



Full wwPDB EM Validation Report ⓘ

May 17, 2025 – 11:10 PM EDT

PDB ID : 7MPJ / pdb_00007mpj
EMDB ID : EMD-23935
Title : Stm1 bound vacant 80S structure isolated from wild-type
Authors : Rai, J.; Zhao, Y.; Li, H.
Deposited on : 2021-05-04
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

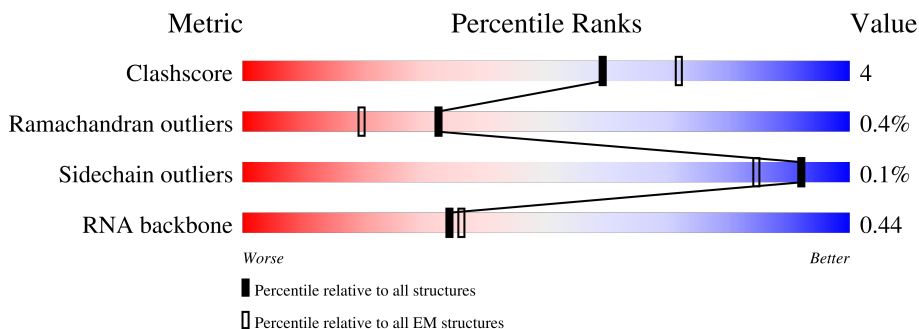
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BA	206	<div> <div>7%</div> <div>81%</div> <div>19%</div> </div>
2	BB	214	<div> <div>14%</div> <div>73%</div> <div>25%</div> </div>
3	BC	217	<div> <div>85%</div> <div>14%</div> </div>
4	BD	223	<div> <div>9%</div> <div>83%</div> <div>17%</div> </div>
5	BE	260	<div> <div>5%</div> <div>80%</div> <div>20%</div> </div>
6	BF	206	<div> <div>7%</div> <div>86%</div> <div>13%</div> </div>
7	BG	226	<div> <div>22%</div> <div>84%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
8	BH	184	
9	BI	188	
10	BJ	185	
11	BK	96	
12	BL	155	
13	BM	121	
14	BN	150	
15	BO	127	
16	BP	124	
17	BQ	141	
18	BR	121	
19	BS	145	
20	BT	141	
21	BU	107	
22	BV	87	
23	BW	129	
24	BX	144	
25	BY	134	
26	BZ	69	
27	Ba	97	
28	Bb	81	
29	Bc	63	
30	Bd	53	
31	Be	60	
32	Bf	57	

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Mol	Chain	Length	Quality of chain
33	Bg	312	
34	Bh	89	
35	B5	1781	
36	A1	3137	
37	A3	121	
38	A4	158	
39	AA	247	
40	AB	386	
41	AC	361	
42	AD	292	
43	AE	156	
44	AF	222	
45	AG	230	
46	AH	190	
47	AI	205	
48	AJ	169	
49	AL	193	
50	AM	136	
51	AN	203	
52	AO	197	
53	AP	175	
54	AQ	185	
55	AR	188	
56	AS	172	
57	AT	159	

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Mol	Chain	Length	Quality of chain
58	AU	100	
59	AV	136	
60	AW	63	
61	AX	121	
62	AY	126	
63	AZ	135	
64	Aa	148	
65	Ab	58	
66	Ac	97	
67	Ad	109	
68	Ae	127	
69	Af	106	
70	Ag	112	
71	Ah	119	
72	Ai	99	
73	Aj	87	
74	Ak	77	
75	Al	50	
76	Am	52	
77	An	25	
78	Ao	105	
79	Ap	91	

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
35	G7M	B5	1575	X	-	-	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 199813 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BH	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	ASN	deletion	UNP P0CX39
BI	?	-	VAL	deletion	UNP P0CX39
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	THR	deletion	UNP P0CX39
BI	?	-	VAL	deletion	UNP P0CX39
BI	?	-	ALA	deletion	UNP P0CX39

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 11 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 13 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BM	121	Total	C	N	O	S	0	0
			913	574	162	175	2		

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 15 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 17 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	BQ	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 18 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BR	121	Total	C	N	O	S	0	0
			975	611	183	179	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	?	-	SER	deletion	UNP P02407
BR	?	-	ASN	deletion	UNP P02407
BR	?	-	GLY	deletion	UNP P02407
BR	?	-	VAL	deletion	UNP P02407

- Molecule 19 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 20 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 21 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 22 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 23 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 24 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 25 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	BY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 26 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	BZ	69	Total	C	N	O	0	0
			558	357	103	98		

- Molecule 27 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 28 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 29 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 30 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 31 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 32 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	57	Total	C	N	O	S	0	0
			454	288	86	77	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bf	97	ALA	LYS	conflict	UNP P05759
Bf	?	-	CYS	deletion	UNP P05759
Bf	?	-	GLY	deletion	UNP P05759
Bf	?	-	ALA	deletion	UNP P05759

- Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 34 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bh	89	Total	C	N	O		0	0
			675	391	137	147			

- Molecule 35 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B5	1781	Total	C	N	O	P	1	0
			37850	16932	6657	12480	1781		

- Molecule 36 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	A1	3137	Total	C	N	O	P	0	0
			67139	30012	12094	21896	3137		

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AB	386	Total	C	N	O	S	0	0
			3078	1953	584	533	8		

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AE	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AI	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	?	-	MET	deletion	UNP P41805
AI	?	-	LEU	deletion	UNP P41805
AI	?	-	SER	deletion	UNP P41805
AI	?	-	CYS	deletion	UNP P41805
AI	?	-	ALA	deletion	UNP P41805
AI	?	-	GLY	deletion	UNP P41805
AI	?	-	ALA	deletion	UNP P41805
AI	?	-	ASP	deletion	UNP P41805
AI	?	-	ARG	deletion	UNP P41805
AI	?	-	LEU	deletion	UNP P41805
AI	?	-	GLN	deletion	UNP P41805
AI	?	-	GLN	deletion	UNP P41805

- Molecule 48 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	AL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AO	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AP	175	Total	C	N	O	0	0
			1388	862	277	249		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	VAL	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	LYS	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	GLU	deletion	UNP P05740
AP	?	-	LYS	deletion	UNP P05740

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	AR	188	Total	C	N	O		
			1521	935	326	260	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AS	172	Total	C	N	O	S		
			1445	930	267	244	4	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AT	159	Total	C	N	O	S		
			1276	805	246	221	4	0	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	AU	100	Total	C	N	O		
			796	516	131	149	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AV	136	Total	C	N	O	S		
			1003	628	189	179	7	0	0

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AW	63	Total	C	N	O	S		
			521	336	102	82	1	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AX	121	Total	C	N	O	S		
			968	623	170	173	2	0	0

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	AY	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	AZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Aa	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	Ab	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ac	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ae	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Af	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	Ak	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 76 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	BJ	1	Total	Mg	0
			1	1	
80	BT	1	Total	Mg	0
			1	1	
80	Be	1	Total	Mg	0
			1	1	
80	B5	122	Total	Mg	0
			122	122	
80	A1	541	Total	Mg	0
			541	541	
80	A3	3	Total	Mg	0
			3	3	
80	A4	18	Total	Mg	0
			18	18	
80	AA	2	Total	Mg	0
			2	2	
80	AB	5	Total	Mg	0
			5	5	

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Mol	Chain	Residues	Atoms		AltConf
80	AC	6	Total 6	Mg 6	0
80	AF	1	Total 1	Mg 1	0
80	AG	1	Total 1	Mg 1	0
80	AI	2	Total 2	Mg 2	0
80	AL	2	Total 2	Mg 2	0
80	AM	1	Total 1	Mg 1	0
80	AN	5	Total 5	Mg 5	0
80	AO	2	Total 2	Mg 2	0
80	AP	2	Total 2	Mg 2	0
80	AQ	3	Total 3	Mg 3	0
80	AR	3	Total 3	Mg 3	0
80	AS	3	Total 3	Mg 3	0
80	AY	1	Total 1	Mg 1	0
80	Aa	3	Total 3	Mg 3	0
80	Ad	2	Total 2	Mg 2	0
80	Ae	3	Total 3	Mg 3	0
80	Af	2	Total 2	Mg 2	0
80	Ai	1	Total 1	Mg 1	0
80	Aj	5	Total 5	Mg 5	0
80	Am	1	Total 1	Mg 1	0
80	Ao	2	Total 2	Mg 2	0

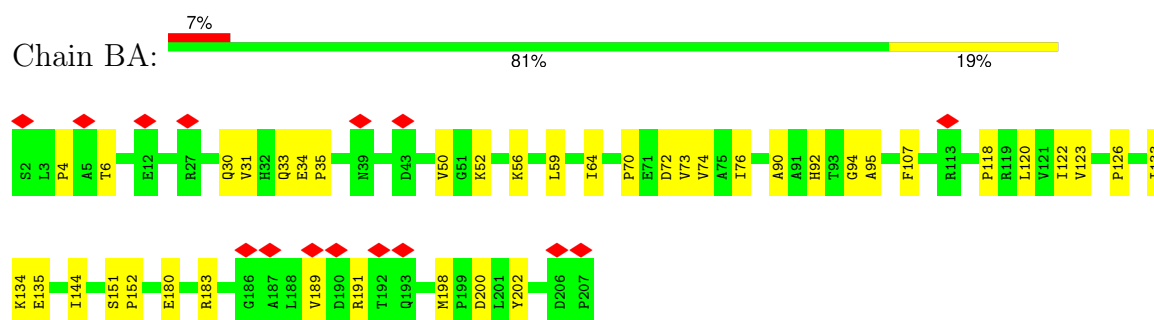
- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Bb	1	Total 1	Zn 1	0
81	Ao	1	Total 1	Zn 1	0

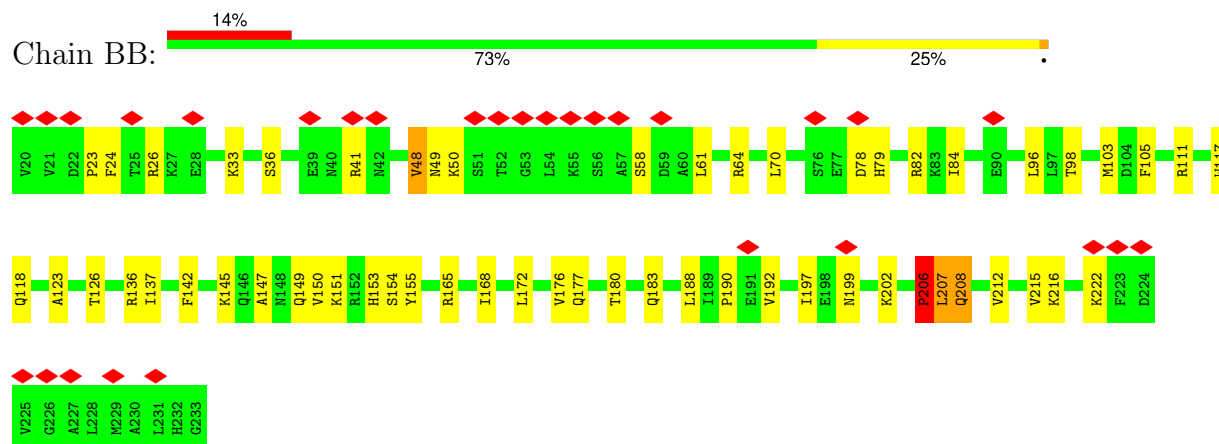
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

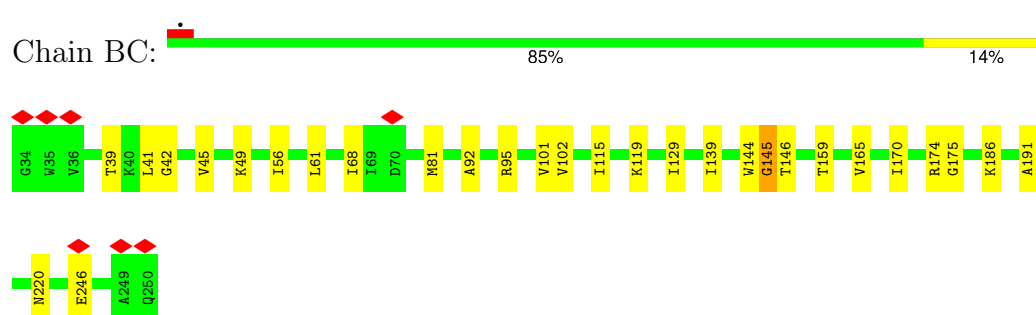
- Molecule 1: 40S ribosomal protein S0-A



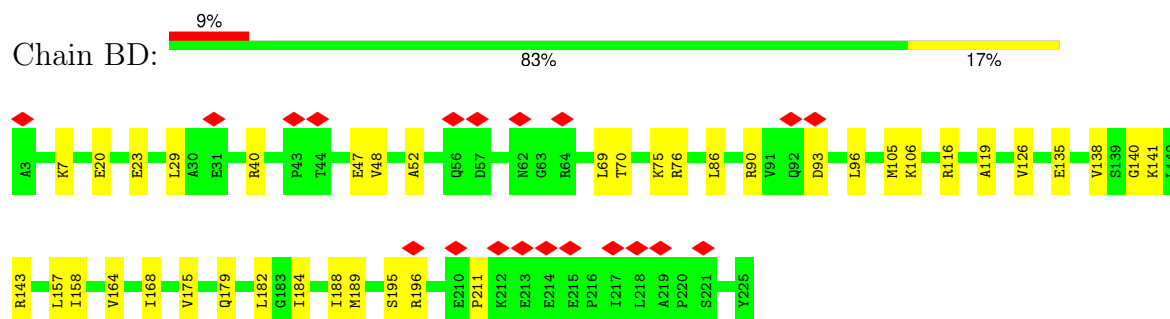
- Molecule 2: 40S ribosomal protein S1-A



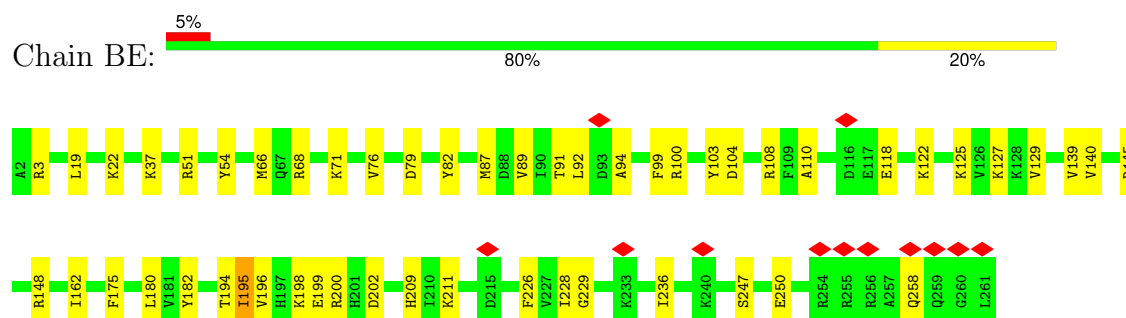
- Molecule 3: 40S ribosomal protein S2



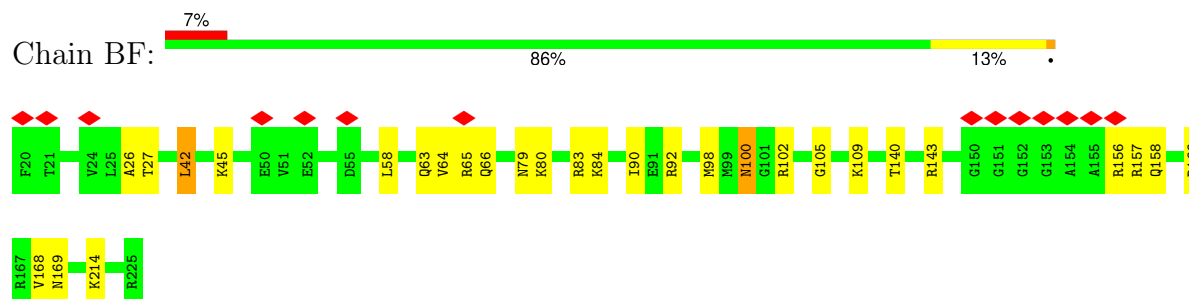
- Molecule 4: 40S ribosomal protein S3



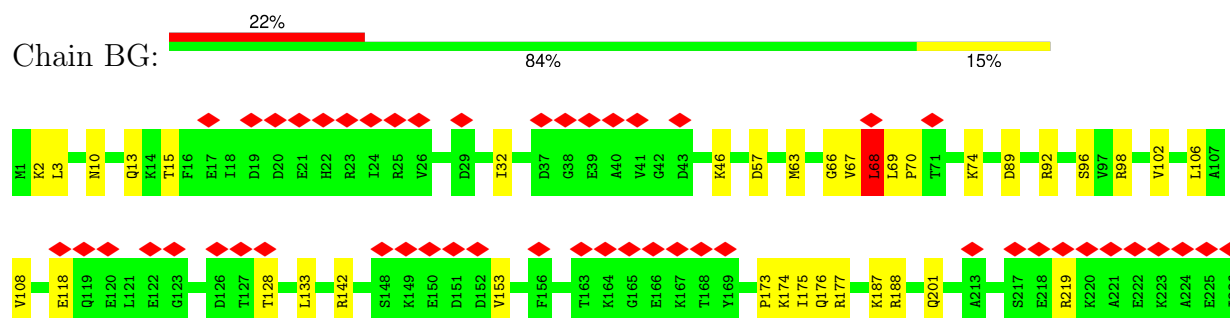
- Molecule 5: 40S ribosomal protein S4-A



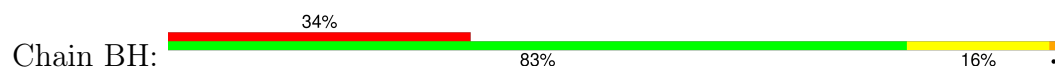
- Molecule 6: 40S ribosomal protein S5

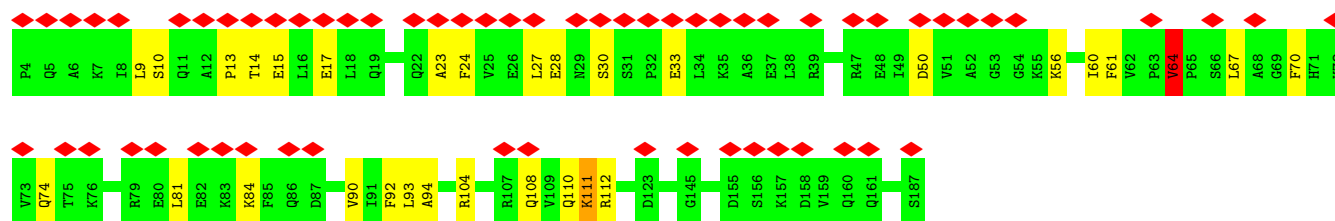


- Molecule 7: 40S ribosomal protein S6-A

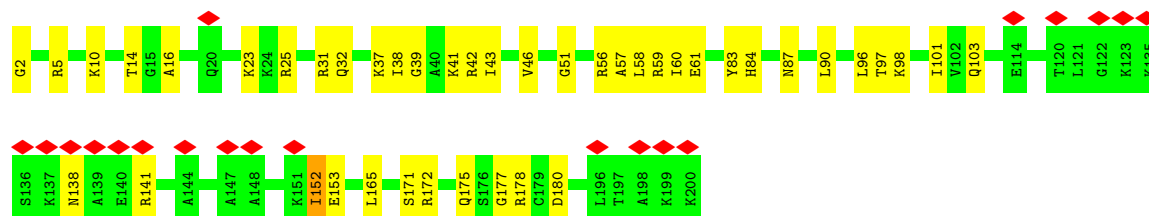
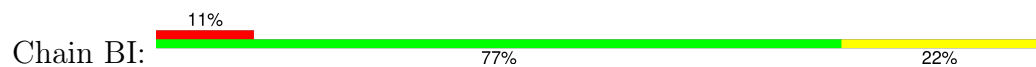


- Molecule 8: 40S ribosomal protein S7-A

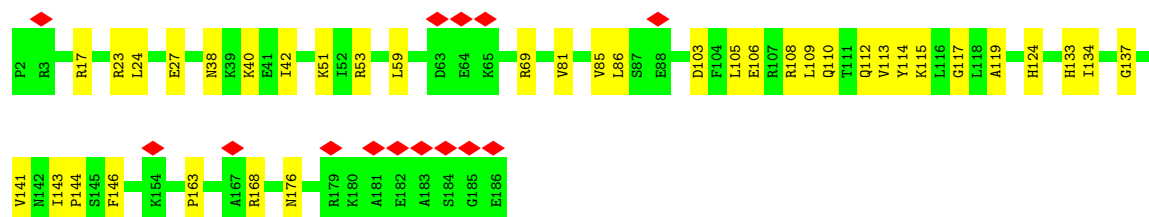
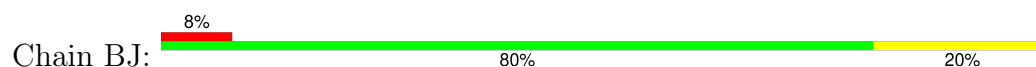




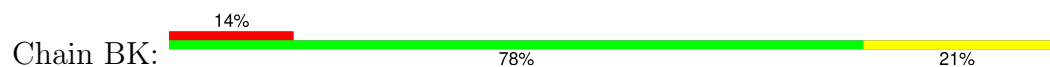
• Molecule 9: 40S ribosomal protein S8-A



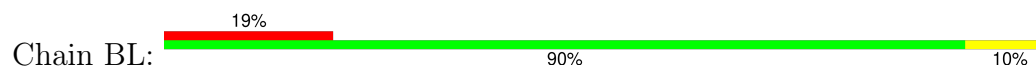
• Molecule 10: 40S ribosomal protein S9-A



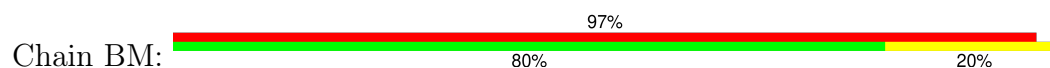
• Molecule 11: 40S ribosomal protein S10-A

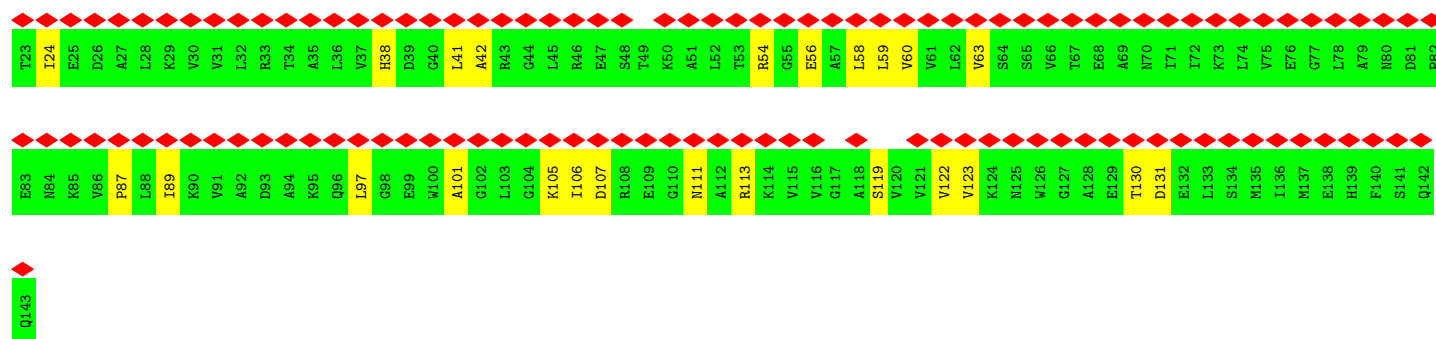


• Molecule 12: 40S ribosomal protein S11-A

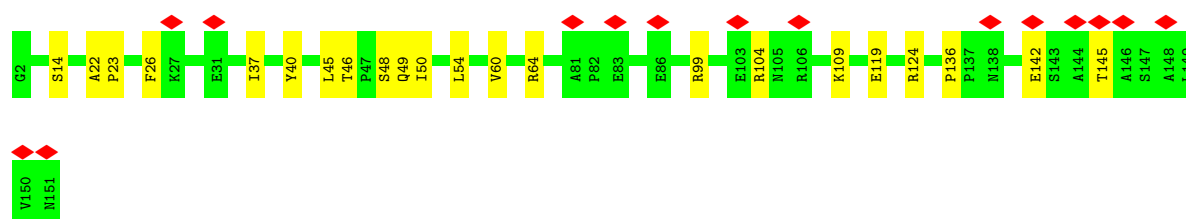
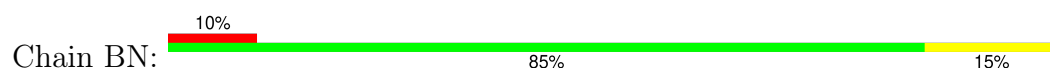


• Molecule 13: 40S ribosomal protein S12

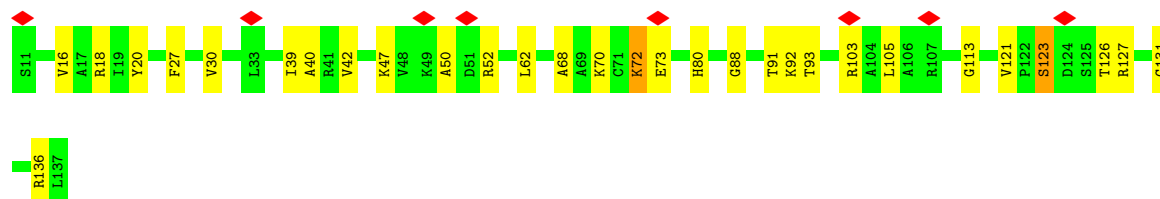
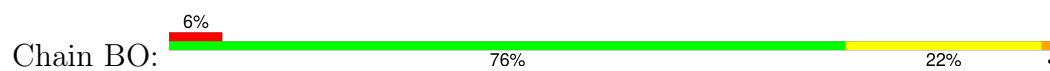




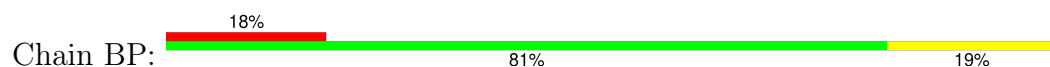
- Molecule 14: 40S ribosomal protein S13



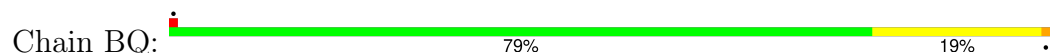
- Molecule 15: 40S ribosomal protein S14-A



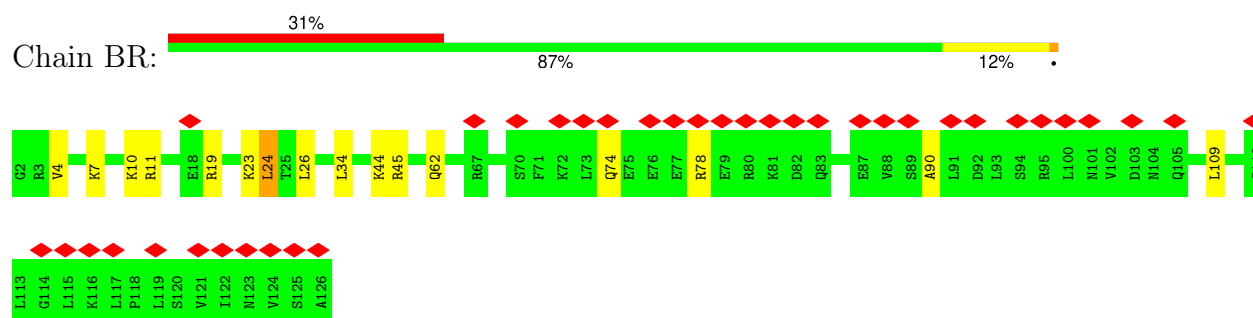
- Molecule 16: 40S ribosomal protein S15



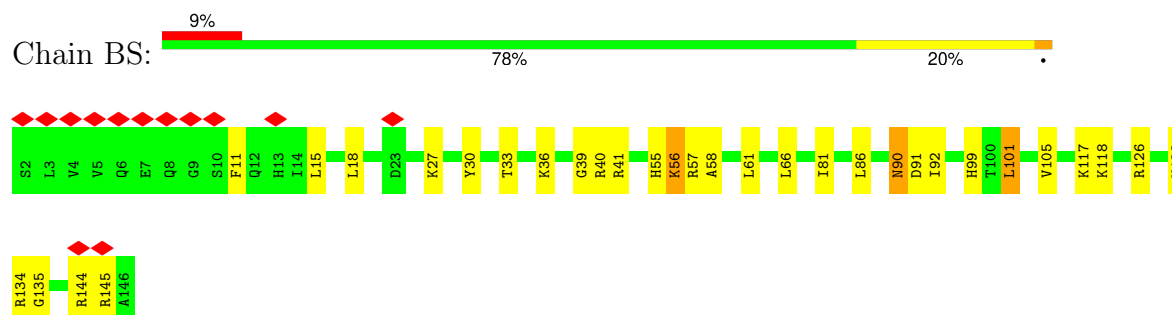
- Molecule 17: 40S ribosomal protein S16-A



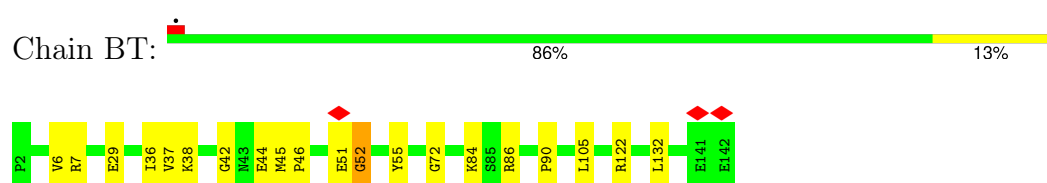
- Molecule 18: 40S ribosomal protein S17-A



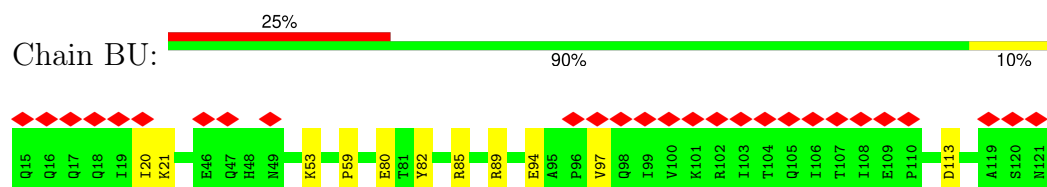
- Molecule 19: 40S ribosomal protein S18-A



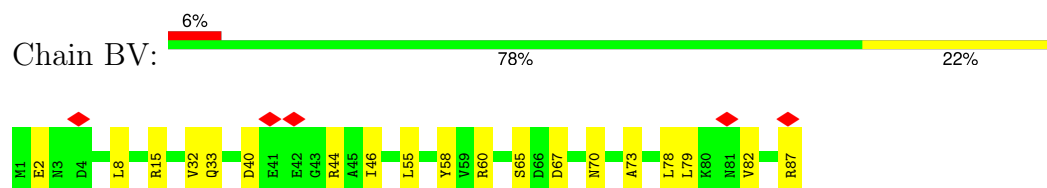
- Molecule 20: 40S ribosomal protein S19-A



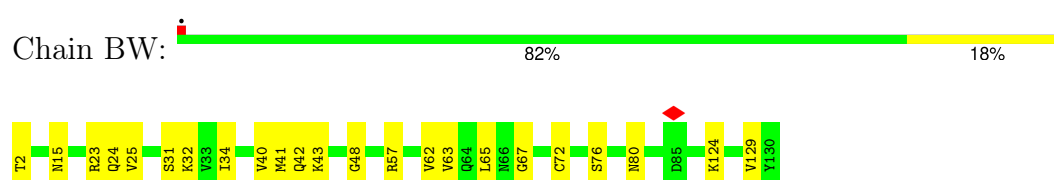
- Molecule 21: 40S ribosomal protein S20




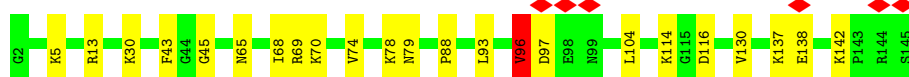
- Molecule 22: 40S ribosomal protein S21-A




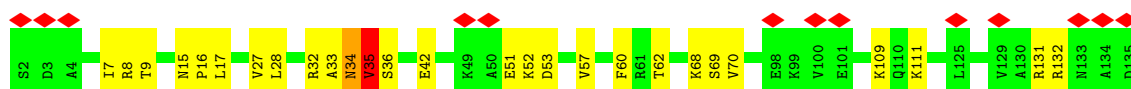
- Molecule 23: 40S ribosomal protein S22-A




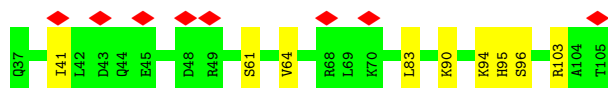
• Molecule 24: 40S ribosomal protein S23-A

Chain BX:  84% 15%


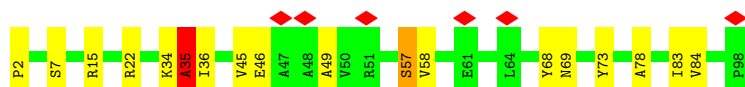
• Molecule 25: 40S ribosomal protein S24-A

Chain BY:  10% 80% 19%


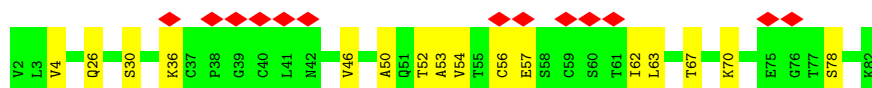
• Molecule 26: 40S ribosomal protein S25-A

Chain BZ:  12% 87% 13%


• Molecule 27: 40S ribosomal protein S26-A

Chain Ba:  6% 81% 16%


• Molecule 28: 40S ribosomal protein S27-A

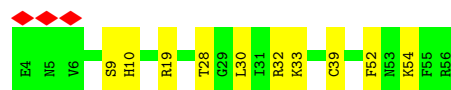
Chain Bb:  16% 80% 20%

• Molecule 29: 40S ribosomal protein S28-A

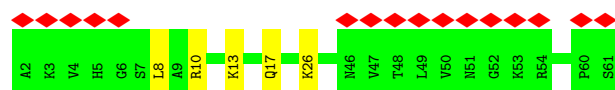
Chain Bc:  14% 90% 10%

• Molecule 30: 40S ribosomal protein S29-A

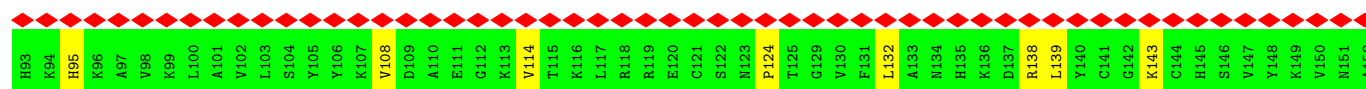
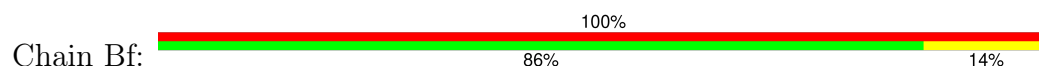
Chain Bd:  6% 81% 19%



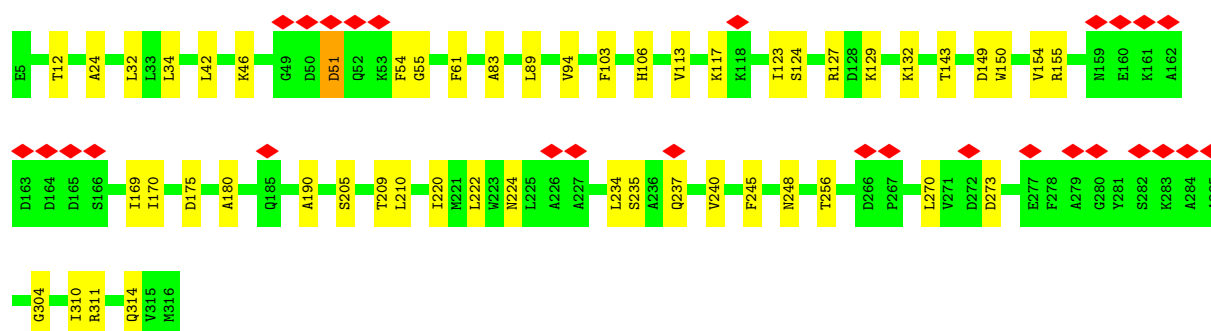
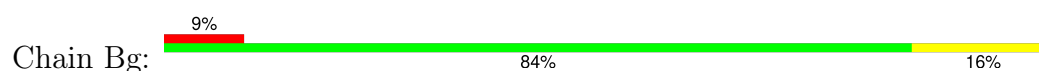
- Molecule 31: 40S ribosomal protein S30-A



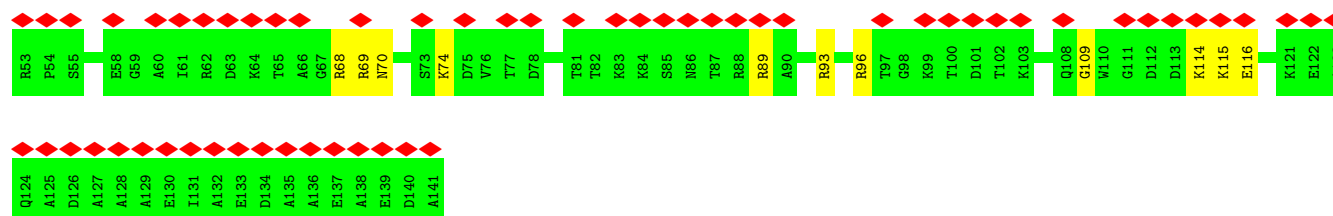
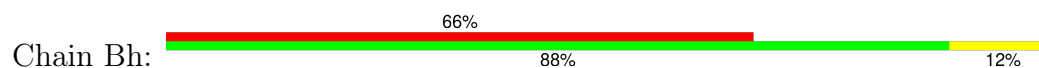
- Molecule 32: 40S ribosomal protein S31



- Molecule 33: Guanine nucleotide-binding protein subunit beta-like protein

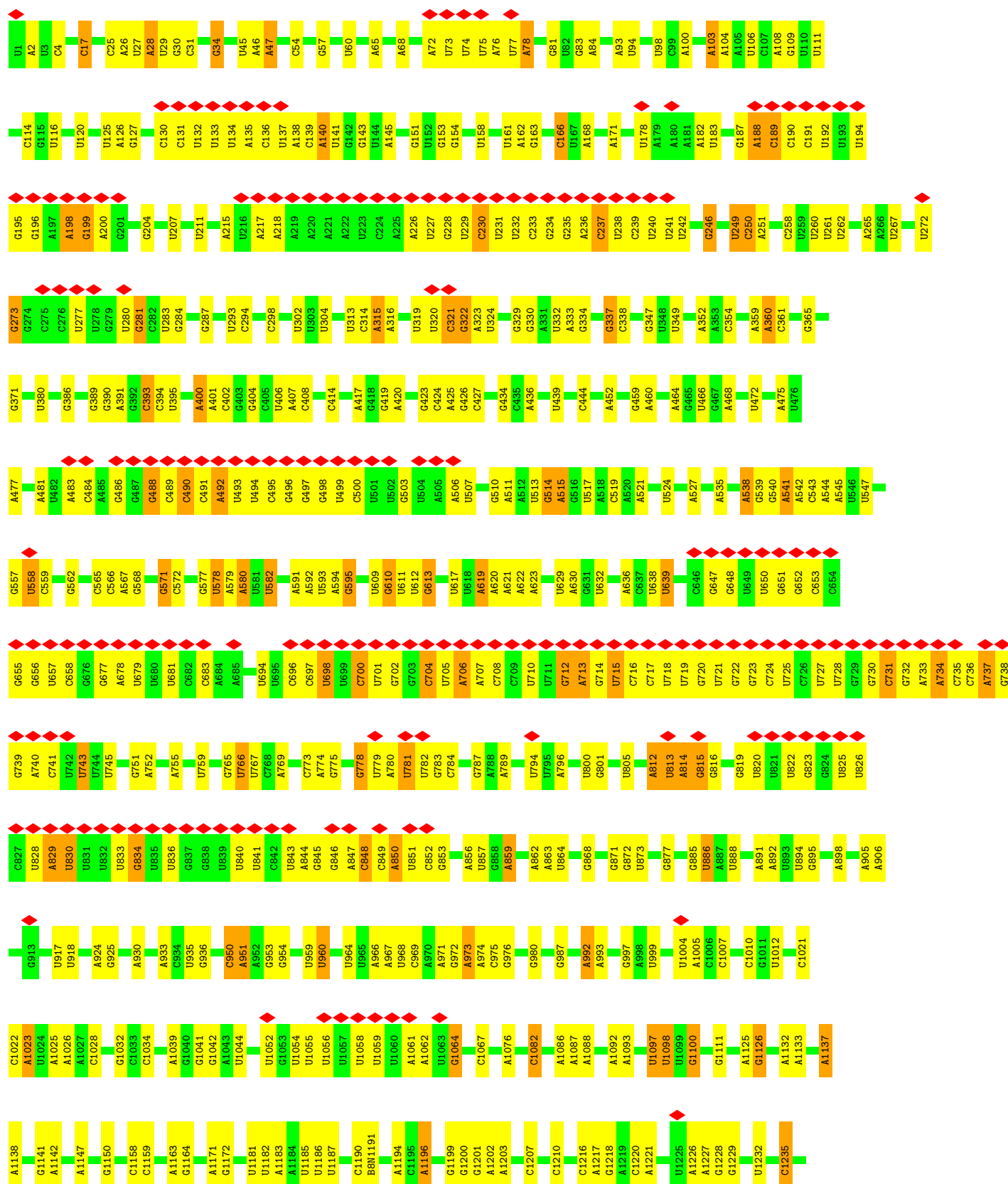


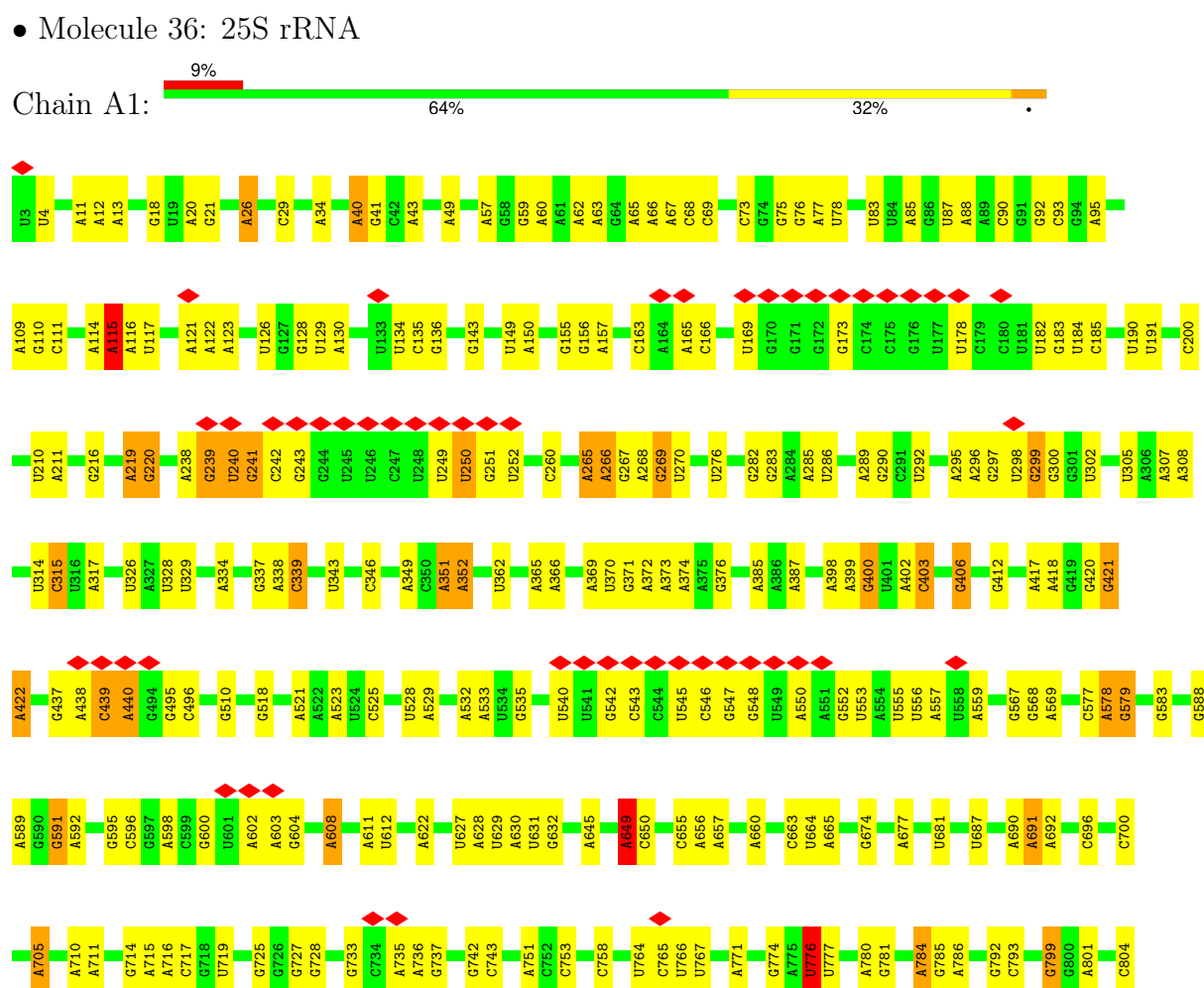
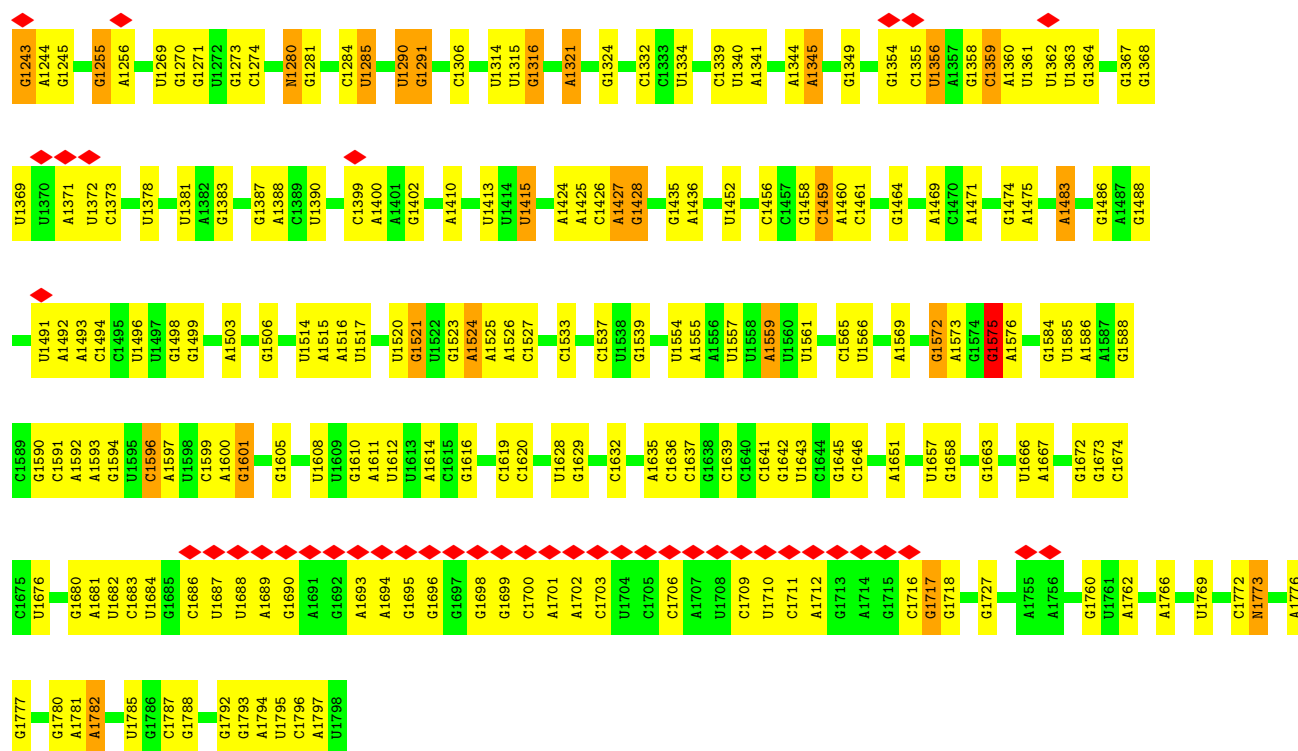
- Molecule 34: Suppressor protein STM1



