



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2025 – 04:31 AM EST

PDB ID : 5J5B  
Title : Structure of the WT E coli ribosome bound to tetracycline  
Authors : Cocozaki, A.; Ferguson, A.  
Deposited on : 2016-04-01  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

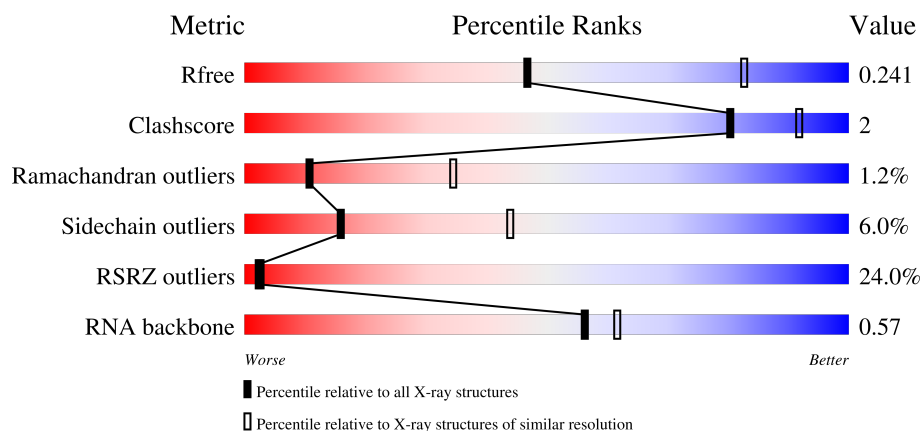
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)
RNA backbone	3690	1037 (3.00-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>8%</div> <div>78%</div> <div>20%</div> </div>
1	BA	1534	<div> <div>27%</div> <div>77%</div> <div>20%</div> </div>
2	AB	224	<div> <div>17%</div> <div>88%</div> <div>11%</div> </div>
2	BB	224	<div> <div>21%</div> <div>86%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
16	AP	82	<div> <div>12%</div> <div>94%</div> <div>6%</div> </div>
16	BP	82	<div> <div>73%</div> <div>89%</div> <div>10%</div> </div>
17	AQ	80	<div> <div>9%</div> <div>78%</div> <div>22%</div> </div>
17	BQ	80	<div> <div>35%</div> <div>75%</div> <div>24%</div> </div>
18	AR	55	<div> <div>9%</div> <div>85%</div> <div>13%</div> </div>
18	BR	55	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
19	AS	79	<div> <div>27%</div> <div>82%</div> <div>14%</div> </div>
19	BS	79	<div> <div>46%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>
20	AT	86	<div> <div>17%</div> <div>91%</div> <div>8%</div> </div>
20	BT	86	<div> <div>52%</div> <div>74%</div> <div>20%</div> <div>5%</div> </div>
21	AU	56	<div> <div>25%</div> <div>88%</div> <div>12%</div> </div>
21	BU	56	<div> <div>20%</div> <div>88%</div> <div>12%</div> </div>
22	C1	56	<div> <div>62%</div> <div>64%</div> <div>30%</div> <div>5%</div> </div>
22	D1	56	<div> <div>4%</div> <div>73%</div> <div>27%</div> </div>
23	C2	51	<div> <div>41%</div> <div>76%</div> <div>22%</div> </div>
23	D2	51	<div> <div>6%</div> <div>80%</div> <div>18%</div> </div>
24	C3	46	<div> <div>80%</div> <div>76%</div> <div>24%</div> </div>
24	D3	46	<div> <div>7%</div> <div>89%</div> <div>11%</div> </div>
25	C4	64	<div> <div>91%</div> <div>86%</div> <div>12%</div> </div>
25	D4	64	<div> <div>2%</div> <div>83%</div> <div>16%</div> </div>
26	C5	38	<div> <div>66%</div> <div>76%</div> <div>21%</div> </div>
26	D5	38	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
27	C0	58	<div> <div>47%</div> <div>88%</div> <div>10%</div> </div>
27	D0	58	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	271	
29	DC	271	
30	CD	209	
30	DD	209	
31	CA	2904	
32	CE	201	
32	DE	201	
33	CF	177	
33	DF	177	
34	CG	176	
34	DG	176	
35	CH	149	
35	DH	149	
36	CJ	134	
36	DJ	134	
37	CK	142	
37	DK	142	
38	CL	123	
38	DL	123	
39	CM	144	
39	DM	144	
40	CN	136	
40	DN	136	

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Mol	Chain	Length	Quality of chain
41	CO	125	<div> <div>56%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
41	DO	125	<div> <div>93%</div> <div>7%</div> </div>
42	CP	117	<div> <div>17%</div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
42	DP	117	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
43	CQ	114	<div> <div>29%</div> <div>89%</div> <div>11%</div> <div>•</div> </div>
43	DQ	114	<div> <div>3%</div> <div>90%</div> <div>10%</div> </div>
44	CR	117	<div> <div>59%</div> <div>88%</div> <div>12%</div> </div>
44	DR	117	<div> <div>0%</div> <div>93%</div> <div>6%</div> <div>•</div> </div>
45	CS	103	<div> <div>50%</div> <div>85%</div> <div>13%</div> <div>• •</div> </div>
45	DS	103	<div> <div>2%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
46	CT	110	<div> <div>69%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
46	DT	110	<div> <div>2%</div> <div>86%</div> <div>14%</div> </div>
47	CU	93	<div> <div>67%</div> <div>75%</div> <div>22%</div> <div>•</div> </div>
47	DU	93	<div> <div>10%</div> <div>90%</div> <div>10%</div> </div>
48	CV	102	<div> <div>68%</div> <div>83%</div> <div>16%</div> <div>•</div> </div>
48	DV	102	<div> <div>5%</div> <div>91%</div> <div>8%</div> <div>•</div> </div>
49	CW	94	<div> <div>22%</div> <div>89%</div> <div>11%</div> </div>
49	DW	94	<div> <div>0%</div> <div>91%</div> <div>9%</div> </div>
50	CX	76	<div> <div>42%</div> <div>95%</div> <div>• •</div> </div>
50	DX	76	<div> <div>0%</div> <div>91%</div> <div>9%</div> </div>
51	CY	77	<div> <div>61%</div> <div>83%</div> <div>17%</div> </div>
51	DY	77	<div> <div>0%</div> <div>90%</div> <div>10%</div> </div>
52	CZ	62	<div> <div>63%</div> <div>92%</div> <div>8%</div> </div>
52	DZ	62	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
53	DI	135	<div> <div>38%</div> <div>71%</div> <div>27%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
54	DA	2904	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1601	-	-	-	X
55	MG	AA	1603	-	-	-	X
55	MG	AA	1605	-	-	-	X
55	MG	AA	1606	-	-	-	X
55	MG	AA	1616	-	-	-	X
55	MG	BA	1638	-	-	-	X
55	MG	BA	1640	-	-	-	X
55	MG	BA	1642	-	-	-	X
55	MG	CA	3055	-	-	-	X
55	MG	CA	3116	-	-	-	X
55	MG	CA	3118	-	-	-	X
55	MG	CA	3121	-	-	-	X
55	MG	CA	3124	-	-	-	X
55	MG	CA	3138	-	-	-	X
55	MG	CA	3140	-	-	-	X
55	MG	CA	3146	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	DA	3124	-	-	-	X
55	MG	DA	3139	-	-	-	X
55	MG	DA	3153	-	-	-	X
55	MG	DA	3172	-	-	-	X
57	MPD	AA	1676	-	-	-	X
58	PUT	AA	1672	-	-	-	X
66	ACY	DA	3196	-	X	-	-

## 2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295188 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32930	14694	6041	10661	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32908	14684	6036	10655	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			
2	BB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			
12	BL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			
14	BN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
22	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
23	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
24	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
25	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
27	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
28	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
30	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	1723	G	A	conflict	GB 939731527
CA	1725	U	C	conflict	GB 939731527
CA	1726	C	G	conflict	GB 939731527
CA	1727	C	A	conflict	GB 939731527
CA	1730	C	U	conflict	GB 939731527
CA	1733	G	U	conflict	GB 939731527
CA	1734	G	C	conflict	GB 939731527
CA	1735	A	G	conflict	GB 939731527

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
32	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
33	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
34	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
35	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 36 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			
36	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
37	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
38	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
39	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
40	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CN	81	4D4	ARG	modified residue	UNP P0ADY7
DN	81	4D4	ARG	modified residue	UNP P0ADY7

- Molecule 41 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
41	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CP	116	Total	C	N	O		0	0	0
			892	552	178	162				
42	DP	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 43 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
43	DQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	CR	117	Total	C	N	O	0	0	0
			947	604	192	151			
44	DR	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 45 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
45	DS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 46 is a protein called 50S ribosomal protein L22.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
46	DT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
47	DU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CV	102	Total	C	N	O	0	0	0
			780	492	146	142			
48	DV	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
49	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 50 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
50	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
52	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	DI	135	Total	C	N	O	S	0	0	0
			1023	649	179	192	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

- Molecule 54 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DA	2897	Total	C	N	O	P	0	11	0
			62423	27855	11485	20176	2907			

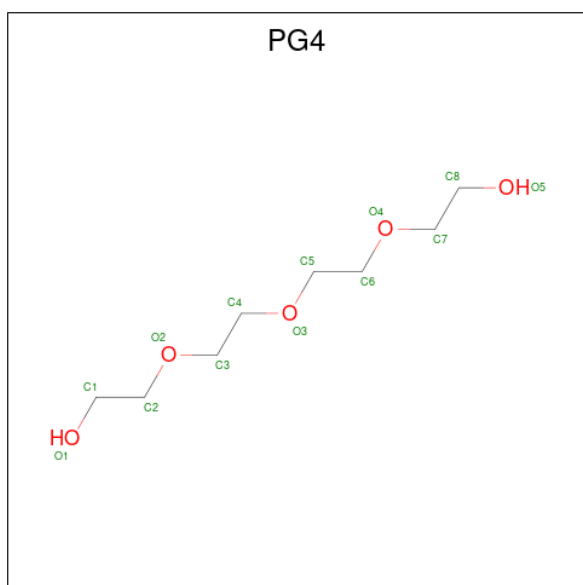
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	1723	G	A	conflict	GB 939731527
DA	1725	U	C	conflict	GB 939731527
DA	1726	C	G	conflict	GB 939731527
DA	1727	C	A	conflict	GB 939731527
DA	1730	C	U	conflict	GB 939731527
DA	1733	G	U	conflict	GB 939731527
DA	1734	G	C	conflict	GB 939731527
DA	1735	A	G	conflict	GB 939731527

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	71	Total	Mg	0	0
			71	71		
55	C3	1	Total	Mg	0	0
			1	1		
55	BA	43	Total	Mg	0	0
			43	43		
55	CB	3	Total	Mg	0	0
			3	3		
55	CA	155	Total	Mg	0	0
			155	155		
55	DD	2	Total	Mg	0	0
			2	2		
55	DM	1	Total	Mg	0	0
			1	1		
55	DR	2	Total	Mg	0	0
			2	2		
55	DB	9	Total	Mg	0	0
			9	9		
55	DA	182	Total	Mg	0	0
			182	182		

- Molecule 56 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



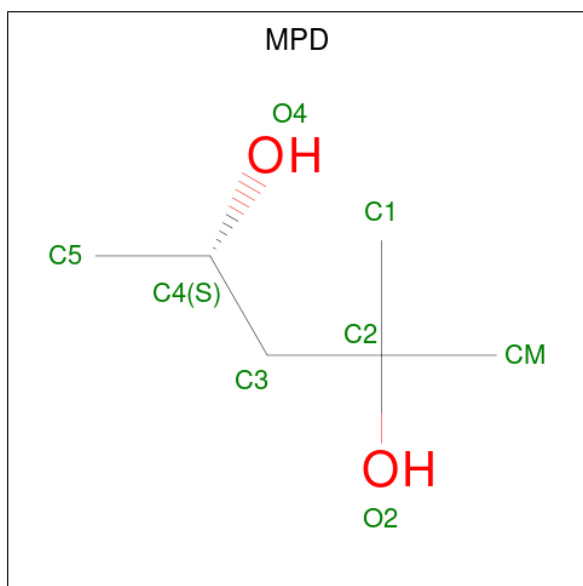
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	C	O	0	0
			13	8	5		
56	BA	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DQ	1	Total	C	O	0	0
			13	8	5		
56	DR	1	Total	C	O	0	0
			13	8	5		
56	DS	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



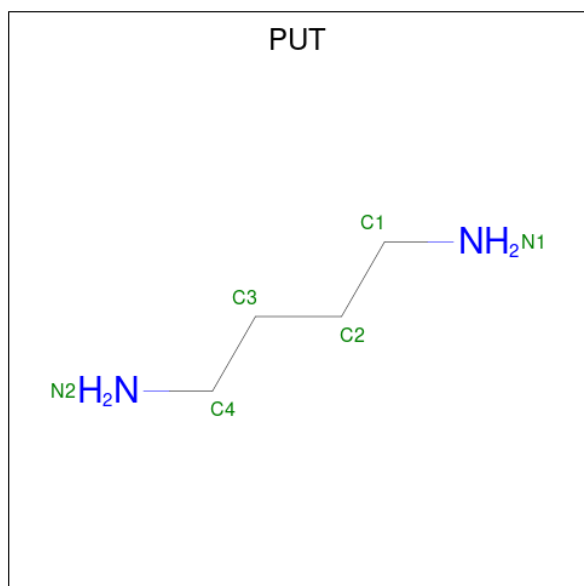
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			8	6	2		
57	AA	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DK	1	Total	C	O	0	0
			8	6	2		
57	DN	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	DS	1	Total C O 8 6 2	0	0
57	DT	1	Total C O 8 6 2	0	0
57	DT	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0

- Molecule 58 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



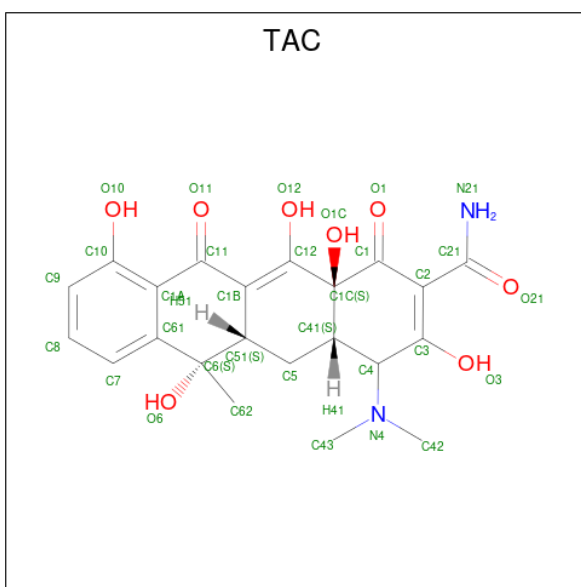
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	1	Total C N 6 4 2	0	0
58	AA	1	Total C N 6 4 2	0	0
58	AA	1	Total C N 6 4 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		

- Molecule 59 is TETRACYCLINE (three-letter code: TAC) (formula:  $C_{22}H_{24}N_2O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total 32	C 22	N 2	O 8	0	0
59	BA	1	Total 32	C 22	N 2	O 8	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AB	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0
60	D5	1	Total Zn 1 1	0	0

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

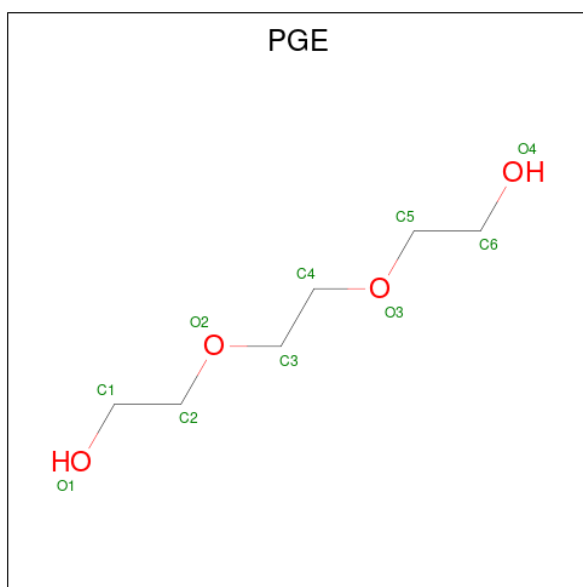
- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





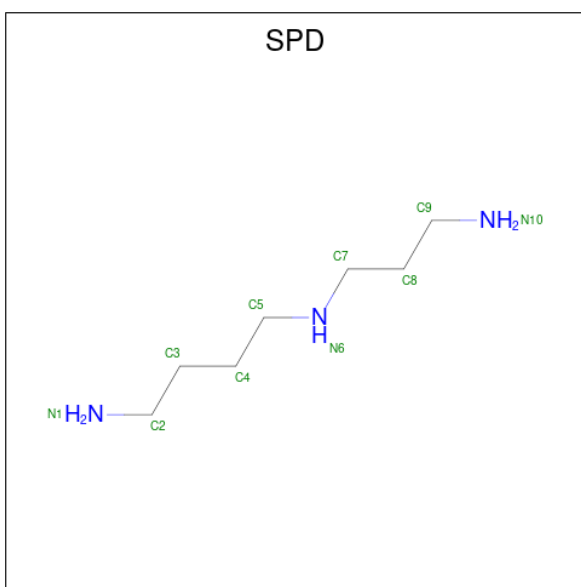
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



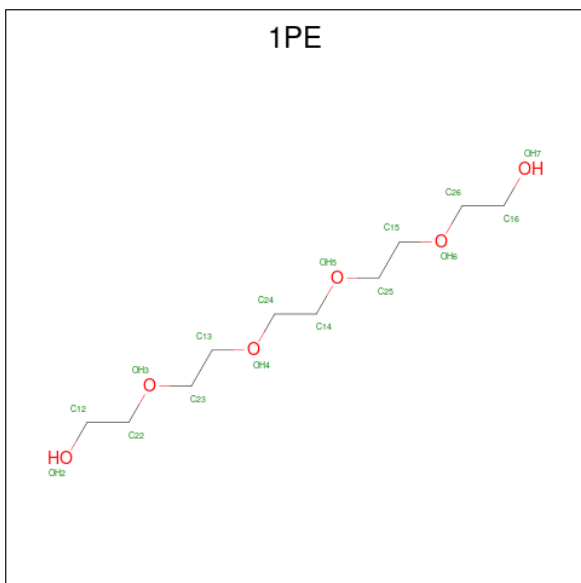
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 64 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



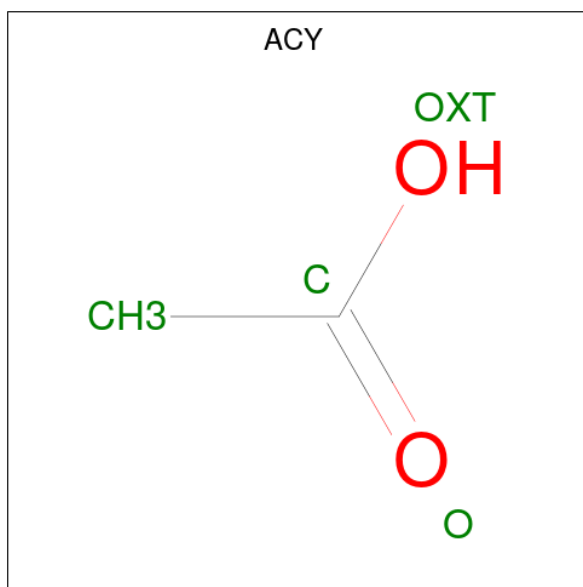
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



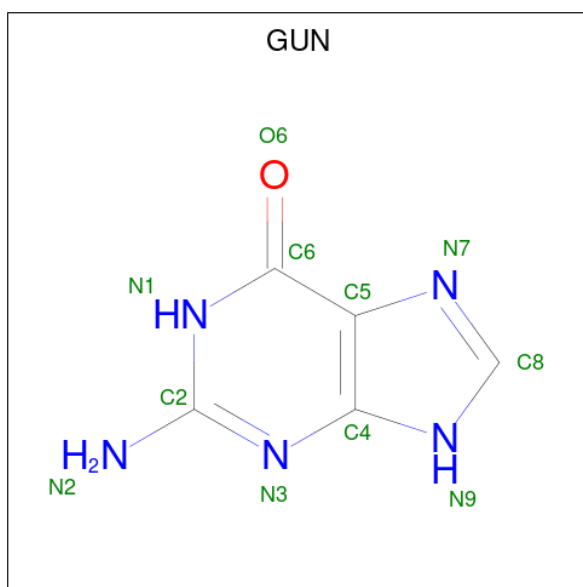
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



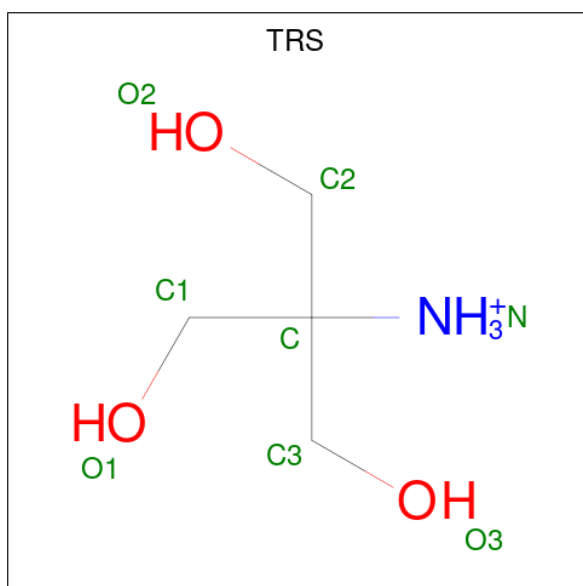
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (three-letter code: GUN) (formula:  $C_5H_5N_5O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
67	DA	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
68	DA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 69 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	AA	507	Total O 507 507	0	0
69	AC	4	Total O 4 4	0	0
69	AD	2	Total O 2 2	0	0
69	AE	4	Total O 4 4	0	0
69	AF	1	Total O 1 1	0	0
69	AG	1	Total O 1 1	0	0
69	AH	1	Total O 1 1	0	0
69	AJ	2	Total O 2 2	0	0
69	AK	5	Total O 5 5	0	0
69	AL	8	Total O 8 8	0	0
69	AM	4	Total O 4 4	0	0
69	AN	5	Total O 5 5	0	0
69	AO	2	Total O 2 2	0	0
69	AP	2	Total O 2 2	0	0
69	AR	1	Total O 1 1	0	0
69	AS	1	Total O 1 1	0	0
69	AT	2	Total O 2 2	0	0
69	AU	3	Total O 3 3	0	0
69	C3	3	Total O 3 3	0	0
69	C4	2	Total O 2 2	0	0
69	BA	287	Total O 287 287	0	0
69	BD	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	BE	1	Total 1	O 1	0	0
69	BF	1	Total 1	O 1	0	0
69	BK	1	Total 1	O 1	0	0
69	BL	3	Total 3	O 3	0	0
69	BN	2	Total 2	O 2	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	3	Total 3	O 3	0	0
69	BR	1	Total 1	O 1	0	0
69	BT	4	Total 4	O 4	0	0
69	BU	2	Total 2	O 2	0	0
69	D1	42	Total 42	O 42	0	0
69	D2	7	Total 7	O 7	0	0
69	D3	24	Total 24	O 24	0	0
69	D4	33	Total 33	O 33	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	27	Total 27	O 27	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	5	Total 5	O 5	0	0
69	CA	692	Total 692	O 692	0	0
69	DC	102	Total 102	O 102	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DD	105	Total 105	O 105	0	0
69	CE	7	Total 7	O 7	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	3	Total 3	O 3	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	63	Total 63	O 63	0	0
69	DF	14	Total 14	O 14	0	0
69	DG	6	Total 6	O 6	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	58	Total 58	O 58	0	0
69	DL	51	Total 51	O 51	0	0
69	DM	62	Total 62	O 62	0	0
69	DN	71	Total 71	O 71	0	0
69	DO	44	Total 44	O 44	0	0
69	DP	35	Total 35	O 35	0	0
69	DQ	27	Total 27	O 27	0	0
69	DR	64	Total 64	O 64	0	0

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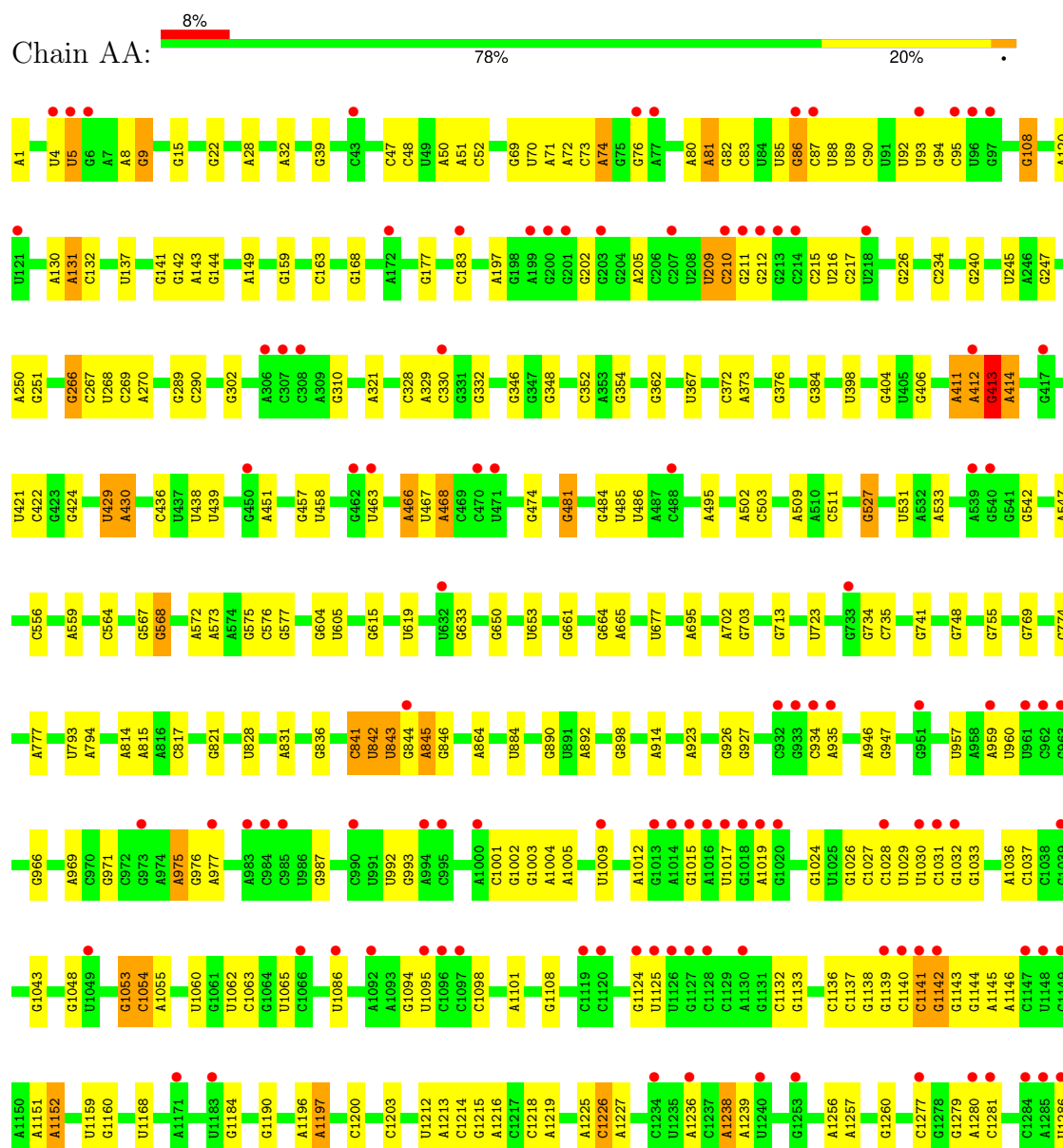
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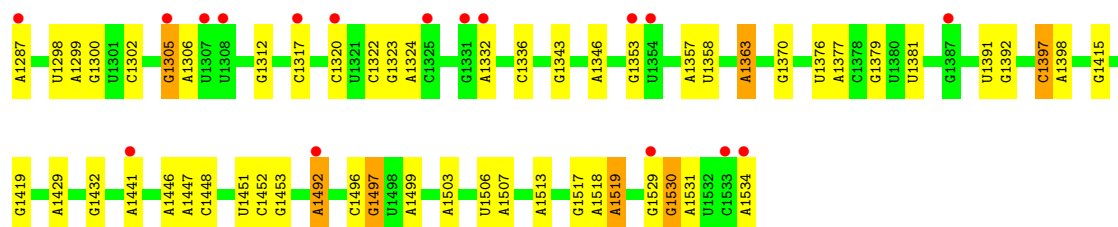
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DS	51	Total 51	O 51	0	0
69	DT	69	Total 69	O 69	0	0
69	DU	17	Total 17	O 17	0	0
69	DV	19	Total 19	O 19	0	0
69	DW	31	Total 31	O 31	0	0
69	DX	30	Total 30	O 30	0	0
69	DY	9	Total 9	O 9	0	0
69	DZ	7	Total 7	O 7	0	0
69	DB	212	Total 212	O 212	0	0
69	DA	4834	Total 4834	O 4834	0	0

### 3 Residue-property plots

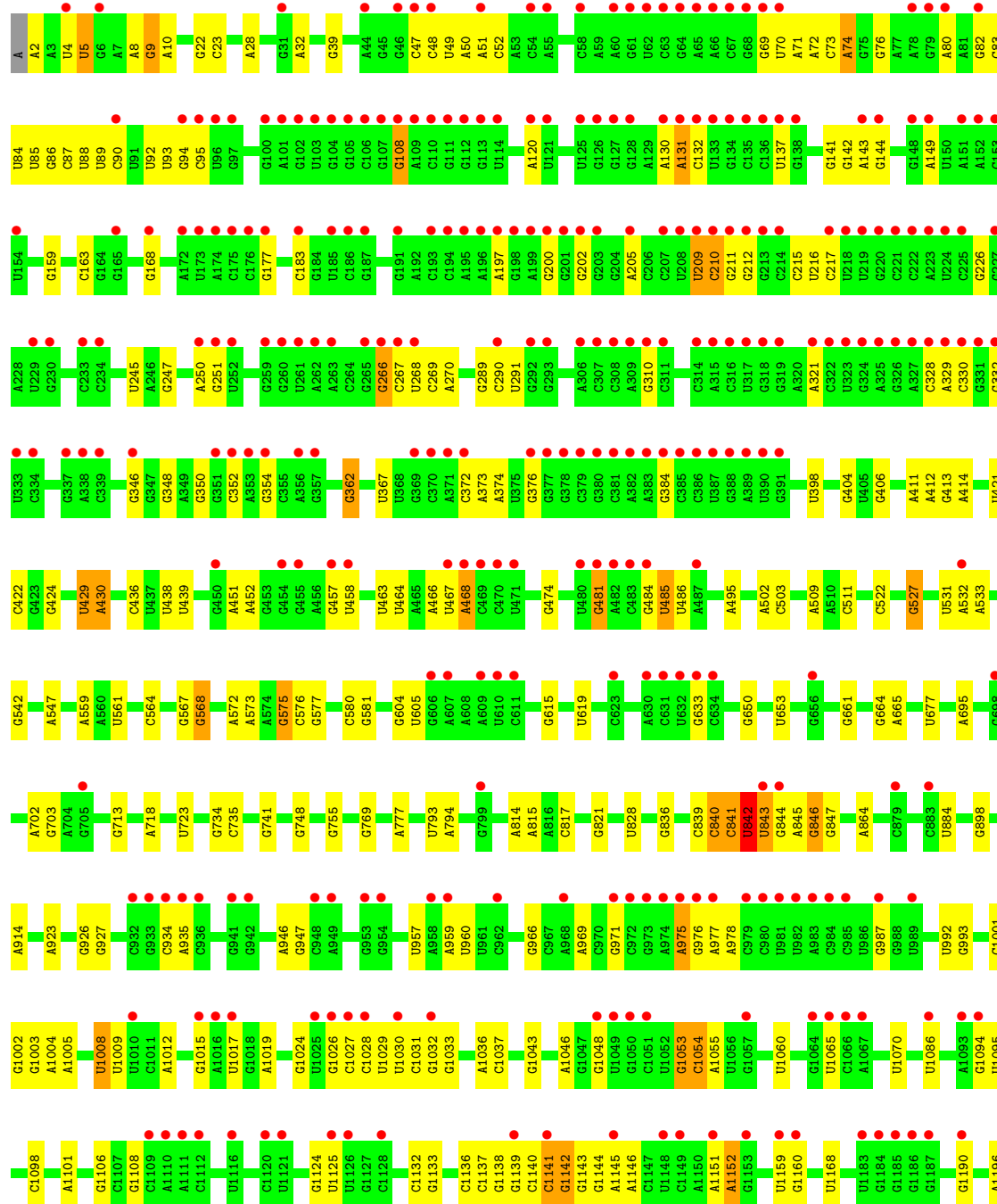
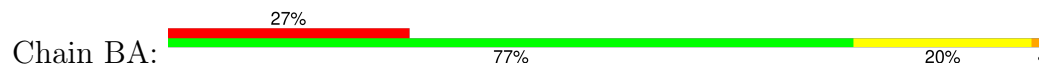
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

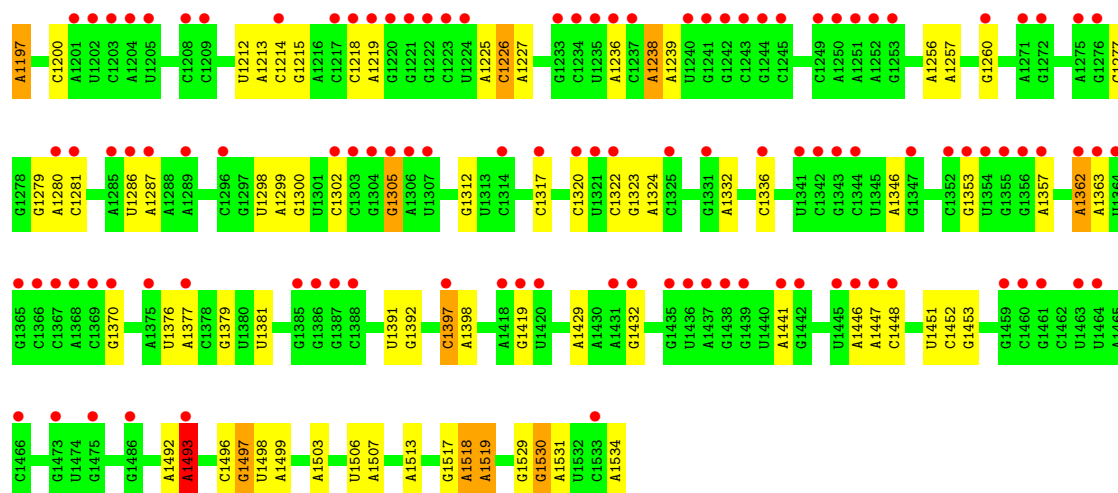
#### • Molecule 1: 16S rRNA



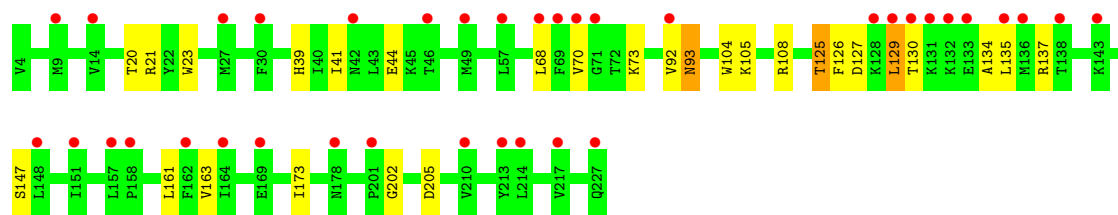
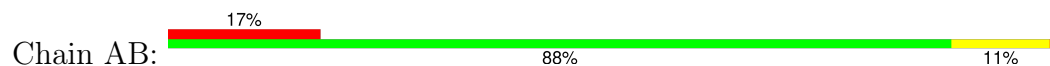


● Molecule 1: 16S rRNA

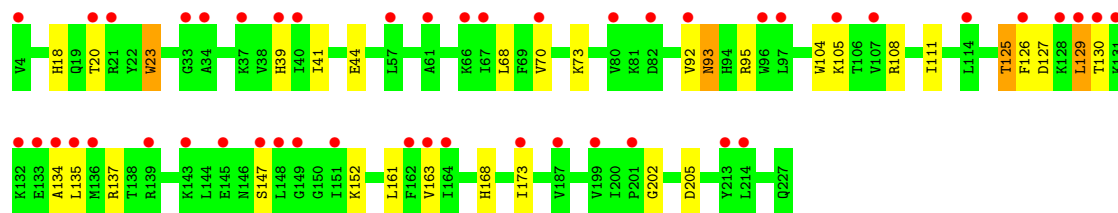
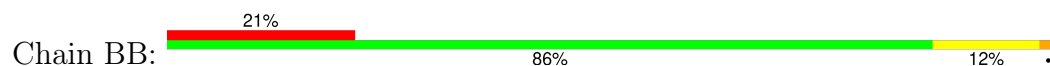




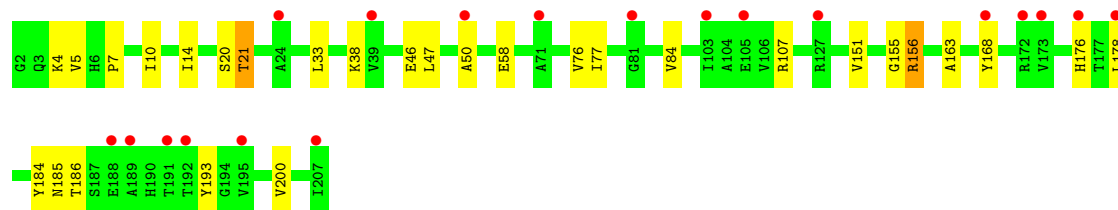
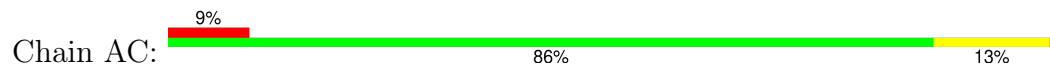
• Molecule 2: 30S ribosomal protein S2



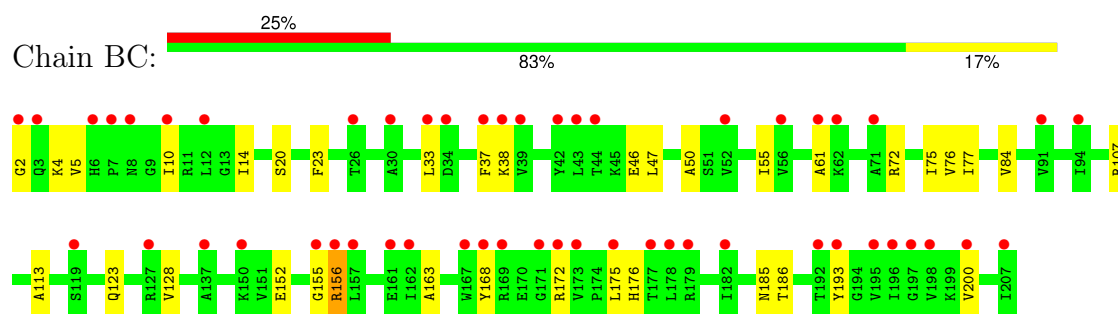
• Molecule 2: 30S ribosomal protein S2



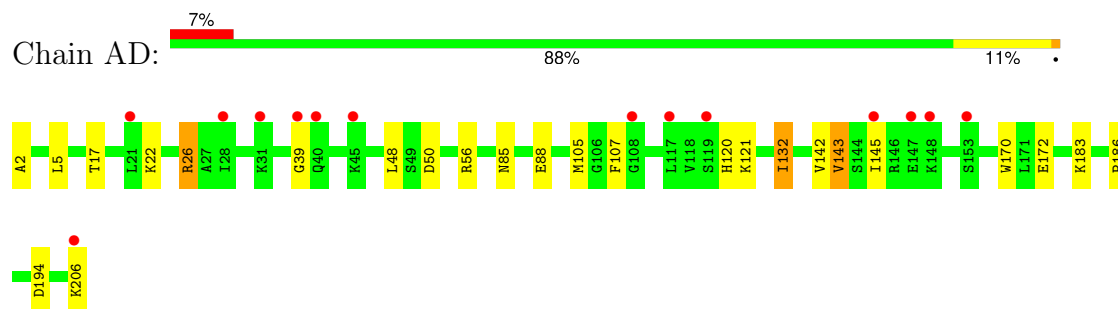
• Molecule 3: 30S ribosomal protein S3



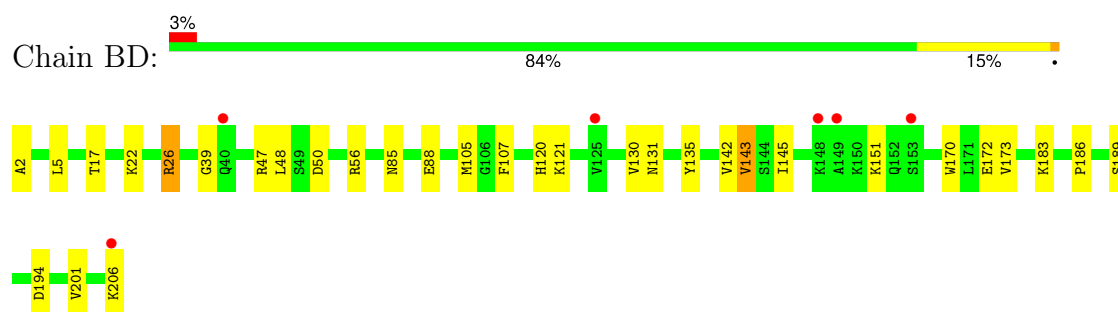
• Molecule 3: 30S ribosomal protein S3



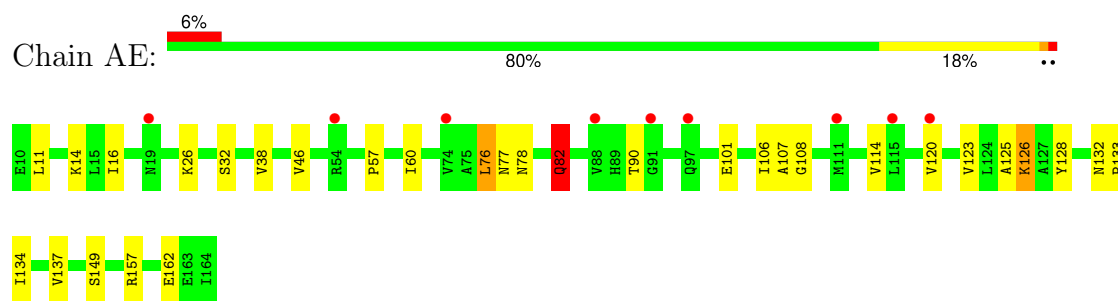
- Molecule 4: 30S ribosomal protein S4



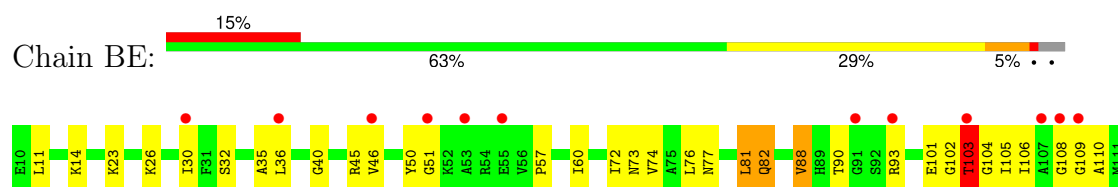
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

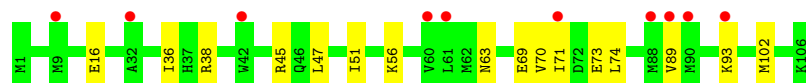
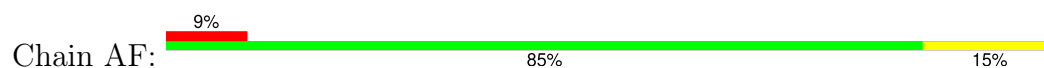


- Molecule 5: 30S ribosomal protein S5

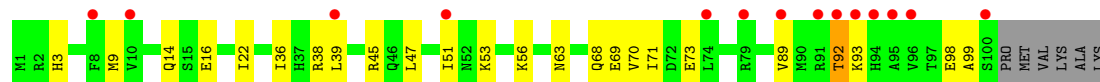




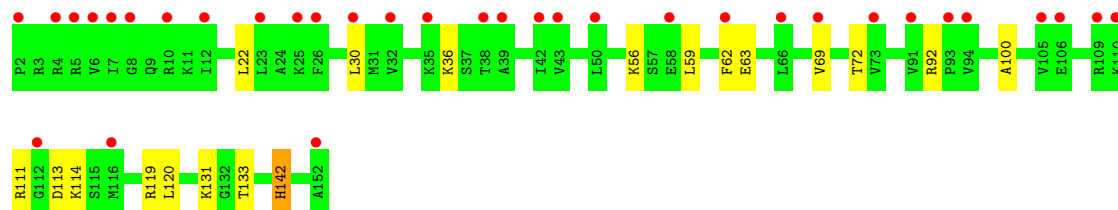
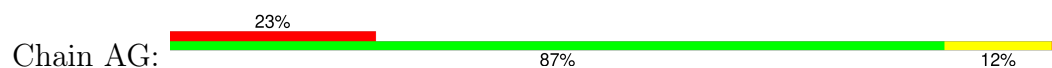
- Molecule 6: 30S ribosomal protein S6



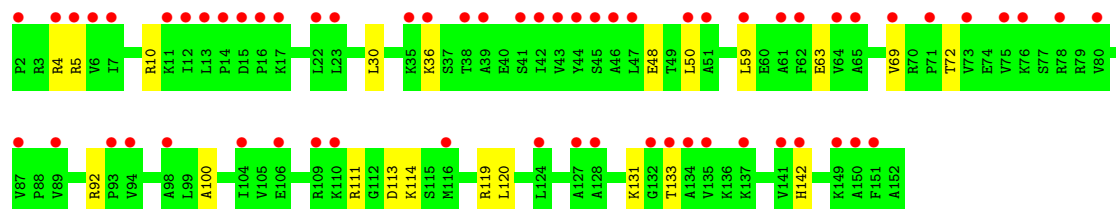
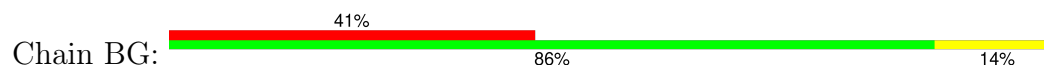
- Molecule 6: 30S ribosomal protein S6



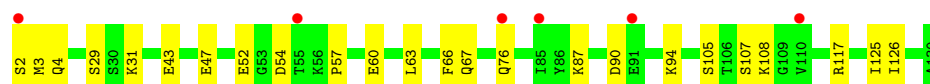
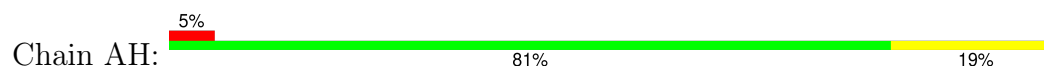
- Molecule 7: 30S ribosomal protein S7



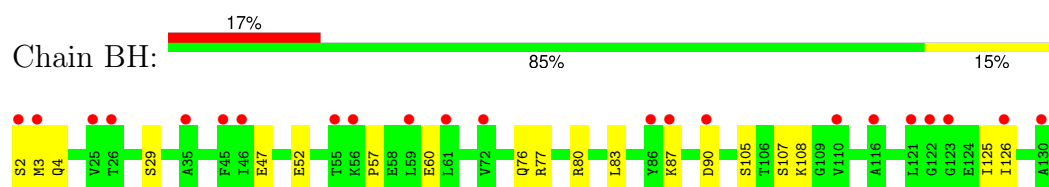
- Molecule 7: 30S ribosomal protein S7



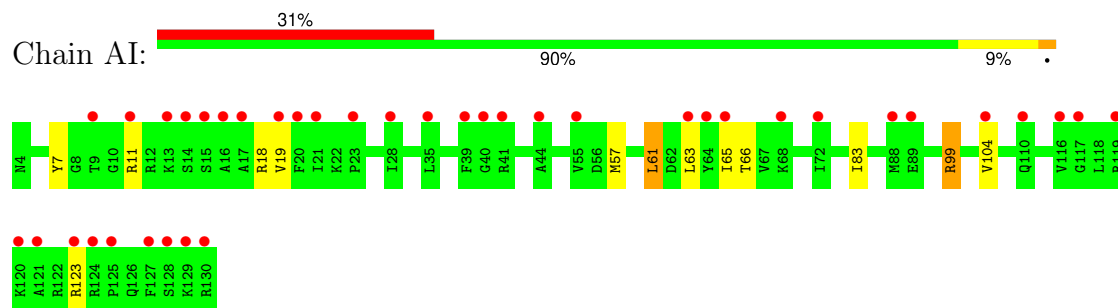
- Molecule 8: 30S ribosomal protein S8



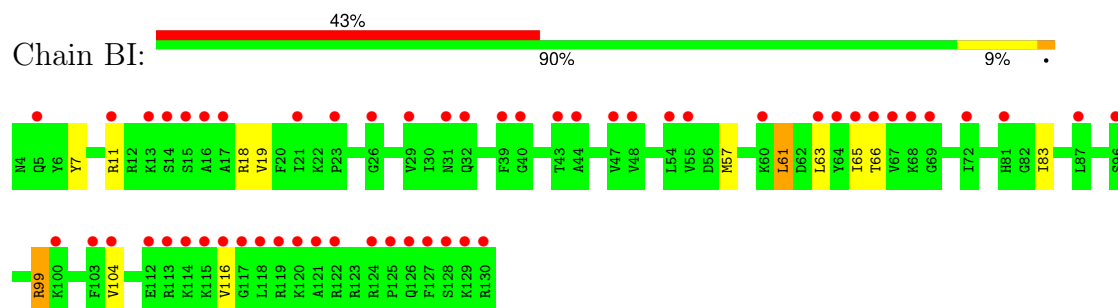
- Molecule 8: 30S ribosomal protein S8



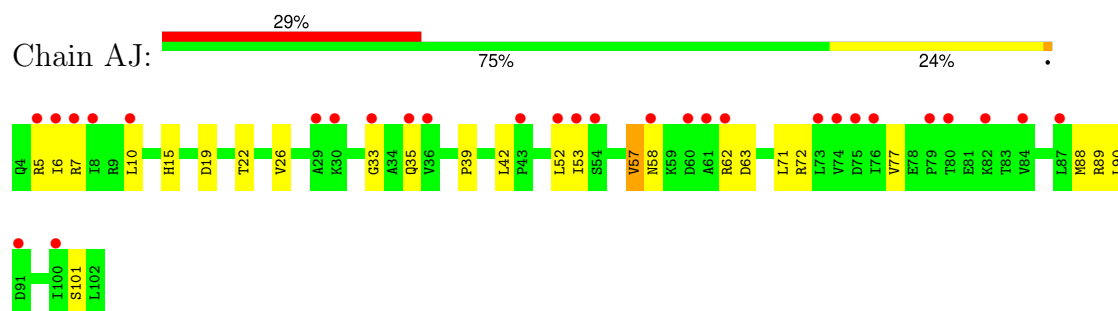
• Molecule 9: 30S ribosomal protein S9



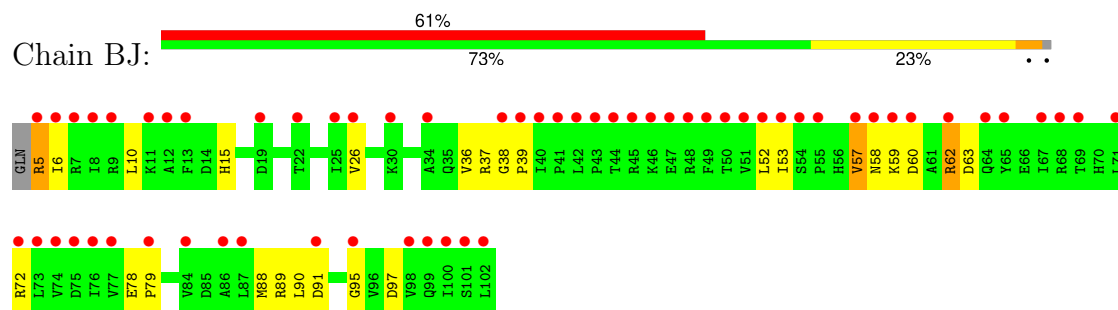
• Molecule 9: 30S ribosomal protein S9



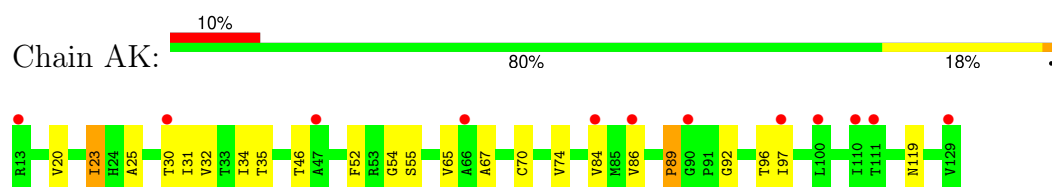
• Molecule 10: 30S ribosomal protein S10



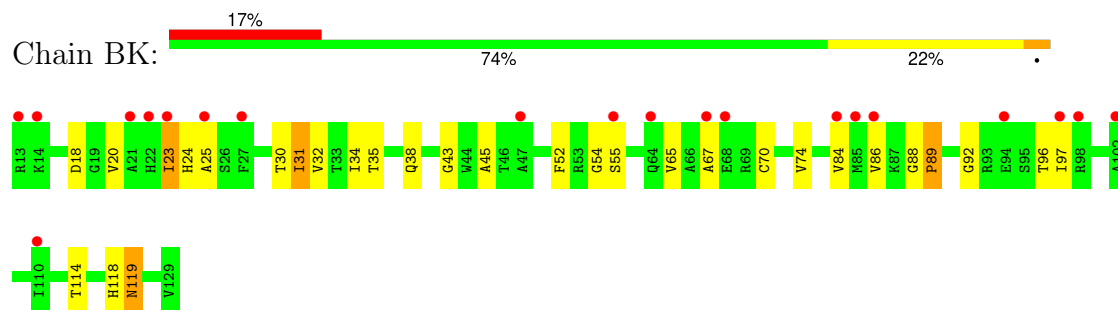
• Molecule 10: 30S ribosomal protein S10



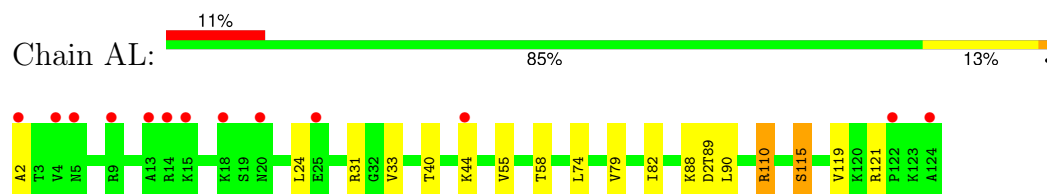
• Molecule 11: 30S ribosomal protein S11



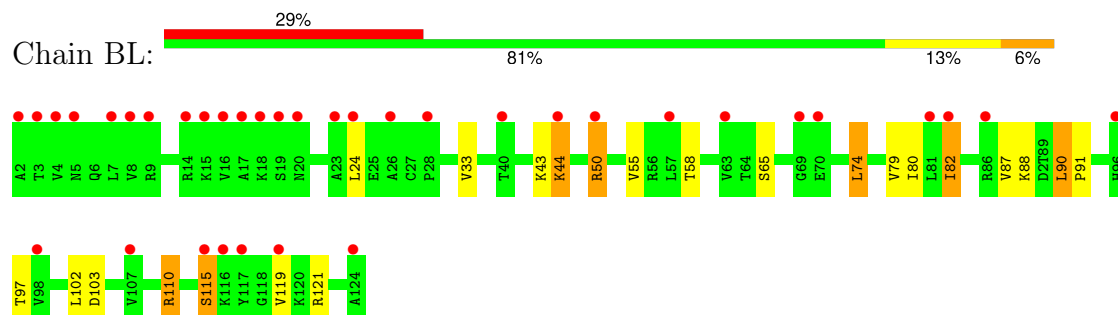
- Molecule 11: 30S ribosomal protein S11



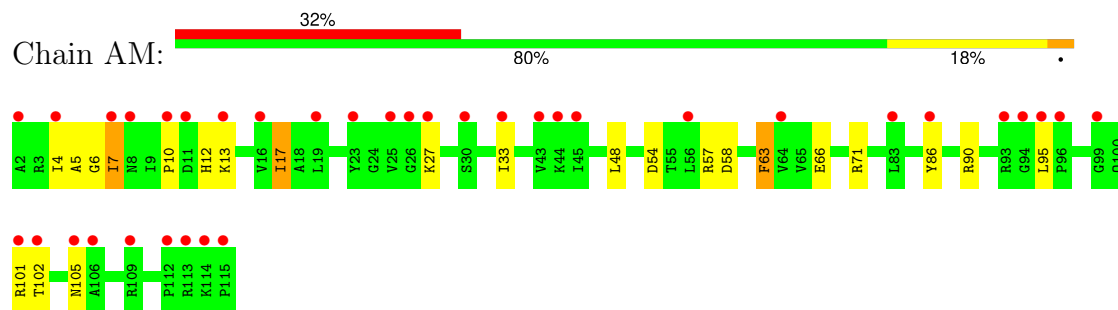
- Molecule 12: 30S ribosomal protein S12



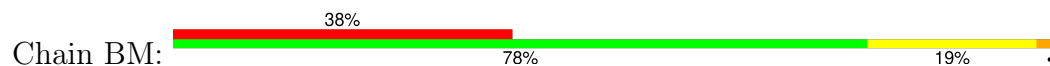
- Molecule 12: 30S ribosomal protein S12



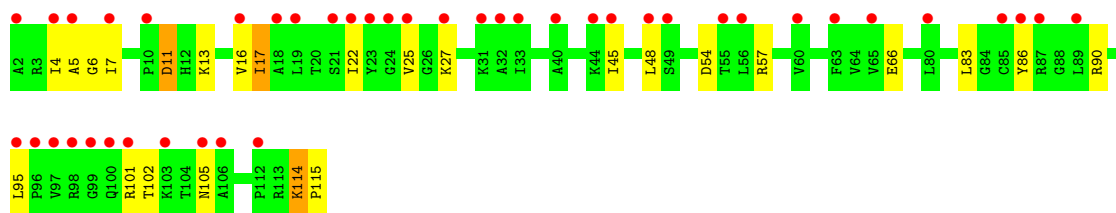
- Molecule 13: 30S ribosomal protein S13



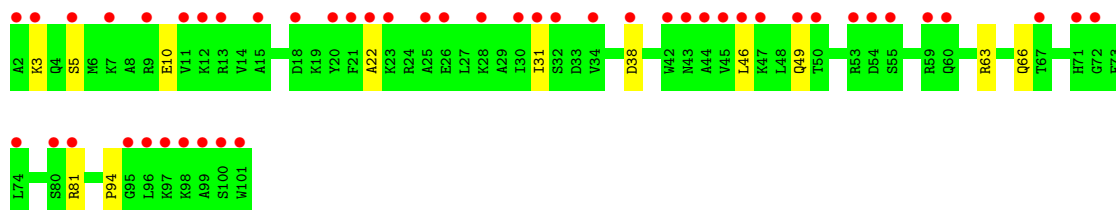
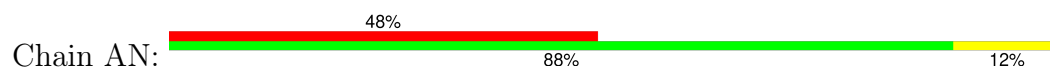
- Molecule 13: 30S ribosomal protein S13



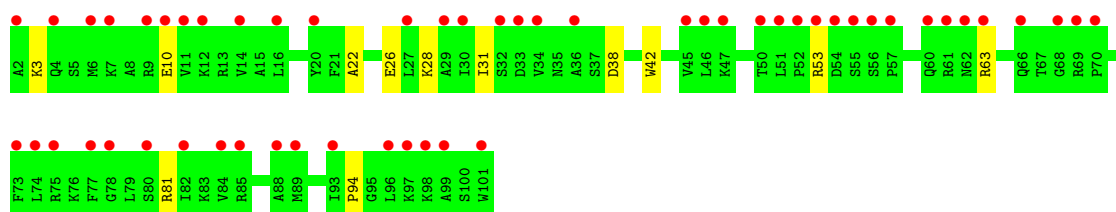




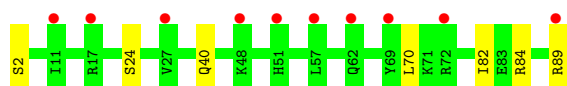
• Molecule 14: 30S ribosomal protein S14



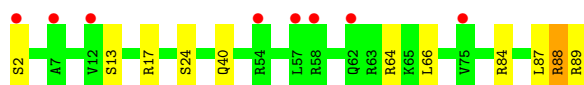
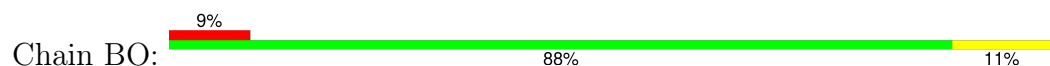
• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15



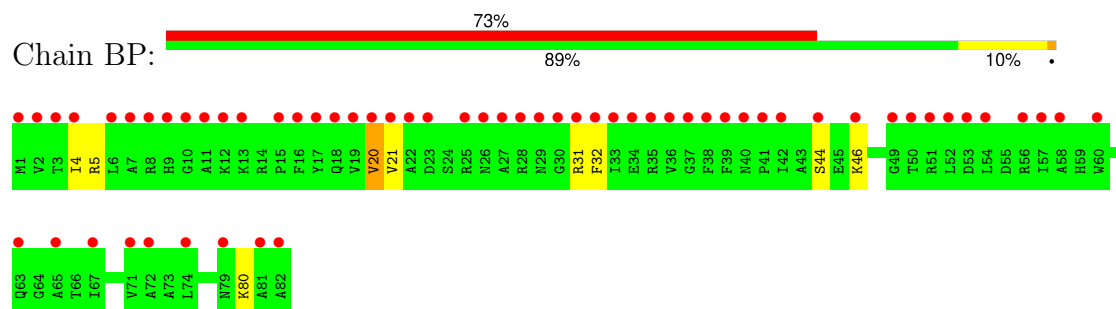
• Molecule 15: 30S ribosomal protein S15



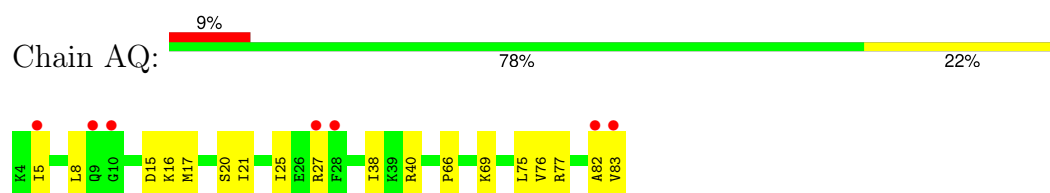
• Molecule 16: 30S ribosomal protein S16



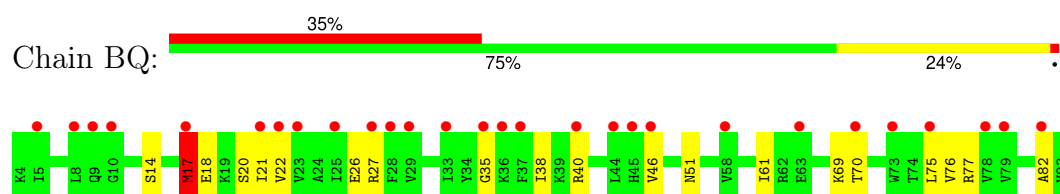
- Molecule 16: 30S ribosomal protein S16



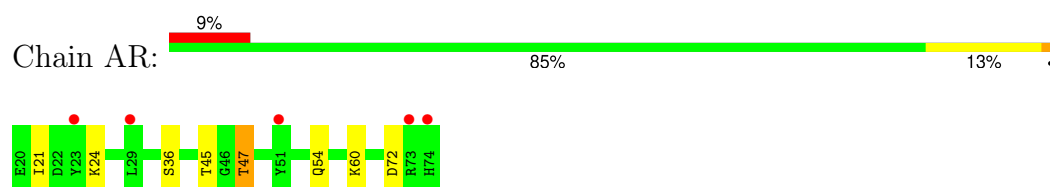
- Molecule 17: 30S ribosomal protein S17



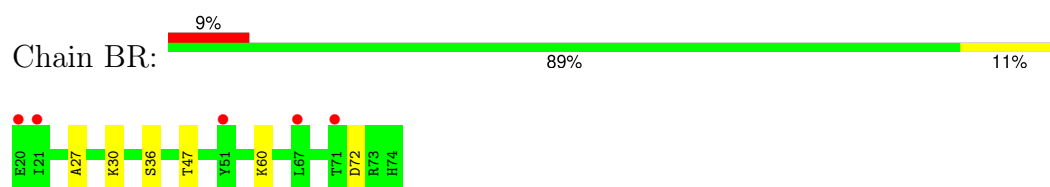
- Molecule 17: 30S ribosomal protein S17



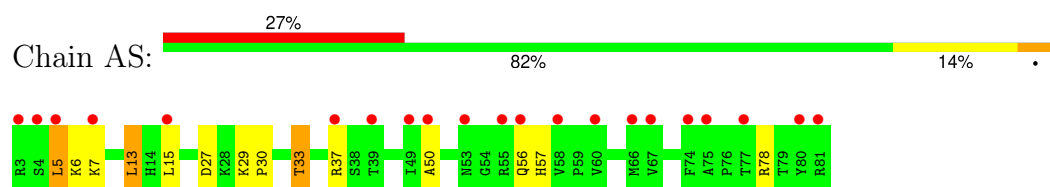
- Molecule 18: 30S ribosomal protein S18



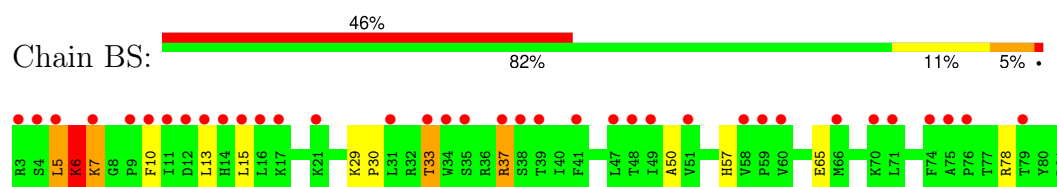
- Molecule 18: 30S ribosomal protein S18



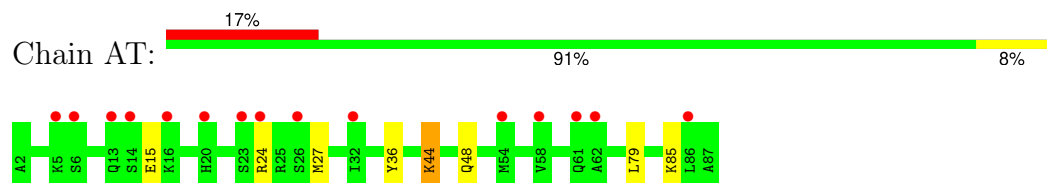
- Molecule 19: 30S ribosomal protein S19



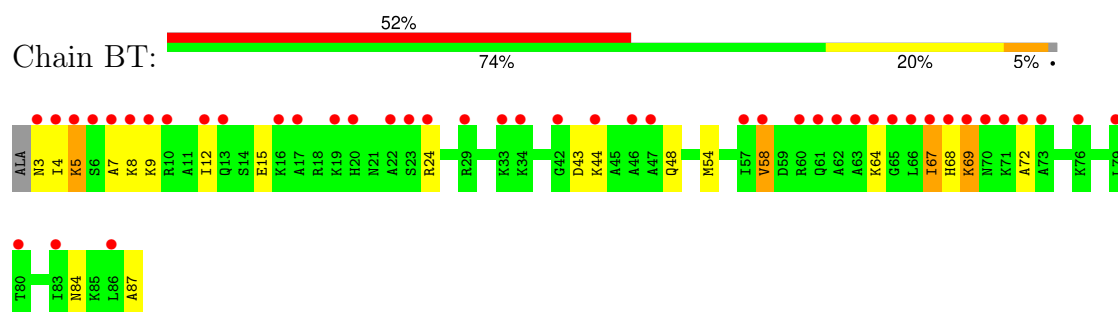
- Molecule 19: 30S ribosomal protein S19



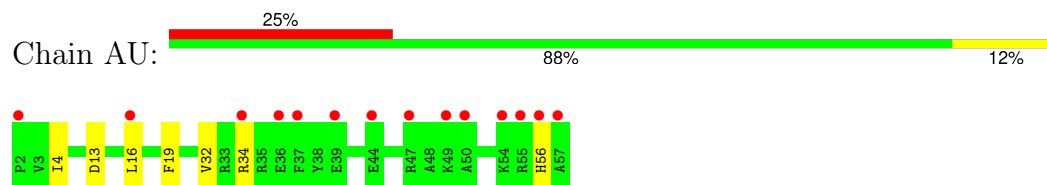
- Molecule 20: 30S ribosomal protein S20



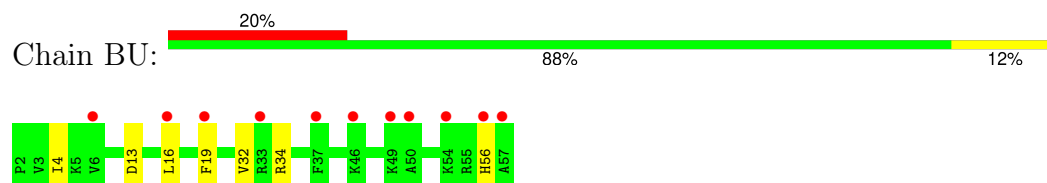
- Molecule 20: 30S ribosomal protein S20



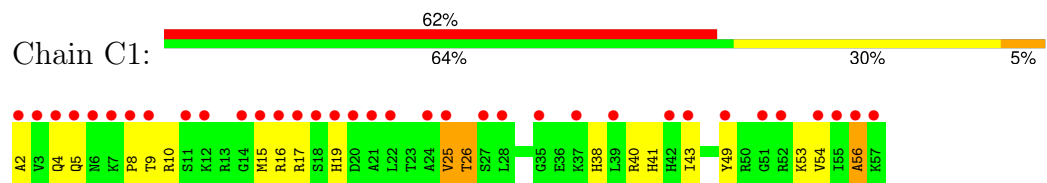
- Molecule 21: 30S ribosomal protein S21



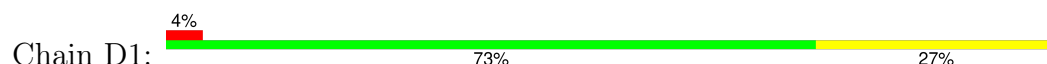
- Molecule 21: 30S ribosomal protein S21

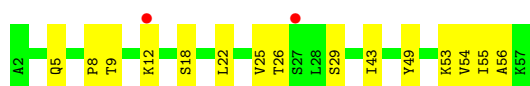


- Molecule 22: 50S ribosomal protein L32

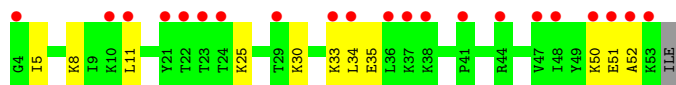
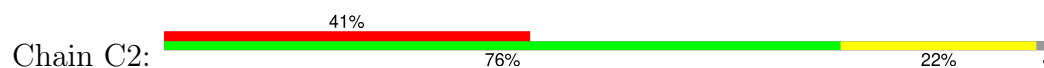


- Molecule 22: 50S ribosomal protein L32

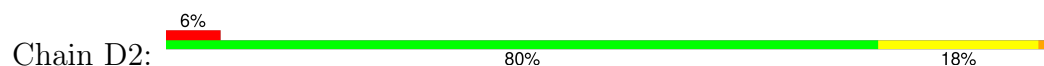




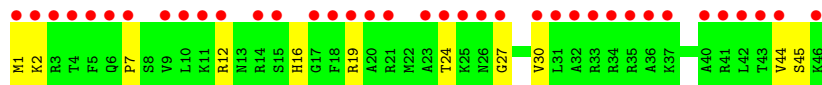
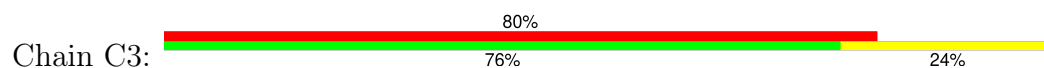
- Molecule 23: 50S ribosomal protein L33



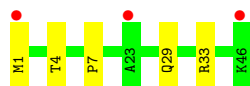
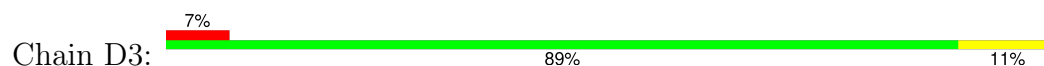
- Molecule 23: 50S ribosomal protein L33



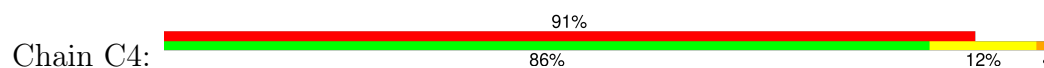
- Molecule 24: 50S ribosomal protein L34



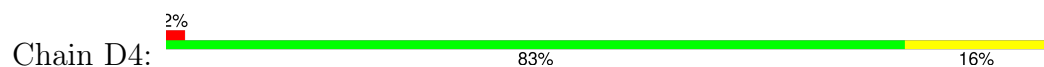
- Molecule 24: 50S ribosomal protein L34

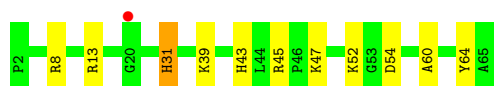


- Molecule 25: 50S ribosomal protein L35

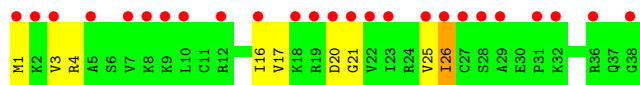
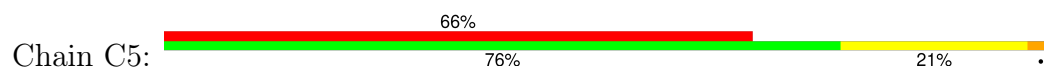


- Molecule 25: 50S ribosomal protein L35





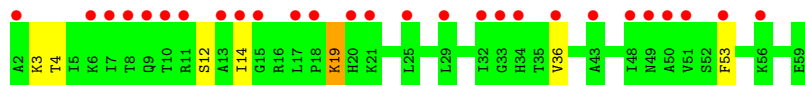
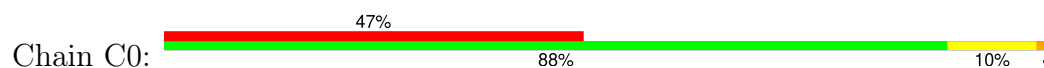
- Molecule 26: 50S ribosomal protein L36



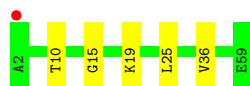
- Molecule 26: 50S ribosomal protein L36



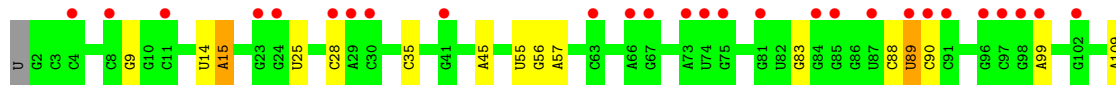
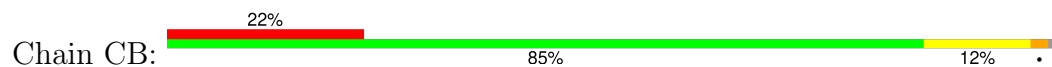
- Molecule 27: 50S ribosomal protein L30



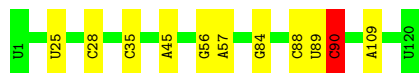
- Molecule 27: 50S ribosomal protein L30



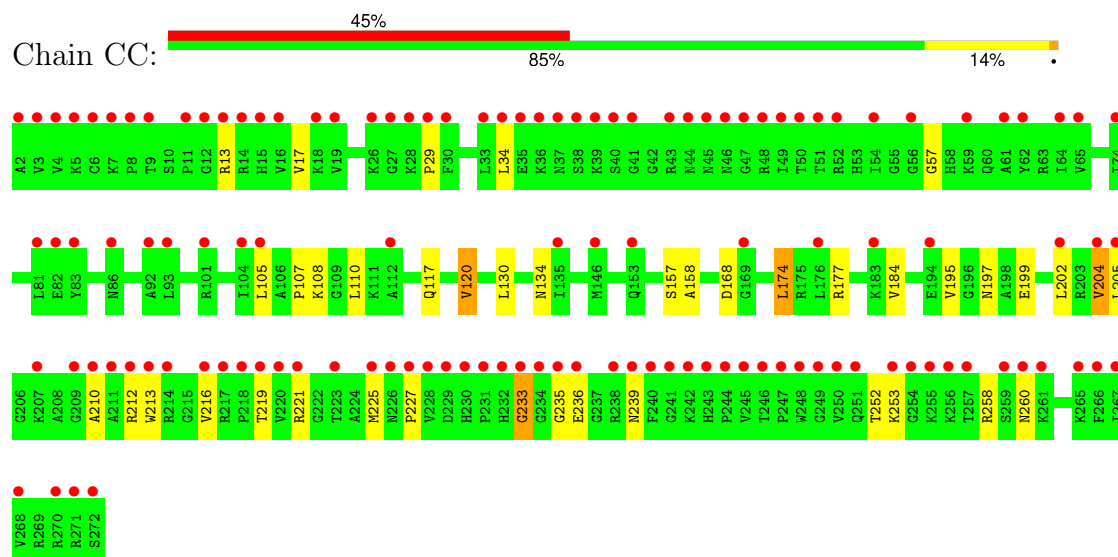
- Molecule 28: 5S rRNA



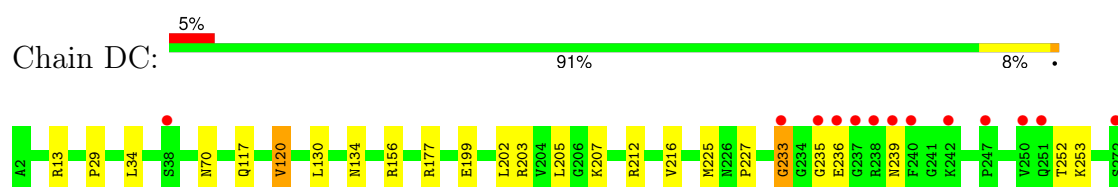
- Molecule 28: 5S rRNA



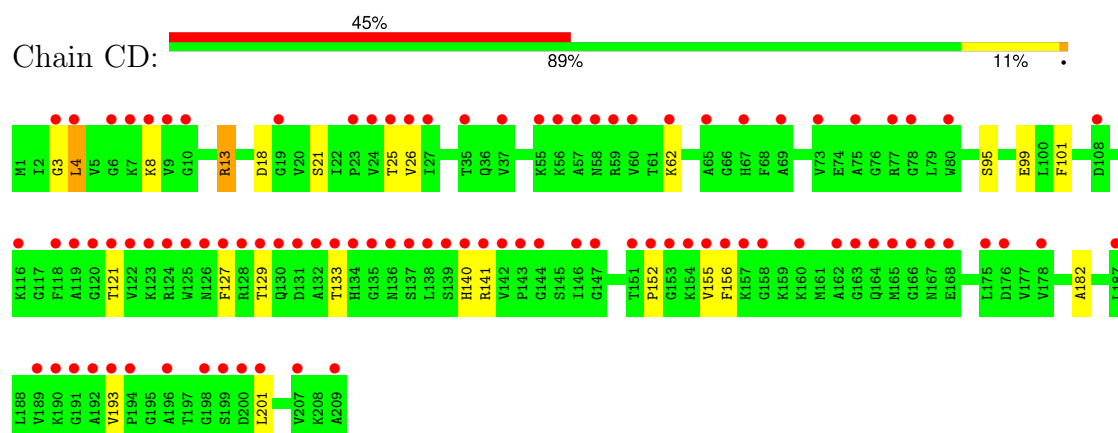
- Molecule 29: 50S ribosomal protein L2



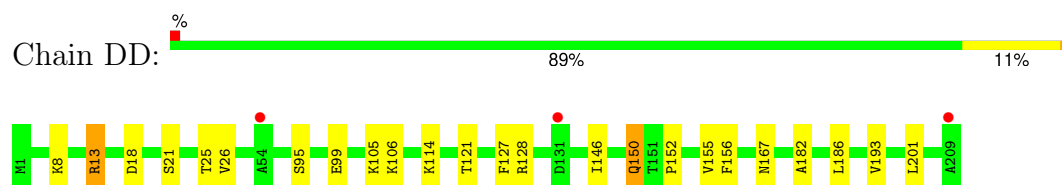
- Molecule 29: 50S ribosomal protein L2



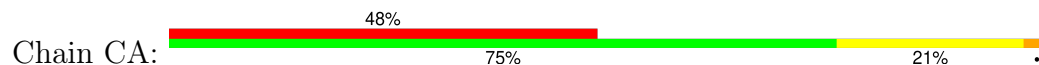
- Molecule 30: 50S ribosomal protein L3

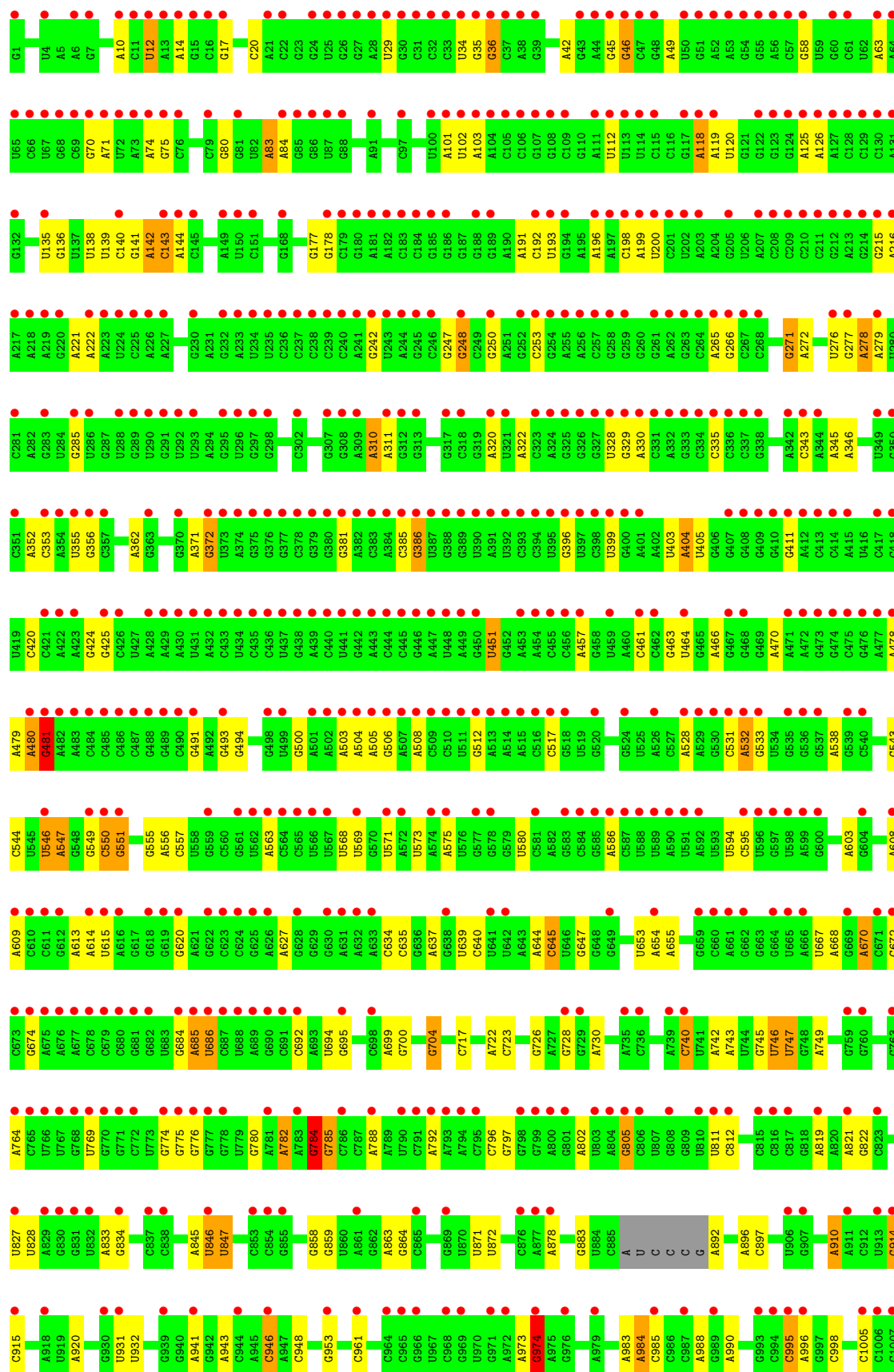


- Molecule 30: 50S ribosomal protein L3



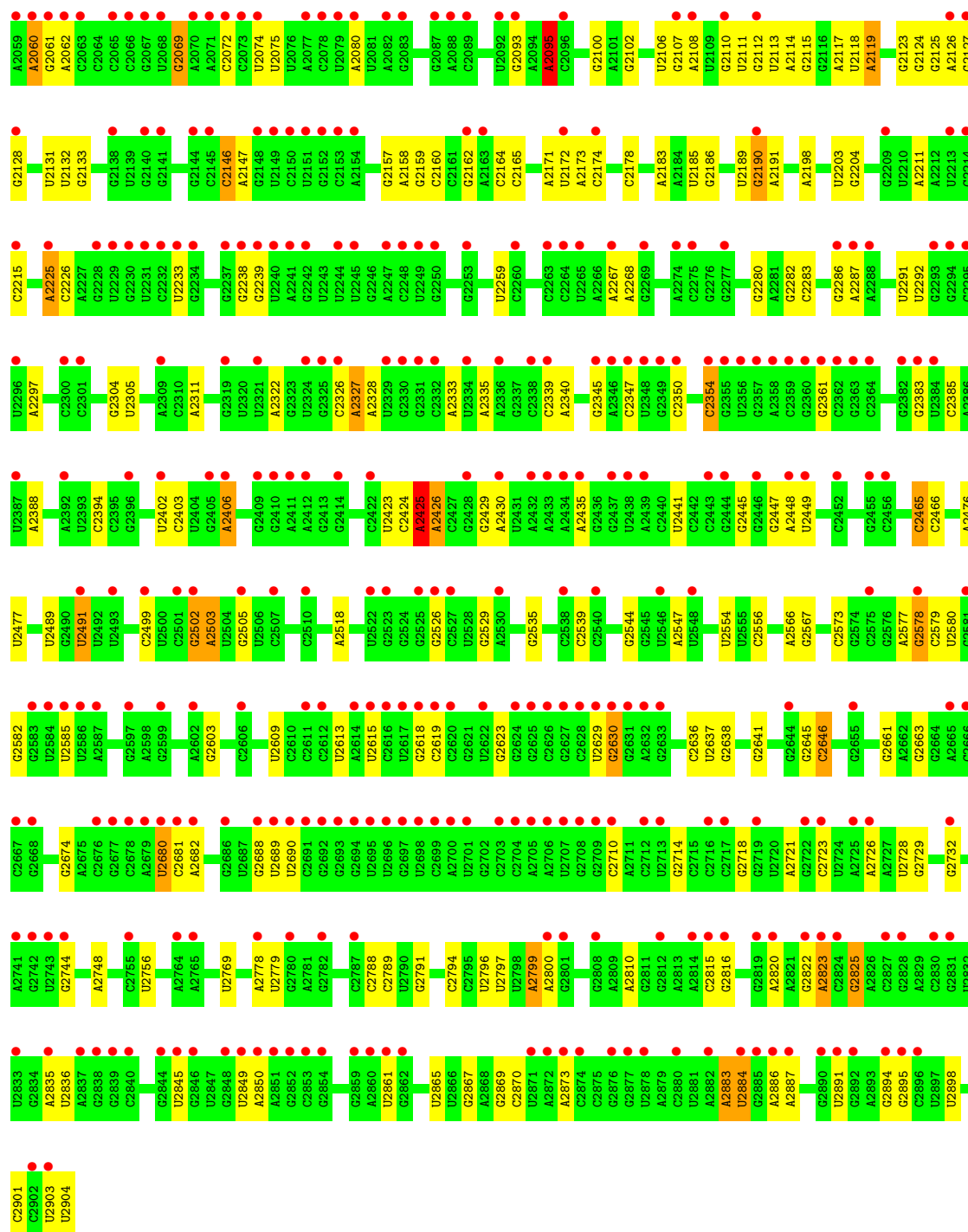
- Molecule 31: 23S rRNA





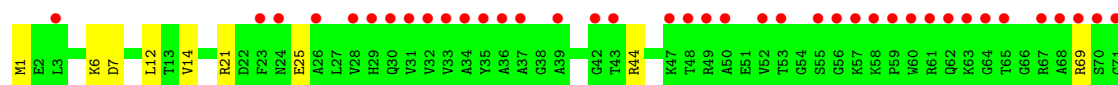


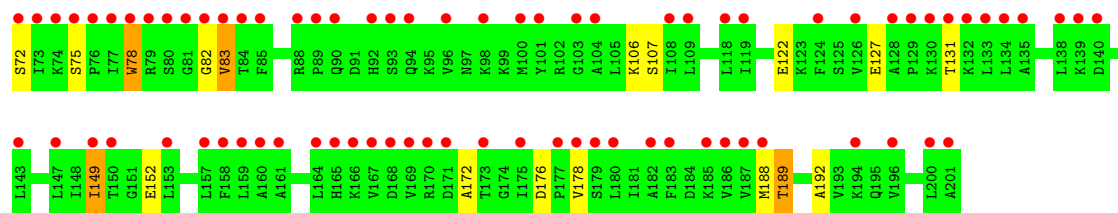




• Molecule 32: 50S ribosomal protein L4

Chain CE:

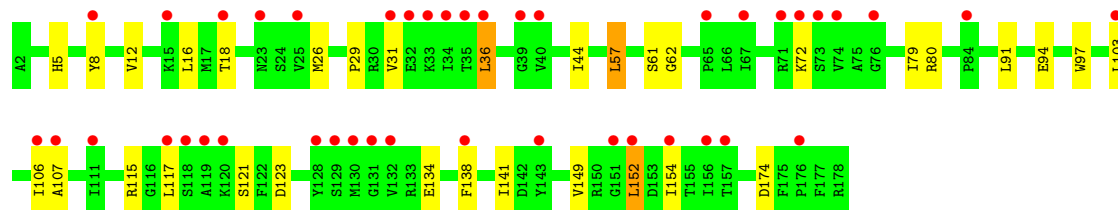
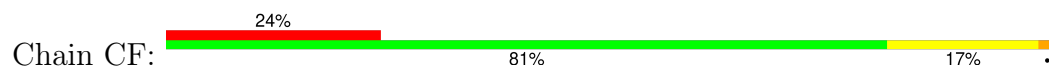




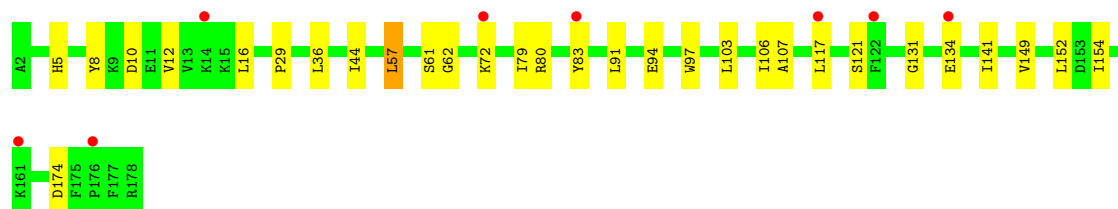
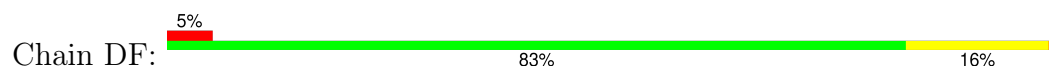
• Molecule 32: 50S ribosomal protein L4



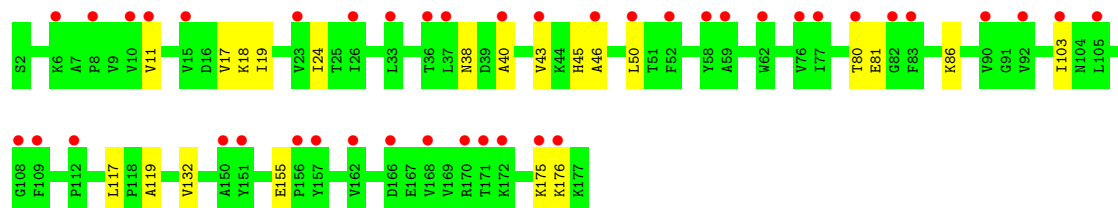
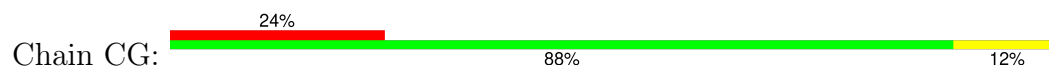
• Molecule 33: 50S ribosomal protein L5



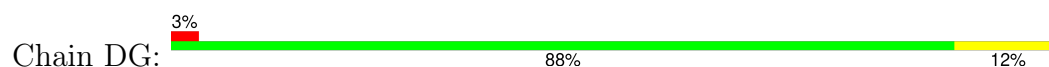
• Molecule 33: 50S ribosomal protein L5



• Molecule 34: 50S ribosomal protein L6

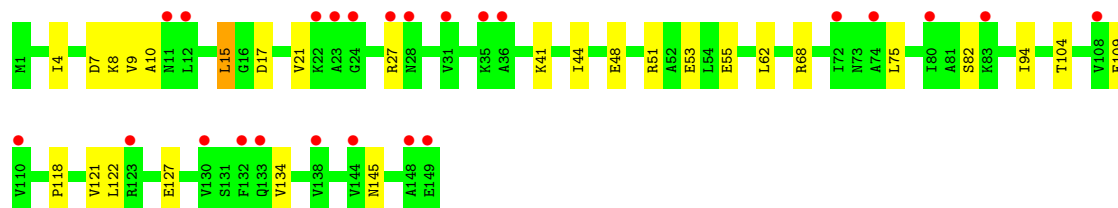
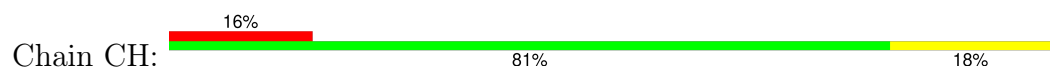


• Molecule 34: 50S ribosomal protein L6

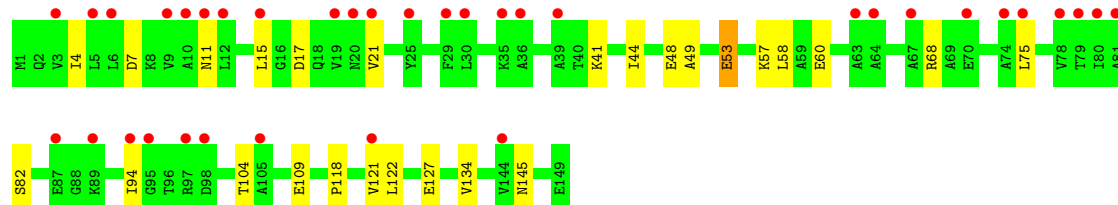
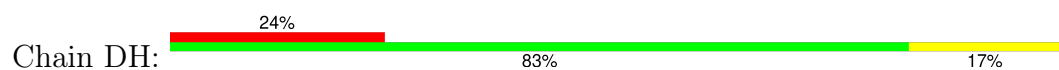




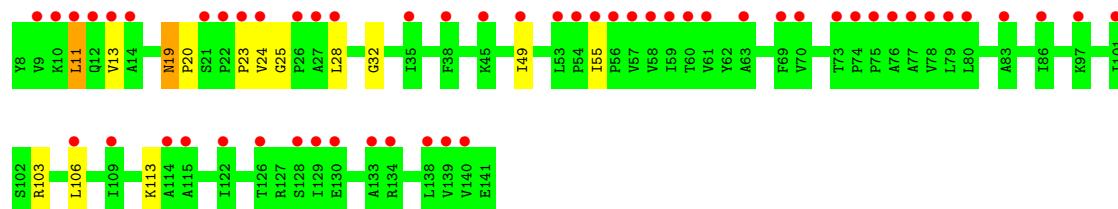
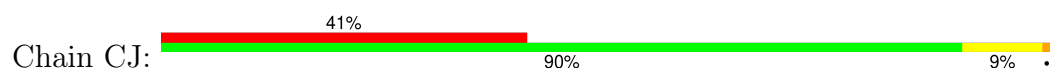
- Molecule 35: 50S ribosomal protein L9



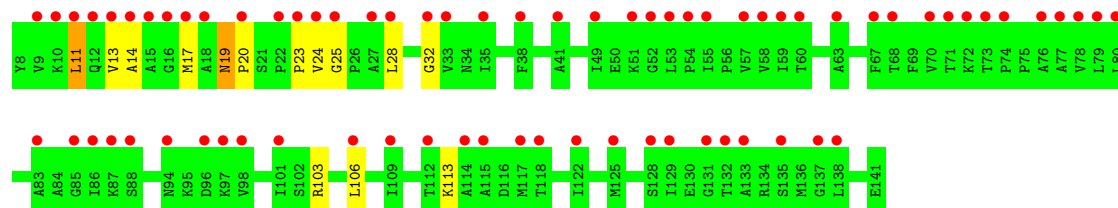
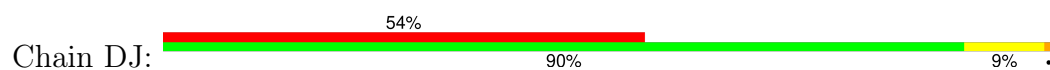
- Molecule 35: 50S ribosomal protein L9



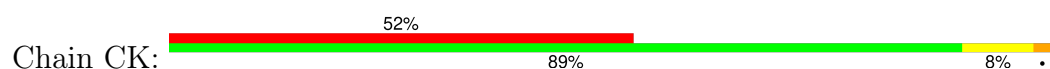
- Molecule 36: 50S ribosomal protein L11

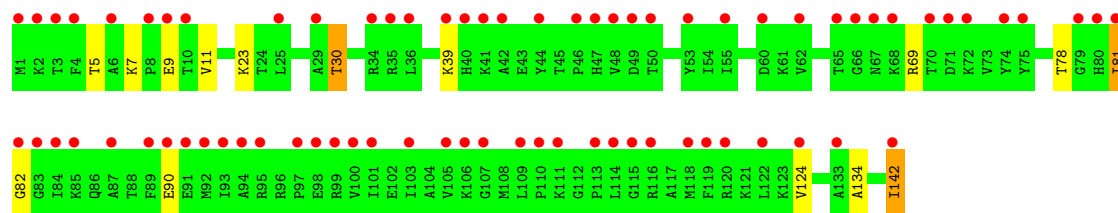


- Molecule 36: 50S ribosomal protein L11



- Molecule 37: 50S ribosomal protein L13





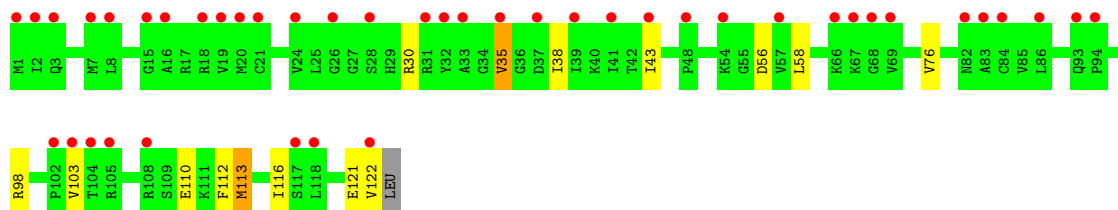
• Molecule 37: 50S ribosomal protein L13

Chain DK: 94% 5% .



• Molecule 38: 50S ribosomal protein L14

Chain CL: 35% 87% 11% ..



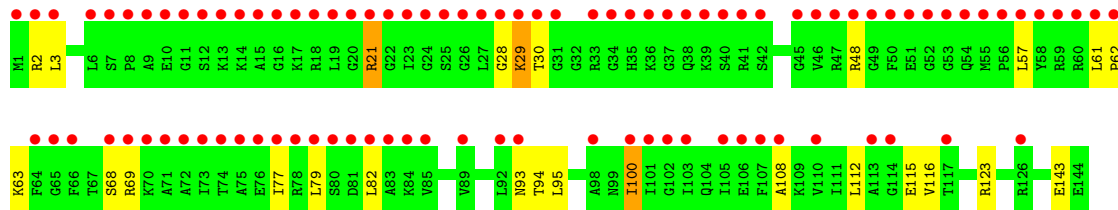
• Molecule 38: 50S ribosomal protein L14

Chain DL: 90% 8% .



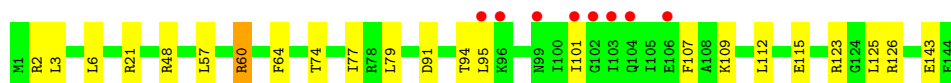
• Molecule 39: 50S ribosomal protein L15

Chain CM: 66% 82% 16% .

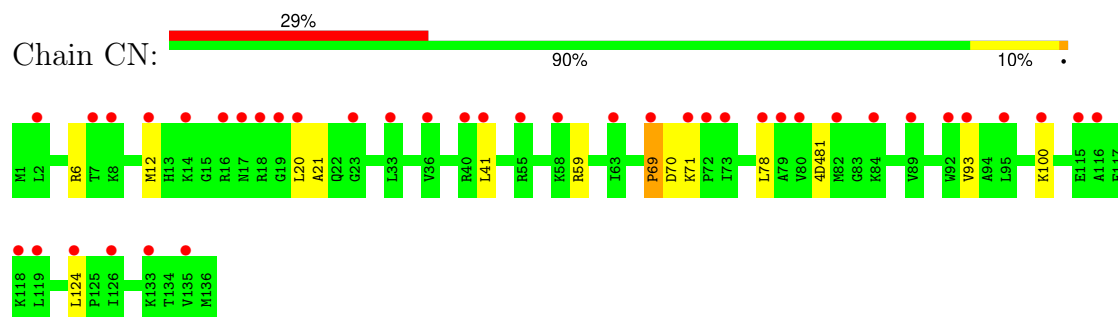


• Molecule 39: 50S ribosomal protein L15

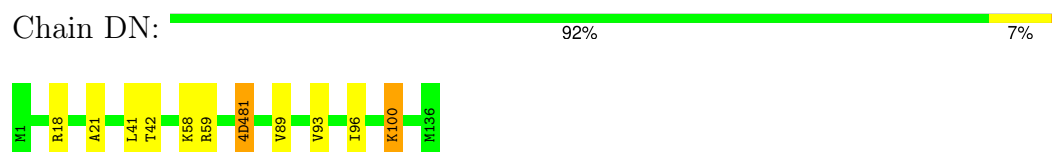
Chain DM: 6% 84% 15% .



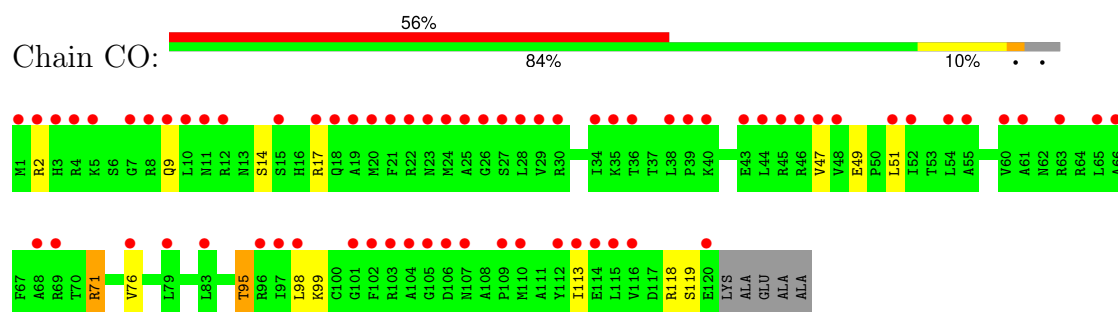
- Molecule 40: 50S ribosomal protein L16



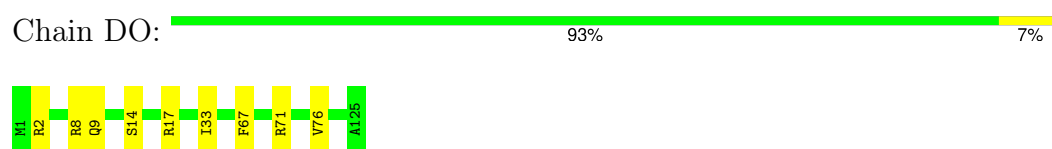
- Molecule 40: 50S ribosomal protein L16



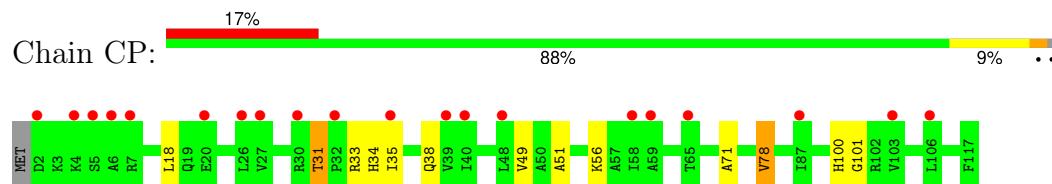
- Molecule 41: 50S ribosomal protein L17



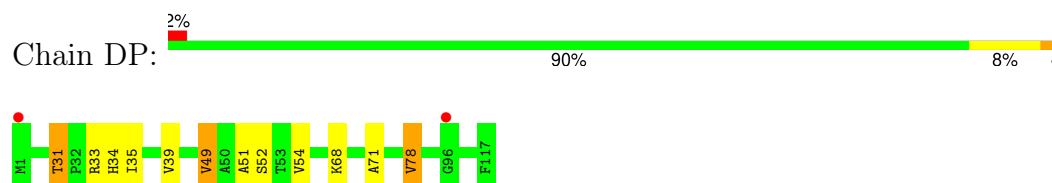
- Molecule 41: 50S ribosomal protein L17



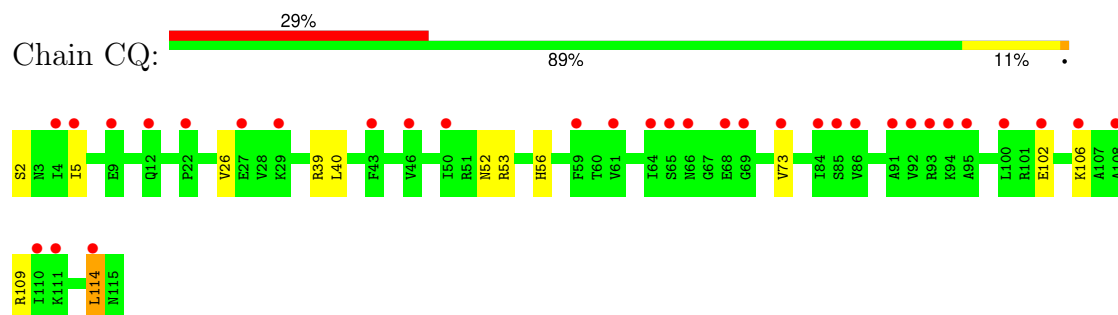
- Molecule 42: 50S ribosomal protein L18



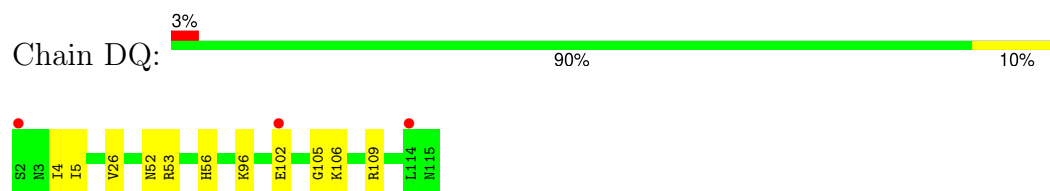
- Molecule 42: 50S ribosomal protein L18



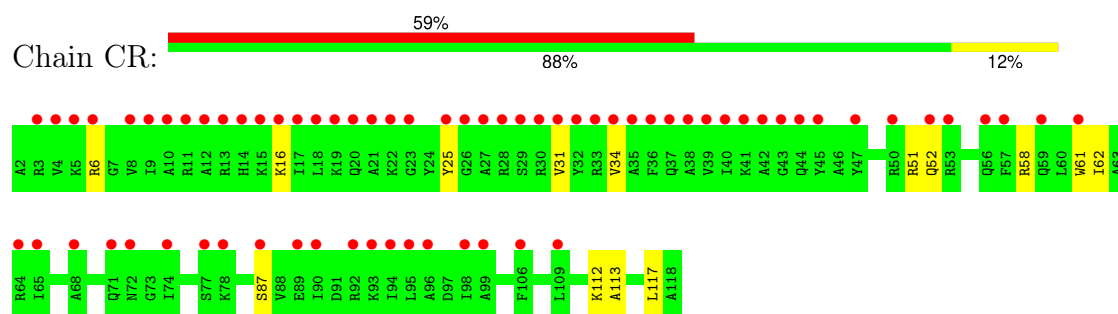
- Molecule 43: 50S ribosomal protein L19



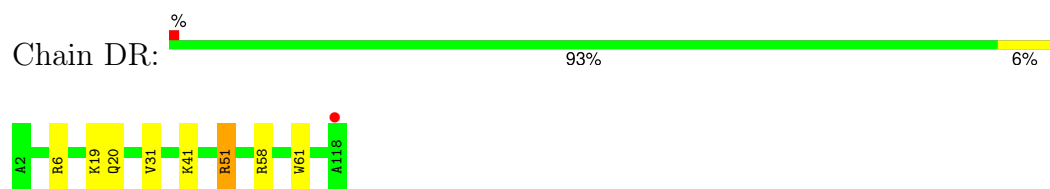
- Molecule 43: 50S ribosomal protein L19



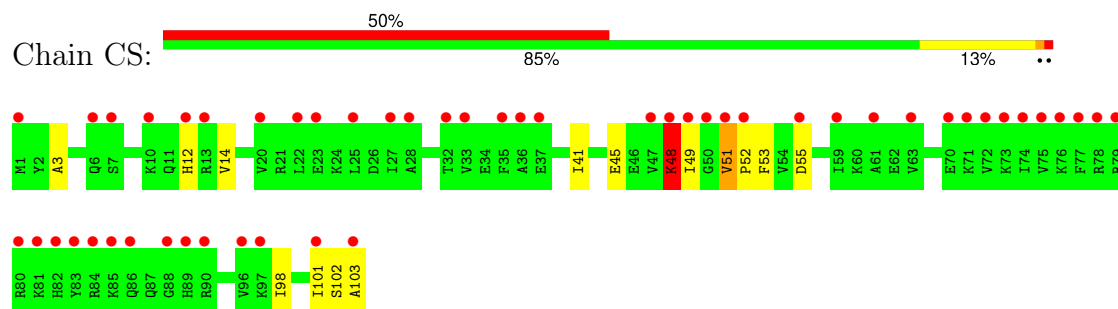
- Molecule 44: 50S ribosomal protein L20



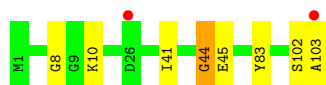
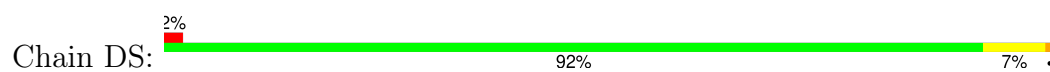
- Molecule 44: 50S ribosomal protein L20



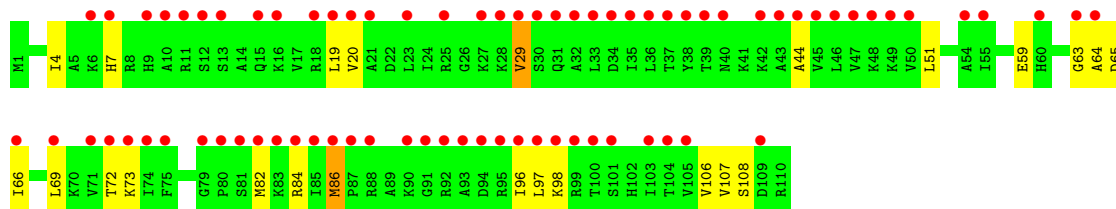
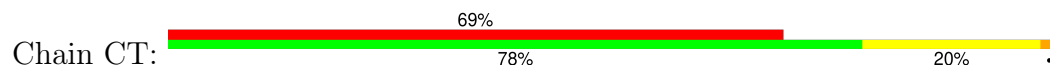
- Molecule 45: 50S ribosomal protein L21



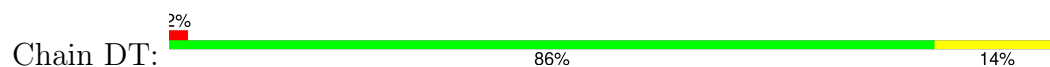
- Molecule 45: 50S ribosomal protein L21



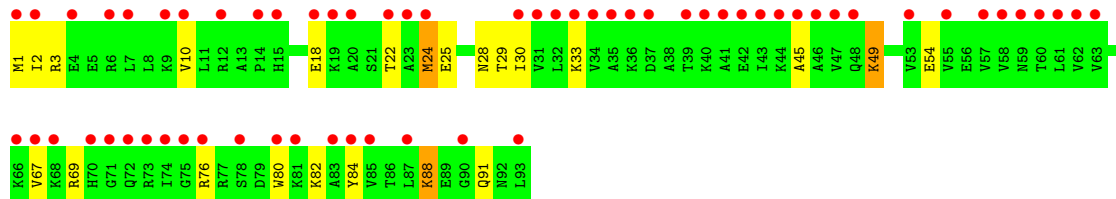
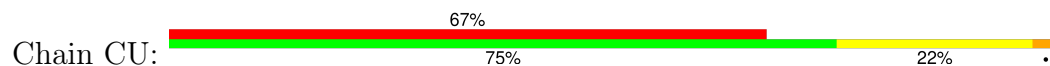
- Molecule 46: 50S ribosomal protein L22



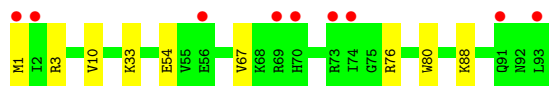
- Molecule 46: 50S ribosomal protein L22



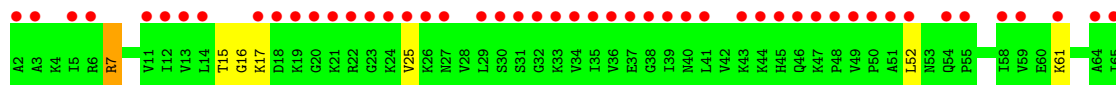
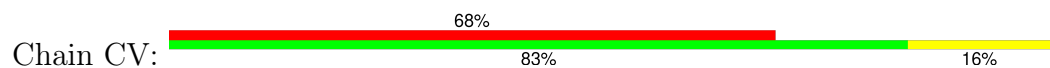
- Molecule 47: 50S ribosomal protein L23

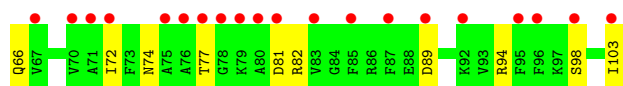


- Molecule 47: 50S ribosomal protein L23

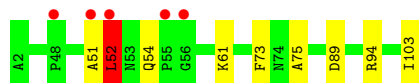


- Molecule 48: 50S ribosomal protein L24

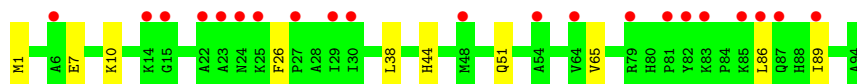




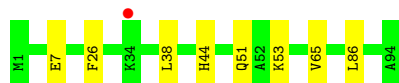
- Molecule 48: 50S ribosomal protein L24



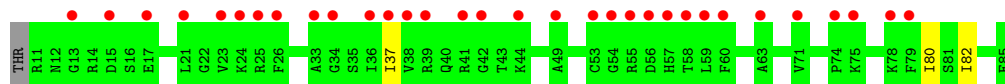
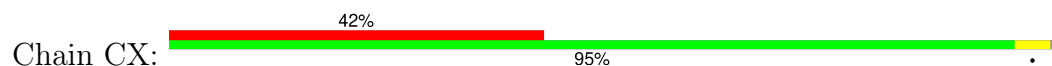
- Molecule 49: 50S ribosomal protein L25



- Molecule 49: 50S ribosomal protein L25



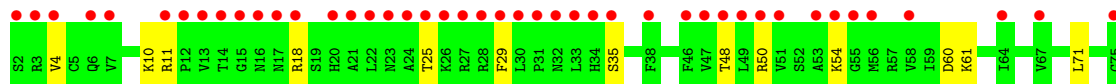
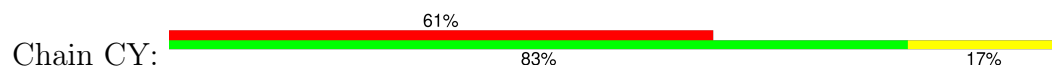
- Molecule 50: 50S ribosomal protein L27



- Molecule 50: 50S ribosomal protein L27



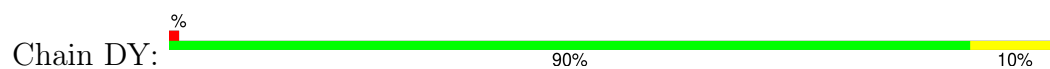
- Molecule 51: 50S ribosomal protein L28



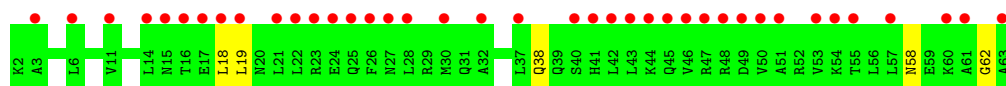




- Molecule 51: 50S ribosomal protein L28



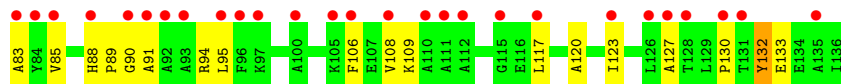
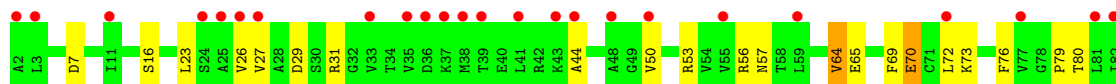
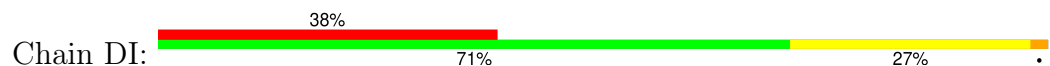
- Molecule 52: 50S ribosomal protein L29



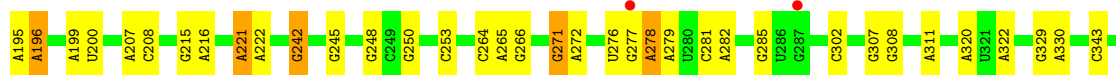
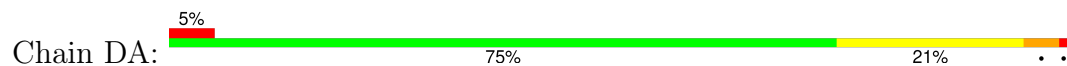
- Molecule 52: 50S ribosomal protein L29



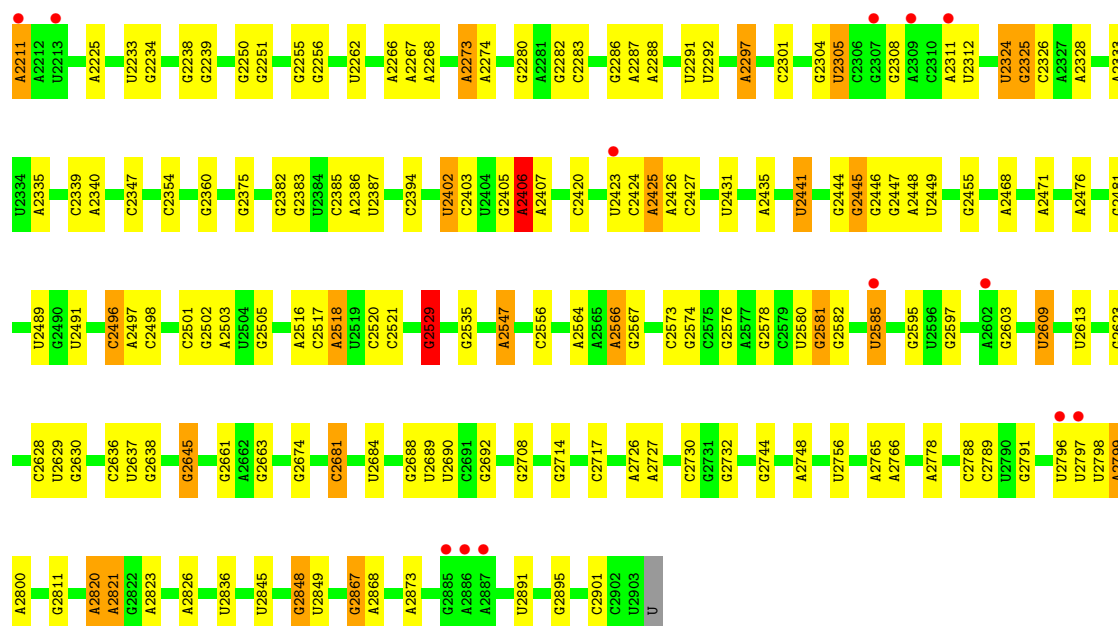
- Molecule 53: 50S ribosomal protein L10



- Molecule 54: 23S rRNA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.31Å 434.58Å 624.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.80 48.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (48.16-2.80) 85.7 (48.16-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.79 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, $R_{free}$	0.209 , 0.219 0.232 , 0.241	Depositor DCC
$R_{free}$ test set	4734 reflections (0.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 93.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	295188	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, OMU, 5MC, 2MA, PSU, TAC, TRS, 5MU, SPD, PEG, MG, 4D4, PGE, 1MG, MPD, ACY, H2U, PUT, OMC, UR3, OMG, EDO, 3TD, D2T, G7M, GUN, 1PE, MEQ, 2MG, PG4, 4OC, 6MZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	1.04	7/36593 (0.0%)	0.86	5/57081 (0.0%)
1	BA	1.05	10/36568 (0.0%)	0.86	5/57042 (0.0%)
2	AB	0.48	0/1784	0.65	0/2403
2	BB	0.48	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.67	0/2225
3	BC	0.47	0/1652	0.67	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.43	0/1665	0.70	0/2227
5	AE	0.48	0/1157	0.77	0/1557
5	BE	0.51	0/1118	0.81	0/1504
6	AF	0.46	0/881	0.69	0/1189
6	BF	0.47	0/835	0.77	0/1128
7	AG	0.45	0/1196	0.61	0/1602
7	BG	0.46	0/1196	0.62	0/1602
8	AH	0.46	0/989	0.71	0/1326
8	BH	0.46	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.66	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.44	0/806	0.67	0/1089
10	BJ	0.48	0/797	0.71	0/1077
11	AK	0.46	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.44	0/960	0.74	0/1286
12	BL	0.47	0/960	0.74	0/1286
13	AM	0.51	0/893	0.72	0/1193
13	BM	0.49	0/893	0.71	0/1193
14	AN	0.46	0/817	0.63	0/1088
14	BN	0.44	0/817	0.63	0/1088
15	AO	0.48	0/722	0.60	0/964
15	BO	0.47	0/722	0.63	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	AP	0.48	0/659	0.70	0/884
16	BP	0.50	0/659	0.76	0/884
17	AQ	0.48	0/658	0.73	0/881
17	BQ	0.51	0/658	0.78	0/881
18	AR	0.53	0/463	0.65	0/621
18	BR	0.50	0/463	0.64	0/621
19	AS	0.47	0/653	0.59	0/877
19	BS	0.45	0/653	0.60	0/877
20	AT	0.48	0/676	0.66	0/895
20	BT	0.52	0/671	0.68	0/888
21	AU	0.45	0/472	0.61	0/627
21	BU	0.43	0/472	0.63	0/627
22	C1	0.49	0/450	0.71	0/599
22	D1	0.61	0/450	0.79	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.51	0/421	0.73	0/561
24	C3	0.46	0/380	0.69	0/498
24	D3	0.55	0/380	0.76	0/498
25	C4	0.46	0/513	0.67	0/676
25	D4	0.56	0/513	0.71	0/676
26	C5	0.43	0/303	0.77	0/397
26	D5	0.53	0/303	0.76	0/397
27	C0	0.52	0/453	0.77	0/605
27	D0	0.62	0/467	0.81	0/623
28	CB	0.98	0/2828	0.88	2/4410 (0.0%)
28	DB	1.12	1/2872 (0.0%)	0.90	0/4478
29	CC	0.45	0/2122	0.76	0/2852
29	DC	0.50	0/2122	0.76	1/2852 (0.0%)
30	CD	0.43	0/1576	0.70	0/2119
30	DD	0.54	0/1576	0.73	0/2119
31	CA	1.07	44/69165 (0.1%)	0.87	17/107896 (0.0%)
32	CE	0.45	0/1571	0.72	0/2113
32	DE	0.52	0/1571	0.72	0/2113
33	CF	0.43	0/1435	0.68	0/1926
33	DF	0.46	0/1435	0.70	0/1926
34	CG	0.42	0/1343	0.66	0/1816
34	DG	0.44	0/1343	0.64	0/1816
35	CH	0.48	0/1121	0.68	0/1515
35	DH	0.48	0/1121	0.68	0/1515
36	CJ	0.48	0/993	0.62	0/1341
36	DJ	0.48	0/993	0.62	0/1341
37	CK	0.43	0/1152	0.70	0/1551
37	DK	0.56	0/1152	0.74	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	CL	0.47	0/947	0.74	0/1268
38	DL	0.54	0/955	0.75	0/1279
39	CM	0.46	0/1062	0.74	1/1413 (0.1%)
39	DM	0.50	0/1062	0.75	1/1413 (0.1%)
40	CN	0.45	0/1081	0.75	1/1443 (0.1%)
40	DN	0.59	0/1092	0.81	0/1457
41	CO	0.46	0/973	0.72	0/1301
41	DO	0.58	0/1006	0.81	0/1345
42	CP	0.43	0/902	0.73	0/1209
42	DP	0.47	0/910	0.73	0/1219
43	CQ	0.41	0/929	0.71	0/1242
43	DQ	0.48	0/929	0.72	0/1242
44	CR	0.48	0/960	0.69	0/1278
44	DR	0.62	0/960	0.76	0/1278
45	CS	0.44	0/829	0.73	0/1107
45	DS	0.55	0/829	0.78	0/1107
46	CT	0.43	0/864	0.74	0/1156
46	DT	0.55	0/864	0.75	0/1156
47	CU	0.44	0/745	0.72	0/994
47	DU	0.48	0/745	0.72	0/994
48	CV	0.45	0/788	0.77	0/1051
48	DV	0.49	0/788	0.77	0/1051
49	CW	0.40	0/766	0.65	0/1025
49	DW	0.50	0/766	0.69	0/1025
50	CX	0.39	0/576	0.65	0/762
50	DX	0.53	0/598	0.73	0/790
51	CY	0.43	0/635	0.73	0/848
51	DY	0.46	0/635	0.72	0/848
52	CZ	0.42	0/502	0.60	0/667
52	DZ	0.43	0/502	0.60	0/667
53	DI	0.51	0/1037	0.74	1/1402 (0.1%)
54	DA	1.27	154/69364 (0.2%)	0.97	25/108207 (0.0%)
All	All	0.98	216/309263 (0.1%)	0.85	59/462195 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
10	BJ	0	1
31	CA	0	12
54	DA	0	89
All	All	0	110

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1020	A	N3-C4	9.99	1.40	1.34
31	CA	1936	A	N9-C4	-9.12	1.32	1.37
31	CA	2095	A	O5'-C5'	-9.03	1.28	1.42
54	DA	539	G	N7-C5	7.80	1.44	1.39
54	DA	195	A	N9-C4	7.60	1.42	1.37
54	DA	12	U	C1'-N1	7.56	1.60	1.48
54	DA	2097	A	O5'-C5'	-7.34	1.31	1.42
54	DA	2050	C	N1-C6	7.33	1.41	1.37
31	CA	769	U	C1'-N1	7.13	1.59	1.48
54	DA	2520	C	N1-C6	7.12	1.41	1.37
54	DA	1286	A	N3-C4	7.07	1.39	1.34
31	CA	12	U	C1'-N1	7.05	1.59	1.48
54	DA	2585	U	C1'-N1	6.98	1.59	1.48
54	DA	2060	A	N3-C4	6.97	1.39	1.34
31	CA	2425	A	C3'-O3'	6.94	1.51	1.42
54	DA	484	C	C1'-N1	6.79	1.58	1.48
1	BA	1493	A	C3'-O3'	6.79	1.51	1.42
31	CA	546	U	C1'-N1	6.78	1.58	1.48
54	DA	1665	A	N7-C5	6.69	1.43	1.39
54	DA	1787	A	N9-C4	6.63	1.41	1.37
1	BA	5	U	C1'-N1	6.53	1.58	1.48
1	BA	1397	C	N1-C2	6.52	1.46	1.40
1	BA	28	A	O5'-C5'	-6.49	1.32	1.42
54	DA	959	A	N3-C4	6.38	1.38	1.34
54	DA	2053	G	C6-N1	6.37	1.44	1.39
54	DA	671	C	C1'-N1	6.34	1.58	1.48
54	DA	1306	C	C1'-N1	6.31	1.58	1.48
31	CA	2225	A	C3'-O3'	6.30	1.50	1.42
54	DA	582	A	N9-C4	6.30	1.41	1.37
54	DA	2547	A	O5'-C5'	-6.23	1.32	1.42
54	DA	998	C	C1'-N1	6.21	1.58	1.48
54	DA	31	C	N1-C6	6.15	1.40	1.37
54	DA	2023	C	N1-C6	6.13	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	28	A	O5'-C5'	-6.11	1.33	1.42
54	DA	1000	A	N3-C4	6.10	1.38	1.34
28	DB	90	C	O5'-C5'	-6.09	1.33	1.42
54	DA	372	G	C3'-O3'	6.09	1.50	1.42
54	DA	727	A	N3-C4	6.08	1.38	1.34
54	DA	2867	G	C3'-O3'	6.07	1.50	1.42
54	DA	579	G	C2'-C1'	-6.04	1.46	1.53
1	BA	1008	U	O5'-C5'	-6.00	1.33	1.42
54	DA	972	A	C6-N6	5.98	1.38	1.33
54	DA	102	U	N1-C2	5.98	1.44	1.38
54	DA	1635	A	N3-C4	5.97	1.38	1.34
54	DA	578	G	N3-C4	5.97	1.39	1.35
54	DA	2547	A	P-O5'	-5.93	1.53	1.59
1	AA	5	U	C1'-N1	5.93	1.57	1.48
54	DA	2518	A	N9-C4	5.93	1.41	1.37
54	DA	2717	C	N1-C6	5.91	1.40	1.37
54	DA	1294	U	O5'-C5'	-5.90	1.33	1.42
54	DA	2297	A	O5'-C5'	-5.90	1.33	1.42
54	DA	984	A	N3-C4	5.90	1.38	1.34
31	CA	253	C	C1'-N1	5.88	1.57	1.48
54	DA	1137	G	N3-C4	5.86	1.39	1.35
54	DA	2756	U	C3'-O3'	5.86	1.50	1.42
54	DA	2044	C	N1-C6	5.85	1.40	1.37
54	DA	1965	C	C1'-N1	5.84	1.57	1.48
1	AA	1397	C	N1-C6	5.82	1.40	1.37
54	DA	2036	C	N1-C6	5.81	1.40	1.37
54	DA	2127	G	C3'-O3'	5.80	1.50	1.42
31	CA	1788	C	C1'-N1	5.80	1.57	1.48
54	DA	2447	G	N3-C4	5.80	1.39	1.35
54	DA	2521	C	N1-C6	5.78	1.40	1.37
31	CA	2619	C	C1'-N1	5.78	1.57	1.48
54	DA	838	C	N1-C6	5.77	1.40	1.37
54	DA	2766	A	N9-C4	5.76	1.41	1.37
54	DA	575	A	N9-C4	5.76	1.41	1.37
54	DA	969	G	C8-N7	-5.76	1.27	1.30
54	DA	1267	U	C2-N3	5.73	1.41	1.37
31	CA	2579	C	C1'-N1	5.73	1.57	1.48
54	DA	1164	C	N1-C6	5.72	1.40	1.37
31	CA	1306	C	C1'-N1	5.72	1.57	1.48
54	DA	2446	G	N3-C4	5.68	1.39	1.35
1	BA	290	C	C1'-N1	5.68	1.57	1.48
54	DA	990	A	N7-C5	5.68	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1534	U	C1'-N1	5.67	1.57	1.48
31	CA	1314	C	C1'-N1	5.65	1.57	1.48
54	DA	1189	A	N9-C4	5.64	1.41	1.37
54	DA	457	A	N3-C4	5.64	1.38	1.34
54	DA	744	U	N1-C6	5.63	1.43	1.38
54	DA	12	U	N1-C2	5.62	1.43	1.38
54	DA	1311	G	C6-N1	5.62	1.43	1.39
54	DA	508	A	N3-C4	5.61	1.38	1.34
54	DA	2426	A	N3-C4	5.61	1.38	1.34
54	DA	1021	A	N9-C4	5.58	1.41	1.37
54	DA	1660	G	O5'-C5'	-5.58	1.33	1.42
31	CA	1658	C	C1'-N1	5.57	1.57	1.48
54	DA	1965	C	C3'-O3'	-5.56	1.34	1.42
54	DA	823	C	N1-C6	5.56	1.40	1.37
1	BA	485	U	N1-C2	5.55	1.43	1.38
54	DA	2576	G	O3'-P	-5.53	1.54	1.61
54	DA	1920	C	C1'-N1	5.53	1.57	1.48
54	DA	2425	A	C3'-O3'	5.52	1.49	1.42
54	DA	2444	G	N7-C5	5.51	1.42	1.39
31	CA	2680	U	C3'-O3'	5.50	1.49	1.42
54	DA	739	A	N3-C4	5.50	1.38	1.34
54	DA	2056	G	C6-N1	5.50	1.43	1.39
1	BA	575	G	C3'-O3'	5.50	1.49	1.42
54	DA	821	A	N3-C4	5.48	1.38	1.34
31	CA	2006	C	C1'-N1	5.46	1.56	1.48
54	DA	2821	A	N3-C4	5.45	1.38	1.34
54	DA	613	A	N9-C4	5.43	1.41	1.37
31	CA	995	C	O5'-C5'	-5.42	1.34	1.42
31	CA	2233	U	C1'-N1	5.42	1.56	1.48
54	DA	561	G	N3-C4	5.41	1.39	1.35
54	DA	810	U	N1-C2	5.39	1.43	1.38
54	DA	1133	A	O5'-C5'	-5.39	1.34	1.42
31	CA	2146	C	C3'-O3'	5.39	1.49	1.42
54	DA	12	U	P-O5'	5.38	1.65	1.59
31	CA	946	C	C1'-N1	5.38	1.56	1.48
31	CA	2823	A	C3'-O3'	5.38	1.49	1.42
1	AA	1203	C	C1'-N1	5.37	1.56	1.48
54	DA	918	A	N3-C4	5.36	1.38	1.34
54	DA	962	G	N3-C4	5.36	1.39	1.35
54	DA	1274	A	N7-C5	-5.36	1.36	1.39
54	DA	469	G	N3-C4	5.36	1.39	1.35
54	DA	196	A	N9-C4	5.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	816	C	N1-C6	5.35	1.40	1.37
54	DA	1270	C	N1-C6	5.35	1.40	1.37
54	DA	2692	G	N3-C4	5.35	1.39	1.35
31	CA	1825	U	C1'-N1	5.35	1.56	1.48
31	CA	404	A	C3'-O3'	5.34	1.49	1.42
54	DA	809	G	N7-C5	5.34	1.42	1.39
54	DA	2730	C	N1-C6	5.34	1.40	1.37
54	DA	653	U	C1'-N1	5.33	1.56	1.48
54	DA	959	A	N9-C4	5.33	1.41	1.37
54	DA	819	A	N3-C4	5.31	1.38	1.34
54	DA	1268	A	N3-C4	5.31	1.38	1.34
54	DA	1664	A	N9-C4	5.31	1.41	1.37
54	DA	613	A	C3'-O3'	5.31	1.49	1.42
31	CA	451	U	C1'-N1	5.30	1.56	1.48
54	DA	2036	C	C1'-N1	5.29	1.56	1.48
31	CA	461	C	C1'-N1	5.29	1.56	1.48
31	CA	653	U	C1'-N1	5.29	1.56	1.48
31	CA	1629	U	C1'-N1	5.27	1.56	1.48
54	DA	1265	A	N9-C4	5.27	1.41	1.37
1	BA	842	U	C3'-O3'	5.27	1.49	1.42
54	DA	2273	A	N3-C4	5.27	1.38	1.34
31	CA	480	A	N9-C4	5.26	1.41	1.37
31	CA	2723	C	C1'-N1	5.26	1.56	1.48
31	CA	557	C	C1'-N1	5.25	1.56	1.48
54	DA	271	G	C3'-O3'	5.25	1.49	1.42
54	DA	27	G	C6-N1	5.23	1.43	1.39
54	DA	2521	C	C1'-N1	5.22	1.56	1.48
1	AA	575	G	C3'-O3'	5.22	1.49	1.42
54	DA	2288	A	N3-C4	5.22	1.38	1.34
54	DA	512	G	N9-C4	5.22	1.42	1.38
31	CA	198	C	C1'-N1	5.21	1.56	1.48
54	DA	264	C	N1-C2	5.20	1.45	1.40
54	DA	2211	A	C3'-O3'	5.20	1.49	1.42
54	DA	1675	C	N1-C6	5.19	1.40	1.37
54	DA	2585	U	N1-C2	5.19	1.43	1.38
31	CA	1771	C	C1'-N1	5.19	1.56	1.48
31	CA	2646	C	C1'-N1	5.18	1.56	1.48
54	DA	2033	A	P-O5'	5.18	1.65	1.59
31	CA	672	C	C1'-N1	5.18	1.56	1.48
54	DA	2901	C	C1'-N1	5.18	1.56	1.48
1	BA	291	U	C1'-N1	5.17	1.56	1.48
31	CA	1971	U	C1'-N1	5.17	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	2354	C	O5'-C5'	-5.17	1.34	1.42
54	DA	1776	G	O5'-C5'	-5.16	1.34	1.42
54	DA	1284	A	N3-C4	5.15	1.38	1.34
54	DA	1965	C	O5'-C5'	-5.15	1.34	1.42
54	DA	2077	A	N3-C4	5.15	1.38	1.34
54	DA	2427	C	N1-C6	5.15	1.40	1.37
54	DA	1584	U	C1'-N1	5.14	1.56	1.48
54	DA	577	G	N3-C4	5.13	1.39	1.35
54	DA	562	U	N1-C6	5.13	1.42	1.38
54	DA	792	A	N3-C4	5.12	1.38	1.34
54	DA	2581	G	C3'-O3'	5.12	1.49	1.42
54	DA	911	A	N3-C4	5.12	1.38	1.34
54	DA	2496	C	O5'-C5'	-5.11	1.34	1.42
54	DA	1030	C	N1-C6	5.11	1.40	1.37
54	DA	581	C	C1'-N1	5.10	1.56	1.48
54	DA	2301	C	C1'-N1	5.10	1.56	1.48
54	DA	585	G	N9-C4	5.10	1.42	1.38
31	CA	2354	C	C1'-N1	5.10	1.56	1.48
31	CA	2465	C	C1'-N1	5.10	1.56	1.48
54	DA	2708	G	N3-C4	5.10	1.39	1.35
54	DA	1704	C	C1'-N1	5.09	1.56	1.48
54	DA	684	G	N3-C4	5.09	1.39	1.35
54	DA	1331	G	N3-C4	5.08	1.39	1.35
1	AA	290	C	C1'-N1	5.08	1.56	1.48
54	DA	353	C	C1'-N1	5.08	1.56	1.48
54	DA	1607	C	N1-C6	5.08	1.40	1.37
31	CA	2756	U	C3'-O3'	5.08	1.49	1.42
54	DA	1335	C	C1'-N1	5.08	1.56	1.48
54	DA	1611	C	N1-C6	5.08	1.40	1.37
54	DA	195	A	N3-C4	5.07	1.37	1.34
31	CA	2215	C	C1'-N1	5.07	1.56	1.48
54	DA	1253	A	O5'-C5'	-5.07	1.34	1.42
54	DA	2406	A	P-O5'	5.07	1.64	1.59
31	CA	2901	C	C1'-N1	5.07	1.56	1.48
54	DA	1644	C	C1'-N1	5.07	1.56	1.48
54	DA	114	U	C1'-N1	5.06	1.56	1.48
54	DA	2455	G	C3'-O3'	-5.06	1.35	1.42
54	DA	465	G	N3-C4	5.06	1.39	1.35
54	DA	2471	A	N3-C4	5.05	1.37	1.34
54	DA	1637	A	N7-C5	5.05	1.42	1.39
31	CA	692	C	C1'-N1	5.04	1.56	1.48
54	DA	12	U	C3'-O3'	5.04	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	15	G	N3-C4	5.04	1.39	1.35
31	CA	2044	C	C1'-N1	5.03	1.56	1.48
31	CA	20	C	C1'-N1	5.03	1.56	1.48
31	CA	1704	C	C1'-N1	5.03	1.56	1.48
54	DA	672	C	N1-C6	5.02	1.40	1.37
54	DA	140	C	C1'-N1	5.01	1.56	1.48
54	DA	1437	C	O5'-C5'	-5.01	1.34	1.42
54	DA	2158	A	C3'-O3'	5.01	1.49	1.42
54	DA	511	U	C1'-N1	5.01	1.56	1.48
54	DA	2585	U	C3'-O3'	5.01	1.49	1.42
54	DA	1999	C	N1-C6	5.01	1.40	1.37
54	DA	2826	A	C8-N7	-5.00	1.28	1.31
54	DA	574	A	O5'-C5'	-5.00	1.34	1.42
54	DA	1020	A	C6-N1	5.00	1.39	1.35
54	DA	2402	U	P-O5'	5.00	1.64	1.59

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.09	116.27	108.20
54	DA	512	G	O4'-C1'-N9	8.48	114.99	108.20
1	AA	413	G	C1'-O4'-C4'	-8.21	103.34	109.90
54	DA	784	G	P-O3'-C3'	7.87	129.15	119.70
40	CN	69	PRO	C-N-CA	7.39	140.17	121.70
54	DA	1936	A	O4'-C1'-N9	7.29	114.03	108.20
1	AA	1	A	OP1-P-OP2	-7.17	108.84	119.60
54	DA	2820	A	P-O3'-C3'	7.12	128.24	119.70
54	DA	892	A	OP1-P-OP2	-7.03	109.05	119.60
53	DI	132	TYR	C-N-CA	7.00	139.21	121.70
31	CA	892	A	OP1-P-OP2	-6.96	109.16	119.60
54	DA	1	G	OP1-P-OP2	-6.87	109.30	119.60
1	BA	1362	A	C1'-O4'-C4'	-6.83	104.44	109.90
31	CA	974	G	N9-C1'-C2'	6.74	122.76	114.00
1	BA	2	A	OP1-P-OP2	-6.69	109.56	119.60
31	CA	271	G	P-O3'-C3'	6.45	127.44	119.70
54	DA	271	G	P-O3'-C3'	6.44	127.42	119.70
1	AA	413	G	O4'-C1'-N9	6.41	113.33	108.20
54	DA	2848	G	O4'-C1'-N9	6.25	113.20	108.20
54	DA	1311	G	O4'-C1'-N9	6.14	113.11	108.20
31	CA	2425	A	P-O3'-C3'	5.95	126.84	119.70
31	CA	512	G	O4'-C1'-N9	5.88	112.90	108.20
31	CA	451	U	C1'-O4'-C4'	-5.87	105.21	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	842	U	P-O3'-C3'	5.84	126.71	119.70
54	DA	1379	U	P-O3'-C3'	5.78	126.63	119.70
39	DM	60	ARG	CG-CD-NE	5.73	123.84	111.80
1	BA	485	U	O4'-C1'-N1	5.70	112.76	108.20
31	CA	1379	U	P-O3'-C3'	5.69	126.53	119.70
31	CA	784	G	P-O3'-C3'	5.69	126.53	119.70
54	DA	704	G	O4'-C1'-N9	5.61	112.69	108.20
54	DA	242	G	C3'-C2'-C1'	-5.59	97.03	101.50
54	DA	2406	A	C5'-C4'-O4'	-5.57	102.41	109.10
54	DA	1434	A	O4'-C1'-N9	5.41	112.53	108.20
54	DA	27	G	O4'-C1'-N9	5.37	112.50	108.20
1	BA	1397	C	C2-N1-C1'	5.35	124.69	118.80
29	DC	156	ARG	CB-CG-CD	-5.33	97.73	111.60
54	DA	1165	A	O4'-C1'-N9	5.33	112.46	108.20
31	CA	2035	G	C1'-O4'-C4'	-5.29	105.67	109.90
31	CA	2095	A	C5'-C4'-C3'	-5.28	107.55	116.00
31	CA	2225	A	P-O3'-C3'	5.25	126.01	119.70
31	CA	704	G	O4'-C1'-N9	5.25	112.40	108.20
31	CA	2825	G	O4'-C1'-N9	5.21	112.37	108.20
54	DA	512	G	C1'-O4'-C4'	-5.20	105.74	109.90
54	DA	2280	G	C4'-C3'-C2'	-5.20	97.40	102.60
31	CA	242	G	C3'-C2'-C1'	-5.19	97.35	101.50
39	CM	68	SER	C-N-CA	5.19	134.67	121.70
54	DA	479	A	C3'-C2'-C1'	-5.18	97.35	101.50
54	DA	2645	G	O4'-C1'-N9	5.18	112.35	108.20
31	CA	2406	A	C5'-C4'-O4'	5.18	115.31	109.10
54	DA	807	U	C4'-C3'-C2'	-5.17	97.43	102.60
1	AA	841	C	P-O3'-C3'	5.14	125.87	119.70
54	DA	1238	G	C4'-C3'-C2'	-5.12	97.48	102.60
28	CB	89	U	O4'-C1'-N1	5.10	112.28	108.20
54	DA	1997	C	C4'-C3'-C2'	-5.10	97.50	102.60
54	DA	2048	G	C8-N9-C4	-5.09	104.36	106.40
31	CA	2447	G	C3'-C2'-C1'	-5.06	97.45	101.50
1	AA	890	G	C3'-C2'-C1'	-5.05	97.46	101.50
54	DA	2447	G	C3'-C2'-C1'	-5.04	97.47	101.50
31	CA	974	G	C3'-C2'-C1'	-5.03	97.47	101.50

There are no chirality outliers.