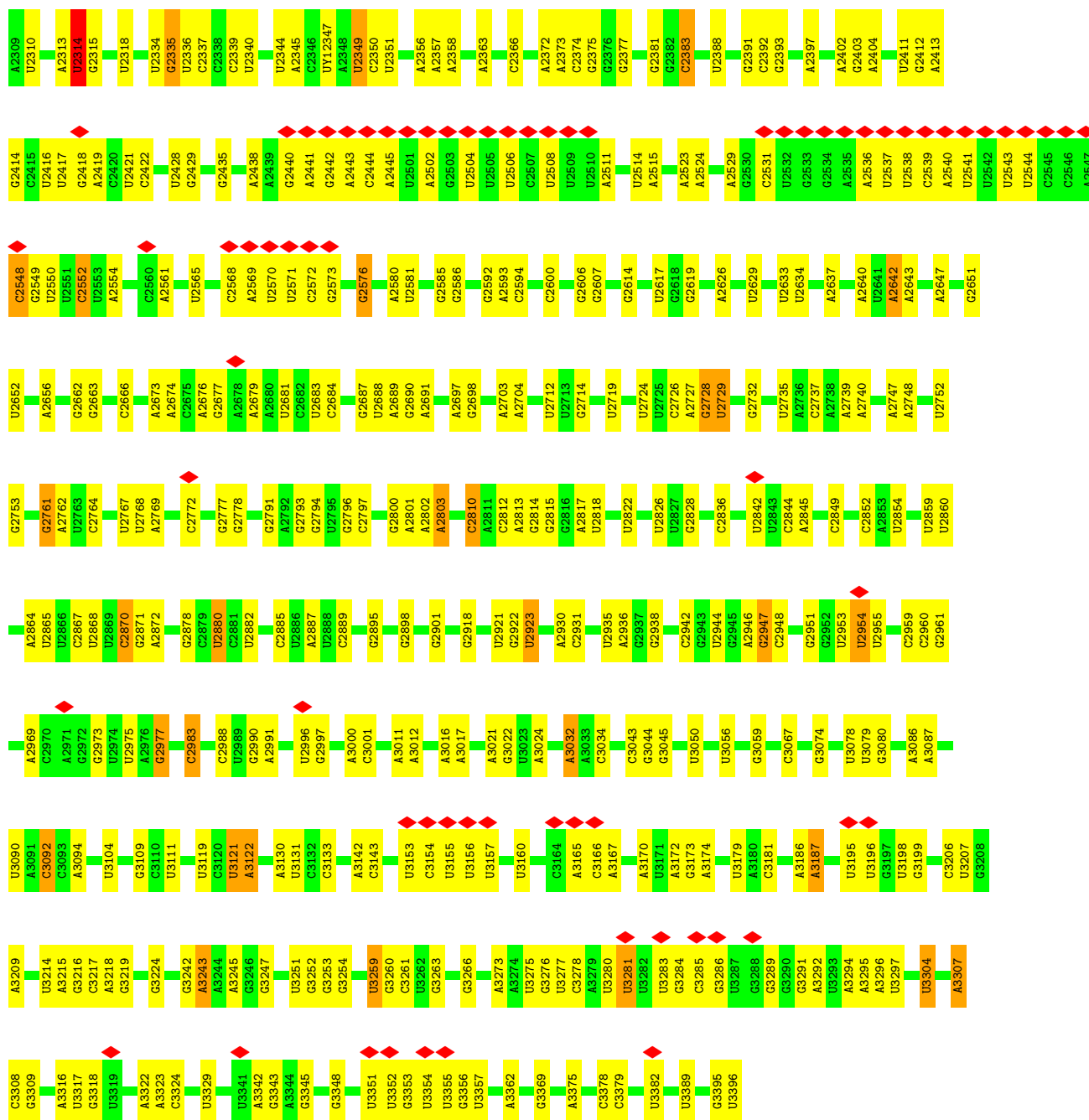
- Molecule 35: 18S rRNA



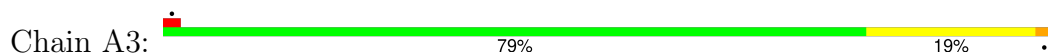






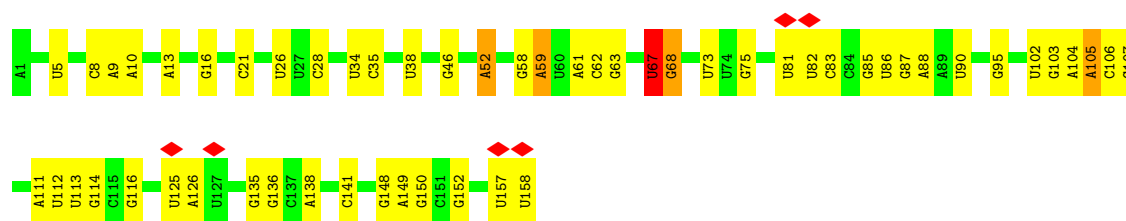


• Molecule 37: 5S rRNA

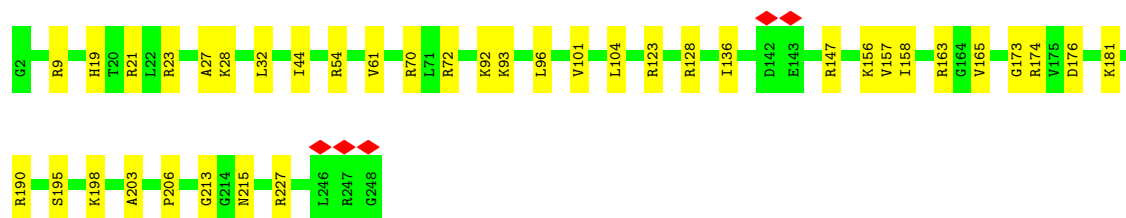
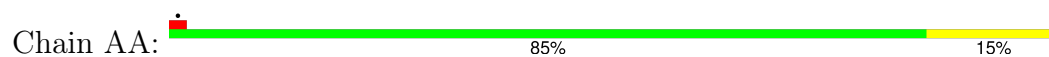


• Molecule 38: 5.8S rRNA

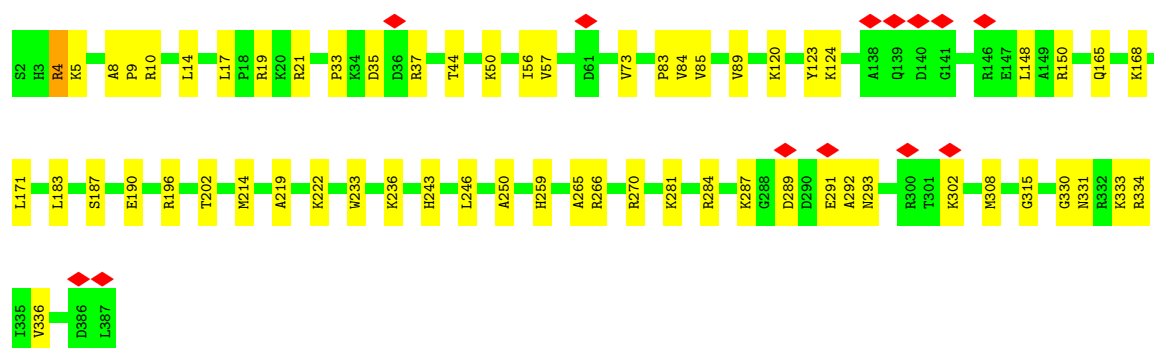
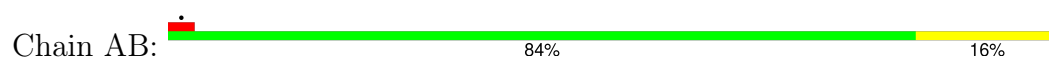




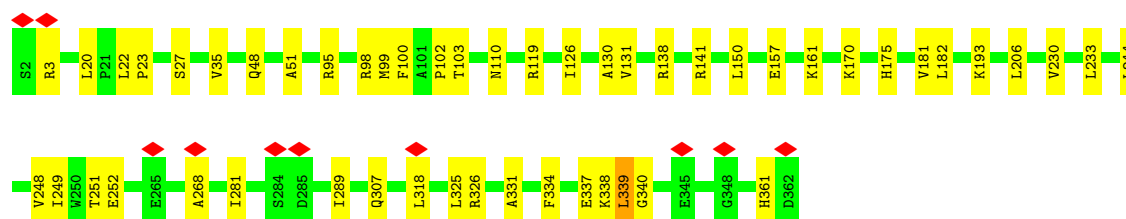
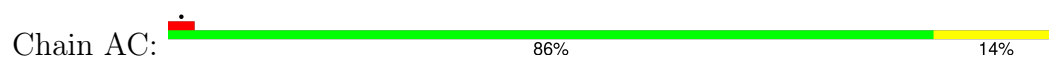
• Molecule 39: 60S ribosomal protein L2-A



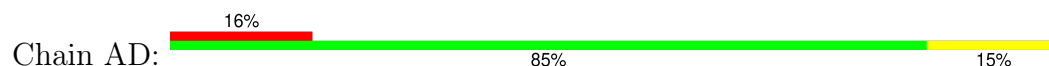
• Molecule 40: 60S ribosomal protein L3

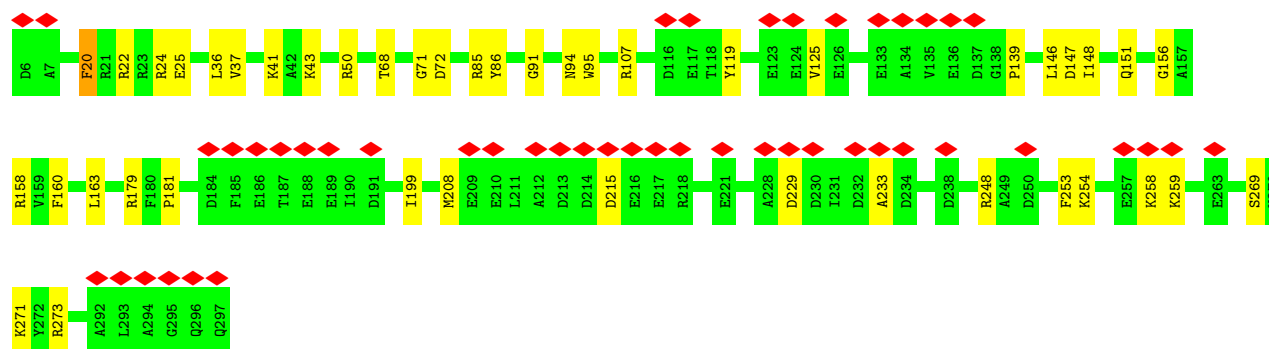


• Molecule 41: 60S ribosomal protein L4-A

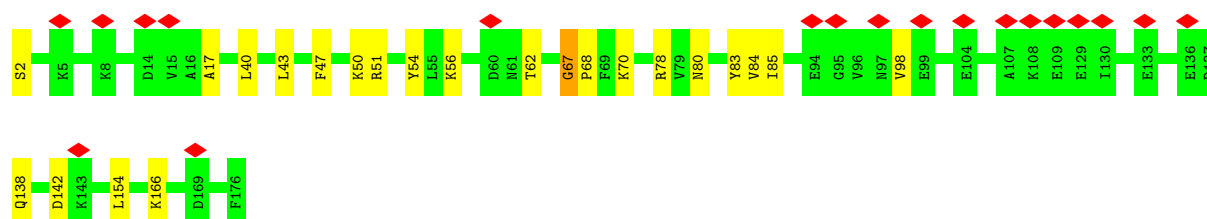
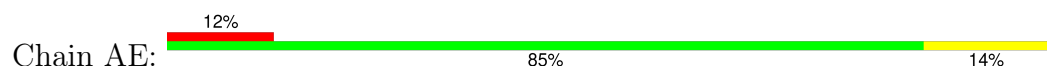


• Molecule 42: 60S ribosomal protein L5

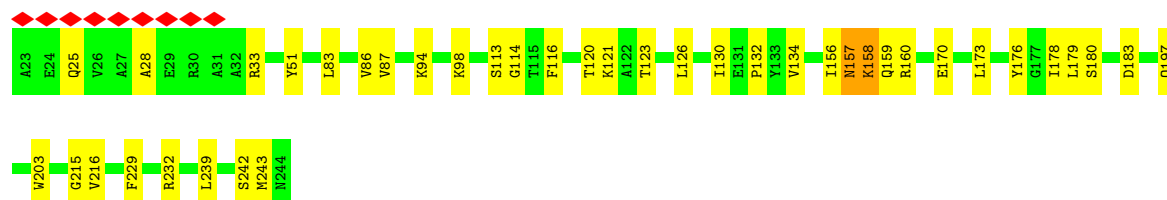
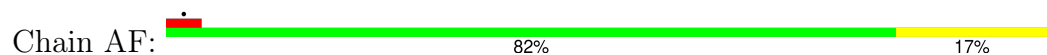




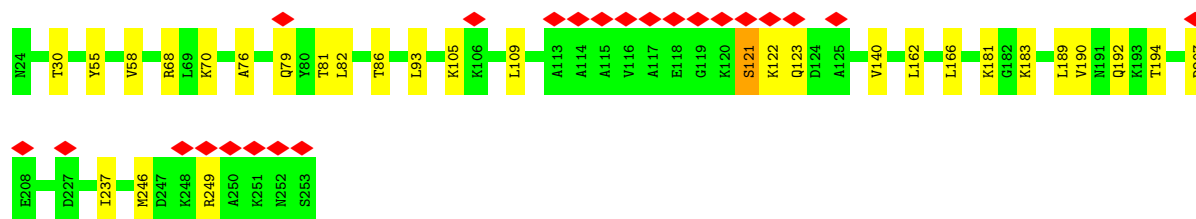
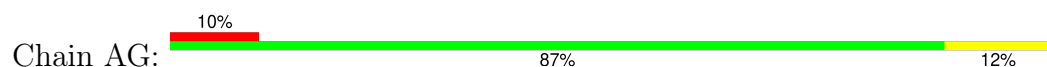
• Molecule 43: 60S ribosomal protein L6-A



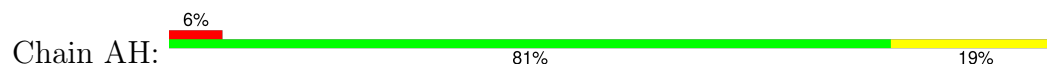
• Molecule 44: 60S ribosomal protein L7-A

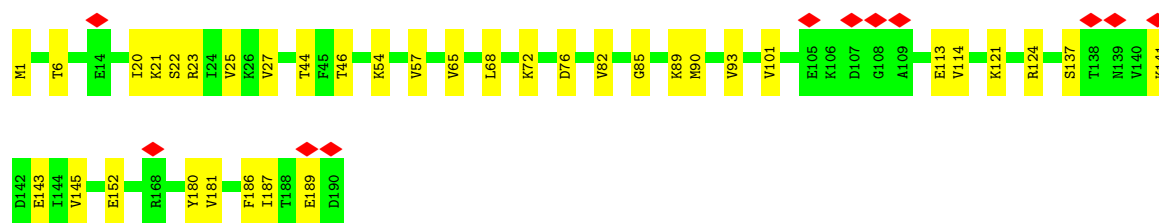


• Molecule 45: 60S ribosomal protein L8-A

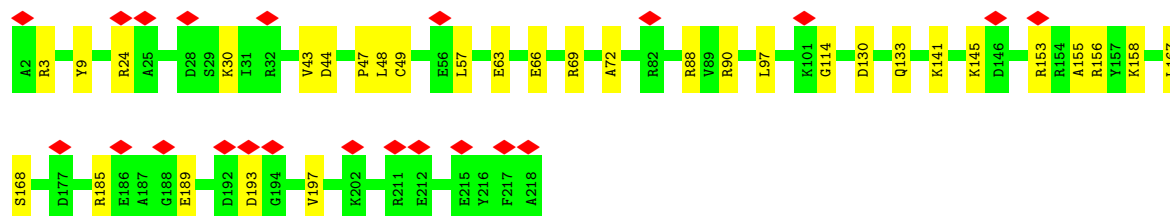
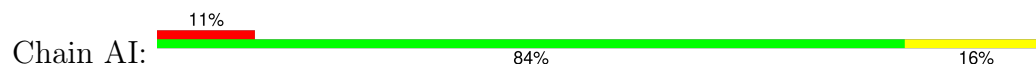


• Molecule 46: 60S ribosomal protein L9-A

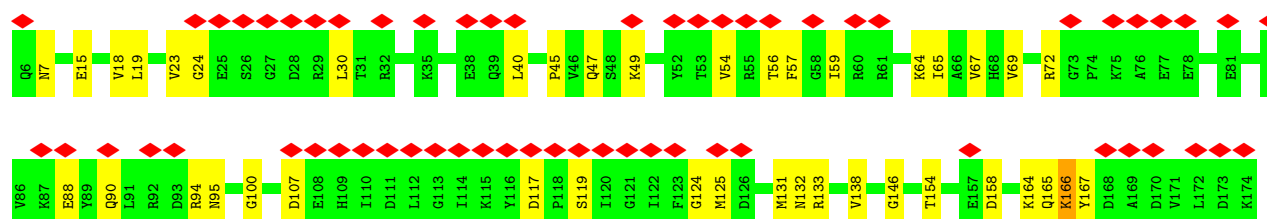
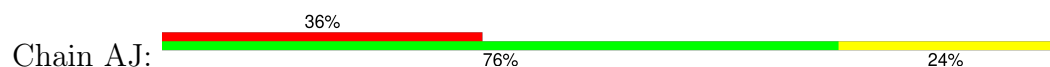




• Molecule 47: 60S ribosomal protein L10



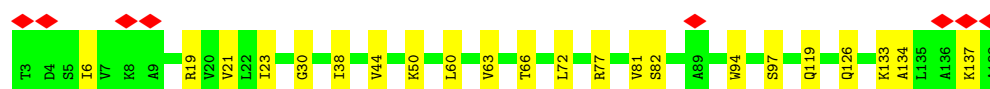
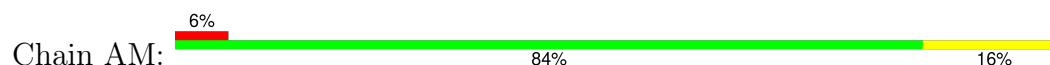
• Molecule 48: 60S ribosomal protein L11-A



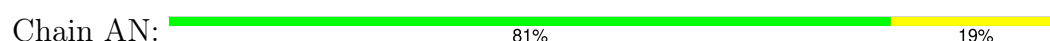
• Molecule 49: 60S ribosomal protein L13-A

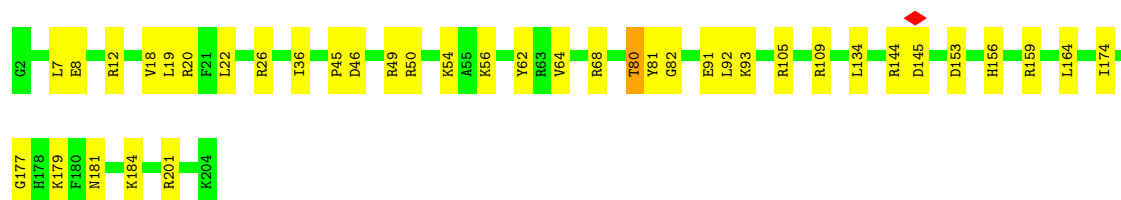


• Molecule 50: 60S ribosomal protein L14-A

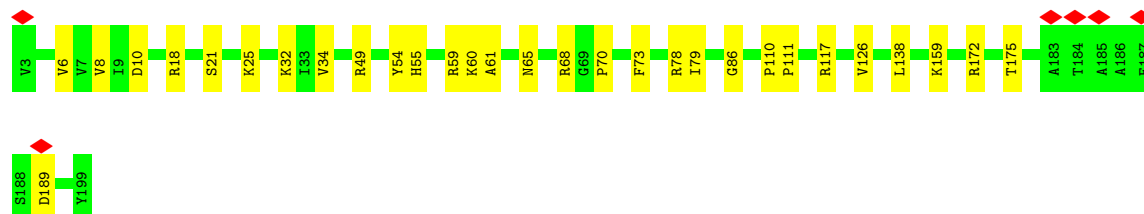
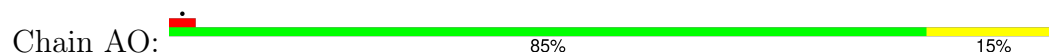


• Molecule 51: 60S ribosomal protein L15-A

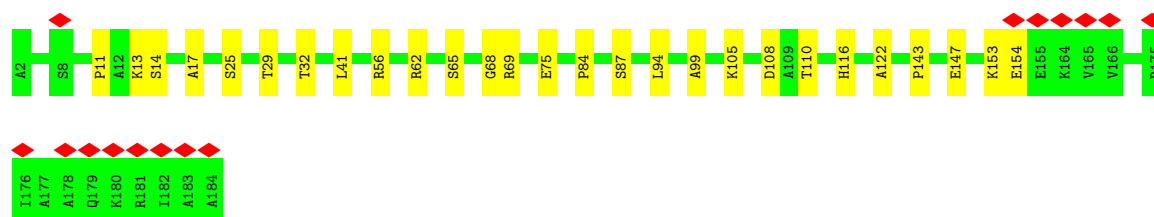
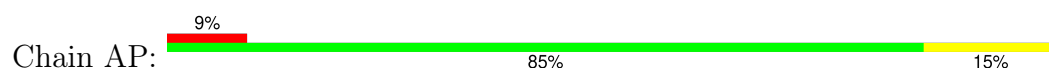




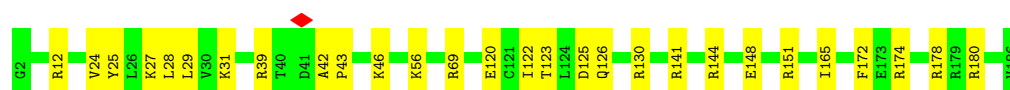
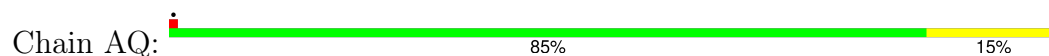
- Molecule 52: 60S ribosomal protein L16-A



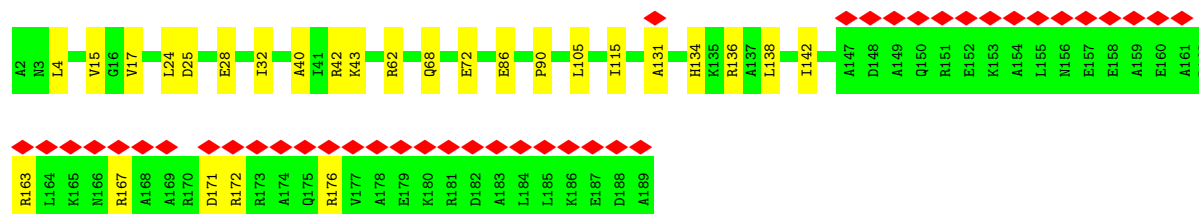
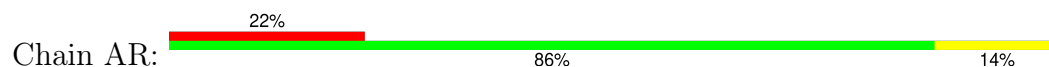
- Molecule 53: 60S ribosomal protein L17-A




- Molecule 54: 60S ribosomal protein L18-A

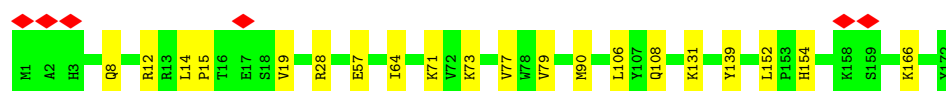


- Molecule 55: 60S ribosomal protein L19-A




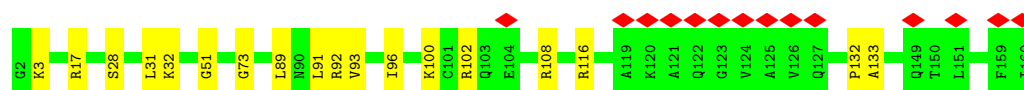
- Molecule 56: 60S ribosomal protein L20-A

Chain AS:  88% 12%




- Molecule 57: 60S ribosomal protein L21-A

Chain AT:  9% 89% 11%




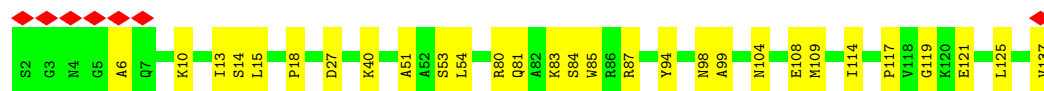
- Molecule 58: 60S ribosomal protein L22-A

Chain AU:  21% 85% 15%



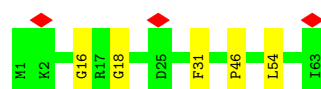
- Molecule 59: 60S ribosomal protein L23-A

Chain AV:  5% 79% 21%




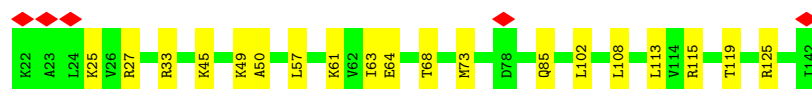
- Molecule 60: 60S ribosomal protein L24-A

Chain AW:  5% 92% 8%




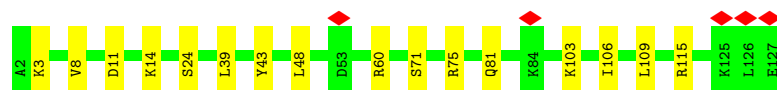
- Molecule 61: 60S ribosomal protein L25

Chain AX:  84% 16%

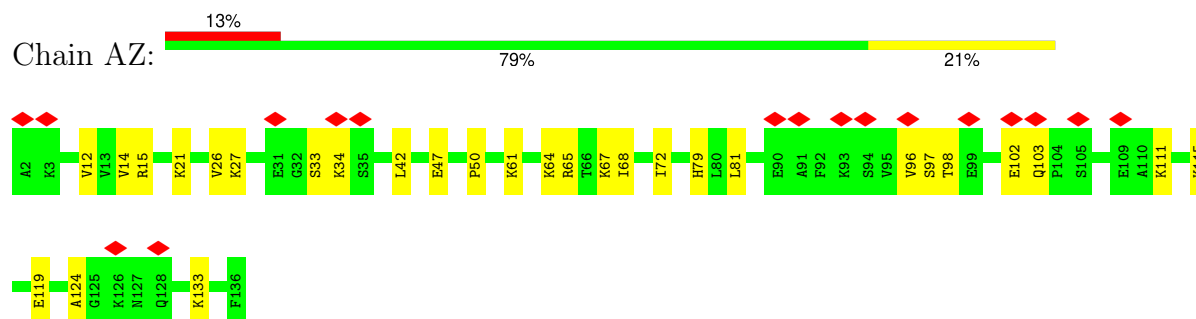


- Molecule 62: 60S ribosomal protein L26-A

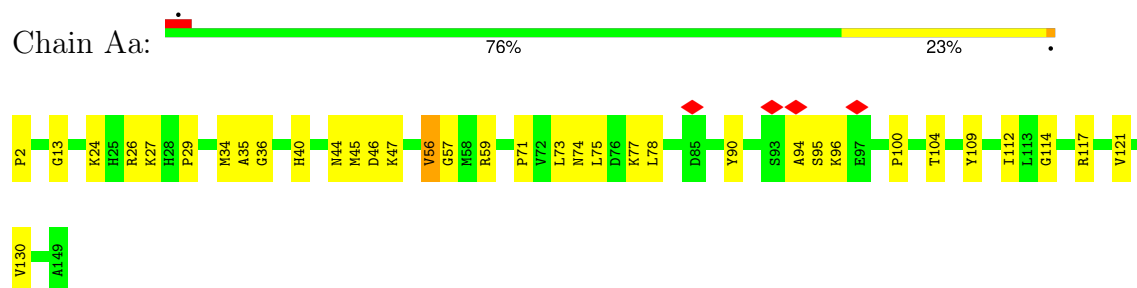
Chain AY:  87% 13%



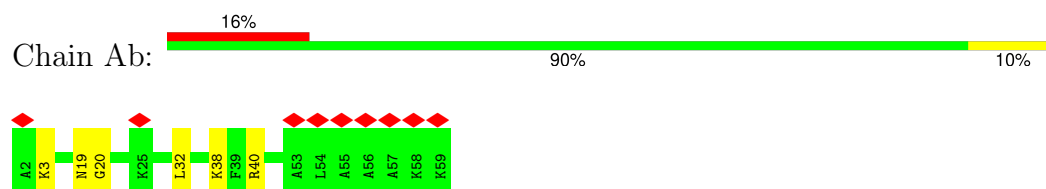
- Molecule 63: 60S ribosomal protein L27-A



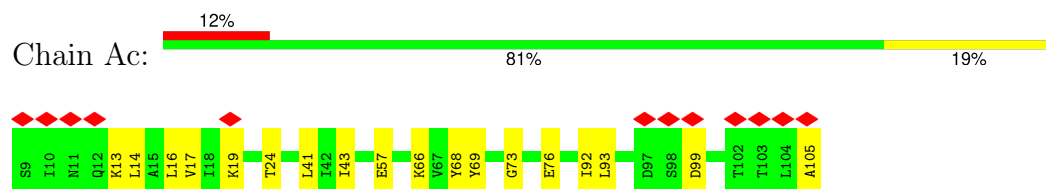
- Molecule 64: 60S ribosomal protein L28



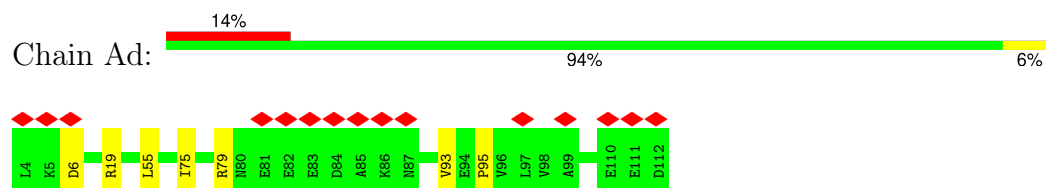
- Molecule 65: 60S ribosomal protein L29



- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32

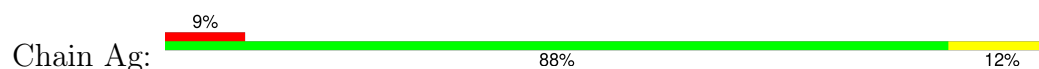




- Molecule 69: 60S ribosomal protein L33-A



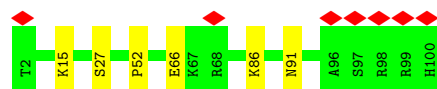
- Molecule 70: 60S ribosomal protein L34-A



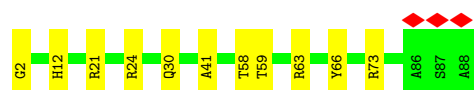
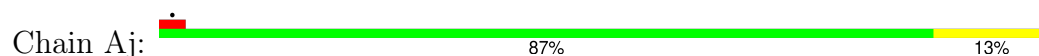
- Molecule 71: 60S ribosomal protein L35-A



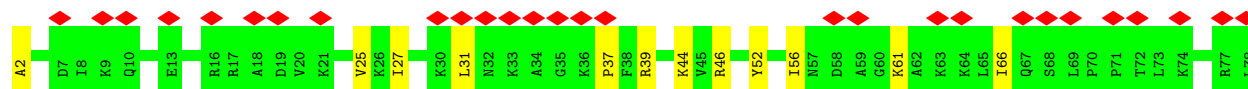
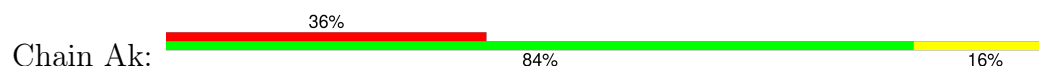
- Molecule 72: 60S ribosomal protein L36-A



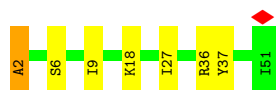
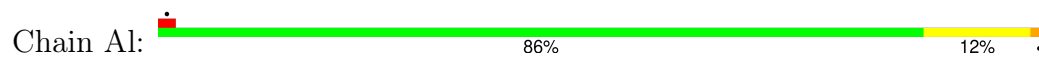
- Molecule 73: 60S ribosomal protein L37-A



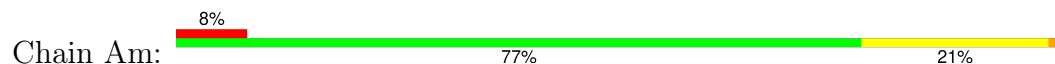
- Molecule 74: 60S ribosomal protein L38



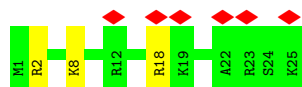
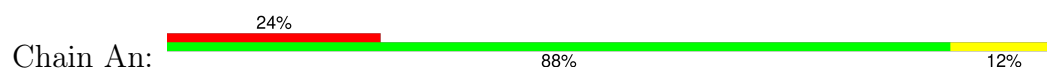
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: 60S ribosomal protein L40-A



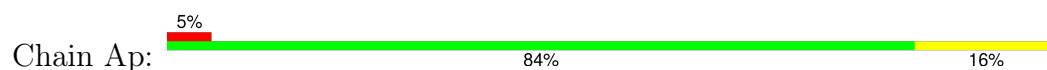
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	289345	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.428	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	463.968, 463.968, 463.968	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, B8N, 5MC, OMU, UR3, OMG, G7M, MG, UY1, HIC, 1MA, OMC, ZN, PSU, A2M, 4AC

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	BA	0.32	0/1653	0.63	0/2261
2	BB	0.34	0/1735	0.86	8/2335 (0.3%)
3	BC	0.35	0/1665	0.69	3/2263 (0.1%)
4	BD	0.34	0/1759	0.68	0/2368
5	BE	0.36	0/2109	0.69	0/2839
6	BF	0.37	0/1629	0.75	0/2202
7	BG	0.28	0/1844	0.68	1/2464 (0.0%)
8	BH	0.33	0/1506	0.76	2/2028 (0.1%)
9	BI	0.38	0/1514	0.82	2/2021 (0.1%)
10	BJ	0.32	0/1519	0.75	0/2035
11	BK	0.36	0/837	0.83	1/1131 (0.1%)
12	BL	0.33	0/1272	0.60	0/1712
13	BM	0.29	0/921	0.83	5/1245 (0.4%)
14	BN	0.32	0/1215	0.71	1/1638 (0.1%)
15	BO	0.37	0/952	0.84	4/1279 (0.3%)
16	BP	0.36	0/1012	0.74	1/1356 (0.1%)
17	BQ	0.39	0/1125	0.70	2/1510 (0.1%)
18	BR	0.36	0/984	0.68	0/1318
19	BS	0.39	0/1211	0.82	1/1628 (0.1%)
20	BT	0.42	0/1113	0.80	5/1494 (0.3%)
21	BU	0.36	0/865	0.64	0/1169
22	BV	0.32	0/692	0.64	0/932
23	BW	0.39	0/1038	0.63	0/1395
24	BX	0.36	0/1139	0.81	2/1518 (0.1%)
25	BY	0.34	0/1087	0.72	1/1449 (0.1%)
26	BZ	0.33	0/566	0.74	0/761
27	Ba	0.41	0/782	0.84	2/1047 (0.2%)
28	Bb	0.29	0/620	0.66	0/838
29	Bc	0.36	0/499	0.68	0/670
30	Bd	0.42	0/452	0.69	2/600 (0.3%)
31	Be	0.29	0/483	0.66	0/643
32	Bf	0.24	0/462	0.69	0/617

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Bg	0.34	0/2454	0.69	2/3340 (0.1%)
34	Bh	0.28	0/678	0.68	0/905
35	B5	0.39	0/41414	0.44	0/64521
36	A1	0.42	1/73484 (0.0%)	0.46	13/114569 (0.0%)
37	A3	0.35	0/2861	0.38	0/4457
38	A4	0.41	0/3723	0.45	1/5794 (0.0%)
39	AA	0.40	0/1912	0.64	0/2569
40	AB	0.41	0/3136	0.71	5/4213 (0.1%)
41	AC	0.38	0/2800	0.72	5/3790 (0.1%)
42	AD	0.31	0/2390	0.65	2/3225 (0.1%)
43	AE	0.33	0/1260	0.59	0/1694
44	AF	0.42	0/1821	0.73	0/2451
45	AG	0.32	0/1830	0.66	0/2469
46	AH	0.32	0/1531	0.62	0/2062
47	AI	0.32	0/1708	0.63	0/2290
48	AJ	0.31	0/1374	0.76	4/1842 (0.2%)
49	AL	0.37	0/1568	0.75	1/2106 (0.0%)
50	AM	0.33	0/1068	0.57	0/1438
51	AN	0.44	0/1757	0.75	0/2354
52	AO	0.41	0/1585	0.66	0/2128
53	AP	0.37	0/1410	0.63	0/1893
54	AQ	0.36	0/1465	0.68	1/1965 (0.1%)
55	AR	0.33	0/1538	0.63	0/2050
56	AS	0.40	0/1481	0.67	0/1990
57	AT	0.37	0/1300	0.69	0/1743
58	AU	0.29	0/812	0.68	1/1099 (0.1%)
59	AV	0.39	0/1018	0.63	0/1369
60	AW	0.34	0/533	0.60	0/707
61	AX	0.36	0/983	0.65	0/1325
62	AY	0.37	0/1004	0.60	0/1341
63	AZ	0.31	0/1118	0.69	2/1497 (0.1%)
64	Aa	0.44	0/1204	0.83	5/1612 (0.3%)
65	Ab	0.30	0/473	0.68	0/629
66	Ac	0.30	0/751	0.62	0/1008
67	Ad	0.33	0/904	0.60	0/1213
68	Ae	0.39	0/1041	0.63	0/1394
69	Af	0.46	0/868	0.66	0/1168
70	Ag	0.41	0/890	0.75	1/1189 (0.1%)
71	Ah	0.34	0/978	0.67	1/1301 (0.1%)
72	Ai	0.37	0/778	0.77	0/1034
73	Aj	0.43	0/696	0.68	0/923
74	Ak	0.32	0/618	0.60	0/826
75	Al	0.38	0/443	0.72	2/588 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Am	0.33	0/423	0.62	1/562 (0.2%)
77	An	0.36	0/234	0.75	0/300
78	Ao	0.33	0/860	0.58	0/1136
79	Ap	0.34	0/701	0.72	2/934 (0.2%)
All	All	0.39	1/211138 (0.0%)	0.56	92/309779 (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
2	BB	0	5
3	BC	0	2
5	BE	0	2
6	BF	0	2
7	BG	0	1
8	BH	0	3
9	BI	0	1
10	BJ	0	3
11	BK	0	3
12	BL	0	1
15	BO	0	1
17	BQ	0	3
19	BS	0	4
20	BT	0	1
24	BX	0	3
25	BY	0	1
27	Ba	0	4
35	B5	3	0
41	AC	0	2
42	AD	0	2
43	AE	0	1
44	AF	0	3
45	AG	0	5
46	AH	0	1
48	AJ	0	2
49	AL	0	2
51	AN	0	2
52	AO	0	1
55	AR	0	1
57	AT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	AZ	0	1
64	Aa	0	1
65	Ab	0	2
70	Ag	0	1
71	Ah	0	1
72	Ai	0	1
All	All	3	70