All (110) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
5	AE	82	GLN	Sidechain
1	BA	1432	G	Sidechain
1	BA	362	G	Sidechain
1	BA	575	G	Sidechain
1	BA	898	G	Sidechain
10	BJ	37	ARG	Mainchain
31	CA	1693	U	Sidechain
31	CA	1777	U	Sidechain
31	CA	1936	A	Sidechain
31	CA	1937	A	Sidechain
31	CA	2267	A	Sidechain
31	CA	2638	G	Sidechain
31	CA	2732	G	Sidechain
31	CA	463	G	Sidechain
31	CA	481	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	805	G	Sidechain
54	DA	1009	A	Sidechain
54	DA	1142	A	Sidechain
54	DA	1236	G	Sidechain
54	DA	1253	A	Sidechain
54	DA	1283	G	Sidechain
54	DA	1311	G	Sidechain
54	DA	1324	G	Sidechain
54	DA	1343	G	Sidechain
54	DA	1425	G	Sidechain
54	DA	15	G	Sidechain
54	DA	1631	G	Sidechain
54	DA	1645	G	Sidechain
54	DA	1666	G	Sidechain
54	DA	1667	G	Sidechain
54	DA	1672	A	Sidechain
54	DA	1681	G	Sidechain
54	DA	1682	G	Sidechain
54	DA	1693	U	Sidechain
54	DA	1753	G	Sidechain
54	DA	1761	C	Sidechain
54	DA	1779	U	Sidechain
54	DA	1802	A	Sidechain

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Mol	Chain	Res	Type	Group
54	DA	1938	A	Sidechain
54	DA	2029	G	Sidechain
54	DA	2037	A	Sidechain
54	DA	2048	G	Sidechain
54	DA	2074	U	Sidechain
54	DA	2078	C	Sidechain
54	DA	221	A	Sidechain
54	DA	2250	G	Sidechain
54	DA	2266	A	Sidechain
54	DA	2267	A	Sidechain
54	DA	2282	G	Sidechain
54	DA	2328	A	Sidechain
54	DA	2375	G	Sidechain
54	DA	2382	G	Sidechain
54	DA	2405	G	Sidechain
54	DA	2468	A	Sidechain
54	DA	2481	G	Sidechain
54	DA	2489	U	Sidechain
54	DA	2497	A	Sidechain
54	DA	250	G	Sidechain
54	DA	2516	A	Sidechain
54	DA	2517	C	Sidechain
54	DA	2529	G	Sidechain
54	DA	2564	A	Sidechain
54	DA	2566	A	Sidechain
54	DA	2581	G	Sidechain
54	DA	2582	G	Sidechain
54	DA	2595	G	Sidechain
54	DA	2597	G	Sidechain
54	DA	2638	G	Sidechain
54	DA	2645	G	Sidechain
54	DA	2688	G	Sidechain
54	DA	27	G	Sidechain
54	DA	2727	A	Sidechain
54	DA	2732	G	Sidechain
54	DA	2848	G	Sidechain
54	DA	307	G	Sidechain
54	DA	308	G	Sidechain
54	DA	395	U	Sidechain
54	DA	452	G	Sidechain
54	DA	463	G	Sidechain
54	DA	464	U	Sidechain

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Mol	Chain	Res	Type	Group
54	DA	481	G	Sidechain
54	DA	512	G	Sidechain
54	DA	555	G	Sidechain
54	DA	575	A	Sidechain
54	DA	577	G	Sidechain
54	DA	58	G	Sidechain
54	DA	630	G	Sidechain
54	DA	675	A	Sidechain
54	DA	690	G	Sidechain
54	DA	700	G	Sidechain
54	DA	704	G	Sidechain
54	DA	726	G	Sidechain
54	DA	727	A	Sidechain
54	DA	728	G	Sidechain
54	DA	748	G	Sidechain
54	DA	774	G	Sidechain
54	DA	775	G	Sidechain
54	DA	800	A	Sidechain
54	DA	805	G	Sidechain
54	DA	858	G	Sidechain
54	DA	910	A	Sidechain
54	DA	956	G	Sidechain
54	DA	959	A	Sidechain
54	DA	980	A	Sidechain
54	DA	984	A	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	90	0
1	BA	32908	0	16580	98	0
2	AB	1753	0	1780	10	0
2	BB	1753	0	1780	14	0
3	AC	1625	0	1696	14	0
3	BC	1625	0	1696	18	0
4	AD	1643	0	1707	13	0
4	BD	1643	0	1707	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	30	0
6	AF	862	0	864	7	0
6	BF	817	0	808	8	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	6	0
9	BI	1022	0	1070	6	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	14	0
11	BK	877	0	887	17	0
12	AL	957	0	1017	7	0
12	BL	957	0	1017	10	0
13	AM	884	0	941	10	0
13	BM	884	0	941	11	0
14	AN	805	0	844	8	0
14	BN	805	0	844	8	0
15	AO	714	0	734	1	0
15	BO	714	0	734	0	0
16	AP	649	0	666	3	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	3	0
19	AS	638	0	665	7	0
19	BS	638	0	665	9	0
20	AT	670	0	719	2	0
20	BT	665	0	714	8	0
21	AU	465	0	491	2	0
21	BU	465	0	491	2	0
22	C1	444	0	458	21	0
22	D1	444	0	458	13	0
23	C2	409	0	440	4	0
23	D2	414	0	442	5	0
24	C3	377	0	418	9	0
24	D3	377	0	418	5	0
25	C4	504	0	572	7	0
25	D4	504	0	572	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C5	302	0	340	7	0
26	D5	302	0	340	1	0
27	C0	449	0	488	3	0
27	D0	463	0	504	1	0
28	CB	2529	0	1281	5	0
28	DB	2569	0	1301	5	0
29	CC	2083	0	2154	17	0
29	DC	2083	0	2154	11	0
30	CD	1565	0	1614	16	0
30	DD	1576	0	1627	16	0
31	CA	62229	0	31318	213	0
32	CE	1552	0	1619	13	0
32	DE	1552	0	1619	11	0
33	CF	1411	0	1444	15	0
33	DF	1411	0	1444	11	0
34	CG	1323	0	1371	9	0
34	DG	1323	0	1371	9	0
35	CH	1110	0	1148	7	0
35	DH	1110	0	1148	6	0
36	CJ	979	0	1028	5	0
36	DJ	979	0	1028	4	0
37	CK	1129	0	1162	10	0
37	DK	1129	0	1162	4	0
38	CL	938	0	1012	8	0
38	DL	946	0	1023	6	0
39	CM	1053	0	1129	16	0
39	DM	1053	0	1129	15	0
40	CN	1075	0	1154	5	0
40	DN	1092	0	1177	7	0
41	CO	960	0	1000	7	0
41	DO	993	0	1034	5	0
42	CP	892	0	923	6	0
42	DP	900	0	935	9	0
43	CQ	917	0	962	7	0
43	DQ	917	0	962	7	0
44	CR	947	0	1019	13	0
44	DR	947	0	1019	9	0
45	CS	816	0	839	8	0
45	DS	816	0	839	5	0
46	CT	857	0	922	12	0
46	DT	857	0	922	10	0
47	CU	739	0	807	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DU	739	0	807	4	0
48	CV	780	0	831	6	0
48	DV	780	0	831	4	0
49	CW	753	0	780	5	0
49	DW	753	0	780	3	0
50	CX	569	0	581	1	0
50	DX	591	0	606	7	0
51	CY	625	0	652	7	0
51	DY	625	0	652	4	0
52	CZ	501	0	531	0	0
52	DZ	501	0	531	1	0
53	DI	1023	0	1052	19	0
54	DA	62423	0	31411	171	0
55	AA	71	0	0	0	0
55	BA	43	0	0	0	0
55	C3	1	0	0	0	0
55	CA	155	0	0	0	0
55	CB	3	0	0	0	0
55	DA	182	0	0	0	0
55	DB	9	0	0	0	0
55	DD	2	0	0	0	0
55	DM	1	0	0	0	0
55	DR	2	0	0	0	0
56	AA	13	0	18	1	0
56	BA	13	0	18	0	0
56	DA	26	0	36	2	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	1	0
57	AA	16	0	28	0	0
57	DA	40	0	70	5	0
57	DE	16	0	28	0	0
57	DK	8	0	14	0	0
57	DN	8	0	14	1	0
57	DS	8	0	14	0	0
57	DT	16	0	28	0	0
58	AA	24	0	48	0	0
58	DA	72	0	144	10	0
59	AA	32	0	21	1	0
59	BA	32	0	21	1	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
61	D3	7	0	10	2	0
61	DA	35	0	50	1	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	0	0
62	D1	4	0	6	0	0
62	DA	36	0	54	2	0
62	DB	8	0	12	1	0
63	D1	10	0	14	2	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	0
63	DD	10	0	14	2	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	4	0
65	DA	32	0	44	0	0
66	DA	12	0	11	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	4	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	5	0	0	0	0
69	AL	8	0	0	0	0
69	AM	4	0	0	1	0
69	AN	5	0	0	1	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	2	0	0	0	0
69	AU	3	0	0	0	0
69	BA	287	0	0	1	0
69	BD	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	1	0	0	0	0
69	BL	3	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	0	0
69	BR	1	0	0	0	0
69	BT	4	0	0	0	0
69	BU	2	0	0	0	0
69	C3	3	0	0	1	0
69	C4	2	0	0	0	0
69	CA	692	0	0	1	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	5	0	0	0	0
69	CE	7	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	3	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	27	0	0	0	0
69	D1	42	0	0	0	0
69	D2	7	0	0	0	0
69	D3	24	0	0	0	0
69	D4	33	0	0	1	0
69	D5	13	0	0	0	0
69	DA	4834	0	0	7	0
69	DB	212	0	0	0	0
69	DC	102	0	0	0	0
69	DD	105	0	0	1	0
69	DE	63	0	0	0	0
69	DF	14	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	58	0	0	0	0
69	DL	51	0	0	0	0
69	DM	62	0	0	0	0
69	DN	71	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DO	44	0	0	0	0
69	DP	35	0	0	0	0
69	DQ	27	0	0	1	0
69	DR	64	0	0	0	0
69	DS	51	0	0	0	0
69	DT	69	0	0	1	0
69	DU	17	0	0	0	0
69	DV	19	0	0	0	0
69	DW	31	0	0	0	0
69	DX	30	0	0	1	0
69	DY	9	0	0	0	0
69	DZ	7	0	0	0	0
All	All	295188	0	194452	1182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (1182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:CS:14:VAL:HG21	45:CS:98:ILE:HG13	1.32	1.05
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.43	0.98
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
47:CU:28:ASN:HD21	47:CU:91:GLN:HB3	1.29	0.96
14:AN:66:GLN:HB2	69:AN:205:HOH:O	1.67	0.95
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.50	0.93
39:CM:82:LEU:HD11	39:CM:116:VAL:HG23	1.52	0.92
45:CS:14:VAL:CG2	45:CS:98:ILE:HG13	1.99	0.90
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	1.86	0.90
39:CM:77:ILE:HD11	39:CM:108:ALA:HB1	1.55	0.89
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.55	0.87
31:CA:1005:C:O2'	37:CK:30:THR:HG21	1.75	0.86
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	1.91	0.86
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.58	0.85
31:CA:2796:U:H3	31:CA:2799:A:H61	1.22	0.85
31:CA:1779:U:H5	31:CA:1784:A:N7	1.74	0.85
1:BA:1305:G:H21	1:BA:1332:A:H2	1.24	0.83
54:DA:2796:U:H3	54:DA:2799:A:H61	1.21	0.83
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.43	0.83
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.14	0.82
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1305:G:H21	1:AA:1332:A:H2	1.23	0.81
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.62	0.81
32:CE:149:ILE:HG12	32:CE:188:MET:HG2	1.62	0.81
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.62	0.81
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.62	0.80
54:DA:2033:A:H5'	69:DA:4112:HOH:O	1.81	0.80
45:CS:14:VAL:HG21	45:CS:98:ILE:CG1	2.11	0.79
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.18	0.79
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.63	0.79
44:DR:20:GLN:CG	56:DR:202:PG4:H42	2.12	0.79
40:DN:18[A]:ARG:HG2	28:DB:90:C:H5'	1.64	0.78
44:DR:20:GLN:HG3	56:DR:202:PG4:H42	1.64	0.78
54:DA:135:U:H3	54:DA:144:A:H61	1.32	0.77
34:DG:24:ILE:HD11	34:DG:43:VAL:HG11	1.66	0.77
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.67	0.77
34:CG:24:ILE:HD11	34:CG:43:VAL:HG11	1.66	0.77
31:CA:135:U:H3	31:CA:144:A:H61	1.33	0.77
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.15	0.77
54:DA:568:U:H1'	54:DA:2030:6MZ:H9C1	1.66	0.77
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.20	0.76
1:BA:664:G:H22	1:BA:741:G:H1	1.34	0.76
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.66	0.76
38:CL:38:ILE:HD11	38:CL:112:PHE:HZ	1.49	0.76
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.68	0.75
1:AA:664:G:H22	1:AA:741:G:H1	1.34	0.75
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.69	0.74
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.70	0.74
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.70	0.73
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.70	0.73
31:CA:528:A:C2	31:CA:2043:C:H4'	2.23	0.73
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.69	0.73
1:AA:842:U:H4'	1:AA:843:U:OP1	1.88	0.73
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.37	0.73
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.23	0.73
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.69	0.73
24:C3:7:PRO:HB2	31:CA:1309:G:H4'	1.71	0.72
54:DA:2127:G:H4'	54:DA:2128:G:OP1	1.90	0.72
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.71	0.71
38:DL:38:ILE:HD11	38:DL:112:PHE:HZ	1.53	0.71
1:AA:73:C:HO2'	1:AA:74:A:H8	1.38	0.70
1:BA:202:G:HO2'	1:BA:468:A:H8	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CT:86:MET:HB2	46:CT:96:ILE:HD11	1.73	0.70
54:DA:1913:A:H4'	54:DA:1913:A:OP1	1.90	0.70
54:DA:2255:G:H21	68:DA:3219:TRS:H12	1.56	0.70
31:CA:1936:A:H2	31:CA:1943:U:N3	1.83	0.70
31:CA:846:U:H1'	31:CA:847:U:H5	1.56	0.70
25:D4:54:ASP:HB3	39:DM:57:LEU:HD22	1.74	0.70
54:DA:2628:C:H5'	58:DA:3195:PUT:H12	1.73	0.69
31:CA:1478:G:H1	31:CA:1513:U:H3	1.39	0.69
53:DI:64:VAL:HG22	53:DI:69:PHE:HB2	1.75	0.69
54:DA:1478:G:H1	54:DA:1513:U:H3	1.38	0.68
2:BB:23:TRP:HB3	2:BB:39:HIS:HE1	1.56	0.68
33:CF:36:LEU:HD21	33:CF:91:LEU:HD11	1.76	0.68
25:C4:60:ALA:O	39:CM:48:ARG:HD2	1.94	0.68
58:DA:3195:PUT:H11	69:DA:5709:HOH:O	1.94	0.68
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.76	0.67
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.09	0.67
22:C1:15:MET:HB3	31:CA:2045:C:O3'	1.94	0.67
51:CY:4:VAL:HG22	51:CY:11:ARG:HG3	1.75	0.67
38:DL:30:ARG:HD2	54:DA:2674:G:H4'	1.76	0.67
48:DV:52:LEU:HB3	48:DV:54:GLN:HB2	1.77	0.67
31:CA:674:G:H1'	32:CE:69:ARG:HD2	1.77	0.67
31:CA:45:G:H5''	31:CA:46:G:H5'	1.76	0.67
42:DP:39:VAL:HB	42:DP:49:VAL:HG23	1.76	0.66
1:BA:73:C:HO2'	1:BA:74:A:H8	1.43	0.66
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.95	0.66
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.94	0.66
22:D1:55:ILE:HD12	41:DO:33:ILE:HD11	1.78	0.66
1:AA:202:G:HO2'	1:AA:468:A:H8	1.44	0.66
39:CM:79:LEU:HD11	39:CM:112:LEU:HD12	1.77	0.66
34:CG:80:THR:HG23	34:CG:81:GLU:H	1.60	0.65
54:DA:45:G:H5''	54:DA:46:G:H5'	1.77	0.65
24:D3:7:PRO:HB2	54:DA:1309:G:H4'	1.78	0.65
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.78	0.65
31:CA:1250:G:H5''	44:CR:6:ARG:HD3	1.79	0.65
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.78	0.64
31:CA:974:G:H8	31:CA:990:A:H62	1.46	0.64
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.97	0.64
1:AA:412:A:H3'	1:AA:413:G:H5'	1.79	0.64
1:BA:841:C:H3'	1:BA:842:U:C5'	2.27	0.64
33:DF:61:SER:HB2	33:DF:91:LEU:HD21	1.79	0.64
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.80	0.64
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.80	0.63
33:CF:61:SER:HB2	33:CF:91:LEU:HD21	1.80	0.63
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.33	0.63
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.80	0.63
54:DA:31:C:O3'	54:DA:1238:G:H5''	1.98	0.63
54:DA:1105:U:H2'	54:DA:1106:G:C8	2.33	0.63
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.80	0.63
38:CL:76:VAL:HG12	43:CQ:73:VAL:HB	1.81	0.63
46:CT:82:MET:HB2	46:CT:98:LYS:HB2	1.79	0.63
39:DM:77:ILE:HD11	39:DM:101:ILE:CG2	2.29	0.63
54:DA:2256:G:H21	56:DA:3193:PG4:H31	1.63	0.63
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.98	0.62
31:CA:17:G:H4'	44:CR:25:TYR:HE2	1.62	0.62
44:DR:20:GLN:HG2	56:DR:202:PG4:H51	1.81	0.62
54:DA:1482:G:H1'	54:DA:1509:A:H61	1.65	0.62
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.47	0.62
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.82	0.62
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.80	0.62
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.82	0.62
24:C3:30:VAL:HG13	31:CA:466:A:H5''	1.81	0.62
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.80	0.62
42:DP:31:THR:HG21	28:DB:28:C:OP1	2.00	0.62
54:DA:788:A:H3'	58:DA:3221:PUT:H41	1.82	0.62
1:BA:209:U:H4'	1:BA:210:C:OP2	2.01	0.61
5:AE:77:ASN:HB2	5:AE:82:GLN:HE22	1.61	0.61
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.82	0.61
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.82	0.61
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.82	0.61
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.65	0.61
63:DD:301:PGE:H12	54:DA:2623:G:OP1	2.01	0.61
54:DA:1847:A:HO2'	54:DA:1848:A:H8	1.48	0.61
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.83	0.61
35:CH:15:LEU:HD22	35:CH:15:LEU:H	1.66	0.61
25:C4:54:ASP:HB3	39:CM:57:LEU:HD22	1.82	0.61
44:DR:20:GLN:HG2	56:DR:202:PG4:H42	1.81	0.60
32:DE:48:THR:HG23	32:DE:88:ARG:NH1	2.16	0.60
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.81	0.60
33:CF:31:VAL:CG1	33:CF:97:TRP:CH2	2.84	0.60
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.83	0.60
46:DT:82:MET:HB2	46:DT:98:LYS:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.36	0.60
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.66	0.60
47:DU:80:TRP:HB3	63:DU:101:PGE:H32	1.84	0.60
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.49	0.60
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.66	0.60
46:CT:59:GLU:HA	46:CT:64:ALA:HA	1.82	0.60
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.67	0.59
1:BA:843:U:H5''	1:BA:843:U:H6	1.67	0.59
31:CA:528:A:H8	31:CA:528:A:H3'	1.67	0.59
1:BA:9:G:H4'	5:BE:109:GLY:H	1.66	0.59
1:BA:978:A:HO2'	1:BA:1322:C:H5	1.51	0.59
31:CA:1779:U:C5	31:CA:1784:A:N7	2.64	0.59
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.68	0.59
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.82	0.59
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.83	0.59
44:DR:31:VAL:HG13	54:DA:580:U:O3'	2.02	0.59
1:BA:1141:C:HO2'	1:BA:1142:G:H8	1.51	0.59
31:CA:528:A:H3'	31:CA:528:A:C8	2.38	0.59
32:DE:33:VAL:HG22	57:DA:3192:MPD:H12	1.84	0.59
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.38	0.59
1:AA:451:A:H61	1:AA:481:G:H5'	1.67	0.59
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.48	0.59
1:AA:202:G:H21	1:AA:466:A:H61	1.51	0.58
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.85	0.58
31:CA:372:G:H5''	51:CY:61:LYS:HD3	1.83	0.58
44:DR:19:LYS:HB3	56:DR:202:PG4:H41	1.85	0.58
31:CA:2728:U:O2'	31:CA:2729:G:H5''	2.04	0.58
1:BA:841:C:H3'	1:BA:842:U:H5''	1.85	0.58
54:DA:2128:G:H1	54:DA:2160:C:H42	1.52	0.58
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.43	0.58
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.86	0.58
22:C1:38:HIS:CE1	31:CA:2884:U:O4	2.54	0.58
5:BE:133:PRO:O	5:BE:137:VAL:HG12	2.02	0.58
54:DA:12:U:H2'	54:DA:12:U:O2	2.04	0.58
1:BA:946:A:H2'	1:BA:947:G:C8	2.38	0.58
41:CO:49:GLU:OE2	41:CO:95:THR:HG22	2.04	0.58
1:AA:946:A:H2'	1:AA:947:G:C8	2.39	0.58
30:DD:114:LYS:HE2	54:DA:2681:C:OP2	2.04	0.58
54:DA:1105:U:H2'	54:DA:1106:G:H8	1.68	0.58
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.86	0.58
35:CH:41:LYS:HA	35:CH:44:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:120:VAL:HG12	29:CC:134:ASN:ND2	2.19	0.57
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.87	0.57
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.86	0.57
1:BA:209:U:H2'	1:BA:209:U:O2	2.03	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.86	0.57
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.33	0.57
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.86	0.57
31:CA:550:C:H2'	31:CA:551:G:H5''	1.86	0.57
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.86	0.57
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.57
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.40	0.57
33:CF:36:LEU:HD21	33:CF:91:LEU:CD1	2.34	0.57
35:CH:27:ARG:HH11	51:CY:60:ASP:HA	1.70	0.57
32:DE:189:THR:HG22	32:DE:192:ALA:H	1.69	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.86	0.57
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.68	0.57
39:CM:28:GLY:O	39:CM:29:LYS:O	2.21	0.57
46:CT:66:ILE:HA	46:CT:69:LEU:HD22	1.87	0.57
47:CU:24:MET:HG2	47:CU:29:THR:O	2.05	0.57
34:DG:42:GLU:HG2	34:DG:55:ARG:HH21	1.68	0.57
1:AA:1141:C:HO2'	1:AA:1142:G:H8	1.52	0.57
29:DC:120:VAL:HG12	29:DC:134:ASN:ND2	2.20	0.57
35:DH:41:LYS:HA	35:DH:44:ILE:HG12	1.86	0.57
1:AA:81:A:H61	1:AA:86:G:H1	1.53	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.69	0.56
22:C1:49:TYR:OH	31:CA:2883:A:OP1	2.22	0.56
1:BA:451:A:H61	1:BA:481:G:H5'	1.69	0.56
22:D1:8:PRO:HG2	54:DA:1264:A:H5'	1.86	0.56
22:C1:19:HIS:CD2	31:CA:2046:G:H1'	2.41	0.56
31:CA:2394:C:H5''	39:CM:63:LYS:HE2	1.88	0.56
30:DD:146:ILE:HD12	30:DD:155:VAL:HG21	1.87	0.56
32:CE:189:THR:HG22	32:CE:192:ALA:H	1.71	0.56
40:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.88	0.56
5:BE:77:ASN:HB2	5:BE:82:GLN:HE22	1.69	0.56
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.70	0.56
39:DM:77:ILE:HD11	39:DM:101:ILE:HG21	1.87	0.56
54:DA:62:U:O4'	57:DA:3203:MPD:H31	2.05	0.56
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.40	0.56
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.56
43:DQ:96:LYS:HE3	69:DQ:306:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:550:C:H2'	54:DA:551:G:H5''	1.87	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.36	0.56
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.53	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.88	0.56
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.86	0.56
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.36	0.55
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.41	0.55
24:D3:4:THR:HG22	54:DA:687:C:H1'	1.88	0.55
31:CA:2304:G:H5'	33:CF:121:SER:HB2	1.88	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
24:C3:30:VAL:CG1	31:CA:466:A:H5''	2.36	0.55
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.71	0.55
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.89	0.55
31:CA:457:A:N1	31:CA:470:A:H5''	2.21	0.55
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.70	0.55
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.87	0.55
54:DA:31:C:O2'	54:DA:1238:G:H5'	2.06	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.88	0.55
1:AA:412:A:H3'	1:AA:413:G:C5'	2.37	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.88	0.55
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.53	0.55
4:BD:85:ASN:HB3	4:BD:88:GLU:HB2	1.89	0.55
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.72	0.55
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.89	0.55
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.88	0.55
54:DA:2297:A:C8	54:DA:2297:A:H5''	2.42	0.55
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.41	0.55
47:CU:22:THR:HA	47:CU:25:GLU:HG2	1.87	0.55
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.88	0.54
28:CB:55:U:H1'	33:CF:26:MET:HG3	1.89	0.54
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.89	0.54
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.88	0.54
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.88	0.54
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.54
27:C0:12:SER:HB3	31:CA:988:A:P	2.47	0.54
43:DQ:106:LYS:HA	43:DQ:109:ARG:HD3	1.90	0.54
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.38	0.54
1:BA:108:G:H5''	1:BA:108:G:N3	2.23	0.54
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.90	0.54
64:DA:3223:SPD:H92	64:DA:3223:SPD:H52	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.90	0.54
24:C3:2:LYS:NZ	69:C3:201:HOH:O	2.40	0.54
25:D4:8:ARG:HD3	54:DA:245:G:O6	2.08	0.54
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.54
44:CR:87:SER:HB3	45:CS:52:PRO:HD3	1.90	0.54
5:BE:35:ALA:O	5:BE:50:TYR:O	2.26	0.54
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.54
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.42	0.54
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.54
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.22	0.54
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.73	0.54
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.90	0.54
47:DU:67:VAL:HG22	47:DU:76:ARG:HG3	1.90	0.54
1:AA:108:G:N3	1:AA:108:G:H5''	2.22	0.53
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.43	0.53
43:CQ:106:LYS:HA	43:CQ:109:ARG:HD3	1.90	0.53
1:AA:1144:G:H21	1:AA:1146:A:H62	1.56	0.53
4:AD:85:ASN:HB3	4:AD:88:GLU:HB2	1.90	0.53
1:BA:374:A:OP1	1:BA:452:A:N1	2.42	0.53
32:CE:149:ILE:HD12	32:CE:172:ALA:HA	1.89	0.53
33:CF:31:VAL:HG11	33:CF:97:TRP:CH2	2.43	0.53
1:AA:209:U:H4'	1:AA:210:C:OP2	2.08	0.53
39:CM:82:LEU:HD11	39:CM:116:VAL:CG2	2.32	0.53
1:BA:1144:G:H21	1:BA:1146:A:H62	1.56	0.53
63:D1:102:PGE:H42	46:DT:23:LEU:HD23	1.91	0.53
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.91	0.53
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.08	0.53
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.90	0.53
35:CH:4:ILE:HD11	35:CH:44:ILE:HG22	1.90	0.53
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.73	0.53
8:BH:29:SER:HB3	8:BH:57:PRO:HB2	1.91	0.53
31:CA:2845:U:H5''	43:CQ:52:ASN:O	2.09	0.53
54:DA:2796:U:H3	54:DA:2799:A:N6	1.97	0.53
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.91	0.53
38:DL:76:VAL:CG2	54:DA:2684:U:H4'	2.38	0.53
53:DI:69:PHE:HB3	53:DI:72:LEU:HD12	1.91	0.53
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.91	0.53
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.91	0.53
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.90	0.53
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.74	0.53
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:328:U:O3'	48:CV:66:GLN:HG3	2.09	0.53
43:DQ:52:ASN:O	54:DA:2845:U:H5''	2.09	0.53
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.91	0.53
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.91	0.53
22:C1:17:ARG:NH2	31:CA:1266:G:OP2	2.42	0.53
25:D4:64:TYR:CE2	54:DA:242:G:H5''	2.44	0.53
31:CA:1936:A:C2	31:CA:1943:U:N3	2.59	0.53
23:D2:8:LYS:HE3	54:DA:2420:C:H5''	1.91	0.52
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.92	0.52
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.08	0.52
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.91	0.52
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.92	0.52
34:DG:175:LYS:HG3	54:DA:2529:G:H4'	1.91	0.52
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.73	0.52
31:CA:2037:A:H2'	31:CA:2038:G:C8	2.44	0.52
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.75	0.52
31:CA:118:A:N3	31:CA:178:G:H1'	2.25	0.52
31:CA:2796:U:H3	31:CA:2799:A:N6	1.99	0.52
30:DD:128:ARG:HG3	69:DA:7413:HOH:O	2.09	0.52
31:CA:2297:A:C8	31:CA:2297:A:H5''	2.45	0.52
34:DG:86:LYS:HG2	34:DG:132:VAL:HG22	1.91	0.52
54:DA:74:A:H5''	54:DA:74:A:N3	2.25	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
31:CA:668:A:H2'	31:CA:670:A:H62	1.75	0.52
34:CG:86:LYS:HG2	34:CG:132:VAL:HG22	1.92	0.52
42:CP:100:HIS:CD2	42:CP:101:GLY:H	2.28	0.52
1:AA:86:G:H21	1:AA:87:C:H41	1.58	0.52
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.91	0.52
47:DU:54:GLU:HB3	47:DU:88:LYS:HD2	1.92	0.52
64:DA:3223:SPD:H92	64:DA:3223:SPD:C5	2.40	0.52
1:AA:845:A:O4'	1:AA:845:A:P	2.68	0.52
11:AK:23:ILE:HD11	11:AK:86:VAL:HG13	1.92	0.52
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.24	0.52
31:CA:699:A:H2'	31:CA:700:G:O4'	2.10	0.52
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.45	0.52
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.93	0.52
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.91	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.74	0.52
32:CE:21:ARG:HD3	32:CE:106:LYS:HB3	1.92	0.52
32:DE:21:ARG:HD3	32:DE:106:LYS:HB3	1.91	0.52
39:DM:79:LEU:HD11	39:DM:112:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DI:44:ALA:HB1	53:DI:95:LEU:HD11	1.91	0.52
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.92	0.51
42:CP:51:ALA:HB3	42:CP:78:VAL:HG13	1.92	0.51
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.76	0.51
1:BA:350:G:H5''	20:BT:3:ASN:HD22	1.76	0.51
29:CC:13:ARG:HD3	31:CA:728:G:H4'	1.92	0.51
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.93	0.51
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.93	0.51
30:DD:25:THR:HG21	30:DD:193:VAL:HG22	1.92	0.51
46:CT:69:LEU:HG	46:CT:107:VAL:HG22	1.92	0.51
54:DA:1853:A:N1	54:DA:2087:G:H1'	2.25	0.51
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.51
11:BK:23:ILE:HD11	11:BK:86:VAL:HG13	1.91	0.51
25:D4:60:ALA:O	39:DM:48:ARG:HD2	2.10	0.51
31:CA:532:A:N1	31:CA:2020:A:H1'	2.25	0.51
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.92	0.51
1:BA:374:A:H5''	1:BA:452:A:N1	2.25	0.51
22:D1:22:LEU:HD23	61:D1:103:PEG:H31	1.91	0.51
31:CA:569:U:H5''	31:CA:821:A:C2	2.46	0.51
47:CU:54:GLU:HB3	47:CU:88:LYS:HD2	1.92	0.51
38:DL:38:ILE:HD11	38:DL:112:PHE:CZ	2.42	0.51
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.92	0.51
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.46	0.51
31:CA:12:U:H2'	31:CA:12:U:O2	2.11	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.93	0.51
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.93	0.51
42:DP:51:ALA:HB3	42:DP:78:VAL:HG13	1.93	0.51
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.46	0.51
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.45	0.51
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.46	0.51
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.93	0.51
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.76	0.51
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.11	0.51
31:CA:674:G:H1'	32:CE:69:ARG:HH11	1.76	0.51
54:DA:1847:A:O2'	54:DA:1848:A:H8	1.93	0.51
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.93	0.50
47:CU:18:GLU:H	47:CU:18:GLU:CD	2.15	0.50
35:DH:4:ILE:HD11	35:DH:44:ILE:HG22	1.93	0.50
1:AA:774:G:H21	56:AA:1670:PG4:H51	1.75	0.50
31:CA:784:G:H5'	31:CA:785:G:OP1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CT:73:LYS:HB2	46:CT:106:VAL:HB	1.92	0.50
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.92	0.50
22:C1:15:MET:SD	31:CA:2045:C:H5''	2.51	0.50
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.93	0.50
37:CK:81:ILE:HG23	37:CK:82:GLY:H	1.77	0.50
53:DI:57:ASN:HB3	53:DI:76:PHE:HB3	1.93	0.50
25:D4:31:HIS:HB2	69:D4:103:HOH:O	2.11	0.50
33:DF:131:GLY:HA3	54:DA:2305:U:H5''	1.94	0.50
34:DG:19:ILE:HG12	34:DG:24:ILE:HG12	1.93	0.50
54:DA:1026:G:H2'	54:DA:1027:A:C8	2.46	0.50
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.93	0.50
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.50
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.93	0.50
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.50
22:C1:16:ARG:HA	31:CA:2046:G:C5'	2.41	0.50
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.77	0.50
25:D4:8:ARG:CD	54:DA:245:G:O6	2.60	0.50
31:CA:17:G:H4'	44:CR:25:TYR:CE2	2.44	0.50
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.92	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.93	0.50
24:C3:16:HIS:CD2	31:CA:464:U:HO2'	2.29	0.50
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.76	0.50
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.92	0.50
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	1.93	0.50
23:D2:25:LYS:HE2	23:D2:30:LYS:O	2.12	0.50
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.12	0.50
18:AR:45:THR:OG1	18:AR:47:THR:HG22	2.12	0.50
31:CA:70:G:H5''	31:CA:112:U:O2	2.12	0.50
31:CA:532:A:N3	31:CA:532:A:H2'	2.26	0.50
42:DP:68:LYS:HB3	61:DP:201:PEG:H22	1.93	0.50
54:DA:1536:C:H4'	54:DA:1537:G:H5''	1.93	0.50
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.94	0.49
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.93	0.49
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.93	0.49
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.94	0.49
40:DN:81[B]:4D4:H9	54:DA:2496:C:OP2	2.12	0.49
50:DX:41[A]:ARG:HG3	54:DA:2386:A:N3	2.26	0.49
54:DA:479:A:N3	54:DA:481:G:H5''	2.26	0.49
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.94	0.49
1:BA:374:A:H5''	1:BA:452:A:C2	2.47	0.49
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CF:44:ILE:HG21	33:CF:79:ILE:HG22	1.94	0.49
54:DA:914:G:H5'	54:DA:914:G:H8	1.78	0.49
24:C3:24:THR:HG23	24:C3:27:GLY:H	1.78	0.49
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.94	0.49
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.93	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.47	0.49
31:CA:2445:2MG:HM21	31:CA:2449:U:O4	2.11	0.49
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.95	0.49
40:CN:21:ALA:HB1	40:CN:100:LYS:HG2	1.94	0.49
53:DI:31:ARG:HB2	53:DI:79:PRO:HG2	1.93	0.49
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.93	0.49
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.47	0.49
54:DA:1433:A:O2'	54:DA:1434:A:H5'	2.12	0.49
1:BA:202:G:H1	1:BA:215:C:H42	1.59	0.49
34:CG:19:ILE:HG12	34:CG:24:ILE:HG12	1.93	0.49
54:DA:789:A:OP1	58:DA:3221:PUT:H12	2.12	0.49
54:DA:2441:U:O2'	64:DA:3223:SPD:H91	2.13	0.49
1:AA:411:A:P	4:AD:26:ARG:HH12	2.36	0.49
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.95	0.49
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.95	0.49
1:BA:76:G:H1	1:BA:93:U:H3	1.61	0.49
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.12	0.49
28:CB:14:U:H2'	28:CB:15:A:H2	1.76	0.49
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.78	0.49
25:C4:25:LYS:HB3	39:CM:62:PRO:HG2	1.94	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.95	0.49
31:CA:2019:A:H4'	44:CR:34:VAL:HG21	1.94	0.49
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.77	0.49
26:C5:1:MET:HB2	31:CA:2526:G:O2'	2.13	0.49
39:DM:21:ARG:HA	54:DA:811:U:H2'	1.95	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.49
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.95	0.49
38:CL:43:ILE:HD12	38:CL:56:ASP:HB2	1.94	0.49
46:CT:4:ILE:HG12	46:CT:106:VAL:HG22	1.94	0.49
1:BA:840:C:H2'	1:BA:841:C:O4'	2.13	0.48
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.93	0.48
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.95	0.48
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.13	0.48
28:DB:84:G:H21	62:DB:211:EDO:H11	1.78	0.48
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.94	0.48
15:AO:82:ILE:HG21	15:AO:89:ARG:OXT	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:381:G:OP1	51:CY:18:ARG:HD3	2.12	0.48
31:CA:479:A:N3	31:CA:481:G:H5''	2.28	0.48
31:CA:998:C:OP2	44:CR:58:ARG:NH2	2.46	0.48
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.78	0.48
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.13	0.48
30:DD:13:ARG:NH1	69:DD:401:HOH:O	2.44	0.48
32:CE:75:SER:O	32:CE:78:TRP:HB2	2.13	0.48
54:DA:837:C:H5	69:DA:6714:HOH:O	1.95	0.48
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	1.95	0.48
22:C1:16:ARG:HA	31:CA:2046:G:H5'	1.95	0.48
2:BB:73:LYS:HD2	2:BB:168:HIS:HD2	1.77	0.48
3:BC:72:ARG:HB3	3:BC:75:ILE:HG22	1.94	0.48
30:DD:99:GLU:HG2	30:DD:182:ALA:HB2	1.94	0.48
34:CG:80:THR:HG23	34:CG:81:GLU:N	2.24	0.48
33:DF:121:SER:HB2	54:DA:2304:G:H5'	1.95	0.48
63:D1:102:PGE:H4	69:DT:313:HOH:O	2.13	0.48
29:CC:177:ARG:HG2	31:CA:1820:U:OP1	2.14	0.48
31:CA:914:G:H8	31:CA:914:G:H5''	1.79	0.48
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.96	0.48
1:AA:413:G:H5''	1:AA:414:A:H5'	1.96	0.48
1:BA:677:U:H3	1:BA:713:G:H22	1.61	0.48
28:CB:14:U:H2'	28:CB:15:A:C2	2.49	0.48
42:DP:31:THR:HG22	42:DP:33:ARG:H	1.79	0.48
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.96	0.48
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.94	0.48
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.95	0.48
31:CA:634:C:H2'	31:CA:635:C:C6	2.49	0.48
46:DT:4:ILE:HG12	46:DT:106:VAL:HG22	1.94	0.48
1:BA:975:A:H8	1:BA:1357:A:HO2'	1.61	0.48
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.93	0.48
38:CL:38:ILE:HD11	38:CL:112:PHE:CZ	2.38	0.48
40:DN:41:LEU:HG	40:DN:96:ILE:HG13	1.96	0.48
46:DT:72:THR:HG21	46:DT:108:SER:HB3	1.95	0.48
53:DI:50:VAL:HG13	53:DI:85:VAL:HG22	1.96	0.48
1:AA:975:A:H8	1:AA:1357:A:HO2'	1.60	0.48
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.49	0.48
31:CA:247:G:H4'	31:CA:386:G:C5	2.49	0.48
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.48	0.48
5:BE:36:LEU:HD21	5:BE:137:VAL:HG11	1.95	0.48
30:DD:150[B]:MEQ:HE2	54:DA:2033:A:O5'	2.14	0.48
33:DF:44:ILE:HG21	33:DF:79:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DT:73:LYS:HB2	46:DT:106:VAL:HB	1.95	0.48
54:DA:1587:G:H2'	54:DA:1588:G:H8	1.79	0.48
1:AA:542:G:H5'	4:AD:39:GLY:HA3	1.96	0.47
36:CJ:19:ASN:H	36:CJ:20:PRO:HD2	1.79	0.47
54:DA:11:C:H2'	54:DA:12:U:H5'	1.95	0.47
54:DA:1172:C:C5	54:DA:1173:U:H1'	2.49	0.47
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.14	0.47
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.96	0.47
33:CF:36:LEU:HB2	33:CF:57:LEU:HD21	1.97	0.47
54:DA:1975:G:H21	63:DA:3224:PGE:C2	2.27	0.47
1:AA:1055:A:H2'	3:AC:156:ARG:HD2	1.96	0.47
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.12	0.47
23:C2:25:LYS:HE2	23:C2:30:LYS:O	2.14	0.47
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.97	0.47
30:DD:8:LYS:HB2	30:DD:201:LEU:HD11	1.96	0.47
13:AM:4:ILE:HD12	13:AM:10:PRO:HG2	1.95	0.47
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.29	0.47
30:DD:105:LYS:NZ	30:DD:106:LYS:HE3	2.30	0.47
38:DL:43:ILE:HD12	38:DL:56:ASP:HB2	1.96	0.47
44:DR:6:ARG:HD3	54:DA:1250:G:H5''	1.95	0.47
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.97	0.47
22:D1:9:THR:HG21	54:DA:2020:A:H5'	1.96	0.47
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.15	0.47
31:CA:2185:U:H2'	31:CA:2186:G:H8	1.79	0.47
33:CF:8:TYR:HA	33:CF:12:VAL:HB	1.97	0.47
51:CY:10:LYS:HE3	51:CY:54:LYS:HG2	1.96	0.47
36:DJ:103:ARG:HA	36:DJ:106:LEU:HD12	1.96	0.47
54:DA:2291:U:H2'	54:DA:2292:U:C6	2.49	0.47
54:DA:789:A:OP1	58:DA:3221:PUT:C1	2.63	0.47
1:AA:269:C:H2'	1:AA:270:A:C8	2.50	0.47
1:AA:677:U:H3	1:AA:713:G:H22	1.63	0.47
1:BA:846:G:H2'	1:BA:847:G:H8	1.79	0.47
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.79	0.47
31:CA:2030:6MZ:C2	31:CA:2499:C:H5''	2.45	0.47
33:DF:8:TYR:HA	33:DF:12:VAL:HB	1.97	0.47
33:DF:36:LEU:HB2	33:DF:57:LEU:HD21	1.96	0.47
35:DH:49:ALA:O	35:DH:53:GLU:HB3	2.15	0.47
42:DP:52:SER:OG	42:DP:54:VAL:HG22	2.14	0.47
48:DV:73:PHE:CE2	48:DV:75:ALA:HA	2.49	0.47
51:DY:10:LYS:HE3	51:DY:54:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:644:A:H2'	54:DA:645:C:O4'	2.14	0.47
54:DA:1975:G:H21	63:DA:3224:PGE:H2	1.79	0.47
1:BA:269:C:H2'	1:BA:270:A:C8	2.50	0.47
32:CE:1:MET:HG2	32:CE:14:VAL:HG23	1.97	0.47
36:DJ:19:ASN:H	36:DJ:20:PRO:HD2	1.80	0.47
54:DA:1182:G:H2'	54:DA:1183:U:O4'	2.15	0.47
22:D1:55:ILE:HD12	41:DO:33:ILE:CD1	2.45	0.47
30:CD:155:VAL:HG21	31:CA:2618:G:H21	1.79	0.47
31:CA:396:G:H1'	51:CY:29:PHE:HB3	1.95	0.47
31:CA:608:A:H2'	31:CA:609:A:C8	2.50	0.47
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.50	0.47
48:CV:74:ASN:HD22	48:CV:77:THR:H	1.63	0.47
42:DP:31:THR:HG21	28:DB:28:C:P	2.54	0.47
54:DA:1236:G:N7	58:DA:3189:PUT:H41	2.30	0.47
22:C1:41:HIS:O	41:CO:99:LYS:HE2	2.14	0.47
24:C3:19:ARG:NH2	31:CA:125:A:OP2	2.38	0.47
27:C0:19:LYS:HE3	31:CA:920:A:OP1	2.14	0.47
2:BB:73:LYS:HD2	2:BB:168:HIS:CD2	2.51	0.47
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.15	0.47
31:CA:310:A:H5''	48:CV:15:THR:HG23	1.96	0.47
31:CA:1936:A:H62	31:CA:1963:U:H3	1.60	0.47
37:DK:69:ARG:O	37:DK:90:GLU:HB2	2.15	0.47
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.97	0.46
1:BA:1055:A:H2'	3:BC:156:ARG:HD2	1.97	0.46
31:CA:193:U:H5	69:CA:3370:HOH:O	1.98	0.46
33:CF:103:LEU:HA	33:CF:107:ALA:HB3	1.97	0.46
32:DE:176:ASP:OD2	32:DE:178:VAL:HG12	2.15	0.46
54:DA:749:A:H4'	54:DA:1271:G:N3	2.29	0.46
54:DA:1180:U:H5''	54:DA:1180:U:H6	1.80	0.46
1:AA:73:C:O2'	1:AA:74:A:H8	1.97	0.46
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.97	0.46
22:C1:2:ALA:N	31:CA:2577:A:H2	2.13	0.46
1:BA:23:C:H5	1:BA:561:U:O4	1.98	0.46
41:CO:47:VAL:O	41:CO:51:LEU:HD23	2.15	0.46
33:DF:103:LEU:HA	33:DF:107:ALA:HB3	1.97	0.46
1:AA:1197:A:H5''	59:AA:1678:TAC:O12	2.15	0.46
1:BA:202:G:H21	1:BA:466:A:H61	1.62	0.46
22:D1:25:VAL:HG11	46:DT:38:TYR:HB2	1.98	0.46
31:CA:846:U:H1'	31:CA:847:U:C5	2.44	0.46
42:CP:31:THR:HG22	42:CP:33:ARG:H	1.79	0.46
48:CV:7:ARG:O	48:CV:25:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.95	0.46
30:CD:62:LYS:HE2	31:CA:2810:A:H5''	1.98	0.46
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.51	0.46
50:DX:39:ARG:NH1	69:DX:101:HOH:O	2.48	0.46
51:DY:61:LYS:HD3	54:DA:372:G:H5''	1.98	0.46
1:AA:76:G:H1	1:AA:93:U:H3	1.62	0.46
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.97	0.46
25:D4:64:TYR:CZ	54:DA:242:G:H5''	2.51	0.46
30:CD:3:GLY:O	30:CD:4:LEU:HD13	2.15	0.46
39:CM:77:ILE:CD1	39:CM:108:ALA:HB1	2.36	0.46
54:DA:102:U:H2'	54:DA:102:U:O2	2.15	0.46
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.50	0.46
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.81	0.46
29:CC:219:THR:O	31:CA:1789:A:H5''	2.15	0.46
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.45	0.46
31:CA:740:C:H5'	31:CA:1784:A:C3'	2.38	0.46
31:CA:749:A:H4'	31:CA:1271:G:N3	2.29	0.46
29:DC:207:LYS:HB2	54:DA:729:G:C6	2.51	0.46
54:DA:57:C:H2'	54:DA:58:G:O4'	2.16	0.46
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.31	0.46
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.97	0.46
22:D1:5:GLN:O	54:DA:2017:U:H4'	2.16	0.46
43:CQ:114:LEU:HD23	43:CQ:114:LEU:H	1.81	0.46
47:CU:45:ALA:O	47:CU:49:LYS:HG2	2.14	0.46
1:BA:376:G:H5''	16:BP:5:ARG:HB2	1.97	0.46
29:CC:235:GLY:HA3	29:CC:239:ASN:HB2	1.97	0.46
31:CA:948:C:H1'	31:CA:984:A:C8	2.50	0.46
31:CA:1250:G:C5'	44:CR:6:ARG:HD3	2.45	0.46
31:CA:2489:U:HO2'	31:CA:2491:U:H5	1.64	0.46
34:CG:80:THR:CG2	34:CG:81:GLU:H	2.27	0.46
44:CR:58:ARG:HA	44:CR:61:TRP:CE3	2.50	0.46
1:AA:438:U:H5'	4:AD:120:HIS:HB3	1.98	0.46
1:AA:1054:C:H5''	1:AA:1054:C:H6	1.80	0.46
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.97	0.46
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.97	0.46
1:BA:310:G:H5''	16:BP:31:ARG:HB2	1.97	0.46
1:BA:438:U:H5'	4:BD:120:HIS:HB3	1.97	0.46
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.16	0.46
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.16	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
30:DD:186:LEU:HD21	43:DQ:4:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:871:U:H2'	54:DA:872:U:C6	2.51	0.46
1:AA:216:U:H2'	1:AA:217:C:C6	2.50	0.46
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.15	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.51	0.46
47:CU:67:VAL:HG22	47:CU:76:ARG:HG3	1.98	0.46
54:DA:722:A:H2'	54:DA:723:C:O4'	2.16	0.46
54:DA:2800:A:C2	54:DA:2895:G:H1'	2.51	0.46
1:BA:846:G:H2'	1:BA:847:G:C8	2.51	0.45
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.80	0.45
31:CA:594:U:H2'	31:CA:595:C:C6	2.51	0.45
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.16	0.45
31:CA:1131:G:OP1	37:CK:82:GLY:HA2	2.16	0.45
36:CJ:103:ARG:HA	36:CJ:106:LEU:HD12	1.96	0.45
54:DA:2070:A:H2'	54:DA:2071:A:O4'	2.16	0.45
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.45
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.32	0.45
30:CD:8:LYS:HB2	30:CD:201:LEU:HD11	1.97	0.45
40:CN:69:PRO:O	40:CN:93:VAL:O	2.34	0.45
42:CP:31:THR:HG22	42:CP:34:HIS:H	1.81	0.45
35:DH:104:THR:HG22	35:DH:109:GLU:HA	1.97	0.45
54:DA:2086:U:H2'	54:DA:2087:G:C8	2.51	0.45
54:DA:2117:A:H61	54:DA:2171:A:H61	1.63	0.45
64:DA:3223:SPD:H82	69:DA:4264:HOH:O	2.16	0.45
1:BA:411:A:P	4:BD:26:ARG:HH12	2.39	0.45
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.52	0.45
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.99	0.45
29:DC:177:ARG:HG2	54:DA:1820:U:OP1	2.17	0.45
29:DC:235:GLY:HA3	29:DC:239:ASN:HB2	1.99	0.45
32:DE:1:MET:HG2	32:DE:14:VAL:HG23	1.97	0.45
41:DO:9:GLN:O	41:DO:17:ARG:HD3	2.17	0.45
54:DA:2628:C:C5'	58:DA:3195:PUT:H12	2.42	0.45
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.97	0.45
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.16	0.45
26:C5:4:ARG:NH1	31:CA:2477:U:O2	2.44	0.45
1:BA:216:U:H2'	1:BA:217:C:C6	2.51	0.45
31:CA:320:A:H2'	32:CE:131:THR:HG21	1.99	0.45
31:CA:1251:C:OP2	44:CR:6:ARG:HD2	2.17	0.45
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.81	0.45
30:DD:152:PRO:HG3	30:DD:156:PHE:CZ	2.52	0.45
45:DS:8:GLY:HA2	54:DA:1161:C:O2'	2.16	0.45
50:DX:37:ILE:HG21	50:DX:80:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:DY:7:VAL:HG23	51:DY:51:VAL:HG12	1.98	0.45
1:AA:376:G:H5''	16:AP:5:ARG:HB2	1.98	0.45
1:AA:845:A:H2'	1:AA:846:G:O4'	2.17	0.45
22:C1:5:GLN:NE2	31:CA:2056:G:H4'	2.31	0.45
1:BA:8:A:H1'	5:BE:108:GLY:HA2	1.97	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.16	0.45
37:CK:69:ARG:O	37:CK:90:GLU:HB3	2.16	0.45
44:DR:58:ARG:HA	44:DR:61:TRP:CE3	2.51	0.45
54:DA:1133:A:N3	58:DA:3212:PUT:H22	2.32	0.45
2:AB:93:ASN:H	2:AB:93:ASN:HD22	1.65	0.45
31:CA:191:A:H2'	31:CA:192:C:C6	2.51	0.45
31:CA:871:U:H2'	31:CA:872:U:C6	2.51	0.45
31:CA:2674:G:H4'	38:CL:30:ARG:HD2	1.99	0.45
44:CR:112:LYS:HD3	45:CS:48:LYS:HG3	1.99	0.45
46:CT:84:ARG:HB2	46:CT:96:ILE:HB	1.99	0.45
32:DE:32:VAL:HG21	39:DM:6:LEU:HD13	1.99	0.45
34:DG:103:ILE:HD11	34:DG:117:LEU:HD21	1.99	0.45
42:DP:35:ILE:HG21	42:DP:71:ALA:HA	1.98	0.45
43:DQ:52:ASN:O	43:DQ:53:ARG:HD3	2.16	0.45
54:DA:1509:A:HO2'	54:DA:1510:G:H8	1.65	0.45
4:AD:172:GLU:HG2	4:AD:183:LYS:HD2	1.99	0.45
2:BB:93:ASN:HD22	2:BB:93:ASN:H	1.65	0.45
31:CA:248:G:H5'	31:CA:250:G:N7	2.31	0.45
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.51	0.45
32:CE:176:ASP:OD2	32:CE:178:VAL:HG12	2.16	0.45
45:CS:49:ILE:HB	45:CS:51:VAL:O	2.17	0.45
47:CU:28:ASN:ND2	47:CU:91:GLN:HB3	2.14	0.45
53:DI:70:GLU:HG2	53:DI:73:LYS:HE3	1.98	0.45
54:DA:136:G:H1	54:DA:143:C:H42	1.65	0.45
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.17	0.45
53:DI:132:TYR:H	53:DI:133:GLU:HB2	1.81	0.45
54:DA:1168:G:H8	54:DA:1168:G:H5''	1.81	0.45
54:DA:2609:U:C5	62:DA:3194:EDO:H12	2.51	0.45
1:AA:202:G:H1	1:AA:215:C:H42	1.64	0.45
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.98	0.45
25:C4:25:LYS:O	39:CM:62:PRO:HD2	2.16	0.45
24:D3:33:ARG:HG3	61:D3:102:PEG:H31	1.99	0.45
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.17	0.45
31:CA:1965:C:H5''	31:CA:1966:A:H2'	1.99	0.45
46:CT:72:THR:HG21	46:CT:108:SER:HB3	1.98	0.45
37:DK:7:LYS:O	37:DK:11:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:DW:38:LEU:HD21	49:DW:65:VAL:HG11	1.99	0.45
54:DA:355:U:H2'	54:DA:356:G:H8	1.82	0.45
4:BD:172:GLU:HG2	4:BD:183:LYS:HD2	1.99	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
31:CA:1775:U:O4	31:CA:1789:A:H2	2.00	0.45
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.17	0.45
54:DA:612:G:H2'	54:DA:614:A:C8	2.52	0.45
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.82	0.44
24:C3:19:ARG:HG3	31:CA:126:A:O5'	2.17	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.32	0.44
31:CA:478:A:H61	31:CA:500:G:H4'	1.81	0.44
54:DA:1283:G:H1'	54:DA:1329:U:O2	2.17	0.44
54:DA:1349:C:O2'	56:DA:3215:PG4:H82	2.16	0.44
25:C4:2:PRO:HD2	31:CA:667:U:O2	2.17	0.44
2:BB:68:LEU:HD11	2:BB:92:VAL:HG23	2.00	0.44
30:CD:13:ARG:HH11	43:CQ:56:HIS:HA	1.83	0.44
29:DC:212:ARG:HD2	29:DC:216:VAL:O	2.18	0.44
33:DF:16:LEU:HD13	33:DF:29:PRO:HD2	1.99	0.44
54:DA:278:A:N3	54:DA:278:A:H2'	2.32	0.44
54:DA:760:G:H4'	54:DA:1776:G:OP1	2.18	0.44
54:DA:1738:G:HO2'	54:DA:1739:A:H8	1.62	0.44
1:AA:957:U:O2	1:AA:959:A:H8	2.01	0.44
2:AB:68:LEU:HD11	2:AB:92:VAL:HG23	1.99	0.44
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.81	0.44
1:BA:957:U:O2	1:BA:959:A:H8	2.01	0.44
31:CA:639:U:H2'	31:CA:640:C:C6	2.52	0.44
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.51	0.44
50:CX:37:ILE:HG21	50:CX:80:ILE:HG21	1.98	0.44
42:DP:31:THR:HG22	42:DP:34:HIS:H	1.80	0.44
1:AA:1053:G:N7	1:AA:1200:C:H5''	2.33	0.44
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.99	0.44
1:BA:1054:C:H5''	1:BA:1054:C:H6	1.83	0.44
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.99	0.44
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.99	0.44
1:AA:9:G:H5'	5:AE:108:GLY:HA3	1.99	0.44
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.51	0.44
9:AI:99:ARG:HG2	9:AI:104:VAL:HG21	1.99	0.44
1:BA:73:C:O2'	1:BA:74:A:H8	1.97	0.44
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.53	0.44
22:D1:9:THR:CG2	54:DA:2020:A:H5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D3:4:THR:HA	54:DA:687:C:O4'	2.16	0.44
29:DC:13:ARG:HD3	54:DA:728:G:H4'	2.00	0.44
29:DC:203:ARG:HH21	29:DC:205:LEU:HD21	1.82	0.44
33:CF:16:LEU:HD13	33:CF:29:PRO:HD2	1.98	0.44
54:DA:1321:A:C2	63:DA:3216:PGE:H12	2.53	0.44
27:C0:53:PHE:CG	28:CB:83:G:H4'	2.53	0.44
27:D0:15:GLY:HA2	54:DA:969:G:O3'	2.17	0.44
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.18	0.44
31:CA:863:A:H2'	31:CA:864:G:C8	2.53	0.44
35:CH:104:THR:HG22	35:CH:109:GLU:HA	1.98	0.44
49:CW:38:LEU:HD21	49:CW:65:VAL:HG11	1.98	0.44
39:DM:60:ARG:HD2	54:DA:2360:G:H1'	2.00	0.44
54:DA:639:U:H2'	54:DA:640:C:C6	2.53	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	2.00	0.44
3:AC:21:THR:HG23	3:AC:58:GLU:HB3	1.99	0.44
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.41	0.44
13:AM:12:HIS:HB3	69:AM:302:HOH:O	2.18	0.44
13:AM:17:ILE:HD12	13:AM:17:ILE:H	1.83	0.44
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	2.00	0.44
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	2.00	0.44
42:CP:35:ILE:HG21	42:CP:71:ALA:HA	1.99	0.44
54:DA:493:G:H2'	54:DA:494:G:O4'	2.18	0.44
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.99	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.82	0.44
29:CC:199:GLU:O	29:CC:202:LEU:HB2	2.18	0.44
29:CC:212:ARG:HD2	29:CC:216:VAL:O	2.18	0.44
31:CA:2051:A:H5'	31:CA:2578:G:O4'	2.18	0.44
54:DA:62:U:H5'	57:DA:3203:MPD:H53	2.00	0.44
54:DA:1831:G:H1'	63:DA:3224:PGE:H22	1.98	0.44
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	2.00	0.44
1:BA:1060:U:H5	3:BC:2:GLY:HA3	1.81	0.44
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.53	0.44
37:CK:7:LYS:O	37:CK:11:VAL:HG23	2.17	0.44
49:CW:51:GLN:HG2	49:CW:86:LEU:HD11	2.00	0.44
36:DJ:11:LEU:HD22	36:DJ:24:VAL:HG23	2.00	0.44
45:DS:41:ILE:HD13	45:DS:103:ALA:HA	1.99	0.44
48:DV:94:ARG:HB3	48:DV:103:ILE:HD12	1.99	0.44
53:DI:85:VAL:HG21	53:DI:90:GLY:O	2.17	0.44
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.18	0.43
22:C1:5:GLN:HG3	31:CA:2054:A:C2	2.53	0.43
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	2.00	0.43
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	2.00	0.43
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.18	0.43
31:CA:528:A:C8	31:CA:528:A:C3'	3.00	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1991:U:H2'	31:CA:1992:G:H5''	2.00	0.43
44:CR:113:ALA:O	44:CR:117:LEU:HD12	2.18	0.43
40:DN:42:THR:HG22	40:DN:93:VAL:HG12	1.99	0.43
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.00	0.43
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.83	0.43
17:AQ:8:LEU:HD13	17:AQ:25:ILE:HG13	2.00	0.43
1:BA:1060:U:H4'	10:BJ:53:ILE:HG23	2.00	0.43
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	2.00	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.47	0.43
31:CA:355:U:H2'	31:CA:356:G:H8	1.83	0.43
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.53	0.43
33:CF:5:HIS:HB2	33:CF:97:TRP:CD1	2.53	0.43
32:DE:84:THR:HG21	54:DA:586:A:H5'	1.99	0.43
54:DA:1394:U:H4'	54:DA:1603:A:H4'	2.00	0.43
1:AA:1060:U:H4'	10:AJ:53:ILE:HG23	2.00	0.43
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	2.00	0.43
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.18	0.43
30:CD:26:VAL:HG21	43:CQ:5:ILE:HG12	2.00	0.43
31:CA:532:A:H4'	31:CA:533:G:C8	2.54	0.43
33:DF:80:ARG:HB3	33:DF:83:TYR:CE1	2.53	0.43
1:AA:604:G:H2'	1:AA:605:U:O4'	2.19	0.43
2:AB:70:VAL:HB	2:AB:163:VAL:HG22	2.00	0.43
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.00	0.43
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.62	0.43
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.34	0.43
34:CG:17:VAL:HG11	34:CG:50:LEU:HD21	2.01	0.43
48:CV:94:ARG:HB3	48:CV:103:ILE:HD12	1.99	0.43
33:DF:5:HIS:HB2	33:DF:97:TRP:CD1	2.54	0.43
54:DA:142:A:H2'	54:DA:143:C:C6	2.53	0.43
54:DA:1424:G:H21	63:DA:3213:PGE:H32	1.84	0.43
54:DA:2031:A:C6	54:DA:2498:OMC:H1'	2.53	0.43
1:AA:1226:C:H2'	13:AM:102:THR:HB	2.00	0.43
12:AL:31:ARG:O	12:AL:58:THR:HG23	2.18	0.43
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.99	0.43
26:C5:17:VAL:HG12	26:C5:26:ILE:HD12	2.01	0.43
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.54	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
36:CJ:11:LEU:HD22	36:CJ:24:VAL:HG23	2.00	0.43
38:CL:113:MET:O	38:CL:116:ILE:HG13	2.18	0.43
54:DA:191:A:H2'	54:DA:192:C:C6	2.53	0.43
54:DA:523:C:H4'	54:DA:540:C:O2	2.19	0.43
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.61	0.43
22:C1:54:VAL:HG21	41:CO:98:LEU:HD22	2.00	0.43
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.54	0.43
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.99	0.43
13:BM:54:ASP:HA	13:BM:57:ARG:HD2	2.00	0.43
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.48	0.43
22:D1:53:LYS:HE3	22:D1:56:ALA:HA	2.00	0.43
29:CC:225:MET:O	29:CC:233:GLY:O	2.36	0.43
31:CA:528:A:C2	31:CA:2042:A:H2'	2.54	0.43
38:CL:103:VAL:O	38:CL:122:VAL:HB	2.18	0.43
39:CM:95:LEU:HD22	39:CM:100:ILE:HG12	1.99	0.43
41:CO:71:ARG:HG3	41:CO:71:ARG:O	2.19	0.43
45:DS:44:GLY:O	45:DS:45:GLU:HG2	2.17	0.43
53:DI:27:VAL:HG13	53:DI:80:THR:HG23	2.00	0.43
53:DI:50:VAL:HG22	53:DI:85:VAL:HG13	2.00	0.43
54:DA:2849:U:H4'	54:DA:2868:A:C2	2.54	0.43
1:BA:502:A:H2'	1:BA:503:C:O4'	2.19	0.43
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	2.01	0.43
31:CA:335:C:H5''	48:CV:82:ARG:HD3	2.01	0.43
31:CA:493:G:H2'	31:CA:494:G:O4'	2.18	0.43
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.54	0.43
31:CA:2728:U:O2'	31:CA:2729:G:H8	2.01	0.43
53:DI:56:ARG:HA	54:DA:1107:G:OP1	2.19	0.43
54:DA:5:A:H2'	54:DA:6:A:C8	2.53	0.43
54:DA:1028:A:N6	54:DA:1125:G:H2'	2.34	0.43
54:DA:1654:A:H1'	54:DA:2823:A:H5'	2.00	0.43
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.19	0.43
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.54	0.43
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.54	0.43
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	2.00	0.43
1:BA:1493:A:H8	1:BA:1493:A:OP2	2.01	0.43
31:CA:83:A:H2	31:CA:103:A:N7	2.17	0.43
31:CA:580:U:O3'	44:CR:31:VAL:HG13	2.19	0.43
31:CA:685:A:H5''	31:CA:774:G:O6	2.19	0.43
33:DF:36:LEU:HD22	33:DF:154:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DK:23:LYS:HE2	37:DK:142:ILE:OXT	2.19	0.43
47:DU:33:LYS:HG3	47:DU:80:TRP:CE3	2.53	0.43
53:DI:26:VAL:HB	53:DI:83:ALA:HB3	2.01	0.43
54:DA:2233:U:H2'	54:DA:2234:G:C8	2.54	0.43
4:BD:105:MET:SD	4:BD:143:VAL:HG22	2.59	0.43
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.19	0.43
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	2.00	0.43
28:CB:28:C:OP1	42:CP:31:THR:HG21	2.17	0.43
31:CA:1168:G:H5''	31:CA:1168:G:H8	1.83	0.43
30:DD:121:THR:HB	30:DD:127:PHE:CD2	2.54	0.43
41:CO:9:GLN:O	41:CO:17:ARG:HD3	2.17	0.43
45:CS:3:ALA:HB3	45:CS:101:ILE:HD12	2.01	0.43
45:DS:10:LYS:HE3	56:DS:202:PG4:H21	2.00	0.43
45:DS:83:TYR:CE1	54:DA:1187:G:H5''	2.54	0.43
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.54	0.43
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.84	0.43
24:D3:29:GLN:HG2	61:D3:102:PEG:H21	2.01	0.43
31:CA:35:G:H2'	31:CA:36:G:O4'	2.19	0.43
31:CA:1936:A:N6	31:CA:1963:U:H3	2.16	0.43
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.84	0.43
34:CG:103:ILE:HD11	34:CG:117:LEU:HD21	2.01	0.43
37:DK:7:LYS:HG2	54:DA:538:A:H4'	2.01	0.43
49:DW:51:GLN:HG2	49:DW:86:LEU:HD11	2.01	0.43
54:DA:1101:U:H2'	54:DA:1102:C:C6	2.54	0.43
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.55	0.42
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.00	0.42
2:BB:104:TRP:O	2:BB:108:ARG:HB2	2.19	0.42
9:BI:99:ARG:HG2	9:BI:104:VAL:HG21	2.00	0.42
34:DG:17:VAL:HG11	34:DG:50:LEU:HD21	2.00	0.42
40:DN:21:ALA:HB1	40:DN:100:LYS:HG2	2.00	0.42
54:DA:2326:C:H3'	69:DA:7768:HOH:O	2.18	0.42
54:DA:2636:C:H2'	54:DA:2637:U:C6	2.53	0.42
61:DA:3200:PEG:H32	69:DA:3799:HOH:O	2.19	0.42
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.00	0.42
1:BA:978:A:O2'	1:BA:1322:C:H5	2.00	0.42
5:BE:74:VAL:HG11	5:BE:144:LEU:HB3	2.01	0.42
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.58	0.42
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	2.00	0.42
31:CA:136:G:H1	31:CA:143:C:H42	1.65	0.42
31:CA:822:G:O6	31:CA:943:A:H2	2.01	0.42
30:DD:13:ARG:HD3	30:DD:21:SER:OG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CF:36:LEU:HD12	33:CF:154:ILE:HG12	2.01	0.42
37:CK:23:LYS:HE3	37:CK:142:ILE:OXT	2.20	0.42
47:CU:33:LYS:HG3	47:CU:80:TRP:CE3	2.55	0.42
49:CW:26:PHE:CE1	49:CW:44:HIS:HA	2.53	0.42
49:DW:26:PHE:CE2	49:DW:44:HIS:HA	2.54	0.42
54:DA:1510:G:H2'	54:DA:1511:G:O4'	2.18	0.42
54:DA:2051:A:H5'	54:DA:2578:G:O4'	2.19	0.42
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.54	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.84	0.42
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	2.01	0.42
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.85	0.42
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.19	0.42
31:CA:2869:G:H2'	31:CA:2870:C:O4'	2.19	0.42
30:DD:167:ASN:O	63:DD:301:PGE:H52	2.20	0.42
45:CS:41:ILE:HD13	45:CS:103:ALA:HA	2.00	0.42
32:DE:48:THR:HG23	32:DE:88:ARG:HH12	1.82	0.42
54:DA:1654:A:C1'	54:DA:2823:A:H5'	2.50	0.42
1:BA:49:U:O2	1:BA:362:G:H1'	2.20	0.42
2:BB:70:VAL:HB	2:BB:163:VAL:HG22	2.00	0.42
54:DA:189:G:N7	62:DA:3197:EDO:H21	2.35	0.42
54:DA:1932:A:H2'	54:DA:1933:G:O4'	2.20	0.42
1:BA:604:G:H2'	1:BA:605:U:O4'	2.20	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.00	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.00	0.42
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	2.01	0.42
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.34	0.42
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.42
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.20	0.42
22:C1:9:THR:CG2	31:CA:2020:A:H5'	2.49	0.42
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.01	0.42
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	2.01	0.42
29:CC:57:GLY:HA2	29:CC:213:TRP:HA	2.00	0.42
31:CA:538:A:H4'	37:CK:7:LYS:HG2	2.02	0.42
31:CA:686:U:H2'	31:CA:788:A:N1	2.34	0.42
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.20	0.42
29:DC:225:MET:O	29:DC:233:GLY:O	2.38	0.42
38:CL:121:GLU:HG2	38:CL:122:VAL:HG23	2.02	0.42
41:DO:67:PHE:O	41:DO:71:ARG:HD2	2.20	0.42
1:AA:502:A:H2'	1:AA:503:C:O4'	2.19	0.42
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:17:ILE:H	13:BM:17:ILE:HD12	1.85	0.42
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.20	0.42
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.54	0.42
33:CF:138:PHE:HE1	33:CF:152:LEU:HD21	1.85	0.42
37:CK:81:ILE:HG23	37:CK:82:GLY:N	2.35	0.42
54:DA:825:A:H5''	58:DA:3222:PUT:H12	2.02	0.42
54:DA:984:A:N3	54:DA:984:A:H2'	2.33	0.42
54:DA:2445:2MG:HM21	54:DA:2449:H2U:O4	2.20	0.42
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.65	0.42
4:AD:105:MET:SD	4:AD:143:VAL:HG22	2.60	0.42
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.55	0.42
1:BA:1322:C:OP1	1:BA:1322:C:O2	2.38	0.42
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.55	0.42
35:CH:68:ARG:HB3	35:CH:134:VAL:HG21	2.02	0.42
46:CT:20:VAL:HG11	46:CT:44:ALA:HA	2.02	0.42
49:CW:86:LEU:HD13	49:CW:89:ILE:HD11	2.01	0.42
48:DV:51:ALA:O	48:DV:52:LEU:HB2	2.19	0.42
54:DA:355:U:H2'	54:DA:356:G:C8	2.55	0.42
2:AB:104:TRP:O	2:AB:108:ARG:HB2	2.20	0.42
5:AE:77:ASN:HB2	5:AE:82:GLN:HE21	1.74	0.42
5:BE:157:ARG:HG2	5:BE:158:GLY:N	2.35	0.42
12:BL:102:LEU:HB3	12:BL:103:ASP:H	1.78	0.42
31:CA:796:C:H2'	31:CA:797:G:C8	2.54	0.42
31:CA:2060:A:N6	32:CE:69:ARG:NH2	2.67	0.42
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.55	0.42
32:CE:178:VAL:HG23	39:CM:3:LEU:HD21	2.02	0.42
39:DM:109:LYS:HG2	39:DM:126:ARG:HB2	2.02	0.42
54:DA:1794:A:H2'	54:DA:1795:C:C6	2.54	0.42
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	2.02	0.42
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.85	0.42
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.43	0.42
25:D4:8:ARG:HG3	54:DA:253:C:N4	2.35	0.42
35:CH:82:SER:HB2	35:CH:94:ILE:HD11	2.02	0.42
49:CW:26:PHE:HE1	49:CW:44:HIS:HA	1.85	0.42
54:DA:747:5MU:O2	54:DA:2014:A:H1'	2.20	0.42
54:DA:1555:G:OP1	58:DA:3218:PUT:H41	2.20	0.42
54:DA:2406:A:H5'	54:DA:2406:A:C8	2.55	0.42
3:AC:156:ARG:HD3	3:AC:193:TYR:O	2.20	0.41
7:AG:72:THR:HG22	7:AG:142:HIS:CE1	2.55	0.41
22:C1:4:GLN:HB3	31:CA:2615:U:H1'	2.02	0.41
5:BE:115:LEU:HG	5:BE:123:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41
25:D4:39:LYS:O	25:D4:43:HIS:HD2	2.03	0.41
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.54	0.41
54:DA:320:A:H4'	54:DA:322:A:N7	2.35	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.56	0.41
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.02	0.41
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	2.03	0.41
5:BE:23:LYS:HB3	5:BE:30:ILE:HG23	2.01	0.41
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.20	0.41
40:CN:41:LEU:HD21	40:CN:124:LEU:HD22	2.02	0.41
43:CQ:52:ASN:O	43:CQ:53:ARG:HD3	2.20	0.41
46:DT:6:LYS:HB2	54:DA:494:G:H4'	2.02	0.41
54:DA:136:G:H1	54:DA:143:C:N4	2.18	0.41
1:AA:302:G:O2'	1:AA:556:C:H5''	2.20	0.41
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.36	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.85	0.41
29:CC:221:ARG:NH1	31:CA:1789:A:OP2	2.53	0.41
31:CA:136:G:H1	31:CA:143:C:N4	2.19	0.41
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.55	0.41
40:CN:71:LYS:HB3	40:CN:93:VAL:O	2.21	0.41
47:CU:82:LYS:HD3	47:CU:84:TYR:CE1	2.55	0.41
44:DR:51:ARG:HH22	54:DA:993:G:P	2.43	0.41
54:DA:1417:C:H5'	54:DA:1588:G:H1'	2.01	0.41
54:DA:1418:G:H2'	54:DA:1579:A:N6	2.35	0.41
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.02	0.41
1:BA:429:U:H1'	1:BA:430:A:H5''	2.03	0.41
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.20	0.41
31:CA:355:U:H2'	31:CA:356:G:C8	2.56	0.41
31:CA:742:A:H2'	31:CA:743:A:C8	2.55	0.41
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.56	0.41
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.56	0.41
53:DI:94:ARG:HG2	53:DI:127:ALA:HA	2.02	0.41
54:DA:1202:G:H1'	57:DA:3192:MPD:HM1	2.02	0.41
54:DA:1430:G:H2'	54:DA:1431:A:O4'	2.20	0.41
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.56	0.41
19:AS:5:LEU:H	19:AS:5:LEU:HG	1.75	0.41
1:BA:131:A:H2'	1:BA:132:C:C6	2.55	0.41
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.69	0.41
25:D4:13:ARG:HH11	54:DA:2394:C:H5'	1.84	0.41
25:D4:47:LYS:HE3	39:DM:64:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41
31:CA:2043:C:H5''	31:CA:2043:C:C6	2.55	0.41
31:CA:2060:A:N6	32:CE:69:ARG:HH21	2.19	0.41
39:CM:123:ARG:HG3	39:CM:143:GLU:HG3	2.03	0.41
46:CT:29:VAL:HG22	46:CT:51:LEU:HD11	2.02	0.41
41:DO:8:ARG:HD3	54:DA:1652:A:OP1	2.19	0.41
54:DA:138:U:H5'	54:DA:139:U:H5'	2.03	0.41
54:DA:602:A:C6	57:DA:3190:MPD:H31	2.56	0.41
54:DA:686:U:H2'	54:DA:788:A:N1	2.35	0.41
54:DA:792:A:N3	54:DA:2072:C:O2'	2.48	0.41
54:DA:2128:G:H1	54:DA:2160:C:N4	2.18	0.41
1:AA:439:U:H5''	4:AD:121:LYS:HD2	2.02	0.41
1:AA:1343:G:O2'	9:AI:123:ARG:HD2	2.20	0.41
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	2.02	0.41
4:BD:130:VAL:HG11	4:BD:135:TYR:CG	2.56	0.41
11:BK:20:VAL:HB	11:BK:35:THR:HG23	2.02	0.41
12:BL:87:VAL:HG11	12:BL:90:LEU:HD22	2.02	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5''	2.01	0.41
31:CA:1364:G:P	51:CY:50:ARG:HH22	2.43	0.41
31:CA:1722:A:N6	31:CA:1738:G:H1'	2.36	0.41
46:CT:69:LEU:HG	46:CT:107:VAL:CG2	2.50	0.41
35:DH:82:SER:HB2	35:DH:94:ILE:HD11	2.02	0.41
54:DA:2097:A:H8	54:DA:2097:A:H5''	1.85	0.41
1:AA:429:U:H1'	1:AA:430:A:H5''	2.02	0.41
6:AF:102:MET:CE	18:AR:24:LYS:HB3	2.50	0.41
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.86	0.41
1:BA:1376:U:H2'	1:BA:1377:A:C8	2.55	0.41
5:BE:82:GLN:HG2	5:BE:149:SER:HA	2.01	0.41
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.03	0.41
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	2.03	0.41
31:CA:811:U:H2'	39:CM:21:ARG:HA	2.02	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.55	0.41
41:CO:95:THR:HG21	41:CO:113:ILE:HD11	2.02	0.41
34:DG:140:VAL:O	34:DG:144:VAL:HG23	2.20	0.41
46:DT:20:VAL:HG11	46:DT:44:ALA:HA	2.03	0.41
54:DA:1515:A:H2'	54:DA:1516:G:O4'	2.20	0.41
54:DA:2038:G:H2'	54:DA:2039:U:O4'	2.21	0.41
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.56	0.41
5:BE:77:ASN:HB2	5:BE:82:GLN:HE21	1.79	0.41
31:CA:910:A:H62	40:CN:12:MET:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2095:A:H5''	31:CA:2095:A:C8	2.54	0.41
31:CA:2898:U:O2	37:CK:134:ALA:HB1	2.20	0.41
35:DH:68:ARG:HB3	35:DH:134:VAL:HG21	2.03	0.41
50:DX:41[A]:ARG:HD2	54:DA:2387:U:H1'	2.03	0.41
50:DX:41[B]:ARG:HD3	50:DX:41[B]:ARG:HA	1.94	0.41
54:DA:1020:A:C2	54:DA:1141:U:C2	3.08	0.41
54:DA:2324:U:H3'	54:DA:2325:G:H5''	2.03	0.41
5:AE:157:ARG:CD	8:AH:43:GLU:O	2.69	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.03	0.41
11:AK:20:VAL:HB	11:AK:35:THR:HG23	2.03	0.41
25:C4:24:HIS:CG	39:CM:61:LEU:HD13	2.56	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.20	0.41
1:BA:841:C:H3'	1:BA:842:U:C4'	2.51	0.41
11:BK:34:ILE:HG12	11:BK:70:CYS:SG	2.60	0.41
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	2.03	0.41
31:CA:547:A:H2'	31:CA:547:A:N3	2.36	0.41
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.55	0.41
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41
31:CA:2641:G:H5''	37:CK:78:THR:HB	2.03	0.41
30:DD:13:ARG:HH11	43:DQ:56:HIS:HA	1.86	0.41
34:CG:38:ASN:HD22	34:CG:40:ALA:HB3	1.86	0.41
36:CJ:49:ILE:HG13	36:CJ:55:ILE:HD13	2.03	0.41
32:DE:23:PHE:HE2	32:DE:25:GLU:HG3	1.86	0.41
32:DE:178:VAL:HG23	39:DM:3:LEU:HD21	2.01	0.41
50:DX:38:VAL:HG12	50:DX:59:LEU:HB2	2.02	0.41
53:DI:132:TYR:N	53:DI:133:GLU:HB2	2.35	0.41
54:DA:2133:G:H21	54:DA:2158:A:N6	2.18	0.41
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.03	0.41
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.85	0.41
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.21	0.41
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.41
1:BA:439:U:H5''	4:BD:121:LYS:HD2	2.02	0.41
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.03	0.41
31:CA:29:U:H6	31:CA:29:U:O5'	2.02	0.41
31:CA:780:G:H2'	31:CA:782:A:N7	2.36	0.41
36:DJ:14:ALA:HB3	36:DJ:17:MET:HB2	2.03	0.41
39:DM:74:THR:HG23	39:DM:107:PHE:HB2	2.02	0.41
40:DN:89:VAL:CG1	57:DN:201:MPD:HM3	2.50	0.41
46:DT:84:ARG:HB2	46:DT:96:ILE:HB	2.02	0.41
51:DY:29:PHE:HB3	54:DA:396:G:H1'	2.03	0.41
53:DI:29:ASP:HB3	53:DI:106:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:207:A:H2'	54:DA:208:C:O4'	2.20	0.41
54:DA:1306:C:H6	54:DA:1306:C:H5''	1.85	0.41
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.21	0.40
1:AA:1141:C:O2'	1:AA:1142:G:H8	2.03	0.40
1:AA:1216:A:H5''	14:AN:5:SER:HB3	2.02	0.40
6:BF:22:ILE:HG23	6:BF:39:LEU:HD11	2.02	0.40
10:BJ:59:LYS:HD2	10:BJ:60:ASP:OD1	2.21	0.40
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.60	0.40
30:DD:26:VAL:HG21	43:DQ:5:ILE:HG12	2.03	0.40
34:DG:50:LEU:HD13	34:DG:72:LEU:HD23	2.02	0.40
39:DM:123:ARG:HG3	39:DM:143:GLU:HG3	2.03	0.40
50:DX:41[A]:ARG:HH12	54:DA:2262:U:H5''	1.85	0.40
53:DI:23:LEU:HD13	53:DI:89:PRO:HD3	2.03	0.40
54:DA:281:C:H2'	54:DA:282:A:C8	2.56	0.40
54:DA:839:U:H2'	54:DA:840:C:C6	2.56	0.40
1:AA:831:A:H5''	2:AB:21:ARG:HD3	2.03	0.40
14:AN:46:LEU:HD22	19:AS:13:LEU:HG	2.02	0.40
1:BA:268:U:H2'	1:BA:269:C:C6	2.56	0.40
1:BA:718:A:H5'	11:BK:119:ASN:HB2	2.04	0.40
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.36	0.40
1:BA:1197:A:H5''	59:BA:1602:TAC:O12	2.21	0.40
9:BI:116:VAL:HG21	10:BJ:62:ARG:HD3	2.04	0.40
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.56	0.40
52:DZ:56:LEU:HA	52:DZ:59:GLU:HG2	2.03	0.40
53:DI:65:GLU:HA	53:DI:70:GLU:HG3	2.02	0.40
53:DI:120:ALA:HA	53:DI:123:ILE:HD11	2.03	0.40
54:DA:2273:A:H2'	54:DA:2274:A:C8	2.55	0.40
1:AA:268:U:H2'	1:AA:269:C:C6	2.56	0.40
11:AK:31:ILE:HG12	11:AK:46:THR:CG2	2.51	0.40
25:C4:52:LYS:HA	25:C4:55:LEU:HD12	2.03	0.40
31:CA:1306:C:H5''	31:CA:1306:C:H6	1.86	0.40
31:CA:1418:G:H2'	31:CA:1579:A:N6	2.36	0.40
39:DM:77:ILE:CD1	39:DM:101:ILE:CG2	2.97	0.40
39:DM:95:LEU:HD11	39:DM:125:LEU:HD21	2.03	0.40
46:DT:72:THR:CG2	46:DT:108:SER:HB3	2.52	0.40
54:DA:1532:A:H5''	54:DA:1532:A:H8	1.86	0.40
54:DA:2339:C:H2'	54:DA:2340:A:C8	2.57	0.40
1:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
1:BA:1322:C:P	19:BS:78:ARG:HH22	2.43	0.40
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	2.04	0.40
12:BL:74:LEU:HD21	12:BL:80:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D1:8:PRO:HD2	54:DA:1263:U:O2'	2.22	0.40
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.86	0.40
31:CA:644:A:H2'	31:CA:645:C:O4'	2.22	0.40
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.70	0.40
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.56	0.40
36:CJ:19:ASN:N	36:CJ:20:PRO:HD2	2.37	0.40
44:CR:58:ARG:HH11	44:CR:62:ILE:HD11	1.86	0.40
38:DL:113:MET:O	38:DL:116:ILE:HG13	2.19	0.40
54:DA:2788:C:H2'	54:DA:2789:C:C6	2.57	0.40
1:AA:567:G:H2'	1:AA:568:G:O4'	2.21	0.40
1:BA:580:C:H2'	1:BA:581:G:O4'	2.22	0.40
19:BS:5:LEU:CD2	19:BS:10:PHE:HB2	2.51	0.40
31:CA:1072:C:H2'	31:CA:1093:G:O6	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	210 (95%)	9 (4%)	3 (1%)	9	30
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	7	24
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	25	56
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	13	39
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	19	48
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	4	15
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	6	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	19	48
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	5	20
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	1	5
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	7	26
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	7	26
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	16	44
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	4	15
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	2	7
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	6	21
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	6	21
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	11	34
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4	17
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	10	32
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	1	3
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	10	32
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	4	16
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	11	34
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	2	8
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	19
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	14
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	3	10
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
29	CC	269/271 (99%)	252 (94%)	12 (4%)	5 (2%)	6	23
29	DC	269/271 (99%)	257 (96%)	10 (4%)	2 (1%)	19	48
30	CD	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
30	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
32	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	8	29
32	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	25	56
33	CF	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	22	51
33	DF	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	22	51
34	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	3	13
34	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	22	51
35	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	3	11
35	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	6	21
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	13
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	13
37	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	19	48
37	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	19	48
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	7	26
38	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	44
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5	20
39	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16	44
40	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	7	26
41	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
42	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
42	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
43	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	42
44	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
45	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	13
45	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	13	39
46	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	6	23
46	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	12	37
47	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
48	CV	100/102 (98%)	91 (91%)	4 (4%)	5 (5%)	1	5
48	DV	100/102 (98%)	96 (96%)	2 (2%)	2 (2%)	6	21
49	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
50	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
50	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
51	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
51	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	26
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2	7
All	All	11406/11629 (98%)	10790 (95%)	484 (4%)	132 (1%)	11	34

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE

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Mol	Chain	Res	Type
3	AC	156	ARG
13	AM	5	ALA
22	C1	25	VAL
2	BB	126	PHE
3	BC	156	ARG
5	BE	51	GLY
10	BJ	38	GLY
10	BJ	91	ASP
13	BM	7	ILE
16	BP	80	LYS
20	BT	5	LYS
29	CC	158	ALA
29	CC	197	ASN
32	CE	83	VAL
34	CG	119	ALA
34	CG	175	LYS
34	CG	176	LYS
35	CH	10	ALA
36	CJ	19	ASN
37	CK	81	ILE
38	CL	35	VAL
39	CM	29	LYS
40	CN	70	ASP
41	CO	118	ARG
47	CU	88	LYS
48	CV	7	ARG
36	DJ	19	ASN
48	DV	52	LEU
10	AJ	57	VAL
13	AM	105	ASN
14	AN	38	ASP
17	AQ	82	ALA
22	C1	56	ALA
23	C2	5	ILE
23	C2	51	GLU
27	C0	4	THR
27	C0	14	ILE
3	BC	61	ALA
5	BE	110	ALA
6	BF	92	THR
6	BF	98	GLU
10	BJ	57	VAL

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Mol	Chain	Res	Type
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
17	BQ	70	THR
17	BQ	82	ALA
19	BS	6	LYS
29	CC	233	GLY
29	CC	253	LYS
29	DC	233	GLY
29	DC	253	LYS
32	CE	82	GLY
34	CG	46	ALA
36	CJ	25	GLY
39	CM	69	ARG
48	CV	16	GLY
48	CV	17	LYS
34	DG	46	ALA
36	DJ	25	GLY
2	AB	125	THR
2	AB	127	ASP
7	AG	56	LYS
11	AK	54	GLY
11	AK	89	PRO
13	AM	7	ILE
22	C1	26	THR
24	C3	45	SER
2	BB	125	THR
2	BB	127	ASP
5	BE	103	THR
10	BJ	95	GLY
11	BK	54	GLY
11	BK	89	PRO
12	BL	44	LYS
14	BN	38	ASP
15	BO	88	ARG
17	BQ	17	MET
17	BQ	18	GLU
19	BS	5	LEU
29	CC	108	LYS
32	CE	6	LYS
35	CH	118	PRO
48	CV	89	ASP

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Mol	Chain	Res	Type
32	DE	6	LYS
35	DH	118	PRO
38	DL	108	ARG
45	DS	44	GLY
48	DV	89	ASP
53	DI	91	ALA
53	DI	109	LYS
53	DI	130	PRO
5	AE	162	GLU
10	BJ	36	VAL
13	BM	4	ILE
35	CH	9	VAL
39	CM	30	THR
41	CO	119	SER
45	CS	55	ASP
46	CT	63	GLY
35	DH	11	ASN
53	DI	70	GLU
53	DI	88	HIS
19	AS	6	LYS
2	BB	95	ARG
5	BE	105	ILE
14	BN	22	ALA
35	CH	8	LYS
35	CH	122	LEU
36	CJ	23	PRO
45	CS	48	LYS
45	CS	53	PHE
35	DH	122	LEU
36	DJ	23	PRO
43	DQ	105	GLY
53	DI	108	VAL
14	AN	22	ALA
16	BP	44	SER
34	CG	45	HIS
38	CL	110	GLU
46	CT	65	ASP
48	CV	52	LEU
52	CZ	62	GLY
37	DK	83	GLY
26	C5	21	GLY
33	CF	62	GLY

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Mol	Chain	Res	Type
36	CJ	32	GLY
33	DF	62	GLY
36	DJ	32	GLY
17	BQ	35	GLY
10	AJ	33	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	173 (93%)	13 (7%)	12	36
2	BB	186/186 (100%)	173 (93%)	13 (7%)	12	36
3	AC	170/170 (100%)	159 (94%)	11 (6%)	14	40
3	BC	170/170 (100%)	156 (92%)	14 (8%)	9	29
4	AD	172/172 (100%)	163 (95%)	9 (5%)	19	50
4	BD	172/172 (100%)	160 (93%)	12 (7%)	12	36
5	AE	118/118 (100%)	106 (90%)	12 (10%)	6	19
5	BE	113/118 (96%)	95 (84%)	18 (16%)	2	7
6	AF	92/92 (100%)	86 (94%)	6 (6%)	14	40
6	BF	87/92 (95%)	77 (88%)	10 (12%)	4	15
7	AG	124/124 (100%)	115 (93%)	9 (7%)	11	34
7	BG	124/124 (100%)	109 (88%)	15 (12%)	4	13
8	AH	104/104 (100%)	93 (89%)	11 (11%)	5	18
8	BH	104/104 (100%)	93 (89%)	11 (11%)	5	18
9	AI	105/105 (100%)	100 (95%)	5 (5%)	21	53
9	BI	105/105 (100%)	100 (95%)	5 (5%)	21	53
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	13	37
10	BJ	86/87 (99%)	78 (91%)	8 (9%)	7	23
11	AK	90/90 (100%)	87 (97%)	3 (3%)	33	67
11	BK	90/90 (100%)	83 (92%)	7 (8%)	10	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	102/102 (100%)	92 (90%)	10 (10%)	6	21
12	BL	102/102 (100%)	90 (88%)	12 (12%)	4	14
13	AM	92/92 (100%)	83 (90%)	9 (10%)	6	21
13	BM	92/92 (100%)	85 (92%)	7 (8%)	11	32
14	AN	83/83 (100%)	82 (99%)	1 (1%)	67	89
14	BN	83/83 (100%)	82 (99%)	1 (1%)	67	89
15	AO	76/76 (100%)	71 (93%)	5 (7%)	14	39
15	BO	76/76 (100%)	65 (86%)	11 (14%)	2	8
16	AP	65/65 (100%)	64 (98%)	1 (2%)	60	86
16	BP	65/65 (100%)	63 (97%)	2 (3%)	35	69
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	7	22
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	5	17
18	AR	48/48 (100%)	47 (98%)	1 (2%)	48	80
18	BR	48/48 (100%)	47 (98%)	1 (2%)	48	80
19	AS	70/70 (100%)	63 (90%)	7 (10%)	6	20
19	BS	70/70 (100%)	65 (93%)	5 (7%)	12	35
20	AT	65/65 (100%)	59 (91%)	6 (9%)	7	24
20	BT	65/65 (100%)	55 (85%)	10 (15%)	2	7
21	AU	48/48 (100%)	44 (92%)	4 (8%)	9	28
21	BU	48/48 (100%)	44 (92%)	4 (8%)	9	28
22	C1	47/47 (100%)	45 (96%)	2 (4%)	25	57
22	D1	47/47 (100%)	44 (94%)	3 (6%)	14	41
23	C2	45/46 (98%)	44 (98%)	1 (2%)	47	79
23	D2	45/46 (98%)	43 (96%)	2 (4%)	24	56
24	C3	38/38 (100%)	37 (97%)	1 (3%)	41	75
24	D3	38/38 (100%)	37 (97%)	1 (3%)	41	75
25	C4	51/51 (100%)	48 (94%)	3 (6%)	16	44
25	D4	51/51 (100%)	48 (94%)	3 (6%)	16	44
26	C5	34/34 (100%)	32 (94%)	2 (6%)	16	44
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	45 (94%)	3 (6%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D0	49/48 (102%)	45 (92%)	4 (8%)	9	29
29	CC	216/216 (100%)	203 (94%)	13 (6%)	16	44
29	DC	216/216 (100%)	210 (97%)	6 (3%)	38	72
30	CD	163/163 (100%)	159 (98%)	4 (2%)	42	75
30	DD	163/163 (100%)	160 (98%)	3 (2%)	54	83
32	CE	165/165 (100%)	152 (92%)	13 (8%)	10	30
32	DE	165/165 (100%)	161 (98%)	4 (2%)	44	77
33	CF	148/148 (100%)	133 (90%)	15 (10%)	6	20
33	DF	148/148 (100%)	137 (93%)	11 (7%)	11	33
34	CG	137/137 (100%)	134 (98%)	3 (2%)	47	79
34	DG	137/137 (100%)	132 (96%)	5 (4%)	30	64
35	CH	114/114 (100%)	101 (89%)	13 (11%)	4	15
35	DH	114/114 (100%)	101 (89%)	13 (11%)	4	15
36	CJ	104/104 (100%)	100 (96%)	4 (4%)	28	62
36	DJ	104/104 (100%)	100 (96%)	4 (4%)	28	62
37	CK	116/116 (100%)	110 (95%)	6 (5%)	19	50
37	DK	116/116 (100%)	114 (98%)	2 (2%)	56	84
38	CL	103/104 (99%)	99 (96%)	4 (4%)	27	61
38	DL	104/104 (100%)	99 (95%)	5 (5%)	21	53
39	CM	103/103 (100%)	97 (94%)	6 (6%)	17	45
39	DM	103/103 (100%)	99 (96%)	4 (4%)	27	61
40	CN	108/108 (100%)	104 (96%)	4 (4%)	29	63
40	DN	109/108 (101%)	106 (97%)	3 (3%)	38	72
41	CO	100/102 (98%)	95 (95%)	5 (5%)	20	51
41	DO	102/102 (100%)	99 (97%)	3 (3%)	37	71
42	CP	86/87 (99%)	80 (93%)	6 (7%)	12	36
42	DP	87/87 (100%)	84 (97%)	3 (3%)	32	66
43	CQ	99/99 (100%)	93 (94%)	6 (6%)	15	43
43	DQ	99/99 (100%)	97 (98%)	2 (2%)	50	81
44	CR	89/89 (100%)	86 (97%)	3 (3%)	32	66
44	DR	89/89 (100%)	87 (98%)	2 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	CS	84/84 (100%)	79 (94%)	5 (6%)	16	44
45	DS	84/84 (100%)	83 (99%)	1 (1%)	67	89
46	CT	93/93 (100%)	88 (95%)	5 (5%)	18	48
46	DT	93/93 (100%)	92 (99%)	1 (1%)	70	90
47	CU	80/80 (100%)	72 (90%)	8 (10%)	6	20
47	DU	80/80 (100%)	77 (96%)	3 (4%)	28	62
48	CV	83/83 (100%)	79 (95%)	4 (5%)	21	53
48	DV	83/83 (100%)	81 (98%)	2 (2%)	44	77
49	CW	78/78 (100%)	75 (96%)	3 (4%)	28	62
49	DW	78/78 (100%)	76 (97%)	2 (3%)	41	75
50	CX	56/58 (97%)	55 (98%)	1 (2%)	54	83
50	DX	58/58 (100%)	57 (98%)	1 (2%)	56	84
51	CY	67/67 (100%)	63 (94%)	4 (6%)	16	44
51	DY	67/67 (100%)	65 (97%)	2 (3%)	36	70
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	11	33
52	DZ	54/54 (100%)	52 (96%)	2 (4%)	29	63
53	DI	103/103 (100%)	98 (95%)	5 (5%)	21	52
All	All	9460/9477 (100%)	8897 (94%)	563 (6%)	16	44

All (563) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	44	GLU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	205	ASP
3	AC	4	LYS

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Mol	Chain	Res	Type
3	AC	14	ILE
3	AC	21	THR
3	AC	33	LEU
3	AC	38	LYS
3	AC	46	GLU
3	AC	107	ARG
3	AC	168	TYR
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
4	AD	5	LEU
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	50	ASP
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	194	ASP
5	AE	11	LEU
5	AE	14	LYS
5	AE	32	SER
5	AE	46	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	82	GLN
5	AE	101	GLU
5	AE	106	ILE
5	AE	123	VAL
5	AE	126	LYS
5	AE	149	SER
6	AF	36	ILE
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	30	LEU
7	AG	36	LYS
7	AG	59	LEU
7	AG	63	GLU
7	AG	92	ARG

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Mol	Chain	Res	Type
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	90	ASP
8	AH	107	SER
8	AH	108	LYS
9	AI	11	ARG
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	99	ARG
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	23	ILE
11	AK	55	SER
11	AK	119	ASN
12	AL	24	LEU
12	AL	40	THR
12	AL	55	VAL
12	AL	74	LEU
12	AL	82	ILE
12	AL	88	LYS
12	AL	90	LEU
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	17	ILE

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Mol	Chain	Res	Type
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
13	AM	71	ARG
13	AM	101	ARG
14	AN	31	ILE
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	84	ARG
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	27	ARG
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	47	THR
19	AS	5	LEU
19	AS	7	LYS
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
20	AT	15	GLU
20	AT	24	ARG
20	AT	27	MET
20	AT	44	LYS
20	AT	48	GLN
20	AT	85	LYS
21	AU	13	ASP
21	AU	16	LEU
21	AU	34	ARG
21	AU	56	HIS
22	C1	10	ARG
22	C1	40	ARG
23	C2	8	LYS
24	C3	1	MET

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Mol	Chain	Res	Type
25	C4	31	HIS
25	C4	45	ARG
25	C4	52	LYS
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	19	LYS
27	C0	36	VAL
2	BB	18	HIS
2	BB	23	TRP
2	BB	44	GLU
2	BB	93	ASN
2	BB	105	LYS
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	205	ASP
3	BC	4	LYS
3	BC	14	ILE
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	55	ILE
3	BC	107	ARG
3	BC	152	GLU
3	BC	168	TYR
3	BC	175	LEU
3	BC	185	ASN
3	BC	186	THR
3	BC	193	TYR
4	BD	5	LEU
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	47	ARG
4	BD	50	ASP
4	BD	142	VAL

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Mol	Chain	Res	Type
4	BD	143	VAL
4	BD	151	LYS
4	BD	173	VAL
4	BD	194	ASP
4	BD	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	32	SER
5	BE	46	VAL
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	151	GLU
5	BE	152	MET
5	BE	157	ARG
5	BE	159	LYS
6	BF	9	MET
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	53	LYS
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	89	VAL
6	BF	93	LYS
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	59	LEU
7	BG	63	GLU

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Mol	Chain	Res	Type
7	BG	72	THR
7	BG	92	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	47	GLU
8	BH	52	GLU
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	90	ASP
8	BH	107	SER
8	BH	108	LYS
9	BI	11	ARG
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	99	ARG
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	23	ILE
11	BK	31	ILE
11	BK	38	GLN
11	BK	55	SER
11	BK	118	HIS
11	BK	119	ASN
12	BL	24	LEU
12	BL	44	LYS
12	BL	50	ARG
12	BL	55	VAL
12	BL	58	THR

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Mol	Chain	Res	Type
12	BL	74	LEU
12	BL	82	ILE
12	BL	88	LYS
12	BL	90	LEU
12	BL	110	ARG
12	BL	115	SER
12	BL	121	ARG
13	BM	11	ASP
13	BM	13	LYS
13	BM	16	VAL
13	BM	17	ILE
13	BM	27	LYS
13	BM	48	LEU
13	BM	101	ARG
14	BN	26	GLU
15	BO	2	SER
15	BO	13	SER
15	BO	17	ARG
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	84	ARG
15	BO	87	LEU
15	BO	88	ARG
15	BO	89	ARG
16	BP	20	VAL
16	BP	46	LYS
17	BQ	17	MET
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	27	ARG
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	75	LEU
18	BR	47	THR
19	BS	6	LYS
19	BS	7	LYS
19	BS	13	LEU
19	BS	33	THR
19	BS	37	ARG

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Mol	Chain	Res	Type
20	BT	15	GLU
20	BT	24	ARG
20	BT	43	ASP
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	16	LEU
21	BU	34	ARG
21	BU	56	HIS
22	D1	18	SER
22	D1	26	THR
22	D1	29	SER
23	D2	5	ILE
23	D2	8	LYS
24	D3	1	MET
25	D4	31	HIS
25	D4	45	ARG
25	D4	52	LYS
27	D0	10	THR
27	D0	19	LYS
27	D0	25	LEU
27	D0	36	VAL
29	CC	117	GLN
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	174	LEU
29	CC	195	VAL
29	CC	204	VAL
29	CC	205	LEU
29	CC	236	GLU
29	CC	252	THR
29	CC	258	ARG
29	CC	260	ASN
30	CD	4	LEU
30	CD	13	ARG

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Mol	Chain	Res	Type
30	CD	18	ASP
30	CD	95	SER
29	DC	70	ASN
29	DC	117	GLN
29	DC	120	VAL
29	DC	130	LEU
29	DC	236	GLU
29	DC	252	THR
30	DD	13	ARG
30	DD	18	ASP
30	DD	95	SER
32	CE	7	ASP
32	CE	12	LEU
32	CE	25	GLU
32	CE	44	ARG
32	CE	72	SER
32	CE	78	TRP
32	CE	83	VAL
32	CE	107	SER
32	CE	122	GLU
32	CE	127	GLU
32	CE	149	ILE
32	CE	152	GLU
32	CE	189	THR
33	CF	18	THR
33	CF	36	LEU
33	CF	57	LEU
33	CF	72	LYS
33	CF	80	ARG
33	CF	94	GLU
33	CF	106	ILE
33	CF	115	ARG
33	CF	117	LEU
33	CF	123	ASP
33	CF	134	GLU
33	CF	141	ILE
33	CF	149	VAL
33	CF	152	LEU
33	CF	174	ASP
34	CG	11	VAL
34	CG	18	LYS
34	CG	155	GLU

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Mol	Chain	Res	Type
35	CH	7	ASP
35	CH	15	LEU
35	CH	17	ASP
35	CH	21	VAL
35	CH	48	GLU
35	CH	51	ARG
35	CH	53	GLU
35	CH	55	GLU
35	CH	62	LEU
35	CH	75	LEU
35	CH	121	VAL
35	CH	127	GLU
35	CH	145	ASN
36	CJ	11	LEU
36	CJ	13	VAL
36	CJ	28	LEU
36	CJ	113	LYS
37	CK	5	THR
37	CK	9	GLU
37	CK	30	THR
37	CK	39	LYS
37	CK	124	VAL
37	CK	142	ILE
38	CL	35	VAL
38	CL	58	LEU
38	CL	98	ARG
38	CL	113	MET
39	CM	2	ARG
39	CM	21	ARG
39	CM	93	ASN
39	CM	94	THR
39	CM	100	ILE
39	CM	115	GLU
40	CN	6	ARG
40	CN	20	LEU
40	CN	59	ARG
40	CN	78	LEU
41	CO	2	ARG
41	CO	14	SER
41	CO	71	ARG
41	CO	76	VAL
41	CO	95	THR

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Mol	Chain	Res	Type
42	CP	18	LEU
42	CP	31	THR
42	CP	38	GLN
42	CP	49	VAL
42	CP	56	LYS
42	CP	78	VAL
43	CQ	2	SER
43	CQ	26	VAL
43	CQ	39	ARG
43	CQ	40	LEU
43	CQ	102	GLU
43	CQ	114	LEU
44	CR	16	LYS
44	CR	51	ARG
44	CR	52	GLN
45	CS	12	HIS
45	CS	45	GLU
45	CS	48	LYS
45	CS	51	VAL
45	CS	102	SER
46	CT	7	HIS
46	CT	19	LEU
46	CT	29	VAL
46	CT	86	MET
46	CT	97	LEU
47	CU	1	MET
47	CU	2	ILE
47	CU	3	ARG
47	CU	10	VAL
47	CU	24	MET
47	CU	30	ILE
47	CU	49	LYS
47	CU	69	ARG
48	CV	61	LYS
48	CV	72	ILE
48	CV	81	ASP
48	CV	98	SER
49	CW	1	MET
49	CW	7	GLU
49	CW	10	LYS
50	CX	82	ILE
51	CY	25	THR

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Mol	Chain	Res	Type
51	CY	35	SER
51	CY	48	THR
51	CY	71	LEU
52	CZ	18	LEU
52	CZ	19	LEU
52	CZ	38	GLN
52	CZ	58	ASN
32	DE	12	LEU
32	DE	107	SER
32	DE	127	GLU
32	DE	189	THR
33	DF	10	ASP
33	DF	57	LEU
33	DF	72	LYS
33	DF	94	GLU
33	DF	106	ILE
33	DF	117	LEU
33	DF	134	GLU
33	DF	141	ILE
33	DF	149	VAL
33	DF	152	LEU
33	DF	174	ASP
34	DG	3	ARG
34	DG	11	VAL
34	DG	18	LYS
34	DG	56	ASP
34	DG	155	GLU
35	DH	7	ASP
35	DH	15	LEU
35	DH	17	ASP
35	DH	21	VAL
35	DH	48	GLU
35	DH	53	GLU
35	DH	57	LYS
35	DH	58	LEU
35	DH	60	GLU
35	DH	75	LEU
35	DH	121	VAL
35	DH	127	GLU
35	DH	145	ASN
36	DJ	11	LEU
36	DJ	13	VAL

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Mol	Chain	Res	Type
36	DJ	28	LEU
36	DJ	113	LYS
37	DK	124	VAL
37	DK	142	ILE
38	DL	58	LEU
38	DL	76	VAL
38	DL	110	GLU
38	DL	113	MET
38	DL	123	LEU
39	DM	2	ARG
39	DM	91	ASP
39	DM	94	THR
39	DM	115	GLU
40	DN	58	LYS
40	DN	59	ARG
40	DN	100	LYS
41	DO	2	ARG
41	DO	14	SER
41	DO	76	VAL
42	DP	31	THR
42	DP	49	VAL
42	DP	78	VAL
43	DQ	26	VAL
43	DQ	102	GLU
44	DR	41	LYS
44	DR	51	ARG
45	DS	102	SER
46	DT	86	MET
47	DU	1	MET
47	DU	3	ARG
47	DU	10	VAL
48	DV	52	LEU
48	DV	61	LYS
49	DW	7	GLU
49	DW	53	LYS
50	DX	82	ILE
51	DY	25	THR
51	DY	35	SER
52	DZ	19	LEU
52	DZ	38	GLN
53	DI	7	ASP
53	DI	16	SER

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Mol	Chain	Res	Type
53	DI	53	ARG
53	DI	64	VAL
53	DI	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	18	HIS
2	AB	93	ASN
2	AB	94	HIS
2	AB	120	GLN
4	AD	136	GLN
5	AE	89	HIS
6	AF	63	ASN
7	AG	97	ASN
7	AG	142	HIS
8	AH	4	GLN
10	AJ	58	ASN
20	AT	48	GLN
20	AT	78	ASN
22	C1	6	ASN
22	C1	38	HIS
2	BB	39	HIS
2	BB	93	ASN
2	BB	94	HIS
2	BB	120	GLN
2	BB	168	HIS
4	BD	131	ASN
5	BE	70	ASN
5	BE	89	HIS
5	BE	122	ASN
7	BG	97	ASN
8	BH	4	GLN
8	BH	38	ASN
17	BQ	51	ASN
20	BT	3	ASN
24	D3	26	ASN
25	D4	43	HIS
29	CC	142	HIS
29	DC	142	HIS
32	CE	115	GLN
33	CF	27	GLN

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Mol	Chain	Res	Type
34	CG	38	ASN
37	CK	138	GLN
42	CP	29	HIS
42	CP	100	HIS
47	CU	28	ASN
48	CV	74	ASN
50	CX	57	HIS
52	CZ	45	GLN
48	DV	54	GLN
53	DI	122	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	239 (15%)	27 (1%)
1	BA	1529/1534 (99%)	246 (16%)	28 (1%)
28	CB	117/120 (97%)	11 (9%)	0
28	DB	119/120 (99%)	9 (7%)	0
31	CA	2892/2904 (99%)	425 (14%)	72 (2%)
54	DA	2880/2904 (99%)	367 (12%)	57 (1%)
All	All	9067/9116 (99%)	1297 (14%)	184 (2%)

All (1297) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A

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Mol	Chain	Res	Type
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	120	A
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	177	G
1	AA	183	C
1	AA	197	A
1	AA	205	A
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	250	A
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	321	A
1	AA	328	C

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Mol	Chain	Res	Type
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	348	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	G
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	436	C
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	509	A
1	AA	511	C
1	AA	527	G7M
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C

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Mol	Chain	Res	Type
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	615	G
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A

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Mol	Chain	Res	Type
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	993	G
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1053	G
1	AA	1054	C
1	AA	1065	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A
1	AA	1124	G
1	AA	1125	U
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1145	A
1	AA	1152	A

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Mol	Chain	Res	Type
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C

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Mol	Chain	Res	Type
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1492	A
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	9	G
1	BA	22	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	80	A
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	86	G
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C
1	BA	92	U
1	BA	94	G
1	BA	95	C
1	BA	108	G

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Mol	Chain	Res	Type
1	BA	120	A
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	177	G
1	BA	183	C
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	245	U
1	BA	247	G
1	BA	250	A
1	BA	251	G
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	348	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	384	G
1	BA	398	U

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Mol	Chain	Res	Type
1	BA	406	G
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	430	A
1	BA	436	C
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	509	A
1	BA	511	C
1	BA	527	G7M
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	615	G
1	BA	633	G
1	BA	650	G
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	695	A
1	BA	702	A

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Mol	Chain	Res	Type
1	BA	703	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	844	G
1	BA	845	A
1	BA	846	G
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	971	G
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	987	G
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G

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Mol	Chain	Res	Type
1	BA	1026	G
1	BA	1027	C
1	BA	1028	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1046	A
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1070	U
1	BA	1086	U
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1142	G
1	BA	1143	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1212	U
1	BA	1213	A

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Mol	Chain	Res	Type
1	BA	1214	C
1	BA	1215	G
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1260	G
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1320	C
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1492	A
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A

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Mol	Chain	Res	Type
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	36	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	63	A
31	CA	71	A
31	CA	74	A
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G

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Mol	Chain	Res	Type
31	CA	142	A
31	CA	143	C
31	CA	196	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	420	C
31	CA	424	G
31	CA	425	G
31	CA	451	U
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	503	A

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Mol	Chain	Res	Type
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C
31	CA	531	C
31	CA	532	A
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	549	G
31	CA	550	C
31	CA	551	G
31	CA	555	G
31	CA	556	A
31	CA	563	A
31	CA	571	U
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A
31	CA	615	U
31	CA	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	654	A
31	CA	655	A
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU
31	CA	775	G
31	CA	776	G

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Mol	Chain	Res	Type
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A
31	CA	883	G
31	CA	896	A
31	CA	897	C
31	CA	910	A
31	CA	914	G
31	CA	915	C
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	961	C
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A

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Mol	Chain	Res	Type
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1070	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1091	G
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	C
31	CA	1171	G
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1210	G
31	CA	1212	G
31	CA	1236	G
31	CA	1238	G
31	CA	1253	A
31	CA	1256	G
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G

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Mol	Chain	Res	Type
31	CA	1301	A
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1328	A
31	CA	1352	U
31	CA	1365	A
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1391	U
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1437	C
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1509	A
31	CA	1510	G
31	CA	1515	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1566	A
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A

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Mol	Chain	Res	Type
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1674	G
31	CA	1695	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1731	G
31	CA	1732	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1816	C
31	CA	1822	C
31	CA	1829	A
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1900	A
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A

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Mol	Chain	Res	Type
31	CA	1972	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A
31	CA	2036	C
31	CA	2043	C
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2102	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A

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Mol	Chain	Res	Type
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2160	C
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2183	A
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2280	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2326	C
31	CA	2327	A
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2388	A

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Mol	Chain	Res	Type
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2476	A
31	CA	2491	U
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2578	G
31	CA	2582	G
31	CA	2585	U
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G

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Mol	Chain	Res	Type
31	CA	2718	G
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2769	U
31	CA	2778	A
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2820	A
31	CA	2835	A
31	CA	2836	U
31	CA	2850	A
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2887	A
31	CA	2891	U
31	CA	2903	U
31	CA	2904	U
28	DB	25	U
28	DB	35	C
28	DB	45	A
28	DB	56	G
28	DB	57	A
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
54	DA	10	A
54	DA	12	U
54	DA	34	U
54	DA	46	G
54	DA	63	A
54	DA	71	A
54	DA	74	A
54	DA	75	G
54	DA	80	G
54	DA	84	A

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Mol	Chain	Res	Type
54	DA	101	A
54	DA	102	U
54	DA	118	A
54	DA	119	A
54	DA	120	U
54	DA	138	U
54	DA	139	U
54	DA	140	C
54	DA	141	G
54	DA	142	A
54	DA	143	C
54	DA	196	A
54	DA	199	A
54	DA	200	U
54	DA	215	G
54	DA	216	A
54	DA	221	A
54	DA	222	A
54	DA	248	G
54	DA	265	A
54	DA	266	G
54	DA	272	A
54	DA	276	U
54	DA	277	G
54	DA	278	A
54	DA	279	A
54	DA	285	G
54	DA	302	C
54	DA	311	A
54	DA	329	G
54	DA	330	A
54	DA	343	C
54	DA	346	A
54	DA	352	A
54	DA	353	C
54	DA	362	A
54	DA	370	G
54	DA	372	G
54	DA	386	G
54	DA	399	U
54	DA	411	G
54	DA	412	A

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Mol	Chain	Res	Type
54	DA	420	C
54	DA	424	G
54	DA	425	G
54	DA	451	U
54	DA	480	A
54	DA	481	G
54	DA	491	G
54	DA	504	A
54	DA	505	A
54	DA	508	A
54	DA	531	C
54	DA	532	A
54	DA	543	G
54	DA	544	C
54	DA	546	U
54	DA	547	A
54	DA	548	G
54	DA	549	G
54	DA	550	C
54	DA	551	G
54	DA	563	A
54	DA	573	U
54	DA	575	A
54	DA	586	A
54	DA	603	A
54	DA	613	A
54	DA	614	A
54	DA	615	U
54	DA	627	A
54	DA	637	A
54	DA	645	C
54	DA	647	G
54	DA	654	A
54	DA	655	A
54	DA	686	U
54	DA	717	C
54	DA	730	A
54	DA	747	5MU
54	DA	764	A
54	DA	765	C
54	DA	775	G
54	DA	776	G

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Mol	Chain	Res	Type
54	DA	782	A
54	DA	784	G
54	DA	785	G
54	DA	790	U
54	DA	792	A
54	DA	805	G
54	DA	812	C
54	DA	827	U
54	DA	828	U
54	DA	858	G
54	DA	859	G
54	DA	860	U
54	DA	878	A
54	DA	883	G
54	DA	885	C
54	DA	896	A
54	DA	897	C
54	DA	910	A
54	DA	914	G
54	DA	915	C
54	DA	927	A
54	DA	931	U
54	DA	932	U
54	DA	946	C
54	DA	961	C
54	DA	974	G
54	DA	983	A
54	DA	996	A
54	DA	1012	U
54	DA	1013	C
54	DA	1022	G
54	DA	1026	G
54	DA	1033	U
54	DA	1040	A
54	DA	1047	G
54	DA	1057	A
54	DA	1061	U
54	DA	1070	A
54	DA	1083	U
54	DA	1088	A
54	DA	1089	A
54	DA	1090	A

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Mol	Chain	Res	Type
54	DA	1091	G
54	DA	1096	A
54	DA	1097	U
54	DA	1112	G
54	DA	1132	U
54	DA	1133	A
54	DA	1135	C
54	DA	1136	G
54	DA	1142	A
54	DA	1168	G
54	DA	1172	C
54	DA	1174	U
54	DA	1175	A
54	DA	1176	U
54	DA	1177	G
54	DA	1180	U
54	DA	1187	G
54	DA	1237	A
54	DA	1238	G
54	DA	1253	A
54	DA	1256	G
54	DA	1271	G
54	DA	1272	A
54	DA	1273	U
54	DA	1300	G
54	DA	1301	A
54	DA	1329	U
54	DA	1352	U
54	DA	1365	A
54	DA	1379	U
54	DA	1383	A
54	DA	1391	U
54	DA	1416	G
54	DA	1417	C
54	DA	1427	A
54	DA	1428	C
54	DA	1434	A
54	DA	1435	G
54	DA	1452	G
54	DA	1453	A
54	DA	1460	U
54	DA	1482	G

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Mol	Chain	Res	Type
54	DA	1490	A
54	DA	1491	G
54	DA	1493	C
54	DA	1494	A
54	DA	1497	U
54	DA	1508	A
54	DA	1509	A
54	DA	1510	G
54	DA	1515	A
54	DA	1523	U
54	DA	1532	A
54	DA	1534	U
54	DA	1535	A
54	DA	1536	C
54	DA	1537	G
54	DA	1566	A
54	DA	1569	A
54	DA	1578	U
54	DA	1583	A
54	DA	1585	C
54	DA	1607	C
54	DA	1608	A
54	DA	1616	A
54	DA	1647	U
54	DA	1648	U
54	DA	1649	G
54	DA	1674	G
54	DA	1715	G
54	DA	1729	U
54	DA	1730	C
54	DA	1731	G
54	DA	1732	C
54	DA	1738	G
54	DA	1744	A
54	DA	1764	C
54	DA	1773	A
54	DA	1782	U
54	DA	1800	C
54	DA	1801	A
54	DA	1808	A
54	DA	1816	C
54	DA	1829	A

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Mol	Chain	Res	Type
54	DA	1869	G
54	DA	1870	C
54	DA	1871	A
54	DA	1872	A
54	DA	1873	G
54	DA	1906	G
54	DA	1907	G
54	DA	1913	A
54	DA	1914	C
54	DA	1929	G
54	DA	1930	G
54	DA	1931	U
54	DA	1937	A
54	DA	1938	A
54	DA	1955	U
54	DA	1965	C
54	DA	1967	C
54	DA	1970	A
54	DA	1972	G
54	DA	1991	U
54	DA	1993	U
54	DA	1997	C
54	DA	2023	C
54	DA	2031	A
54	DA	2033	A
54	DA	2043	C
54	DA	2055	C
54	DA	2056	G
54	DA	2060	A
54	DA	2061	G
54	DA	2062	A
54	DA	2069	G7M
54	DA	2097	A
54	DA	2100	G
54	DA	2102	G
54	DA	2105	U
54	DA	2111	U
54	DA	2112	G
54	DA	2113	U
54	DA	2116	G
54	DA	2117	A
54	DA	2118	U

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Mol	Chain	Res	Type
54	DA	2119	A
54	DA	2120	G
54	DA	2123	G
54	DA	2125	G
54	DA	2126	A
54	DA	2128	G
54	DA	2131	U
54	DA	2132	U
54	DA	2133	G
54	DA	2134	A
54	DA	2135	A
54	DA	2145	C
54	DA	2146	C
54	DA	2148	G
54	DA	2158	A
54	DA	2159	G
54	DA	2160	C
54	DA	2161	C
54	DA	2162	G
54	DA	2163	A
54	DA	2164	C
54	DA	2165	C
54	DA	2167	U
54	DA	2168	G
54	DA	2169	A
54	DA	2170	A
54	DA	2171	A
54	DA	2172	U
54	DA	2173	A
54	DA	2177	C
54	DA	2178	C
54	DA	2179	C
54	DA	2181	U
54	DA	2183	A
54	DA	2185	U
54	DA	2190	G
54	DA	2198	A
54	DA	2204	G
54	DA	2211	A
54	DA	2225	A
54	DA	2238	G
54	DA	2239	G

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Mol	Chain	Res	Type
54	DA	2268	A
54	DA	2283	C
54	DA	2286	G
54	DA	2287	A
54	DA	2305	U
54	DA	2308	G
54	DA	2312	U
54	DA	2324	U
54	DA	2325	G
54	DA	2333	A
54	DA	2335	A
54	DA	2347	C
54	DA	2383	G
54	DA	2385	C
54	DA	2402	U
54	DA	2403	C
54	DA	2406	A
54	DA	2407	A
54	DA	2423	U
54	DA	2424	C
54	DA	2425	A
54	DA	2431	U
54	DA	2435	A
54	DA	2441	U
54	DA	2448	A
54	DA	2476	A
54	DA	2491	U
54	DA	2502	G
54	DA	2505	G
54	DA	2518	A
54	DA	2529	G
54	DA	2535	G
54	DA	2547	A
54	DA	2556	C
54	DA	2566	A
54	DA	2567	G
54	DA	2573	C
54	DA	2574	G
54	DA	2585	U
54	DA	2603	G
54	DA	2609	U
54	DA	2613	U

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Mol	Chain	Res	Type
54	DA	2629	U
54	DA	2630	G
54	DA	2661	G
54	DA	2663	G
54	DA	2689	U
54	DA	2690	U
54	DA	2714	G
54	DA	2726	A
54	DA	2744	G
54	DA	2748	A
54	DA	2765	A
54	DA	2778	A
54	DA	2791	G
54	DA	2798	U
54	DA	2799	A
54	DA	2811	G
54	DA	2820	A
54	DA	2821	A
54	DA	2836	U
54	DA	2867	G
54	DA	2891	U

All (184) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	209	U
1	AA	413	G
1	AA	429	U
1	AA	485	U
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	793	U
1	AA	841	C
1	AA	842	U
1	AA	884	U
1	AA	992	U
1	AA	1086	U

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Mol	Chain	Res	Type
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	429	U
1	BA	485	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1362	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
31	CA	83	A
31	CA	101	A
31	CA	138	U
31	CA	141	G

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Mol	Chain	Res	Type
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	221	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	403	U
31	CA	404	A
31	CA	451	U
31	CA	503	A
31	CA	506	G
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1046	A
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1141	U
31	CA	1253	A
31	CA	1286	A
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C

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Mol	Chain	Res	Type
31	CA	1647	U
31	CA	1730	C
31	CA	1786	A
31	CA	1870	C
31	CA	1871	A
31	CA	2035	G
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2225	A
31	CA	2282	G
31	CA	2286	G
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2430	A
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2797	U
31	CA	2849	U
31	CA	2873	A
54	DA	138	U
54	DA	141	G
54	DA	199	A
54	DA	271	G
54	DA	278	A
54	DA	370	G
54	DA	403	U
54	DA	503	A
54	DA	620	G
54	DA	764	A
54	DA	784	G
54	DA	859	G
54	DA	961	C
54	DA	984	A
54	DA	1061	U
54	DA	1069	A

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Mol	Chain	Res	Type
54	DA	1070	A
54	DA	1087	G
54	DA	1088	A
54	DA	1089	A
54	DA	1128	G
54	DA	1141	U
54	DA	1142	A
54	DA	1175	A
54	DA	1253	A
54	DA	1286	A
54	DA	1300	G
54	DA	1320	C
54	DA	1490	A
54	DA	1497	U
54	DA	1509	A
54	DA	1535	A
54	DA	1607	C
54	DA	1647	U
54	DA	1730	C
54	DA	1870	C
54	DA	1871	A
54	DA	1936	A
54	DA	2097	A
54	DA	2119	A
54	DA	2127	G
54	DA	2146	C
54	DA	2157	G
54	DA	2158	A
54	DA	2164	C
54	DA	2172	U
54	DA	2286	G
54	DA	2311	A
54	DA	2324	U
54	DA	2406	A
54	DA	2423	U
54	DA	2501	C
54	DA	2585	U
54	DA	2681	C
54	DA	2797	U
54	DA	2798	U
54	DA	2873	A