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2281	A2M	O3'-P	5.15	1.61	1.56

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	266	A	OP1-P-OP2	-13.71	78.48	119.60
36	A1	1948	G	O5'-P-OP1	-11.65	73.04	108.00
36	A1	266	A	O5'-P-OP1	-11.17	74.49	108.00
36	A1	265	A	OP2-P-O3'	-11.02	74.95	108.00
36	A1	1947	G	OP2-P-O3'	-9.98	78.07	108.00
40	AB	168	LYS	CA-C-N	9.26	154.35	121.59
40	AB	168	LYS	C-N-CA	9.26	154.35	121.59
36	A1	1947	G	OP1-P-O3'	-8.94	81.19	108.00
36	A1	266	A	O5'-P-OP2	8.84	134.52	108.00
36	A1	1948	G	O5'-P-OP2	-8.57	82.28	108.00
2	BB	147	ALA	CA-C-N	8.13	137.06	121.54
2	BB	147	ALA	C-N-CA	8.13	137.06	121.54
36	A1	265	A	OP1-P-O3'	7.95	131.84	108.00
11	BK	63	TYR	N-CA-C	7.76	122.11	111.71
64	Aa	47	LYS	CA-C-N	7.59	136.03	121.54
64	Aa	47	LYS	C-N-CA	7.59	136.03	121.54
15	BO	50	ALA	CA-C-N	7.18	133.81	122.61
15	BO	50	ALA	C-N-CA	7.18	133.81	122.61
16	BP	101	ALA	N-CA-C	6.86	119.59	111.02
36	A1	115	A	O5'-P-OP1	6.76	128.28	108.00
7	BG	68	LEU	CA-CB-CG	6.60	139.41	116.30
36	A1	1948	G	OP1-P-OP2	6.55	139.25	119.60
20	BT	52	GLY	CA-C-N	6.48	133.92	121.54
20	BT	52	GLY	C-N-CA	6.48	133.92	121.54
3	BC	145	GLY	CA-C-N	6.41	133.78	121.54
3	BC	145	GLY	C-N-CA	6.41	133.78	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Ba	35	ALA	CA-C-N	6.33	133.36	121.97
27	Ba	35	ALA	C-N-CA	6.33	133.36	121.97
64	Aa	56	VAL	N-CA-C	-6.31	96.21	109.34
15	BO	72	LYS	CA-C-N	6.31	137.62	126.45
15	BO	72	LYS	C-N-CA	6.31	137.62	126.45
49	AL	48	PRO	N-CA-C	6.21	125.27	112.47
41	AC	181	VAL	CA-C-N	6.17	133.33	121.54
41	AC	181	VAL	C-N-CA	6.17	133.33	121.54
36	A1	406	G	O4'-C1'-N9	6.11	117.37	108.20
8	BH	64	VAL	CA-CB-CG1	6.08	120.74	110.40
41	AC	337	GLU	CA-C-N	6.00	133.00	121.54
41	AC	337	GLU	C-N-CA	6.00	133.00	121.54
3	BC	146	THR	N-CA-C	-6.00	98.03	110.80
9	BI	152	ILE	CB-CA-C	5.96	116.77	111.71
33	Bg	117	LYS	CA-C-N	5.90	136.57	125.66
33	Bg	117	LYS	C-N-CA	5.90	136.57	125.66
14	BN	22	ALA	C-N-CD	-5.82	107.79	120.60
17	BQ	31	VAL	CA-C-N	5.79	132.60	121.54
17	BQ	31	VAL	C-N-CA	5.79	132.60	121.54
64	Aa	77	LYS	CA-C-N	5.75	132.53	121.54
64	Aa	77	LYS	C-N-CA	5.75	132.53	121.54
25	BY	35	VAL	CG1-CB-CG2	-5.74	98.17	110.80
24	BX	96	VAL	CA-C-N	5.71	132.45	121.54
24	BX	96	VAL	C-N-CA	5.71	132.45	121.54
63	AZ	102	GLU	CA-C-N	5.71	135.72	121.80
63	AZ	102	GLU	C-N-CA	5.71	135.72	121.80
13	BM	105	LYS	CA-C-N	5.65	128.17	120.77
13	BM	105	LYS	C-N-CA	5.65	128.17	120.77
20	BT	29	GLU	CA-CB-CG	5.65	125.40	114.10
13	BM	89	ILE	N-CA-C	-5.59	107.37	112.96
36	A1	1314	C	C2'-C3'-O3'	5.53	122.00	113.70
13	BM	38	HIS	CA-C-N	5.53	132.10	121.54
13	BM	38	HIS	C-N-CA	5.53	132.10	121.54
79	Ap	51	ALA	CA-C-N	5.52	132.08	121.54
79	Ap	51	ALA	C-N-CA	5.52	132.08	121.54
30	Bd	9	SER	CA-C-N	5.43	136.00	122.74
30	Bd	9	SER	C-N-CA	5.43	136.00	122.74
40	AB	4	ARG	CA-C-N	5.36	131.77	121.54
40	AB	4	ARG	C-N-CA	5.36	131.77	121.54
41	AC	182	LEU	CA-CB-CG	5.36	135.04	116.30
70	Ag	96	GLU	N-CA-CB	5.30	118.50	110.28
75	Al	2	ALA	CA-C-N	5.30	131.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	Al	2	ALA	C-N-CA	5.30	131.66	121.54
2	BB	176	VAL	CA-C-N	5.27	131.60	121.54
2	BB	176	VAL	C-N-CA	5.27	131.60	121.54
2	BB	48	VAL	CA-C-N	5.26	134.29	122.19
2	BB	48	VAL	C-N-CA	5.26	134.29	122.19
54	AQ	180	ARG	CA-CB-CG	5.25	124.59	114.10
38	A4	67	U	C2'-C3'-O3'	5.24	121.56	113.70
2	BB	206	PRO	CA-C-N	5.22	131.51	121.54
2	BB	206	PRO	C-N-CA	5.22	131.51	121.54
42	AD	229	ASP	CA-C-N	5.22	131.51	121.54
42	AD	229	ASP	C-N-CA	5.22	131.51	121.54
76	Am	79	GLU	CA-CB-CG	5.17	124.44	114.10
48	AJ	94	ARG	CA-C-N	5.16	131.40	121.54
48	AJ	94	ARG	C-N-CA	5.16	131.40	121.54
40	AB	10	ARG	CG-CD-NE	-5.16	100.64	112.00
9	BI	61	GLU	CA-CB-CG	5.16	124.42	114.10
19	BS	117	LYS	CA-CB-CG	5.13	124.36	114.10
71	Ah	10	ARG	CA-CB-CG	5.13	124.35	114.10
8	BH	28	GLU	N-CA-CB	5.12	117.99	110.57
20	BT	38	LYS	CA-C-N	5.06	131.20	121.54
20	BT	38	LYS	C-N-CA	5.06	131.20	121.54
48	AJ	167	TYR	CA-C-N	5.02	131.13	121.54
48	AJ	167	TYR	C-N-CA	5.02	131.13	121.54
58	AU	89	LEU	CA-CB-CG	5.00	133.81	116.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	B5	1575	G7M	C2',C3',C4'

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	AC	130	ALA	Peptide
41	AC	318	LEU	Peptide
42	AD	258	LYS	Peptide
42	AD	43	LYS	Peptide
43	AE	67	GLY	Peptide
44	AF	157	ASN	Peptide
44	AF	215	GLY	Peptide
44	AF	232	ARG	Peptide
45	AG	121	SER	Peptide

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Mol	Chain	Res	Type	Group
45	AG	123	GLN	Peptide
45	AG	30	THR	Peptide
45	AG	76	ALA	Peptide
45	AG	79	GLN	Peptide
46	AH	21	LYS	Peptide
48	AJ	164	LYS	Peptide
48	AJ	166	LYS	Peptide
49	AL	47	ALA	Peptide
49	AL	75	PHE	Peptide
51	AN	80	THR	Peptide
51	AN	92	LEU	Peptide
52	AO	110[A]	PRO	Peptide
55	AR	131	ALA	Peptide
57	AT	17	ARG	Peptide
63	AZ	124	ALA	Peptide
64	Aa	46	ASP	Peptide
65	Ab	19	ASN	Peptide
65	Ab	20	GLY	Peptide
70	Ag	80	ARG	Peptide
71	Ah	90	ARG	Peptide
72	Ai	27	SER	Peptide
2	BB	177	GLN	Peptide
2	BB	206	PRO	Peptide
2	BB	208	GLN	Peptide
2	BB	212	VAL	Peptide
2	BB	222	LYS	Peptide
3	BC	144	TRP	Peptide
3	BC	145	GLY	Peptide
5	BE	195	ILE	Peptide
5	BE	199	GLU	Peptide
6	BF	100	ASN	Peptide
6	BF	42	LEU	Peptide
7	BG	68	LEU	Peptide
8	BH	110	GLN	Peptide
8	BH	111	LYS	Peptide
8	BH	64	VAL	Peptide
9	BI	51	GLY	Peptide
10	BJ	117	GLY	Peptide
10	BJ	137	GLY	Peptide
10	BJ	163	PRO	Peptide
11	BK	2	LEU	Peptide
11	BK	53	GLY	Peptide

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Mol	Chain	Res	Type	Group
11	BK	63	TYR	Peptide
12	BL	5	LEU	Peptide
15	BO	123	SER	Peptide
17	BQ	32	ASN	Peptide
17	BQ	33	GLY	Peptide
17	BQ	40	GLU	Peptide
19	BS	101	LEU	Peptide
19	BS	56	LYS	Peptide
19	BS	81	ILE	Peptide
19	BS	90	ASN	Peptide
20	BT	51	GLU	Peptide
24	BX	138	GLU	Peptide
24	BX	88	PRO	Peptide
24	BX	96	VAL	Peptide
25	BY	34	ASN	Peptide
27	Ba	34	LYS	Peptide
27	Ba	35	ALA	Peptide
27	Ba	57	SER	Peptide
27	Ba	7	SER	Peptide

5.2 Too-close contacts

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	BA	1612	0	1623	29	0
2	BB	1709	0	1784	37	0
3	BC	1635	0	1723	18	0
4	BD	1734	0	1817	26	0
5	BE	2068	0	2154	34	0
6	BF	1609	0	1675	20	0
7	BG	1820	0	1917	25	0
8	BH	1481	0	1572	18	0
9	BI	1489	0	1525	33	0
10	BJ	1494	0	1573	21	0
11	BK	817	0	804	12	0
12	BL	1244	0	1314	11	0
13	BM	913	0	955	13	0
14	BN	1192	0	1255	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	BO	941	0	979	21	0
16	BP	991	0	1035	15	0
17	BQ	1105	0	1166	18	0
18	BR	975	0	1039	12	0
19	BS	1192	0	1222	24	0
20	BT	1095	0	1114	14	0
21	BU	855	0	917	10	0
22	BV	684	0	671	15	0
23	BW	1021	0	1060	16	0
24	BX	1121	0	1196	14	0
25	BY	1073	0	1132	19	0
26	BZ	558	0	598	6	0
27	Ba	769	0	818	11	0
28	Bb	610	0	631	10	0
29	Bc	497	0	535	5	0
30	Bd	442	0	432	7	0
31	Be	475	0	525	4	0
32	Bf	454	0	468	5	0
33	Bg	2401	0	2356	29	0
34	Bh	675	0	654	10	0
35	B5	37850	0	19060	265	0
36	A1	67139	0	33772	380	0
37	A3	2579	0	1304	10	0
38	A4	3353	0	1696	19	0
39	AA	1878	0	1945	26	0
40	AB	3078	0	3149	46	0
41	AC	2748	0	2859	35	0
42	AD	2341	0	2290	27	0
43	AE	1239	0	1326	16	0
44	AF	1784	0	1862	22	0
45	AG	1798	0	1894	15	0
46	AH	1510	0	1576	23	0
47	AI	1672	0	1711	21	0
48	AJ	1353	0	1383	23	0
49	AL	1543	0	1608	9	0
50	AM	1053	0	1149	14	0
51	AN	1720	0	1779	31	0
52	AO	1555	0	1659	21	0
53	AP	1388	0	1423	20	0
54	AQ	1441	0	1543	19	0
55	AR	1521	0	1617	15	0
56	AS	1445	0	1487	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AT	1276	0	1323	14	0
58	AU	796	0	812	8	0
59	AV	1003	0	1048	21	0
60	AW	521	0	551	3	0
61	AX	968	0	1036	13	0
62	AY	993	0	1081	8	0
63	AZ	1092	0	1155	16	0
64	Aa	1173	0	1215	23	0
65	Ab	462	0	491	3	0
66	Ac	743	0	797	11	0
67	Ad	890	0	938	4	0
68	Ae	1020	0	1089	11	0
69	Af	850	0	880	4	0
70	Ag	880	0	945	9	0
71	Ah	969	0	1078	6	0
72	Ai	771	0	849	4	0
73	Aj	681	0	687	9	0
74	Ak	612	0	682	8	0
75	Al	436	0	474	6	0
76	Am	417	0	459	9	0
77	An	233	0	284	5	0
78	Ao	847	0	914	7	0
79	Ap	694	0	738	9	0
80	A1	541	0	0	0	0
80	A3	3	0	0	0	0
80	A4	18	0	0	0	0
80	AA	2	0	0	0	0
80	AB	5	0	0	0	0
80	AC	6	0	0	0	0
80	AF	1	0	0	0	0
80	AG	1	0	0	0	0
80	AI	2	0	0	0	0
80	AL	2	0	0	0	0
80	AM	1	0	0	0	0
80	AN	5	0	0	0	0
80	AO	2	0	0	0	0
80	AP	2	0	0	0	0
80	AQ	3	0	0	0	0
80	AR	3	0	0	0	0
80	AS	3	0	0	0	0
80	AY	1	0	0	0	0
80	Aa	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Ad	2	0	0	0	0
80	Ae	3	0	0	0	0
80	Af	2	0	0	0	0
80	Ai	1	0	0	0	0
80	Aj	5	0	0	0	0
80	Am	1	0	0	0	0
80	Ao	2	0	0	0	0
80	B5	122	0	0	0	0
80	BJ	1	0	0	0	0
80	BT	1	0	0	0	0
80	Be	1	0	0	0	0
81	Ao	1	0	0	0	0
81	Bb	1	0	0	0	0
All	All	199813	0	147857	1474	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 4.