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

76 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
54	OMG	DA	2251	54	19,26,27	0.95	1 (5%)	21,38,41	0.63	0
31	OMC	CA	2498	55,31	19,22,23	0.46	0	25,31,34	0.47	0
54	PSU	DA	746	55,54	18,21,22	0.99	2 (11%)	21,30,33	0.50	0
40	4D4	DN	81[A]	-	9,11,12	2.24	2 (22%)	7,13,15	2.34	2 (28%)
54	2MA	DA	2503	55,54	17,25,26	0.91	1 (5%)	16,37,40	2.23	1 (6%)
31	6MZ	CA	1618	31	17,25,26	1.01	1 (5%)	15,36,39	1.10	2 (13%)
40	4D4	CN	81	40	9,11,12	2.10	2 (22%)	7,13,15	2.62	2 (28%)
31	5MC	CA	1962	31	19,22,23	0.24	0	26,32,35	0.37	0
31	PSU	CA	2605	31	18,21,22	0.33	0	21,30,33	0.56	0
54	6MZ	DA	1618	54	17,25,26	0.99	0	15,36,39	1.80	2 (13%)
54	3TD	DA	1915	54	19,22,23	0.54	0	23,32,35	0.85	1 (4%)
30	MEQ	DD	150[A]	30	8,9,10	0.55	0	5,10,12	0.45	0
1	G7M	BA	527	1	20,26,27	0.94	1 (5%)	16,39,42	2.11	1 (6%)
31	2MG	CA	1835	31	18,26,27	0.95	1 (5%)	16,38,41	0.52	0
31	PSU	CA	2457	31	18,21,22	0.44	0	21,30,33	0.46	0
31	G7M	CA	2069	31	20,26,27	0.82	1 (5%)	16,39,42	0.98	1 (6%)
1	2MG	AA	1516	1	18,26,27	0.89	0	16,38,41	0.73	0
54	OMC	DA	2498	55,54	19,22,23	0.40	0	25,31,34	0.56	0
54	6MZ	DA	2030	54	17,25,26	0.94	1 (5%)	15,36,39	0.92	1 (6%)
31	2MG	CA	2445	31	18,26,27	0.92	0	16,38,41	0.65	0
54	PSU	DA	2504	54	18,21,22	0.63	0	21,30,33	0.45	0
1	G7M	AA	527	1	20,26,27	0.78	0	16,39,42	1.81	1 (6%)
54	PSU	DA	1917	54	18,21,22	0.40	0	21,30,33	0.50	0
54	1MG	DA	745	54	19,26,27	1.51	2 (10%)	18,39,42	0.74	1 (5%)
31	PSU	CA	746	55,31	18,21,22	0.63	1 (5%)	21,30,33	0.44	0
1	MA6	BA	1519	1	19,26,27	0.81	0	18,38,41	1.32	2 (11%)
31	PSU	CA	955	31	18,21,22	0.29	0	21,30,33	0.53	0
12	D2T	AL	89	12	8,9,10	1.32	1 (12%)	6,11,13	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	BA	1402	1	20,23,24	0.41	0	25,32,35	0.52	0
31	6MZ	CA	2030	31	17,25,26	0.91	0	15,36,39	1.07	2 (13%)
1	2MG	BA	1516	1	18,26,27	0.83	0	16,38,41	0.71	0
31	1MG	CA	745	31	19,26,27	1.34	3 (15%)	18,39,42	0.64	0
31	OMG	CA	2251	31	19,26,27	0.79	0	21,38,41	0.64	0
1	2MG	BA	966	55,1	18,26,27	0.80	0	16,38,41	0.54	0
31	OMU	CA	2552	31	19,22,23	0.31	0	25,31,34	0.31	0
1	5MC	AA	1407	1	19,22,23	0.34	0	26,32,35	0.46	0
1	MA6	AA	1518	1	19,26,27	0.93	0	18,38,41	1.00	0
31	PSU	CA	1917	31	18,21,22	0.34	0	21,30,33	0.44	0
54	PSU	DA	955	54	18,21,22	0.63	1 (5%)	21,30,33	0.63	0
40	4D4	DN	81[B]	-	9,11,12	1.49	1 (11%)	7,13,15	2.64	2 (28%)
54	PSU	DA	2604	54	18,21,22	0.55	0	21,30,33	0.65	0
1	2MG	AA	966	1	18,26,27	0.76	0	16,38,41	0.67	0
54	OMU	DA	2552	54	19,22,23	0.34	0	25,31,34	0.36	0
54	PSU	DA	2605	54	18,21,22	0.40	0	21,30,33	0.58	0
31	3TD	CA	1915	31	19,22,23	0.50	0	23,32,35	0.80	1 (4%)
30	MEQ	DD	150[B]	30	8,9,10	1.96	1 (12%)	5,10,12	1.71	1 (20%)
54	5MU	DA	747	54	19,22,23	0.46	0	27,32,35	0.44	0
1	PSU	BA	516	1	18,21,22	0.39	0	21,30,33	0.45	0
31	5MU	CA	1939	31	19,22,23	0.48	0	27,32,35	0.41	0
31	2MA	CA	2503	31	17,25,26	0.91	1 (5%)	16,37,40	2.25	1 (6%)
54	G7M	DA	2069	54	20,26,27	0.71	1 (5%)	16,39,42	0.91	1 (6%)
54	PSU	DA	2457	54	18,21,22	0.41	0	21,30,33	0.43	0
54	5MC	DA	1962	54	19,22,23	0.45	0	26,32,35	0.49	0
1	2MG	BA	1207	1	18,26,27	0.81	0	16,38,41	0.61	0
1	4OC	AA	1402	1	20,23,24	0.30	0	25,32,35	0.52	0
31	PSU	CA	2504	31	18,21,22	0.40	0	21,30,33	0.47	0
1	5MC	AA	967	1	19,22,23	0.29	0	26,32,35	0.37	0
54	5MU	DA	1939	54	19,22,23	0.34	0	27,32,35	0.41	0
54	H2U	DA	2449	54	18,21,22	0.47	0	19,30,33	0.50	0
1	PSU	AA	516	55,1	18,21,22	0.28	0	21,30,33	0.45	0
54	2MG	DA	1835	54	18,26,27	0.86	1 (5%)	16,38,41	0.63	0
1	5MC	BA	967	1	19,22,23	0.27	0	26,32,35	0.36	0
30	MEQ	CD	150	30	7,8,10	0.39	0	4,9,12	0.38	0
54	2MG	DA	2445	54	18,26,27	0.91	0	16,38,41	0.85	1 (6%)
54	PSU	DA	2580	54	18,21,22	0.78	1 (5%)	21,30,33	0.69	0
31	5MU	CA	747	31	19,22,23	0.34	0	27,32,35	0.38	0
1	2MG	AA	1207	1	18,26,27	0.82	0	16,38,41	0.63	0
1	UR3	BA	1498	1	19,22,23	0.51	0	26,32,35	0.84	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	PSU	CA	1911	31	18,21,22	0.27	0	21,30,33	0.40	0
1	5MC	BA	1407	1	19,22,23	0.31	0	26,32,35	0.45	0
31	PSU	CA	2580	31	18,21,22	0.40	0	21,30,33	0.68	1 (4%)
1	MA6	AA	1519	1	19,26,27	0.82	0	18,38,41	1.36	2 (11%)
1	MA6	BA	1518	1	19,26,27	0.91	0	18,38,41	1.03	1 (5%)
54	PSU	DA	1911	54	18,21,22	0.30	0	21,30,33	0.39	0
1	UR3	AA	1498	1	19,22,23	0.29	0	26,32,35	0.35	0
12	D2T	BL	89	12	8,9,10	0.77	0	6,11,13	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	OMG	DA	2251	54	-	1/5/27/28	0/3/3/3
31	OMC	CA	2498	55,31	-	0/9/27/28	0/2/2/2
54	PSU	DA	746	55,54	-	2/7/25/26	0/2/2/2
40	4D4	DN	81[A]	-	-	0/11/12/14	-
54	2MA	DA	2503	55,54	-	1/3/25/26	0/3/3/3
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
40	4D4	CN	81	40	-	1/11/12/14	-
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
30	MEQ	DD	150[A]	30	-	3/8/9/11	-
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	G7M	CA	2069	31	-	1/3/25/26	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
54	OMC	DA	2498	55,54	-	0/9/27/28	0/2/2/2
54	6MZ	DA	2030	54	-	2/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
54	PSU	DA	2504	54	-	1/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	55,31	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	BA	1519	1	-	1/7/29/30	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	2/7/12/14	-
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	1/5/27/28	0/3/3/3
1	2MG	BA	966	55,1	-	0/5/27/28	0/3/3/3
31	OMU	CA	2552	31	-	1/9/27/28	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
40	4D4	DN	81[B]	-	-	2/11/12/14	-
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
54	OMU	DA	2552	54	-	1/9/27/28	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
30	MEQ	DD	150[B]	30	-	4/8/9/11	-
54	5MU	DA	747	54	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	1/3/25/26	0/3/3/3
54	G7M	DA	2069	54	-	1/3/25/26	0/3/3/3
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
54	5MC	DA	1962	54	-	2/7/25/26	0/2/2/2
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
54	5MU	DA	1939	54	-	0/7/25/26	0/2/2/2
54	H2U	DA	2449	54	-	1/7/38/39	0/2/2/2
1	PSU	AA	516	55,1	-	0/7/25/26	0/2/2/2
54	2MG	DA	1835	54	-	2/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
30	MEQ	CD	150	30	-	2/6/7/11	-
54	2MG	DA	2445	54	-	0/5/27/28	0/3/3/3
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	1/7/29/30	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	DN	81[A]	4D4	CZ-NE	6.08	1.45	1.33
40	CN	81	4D4	CZ-NE	5.62	1.44	1.33
30	DD	150[B]	MEQ	CB-CA	5.34	1.61	1.53
31	CA	745	1MG	C2-N1	4.51	1.45	1.37
54	DA	745	1MG	C2-N1	4.43	1.45	1.37
40	DN	81[B]	4D4	CZ-NE	3.84	1.40	1.33
31	CA	2069	G7M	C1'-N9	-3.16	1.41	1.50
54	DA	745	1MG	C8-N7	-2.91	1.30	1.34
54	DA	746	PSU	O4'-C1'	-2.77	1.40	1.43
12	AL	89	D2T	CB-SB	2.71	1.85	1.82
40	DN	81[A]	4D4	CZ-NH1	2.58	1.43	1.34
54	DA	746	PSU	C2'-C1'	-2.57	1.50	1.53
40	CN	81	4D4	CZ-NH1	2.52	1.43	1.34
54	DA	2580	PSU	O4'-C1'	-2.50	1.40	1.43
54	DA	2251	OMG	C5-C6	-2.46	1.42	1.47
31	CA	746	PSU	O4'-C1'	-2.36	1.40	1.43
54	DA	2069	G7M	C1'-N9	-2.30	1.44	1.50
31	CA	2503	2MA	C8-N7	-2.22	1.31	1.34
54	DA	1835	2MG	C8-N7	-2.22	1.31	1.34
1	BA	527	G7M	C1'-N9	-2.18	1.44	1.50
31	CA	745	1MG	C8-N7	-2.17	1.31	1.34
54	DA	2503	2MA	C8-N7	-2.14	1.31	1.34
31	CA	1618	6MZ	C6-C5	-2.12	1.41	1.44
54	DA	955	PSU	C2'-C1'	-2.07	1.50	1.53
31	CA	1835	2MG	C8-N7	-2.05	1.31	1.34
54	DA	2030	6MZ	C6-C5	-2.01	1.41	1.44
31	CA	745	1MG	O4'-C1'	2.00	1.43	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	C4-N3-C2	-8.68	116.64	123.30
54	DA	2503	2MA	C4-N3-C2	-8.43	116.83	123.30
1	BA	527	G7M	O4'-C1'-N9	7.94	119.28	108.75
1	AA	527	G7M	O4'-C1'-N9	6.83	117.80	108.75
54	DA	1618	6MZ	C9-N6-C6	6.07	128.48	122.85
40	CN	81	4D4	NE-CZ-NH2	5.77	130.58	120.67
40	DN	81[B]	4D4	NE-CZ-NH2	5.66	130.39	120.67
40	DN	81[A]	4D4	NE-CZ-NH2	5.22	129.64	120.67
1	AA	1519	MA6	N1-C6-N6	-4.13	112.06	116.83
1	BA	1519	MA6	N1-C6-N6	-3.98	112.24	116.83
30	DD	150[B]	MEQ	CB-CG-CD	3.81	121.55	113.06
40	DN	81[B]	4D4	NH1-CZ-NE	-3.77	110.70	119.27
31	CA	2069	G7M	O4'-C1'-N9	3.66	113.59	108.75
40	CN	81	4D4	NH1-CZ-NE	-3.37	111.61	119.27
54	DA	1915	3TD	C1'-C5-C4	3.35	122.70	117.61
54	DA	2069	G7M	O4'-C1'-N9	3.23	113.03	108.75
1	BA	1498	UR3	C4-N3-C2	-3.15	122.04	124.58
31	CA	1915	3TD	C1'-C5-C4	3.10	122.31	117.61
31	CA	1618	6MZ	C9-N6-C6	3.03	125.66	122.85
40	DN	81[A]	4D4	NH1-CZ-NE	-2.81	112.87	119.27
31	CA	1618	6MZ	C2-N1-C6	2.64	118.64	116.60
31	CA	2030	6MZ	C2-N1-C6	2.56	118.58	116.60
1	AA	1519	MA6	C2-N1-C6	-2.51	114.37	116.84
54	DA	2030	6MZ	C2-N1-C6	2.48	118.52	116.60
54	DA	1618	6MZ	C2-N1-C6	2.45	118.50	116.60
1	BA	1519	MA6	C2-N1-C6	-2.30	114.58	116.84
54	DA	2445	2MG	O6-C6-C5	2.28	128.84	124.32
1	BA	1518	MA6	N1-C6-N6	-2.18	114.31	116.83
31	CA	2030	6MZ	C9-N6-C6	2.16	124.85	122.85
54	DA	745	1MG	O4'-C4'-C3'	-2.10	100.99	105.15
31	CA	2580	PSU	O4'-C1'-C2'	2.09	108.04	105.15

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
12	AL	89	D2T	SB-CB-CG-OD2
1	BA	527	G7M	O4'-C4'-C5'-O5'
12	BL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
12	BL	89	D2T	CA-CB-CG-OD2
30	CD	150	MEQ	C-CA-CB-CG
31	CA	2251	OMG	C1'-C2'-O2'-CM2
30	DD	150[B]	MEQ	N-CA-CB-CG
30	DD	150[B]	MEQ	C-CA-CB-CG
40	DN	81[B]	4D4	CA-CB-CG-CD
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
30	DD	150[A]	MEQ	OE1-CD-CG-CB
30	DD	150[A]	MEQ	NE2-CD-CG-CB
30	CD	150	MEQ	CA-CB-CG-CD
40	DN	81[B]	4D4	OB-CB-CG-CD
54	DA	2030	6MZ	O4'-C4'-C5'-O5'
54	DA	2030	6MZ	C3'-C4'-C5'-O5'
30	DD	150[A]	MEQ	CA-CB-CG-CD
31	CA	1835	2MG	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
31	CA	1835	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	C5-C6-N6-C9
1	BA	1519	MA6	C5-C6-N6-C9
54	DA	2069	G7M	C4'-C5'-O5'-P
54	DA	1835	2MG	O4'-C4'-C5'-O5'
54	DA	1835	2MG	C3'-C4'-C5'-O5'
54	DA	2503	2MA	C4'-C5'-O5'-P
30	DD	150[B]	MEQ	OE1-CD-NE2-CE
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
31	CA	2069	G7M	C4'-C5'-O5'-P
30	DD	150[B]	MEQ	CA-CB-CG-CD
31	CA	2503	2MA	C4'-C5'-O5'-P
31	CA	2504	PSU	O4'-C4'-C5'-O5'
40	CN	81	4D4	CG-CD-NE-CZ
12	BL	89	D2T	SB-CB-CG-OD2
54	DA	2251	OMG	C1'-C2'-O2'-CM2
31	CA	746	PSU	O4'-C1'-C5-C6
54	DA	746	PSU	O4'-C1'-C5-C6
31	CA	2552	OMU	C3'-C2'-O2'-CM2
54	DA	2504	PSU	O4'-C4'-C5'-O5'
31	CA	746	PSU	C2'-C1'-C5-C6
54	DA	746	PSU	C2'-C1'-C5-C6
54	DA	2552	OMU	C3'-C2'-O2'-CM2
54	DA	1962	5MC	O4'-C4'-C5'-O5'
54	DA	2449	H2U	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
54	DA	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	DA	2498	OMC	1	0
54	DA	2030	6MZ	1	0
31	CA	2445	2MG	1	0
1	BA	1519	MA6	1	0
31	CA	2030	6MZ	2	0
1	AA	1518	MA6	1	0
40	DN	81[B]	4D4	1	0
30	DD	150[B]	MEQ	1	0
54	DA	747	5MU	1	0
31	CA	2503	2MA	1	0
54	DA	2449	H2U	1	0
54	DA	2445	2MG	1	0
31	CA	747	5MU	1	0
1	AA	1519	MA6	1	0
1	BA	1518	MA6	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 554 ligands modelled in this entry, 472 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	PG4	DQ	202	-	12,12,12	0.15	0	11,11,11	0.16	0
67	GUN	DA	3210	-	7,12,12	0.72	0	8,17,17	0.82	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	MPD	AA	1676	-	7,7,7	0.54	0	9,10,10	0.45	0
57	MPD	DN	201	-	7,7,7	1.01	1 (14%)	9,10,10	0.63	0
57	MPD	DT	202	-	7,7,7	0.75	0	9,10,10	0.43	0
61	PEG	DA	3225	-	6,6,6	0.50	0	5,5,5	0.27	0
56	PG4	DS	202	-	12,12,12	0.48	0	11,11,11	0.43	0
58	PUT	AA	1674	-	5,5,5	0.15	0	4,4,4	0.14	0
62	EDO	DA	3194	-	3,3,3	0.60	0	2,2,2	0.12	0
58	PUT	AA	1673	-	5,5,5	0.15	0	4,4,4	0.15	0
58	PUT	DA	3211	-	5,5,5	0.31	0	4,4,4	0.20	0
58	PUT	DA	3212	-	5,5,5	0.37	0	4,4,4	0.33	0
61	PEG	DA	3199	-	6,6,6	0.30	0	5,5,5	0.20	0
57	MPD	DA	3190	-	7,7,7	0.44	0	9,10,10	0.51	0
63	PGE	DU	101	-	9,9,9	0.25	0	8,8,8	0.37	0
63	PGE	D3	101	-	9,9,9	0.29	0	8,8,8	0.23	0
61	PEG	DP	201	-	6,6,6	0.30	0	5,5,5	0.15	0
63	PGE	DA	3213	-	9,9,9	0.17	0	8,8,8	0.18	0
58	PUT	DA	3002	-	5,5,5	0.20	0	4,4,4	0.07	0
66	ACY	DA	3191	-	3,3,3	1.01	0	3,3,3	0.90	0
58	PUT	DA	3204	-	5,5,5	0.35	0	4,4,4	0.30	0
56	PG4	DR	202	-	12,12,12	0.43	0	11,11,11	0.54	0
57	MPD	DT	201	-	7,7,7	0.57	0	9,10,10	0.19	0
65	1PE	DA	3185	-	15,15,15	0.16	0	14,14,14	0.16	0
64	SPD	DA	3223	-	9,9,9	0.17	0	8,8,8	0.69	0
62	EDO	DA	3004	-	3,3,3	0.67	0	2,2,2	0.18	0
63	PGE	DA	3186	-	9,9,9	0.35	0	8,8,8	0.56	0
61	PEG	DA	3217	-	6,6,6	0.30	0	5,5,5	0.08	0
57	MPD	DE	301	-	7,7,7	0.79	0	9,10,10	0.81	0
62	EDO	D1	101	-	3,3,3	0.61	0	2,2,2	0.19	0
63	PGE	DA	3224	-	9,9,9	0.25	0	8,8,8	0.17	0
64	SPD	DA	3205	-	9,9,9	0.24	0	8,8,8	0.19	0
62	EDO	DB	211	-	3,3,3	0.54	0	2,2,2	0.22	0
58	PUT	DA	3221	-	5,5,5	0.46	0	4,4,4	0.65	0
62	EDO	DA	3001	-	3,3,3	0.77	0	2,2,2	0.15	0
58	PUT	DA	3218	-	5,5,5	0.12	0	4,4,4	0.10	0
62	EDO	DA	3198	-	3,3,3	0.62	0	2,2,2	0.39	0
64	SPD	DA	3187	-	9,9,9	0.15	0	8,8,8	0.43	0
58	PUT	AA	1675	-	5,5,5	0.20	0	4,4,4	0.23	0
57	MPD	DA	3209	-	7,7,7	0.64	0	9,10,10	0.42	0
58	PUT	DA	3184	-	5,5,5	0.23	0	4,4,4	0.17	0
66	ACY	DA	3196	-	3,3,3	2.60	1 (33%)	3,3,3	2.25	2 (66%)
63	PGE	D1	102	-	9,9,9	0.29	0	8,8,8	0.30	0
57	MPD	DA	3192	-	7,7,7	0.64	0	9,10,10	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	PG4	BA	1601	-	12,12,12	0.21	0	11,11,11	0.22	0
61	PEG	DA	3200	-	6,6,6	0.51	0	5,5,5	0.28	0
58	PUT	AA	1672	-	5,5,5	0.22	0	4,4,4	0.19	0
61	PEG	DQ	201	-	6,6,6	0.21	0	5,5,5	0.15	0
64	SPD	DA	3183	-	9,9,9	0.12	0	8,8,8	0.20	0
61	PEG	D3	102	-	6,6,6	0.33	0	5,5,5	0.24	0
61	PEG	DA	3226	-	6,6,6	0.43	0	5,5,5	0.27	0
66	ACY	DA	3201	-	3,3,3	0.98	0	3,3,3	0.93	0
58	PUT	DA	3195	-	5,5,5	0.31	0	4,4,4	0.55	0
61	PEG	DL	201	-	6,6,6	0.13	0	5,5,5	0.12	0
63	PGE	DS	201	-	9,9,9	0.49	0	8,8,8	0.48	0
58	PUT	DA	3220	-	5,5,5	0.18	0	4,4,4	0.14	0
62	EDO	DA	3003	-	3,3,3	0.70	0	2,2,2	0.17	0
63	PGE	DA	3216	-	9,9,9	0.15	0	8,8,8	0.25	0
62	EDO	DA	3197	-	3,3,3	0.58	0	2,2,2	0.27	0
56	PG4	DA	3193	-	12,12,12	0.30	0	11,11,11	0.43	0
65	1PE	DA	3202	-	15,15,15	0.35	0	14,14,14	0.39	0
68	TRS	DA	3219	-	7,7,7	0.36	0	9,9,9	0.36	0
58	PUT	DA	3189	-	5,5,5	0.47	0	4,4,4	0.45	0
59	TAC	BA	1602	55	34,35,35	0.42	0	43,58,58	1.10	2 (4%)
57	MPD	DK	201	-	7,7,7	0.68	0	9,10,10	0.25	0
58	PUT	DA	3188	-	5,5,5	0.44	0	4,4,4	0.28	0
56	PG4	DA	3215	-	12,12,12	0.16	0	11,11,11	0.13	0
62	EDO	DA	3207	-	3,3,3	0.65	0	2,2,2	0.21	0
57	MPD	DS	203	-	7,7,7	0.42	0	9,10,10	0.73	0
62	EDO	DB	210	-	3,3,3	0.54	0	2,2,2	0.26	0
63	PGE	DD	301	-	9,9,9	0.29	0	8,8,8	0.32	0
57	MPD	DA	3206	-	7,7,7	0.95	1 (14%)	9,10,10	0.55	0
57	MPD	DE	302	-	7,7,7	0.82	0	9,10,10	0.53	0
62	EDO	DA	3208	-	3,3,3	0.54	0	2,2,2	0.34	0
58	PUT	DA	3222	-	5,5,5	0.30	0	4,4,4	0.29	0
59	TAC	AA	1678	55	34,35,35	0.50	0	43,58,58	1.03	2 (4%)
57	MPD	AA	1671	-	7,7,7	0.64	0	9,10,10	0.50	0
62	EDO	DA	3214	-	3,3,3	0.60	0	2,2,2	0.27	0
61	PEG	D1	103	-	6,6,6	0.42	0	5,5,5	0.15	0
56	PG4	AA	1670	-	12,12,12	0.26	0	11,11,11	0.41	0
57	MPD	DA	3203	-	7,7,7	0.84	0	9,10,10	0.66	0
61	PEG	AL	201	-	6,6,6	0.26	0	5,5,5	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PG4	DQ	202	-	-	1/10/10/10	-
67	GUN	DA	3210	-	-	-	0/2/2/2
57	MPD	AA	1676	-	-	1/5/5/5	-
57	MPD	DN	201	-	-	3/5/5/5	-
57	MPD	DT	202	-	-	3/5/5/5	-
61	PEG	DA	3225	-	-	2/4/4/4	-
56	PG4	DS	202	-	-	2/10/10/10	-
58	PUT	AA	1674	-	-	0/3/3/3	-
62	EDO	DA	3194	-	-	1/1/1/1	-
58	PUT	AA	1673	-	-	0/3/3/3	-
58	PUT	DA	3211	-	-	0/3/3/3	-
58	PUT	DA	3212	-	-	1/3/3/3	-
61	PEG	DA	3199	-	-	3/4/4/4	-
57	MPD	DA	3190	-	-	2/5/5/5	-
63	PGE	DU	101	-	-	4/7/7/7	-
63	PGE	D3	101	-	-	2/7/7/7	-
61	PEG	DP	201	-	-	2/4/4/4	-
63	PGE	DA	3213	-	-	3/7/7/7	-
58	PUT	DA	3002	-	-	0/3/3/3	-
58	PUT	DA	3204	-	-	1/3/3/3	-
56	PG4	DR	202	-	-	6/10/10/10	-
57	MPD	DT	201	-	-	2/5/5/5	-
65	1PE	DA	3185	-	-	5/13/13/13	-
64	SPD	DA	3223	-	-	4/7/7/7	-
62	EDO	DA	3004	-	-	0/1/1/1	-
63	PGE	DA	3186	-	-	4/7/7/7	-
61	PEG	DA	3217	-	-	3/4/4/4	-
57	MPD	DE	301	-	-	5/5/5/5	-
62	EDO	D1	101	-	-	0/1/1/1	-
63	PGE	DA	3224	-	-	4/7/7/7	-
64	SPD	DA	3205	-	-	5/7/7/7	-
62	EDO	DB	211	-	-	0/1/1/1	-
58	PUT	DA	3221	-	-	1/3/3/3	-
62	EDO	DA	3001	-	-	1/1/1/1	-
58	PUT	DA	3218	-	-	0/3/3/3	-
62	EDO	DA	3198	-	-	1/1/1/1	-
64	SPD	DA	3187	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PUT	AA	1675	-	-	1/3/3/3	-
57	MPD	DA	3209	-	-	1/5/5/5	-
58	PUT	DA	3184	-	-	0/3/3/3	-
63	PGE	D1	102	-	-	4/7/7/7	-
57	MPD	DA	3192	-	-	2/5/5/5	-
56	PG4	BA	1601	-	-	0/10/10/10	-
61	PEG	DA	3200	-	-	3/4/4/4	-
58	PUT	AA	1672	-	-	0/3/3/3	-
61	PEG	DQ	201	-	-	2/4/4/4	-
64	SPD	DA	3183	-	-	1/7/7/7	-
61	PEG	D3	102	-	-	2/4/4/4	-
61	PEG	DA	3226	-	-	0/4/4/4	-
58	PUT	DA	3195	-	-	1/3/3/3	-
61	PEG	DL	201	-	-	2/4/4/4	-
63	PGE	DS	201	-	-	3/7/7/7	-
58	PUT	DA	3220	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	0/1/1/1	-
63	PGE	DA	3216	-	-	4/7/7/7	-
62	EDO	DA	3197	-	-	0/1/1/1	-
56	PG4	DA	3193	-	-	8/10/10/10	-
65	1PE	DA	3202	-	-	8/13/13/13	-
68	TRS	DA	3219	-	-	0/9/9/9	-
58	PUT	DA	3189	-	-	0/3/3/3	-
59	TAC	BA	1602	55	-	6/8/74/74	0/4/4/4
57	MPD	DK	201	-	-	2/5/5/5	-
58	PUT	DA	3188	-	-	0/3/3/3	-
56	PG4	DA	3215	-	-	4/10/10/10	-
62	EDO	DA	3207	-	-	0/1/1/1	-
57	MPD	DS	203	-	-	0/5/5/5	-
62	EDO	DB	210	-	-	0/1/1/1	-
63	PGE	DD	301	-	-	4/7/7/7	-
57	MPD	DA	3206	-	-	2/5/5/5	-
57	MPD	DE	302	-	-	1/5/5/5	-
62	EDO	DA	3208	-	-	0/1/1/1	-
58	PUT	DA	3222	-	-	1/3/3/3	-
59	TAC	AA	1678	55	-	4/8/74/74	0/4/4/4
57	MPD	AA	1671	-	-	1/5/5/5	-
62	EDO	DA	3214	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PEG	D1	103	-	-	1/4/4/4	-
56	PG4	AA	1670	-	-	4/10/10/10	-
57	MPD	DA	3203	-	-	1/5/5/5	-
61	PEG	AL	201	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	4.29	1.40	1.22
57	DN	201	MPD	C3-C2	2.23	1.60	1.54
57	DA	3206	MPD	C3-C2	2.09	1.60	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	1602	TAC	C5-C41-C4	-5.40	105.94	113.73
59	AA	1678	TAC	C5-C41-C4	-5.03	106.46	113.73
66	DA	3196	ACY	OXT-C-CH3	2.95	127.42	115.05
59	BA	1602	TAC	O3-C3-C2	-2.61	118.57	122.93
66	DA	3196	ACY	O-C-CH3	-2.50	112.27	122.53
59	AA	1678	TAC	O3-C3-C2	-2.42	118.88	122.93

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1676	MPD	C2-C3-C4-O4
57	DE	301	MPD	C1-C2-C3-C4
57	DE	301	MPD	O2-C2-C3-C4
57	DE	301	MPD	C2-C3-C4-O4
57	DE	301	MPD	C2-C3-C4-C5
57	DN	201	MPD	CM-C2-C3-C4
57	DT	202	MPD	C2-C3-C4-C5
57	DA	3190	MPD	C2-C3-C4-O4
57	DA	3190	MPD	C2-C3-C4-C5
59	AA	1678	TAC	C3-C4-N4-C42
59	AA	1678	TAC	C3-C4-N4-C43
59	AA	1678	TAC	C41-C4-N4-C42
59	BA	1602	TAC	C1-C2-C21-O21
59	BA	1602	TAC	C1-C2-C21-N21
59	BA	1602	TAC	C3-C2-C21-O21

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Mol	Chain	Res	Type	Atoms
59	BA	1602	TAC	C3-C2-C21-N21
59	BA	1602	TAC	C41-C4-N4-C42
56	DR	202	PG4	O3-C5-C6-O4
65	DA	3202	1PE	OH6-C15-C25-OH5
64	DA	3205	SPD	C3-C4-C5-N6
63	DA	3213	PGE	O2-C3-C4-O3
56	DR	202	PG4	O2-C3-C4-O3
56	DA	3193	PG4	O3-C5-C6-O4
63	DA	3186	PGE	O3-C5-C6-O4
65	DA	3202	1PE	OH4-C13-C23-OH3
56	DS	202	PG4	O4-C7-C8-O5
65	DA	3185	1PE	OH2-C12-C22-OH3
56	DQ	202	PG4	O1-C1-C2-O2
63	DU	101	PGE	O3-C5-C6-O4
58	DA	3195	PUT	C1-C2-C3-C4
63	DS	201	PGE	O3-C5-C6-O4
64	DA	3205	SPD	C4-C5-N6-C7
64	DA	3205	SPD	C8-C7-N6-C5
61	D1	103	PEG	O2-C3-C4-O4
61	DL	201	PEG	O2-C3-C4-O4
61	DA	3199	PEG	O2-C3-C4-O4
63	DA	3186	PGE	O1-C1-C2-O2
63	DA	3224	PGE	O3-C5-C6-O4
65	DA	3202	1PE	OH2-C12-C22-OH3
62	DA	3194	EDO	O1-C1-C2-O2
64	DA	3205	SPD	C2-C3-C4-C5
58	DA	3204	PUT	C1-C2-C3-C4
61	DA	3200	PEG	O2-C3-C4-O4
63	DA	3224	PGE	O1-C1-C2-O2
63	DD	301	PGE	O2-C3-C4-O3
58	DA	3222	PUT	C1-C2-C3-C4
61	DA	3217	PEG	O2-C3-C4-O4
56	DR	202	PG4	C5-C6-O4-C7
56	DR	202	PG4	C6-C5-O3-C4
58	DA	3212	PUT	C1-C2-C3-C4
63	DU	101	PGE	O1-C1-C2-O2
56	DA	3193	PG4	C1-C2-O2-C3
61	DP	201	PEG	C1-C2-O2-C3
61	DL	201	PEG	C4-C3-O2-C2
56	AA	1670	PG4	C4-C3-O2-C2
65	DA	3185	1PE	C12-C22-OH3-C23
61	AL	201	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
63	D3	101	PGE	C3-C4-O3-C5
56	DA	3215	PG4	C1-C2-O2-C3
56	DA	3215	PG4	C3-C4-O3-C5
63	DA	3213	PGE	C4-C3-O2-C2
56	AA	1670	PG4	C3-C4-O3-C5
56	DA	3193	PG4	C4-C3-O2-C2
61	DA	3200	PEG	C1-C2-O2-C3
61	DA	3199	PEG	C1-C2-O2-C3
61	DA	3199	PEG	O1-C1-C2-O2
61	DA	3217	PEG	O1-C1-C2-O2
63	DD	301	PGE	O3-C5-C6-O4
64	DA	3223	SPD	C4-C5-N6-C7
65	DA	3202	1PE	C16-C26-OH6-C15
61	DA	3225	PEG	C1-C2-O2-C3
61	DA	3225	PEG	C4-C3-O2-C2
65	DA	3202	1PE	C12-C22-OH3-C23
61	DP	201	PEG	C4-C3-O2-C2
56	DA	3215	PG4	C8-C7-O4-C6
63	DD	301	PGE	C4-C3-O2-C2
56	AA	1670	PG4	C5-C6-O4-C7
56	DR	202	PG4	C4-C3-O2-C2
65	DA	3185	1PE	C16-C26-OH6-C15
56	AA	1670	PG4	O1-C1-C2-O2
57	DA	3203	MPD	O2-C2-C3-C4
61	DA	3200	PEG	C4-C3-O2-C2
57	DE	302	MPD	C2-C3-C4-O4
57	DA	3192	MPD	C2-C3-C4-O4
65	DA	3185	1PE	C24-C14-OH5-C25
57	DE	301	MPD	CM-C2-C3-C4
57	DN	201	MPD	C1-C2-C3-C4
57	DT	201	MPD	C1-C2-C3-C4
59	AA	1678	TAC	C41-C4-N4-C43
59	BA	1602	TAC	C3-C4-N4-C43
63	DA	3224	PGE	C1-C2-O2-C3
63	DA	3216	PGE	C3-C4-O3-C5
61	DA	3217	PEG	C1-C2-O2-C3
58	AA	1675	PUT	C1-C2-C3-C4
64	DA	3205	SPD	N6-C7-C8-C9
63	DA	3216	PGE	C4-C3-O2-C2
62	DA	3001	EDO	O1-C1-C2-O2
63	DA	3224	PGE	C3-C4-O3-C5
57	DA	3192	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
63	D1	102	PGE	O3-C5-C6-O4
56	DR	202	PG4	C3-C4-O3-C5
56	DA	3193	PG4	C3-C4-O3-C5
58	DA	3221	PUT	C1-C2-C3-C4
64	DA	3223	SPD	C3-C4-C5-N6
61	AL	201	PEG	C4-C3-O2-C2
62	DA	3198	EDO	O1-C1-C2-O2
63	DA	3186	PGE	C3-C4-O3-C5
63	D1	102	PGE	C3-C4-O3-C5
63	DS	201	PGE	C6-C5-O3-C4
65	DA	3202	1PE	C15-C25-OH5-C14
63	D1	102	PGE	C4-C3-O2-C2
56	DA	3193	PG4	C6-C5-O3-C4
63	DU	101	PGE	C6-C5-O3-C4
56	DS	202	PG4	O2-C3-C4-O3
63	DA	3186	PGE	C4-C3-O2-C2
56	DA	3193	PG4	C8-C7-O4-C6
56	DA	3193	PG4	O4-C7-C8-O5
63	DD	301	PGE	C3-C4-O3-C5
64	DA	3183	SPD	C8-C7-N6-C5
63	DA	3216	PGE	C1-C2-O2-C3
61	D3	102	PEG	C1-C2-O2-C3
63	DU	101	PGE	O2-C3-C4-O3
64	DA	3223	SPD	C8-C7-N6-C5
65	DA	3185	1PE	C13-C23-OH3-C22
56	DA	3215	PG4	O1-C1-C2-O2
61	DQ	201	PEG	O1-C1-C2-O2
63	D3	101	PGE	C4-C3-O2-C2
63	DA	3216	PGE	O2-C3-C4-O3
56	DA	3193	PG4	O2-C3-C4-O3
57	DK	201	MPD	O2-C2-C3-C4
57	DT	202	MPD	O2-C2-C3-C4
57	DA	3206	MPD	O2-C2-C3-C4
57	AA	1671	MPD	C2-C3-C4-O4
57	DK	201	MPD	C2-C3-C4-O4
57	DN	201	MPD	C2-C3-C4-O4
57	DT	202	MPD	C2-C3-C4-O4
57	DA	3209	MPD	C2-C3-C4-O4
61	DQ	201	PEG	C1-C2-O2-C3
61	D3	102	PEG	O1-C1-C2-O2
57	DT	201	MPD	CM-C2-C3-C4
57	DA	3206	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
65	DA	3202	1PE	C14-C24-OH4-C13
64	DA	3223	SPD	C7-C8-C9-N10
63	DS	201	PGE	O2-C3-C4-O3
63	D1	102	PGE	O2-C3-C4-O3
63	DA	3213	PGE	O1-C1-C2-O2
65	DA	3202	1PE	OH5-C14-C24-OH4

There are no ring outliers.

32 monomers are involved in 50 short contacts:

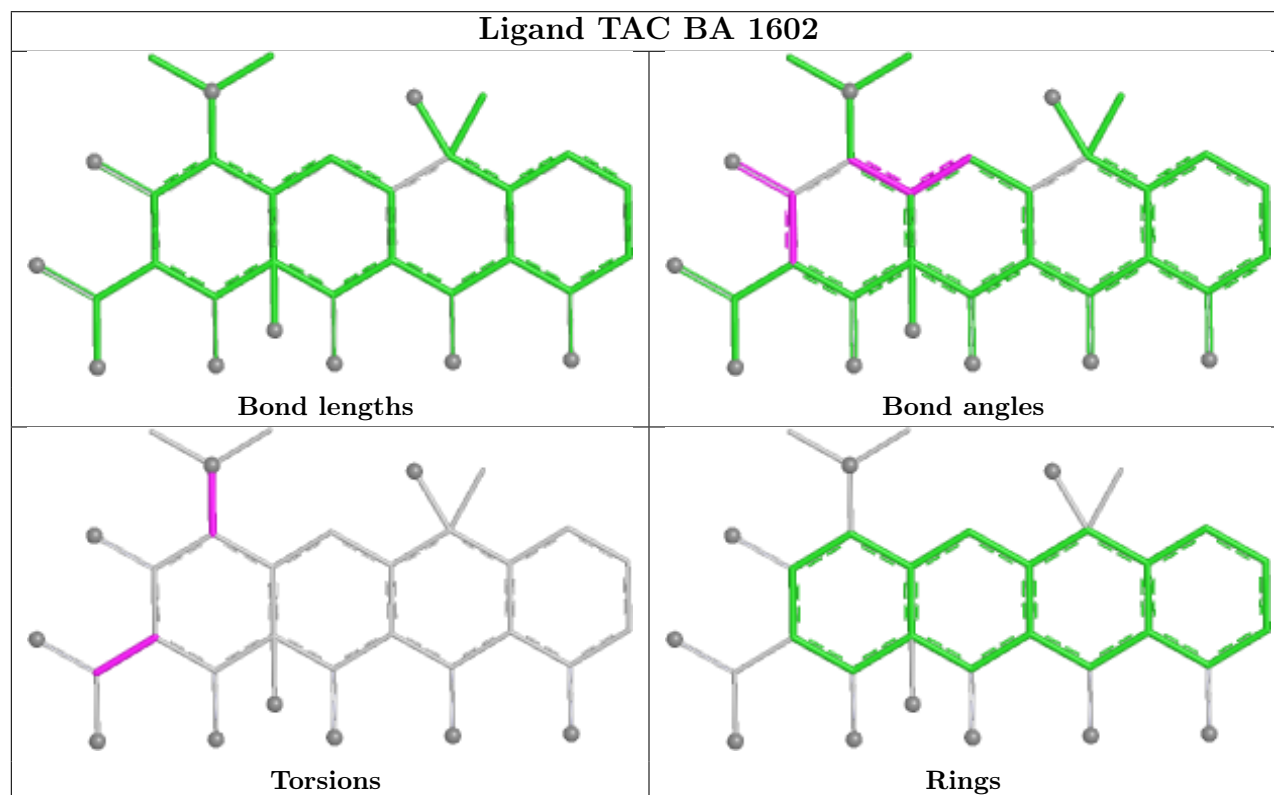
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DN	201	MPD	1	0
56	DS	202	PG4	1	0
62	DA	3194	EDO	1	0
58	DA	3212	PUT	1	0
57	DA	3190	MPD	1	0
63	DU	101	PGE	1	0
61	DP	201	PEG	1	0
63	DA	3213	PGE	1	0
56	DR	202	PG4	5	0
64	DA	3223	SPD	4	0
63	DA	3224	PGE	3	0
62	DB	211	EDO	1	0
58	DA	3221	PUT	3	0
58	DA	3218	PUT	1	0
63	D1	102	PGE	2	0
57	DA	3192	MPD	2	0
61	DA	3200	PEG	1	0
61	D3	102	PEG	2	0
58	DA	3195	PUT	3	0
63	DA	3216	PGE	1	0
62	DA	3197	EDO	1	0
56	DA	3193	PG4	1	0
68	DA	3219	TRS	1	0
58	DA	3189	PUT	1	0
59	BA	1602	TAC	1	0
56	DA	3215	PG4	1	0
63	DD	301	PGE	2	0
58	DA	3222	PUT	1	0
59	AA	1678	TAC	1	0
61	D1	103	PEG	1	0
56	AA	1670	PG4	1	0

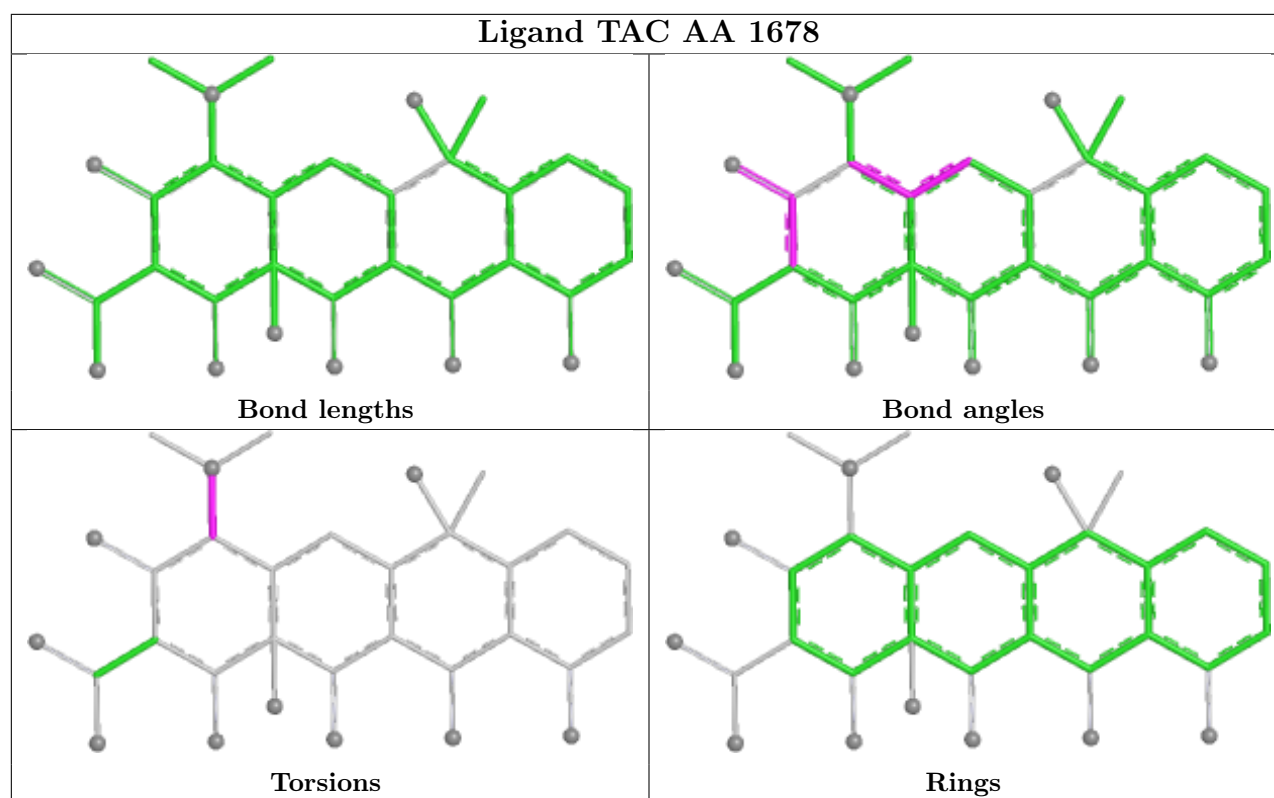
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DA	3203	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1523/1534 (99%)	0.73	126 (8%) 19 14	43, 97, 239, 285	0
1	BA	1522/1534 (99%)	1.48	413 (27%) 2 2	52, 139, 267, 278	0
2	AB	224/224 (100%)	1.18	37 (16%) 5 5	78, 123, 207, 275	0
2	BB	224/224 (100%)	1.41	47 (20%) 3 3	93, 139, 208, 261	0
3	AC	206/206 (100%)	0.87	19 (9%) 16 12	73, 101, 135, 157	0
3	BC	206/206 (100%)	1.45	52 (25%) 2 2	103, 141, 180, 219	0
4	AD	205/205 (100%)	0.82	14 (6%) 25 19	53, 96, 127, 158	0
4	BD	205/205 (100%)	0.65	6 (2%) 54 45	53, 77, 106, 135	0
5	AE	155/155 (100%)	0.71	9 (5%) 30 23	60, 87, 139, 174	0
5	BE	150/155 (96%)	1.27	24 (16%) 6 5	71, 91, 142, 229	0
6	AF	106/106 (100%)	0.81	10 (9%) 15 12	72, 97, 120, 134	0
6	BF	100/106 (94%)	1.04	14 (14%) 7 7	79, 112, 139, 147	0
7	AG	151/151 (100%)	1.46	34 (22%) 3 3	99, 128, 157, 169	0
7	BG	151/151 (100%)	1.89	62 (41%) 1 1	139, 193, 209, 220	0
8	AH	129/129 (100%)	0.75	6 (4%) 37 30	66, 85, 113, 128	0
8	BH	129/129 (100%)	1.29	22 (17%) 5 4	86, 110, 145, 164	0
9	AI	127/127 (100%)	1.58	39 (30%) 1 1	85, 123, 161, 188	0
9	BI	127/127 (100%)	2.17	54 (42%) 1 1	130, 168, 201, 223	0
10	AJ	99/99 (100%)	1.63	29 (29%) 1 2	85, 111, 142, 157	0
10	BJ	98/99 (98%)	2.44	60 (61%) 0 0	132, 163, 188, 200	0
11	AK	117/117 (100%)	0.91	12 (10%) 13 10	52, 102, 138, 153	0
11	BK	117/117 (100%)	1.25	20 (17%) 5 4	73, 109, 139, 160	0
12	AL	122/123 (99%)	0.71	13 (10%) 12 10	48, 66, 99, 126	0
12	BL	122/123 (99%)	1.52	36 (29%) 1 2	75, 91, 112, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	114/114 (100%)	1.59	36 (31%)	1	1	90, 118, 167, 184	0
13	BM	114/114 (100%)	1.86	43 (37%)	1	1	195, 228, 237, 241	0
14	AN	100/100 (100%)	2.05	48 (48%)	0	1	82, 108, 198, 210	0
14	BN	100/100 (100%)	2.19	54 (54%)	0	0	125, 173, 232, 242	0
15	AO	88/88 (100%)	0.74	10 (11%)	11	9	63, 87, 108, 128	0
15	BO	88/88 (100%)	1.04	8 (9%)	16	12	75, 105, 125, 144	0
16	AP	82/82 (100%)	1.02	10 (12%)	10	8	60, 79, 114, 133	0
16	BP	82/82 (100%)	2.85	60 (73%)	0	0	89, 105, 151, 161	0
17	AQ	80/80 (100%)	0.82	7 (8%)	17	13	63, 79, 114, 136	0
17	BQ	80/80 (100%)	1.77	28 (35%)	1	1	94, 119, 143, 147	0
18	AR	55/55 (100%)	0.99	5 (9%)	16	12	68, 91, 126, 154	0
18	BR	55/55 (100%)	1.03	5 (9%)	16	12	71, 89, 123, 150	0
19	AS	79/79 (100%)	1.61	21 (26%)	2	2	94, 109, 146, 153	0
19	BS	79/79 (100%)	2.15	36 (45%)	1	1	206, 223, 234, 242	0
20	AT	86/86 (100%)	1.28	15 (17%)	5	4	67, 79, 116, 132	0
20	BT	85/86 (98%)	2.37	45 (52%)	0	0	101, 121, 164, 175	0
21	AU	56/56 (100%)	1.26	14 (25%)	2	2	80, 118, 156, 170	0
21	BU	56/56 (100%)	1.12	11 (19%)	4	4	75, 100, 143, 156	0
22	C1	56/56 (100%)	2.79	35 (62%)	0	0	94, 138, 164, 182	0
22	D1	56/56 (100%)	0.30	2 (3%)	46	38	20, 41, 64, 95	0
23	C2	50/51 (98%)	2.10	21 (42%)	1	1	126, 141, 153, 175	0
23	D2	51/51 (100%)	0.47	3 (5%)	29	22	49, 63, 89, 104	0
24	C3	46/46 (100%)	3.08	37 (80%)	0	0	99, 109, 119, 131	0
24	D3	46/46 (100%)	0.46	3 (6%)	26	20	30, 42, 56, 99	0
25	C4	64/64 (100%)	3.76	58 (90%)	0	0	105, 121, 134, 140	0
25	D4	64/64 (100%)	0.27	1 (1%)	70	63	34, 41, 52, 63	0
26	C5	38/38 (100%)	2.69	25 (65%)	0	0	100, 114, 124, 134	0
26	D5	38/38 (100%)	0.41	1 (2%)	57	49	31, 46, 62, 82	0
27	C0	58/58 (100%)	2.08	27 (46%)	0	1	98, 113, 132, 135	0
27	D0	58/58 (100%)	0.39	1 (1%)	69	61	25, 35, 50, 72	2 (3%)
28	CB	118/120 (98%)	1.51	27 (22%)	2	3	132, 189, 251, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	120/120 (100%)	-0.09	0 100 100	29, 56, 101, 148	0
29	CC	271/271 (100%)	2.18	123 (45%) 1 1	80, 112, 146, 165	0
29	DC	271/271 (100%)	0.06	13 (4%) 36 29	28, 56, 84, 100	0
30	CD	208/209 (99%)	2.00	94 (45%) 1 1	86, 121, 156, 181	0
30	DD	208/209 (99%)	-0.19	3 (1%) 73 66	18, 39, 67, 88	0
31	CA	2876/2904 (99%)	2.08	1380 (47%) 0 1	71, 170, 260, 285	0
32	CE	201/201 (100%)	2.45	116 (57%) 0 0	112, 159, 194, 210	0
32	DE	201/201 (100%)	0.08	3 (1%) 71 64	24, 55, 100, 139	0
33	CF	177/177 (100%)	1.48	42 (23%) 2 3	198, 211, 219, 226	0
33	DF	177/177 (100%)	0.76	8 (4%) 39 31	50, 79, 125, 137	0
34	CG	176/176 (100%)	1.44	42 (23%) 2 3	130, 170, 205, 215	0
34	DG	176/176 (100%)	0.35	6 (3%) 48 40	42, 70, 97, 139	0
35	CH	149/149 (100%)	1.26	24 (16%) 5 5	84, 151, 170, 180	0
35	DH	149/149 (100%)	1.46	36 (24%) 2 2	74, 150, 187, 199	0
36	CJ	134/134 (100%)	2.07	55 (41%) 1 1	227, 245, 255, 263	0
36	DJ	134/134 (100%)	2.33	72 (53%) 0 0	196, 220, 229, 237	0
37	CK	142/142 (100%)	2.19	74 (52%) 0 0	95, 117, 152, 194	0
37	DK	142/142 (100%)	-0.37	0 100 100	19, 34, 58, 72	0
38	CL	122/123 (99%)	1.74	43 (35%) 1 1	90, 109, 141, 158	0
38	DL	123/123 (100%)	-0.23	0 100 100	28, 43, 70, 106	0
39	CM	144/144 (100%)	2.90	95 (65%) 0 0	104, 151, 201, 235	0
39	DM	144/144 (100%)	0.34	8 (5%) 31 24	18, 55, 84, 116	0
40	CN	135/136 (99%)	1.64	40 (29%) 1 2	92, 112, 142, 180	0
40	DN	135/136 (99%)	-0.28	0 100 100	16, 39, 67, 86	1 (0%)
41	CO	120/125 (96%)	2.45	70 (58%) 0 0	101, 123, 143, 177	0
41	DO	125/125 (100%)	-0.29	0 100 100	24, 36, 65, 108	0
42	CP	116/117 (99%)	1.44	20 (17%) 5 4	139, 162, 177, 181	0
42	DP	117/117 (100%)	0.23	2 (1%) 69 61	36, 56, 84, 93	0
43	CQ	114/114 (100%)	1.69	33 (28%) 1 2	100, 117, 149, 164	0
43	DQ	114/114 (100%)	0.03	3 (2%) 57 49	30, 49, 77, 109	0
44	CR	117/117 (100%)	2.57	69 (58%) 0 0	89, 122, 157, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	DR	117/117 (100%)	-0.43	1 (0%) 81 75	18, 29, 48, 72	0
45	CS	103/103 (100%)	2.45	51 (49%) 0 1	107, 133, 172, 185	0
45	DS	103/103 (100%)	-0.21	2 (1%) 66 58	19, 41, 69, 91	0
46	CT	110/110 (100%)	2.63	76 (69%) 0 0	99, 127, 167, 182	0
46	DT	110/110 (100%)	-0.18	2 (1%) 67 60	19, 33, 60, 116	0
47	CU	93/93 (100%)	2.62	62 (66%) 0 0	123, 147, 176, 185	0
47	DU	93/93 (100%)	0.53	9 (9%) 15 11	31, 53, 109, 124	0
48	CV	102/102 (100%)	2.75	69 (67%) 0 0	113, 161, 198, 209	0
48	DV	102/102 (100%)	0.38	5 (4%) 36 28	42, 60, 121, 157	0
49	CW	94/94 (100%)	1.32	21 (22%) 3 3	116, 137, 156, 161	0
49	DW	94/94 (100%)	-0.08	1 (1%) 77 71	31, 51, 76, 86	0
50	CX	75/76 (98%)	1.96	32 (42%) 1 1	103, 126, 140, 170	0
50	DX	76/76 (100%)	-0.04	1 (1%) 74 67	18, 39, 64, 104	1 (1%)
51	CY	77/77 (100%)	2.53	47 (61%) 0 0	97, 117, 142, 161	0
51	DY	77/77 (100%)	0.07	1 (1%) 74 67	38, 54, 88, 103	0
52	CZ	62/62 (100%)	2.38	39 (62%) 0 0	127, 163, 175, 186	0
52	DZ	62/62 (100%)	0.52	3 (4%) 36 29	48, 70, 103, 126	0
53	DI	135/135 (100%)	1.85	51 (37%) 1 1	78, 150, 197, 207	1 (0%)
54	DA	2873/2904 (98%)	-0.10	142 (4%) 36 28	17, 44, 217, 299	11 (0%)
All	All	20633/20745 (99%)	1.15	4944 (23%) 2 3	16, 108, 239, 299	16 (0%)

All (4944) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	5	ARG	12.5
41	CO	46	ARG	9.6
10	BJ	74	VAL	9.0
9	BI	124	ARG	8.9
9	BI	16	ALA	8.8
39	CM	100	ILE	8.8
20	BT	4	ILE	8.7
22	C1	2	ALA	8.6
37	CK	81	ILE	8.4
45	CS	81	LYS	8.4
25	C4	28	ASN	8.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
46	CT	43	ALA	8.1
39	CM	27	LEU	8.1
39	CM	80	SER	8.1
7	AG	4	ARG	8.1
47	CU	36	LYS	8.0
30	CD	126	ASN	8.0
47	CU	43	ILE	8.0
45	CS	78	ARG	7.9
12	AL	124	ALA	7.8
32	CE	104	ALA	7.8
54	DA	2120	G	7.8
32	CE	73	ILE	7.8
14	AN	21	PHE	7.8
29	CC	234	GLY	7.8
7	BG	4	ARG	7.7
25	C4	39	LYS	7.6
1	BA	211	G	7.5
1	AA	121	U	7.4
39	CM	101	ILE	7.4
31	CA	331	C	7.4
36	DJ	54	PRO	7.4
29	CC	242	LYS	7.3
45	CS	80	ARG	7.2
22	C1	5	GLN	7.1
45	CS	82	HIS	7.1
48	CV	80	ALA	7.1
39	CM	30	THR	6.9
24	C3	42	LEU	6.8
16	BP	17	TYR	6.8
25	C4	15	LYS	6.8
39	CM	81	ASP	6.8
21	BU	57	ALA	6.8
29	CC	228	VAL	6.7
39	CM	29	LYS	6.7
19	BS	12	ASP	6.7
25	C4	37	ALA	6.7
20	BT	5	LYS	6.7
31	CA	1238	G	6.7
31	CA	1984	G	6.7
22	C1	3	VAL	6.6
48	CV	13	VAL	6.6
32	CE	33	VAL	6.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	75	G	6.5
23	C2	24	THR	6.5
39	CM	35	HIS	6.5
1	BA	983	A	6.4
46	CT	83	LYS	6.4
22	C1	21	ALA	6.4
29	CC	30	PHE	6.4
36	DJ	55	ILE	6.4
19	BS	37	ARG	6.4
53	DI	38	MET	6.3
9	BI	14	SER	6.3
30	CD	128	ARG	6.3
41	CO	25	ALA	6.3
53	DI	126	LEU	6.3
25	C4	41	LYS	6.3
9	BI	125	PRO	6.3
30	CD	26	VAL	6.3
1	BA	121	U	6.2
30	CD	154	LYS	6.2
9	BI	117	GLY	6.2
31	CA	386	G	6.2
31	CA	2172	U	6.1
39	CM	19	LEU	6.1
31	CA	411	G	6.1
48	DV	56	GLY	6.1
48	CV	31	SER	6.1
45	CS	83	TYR	6.1
44	CR	8	VAL	6.1
37	CK	42	ALA	6.1
8	AH	2	SER	6.1
16	BP	20	VAL	6.1
44	CR	37	GLN	6.1
9	BI	116	VAL	6.0
31	CA	2691	C	6.0
36	DJ	53	LEU	6.0
22	C1	6	ASN	6.0
21	AU	57	ALA	5.9
29	CC	236	GLU	5.9
45	CS	73	LYS	5.9
1	BA	212	G	5.9
46	CT	97	LEU	5.9
38	CL	122	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
31	CA	183	C	5.9
29	CC	12	GLY	5.9
29	CC	47	GLY	5.9
44	CR	33	ARG	5.8
45	CS	75	VAL	5.8
54	DA	2141	G	5.8
25	C4	60	ALA	5.8
44	CR	28	ARG	5.8
31	CA	2666	C	5.8
44	CR	29	SER	5.8
10	BJ	41	PRO	5.7
32	CE	67	ARG	5.7
2	BB	187	VAL	5.7
26	C5	3	VAL	5.7
25	C4	61	CYS	5.7
31	CA	68	G	5.7
31	CA	2677	G	5.7
24	C3	1	MET	5.7
25	C4	40	ARG	5.6
31	CA	1215	G	5.6
31	CA	2693	G	5.6
13	BM	10	PRO	5.6
39	CM	8	PRO	5.6
14	BN	97	LYS	5.6
32	CE	32	VAL	5.6
39	CM	71	ALA	5.6
20	BT	72	ALA	5.6
39	CM	72	ALA	5.6
10	BJ	8	ILE	5.6
29	CC	212	ARG	5.6
31	CA	1216	G	5.6
54	DA	2172	U	5.6
39	CM	92	LEU	5.6
10	BJ	26	VAL	5.6
25	C4	43	HIS	5.6
39	CM	53	GLY	5.6
36	DJ	13	VAL	5.5
44	CR	9	ILE	5.5
40	CN	41	LEU	5.5
48	CV	35	ILE	5.5
1	AA	1148	U	5.5
24	D3	46	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
2	AB	30	PHE	5.5
45	CS	27	ILE	5.5
1	BA	202	G	5.5
31	CA	2383	G	5.5
32	CE	36	ALA	5.5
50	CX	54	GLY	5.5
44	CR	6	ARG	5.5
45	CS	77	PHE	5.5
31	CA	330	A	5.5
36	CJ	23	PRO	5.5
1	BA	108	G	5.4
31	CA	33	C	5.4
36	DJ	24	VAL	5.4
39	CM	15	ALA	5.4
45	CS	84	ARG	5.4
9	BI	68	LYS	5.4
44	CR	13	ARG	5.4
5	BE	91	GLY	5.4
2	BB	132	LYS	5.4
35	DH	11	ASN	5.4
24	C3	31	LEU	5.4
46	CT	82	MET	5.4
9	AI	17	ALA	5.4
44	CR	38	ALA	5.4
8	BH	2	SER	5.4
19	BS	49	ILE	5.3
1	BA	201	G	5.3
31	CA	776	G	5.3
17	BQ	29	VAL	5.3
22	C1	7	LYS	5.3
16	BP	2	VAL	5.3
51	CY	24	ALA	5.3
41	CO	18	GLN	5.3
9	BI	127	PHE	5.3
39	CM	75	ALA	5.3
9	BI	128	SER	5.2
31	CA	1986	C	5.2
32	CE	69	ARG	5.2
33	CF	156	ILE	5.2
39	CM	36	LYS	5.2
20	BT	13	GLN	5.2
54	DA	2110	G	5.2

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Mol	Chain	Res	Type	RSRZ
31	CA	125	A	5.2
44	CR	11	ARG	5.2
53	DI	83	ALA	5.2
31	CA	2363	G	5.2
46	CT	85	ILE	5.2
48	CV	39	ILE	5.2
1	BA	470	C	5.2
31	CA	32	C	5.2
16	BP	52	LEU	5.2
1	BA	325	A	5.2
44	CR	22	LYS	5.2
32	CE	28	VAL	5.1
36	CJ	13	VAL	5.1
47	CU	34	VAL	5.1
9	BI	119	ARG	5.1
13	BM	96	PRO	5.1
29	CC	241	GLY	5.1
31	CA	2406	A	5.1
39	CM	107	PHE	5.1
31	CA	1068	G	5.1
25	C4	29	LEU	5.1
25	C4	55	LEU	5.1
32	CE	164	LEU	5.1
25	C4	3	LYS	5.1
3	BC	26	THR	5.1
37	CK	84	ILE	5.1
24	C3	27	GLY	5.1
29	CC	233	GLY	5.1
25	C4	57	LEU	5.1
1	BA	1242	G	5.1
28	CB	98	G	5.1
31	CA	329	G	5.1
31	CA	2067	G	5.1
31	CA	2525	G	5.1
31	CA	1958	C	5.1
35	DH	12	LEU	5.1
30	CD	132	ALA	5.1
44	CR	10	ALA	5.1
31	CA	12	U	5.1
32	CE	65	THR	5.1
43	DQ	2	SER	5.1
48	CV	67	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
25	C4	46	PRO	5.0
39	CM	51	GLU	5.0
48	CV	36	VAL	5.0
1	BA	260	G	5.0
44	CR	35	ALA	5.0
18	BR	51	TYR	5.0
7	BG	43	VAL	5.0
45	CS	76	LYS	5.0
16	BP	27	ALA	5.0
31	CA	805	G	5.0
7	AG	109	ARG	5.0
31	CA	1214	A	5.0
1	AA	1030	U	5.0
31	CA	2690	U	5.0
19	BS	35	SER	5.0
48	CV	5	ILE	5.0
37	CK	119	PHE	5.0
53	DI	96	PHE	5.0
39	CM	84	LYS	5.0
42	CP	48	LEU	5.0
44	CR	44	GLN	5.0
46	CT	86	MET	4.9
9	AI	20	PHE	4.9
29	CC	238	ARG	4.9
29	CC	37	ASN	4.9
31	CA	2402	U	4.9
1	BA	134	G	4.9
31	CA	1213	A	4.9
29	CC	248	TRP	4.9
39	CM	114	GLY	4.9
32	CE	178	VAL	4.9
46	CT	47	VAL	4.9
1	BA	307	C	4.9
1	BA	330	C	4.9
3	AC	207	ILE	4.9
16	BP	57	ILE	4.9
39	DM	104	GLN	4.9
53	DI	93	ALA	4.9
26	C5	18	LYS	4.9
1	BA	1386	G	4.9
46	CT	99	ARG	4.9
20	BT	66	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
45	CS	72	VAL	4.9
29	CC	243	HIS	4.9
52	CZ	45	GLN	4.9
51	CY	49	LEU	4.9
1	BA	1067	A	4.9
39	CM	45	GLY	4.9
54	DA	2886[A]	A	4.9
19	BS	76	PRO	4.9
47	CU	74	ILE	4.9
26	C5	10	LEU	4.8
47	CU	61	LEU	4.8
31	CA	1985	C	4.8
1	BA	306	A	4.8
53	DI	131	THR	4.8
26	C5	21	GLY	4.8
29	CC	231	PRO	4.8
23	C2	37	LYS	4.8
25	C4	36	LYS	4.8
12	AL	2	ALA	4.8
31	CA	327	G	4.8
5	BE	109	GLY	4.8
45	CS	96	VAL	4.8
51	CY	54	LYS	4.8
1	BA	135	C	4.8
19	BS	71	LEU	4.8
10	AJ	74	VAL	4.8
32	CE	64	GLY	4.8
31	CA	1647	U	4.8
13	BM	27	LYS	4.8
26	C5	2	LYS	4.8
31	CA	2410	G	4.8
43	CQ	84	ILE	4.8
45	CS	86	GLN	4.8
29	CC	27	GLY	4.7
3	BC	162	ILE	4.7
20	BT	67	ILE	4.7
51	CY	35	SER	4.7
18	BR	20	GLU	4.7
2	BB	130	THR	4.7
52	CZ	57	LEU	4.7
54	DA	277	G	4.7
25	C4	7	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
39	CM	26	GLY	4.7
39	CM	49	GLY	4.7
30	CD	8	LYS	4.7
7	AG	7	ILE	4.7
9	AI	21	ILE	4.7
41	CO	28	LEU	4.7
32	CE	34	ALA	4.7
37	CK	6	ALA	4.7
29	CC	9	THR	4.7
2	BB	136	MET	4.7
31	CA	326	G	4.7
31	CA	1202	G	4.7
31	CA	1236	G	4.7
23	D2	54	ILE	4.7
47	DU	70	HIS	4.7
31	CA	767	U	4.7
10	BJ	50	THR	4.7
47	CU	62	VAL	4.7
31	CA	2502	G	4.7
46	CT	46	LEU	4.7
51	CY	30	LEU	4.7
31	CA	1251	C	4.7
2	BB	34	ALA	4.7
16	BP	18	GLN	4.7
34	CG	172	LYS	4.7
39	CM	70	LYS	4.7
41	CO	105	GLY	4.6
45	CS	50	GLY	4.6
25	C4	4	ILE	4.6
48	CV	12	ILE	4.6
13	BM	19	LEU	4.6
29	CC	61	ALA	4.6
45	CS	36	ALA	4.6
52	CZ	32	ALA	4.6
25	C4	14	PHE	4.6
1	BA	203	G	4.6
31	CA	412	A	4.6
14	BN	47	LYS	4.6
27	C0	56	LYS	4.6
29	CC	223	THR	4.6
32	CE	63	LYS	4.6
39	CM	20	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
41	CO	1	MET	4.6
51	CY	4	VAL	4.6
1	BA	632	U	4.6
1	BA	982	U	4.6
36	CJ	122	ILE	4.6
31	CA	1252	G	4.6
13	BM	89	LEU	4.6
36	CJ	80	LEU	4.6
37	CK	25	LEU	4.6
46	CT	44	ALA	4.6
9	BI	129	LYS	4.6
25	C4	25	LYS	4.6
27	C0	15	GLY	4.6
36	CJ	55	ILE	4.6
32	CE	177	PRO	4.6
44	CR	30	ARG	4.6
7	BG	106	GLU	4.6
39	CM	10	GLU	4.6
14	AN	54	ASP	4.6
32	CE	96	VAL	4.6
2	BB	67	ILE	4.6
3	BC	193	TYR	4.6
10	BJ	76	ILE	4.6
19	BS	33	THR	4.6
29	CC	227	PRO	4.5
31	CA	2891	U	4.5
1	BA	1219	A	4.5
30	CD	160	LYS	4.5
1	BA	63	C	4.5
32	CE	50	ALA	4.5
1	BA	1064	G	4.5
1	BA	1305	G	4.5
10	AJ	75	ASP	4.5
29	CC	229	ASP	4.5
31	CA	1300	G	4.5
29	CC	245	VAL	4.5
36	DJ	78	VAL	4.5
7	BG	5	ARG	4.5
22	C1	11	SER	4.5
32	CE	75	SER	4.5
20	AT	20	HIS	4.5
48	CV	26	LYS	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	2358	A	4.5
1	BA	1302	C	4.5
13	AM	105	ASN	4.5
46	CT	45	VAL	4.5
19	AS	49	ILE	4.5
32	CE	134	LEU	4.5
45	CS	79	ARG	4.5
46	CT	84	ARG	4.5
1	AA	1127	G	4.5
16	BP	12	LYS	4.5
31	CA	387	U	4.5
31	CA	810	U	4.5
3	BC	30	ALA	4.5
36	DJ	138	LEU	4.5
31	CA	2364	C	4.5
29	CC	251	GLN	4.5
38	CL	94	PRO	4.5
32	CE	77	ILE	4.5
32	CE	175	ILE	4.5
39	CM	23	ILE	4.5
27	C0	29	LEU	4.5
31	CA	1322	A	4.5
23	C2	21	TYR	4.5
31	CA	2000	C	4.5
1	BA	1065	U	4.4
31	CA	2245	U	4.4
36	DJ	9	VAL	4.4
31	CA	30	G	4.4
31	CA	1250	G	4.4
14	AN	97	LYS	4.4
25	C4	35	LYS	4.4
37	CK	111	LYS	4.4
3	BC	192	THR	4.4
25	C4	22	PHE	4.4
31	CA	1518	C	4.4
36	DJ	76	ALA	4.4
14	BN	96	LEU	4.4
1	BA	209	U	4.4
31	CA	34	U	4.4
31	CA	1217	U	4.4
2	BB	131	LYS	4.4
30	CD	157	LYS	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
29	CC	8	PRO	4.4
50	CX	56	ASP	4.4
24	C3	36	ALA	4.4
43	CQ	95	ALA	4.4
36	CJ	11	LEU	4.4
53	DI	95	LEU	4.4
1	BA	352	C	4.4
11	BK	14	LYS	4.4
51	CY	26	LYS	4.4
1	BA	1049	U	4.4
32	CE	30	GLN	4.4
1	BA	1355	G	4.4
29	CC	210	ALA	4.4
31	CA	801	G	4.4
31	CA	1324	G	4.4
45	CS	49	ILE	4.4
29	CC	34	LEU	4.4
31	CA	53	A	4.4
36	CJ	24	VAL	4.4
41	CO	43	GLU	4.4
32	CE	70	SER	4.4
32	CE	72	SER	4.4
30	CD	10	GLY	4.4
31	CA	623	C	4.4
36	CJ	74	PRO	4.4
31	CA	1325	U	4.4
29	CC	240	PHE	4.4
16	BP	4	ILE	4.3
16	BP	42	ILE	4.3
26	C5	26	ILE	4.3
29	CC	261	LYS	4.3
29	CC	265	LYS	4.3
40	CN	84	LYS	4.3
50	CX	38	VAL	4.3
6	BF	100	SER	4.3
20	BT	6	SER	4.3
31	CA	1377	G	4.3
31	CA	1653	G	4.3
39	CM	52	GLY	4.3
31	CA	2713	U	4.3
31	CA	765	C	4.3
31	CA	2362	C	4.3