All (1474) 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)
36:A1:437:G:H1	36:A1:622:A:N6	1.61	0.98
35:B5:868:G:H1	35:B5:960:U:H3	1.06	0.97
35:B5:1588:G:H1	35:B5:1608:U:H3	1.08	0.94
36:A1:3348:G:H1	36:A1:3357:U:H3	1.10	0.94
23:BW:2:THR:N	35:B5:1034:C:HO2'	1.71	0.87
36:A1:437:G:H1	36:A1:622:A:H61	0.87	0.87
36:A1:2257:C:N4	36:A1:2259:A:C5	2.50	0.79
18:BR:24:LEU:HB3	18:BR:34:LEU:HD11	1.67	0.76
36:A1:2257:C:H42	36:A1:2259:A:N6	1.85	0.74
36:A1:2257:C:C4	36:A1:2259:A:N7	2.55	0.74
44:AF:87:VAL:HG11	44:AF:243:MET:HE1	1.72	0.71
59:AV:81:GLN:O	59:AV:98:ASN:ND2	2.23	0.71
5:BE:87:MET:HE1	5:BE:236:ILE:HD13	1.72	0.70
16:BP:58:LYS:HZ1	35:B5:1243:G:H1	1.38	0.69
17:BQ:14:LYS:NZ	35:B5:1610:G:N7	2.41	0.69
36:A1:2257:C:N4	36:A1:2259:A:N6	2.40	0.69
36:A1:2969:A:N7	39:AA:215:ASN:ND2	2.41	0.69
40:AB:291:GLU:HG3	40:AB:302:LYS:HD2	1.75	0.69
36:A1:1213:G:H4'	56:AS:90:MET:HG3	1.74	0.69
4:BD:141:LYS:HE2	4:BD:179:GLN:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B5:1585:U:H3	35:B5:1611:A:H2	1.40	0.68
41:AC:334:PHE:HA	41:AC:339:LEU:HD12	1.75	0.68
45:AG:81:THR:HG21	45:AG:181:LYS:HG3	1.75	0.68
35:B5:1339:C:O2'	35:B5:1341:A:N7	2.27	0.67
36:A1:3343:G:H21	36:A1:3362:A:H2	1.43	0.67
35:B5:514:G:H1	35:B5:543:C:H5	1.41	0.67
6:BF:64:VAL:HG23	6:BF:65:ARG:HG2	1.77	0.66
19:BS:144:ARG:HH22	35:B5:1171:A:H5''	1.59	0.66
36:A1:2673:A:H5''	48:AJ:95:ASN:HD22	1.59	0.66
35:B5:1356:U:H3	35:B5:1367:G:H1	1.41	0.66
36:A1:1317:A:O2'	52:AO:18[A]:ARG:NH2	2.28	0.66
41:AC:99:MET:HE3	41:AC:102:PRO:HA	1.77	0.66
33:Bg:89:LEU:HB2	33:Bg:103:PHE:HB2	1.77	0.65
36:A1:1448:U:H2'	36:A1:1449:A2M:H8	1.78	0.65
35:B5:1291:G:H22	35:B5:1324:G:H22	1.45	0.65
36:A1:687:U:OP2	49:AL:36:ARG:NH2	2.30	0.65
36:A1:2257:C:N4	36:A1:2259:A:C6	2.64	0.65
36:A1:2257:C:N4	36:A1:2259:A:H62	1.95	0.65
48:AJ:15:GLU:OE1	48:AJ:72:ARG:NH1	2.28	0.65
15:BO:16:VAL:O	15:BO:30:VAL:HA	1.97	0.65
9:BI:37:LYS:HB2	9:BI:59:ARG:HG2	1.79	0.64
23:BW:31:SER:H	23:BW:34:ILE:HD12	1.61	0.64
40:AB:50:LYS:NZ	40:AB:330:GLY:O	2.30	0.64
36:A1:2392:C:O2'	40:AB:266:ARG:NH2	2.29	0.64
36:A1:2176:U:OP1	39:AA:54:ARG:NH2	2.30	0.64
48:AJ:133:ARG:NH2	48:AJ:158:ASP:OD2	2.31	0.64
57:AT:73:GLY:HA2	57:AT:89:LEU:O	1.98	0.64
36:A1:2673:A:N1	36:A1:2681:U:C4	2.66	0.64
42:AD:148:ILE:HB	42:AD:151:GLN:HE21	1.62	0.64
16:BP:18:ARG:NH1	19:BS:90:ASN:O	2.32	0.63
6:BF:98:MET:HE1	35:B5:1610:G:H4'	1.81	0.63
51:AN:159:ARG:HB3	51:AN:164:LEU:HB2	1.81	0.63
9:BI:84:HIS:HE2	9:BI:97:THR:HG1	1.48	0.62
36:A1:792:G:H5''	64:Aa:2:PRO:HG3	1.80	0.62
36:A1:2366:C:OP1	40:AB:259:HIS:NE2	2.31	0.62
41:AC:110:ASN:HD22	51:AN:201:ARG:HB3	1.65	0.62
36:A1:178:U:O4	36:A1:238:A:N7	2.31	0.62
52:AO:61[A]:ALA:HA	52:AO:70[A]:PRO:HD2	1.80	0.62
3:BC:56:ILE:HG23	3:BC:61:LEU:HB2	1.82	0.61
36:A1:3297:U:O4	40:AB:124:LYS:NZ	2.34	0.61
58:AU:56:VAL:HG22	58:AU:65:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:101:VAL:HG22	3:BC:115:ILE:HG12	1.82	0.61
10:BJ:119:ALA:O	10:BJ:124:HIS:ND1	2.33	0.61
8:BH:50:ASP:HA	8:BH:56:LYS:HG2	1.82	0.61
24:BX:70:LYS:NZ	35:B5:567:A:OP1	2.33	0.61
26:BZ:95:HIS:ND1	26:BZ:96:SER:O	2.32	0.61
53:AP:122:ALA:HB3	53:AP:143:PRO:HB2	1.81	0.61
21:BU:82:TYR:HB3	30:Bd:52:PHE:HB3	1.83	0.61
41:AC:20:LEU:HD11	41:AC:252:GLU:HG3	1.82	0.61
4:BD:164:VAL:HA	4:BD:168:ILE:HD12	1.83	0.60
5:BE:54:TYR:O	25:BY:15:ASN:ND2	2.34	0.60
5:BE:129:VAL:HG22	5:BE:139:VAL:HG12	1.83	0.60
48:AJ:88:GLU:O	48:AJ:90:GLN:NE2	2.33	0.60
13:BM:42:ALA:HB3	13:BM:122:VAL:HB	1.82	0.60
35:B5:992:A:O2'	35:B5:1785:U:O2	2.19	0.60
36:A1:714:G:HO2'	36:A1:753:C:HO2'	1.49	0.60
2:BB:168:ILE:HG12	2:BB:197:ILE:HD12	1.83	0.60
17:BQ:32:ASN:O	17:BQ:68:ARG:NH1	2.34	0.60
18:BR:7:LYS:HD2	18:BR:11:ARG:HH21	1.66	0.60
25:BY:34:ASN:O	35:B5:521:A:O2'	2.19	0.60
36:A1:1613:A:OP1	74:Ak:2:ALA:N	2.33	0.60
39:AA:104:LEU:HD22	39:AA:136:ILE:HD11	1.83	0.60
44:AF:173:LEU:HB3	44:AF:178:ILE:HB	1.82	0.60
13:BM:60:VAL:HG12	13:BM:122:VAL:HG22	1.84	0.60
36:A1:728:G:H5''	54:AQ:43:PRO:HB2	1.83	0.60
60:AW:46:PRO:HB2	60:AW:54:LEU:HD23	1.83	0.60
34:Bh:70:ASN:C	34:Bh:70:ASN:HD22	2.09	0.60
35:B5:1159:C:N4	35:B5:1285:U:OP1	2.35	0.60
36:A1:1193:A:OP2	52:AO:49[A]:ARG:NH1	2.35	0.60
36:A1:1389:G:H5''	68:Ae:101:SER:HB3	1.82	0.60
40:AB:287:LYS:O	40:AB:293:ASN:ND2	2.35	0.60
36:A1:2138:A:HO2'	73:Aj:2:GLY:N	1.99	0.60
42:AD:50:ARG:NH1	42:AD:147:ASP:OD2	2.35	0.60
36:A1:1348:U:OP1	54:AQ:39:ARG:NH1	2.34	0.60
66:Ac:41:LEU:HD13	66:Ac:66:LYS:HZ2	1.67	0.60
7:BG:70:PRO:HA	7:BG:98:ARG:HH22	1.67	0.59
55:AR:68:GLN:NE2	55:AR:72:GLU:OE2	2.35	0.59
35:B5:812:A:H62	35:B5:859:A:H5'	1.67	0.59
10:BJ:106:GLU:O	10:BJ:112:GLN:NE2	2.34	0.59
36:A1:1940:G:H21	36:A1:3362:A:H8	1.51	0.59
39:AA:27:ALA:O	39:AA:128:ARG:NH2	2.32	0.59
27:Ba:15:ARG:NH1	35:B5:936:G:N7	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BJ:176:ASN:ND2	35:B5:511:A:OP2	2.36	0.59
33:Bg:149:ASP:H	33:Bg:175:ASP:HB3	1.67	0.59
36:A1:1656:A:OP2	70:Ag:37:LYS:NZ	2.36	0.59
36:A1:2953:U:H2'	36:A1:2954:U:H2'	1.85	0.59
6:BF:140:THR:HA	6:BF:214:LYS:HD2	1.85	0.59
9:BI:10:LYS:NZ	35:B5:322:G:O2'	2.36	0.59
14:BN:46:THR:HB	14:BN:49:GLN:HG3	1.85	0.59
36:A1:1054:A:H5''	36:A1:2637:A:H61	1.68	0.59
4:BD:138:VAL:HG22	4:BD:184:ILE:HG22	1.84	0.59
36:A1:837:A:OP2	79:Ap:4:ARG:NH1	2.35	0.59
36:A1:838:G:O6	79:Ap:4:ARG:NH2	2.35	0.59
36:A1:3090:U:OP1	40:AB:270:ARG:NH2	2.33	0.59
36:A1:804:C:OP1	41:AC:98:ARG:NH2	2.36	0.59
36:A1:985:U:H5''	44:AF:98:LYS:HE2	1.85	0.59
36:A1:1639:C:OP2	70:Ag:74:ARG:NH2	2.26	0.58
79:Ap:38:ASP:HA	79:Ap:45:LYS:HA	1.85	0.58
8:BH:64:VAL:HG22	8:BH:94:ALA:HB1	1.84	0.58
14:BN:104:ARG:NH2	35:B5:951:A:OP1	2.36	0.58
15:BO:52:ARG:HD3	35:B5:905:A:H5''	1.85	0.58
17:BQ:41:PRO:HG2	17:BQ:44:LEU:HB2	1.85	0.58
35:B5:538:A:H5'	35:B5:543:C:H42	1.67	0.58
36:A1:302:U:H5''	51:AN:179:LYS:HE3	1.85	0.58
36:A1:3343:G:O2'	36:A1:3362:A:N6	2.35	0.58
63:AZ:26:VAL:HG11	63:AZ:96:VAL:HG23	1.84	0.58
36:A1:67:A:O2'	36:A1:315:C:O2	2.22	0.58
36:A1:352:A:H61	36:A1:365:A:H5''	1.68	0.58
55:AR:86:GLU:HG2	55:AR:90:PRO:HA	1.85	0.58
36:A1:289:A:O2'	51:AN:93:LYS:O	2.21	0.58
5:BE:200:ARG:NH2	5:BE:202:ASP:OD1	2.37	0.58
35:B5:829:A:H4'	35:B5:830:U:H5'	1.85	0.58
36:A1:2673:A:OP1	48:AJ:95:ASN:ND2	2.37	0.58
36:A1:2878:G:H5''	40:AB:5:LYS:HE2	1.84	0.58
36:A1:3309:G:H1'	53:AP:69:ARG:HD2	1.83	0.58
46:AH:101:VAL:HG22	46:AH:114:VAL:HG22	1.86	0.58
7:BG:3:LEU:O	7:BG:15:THR:HA	2.04	0.58
10:BJ:168:ARG:NH1	35:B5:535:A:OP1	2.35	0.58
13:BM:63:VAL:HB	13:BM:119:SER:HA	1.85	0.58
35:B5:1171:A:H2'	35:B5:1172:G:C8	2.38	0.58
33:Bg:270:LEU:HD21	33:Bg:273:ASP:HB2	1.85	0.58
36:A1:1361:U:O2	44:AF:159:GLN:NE2	2.37	0.58
46:AH:90:MET:HE3	46:AH:181:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:31:VAL:HA	1:BA:34:GLU:HG3	1.84	0.58
36:A1:1483:G:O6	70:Ag:4:ARG:NH2	2.36	0.58
36:A1:2600:C:OP1	51:AN:93:LYS:NZ	2.37	0.58
40:AB:219:ALA:HB2	40:AB:336:VAL:HG23	1.86	0.58
27:Ba:45:VAL:HG12	27:Ba:46:GLU:HG2	1.85	0.58
73:Aj:21:ARG:NH2	73:Aj:41:ALA:O	2.28	0.58
13:BM:107:ASP:HB2	13:BM:113:ARG:HH22	1.69	0.57
36:A1:3034:C:H5	46:AH:121:LYS:H	1.51	0.57
59:AV:109:MET:HE1	59:AV:114:ILE:HG12	1.85	0.57
10:BJ:17:ARG:O	10:BJ:23:ARG:NH2	2.37	0.57
33:Bg:123:ILE:HG21	33:Bg:169:ILE:HG21	1.84	0.57
46:AH:93:VAL:HG22	76:Am:82:LEU:HB3	1.85	0.57
35:B5:517:U:H3	35:B5:535:A:H61	1.52	0.57
1:BA:30:GLN:NE2	1:BA:151:SER:O	2.38	0.57
12:BL:73:GLY:HA3	12:BL:86:ILE:HD12	1.87	0.57
18:BR:10:LYS:NZ	35:B5:1316:G:O2'	2.38	0.57
19:BS:15:LEU:HD12	19:BS:66:LEU:HD21	1.87	0.57
25:BY:32:ARG:NH2	25:BY:33:ALA:O	2.37	0.57
36:A1:2748:A:H1'	42:AD:36:LEU:HD23	1.87	0.57
39:AA:101:VAL:HG22	39:AA:165:VAL:HG22	1.86	0.57
45:AG:121:SER:OG	45:AG:122:LYS:N	2.38	0.57
4:BD:143:ARG:HH22	35:B5:558:U:H3	1.52	0.57
36:A1:297:G:O6	51:AN:12:ARG:NH1	2.36	0.57
36:A1:1132:C:H2'	36:A1:1133:A2M:H8	1.86	0.57
36:A1:3308:C:N3	53:AP:69:ARG:NH1	2.52	0.57
49:AL:74:GLY:O	49:AL:101:ARG:NH1	2.38	0.57
9:BI:98:LYS:NZ	35:B5:329:G:OP1	2.38	0.57
51:AN:8:GLU:OE2	51:AN:12:ARG:NH2	2.37	0.57
7:BG:201:GLN:NE2	35:B5:125:U:OP1	2.35	0.57
24:BX:69:ARG:NH2	35:B5:568:G:N7	2.52	0.57
36:A1:904:A:OP2	73:Aj:30:GLN:NE2	2.36	0.57
36:A1:2864:A:H5''	47:AI:114:GLY:HA3	1.86	0.57
38:A4:141:C:OP1	51:AN:109:ARG:NH2	2.38	0.57
2:BB:58:SER:HA	2:BB:61:LEU:HD12	1.86	0.57
19:BS:61:LEU:HD23	19:BS:66:LEU:HD12	1.87	0.57
36:A1:2257:C:C5	36:A1:2259:A:N7	2.73	0.57
71:Ah:73:LYS:O	71:Ah:76:GLN:NE2	2.38	0.57
74:Ak:25:VAL:HG21	74:Ak:66:ILE:HD13	1.86	0.57
26:BZ:61:SER:H	26:BZ:64:VAL:HB	1.70	0.57
36:A1:845:G:H21	36:A1:848:A:H2	1.53	0.57
2:BB:61:LEU:HD13	2:BB:96:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BI:16:ALA:HB2	35:B5:354:C:H5''	1.86	0.56
48:AJ:49:LYS:HG3	48:AJ:64:LYS:HD3	1.86	0.56
59:AV:80:ARG:NH1	59:AV:117:PRO:O	2.36	0.56
74:Ak:31:LEU:HA	74:Ak:37:PRO:HA	1.85	0.56
6:BF:92:ARG:NH2	6:BF:169:ASN:OD1	2.34	0.56
14:BN:109:LYS:HD2	35:B5:975:C:H5''	1.87	0.56
22:BV:55:LEU:HD13	22:BV:65:SER:HB2	1.87	0.56
6:BF:63:GLN:HE22	6:BF:66:GLN:HB2	1.69	0.56
36:A1:2895:G:O2'	76:Am:100:TYR:O	2.22	0.56
15:BO:126:THR:HG21	35:B5:888:U:H1'	1.88	0.56
21:BU:20:ILE:HG21	21:BU:97:VAL:HB	1.86	0.56
35:B5:972:G:O2'	36:A1:847:A:N6	2.39	0.56
50:AM:60:LEU:HD13	56:AS:152:LEU:HD11	1.86	0.56
21:BU:53:LYS:HD3	35:B5:1345:A:H5'	1.87	0.56
23:BW:15:ASN:ND2	23:BW:72:CYS:O	2.38	0.56
36:A1:2901:G:O2'	36:A1:3024:A:N1	2.37	0.56
19:BS:18:LEU:HD21	19:BS:101:LEU:HD13	1.87	0.56
20:BT:86:ARG:NH2	35:B5:1601:G:OP1	2.29	0.56
36:A1:1156:C:OP2	44:AF:94:LYS:NZ	2.37	0.56
19:BS:135:GLY:HA3	35:B5:1559:A:H5''	1.88	0.56
39:AA:92:LYS:HE3	39:AA:93:LYS:HE3	1.87	0.56
1:BA:59:LEU:HD22	22:BV:79:LEU:HD11	1.88	0.56
2:BB:36:SER:OG	2:BB:41:ARG:NH2	2.39	0.56
21:BU:59:PRO:HG3	35:B5:1381:U:H4'	1.88	0.56
36:A1:860:G:OP1	79:Ap:17:ARG:NH1	2.38	0.56
36:A1:1390:A:N6	36:A1:1418:A:O2'	2.38	0.56
51:AN:46:ASP:OD1	51:AN:50:ARG:NH2	2.34	0.56
54:AQ:120:GLU:OE2	54:AQ:130:ARG:NH1	2.38	0.56
36:A1:93:C:OP2	36:A1:2764:C:O2'	2.23	0.55
40:AB:214:MET:HE2	40:AB:281:LYS:HE2	1.88	0.55
79:Ap:36:ARG:HG2	79:Ap:48:LYS:HE2	1.88	0.55
36:A1:1682:U:O4	58:AU:90:ARG:NH1	2.39	0.55
39:AA:173:GLY:O	39:AA:176:ASP:HB2	2.06	0.55
41:AC:361:HIS:O	56:AS:28:ARG:NH2	2.39	0.55
46:AH:72:LYS:NZ	46:AH:76:ASP:OD2	2.40	0.55
54:AQ:174:ARG:HA	54:AQ:178:ARG:HG2	1.88	0.55
7:BG:187:LYS:NZ	35:B5:139:C:O2'	2.40	0.55
36:A1:90:C:OP1	64:Aa:59:ARG:NH1	2.35	0.55
36:A1:126:U:OP1	51:AN:144:ARG:NH1	2.38	0.55
35:B5:1777:G:N7	77:An:8:LYS:NZ	2.53	0.55
36:A1:114:A:OP1	51:AN:54:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A1:807:A2M:H62	36:A1:934:G:H22	1.54	0.55
36:A1:1010:G:N2	47:AI:193:ASP:OD2	2.39	0.55
36:A1:1233:G:N2	36:A1:1263:A:OP2	2.39	0.55
45:AG:183:LYS:HB2	45:AG:194:THR:HG23	1.88	0.55
5:BE:19:LEU:HB2	5:BE:51:ARG:HH22	1.72	0.55
35:B5:895:G:H1	35:B5:917:U:H3	1.54	0.55
54:AQ:123:THR:OG1	54:AQ:125:ASP:OD1	2.24	0.55
66:Ac:17:VAL:HG11	66:Ac:92:ILE:HD12	1.87	0.55
2:BB:26:ARG:O	2:BB:50:LYS:N	2.39	0.55
16:BP:129:GLY:HA3	34:Bh:74:LYS:HD2	1.87	0.55
19:BS:41:ARG:NH1	35:B5:1565:C:OP1	2.35	0.55
19:BS:145:ARG:NH1	35:B5:1569:A:O2'	2.40	0.55
59:AV:15:LEU:HD13	59:AV:51:ALA:HB3	1.89	0.55
66:Ac:73:GLY:N	66:Ac:76:GLU:OE2	2.35	0.55
21:BU:21:LYS:NZ	21:BU:94:GLU:OE2	2.39	0.55
28:Bb:56:CYS:SG	28:Bb:57:GLU:N	2.79	0.55
4:BD:157:LEU:HD23	4:BD:189:MET:HB2	1.89	0.55
51:AN:177:GLY:O	51:AN:184:LYS:NZ	2.39	0.55
9:BI:32:GLN:OE1	35:B5:1727:G:N2	2.33	0.55
59:AV:85:TRP:NE1	59:AV:121:GLU:OE2	2.37	0.55
1:BA:122:ILE:HA	1:BA:144:ILE:O	2.06	0.55
7:BG:13:GLN:NE2	35:B5:151:G:N3	2.55	0.55
14:BN:124:ARG:NH2	35:B5:967:A:OP2	2.38	0.55
34:Bh:89:ARG:NH1	35:B5:1190:C:OP1	2.39	0.55
36:A1:655:C:H5''	68:Ae:26:HIS:HB3	1.89	0.55
36:A1:2115:G:H22	36:A1:2120:A:H1'	1.71	0.55
62:AY:48:LEU:HD13	62:AY:115:ARG:HH21	1.72	0.55
78:Ao:38:GLN:HA	78:Ao:41:ARG:HE	1.71	0.55
6:BF:143:ARG:NH1	29:Bc:57:MET:SD	2.80	0.54
3:BC:175:GLY:O	10:BJ:53:ARG:NH2	2.41	0.54
36:A1:26:A:N3	36:A1:328:U:O2'	2.37	0.54
36:A1:128:G:H5''	61:AX:45:LYS:HZ1	1.71	0.54
36:A1:351:A:N6	75:Al:37:TYR:O	2.40	0.54
36:A1:1322:U:O2	56:AS:108:GLN:NE2	2.38	0.54
38:A4:21:C:OP1	41:AC:193:LYS:NZ	2.35	0.54
35:B5:321:C:N4	35:B5:1667:A:OP1	2.40	0.54
35:B5:1483:A:OP2	35:B5:1521:G:N2	2.37	0.54
41:AC:35:VAL:HG21	41:AC:244:LEU:HD21	1.89	0.54
43:AE:43:LEU:HD11	43:AE:85:ILE:HG13	1.90	0.54
2:BB:70:LEU:HD22	2:BB:84:ILE:HD11	1.89	0.54
3:BC:81:MET:HE1	3:BC:186:LYS:HG2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:92:LEU:HD13	25:BY:17:LEU:HD11	1.89	0.54
35:B5:103:A:OP2	35:B5:360:A:N6	2.38	0.54
35:B5:1126:OMG:OP2	77:An:18:ARG:NH2	2.40	0.54
53:AP:13:LYS:NZ	53:AP:154:GLU:OE2	2.40	0.54
61:AX:25:LYS:HB3	61:AX:27:ARG:HE	1.73	0.54
61:AX:50:ALA:HB1	71:Ah:66:VAL:HG11	1.88	0.54
35:B5:490:C:N4	35:B5:492:A:O4'	2.41	0.54
47:AI:130:ASP:OD2	47:AI:133:GLN:NE2	2.41	0.54
2:BB:111:ARG:HH12	35:B5:930:A:H1'	1.72	0.54
15:BO:131:GLY:O	27:Ba:22:ARG:NH2	2.41	0.54
20:BT:72:GLY:HA3	35:B5:1498:G:H5''	1.89	0.54
1:BA:72:ASP:HB2	1:BA:118:PRO:HA	1.89	0.54
33:Bg:127:ARG:HA	33:Bg:150:TRP:HB2	1.88	0.54
35:B5:976:G:N1	35:B5:1023:A:O2'	2.39	0.54
36:A1:1062:A:O2'	57:AT:108:ARG:NH1	2.40	0.54
41:AC:338:LYS:O	41:AC:340:GLY:N	2.41	0.54
43:AE:40:LEU:HD11	43:AE:54:TYR:HB2	1.90	0.54
1:BA:52:LYS:HE3	22:BV:82:VAL:HA	1.90	0.54
6:BF:156:ARG:HE	6:BF:157:ARG:H	1.55	0.54
56:AS:77:VAL:HG11	56:AS:106:LEU:HD22	1.90	0.54
35:B5:228:G:N2	35:B5:230:C:OP1	2.40	0.53
36:A1:1695:U:O2'	36:A1:1749:A:N1	2.36	0.53
36:A1:2193:U:H5''	36:A1:2194:G:H5'	1.89	0.53
46:AH:6:THR:HG21	46:AH:65:VAL:HG13	1.90	0.53
6:BF:26:ALA:HB2	17:BQ:26:LYS:HG3	1.89	0.53
22:BV:15:ARG:NH1	22:BV:33:GLN:OE1	2.37	0.53
35:B5:704:C:O2'	35:B5:734:A:N6	2.41	0.53
36:A1:412:G:OP1	53:AP:62:ARG:NH1	2.41	0.53
36:A1:2767:U:O2'	78:Ao:30:ALA:O	2.25	0.53
36:A1:3021:A:H61	36:A1:3032:A:H3'	1.73	0.53
36:A1:3050:U:O2'	60:AW:16:GLY:O	2.22	0.53
36:A1:3348:G:N2	36:A1:3357:U:O2	2.30	0.53
39:AA:96:LEU:O	79:Ap:87:ARG:NH1	2.36	0.53
45:AG:68:ARG:NH1	45:AG:237:ILE:O	2.41	0.53
35:B5:198:A:H3'	35:B5:199:G:H8	1.73	0.53
36:A1:2548:C:OP2	39:AA:93:LYS:NZ	2.40	0.53
40:AB:187:SER:O	40:AB:190:GLU:N	2.41	0.53
76:Am:91:CYS:HA	76:Am:124:LYS:HD3	1.90	0.53
4:BD:23:GLU:OE1	11:BK:61:TRP:NE1	2.35	0.53
5:BE:103:TYR:O	5:BE:182:TYR:OH	2.25	0.53
12:BL:152:GLN:HB3	14:BN:136:PRO:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AQ:25:TYR:HA	54:AQ:28:LEU:HD12	1.89	0.53
23:BW:80:ASN:OD1	23:BW:124:LYS:NZ	2.37	0.53
36:A1:3285:C:H2'	36:A1:3286:G:H8	1.73	0.53
64:Aa:112:ILE:HB	64:Aa:130:VAL:HG12	1.91	0.53
5:BE:68:ARG:HE	5:BE:76:VAL:HG11	1.72	0.53
22:BV:67:ASP:OD2	22:BV:87:ARG:NH1	2.41	0.53
36:A1:2150:G:O2'	36:A1:2189:U:OP1	2.26	0.53
2:BB:142:PHE:HB2	2:BB:208:GLN:HG3	1.89	0.53
4:BD:29:LEU:HD21	4:BD:69:LEU:HD11	1.90	0.53
6:BF:166:ARG:HH12	35:B5:1163:A:H4'	1.73	0.53
7:BG:10:ASN:HB3	7:BG:128:THR:HA	1.91	0.53
13:BM:101:ALA:O	13:BM:111:ASN:ND2	2.42	0.53
33:Bg:32:LEU:HD21	33:Bg:94:VAL:HG11	1.91	0.53
36:A1:1592:G:OP1	70:Ag:58:ARG:NH2	2.35	0.53
36:A1:2261:G:OP1	36:A1:2306:C:N4	2.42	0.53
39:AA:19:HIS:O	39:AA:23:ARG:NH1	2.42	0.53
5:BE:22:LYS:N	35:B5:773:C:OP1	2.41	0.53
9:BI:23:LYS:NZ	35:B5:391:A:OP2	2.41	0.53
36:A1:296:A:OP1	72:Ai:86:LYS:NZ	2.41	0.53
36:A1:2880:PSU:H5'	40:AB:236:LYS:HD3	1.90	0.53
37:A3:6:C:O2'	42:AD:50:ARG:NH2	2.41	0.53
52:AO:79[A]:ILE:HG21	52:AO:138[A]:LEU:HD11	1.90	0.53
55:AR:115:ILE:HD11	55:AR:142:ILE:HG23	1.90	0.53
20:BT:6:VAL:HG21	20:BT:132:LEU:HB3	1.90	0.53
35:B5:1773:4AC:H5	77:An:2:ARG:HH21	1.73	0.53
36:A1:1613:A:OP2	74:Ak:46:ARG:NH1	2.37	0.53
36:A1:2642:A:OP2	57:AT:3:LYS:NZ	2.42	0.53
2:BB:118:GLN:OE1	2:BB:208:GLN:NE2	2.42	0.53
5:BE:94:ALA:HB1	25:BY:16:PRO:HB2	1.91	0.53
7:BG:89:ASP:OD1	35:B5:395:U:O2'	2.27	0.53
12:BL:38:ALA:O	35:B5:246:G:N2	2.40	0.53
27:Ba:78:ALA:HA	27:Ba:83:ILE:HD12	1.91	0.53
30:Bd:33:LYS:HE3	35:B5:1594:G:H5'	1.91	0.53
36:A1:674:G:O6	54:AQ:56:LYS:NZ	2.42	0.53
36:A1:1342:C:H5''	54:AQ:12:ARG:HG2	1.90	0.53
36:A1:2836:C:H5	36:A1:2852:C:H42	1.57	0.53
42:AD:20:PHE:O	42:AD:24:ARG:NH2	2.42	0.53
9:BI:31:ARG:NH1	35:B5:332:U:OP1	2.42	0.52
12:BL:101:GLU:OE1	24:BX:13:ARG:NH2	2.42	0.52
35:B5:488:G:H3'	35:B5:492:A:H62	1.73	0.52
63:AZ:115:LYS:NZ	63:AZ:119:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BI:172:ARG:NH1	35:B5:330:G:OP2	2.42	0.52
33:Bg:12:THR:HG22	33:Bg:311:ARG:HG2	1.91	0.52
38:A4:103:G:OP2	38:A4:105:A:O2'	2.24	0.52
72:AI:66:GLU:OE2	72:AI:91:ASN:ND2	2.42	0.52
1:BA:189:VAL:O	22:BV:44:ARG:NH2	2.42	0.52
11:BK:1:MET:HG3	35:B5:1216:C:H5''	1.91	0.52
17:BQ:136:SER:HB3	35:B5:1586:A:H5''	1.91	0.52
18:BR:74:GLN:OE1	18:BR:78:ARG:NH1	2.41	0.52
19:BS:27:LYS:HE3	19:BS:55:HIS:HA	1.90	0.52
42:AD:95:TRP:HA	42:AD:158:ARG:HG2	1.91	0.52
48:AJ:19:LEU:HD22	48:AJ:125:MET:HE2	1.91	0.52
7:BG:188:ARG:NH1	35:B5:284:G:N7	2.57	0.52
12:BL:80:MET:SD	35:B5:324:U:O2'	2.66	0.52
12:BL:124:THR:HB	12:BL:141:LYS:HB3	1.92	0.52
36:A1:1181:U:O4	52:AO:21[A]:SER:OG	2.27	0.52
36:A1:1281:G:N2	36:A1:1282:G:O6	2.42	0.52
36:A1:1740:U:H1'	36:A1:1741:A:H2	1.74	0.52
36:A1:3329:U:H5''	40:AB:308:MET:HE2	1.92	0.52
36:A1:1019:G:N2	36:A1:1034:U:OP1	2.42	0.52
36:A1:2885:C:OP1	52:AO:59[A]:ARG:NH1	2.43	0.52
36:A1:3206:C:OP1	56:AS:166:LYS:NZ	2.43	0.52
1:BA:92:HIS:ND1	1:BA:202:TYR:OH	2.38	0.52
48:AJ:117:ASP:OD1	48:AJ:119:SER:OG	2.26	0.52
18:BR:26:LEU:HD21	18:BR:62:GLN:HG3	1.92	0.52
25:BY:51:GLU:HG3	25:BY:53:ASP:H	1.74	0.52
36:A1:437:G:C6	36:A1:622:A:N6	2.76	0.52
36:A1:1047:A:N3	36:A1:2633:U:O2'	2.40	0.52
36:A1:1385:C:OP1	41:AC:141:ARG:NH1	2.43	0.52
36:A1:2185:G:O2'	36:A1:2314:PSU:OP2	2.23	0.52
47:AI:66:GLU:OE2	47:AI:69:ARG:NH2	2.43	0.52
59:AV:10:LYS:HD3	59:AV:125:LEU:HD22	1.92	0.52
63:AZ:50:PRO:HD3	63:AZ:68:ILE:HG12	1.92	0.52
13:BM:97:LEU:O	13:BM:101:ALA:HB3	2.10	0.52
30:Bd:10:HIS:ND1	35:B5:1452:U:OP1	2.42	0.52
33:Bg:154:VAL:O	33:Bg:155:ARG:NE	2.42	0.52
33:Bg:235:SER:OG	33:Bg:237:GLN:OE1	2.26	0.52
36:A1:966:PSU:OP1	64:Aa:44:ASN:ND2	2.42	0.52
36:A1:2179:C:O2'	39:AA:174:ARG:NH2	2.42	0.52
40:AB:4:ARG:HH21	40:AB:8:ALA:HB3	1.74	0.52
45:AG:162:LEU:HA	51:AN:7:LEU:HD21	1.91	0.52
6:BF:79:ASN:OD1	6:BF:83:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:175:ILE:HG12	35:B5:78:A:H1'	1.92	0.52
17:BQ:10:PHE:HA	17:BQ:18:ALA:O	2.10	0.52
36:A1:3045:G:OP1	40:AB:19:ARG:NH2	2.41	0.52
4:BD:93:ASP:HB3	4:BD:96:LEU:HD13	1.92	0.51
16:BP:126:VAL:HG11	35:B5:1459:C:H4'	1.92	0.51
36:A1:149:U:OP1	51:AN:49:ARG:NH1	2.41	0.51
36:A1:1367:G:OP1	68:Ae:45:ARG:NH2	2.42	0.51
37:A3:55:A:O4'	48:AJ:7:ASN:ND2	2.43	0.51
48:AJ:132:ASN:OD1	48:AJ:132:ASN:N	2.43	0.51
13:BM:54:ARG:NH2	13:BM:56:GLU:OE2	2.43	0.51
15:BO:121:VAL:O	35:B5:886:U:O2'	2.22	0.51
42:AD:119:TYR:OH	42:AD:139:PRO:O	2.23	0.51
46:AH:85:GLY:HA3	46:AH:187:ILE:HD12	1.92	0.51
46:AH:89:LYS:HG2	46:AH:145:VAL:HG22	1.93	0.51
52:AO:73[A]:PHE:HB3	52:AO:78[A]:ARG:HB3	1.92	0.51
59:AV:87:ARG:HH22	59:AV:137:VAL:HG21	1.75	0.51
11:BK:27:PHE:HB3	11:BK:40:LEU:HD12	1.93	0.51
16:BP:47:ARG:NH2	35:B5:1555:A:OP2	2.44	0.51
33:Bg:42:LEU:HB2	33:Bg:61:PHE:HB2	1.92	0.51
35:B5:29:U:H2'	35:B5:30:G:H8	1.76	0.51
36:A1:985:U:H2'	36:A1:986:PSU:H6	1.76	0.51
48:AJ:23:VAL:HB	48:AJ:30:LEU:HD12	1.91	0.51
78:Ao:38:GLN:HB2	78:Ao:41:ARG:HH21	1.75	0.51
8:BH:112:ARG:NH2	35:B5:639:U:OP1	2.43	0.51
13:BM:106:ILE:O	13:BM:113:ARG:NH2	2.43	0.51
21:BU:80:GLU:HG2	30:Bd:54:LYS:HD3	1.90	0.51
25:BY:57:VAL:HB	25:BY:60:PHE:HE2	1.75	0.51
36:A1:1769:G:O2'	58:AU:99:LYS:NZ	2.43	0.51
41:AC:230:VAL:HA	41:AC:233:LEU:HD13	1.92	0.51
1:BA:64:ILE:HG23	1:BA:73:VAL:HG11	1.92	0.51
1:BA:107:PHE:HB2	1:BA:135:GLU:HG2	1.91	0.51
8:BH:9:LEU:HD21	8:BH:17:GLU:HG3	1.92	0.51
36:A1:2768:U:H2'	36:A1:2769:A:H8	1.76	0.51
50:AM:19:ARG:NH1	50:AM:66:THR:O	2.41	0.51
52:AO:65[A]:ASN:HB3	52:AO:68[A]:ARG:HG2	1.91	0.51
54:AQ:122:ILE:HG23	54:AQ:126:GLN:HB2	1.92	0.51
78:Ao:28:TYR:HB3	78:Ao:69:VAL:HB	1.93	0.51
8:BH:104:ARG:NH1	35:B5:805:U:O4	2.44	0.51
35:B5:371:G:N2	35:B5:612:U:O2	2.43	0.51
36:A1:831:G:O2'	36:A1:1864:A:N3	2.38	0.51
2:BB:111:ARG:NH2	35:B5:930:A:N3	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Bg:222:LEU:HD23	33:Bg:234:LEU:HD13	1.92	0.51
35:B5:1474:G:H2'	35:B5:1475:A:C8	2.45	0.51
36:A1:912:G:OP2	39:AA:9:ARG:NH1	2.44	0.51
36:A1:3309:G:O6	40:AB:21:ARG:NH2	2.44	0.51
48:AJ:54:VAL:HG23	48:AJ:56:THR:H	1.75	0.51
9:BI:5:ARG:NH2	35:B5:334:G:O6	2.43	0.51
35:B5:47:A:N7	35:B5:98:U:O2'	2.44	0.51
36:A1:1245:A:O2'	36:A1:1247:U:OP1	2.29	0.51
36:A1:1696:A:H2'	36:A1:1697:A:C8	2.46	0.51
1:BA:134:LYS:NZ	35:B5:1321:A:N7	2.59	0.51
3:BC:56:ILE:HA	3:BC:61:LEU:HD12	1.93	0.51
11:BK:10:LYS:HA	11:BK:13:GLN:HG2	1.93	0.51
14:BN:48:SER:OG	35:B5:868:G:N2	2.41	0.51
35:B5:1023:A:OP1	35:B5:1126:OMG:N2	2.37	0.51
35:B5:1196:A:OP2	35:B5:1464:G:N2	2.43	0.51
36:A1:95:A:H5''	64:Aa:34:MET:HB2	1.92	0.51
36:A1:799:G:O2'	49:AL:18:TRP:NE1	2.44	0.51
36:A1:1129:A:H2'	36:A1:1130:A:C8	2.46	0.51
36:A1:3121:U:H1'	36:A1:3122:A:H5''	1.93	0.51
1:BA:180:GLU:OE1	1:BA:191:ARG:NH2	2.43	0.50
10:BJ:108:ARG:NH1	10:BJ:110:GLN:OE1	2.44	0.50
18:BR:45:ARG:NH1	35:B5:1332:C:OP2	2.43	0.50
34:Bh:93:ARG:NH1	35:B5:1427:A:OP2	2.41	0.50
35:B5:698:U:H3	35:B5:741:C:N4	2.09	0.50
35:B5:1022:C:H4'	35:B5:1125:A:H61	1.76	0.50
35:B5:1688:U:H3	35:B5:1712:A:H61	1.59	0.50
36:A1:115:A:H2'	36:A1:265:A:C2	2.46	0.50
9:BI:57:ALA:HB2	9:BI:177:GLY:HA2	1.92	0.50
33:Bg:240:VAL:HG22	33:Bg:256:THR:HG22	1.93	0.50
42:AD:125:VAL:HG11	42:AD:199:ILE:HG21	1.92	0.50
55:AR:167:ARG:HE	55:AR:171:ASP:HB2	1.76	0.50
9:BI:46:VAL:HG21	9:BI:56:ARG:HE	1.76	0.50
9:BI:141:ARG:NH2	35:B5:196:G:O6	2.43	0.50
23:BW:40:VAL:HA	23:BW:43:LYS:HE3	1.93	0.50
35:B5:1488:G:O2'	35:B5:1494:C:O2	2.26	0.50
39:AA:147:ARG:HG2	39:AA:157:VAL:HG22	1.94	0.50
57:AT:51:GLY:HA3	57:AT:92:ARG:HG3	1.93	0.50
7:BG:66:GLY:HA3	35:B5:1681:A:H1'	1.93	0.50
23:BW:15:ASN:ND2	23:BW:72:CYS:SG	2.84	0.50
32:Bf:138:ARG:NH1	35:B5:1235:C:O2	2.42	0.50
36:A1:2882:U:H5	40:AB:4:ARG:HH11	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BY:109:LYS:NZ	35:B5:459:G:OP1	2.36	0.50
33:Bg:180:ALA:HB3	33:Bg:190:ALA:HB3	1.94	0.50
38:A4:52:A:H62	75:A1:27:ILE:HD13	1.74	0.50
59:AV:18:PRO:HA	59:AV:51:ALA:HA	1.93	0.50
15:BO:88:GLY:O	15:BO:92:LYS:NZ	2.32	0.50
35:B5:814:A:O2'	35:B5:816:G:OP2	2.29	0.50
36:A1:1472:U:H5'	55:AR:4:LEU:HB2	1.94	0.50
39:AA:32:LEU:HD13	39:AA:163:ARG:HD3	1.94	0.50
46:AH:20:ILE:HG12	46:AH:25:VAL:HG13	1.93	0.50
66:Ac:24:THR:HG23	66:Ac:93:LEU:HD11	1.94	0.50
9:BI:2:GLY:N	35:B5:393:C:OP2	2.45	0.50
25:BY:9:THR:OG1	35:B5:781:U:OP2	2.29	0.50
36:A1:1192:C:N4	36:A1:1301:A:O2'	2.45	0.50
50:AM:38:ILE:HA	50:AM:44:VAL:HG12	1.94	0.50
52:AO:172[A]:ARG:HA	52:AO:175[A]:THR:HG22	1.93	0.50
64:Aa:56:VAL:HG12	64:Aa:57:GLY:H	1.77	0.50
79:Ap:7:LYS:O	79:Ap:27:LYS:NZ	2.43	0.50
2:BB:180:THR:O	2:BB:183:GLN:N	2.45	0.50
8:BH:108:GLN:NE2	35:B5:743:U:O4'	2.44	0.50
28:Bb:53:ALA:HB1	28:Bb:62:ILE:HG22	1.93	0.50
35:B5:472:U:O2'	35:B5:769:A:N3	2.44	0.50
35:B5:714:G:H2'	35:B5:715:U:H4'	1.93	0.50
36:A1:297:G:H4'	36:A1:299:G:H5'	1.93	0.50
36:A1:627:U:H2'	36:A1:628:A:C8	2.47	0.50
36:A1:3242:G:O6	40:AB:150:ARG:NH1	2.45	0.50
5:BE:247:SER:OG	5:BE:250:GLU:OE1	2.29	0.50
22:BV:79:LEU:HD13	22:BV:82:VAL:HG21	1.92	0.50
32:Bf:108:VAL:HG13	32:Bf:114:VAL:HG12	1.93	0.50
35:B5:924:A:H2'	35:B5:925:G:C8	2.46	0.50
35:B5:973:A:H4'	36:A1:848:A:C8	2.47	0.50
35:B5:1533:C:H4'	35:B5:1539:G:C6	2.46	0.50
36:A1:362:U:O4	73:Aj:24:ARG:NH2	2.44	0.50
36:A1:1530:U:HO2'	38:A4:114:G:HO2'	1.57	0.50
36:A1:3092:C:O2'	36:A1:3094:A:OP2	2.24	0.50
36:A1:3186:A:N3	46:AH:44:THR:OG1	2.43	0.50
37:A3:1:G:N3	42:AD:269:SER:OG	2.42	0.50
2:BB:199:ASN:HA	2:BB:202:LYS:HE3	1.93	0.49
43:AE:138:GLN:HE21	43:AE:142:ASP:CG	2.20	0.49
51:AN:181:ASN:HA	51:AN:184:LYS:HE2	1.94	0.49
1:BA:183:ARG:O	22:BV:44:ARG:NH1	2.46	0.49
51:AN:20:ARG:HH12	72:Ai:52:PRO:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AY:11:ASP:HB3	62:AY:14:LYS:HB2	1.94	0.49
16:BP:124:THR:HB	35:B5:1182:U:H4'	1.94	0.49
25:BY:131:ARG:NH2	35:B5:154:G:OP2	2.45	0.49
35:B5:980:G:H4'	35:B5:1776:A:H4'	1.93	0.49
36:A1:784:A:OP2	54:AQ:69:ARG:NH1	2.37	0.49
42:AD:37:VAL:HG12	57:AT:31:LEU:HD21	1.93	0.49
35:B5:34:G:O2'	35:B5:515:A:O2'	2.29	0.49
36:A1:292:U:OP2	51:AN:68:ARG:NH2	2.45	0.49
38:A4:103:G:H4'	73:Aj:21:ARG:HG3	1.93	0.49
53:AP:56:ARG:NH1	53:AP:75:GLU:OE2	2.45	0.49
64:Aa:95:SER:OG	64:Aa:96:LYS:O	2.29	0.49
69:Af:6:ARG:NH1	69:Af:8:TYR:O	2.45	0.49
70:Ag:57:LEU:HB3	70:Ag:61:GLN:HB2	1.93	0.49
10:BJ:59:LEU:HD22	10:BJ:69:ARG:HA	1.94	0.49
10:BJ:110:GLN:HB2	10:BJ:144:PRO:HB3	1.94	0.49
23:BW:23:ARG:HG3	28:Bb:4:VAL:HG22	1.93	0.49
36:A1:655:C:H2'	36:A1:656:A:H8	1.77	0.49
61:AX:115:ARG:NH2	61:AX:119:THR:OG1	2.40	0.49
63:AZ:33:SER:OG	63:AZ:34:LYS:N	2.46	0.49
64:Aa:36:GLY:HA3	64:Aa:40:HIS:CE1	2.48	0.49
1:BA:6:THR:O	1:BA:191:ARG:NH1	2.45	0.49
20:BT:122:ARG:NH1	35:B5:1499:G:OP1	2.45	0.49
36:A1:2683:U:H5'	48:AJ:18:VAL:HG11	1.93	0.49
46:AH:113:GLU:HA	46:AH:124:ARG:O	2.13	0.49
49:AL:48:PRO:HB2	71:Ah:117:ALA:HB2	1.93	0.49
5:BE:100:ARG:HH21	5:BE:118:GLU:HG2	1.77	0.49
6:BF:42:LEU:O	6:BF:45:LYS:N	2.42	0.49
27:Ba:2:PRO:HB3	35:B5:1142:A:H5''	1.93	0.49
29:Bc:9:LEU:HB3	29:Bc:33:LEU:HD12	1.94	0.49
5:BE:175:PHE:HE2	5:BE:198:LYS:HD3	1.78	0.49
8:BH:14:THR:OG1	8:BH:15:GLU:OE1	2.30	0.49
10:BJ:85:VAL:HG13	10:BJ:103:ASP:HB3	1.95	0.49
33:Bg:209:THR:OG1	33:Bg:224:ASN:OD1	2.31	0.49
33:Bg:220:ILE:HB	33:Bg:234:LEU:HB2	1.94	0.49
35:B5:700:C:H1'	35:B5:740:A:H61	1.78	0.49
36:A1:649:A2M:OP2	36:A1:2868:U:O2'	2.30	0.49
38:A4:58:G:O6	73:Aj:63:ARG:NH2	2.46	0.49
5:BE:145:ARG:HD2	5:BE:162:ILE:HD13	1.95	0.49
5:BE:196:VAL:N	5:BE:209:HIS:O	2.42	0.49
8:BH:81:LEU:HD23	8:BH:90:VAL:HG21	1.95	0.49
15:BO:123:SER:O	35:B5:885:G:N2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BP:52:LYS:NZ	35:B5:1554:U:O2'	2.43	0.49
36:A1:123:A:OP1	45:AG:105:LYS:NZ	2.37	0.49
36:A1:608:A:O3'	41:AC:326:ARG:NH1	2.46	0.49
36:A1:1447:G:N7	53:AP:25:SER:OG	2.37	0.49
2:BB:137:ILE:HG21	2:BB:172:LEU:HD22	1.94	0.49
3:BC:170:ILE:HB	3:BC:197:TYR:HB2	1.95	0.49
11:BK:7:ASP:HA	11:BK:10:LYS:HG2	1.93	0.49
24:BX:96:VAL:O	24:BX:142:LYS:NZ	2.36	0.49
34:Bh:114:LYS:HB2	34:Bh:115:LYS:HD2	1.95	0.49
35:B5:162:A:H3'	35:B5:163:G:H21	1.77	0.49
35:B5:1220:C:H2'	35:B5:1221:A:H8	1.76	0.49
35:B5:1354:G:O6	35:B5:1369:U:O4	2.31	0.49
36:A1:776:PSU:N1	36:A1:2719:U:O2	2.36	0.49
3:BC:119:LYS:HE3	35:B5:1291:G:H5'	1.95	0.48
35:B5:1628:U:H2'	35:B5:1629:G:C8	2.48	0.48
36:A1:598:A:H4'	41:AC:325:LEU:HD13	1.95	0.48
36:A1:727:G:OP2	36:A1:742:G:N2	2.45	0.48
36:A1:1149:G:OP2	69:Af:21:ARG:NH2	2.40	0.48
36:A1:1779:C:N4	36:A1:2102:U:OP1	2.44	0.48
1:BA:35:PRO:O	1:BA:52:LYS:NZ	2.37	0.48
15:BO:52:ARG:NH1	35:B5:905:A:O3'	2.46	0.48
24:BX:5:LYS:NZ	35:B5:612:U:OP2	2.45	0.48
35:B5:1207:C:H42	35:B5:1456:C:H5	1.61	0.48
36:A1:115:A:OP1	36:A1:115:A:H4'	2.09	0.48
1:BA:123:VAL:HG21	1:BA:133:ILE:HD11	1.96	0.48
2:BB:33:LYS:O	2:BB:98:THR:OG1	2.29	0.48
14:BN:14:SER:HB3	35:B5:959:U:H5''	1.94	0.48
16:BP:90:ILE:HD13	16:BP:109:PRO:HA	1.95	0.48
20:BT:44:GLU:HG2	20:BT:45:MET:HG2	1.96	0.48
35:B5:871:G:H2'	35:B5:872:G:C8	2.47	0.48
36:A1:631:U:H2'	36:A1:632:G:C8	2.49	0.48
36:A1:3324:C:OP1	67:Ad:19:ARG:NH1	2.44	0.48
41:AC:3:ARG:NH1	41:AC:27:SER:OG	2.46	0.48
44:AF:160:ARG:HG3	44:AF:203:TRP:CD2	2.48	0.48
4:BD:106:LYS:HG3	4:BD:175:VAL:HG22	1.94	0.48
6:BF:80:LYS:HB2	6:BF:83:ARG:HG3	1.95	0.48
11:BK:24:LYS:HG2	11:BK:26:ASP:HB2	1.94	0.48
14:BN:40:TYR:HB3	14:BN:45:LEU:HD12	1.96	0.48
17:BQ:40:GLU:OE2	17:BQ:45:ARG:NH2	2.44	0.48
20:BT:105:LEU:HD13	20:BT:122:ARG:HD3	1.95	0.48
26:BZ:90:LYS:NZ	26:BZ:103:ARG:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A1:1831:U:O2'	38:A4:114:G:OP1	2.26	0.48
45:AG:246:MET:SD	45:AG:249:ARG:NH2	2.87	0.48
52:AO:189[A]:ASP:OD1	52:AO:189[A]:ASP:N	2.47	0.48
3:BC:92:ALA:HB1	35:B5:1425:A:H4'	1.95	0.48
4:BD:211:PRO:HG3	18:BR:19:ARG:HB2	1.95	0.48
16:BP:127:ARG:HE	16:BP:130:ARG:HH21	1.62	0.48
24:BX:30:LYS:NZ	35:B5:1132:A:OP1	2.40	0.48
36:A1:655:C:H2'	36:A1:656:A:C8	2.48	0.48
36:A1:664:U:H2'	36:A1:665:A:C8	2.48	0.48
36:A1:816:A:H5'	36:A1:906:A:H61	1.78	0.48
40:AB:14:LEU:HA	40:AB:17:LEU:HD13	1.96	0.48
9:BI:98:LYS:HB3	35:B5:329:G:H5''	1.95	0.48
9:BI:171:SER:HB2	9:BI:180:ASP:HB2	1.95	0.48
9:BI:178:ARG:NH1	35:B5:207:U:O2	2.36	0.48
13:BM:59:LEU:HB2	13:BM:123:VAL:HB	1.95	0.48
15:BO:91:THR:HG23	15:BO:93:THR:H	1.77	0.48
39:AA:70:ARG:HH11	39:AA:72:ARG:NH2	2.11	0.48
51:AN:62:TYR:HD2	51:AN:134:LEU:HD13	1.78	0.48
75:A1:6:SER:HB3	75:A1:9:ILE:HG12	1.95	0.48
7:BG:92:ARG:NH2	35:B5:1674:C:OP1	2.47	0.48
10:BJ:141:VAL:HG12	10:BJ:143:ILE:H	1.79	0.48
17:BQ:113:ASP:OD1	17:BQ:115:THR:OG1	2.32	0.48
33:Bg:46:LYS:O	33:Bg:55:GLY:HA2	2.14	0.48
35:B5:1291:G:H1	35:B5:1324:G:H1	1.61	0.48
36:A1:1564:U:O2'	36:A1:1576:G:O6	2.27	0.48
61:AX:57:LEU:HD12	61:AX:61:LYS:HB3	1.96	0.48
2:BB:61:LEU:HA	2:BB:64:ARG:HH11	1.78	0.48
5:BE:180:LEU:HA	5:BE:194:THR:HG22	1.96	0.48
5:BE:182:TYR:HB2	5:BE:228:ILE:HD13	1.95	0.48
7:BG:57:ASP:HA	7:BG:106:LEU:HA	1.94	0.48
15:BO:47:LYS:NZ	15:BO:62:LEU:O	2.46	0.48
22:BV:73:ALA:HB1	22:BV:78:LEU:HB2	1.96	0.48
35:B5:315:A:N1	35:B5:349:U:O2'	2.43	0.48
36:A1:591:G:O2'	43:AE:17:ALA:O	2.28	0.48
36:A1:2854:U:OP2	47:AI:3:ARG:NH2	2.47	0.48
38:A4:107:G:H4'	38:A4:138:A:H5'	1.96	0.48
35:B5:778:G:H2'	35:B5:779:U:H2'	1.96	0.48
35:B5:1055:U:O2	35:B5:1064:G:O6	2.31	0.48
36:A1:343:U:H1'	41:AC:95:ARG:HG3	1.96	0.48
36:A1:2960:C:H2'	36:A1:2961:G:C8	2.49	0.48
36:A1:3243:A:OP1	52:AO:159[A]:LYS:NZ	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AC:281:ILE:HD12	54:AQ:29:LEU:HG	1.94	0.48
56:AS:8:GLN:HB3	56:AS:64:ILE:HD11	1.94	0.48
8:BH:61:PHE:HA	8:BH:93:LEU:O	2.14	0.48
9:BI:14:THR:O	35:B5:347:G:N2	2.47	0.48
16:BP:20:VAL:HG13	16:BP:24:LYS:HD2	1.96	0.48
36:A1:629:U:H2'	36:A1:630:A:C8	2.48	0.48
36:A1:2228:A:H2'	36:A1:2229:A:C8	2.49	0.48
36:A1:3379:C:H4'	40:AB:315:GLY:HA2	1.96	0.48
42:AD:215:ASP:OD1	42:AD:215:ASP:N	2.45	0.48
73:Aj:66:TYR:OH	73:Aj:73:ARG:NH2	2.47	0.48
35:B5:800:U:H2'	35:B5:801:G:C8	2.49	0.47
36:A1:2146:C:H5''	39:AA:203:ALA:HB1	1.95	0.47
39:AA:195:SER:O	39:AA:198:LYS:NZ	2.39	0.47
40:AB:85:VAL:HG22	40:AB:202:THR:HG22	1.95	0.47
44:AF:25:GLN:HG3	44:AF:28:ALA:HB3	1.95	0.47
70:Ag:29:ILE:HD11	70:Ag:31:ARG:HH21	1.78	0.47
7:BG:174:LYS:HG3	35:B5:78:A:H2	1.78	0.47
14:BN:37:ILE:HG23	14:BN:50:ILE:HG21	1.97	0.47
19:BS:86:LEU:HD22	19:BS:99:HIS:HB2	1.95	0.47
36:A1:307:A:H2'	36:A1:308:A:C8	2.49	0.47
36:A1:2213:A:H2'	36:A1:2214:A:C8	2.49	0.47
44:AF:83:LEU:HD11	44:AF:116:PHE:HB3	1.95	0.47
48:AJ:57:PHE:HB2	48:AJ:59:ILE:HG12	1.96	0.47
79:Ap:30:GLU:HA	79:Ap:33:GLN:HG2	1.96	0.47
14:BN:99:ARG:NH2	14:BN:119:GLU:OE2	2.48	0.47
15:BO:18:ARG:HD3	35:B5:918:U:H4'	1.97	0.47
33:Bg:205:SER:HB3	33:Bg:210:LEU:HB2	1.96	0.47
35:B5:591:A:H2'	35:B5:592:A:C8	2.50	0.47
36:A1:437:G:N1	36:A1:622:A:N6	2.34	0.47
42:AD:156:GLY:HA2	42:AD:181:PRO:HD3	1.97	0.47
47:AI:88:ARG:HG2	47:AI:90:ARG:HG2	1.97	0.47
51:AN:56:LYS:NZ	51:AN:145:ASP:OD2	2.47	0.47
53:AP:153:LYS:HB2	53:AP:153:LYS:HE2	1.71	0.47
17:BQ:33:GLY:HA3	20:BT:7:ARG:HD3	1.97	0.47
33:Bg:304:GLY:HA2	33:Bg:310:ILE:HA	1.96	0.47
35:B5:1125:A:OP1	77:An:18:ARG:NH1	2.39	0.47
36:A1:717:C:OP1	36:A1:751:A:O2'	2.29	0.47
36:A1:2991:A:O3'	40:AB:21:ARG:NH2	2.47	0.47
43:AE:62:THR:HG21	43:AE:78:ARG:HD2	1.96	0.47
52:AO:126[A]:VAL:O	56:AS:154:HIS:NE2	2.45	0.47
73:Aj:58:THR:OG1	73:Aj:59:THR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BJ:109:LEU:HB2	10:BJ:146:PHE:HB3	1.95	0.47
15:BO:68:ALA:HB2	15:BO:105:LEU:HD12	1.95	0.47
19:BS:126:ARG:HB2	19:BS:133:VAL:HG12	1.97	0.47
28:Bb:36:LYS:HG3	28:Bb:78:SER:HB3	1.96	0.47
34:Bh:96:ARG:H	35:B5:1274:C:H5	1.63	0.47
36:A1:3016:A:H2'	36:A1:3017:A:C8	2.50	0.47
36:A1:3166:C:H2'	36:A1:3167:A:H8	1.79	0.47
44:AF:170:GLU:HG3	44:AF:179:LEU:HD23	1.96	0.47
52:AO:6[A]:VAL:HG12	52:AO:32[A]:LYS:HB2	1.96	0.47
1:BA:73:VAL:HG13	1:BA:120:LEU:HD23	1.97	0.47
5:BE:71:LYS:HG3	5:BE:91:THR:HB	1.96	0.47
14:BN:142:GLU:OE2	14:BN:145:THR:OG1	2.30	0.47
35:B5:1097:U:H4'	35:B5:1098:U:H5''	1.96	0.47
36:A1:421:G:O6	36:A1:2383:C:O2'	2.30	0.47
36:A1:1446:A:H5''	53:AP:65:SER:HB2	1.96	0.47
61:AX:68:THR:HA	61:AX:73:MET:HE3	1.97	0.47
16:BP:67:ALA:HB2	16:BP:73:PRO:HA	1.97	0.47
24:BX:78:LYS:HG3	24:BX:79:ASN:HB2	1.97	0.47
36:A1:824:C:H5''	39:AA:21:ARG:HD3	1.96	0.47
58:AU:14:THR:HG23	58:AU:66:VAL:HG22	1.96	0.47
59:AV:27:ASP:OD1	59:AV:27:ASP:N	2.45	0.47
17:BQ:129:PHE:O	17:BQ:137:ARG:NH1	2.47	0.47
18:BR:4:VAL:HG22	35:B5:1402:G:H4'	1.96	0.47
35:B5:1041:G:H2'	35:B5:1042:G:C8	2.50	0.47
36:A1:219:A:HO2'	36:A1:220:G:H21	1.62	0.47
36:A1:2732:G:H5'	36:A1:2761:G:H5''	1.97	0.47
42:AD:50:ARG:NH2	42:AD:72:ASP:OD2	2.44	0.47
43:AE:80:ASN:HB3	43:AE:83:TYR:HD1	1.80	0.47
47:AI:30:LYS:HD2	47:AI:63:GLU:HG3	1.97	0.47
50:AM:23:ILE:O	50:AM:30:GLY:N	2.46	0.47
50:AM:50:LYS:NZ	50:AM:82:SER:OG	2.47	0.47
62:AY:39:LEU:HD22	62:AY:43:TYR:HE2	1.78	0.47
3:BC:139:ILE:HD13	3:BC:191:ALA:HB1	1.97	0.47
4:BD:195:SER:OG	4:BD:196:ARG:N	2.48	0.47
9:BI:25:ARG:HA	35:B5:400:A:H5''	1.96	0.47
9:BI:178:ARG:NH2	35:B5:258:C:O2	2.47	0.47
11:BK:91:TYR:HA	11:BK:92:ILE:HA	1.65	0.47
36:A1:3261:C:OP1	50:AM:126:GLN:NE2	2.43	0.47
45:AG:82:LEU:HG	45:AG:86:THR:HG23	1.97	0.47
48:AJ:165:GLN:CD	48:AJ:166:LYS:H	2.23	0.47
50:AM:94:TRP:O	50:AM:97:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AO:54[A]:TYR:OH	52:AO:73[A]:PHE:O	2.32	0.47
1:BA:126:PRO:HG2	1:BA:151:SER:HB2	1.97	0.47
8:BH:30:SER:OG	8:BH:33:GLU:OE2	2.29	0.47
10:BJ:105:LEU:HD13	10:BJ:108:ARG:HD2	1.96	0.47
23:BW:24:GLN:HA	23:BW:63:VAL:O	2.14	0.47
36:A1:250:U:H5''	36:A1:251:G:H8	1.80	0.47
46:AH:186:PHE:HB2	46:AH:189:GLU:HB2	1.97	0.47
76:Am:92:ASP:OD1	76:Am:126:LYS:NZ	2.48	0.47
1:BA:56:LYS:NZ	22:BV:70:ASN:OD1	2.36	0.46
4:BD:140:GLY:HA3	4:BD:182:LEU:HD12	1.97	0.46
5:BE:127:LYS:N	5:BE:140:VAL:O	2.42	0.46
7:BG:133:LEU:O	35:B5:166:C:O2'	2.30	0.46
36:A1:528:U:H2'	36:A1:529:A:C8	2.50	0.46
36:A1:1385:C:O2	43:AE:2:SER:N	2.48	0.46
36:A1:2155:G:O3'	39:AA:227:ARG:NH2	2.47	0.46
64:Aa:71:PRO:HB2	64:Aa:109:TYR:HA	1.97	0.46
2:BB:111:ARG:HB3	27:Ba:68:TYR:HB2	1.97	0.46
4:BD:52:ALA:O	4:BD:90:ARG:HA	2.15	0.46
5:BE:104:ASP:HB3	5:BE:110:ALA:HB2	1.96	0.46
36:A1:366:A:OP1	41:AC:95:ARG:NH1	2.41	0.46
36:A1:743:C:N3	54:AQ:141:ARG:NH2	2.50	0.46
36:A1:2810:C:OP2	36:A1:2955:U:O2'	2.31	0.46
9:BI:41:LYS:HG3	9:BI:60:ILE:HG22	1.97	0.46
35:B5:131:C:H2'	35:B5:132:U:H3'	1.96	0.46
35:B5:813:U:O2'	35:B5:815:G:OP1	2.33	0.46
36:A1:406:G:OP1	36:A1:1415:U:O2'	2.32	0.46
36:A1:1551:C:O2'	36:A1:2170:U:O2'	2.30	0.46
36:A1:2768:U:H2'	36:A1:2769:A:C8	2.51	0.46
42:AD:107:ARG:HD2	42:AD:248:ARG:HG2	1.96	0.46
44:AF:120:THR:HB	57:AT:132:PRO:HB2	1.97	0.46
79:Ap:46:THR:OG1	79:Ap:57:CYS:SG	2.65	0.46
2:BB:126:THR:HG1	2:BB:136:ARG:HE	1.64	0.46
9:BI:172:ARG:HE	9:BI:175:GLN:HG3	1.81	0.46
17:BQ:132:LYS:HG2	17:BQ:138:PHE:HE1	1.80	0.46
28:Bb:30:SER:OG	35:B5:959:U:OP1	2.34	0.46
35:B5:580:A:O2'	35:B5:582:U:OP1	2.32	0.46
35:B5:1291:G:H22	35:B5:1324:G:N2	2.11	0.46
35:B5:1672:G:H2'	35:B5:1673:G:C8	2.50	0.46
36:A1:996:A:N3	37:A3:80:G:O2'	2.48	0.46
67:Ad:55:LEU:HB2	67:Ad:95:PRO:HD3	1.96	0.46
23:BW:42:GLN:NE2	23:BW:48:GLY:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B5:31:C:O2'	35:B5:547:U:OP1	2.34	0.46
35:B5:189:C:O2	35:B5:196:G:N2	2.42	0.46
35:B5:891:A:H2'	35:B5:892:A:C8	2.51	0.46
35:B5:1717:G:H2'	35:B5:1718:G:C8	2.51	0.46
36:A1:990:PSU:H5'	57:AT:100:LYS:HE2	1.97	0.46
36:A1:1246:G:O2'	36:A1:1248:C:OP1	2.31	0.46
36:A1:1810:A:OP2	63:AZ:61:LYS:NZ	2.45	0.46
49:AL:46:ILE:HD11	49:AL:51:LEU:HA	1.98	0.46
16:BP:17:TYR:HB2	16:BP:25:LEU:HD11	1.96	0.46
35:B5:1359:C:H2'	35:B5:1360:A:C8	2.50	0.46
44:AF:180:SER:H	44:AF:183:ASP:HB2	1.81	0.46
63:AZ:21:LYS:HD3	63:AZ:47:GLU:HA	1.97	0.46
2:BB:123:ALA:HB2	2:BB:165:ARG:HG2	1.97	0.46
17:BQ:29:ILE:HD13	17:BQ:52:LEU:HD21	1.98	0.46
36:A1:1950:U:H3	36:A1:2096:A:H61	1.63	0.46
39:AA:28:LYS:HB3	39:AA:123:ARG:HB3	1.97	0.46
53:AP:11:PRO:HA	53:AP:14:SER:HB2	1.96	0.46
14:BN:54:LEU:HB3	14:BN:60:VAL:HB	1.98	0.46
16:BP:41:VAL:HG22	16:BP:84:ILE:HD13	1.97	0.46
36:A1:1925:U:O2'	36:A1:1927:G:N7	2.48	0.46
40:AB:289:ASP:OD1	40:AB:289:ASP:N	2.43	0.46
44:AF:86:VAL:O	44:AF:114:GLY:HA2	2.16	0.46
53:AP:32:THR:HG21	53:AP:87:SER:HB3	1.96	0.46
1:BA:126:PRO:HB2	1:BA:152:PRO:HG2	1.98	0.46
13:BM:24:ILE:HD13	13:BM:87:PRO:HB2	1.98	0.46
36:A1:860:G:H5'	36:A1:861:C:H5''	1.97	0.46
36:A1:2160:G:H2'	36:A1:2161:G:C8	2.51	0.46
36:A1:3067:C:H3'	55:AR:62:ARG:HH12	1.80	0.46
36:A1:3094:A:OP1	59:AV:14:SER:OG	2.32	0.46
36:A1:3252:G:H2'	36:A1:3253:G:C8	2.51	0.46
40:AB:35:ASP:OD2	40:AB:37:ARG:NH2	2.49	0.46
66:Ac:13:LYS:NZ	66:Ac:105:ALA:O	2.44	0.46
78:Ao:25:VAL:HG22	78:Ao:72:LEU:HD13	1.97	0.46
9:BI:87:ASN:HB3	9:BI:90:LEU:HG	1.97	0.46
15:BO:40:ALA:HB2	15:BO:70:LYS:HG2	1.97	0.46
30:Bd:19:ARG:HD2	30:Bd:32:ARG:HD3	1.98	0.46
34:Bh:68:ARG:NH1	35:B5:1460:A:OP2	2.47	0.46
35:B5:1524:A:H2'	35:B5:1525:A:C8	2.51	0.46
36:A1:2697:A:H2'	36:A1:2698:G:C8	2.51	0.46
37:A3:73:C:H41	56:AS:19:VAL:HG21	1.81	0.46
2:BB:103:MET:HE3	2:BB:215:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:207:LEU:HD23	2:BB:207:LEU:HA	1.83	0.45
32:Bf:95:HIS:NE2	35:B5:1232:U:O4	2.40	0.45
36:A1:1699:A:H2'	36:A1:1700:G:C8	2.52	0.45
36:A1:3119:U:H4'	76:Am:104:PRO:HG3	1.98	0.45
52:AO:60[A]:LYS:HE2	52:AO:60[A]:LYS:HB3	1.81	0.45
62:AY:71:SER:N	62:AY:81:GLN:O	2.49	0.45
66:Ac:16:LEU:HG	66:Ac:19:LYS:HE3	1.98	0.45
1:BA:90:ALA:HA	1:BA:95:ALA:HB3	1.97	0.45
4:BD:7:LYS:NZ	21:BU:113:ASP:OD2	2.48	0.45
10:BJ:24:LEU:HD22	35:B5:591:A:H5''	1.98	0.45
19:BS:27:LYS:HA	19:BS:57:ARG:HA	1.98	0.45
35:B5:65:A:H2	35:B5:84:A:H62	1.64	0.45
35:B5:513:U:H2'	35:B5:514:G:C8	2.50	0.45
35:B5:877:G:H22	35:B5:951:A:H2	1.65	0.45
35:B5:1641:C:H2'	35:B5:1642:G:C8	2.52	0.45
36:A1:1125:U:O2'	36:A1:2643:A:N1	2.49	0.45
36:A1:2726:C:H3'	36:A1:2728:G:H21	1.80	0.45
49:AL:185:LYS:HA	49:AL:188:ARG:HG2	1.98	0.45
51:AN:18:VAL:HG13	51:AN:19:LEU:HD12	1.97	0.45
54:AQ:31:LYS:HE3	54:AQ:31:LYS:HB2	1.70	0.45
4:BD:70:THR:HA	4:BD:86:LEU:HD13	1.98	0.45
14:BN:23:PRO:HD2	14:BN:26:PHE:HB2	1.97	0.45
33:Bg:51:ASP:OD1	33:Bg:51:ASP:N	2.48	0.45
35:B5:953:G:H2'	35:B5:954:G:C8	2.52	0.45
36:A1:12:A:H2'	36:A1:13:A:C8	2.52	0.45
36:A1:860:G:C5	39:AA:181:LYS:HB2	2.51	0.45
36:A1:1134:G:O2'	36:A1:2642:A:N3	2.39	0.45
39:AA:70:ARG:HH11	39:AA:72:ARG:HH22	1.65	0.45
46:AH:141:LYS:HD2	46:AH:141:LYS:HA	1.74	0.45
48:AJ:107:ASP:HB3	48:AJ:124:GLY:HA2	1.99	0.45
62:AY:106:ILE:HG21	62:AY:109:LEU:HD23	1.99	0.45
2:BB:153:HIS:HE1	35:B5:1044:U:H5''	1.81	0.45
8:BH:70:PHE:O	8:BH:74:GLN:HB2	2.16	0.45
22:BV:2:GLU:HG3	22:BV:8:LEU:HA	1.97	0.45
35:B5:971:A:N1	36:A1:846:A:N6	2.65	0.45
36:A1:2141:U:H5'	36:A1:2977:G:H4'	1.99	0.45
45:AG:70:LYS:HA	45:AG:70:LYS:HD2	1.82	0.45
47:AI:49:CYS:HB3	47:AI:168:SER:HB3	1.99	0.45
54:AQ:165:ILE:HD11	54:AQ:172:PHE:HB3	1.99	0.45
76:Am:79:GLU:HG3	76:Am:82:LEU:HD12	1.98	0.45
4:BD:40:ARG:NH2	4:BD:47:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:135:GLU:HB2	4:BD:157:LEU:HD11	1.97	0.45
20:BT:36:ILE:HG13	20:BT:37:VAL:HG13	1.98	0.45
35:B5:813:U:O2	55:AR:163:ARG:NH2	2.49	0.45
36:A1:710:A:H2'	36:A1:711:A:C8	2.52	0.45
36:A1:1724:U:H1'	36:A1:1725:C:C6	2.52	0.45
36:A1:2223:A:H2'	36:A1:2224:A:C8	2.51	0.45
36:A1:2357:A:H2'	36:A1:2358:A:C8	2.51	0.45
38:A4:149:A:H2'	38:A4:150:G:C8	2.52	0.45
55:AR:134:HIS:HE1	55:AR:136:ARG:HE	1.64	0.45
64:Aa:104:THR:HG22	64:Aa:109:TYR:HB2	1.98	0.45
74:Ak:44:LYS:HA	74:Ak:52:TYR:O	2.17	0.45
76:Am:104:PRO:HG2	76:Am:107:ALA:HB2	1.98	0.45
10:BJ:113:VAL:HG12	10:BJ:119:ALA:HB2	1.98	0.45
22:BV:40:ASP:HB3	22:BV:46:ILE:HD11	1.97	0.45
25:BY:62:THR:HA	25:BY:69:SER:HA	1.99	0.45
36:A1:1144:U:OP1	36:A1:1367:G:O2'	2.30	0.45
36:A1:1176:C:H2'	36:A1:1177:G:N2	2.32	0.45
36:A1:1191:U:H3'	76:Am:113:ARG:HH12	1.81	0.45
36:A1:1637:A:H4'	63:AZ:15:ARG:HB3	1.98	0.45
36:A1:2666:C:OP2	36:A1:2687:G:N1	2.45	0.45
38:A4:135:G:H5''	61:AX:49:LYS:HD3	1.97	0.45
40:AB:222:LYS:HD3	40:AB:331:ASN:HB3	1.98	0.45
41:AC:289:ILE:HD13	54:AQ:125:ASP:HB2	1.99	0.45
51:AN:22:LEU:HD23	51:AN:26:ARG:HH21	1.80	0.45
59:AV:80:ARG:HB2	59:AV:99:ALA:HB3	1.99	0.45
23:BW:76:SER:H	35:B5:1100:G:HO2'	1.59	0.45
36:A1:76:G:N7	49:AL:101:ARG:HB3	2.32	0.45
36:A1:1303:A:N3	36:A1:2885:C:O2'	2.40	0.45
36:A1:2662:G:H2'	36:A1:2663:G:C8	2.51	0.45
71:Ah:85:THR:HB	71:Ah:88:LEU:HB2	1.97	0.45
3:BC:159:THR:O	3:BC:220:ASN:ND2	2.50	0.45
36:A1:1243:G:N2	36:A1:1248:C:OP2	2.40	0.45
36:A1:1799:A:H2'	36:A1:1800:A:C8	2.52	0.45
36:A1:3252:G:H2'	36:A1:3253:G:H8	1.82	0.45
38:A4:59:A:H1'	61:AX:61:LYS:HE2	1.99	0.45
41:AC:206:LEU:HB3	41:AC:248:VAL:HG22	1.99	0.45
2:BB:150:VAL:HG23	35:B5:1067:C:H5''	1.99	0.45
6:BF:84:LYS:NZ	35:B5:1614:A:OP2	2.45	0.45
33:Bg:89:LEU:HD21	33:Bg:124:SER:HB3	1.98	0.45
35:B5:1087:A:H2'	35:B5:1088:A:C8	2.51	0.45
36:A1:3266:G:OP2	43:AE:70:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:AB:148:LEU:HD13	40:AB:196:ARG:HE	1.82	0.45
23:BW:41:MET:HG2	23:BW:129:VAL:HG21	1.98	0.45
36:A1:656:A:H2'	36:A1:657:A:C8	2.51	0.45
36:A1:1188:U:OP1	36:A1:1210:U:O2'	2.26	0.45
36:A1:3259:U:H5''	36:A1:3261:C:H5	1.82	0.45
36:A1:3295:A:H2'	36:A1:3296:A:C8	2.52	0.45
43:AE:154:LEU:HD12	50:AM:119:GLN:HG2	1.99	0.45
53:AP:108:ASP:OD1	53:AP:110:THR:OG1	2.35	0.45
59:AV:27:ASP:HB3	59:AV:109:MET:HE3	1.99	0.45
69:Af:14:LEU:HD11	69:Af:31:LYS:HB2	1.98	0.45
35:B5:751:G:H2'	35:B5:752:A:H8	1.82	0.44
36:A1:696:C:OP2	41:AC:119:ARG:NH2	2.47	0.44
36:A1:821:U:H2'	36:A1:822:G:H8	1.82	0.44
36:A1:3322:A:H2'	36:A1:3323:A:C8	2.52	0.44
47:AI:153:ARG:HG3	47:AI:156:ARG:HH11	1.82	0.44
60:AW:18:GLY:HA3	60:AW:31:PHE:O	2.17	0.44
63:AZ:97:SER:OG	63:AZ:98:THR:N	2.50	0.44
1:BA:200:ASP:OD2	18:BR:90:ALA:N	2.51	0.44
3:BC:49:LYS:HE3	3:BC:246:GLU:HG3	1.99	0.44
4:BD:126:VAL:HG11	4:BD:188:ILE:HG12	1.98	0.44
23:BW:31:SER:HB3	35:B5:636:A:H5''	1.99	0.44
36:A1:2852:C:N3	47:AI:158:LYS:NZ	2.66	0.44
46:AH:57:VAL:HG23	46:AH:68:LEU:HD13	1.99	0.44
47:AI:57:LEU:HD12	47:AI:130:ASP:HA	1.99	0.44
23:BW:25:VAL:HG13	23:BW:65:LEU:HD11	2.00	0.44
24:BX:43:PHE:O	24:BX:45:GLY:N	2.50	0.44
35:B5:29:U:H2'	35:B5:30:G:C8	2.53	0.44
35:B5:1619:C:H2'	35:B5:1620:C:H6	1.81	0.44
41:AC:161:LYS:HA	41:AC:161:LYS:HD2	1.80	0.44
44:AF:239:LEU:O	44:AF:242:SER:OG	2.31	0.44
47:AI:48:LEU:HD11	47:AI:167:LEU:HD12	1.98	0.44
6:BF:42:LEU:HD21	6:BF:90:ILE:HG21	1.99	0.44
15:BO:127:ARG:NH2	35:B5:1787:C:OP1	2.50	0.44
19:BS:145:ARG:HA	34:Bh:69:ARG:HH22	1.83	0.44
24:BX:114:LYS:HD2	35:B5:571:G:H4'	1.99	0.44
35:B5:1591:C:H2'	35:B5:1592:A:C8	2.52	0.44
36:A1:976:U:P	54:AQ:144:ARG:HH22	2.41	0.44
36:A1:2617:U:H3'	65:Ab:3:LYS:HD2	1.98	0.44
39:AA:206:PRO:HG3	39:AA:213:GLY:HA3	1.99	0.44
42:AD:22:ARG:HA	42:AD:25:GLU:HB2	1.98	0.44
42:AD:41:LYS:HD2	57:AT:93:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AI:44:ASP:OD2	47:AI:185:ARG:NE	2.51	0.44
47:AI:47:PRO:HD2	47:AI:141:LYS:HA	1.99	0.44
3:BC:102:VAL:HG11	3:BC:129:ILE:HG13	1.99	0.44
4:BD:48:VAL:HB	4:BD:86:LEU:HG	1.99	0.44
9:BI:25:ARG:NH2	35:B5:386:G:OP2	2.38	0.44
23:BW:25:VAL:O	23:BW:62:VAL:HA	2.18	0.44
25:BY:60:PHE:HA	25:BY:70:VAL:O	2.17	0.44
31:Be:13:LYS:O	31:Be:17:GLN:HG2	2.18	0.44
46:AH:137:SER:HB2	46:AH:143:GLU:HB3	1.99	0.44
52:AO:8[A]:VAL:HG13	52:AO:34[A]:VAL:HG13	2.00	0.44
64:Aa:73:LEU:HB3	64:Aa:112:ILE:HD13	2.00	0.44
66:Ac:99:ASP:OD1	66:Ac:99:ASP:N	2.45	0.44
35:B5:1642:G:H2'	35:B5:1643:U:H6	1.83	0.44
36:A1:40:A:H5''	64:Aa:35:ALA:HB1	1.98	0.44
36:A1:3000:A:H2'	36:A1:3001:C:C6	2.53	0.44
68:Ae:126:LEU:HB3	68:Ae:128:LEU:HG	1.99	0.44
6:BF:109:LYS:HE3	6:BF:109:LYS:HB2	1.79	0.44
8:BH:60:ILE:HB	8:BH:92:PHE:HA	1.98	0.44
20:BT:42:GLY:HA2	20:BT:84:LYS:HG3	1.99	0.44
35:B5:894:U:H2'	35:B5:895:G:C8	2.53	0.44
36:A1:872:U:O2'	36:A1:1908:A:OP1	2.35	0.44
36:A1:1020:G:H3'	36:A1:1021:G:H8	1.81	0.44
36:A1:2258:U:H2'	36:A1:2259:A:C8	2.53	0.44
36:A1:3133:C:H5'	52:AO:55[A]:HIS:HE1	1.82	0.44
40:AB:171:LEU:HD21	40:AB:333:LYS:HB3	1.99	0.44
48:AJ:47:GLN:HG2	48:AJ:67:VAL:HG12	1.99	0.44
58:AU:80:THR:HG21	58:AU:95:PHE:CD2	2.53	0.44
6:BF:98:MET:HE3	6:BF:105:GLY:O	2.18	0.44
8:BH:24:PHE:HA	8:BH:27:LEU:HG	1.99	0.44
13:BM:41:LEU:HD12	13:BM:41:LEU:HA	1.87	0.44
20:BT:86:ARG:NH1	20:BT:90:PRO:O	2.47	0.44
25:BY:7:ILE:HG13	25:BY:27:VAL:HG13	1.99	0.44
36:A1:63:A:N3	36:A1:78:U:O2'	2.48	0.44
36:A1:577:C:O2'	36:A1:579:G:OP1	2.30	0.44
36:A1:578:A:O2'	41:AC:331:ALA:O	2.31	0.44
38:A4:8:C:H2'	38:A4:9:A:C8	2.53	0.44
39:AA:19:HIS:ND1	39:AA:190:ARG:O	2.47	0.44
42:AD:160:PHE:HA	42:AD:163:LEU:HB3	1.98	0.44
44:AF:156:ILE:N	44:AF:158:LYS:O	2.46	0.44
68:Ae:118:LYS:HZ3	68:Ae:120:THR:HG22	1.83	0.44
76:Am:78:ILE:HG12	76:Am:83:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:20:GLU:OE1	4:BD:76:ARG:NE	2.46	0.44
19:BS:56:LYS:O	19:BS:58:ALA:N	2.49	0.44
33:Bg:54:PHE:HE2	33:Bg:314:GLN:HE21	1.66	0.44
35:B5:54:C:O2'	35:B5:459:G:N7	2.42	0.44
36:A1:1203:A:H61	36:A1:1300:G:H2'	1.82	0.44
36:A1:1384:U:H5'	41:AC:138:ARG:NH1	2.33	0.44
36:A1:1601:U:OP1	55:AR:42:ARG:NH2	2.45	0.44
36:A1:1717:U:H2'	36:A1:1718:G:C8	2.53	0.44
41:AC:98:ARG:NH1	41:AC:100:PHE:HA	2.33	0.44
48:AJ:131:MET:HB3	48:AJ:131:MET:HE3	1.72	0.44
50:AM:72:LEU:HD21	50:AM:81:VAL:HG22	2.00	0.44
55:AR:40:ALA:HA	55:AR:43:LYS:HE2	2.00	0.44
58:AU:16:THR:OG1	58:AU:102:GLU:OE1	2.36	0.44
61:AX:108:LEU:HD23	61:AX:125:ARG:HD3	2.00	0.44
2:BB:117:TRP:HB3	2:BB:153:HIS:HA	2.00	0.43
4:BD:143:ARG:HD3	34:Bh:109:GLY:HA2	1.99	0.43
5:BE:37:LYS:NZ	35:B5:298:C:OP2	2.51	0.43
18:BR:7:LYS:N	35:B5:1316:G:OP1	2.48	0.43
20:BT:52:GLY:HA2	20:BT:55:TYR:HD2	1.82	0.43
23:BW:57:ARG:NE	28:Bb:26:GLN:HE21	2.16	0.43
35:B5:1592:A:H2'	35:B5:1593:A:C8	2.53	0.43
36:A1:821:U:H2'	36:A1:822:G:C8	2.53	0.43
39:AA:44:ILE:O	39:AA:61:VAL:HA	2.18	0.43
46:AH:22:SER:OG	46:AH:23:ARG:N	2.51	0.43
47:AI:72:ALA:HB2	47:AI:155:ALA:HB2	2.00	0.43
55:AR:24:LEU:HD23	55:AR:32:ILE:HG21	2.00	0.43
58:AU:19:VAL:HG21	58:AU:30:PRO:HB3	1.99	0.43
2:BB:145:LYS:HG2	2:BB:154:SER:HB2	2.00	0.43
11:BK:64:TYR:OH	35:B5:1435:G:O6	2.27	0.43
13:BM:130:THR:HG22	13:BM:131:ASP:H	1.82	0.43
24:BX:93:LEU:HD21	31:Be:8:LEU:HD13	1.98	0.43
25:BY:111:LYS:HA	25:BY:111:LYS:HD2	1.86	0.43
27:Ba:35:ALA:C	27:Ba:73:TYR:O	2.61	0.43
28:Bb:67:THR:OG1	28:Bb:70:LYS:O	2.36	0.43
33:Bg:132:LYS:HG2	33:Bg:143:THR:HG23	1.99	0.43
35:B5:17:C:O2'	35:B5:1137:A:N1	2.46	0.43
35:B5:1273:G:H4'	35:B5:1274:C:H3'	2.00	0.43
36:A1:20:A:H2'	36:A1:21:G:C8	2.54	0.43
36:A1:1596:C:H2'	36:A1:1597:C:C6	2.53	0.43
36:A1:2335:G:N2	36:A1:2339:C:O2'	2.51	0.43
36:A1:2988:C:OP1	52:AO:65[A]:ASN:ND2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A1:3214:U:H4'	69:Af:3:GLU:HG2	2.01	0.43
40:AB:84:VAL:O	40:AB:202:THR:HA	2.18	0.43
41:AC:170:LYS:HD3	41:AC:175:HIS:HD2	1.83	0.43
51:AN:80:THR:HG22	51:AN:82:GLY:N	2.34	0.43
53:AP:29:THR:HA	53:AP:32:THR:HG22	1.99	0.43
5:BE:100:ARG:HH12	5:BE:122:LYS:HA	1.83	0.43
9:BI:138:ASN:OD1	9:BI:141:ARG:NH2	2.51	0.43
19:BS:11:PHE:HB2	26:BZ:41:ILE:HD13	2.00	0.43
35:B5:1354:G:O6	35:B5:1369:U:C4	2.71	0.43
36:A1:240:U:O2'	36:A1:241:G:N7	2.50	0.43
36:A1:417:A:H2'	36:A1:418:A:C8	2.53	0.43
36:A1:876:A2M:H5''	36:A1:1890:U:H5''	2.00	0.43
36:A1:3280:U:O2'	36:A1:3281:U:O5'	2.32	0.43
38:A4:141:C:O3'	51:AN:62:TYR:OH	2.36	0.43
43:AE:40:LEU:O	43:AE:51:ARG:HA	2.18	0.43
48:AJ:138:VAL:O	48:AJ:146:GLY:N	2.50	0.43
64:Aa:90:TYR:CG	64:Aa:100:PRO:HG3	2.54	0.43
68:Ae:126:LEU:HD23	68:Ae:126:LEU:HA	1.90	0.43
1:BA:191:ARG:HE	1:BA:191:ARG:HB3	1.67	0.43
36:A1:873:C:H3'	36:A1:874:U:H4'	2.01	0.43
36:A1:1466:G:N2	36:A1:1510:G:H5''	2.33	0.43
36:A1:2160:G:H2'	36:A1:2161:G:H8	1.83	0.43
41:AC:150:LEU:HD23	41:AC:249:ILE:HG12	2.00	0.43
42:AD:179:ARG:HA	42:AD:179:ARG:HD3	1.85	0.43
56:AS:79:VAL:HG13	56:AS:90:MET:HB3	1.99	0.43
59:AV:104:ASN:OD1	59:AV:108:GLU:N	2.48	0.43
7:BG:177:ARG:NH2	35:B5:143:G:O6	2.41	0.43
9:BI:42:ARG:HB3	9:BI:58:LEU:O	2.18	0.43
10:BJ:115:LYS:HA	10:BJ:115:LYS:HD3	1.75	0.43
15:BO:80:HIS:HA	15:BO:113:GLY:O	2.19	0.43
35:B5:1291:G:N2	35:B5:1324:G:H22	2.13	0.43
53:AP:84:PRO:HB2	53:AP:87:SER:HB2	2.01	0.43
59:AV:54:LEU:HD21	59:AV:119:GLY:HA3	2.00	0.43
78:Ao:15:LYS:HA	78:Ao:18:ARG:HG3	2.00	0.43
2:BB:23:PRO:HA	2:BB:26:ARG:HD3	2.00	0.43
4:BD:75:LYS:NZ	11:BK:14:TYR:OH	2.42	0.43
5:BE:211:LYS:HE3	5:BE:211:LYS:HB3	1.91	0.43
35:B5:1525:A:H2'	35:B5:1526:A:C8	2.54	0.43
36:A1:339:C:OP1	36:A1:1380:G:O2'	2.34	0.43
36:A1:963:G:O2'	64:Aa:29:PRO:O	2.34	0.43
36:A1:2218:G:H2'	36:A1:2219:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A1:2428:U:H2'	36:A1:2429:G:H8	1.83	0.43
36:A1:2565:U:O2	36:A1:2576:G:O6	2.37	0.43
36:A1:2767:U:H2'	36:A1:2768:U:C6	2.53	0.43
36:A1:2931:C:H5''	59:AV:40:LYS:HD3	2.01	0.43
38:A4:9:A:H2'	38:A4:10:A:C8	2.54	0.43
46:AH:1:MET:HE3	56:AS:139:TYR:HA	1.99	0.43
51:AN:159:ARG:HA	51:AN:164:LEU:HD12	2.00	0.43
56:AS:12:ARG:NH2	56:AS:57:GLU:OE1	2.51	0.43
14:BN:64:ARG:HH22	35:B5:862:A:H8	1.67	0.43
15:BO:136:ARG:HH21	35:B5:1785:U:H5''	1.83	0.43
16:BP:32:ASP:HA	16:BP:35:LYS:HE3	2.00	0.43
30:Bd:32:ARG:NH2	35:B5:1596:C:O2	2.52	0.43
35:B5:968:U:H2'	35:B5:969:C:O4'	2.19	0.43
41:AC:3:ARG:HD2	41:AC:3:ARG:HA	1.75	0.43
41:AC:22:LEU:HA	41:AC:23:PRO:HD3	1.79	0.43
45:AG:109:LEU:HD23	45:AG:109:LEU:HA	1.88	0.43
48:AJ:24:GLY:HA2	48:AJ:65:ILE:HB	2.00	0.43
48:AJ:45:PRO:HB3	48:AJ:69:VAL:HB	2.00	0.43
1:BA:30:GLN:HE21	1:BA:33:GLN:HG2	1.83	0.43
4:BD:116:ARG:NH1	34:Bh:116:GLU:OE2	2.40	0.43
35:B5:140:A:N6	35:B5:281:G:OP2	2.52	0.43
35:B5:393:C:H2'	35:B5:394:C:C6	2.53	0.43
35:B5:610:G:O2'	35:B5:613:G:O2'	2.35	0.43
36:A1:1666:G:H2'	36:A1:1667:A:H8	1.84	0.43
41:AC:99:MET:HE3	41:AC:103:THR:H	1.83	0.43
47:AI:9:TYR:HB3	47:AI:97:LEU:HD22	2.01	0.43
1:BA:76:ILE:HB	1:BA:123:VAL:HG12	2.01	0.43
7:BG:142:ARG:HD2	7:BG:153:VAL:HG11	2.01	0.43
19:BS:41:ARG:NH2	20:BT:36:ILE:O	2.52	0.43
27:Ba:57:SER:OG	27:Ba:58:VAL:O	2.32	0.43
33:Bg:155:ARG:HB2	33:Bg:170:ILE:HG13	2.01	0.43
35:B5:490:C:C5	35:B5:492:A:H5''	2.54	0.43
36:A1:900:G:H1'	36:A1:1589:A:N6	2.33	0.43
36:A1:1076:C:H4'	65:Ab:38:LYS:HG2	2.01	0.43
36:A1:1311:G:N2	52:AO:86[A]:GLY:O	2.31	0.43
36:A1:1810:A:H2'	36:A1:1811:G:C8	2.53	0.43
36:A1:2258:U:H2'	36:A1:2259:A:H8	1.82	0.43
37:A3:2:G:H5'	42:AD:273:ARG:HD2	2.01	0.43
38:A4:67:U:H2'	38:A4:68:G:H8	1.84	0.43
43:AE:40:LEU:HD13	43:AE:84:VAL:HG11	2.00	0.43
46:AH:27:VAL:HG12	46:AH:82:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AS:71:LYS:O	56:AS:73:LYS:NZ	2.52	0.43
75:AI:36:ARG:HE	75:AI:36:ARG:HB3	1.70	0.43
2:BB:70:LEU:HD13	2:BB:84:ILE:HG13	2.01	0.43
3:BC:95:ARG:NH2	35:B5:1290:PSU:OP1	2.50	0.43
6:BF:100:ASN:O	6:BF:102:ARG:N	2.52	0.43
35:B5:250:C:H2'	35:B5:251:A:H8	1.84	0.43
36:A1:314:U:H2'	36:A1:315:C:C6	2.53	0.43
36:A1:400:G:H5''	36:A1:403:C:H1'	2.01	0.43
36:A1:2428:U:H2'	36:A1:2429:G:C8	2.54	0.43
40:AB:33:PRO:HD2	40:AB:44:THR:HB	2.01	0.43
45:AG:189:LEU:HD12	45:AG:190:VAL:HG13	2.01	0.43
53:AP:116:HIS:NE2	53:AP:147:GLU:OE1	2.51	0.43
62:AY:60:ARG:HB2	62:AY:103:LYS:HB3	2.00	0.43
63:AZ:12:VAL:HB	63:AZ:81:LEU:HB3	2.01	0.43
24:BX:74:VAL:HG11	24:BX:104:LEU:HD11	2.01	0.42
35:B5:1280:4AC:H2'	35:B5:1281:G:H8	1.84	0.42
36:A1:567:G:H2'	36:A1:568:G:C8	2.54	0.42
36:A1:600:G:N2	36:A1:603:A:OP2	2.52	0.42
36:A1:1308:A:N1	36:A1:2381:G:O2'	2.47	0.42
36:A1:1497:C:H2'	36:A1:1498:A:C8	2.53	0.42
36:A1:2683:U:H2'	36:A1:2684:C:C6	2.54	0.42
36:A1:3044:G:H2'	36:A1:3045:G:C8	2.54	0.42
41:AC:126:ILE:HG12	41:AC:233:LEU:HD23	2.01	0.42
42:AD:68:THR:OG1	42:AD:71:GLY:O	2.30	0.42
54:AQ:148:GLU:OE2	54:AQ:151:ARG:NE	2.52	0.42
56:AS:14:LEU:HA	56:AS:15:PRO:HD3	1.88	0.42
57:AT:91:LEU:HD12	57:AT:96:ILE:HD11	2.00	0.42
5:BE:79:ASP:HB3	5:BE:82:TYR:HB2	2.01	0.42
5:BE:195:ILE:HG13	5:BE:196:VAL:C	2.44	0.42
8:BH:67:LEU:HD21	8:BH:94:ALA:HB2	2.01	0.42
9:BI:43:ILE:HA	9:BI:56:ARG:O	2.19	0.42
19:BS:30:TYR:HE1	19:BS:40:ARG:HD3	1.83	0.42
35:B5:319:U:H4'	35:B5:323:A:C8	2.55	0.42
35:B5:712:G:H5''	35:B5:713:A:H8	1.83	0.42
36:A1:2282:U:OP1	36:A1:2973:G:O2'	2.29	0.42
52:AO:25[A]:LYS:HA	52:AO:25[A]:LYS:HD3	1.89	0.42
55:AR:25:ASP:HB3	55:AR:28:GLU:HB2	2.00	0.42
56:AS:131:LYS:HE2	56:AS:131:LYS:HB2	1.74	0.42
2:BB:153:HIS:HD2	2:BB:155:TYR:CD2	2.37	0.42
3:BC:45:VAL:HG21	3:BC:68:ILE:HG23	2.01	0.42
8:BH:108:GLN:HG3	35:B5:743:U:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BI:83:TYR:HB3	9:BI:101:ILE:HB	2.00	0.42
12:BL:109:VAL:HG22	12:BL:137:PHE:HB2	2.00	0.42
25:BY:8:ARG:HH12	25:BY:28:LEU:HG	1.84	0.42
35:B5:751:G:H2'	35:B5:752:A:C8	2.54	0.42
36:A1:269:G:H8	36:A1:270:U:H5	1.68	0.42
36:A1:1405:U:OP2	68:Ae:59:SER:OG	2.28	0.42
36:A1:1786:G:H2'	36:A1:1787:A:C8	2.55	0.42
36:A1:2349:PSU:O2'	36:A1:3307:A:N3	2.52	0.42
43:AE:56:LYS:HB2	43:AE:98:VAL:HG11	2.01	0.42
48:AJ:100:GLY:HA3	48:AJ:154:THR:HG22	2.01	0.42
49:AL:3:ILE:HG21	64:Aa:45:MET:HE3	2.00	0.42
63:AZ:64:LYS:HA	63:AZ:67:LYS:HG2	2.01	0.42
65:Ab:32:LEU:HD13	65:Ab:40:ARG:HG2	2.00	0.42
7:BG:15:THR:HG21	35:B5:153:G:H4'	2.02	0.42
9:BI:38:ILE:HG12	9:BI:96:LEU:HD11	2.00	0.42
22:BV:58:TYR:HE1	35:B5:1082:C:H4'	1.84	0.42
33:Bg:248:ASN:OD1	33:Bg:248:ASN:N	2.53	0.42
35:B5:848:C:N3	35:B5:850:A:N6	2.66	0.42
36:A1:418:A:N1	38:A4:5:U:H5	2.16	0.42
36:A1:1468:A:N1	36:A1:1880:U:O2'	2.45	0.42
42:AD:91:GLY:O	42:AD:94:ASN:ND2	2.53	0.42
44:AF:130:ILE:HD12	44:AF:134:VAL:HG11	2.02	0.42
55:AR:105:LEU:HD23	55:AR:138:LEU:HD23	2.01	0.42
63:AZ:133:LYS:HB3	63:AZ:133:LYS:HE2	1.83	0.42
1:BA:50:VAL:HG22	18:BR:109:LEU:HD21	2.01	0.42
1:BA:70:PRO:HB2	1:BA:94:GLY:HA3	2.01	0.42
9:BI:58:LEU:HD21	35:B5:1676:U:H5''	2.01	0.42
10:BJ:27:GLU:HB3	10:BJ:42:ILE:HD13	2.00	0.42
19:BS:39:GLY:H	35:B5:1566:U:H5''	1.83	0.42
27:Ba:84:VAL:O	35:B5:1797:A:N6	2.51	0.42
35:B5:237:C:N4	35:B5:834:G:OP2	2.52	0.42
35:B5:950:C:O2'	35:B5:951:A:OP1	2.37	0.42
36:A1:2392:C:H1'	40:AB:266:ARG:HH21	1.85	0.42
36:A1:2647:A:O3'	47:AI:24:ARG:NH2	2.53	0.42
40:AB:292:ALA:HB2	40:AB:302:LYS:HD3	2.02	0.42
50:AM:134:ALA:HA	50:AM:137:LYS:HE3	2.02	0.42
36:A1:2152:A:H2'	36:A1:2153:U:C6	2.55	0.42
36:A1:2812:C:H2'	36:A1:2813:A:C8	2.54	0.42
37:A3:118:A:H5''	42:AD:253:PHE:CZ	2.54	0.42
40:AB:123:TYR:CZ	40:AB:124:LYS:HG3	2.55	0.42
40:AB:284:ARG:NH1	40:AB:293:ASN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ac:43:ILE:HG12	66:Ac:68:TYR:HB3	2.02	0.42
12:BL:2:SER:O	12:BL:2:SER:OG	2.34	0.42
18:BR:44:LYS:NZ	35:B5:1387:G:N7	2.54	0.42
19:BS:30:TYR:O	19:BS:33:THR:OG1	2.35	0.42
26:BZ:83:LEU:HD23	26:BZ:83:LEU:HA	1.85	0.42
27:Ba:35:ALA:O	27:Ba:73:TYR:O	2.37	0.42
35:B5:702:G:O6	35:B5:737:A:N6	2.52	0.42
35:B5:1515:A:O2'	35:B5:1517:U:OP2	2.30	0.42
36:A1:1493:G:O6	75:A1:2:ALA:N	2.53	0.42
36:A1:2413:A:H2'	36:A1:2414:G:H8	1.84	0.42
36:A1:3111:U:O2'	46:AH:152:GLU:OE2	2.34	0.42
44:AF:123:THR:HG23	44:AF:126:LEU:HD12	2.01	0.42
51:AN:45:PRO:O	51:AN:49:ARG:HG2	2.19	0.42
53:AP:17:ALA:HB1	53:AP:94:LEU:HD22	2.02	0.42
54:AQ:42:ALA:O	54:AQ:46:LYS:NZ	2.50	0.42
63:AZ:14:VAL:HB	70:Ag:86:LYS:HG3	2.01	0.42
63:AZ:27:LYS:HB3	63:AZ:42:LEU:HB2	2.02	0.42
64:Aa:104:THR:HG21	64:Aa:112:ILE:HD11	2.02	0.42
1:BA:198:MET:HG2	1:BA:200:ASP:H	1.84	0.42
3:BC:174:ARG:HA	3:BC:195:ASP:OD2	2.19	0.42
19:BS:41:ARG:HE	20:BT:46:PRO:HD3	1.85	0.42
28:Bb:56:CYS:HB2	28:Bb:63:LEU:HD11	2.01	0.42
35:B5:1220:C:H2'	35:B5:1221:A:C8	2.54	0.42
36:A1:2356:A:H61	36:A1:2983:C:H5	1.67	0.42
44:AF:121:LYS:HB2	57:AT:133:ALA:HB3	2.02	0.42
63:AZ:15:ARG:HG3	63:AZ:79:HIS:CD2	2.54	0.42
78:Ao:72:LEU:O	78:Ao:80:ARG:HA	2.19	0.42
2:BB:24:PHE:HZ	15:BO:39:ILE:HA	1.85	0.42
4:BD:40:ARG:HB2	4:BD:47:GLU:HG2	2.01	0.42
4:BD:105:MET:HE1	4:BD:119:ALA:HB2	2.01	0.42
5:BE:19:LEU:HD11	5:BE:108:ARG:HD2	2.02	0.42
11:BK:59:PHE:CZ	11:BK:62:GLN:HA	2.55	0.42
19:BS:36:LYS:HB3	19:BS:105:VAL:HG21	2.02	0.42
35:B5:108:A:H2'	35:B5:109:G:C8	2.55	0.42
35:B5:1164:G:O2'	35:B5:1612:U:O2	2.35	0.42
36:A1:595:G:OP1	44:AF:33:ARG:NH1	2.40	0.42
36:A1:1345:G:N2	41:AC:307:GLN:OE1	2.50	0.42
36:A1:2366:C:H5'	40:AB:259:HIS:CE1	2.55	0.42
36:A1:3214:U:H6	43:AE:166:LYS:HE2	1.85	0.42
45:AG:55:TYR:HA	45:AG:58:VAL:HG12	2.01	0.42
47:AI:145:LYS:HE3	47:AI:167:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AM:21:VAL:HB	50:AM:63:VAL:HG13	2.02	0.42
53:AP:94:LEU:HA	53:AP:94:LEU:HD23	1.75	0.42
74:Ak:56:ILE:HD12	74:Ak:61:LYS:HE2	2.01	0.42
2:BB:48:VAL:HB	2:BB:49:ASN:H	1.65	0.42
2:BB:78:ASP:OD1	2:BB:79:HIS:ND1	2.53	0.42
5:BE:100:ARG:NH2	5:BE:118:GLU:O	2.52	0.42
6:BF:158:GLN:HG2	29:Bc:65:ARG:HH22	1.85	0.42
12:BL:133:LYS:HB2	35:B5:337:G:H3'	2.02	0.42
21:BU:20:ILE:HD13	21:BU:97:VAL:HB	2.02	0.42
35:B5:706:A:H62	35:B5:731:C:H2'	1.85	0.42
35:B5:1132:A:H2'	35:B5:1133:A:C8	2.55	0.42
36:A1:1495:U:H5	36:A1:1835:A:N1	2.17	0.42
36:A1:3187:A:H5'	46:AH:22:SER:HB2	2.02	0.42
47:AI:43:VAL:HG21	47:AI:197:VAL:HB	2.00	0.42
62:AY:3:LYS:HD2	62:AY:8:VAL:HG23	2.01	0.42
2:BB:82:ARG:HG2	2:BB:105:PHE:CE1	2.55	0.41
2:BB:82:ARG:NH1	2:BB:188:LEU:O	2.40	0.41
2:BB:136:ARG:HB3	2:BB:216:LYS:HG3	2.02	0.41
2:BB:190:PRO:HG2	2:BB:192:VAL:HG23	2.02	0.41
5:BE:3:ARG:HB3	35:B5:93:A:H1'	2.02	0.41
7:BG:74:LYS:HA	7:BG:96:SER:HA	2.02	0.41
7:BG:188:ARG:HD3	35:B5:283:U:H5''	2.02	0.41
24:BX:68:ILE:HD13	31:Be:10:ARG:HH22	1.84	0.41
36:A1:2253:G:H1	36:A1:2263:C:H5	1.67	0.41
36:A1:2279:A:OP2	36:A1:2304:C:N4	2.47	0.41
36:A1:2947:G:N3	40:AB:250:ALA:HB1	2.35	0.41
43:AE:47:PHE:HB3	43:AE:50:LYS:HG3	2.02	0.41
44:AF:51:TYR:OH	44:AF:183:ASP:OD1	2.34	0.41
59:AV:84:SER:HA	59:AV:94:TYR:HB3	2.02	0.41
66:Ac:14:LEU:HD21	66:Ac:43:ILE:HD13	2.02	0.41
66:Ac:57:GLU:OE1	66:Ac:69:TYR:OH	2.37	0.41
7:BG:2:LYS:O	7:BG:108:VAL:HA	2.20	0.41
17:BQ:47:LYS:HD2	17:BQ:47:LYS:HA	1.83	0.41
22:BV:32:VAL:HG22	22:BV:60:ARG:HD2	2.01	0.41
32:Bf:132:LEU:HD12	32:Bf:139:LEU:HB3	2.03	0.41
33:Bg:222:LEU:HD11	33:Bg:245:PHE:HZ	1.85	0.41
35:B5:739:G:OP2	35:B5:739:G:N2	2.43	0.41
36:A1:239:G:N2	71:Ah:94:LYS:O	2.53	0.41
36:A1:1661:G:H2'	36:A1:1662:G:C8	2.54	0.41
36:A1:1785:U:H2'	36:A1:1786:G:C8	2.55	0.41
42:AD:85:ARG:HH12	42:AD:254:LYS:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:AF:87:VAL:HA	44:AF:113:SER:O	2.19	0.41
45:AG:190:VAL:HG23	45:AG:192:GLN:HG2	2.02	0.41
47:AI:189:GLU:N	47:AI:189:GLU:OE1	2.53	0.41
51:AN:153:ASP:HB3	51:AN:156:HIS:HD2	1.86	0.41
53:AP:41:LEU:HD21	53:AP:99:ALA:HB2	2.03	0.41
68:Ae:9:ILE:HG12	68:Ae:63:THR:HB	2.02	0.41
3:BC:41:LEU:HD13	3:BC:61:LEU:HD13	2.01	0.41
5:BE:148:ARG:HD2	35:B5:125:U:H5'	2.02	0.41
5:BE:180:LEU:N	5:BE:229:GLY:O	2.53	0.41
7:BG:102:VAL:HG13	7:BG:106:LEU:HD12	2.01	0.41
10:BJ:38:ASN:HB3	10:BJ:40:LYS:H	1.85	0.41
25:BY:35:VAL:HG23	25:BY:36:SER:H	1.86	0.41
25:BY:132:ARG:NH1	35:B5:154:G:OP2	2.53	0.41
26:BZ:94:LYS:HB3	26:BZ:94:LYS:HE3	1.78	0.41
36:A1:2152:A:H2'	36:A1:2153:U:H6	1.85	0.41
40:AB:83:PRO:O	40:AB:165:GLN:NE2	2.49	0.41
46:AH:186:PHE:HD2	46:AH:189:GLU:HG3	1.84	0.41
61:AX:63:ILE:HD12	61:AX:102:LEU:HD12	2.02	0.41
63:AZ:61:LYS:O	63:AZ:65:ARG:HG2	2.21	0.41
74:Ak:27:ILE:HG12	74:Ak:39:ARG:HH21	1.85	0.41
5:BE:66:MET:HE3	5:BE:66:MET:HB3	1.96	0.41
5:BE:89:VAL:HA	5:BE:99:PHE:O	2.20	0.41
9:BI:152:ILE:HG13	9:BI:153:GLU:H	1.84	0.41
21:BU:89:ARG:HH12	35:B5:1383:G:P	2.43	0.41
33:Bg:129:LYS:HB2	33:Bg:129:LYS:HE3	1.80	0.41
35:B5:27:U:H2'	35:B5:28:A2M:H8	2.02	0.41
36:A1:945:C:H2'	36:A1:946:U:C6	2.56	0.41
36:A1:966:PSU:H2'	36:A1:967:A:C8	2.55	0.41
36:A1:1404:G:OP2	68:Ae:11:LYS:NZ	2.48	0.41
36:A1:1782:U:O2'	36:A1:1858:A:OP1	2.36	0.41
36:A1:2880:PSU:H1'	40:AB:250:ALA:HB3	2.02	0.41
50:AM:133:LYS:HE2	50:AM:133:LYS:HB3	1.84	0.41
52:AO:10[A]:ASP:HB2	52:AO:117[A]:ARG:HB3	2.02	0.41
55:AR:15:VAL:HG23	55:AR:17:VAL:HG22	2.03	0.41
1:BA:74:VAL:HG23	1:BA:118:PRO:HB3	2.03	0.41
3:BC:39:THR:O	3:BC:42:GLY:N	2.54	0.41
7:BG:174:LYS:NZ	7:BG:176:GLN:OE1	2.53	0.41
15:BO:42:VAL:HG11	15:BO:47:LYS:HZ1	1.85	0.41
17:BQ:69:VAL:HG11	17:BQ:81:ILE:HD11	2.03	0.41
25:BY:42:GLU:HG3	25:BY:52:LYS:HE2	2.02	0.41
33:Bg:83:ALA:HB2	33:Bg:113:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B5:293:U:H2'	35:B5:294:C:C6	2.56	0.41
35:B5:712:G:H5''	35:B5:713:A:C8	2.55	0.41
35:B5:1474:G:H2'	35:B5:1475:A:H8	1.84	0.41
35:B5:1594:G:OP2	35:B5:1596:C:N4	2.51	0.41
36:A1:41:G:N2	36:A1:2803:A:H62	2.19	0.41
36:A1:87:U:H2'	36:A1:88:A:C8	2.55	0.41
36:A1:129:U:H2'	36:A1:130:A:C8	2.56	0.41
36:A1:289:A:H2'	36:A1:290:G:H8	1.86	0.41
36:A1:1523:U:H5'	61:AX:113:LEU:HB3	2.02	0.41
36:A1:1565:G:N2	36:A1:1811:G:OP1	2.53	0.41
36:A1:1889:G:OP1	40:AB:246:LEU:N	2.47	0.41
36:A1:3199:G:H4'	50:AM:6:ILE:HD13	2.02	0.41
37:A3:94:C:H2'	37:A3:95:A:C8	2.55	0.41
41:AC:157:GLU:HG3	41:AC:251:THR:HG21	2.03	0.41
43:AE:40:LEU:HB3	43:AE:84:VAL:HG13	2.01	0.41
43:AE:67:GLY:HA2	43:AE:68:PRO:HD3	1.91	0.41
44:AF:176:TYR:CZ	44:AF:197:GLN:HG2	2.55	0.41
68:Ae:66:LEU:HD23	68:Ae:72:LYS:HG3	2.03	0.41
7:BG:219:ARG:HH22	35:B5:242:U:P	2.43	0.41
9:BI:39:GLY:O	9:BI:59:ARG:HB3	2.20	0.41
28:Bb:50:ALA:O	28:Bb:52:THR:N	2.52	0.41
29:Bc:42:ARG:HE	29:Bc:42:ARG:HB3	1.75	0.41
36:A1:182:U:H2'	36:A1:183:G:H8	1.85	0.41
36:A1:1497:C:H2'	36:A1:1498:A:H8	1.86	0.41
42:AD:208:MET:HE3	42:AD:233:ALA:HA	2.03	0.41
47:AI:30:LYS:HD2	47:AI:63:GLU:HA	2.03	0.41
71:Ah:31:LEU:HB3	71:Ah:44:ILE:HD13	2.02	0.41
75:Al:18:LYS:HB2	75:Al:18:LYS:HE3	1.90	0.41
2:BB:61:LEU:HD23	2:BB:64:ARG:HD2	2.02	0.41
2:BB:149:GLN:HE21	2:BB:151:LYS:HG3	1.86	0.41
9:BI:103:GLN:HA	9:BI:165:LEU:O	2.21	0.41
15:BO:103:ARG:HG3	27:Ba:49:ALA:HB2	2.02	0.41
19:BS:41:ARG:NE	20:BT:46:PRO:HD3	2.36	0.41
19:BS:134:ARG:HD3	35:B5:1559:A:C5	2.55	0.41
35:B5:891:A:H2'	35:B5:892:A:H8	1.86	0.41
35:B5:1772:C:H2'	35:B5:1773:4AC:H6	2.02	0.41
36:A1:1659:U:H2'	36:A1:1660:C:C6	2.56	0.41
36:A1:1798:A:H2'	36:A1:1799:A:C8	2.56	0.41
36:A1:1846:C:OP1	36:A1:1849:C:N4	2.50	0.41
36:A1:3160:U:H5''	36:A1:3396:U:H3'	2.03	0.41
46:AH:90:MET:HA	46:AH:180:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AY:24:SER:HB3	62:AY:75:ARG:HH11	1.84	0.41
6:BF:58:LEU:HD22	6:BF:168:VAL:HG23	2.03	0.41
10:BJ:51:LYS:HE3	10:BJ:51:LYS:HB2	1.88	0.41
10:BJ:114:TYR:HA	10:BJ:119:ALA:HB3	2.03	0.41
31:Be:26:LYS:HB3	31:Be:26:LYS:HE3	1.84	0.41
33:Bg:106:HIS:CE1	33:Bg:132:LYS:HG3	2.56	0.41
35:B5:273:G:O6	35:B5:283:U:O2	2.39	0.41
36:A1:184:U:H2'	36:A1:185:C:C6	2.56	0.41
36:A1:525:C:OP2	50:AM:77:ARG:NH2	2.51	0.41
36:A1:705:A:N7	64:Aa:74:ASN:ND2	2.57	0.41
36:A1:792:G:H2'	36:A1:793:C:C6	2.56	0.41
36:A1:943:U:H3'	64:Aa:13:GLY:HA2	2.02	0.41
36:A1:1047:A:H2'	36:A1:1048:A:C8	2.56	0.41
36:A1:1836:C:O2'	36:A1:1842:A:N1	2.46	0.41
36:A1:1915:A:H2'	36:A1:1916:U:C6	2.56	0.41
37:A3:71:G:H2'	37:A3:72:A:C8	2.55	0.41
42:AD:85:ARG:NH2	42:AD:86:TYR:OH	2.51	0.41
44:AF:132:PRO:HA	44:AF:229:PHE:CG	2.55	0.41
57:AT:102:ARG:HA	57:AT:102:ARG:HD2	1.70	0.41
59:AV:15:LEU:HD23	59:AV:53:SER:HB2	2.01	0.41
61:AX:64:GLU:OE1	61:AX:85:GLN:NE2	2.53	0.41
2:BB:33:LYS:HB3	2:BB:41:ARG:HD2	2.03	0.41
5:BE:125:LYS:HB2	5:BE:226:PHE:CD1	2.56	0.41
7:BG:46:LYS:NZ	7:BG:118:GLU:OE1	2.38	0.41
8:BH:10:SER:O	8:BH:10:SER:OG	2.33	0.41
8:BH:23:ALA:HB1	8:BH:84:LYS:HD2	2.03	0.41
11:BK:60:SER:HB3	11:BK:65:TYR:HE1	1.86	0.41
16:BP:108:ARG:HH22	19:BS:118:LYS:HG2	1.84	0.41
17:BQ:95:LYS:HD2	17:BQ:96:TYR:CZ	2.56	0.41
24:BX:65:ASN:ND2	24:BX:116:ASP:OD2	2.48	0.41
35:B5:407:A:H2'	35:B5:408:C:C6	2.56	0.41
36:A1:691:A:N1	38:A4:28:C:O2'	2.45	0.41
36:A1:1096:U:OP2	57:AT:116:ARG:NH1	2.51	0.41
36:A1:1108:U:H2'	36:A1:1109:U:C6	2.56	0.41
36:A1:1261:G:H5'	36:A1:1262:G:H5'	2.02	0.41
36:A1:1913:A:N3	36:A1:2120:A:H2'	2.36	0.41
36:A1:2127:U:O2'	36:A1:2301:U:OP1	2.28	0.41
36:A1:2350:C:H5''	53:AP:68:GLY:HA3	2.02	0.41
36:A1:2552:C:N4	66:Ac:57:GLU:OE2	2.43	0.41
36:A1:2592:G:H4'	36:A1:2594:C:C2	2.55	0.41
36:A1:2747:A:H2'	36:A1:2748:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A4:26:U:O2'	41:AC:51:ALA:O	2.34	0.41
40:AB:57:VAL:HG22	40:AB:73:VAL:HG22	2.03	0.41
40:AB:233:TRP:CD1	40:AB:265:ALA:HB1	2.56	0.41
41:AC:48:GLN:HE21	41:AC:48:GLN:HB3	1.64	0.41
45:AG:93:LEU:HD11	45:AG:207:ASP:HB3	2.02	0.41
53:AP:105:LYS:HE2	53:AP:105:LYS:HB2	1.77	0.41
59:AV:6:ALA:HB1	59:AV:125:LEU:HG	2.03	0.41
59:AV:81:GLN:HG2	59:AV:83:LYS:H	1.86	0.41
67:Ad:6:ASP:OD2	67:Ad:79:ARG:NH2	2.53	0.41
67:Ad:75:ILE:HG12	67:Ad:93:VAL:HG22	2.02	0.41
70:Ag:16:ARG:HG2	70:Ag:37:LYS:HD3	2.03	0.41
70:Ag:103:LYS:HE3	70:Ag:103:LYS:HB3	1.85	0.41
4:BD:158:ILE:HD13	4:BD:158:ILE:HA	1.87	0.41
13:BM:58:LEU:HG	13:BM:59:LEU:HG	2.02	0.41
15:BO:72:LYS:O	15:BO:73:GLU:HG2	2.20	0.41
22:BV:73:ALA:HB3	22:BV:79:LEU:HD12	2.03	0.41
35:B5:406:U:H2'	35:B5:407:A:C8	2.56	0.41
35:B5:593:U:H4'	35:B5:595:G:H4'	2.01	0.41
35:B5:1229:G:N2	35:B5:1255:G:O2'	2.54	0.41
36:A1:87:U:H2'	36:A1:88:A:H8	1.86	0.41
36:A1:439:C:O2'	36:A1:440:A:O4'	2.39	0.41
36:A1:1580:A:H2	61:AX:33:ARG:HD3	1.86	0.41
36:A1:1750:A:OP1	74:Ak:44:LYS:NZ	2.37	0.41
40:AB:120:LYS:HA	40:AB:120:LYS:HD3	1.89	0.41
42:AD:271:LYS:HB2	42:AD:271:LYS:HE3	1.85	0.41
5:BE:200:ARG:HH22	35:B5:246:G:H5'	1.85	0.40
12:BL:17:PRO:O	35:B5:249:U:N3	2.40	0.40
17:BQ:46:PHE:HA	17:BQ:49:TYR:HB2	2.03	0.40
21:BU:85:ARG:HH22	35:B5:1334:U:H4'	1.85	0.40
23:BW:32:LYS:NZ	35:B5:805:U:OP1	2.52	0.40
35:B5:629:U:H2'	35:B5:630:A:C8	2.56	0.40
35:B5:647:G:N2	35:B5:648:G:O6	2.54	0.40
35:B5:1773:4AC:H5	77:An:2:ARG:NH2	2.35	0.40
35:B5:1787:C:H2'	35:B5:1788:G:C8	2.56	0.40
36:A1:2113:A:O2'	36:A1:2116:G:N7	2.47	0.40
40:AB:56:ILE:O	40:AB:73:VAL:HA	2.22	0.40
45:AG:140:VAL:HG22	45:AG:166:LEU:HD21	2.03	0.40
54:AQ:24:VAL:HA	54:AQ:27:LYS:HD2	2.03	0.40
55:AR:172:ARG:HG2	55:AR:176:ARG:HD3	2.03	0.40
64:Aa:24:LYS:O	64:Aa:26:ARG:HG2	2.21	0.40
8:BH:13:PRO:HA	8:BH:14:THR:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BJ:81:VAL:HG23	10:BJ:86:LEU:HD23	2.02	0.40
24:BX:130:VAL:HG11	24:BX:142:LYS:HA	2.04	0.40
25:BY:62:THR:OG1	25:BY:68:LYS:O	2.37	0.40
33:Bg:24:ALA:HB3	33:Bg:34:LEU:HB3	2.03	0.40
35:B5:698:U:N3	35:B5:741:C:C4	2.89	0.40
35:B5:1183:A:N3	35:B5:1210:C:O2'	2.46	0.40
36:A1:528:U:H2'	36:A1:529:A:H8	1.86	0.40
36:A1:596:C:O2	41:AC:326:ARG:NE	2.54	0.40
36:A1:700:C:OP1	49:AL:65:TYR:OH	2.28	0.40
36:A1:716:A:C6	64:Aa:117:ARG:HG3	2.57	0.40
36:A1:1054:A:H5''	36:A1:2637:A:N6	2.34	0.40
36:A1:3043:C:H5'	40:AB:9:PRO:HG2	2.03	0.40
36:A1:3304:U:H1'	40:AB:334:ARG:HH21	1.87	0.40
39:AA:156:LYS:HG2	39:AA:158:ILE:HG23	2.03	0.40
59:AV:13:ILE:HG23	59:AV:85:TRP:CG	2.56	0.40
59:AV:125:LEU:HD12	59:AV:125:LEU:HA	1.97	0.40
63:AZ:72:ILE:HG12	63:AZ:111:LYS:HG3	2.03	0.40
64:Aa:27:LYS:HA	64:Aa:27:LYS:HD2	1.95	0.40
15:BO:20:TYR:HB3	15:BO:27:PHE:HB2	2.03	0.40
35:B5:992:A:C2	35:B5:1012:U:N3	2.79	0.40
35:B5:1561:U:H4'	35:B5:1599:C:H4'	2.03	0.40
36:A1:63:A:H5''	51:AN:174:ILE:HG21	2.02	0.40
36:A1:1405:U:H5'	68:Ae:58:GLY:HA2	2.02	0.40
36:A1:1675:G:H2'	36:A1:1676:A:H8	1.87	0.40
36:A1:2219:A:H2'	36:A1:2220:A2M:C8	2.51	0.40
40:AB:302:LYS:HD3	40:AB:302:LYS:HA	1.84	0.40
46:AH:46:THR:HG22	46:AH:54:LYS:HB2	2.02	0.40
48:AJ:40:LEU:HD23	48:AJ:125:MET:HE1	2.03	0.40
3:BC:165:VAL:HG11	3:BC:210:THR:HA	2.02	0.40
6:BF:27:THR:HG23	17:BQ:28:LEU:HA	2.03	0.40
17:BQ:7:VAL:HG12	17:BQ:95:LYS:HE3	2.04	0.40
29:Bc:33:LEU:HD11	29:Bc:53:ILE:HD13	2.04	0.40
30:Bd:30:LEU:HA	30:Bd:39:CYS:HA	2.04	0.40
36:A1:29:C:H4'	36:A1:62:A:H4'	2.04	0.40
36:A1:178:U:H5'	36:A1:241:G:H22	1.86	0.40
36:A1:692:A:OP1	51:AN:201:ARG:NH2	2.40	0.40
37:A3:36:C:H2'	37:A3:37:G:C8	2.57	0.40
42:AD:146:LEU:HD22	42:AD:163:LEU:HD13	2.04	0.40
51:AN:36:ILE:HD11	51:AN:105:ARG:HB3	2.03	0.40
51:AN:36:ILE:HG12	51:AN:64:VAL:HG23	2.04	0.40
57:AT:28:SER:O	57:AT:32:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AU:43:VAL:HG13	58:AU:49:ASN:HB3	2.04	0.40
7:BG:32:ILE:HD11	7:BG:63:MET:HB3	2.02	0.40
11:BK:23:ALA:O	11:BK:64:TYR:HB2	2.22	0.40
12:BL:40:LEU:HG	35:B5:246:G:N3	2.37	0.40
28:Bb:46:VAL:HG22	28:Bb:54:VAL:HG11	2.03	0.40
32:Bf:124:PRO:HD2	32:Bf:143:LYS:HG2	2.03	0.40
35:B5:188:A:N7	35:B5:189:C:N4	2.70	0.40
36:A1:73:C:C4	72:Ai:15:LYS:HD3	2.56	0.40
36:A1:276:U:O2'	51:AN:91:GLU:OE2	2.33	0.40
36:A1:422:A:C2	36:A1:2363:A:H4'	2.56	0.40
36:A1:901:G:OP1	73:Aj:12:HIS:NE2	2.53	0.40
36:A1:1378:U:H2'	36:A1:1379:G:H8	1.87	0.40
36:A1:2261:G:O2'	36:A1:2263:C:N4	2.54	0.40
36:A1:2344:U:H2'	36:A1:2345:A:C8	2.55	0.40
36:A1:3291:G:H2'	36:A1:3292:A:C8	2.57	0.40
40:AB:183:LEU:HD23	40:AB:183:LEU:HA	1.90	0.40
57:AT:89:LEU:HD23	57:AT:91:LEU:HD11	2.04	0.40
64:Aa:75:LEU:HD13	64:Aa:114:GLY:HA2	2.03	0.40
64:Aa:94:ALA:HB2	64:Aa:121:VAL:HG22	2.04	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 PDB entries followed by that with respect to all EM entries.

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	
1	BA	204/206 (99%)	184 (90%)	19 (9%)	1 (0%)	25	49
2	BB	212/214 (99%)	178 (84%)	32 (15%)	2 (1%)	14	35
3	BC	215/217 (99%)	196 (91%)	19 (9%)	0	100	100
4	BD	221/223 (99%)	208 (94%)	13 (6%)	0	100	100
5	BE	258/260 (99%)	236 (92%)	22 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BF	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
7	BG	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	7	18
8	BH	182/184 (99%)	165 (91%)	16 (9%)	1 (0%)	25	49
9	BI	184/188 (98%)	160 (87%)	24 (13%)	0	100	100
10	BJ	183/185 (99%)	166 (91%)	15 (8%)	2 (1%)	12	30
11	BK	94/96 (98%)	84 (89%)	10 (11%)	0	100	100
12	BL	153/155 (99%)	141 (92%)	12 (8%)	0	100	100
13	BM	119/121 (98%)	89 (75%)	30 (25%)	0	100	100
14	BN	148/150 (99%)	141 (95%)	7 (5%)	0	100	100
15	BO	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
16	BP	122/124 (98%)	109 (89%)	11 (9%)	2 (2%)	8	21
17	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	19	42
18	BR	117/121 (97%)	107 (92%)	8 (7%)	2 (2%)	7	20
19	BS	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	9	24
20	BT	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
21	BU	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
22	BV	83/87 (95%)	75 (90%)	8 (10%)	0	100	100
23	BW	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	38
24	BX	142/144 (99%)	120 (84%)	19 (13%)	3 (2%)	5	15
25	BY	132/134 (98%)	124 (94%)	7 (5%)	1 (1%)	16	38
26	BZ	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
27	Ba	95/97 (98%)	78 (82%)	15 (16%)	2 (2%)	5	15
28	Bb	79/81 (98%)	66 (84%)	13 (16%)	0	100	100
29	Bc	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
30	Bd	51/53 (96%)	51 (100%)	0	0	100	100
31	Be	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
32	Bf	53/57 (93%)	39 (74%)	14 (26%)	0	100	100
33	Bg	310/312 (99%)	273 (88%)	36 (12%)	1 (0%)	37	61
34	Bh	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
39	AA	245/247 (99%)	233 (95%)	12 (5%)	0	100	100
40	AB	383/386 (99%)	364 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	AC	359/361 (99%)	329 (92%)	27 (8%)	3 (1%)	16	38
42	AD	290/292 (99%)	268 (92%)	20 (7%)	2 (1%)	19	42
43	AE	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
44	AF	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	14	35
45	AG	228/230 (99%)	214 (94%)	14 (6%)	0	100	100
46	AH	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
47	AI	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
48	AJ	167/169 (99%)	147 (88%)	20 (12%)	0	100	100
49	AL	191/193 (99%)	169 (88%)	19 (10%)	3 (2%)	8	21
50	AM	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
51	AN	201/203 (99%)	183 (91%)	17 (8%)	1 (0%)	25	49
52	AO	195/197 (99%)	191 (98%)	3 (2%)	1 (0%)	25	49
53	AP	171/175 (98%)	167 (98%)	4 (2%)	0	100	100
54	AQ	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
55	AR	186/188 (99%)	179 (96%)	7 (4%)	0	100	100
56	AS	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
57	AT	157/159 (99%)	145 (92%)	12 (8%)	0	100	100
58	AU	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
59	AV	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
60	AW	61/63 (97%)	61 (100%)	0	0	100	100
61	AX	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
62	AY	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
63	AZ	133/135 (98%)	120 (90%)	12 (9%)	1 (1%)	16	38
64	Aa	146/148 (99%)	123 (84%)	22 (15%)	1 (1%)	19	42
65	Ab	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
66	Ac	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
67	Ad	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
68	Ae	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
69	Af	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
70	Ag	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
71	Ah	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	14	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Ai	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
73	Aj	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
74	Ak	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
75	Al	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
76	Am	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
77	An	23/25 (92%)	23 (100%)	0	0	100	100
78	Ao	103/105 (98%)	90 (87%)	13 (13%)	0	100	100
79	Ap	89/91 (98%)	83 (93%)	5 (6%)	1 (1%)	12	30
All	All	10956/11121 (98%)	10097 (92%)	818 (8%)	41 (0%)	32	55