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Mol	Chain	Res	Type	RSRZ
11	BK	21	ALA	4.3
35	DH	25	TYR	4.3
41	CO	113	ILE	4.3
50	CX	44	LYS	4.3
36	CJ	56	PRO	4.3
31	CA	508	A	4.3
54	DA	1847	A	4.3
1	BA	213	G	4.3
32	CE	62	GLN	4.3
29	CC	213	TRP	4.3
31	CA	1066	U	4.3
9	BI	44	ALA	4.3
29	CC	64	ILE	4.3
29	CC	255	LYS	4.3
31	CA	1547	C	4.3
31	CA	2066	C	4.3
47	CU	10	VAL	4.3
48	CV	20	GLY	4.3
22	D1	27	SER	4.3
31	CA	504	A	4.3
31	CA	2665	A	4.3
31	CA	2820	A	4.3
39	CM	64	PHE	4.3
16	AP	4	ILE	4.3
47	CU	32	LEU	4.3
48	CV	47	LYS	4.3
1	BA	102	G	4.3
1	BA	942	G	4.3
29	CC	48	ARG	4.3
9	BI	48	VAL	4.3
54	DA	1087	G	4.3
1	BA	1243	C	4.3
31	CA	2045	C	4.3
16	BP	30	GLY	4.3
30	CD	166	GLY	4.3
14	AN	101	TRP	4.3
1	BA	223	A	4.3
24	C3	20	ALA	4.3
47	CU	73	ARG	4.3
29	CC	216	VAL	4.2
31	CA	355	U	4.2
31	CA	2449	U	4.2

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Mol	Chain	Res	Type	RSRZ
1	BA	933	G	4.2
31	CA	180	G	4.2
31	CA	446	G	4.2
31	CA	729	G	4.2
31	CA	1381	G	4.2
51	CY	31	PRO	4.2
1	BA	186	C	4.2
6	AF	61	LEU	4.2
41	CO	10	LEU	4.2
38	CL	3	GLN	4.2
12	BL	86	ARG	4.2
51	CY	28	ARG	4.2
29	CC	220	VAL	4.2
45	CS	51	VAL	4.2
9	AI	89	GLU	4.2
32	CE	81	GLY	4.2
29	CC	28	LYS	4.2
31	CA	128	C	4.2
31	CA	510	C	4.2
54	DA	2125	G	4.2
14	BN	9	ARG	4.2
47	CU	46	ALA	4.2
16	BP	36	VAL	4.2
26	C5	31	PRO	4.2
29	CC	46	ASN	4.2
31	CA	150	U	4.2
51	CY	16	ASN	4.2
30	CD	144	GLY	4.2
31	CA	501	A	4.2
31	CA	829	A	4.2
48	CV	21	LYS	4.2
32	CE	200	LEU	4.2
36	DJ	79	LEU	4.2
15	BO	58	ARG	4.2
44	CR	59	GLN	4.2
25	C4	58	VAL	4.2
45	DS	103	ALA	4.2
31	CA	31	C	4.2
31	CA	1644	C	4.2
31	CA	1764	C	4.2
46	CT	20	VAL	4.2
47	CU	58	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	BA	107	G	4.2
31	CA	117	G	4.2
54	DA	2152	G	4.2
17	BQ	70	THR	4.2
31	CA	615	U	4.2
1	BA	109	A	4.2
7	AG	23	LEU	4.2
9	AI	127	PHE	4.2
31	CA	1205	A	4.2
31	CA	1237	A	4.2
31	CA	2860	A	4.2
54	DA	654	A	4.2
54	DA	1084	A	4.2
20	BT	57	ILE	4.2
6	BF	91	ARG	4.2
32	CE	52	VAL	4.2
50	CX	23	VAL	4.2
2	AB	130	THR	4.1
46	CT	100	THR	4.1
1	BA	1218	C	4.1
31	CA	16	C	4.1
31	CA	791	C	4.1
1	BA	378	G	4.1
31	CA	46	G	4.1
31	CA	1210	G	4.1
31	CA	1235	G	4.1
17	BQ	8	LEU	4.1
20	BT	86	LEU	4.1
32	CE	138	LEU	4.1
52	CZ	18	LEU	4.1
29	CC	49	ILE	4.1
36	DJ	59	ILE	4.1
20	BT	10	ARG	4.1
35	CH	27	ARG	4.1
1	AA	306	A	4.1
1	BA	389	A	4.1
31	CA	126	A	4.1
31	CA	1253	A	4.1
31	CA	1598	A	4.1
31	CA	2725	A	4.1
26	C5	7	VAL	4.1
48	CV	70	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
24	C3	4	THR	4.1
41	CO	109	PRO	4.1
1	BA	110	C	4.1
19	BS	13	LEU	4.1
31	CA	257	C	4.1
9	BI	31	ASN	4.1
1	BA	208	U	4.1
31	CA	596	U	4.1
31	CA	2861	U	4.1
39	CM	21	ARG	4.1
31	CA	1239	G	4.1
31	CA	1374	G	4.1
31	CA	2046	G	4.1
13	AM	106	ALA	4.1
30	CD	142	VAL	4.1
45	CS	28	ALA	4.1
47	CU	83	ALA	4.1
9	AI	129	LYS	4.1
10	BJ	59	LYS	4.1
32	CE	80	SER	4.1
41	CO	7	GLY	4.1
36	CJ	69	PHE	4.1
37	CK	47	HIS	4.1
38	CL	35	VAL	4.1
40	CN	36	VAL	4.1
42	CP	103	VAL	4.1
44	CR	39	VAL	4.1
48	CV	3	ALA	4.1
47	CU	33	LYS	4.1
1	BA	104	G	4.1
31	CA	1380	G	4.1
54	DA	1091	G	4.1
1	AA	1019	A	4.1
40	CN	72	PRO	4.1
24	C3	24	THR	4.1
29	CC	33	LEU	4.1
29	CC	38	SER	4.1
10	BJ	100	ILE	4.1
19	BS	11	ILE	4.1
50	CX	36	ILE	4.1
36	CJ	140	VAL	4.1
36	CJ	14	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
31	CA	433	C	4.1
5	BE	140	THR	4.0
1	BA	65	A	4.0
31	CA	256	A	4.0
31	CA	480	A	4.0
54	DA	1090	A	4.0
29	CC	221	ARG	4.0
31	CA	308	G	4.0
51	CY	3	ARG	4.0
44	CR	34	VAL	4.0
36	CJ	76	ALA	4.0
41	CO	40	LYS	4.0
39	CM	38	GLN	4.0
22	C1	8	PRO	4.0
25	C4	63	PRO	4.0
1	BA	106	C	4.0
13	AM	33	ILE	4.0
44	CR	26	GLY	4.0
32	CE	78	TRP	4.0
2	AB	132	LYS	4.0
30	CD	122	VAL	4.0
31	CA	26	G	4.0
35	DH	63	ALA	4.0
27	C0	18	PRO	4.0
31	CA	1778	U	4.0
39	CM	56	PRO	4.0
35	CH	132	PHE	4.0
39	CM	59	ARG	4.0
1	BA	379	C	4.0
14	BN	98	LYS	4.0
36	DJ	10	LYS	4.0
41	CO	29	VAL	4.0
45	CS	71	LYS	4.0
1	AA	1092	A	4.0
31	CA	2071	A	4.0
41	CO	24	MET	4.0
47	CU	35	ALA	4.0
10	BJ	73	LEU	4.0
24	C3	10	LEU	4.0
47	CU	7	LEU	4.0
52	CZ	14	LEU	4.0
1	AA	963	G	4.0

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Mol	Chain	Res	Type	RSRZ
1	BA	200	G	4.0
31	CA	474	G	4.0
31	CA	2742	G	4.0
31	CA	2780	G	4.0
41	CO	22	ARG	4.0
39	CM	24	GLY	4.0
48	CV	77	THR	4.0
1	BA	222	C	4.0
2	AB	27	MET	4.0
5	BE	46	VAL	4.0
16	BP	9	HIS	4.0
52	DZ	63	ALA	4.0
31	CA	182	A	4.0
31	CA	2706	A	4.0
11	BK	97	ILE	4.0
14	BN	93	ILE	4.0
44	CR	65	ILE	4.0
3	BC	2	GLY	4.0
37	CK	71	ASP	4.0
39	CM	102	GLY	4.0
1	AA	933	G	3.9
1	BA	380	G	3.9
12	AL	15	LYS	3.9
25	C4	47	LYS	3.9
31	CA	1332	G	3.9
39	CM	74	THR	3.9
48	CV	44	LYS	3.9
47	CU	47	VAL	3.9
48	CV	25	VAL	3.9
7	BG	39	ALA	3.9
25	C4	65	ALA	3.9
27	D0	2[A]	ALA	3.9
29	CC	205	LEU	3.9
31	CA	61	C	3.9
31	CA	1233	C	3.9
31	CA	1600	C	3.9
39	CM	61	LEU	3.9
11	AK	110	ILE	3.9
16	BP	26	ASN	3.9
37	CK	142	ILE	3.9
42	CP	87	ILE	3.9
51	CY	48	THR	3.9

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Mol	Chain	Res	Type	RSRZ
19	AS	58	VAL	3.9
31	CA	2061	G	3.9
13	BM	22	ILE	3.9
15	BO	62	GLN	3.9
31	CA	57	C	3.9
31	CA	1323	C	3.9
31	CA	2527	C	3.9
54	DA	143	C	3.9
39	CM	28	GLY	3.9
39	CM	39	LYS	3.9
46	CT	98	LYS	3.9
48	CV	24	LYS	3.9
22	C1	15	MET	3.9
31	CA	354	A	3.9
31	CA	626	A	3.9
31	CA	804	A	3.9
31	CA	392	U	3.9
48	CV	59	VAL	3.9
12	BL	26	ALA	3.9
25	C4	27	ALA	3.9
32	CE	161	ALA	3.9
41	CO	68	ALA	3.9
52	CZ	61	ALA	3.9
19	BS	14	HIS	3.9
37	CK	109	LEU	3.9
51	CY	22	LEU	3.9
22	C1	55	ILE	3.9
30	CD	146	ILE	3.9
43	CQ	85	SER	3.9
31	CA	289	G	3.9
31	CA	1248	G	3.9
31	CA	1444	G	3.9
52	CZ	30	MET	3.9
1	BA	136	C	3.9
1	BA	210	C	3.9
31	CA	2073	C	3.9
48	CV	49	VAL	3.9
1	AA	994	A	3.9
1	AA	1441	A	3.9
31	CA	675	A	3.9
13	BM	106	ALA	3.9
7	BG	93	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
16	BP	51	ARG	3.9
46	CT	11	ARG	3.9
32	CE	101	TYR	3.9
16	BP	16	PHE	3.9
36	DJ	117	MET	3.9
36	DJ	131	GLY	3.9
29	CC	239	ASN	3.9
41	CO	23	ASN	3.9
1	BA	326	G	3.9
31	CA	248	G	3.9
31	CA	2526	G	3.9
31	CA	2692	G	3.9
36	CJ	70	VAL	3.8
1	BA	308	C	3.8
1	BA	1217	C	3.8
10	BJ	42	LEU	3.8
31	CA	237	C	3.8
31	CA	678	C	3.8
32	CE	131	THR	3.8
47	CU	93	LEU	3.8
1	AA	1017	U	3.8
1	BA	1151	A	3.8
1	BA	1201	A	3.8
31	CA	477	A	3.8
31	CA	1321	A	3.8
31	CA	2800	A	3.8
24	C3	35	ARG	3.8
40	CN	40	ARG	3.8
46	CT	16	LYS	3.8
37	CK	48	VAL	3.8
39	CM	46	VAL	3.8
11	BK	94	GLU	3.8
19	BS	15	LEU	3.8
33	CF	32	GLU	3.8
51	CY	25	THR	3.8
31	CA	1382	G	3.8
31	CA	1651	G	3.8
31	CA	2444	G	3.8
1	AA	984	C	3.8
1	BA	984	C	3.8
1	BA	1066	C	3.8
10	AJ	6	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
26	C5	23	ILE	3.8
31	CA	236	C	3.8
31	CA	1289	C	3.8
31	CA	2072	C	3.8
44	CR	17	ILE	3.8
45	CS	35	PHE	3.8
15	AO	69	TYR	3.8
46	CT	15	GLN	3.8
39	DM	102	GLY	3.8
52	CZ	53	VAL	3.8
41	CO	44	LEU	3.8
41	CO	104	ALA	3.8
12	BL	14	ARG	3.8
29	DC	238	ARG	3.8
24	C3	46	LYS	3.8
2	BB	201	PRO	3.8
3	BC	196	ILE	3.8
6	BF	93	LYS	3.8
1	AA	96	U	3.8
7	BG	62	PHE	3.8
31	CA	67	U	3.8
41	CO	21	PHE	3.8
54	DA	2797	U	3.8
1	BA	113	G	3.8
31	CA	105	C	3.8
31	CA	394	C	3.8
31	CA	672	C	3.8
31	CA	830	G	3.8
31	CA	1708	C	3.8
31	CA	2862	G	3.8
3	BC	197	GLY	3.8
25	C4	56	GLY	3.8
31	CA	677	A	3.8
36	DJ	12	GLN	3.8
54	DA	2142	A	3.8
50	CX	53	CYS	3.8
30	CD	155	VAL	3.8
39	CM	42	SER	3.8
7	BG	13	LEU	3.8
36	DJ	80	LEU	3.8
52	CZ	22	LEU	3.8
11	AK	66	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
9	BI	122	ARG	3.8
24	C3	2	LYS	3.8
29	CC	52	ARG	3.8
39	CM	14	LYS	3.8
39	CM	78	ARG	3.8
23	C2	22	THR	3.8
53	DI	128	THR	3.8
29	CC	225	MET	3.8
22	C1	4	GLN	3.8
1	BA	948	C	3.8
31	CA	624	C	3.8
31	CA	1305	C	3.8
31	CA	1349	C	3.8
31	CA	1606	C	3.8
31	CA	2260	C	3.8
31	CA	2873	A	3.8
39	CM	3	LEU	3.8
1	AA	1018	G	3.8
31	CA	54	G	3.8
31	CA	481	G	3.8
31	CA	536	G	3.8
31	CA	2107	G	3.8
3	BC	137	ALA	3.7
19	AS	75	ALA	3.7
22	C1	12	LYS	3.7
30	CD	57	ALA	3.7
32	CE	37	ALA	3.7
43	CQ	91	ALA	3.7
25	C4	17	THR	3.7
53	DI	106	PHE	3.7
27	C0	9	GLN	3.7
41	CO	9	GLN	3.7
3	BC	168	TYR	3.7
9	BI	67	VAL	3.7
22	C1	25	VAL	3.7
36	DJ	70	VAL	3.7
7	BG	35	LYS	3.7
10	BJ	46	LYS	3.7
16	BP	46	LYS	3.7
20	BT	64	LYS	3.7
20	BT	76	LYS	3.7
25	C4	5	LYS	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	482	A	3.7
1	BA	985	C	3.7
1	BA	1363	A	3.7
31	CA	225	C	3.7
31	CA	426	C	3.7
31	CA	676	A	3.7
31	CA	1302	A	3.7
1	BA	1387	G	3.7
10	BJ	44	THR	3.7
10	BJ	69	THR	3.7
30	CD	25	THR	3.7
31	CA	356	G	3.7
31	CA	388	G	3.7
31	CA	410	G	3.7
31	CA	442	G	3.7
31	CA	1277	G	3.7
29	CC	235	GLY	3.7
32	CE	143	LEU	3.7
32	CE	147	LEU	3.7
36	CJ	28	LEU	3.7
10	BJ	98	VAL	3.7
22	C1	54	VAL	3.7
23	C2	47	VAL	3.7
25	C4	50	VAL	3.7
37	CK	74	TYR	3.7
52	CZ	50	VAL	3.7
54	DA	2109	U	3.7
14	BN	12	LYS	3.7
16	BP	7	ALA	3.7
32	CE	39	ALA	3.7
36	CJ	129	ILE	3.7
44	CR	27	ALA	3.7
49	CW	22	ALA	3.7
1	AA	962	C	3.7
1	AA	1128	C	3.7
1	AA	1149	C	3.7
1	BA	175	C	3.7
2	AB	42	ASN	3.7
32	CE	85	PHE	3.7
47	CU	60	THR	3.7
1	BA	68	G	3.7
1	BA	1461	G	3.7

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Mol	Chain	Res	Type	RSRZ
13	AM	11	ASP	3.7
14	BN	54	ASP	3.7
29	CC	254	GLY	3.7
3	BC	43	LEU	3.7
31	CA	389	G	3.7
31	CA	989	G	3.7
31	CA	1983	G	3.7
36	DJ	57	VAL	3.7
41	CO	47	VAL	3.7
48	CV	83	VAL	3.7
20	BT	69	LYS	3.7
31	CA	448	U	3.7
31	CA	2522	U	3.7
31	CA	2629	U	3.7
41	CO	4	ARG	3.7
16	BP	22	ALA	3.7
24	C3	23	ALA	3.7
32	CE	135	ALA	3.7
7	AG	62	PHE	3.7
27	C0	53	PHE	3.7
36	CJ	38	PHE	3.7
25	C4	38	THR	3.7
27	C0	10	THR	3.7
31	CA	2020	A	3.7
31	CA	2070	A	3.7
1	BA	322	C	3.7
1	BA	328	C	3.7
1	BA	381	C	3.7
31	CA	444	C	3.7
29	CC	202	LEU	3.7
46	CT	19	LEU	3.7
8	BH	110	VAL	3.7
10	BJ	60	ASP	3.7
14	BN	45	VAL	3.7
47	CU	19	LYS	3.7
48	CV	43	LYS	3.7
44	CR	50	ARG	3.7
1	BA	198	G	3.7
1	BA	1220	G	3.7
1	BA	1222	G	3.7
1	BA	1432	G	3.7
31	CA	325	G	3.7

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Mol	Chain	Res	Type	RSRZ
31	CA	333	G	3.7
31	CA	408	G	3.7
31	CA	583	G	3.7
1	BA	1364	U	3.7
25	C4	59	ILE	3.7
14	AN	22	ALA	3.7
31	CA	390	U	3.7
24	C3	7	PRO	3.6
29	CC	247	PRO	3.6
36	DJ	23	PRO	3.6
39	CM	50	PHE	3.6
2	BB	20	THR	3.6
36	CJ	126	THR	3.6
34	CG	33	LEU	3.6
36	DJ	106	LEU	3.6
1	BA	101	A	3.6
31	CA	127	A	3.6
51	CY	47	VAL	3.6
1	BA	1369	C	3.6
2	BB	21	ARG	3.6
16	BP	25	ARG	3.6
31	CA	413	C	3.6
44	CR	52	GLN	3.6
44	CR	3	ARG	3.6
44	CR	90	ILE	3.6
14	AN	25	ALA	3.6
37	CK	94	ALA	3.6
20	BT	68	HIS	3.6
36	CJ	54	PRO	3.6
44	CR	106	PHE	3.6
1	BA	112	G	3.6
31	CA	379	G	3.6
31	CA	409	G	3.6
31	CA	1770	G	3.6
31	CA	2242	G	3.6
31	CA	2409	G	3.6
6	BF	39	LEU	3.6
22	C1	28	LEU	3.6
9	BI	100	LYS	3.6
23	C2	23	THR	3.6
43	CQ	94	LYS	3.6
50	CX	24	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
9	AI	124	ARG	3.6
20	AT	61	GLN	3.6
37	CK	34	ARG	3.6
10	BJ	6	ILE	3.6
29	CC	54	ILE	3.6
31	CA	1067	A	3.6
31	CA	2346	A	3.6
42	CP	40	ILE	3.6
1	BA	339	C	3.6
2	BB	134	ALA	3.6
25	C4	48	ALA	3.6
30	CD	65	ALA	3.6
31	CA	1161	C	3.6
36	DJ	14	ALA	3.6
46	CT	38	TYR	3.6
13	AM	96	PRO	3.6
29	CC	11	PRO	3.6
30	CD	156	PHE	3.6
1	BA	103	U	3.6
31	CA	1326	U	3.6
31	CA	1375	U	3.6
31	CA	2438	U	3.6
54	DA	2585	U	3.6
27	C0	17	LEU	3.6
32	CE	132	LYS	3.6
37	CK	72	LYS	3.6
48	CV	14	LEU	3.6
51	CY	14	THR	3.6
37	CK	79	GLY	3.6
39	CM	37	GLY	3.6
1	BA	1356	G	3.6
10	BJ	57	VAL	3.6
11	BK	84	VAL	3.6
30	CD	9	VAL	3.6
31	CA	381	G	3.6
31	CA	1355	G	3.6
24	C3	14	ARG	3.6
52	CZ	23	ARG	3.6
10	AJ	53	ILE	3.6
41	CO	34	ILE	3.6
43	CQ	110	ILE	3.6
9	BI	121	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
16	BP	82	ALA	3.6
20	BT	63	ALA	3.6
53	DI	2	ALA	3.6
31	CA	443	A	3.6
31	CA	1353	A	3.6
31	CA	2872	A	3.6
1	BA	1366	C	3.6
31	CA	565	C	3.6
31	CA	1306	C	3.6
31	CA	1350	C	3.6
31	CA	2628	C	3.6
31	CA	931	U	3.6
31	CA	2833	U	3.6
33	DF	117	LEU	3.6
38	CL	66	LYS	3.6
7	BG	38	THR	3.6
36	DJ	118	THR	3.6
29	CC	250	VAL	3.6
47	CU	30	ILE	3.6
48	CV	58	ILE	3.6
29	CC	112	ALA	3.6
31	CA	250	G	3.6
31	CA	1331	G	3.6
31	CA	1573	G	3.6
31	CA	2708	G	3.6
16	AP	17	TYR	3.6
24	C3	5	PHE	3.6
29	DC	240	PHE	3.6
34	CG	157	TYR	3.6
1	AA	1016	A	3.5
1	BA	353	A	3.5
2	BB	135	LEU	3.6
3	BC	175	LEU	3.6
48	CV	33	LYS	3.6
34	DG	173	GLU	3.5
1	BA	261	U	3.5
31	CA	11	C	3.5
31	CA	198	C	3.5
31	CA	318	C	3.5
31	CA	385	C	3.5
31	CA	455	C	3.5
31	CA	1396	U	3.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1612	C	3.5
31	CA	2244	U	3.5
47	DU	1	MET	3.5
5	BE	157	ARG	3.5
24	C3	9	VAL	3.5
36	CJ	58	VAL	3.5
41	CO	27	SER	3.5
48	CV	65	ILE	3.5
52	CZ	15	ASN	3.5
12	BL	124	ALA	3.5
9	AI	125	PRO	3.5
10	AJ	73	LEU	3.5
12	BL	117	TYR	3.5
40	CN	118	LYS	3.5
51	CY	77	LYS	3.5
30	CD	138	LEU	3.5
44	CR	18	LEU	3.5
17	BQ	63	GLU	3.5
31	CA	690	G	3.5
31	CA	1266	G	3.5
31	CA	1407	G	3.5
31	CA	1767	G	3.5
31	CA	2455	G	3.5
54	DA	2140	G	3.5
33	CF	130	MET	3.5
1	BA	196	A	3.5
31	CA	1359	A	3.5
7	AG	43	VAL	3.5
18	AR	73	ARG	3.5
36	DJ	58	VAL	3.5
50	CX	13	GLY	3.5
31	CA	328	U	3.5
31	CA	1406	U	3.5
17	BQ	21	ILE	3.5
1	BA	1203	C	3.5
31	CA	76	C	3.5
32	CE	90	GLN	3.5
7	BG	134	ALA	3.5
20	AT	62	ALA	3.5
20	BT	73	ALA	3.5
32	CE	182	ALA	3.5
44	DR	118	ALA	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
46	CT	42	LYS	3.5
36	DJ	11	LEU	3.5
29	CC	217	ARG	3.5
35	CH	108	VAL	3.5
47	CU	67	VAL	3.5
1	BA	64	G	3.5
1	BA	331	G	3.5
31	CA	242	G	3.5
31	CA	377	G	3.5
31	CA	505	A	3.5
31	CA	619	G	3.5
31	CA	1311	G	3.5
31	CA	1378	A	3.5
31	CA	2618	G	3.5
37	CK	103	ILE	3.5
54	DA	549	G	3.5
31	CA	1709	U	3.5
31	CA	2249	U	3.5
47	CU	72	GLN	3.5
12	BL	18	LYS	3.5
23	C2	10	LYS	3.5
30	DD	54	ALA	3.5
30	CD	23	PRO	3.5
31	CA	680	C	3.5
31	CA	2712	C	3.5
50	CX	60	PHE	3.5
54	DA	2174	C	3.5
52	CZ	43	LEU	3.5
13	AM	109	ARG	3.5
41	CO	8	ARG	3.5
46	DT	110	ARG	3.5
5	BE	108	GLY	3.5
16	BP	21	VAL	3.5
17	BQ	46	VAL	3.5
29	CC	41	GLY	3.5
29	CC	65	VAL	3.5
29	CC	249	GLY	3.5
16	BP	50	THR	3.5
1	AA	1240	U	3.5
1	BA	218	U	3.5
1	BA	219	U	3.5
1	BA	390	U	3.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1779	U	3.5
31	CA	2689	U	3.5
31	CA	1328	A	3.5
31	CA	1572	A	3.5
31	CA	2019	A	3.5
39	CM	83	ALA	3.5
1	BA	1026	G	3.5
1	BA	1221	G	3.5
31	CA	259	G	3.5
31	CA	512	G	3.5
31	CA	2697	G	3.5
31	CA	2844	G	3.5
31	CA	2895	G	3.5
36	DJ	135	SER	3.5
54	DA	548	G	3.5
29	CC	86	ASN	3.5
1	AA	1031	C	3.5
31	CA	335	C	3.5
31	CA	1615	C	3.5
19	AS	3	ARG	3.5
29	CC	62	TYR	3.5
36	DJ	96	ASP	3.4
7	AG	8	GLY	3.4
7	AG	32	VAL	3.4
10	BJ	84	VAL	3.4
25	C4	9	GLY	3.4
26	C5	22	VAL	3.4
26	C5	38	GLY	3.4
37	CK	105	VAL	3.4
16	BP	67	ILE	3.4
36	DJ	129	ILE	3.4
37	CK	93	ILE	3.4
7	BG	133	THR	3.4
30	CD	62	LYS	3.4
32	CE	57	LYS	3.4
1	BA	981	U	3.4
1	BA	1307	U	3.4
12	BL	2	ALA	3.4
16	BP	11	ALA	3.4
16	BP	39	PHE	3.4
31	CA	1209	U	3.4
31	CA	1599	U	3.4

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Mol	Chain	Res	Type	RSRZ
36	CJ	79	LEU	3.4
36	DJ	20	PRO	3.4
36	DJ	133	ALA	3.4
40	CN	92	TRP	3.4
42	CP	6	ALA	3.4
46	CT	64	ALA	3.4
10	BJ	54	SER	3.4
13	AM	30	SER	3.4
31	CA	309	A	3.4
31	CA	382	A	3.4
31	CA	482	A	3.4
31	CA	575	A	3.4
29	CC	43	ARG	3.4
1	BA	111	G	3.4
1	BA	220	G	3.4
31	CA	831	G	3.4
31	CA	1430	G	3.4
44	CR	25	TYR	3.4
29	CC	204	VAL	3.4
1	BA	207	C	3.4
28	CB	97	C	3.4
31	CA	517	C	3.4
31	CA	581	C	3.4
31	CA	795	C	3.4
31	CA	994	C	3.4
31	CA	1646	C	3.4
31	CA	2078	C	3.4
46	CT	94	ASP	3.4
47	CU	2	ILE	3.4
48	CV	89	ASP	3.4
49	CW	89	ILE	3.4
14	AN	12	LYS	3.4
19	BS	17	LYS	3.4
47	CU	81	LYS	3.4
23	C2	34	LEU	3.4
23	C2	36	LEU	3.4
25	C4	44	LEU	3.4
33	CF	103	LEU	3.4
51	CY	33	LEU	3.4
32	CE	60	TRP	3.4
1	BA	4	U	3.4
31	CA	235	U	3.4

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Mol	Chain	Res	Type	RSRZ
10	BJ	58	ASN	3.4
35	DH	20	ASN	3.4
41	CO	11	ASN	3.4
1	AA	1280	A	3.4
31	CA	103	A	3.4
31	CA	614	A	3.4
31	CA	1156	A	3.4
7	AG	6	VAL	3.4
13	BM	86	TYR	3.4
16	BP	33	ILE	3.4
32	CE	119	ILE	3.4
48	CV	17	LYS	3.4
1	BA	79	G	3.4
1	BA	377	G	3.4
31	CA	396	G	3.4
31	CA	1131	G	3.4
31	CA	1341	G	3.4
31	CA	1356	G	3.4
31	CA	1360	G	3.4
31	CA	1622	G	3.4
31	CA	1643	G	3.4
31	CA	69	C	3.4
31	CA	995	C	3.4
31	CA	1005	C	3.4
31	CA	1314	C	3.4
31	CA	2616	C	3.4
10	BJ	71	LEU	3.4
36	CJ	106	LEU	3.4
36	CJ	138	LEU	3.4
16	AP	16	PHE	3.4
51	CY	56	MET	3.4
31	CA	1769	U	3.4
48	CV	6	ARG	3.4
36	DJ	128	SER	3.4
18	BR	21	ILE	3.4
30	CD	60	VAL	3.4
32	CE	196	VAL	3.4
34	CG	10	VAL	3.4
41	CO	97	ILE	3.4
43	CQ	92	VAL	3.4
53	DI	33	VAL	3.4
43	CQ	68	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	BA	1441	A	3.4
9	BI	120	LYS	3.4
20	AT	16	LYS	3.4
31	CA	222	A	3.4
31	CA	391	A	3.4
31	CA	1262	A	3.4
31	CA	1393	A	3.4
31	CA	1548	A	3.4
31	CA	2126	A	3.4
31	CA	2411	A	3.4
32	CE	47	LYS	3.4
53	DI	90	GLY	3.4
42	CP	2	ASP	3.4
30	CD	201	LEU	3.4
46	CT	36	LEU	3.4
48	CV	29	LEU	3.4
6	AF	88	MET	3.4
7	AG	116	MET	3.4
39	CM	1	MET	3.4
30	CD	121	THR	3.4
1	BA	1253	G	3.4
1	BA	1343	G	3.4
20	BT	61	GLN	3.4
29	DC	251	GLN	3.4
31	CA	264	C	3.4
31	CA	679	C	3.4
31	CA	1480	C	3.4
31	CA	2676	C	3.4
31	CA	2874	C	3.4
54	DA	2175	C	3.4
22	C1	16	ARG	3.4
41	CO	3	HIS	3.4
42	CP	7	ARG	3.4
31	CA	1513	U	3.4
31	CA	2743	U	3.4
22	C1	27	SER	3.4
23	C2	53	LYS	3.4
30	CD	55	LYS	3.4
32	CE	55	SER	3.4
35	CH	11	ASN	3.4
36	CJ	128	SER	3.4
44	CR	78	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
48	CV	37	GLU	3.4
39	CM	58	TYR	3.3
1	BA	199	A	3.3
31	CA	219	A	3.3
31	CA	241	A	3.3
31	CA	332	A	3.3
39	CM	55	MET	3.3
54	DA	1085	A	3.3
30	CD	118	PHE	3.3
13	BM	18	ALA	3.3
46	CT	39	THR	3.3
41	CO	2	ARG	3.3
51	CY	18	ARG	3.3
16	BP	60	TRP	3.3
31	CA	240	C	3.3
31	CA	393	C	3.3
9	AI	19	VAL	3.3
14	BN	82	ILE	3.3
20	BT	12	ILE	3.3
23	C2	48	ILE	3.3
31	CA	1	G	3.3
31	CA	124	G	3.3
31	CA	438	G	3.3
31	CA	774	G	3.3
31	CA	1195	G	3.3
31	CA	1826	G	3.3
31	CA	2238	G	3.3
31	CA	288	U	3.3
31	CA	2079	U	3.3
51	CY	15	GLY	3.3
2	BB	147	SER	3.3
22	C1	18	SER	3.3
32	CE	93	SER	3.3
39	CM	25	SER	3.3
33	CF	152	LEU	3.3
44	CR	47	TYR	3.3
51	CY	29	PHE	3.3
14	BN	57	PRO	3.3
25	C4	54	ASP	3.3
1	AA	1492	A	3.3
1	BA	974	A	3.3
11	AK	47	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
30	CD	119	ALA	3.3
38	CL	33	ALA	3.3
46	CT	87	PRO	3.3
31	CA	432	A	3.3
31	CA	631	A	3.3
31	CA	764	A	3.3
30	CD	123	LYS	3.3
50	CX	78	LYS	3.3
7	BG	42	ILE	3.3
11	BK	110	ILE	3.3
27	C0	32	ILE	3.3
33	CF	154	ILE	3.3
40	CN	73	ILE	3.3
44	CR	31	VAL	3.3
51	CY	13	VAL	3.3
29	CC	209	GLY	3.3
31	CA	383	C	3.3
31	CA	445	C	3.3
31	CA	1319	C	3.3
36	DJ	52	GLY	3.3
1	BA	133	U	3.3
31	CA	434	U	3.3
36	DJ	94	ASN	3.3
29	DC	272	SER	3.3
39	CM	40	SER	3.3
1	BA	1050	G	3.3
16	BP	32	PHE	3.3
31	CA	2027	G	3.3
31	CA	2056	G	3.3
36	DJ	38	PHE	3.3
2	AB	201	PRO	3.3
37	CK	97	PRO	3.3
15	AO	72	ARG	3.3
29	CC	50	THR	3.3
34	CG	36	THR	3.3
1	BA	151	A	3.3
1	BA	250	A	3.3
1	BA	1236	A	3.3
29	CC	5	LYS	3.3
31	CA	515	A	3.3
31	CA	2059	A	3.3
44	CR	5	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
44	CR	15	LYS	3.3
50	CX	37	ILE	3.3
7	BG	64	VAL	3.3
14	AN	45	VAL	3.3
10	BJ	38	GLY	3.3
20	BT	65	GLY	3.3
7	AG	106	GLU	3.3
31	CA	2871	U	3.3
1	BA	962	C	3.3
16	AP	39	PHE	3.3
31	CA	179	C	3.3
31	CA	336	C	3.3
31	CA	456	C	3.3
31	CA	806	C	3.3
31	CA	946	C	3.3
31	CA	2699	C	3.3
32	CE	158	PHE	3.3
46	CT	101	SER	3.3
54	DA	1172	C	3.3
13	AM	112	PRO	3.3
22	C1	24	ALA	3.3
32	CE	128	ALA	3.3
40	CN	79	ALA	3.3
41	CO	63	ARG	3.3
53	DI	25	ALA	3.3
1	AA	1039	G	3.3
1	AA	1305	G	3.3
1	BA	165	G	3.3
1	BA	187	G	3.3
1	BA	633	G	3.3
2	BB	82	ASP	3.3
7	BG	137	LYS	3.3
16	BP	23	ASP	3.3
31	CA	55	G	3.3
31	CA	254	G	3.3
31	CA	380	G	3.3
31	CA	1026	G	3.3
31	CA	1138	G	3.3
31	CA	1212	G	3.3
31	CA	1358	G	3.3
31	CA	1368	G	3.3
12	BL	4	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
45	CS	20	VAL	3.3
53	DI	26	VAL	3.3
1	BA	315	A	3.3
31	CA	1525	A	3.3
31	CA	1616	A	3.3
16	BP	6	LEU	3.3
39	CM	11	GLY	3.3
40	CN	20	LEU	3.3
47	CU	87	LEU	3.3
12	BL	70	GLU	3.3
1	BA	137	U	3.2
30	CD	136	ASN	3.2
35	CH	23	ALA	3.2
39	CM	108	ALA	3.2
44	CR	42	ALA	3.2
1	BA	54	C	3.2
1	BA	132	C	3.2
1	BA	214	C	3.2
1	BA	221	C	3.2
1	BA	267	C	3.2
1	BA	1388	C	3.2
42	CP	4	LYS	3.2
48	CV	61	LYS	3.2
54	DA	1104	C	3.2
54	DA	2153	C	3.2
24	C3	43	THR	3.2
30	DD	131	ASP	3.2
32	CE	168	ASP	3.2
7	BG	80	VAL	3.2
10	BJ	51	VAL	3.2
14	BN	101	TRP	3.2
31	CA	7	G	3.2
31	CA	771	G	3.2
31	CA	974	G	3.2
31	CA	1288	G	3.2
31	CA	1429	G	3.2
31	CA	1645	G	3.2
31	CA	2127	G	3.2
31	CA	2405	G	3.2
31	CA	2627	G	3.2
33	CF	131	GLY	3.2
1	BA	1110	A	3.2

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Mol	Chain	Res	Type	RSRZ
31	CA	507	A	3.2
31	CA	2062	A	3.2
54	DA	2163	A	3.2
10	BJ	62	ARG	3.2
9	BI	17	ALA	3.2
29	DC	239	ASN	3.2
37	CK	120	ARG	3.2
1	BA	173	U	3.2
5	BE	103	THR	3.2
14	BN	60	GLN	3.2
7	AG	105	VAL	3.2
10	AJ	80	THR	3.2
30	CD	133	THR	3.2
32	CE	169	VAL	3.2
51	CY	34	HIS	3.2
31	CA	37	C	3.2
31	CA	211	C	3.2
31	CA	239	C	3.2
31	CA	509	C	3.2
39	CM	79	LEU	3.2
9	AI	117	GLY	3.2
30	CD	6	GLY	3.2
10	BJ	49	PHE	3.2
1	AA	1015	G	3.2
1	BA	324	G	3.2
1	BA	354	G	3.2
1	BA	935	A	3.2
14	BN	70	PRO	3.2
21	AU	2	PRO	3.2
24	C3	3	ARG	3.2
29	CC	253	LYS	3.2
31	CA	215	G	3.2
31	CA	252	G	3.2
31	CA	597	G	3.2
31	CA	616	A	3.2
31	CA	1271	G	3.2
31	CA	1361	G	3.2
31	CA	1597	A	3.2
39	CM	13	LYS	3.2
41	CO	39	PRO	3.2
43	CQ	111	LYS	3.2
7	BG	65	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
9	AI	16	ALA	3.2
48	CV	64	ALA	3.2
1	AA	1086	U	3.2
9	BI	15	SER	3.2
31	CA	431	U	3.2
31	CA	2615	U	3.2
36	CJ	59	ILE	3.2
53	DI	24	SER	3.2
54	DA	2151	U	3.2
10	BJ	77	VAL	3.2
11	AK	84	VAL	3.2
20	AT	58	VAL	3.2
40	CN	89	VAL	3.2
51	DY	20	HIS	3.2
37	CK	36	LEU	3.2
48	CV	52	LEU	3.2
25	D4	20	GLY	3.2
32	CE	42	GLY	3.2
1	AA	330	C	3.2
1	BA	67	C	3.2
17	BQ	73	TRP	3.2
31	CA	343	C	3.2
31	CA	968	C	3.2
31	CA	1605	C	3.2
31	CA	1957	C	3.2
14	BN	73	PHE	3.2
14	BN	52	PRO	3.2
29	CC	29	PRO	3.2
36	DJ	115	ALA	3.2
1	BA	174	A	3.2
31	CA	514	A	3.2
31	CA	794	A	3.2
31	CA	1654	A	3.2
51	CY	64	ILE	3.2
1	AA	540	G	3.2
1	BA	1244	G	3.2
31	CA	27	G	3.2
19	BS	58	VAL	3.2
20	AT	6	SER	3.2
31	CA	1240	U	3.2
31	CA	1971	U	3.2
36	CJ	78	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
37	CK	40	HIS	3.2
46	CT	71	VAL	3.2
2	AB	135	LEU	3.2
2	BB	129	LEU	3.2
8	AH	76	GLN	3.2
10	BJ	52	LEU	3.2
14	AN	42	TRP	3.2
7	BG	109	ARG	3.2
19	BS	3	ARG	3.2
25	C4	12	LYS	3.2
32	CE	74	LYS	3.2
36	CJ	10	LYS	3.2
1	AA	95	C	3.2
1	AA	1281	C	3.2
1	BA	1320	C	3.2
10	BJ	39	PRO	3.2
31	CA	129	C	3.2
31	CA	184	C	3.2
31	CA	1208	C	3.2
31	CA	1607	C	3.2
31	CA	2443	C	3.2
31	CA	2667	C	3.2
53	DI	130	PRO	3.2
34	CG	46	ALA	3.1
9	BI	72	ILE	3.1
40	CN	126	ILE	3.1
44	CR	40	ILE	3.1
6	AF	89	VAL	3.1
17	BQ	23	VAL	3.1
20	BT	79	LEU	3.1
25	C4	33	LEU	3.1
32	CE	83	VAL	3.1
53	DI	55	VAL	3.1
31	CA	101	A	3.1
31	CA	2741	A	3.1
12	BL	19	SER	3.1
14	AN	100	SER	3.1
17	BQ	9	GLN	3.1
19	AS	56	GLN	3.1
31	CA	234	U	3.1
31	CA	1956	U	3.1
54	DA	1083	U	3.1

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Mol	Chain	Res	Type	RSRZ
12	BL	3	THR	3.1
3	BC	155	GLY	3.1
29	DC	233	GLY	3.1
39	CM	22	GLY	3.1
1	BA	1385	G	3.1
31	CA	51	G	3.1
31	CA	585	G	3.1
31	CA	625	G	3.1
31	CA	1245	G	3.1
31	CA	1346	G	3.1
31	CA	1623	G	3.1
31	CA	1631	G	3.1
31	CA	1721	G	3.1
31	CA	2209	G	3.1
31	CA	2877	G	3.1
6	BF	8	PHE	3.1
7	BG	15	ASP	3.1
14	BN	7	LYS	3.1
17	BQ	37	PHE	3.1
19	BS	21	LYS	3.1
24	C3	18	PHE	3.1
30	CD	131	ASP	3.1
35	CH	83	LYS	3.1
32	CE	76	PRO	3.1
48	CV	55	PRO	3.1
11	BK	47	ALA	3.1
36	CJ	114	ALA	3.1
46	CT	96	ILE	3.1
53	DI	123	ILE	3.1
1	BA	979	C	3.1
1	BA	1245	C	3.1
31	CA	151	C	3.1
31	CA	837	C	3.1
31	CA	2150	C	3.1
31	CA	2275	C	3.1
31	CA	2678	C	3.1
9	AI	104	VAL	3.1
10	BJ	102	LEU	3.1
36	CJ	53	LEU	3.1
40	CN	78	LEU	3.1
51	CY	51	VAL	3.1
51	CY	6	GLN	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AA	959	A	3.1
1	AA	1183	U	3.1
1	BA	1418	A	3.1
3	BC	177	THR	3.1
31	CA	74	A	3.1
31	CA	104	A	3.1
31	CA	457	A	3.1
31	CA	790	U	3.1
31	CA	1244	A	3.1
31	CA	1301	A	3.1
31	CA	2412	A	3.1
31	CA	2585	U	3.1
32	CE	43	THR	3.1
36	CJ	73	THR	3.1
39	CM	7	SER	3.1
32	CE	56	GLY	3.1
39	CM	34	GLY	3.1
12	AL	14	ARG	3.1
16	BP	8	ARG	3.1
21	AU	37	PHE	3.1
35	DH	29	PHE	3.1
39	CM	60	ARG	3.1
37	CK	49	ASP	3.1
1	BA	61	G	3.1
1	BA	100	G	3.1
14	AN	99	ALA	3.1
14	BN	29	ALA	3.1
16	BP	81	ALA	3.1
31	CA	317	G	3.1
31	CA	1136	G	3.1
31	CA	2012	G	3.1
2	AB	151	ILE	3.1
17	BQ	5	ILE	3.1
17	BQ	25	ILE	3.1
9	BI	118	LEU	3.1
32	CE	3	LEU	3.1
50	CX	21	LEU	3.1
45	CS	12	HIS	3.1
1	AA	932	C	3.1
31	CA	584	C	3.1
31	CA	660	C	3.1
31	CA	1290	C	3.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1437	C	3.1
31	CA	1625	C	3.1
30	CD	130	GLN	3.1
24	C3	25	LYS	3.1
36	DJ	51	LYS	3.1
44	CR	16	LYS	3.1
2	AB	46	THR	3.1
13	BM	99	GLY	3.1
20	BT	80	THR	3.1
29	CC	219	THR	3.1
34	CG	80	THR	3.1
38	CL	15	GLY	3.1
32	CE	49	ARG	3.1
32	CE	179	SER	3.1
41	CO	36	THR	3.1
1	AA	4	U	3.1
2	BB	126	PHE	3.1
3	BC	156	ARG	3.1
31	CA	686	U	3.1
31	CA	1234	U	3.1
31	CA	1880	U	3.1
31	CA	324	A	3.1
31	CA	2060	A	3.1
31	CA	2435	A	3.1
31	CA	2448	A	3.1
31	CA	2602	A	3.1
31	CA	2882	A	3.1
47	CU	37	ASP	3.1
30	CD	192	ALA	3.1
14	AN	96	LEU	3.1
41	CO	83	LEU	3.1
45	CS	22	LEU	3.1
14	BN	11	VAL	3.1
1	BA	105	G	3.1
1	BA	1442	G	3.1
31	CA	518	G	3.1
31	CA	535	G	3.1
31	CA	539	G	3.1
31	CA	659	G	3.1
31	CA	1371	G	3.1
31	CA	1524	G	3.1
54	DA	2133	G	3.1

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Mol	Chain	Res	Type	RSRZ
9	AI	64	TYR	3.1
12	BL	15	LYS	3.1
37	CK	44	TYR	3.1
20	BT	3	ASN	3.1
9	AI	119	ARG	3.1
34	CG	170	ARG	3.1
37	CK	83	GLY	3.1
39	CM	41	ARG	3.1
1	AA	470	C	3.1
1	BA	234	C	3.1
1	BA	1367	C	3.1
25	C4	6	THR	3.1
31	CA	673	C	3.1
31	CA	1293	C	3.1
16	BP	15	PRO	3.1
31	CA	2324	U	3.1
2	AB	136	MET	3.1
21	AU	36	GLU	3.1
1	AA	199	A	3.1
1	AA	1130	A	3.1
1	BA	66	A	3.1
1	BA	609	A	3.1
2	BB	164	ILE	3.1
7	BG	128	ALA	3.1
10	BJ	25	ILE	3.1
22	C1	20	ASP	3.1
31	CA	52	A	3.1
31	CA	1307	A	3.1
36	DJ	15	ALA	3.1
36	DJ	35	ILE	3.1
36	DJ	109	ILE	3.1
48	CV	103	ILE	3.1
16	BP	74	LEU	3.0
14	AN	11	VAL	3.0
16	AP	71	VAL	3.0
36	CJ	9	VAL	3.0
51	CY	67	VAL	3.0
53	DI	77	VAL	3.0
25	C4	26	HIS	3.0
9	BI	130	ARG	3.0
10	BJ	45	ARG	3.0
10	BJ	72	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
24	C3	6	GLN	3.0
39	CM	69	ARG	3.0
44	CR	20	GLN	3.0
49	CW	87	GLN	3.0
41	CO	107	ASN	3.0
1	AA	201	G	3.0
1	BA	332	G	3.0
27	C0	8	THR	3.0
28	CB	102	G	3.0
31	CA	15	G	3.0
31	CA	185	G	3.0
31	CA	245	G	3.0
31	CA	291	G	3.0
31	CA	338	G	3.0
31	CA	376	G	3.0
31	CA	682	G	3.0
31	CA	799	G	3.0
31	CA	808	G	3.0
31	CA	953	G	3.0
31	CA	1137	G	3.0
31	CA	2250	G	3.0
31	CA	2894	G	3.0
37	CK	70	THR	3.0
52	CZ	16	THR	3.0
32	CE	89	PRO	3.0
38	CL	48	PRO	3.0
1	BA	932	C	3.0
1	BA	1159	U	3.0
11	AK	97	ILE	3.0
14	AN	31	ILE	3.0
31	CA	29	U	3.0
31	CA	1320	C	3.0
31	CA	1493	C	3.0
31	CA	1658	C	3.0
33	CF	34	ILE	3.0
13	BM	40	ALA	3.0
27	C0	13	ALA	3.0
32	CE	68	ALA	3.0
39	CM	106	GLU	3.0
43	CQ	9	GLU	3.0
46	CT	10	ALA	3.0
14	BN	46	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
32	CE	153	LEU	3.0
53	DI	117	LEU	3.0
2	AB	210	VAL	3.0
3	BC	173	VAL	3.0
4	BD	125	VAL	3.0
7	BG	135	VAL	3.0
31	CA	118	A	3.0
31	CA	532	A	3.0
31	CA	1354	A	3.0
54	DA	1086	A	3.0
22	C1	37	LYS	3.0
25	C4	19	LYS	3.0
41	CO	5	LYS	3.0
47	CU	66	LYS	3.0
10	BJ	7	ARG	3.0
29	CC	101	ARG	3.0
39	CM	18	ARG	3.0
48	CV	38	GLY	3.0
29	CC	257	THR	3.0
33	CF	157	THR	3.0
9	AI	72	ILE	3.0
29	CC	104	ILE	3.0
14	BN	2	ALA	3.0
20	BT	22	ALA	3.0
30	CD	168	GLU	3.0
46	CT	30	SER	3.0
46	CT	32	ALA	3.0
1	BA	351	G	3.0
1	BA	1241	G	3.0
31	CA	107	G	3.0
31	CA	214	G	3.0
31	CA	312	G	3.0
31	CA	1065	U	3.0
31	CA	1719	G	3.0
31	CA	1865	U	3.0
31	CA	2695	U	3.0
31	CA	2707	U	3.0
54	DA	141	G	3.0
54	DA	1093	G	3.0
54	DA	2186	G	3.0
1	BA	314	C	3.0
1	BA	631	C	3.0

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Mol	Chain	Res	Type	RSRZ
7	AG	94	VAL	3.0
9	BI	104	VAL	3.0
9	BI	114	LYS	3.0
11	BK	86	VAL	3.0
14	AN	23	LYS	3.0
19	BS	51	VAL	3.0
29	DC	250	VAL	3.0
30	CD	116	LYS	3.0
30	CD	200	ASP	3.0
31	CA	143	C	3.0
31	CA	268	C	3.0
31	CA	351	C	3.0
31	CA	531	C	3.0
31	CA	786	C	3.0
31	CA	1774	C	3.0
31	CA	2717	C	3.0
46	CT	6	LYS	3.0
50	CX	15	ASP	3.0
51	CY	7	VAL	3.0
27	C0	20	HIS	3.0
52	CZ	41	HIS	3.0
1	BA	1252	A	3.0
1	BA	1362	A	3.0
31	CA	439	A	3.0
31	CA	1285	A	3.0
31	CA	1552	A	3.0
5	BE	112	ARG	3.0
13	AM	113	ARG	3.0
14	AN	53	ARG	3.0
24	C3	33	ARG	3.0
25	C4	42	ARG	3.0
29	CC	153	GLN	3.0
34	CG	108	GLY	3.0
37	CK	118	MET	3.0
3	BC	44	THR	3.0
7	BG	12	ILE	3.0
14	AN	43	ASN	3.0
14	AN	67	THR	3.0
19	AS	39	THR	3.0
32	CE	173	THR	3.0
40	CN	69	PRO	3.0
20	BT	83	ILE	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	AB	148	LEU	3.0
30	CD	4	LEU	3.0
52	CZ	21	LEU	3.0
52	CZ	42	LEU	3.0
3	BC	161	GLU	3.0
14	BN	99	ALA	3.0
20	BT	7	ALA	3.0
29	CC	211	ALA	3.0
20	BT	16	LYS	3.0
29	CC	26	LYS	3.0
32	CE	139	LYS	3.0
48	CV	79	LYS	3.0
31	CA	2321	U	3.0
31	CA	2384	U	3.0
32	CE	31	VAL	3.0
54	DA	12	U	3.0
45	DS	26	ASP	3.0
1	BA	266	G	3.0
1	BA	318	G	3.0
9	BI	11	ARG	3.0
14	AN	13	ARG	3.0
14	BN	53	ARG	3.0
18	AR	74	HIS	3.0
27	C0	11	ARG	3.0
30	CD	59	ARG	3.0
31	CA	88	G	3.0
31	CA	106	C	3.0
31	CA	188	G	3.0
31	CA	993	G	3.0
31	CA	1211	C	3.0
31	CA	1339	G	3.0
31	CA	1574	C	3.0
31	CA	1642	G	3.0
31	CA	1996	C	3.0
31	CA	2214	C	3.0
32	CE	61	ARG	3.0
37	CK	116	ARG	3.0
54	DA	1074	G	3.0
19	AS	74	PHE	3.0
32	CE	82	GLY	3.0
33	CF	76	GLY	3.0
1	BA	172	A	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	338	A	3.0
31	CA	144	A	3.0
31	CA	788	A	3.0
31	CA	979	A	3.0
31	CA	1008	A	3.0
31	CA	1275	A	3.0
31	CA	1652	A	3.0
33	DF	83	TYR	3.0
48	DV	55	PRO	3.0
10	BJ	67	ILE	3.0
46	CT	74	ILE	3.0
5	BE	115	LEU	3.0
6	BF	92	THR	3.0
32	CE	159	LEU	3.0
36	DJ	28	LEU	3.0
41	CO	54	LEU	3.0
4	AD	206	LYS	3.0
10	BJ	11	LYS	3.0
35	DH	74	ALA	3.0
39	CM	17	LYS	3.0
40	CN	71	LYS	3.0
41	CO	19	ALA	3.0
44	CR	12	ALA	3.0
48	CV	2	ALA	3.0
2	AB	14	VAL	3.0
9	AI	116	VAL	3.0
19	AS	60	VAL	3.0
30	CD	137	SER	3.0
32	CE	167	VAL	3.0
47	CU	57	VAL	3.0
1	AA	1126	U	2.9
31	CA	566	U	2.9
31	CA	2584	U	2.9
14	AN	71	HIS	2.9
40	CN	16	ARG	2.9
48	CV	22	ARG	2.9
24	D3	1	MET	2.9
25	C4	20	GLY	2.9
25	C4	53	GLY	2.9
1	AA	1096	C	2.9
1	BA	95	C	2.9
1	BA	980	C	2.9

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Mol	Chain	Res	Type	RSRZ
31	CA	475	C	2.9
31	CA	2089	C	2.9
31	CA	2174	C	2.9
54	DA	2150	C	2.9
54	DA	2165	C	2.9
1	AA	1020	G	2.9
1	BA	391	G	2.9
1	BA	484	G	2.9
1	BA	1032	G	2.9
9	BI	23	PRO	2.9
22	C1	49	TYR	2.9
25	C4	2	PRO	2.9
25	C4	64	TYR	2.9
31	CA	39	G	2.9
31	CA	425	G	2.9
31	CA	577	G	2.9
31	CA	775	G	2.9
31	CA	969	G	2.9
31	CA	1364	G	2.9
31	CA	2630	G	2.9
31	CA	2838	G	2.9
31	CA	2885	G	2.9
31	CA	2890	G	2.9
43	CQ	5	ILE	2.9
54	DA	2124	G	2.9
54	DA	2127	G	2.9
1	BA	1016	A	2.9
7	BG	23	LEU	2.9
7	BG	50	LEU	2.9
30	CD	187	LEU	2.9
31	CA	14	A	2.9
31	CA	203	A	2.9
31	CA	472	A	2.9
31	CA	513	A	2.9
31	CA	911	A	2.9
31	CA	1327	A	2.9
31	CA	2850	A	2.9
54	DA	1080	A	2.9
54	DA	2311	A	2.9
4	AD	148	LYS	2.9
14	AN	98	LYS	2.9
12	BL	17	ALA	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
47	CU	41	ALA	2.9
14	AN	26	GLU	2.9
29	CC	260	ASN	2.9
17	BQ	79	VAL	2.9
29	CC	268	VAL	2.9
33	CF	25	VAL	2.9
34	CG	76	VAL	2.9
34	CG	168	VAL	2.9
12	BL	115	SER	2.9
19	BS	38	SER	2.9
24	C3	41	ARG	2.9
32	CE	79	ARG	2.9
33	CF	118	SER	2.9
50	CX	41	ARG	2.9
31	CA	1466	U	2.9
31	CA	1624	U	2.9
41	CO	20	MET	2.9
54	DA	1078	U	2.9
41	CO	102	PHE	2.9
30	CD	135	GLY	2.9
33	CF	67	ILE	2.9
43	CQ	64	ILE	2.9
47	DU	2	ILE	2.9
18	AR	23	TYR	2.9
20	AT	5	LYS	2.9
3	AC	191	THR	2.9
20	BT	46	ALA	2.9
30	CD	75	ALA	2.9
31	CA	109	C	2.9
31	CA	876	C	2.9
31	CA	1639	C	2.9
31	CA	2452	C	2.9
34	CG	171	THR	2.9
41	CO	55	ALA	2.9
1	BA	97	G	2.9
1	BA	384	G	2.9
1	BA	1204	A	2.9
1	BA	1304	G	2.9
3	AC	105	GLU	2.9
6	BF	10	VAL	2.9
12	BL	16	VAL	2.9
24	C3	30	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
26	C5	25	VAL	2.9
30	CD	37	VAL	2.9
31	CA	227	A	2.9
31	CA	473	G	2.9
31	CA	561	G	2.9
31	CA	618	G	2.9
31	CA	777	G	2.9
31	CA	781	A	2.9
31	CA	1309	G	2.9
31	CA	1337	G	2.9
31	CA	1475	G	2.9
31	CA	1555	G	2.9
31	CA	1609	A	2.9
31	CA	1811	G	2.9
31	CA	1959	G	2.9
31	CA	2087	G	2.9
31	CA	2632	A	2.9
47	CU	31	VAL	2.9
29	CC	232	HIS	2.9
48	CV	30	SER	2.9
1	BA	458	U	2.9
1	BA	1183	U	2.9
31	CA	224	U	2.9
31	CA	1199	U	2.9
31	CA	1468	U	2.9
31	CA	1963	U	2.9
46	CT	79	GLY	2.9
49	CW	15	GLY	2.9
3	AC	103	ILE	2.9
3	BC	94	ILE	2.9
7	BG	2	PRO	2.9
7	BG	7	ILE	2.9
14	BN	66	GLN	2.9
29	CC	218	PRO	2.9
35	DH	80	ILE	2.9
39	CM	6	LEU	2.9
39	CM	57	LEU	2.9
42	CP	32	PRO	2.9
45	CS	52	PRO	2.9
45	CS	48	LYS	2.9
20	BT	62	ALA	2.9
34	CG	40	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
35	DH	10	ALA	2.9
53	DI	111	ALA	2.9
30	CD	129	THR	2.9
17	AQ	83	VAL	2.9
29	CC	19	VAL	2.9
36	CJ	130	GLU	2.9
45	CS	33	VAL	2.9
45	CS	37	GLU	2.9
45	CS	63	VAL	2.9
1	AA	1140	C	2.9
1	AA	1317	C	2.9
1	BA	469	C	2.9
29	CC	13	ARG	2.9
31	CA	267	C	2.9
31	CA	1092	C	2.9
31	CA	1117	C	2.9
31	CA	1454	C	2.9
31	CA	1752	C	2.9
31	CA	2248	C	2.9
31	CA	2710	C	2.9
39	CM	47	ARG	2.9
1	AA	1236	A	2.9
1	BA	60	A	2.9
1	BA	959	A	2.9
1	BA	1251	A	2.9
31	CA	1469	A	2.9
31	CA	1566	A	2.9
31	CA	1744	A	2.9
31	CA	2392	A	2.9
54	DA	144	A	2.9
54	DA	1077	A	2.9
54	DA	1103	A	2.9
9	BI	81	HIS	2.9
47	CU	80	TRP	2.9
51	CY	20	HIS	2.9
1	AA	1124	G	2.9
1	BA	46	G	2.9
1	BA	454	G	2.9
1	BA	1094	G	2.9
31	CA	123	G	2.9
31	CA	186	G	2.9
31	CA	669	G	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	1296	G	2.9
31	CA	1426	G	2.9
31	CA	2128	G	2.9
31	CA	2230	G	2.9
31	CA	2709	G	2.9
31	CA	2812	G	2.9
51	CY	46	PHE	2.9
41	CO	15	SER	2.9
54	DA	2121	G	2.9
45	CS	88	GLY	2.9
1	BA	1240	U	2.9
9	AI	35	LEU	2.9
13	BM	4	ILE	2.9
19	BS	31	LEU	2.9
26	C5	9	LYS	2.9
30	CD	7	LYS	2.9
32	CE	108	ILE	2.9
31	CA	1379	U	2.9
31	CA	2845	U	2.9
37	CK	85	LYS	2.9
40	CN	100	LYS	2.9
46	CT	73	LYS	2.9
39	CM	54	GLN	2.9
8	BH	130	ALA	2.9
11	BK	67	ALA	2.9
35	DH	64	ALA	2.9
44	CR	32	TYR	2.9
19	BS	39	THR	2.9
22	C1	9	THR	2.9
41	CO	116	VAL	2.9
46	CT	29	VAL	2.9
8	BH	3	MET	2.9
20	BT	60	ARG	2.9
47	CU	76	ARG	2.9
52	CZ	48	ARG	2.9
16	BP	29	ASN	2.9
1	AA	995	C	2.8
16	BP	38	PHE	2.8
1	BA	195	A	2.8
1	BA	327	A	2.8
1	BA	334	C	2.8
1	BA	382	A	2.8

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Mol	Chain	Res	Type	RSRZ
1	BA	383	A	2.8
1	BA	532	A	2.8
1	BA	1028	C	2.8
1	BA	1280	A	2.8
1	BA	1281	C	2.8
1	BA	1368	A	2.8
1	BA	1460	C	2.8
31	CA	320	A	2.8
31	CA	353	C	2.8
31	CA	1007	C	2.8
31	CA	1395	A	2.8
31	CA	1626	A	2.8
31	CA	2510	C	2.8
54	DA	1420	A	2.8
7	BG	17	LYS	2.8
13	BM	45	ILE	2.8
14	AN	7	LYS	2.8
14	BN	80	SER	2.8
18	BR	67	LEU	2.8
21	AU	16	LEU	2.8
29	CC	59	LYS	2.8
29	CC	256	LYS	2.8
29	CC	267	ILE	2.8
32	CE	130	LYS	2.8
36	DJ	137	GLY	2.8
37	CK	106	LYS	2.8
44	CR	87	SER	2.8
52	CZ	6	LEU	2.8
53	DI	59	LEU	2.8
1	BA	69	G	2.8
1	BA	319	G	2.8
16	BP	53	ASP	2.8
1	BA	471	U	2.8
1	BA	1235	U	2.8
31	CA	263	G	2.8
31	CA	476	G	2.8
31	CA	695	G	2.8
31	CA	1369	G	2.8
31	CA	1425	G	2.8
31	CA	2029	G	2.8
31	CA	2583	G	2.8
31	CA	2732	G	2.8