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	AC	339	LEU
49	AL	48	PRO
49	AL	76	THR
51	AN	81	TYR
52	AO	111[A]	PRO
64	Aa	78	LEU
2	BB	206	PRO
2	BB	207	LEU
7	BG	173	PRO
8	BH	111	LYS
10	BJ	134	ILE
16	BP	125	PRO
19	BS	91	ASP
24	BX	97	ASP
42	AD	20	PHE
49	AL	63	VAL
1	BA	4	PRO
7	BG	68	LEU
10	BJ	133	HIS
27	Ba	35	ALA
27	Ba	36	ILE
42	AD	259	LYS
18	BR	23	LYS
18	BR	24	LEU
24	BX	137	LYS
41	AC	268	ALA

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Mol	Chain	Res	Type
71	Ah	91	ALA
79	Ap	52	ALA
44	AF	158	LYS
17	BQ	33	GLY
24	BX	96	VAL
33	Bg	51	ASP
7	BG	69	LEU
19	BS	92	ILE
44	AF	216	VAL
16	BP	126	VAL
63	AZ	103	GLN
7	BG	67	VAL
41	AC	131	VAL
23	BW	67	GLY
25	BY	35	VAL

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 PDB entries followed by that with respect to all EM entries.

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	
1	BA	173/173 (100%)	173 (100%)	0	100	100
2	BB	191/191 (100%)	191 (100%)	0	100	100
3	BC	176/176 (100%)	176 (100%)	0	100	100
4	BD	182/182 (100%)	182 (100%)	0	100	100
5	BE	221/221 (100%)	220 (100%)	1 (0%)	86	95
6	BF	173/173 (100%)	173 (100%)	0	100	100
7	BG	193/193 (100%)	193 (100%)	0	100	100
8	BH	165/165 (100%)	165 (100%)	0	100	100
9	BI	150/150 (100%)	150 (100%)	0	100	100
10	BJ	158/158 (100%)	158 (100%)	0	100	100
11	BK	89/89 (100%)	89 (100%)	0	100	100
12	BL	136/136 (100%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	BM	98/98 (100%)	98 (100%)	0	100	100
14	BN	127/127 (100%)	127 (100%)	0	100	100
15	BO	96/96 (100%)	96 (100%)	0	100	100
16	BP	104/104 (100%)	104 (100%)	0	100	100
17	BQ	117/117 (100%)	117 (100%)	0	100	100
18	BR	110/110 (100%)	110 (100%)	0	100	100
19	BS	128/128 (100%)	128 (100%)	0	100	100
20	BT	113/113 (100%)	113 (100%)	0	100	100
21	BU	100/100 (100%)	100 (100%)	0	100	100
22	BV	74/74 (100%)	74 (100%)	0	100	100
23	BW	110/110 (100%)	110 (100%)	0	100	100
24	BX	119/119 (100%)	119 (100%)	0	100	100
25	BY	112/112 (100%)	112 (100%)	0	100	100
26	BZ	61/61 (100%)	61 (100%)	0	100	100
27	Ba	83/83 (100%)	82 (99%)	1 (1%)	67	86
28	Bb	70/70 (100%)	70 (100%)	0	100	100
29	Bc	56/56 (100%)	56 (100%)	0	100	100
30	Bd	47/47 (100%)	46 (98%)	1 (2%)	48	76
31	Be	51/51 (100%)	51 (100%)	0	100	100
32	Bf	49/49 (100%)	49 (100%)	0	100	100
33	Bg	256/257 (100%)	256 (100%)	0	100	100
34	Bh	68/68 (100%)	68 (100%)	0	100	100
39	AA	189/189 (100%)	189 (100%)	0	100	100
40	AB	319/321 (99%)	318 (100%)	1 (0%)	91	97
41	AC	288/288 (100%)	288 (100%)	0	100	100
42	AD	241/241 (100%)	241 (100%)	0	100	100
43	AE	134/134 (100%)	134 (100%)	0	100	100
44	AF	186/186 (100%)	185 (100%)	1 (0%)	86	95
45	AG	189/189 (100%)	189 (100%)	0	100	100
46	AH	170/170 (100%)	170 (100%)	0	100	100
47	AI	176/176 (100%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	AJ	147/147 (100%)	147 (100%)	0	100	100
49	AL	154/154 (100%)	154 (100%)	0	100	100
50	AM	107/107 (100%)	107 (100%)	0	100	100
51	AN	175/175 (100%)	175 (100%)	0	100	100
52	AO	160/160 (100%)	160 (100%)	0	100	100
53	AP	141/141 (100%)	141 (100%)	0	100	100
54	AQ	150/150 (100%)	150 (100%)	0	100	100
55	AR	153/153 (100%)	153 (100%)	0	100	100
56	AS	156/156 (100%)	156 (100%)	0	100	100
57	AT	136/136 (100%)	136 (100%)	0	100	100
58	AU	87/87 (100%)	87 (100%)	0	100	100
59	AV	104/104 (100%)	104 (100%)	0	100	100
60	AW	55/55 (100%)	55 (100%)	0	100	100
61	AX	105/105 (100%)	105 (100%)	0	100	100
62	AY	109/109 (100%)	109 (100%)	0	100	100
63	AZ	115/115 (100%)	115 (100%)	0	100	100
64	Aa	118/118 (100%)	118 (100%)	0	100	100
65	Ab	46/46 (100%)	46 (100%)	0	100	100
66	Ac	81/81 (100%)	81 (100%)	0	100	100
67	Ad	96/96 (100%)	96 (100%)	0	100	100
68	Ae	109/109 (100%)	109 (100%)	0	100	100
69	Af	90/90 (100%)	90 (100%)	0	100	100
70	Ag	95/95 (100%)	95 (100%)	0	100	100
71	Ah	104/104 (100%)	104 (100%)	0	100	100
72	Ai	81/81 (100%)	81 (100%)	0	100	100
73	Aj	70/70 (100%)	70 (100%)	0	100	100
74	Ak	68/68 (100%)	68 (100%)	0	100	100
75	Al	45/45 (100%)	45 (100%)	0	100	100
76	Am	47/47 (100%)	47 (100%)	0	100	100
77	An	23/23 (100%)	23 (100%)	0	100	100
78	Ao	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	Ap	71/71 (100%)	71 (100%)	0	100	100
All	All	9336/9339 (100%)	9331 (100%)	5 (0%)	92	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	BE	258	GLN
27	Ba	69	ASN
30	Bd	28	THR
40	AB	89	VAL
44	AF	157	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	30	GLN
1	BA	163	ASN
2	BB	199	ASN
3	BC	110	HIS
3	BC	220	ASN
4	BD	159	HIS
4	BD	162	GLN
4	BD	165	ASN
5	BE	258	GLN
6	BF	34	GLN
6	BF	37	GLN
6	BF	66	GLN
6	BF	103	ASN
6	BF	104	ASN
6	BF	131	GLN
7	BG	197	ASN
8	BH	11	GLN
8	BH	42	GLN
11	BK	28	ASN
11	BK	47	GLN
14	BN	138	ASN
14	BN	151	ASN
15	BO	12	GLN
16	BP	15	HIS
16	BP	103	ASN
19	BS	25	ASN

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Mol	Chain	Res	Type
20	BT	25	GLN
20	BT	64	HIS
20	BT	127	ASN
21	BU	33	GLN
23	BW	70	ASN
26	BZ	44	GLN
28	Bb	9	HIS
32	Bf	123	ASN
33	Bg	182	ASN
33	Bg	314	GLN
39	AA	47	GLN
39	AA	205	ASN
40	AB	121	ASN
40	AB	224	HIS
41	AC	9	HIS
41	AC	110	ASN
41	AC	116	ASN
41	AC	175	HIS
41	AC	260	GLN
41	AC	316	ASN
42	AD	32	GLN
42	AD	90	HIS
42	AD	151	GLN
42	AD	206	GLN
44	AF	25	GLN
44	AF	64	GLN
44	AF	80	GLN
44	AF	197	GLN
45	AG	191	ASN
45	AG	221	ASN
46	AH	96	HIS
46	AH	125	ASN
46	AH	149	ASN
46	AH	163	GLN
47	AI	59	GLN
47	AI	92	HIS
47	AI	175	ASN
47	AI	209	ASN
48	AJ	68	HIS
48	AJ	95	ASN
48	AJ	109	HIS
49	AL	12	ASN

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Mol	Chain	Res	Type
49	AL	106	GLN
50	AM	56	GLN
51	AN	95	GLN
51	AN	138	GLN
52	AO	122[A]	GLN
53	AP	50	GLN
53	AP	133	HIS
53	AP	137	ASN
53	AP	172	GLN
53	AP	179	GLN
54	AQ	126	GLN
56	AS	3	HIS
57	AT	5	HIS
57	AT	131	GLN
57	AT	134	GLN
58	AU	87	ASN
58	AU	101	ASN
59	AV	98	ASN
60	AW	42	GLN
61	AX	85	GLN
63	AZ	122	HIS
63	AZ	127	ASN
64	Aa	14	HIS
64	Aa	120	ASN
67	Ad	57	GLN
68	Ae	20	HIS
68	Ae	49	ASN
68	Ae	60	ASN
74	Ak	67	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	B5	1779/1781 (99%)	474 (26%)	12 (0%)
36	A1	3131/3137 (99%)	709 (22%)	17 (0%)
37	A3	120/121 (99%)	13 (10%)	0
38	A4	156/158 (98%)	37 (23%)	1 (0%)
All	All	5186/5197 (99%)	1233 (23%)	30 (0%)

All (1233) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	B5	2	A
35	B5	4	C
35	B5	17	C
35	B5	25	C
35	B5	26	A
35	B5	34	G
35	B5	45	U
35	B5	46	A
35	B5	47	A
35	B5	57	G
35	B5	60	U
35	B5	68	A
35	B5	72	A
35	B5	73	U
35	B5	74	U
35	B5	75	U
35	B5	76	A
35	B5	77	U
35	B5	78	A
35	B5	81	G
35	B5	83	G
35	B5	94	U
35	B5	103	A
35	B5	104	A
35	B5	111	U
35	B5	114	C
35	B5	116	U
35	B5	126	A
35	B5	127	G
35	B5	130	C
35	B5	133	U
35	B5	134	U
35	B5	135	A
35	B5	136	C
35	B5	137	U
35	B5	138	A
35	B5	140	A
35	B5	141	U
35	B5	145	A
35	B5	158	U
35	B5	161	U
35	B5	166	C
35	B5	168	A

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Mol	Chain	Res	Type
35	B5	171	A
35	B5	178	U
35	B5	182	A
35	B5	183	U
35	B5	188	A
35	B5	189	C
35	B5	190	C
35	B5	191	C
35	B5	192	U
35	B5	194	U
35	B5	195	G
35	B5	198	A
35	B5	199	G
35	B5	200	A
35	B5	204	G
35	B5	215	A
35	B5	217	A
35	B5	218	A
35	B5	226	A
35	B5	227	U
35	B5	229	U
35	B5	230	C
35	B5	231	U
35	B5	232	U
35	B5	233	C
35	B5	234	G
35	B5	235	G
35	B5	236	A
35	B5	237	C
35	B5	238	U
35	B5	239	C
35	B5	240	U
35	B5	241	U
35	B5	246	G
35	B5	249	U
35	B5	250	C
35	B5	260	U
35	B5	261	U
35	B5	262	U
35	B5	265	A
35	B5	267	U
35	B5	272	U

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Mol	Chain	Res	Type
35	B5	273	G
35	B5	277	U
35	B5	280	U
35	B5	281	G
35	B5	287	G
35	B5	304	U
35	B5	313	U
35	B5	314	C
35	B5	315	A
35	B5	316	A
35	B5	320	U
35	B5	321	C
35	B5	322	G
35	B5	333	A
35	B5	337	G
35	B5	338	C
35	B5	352	A
35	B5	359	A
35	B5	360	A
35	B5	361	C
35	B5	365	G
35	B5	380	U
35	B5	389	G
35	B5	390	G
35	B5	393	C
35	B5	400	A
35	B5	401	A
35	B5	402	C
35	B5	404	G
35	B5	417	A
35	B5	419	G
35	B5	423	G
35	B5	424	C
35	B5	425	A
35	B5	426	G
35	B5	427	C
35	B5	434	G
35	B5	439	U
35	B5	444	C
35	B5	452	A
35	B5	460	A
35	B5	464	A

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Mol	Chain	Res	Type
35	B5	468	A
35	B5	475	A
35	B5	477	A
35	B5	481	A
35	B5	483	A
35	B5	484	C
35	B5	486	G
35	B5	488	G
35	B5	489	C
35	B5	490	C
35	B5	491	C
35	B5	492	A
35	B5	493	U
35	B5	494	U
35	B5	495	C
35	B5	496	G
35	B5	497	G
35	B5	498	G
35	B5	499	U
35	B5	500	C
35	B5	503	G
35	B5	506	A
35	B5	507	U
35	B5	510	G
35	B5	514	G
35	B5	515	A
35	B5	519	C
35	B5	524	U
35	B5	527	A
35	B5	538	A
35	B5	539	G
35	B5	540	G
35	B5	541	A2M
35	B5	542	A
35	B5	544	A
35	B5	545	A
35	B5	557	G
35	B5	558	U
35	B5	559	C
35	B5	565	C
35	B5	566	C
35	B5	571	G

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Mol	Chain	Res	Type
35	B5	572	C
35	B5	577	G
35	B5	578	OMU
35	B5	579	A
35	B5	580	A
35	B5	582	U
35	B5	594	A
35	B5	595	G
35	B5	609	U
35	B5	610	G
35	B5	611	U
35	B5	613	G
35	B5	617	U
35	B5	619	A2M
35	B5	620	A
35	B5	621	A
35	B5	622	A
35	B5	623	A
35	B5	638	U
35	B5	639	U
35	B5	650	U
35	B5	651	G
35	B5	652	G
35	B5	653	C
35	B5	655	G
35	B5	656	G
35	B5	657	U
35	B5	658	C
35	B5	677	G
35	B5	678	A
35	B5	679	U
35	B5	681	U
35	B5	683	C
35	B5	694	U
35	B5	696	C
35	B5	697	C
35	B5	698	U
35	B5	700	C
35	B5	701	U
35	B5	704	C
35	B5	705	U
35	B5	706	A

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Mol	Chain	Res	Type
35	B5	707	A
35	B5	708	C
35	B5	710	U
35	B5	712	G
35	B5	713	A
35	B5	715	U
35	B5	716	C
35	B5	717	C
35	B5	718	U
35	B5	719	U
35	B5	720	G
35	B5	721	U
35	B5	722	G
35	B5	723	G
35	B5	724	C
35	B5	725	U
35	B5	727	U
35	B5	728	U
35	B5	730	G
35	B5	731	C
35	B5	732	G
35	B5	733	A
35	B5	734	A
35	B5	735	C
35	B5	736	C
35	B5	737	A
35	B5	738	G
35	B5	743	U
35	B5	745	U
35	B5	755	A
35	B5	765	G
35	B5	766	PSU
35	B5	767	U
35	B5	774	A
35	B5	775	G
35	B5	778	G
35	B5	780	A
35	B5	781	U
35	B5	782	U
35	B5	783	G
35	B5	784	C
35	B5	787	G

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Mol	Chain	Res	Type
35	B5	789	A
35	B5	794	U
35	B5	812	A
35	B5	813	U
35	B5	814	A
35	B5	815	G
35	B5	819	G
35	B5	820	U
35	B5	822	U
35	B5	823	G
35	B5	825	U
35	B5	826	U
35	B5	828	U
35	B5	829	A
35	B5	830	U
35	B5	833	U
35	B5	834	G
35	B5	836	U
35	B5	840	U
35	B5	841	U
35	B5	843	U
35	B5	844	A
35	B5	845	G
35	B5	846	G
35	B5	847	A
35	B5	848	C
35	B5	849	C
35	B5	850	A
35	B5	851	U
35	B5	852	C
35	B5	853	G
35	B5	856	A
35	B5	857	U
35	B5	859	A
35	B5	863	A
35	B5	864	U
35	B5	873	U
35	B5	886	U
35	B5	898	A
35	B5	906	A
35	B5	933	A
35	B5	935	U

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Mol	Chain	Res	Type
35	B5	951	A
35	B5	960	U
35	B5	964	U
35	B5	966	A
35	B5	973	A
35	B5	987	G
35	B5	992	A
35	B5	993	A
35	B5	997	G
35	B5	1004	U
35	B5	1005	A
35	B5	1010	C
35	B5	1021	C
35	B5	1023	A
35	B5	1025	A
35	B5	1026	A
35	B5	1028	C
35	B5	1032	G
35	B5	1039	A
35	B5	1052	U
35	B5	1054	U
35	B5	1056	U
35	B5	1058	U
35	B5	1059	U
35	B5	1061	A
35	B5	1062	A
35	B5	1064	G
35	B5	1076	A
35	B5	1082	C
35	B5	1086	A
35	B5	1092	A
35	B5	1093	A
35	B5	1097	U
35	B5	1098	U
35	B5	1100	G
35	B5	1111	G
35	B5	1137	A
35	B5	1138	A
35	B5	1141	G
35	B5	1147	A
35	B5	1150	G
35	B5	1158	C

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Mol	Chain	Res	Type
35	B5	1185	U
35	B5	1186	U
35	B5	1194	A
35	B5	1196	A
35	B5	1199	G
35	B5	1200	G
35	B5	1201	G
35	B5	1202	A
35	B5	1203	A
35	B5	1217	A
35	B5	1218	G
35	B5	1226	A
35	B5	1227	A
35	B5	1228	G
35	B5	1235	C
35	B5	1243	G
35	B5	1244	A
35	B5	1245	G
35	B5	1255	G
35	B5	1256	A
35	B5	1270	G
35	B5	1284	C
35	B5	1285	U
35	B5	1291	G
35	B5	1306	C
35	B5	1314	U
35	B5	1315	U
35	B5	1316	G
35	B5	1321	A
35	B5	1340	U
35	B5	1344	A
35	B5	1345	A
35	B5	1349	G
35	B5	1355	C
35	B5	1356	U
35	B5	1358	G
35	B5	1359	C
35	B5	1361	U
35	B5	1362	U
35	B5	1363	U
35	B5	1364	G
35	B5	1368	G

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Mol	Chain	Res	Type
35	B5	1371	A
35	B5	1372	U
35	B5	1373	C
35	B5	1378	U
35	B5	1388	A
35	B5	1390	U
35	B5	1399	C
35	B5	1400	A
35	B5	1410	A
35	B5	1413	U
35	B5	1415	PSU
35	B5	1424	A
35	B5	1426	C
35	B5	1427	A
35	B5	1428	OMG
35	B5	1436	A
35	B5	1459	C
35	B5	1461	C
35	B5	1469	A
35	B5	1471	A
35	B5	1483	A
35	B5	1486	G
35	B5	1491	U
35	B5	1492	A
35	B5	1493	A
35	B5	1496	U
35	B5	1503	A
35	B5	1506	G
35	B5	1514	U
35	B5	1516	A
35	B5	1520	U
35	B5	1521	G
35	B5	1523	G
35	B5	1524	A
35	B5	1527	C
35	B5	1537	C
35	B5	1557	U
35	B5	1559	A
35	B5	1572	OMG
35	B5	1573	A
35	B5	1575	G7M
35	B5	1576	A

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Mol	Chain	Res	Type
35	B5	1584	G
35	B5	1590	G
35	B5	1596	C
35	B5	1597	A
35	B5	1600	A
35	B5	1601	G
35	B5	1605	G
35	B5	1616	G
35	B5	1632	C
35	B5	1635	A
35	B5	1636	C
35	B5	1637	C
35	B5	1646	C
35	B5	1651	A
35	B5	1657	U
35	B5	1658	G
35	B5	1663	G
35	B5	1666	U
35	B5	1680	G
35	B5	1682	U
35	B5	1683	C
35	B5	1684	U
35	B5	1686	C
35	B5	1687	U
35	B5	1689	A
35	B5	1690	G
35	B5	1693	A
35	B5	1694	A
35	B5	1695	G
35	B5	1696	G
35	B5	1698	G
35	B5	1699	G
35	B5	1700	C
35	B5	1701	A
35	B5	1702	A
35	B5	1703	C
35	B5	1706	C
35	B5	1709	C
35	B5	1710	U
35	B5	1711	C
35	B5	1716	C
35	B5	1717	G

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Mol	Chain	Res	Type
35	B5	1760	G
35	B5	1762	A
35	B5	1766	A
35	B5	1769	U
35	B5	1780	G
35	B5	1782	MA6
35	B5	1792	G
35	B5	1793	G
35	B5	1794	A
35	B5	1795	U
35	B5	1796	C
36	A1	4	U
36	A1	11	A
36	A1	18	G
36	A1	26	A
36	A1	34	A
36	A1	40	A
36	A1	43	A
36	A1	49	A
36	A1	57	A
36	A1	59	G
36	A1	60	A
36	A1	65	A
36	A1	66	A
36	A1	68	C
36	A1	69	C
36	A1	75	G
36	A1	77	A
36	A1	83	U
36	A1	85	A
36	A1	92	G
36	A1	109	A
36	A1	110	G
36	A1	111	C
36	A1	115	A
36	A1	116	A
36	A1	117	U
36	A1	121	A
36	A1	122	A
36	A1	134	U
36	A1	135	C
36	A1	136	G

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Mol	Chain	Res	Type
36	A1	143	G
36	A1	150	A
36	A1	155	G
36	A1	156	G
36	A1	157	A
36	A1	163	C
36	A1	165	A
36	A1	166	C
36	A1	169	U
36	A1	173	G
36	A1	190	U
36	A1	191	U
36	A1	200	C
36	A1	210	U
36	A1	211	A
36	A1	216	G
36	A1	219	A
36	A1	220	G
36	A1	239	G
36	A1	240	U
36	A1	241	G
36	A1	242	C
36	A1	243	G
36	A1	249	U
36	A1	250	U
36	A1	252	U
36	A1	260	C
36	A1	266	A
36	A1	267	G
36	A1	268	A
36	A1	269	G
36	A1	283	G
36	A1	285	A
36	A1	286	U
36	A1	295	A
36	A1	298	U
36	A1	299	G
36	A1	300	G
36	A1	305	U
36	A1	315	C
36	A1	317	A
36	A1	326	U

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Mol	Chain	Res	Type
36	A1	329	U
36	A1	334	A
36	A1	337	G
36	A1	338	A
36	A1	339	C
36	A1	346	C
36	A1	349	A
36	A1	351	A
36	A1	352	A
36	A1	369	A
36	A1	370	U
36	A1	371	G
36	A1	372	A
36	A1	373	A
36	A1	374	A
36	A1	376	G
36	A1	385	A
36	A1	387	A
36	A1	398	A
36	A1	399	A
36	A1	400	G
36	A1	402	A
36	A1	403	C
36	A1	420	G
36	A1	421	G
36	A1	422	A
36	A1	438	A
36	A1	440	A
36	A1	495	G
36	A1	496	C
36	A1	510	G
36	A1	518	G
36	A1	521	A
36	A1	523	A
36	A1	532	A
36	A1	533	A
36	A1	535	G
36	A1	540	U
36	A1	542	G
36	A1	543	C
36	A1	545	U
36	A1	546	C

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Mol	Chain	Res	Type
36	A1	547	G
36	A1	548	G
36	A1	550	A
36	A1	552	G
36	A1	553	U
36	A1	555	U
36	A1	556	U
36	A1	557	A
36	A1	559	A
36	A1	569	A
36	A1	578	A
36	A1	579	G
36	A1	583	G
36	A1	588	G
36	A1	589	A
36	A1	591	G
36	A1	592	A
36	A1	602	A
36	A1	604	G
36	A1	608	A
36	A1	611	A
36	A1	612	U
36	A1	649	A2M
36	A1	660	A
36	A1	677	A
36	A1	681	U
36	A1	690	A
36	A1	691	A
36	A1	705	A
36	A1	715	A
36	A1	719	U
36	A1	725	G
36	A1	733	G
36	A1	735	A
36	A1	736	A
36	A1	737	G
36	A1	758	C
36	A1	764	U
36	A1	765	C
36	A1	766	U
36	A1	767	U
36	A1	771	A

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Mol	Chain	Res	Type
36	A1	774	G
36	A1	776	PSU
36	A1	777	U
36	A1	780	A
36	A1	781	G
36	A1	784	A
36	A1	785	G
36	A1	786	A
36	A1	799	G
36	A1	801	A
36	A1	806	A
36	A1	807	A2M
36	A1	808	A
36	A1	813	G
36	A1	817	A2M
36	A1	818	C
36	A1	830	A
36	A1	844	G
36	A1	848	A
36	A1	849	C
36	A1	857	G
36	A1	861	C
36	A1	862	U
36	A1	865	U
36	A1	874	U
36	A1	879	U
36	A1	881	C
36	A1	896	A
36	A1	897	U
36	A1	907	G
36	A1	908	OMG
36	A1	909	G
36	A1	914	A
36	A1	915	A
36	A1	916	G
36	A1	917	A
36	A1	920	A
36	A1	921	A
36	A1	923	C
36	A1	924	G
36	A1	925	A
36	A1	934	G

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Mol	Chain	Res	Type
36	A1	937	G
36	A1	944	C
36	A1	959	C
36	A1	960	PSU
36	A1	962	A
36	A1	963	G
36	A1	970	A
36	A1	979	U
36	A1	980	A
36	A1	981	U
36	A1	982	C
36	A1	984	G
36	A1	991	G
36	A1	995	U
36	A1	1002	A
36	A1	1006	A
36	A1	1010	G
36	A1	1016	C
36	A1	1017	C
36	A1	1018	G
36	A1	1019	G
36	A1	1022	U
36	A1	1023	C
36	A1	1031	C
36	A1	1032	C
36	A1	1033	U
36	A1	1034	U
36	A1	1035	G
36	A1	1041	U
36	A1	1045	C
36	A1	1047	A
36	A1	1049	C
36	A1	1063	G
36	A1	1064	A
36	A1	1066	G
36	A1	1068	C
36	A1	1072	G
36	A1	1074	U
36	A1	1081	U
36	A1	1087	G
36	A1	1094	U
36	A1	1097	G

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Mol	Chain	Res	Type
36	A1	1098	A
36	A1	1099	A
36	A1	1103	A
36	A1	1104	G
36	A1	1117	G
36	A1	1131	G
36	A1	1132	C
36	A1	1135	A
36	A1	1144	U
36	A1	1153	A
36	A1	1154	A
36	A1	1155	C
36	A1	1159	A
36	A1	1178	G
36	A1	1180	A
36	A1	1181	U
36	A1	1182	A
36	A1	1189	C
36	A1	1191	U
36	A1	1192	C
36	A1	1196	C
36	A1	1200	A
36	A1	1201	C
36	A1	1202	A
36	A1	1208	U
36	A1	1222	G
36	A1	1223	A
36	A1	1227	C
36	A1	1228	C
36	A1	1231	A
36	A1	1232	C
36	A1	1233	G
36	A1	1235	U
36	A1	1236	G
36	A1	1237	G
36	A1	1239	C
36	A1	1240	A
36	A1	1241	U
36	A1	1242	G
36	A1	1243	G
36	A1	1244	A
36	A1	1245	A