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Mol	Chain	Res	Type	RSRZ
54	DA	846[A]	U	2.8
54	DA	1738	G	2.8
6	BF	95	ALA	2.8
7	BG	98	ALA	2.8
20	BT	17	ALA	2.8
32	CE	201	ALA	2.8
2	BB	92	VAL	2.8
37	CK	100	VAL	2.8
42	CP	27	VAL	2.8
14	AN	59	ARG	2.8
36	DJ	68	THR	2.8
47	CU	6	ARG	2.8
50	CX	55	ARG	2.8
9	BI	39	PHE	2.8
19	AS	53	ASN	2.8
22	C1	19	HIS	2.8
43	CQ	59	PHE	2.8
43	CQ	66	ASN	2.8
50	CX	26	PHE	2.8
51	CY	38	PHE	2.8
6	AF	42	TRP	2.8
16	BP	13	LYS	2.8
35	DH	89	LYS	2.8
44	CR	19	LYS	2.8
13	AM	99	GLY	2.8
37	CK	82	GLY	2.8
37	CK	122	LEU	2.8
45	CS	74	ILE	2.8
53	DI	82	ILE	2.8
3	BC	7	PRO	2.8
34	CG	156	PRO	2.8
1	AA	1119	C	2.8
1	BA	1322	C	2.8
14	BN	55	SER	2.8
31	CA	111	A	2.8
31	CA	197	A	2.8
31	CA	207	A	2.8
31	CA	265	A	2.8
31	CA	564	C	2.8
31	CA	740	C	2.8
31	CA	793	A	2.8
31	CA	854	C	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	1287	A	2.8
31	CA	1386	C	2.8
31	CA	1461	C	2.8
31	CA	1997	C	2.8
31	CA	2326	C	2.8
36	DJ	88	SER	2.8
38	CL	28	SER	2.8
52	CZ	40	SER	2.8
44	CR	56	GLN	2.8
32	DE	7	ASP	2.8
1	BA	1321	U	2.8
1	BA	1354	U	2.8
7	BG	51	ALA	2.8
29	CC	92	ALA	2.8
31	CA	276	U	2.8
31	CA	1119	U	2.8
31	CA	1294	U	2.8
31	CA	1340	U	2.8
31	CA	1390	U	2.8
31	CA	1758	U	2.8
40	CN	116	ALA	2.8
41	CO	66	ALA	2.8
54	DA	546	U	2.8
36	CJ	139	VAL	2.8
38	CL	21	CYS	2.8
48	CV	11	VAL	2.8
52	CZ	46	VAL	2.8
10	BJ	48	ARG	2.8
29	CC	83	TYR	2.8
33	CF	128	TYR	2.8
44	CR	45	TYR	2.8
1	AA	97	G	2.8
1	BA	481	G	2.8
1	BA	941	G	2.8
1	BA	976	G	2.8
1	BA	1370	G	2.8
2	BB	133	GLU	2.8
10	BJ	47	GLU	2.8
29	CC	246	THR	2.8
31	CA	258	G	2.8
31	CA	297	G	2.8
31	CA	488	G	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	649	G	2.8
31	CA	1218	G	2.8
31	CA	2010	G	2.8
31	CA	2361	G	2.8
31	CA	2633	G	2.8
31	CA	2688	G	2.8
31	CA	2801	G	2.8
36	DJ	71	THR	2.8
43	CQ	27	GLU	2.8
44	CR	57	PHE	2.8
14	AN	47	LYS	2.8
37	CK	39	LYS	2.8
46	CT	90	LYS	2.8
4	AD	21	LEU	2.8
5	BE	30	ILE	2.8
7	BG	124	LEU	2.8
12	BL	24	LEU	2.8
13	AM	19	LEU	2.8
19	BS	47	LEU	2.8
29	CC	45	ASN	2.8
29	CC	105	LEU	2.8
33	CF	117	LEU	2.8
41	CO	79	LEU	2.8
22	C1	35	GLY	2.8
35	CH	24	GLY	2.8
46	CT	63	GLY	2.8
7	BG	16	PRO	2.8
33	CF	84	PRO	2.8
9	AI	14	SER	2.8
14	AN	55	SER	2.8
43	CQ	12	GLN	2.8
46	CT	81	SER	2.8
1	BA	217	C	2.8
1	BA	316	C	2.8
3	BC	200	VAL	2.8
31	CA	22	C	2.8
31	CA	196	A	2.8
31	CA	208	C	2.8
31	CA	238	C	2.8
31	CA	435	C	2.8
31	CA	447	A	2.8
31	CA	944	C	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	1261	C	2.8
31	CA	1330	C	2.8
31	CA	1387	A	2.8
31	CA	1526	C	2.8
31	CA	1789	A	2.8
31	CA	2241	A	2.8
31	CA	2538	C	2.8
31	CA	2681	C	2.8
47	CU	1	MET	2.8
50	CX	63	ALA	2.8
53	DI	92	ALA	2.8
13	BM	98	ARG	2.8
35	CH	138	VAL	2.8
1	BA	224	U	2.8
31	CA	1621	U	2.8
36	DJ	112	THR	2.8
23	C2	33	LYS	2.8
30	CD	127	PHE	2.8
48	CV	19	LYS	2.8
2	AB	68	LEU	2.8
7	BG	59	LEU	2.8
11	AK	100	LEU	2.8
35	DH	15	LEU	2.8
53	DI	72	LEU	2.8
1	AA	450	G	2.8
1	AA	1353	G	2.8
1	BA	177	G	2.8
7	AG	42	ILE	2.8
31	CA	350	G	2.8
31	CA	372	G	2.8
31	CA	1197	G	2.8
39	CM	77	ILE	2.8
17	BQ	35	GLY	2.8
20	BT	70	ASN	2.8
37	CK	115	GLY	2.8
41	CO	26	GLY	2.8
49	CW	81	PRO	2.8
7	BG	73	VAL	2.8
7	BG	94	VAL	2.8
16	BP	65	ALA	2.8
19	BS	4	SER	2.8
44	CR	21	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
48	CV	71	ALA	2.8
51	CY	11	ARG	2.8
1	BA	197	A	2.8
31	CA	574	A	2.8
31	CA	685	A	2.8
31	CA	735	A	2.8
31	CA	1571	A	2.8
31	CA	1785	A	2.8
31	CA	2054	A	2.8
54	DA	2108	A	2.8
1	BA	185	U	2.8
1	BA	372	C	2.8
1	BA	634	C	2.8
18	AR	51	TYR	2.8
7	BG	76	LYS	2.8
9	AI	68	LYS	2.8
31	CA	337	C	2.8
31	CA	418	C	2.8
31	CA	587	C	2.8
31	CA	687	C	2.8
31	CA	1049	C	2.8
31	CA	1291	C	2.8
31	CA	1345	C	2.8
31	CA	1467	U	2.8
31	CA	1775	U	2.8
31	CA	2006	C	2.8
31	CA	2704	C	2.8
54	DA	885	C	2.8
54	DA	1105	U	2.8
14	BN	50	THR	2.8
23	C2	51	GLU	2.8
35	DH	87	GLU	2.8
38	CL	67	LYS	2.8
40	CN	133	LYS	2.8
36	DJ	67	PHE	2.8
37	CK	89	PHE	2.8
48	CV	85	PHE	2.8
2	AB	157	LEU	2.8
53	DI	41	LEU	2.8
2	BB	151	ILE	2.8
13	AM	4	ILE	2.8
29	CC	230	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
44	CR	14	HIS	2.8
8	BH	123	GLY	2.8
43	CQ	69	GLY	2.8
16	BP	41	PRO	2.7
19	BS	9	PRO	2.7
32	CE	59	PRO	2.7
37	CK	1	MET	2.7
49	CW	48	MET	2.7
1	BA	1365	G	2.7
17	AQ	9	GLN	2.7
28	CB	24	G	2.7
31	CA	400	G	2.7
31	CA	1992	G	2.7
31	CA	2035	G	2.7
54	DA	1056	G	2.7
5	BE	120	VAL	2.7
26	C5	12	ARG	2.7
35	CH	110	VAL	2.7
37	CK	133	ALA	2.7
38	CL	57	VAL	2.7
38	CL	83	ALA	2.7
41	CO	60	VAL	2.7
46	CT	95	ARG	2.7
48	CV	75	ALA	2.7
4	BD	153	SER	2.7
2	AB	131	LYS	2.7
16	AP	12	LYS	2.7
13	AM	86	TYR	2.7
14	AN	20	TYR	2.7
1	AA	632	U	2.7
1	BA	1126	U	2.7
14	BN	77	PHE	2.7
31	CA	1201	U	2.7
31	CA	1551	A	2.7
31	CA	1762	A	2.7
31	CA	2240	U	2.7
37	CK	9	GLU	2.7
39	CM	82	LEU	2.7
45	CS	70	GLU	2.7
31	CA	63	A	2.7
31	CA	590	A	2.7
31	CA	2530	A	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	2887	A	2.7
46	CT	37	THR	2.7
48	CV	41	LEU	2.7
54	DA	1089	A	2.7
54	DA	2111	U	2.7
54	DA	2119	A	2.7
2	AB	164	ILE	2.7
10	BJ	40	ILE	2.7
26	C5	16	ILE	2.7
46	CT	55	ILE	2.7
31	CA	47	C	2.7
31	CA	130	C	2.7
31	CA	145	C	2.7
31	CA	1135	C	2.7
31	CA	1178	C	2.7
31	CA	1348	C	2.7
31	CA	1351	C	2.7
31	CA	1604	C	2.7
31	CA	1771	C	2.7
31	CA	2047	C	2.7
31	CA	2065	C	2.7
54	DA	1092	C	2.7
16	BP	10	GLY	2.7
30	CD	3	GLY	2.7
29	CC	226	ASN	2.7
32	CE	24	ASN	2.7
3	AC	127	ARG	2.7
10	BJ	9	ARG	2.7
29	CC	271	ARG	2.7
34	DG	170	ARG	2.7
2	BB	107	VAL	2.7
3	BC	71	ALA	2.7
4	BD	40	GLN	2.7
9	BI	126	GLN	2.7
13	AM	16	VAL	2.7
27	C0	36	VAL	2.7
34	CG	162	VAL	2.7
36	CJ	57	VAL	2.7
36	CJ	83	ALA	2.7
48	CV	46	GLN	2.7
27	C0	6	LYS	2.7
37	CK	2	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
45	CS	7	SER	2.7
1	AA	203	G	2.7
1	BA	292	G	2.7
1	BA	346	G	2.7
1	BA	1347	G	2.7
1	BA	1353	G	2.7
28	CB	23	G	2.7
31	CA	108	G	2.7
31	CA	1160	G	2.7
31	CA	1627	G	2.7
31	CA	1954	G	2.7
31	CA	2140	G	2.7
31	CA	2319	G	2.7
31	CA	2382	G	2.7
31	CA	2694	G	2.7
2	AB	69	PHE	2.7
32	CE	183	PHE	2.7
41	CO	98	LEU	2.7
2	AB	213	TYR	2.7
16	BP	3	THR	2.7
36	CJ	101	ILE	2.7
36	CJ	109	ILE	2.7
31	CA	65	U	2.7
31	CA	293	U	2.7
31	CA	1391	U	2.7
31	CA	2149	U	2.7
46	CT	7	HIS	2.7
54	DA	139	U	2.7
1	BA	1250	A	2.7
1	BA	1285	A	2.7
31	CA	218	A	2.7
31	CA	528	A	2.7
31	CA	654	A	2.7
31	CA	1254	A	2.7
31	CA	1272	A	2.7
31	CA	1365	A	2.7
31	CA	2058	A	2.7
33	DF	176	PRO	2.7
37	CK	46	PRO	2.7
39	CM	65	GLY	2.7
51	CY	12	PRO	2.7
38	CL	7	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	AA	307	C	2.7
31	CA	66	C	2.7
31	CA	209	C	2.7
31	CA	1200	C	2.7
31	CA	1297	C	2.7
31	CA	2050	C	2.7
31	CA	2896	C	2.7
16	BP	35	ARG	2.7
21	AU	55	ARG	2.7
24	C3	26	ASN	2.7
30	CD	77	ARG	2.7
38	CL	82	ASN	2.7
46	CT	40	ASN	2.7
50	CX	25	ARG	2.7
52	CZ	27	ASN	2.7
13	BM	25	VAL	2.7
21	BU	6	VAL	2.7
33	CF	40	VAL	2.7
35	CH	74	ALA	2.7
38	CL	24	VAL	2.7
24	C3	37	LYS	2.7
2	AB	214	LEU	2.7
8	BH	59	LEU	2.7
32	CE	23	PHE	2.7
34	CG	105	LEU	2.7
40	CN	2	LEU	2.7
41	CO	38	LEU	2.7
14	AN	80	SER	2.7
26	C5	28	SER	2.7
9	AI	28	ILE	2.7
41	CO	114	GLU	2.7
46	CT	35	ILE	2.7
10	BJ	75	ASP	2.7
50	CX	17	GLU	2.7
53	DI	84	TYR	2.7
1	AA	1354	U	2.7
1	BA	96	U	2.7
1	BA	333	U	2.7
1	BA	987	G	2.7
1	BA	1086	U	2.7
4	AD	39	GLY	2.7
28	CB	85	G	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	642	U	2.7
31	CA	662	G	2.7
31	CA	1292	G	2.7
31	CA	1352	U	2.7
31	CA	1443	U	2.7
31	CA	1661	G	2.7
31	CA	1753	G	2.7
31	CA	1812	U	2.7
31	CA	2491	U	2.7
31	CA	2884	U	2.7
48	CV	23	GLY	2.7
1	BA	371	A	2.7
13	AM	101	ARG	2.7
15	AO	17	ARG	2.7
26	C5	36	ARG	2.7
31	CA	13	A	2.7
31	CA	149	A	2.7
31	CA	311	A	2.7
31	CA	344	A	2.7
31	CA	599	A	2.7
31	CA	1367	A	2.7
31	CA	1453	A	2.7
31	CA	1603	A	2.7
45	CS	90	ARG	2.7
8	AH	110	VAL	2.7
8	BH	116	ALA	2.7
20	BT	19	LYS	2.7
23	D2	10	LYS	2.7
10	AJ	58	ASN	2.7
12	AL	20	ASN	2.7
24	C3	40	ALA	2.7
25	C4	23	LYS	2.7
29	CC	16	VAL	2.7
29	CC	36	LYS	2.7
33	CF	72	LYS	2.7
34	CG	59	ALA	2.7
36	DJ	41	ALA	2.7
36	DJ	77	ALA	2.7
37	CK	124	VAL	2.7
47	CU	9	LYS	2.7
37	CK	67	ASN	2.7
48	DV	51	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
51	CY	23	ASN	2.7
51	CY	53	ALA	2.7
15	AO	62	GLN	2.7
31	CA	550	C	2.7
31	CA	1295	C	2.7
31	CA	1451	C	2.7
31	CA	1463	C	2.7
31	CA	2096	C	2.7
31	CA	2300	C	2.7
14	BN	74	LEU	2.7
7	BG	151	PHE	2.7
22	C1	43	ILE	2.7
27	C0	48	ILE	2.7
29	CC	35	GLU	2.7
29	DC	38	SER	2.7
42	CP	5	SER	2.7
14	BN	6	MET	2.7
33	CF	35	THR	2.7
13	AM	94	GLY	2.7
32	CE	103	GLY	2.7
7	AG	10	ARG	2.6
12	BL	9	ARG	2.6
24	C3	21	ARG	2.6
28	CB	74	U	2.7
31	CA	102	U	2.7
31	CA	803	U	2.7
31	CA	1460	U	2.7
31	CA	1825	U	2.7
31	CA	1827	U	2.7
31	CA	2387	U	2.7
6	AF	93	LYS	2.6
7	BG	110	LYS	2.6
29	CC	39	LYS	2.6
45	CS	85	LYS	2.6
5	BE	114	VAL	2.6
13	BM	97	VAL	2.6
16	BP	19	VAL	2.6
19	BS	60	VAL	2.6
32	CE	186	VAL	2.6
34	CG	92	VAL	2.6
40	CN	80	VAL	2.6
1	BA	94	G	2.6

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Mol	Chain	Res	Type	RSRZ
1	BA	357	G	2.6
1	BA	1276	G	2.6
13	BM	32	ALA	2.6
14	AN	15	ALA	2.6
31	CA	205	G	2.6
31	CA	768	G	2.6
31	CA	1093	G	2.6
31	CA	1766	G	2.6
31	CA	1862	G	2.6
31	CA	2004	G	2.6
31	CA	2357	G	2.6
31	CA	2822	G	2.6
34	CG	150	ALA	2.6
44	CR	99	ALA	2.6
52	CZ	63	ALA	2.6
54	DA	2107	G	2.6
1	BA	205	A	2.6
1	BA	329	A	2.6
31	CA	223	A	2.6
31	CA	1046	A	2.6
31	CA	1439	A	2.6
31	CA	1637	A	2.6
31	CA	2823	A	2.6
46	CT	31	GLN	2.6
54	DA	613	A	2.6
16	BP	79	ASN	2.6
51	CY	17	ASN	2.6
14	BN	16	LEU	2.6
40	CN	95	LEU	2.6
17	BQ	28	PHE	2.6
29	CC	266	PHE	2.6
1	BA	194	C	2.6
13	BM	7	ILE	2.6
28	CB	28	C	2.6
31	CA	246	C	2.6
31	CA	1006	C	2.6
31	CA	1357	C	2.6
31	CA	1788	C	2.6
31	CA	1879	C	2.6
31	CA	2021	C	2.6
31	CA	2824	C	2.6
31	CA	2827	C	2.6

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Mol	Chain	Res	Type	RSRZ
34	CG	103	ILE	2.6
54	DA	1211	C	2.6
8	AH	91	GLU	2.6
29	CC	194	GLU	2.6
41	CO	110	MET	2.6
42	CP	20	GLU	2.6
29	CC	15	HIS	2.6
8	BH	122	GLY	2.6
19	AS	77	THR	2.6
40	CN	19	GLY	2.6
51	CY	78	TYR	2.6
45	CS	13	ARG	2.6
51	CY	50	ARG	2.6
13	BM	103	LYS	2.6
33	DF	14	LYS	2.6
34	CG	176	LYS	2.6
34	DG	44	LYS	2.6
1	BA	114	U	2.6
1	BA	323	U	2.6
5	AE	120	VAL	2.6
30	CD	207	VAL	2.6
31	CA	641	U	2.6
31	CA	2696	U	2.6
38	CL	19	VAL	2.6
54	DA	1081	U	2.6
54	DA	2149	U	2.6
36	DJ	63	ALA	2.6
34	CG	62	TRP	2.6
2	AB	129	LEU	2.6
10	BJ	64	GLN	2.6
14	BN	27	LEU	2.6
19	BS	16	LEU	2.6
44	CR	72	ASN	2.6
1	BA	949	A	2.6
1	BA	975	A	2.6
3	BC	207	ILE	2.6
27	C0	7	ILE	2.6
31	CA	73	A	2.6
31	CA	415	A	2.6
31	CA	666	A	2.6
31	CA	972	A	2.6
31	CA	1247	A	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	1635	A	2.6
31	CA	1938	A	2.6
31	CA	2267	A	2.6
44	CR	98	ILE	2.6
48	CV	72	ILE	2.6
53	DI	11	ILE	2.6
1	AA	76	G	2.6
1	BA	31	G	2.6
1	BA	265	G	2.6
1	BA	844	G	2.6
31	CA	45	G	2.6
31	CA	285	G	2.6
31	CA	770	G	2.6
31	CA	1232	G	2.6
31	CA	1478	G	2.6
31	CA	2032	G	2.6
31	CA	2269	G	2.6
31	CA	2599	G	2.6
31	CA	2808	G	2.6
54	DA	2116	G	2.6
54	DA	2138	G	2.6
35	CH	149	GLU	2.6
1	AA	1147	C	2.6
1	BA	176	C	2.6
28	CB	90	C	2.6
2	AB	71	GLY	2.6
29	DC	247	PRO	2.6
31	CA	1499	C	2.6
31	CA	1556	C	2.6
36	DJ	73	THR	2.6
39	CM	16	GLY	2.6
9	AI	130	ARG	2.6
14	BN	63	ARG	2.6
46	CT	72	THR	2.6
32	CE	166	LYS	2.6
44	CR	41	LYS	2.6
47	CU	44	LYS	2.6
49	CW	25	LYS	2.6
7	BG	6	VAL	2.6
17	BQ	22	VAL	2.6
47	CU	85	VAL	2.6
1	BA	268	U	2.6

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Mol	Chain	Res	Type	RSRZ
30	CD	69	ALA	2.6
35	DH	67	ALA	2.6
39	CM	98	ALA	2.6
4	AD	117	LEU	2.6
10	BJ	87	LEU	2.6
19	BS	5	LEU	2.6
25	C4	62	LEU	2.6
41	CO	51	LEU	2.6
54	DA	138	U	2.6
36	DJ	86	ILE	2.6
52	CZ	26	PHE	2.6
12	BL	20	ASN	2.6
13	AM	8	ASN	2.6
16	BP	40	ASN	2.6
17	BQ	17	MET	2.6
48	CV	27	ASN	2.6
1	BA	262	A	2.6
28	CB	29	A	2.6
31	CA	56	A	2.6
31	CA	181	A	2.6
31	CA	244	A	2.6
31	CA	255	A	2.6
31	CA	608	A	2.6
31	CA	633	A	2.6
31	CA	1596	A	2.6
31	CA	2726	A	2.6
54	DA	2184	A	2.6
7	BG	71	PRO	2.6
25	C4	24	HIS	2.6
30	CD	143	PRO	2.6
39	CM	62	PRO	2.6
46	CT	80	PRO	2.6
47	CU	70	HIS	2.6
53	DI	88	HIS	2.6
5	AE	91	GLY	2.6
5	BE	93	ARG	2.6
41	CO	69	ARG	2.6
47	CU	40	LYS	2.6
52	CZ	47	ARG	2.6
28	CB	84	G	2.6
31	CA	551	G	2.6
31	CA	600	G	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	674	G	2.6
31	CA	1441	G	2.6
31	CA	1511	G	2.6
31	CA	1517	G	2.6
31	CA	1828	G	2.6
31	CA	1842	G	2.6
31	CA	1873	G	2.6
42	CP	65	THR	2.6
10	AJ	54	SER	2.6
13	BM	21	SER	2.6
14	AN	32	SER	2.6
1	AA	1141	C	2.6
1	BA	153	C	2.6
1	BA	1344	C	2.6
10	AJ	91	ASP	2.6
31	CA	140	C	2.6
31	CA	253	C	2.6
31	CA	1399	C	2.6
31	CA	2347	C	2.6
3	BC	195	VAL	2.6
24	C3	44	VAL	2.6
3	BC	178	LEU	2.6
9	BI	63	LEU	2.6
13	BM	95	LEU	2.6
24	C3	32	ALA	2.6
41	CO	115	LEU	2.6
43	CQ	108	ALA	2.6
48	CV	51	ALA	2.6
1	AA	1125	U	2.6
1	BA	1017	U	2.6
17	BQ	33	ILE	2.6
31	CA	511	U	2.6
31	CA	1648	U	2.6
31	CA	2296	U	2.6
31	CA	2334	U	2.6
39	CM	105	ILE	2.6
45	CS	6	GLN	2.6
46	CT	66	ILE	2.6
33	CF	23	ASN	2.6
20	BT	34	LYS	2.6
29	CC	244	PRO	2.6
37	CK	113	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
50	CX	75	LYS	2.6
3	BC	171	GLY	2.6
3	BC	172	ARG	2.6
16	BP	49	GLY	2.6
20	BT	24	ARG	2.6
47	DU	69	ARG	2.6
1	BA	977	A	2.6
31	CA	71	A	2.6
31	CA	216	A	2.6
31	CA	483	A	2.6
31	CA	586	A	2.6
31	CA	792	A	2.6
31	CA	1808	A	2.6
31	CA	1981	A	2.6
31	CA	2154	A	2.6
31	CA	2274	A	2.6
31	CA	2587	A	2.6
31	CA	2705	A	2.6
54	DA	2602	A	2.6
9	BI	64	TYR	2.6
10	BJ	22	THR	2.6
10	BJ	65	TYR	2.6
30	CD	151	THR	2.6
37	CK	3	THR	2.6
37	CK	50	THR	2.6
3	BC	119	SER	2.6
12	AL	4	VAL	2.6
19	AS	4	SER	2.6
33	CF	74	VAL	2.6
35	DH	144	VAL	2.6
3	BC	34	ASP	2.6
15	BO	57	LEU	2.6
26	C5	29	ALA	2.5
38	CL	16	ALA	2.5
42	CP	106	LEU	2.6
46	CT	23	LEU	2.6
53	DI	91	ALA	2.5
1	AA	844	G	2.5
1	AA	1284	C	2.5
1	BA	1249	C	2.5
1	BA	1296	C	2.5
1	BA	1336	C	2.5

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Mol	Chain	Res	Type	RSRZ
1	BA	1342	C	2.5
31	CA	60	G	2.5
31	CA	86	G	2.5
31	CA	189	G	2.5
31	CA	261	G	2.5
31	CA	307	G	2.5
31	CA	440	C	2.5
31	CA	620	G	2.5
31	CA	798	G	2.5
31	CA	1370	C	2.5
31	CA	1388	G	2.5
31	CA	1514	G	2.5
31	CA	1806	C	2.5
31	CA	1934	C	2.5
31	CA	2620	C	2.5
31	CA	2631	G	2.5
54	DA	1062	G	2.5
54	DA	1100	C	2.5
54	DA	2143	C	2.5
3	BC	10	ILE	2.5
13	BM	33	ILE	2.5
29	CC	135	ILE	2.5
37	CK	92	MET	2.5
38	CL	41	ILE	2.5
2	BB	96	TRP	2.5
1	BA	1341	U	2.5
31	CA	25	U	2.5
31	CA	906	U	2.5
54	DA	1094	U	2.5
54	DA	1497	U	2.5
20	BT	33	LYS	2.5
39	CM	93	ASN	2.5
46	CT	48	LYS	2.5
47	CU	59	ASN	2.5
3	BC	179	ARG	2.5
5	BE	116	GLU	2.5
11	AK	13	ARG	2.5
11	BK	13	ARG	2.5
22	C1	17	ARG	2.5
30	CD	141	ARG	2.5
32	CE	88	ARG	2.5
32	CE	165	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
29	CC	169	GLY	2.5
30	CD	147	GLY	2.5
38	CL	26	GLY	2.5
2	AB	70	VAL	2.5
3	AC	192	THR	2.5
30	CD	189	VAL	2.5
43	CQ	61	VAL	2.5
46	CT	104	THR	2.5
47	CU	22	THR	2.5
1	BA	131	A	2.5
1	BA	1093	A	2.5
1	BA	1145	A	2.5
1	BA	1437	A	2.5
5	AE	115	LEU	2.5
9	BI	54	LEU	2.5
18	AR	29	LEU	2.5
31	CA	213	A	2.5
31	CA	1304	A	2.5
31	CA	1308	A	2.5
31	CA	1634	A	2.5
32	CE	109	LEU	2.5
20	BT	47	ALA	2.5
36	DJ	18	ALA	2.5
46	CT	93	ALA	2.5
47	CU	45	ALA	2.5
41	CO	106	ASP	2.5
9	AI	39	PHE	2.5
10	BJ	53	ILE	2.5
35	CH	80	ILE	2.5
36	DJ	122	ILE	2.5
47	DU	74	ILE	2.5
30	CD	125	TRP	2.5
1	BA	1112	C	2.5
31	CA	201	C	2.5
31	CA	1167	C	2.5
31	CA	2787	C	2.5
1	AA	86	G	2.5
1	AA	1387	G	2.5
1	BA	259	G	2.5
1	BA	457	G	2.5
1	BA	1160	G	2.5
2	AB	143	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
7	BG	36	LYS	2.5
9	AI	13	LYS	2.5
31	CA	122	G	2.5
31	CA	591	U	2.5
31	CA	684	G	2.5
31	CA	688	U	2.5
31	CA	1033	U	2.5
31	CA	1206	G	2.5
31	CA	1554	U	2.5
31	CA	1714	U	2.5
31	CA	1718	G	2.5
31	CA	1807	G	2.5
31	CA	1903	G	2.5
31	CA	2162	G	2.5
31	CA	2190	G	2.5
34	CG	175	LYS	2.5
38	CL	84	CYS	2.5
54	DA	1171	G	2.5
7	BG	78	ARG	2.5
13	BM	87	ARG	2.5
14	BN	85	ARG	2.5
16	BP	28	ARG	2.5
24	C3	12	ARG	2.5
29	CC	270	ARG	2.5
38	CL	105	ARG	2.5
13	BM	105	ASN	2.5
14	BN	10	GLU	2.5
46	CT	9	HIS	2.5
30	CD	198	GLY	2.5
3	AC	39	VAL	2.5
3	BC	91	VAL	2.5
7	BG	22	LEU	2.5
14	BN	34	VAL	2.5
16	BP	71	VAL	2.5
22	C1	39	LEU	2.5
35	DH	78	VAL	2.5
40	CN	124	LEU	2.5
32	CE	35	TYR	2.5
49	CW	82	TYR	2.5
21	AU	50	ALA	2.5
51	CY	21	ALA	2.5
9	BI	21	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
29	CC	272	SER	2.5
42	CP	58	ILE	2.5
1	AA	539	A	2.5
1	BA	1275	A	2.5
1	BA	1377	A	2.5
31	CA	429	A	2.5
31	CA	503	A	2.5
31	CA	1528	A	2.5
31	CA	2003	A	2.5
54	DA	2183	A	2.5
20	AT	13	GLN	2.5
20	BT	8	LYS	2.5
23	D2	53	LYS	2.5
26	C5	32	LYS	2.5
35	CH	35	LYS	2.5
37	CK	41	LYS	2.5
2	BB	139	ARG	2.5
24	C3	34	ARG	2.5
38	CL	31	ARG	2.5
39	CM	48	ARG	2.5
41	CO	45	ARG	2.5
1	AA	961	U	2.5
7	AG	2	PRO	2.5
7	BG	14	PRO	2.5
10	AJ	79	PRO	2.5
31	CA	100	U	2.5
31	CA	349	U	2.5
31	CA	1438	U	2.5
31	CA	2213	U	2.5
54	DA	1082	U	2.5
54	DA	2118	U	2.5
54	DA	2423	U	2.5
1	BA	225	C	2.5
1	BA	1448	C	2.5
2	BB	145	GLU	2.5
3	AC	188	GLU	2.5
12	AL	25	GLU	2.5
20	BT	42	GLY	2.5
28	CB	91	C	2.5
31	CA	486	C	2.5
31	CA	516	C	2.5
31	CA	812	C	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1472	C	2.5
31	CA	1706	C	2.5
31	CA	1732	C	2.5
31	CA	2001	C	2.5
31	CA	2716	C	2.5
47	CU	15	HIS	2.5
47	CU	75	GLY	2.5
47	CU	90	GLY	2.5
48	CV	78	GLY	2.5
49	CW	24	ASN	2.5
51	CY	32	ASN	2.5
1	AA	211	G	2.5
1	AA	1032	G	2.5
1	AA	1142	G	2.5
1	BA	376	G	2.5
1	BA	1331	G	2.5
3	BC	39	VAL	2.5
6	BF	89	VAL	2.5
7	AG	30	LEU	2.5
7	BG	69	VAL	2.5
7	BG	87	VAL	2.5
13	BM	56	LEU	2.5
14	AN	34	VAL	2.5
19	AS	5	LEU	2.5
20	BT	58	VAL	2.5
30	CD	178	VAL	2.5
31	CA	530	G	2.5
31	CA	622	G	2.5
31	CA	1479	G	2.5
31	CA	2414	G	2.5
31	CA	2819	G	2.5
31	CA	2828	G	2.5
31	CA	2848	G	2.5
31	CA	2876	G	2.5
35	CH	31	VAL	2.5
35	DH	6	LEU	2.5
47	CU	55	VAL	2.5
54	DA	361	G	2.5
14	AN	50	THR	2.5
32	CE	84	THR	2.5
13	BM	2	ALA	2.5
35	DH	39	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
38	CL	2	ILE	2.5
19	BS	10	PHE	2.5
14	BN	56	SER	2.5
10	AJ	60	ASP	2.5
45	CS	55	ASP	2.5
9	BI	32	GLN	2.5
36	CJ	12	GLN	2.5
1	AA	977	A	2.5
1	AA	1014	A	2.5
1	AA	1285	A	2.5
28	CB	99	A	2.5
31	CA	689	A	2.5
31	CA	1937	A	2.5
31	CA	2287	A	2.5
31	CA	2700	A	2.5
31	CA	2765	A	2.5
54	DA	362	A	2.5
16	BP	31	ARG	2.5
36	CJ	22	PRO	2.5
6	BF	94	HIS	2.5
30	CD	134	HIS	2.5
1	BA	1125	U	2.5
1	BA	1205	U	2.5
31	CA	72	U	2.5
31	CA	202	U	2.5
31	CA	562	U	2.5
31	CA	1258	U	2.5
41	CO	101	GLY	2.5
48	CV	32	GLY	2.5
51	CY	76	GLU	2.5
54	DA	1415	U	2.5
54	DA	2796	U	2.5
8	BH	121	LEU	2.5
29	CC	93	LEU	2.5
32	CE	133	LEU	2.5
44	CR	109	LEU	2.5
52	CZ	19	LEU	2.5
52	CZ	37	LEU	2.5
7	BG	75	VAL	2.5
14	BN	84	VAL	2.5
15	BO	12	VAL	2.5
30	CD	58	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
30	CD	193	VAL	2.5
33	CF	31	VAL	2.5
41	CO	76	VAL	2.5
43	CQ	73	VAL	2.5
44	CR	4	VAL	2.5
53	DI	35	VAL	2.5
1	AA	934	C	2.5
1	BA	1208	C	2.5
1	BA	1209	C	2.5
1	BA	1352	C	2.5
2	AB	9	MET	2.5
6	AF	90	MET	2.5
11	BK	85	MET	2.5
26	C5	1	MET	2.5
31	CA	484	C	2.5
31	CA	485	C	2.5
31	CA	698	C	2.5
31	CA	736	C	2.5
31	CA	772	C	2.5
31	CA	1278	C	2.5
31	CA	1404	C	2.5
31	CA	1446	C	2.5
31	CA	1790	C	2.5
31	CA	1837	C	2.5
31	CA	2264	C	2.5
31	CA	2840	C	2.5
54	DA	1577	C	2.5
14	BN	30	ILE	2.5
53	DI	44	ALA	2.5
1	AA	212	G	2.4
1	AA	733	G	2.4
1	BA	1419	G	2.4
1	BA	1473	G	2.4
2	BB	143	LYS	2.4
7	AG	25	LYS	2.4
21	AU	54	LYS	2.4
25	C4	16	LYS	2.4
29	CC	7	LYS	2.4
31	CA	81	G	2.4
31	CA	85	G	2.4
31	CA	132	G	2.4
31	CA	194	G	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	489	G	2.4
31	CA	907	G	2.4
31	CA	1465	G	2.4
31	CA	1619	G	2.4
31	CA	1620	G	2.4
31	CA	1628	G	2.4
31	CA	1743	G	2.4
31	CA	2148	G	2.4
31	CA	2293	G	2.4
31	CA	2349	G	2.4
31	CA	2360	G	2.4
40	CN	58	LYS	2.4
53	DI	43	LYS	2.4
54	DA	1875	G	2.4
8	BH	90	ASP	2.4
10	AJ	62	ARG	2.4
19	AS	55	ARG	2.4
39	CM	33	ARG	2.4
40	CN	18	ARG	2.4
41	CO	103	ARG	2.4
13	BM	112	PRO	2.4
36	CJ	75	PRO	2.4
43	CQ	22	PRO	2.4
49	CW	27	PRO	2.4
1	BA	44	A	2.4
31	CA	6	A	2.4
31	CA	91	A	2.4
31	CA	226	A	2.4
31	CA	453	A	2.4
31	CA	941	A	2.4
31	CA	996	A	2.4
31	CA	1134	A	2.4
31	CA	1143	A	2.4
31	CA	1383	A	2.4
31	CA	2088	A	2.4
31	CA	2163	A	2.4
31	CA	2288	A	2.4
31	CA	2835	A	2.4
31	CA	2851	A	2.4
37	CK	66	GLY	2.4
44	CR	23	GLY	2.4
45	CS	89	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
9	BI	87	LEU	2.4
34	CG	50	LEU	2.4
13	AM	25	VAL	2.4
19	BS	66	MET	2.4
20	AT	54	MET	2.4
29	CC	6	CYS	2.4
31	CA	50	U	2.4
31	CA	373	U	2.4
31	CA	459	U	2.4
31	CA	766	U	2.4
31	CA	1636	U	2.4
35	DH	9	VAL	2.4
51	CY	58	VAL	2.4
52	CZ	11	VAL	2.4
10	AJ	76	ILE	2.4
23	C2	52	ALA	2.4
26	C5	5	ALA	2.4
30	CD	209	ALA	2.4
30	DD	209	ALA	2.4
35	DH	36	ALA	2.4
44	CR	96	ALA	2.4
53	DI	48	ALA	2.4
53	DI	112	ALA	2.4
8	AH	55	THR	2.4
12	AL	18	LYS	2.4
35	CH	22	LYS	2.4
37	CK	4	PHE	2.4
52	CZ	54	LYS	2.4
1	AA	985	C	2.4
1	AA	1120	C	2.4
1	BA	483	C	2.4
1	BA	623	C	2.4
1	BA	1533	C	2.4
8	BH	86	TYR	2.4
31	CA	323	C	2.4
17	BQ	27	ARG	2.4
29	CC	214	ARG	2.4
32	CE	170	ARG	2.4
37	CK	99	ARG	2.4
41	CO	96	ARG	2.4
3	BC	3	GLN	2.4
20	AT	14	SER	2.4

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Mol	Chain	Res	Type	RSRZ
29	CC	259	SER	2.4
33	CF	129	SER	2.4
37	CK	8	PRO	2.4
52	CZ	49	ASP	2.4
1	BA	251	G	2.4
1	BA	799	G	2.4
31	CA	17	G	2.4
31	CA	232	G	2.4
31	CA	295	G	2.4
31	CA	407	G	2.4
31	CA	1091	G	2.4
31	CA	1185	G	2.4
31	CA	1225	G	2.4
31	CA	1464	G	2.4
31	CA	1702	G	2.4
31	CA	2152	G	2.4
31	CA	2237	G	2.4
31	CA	2625	G	2.4
31	CA	2719	G	2.4
31	CA	2859	G	2.4
54	DA	1099	G	2.4
3	AC	81	GLY	2.4
14	BN	68	GLY	2.4
25	C4	21	GLY	2.4
30	CD	67	HIS	2.4
33	CF	151	GLY	2.4
35	DH	5	LEU	2.4
2	BB	199	VAL	2.4
16	AP	21	VAL	2.4
17	BQ	58	VAL	2.4
40	CN	93	VAL	2.4
1	BA	80	A	2.4
1	BA	968	A	2.4
31	CA	342	A	2.4
31	CA	422	A	2.4
31	CA	918	A	2.4
31	CA	1241	A	2.4
31	CA	1385	A	2.4
31	CA	1569	A	2.4
31	CA	1805	A	2.4
31	CA	1960	A	2.4
31	CA	2013	A	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	2108	A	2.4
54	DA	2154	A	2.4
1	BA	229	U	2.4
1	BA	467	U	2.4
31	CA	567	U	2.4
31	CA	2151	U	2.4
33	CF	106	ILE	2.4
34	CG	26	ILE	2.4
6	AF	32	ALA	2.4
10	AJ	61	ALA	2.4
11	BK	25	ALA	2.4
46	CT	54	ALA	2.4
47	CU	20	ALA	2.4
46	CT	75	PHE	2.4
11	AK	30	THR	2.4
29	CC	51	THR	2.4
38	CL	104	THR	2.4
39	CM	117	THR	2.4
47	CU	39	THR	2.4
9	BI	113	ARG	2.4
25	C4	45	ARG	2.4
29	CC	14	ARG	2.4
39	CM	2	ARG	2.4
41	CO	12	ARG	2.4
42	CP	30	ARG	2.4
1	BA	385	C	2.4
1	BA	1141	C	2.4
31	CA	421	C	2.4
31	CA	595	C	2.4
31	CA	823	C	2.4
31	CA	1362	C	2.4
31	CA	1656	C	2.4
31	CA	2153	C	2.4
31	CA	2815	C	2.4
54	DA	1052	C	2.4
54	DA	2178	C	2.4
5	AE	97	GLN	2.4
14	AN	60	GLN	2.4
10	AJ	43	PRO	2.4
9	AI	63	LEU	2.4
10	BJ	19	ASP	2.4
33	CF	73	SER	2.4

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Mol	Chain	Res	Type	RSRZ
39	CM	68	SER	2.4
16	BP	54	LEU	2.4
29	CC	176	LEU	2.4
38	CL	8	LEU	2.4
48	CV	81	ASP	2.4
53	DI	36	ASP	2.4
3	AC	176	HIS	2.4
9	AI	40	GLY	2.4
9	BI	69	GLY	2.4
11	BK	22	HIS	2.4
2	AB	133	GLU	2.4
7	AG	73	VAL	2.4
10	AJ	84	VAL	2.4
14	BN	14	VAL	2.4
21	AU	44	GLU	2.4
29	CC	3	VAL	2.4
39	DM	106	GLU	2.4
43	CQ	102	GLU	2.4
52	CZ	17	GLU	2.4
52	CZ	24	GLU	2.4
53	DI	108	VAL	2.4
9	BI	115	LYS	2.4
27	C0	14	ILE	2.4
31	CA	35	G	2.4
31	CA	630	G	2.4
31	CA	664	G	2.4
31	CA	763	G	2.4
31	CA	1421	G	2.4
31	CA	1516	G	2.4
31	CA	1537	G	2.4
31	CA	1660	G	2.4
31	CA	1930	G	2.4
31	CA	2331	G	2.4
31	CA	2523	G	2.4
31	CA	2722	G	2.4
31	CA	2782	G	2.4
36	CJ	35	ILE	2.4
42	CP	35	ILE	2.4
45	CS	59	ILE	2.4
46	CT	103	ILE	2.4
54	DA	879	G	2.4
29	DC	242	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
14	AN	2	ALA	2.4
35	DH	81	ALA	2.4
1	BA	152	A	2.4
1	BA	1025	U	2.4
11	BK	27	PHE	2.4
3	BC	8	ASN	2.4
31	CA	193	U	2.4
31	CA	262	A	2.4
31	CA	665	U	2.4
31	CA	783	A	2.4
31	CA	821	A	2.4
31	CA	913	U	2.4
31	CA	1249	U	2.4
31	CA	1427	A	2.4
31	CA	1630	A	2.4
31	CA	1655	A	2.4
31	CA	1864	U	2.4
31	CA	2233	U	2.4
31	CA	2247	A	2.4
31	CA	2433	A	2.4
31	CA	2614	A	2.4
34	CG	83	PHE	2.4
48	CV	95	PHE	2.4
50	CX	79	PHE	2.4
54	DA	1073	A	2.4
32	CE	150	THR	2.4
25	C4	30	ARG	2.4
26	C5	19	ARG	2.4
41	CO	112	TYR	2.4
50	CX	39	ARG	2.4
10	BJ	99	GLN	2.4
14	BN	4	GLN	2.4
16	BP	63	GLN	2.4
33	CF	36	LEU	2.4
42	CP	26	LEU	2.4
52	CZ	28	LEU	2.4
25	C4	49	MET	2.4
1	AA	1066	C	2.4
12	BL	96	HIS	2.4
14	AN	18	ASP	2.4
14	BN	78	GLY	2.4
17	BQ	10	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
29	CC	56	GLY	2.4
30	CD	153	GLY	2.4
31	CA	115	C	2.4
31	CA	210	C	2.4
31	CA	417	C	2.4
31	CA	610	C	2.4
31	CA	692	C	2.4
31	CA	1768	C	2.4
31	CA	2063	C	2.4
31	CA	2830	C	2.4
38	CL	117	SER	2.4
54	DA	1102	C	2.4
3	BC	198	VAL	2.4
11	AK	129	VAL	2.4
35	CH	144	VAL	2.4
36	DJ	33	VAL	2.4
41	CO	48	VAL	2.4
46	CT	105	VAL	2.4
4	BD	148	LYS	2.4
12	BL	44	LYS	2.4
25	C4	52	LYS	2.4
32	CE	185	LYS	2.4
37	CK	68	LYS	2.4
44	CR	93	LYS	2.4
49	CW	14	LYS	2.4
7	AG	152	ALA	2.4
10	BJ	86	ALA	2.4
36	DJ	114	ALA	2.4
1	AA	213	G	2.4
1	AA	973	G	2.4
1	AA	1095	U	2.4
1	BA	656	G	2.4
1	BA	1139	G	2.4
1	BA	1202	U	2.4
3	BC	127	ARG	2.4
5	AE	19	ASN	2.4
10	AJ	5	ARG	2.4
19	AS	81	ARG	2.4
19	BS	79	THR	2.4
20	AT	24	ARG	2.4
20	BT	29	ARG	2.4
1	BA	321	A	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	38	A	2.4
31	CA	363	G	2.4
31	CA	375	G	2.4
31	CA	464	U	2.4
31	CA	506	G	2.4
31	CA	533	G	2.4
31	CA	549	G	2.4
31	CA	769	U	2.4
31	CA	832	U	2.4
31	CA	846	U	2.4
31	CA	1458	U	2.4
31	CA	1481	U	2.4
31	CA	739	A	2.4
31	CA	869	G	2.4
31	CA	877	A	2.4
31	CA	930	G	2.4
31	CA	1106	G	2.4
31	CA	1139	G	2.4
31	CA	1263	U	2.4
31	CA	1546	G	2.4
31	CA	1763	G	2.4
31	CA	1765	U	2.4
31	CA	1777	U	2.4
31	CA	2239	G	2.4
31	CA	2286	G	2.4
31	CA	2345	G	2.4
31	CA	2581	G	2.4
31	CA	2816	G	2.4
31	CA	2846	G	2.4
39	CM	126	ARG	2.4
54	DA	363	G	2.4
54	DA	1416	G	2.4
54	DA	2213	U	2.4
54	DA	2126	A	2.4
54	DA	2135	A	2.4
54	DA	2885[A]	G	2.4
7	BG	44	TYR	2.3
7	AG	66	LEU	2.3
22	C1	22	LEU	2.3
32	CE	129	PRO	2.3
38	CL	86	LEU	2.3
16	BP	1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
29	CC	146	MET	2.3
38	CL	1	MET	2.3
40	CN	12	MET	2.3
29	DC	235	GLY	2.3
30	CD	78	GLY	2.3
36	DJ	25	GLY	2.3
2	BB	37	LYS	2.3
7	AG	110	LYS	2.3
10	AJ	30	LYS	2.3
13	AM	64	VAL	2.3
22	C1	57	LYS	2.3
26	C5	8	LYS	2.3
30	CD	190	LYS	2.3
34	CG	11	VAL	2.3
34	CG	166	ASP	2.3
35	CH	130	VAL	2.3
37	CK	60	ASP	2.3
39	CM	85	VAL	2.3
39	CM	89	VAL	2.3
42	CP	39	VAL	2.3
44	CR	61	TRP	2.3
45	CS	47	VAL	2.3
46	CT	27	LYS	2.3
2	BB	173	ILE	2.3
9	BI	65	ILE	2.3
13	AM	7	ILE	2.3
1	AA	183	C	2.3
1	BA	370	C	2.3
1	BA	883	C	2.3
1	BA	1325	C	2.3
31	CA	79	C	2.3
31	CA	1104	C	2.3
31	CA	1118	C	2.3
31	CA	1363	C	2.3
31	CA	1462	C	2.3
31	CA	2354	C	2.3
31	CA	2499	C	2.3
31	CA	2611	C	2.3
54	DA	1072	C	2.3
3	AC	71	ALA	2.3
10	BJ	34	ALA	2.3
13	AM	2	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
13	BM	63	PHE	2.3
16	AP	7	ALA	2.3
36	CJ	63	ALA	2.3
47	CU	23	ALA	2.3
48	CV	87	PHE	2.3
49	CW	23	ALA	2.3
53	DI	100	ALA	2.3
53	DI	135	ALA	2.3
3	BC	169	ARG	2.3
12	AL	9	ARG	2.3
17	AQ	27	ARG	2.3
37	CK	35	ARG	2.3
38	CL	18	ARG	2.3
46	CT	25	ARG	2.3
47	DU	73	ARG	2.3
36	CJ	60	THR	2.3
37	CK	10	THR	2.3
1	AA	471	U	2.3
1	BA	1464	U	2.3
31	CA	292	U	2.3
31	CA	441	U	2.3
31	CA	598	U	2.3
31	CA	2701	U	2.3
19	AS	80	TYR	2.3
31	CA	44	A	2.3
31	CA	131	A	2.3
31	CA	401	A	2.3
31	CA	502	A	2.3
31	CA	800	A	2.3
31	CA	1127	A	2.3
31	CA	1144	A	2.3
31	CA	1373	A	2.3
31	CA	1494	A	2.3
31	CA	1614	A	2.3
31	CA	2336	A	2.3
31	CA	2837	A	2.3
54	DA	2134	A	2.3
1	AA	200	G	2.3
1	AA	417	G	2.3
1	BA	698	G	2.3
1	BA	1233	G	2.3
9	AI	110	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
9	BI	5	GLN	2.3
31	CA	36	G	2.3
31	CA	212	G	2.3
31	CA	491	G	2.3
31	CA	537	G	2.3
31	CA	638	G	2.3
31	CA	760	G	2.3
31	CA	855	G	2.3
31	CA	1107	G	2.3
31	CA	1168	G	2.3
31	CA	1310	G	2.3
31	CA	1408	G	2.3
31	CA	1682	G	2.3
31	CA	1710	G	2.3
31	CA	1975	G	2.3
31	CA	2446	G	2.3
31	CA	2744	G	2.3
32	CE	94	GLN	2.3
44	CR	71	GLN	2.3
5	BE	129	GLY	2.3
7	AG	112	GLY	2.3
13	AM	13	LYS	2.3
13	AM	26	GLY	2.3
14	AN	72	GLY	2.3
25	C4	18	GLY	2.3
27	C0	34	HIS	2.3
32	CE	29	HIS	2.3
33	DF	72	LYS	2.3
40	CN	14	LYS	2.3
2	AB	217	VAL	2.3
8	BH	25	VAL	2.3
10	AJ	36	VAL	2.3
12	BL	119	VAL	2.3
43	CQ	46	VAL	2.3
4	AD	145	ILE	2.3
8	BH	46	ILE	2.3
9	AI	65	ILE	2.3
13	AM	45	ILE	2.3
39	CM	73	ILE	2.3
39	CM	103	ILE	2.3
9	AI	128	SER	2.3
10	BJ	91	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
14	BN	32	SER	2.3
36	CJ	21	SER	2.3
39	CM	76	GLU	2.3
46	CT	13	SER	2.3
47	CU	42	GLU	2.3
3	BC	37	PHE	2.3
7	AG	39	ALA	2.3
19	BS	75	ALA	2.3
37	CK	87	ALA	2.3
42	CP	59	ALA	2.3
44	CR	68	ALA	2.3
45	CS	61	ALA	2.3
49	CW	6	ALA	2.3
9	AI	123	ARG	2.3
44	CR	92	ARG	2.3
49	CW	79	ARG	2.3
1	BA	1120	C	2.3
1	BA	1317	C	2.3
1	BA	1466	C	2.3
31	CA	671	C	2.3
31	CA	1498	C	2.3
31	CA	2044	C	2.3
31	CA	2263	C	2.3
31	CA	2612	C	2.3
31	CA	2902	C	2.3
9	BI	66	THR	2.3
23	C2	29	THR	2.3
36	DJ	132	THR	2.3
8	BH	61	LEU	2.3
26	C5	27	CYS	2.3
32	CE	118	LEU	2.3
39	DM	99	ASN	2.3
40	CN	119	LEU	2.3
53	DI	3	LEU	2.3
1	AA	1049	U	2.3
1	AA	1286	U	2.3
1	BA	62	U	2.3
2	BB	213	TYR	2.3
31	CA	113	U	2.3
31	CA	1224	U	2.3
31	CA	2068	U	2.3
48	CV	50	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
37	CK	75	TYR	2.3
7	BG	11	LYS	2.3
17	BQ	36	LYS	2.3
32	CE	194	LYS	2.3
45	CS	10	LYS	2.3
46	CT	49	LYS	2.3
1	BA	263	A	2.3
3	AC	195	VAL	2.3
5	BE	51	GLY	2.3
9	BI	29	VAL	2.3
9	BI	40	GLY	2.3
15	AO	51	HIS	2.3
22	C1	14	GLY	2.3
31	CA	423	A	2.3
31	CA	454	A	2.3
31	CA	478	A	2.3
31	CA	592	A	2.3
31	CA	2764	A	2.3
33	CF	39	GLY	2.3
48	CV	34	VAL	2.3
54	DA	1722	A	2.3
54	DA	2117	A	2.3
1	AA	951	G	2.3
1	AA	1013	G	2.3
1	BA	138	G	2.3
1	BA	973	G	2.3
1	BA	1184	G	2.3
1	BA	1190	G	2.3
31	CA	313	G	2.3
31	CA	559	G	2.3
31	CA	759	G	2.3
31	CA	1186	G	2.3
31	CA	1259	G	2.3
31	CA	1435	G	2.3
31	CA	1950	G	2.3
31	CA	2294	G	2.3
31	CA	2655	G	2.3
31	CA	2839	G	2.3
31	CA	2854	G	2.3
34	CG	109	PHE	2.3
35	DH	70	GLU	2.3
37	CK	90	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
41	CO	120	GLU	2.3
7	BG	61	ALA	2.3
16	BP	44	SER	2.3
20	AT	26	SER	2.3
24	D3	23	ALA	2.3
47	CU	78	SER	2.3
12	BL	50	ARG	2.3
21	AU	47	ARG	2.3
40	CN	55	ARG	2.3
44	CR	64	ARG	2.3
2	BB	114	LEU	2.3
3	BC	157	LEU	2.3
13	BM	48	LEU	2.3
40	CN	82	MET	2.3
5	BE	131	THR	2.3
9	AI	9	THR	2.3
35	DH	79	THR	2.3
45	CS	32	THR	2.3
1	AA	308	C	2.3
1	BA	233	C	2.3
1	BA	1303	C	2.3
9	AI	23	PRO	2.3
31	CA	281	C	2.3
31	CA	490	C	2.3
31	CA	611	C	2.3
31	CA	915	C	2.3
31	CA	2295	C	2.3
33	CF	65	PRO	2.3
38	CL	102	PRO	2.3
54	DA	2096	C	2.3
2	BB	66	LYS	2.3
3	BC	150	LYS	2.3
12	BL	5	ASN	2.3
14	AN	3	LYS	2.3
43	CQ	29	LYS	2.3
1	BA	252	U	2.3
1	BA	1030	U	2.3
1	BA	1224	U	2.3
1	BA	1436	U	2.3
31	CA	499	U	2.3
31	CA	811	U	2.3
31	CA	1476	U	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	2231	U	2.3
54	DA	360	U	2.3
54	DA	2139	U	2.3
3	BC	52	VAL	2.3
12	BL	107	VAL	2.3
17	AQ	10	GLY	2.3
46	CT	60	HIS	2.3
51	CY	75	GLY	2.3
33	CF	111	ILE	2.3
35	CH	72	ILE	2.3
1	AA	983	A	2.3
1	BA	607	A	2.3
1	BA	958	A	2.3
8	BH	45	PHE	2.3
19	BS	34	TRP	2.3
3	AC	189	ALA	2.3
5	BE	107	ALA	2.3
10	BJ	12	ALA	2.3
29	CC	82	GLU	2.3
31	CA	21	A	2.3
31	CA	279	A	2.3
31	CA	563	A	2.3
31	CA	632	A	2.3
31	CA	1084	A	2.3
31	CA	1129	A	2.3
31	CA	1490	A	2.3
31	CA	1772	A	2.3
31	CA	1780	A	2.3
31	CA	2082	A	2.3
31	CA	2434	A	2.3
31	CA	2778	A	2.3
31	CA	2886	A	2.3
40	CN	115	GLU	2.3
54	DA	142	A	2.3
54	DA	2147	A	2.3
14	BN	61	ARG	2.3
22	C1	56	ALA	2.3
41	CO	30	ARG	2.3
43	CQ	93	ARG	2.3
14	AN	38	ASP	2.3
1	AA	1331	G	2.3
1	BA	6	G	2.3

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Mol	Chain	Res	Type	RSRZ
1	BA	168	G	2.3
1	BA	230	G	2.3
1	BA	388	G	2.3
1	BA	1439	G	2.3
3	BC	33	LEU	2.3
27	C0	25	LEU	2.3
31	CA	168	G	2.3
31	CA	220	G	2.3
31	CA	230	G	2.3
31	CA	277	G	2.3
31	CA	520	G	2.3
31	CA	612	G	2.3
31	CA	1445	G	2.3
31	CA	1455	G	2.3
31	CA	1814	G	2.3
31	CA	2325	G	2.3
31	CA	2355	G	2.3
31	CA	2428	G	2.3
31	CA	2624	G	2.3
31	CA	2644	G	2.3
9	AI	120	LYS	2.3
9	BI	43	THR	2.3
10	BJ	79	PRO	2.3
13	AM	27	LYS	2.3
13	AM	115	PRO	2.3
13	BM	44	LYS	2.3
29	CC	18	LYS	2.3
32	CE	58	LYS	2.3
33	DF	161	LYS	2.3
36	CJ	26	PRO	2.3
36	CJ	97	LYS	2.3
36	DJ	60	THR	2.3
53	DI	37	LYS	2.3
53	DI	39	THR	2.3
1	AA	210	C	2.2
1	AA	1277	C	2.2
4	AD	108	GLY	2.2
11	AK	86	VAL	2.2
11	BK	64	GLN	2.2
1	BA	317	U	2.2
1	BA	386	C	2.2
1	BA	972	C	2.2

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Mol	Chain	Res	Type	RSRZ
2	BB	4	VAL	2.2
2	BB	33	GLY	2.2
1	BA	1116	U	2.2
17	BQ	45	HIS	2.2
22	C1	42	HIS	2.2
28	CB	63	C	2.2
30	CD	73	VAL	2.2
31	CA	815	C	2.2
31	CA	1045	C	2.2
31	CA	1064	C	2.2
31	CA	1255	U	2.2
31	CA	1257	C	2.2
31	CA	1638	C	2.2
31	CA	1961	C	2.2
31	CA	2055	C	2.2
34	CG	82	GLY	2.2
34	CG	90	VAL	2.2
37	CK	53	TYR	2.2
30	CD	140	HIS	2.2
31	CA	378	C	2.2
31	CA	437	U	2.2
31	CA	540	C	2.2
36	CJ	86	ILE	2.2
37	CK	107	GLY	2.2
38	CL	39	ILE	2.2
39	CM	31	GLY	2.2
53	DI	27	VAL	2.2
31	CA	2680	U	2.2
31	CA	2878	U	2.2
54	DA	2161	C	2.2
3	BC	167	TRP	2.2
10	BJ	68	ARG	2.2
13	AM	93	ARG	2.2
14	AN	9	ARG	2.2
35	CH	148	ALA	2.2
36	DJ	83	ALA	2.2
37	CK	91	GLU	2.2
45	CS	103	ALA	2.2
1	AA	1534	A	2.2
1	BA	55	A	2.2
1	BA	149	A	2.2
1	BA	468	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1287	A	2.2
9	AI	88	MET	2.2
31	CA	10	A	2.2
31	CA	609	A	2.2
31	CA	878	A	2.2
31	CA	1133	A	2.2
31	CA	2033	A	2.2
31	CA	2682	A	2.2
54	DA	2176	A	2.2
7	BG	47	LEU	2.2
43	CQ	65	SER	2.2
50	CX	59	LEU	2.2
2	BB	128	LYS	2.2
4	AD	31	LYS	2.2
4	BD	206	LYS	2.2
12	AL	44	LYS	2.2
13	AM	44	LYS	2.2
15	AO	48	LYS	2.2
22	D1	12	LYS	2.2
23	C2	38	LYS	2.2
24	C3	11	LYS	2.2
11	AK	111	THR	2.2
32	CE	48	THR	2.2
37	CK	65	THR	2.2
1	AA	6	G	2.2
1	BA	310	G	2.2
1	BA	455	G	2.2
1	BA	1185	G	2.2
1	BA	1438	G	2.2
2	AB	178	ASN	2.2
9	BI	47	VAL	2.2
10	AJ	8	ILE	2.2
10	AJ	33	GLY	2.2
11	AK	90	GLY	2.2
13	BM	24	GLY	2.2
13	BM	100	GLN	2.2
20	AT	32	ILE	2.2
27	C0	51	VAL	2.2
31	CA	467	G	2.2
31	CA	498	G	2.2
31	CA	628	G	2.2
31	CA	728	G	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1317	G	2.2
31	CA	2110	G	2.2
32	CE	187	VAL	2.2
34	CG	77	ILE	2.2
44	CR	94	ILE	2.2
38	CL	32	TYR	2.2
1	BA	843	U	2.2
1	BA	1148	U	2.2
7	AG	26	PHE	2.2
31	CA	321	U	2.2
31	CA	395	U	2.2
31	CA	2074	U	2.2
31	CA	2546	U	2.2
31	CA	2586	U	2.2
1	AA	207	C	2.2
1	BA	290	C	2.2
1	BA	936	C	2.2
15	BO	54	ARG	2.2
21	AU	34	ARG	2.2
30	CD	124	ARG	2.2
31	CA	1675	C	2.2
31	CA	2215	C	2.2
31	CA	2359	C	2.2
36	CJ	134	ARG	2.2
41	CO	17	ARG	2.2
4	AD	147	GLU	2.2
11	BK	102	ALA	2.2
13	BM	5	ALA	2.2
17	BQ	82	ALA	2.2
21	AU	39	GLU	2.2
29	CC	2	ALA	2.2
30	CD	162	ALA	2.2
32	CE	26	ALA	2.2
32	DE	201	ALA	2.2
35	DH	105	ALA	2.2
7	BG	116	MET	2.2
5	BE	36	LEU	2.2
32	CE	180	LEU	2.2
43	CQ	100	LEU	2.2
44	CR	95	LEU	2.2
2	AB	128	LYS	2.2
8	BH	56	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
14	AN	28	LYS	2.2
14	BN	33	ASP	2.2
29	CC	183	LYS	2.2
32	CE	98	LYS	2.2
33	CF	33	LYS	2.2
43	CQ	106	LYS	2.2
52	CZ	60	LYS	2.2
53	DI	105	LYS	2.2
1	AA	1287	A	2.2
1	BA	130	A	2.2
1	BA	356	A	2.2
1	BA	487	A	2.2
1	BA	1375	A	2.2
4	AD	119	SER	2.2
14	AN	5	SER	2.2
20	AT	23	SER	2.2
30	CD	139	SER	2.2
5	BE	150	PRO	2.2
30	CD	194	PRO	2.2
31	CA	199	A	2.2
31	CA	233	A	2.2
31	CA	428	A	2.2
31	CA	572	A	2.2
31	CA	1027	A	2.2
31	CA	1194	A	2.2
31	CA	1669	A	2.2
31	CA	1784	A	2.2
31	CA	1854	A	2.2
31	CA	2005	A	2.2
31	CA	2077	A	2.2
31	CA	2432	A	2.2
31	CA	2679	A	2.2
33	CF	176	PRO	2.2
54	DA	1098	A	2.2
8	BH	26	THR	2.2
16	AP	50	THR	2.2
18	BR	71	THR	2.2
30	CD	35	THR	2.2
2	BB	70	VAL	2.2
2	BB	163	VAL	2.2
7	BG	104	ILE	2.2
9	AI	55	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
9	BI	55	VAL	2.2
11	BK	23	ILE	2.2
13	AM	43	VAL	2.2
13	BM	60	VAL	2.2
17	AQ	5	ILE	2.2
35	DH	3	VAL	2.2
36	DJ	49	ILE	2.2
37	CK	55	ILE	2.2
36	DJ	16	GLY	2.2
39	CM	110	VAL	2.2
49	CW	30	ILE	2.2
16	BP	37	GLY	2.2
46	CT	91	GLY	2.2
47	CU	63	VAL	2.2
38	CL	93	GLN	2.2
13	BM	23	TYR	2.2
2	AB	162	PHE	2.2
9	AI	11	ARG	2.2
10	BJ	13	PHE	2.2
11	BK	98	ARG	2.2
19	BS	41	PHE	2.2
19	BS	74	PHE	2.2
25	C4	8	ARG	2.2
46	CT	18	ARG	2.2
48	CV	96	PHE	2.2
1	AA	462	G	2.2
1	AA	1253	G	2.2
1	BA	227	G	2.2
1	BA	480	U	2.2
1	BA	606	G	2.2
1	BA	989	U	2.2
1	BA	1048	G	2.2
1	BA	1121	U	2.2
1	BA	1286	U	2.2
5	BE	53	ALA	2.2
7	BG	46	ALA	2.2
11	BK	68	GLU	2.2
14	BN	89	MET	2.2
28	CB	67	G	2.2
31	CA	24	G	2.2
31	CA	283	G	2.2
31	CA	290	U	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	296	U	2.2
31	CA	399	U	2.2
31	CA	939	G	2.2
31	CA	1099	G	2.2
31	CA	1482	G	2.2
31	CA	1483	G	2.2
31	CA	1613	G	2.2
31	CA	1662	U	2.2
31	CA	1863	G	2.2
31	CA	1878	G	2.2
31	CA	2034	U	2.2
31	CA	2093	G	2.2
31	CA	2265	U	2.2
31	CA	2277	G	2.2
31	CA	2348	U	2.2
31	CA	2505	G	2.2
31	CA	2686	G	2.2
31	CA	2698	U	2.2
54	DA	1061	U	2.2
54	DA	1065	U	2.2
54	DA	2112	G	2.2
54	DA	2190	G	2.2
12	BL	81	LEU	2.2
14	BN	51	LEU	2.2
39	DM	95	LEU	2.2
1	AA	43	C	2.2
1	AA	87	C	2.2
1	AA	990	C	2.2
1	AA	1097	C	2.2
1	BA	183	C	2.2
1	BA	611	C	2.2
1	BA	1051	C	2.2
1	BA	1109	C	2.2
21	BU	46	LYS	2.2
21	BU	54	LYS	2.2
28	CB	4	C	2.2
31	CA	461	C	2.2
31	CA	1075	C	2.2
31	CA	1428	C	2.2
31	CA	1816	C	2.2
31	CA	2540	C	2.2
31	CA	2626	C	2.2

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Mol	Chain	Res	Type	RSRZ
34	CG	6	LYS	2.2
36	DJ	97	LYS	2.2
13	AM	10	PRO	2.2
30	CD	152	PRO	2.2
1	BA	51	A	2.2
1	BA	1289	A	2.2
6	AF	71	ILE	2.2
6	BF	96	VAL	2.2
7	BG	89	VAL	2.2
7	BG	141	VAL	2.2
12	BL	63	VAL	2.2
13	BM	65	VAL	2.2
30	CD	24	VAL	2.2
31	CA	374	A	2.2
31	CA	384	A	2.2
31	CA	861	A	2.2
31	CA	1189	A	2.2
31	CA	1246	A	2.2
32	CE	53	THR	2.2
32	CE	149	ILE	2.2
33	CF	132	VAL	2.2
34	CG	15	VAL	2.2
35	DH	19	VAL	2.2
37	CK	101	ILE	2.2
49	CW	29	ILE	2.2
54	DA	404[A]	A	2.2
54	DA	2211	A	2.2
27	C0	33	GLY	2.2
32	CE	71	GLY	2.2
36	DJ	85	GLY	2.2
40	CN	23	GLY	2.2
44	CR	43	GLY	2.2
3	BC	6	HIS	2.2
48	CV	45	HIS	2.2
48	CV	54	GLN	2.2
52	CZ	25	GLN	2.2
12	AL	5	ASN	2.2
14	BN	75	ARG	2.2
19	AS	37	ARG	2.2
21	BU	33	ARG	2.2
30	CD	167	ASN	2.2
33	CF	143	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
37	CK	95	ARG	2.2
40	CN	17	ASN	2.2
48	CV	40	ASN	2.2
36	DJ	17	MET	2.2
47	CU	24	MET	2.2
7	BG	150	ALA	2.2
9	AI	121	ALA	2.2
16	BP	72	ALA	2.2
27	C0	50	ALA	2.2
36	DJ	27	ALA	2.2
53	DI	110	ALA	2.2
53	DI	127	ALA	2.2
3	BC	12	LEU	2.2
14	AN	46	LEU	2.2
20	AT	86	LEU	2.2
1	AA	218	U	2.2
1	BA	610	U	2.2
1	BA	1463	U	2.2
3	BC	38	LYS	2.2
3	BC	62	LYS	2.2
5	BE	159	LYS	2.2
31	CA	589	U	2.2
31	CA	1720	U	2.2
31	CA	1995	U	2.2
33	DF	134	GLU	2.2
41	CO	35	LYS	2.2
52	DZ	8	GLU	2.2
54	DA	1058	U	2.2
1	BA	293	G	2.2
1	BA	705	G	2.2
1	BA	971	G	2.2
1	BA	1015	G	2.2
1	BA	1272	G	2.2
1	BA	1435	G	2.2
1	BA	1486	G	2.2
28	CB	96	G	2.2
31	CA	48	G	2.2
31	CA	266	G	2.2
31	CA	450	G	2.2
31	CA	524	G	2.2
31	CA	604	G	2.2
31	CA	1022	G	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1041	G	2.2
31	CA	1193	G	2.2
31	CA	1334	G	2.2
31	CA	1500	G	2.2
31	CA	1674	G	2.2
34	CG	8	PRO	2.2
48	CV	48	PRO	2.2
54	DA	1106	G	2.2
54	DA	2148	G	2.2
1	AA	1320	C	2.2
28	CB	8	C	2.2
31	CA	192	C	2.2
31	CA	817	C	2.2
31	CA	853	C	2.2
31	CA	865	C	2.2
31	CA	964	C	2.2
31	CA	1270	C	2.2
31	CA	1793	C	2.2
31	CA	2145	C	2.2
31	CA	2703	C	2.2
54	DA	1732	C	2.2
14	AN	30	ILE	2.2
15	AO	11	ILE	2.2
34	DG	24	ILE	2.2
39	DM	101	ILE	2.2
39	DM	103	ILE	2.2
43	CQ	4	ILE	2.2
43	CQ	50	ILE	2.2
44	CR	74	ILE	2.2
46	CT	12	SER	2.2
48	CV	98	SER	2.2
51	CY	2	SER	2.2
7	AG	69	VAL	2.2
15	BO	75	VAL	2.2
19	AS	67	VAL	2.2
32	CE	126	VAL	2.2
40	CN	135	VAL	2.2
50	CX	71	VAL	2.2
7	AG	38	THR	2.1
7	BG	132	GLY	2.1
23	C2	4	GLY	2.1
20	BT	20	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	AA	935	A	2.1
1	BA	120	A	2.1
1	BA	143	A	2.1
2	AB	227	GLN	2.1
14	AN	49	GLN	2.1
21	BU	37	PHE	2.1
31	CA	28	A	2.1
31	CA	526	A	2.1
31	CA	529	A	2.1
31	CA	661	A	2.1
31	CA	1142	A	2.1
31	CA	1477	A	2.1
31	CA	2080	A	2.1
31	CA	2439	A	2.1
33	CF	71	ARG	2.1
47	CU	12	ARG	2.1
5	AE	111	MET	2.1
19	AS	66	MET	2.1
34	CG	151	TYR	2.1
42	DP	1	MET	2.1
2	AB	57	LEU	2.1
2	BB	57	LEU	2.1
3	BC	61	ALA	2.1
4	AD	45	LYS	2.1
8	BH	35	ALA	2.1
10	AJ	87	LEU	2.1
13	AM	114	LYS	2.1
13	BM	80	LEU	2.1
14	BN	36	ALA	2.1
19	AS	7	LYS	2.1
19	AS	15	LEU	2.1
20	BT	44	LYS	2.1
21	BU	50	ALA	2.1
30	CD	56	LYS	2.1
34	CG	37	LEU	2.1
36	CJ	27	ALA	2.1
45	CS	97	LYS	2.1
46	CT	33	LEU	2.1
48	CV	92	LYS	2.1
45	CS	23	GLU	2.1
1	AA	463	U	2.1
1	AA	1009	U	2.1