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Mol	Chain	Res	Type
36	A1	1246	G
36	A1	1247	U
36	A1	1248	C
36	A1	1249	G
36	A1	1250	G
36	A1	1251	A
36	A1	1252	A
36	A1	1263	A
36	A1	1268	G
36	A1	1270	A
36	A1	1271	A
36	A1	1272	C
36	A1	1273	A
36	A1	1277	C
36	A1	1281	G
36	A1	1282	G
36	A1	1283	C
36	A1	1286	A
36	A1	1287	A
36	A1	1292	C
36	A1	1305	U
36	A1	1307	G
36	A1	1309	U
36	A1	1315	U
36	A1	1317	A
36	A1	1318	A
36	A1	1332	A
36	A1	1348	U
36	A1	1349	G
36	A1	1350	A
36	A1	1351	U
36	A1	1352	A
36	A1	1353	U
36	A1	1354	G
36	A1	1355	A
36	A1	1356	U
36	A1	1357	G
36	A1	1386	A
36	A1	1392	G
36	A1	1399	A
36	A1	1400	G
36	A1	1408	G

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Mol	Chain	Res	Type
36	A1	1417	G
36	A1	1418	A
36	A1	1419	A
36	A1	1434	G
36	A1	1437	OMC
36	A1	1443	G
36	A1	1450	OMG
36	A1	1455	U
36	A1	1460	A
36	A1	1465	A
36	A1	1469	C
36	A1	1477	A
36	A1	1481	A
36	A1	1487	G
36	A1	1496	C
36	A1	1508	C
36	A1	1511	U
36	A1	1524	A
36	A1	1536	G
36	A1	1539	A
36	A1	1548	C
36	A1	1553	U
36	A1	1555	U
36	A1	1557	A
36	A1	1558	A
36	A1	1561	G
36	A1	1562	C
36	A1	1564	U
36	A1	1565	G
36	A1	1566	A
36	A1	1567	U
36	A1	1570	U
36	A1	1572	U
36	A1	1574	C
36	A1	1575	A
36	A1	1576	G
36	A1	1577	G
36	A1	1583	A
36	A1	1587	A
36	A1	1589	A
36	A1	1590	G
36	A1	1593	A

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Mol	Chain	Res	Type
36	A1	1605	A
36	A1	1621	A
36	A1	1628	C
36	A1	1629	U
36	A1	1630	U
36	A1	1641	U
36	A1	1642	A
36	A1	1643	A
36	A1	1645	U
36	A1	1657	C
36	A1	1664	G
36	A1	1714	A
36	A1	1724	U
36	A1	1730	G
36	A1	1736	G
36	A1	1741	A
36	A1	1742	U
36	A1	1750	A
36	A1	1751	G
36	A1	1761	C
36	A1	1762	C
36	A1	1763	U
36	A1	1764	U
36	A1	1765	U
36	A1	1766	G
36	A1	1778	G
36	A1	1780	G
36	A1	1797	A
36	A1	1813	A
36	A1	1814	A
36	A1	1815	U
36	A1	1816	A
36	A1	1817	G
36	A1	1820	U
36	A1	1821	U
36	A1	1834	U
36	A1	1839	A
36	A1	1842	A
36	A1	1846	C
36	A1	1848	G
36	A1	1849	C
36	A1	1858	A

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Mol	Chain	Res	Type
36	A1	1860	G
36	A1	1866	C
36	A1	1867	A
36	A1	1878	G
36	A1	1880	U
36	A1	1886	A
36	A1	1890	U
36	A1	1893	A
36	A1	1897	G
36	A1	1906	G
36	A1	1908	A
36	A1	1932	A
36	A1	1934	G
36	A1	1947	G
36	A1	1948	G
36	A1	1949	G
36	A1	1951	C
36	A1	1952	G
36	A1	1953	G
36	A1	2094	C
36	A1	2095	G
36	A1	2096	A
36	A1	2112	U
36	A1	2114	C
36	A1	2121	G
36	A1	2122	G
36	A1	2131	A
36	A1	2140	U
36	A1	2142	1MA
36	A1	2144	A
36	A1	2158	A
36	A1	2159	U
36	A1	2160	G
36	A1	2162	U
36	A1	2164	A
36	A1	2165	G
36	A1	2169	G
36	A1	2170	U
36	A1	2171	G
36	A1	2176	U
36	A1	2187	G
36	A1	2188	A

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Mol	Chain	Res	Type
36	A1	2192	C
36	A1	2195	C
36	A1	2197	OMC
36	A1	2205	U
36	A1	2206	G
36	A1	2207	A
36	A1	2209	U
36	A1	2210	G
36	A1	2213	A
36	A1	2225	U
36	A1	2244	A
36	A1	2249	G
36	A1	2250	G
36	A1	2256	A
36	A1	2257	C
36	A1	2258	U
36	A1	2260	PSU
36	A1	2266	PSU
36	A1	2268	U
36	A1	2269	U
36	A1	2270	A
36	A1	2272	G
36	A1	2273	G
36	A1	2274	U
36	A1	2280	A2M
36	A1	2281	A2M
36	A1	2282	U
36	A1	2287	C
36	A1	2288	OMG
36	A1	2304	C
36	A1	2307	G
36	A1	2308	C
36	A1	2310	U
36	A1	2313	A
36	A1	2314	PSU
36	A1	2315	G
36	A1	2318	U
36	A1	2334	U
36	A1	2335	G
36	A1	2336	U
36	A1	2372	A
36	A1	2373	A

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Mol	Chain	Res	Type
36	A1	2374	C
36	A1	2375	G
36	A1	2377	G
36	A1	2383	C
36	A1	2388	U
36	A1	2391	G
36	A1	2393	G
36	A1	2397	A
36	A1	2402	A
36	A1	2403	G
36	A1	2404	A
36	A1	2411	U
36	A1	2412	G
36	A1	2418	G
36	A1	2419	A
36	A1	2422	C
36	A1	2435	G
36	A1	2438	A
36	A1	2440	G
36	A1	2441	A
36	A1	2442	G
36	A1	2443	A
36	A1	2444	C
36	A1	2445	A
36	A1	2502	A
36	A1	2504	U
36	A1	2506	U
36	A1	2508	U
36	A1	2511	A
36	A1	2514	U
36	A1	2515	A
36	A1	2523	A
36	A1	2524	A
36	A1	2529	A
36	A1	2531	C
36	A1	2536	A
36	A1	2537	U
36	A1	2538	U
36	A1	2539	C
36	A1	2540	A
36	A1	2541	U
36	A1	2543	U

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Mol	Chain	Res	Type
36	A1	2544	U
36	A1	2548	C
36	A1	2549	G
36	A1	2550	U
36	A1	2552	C
36	A1	2554	A
36	A1	2561	A
36	A1	2568	C
36	A1	2569	A
36	A1	2570	U
36	A1	2571	U
36	A1	2572	C
36	A1	2573	G
36	A1	2576	G
36	A1	2580	A
36	A1	2581	U
36	A1	2585	G
36	A1	2586	G
36	A1	2593	A
36	A1	2606	G
36	A1	2607	G
36	A1	2614	G
36	A1	2626	A
36	A1	2629	U
36	A1	2642	A
36	A1	2651	G
36	A1	2652	U
36	A1	2656	A
36	A1	2674	A
36	A1	2676	A
36	A1	2677	G
36	A1	2679	A
36	A1	2688	U
36	A1	2689	A
36	A1	2690	G
36	A1	2691	A
36	A1	2703	A
36	A1	2704	A
36	A1	2712	U
36	A1	2714	G
36	A1	2727	A
36	A1	2728	G

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Mol	Chain	Res	Type
36	A1	2729	OMU
36	A1	2737	C
36	A1	2739	A
36	A1	2740	A
36	A1	2752	U
36	A1	2753	G
36	A1	2761	G
36	A1	2762	A
36	A1	2772	C
36	A1	2777	G
36	A1	2778	G
36	A1	2794	G
36	A1	2796	G
36	A1	2797	C
36	A1	2800	G
36	A1	2801	A
36	A1	2802	A
36	A1	2803	A
36	A1	2810	C
36	A1	2814	G
36	A1	2817	A
36	A1	2818	U
36	A1	2822	U
36	A1	2828	G
36	A1	2842	U
36	A1	2844	C
36	A1	2845	A
36	A1	2849	C
36	A1	2859	U
36	A1	2860	U
36	A1	2867	C
36	A1	2871	G
36	A1	2872	A
36	A1	2887	A
36	A1	2889	C
36	A1	2898	G
36	A1	2918	G
36	A1	2923	PSU
36	A1	2930	A
36	A1	2935	U
36	A1	2936	A
36	A1	2938	G

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Mol	Chain	Res	Type
36	A1	2942	C
36	A1	2947	G
36	A1	2951	G
36	A1	2954	U
36	A1	2977	G
36	A1	2983	C
36	A1	2990	G
36	A1	2996	U
36	A1	2997	G
36	A1	3011	A
36	A1	3012	A
36	A1	3022	G
36	A1	3032	A
36	A1	3056	U
36	A1	3059	G
36	A1	3074	G
36	A1	3078	U
36	A1	3079	U
36	A1	3080	G
36	A1	3086	A
36	A1	3087	A
36	A1	3092	C
36	A1	3104	U
36	A1	3109	G
36	A1	3122	A
36	A1	3130	A
36	A1	3131	U
36	A1	3142	A
36	A1	3143	C
36	A1	3153	U
36	A1	3154	C
36	A1	3155	U
36	A1	3156	U
36	A1	3157	U
36	A1	3165	A
36	A1	3170	A
36	A1	3172	A
36	A1	3173	G
36	A1	3174	A
36	A1	3179	U
36	A1	3181	C
36	A1	3187	A

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Mol	Chain	Res	Type
36	A1	3195	U
36	A1	3196	U
36	A1	3198	U
36	A1	3207	U
36	A1	3209	A
36	A1	3215	A
36	A1	3216	G
36	A1	3217	C
36	A1	3218	A
36	A1	3219	G
36	A1	3224	G
36	A1	3243	A
36	A1	3245	A
36	A1	3247	G
36	A1	3251	U
36	A1	3254	G
36	A1	3259	U
36	A1	3260	G
36	A1	3263	G
36	A1	3273	A
36	A1	3275	U
36	A1	3276	G
36	A1	3277	U
36	A1	3278	C
36	A1	3281	U
36	A1	3283	U
36	A1	3284	G
36	A1	3289	G
36	A1	3294	A
36	A1	3304	U
36	A1	3307	A
36	A1	3316	A
36	A1	3317	U
36	A1	3318	G
36	A1	3342	A
36	A1	3345	G
36	A1	3351	U
36	A1	3352	U
36	A1	3353	G
36	A1	3354	U
36	A1	3355	U
36	A1	3356	G

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Mol	Chain	Res	Type
36	A1	3369	G
36	A1	3375	A
36	A1	3378	C
36	A1	3382	U
36	A1	3389	U
36	A1	3395	G
37	A3	11	A
37	A3	13	A
37	A3	35	C
37	A3	49	G
37	A3	52	G
37	A3	54	U
37	A3	55	A
37	A3	65	G
37	A3	73	C
37	A3	76	A
37	A3	99	G
37	A3	102	A
37	A3	112	G
38	A4	13	A
38	A4	16	G
38	A4	34	U
38	A4	35	C
38	A4	38	U
38	A4	46	G
38	A4	52	A
38	A4	59	A
38	A4	61	A
38	A4	62	C
38	A4	63	G
38	A4	68	G
38	A4	75	G
38	A4	81	U
38	A4	82	U
38	A4	83	C
38	A4	85	G
38	A4	86	U
38	A4	87	G
38	A4	88	A
38	A4	90	U
38	A4	95	G
38	A4	102	U

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Mol	Chain	Res	Type
38	A4	104	A
38	A4	105	A
38	A4	106	C
38	A4	111	A
38	A4	112	U
38	A4	113	U
38	A4	116	G
38	A4	125	U
38	A4	126	A
38	A4	136	G
38	A4	148	G
38	A4	152	G
38	A4	157	U
38	A4	158	U

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	B5	187	G
35	B5	272	U
35	B5	488	G
35	B5	489	C
35	B5	847	A
35	B5	950	C
35	B5	1344	A
35	B5	1358	G
35	B5	1458	G
35	B5	1572	OMG
35	B5	1600	A
35	B5	1645	G
36	A1	115	A
36	A1	267	G
36	A1	282	G
36	A1	439	C
36	A1	588	G
36	A1	873	C
36	A1	916	G
36	A1	1032	C
36	A1	1280	C
36	A1	1314	C
36	A1	1354	G
36	A1	1575	A

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Mol	Chain	Res	Type
36	A1	2372	A
36	A1	2585	G
36	A1	2801	A
36	A1	2870	5MC
36	A1	3121	U
38	A4	67	U

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

110 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	$\# Z > 2$
35	OMG	B5	1126	35	19,26,27	0.90	1 (5%)	21,38,41	1.12	1 (4%)
36	OMC	A1	1437	80,36	19,22,23	0.84	1 (5%)	25,31,34	1.54	4 (16%)
36	A2M	A1	817	80,36	18,25,26	0.85	0	20,36,39	1.41	2 (10%)
36	PSU	A1	2826	80,36	18,21,22	1.54	5 (27%)	21,30,33	2.35	5 (23%)
36	PSU	A1	966	80,36	18,21,22	1.45	5 (27%)	21,30,33	2.08	4 (19%)
36	OMC	A1	650	80,36	19,22,23	0.78	1 (5%)	25,31,34	0.89	0
36	A2M	A1	2640	36	18,25,26	0.85	1 (5%)	20,36,39	1.14	2 (10%)
36	PSU	A1	2880	36	18,21,22	1.55	6 (33%)	21,30,33	2.09	5 (23%)
35	A2M	B5	436	35	18,25,26	0.79	0	20,36,39	1.53	4 (20%)
35	MA6	B5	1781	35	19,26,27	1.00	1 (5%)	18,38,41	2.19	3 (16%)
35	PSU	B5	999	35	18,21,22	1.41	3 (16%)	21,30,33	2.03	3 (14%)
36	1MA	A1	2142	80,36	17,25,26	1.36	2 (11%)	17,37,40	1.33	3 (17%)
36	OMG	A1	1450	36	19,26,27	1.03	1 (5%)	21,38,41	1.04	1 (4%)
36	OMG	A1	2288	36	19,26,27	1.01	1 (5%)	21,38,41	1.01	2 (9%)
35	PSU	B5	759	35	18,21,22	1.51	4 (22%)	21,30,33	2.07	4 (19%)
36	PSU	A1	990	36	18,21,22	1.48	3 (16%)	21,30,33	2.13	3 (14%)
35	OMG	B5	562	35	19,26,27	0.95	1 (5%)	21,38,41	1.11	2 (9%)
35	OMU	B5	578	35	19,22,23	1.21	3 (15%)	25,31,34	1.88	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A2M	B5	619	80,35	18,25,26	0.84	0	20,36,39	1.66	3 (15%)
36	OMU	A1	2417	36	19,22,23	1.41	3 (15%)	25,31,34	1.86	4 (16%)
38	PSU	A4	73	38	18,21,22	1.50	4 (22%)	21,30,33	2.13	4 (19%)
36	PSU	A1	2865	36	18,21,22	1.46	5 (27%)	21,30,33	2.07	3 (14%)
35	PSU	B5	120	35	18,21,22	1.47	4 (22%)	21,30,33	2.01	4 (19%)
36	A2M	A1	2280	80,36	18,25,26	0.77	0	20,36,39	1.26	3 (15%)
36	OMG	A1	908	36	19,26,27	0.97	1 (5%)	21,38,41	1.53	5 (23%)
36	PSU	A1	2260	36	18,21,22	1.51	3 (16%)	21,30,33	1.98	4 (19%)
36	PSU	A1	2129	36	18,21,22	1.57	4 (22%)	21,30,33	2.17	4 (19%)
35	MA6	B5	1782	80,35	19,26,27	0.91	1 (5%)	18,38,41	2.16	4 (22%)
35	PSU	B5	632	35	18,21,22	1.61	5 (27%)	21,30,33	2.10	4 (19%)
36	PSU	A1	2923	36	18,21,22	1.45	4 (22%)	21,30,33	2.07	3 (14%)
36	PSU	A1	2944	80,36	18,21,22	1.55	5 (27%)	21,30,33	2.12	6 (28%)
35	A2M	B5	796	35	18,25,26	0.85	0	20,36,39	1.32	2 (10%)
35	4AC	B5	1280	35	21,24,25	1.01	2 (9%)	28,34,37	2.58	8 (28%)
36	PSU	A1	1042	36	18,21,22	1.47	3 (16%)	21,30,33	1.99	4 (19%)
36	OMC	A1	2337	36	19,22,23	0.74	1 (5%)	25,31,34	0.96	1 (4%)
35	A2M	B5	541	35	18,25,26	0.82	0	20,36,39	1.28	2 (10%)
36	PSU	A1	1124	36	18,21,22	1.56	4 (22%)	21,30,33	2.10	4 (19%)
36	PSU	A1	2133	36	18,21,22	1.70	4 (22%)	21,30,33	2.33	5 (23%)
35	OMC	B5	1639	35	19,22,23	0.83	0	25,31,34	0.80	1 (4%)
36	PSU	A1	2266	36	18,21,22	1.43	4 (22%)	21,30,33	2.13	5 (23%)
35	A2M	B5	974	35	18,25,26	0.79	0	20,36,39	1.15	2 (10%)
36	PSU	A1	960	36	18,21,22	1.48	4 (22%)	21,30,33	2.08	4 (19%)
35	A2M	B5	28	80,35	18,25,26	0.82	0	20,36,39	1.38	3 (15%)
36	A2M	A1	1449	80,36	18,25,26	0.83	0	20,36,39	1.32	1 (5%)
36	OMC	A1	2948	80,36	19,22,23	0.85	1 (5%)	25,31,34	1.31	3 (12%)
36	PSU	A1	2975	36	18,21,22	1.51	4 (22%)	21,30,33	2.17	4 (19%)
35	G7M	B5	1575	35	20,26,27	2.53	4 (20%)	16,39,42	1.23	1 (6%)
36	PSU	A1	2735	36	18,21,22	1.49	5 (27%)	21,30,33	2.08	4 (19%)
36	PSU	A1	1110	36	18,21,22	1.52	4 (22%)	21,30,33	2.25	4 (19%)
36	PSU	A1	2351	36	18,21,22	1.55	4 (22%)	21,30,33	2.04	4 (19%)
36	PSU	A1	986	36	18,21,22	1.58	4 (22%)	21,30,33	1.96	5 (23%)
35	PSU	B5	302	35	18,21,22	1.50	4 (22%)	21,30,33	2.16	4 (19%)
35	OMG	B5	1428	80,35	19,26,27	0.94	1 (5%)	21,38,41	1.13	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	PSU	A1	1056	36	18,21,22	1.59	4 (22%)	21,30,33	2.13	4 (19%)
35	A2M	B5	420	35	18,25,26	0.79	0	20,36,39	1.35	2 (10%)
36	OMG	A1	805	36	19,26,27	0.90	1 (5%)	21,38,41	1.26	3 (14%)
36	PSU	A1	2191	36	18,21,22	1.57	4 (22%)	21,30,33	2.31	5 (23%)
36	OMC	A1	663	36	19,22,23	0.83	1 (5%)	25,31,34	0.97	1 (4%)
35	PSU	B5	1181	35	18,21,22	1.56	4 (22%)	21,30,33	2.06	3 (14%)
36	PSU	A1	2314	36	18,21,22	1.48	3 (16%)	21,30,33	2.01	3 (14%)
36	OMG	A1	2815	36	19,26,27	0.99	1 (5%)	21,38,41	1.08	2 (9%)
35	PSU	B5	1290	35	18,21,22	1.62	5 (27%)	21,30,33	2.26	3 (14%)
35	OMG	B5	1572	35	19,26,27	0.94	1 (5%)	21,38,41	1.12	2 (9%)
36	OMG	A1	2619	80,36	19,26,27	0.89	1 (5%)	21,38,41	1.06	2 (9%)
35	OMC	B5	414	35	19,22,23	0.80	0	25,31,34	0.82	1 (4%)
36	OMG	A1	867	36	19,26,27	0.85	1 (5%)	21,38,41	1.13	2 (9%)
36	PSU	A1	1052	80,36	18,21,22	1.48	4 (22%)	21,30,33	2.13	4 (19%)
36	OMC	A1	2197	80,36	19,22,23	0.79	0	25,31,34	0.89	1 (4%)
36	5MC	A1	2278	80,36	19,22,23	1.43	3 (15%)	26,32,35	1.38	3 (11%)
36	OMU	A1	1888	80,36	19,22,23	1.29	3 (15%)	25,31,34	1.93	4 (16%)
36	OMU	A1	2421	36	19,22,23	1.34	3 (15%)	25,31,34	1.90	4 (16%)
35	4AC	B5	1773	35	21,24,25	1.08	3 (14%)	28,34,37	2.76	7 (25%)
36	A2M	A1	2281	80,36	18,25,26	0.75	0	20,36,39	2.32	5 (25%)
36	A2M	A1	1133	80,36	18,25,26	0.84	1 (5%)	20,36,39	1.32	2 (10%)
36	OMU	A1	2921	80,36	19,22,23	1.27	3 (15%)	25,31,34	1.89	5 (20%)
35	A2M	B5	100	80,35	18,25,26	0.84	1 (5%)	20,36,39	1.15	2 (10%)
35	PSU	B5	766	35	18,21,22	1.50	5 (27%)	21,30,33	2.14	5 (23%)
36	PSU	A1	2349	80,36	18,21,22	1.55	4 (22%)	21,30,33	2.00	4 (19%)
35	PSU	B5	211	35	18,21,22	1.51	4 (22%)	21,30,33	2.11	3 (14%)
37	PSU	A3	50	37	18,21,22	1.47	4 (22%)	21,30,33	2.09	3 (14%)
36	OMU	A1	2729	36	19,22,23	1.40	4 (21%)	25,31,34	1.71	7 (28%)
36	A2M	A1	807	36	18,25,26	0.92	1 (5%)	20,36,39	2.05	5 (25%)
35	PSU	B5	466	35	18,21,22	1.53	4 (22%)	21,30,33	2.03	5 (23%)
36	1MA	A1	645	80,36	17,25,26	1.22	2 (11%)	17,37,40	1.20	2 (11%)
36	A2M	A1	2946	80,36	18,25,26	0.81	0	20,36,39	1.51	4 (20%)
35	PSU	B5	1187	35	18,21,22	1.52	4 (22%)	21,30,33	2.07	3 (14%)
36	A2M	A1	649	36	18,25,26	0.78	0	20,36,39	1.31	2 (10%)
36	PSU	A1	2264	36	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	A2M	A1	876	36	18,25,26	0.80	0	20,36,39	1.26	2 (10%)
36	PSU	A1	2340	80,36	18,21,22	1.65	4 (22%)	21,30,33	2.07	4 (19%)
35	PSU	B5	106	35	18,21,22	1.52	4 (22%)	21,30,33	2.08	3 (14%)
36	OMU	A1	898	36	19,22,23	1.37	4 (21%)	25,31,34	1.87	5 (20%)
35	OMU	B5	1269	80,35	19,22,23	1.34	4 (21%)	25,31,34	1.97	7 (28%)
35	OMC	B5	1007	35	19,22,23	0.90	1 (5%)	25,31,34	1.40	3 (12%)
36	OMC	A1	2959	36	19,22,23	0.79	0	25,31,34	0.99	1 (4%)
35	PSU	B5	1415	35	18,21,22	1.63	4 (22%)	21,30,33	2.12	4 (19%)
35	OMG	B5	1271	35	19,26,27	0.90	1 (5%)	21,38,41	1.11	2 (9%)
35	B8N	B5	1191	35	25,29,30	0.91	1 (4%)	28,42,45	1.72	4 (14%)
36	A2M	A1	2220	36	18,25,26	0.80	1 (5%)	20,36,39	1.59	2 (10%)
36	OMG	A1	2922	36	19,26,27	0.89	1 (5%)	21,38,41	1.03	2 (9%)
36	PSU	A1	2416	80,36	18,21,22	1.56	5 (27%)	21,30,33	2.15	4 (19%)
36	UR3	A1	2634	80,36	19,22,23	0.94	1 (5%)	26,32,35	1.79	3 (11%)
36	OMG	A1	2793	36	19,26,27	0.96	1 (5%)	21,38,41	1.10	2 (9%)
36	5MC	A1	2870	80,36	19,22,23	1.38	3 (15%)	26,32,35	1.58	6 (23%)
36	UY1	A1	2347	36	19,22,23	2.69	3 (15%)	21,31,34	2.67	4 (19%)
36	OMU	A1	2724	36	19,22,23	1.29	3 (15%)	25,31,34	1.75	5 (20%)
36	PSU	A1	1004	36	18,21,22	1.46	4 (22%)	21,30,33	2.07	3 (14%)
36	PSU	A1	776	36	18,21,22	1.55	4 (22%)	21,30,33	2.39	6 (28%)
36	OMG	A1	2791	36	19,26,27	0.95	1 (5%)	21,38,41	1.08	2 (9%)
40	HIC	AB	243	40	8,11,12	1.43	1 (12%)	5,14,16	0.77	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
35	OMG	B5	1126	35	-	0/5/27/28	0/3/3/3
36	OMC	A1	1437	80,36	-	3/9/27/28	0/2/2/2
36	A2M	A1	817	80,36	-	1/5/27/28	0/3/3/3
36	PSU	A1	2826	80,36	-	0/7/25/26	0/2/2/2
36	PSU	A1	966	80,36	-	0/7/25/26	0/2/2/2
36	OMC	A1	650	80,36	-	0/9/27/28	0/2/2/2
36	A2M	A1	2640	36	-	1/5/27/28	0/3/3/3
36	PSU	A1	2880	36	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A2M	B5	436	35	-	0/5/27/28	0/3/3/3
35	MA6	B5	1781	35	-	0/7/29/30	0/3/3/3
35	PSU	B5	999	35	-	0/7/25/26	0/2/2/2
36	1MA	A1	2142	80,36	-	2/3/25/26	0/3/3/3
36	OMG	A1	1450	36	-	2/5/27/28	0/3/3/3
36	OMG	A1	2288	36	-	2/5/27/28	0/3/3/3
35	PSU	B5	759	35	-	0/7/25/26	0/2/2/2
36	PSU	A1	990	36	-	0/7/25/26	0/2/2/2
35	OMG	B5	562	35	-	0/5/27/28	0/3/3/3
35	OMU	B5	578	35	-	0/9/27/28	0/2/2/2
35	A2M	B5	619	80,35	-	2/5/27/28	0/3/3/3
36	OMU	A1	2417	36	-	1/9/27/28	0/2/2/2
38	PSU	A4	73	38	-	0/7/25/26	0/2/2/2
36	PSU	A1	2865	36	-	0/7/25/26	0/2/2/2
35	PSU	B5	120	35	-	0/7/25/26	0/2/2/2
36	A2M	A1	2280	80,36	-	2/5/27/28	0/3/3/3
36	OMG	A1	908	36	-	3/5/27/28	0/3/3/3
36	PSU	A1	2260	36	-	2/7/25/26	0/2/2/2
36	PSU	A1	2129	36	-	0/7/25/26	0/2/2/2
35	MA6	B5	1782	80,35	-	3/7/29/30	0/3/3/3
35	PSU	B5	632	35	-	0/7/25/26	0/2/2/2
36	PSU	A1	2923	36	-	5/7/25/26	0/2/2/2
36	PSU	A1	2944	80,36	-	0/7/25/26	0/2/2/2
35	A2M	B5	796	35	-	0/5/27/28	0/3/3/3
35	4AC	B5	1280	35	-	3/11/29/30	0/2/2/2
36	PSU	A1	1042	36	-	0/7/25/26	0/2/2/2
36	OMC	A1	2337	36	-	0/9/27/28	0/2/2/2
35	A2M	B5	541	35	-	3/5/27/28	0/3/3/3
36	PSU	A1	1124	36	-	2/7/25/26	0/2/2/2
36	PSU	A1	2133	36	-	0/7/25/26	0/2/2/2
35	OMC	B5	1639	35	-	1/9/27/28	0/2/2/2
36	PSU	A1	2266	36	-	3/7/25/26	0/2/2/2
35	A2M	B5	974	35	-	0/5/27/28	0/3/3/3
36	PSU	A1	960	36	-	1/7/25/26	0/2/2/2
35	A2M	B5	28	80,35	-	0/5/27/28	0/3/3/3
36	A2M	A1	1449	80,36	-	0/5/27/28	0/3/3/3
36	OMC	A1	2948	80,36	-	0/9/27/28	0/2/2/2
36	PSU	A1	2975	36	-	0/7/25/26	0/2/2/2
35	G7M	B5	1575	35	3/3/5/5	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PSU	A1	2735	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	1110	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	2351	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	986	36	-	0/7/25/26	0/2/2/2
35	PSU	B5	302	35	-	1/7/25/26	0/2/2/2
35	OMG	B5	1428	80,35	-	3/5/27/28	0/3/3/3
36	PSU	A1	1056	36	-	0/7/25/26	0/2/2/2
35	A2M	B5	420	35	-	0/5/27/28	0/3/3/3
36	OMG	A1	805	36	-	0/5/27/28	0/3/3/3
36	PSU	A1	2191	36	-	0/7/25/26	0/2/2/2
36	OMC	A1	663	36	-	0/9/27/28	0/2/2/2
35	PSU	B5	1181	35	-	0/7/25/26	0/2/2/2
36	PSU	A1	2314	36	-	3/7/25/26	0/2/2/2
36	OMG	A1	2815	36	-	0/5/27/28	0/3/3/3
35	PSU	B5	1290	35	-	0/7/25/26	0/2/2/2
35	OMG	B5	1572	35	-	0/5/27/28	0/3/3/3
36	OMG	A1	2619	80,36	-	1/5/27/28	0/3/3/3
35	OMC	B5	414	35	-	0/9/27/28	0/2/2/2
36	OMG	A1	867	36	-	0/5/27/28	0/3/3/3
36	PSU	A1	1052	80,36	-	2/7/25/26	0/2/2/2
36	OMC	A1	2197	80,36	-	6/9/27/28	0/2/2/2
36	5MC	A1	2278	80,36	-	0/7/25/26	0/2/2/2
36	OMU	A1	1888	80,36	-	0/9/27/28	0/2/2/2
36	OMU	A1	2421	36	-	0/9/27/28	0/2/2/2
35	4AC	B5	1773	35	-	4/11/29/30	0/2/2/2
36	A2M	A1	2281	80,36	-	1/5/27/28	0/3/3/3
36	A2M	A1	1133	80,36	-	0/5/27/28	0/3/3/3
36	OMU	A1	2921	80,36	-	0/9/27/28	0/2/2/2
35	A2M	B5	100	80,35	-	1/5/27/28	0/3/3/3
35	PSU	B5	766	35	-	1/7/25/26	0/2/2/2
36	PSU	A1	2349	80,36	-	0/7/25/26	0/2/2/2
35	PSU	B5	211	35	-	0/7/25/26	0/2/2/2
37	PSU	A3	50	37	-	1/7/25/26	0/2/2/2
36	OMU	A1	2729	36	-	3/9/27/28	0/2/2/2
36	A2M	A1	807	36	-	3/5/27/28	0/3/3/3
35	PSU	B5	466	35	-	0/7/25/26	0/2/2/2
36	1MA	A1	645	80,36	-	0/3/25/26	0/3/3/3
36	A2M	A1	2946	80,36	-	1/5/27/28	0/3/3/3
35	PSU	B5	1187	35	-	0/7/25/26	0/2/2/2
36	A2M	A1	649	36	-	0/5/27/28	0/3/3/3
36	PSU	A1	2264	36	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	A2M	A1	876	36	-	0/5/27/28	0/3/3/3
36	PSU	A1	2340	80,36	-	1/7/25/26	0/2/2/2
35	PSU	B5	106	35	-	0/7/25/26	0/2/2/2
36	OMU	A1	898	36	-	0/9/27/28	0/2/2/2
35	OMU	B5	1269	80,35	-	2/9/27/28	0/2/2/2
35	OMC	B5	1007	35	-	1/9/27/28	0/2/2/2
36	OMC	A1	2959	36	-	0/9/27/28	0/2/2/2
35	PSU	B5	1415	35	-	1/7/25/26	0/2/2/2
35	OMG	B5	1271	35	-	0/5/27/28	0/3/3/3
35	B8N	B5	1191	35	-	0/16/34/35	0/2/2/2
36	A2M	A1	2220	36	-	0/5/27/28	0/3/3/3
36	OMG	A1	2922	36	-	1/5/27/28	0/3/3/3
36	PSU	A1	2416	80,36	-	0/7/25/26	0/2/2/2
36	UR3	A1	2634	80,36	-	0/7/25/26	0/2/2/2
36	OMG	A1	2793	36	-	0/5/27/28	0/3/3/3
36	5MC	A1	2870	80,36	-	4/7/25/26	0/2/2/2
36	UY1	A1	2347	36	-	2/9/27/28	0/2/2/2
36	OMU	A1	2724	36	-	0/9/27/28	0/2/2/2
36	PSU	A1	1004	36	-	0/7/25/26	0/2/2/2
36	PSU	A1	776	36	-	3/7/25/26	0/2/2/2
36	OMG	A1	2791	36	-	0/5/27/28	0/3/3/3
40	HIC	AB	243	40	-	2/5/6/8	0/1/1/1

All (264) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2347	UY1	C6-C5	10.10	1.46	1.35
35	B5	1575	G7M	C8-N9	7.98	1.47	1.33
35	B5	1575	G7M	C8-N7	5.66	1.43	1.33
36	A1	2278	5MC	C5-C4	4.76	1.47	1.44
36	A1	2142	1MA	C2-N3	4.38	1.34	1.28
35	B5	1575	G7M	C5-C4	4.27	1.47	1.39
36	A1	2870	5MC	C5-C4	3.89	1.47	1.44
36	A1	2417	OMU	C4-N3	-3.73	1.32	1.38
36	A1	1056	PSU	C6-C5	3.69	1.39	1.35
36	A1	2260	PSU	C6-C5	3.68	1.39	1.35
37	A3	50	PSU	C6-C5	3.66	1.39	1.35
36	A1	2133	PSU	C4-N3	-3.64	1.32	1.38
36	A1	2314	PSU	C6-C5	3.54	1.39	1.35
36	A1	2191	PSU	C4-N3	-3.53	1.32	1.38
36	A1	776	PSU	C4-N3	-3.53	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2416	PSU	C4-N3	-3.53	1.32	1.38
40	AB	243	HIC	CD2-NE2	-3.52	1.33	1.38
36	A1	1450	OMG	C6-N1	-3.47	1.32	1.37
36	A1	2944	PSU	C4-N3	-3.45	1.32	1.38
35	B5	632	PSU	C4-N3	-3.42	1.32	1.38
36	A1	2347	UY1	C4-N3	-3.41	1.32	1.38
35	B5	1181	PSU	C6-C5	3.40	1.39	1.35
36	A1	898	OMU	C4-N3	-3.39	1.32	1.38
36	A1	986	PSU	C6-C5	3.37	1.39	1.35
36	A1	2880	PSU	C4-N3	-3.36	1.32	1.38
36	A1	2264	PSU	C6-C5	3.35	1.39	1.35
35	B5	466	PSU	C4-N3	-3.34	1.32	1.38
36	A1	1042	PSU	C6-C5	3.34	1.39	1.35
35	B5	1415	PSU	C6-C5	3.34	1.39	1.35
35	B5	1181	PSU	C4-N3	-3.33	1.32	1.38
36	A1	2340	PSU	C6-C5	3.33	1.39	1.35
36	A1	2351	PSU	C4-N3	-3.32	1.32	1.38
35	B5	1290	PSU	C2-N1	-3.32	1.32	1.36
36	A1	2129	PSU	C4-N3	-3.32	1.32	1.38
36	A1	2133	PSU	C6-C5	3.32	1.39	1.35
35	B5	1187	PSU	C4-N3	-3.31	1.32	1.38
36	A1	2340	PSU	C4-N3	-3.31	1.32	1.38
36	A1	1124	PSU	C4-N3	-3.30	1.32	1.38
36	A1	2288	OMG	C6-N1	-3.29	1.32	1.37
36	A1	645	1MA	C2-N3	3.28	1.32	1.28
36	A1	2421	OMU	C4-N3	-3.28	1.33	1.38
36	A1	986	PSU	C4-N3	-3.26	1.32	1.38
36	A1	2815	OMG	C6-N1	-3.25	1.32	1.37
36	A1	2191	PSU	C6-C5	3.25	1.38	1.35
36	A1	2266	PSU	C6-C5	3.24	1.38	1.35
36	A1	2349	PSU	C4-N3	-3.23	1.32	1.38
36	A1	2133	PSU	C2-N3	-3.23	1.32	1.37
36	A1	960	PSU	C4-N3	-3.22	1.32	1.38
35	B5	1290	PSU	C4-N3	-3.22	1.32	1.38
36	A1	1110	PSU	C4-N3	-3.22	1.32	1.38
35	B5	211	PSU	C4-N3	-3.20	1.32	1.38
36	A1	2975	PSU	C4-N3	-3.19	1.32	1.38
36	A1	990	PSU	C6-C5	3.19	1.38	1.35
36	A1	2729	OMU	C4-N3	-3.17	1.33	1.38
36	A1	1042	PSU	C4-N3	-3.16	1.32	1.38
36	A1	2826	PSU	C4-N3	-3.16	1.32	1.38
35	B5	106	PSU	C4-N3	-3.14	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2735	PSU	C4-N3	-3.14	1.33	1.38
36	A1	1056	PSU	C4-N3	-3.13	1.33	1.38
36	A1	776	PSU	C2-N3	-3.12	1.32	1.37
36	A1	1052	PSU	C4-N3	-3.11	1.33	1.38
36	A1	2791	OMG	C6-N1	-3.11	1.33	1.37
35	B5	466	PSU	C6-C5	3.11	1.38	1.35
35	B5	1269	OMU	C4-N3	-3.10	1.33	1.38
35	B5	1415	PSU	C4-N3	-3.08	1.33	1.38
36	A1	776	PSU	C6-C5	3.08	1.38	1.35
38	A4	73	PSU	C6-C5	3.07	1.38	1.35
36	A1	1124	PSU	C6-C5	3.07	1.38	1.35
36	A1	2975	PSU	C6-C5	3.05	1.38	1.35
35	B5	1428	OMG	C6-N1	-3.05	1.33	1.37
36	A1	2129	PSU	C6-C5	3.05	1.38	1.35
36	A1	2724	OMU	C4-N3	-3.04	1.33	1.38
36	A1	2351	PSU	C6-C5	3.03	1.38	1.35
36	A1	990	PSU	C4-N3	-3.03	1.33	1.38
36	A1	2870	5MC	C6-C5	3.03	1.39	1.34
35	B5	999	PSU	C6-C5	3.02	1.38	1.35
38	A4	73	PSU	C4-N3	-3.01	1.33	1.38
35	B5	766	PSU	C4-N3	-3.01	1.33	1.38
36	A1	2921	OMU	C4-N3	-3.00	1.33	1.38
35	B5	562	OMG	C6-N1	-2.99	1.33	1.37
35	B5	211	PSU	C6-C5	2.98	1.38	1.35
36	A1	2923	PSU	C4-N3	-2.98	1.33	1.38
36	A1	986	PSU	C2-N3	-2.97	1.32	1.37
36	A1	2865	PSU	C4-N3	-2.97	1.33	1.38
35	B5	759	PSU	C4-N3	-2.96	1.33	1.38
36	A1	1004	PSU	C6-C5	2.96	1.38	1.35
36	A1	2340	PSU	C2-N3	-2.96	1.32	1.37
35	B5	120	PSU	C4-N3	-2.95	1.33	1.38
36	A1	1052	PSU	C6-C5	2.94	1.38	1.35
35	B5	120	PSU	C6-C5	2.94	1.38	1.35
36	A1	1004	PSU	C4-N3	-2.93	1.33	1.38
35	B5	302	PSU	C4-N3	-2.92	1.33	1.38
36	A1	2880	PSU	C2-N3	-2.90	1.32	1.37
36	A1	2351	PSU	C2-N3	-2.89	1.32	1.37
36	A1	2264	PSU	C4-N3	-2.88	1.33	1.38
36	A1	2314	PSU	C4-N3	-2.87	1.33	1.38
36	A1	2793	OMG	C6-N1	-2.87	1.33	1.37
35	B5	1271	OMG	C6-N1	-2.86	1.33	1.37
36	A1	966	PSU	C4-N3	-2.85	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B5	999	PSU	C4-N3	-2.85	1.33	1.38
36	A1	2729	OMU	C5-C4	-2.85	1.37	1.43
36	A1	2729	OMU	C2-N3	-2.85	1.33	1.38
36	A1	2347	UY1	C2-N3	-2.85	1.32	1.37
36	A1	805	OMG	C6-N1	-2.84	1.33	1.37
36	A1	960	PSU	O4'-C1'	-2.83	1.39	1.43
37	A3	50	PSU	C4-N3	-2.83	1.33	1.38
36	A1	966	PSU	C6-C5	2.83	1.38	1.35
36	A1	2260	PSU	C4-N3	-2.82	1.33	1.38
36	A1	2349	PSU	C6-C5	2.81	1.38	1.35
35	B5	1781	MA6	C6-C5	2.81	1.49	1.44
35	B5	632	PSU	C2-N1	-2.80	1.33	1.36
35	B5	1415	PSU	C2-N1	-2.79	1.33	1.36
35	B5	759	PSU	C6-C5	2.79	1.38	1.35
36	A1	2826	PSU	C2-N1	-2.79	1.33	1.36
35	B5	106	PSU	C6-C5	2.79	1.38	1.35
36	A1	2619	OMG	C6-N1	-2.79	1.33	1.37
36	A1	2421	OMU	C2-N3	-2.79	1.33	1.38
35	B5	766	PSU	C6-C5	2.79	1.38	1.35
35	B5	302	PSU	C2-N3	-2.78	1.32	1.37
35	B5	466	PSU	C2-N3	-2.78	1.32	1.37
35	B5	1126	OMG	C6-N1	-2.77	1.33	1.37
36	A1	2417	OMU	C2-N3	-2.77	1.33	1.38
35	B5	1572	OMG	C6-N1	-2.77	1.33	1.37
36	A1	1888	OMU	C4-N3	-2.77	1.33	1.38
35	B5	1187	PSU	C6-C5	2.76	1.38	1.35
36	A1	2921	OMU	C2-N3	-2.75	1.33	1.38
36	A1	1052	PSU	C2-N3	-2.75	1.32	1.37
36	A1	2735	PSU	C6-C5	2.75	1.38	1.35
35	B5	1191	B8N	C6-C5	2.74	1.39	1.35
36	A1	2340	PSU	C2-N1	-2.74	1.33	1.36
35	B5	1290	PSU	C6-C5	2.73	1.38	1.35
36	A1	2944	PSU	C2-N3	-2.72	1.33	1.37
35	B5	632	PSU	C2-N3	-2.72	1.33	1.37
36	A1	2266	PSU	C4-N3	-2.72	1.33	1.38
36	A1	867	OMG	C6-N1	-2.72	1.33	1.37
35	B5	302	PSU	C6-C5	2.72	1.38	1.35
36	A1	1110	PSU	C6-C5	2.70	1.38	1.35
36	A1	2944	PSU	C6-C5	2.69	1.38	1.35
36	A1	2922	OMG	C6-N1	-2.68	1.33	1.37
35	B5	1415	PSU	C2-N3	-2.67	1.33	1.37
36	A1	2278	5MC	C6-C5	2.66	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B5	578	OMU	C4-N3	-2.65	1.34	1.38
36	A1	2975	PSU	C2-N3	-2.64	1.33	1.37
36	A1	2865	PSU	C6-C5	2.63	1.38	1.35
36	A1	1056	PSU	C2-N3	-2.61	1.33	1.37
35	B5	1575	G7M	C6-N1	-2.60	1.33	1.37
35	B5	759	PSU	C2-N1	-2.60	1.33	1.36
35	B5	1187	PSU	C2-N3	-2.60	1.33	1.37
35	B5	211	PSU	C2-N3	-2.59	1.33	1.37
35	B5	632	PSU	C6-C5	2.59	1.38	1.35
36	A1	2724	OMU	C5-C4	-2.58	1.38	1.43
36	A1	2416	PSU	C2-N3	-2.58	1.33	1.37
36	A1	2133	PSU	C2-N1	-2.58	1.33	1.36
36	A1	645	1MA	C6-N6	2.57	1.34	1.27
36	A1	898	OMU	C5-C4	-2.56	1.38	1.43
36	A1	1888	OMU	C2-N3	-2.56	1.33	1.38
36	A1	2417	OMU	C5-C4	-2.56	1.38	1.43
36	A1	898	OMU	C2-N3	-2.56	1.33	1.38
36	A1	908	OMG	C6-N1	-2.55	1.33	1.37
36	A1	2129	PSU	C2-N3	-2.55	1.33	1.37
36	A1	2416	PSU	C6-C5	2.54	1.38	1.35
38	A4	73	PSU	C2-N3	-2.54	1.33	1.37
35	B5	106	PSU	C2-N3	-2.54	1.33	1.37
35	B5	1782	MA6	C6-C5	2.54	1.48	1.44
36	A1	2880	PSU	C6-C5	2.53	1.38	1.35
35	B5	578	OMU	C2-N3	-2.52	1.33	1.38
35	B5	766	PSU	C2-N3	-2.52	1.33	1.37
36	A1	1124	PSU	C2-N3	-2.52	1.33	1.37
36	A1	2142	1MA	C6-N6	2.52	1.34	1.27
35	B5	759	PSU	C2-N3	-2.51	1.33	1.37
35	B5	1269	OMU	C2-N3	-2.49	1.33	1.38
35	B5	302	PSU	C2-N1	-2.49	1.33	1.36
35	B5	1773	4AC	C4-N4	-2.49	1.36	1.39
38	A4	73	PSU	C2-N1	-2.48	1.33	1.36
35	B5	120	PSU	C2-N3	-2.47	1.33	1.37
36	A1	2416	PSU	C2-N1	-2.47	1.33	1.36
36	A1	1110	PSU	C2-N3	-2.45	1.33	1.37
36	A1	1042	PSU	C2-N3	-2.45	1.33	1.37
36	A1	2921	OMU	C5-C4	-2.45	1.38	1.43
36	A1	990	PSU	C2-N3	-2.44	1.33	1.37
36	A1	2349	PSU	C2-N3	-2.44	1.33	1.37
36	A1	2129	PSU	C2-N1	-2.44	1.33	1.36
36	A1	1888	OMU	C5-C4	-2.44	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	1110	PSU	C2-N1	-2.43	1.33	1.36
35	B5	106	PSU	C2-N1	-2.42	1.33	1.36
36	A1	2826	PSU	C2-N3	-2.41	1.33	1.37
36	A1	2724	OMU	C2-N3	-2.41	1.33	1.38
35	B5	1290	PSU	C2-N3	-2.40	1.33	1.37
36	A1	2923	PSU	C6-C5	2.40	1.37	1.35
35	B5	1280	4AC	C4-N4	-2.39	1.36	1.39
36	A1	2826	PSU	C6-C5	2.39	1.37	1.35
36	A1	2191	PSU	C2-N3	-2.38	1.33	1.37
35	B5	1187	PSU	C2-N1	-2.37	1.33	1.36
36	A1	2865	PSU	C2-N1	-2.37	1.33	1.36
35	B5	1181	PSU	C2-N3	-2.37	1.33	1.37
35	B5	120	PSU	C2-N1	-2.36	1.33	1.36
36	A1	2349	PSU	C2-N1	-2.36	1.33	1.36
36	A1	2870	5MC	C6-N1	-2.34	1.34	1.38
36	A1	1056	PSU	C2-N1	-2.33	1.33	1.36
36	A1	2278	5MC	C6-N1	-2.33	1.34	1.38
36	A1	966	PSU	C2-N1	-2.33	1.33	1.36
36	A1	2735	PSU	C2-N3	-2.32	1.33	1.37
36	A1	2735	PSU	C2-N1	-2.31	1.33	1.36
36	A1	966	PSU	C2-N3	-2.31	1.33	1.37
36	A1	2880	PSU	C2-N1	-2.30	1.33	1.36
36	A1	2944	PSU	O4'-C1'	-2.29	1.40	1.43
35	B5	766	PSU	C2-N1	-2.29	1.33	1.36
36	A1	2260	PSU	C2-N3	-2.29	1.33	1.37
35	B5	632	PSU	C6-N1	-2.29	1.32	1.36
36	A1	2191	PSU	C2-N1	-2.28	1.33	1.36
36	A1	1004	PSU	C2-N3	-2.28	1.33	1.37
36	A1	2421	OMU	C5-C4	-2.26	1.38	1.43
36	A1	650	OMC	C5-C4	-2.24	1.37	1.42
35	B5	1007	OMC	C5-C4	-2.23	1.37	1.42
36	A1	2944	PSU	C2-N1	-2.22	1.33	1.36
35	B5	999	PSU	C2-N3	-2.22	1.33	1.37
35	B5	1290	PSU	C6-N1	-2.21	1.32	1.36
36	A1	1133	A2M	O4'-C1'	2.21	1.43	1.40
36	A1	2923	PSU	C2-N1	-2.21	1.33	1.36
36	A1	1437	OMC	C5-C4	-2.21	1.37	1.42
36	A1	1124	PSU	C2-N1	-2.20	1.33	1.36
35	B5	1269	OMU	C2-N1	2.20	1.41	1.38
36	A1	663	OMC	C5-C4	-2.20	1.37	1.42
36	A1	2416	PSU	C6-N1	-2.19	1.32	1.36
36	A1	2634	UR3	C5-C4	-2.19	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	966	PSU	C6-N1	-2.19	1.32	1.36
36	A1	2264	PSU	C2-N3	-2.18	1.33	1.37
36	A1	776	PSU	O4'-C1'	-2.18	1.40	1.43
36	A1	807	A2M	O4'-C1'	2.18	1.43	1.40
35	B5	1773	4AC	C7-N4	-2.17	1.32	1.37
36	A1	2923	PSU	C2-N3	-2.16	1.33	1.37
36	A1	2729	OMU	C2-N1	2.16	1.41	1.38
36	A1	1004	PSU	C2-N1	-2.16	1.33	1.36
36	A1	2865	PSU	C2-N3	-2.16	1.33	1.37
36	A1	2266	PSU	C2-N3	-2.15	1.33	1.37
35	B5	211	PSU	C2-N1	-2.15	1.33	1.36
36	A1	2220	A2M	O4'-C1'	2.14	1.43	1.40
36	A1	960	PSU	C2-N3	-2.13	1.34	1.37
35	B5	466	PSU	C2-N1	-2.13	1.33	1.36
35	B5	1269	OMU	C5-C4	-2.13	1.39	1.43
36	A1	2865	PSU	O4'-C1'	-2.13	1.40	1.43
36	A1	2735	PSU	C6-N1	-2.12	1.32	1.36
35	B5	1773	4AC	C6-N1	-2.12	1.33	1.38
35	B5	766	PSU	O4'-C1'	-2.12	1.40	1.43
36	A1	986	PSU	C2-N1	-2.12	1.33	1.36
36	A1	2314	PSU	O4'-C1'	-2.12	1.40	1.43
36	A1	2640	A2M	O4'-C1'	2.12	1.43	1.40
36	A1	2826	PSU	C6-N1	-2.11	1.32	1.36
35	B5	1181	PSU	C2-N1	-2.10	1.33	1.36
36	A1	898	OMU	C2-N1	2.10	1.41	1.38
36	A1	2880	PSU	O4'-C1'	-2.09	1.41	1.43
36	A1	2266	PSU	C4-C5	2.09	1.50	1.44
36	A1	1052	PSU	C2-N1	-2.08	1.33	1.36
36	A1	2351	PSU	C2-N1	-2.08	1.34	1.36
36	A1	2975	PSU	C2-N1	-2.07	1.34	1.36
35	B5	578	OMU	C5-C4	-2.06	1.39	1.43
35	B5	100	A2M	O4'-C1'	2.06	1.43	1.40
37	A3	50	PSU	C2-N1	-2.03	1.34	1.36
36	A1	960	PSU	C2-N1	-2.02	1.34	1.36
37	A3	50	PSU	C2-N3	-2.02	1.34	1.37
36	A1	2337	OMC	C5-C4	-2.01	1.38	1.42
35	B5	1280	4AC	C6-N1	-2.00	1.33	1.38
36	A1	2880	PSU	C6-N1	-2.00	1.33	1.36
36	A1	2948	OMC	C5-C4	-2.00	1.38	1.42