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Mol	Chain	Res	Type	RSRZ
1	BA	1445	U	2.1
31	CA	87	U	2.1
31	CA	243	U	2.1
31	CA	588	U	2.1
31	CA	1198	U	2.1
31	CA	1400	U	2.1
31	CA	1442	U	2.1
31	CA	2017	U	2.1
31	CA	2092	U	2.1
54	DA	2130	U	2.1
2	AB	158	PRO	2.1
34	CG	112	PRO	2.1
48	DV	48	PRO	2.1
29	CC	74	ILE	2.1
2	BB	80	VAL	2.1
7	AG	91	VAL	2.1
12	BL	98	VAL	2.1
13	BM	16	VAL	2.1
15	AO	27	VAL	2.1
26	C5	20	ASP	2.1
30	CD	108	ASP	2.1
30	CD	176	ASP	2.1
34	CG	23	VAL	2.1
9	AI	15	SER	2.1
30	CD	163	GLY	2.1
44	CR	77	SER	2.1
1	AA	1325	C	2.1
1	BA	82	G	2.1
1	BA	126	G	2.1
1	BA	144	G	2.1
1	BA	337	G	2.1
1	BA	369	G	2.1
1	BA	934	C	2.1
1	BA	1057	G	2.1
1	BA	1237	C	2.1
1	BA	1459	G	2.1
12	BL	40	THR	2.1
13	AM	102	THR	2.1
22	C1	52	ARG	2.1
28	CB	41	G	2.1
31	CA	298	G	2.1
31	CA	357	C	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	468	G	2.1
31	CA	838	C	2.1
31	CA	914	G	2.1
31	CA	961	C	2.1
31	CA	971	G	2.1
31	CA	987	C	2.1
31	CA	1376	C	2.1
31	CA	1389	G	2.1
31	CA	1416	G	2.1
31	CA	1512	C	2.1
31	CA	1611	C	2.1
31	CA	2040	G	2.1
31	CA	2144	G	2.1
31	CA	2228	G	2.1
31	CA	2396	G	2.1
31	CA	2437	G	2.1
31	CA	2606	C	2.1
31	CA	2619	C	2.1
31	CA	2892	G	2.1
46	CT	92	ARG	2.1
50	CX	57	HIS	2.1
51	CY	27	ARG	2.1
54	DA	359	G	2.1
9	BI	103	PHE	2.1
2	BB	214	LEU	2.1
7	AG	50	LEU	2.1
9	BI	60	LYS	2.1
1	AA	77	A	2.1
1	AA	172	A	2.1
1	AA	412	A	2.1
1	AA	1000	A	2.1
1	BA	309	A	2.1
1	BA	1431	A	2.1
1	BA	1447	A	2.1
7	BG	127	ALA	2.1
9	AI	44	ALA	2.1
12	AL	13	ALA	2.1
14	AN	44	ALA	2.1
14	AN	74	LEU	2.1
15	BO	7	ALA	2.1
17	BQ	44	LEU	2.1
17	BQ	75	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
20	BT	71	LYS	2.1
36	DJ	72	LYS	2.1
36	DJ	87	LYS	2.1
40	CN	8	LYS	2.1
36	CJ	115	ALA	2.1
36	CJ	133	ALA	2.1
39	CM	113	ALA	2.1
40	CN	33	LEU	2.1
47	CU	68	LYS	2.1
47	DU	93	LEU	2.1
49	CW	86	LEU	2.1
53	DI	97	LYS	2.1
28	CB	66	A	2.1
28	CB	73	A	2.1
31	CA	64	A	2.1
31	CA	119	A	2.1
31	CA	449	A	2.1
31	CA	1276	A	2.1
31	CA	1553	A	2.1
31	CA	1773	A	2.1
31	CA	2015	A	2.1
31	CA	2309	A	2.1
31	CA	2814	A	2.1
41	CO	61	ALA	2.1
50	CX	33	ALA	2.1
54	DA	2097	A	2.1
27	C0	49	ASN	2.1
35	CH	28	ASN	2.1
9	BI	112	GLU	2.1
29	DC	236	GLU	2.1
43	DQ	102	GLU	2.1
44	CR	89	GLU	2.1
47	DU	56	GLU	2.1
1	AA	5	U	2.1
1	AA	93	U	2.1
1	AA	1308	U	2.1
1	BA	1420	U	2.1
12	BL	28	PRO	2.1
28	CB	87	U	2.1
31	CA	4	U	2.1
31	CA	112	U	2.1
31	CA	200	U	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	286	U	2.1
31	CA	546	U	2.1
31	CA	1203	U	2.1
31	CA	2356	U	2.1
31	CA	2548	U	2.1
31	CA	2849	U	2.1
31	CA	2903	U	2.1
36	DJ	22	PRO	2.1
54	DA	1176	U	2.1
2	BB	40	ILE	2.1
12	BL	82	ILE	2.1
34	CG	43	VAL	2.1
36	DJ	98	VAL	2.1
38	CL	103	VAL	2.1
43	CQ	86	VAL	2.1
46	CT	50	VAL	2.1
49	CW	64	VAL	2.1
53	DI	85	VAL	2.1
6	AF	9	MET	2.1
10	AJ	7	ARG	2.1
16	BP	56	ARG	2.1
22	C1	51	GLY	2.1
30	CD	120	GLY	2.1
35	DH	97	ARG	2.1
38	CL	68	GLY	2.1
42	DP	96	GLY	2.1
45	CS	1	MET	2.1
46	CT	109	ASP	2.1
53	DI	115	GLY	2.1
2	AB	138	THR	2.1
8	BH	55	THR	2.1
20	BT	23	SER	2.1
30	CD	199	SER	2.1
32	CE	92	HIS	2.1
34	CG	52	PHE	2.1
50	CX	58	THR	2.1
50	DX	10	THR	2.1
4	AD	40	GLN	2.1
9	BI	13	LYS	2.1
12	BL	116	LYS	2.1
19	BS	7	LYS	2.1
21	AU	49	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
21	BU	49	LYS	2.1
27	C0	21	LYS	2.1
33	CF	120	LYS	2.1
46	CT	28	LYS	2.1
10	AJ	52	LEU	2.1
12	BL	7	LEU	2.1
13	AM	56	LEU	2.1
23	C2	11	LEU	2.1
35	DH	75	LEU	2.1
41	CO	65	LEU	2.1
43	CQ	114	LEU	2.1
53	DI	81	LEU	2.1
1	AA	488	C	2.1
1	BA	1214	C	2.1
3	AC	24	ALA	2.1
12	BL	23	ALA	2.1
16	BP	58	ALA	2.1
27	C0	2	ALA	2.1
28	CB	11	C	2.1
28	CB	30	C	2.1
31	CA	97	C	2.1
31	CA	334	C	2.1
31	CA	398	C	2.1
31	CA	462	C	2.1
31	CA	1298	C	2.1
31	CA	2232	C	2.1
31	CA	2338	C	2.1
31	CA	2501	C	2.1
31	CA	2507	C	2.1
31	CA	2853	C	2.1
31	CA	2880	C	2.1
46	CT	21	ALA	2.1
48	CV	76	ALA	2.1
50	CX	49	ALA	2.1
54	DA	544	C	2.1
3	AC	168	TYR	2.1
14	BN	20	TYR	2.1
1	BA	191	G	2.1
1	BA	450	G	2.1
1	BA	1187	G	2.1
1	BA	1260	G	2.1
1	BA	1475	G	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	43	G	2.1
31	CA	178	G	2.1
31	CA	1418	G	2.1
31	CA	1756	G	2.1
31	CA	2038	G	2.1
31	CA	2083	G	2.1
31	CA	2112	G	2.1
31	CA	2138	G	2.1
31	CA	2234	G	2.1
31	CA	2253	G	2.1
31	CA	2831	G	2.1
31	CA	2852	G	2.1
54	DA	287	G	2.1
14	BN	62	ASN	2.1
16	BP	34	GLU	2.1
34	DG	104	ASN	2.1
1	BA	78	A	2.1
1	BA	630	A	2.1
1	BA	1111	A	2.1
1	BA	1446	A	2.1
31	CA	217	A	2.1
31	CA	1204	A	2.1
31	CA	1640	A	2.1
31	CA	1679	A	2.1
31	CA	2430	A	2.1
54	DA	1095	A	2.1
54	DA	2170	A	2.1
54	DA	2309	A	2.1
54	DA	2887[A]	A	2.1
10	BJ	43	PRO	2.1
12	AL	122	PRO	2.1
3	BC	182	ILE	2.1
26	D5	26	ILE	2.1
30	CD	27	ILE	2.1
41	CO	52	ILE	2.1
1	BA	70	U	2.1
1	BA	1010	U	2.1
31	CA	1712	U	2.1
31	CA	2329	U	2.1
54	DA	1173	U	2.1
2	AB	92	VAL	2.1
5	AE	74	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
35	DH	21	VAL	2.1
53	DI	50	VAL	2.1
2	AB	49	MET	2.1
2	BB	149	GLY	2.1
3	AC	172	ARG	2.1
12	BL	69	GLY	2.1
14	AN	95	GLY	2.1
24	C3	17	GLY	2.1
24	C3	19	ARG	2.1
29	DC	237	GLY	2.1
30	CD	19	GLY	2.1
32	CE	100	MET	2.1
46	CT	88	ARG	2.1
50	CX	34	GLY	2.1
51	CY	55	GLY	2.1
10	AJ	82	LYS	2.1
21	BU	19	PHE	2.1
39	CM	66	PHE	2.1
33	CF	18	THR	2.1
34	DG	114	ASP	2.1
52	CZ	44	LYS	2.1
3	AC	178	LEU	2.1
4	AD	153	SER	2.1
10	AJ	10	LEU	2.1
12	BL	57	LEU	2.1
13	AM	83	LEU	2.1
21	BU	16	LEU	2.1
30	CD	164	GLN	2.1
30	CD	175	LEU	2.1
46	CT	69	LEU	2.1
47	CU	48	GLN	2.1
48	DV	52	LEU	2.1
52	CZ	55	THR	2.1
35	CH	133	GLN	2.1
3	AC	50	ALA	2.1
14	BN	88	ALA	2.1
17	AQ	82	ALA	2.1
19	AS	50	ALA	2.1
32	CE	160	ALA	2.1
33	CF	107	ALA	2.1
33	CF	119	ALA	2.1
39	CM	9	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
49	CW	54	ALA	2.1
52	CZ	3	ALA	2.1
47	CU	84	TYR	2.1
1	AA	1533	C	2.1
1	BA	48	C	2.1
1	BA	58	C	2.1
1	BA	311	C	2.1
1	BA	1223	C	2.1
1	BA	1234	C	2.1
1	BA	1314	C	2.1
31	CA	436	C	2.1
31	CA	691	C	2.1
31	CA	816	C	2.1
31	CA	1804	C	2.1
31	CA	1843	C	2.1
31	CA	2301	C	2.1
31	CA	2332	C	2.1
31	CA	2755	C	2.1
47	CU	18	GLU	2.1
10	BJ	55	PRO	2.1
37	CK	110	PRO	2.1
47	CU	14	PRO	2.1
4	AD	28	ILE	2.1
35	DH	94	ILE	2.1
36	CJ	49	ILE	2.1
1	AA	1171	A	2.1
1	AA	1529	G	2.1
1	BA	148	G	2.1
1	BA	954	G	2.1
1	BA	1153	G	2.1
1	BA	1186	G	2.1
1	BA	1306	A	2.1
28	CB	75	G	2.1
31	CA	370	G	2.1
31	CA	1069	A	2.1
31	CA	1471	G	2.1
31	CA	1568	G	2.1
31	CA	1608	A	2.1
31	CA	1659	G	2.1
31	CA	2141	G	2.1
31	CA	2225	A	2.1
31	CA	2597	G	2.1

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Mol	Chain	Res	Type	RSRZ
54	DA	1583	A	2.1
54	DA	1731	G	2.1
54	DA	2307	G	2.1
3	AC	173	VAL	2.1
8	BH	72	VAL	2.1
13	BM	85	CYS	2.1
38	CL	69	VAL	2.1
1	BA	154	U	2.1
5	AE	54	ARG	2.1
9	AI	41	ARG	2.1
14	AN	81	ARG	2.1
14	BN	69	ARG	2.1
17	BQ	40	ARG	2.1
32	CE	188	MET	2.1
36	DJ	125	MET	2.1
38	CL	20	MET	2.1
28	CB	89	U	2.1
31	CA	135	U	2.1
31	CA	397	U	2.1
31	CA	569	U	2.1
31	CA	571	U	2.1
31	CA	827	U	2.1
31	CA	1018	U	2.1
31	CA	1602	U	2.1
31	CA	1751	U	2.1
31	CA	2229	U	2.1
31	CA	2493	U	2.1
54	DA	545	U	2.1
54	DA	653	U	2.1
54	DA	2166	U	2.1
54	DA	2189	U	2.1
7	AG	35	LYS	2.1
29	CC	207	LYS	2.1
30	CD	158	GLY	2.1
35	DH	35	LYS	2.1
36	CJ	45	LYS	2.1
49	DW	34	LYS	2.1
2	BB	39	HIS	2.1
17	AQ	28	PHE	2.1
32	CE	124	PHE	2.1
29	CC	81	LEU	2.0
32	CE	157	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
32	DE	165	HIS	2.1
37	CK	80	HIS	2.1
19	BS	48	THR	2.0
32	CE	140	ASP	2.0
38	CL	37	ASP	2.0
40	CN	7	THR	2.0
46	CT	34	ASP	2.0
47	DU	91	GLN	2.0
48	CV	18	ASP	2.0
4	BD	149	ALA	2.0
7	BG	41	SER	2.0
10	AJ	29	ALA	2.0
10	BJ	101	SER	2.0
13	BM	49	SER	2.0
24	C3	15	SER	2.0
27	C0	43	ALA	2.0
34	CG	58	TYR	2.0
2	AB	169	GLU	2.0
7	AG	58	GLU	2.0
47	CU	4	GLU	2.0
6	BF	51	ILE	2.0
8	AH	85	ILE	2.0
10	AJ	100	ILE	2.0
23	C2	41	PRO	2.0
36	DJ	74	PRO	2.0
38	CL	43	ILE	2.0
40	CN	63	ILE	2.0
50	CX	74	PRO	2.0
1	AA	214	C	2.0
1	BA	879	C	2.0
1	BA	1027	C	2.0
3	BC	56	VAL	2.0
6	AF	60	VAL	2.0
31	CA	414	C	2.0
31	CA	965	C	2.0
31	CA	2339	C	2.0
31	CA	2456	C	2.0
31	CA	2575	C	2.0
31	CA	2723	C	2.0
10	BJ	5	ARG	2.0
13	BM	101	ARG	2.0
23	C2	44	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
35	CH	123	ARG	2.0
35	DH	121	VAL	2.0
36	CJ	61	VAL	2.0
37	CK	62	VAL	2.0
44	CR	53	ARG	2.0
47	CU	53	VAL	2.0
2	BB	105	LYS	2.0
8	BH	87	LYS	2.0
10	BJ	30	LYS	2.0
13	BM	31	LYS	2.0
20	BT	9	LYS	2.0
23	C2	50	LYS	2.0
39	DM	96	LYS	2.0
52	DZ	2	LYS	2.0
1	AA	1332	A	2.0
1	BA	1271	A	2.0
1	BA	1357	A	2.0
1	BA	1493	A	2.0
9	BI	26	GLY	2.0
30	CD	191	GLY	2.0
31	CA	84	A	2.0
31	CA	430	A	2.0
31	CA	471	A	2.0
31	CA	819	A	2.0
31	CA	1264	A	2.0
31	CA	1284	A	2.0
31	CA	1420	A	2.0
31	CA	1711	A	2.0
47	CU	71	GLY	2.0
54	DA	1067	A	2.0
1	AA	1307	U	2.0
1	BA	125	U	2.0
1	BA	387	U	2.0
2	BB	97	LEU	2.0
6	BF	74	LEU	2.0
15	AO	57	LEU	2.0
33	DF	122	PHE	2.0
31	CA	114	U	2.0
1	AA	1139	G	2.0
1	BA	127	G	2.0
1	BA	128	G	2.0
1	BA	953	G	2.0

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Mol	Chain	Res	Type	RSRZ
7	BG	142	HIS	2.0
31	CA	2617	U	2.0
31	CA	2622	U	2.0
37	CK	114	LEU	2.0
28	CB	81	G	2.0
31	CA	58	G	2.0
31	CA	70	G	2.0
31	CA	493	G	2.0
31	CA	578	G	2.0
31	CA	681	G	2.0
31	CA	778	G	2.0
31	CA	834	G	2.0
31	CA	966	G	2.0
31	CA	976	G	2.0
31	CA	1036	G	2.0
31	CA	1087	G	2.0
31	CA	1166	G	2.0
31	CA	1227	G	2.0
31	CA	1256	G	2.0
31	CA	1857	G	2.0
31	CA	1875	G	2.0
31	CA	2330	G	2.0
31	CA	2578	G	2.0
31	CA	2668	G	2.0
2	BB	61	ALA	2.0
10	AJ	35	GLN	2.0
13	BM	55	THR	2.0
30	CD	196	ALA	2.0
32	CE	171	ASP	2.0
35	CH	36	ALA	2.0
35	DH	98	ASP	2.0
36	CJ	77	ALA	2.0
37	CK	29	ALA	2.0
52	CZ	51	ALA	2.0
7	BG	45	SER	2.0
9	BI	96	SER	2.0
11	BK	55	SER	2.0
15	BO	2	SER	2.0
29	CC	40	SER	2.0
39	CM	12	SER	2.0
3	BC	42	TYR	2.0
5	BE	55	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
13	AM	23	TYR	2.0
33	CF	8	TYR	2.0
7	AG	12	ILE	2.0
7	AG	93	PRO	2.0
8	BH	126	ILE	2.0
19	BS	59	PRO	2.0
25	C4	32	ILE	2.0
36	DJ	101	ILE	2.0
37	CK	98	GLU	2.0
45	CS	101	ILE	2.0
29	CC	44	ASN	2.0
30	CD	165	MET	2.0
46	DT	82	MET	2.0
5	AE	88	VAL	2.0
5	BE	136	VAL	2.0
6	BF	79	ARG	2.0
7	BG	149	LYS	2.0
12	BL	8	VAL	2.0
15	AO	89	ARG	2.0
16	AP	20	VAL	2.0
17	BQ	78	VAL	2.0
19	BS	70	LYS	2.0
29	CC	4	VAL	2.0
33	CF	15	LYS	2.0
38	CL	54	LYS	2.0
38	CL	108	ARG	2.0
49	CW	83	LYS	2.0
49	CW	85	LYS	2.0
30	CD	80	TRP	2.0
2	BB	148	LEU	2.0
2	BB	162	PHE	2.0
10	BJ	95	GLY	2.0
13	AM	95	LEU	2.0
33	CF	138	PHE	2.0
35	CH	12	LEU	2.0
35	DH	30	LEU	2.0
35	DH	95	GLY	2.0
36	DJ	32	GLY	2.0
38	CL	118	LEU	2.0
43	CQ	43	PHE	2.0
43	DQ	114	LEU	2.0
44	CR	36	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
45	CS	25	LEU	2.0
50	CX	42	GLY	2.0
1	AA	1028	C	2.0
1	AA	1234	C	2.0
1	BA	47	C	2.0
1	BA	90	C	2.0
1	BA	193	C	2.0
1	BA	1128	C	2.0
1	BA	1149	C	2.0
1	BA	1397	C	2.0
21	AU	56	HIS	2.0
21	BU	56	HIS	2.0
31	CA	302	C	2.0
31	CA	487	C	2.0
31	CA	985	C	2.0
31	CA	1229	C	2.0
31	CA	1315	C	2.0
31	CA	2350	C	2.0
31	CA	2422	C	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	2MG	BA	966	24/25	0.63	0.15	149,156,167,168	0
31	PSU	CA	1911	20/21	0.70	0.11	127,137,139,140	0
31	PSU	CA	1917	20/21	0.70	0.13	120,125,134,134	0
31	2MA	CA	2503	23/24	0.71	0.24	107,109,110,110	0
1	2MG	BA	1207	24/25	0.72	0.13	150,152,156,160	0
1	5MC	BA	967	21/22	0.73	0.16	149,158,161,161	0
31	PSU	CA	746	20/21	0.76	0.16	116,118,119,120	0
31	3TD	CA	1915	21/22	0.76	0.11	149,155,157,158	0
31	PSU	CA	2504	20/21	0.77	0.18	93,103,106,106	0
31	PSU	CA	2580	20/21	0.78	0.15	93,99,101,101	0
31	PSU	CA	955	20/21	0.81	0.16	100,105,108,108	0
31	PSU	CA	2457	20/21	0.83	0.13	96,97,99,99	0
31	6MZ	CA	1618	23/24	0.83	0.17	134,138,143,145	0
31	6MZ	CA	2030	23/24	0.84	0.16	101,104,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	BA	516	20/21	0.85	0.11	80,89,91,94	0
54	3TD	DA	1915	21/22	0.85	0.12	105,110,116,117	0
30	MEQ	CD	150	9/11	0.86	0.20	92,98,133,136	0
31	5MU	CA	1939	21/22	0.86	0.16	70,77,78,80	0
54	PSU	DA	1917	20/21	0.86	0.10	80,84,91,91	0
40	4D4	CN	81	12/13	0.86	0.17	108,112,131,132	0
31	OMU	CA	2552	21/22	0.87	0.23	88,92,94,95	0
12	D2T	AL	89	10/11	0.87	0.14	60,63,71,72	0
1	5MC	BA	1407	21/22	0.87	0.14	98,109,111,115	0
1	2MG	BA	1516	24/25	0.87	0.13	79,86,93,95	0
12	D2T	BL	89	10/11	0.87	0.16	83,85,93,94	0
31	OMG	CA	2251	24/25	0.88	0.16	85,90,93,93	0
31	5MC	CA	1962	21/22	0.88	0.13	70,77,80,82	0
31	OMC	CA	2498	21/22	0.88	0.18	91,94,95,95	0
1	2MG	AA	1207	24/25	0.88	0.11	99,103,105,108	0
31	G7M	CA	2069	24/25	0.88	0.20	102,104,108,109	0
31	2MG	CA	1835	24/25	0.89	0.14	71,73,76,77	0
31	1MG	CA	745	24/25	0.89	0.15	103,107,111,114	0
1	4OC	BA	1402	22/23	0.89	0.12	74,77,79,80	0
31	PSU	CA	2605	20/21	0.89	0.12	79,81,83,84	0
31	5MU	CA	747	21/22	0.89	0.13	116,120,122,123	0
1	G7M	BA	527	24/25	0.89	0.12	70,73,78,79	0
1	UR3	BA	1498	21/22	0.89	0.12	84,87,94,94	0
31	2MG	CA	2445	24/25	0.90	0.21	97,100,102,102	0
1	MA6	BA	1518	24/25	0.90	0.13	84,86,92,93	0
54	PSU	DA	1911	20/21	0.90	0.09	83,90,91,92	0
1	2MG	AA	966	24/25	0.91	0.12	79,84,91,91	0
30	MEQ	DD	150[B]	10/11	0.92	0.13	25,29,41,41	10
1	G7M	AA	527	24/25	0.92	0.10	55,58,62,63	0
1	PSU	AA	516	20/21	0.92	0.10	76,78,82,82	0
1	MA6	BA	1519	24/25	0.92	0.12	80,82,87,88	0
30	MEQ	DD	150[A]	10/11	0.92	0.13	17,22,27,29	10
1	5MC	AA	967	21/22	0.93	0.12	74,88,90,91	0
54	PSU	DA	2604	20/21	0.94	0.10	36,42,53,53	0
40	4D4	DN	81[A]	12/13	0.94	0.15	30,36,49,50	9
40	4D4	DN	81[B]	12/13	0.94	0.15	26,28,31,32	9
1	5MC	AA	1407	21/22	0.95	0.08	51,52,54,55	0
1	UR3	AA	1498	21/22	0.95	0.09	54,56,61,63	0
1	MA6	AA	1518	24/25	0.95	0.10	50,54,56,57	0
54	5MU	DA	1939	21/22	0.96	0.09	31,36,38,39	0
54	5MC	DA	1962	21/22	0.96	0.09	44,46,49,50	0
54	OMU	DA	2552	21/22	0.96	0.10	35,37,44,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	2MG	DA	1835	24/25	0.96	0.09	53,55,56,58	0
54	PSU	DA	2605	20/21	0.96	0.09	33,42,46,46	0
1	MA6	AA	1519	24/25	0.96	0.10	53,56,61,65	0
1	2MG	AA	1516	24/25	0.96	0.10	52,54,56,57	0
1	4OC	AA	1402	22/23	0.96	0.08	52,59,61,62	0
54	PSU	DA	2580	20/21	0.97	0.09	24,30,36,37	0
54	5MU	DA	747	21/22	0.97	0.06	26,28,32,37	0
54	2MG	DA	2445	24/25	0.97	0.09	14,25,28,29	0
54	2MA	DA	2503	23/24	0.97	0.08	26,42,46,47	0
54	PSU	DA	2504	20/21	0.97	0.14	45,53,56,57	0
54	PSU	DA	746	20/21	0.97	0.07	28,30,33,36	0
54	PSU	DA	955	20/21	0.98	0.07	25,26,29,30	0
54	6MZ	DA	1618	23/24	0.98	0.07	25,28,31,33	0
54	6MZ	DA	2030	23/24	0.98	0.06	13,23,28,28	0
54	G7M	DA	2069	24/25	0.98	0.08	24,30,37,38	0
54	OMG	DA	2251	24/25	0.98	0.07	23,27,30,30	0
54	1MG	DA	745	24/25	0.98	0.05	19,26,31,33	0
54	H2U	DA	2449	20/21	0.98	0.08	24,27,28,32	0
54	PSU	DA	2457	20/21	0.98	0.06	20,28,30,31	0
54	OMC	DA	2498	21/22	0.98	0.06	21,22,27,29	0

### 6.3 Carbohydrates

There are no monosaccharides in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3129	1/1	-0.09	0.38	118,118,118,118	0
55	MG	CA	3145	1/1	-0.07	0.34	234,234,234,234	0
55	MG	CA	3109	1/1	-0.06	0.37	175,175,175,175	0
55	MG	CA	3138	1/1	-0.05	0.44	125,125,125,125	0
55	MG	AA	1622	1/1	0.07	0.40	119,119,119,119	0
55	MG	DA	3168	1/1	0.12	0.34	109,109,109,109	0
55	MG	CA	3004	1/1	0.13	0.27	243,243,243,243	0
55	MG	BA	1642	1/1	0.16	0.45	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3123	1/1	0.17	0.21	199,199,199,199	0
55	MG	CA	3131	1/1	0.18	0.30	145,145,145,145	0
55	MG	CA	3060	1/1	0.23	0.20	256,256,256,256	0
55	MG	CA	3140	1/1	0.27	0.48	91,91,91,91	0
55	MG	BA	1638	1/1	0.30	0.43	175,175,175,175	0
55	MG	CA	3121	1/1	0.31	0.44	125,125,125,125	0
55	MG	CA	3153	1/1	0.31	0.34	138,138,138,138	0
55	MG	CA	3037	1/1	0.31	0.18	256,256,256,256	0
55	MG	CA	3025	1/1	0.33	0.30	180,180,180,180	0
55	MG	CA	3139	1/1	0.34	0.30	128,128,128,128	0
55	MG	CA	3001	1/1	0.35	0.23	258,258,258,258	0
55	MG	CA	3076	1/1	0.40	0.22	246,246,246,246	0
55	MG	CA	3146	1/1	0.40	1.20	76,76,76,76	1
55	MG	CA	3110	1/1	0.41	0.40	141,141,141,141	0
55	MG	CA	3033	1/1	0.41	0.24	246,246,246,246	0
55	MG	CA	3132	1/1	0.42	0.33	129,129,129,129	0
55	MG	CA	3074	1/1	0.42	0.26	243,243,243,243	0
55	MG	CA	3059	1/1	0.43	0.17	240,240,240,240	0
55	MG	CA	3103	1/1	0.44	0.21	260,260,260,260	0
55	MG	BA	1629	1/1	0.45	0.36	124,124,124,124	0
55	MG	CA	3066	1/1	0.46	0.13	284,284,284,284	0
55	MG	BA	1643	1/1	0.46	0.20	134,134,134,134	0
55	MG	CA	3122	1/1	0.47	0.33	182,182,182,182	0
55	MG	CA	3151	1/1	0.47	0.26	209,209,209,209	0
55	MG	CA	3118	1/1	0.47	0.45	123,123,123,123	0
55	MG	CA	3155	1/1	0.47	0.22	240,240,240,240	0
55	MG	BA	1605	1/1	0.47	0.16	250,250,250,250	0
55	MG	CA	3128	1/1	0.49	0.35	135,135,135,135	0
55	MG	CA	3119	1/1	0.50	0.20	188,188,188,188	0
55	MG	CA	3130	1/1	0.51	0.24	101,101,101,101	0
55	MG	CA	3141	1/1	0.51	0.32	115,115,115,115	0
55	MG	AA	1608	1/1	0.54	0.40	97,97,97,97	0
55	MG	AA	1603	1/1	0.54	0.48	110,110,110,110	0
55	MG	CA	3007	1/1	0.55	0.19	175,175,175,175	0
55	MG	CA	3125	1/1	0.56	0.35	120,120,120,120	0
55	MG	CA	3116	1/1	0.56	0.43	101,101,101,101	0
55	MG	CA	3124	1/1	0.56	0.40	127,127,127,127	0
55	MG	CA	3147	1/1	0.56	0.68	80,80,80,80	1
55	MG	CA	3020	1/1	0.57	0.35	269,269,269,269	0
55	MG	AA	1606	1/1	0.58	0.44	108,108,108,108	0
55	MG	DA	3139	1/1	0.59	0.85	58,58,58,58	1
55	MG	CA	3006	1/1	0.59	0.11	242,242,242,242	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3002	1/1	0.60	0.32	278,278,278,278	0
55	MG	BA	1608	1/1	0.61	0.22	243,243,243,243	0
55	MG	BA	1641	1/1	0.61	0.27	98,98,98,98	0
55	MG	CA	3134	1/1	0.61	0.31	99,99,99,99	0
55	MG	CA	3072	1/1	0.62	0.28	255,255,255,255	0
55	MG	CA	3105	1/1	0.62	0.31	92,92,92,92	0
55	MG	AA	1628	1/1	0.63	0.19	142,142,142,142	0
55	MG	BA	1626	1/1	0.63	0.16	264,264,264,264	0
55	MG	DA	3180	1/1	0.63	0.22	99,99,99,99	0
55	MG	CA	3031	1/1	0.64	0.16	257,257,257,257	0
55	MG	CA	3154	1/1	0.64	0.27	200,200,200,200	0
55	MG	CA	3127	1/1	0.64	0.18	85,85,85,85	0
55	MG	DA	3145	1/1	0.65	0.23	111,111,111,111	0
55	MG	CA	3133	1/1	0.65	0.26	194,194,194,194	0
55	MG	AA	1609	1/1	0.65	0.31	96,96,96,96	0
55	MG	CA	3013	1/1	0.66	0.20	251,251,251,251	0
55	MG	AA	1605	1/1	0.66	0.46	97,97,97,97	0
55	MG	BA	1606	1/1	0.66	0.14	190,190,190,190	0
55	MG	CA	3046	1/1	0.66	0.30	228,228,228,228	0
55	MG	DA	3172	1/1	0.66	0.41	86,86,86,86	0
55	MG	CA	3030	1/1	0.66	0.14	128,128,128,128	0
55	MG	CA	3149	1/1	0.67	0.33	73,73,73,73	0
55	MG	CA	3009	1/1	0.67	0.18	217,217,217,217	0
55	MG	DB	207	1/1	0.67	0.26	99,99,99,99	0
55	MG	BA	1627	1/1	0.67	0.20	264,264,264,264	0
55	MG	CA	3114	1/1	0.68	0.30	102,102,102,102	0
55	MG	CA	3104	1/1	0.68	0.23	252,252,252,252	0
55	MG	AA	1661	1/1	0.68	0.20	182,182,182,182	0
55	MG	CA	3067	1/1	0.68	0.14	239,239,239,239	0
55	MG	CA	3061	1/1	0.68	0.16	227,227,227,227	0
55	MG	CA	3055	1/1	0.69	0.55	94,94,94,94	0
55	MG	AA	1626	1/1	0.69	0.39	104,104,104,104	0
55	MG	CA	3036	1/1	0.69	0.21	235,235,235,235	0
55	MG	DA	3176	1/1	0.69	0.33	91,91,91,91	0
55	MG	CA	3098	1/1	0.69	0.21	231,231,231,231	0
62	EDO	DA	3004	4/4	0.69	0.33	112,113,114,114	0
55	MG	AA	1654	1/1	0.70	0.30	241,241,241,241	0
55	MG	CA	3032	1/1	0.70	0.24	194,194,194,194	0
55	MG	DA	3159	1/1	0.70	0.27	74,74,74,74	0
55	MG	AA	1616	1/1	0.70	0.45	94,94,94,94	0
63	PGE	D1	102	10/10	0.70	0.34	89,92,93,93	0
55	MG	CA	3054	1/1	0.71	0.18	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MPD	DE	301	8/8	0.71	0.25	98,102,104,105	0
55	MG	BA	1631	1/1	0.71	0.26	151,151,151,151	0
55	MG	CA	3091	1/1	0.71	0.19	202,202,202,202	0
55	MG	DR	203	1/1	0.72	0.24	108,108,108,108	0
55	MG	CA	3021	1/1	0.72	0.35	182,182,182,182	0
55	MG	DA	3179	1/1	0.72	0.22	100,100,100,100	0
55	MG	AA	1601	1/1	0.72	0.59	100,100,100,100	0
55	MG	CA	3136	1/1	0.72	0.31	156,156,156,156	0
55	MG	CA	3117	1/1	0.72	0.28	85,85,85,85	0
55	MG	CA	3027	1/1	0.72	0.17	277,277,277,277	0
68	TRS	DA	3219	8/8	0.72	0.26	95,98,100,101	0
55	MG	AA	1614	1/1	0.73	0.31	126,126,126,126	0
55	MG	AA	1611	1/1	0.73	0.24	88,88,88,88	0
55	MG	CA	3062	1/1	0.73	0.22	196,196,196,196	0
55	MG	CA	3079	1/1	0.73	0.26	177,177,177,177	0
57	MPD	AA	1676	8/8	0.73	0.43	97,99,100,103	0
55	MG	DA	3147	1/1	0.73	0.36	98,98,98,98	0
55	MG	DA	3148	1/1	0.73	0.24	123,123,123,123	0
55	MG	AA	1617	1/1	0.73	0.38	93,93,93,93	0
67	GUN	DA	3210	11/11	0.73	0.19	66,68,71,71	0
55	MG	CA	3038	1/1	0.73	0.15	154,154,154,154	0
61	PEG	DQ	201	7/7	0.74	0.24	104,105,105,106	0
55	MG	DA	3167	1/1	0.74	0.33	80,80,80,80	0
55	MG	DB	209	1/1	0.74	0.35	87,87,87,87	0
66	ACY	DA	3196	4/4	0.74	0.27	79,80,80,80	0
55	MG	AA	1619	1/1	0.74	0.22	94,94,94,94	0
55	MG	AA	1679	1/1	0.74	0.19	163,163,163,163	0
58	PUT	AA	1672	6/6	0.75	0.42	98,98,100,101	0
55	MG	DA	3173	1/1	0.75	0.33	77,77,77,77	0
55	MG	CA	3106	1/1	0.75	0.35	83,83,83,83	0
55	MG	DA	3124	1/1	0.75	0.44	102,102,102,102	0
55	MG	CA	3137	1/1	0.75	0.23	95,95,95,95	0
55	MG	CA	3008	1/1	0.75	0.22	244,244,244,244	0
55	MG	C3	101	1/1	0.75	0.37	299,299,299,299	0
55	MG	DA	3153	1/1	0.76	0.41	100,100,100,100	0
55	MG	DA	3182	1/1	0.76	0.25	65,65,65,65	0
55	MG	BA	1640	1/1	0.76	0.48	101,101,101,101	0
55	MG	BA	1625	1/1	0.76	0.28	231,231,231,231	0
55	MG	AA	1624	1/1	0.76	0.28	92,92,92,92	0
58	PUT	AA	1674	6/6	0.76	0.33	88,90,91,91	0
55	MG	DA	3063	1/1	0.77	0.14	219,219,219,219	0
55	MG	CA	3144	1/1	0.77	0.19	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3053	1/1	0.77	0.10	134,134,134,134	0
55	MG	CA	3120	1/1	0.77	0.25	75,75,75,75	0
55	MG	CA	3070	1/1	0.77	0.10	188,188,188,188	0
61	PEG	DP	201	7/7	0.77	0.18	90,92,94,94	0
55	MG	BA	1639	1/1	0.78	0.26	88,88,88,88	0
55	MG	DA	3122	1/1	0.78	0.39	86,86,86,86	0
55	MG	BA	1644	1/1	0.78	0.14	87,87,87,87	0
62	EDO	DB	210	4/4	0.78	0.31	76,77,77,78	0
55	MG	DA	3163	1/1	0.78	0.28	76,76,76,76	0
55	MG	CB	203	1/1	0.78	0.12	146,146,146,146	0
55	MG	CA	3071	1/1	0.78	0.14	257,257,257,257	0
55	MG	DA	3171	1/1	0.78	0.17	83,83,83,83	0
55	MG	CA	3089	1/1	0.78	0.17	209,209,209,209	0
55	MG	CA	3077	1/1	0.79	0.19	189,189,189,189	0
55	MG	CA	3075	1/1	0.79	0.16	215,215,215,215	0
55	MG	CA	3081	1/1	0.79	0.24	153,153,153,153	0
55	MG	BA	1632	1/1	0.79	0.17	219,219,219,219	0
55	MG	DA	3134	1/1	0.80	0.14	65,65,65,65	0
57	MPD	DT	201	8/8	0.80	0.30	85,87,92,92	0
55	MG	AA	1615	1/1	0.80	0.31	81,81,81,81	0
55	MG	DA	3130	1/1	0.80	0.29	81,81,81,81	0
55	MG	CA	3112	1/1	0.81	0.41	77,77,77,77	0
55	MG	CA	3082	1/1	0.81	0.19	229,229,229,229	0
55	MG	CA	3115	1/1	0.81	0.39	76,76,76,76	0
61	PEG	DA	3217	7/7	0.81	0.35	92,95,99,99	0
55	MG	CA	3012	1/1	0.81	0.14	134,134,134,134	0
55	MG	AA	1647	1/1	0.81	0.14	201,201,201,201	0
55	MG	CA	3107	1/1	0.81	0.28	90,90,90,90	0
63	PGE	D3	101	10/10	0.81	0.24	82,83,87,87	0
55	MG	AA	1630	1/1	0.81	0.13	124,124,124,124	0
55	MG	BA	1609	1/1	0.81	0.24	172,172,172,172	0
58	PUT	AA	1673	6/6	0.81	0.21	122,122,123,123	0
57	MPD	DA	3203	8/8	0.82	0.26	89,92,98,99	0
55	MG	DA	3143	1/1	0.82	0.37	93,93,93,93	0
55	MG	CA	3093	1/1	0.82	0.21	151,151,151,151	0
55	MG	DA	3146	1/1	0.82	0.16	73,73,73,73	0
58	PUT	AA	1675	6/6	0.82	0.22	82,83,84,84	0
59	TAC	BA	1602	32/32	0.82	0.16	170,172,172,172	0
55	MG	CA	3108	1/1	0.82	0.16	72,72,72,72	0
55	MG	AA	1610	1/1	0.82	0.37	97,97,97,97	0
55	MG	BA	1635	1/1	0.82	0.17	226,226,226,226	0
61	PEG	DA	3225	7/7	0.82	0.28	60,63,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3126	1/1	0.82	0.23	70,70,70,70	0
56	PG4	DR	202	13/13	0.82	0.25	55,64,74,75	0
55	MG	CA	3083	1/1	0.82	0.14	209,209,209,209	0
55	MG	AA	1642	1/1	0.82	0.26	153,153,153,153	0
57	MPD	DE	302	8/8	0.82	0.30	92,94,95,96	0
55	MG	CA	3003	1/1	0.82	0.22	218,218,218,218	0
57	MPD	DT	202	8/8	0.82	0.32	88,89,90,92	0
60	ZN	AB	301	1/1	0.83	0.10	198,198,198,198	0
57	MPD	DK	201	8/8	0.83	0.19	91,92,94,95	0
57	MPD	DN	201	8/8	0.83	0.19	83,88,90,91	0
63	PGE	DU	101	10/10	0.83	0.19	62,68,78,78	0
55	MG	AA	1602	1/1	0.83	0.25	82,82,82,82	0
55	MG	CA	3056	1/1	0.83	0.14	119,119,119,119	0
55	MG	CA	3058	1/1	0.83	0.17	137,137,137,137	0
55	MG	CA	3148	1/1	0.84	0.42	80,80,80,80	0
55	MG	DA	3131	1/1	0.84	0.29	85,85,85,85	0
55	MG	AA	1636	1/1	0.84	0.15	103,103,103,103	0
55	MG	DA	3136	1/1	0.84	0.10	100,100,100,100	0
55	MG	CA	3142	1/1	0.84	0.20	85,85,85,85	0
55	MG	DA	3178	1/1	0.84	0.33	100,100,100,100	0
55	MG	DA	3161	1/1	0.84	0.23	69,69,69,69	0
62	EDO	DA	3003	4/4	0.84	0.34	47,49,50,50	0
55	MG	DA	3162	1/1	0.84	0.15	70,70,70,70	0
62	EDO	DA	3208	4/4	0.84	0.37	88,90,91,91	0
57	MPD	DA	3209	8/8	0.84	0.26	65,68,71,72	0
55	MG	DB	206	1/1	0.84	0.22	106,106,106,106	0
56	PG4	BA	1601	13/13	0.84	0.16	90,95,98,99	0
56	PG4	DQ	202	13/13	0.84	0.15	62,65,71,71	0
66	ACY	DA	3201	4/4	0.84	0.23	53,56,57,57	0
55	MG	CA	3101	1/1	0.84	0.13	115,115,115,115	0
58	PUT	DA	3221	6/6	0.84	0.20	45,46,49,51	0
55	MG	CA	3011	1/1	0.85	0.16	120,120,120,120	0
57	MPD	DA	3206	8/8	0.85	0.24	93,94,95,95	0
61	PEG	AL	201	7/7	0.85	0.15	78,79,82,82	0
55	MG	AA	1623	1/1	0.85	0.18	74,74,74,74	0
55	MG	CA	3005	1/1	0.85	0.12	224,224,224,224	0
55	MG	AA	1621	1/1	0.85	0.38	88,88,88,88	0
55	MG	CA	3063	1/1	0.85	0.23	257,257,257,257	0
55	MG	DB	205	1/1	0.85	0.16	64,64,64,64	0
57	MPD	DA	3192	8/8	0.85	0.30	68,72,74,74	0
55	MG	DA	3135	1/1	0.86	0.29	73,73,73,73	0
55	MG	AA	1604	1/1	0.86	0.31	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3128	1/1	0.86	0.30	73,73,73,73	0
63	PGE	DD	301	10/10	0.86	0.18	63,66,69,69	0
55	MG	CA	3017	1/1	0.86	0.15	124,124,124,124	0
55	MG	DA	3123	1/1	0.86	0.32	83,83,83,83	0
56	PG4	DA	3193	13/13	0.86	0.19	59,61,70,71	0
55	MG	DA	3133	1/1	0.86	0.23	70,70,70,70	0
55	MG	AA	1677	1/1	0.86	0.21	78,78,78,78	0
55	MG	CA	3057	1/1	0.87	0.11	128,128,128,128	0
55	MG	DA	3127	1/1	0.87	0.35	71,71,71,71	0
61	PEG	DA	3226	7/7	0.87	0.19	55,59,63,64	0
55	MG	DA	3175	1/1	0.87	0.25	85,85,85,85	0
55	MG	CA	3039	1/1	0.87	0.10	124,124,124,124	0
55	MG	DA	3129	1/1	0.87	0.50	69,69,69,69	0
62	EDO	DA	3207	4/4	0.87	0.29	57,58,59,59	0
55	MG	CA	3126	1/1	0.87	0.23	78,78,78,78	0
55	MG	DA	3166	1/1	0.87	0.23	92,92,92,92	0
59	TAC	AA	1678	32/32	0.87	0.13	64,73,81,82	0
55	MG	BA	1610	1/1	0.87	0.14	119,119,119,119	0
56	PG4	AA	1670	13/13	0.87	0.13	80,86,94,94	0
63	PGE	DA	3213	10/10	0.87	0.16	83,85,89,89	0
63	PGE	DA	3216	10/10	0.87	0.17	57,60,68,70	0
57	MPD	DA	3190	8/8	0.87	0.20	87,88,89,93	0
61	PEG	D3	102	7/7	0.87	0.52	73,79,82,82	0
55	MG	CA	3150	1/1	0.87	0.23	80,80,80,80	0
55	MG	AA	1660	1/1	0.87	0.20	275,275,275,275	0
58	PUT	DA	3195	6/6	0.88	0.26	49,55,59,60	0
55	MG	CA	3090	1/1	0.88	0.09	106,106,106,106	0
55	MG	DA	3181	1/1	0.88	0.15	58,58,58,58	0
55	MG	CA	3015	1/1	0.88	0.17	143,143,143,143	0
55	MG	DA	3125	1/1	0.88	0.32	84,84,84,84	0
65	1PE	DA	3202	16/16	0.88	0.18	52,59,65,67	0
55	MG	BA	1618	1/1	0.88	0.16	144,144,144,144	0
55	MG	DA	3151	1/1	0.88	0.09	54,54,54,54	0
55	MG	CA	3022	1/1	0.88	0.12	142,142,142,142	0
55	MG	DA	3154	1/1	0.88	0.45	58,58,58,58	0
57	MPD	AA	1671	8/8	0.89	0.22	96,98,99,101	0
55	MG	DA	3170	1/1	0.89	0.15	80,80,80,80	0
62	EDO	DA	3214	4/4	0.89	0.19	74,74,74,75	0
55	MG	AA	1665	1/1	0.89	0.12	158,158,158,158	0
55	MG	CA	3065	1/1	0.89	0.12	119,119,119,119	0
55	MG	BA	1611	1/1	0.89	0.11	191,191,191,191	0
63	PGE	DS	201	10/10	0.89	0.11	61,66,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3024	1/1	0.89	0.16	104,104,104,104	0
55	MG	DA	3138	1/1	0.89	0.31	80,80,80,80	0
55	MG	AA	1657	1/1	0.89	0.17	144,144,144,144	0
64	SPD	DA	3205	10/10	0.89	0.24	76,83,85,85	0
58	PUT	DA	3204	6/6	0.89	0.20	63,65,68,69	0
58	PUT	DA	3218	6/6	0.89	0.20	73,74,75,75	0
62	EDO	DA	3001	4/4	0.89	0.25	74,76,76,77	0
55	MG	DA	3132	1/1	0.89	0.31	66,66,66,66	0
56	PG4	DA	3215	13/13	0.89	0.18	91,98,100,100	0
56	PG4	DS	202	13/13	0.90	0.12	49,51,61,62	0
55	MG	CA	3152	1/1	0.90	0.19	87,87,87,87	0
55	MG	CA	3099	1/1	0.90	0.13	101,101,101,101	0
55	MG	CA	3100	1/1	0.90	0.07	135,135,135,135	0
62	EDO	DA	3194	4/4	0.90	0.20	60,61,62,63	0
62	EDO	DA	3197	4/4	0.90	0.16	66,66,67,67	0
62	EDO	DA	3198	4/4	0.90	0.20	53,55,55,55	0
55	MG	CA	3111	1/1	0.90	0.22	91,91,91,91	0
58	PUT	DA	3211	6/6	0.90	0.19	57,65,66,66	0
55	MG	DR	201	1/1	0.90	0.23	55,55,55,55	0
58	PUT	DA	3220	6/6	0.90	0.24	93,96,99,100	0
55	MG	AA	1618	1/1	0.90	0.47	81,81,81,81	0
55	MG	CA	3068	1/1	0.90	0.09	107,107,107,107	0
55	MG	AA	1627	1/1	0.90	0.28	88,88,88,88	0
55	MG	BA	1620	1/1	0.90	0.11	97,97,97,97	0
55	MG	CA	3092	1/1	0.90	0.09	113,113,113,113	0
55	MG	DA	3013	1/1	0.90	0.12	67,67,67,67	0
63	PGE	DA	3224	10/10	0.90	0.21	79,85,88,88	0
64	SPD	DA	3183	10/10	0.90	0.18	48,57,60,60	0
55	MG	DA	3027	1/1	0.90	0.22	76,76,76,76	0
65	1PE	DA	3185	16/16	0.90	0.14	42,50,62,64	0
55	MG	DA	3045	1/1	0.90	0.09	90,90,90,90	0
61	PEG	DA	3200	7/7	0.90	0.31	56,57,59,61	0
55	MG	DA	3164	1/1	0.90	0.25	75,75,75,75	0
55	MG	AA	1607	1/1	0.90	0.35	91,91,91,91	0
55	MG	AA	1612	1/1	0.90	0.18	65,65,65,65	0
61	PEG	DA	3199	7/7	0.91	0.23	62,66,69,69	0
58	PUT	DA	3189	6/6	0.91	0.15	38,44,47,47	0
55	MG	BA	1619	1/1	0.91	0.09	122,122,122,122	0
55	MG	DB	208	1/1	0.91	0.22	66,66,66,66	0
55	MG	DD	303	1/1	0.91	0.11	53,53,53,53	0
62	EDO	D1	101	4/4	0.91	0.12	63,64,67,70	0
55	MG	BA	1614	1/1	0.91	0.19	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3047	1/1	0.91	0.08	94,94,94,94	0
55	MG	CA	3143	1/1	0.91	0.08	85,85,85,85	0
55	MG	DA	3177	1/1	0.91	0.35	84,84,84,84	0
64	SPD	DA	3223	10/10	0.91	0.18	39,42,46,46	0
55	MG	DA	3165	1/1	0.91	0.20	74,74,74,74	0
55	MG	CA	3135	1/1	0.91	0.22	90,90,90,90	0
55	MG	DA	3152	1/1	0.91	0.17	43,43,43,43	0
55	MG	DA	3112	1/1	0.91	0.31	291,291,291,291	0
55	MG	DA	3169	1/1	0.91	0.26	72,72,72,72	0
58	PUT	DA	3184	6/6	0.91	0.23	45,45,47,48	0
55	MG	DA	3160	1/1	0.92	0.10	56,56,56,56	0
55	MG	CA	3088	1/1	0.92	0.17	90,90,90,90	0
55	MG	DA	3142	1/1	0.92	0.21	73,73,73,73	0
62	EDO	DB	211	4/4	0.92	0.16	74,74,75,75	0
55	MG	CA	3029	1/1	0.92	0.10	113,113,113,113	0
55	MG	AA	1656	1/1	0.92	0.08	124,124,124,124	0
55	MG	CA	3019	1/1	0.92	0.08	102,102,102,102	0
55	MG	CA	3044	1/1	0.92	0.10	93,93,93,93	0
61	PEG	DL	201	7/7	0.92	0.13	69,70,71,71	0
55	MG	DA	3121	1/1	0.92	0.30	90,90,90,90	0
55	MG	AA	1620	1/1	0.92	0.14	67,67,67,67	0
55	MG	CA	3026	1/1	0.92	0.15	123,123,123,123	0
55	MG	CA	3034	1/1	0.92	0.26	144,144,144,144	0
55	MG	AA	1664	1/1	0.92	0.09	161,161,161,161	0
55	MG	CA	3087	1/1	0.92	0.08	91,91,91,91	0
55	MG	AA	1655	1/1	0.93	0.07	100,100,100,100	0
55	MG	BA	1616	1/1	0.93	0.13	136,136,136,136	0
55	MG	CA	3040	1/1	0.93	0.10	71,71,71,71	0
55	MG	CA	3073	1/1	0.93	0.12	197,197,197,197	0
55	MG	CA	3023	1/1	0.93	0.08	134,134,134,134	0
55	MG	AA	1625	1/1	0.93	0.14	63,63,63,63	0
55	MG	AA	1633	1/1	0.93	0.07	110,110,110,110	0
55	MG	DA	3150	1/1	0.93	0.07	51,51,51,51	0
55	MG	DA	3005	1/1	0.93	0.09	69,69,69,69	0
55	MG	CA	3096	1/1	0.93	0.10	117,117,117,117	0
55	MG	CA	3048	1/1	0.93	0.07	92,92,92,92	0
55	MG	BA	1603	1/1	0.93	0.14	95,95,95,95	0
55	MG	DA	3158	1/1	0.93	0.10	55,55,55,55	0
55	MG	CA	3035	1/1	0.93	0.21	201,201,201,201	0
55	MG	DA	3065	1/1	0.93	0.30	59,59,59,59	0
55	MG	AA	1658	1/1	0.93	0.09	83,83,83,83	0
55	MG	DA	3118	1/1	0.93	0.12	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	CA	3028	1/1	0.93	0.21	172,172,172,172	0
61	PEG	D1	103	7/7	0.93	0.22	57,60,61,63	0
55	MG	AA	1649	1/1	0.94	0.06	58,58,58,58	0
58	PUT	DA	3222	6/6	0.94	0.16	46,49,51,52	0
55	MG	AA	1613	1/1	0.94	0.38	68,68,68,68	0
55	MG	CA	3016	1/1	0.94	0.06	106,106,106,106	0
55	MG	CA	3049	1/1	0.94	0.09	81,81,81,81	0
55	MG	CB	202	1/1	0.94	0.11	128,128,128,128	0
55	MG	DA	3141	1/1	0.94	0.14	82,82,82,82	0
64	SPD	DA	3187	10/10	0.94	0.15	32,35,43,46	0
58	PUT	DA	3188	6/6	0.94	0.10	30,31,33,39	0
55	MG	CA	3097	1/1	0.94	0.10	110,110,110,110	0
55	MG	DA	3099	1/1	0.94	0.07	81,81,81,81	0
55	MG	CA	3018	1/1	0.94	0.08	78,78,78,78	0
66	ACY	DA	3191	4/4	0.94	0.11	55,55,56,57	0
55	MG	BA	1636	1/1	0.94	0.10	112,112,112,112	0
58	PUT	DA	3212	6/6	0.94	0.32	47,53,59,60	0
55	MG	CA	3064	1/1	0.94	0.10	107,107,107,107	0
55	MG	AA	1632	1/1	0.94	0.12	110,110,110,110	0
55	MG	BA	1637	1/1	0.95	0.08	99,99,99,99	0
55	MG	CB	201	1/1	0.95	0.08	157,157,157,157	0
55	MG	CA	3042	1/1	0.95	0.09	92,92,92,92	0
55	MG	DA	3144	1/1	0.95	0.09	65,65,65,65	0
55	MG	CA	3095	1/1	0.95	0.07	112,112,112,112	0
55	MG	BA	1628	1/1	0.95	0.12	97,97,97,97	0
55	MG	CA	3080	1/1	0.95	0.07	120,120,120,120	0
55	MG	CA	3045	1/1	0.95	0.08	142,142,142,142	0
55	MG	DA	3149	1/1	0.95	0.32	66,66,66,66	0
55	MG	CA	3069	1/1	0.95	0.05	95,95,95,95	0
55	MG	DA	3038	1/1	0.95	0.12	27,27,27,27	0
55	MG	DA	3043	1/1	0.95	0.07	34,34,34,34	0
55	MG	AA	1635	1/1	0.95	0.07	96,96,96,96	0
55	MG	DA	3053	1/1	0.95	0.09	78,78,78,78	0
55	MG	DA	3156	1/1	0.95	0.30	74,74,74,74	0
55	MG	DA	3157	1/1	0.95	0.17	69,69,69,69	0
55	MG	BA	1623	1/1	0.95	0.19	37,37,37,37	0
55	MG	AA	1634	1/1	0.95	0.08	106,106,106,106	0
55	MG	DA	3081	1/1	0.95	0.09	94,94,94,94	0
55	MG	DA	3097	1/1	0.95	0.08	45,45,45,45	0
55	MG	AA	1639	1/1	0.95	0.08	120,120,120,120	0
55	MG	DA	3137	1/1	0.95	0.19	55,55,55,55	0
55	MG	DA	3100	1/1	0.95	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1607	1/1	0.95	0.07	118,118,118,118	0
55	MG	DA	3230	1/1	0.96	0.09	37,37,37,37	0
55	MG	CA	3085	1/1	0.96	0.14	82,82,82,82	0
55	MG	AA	1651	1/1	0.96	0.07	68,68,68,68	0
55	MG	BA	1633	1/1	0.96	0.05	57,57,57,57	0
55	MG	BA	1613	1/1	0.96	0.06	54,54,54,54	0
55	MG	DA	3140	1/1	0.96	0.07	43,43,43,43	0
55	MG	DA	3114	1/1	0.96	0.14	59,59,59,59	0
55	MG	DA	3006	1/1	0.96	0.05	60,60,60,60	0
55	MG	CA	3113	1/1	0.96	0.19	57,57,57,57	0
55	MG	DA	3016	1/1	0.96	0.07	62,62,62,62	0
55	MG	AA	1669	1/1	0.96	0.07	109,109,109,109	0
55	MG	DA	3029	1/1	0.96	0.07	49,49,49,49	0
55	MG	DA	3036	1/1	0.96	0.08	41,41,41,41	0
60	ZN	C5	101	1/1	0.96	0.06	139,139,139,139	0
63	PGE	DA	3186	10/10	0.96	0.10	29,33,36,37	0
55	MG	CA	3102	1/1	0.96	0.07	115,115,115,115	0
57	MPD	DS	203	8/8	0.96	0.14	36,40,42,44	0
55	MG	CA	3050	1/1	0.96	0.07	102,102,102,102	0
55	MG	CA	3051	1/1	0.96	0.05	82,82,82,82	0
55	MG	DA	3174	1/1	0.96	0.13	79,79,79,79	0
55	MG	BA	1621	1/1	0.96	0.09	103,103,103,103	0
55	MG	CA	3094	1/1	0.96	0.09	73,73,73,73	0
55	MG	BA	1604	1/1	0.96	0.05	99,99,99,99	0
55	MG	DA	3080	1/1	0.96	0.08	105,105,105,105	0
55	MG	DA	3155	1/1	0.96	0.32	71,71,71,71	0
55	MG	BA	1624	1/1	0.96	0.06	97,97,97,97	0
55	MG	DA	3084	1/1	0.96	0.08	44,44,44,44	0
55	MG	DA	3091	1/1	0.96	0.06	28,28,28,28	0
55	MG	DA	3227	1/1	0.96	0.08	52,52,52,52	0
55	MG	CA	3084	1/1	0.97	0.05	75,75,75,75	0
55	MG	BA	1615	1/1	0.97	0.09	70,70,70,70	0
55	MG	CA	3086	1/1	0.97	0.05	93,93,93,93	0
55	MG	AA	1640	1/1	0.97	0.05	61,61,61,61	0
55	MG	AA	1641	1/1	0.97	0.07	81,81,81,81	0
55	MG	DA	3007	1/1	0.97	0.08	111,111,111,111	0
55	MG	DA	3009	1/1	0.97	0.10	89,89,89,89	0
55	MG	CA	3078	1/1	0.97	0.08	134,134,134,134	0
55	MG	DA	3096	1/1	0.97	0.12	51,51,51,51	0
58	PUT	DA	3002	6/6	0.97	0.11	39,41,44,47	0
55	MG	DD	302	1/1	0.97	0.05	53,53,53,53	0
55	MG	AA	1663	1/1	0.97	0.06	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1612	1/1	0.97	0.07	101,101,101,101	0
55	MG	AA	1638	1/1	0.97	0.06	94,94,94,94	0
55	MG	CA	3014	1/1	0.97	0.18	71,71,71,71	0
55	MG	AA	1644	1/1	0.97	0.10	83,83,83,83	0
55	MG	DA	3120	1/1	0.97	0.14	48,48,48,48	0
55	MG	AA	1643	1/1	0.98	0.04	64,64,64,64	0
55	MG	DA	3068	1/1	0.98	0.07	67,67,67,67	0
55	MG	DA	3073	1/1	0.98	0.05	45,45,45,45	0
55	MG	DA	3074	1/1	0.98	0.05	32,32,32,32	0
55	MG	DA	3076	1/1	0.98	0.04	25,25,25,25	0
55	MG	AA	1637	1/1	0.98	0.04	49,49,49,49	0
55	MG	AA	1645	1/1	0.98	0.04	48,48,48,48	0
55	MG	DA	3083	1/1	0.98	0.04	60,60,60,60	0
55	MG	AA	1667	1/1	0.98	0.07	51,51,51,51	0
55	MG	DA	3086	1/1	0.98	0.03	41,41,41,41	0
55	MG	DA	3090	1/1	0.98	0.06	21,21,21,21	0
55	MG	CA	3052	1/1	0.98	0.14	96,96,96,96	0
55	MG	DA	3095	1/1	0.98	0.10	38,38,38,38	0
55	MG	CA	3010	1/1	0.98	0.09	99,99,99,99	0
55	MG	DA	3017	1/1	0.98	0.09	56,56,56,56	0
55	MG	DA	3022	1/1	0.98	0.06	50,50,50,50	0
55	MG	CA	3041	1/1	0.98	0.07	90,90,90,90	0
55	MG	DA	3102	1/1	0.98	0.04	52,52,52,52	0
55	MG	DA	3108	1/1	0.98	0.04	39,39,39,39	0
55	MG	AA	1652	1/1	0.98	0.17	40,40,40,40	0
55	MG	DA	3032	1/1	0.98	0.05	34,34,34,34	0
55	MG	DA	3033	1/1	0.98	0.05	19,19,19,19	0
55	MG	DB	204	1/1	0.98	0.04	65,65,65,65	0
55	MG	CA	3043	1/1	0.98	0.08	73,73,73,73	0
55	MG	DA	3041	1/1	0.98	0.04	50,50,50,50	0
55	MG	DA	3042	1/1	0.98	0.11	28,28,28,28	0
60	ZN	D5	101	1/1	0.98	0.03	55,55,55,55	0
55	MG	BA	1622	1/1	0.98	0.06	82,82,82,82	0
55	MG	AA	1653	1/1	0.98	0.04	81,81,81,81	0
55	MG	DA	3049	1/1	0.98	0.05	31,31,31,31	0
55	MG	DA	3050	1/1	0.98	0.04	35,35,35,35	0
55	MG	DA	3052	1/1	0.98	0.05	33,33,33,33	0
55	MG	AA	1646	1/1	0.98	0.04	53,53,53,53	0
55	MG	BA	1634	1/1	0.98	0.06	66,66,66,66	0
55	MG	DA	3064	1/1	0.98	0.10	63,63,63,63	0
55	MG	DA	3044	1/1	0.99	0.06	36,36,36,36	0
55	MG	DA	3098	1/1	0.99	0.03	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3011	1/1	0.99	0.07	24,24,24,24	0
55	MG	DA	3046	1/1	0.99	0.07	47,47,47,47	0
55	MG	DA	3101	1/1	0.99	0.02	30,30,30,30	0
55	MG	DA	3012	1/1	0.99	0.04	39,39,39,39	0
55	MG	DA	3103	1/1	0.99	0.04	46,46,46,46	0
55	MG	DA	3104	1/1	0.99	0.02	59,59,59,59	0
55	MG	DA	3105	1/1	0.99	0.06	31,31,31,31	0
55	MG	DA	3106	1/1	0.99	0.06	32,32,32,32	0
55	MG	DB	201	1/1	0.99	0.10	63,63,63,63	0
55	MG	DA	3109	1/1	0.99	0.04	29,29,29,29	0
55	MG	DA	3111	1/1	0.99	0.06	38,38,38,38	0
55	MG	DA	3015	1/1	0.99	0.02	17,17,17,17	0
55	MG	DB	203	1/1	0.99	0.03	37,37,37,37	0
55	MG	DA	3115	1/1	0.99	0.06	35,35,35,35	0
55	MG	DA	3116	1/1	0.99	0.07	45,45,45,45	0
55	MG	DA	3054	1/1	0.99	0.03	47,47,47,47	0
55	MG	DA	3119	1/1	0.99	0.05	53,53,53,53	0
55	MG	DA	3055	1/1	0.99	0.09	55,55,55,55	0
55	MG	DA	3056	1/1	0.99	0.06	39,39,39,39	0
55	MG	DA	3057	1/1	0.99	0.04	49,49,49,49	0
55	MG	DA	3061	1/1	0.99	0.03	19,19,19,19	0
55	MG	DA	3062	1/1	0.99	0.02	33,33,33,33	0
55	MG	AA	1662	1/1	0.99	0.07	84,84,84,84	0
55	MG	DA	3021	1/1	0.99	0.04	55,55,55,55	0
55	MG	BA	1630	1/1	0.99	0.05	101,101,101,101	0
55	MG	DA	3229	1/1	0.99	0.03	38,38,38,38	0
55	MG	DA	3066	1/1	0.99	0.03	22,22,22,22	0
55	MG	DA	3023	1/1	0.99	0.08	27,27,27,27	0
55	MG	DA	3069	1/1	0.99	0.04	36,36,36,36	0
55	MG	DA	3070	1/1	0.99	0.12	54,54,54,54	0
55	MG	DA	3071	1/1	0.99	0.05	90,90,90,90	0
55	MG	AA	1629	1/1	0.99	0.05	82,82,82,82	0
55	MG	DA	3028	1/1	0.99	0.03	41,41,41,41	0
55	MG	DA	3075	1/1	0.99	0.06	39,39,39,39	0
55	MG	AA	1650	1/1	0.99	0.04	75,75,75,75	0
55	MG	DA	3077	1/1	0.99	0.02	22,22,22,22	0
55	MG	DA	3078	1/1	0.99	0.04	32,32,32,32	0
55	MG	DA	3079	1/1	0.99	0.07	76,76,76,76	0
55	MG	AA	1659	1/1	0.99	0.03	73,73,73,73	0
55	MG	AA	1666	1/1	0.99	0.03	54,54,54,54	0
55	MG	DA	3082	1/1	0.99	0.03	57,57,57,57	0
55	MG	AA	1631	1/1	0.99	0.04	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3037	1/1	0.99	0.06	26,26,26,26	0
55	MG	DA	3085	1/1	0.99	0.07	45,45,45,45	0
55	MG	DM	201	1/1	0.99	0.05	55,55,55,55	0
55	MG	DA	3087	1/1	0.99	0.04	45,45,45,45	0
55	MG	DA	3088	1/1	0.99	0.04	56,56,56,56	0
55	MG	DA	3089	1/1	0.99	0.03	46,46,46,46	0
55	MG	DA	3040	1/1	0.99	0.05	30,30,30,30	0
55	MG	AA	1648	1/1	0.99	0.04	63,63,63,63	0
55	MG	DA	3092	1/1	0.99	0.03	18,18,18,18	0
55	MG	DA	3093	1/1	0.99	0.04	31,31,31,31	0
55	MG	DA	3094	1/1	0.99	0.04	25,25,25,25	0
55	MG	DA	3008	1/1	0.99	0.04	73,73,73,73	0
55	MG	BA	1645	1/1	0.99	0.06	87,87,87,87	0
55	MG	DA	3020	1/1	1.00	0.17	11,11,11,11	0
55	MG	DA	3034	1/1	1.00	0.02	29,29,29,29	0
55	MG	DA	3035	1/1	1.00	0.04	20,20,20,20	0
55	MG	DB	202	1/1	1.00	0.06	33,33,33,33	0
55	MG	DA	3014	1/1	1.00	0.08	24,24,24,24	0
55	MG	DA	3010	1/1	1.00	0.04	24,24,24,24	0
55	MG	DA	3058	1/1	1.00	0.08	37,37,37,37	0
55	MG	DA	3107	1/1	1.00	0.07	39,39,39,39	0
55	MG	DA	3059	1/1	1.00	0.05	32,32,32,32	0
55	MG	DA	3060	1/1	1.00	0.02	29,29,29,29	0
55	MG	DA	3110	1/1	1.00	0.02	20,20,20,20	0
55	MG	DA	3039	1/1	1.00	0.04	27,27,27,27	0
55	MG	DA	3024	1/1	1.00	0.08	42,42,42,42	0
55	MG	DA	3113	1/1	1.00	0.04	25,25,25,25	0
55	MG	DA	3025	1/1	1.00	0.06	26,26,26,26	0
55	MG	DA	3026	1/1	1.00	0.03	29,29,29,29	0
55	MG	AA	1668	1/1	1.00	0.06	40,40,40,40	0
55	MG	DA	3117	1/1	1.00	0.08	32,32,32,32	0
55	MG	BA	1617	1/1	1.00	0.04	65,65,65,65	0
55	MG	DA	3067	1/1	1.00	0.02	51,51,51,51	0
55	MG	DA	3018	1/1	1.00	0.03	29,29,29,29	0
55	MG	DA	3030	1/1	1.00	0.02	14,14,14,14	0
55	MG	DA	3047	1/1	1.00	0.04	34,34,34,34	0
55	MG	DA	3048	1/1	1.00	0.02	47,47,47,47	0
55	MG	DA	3072	1/1	1.00	0.08	49,49,49,49	0
55	MG	DA	3031	1/1	1.00	0.02	35,35,35,35	0
55	MG	DA	3019	1/1	1.00	0.04	47,47,47,47	0
55	MG	DA	3051	1/1	1.00	0.03	24,24,24,24	0
55	MG	DA	3228	1/1	1.00	0.02	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.