All (367) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1773	4AC	N4-C4-N3	10.22	130.45	113.87
35	B5	1280	4AC	N4-C4-N3	9.10	128.63	113.87
36	A1	2133	PSU	N1-C2-N3	7.96	123.57	115.17
36	A1	2826	PSU	N1-C2-N3	7.46	123.04	115.17
36	A1	2347	UY1	C6-C5-C4	-7.33	113.23	118.17
36	A1	2191	PSU	N1-C2-N3	7.18	122.75	115.17
36	A1	1110	PSU	N1-C2-N3	7.14	122.70	115.17
35	B5	1773	4AC	C5-C4-N4	-7.14	110.91	122.94
36	A1	2347	UY1	N1-C2-N3	6.93	122.48	115.17
36	A1	2634	UR3	C4-N3-C2	-6.91	119.02	124.58
36	A1	1124	PSU	N1-C2-N3	6.86	122.41	115.17
35	B5	1781	MA6	C2-N1-C6	6.80	123.51	116.84
36	A1	990	PSU	N1-C2-N3	6.79	122.33	115.17
36	A1	1052	PSU	N1-C2-N3	6.75	122.28	115.17
36	A1	2129	PSU	N1-C2-N3	6.71	122.24	115.17
36	A1	2975	PSU	N1-C2-N3	6.69	122.22	115.17
35	B5	1181	PSU	N1-C2-N3	6.68	122.22	115.17
35	B5	106	PSU	N1-C2-N3	6.64	122.17	115.17
35	B5	1290	PSU	N1-C2-N3	6.62	122.15	115.17
36	A1	2416	PSU	N1-C2-N3	6.61	122.14	115.17
37	A3	50	PSU	N1-C2-N3	6.61	122.14	115.17
35	B5	302	PSU	N1-C2-N3	6.58	122.11	115.17
36	A1	1056	PSU	N1-C2-N3	6.57	122.10	115.17
38	A4	73	PSU	N1-C2-N3	6.57	122.09	115.17
35	B5	1415	PSU	N1-C2-N3	6.54	122.07	115.17
35	B5	211	PSU	N1-C2-N3	6.54	122.07	115.17
36	A1	2865	PSU	N1-C2-N3	6.51	122.04	115.17
36	A1	2264	PSU	N1-C2-N3	6.51	122.04	115.17
36	A1	1042	PSU	N1-C2-N3	6.50	122.02	115.17
35	B5	632	PSU	N1-C2-N3	6.49	122.02	115.17
36	A1	2735	PSU	N1-C2-N3	6.48	122.00	115.17
35	B5	759	PSU	N1-C2-N3	6.48	122.00	115.17
36	A1	2266	PSU	N1-C2-N3	6.46	121.98	115.17
36	A1	2944	PSU	N1-C2-N3	6.45	121.97	115.17
36	A1	2314	PSU	N1-C2-N3	6.44	121.96	115.17
36	A1	960	PSU	N1-C2-N3	6.44	121.96	115.17
36	A1	2923	PSU	N1-C2-N3	6.43	121.95	115.17
35	B5	1187	PSU	N1-C2-N3	6.43	121.95	115.17
35	B5	766	PSU	N1-C2-N3	6.43	121.95	115.17
36	A1	1004	PSU	N1-C2-N3	6.37	121.89	115.17
35	B5	466	PSU	N1-C2-N3	6.36	121.88	115.17
36	A1	776	PSU	N1-C2-N3	6.36	121.87	115.17
35	B5	1782	MA6	C2-N1-C6	6.35	123.06	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	999	PSU	N1-C2-N3	6.33	121.85	115.17
35	B5	120	PSU	N1-C2-N3	6.27	121.78	115.17
36	A1	986	PSU	N1-C2-N3	6.22	121.73	115.17
36	A1	2351	PSU	N1-C2-N3	6.20	121.70	115.17
36	A1	2880	PSU	N1-C2-N3	6.18	121.69	115.17
36	A1	2349	PSU	N1-C2-N3	6.14	121.64	115.17
36	A1	2340	PSU	N1-C2-N3	6.09	121.59	115.17
36	A1	966	PSU	N1-C2-N3	6.01	121.51	115.17
36	A1	2281	A2M	C4'-O4'-C1'	-6.00	104.43	109.92
35	B5	1191	B8N	C4-N3-C2	-6.00	118.23	125.62
36	A1	2260	PSU	N1-C2-N3	5.91	121.40	115.17
35	B5	1280	4AC	C5-C4-N4	-5.68	113.38	122.94
36	A1	2281	A2M	O4'-C1'-N9	5.37	115.87	108.75
36	A1	776	PSU	C4-N3-C2	-5.26	119.12	126.37
35	B5	1290	PSU	O2-C2-N1	-5.21	117.42	122.79
35	B5	578	OMU	C4-N3-C2	-5.11	120.27	126.61
36	A1	2421	OMU	C4-N3-C2	-5.10	120.29	126.61
36	A1	1888	OMU	C4-N3-C2	-4.98	120.43	126.61
36	A1	2191	PSU	C4-N3-C2	-4.96	119.54	126.37
36	A1	2220	A2M	N3-C2-N1	-4.95	121.96	128.67
36	A1	807	A2M	C4'-O4'-C1'	-4.91	105.43	109.92
36	A1	2417	OMU	C4-N3-C2	-4.76	120.70	126.61
35	B5	1280	4AC	CM7-C7-N4	4.74	122.92	115.27
36	A1	2921	OMU	C4-N3-C2	-4.69	120.79	126.61
36	A1	898	OMU	C4-N3-C2	-4.63	120.86	126.61
36	A1	2826	PSU	C4-N3-C2	-4.62	120.00	126.37
36	A1	2417	OMU	C5-C4-N3	4.62	121.27	114.80
36	A1	2826	PSU	O2-C2-N1	-4.60	118.04	122.79
36	A1	2870	5MC	C5-C6-N1	-4.60	118.32	123.31
36	A1	817	A2M	N3-C2-N1	-4.59	122.45	128.67
36	A1	1110	PSU	C4-N3-C2	-4.58	120.06	126.37
36	A1	2944	PSU	C4-N3-C2	-4.51	120.16	126.37
35	B5	1269	OMU	C4-N3-C2	-4.51	121.02	126.61
36	A1	1888	OMU	C5-C4-N3	4.46	121.05	114.80
35	B5	1782	MA6	N3-C2-N1	-4.46	122.62	128.67
36	A1	2129	PSU	C4-N3-C2	-4.46	120.23	126.37
35	B5	619	A2M	O4'-C1'-N9	-4.42	102.89	108.75
36	A1	2421	OMU	N3-C2-N1	4.41	120.63	114.89
36	A1	966	PSU	C4-N3-C2	-4.40	120.31	126.37
35	B5	578	OMU	C5-C4-N3	4.38	120.93	114.80
35	B5	1290	PSU	C4-N3-C2	-4.33	120.41	126.37
36	A1	2921	OMU	C5-C4-N3	4.31	120.84	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2880	PSU	C4-N3-C2	-4.30	120.44	126.37
36	A1	2416	PSU	O2-C2-N1	-4.30	118.36	122.79
36	A1	2921	OMU	N3-C2-N1	4.29	120.48	114.89
36	A1	960	PSU	C4-N3-C2	-4.29	120.47	126.37
35	B5	211	PSU	C4-N3-C2	-4.28	120.48	126.37
36	A1	2264	PSU	C4-N3-C2	-4.27	120.48	126.37
35	B5	766	PSU	C4-N3-C2	-4.26	120.50	126.37
36	A1	2421	OMU	C5-C4-N3	4.22	120.72	114.80
36	A1	2340	PSU	O2-C2-N1	-4.21	118.44	122.79
36	A1	898	OMU	C5-C4-N3	4.21	120.69	114.80
36	A1	1052	PSU	C4-N3-C2	-4.18	120.61	126.37
35	B5	1773	4AC	CM7-C7-N4	4.18	122.01	115.27
36	A1	2417	OMU	N3-C2-N1	4.17	120.32	114.89
35	B5	302	PSU	C4-N3-C2	-4.16	120.64	126.37
36	A1	2416	PSU	C4-N3-C2	-4.15	120.65	126.37
35	B5	1781	MA6	N3-C2-N1	-4.15	123.04	128.67
35	B5	632	PSU	C4-N3-C2	-4.14	120.67	126.37
36	A1	2975	PSU	C4-N3-C2	-4.13	120.68	126.37
36	A1	2266	PSU	C4-N3-C2	-4.12	120.69	126.37
36	A1	1888	OMU	N3-C2-N1	4.12	120.26	114.89
36	A1	990	PSU	C4-N3-C2	-4.12	120.69	126.37
35	B5	999	PSU	C4-N3-C2	-4.12	120.69	126.37
36	A1	898	OMU	N3-C2-N1	4.11	120.25	114.89
36	A1	2724	OMU	C4-N3-C2	-4.11	121.51	126.61
35	B5	1007	OMC	O2-C2-N3	-4.10	115.87	122.33
36	A1	2865	PSU	C4-N3-C2	-4.09	120.74	126.37
35	B5	420	A2M	N3-C2-N1	-4.08	123.13	128.67
35	B5	766	PSU	O2-C2-N1	-4.08	118.59	122.79
36	A1	1004	PSU	C4-N3-C2	-4.07	120.76	126.37
36	A1	2735	PSU	O2-C2-N1	-4.07	118.59	122.79
36	A1	1004	PSU	O2-C2-N1	-4.04	118.62	122.79
35	B5	1187	PSU	C4-N3-C2	-4.03	120.82	126.37
36	A1	1437	OMC	O2-C2-N3	-4.03	115.98	122.33
36	A1	2948	OMC	O2-C2-N3	-4.03	115.98	122.33
36	A1	2133	PSU	C4-N3-C2	-4.02	120.83	126.37
36	A1	1056	PSU	C4-N3-C2	-4.01	120.84	126.37
36	A1	2278	5MC	O2-C2-N3	-4.00	116.02	122.33
37	A3	50	PSU	C4-N3-C2	-4.00	120.86	126.37
36	A1	1449	A2M	N3-C2-N1	-4.00	123.25	128.67
36	A1	1056	PSU	O2-C2-N1	-4.00	118.67	122.79
35	B5	302	PSU	O2-C2-N1	-3.97	118.69	122.79
35	B5	1269	OMU	N3-C2-N1	3.97	120.06	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	73	PSU	C4-N3-C2	-3.97	120.90	126.37
36	A1	2975	PSU	O2-C2-N1	-3.97	118.70	122.79
36	A1	2724	OMU	C5-C4-N3	3.97	120.35	114.80
36	A1	649	A2M	N3-C2-N1	-3.96	123.29	128.67
35	B5	466	PSU	C4-N3-C2	-3.96	120.91	126.37
35	B5	578	OMU	N3-C2-N1	3.95	120.04	114.89
36	A1	2314	PSU	C4-N3-C2	-3.95	120.93	126.37
35	B5	1415	PSU	O2-C2-N1	-3.95	118.72	122.79
36	A1	2281	A2M	N3-C2-N1	-3.94	123.33	128.67
35	B5	1181	PSU	C4-N3-C2	-3.93	120.96	126.37
35	B5	436	A2M	N3-C2-N1	-3.93	123.34	128.67
36	A1	2347	UY1	O2-C2-N1	-3.92	118.74	122.79
35	B5	974	A2M	N3-C2-N1	-3.91	123.37	128.67
36	A1	776	PSU	C5-C6-N1	-3.89	116.73	122.14
36	A1	2129	PSU	O2-C2-N1	-3.89	118.78	122.79
35	B5	759	PSU	C4-N3-C2	-3.89	121.02	126.37
36	A1	2634	UR3	C5-C4-N3	3.87	120.14	115.04
35	B5	106	PSU	C4-N3-C2	-3.87	121.03	126.37
35	B5	1269	OMU	C5-C4-N3	3.86	120.21	114.80
36	A1	2923	PSU	O2-C2-N1	-3.85	118.81	122.79
35	B5	796	A2M	N3-C2-N1	-3.85	123.45	128.67
36	A1	2735	PSU	C4-N3-C2	-3.84	121.08	126.37
36	A1	2923	PSU	C4-N3-C2	-3.84	121.08	126.37
35	B5	28	A2M	N3-C2-N1	-3.84	123.47	128.67
35	B5	120	PSU	C4-N3-C2	-3.83	121.09	126.37
36	A1	2349	PSU	C4-N3-C2	-3.83	121.10	126.37
35	B5	541	A2M	N3-C2-N1	-3.81	123.50	128.67
36	A1	1124	PSU	C4-N3-C2	-3.78	121.16	126.37
36	A1	2640	A2M	N3-C2-N1	-3.78	123.55	128.67
36	A1	2349	PSU	O2-C2-N1	-3.77	118.90	122.79
36	A1	1042	PSU	C4-N3-C2	-3.77	121.17	126.37
36	A1	2729	OMU	N3-C2-N1	3.74	119.76	114.89
35	B5	100	A2M	N3-C2-N1	-3.73	123.61	128.67
35	B5	759	PSU	O2-C2-N1	-3.72	118.95	122.79
36	A1	2351	PSU	O2-C2-N1	-3.72	118.95	122.79
36	A1	2351	PSU	C4-N3-C2	-3.70	121.28	126.37
36	A1	2865	PSU	O2-C2-N1	-3.69	118.98	122.79
36	A1	2729	OMU	C5-C4-N3	3.69	119.97	114.80
38	A4	73	PSU	O2-C2-N1	-3.69	118.98	122.79
35	B5	1781	MA6	C4-C5-N7	-3.67	105.46	109.34
35	B5	1269	OMU	C1'-N1-C2	3.67	124.18	117.59
37	A3	50	PSU	O2-C2-N1	-3.67	119.01	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	106	PSU	O2-C2-N1	-3.66	119.02	122.79
35	B5	1415	PSU	C4-N3-C2	-3.66	121.33	126.37
36	A1	876	A2M	N3-C2-N1	-3.66	123.71	128.67
36	A1	1110	PSU	O2-C2-N1	-3.65	119.02	122.79
35	B5	619	A2M	N3-C2-N1	-3.63	123.75	128.67
36	A1	2191	PSU	O2-C2-N1	-3.62	119.06	122.79
35	B5	1187	PSU	O2-C2-N1	-3.60	119.08	122.79
35	B5	632	PSU	O2-C2-N1	-3.59	119.09	122.79
36	A1	2340	PSU	C4-N3-C2	-3.58	121.44	126.37
36	A1	2260	PSU	C4-N3-C2	-3.54	121.49	126.37
36	A1	2264	PSU	O2-C2-N1	-3.54	119.14	122.79
36	A1	2729	OMU	C4-N3-C2	-3.53	122.23	126.61
35	B5	1782	MA6	C4-C5-N7	-3.53	105.61	109.34
36	A1	807	A2M	O4'-C1'-N9	3.53	113.42	108.75
36	A1	2921	OMU	O4-C4-C5	-3.51	119.11	125.16
36	A1	2724	OMU	N3-C2-N1	3.50	119.45	114.89
36	A1	2260	PSU	C6-C5-C4	-3.49	115.82	118.17
36	A1	960	PSU	O2-C2-N1	-3.41	119.27	122.79
35	B5	1280	4AC	C6-C5-C4	3.41	121.11	117.00
35	B5	211	PSU	O2-C2-N1	-3.39	119.29	122.79
36	A1	2347	UY1	C4-N3-C2	-3.39	121.71	126.37
36	A1	898	OMU	O4-C4-C5	-3.38	119.33	125.16
36	A1	990	PSU	O2-C2-N1	-3.38	119.30	122.79
36	A1	807	A2M	O4'-C4'-C5'	3.34	120.04	109.33
36	A1	2133	PSU	O2-C2-N3	-3.32	115.96	121.86
36	A1	1888	OMU	O4-C4-C5	-3.32	119.44	125.16
35	B5	120	PSU	O2-C2-N1	-3.31	119.38	122.79
35	B5	1773	4AC	C6-C5-C4	3.31	120.98	117.00
36	A1	1437	OMC	CM2-O2'-C2'	3.30	122.95	114.47
36	A1	2880	PSU	O2-C2-N1	-3.30	119.38	122.79
35	B5	999	PSU	O2-C2-N1	-3.29	119.39	122.79
36	A1	966	PSU	O2-C2-N1	-3.29	119.39	122.79
36	A1	1052	PSU	O2-C2-N1	-3.29	119.40	122.79
36	A1	1133	A2M	N3-C2-N1	-3.27	124.23	128.67
36	A1	2142	1MA	C5-C6-N1	3.25	118.63	113.95
35	B5	578	OMU	O4-C4-C5	-3.24	119.57	125.16
35	B5	1181	PSU	O2-C2-N1	-3.24	119.45	122.79
36	A1	807	A2M	C4-C5-N7	-3.24	105.92	109.34
36	A1	908	OMG	CM2-O2'-C2'	3.23	122.77	114.47
36	A1	986	PSU	C4-N3-C2	-3.22	121.93	126.37
36	A1	2266	PSU	O2-C2-N1	-3.21	119.48	122.79
36	A1	2946	A2M	N3-C2-N1	-3.21	124.32	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2421	OMU	O4-C4-C5	-3.20	119.64	125.16
36	A1	867	OMG	C8-N7-C5	3.20	107.99	102.55
36	A1	908	OMG	O2'-C2'-C1'	3.18	115.16	109.00
36	A1	2280	A2M	N3-C2-N1	-3.17	124.38	128.67
35	B5	1575	G7M	CN7-N7-C8	-3.15	110.26	125.43
36	A1	1124	PSU	O2-C2-N1	-3.15	119.54	122.79
35	B5	1191	B8N	C31-N3-C2	3.14	122.28	117.64
36	A1	2314	PSU	O2-C2-N1	-3.13	119.56	122.79
36	A1	2724	OMU	O4-C4-C5	-3.12	119.78	125.16
35	B5	1191	B8N	N3-C2-N1	3.11	120.52	116.72
36	A1	876	A2M	C4-C5-N7	-3.09	106.07	109.34
36	A1	2959	OMC	O2-C2-N3	-3.09	117.47	122.33
36	A1	1437	OMC	C1'-N1-C2	3.07	125.22	118.44
35	B5	1269	OMU	O4-C4-C5	-3.04	119.92	125.16
36	A1	2870	5MC	O2-C2-N3	-3.04	117.54	122.33
36	A1	2417	OMU	O4-C4-C5	-3.01	119.97	125.16
36	A1	966	PSU	C6-C5-C4	-3.01	116.14	118.17
36	A1	805	OMG	C8-N7-C5	3.00	107.65	102.55
36	A1	2815	OMG	C8-N7-C5	3.00	107.65	102.55
36	A1	2278	5MC	C5-C4-N3	-2.98	118.70	121.75
36	A1	776	PSU	O2-C2-N1	-2.98	119.72	122.79
36	A1	807	A2M	N3-C2-N1	-2.97	124.64	128.67
36	A1	2619	OMG	C8-N7-C5	2.97	107.61	102.55
36	A1	2944	PSU	O2-C2-N1	-2.95	119.75	122.79
35	B5	1280	4AC	C5-C4-N3	-2.95	117.99	122.60
35	B5	1415	PSU	C6-C5-C4	-2.94	116.19	118.17
36	A1	2791	OMG	C8-N7-C5	2.94	107.55	102.55
36	A1	986	PSU	C6-C5-C4	-2.94	116.19	118.17
35	B5	1007	OMC	C1'-N1-C2	2.93	124.91	118.44
35	B5	1280	4AC	O7-C7-N4	-2.92	117.31	121.90
36	A1	2340	PSU	C6-C5-C4	-2.91	116.21	118.17
36	A1	1133	A2M	C4-C5-N7	-2.91	106.26	109.34
36	A1	2351	PSU	C6-C5-C4	-2.90	116.21	118.17
36	A1	776	PSU	O4-C4-C5	-2.89	116.81	124.01
36	A1	2793	OMG	C8-N7-C5	2.89	107.46	102.55
35	B5	28	A2M	O4'-C1'-N9	2.87	112.55	108.75
35	B5	1007	OMC	O2-C2-N1	2.87	124.52	118.90
36	A1	2870	5MC	C5-C4-N3	-2.86	118.82	121.75
35	B5	1126	OMG	C8-N7-C5	2.86	107.41	102.55
36	A1	2948	OMC	C1'-N1-C2	2.86	124.75	118.44
35	B5	562	OMG	C8-N7-C5	2.84	107.39	102.55
35	B5	436	A2M	C4'-O4'-C1'	2.83	112.52	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2946	A2M	O4'-C1'-N9	2.81	112.48	108.75
36	A1	2278	5MC	C5-C6-N1	-2.81	120.26	123.31
36	A1	2260	PSU	O2-C2-N1	-2.81	119.89	122.79
36	A1	2142	1MA	N1-C2-N3	-2.80	122.40	125.90
36	A1	2946	A2M	O2'-C2'-C1'	2.79	114.40	109.00
35	B5	1773	4AC	O7-C7-N4	-2.78	117.53	121.90
36	A1	2729	OMU	C6-N1-C2	-2.78	117.62	121.00
36	A1	1437	OMC	O2-C2-N1	2.77	124.33	118.90
36	A1	2337	OMC	O2-C2-N3	-2.75	118.00	122.33
36	A1	2724	OMU	C1'-N1-C2	2.73	122.49	117.59
36	A1	2266	PSU	C6-C5-C4	-2.73	116.33	118.17
35	B5	436	A2M	O4'-C1'-N9	2.72	112.35	108.75
35	B5	1271	OMG	C8-N7-C5	2.71	107.17	102.55
36	A1	2142	1MA	C8-N7-C5	2.71	107.16	102.55
36	A1	2191	PSU	C5-C6-N1	-2.70	118.39	122.14
38	A4	73	PSU	C6-C5-C4	-2.70	116.35	118.17
36	A1	1042	PSU	O2-C2-N1	-2.69	120.01	122.79
36	A1	1450	OMG	C8-N7-C5	2.69	107.13	102.55
36	A1	986	PSU	O2-C2-N1	-2.69	120.02	122.79
36	A1	2922	OMG	C8-N7-C5	2.67	107.09	102.55
36	A1	2729	OMU	C1'-N1-C2	2.65	122.35	117.59
35	B5	302	PSU	C6-C5-C4	-2.65	116.39	118.17
35	B5	1428	OMG	C8-N7-C5	2.64	107.05	102.55
36	A1	908	OMG	C8-N7-C5	2.63	107.02	102.55
36	A1	2288	OMG	C8-N7-C5	2.60	106.97	102.55
35	B5	796	A2M	C4-C5-N7	-2.55	106.64	109.34
35	B5	1773	4AC	C5-C4-N3	-2.55	118.61	122.60
35	B5	120	PSU	C6-C5-C4	-2.53	116.47	118.17
35	B5	420	A2M	C4-C5-N7	-2.50	106.69	109.34
35	B5	466	PSU	O2-C2-N1	-2.50	120.21	122.79
36	A1	2870	5MC	C1'-N1-C6	2.47	125.22	121.15
35	B5	578	OMU	O2-C2-N1	-2.47	119.58	122.80
35	B5	619	A2M	C4-C5-N7	-2.47	106.73	109.34
35	B5	1572	OMG	C8-N7-C5	2.46	106.74	102.55
36	A1	645	1MA	C5-C6-N1	2.46	117.49	113.95
36	A1	2946	A2M	C4-C5-N7	-2.46	106.74	109.34
36	A1	2880	PSU	C6-C5-C4	-2.45	116.52	118.17
36	A1	2729	OMU	O4-C4-C5	-2.45	120.93	125.16
36	A1	2729	OMU	O2-C2-N3	-2.45	116.97	121.49
35	B5	541	A2M	C4-C5-N7	-2.44	106.76	109.34
36	A1	898	OMU	C1'-N1-C2	2.43	121.96	117.59
35	B5	28	A2M	C4-C5-N7	-2.43	106.77	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2870	5MC	CM5-C5-C4	-2.41	116.55	120.51
35	B5	1773	4AC	C1'-N1-C2	2.40	123.75	118.44
35	B5	562	OMG	C5-C6-N1	2.40	118.65	114.07
35	B5	414	OMC	O2-C2-N3	-2.39	118.57	122.33
36	A1	2280	A2M	C4-C5-N7	-2.39	106.81	109.34
36	A1	2288	OMG	C5-C6-N1	2.38	118.61	114.07
35	B5	974	A2M	C4-C5-N7	-2.38	106.83	109.34
35	B5	1280	4AC	O2-C2-N3	-2.37	118.59	122.33
35	B5	436	A2M	C4-C5-N7	-2.36	106.84	109.34
36	A1	2266	PSU	O4'-C1'-C2'	2.35	108.41	105.15
36	A1	2281	A2M	C2'-C1'-N9	-2.35	107.34	112.56
36	A1	908	OMG	O4'-C1'-N9	-2.33	105.65	108.75
36	A1	645	1MA	C8-N7-C5	2.32	106.50	102.55
36	A1	2826	PSU	C5-C6-N1	-2.31	118.93	122.14
36	A1	2948	OMC	O2-C2-N1	2.31	123.43	118.90
36	A1	2640	A2M	C4-C5-N7	-2.31	106.90	109.34
36	A1	663	OMC	O2-C2-N3	-2.30	118.71	122.33
35	B5	1269	OMU	O2-C2-N3	-2.29	117.26	121.49
36	A1	805	OMG	C5-C6-N1	2.29	118.43	114.07
36	A1	2220	A2M	O4'-C1'-N9	2.28	111.77	108.75
35	B5	1639	OMC	O2-C2-N3	-2.28	118.73	122.33
36	A1	776	PSU	O4'-C1'-C2'	2.28	108.31	105.15
36	A1	2870	5MC	N1-C2-N3	2.28	122.75	118.80
36	A1	2791	OMG	C5-C6-N1	2.27	118.41	114.07
36	A1	2815	OMG	C5-C6-N1	2.27	118.40	114.07
36	A1	2133	PSU	O2-C2-N1	-2.27	120.45	122.79
36	A1	2264	PSU	C5-C6-N1	-2.24	119.03	122.14
36	A1	2129	PSU	C5-C6-N1	-2.24	119.03	122.14
36	A1	1056	PSU	C6-C5-C4	-2.24	116.66	118.17
35	B5	466	PSU	O2-C2-N3	-2.23	117.89	121.86
36	A1	2944	PSU	C5-C6-N1	-2.23	119.05	122.14
36	A1	2197	OMC	O2-C2-N3	-2.23	118.82	122.33
36	A1	2349	PSU	C6-C5-C4	-2.22	116.67	118.17
35	B5	100	A2M	C4-C5-N7	-2.22	106.99	109.34
36	A1	2634	UR3	C3U-N3-C4	2.22	120.94	117.87
36	A1	867	OMG	C5-C6-N1	2.21	118.29	114.07
36	A1	2416	PSU	C5-C6-N1	-2.21	119.08	122.14
36	A1	2880	PSU	O4'-C1'-C2'	2.20	108.20	105.15
36	A1	1042	PSU	O2-C2-N3	-2.19	117.96	121.86
35	B5	1572	OMG	C5-C6-N1	2.19	118.25	114.07
36	A1	2280	A2M	N6-C6-N1	2.19	123.02	118.33
36	A1	2921	OMU	O2-C2-N1	-2.19	119.95	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B5	1191	B8N	O36-C34-O35	-2.18	119.14	124.08
36	A1	2619	OMG	C5-C6-N1	2.18	118.22	114.07
36	A1	2281	A2M	C4-C5-N7	-2.17	107.04	109.34
36	A1	649	A2M	C2'-C1'-N9	2.16	117.35	112.56
36	A1	2975	PSU	C6-C5-C4	-2.15	116.72	118.17
36	A1	908	OMG	C5-C6-N1	2.15	118.17	114.07
36	A1	1124	PSU	O2-C2-N3	-2.14	118.05	121.86
35	B5	759	PSU	C6-C5-C4	-2.14	116.73	118.17
35	B5	766	PSU	O4'-C1'-C2'	2.13	108.11	105.15
35	B5	1280	4AC	C1'-N1-C2	2.12	123.13	118.44
36	A1	2922	OMG	C5-C6-N1	2.12	118.12	114.07
36	A1	2793	OMG	CM2-O2'-C2'	-2.11	109.05	114.47
36	A1	2944	PSU	O4'-C1'-C2'	2.10	108.06	105.15
35	B5	632	PSU	C6-C5-C4	-2.10	116.76	118.17
35	B5	466	PSU	C6-C5-C4	-2.09	116.77	118.17
36	A1	805	OMG	O6-C6-C5	-2.09	120.19	124.32
36	A1	2826	PSU	O4'-C1'-C2'	2.08	108.03	105.15
36	A1	2191	PSU	O2-C2-N3	-2.07	118.18	121.86
35	B5	1271	OMG	O6-C6-C5	-2.07	120.21	124.32
36	A1	2133	PSU	C6-N1-C2	-2.06	120.78	122.69
36	A1	817	A2M	C4-C5-N7	-2.06	107.16	109.34
36	A1	2735	PSU	C6-C5-C4	-2.05	116.79	118.17
36	A1	986	PSU	O2-C2-N3	-2.04	118.24	121.86
36	A1	1052	PSU	C5-C6-N1	-2.04	119.31	122.14
35	B5	1782	MA6	C10-N6-C6	2.03	125.00	119.40
35	B5	1269	OMU	C1'-N1-C6	-2.02	116.46	120.78
36	A1	1110	PSU	O2-C2-N3	-2.02	118.28	121.86
36	A1	2944	PSU	O2-C2-N3	-2.02	118.28	121.86
36	A1	960	PSU	C5-C6-N1	-2.02	119.34	122.14
35	B5	766	PSU	C5-C6-N1	-2.00	119.36	122.14

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	B5	1575	G7M	C2'
35	B5	1575	G7M	C3'
35	B5	1575	G7M	C4'

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	AB	243	HIC	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
40	AB	243	HIC	CA-CB-CG-CD2
35	B5	619	A2M	O4'-C4'-C5'-O5'
35	B5	1280	4AC	N3-C4-N4-C7
35	B5	1280	4AC	O7-C7-N4-C4
35	B5	1280	4AC	CM7-C7-N4-C4
35	B5	1773	4AC	N3-C4-N4-C7
35	B5	1782	MA6	C5-C6-N6-C10
36	A1	776	PSU	C2'-C1'-C5-C4
36	A1	776	PSU	C2'-C1'-C5-C6
36	A1	807	A2M	O4'-C4'-C5'-O5'
36	A1	807	A2M	C3'-C4'-C5'-O5'
36	A1	908	OMG	O4'-C4'-C5'-O5'
36	A1	908	OMG	C1'-C2'-O2'-CM2
36	A1	1437	OMC	C1'-C2'-O2'-CM2
36	A1	1450	OMG	O4'-C4'-C5'-O5'
36	A1	2197	OMC	C2'-C1'-N1-C2
36	A1	2197	OMC	C2'-C1'-N1-C6
36	A1	2260	PSU	O4'-C1'-C5-C4
36	A1	2260	PSU	O4'-C1'-C5-C6
36	A1	2266	PSU	O4'-C1'-C5-C4
36	A1	2266	PSU	O4'-C1'-C5-C6
36	A1	2288	OMG	O4'-C4'-C5'-O5'
36	A1	2417	OMU	C1'-C2'-O2'-CM2
36	A1	2619	OMG	C1'-C2'-O2'-CM2
36	A1	2640	A2M	C1'-C2'-O2'-CM'
36	A1	2729	OMU	O4'-C4'-C5'-O5'
36	A1	2923	PSU	O4'-C1'-C5-C4
36	A1	2923	PSU	O4'-C1'-C5-C6
36	A1	2946	A2M	C1'-C2'-O2'-CM'
35	B5	619	A2M	C3'-C4'-C5'-O5'
35	B5	1575	G7M	C3'-C4'-C5'-O5'
35	B5	1782	MA6	O4'-C4'-C5'-O5'
36	A1	1450	OMG	C3'-C4'-C5'-O5'
36	A1	2729	OMU	C3'-C4'-C5'-O5'
36	A1	2923	PSU	O4'-C4'-C5'-O5'
35	B5	1269	OMU	O4'-C1'-N1-C2
35	B5	541	A2M	O4'-C4'-C5'-O5'
36	A1	908	OMG	C3'-C4'-C5'-O5'
36	A1	1052	PSU	O4'-C4'-C5'-O5'
36	A1	2142	1MA	C3'-C4'-C5'-O5'
36	A1	2197	OMC	O4'-C4'-C5'-O5'
36	A1	2314	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
36	A1	2923	PSU	C3'-C4'-C5'-O5'
35	B5	541	A2M	C3'-C4'-C5'-O5'
36	A1	2142	1MA	O4'-C4'-C5'-O5'
36	A1	2288	OMG	C3'-C4'-C5'-O5'
36	A1	2314	PSU	C3'-C4'-C5'-O5'
35	B5	1428	OMG	O4'-C4'-C5'-O5'
36	A1	2280	A2M	C3'-C4'-C5'-O5'
35	B5	1782	MA6	C3'-C4'-C5'-O5'
36	A1	2197	OMC	C3'-C4'-C5'-O5'
36	A1	2280	A2M	O4'-C4'-C5'-O5'
36	A1	817	A2M	C4'-C5'-O5'-P
36	A1	2314	PSU	C4'-C5'-O5'-P
36	A1	2870	5MC	C2'-C1'-N1-C6
36	A1	2347	UY1	C3'-C4'-C5'-O5'
35	B5	1269	OMU	O4'-C1'-N1-C6
35	B5	1773	4AC	O7-C7-N4-C4
35	B5	1773	4AC	CM7-C7-N4-C4
36	A1	1124	PSU	C3'-C4'-C5'-O5'
36	A1	2870	5MC	O4'-C1'-N1-C6
36	A1	2870	5MC	C2'-C1'-N1-C2
35	B5	100	A2M	O4'-C4'-C5'-O5'
35	B5	541	A2M	C4'-C5'-O5'-P
36	A1	2281	A2M	C3'-C2'-O2'-CM'
36	A1	776	PSU	C4'-C5'-O5'-P
36	A1	2266	PSU	C4'-C5'-O5'-P
36	A1	2923	PSU	C4'-C5'-O5'-P
36	A1	960	PSU	O4'-C1'-C5-C4
36	A1	2870	5MC	O4'-C1'-N1-C2
35	B5	1575	G7M	O4'-C4'-C5'-O5'
36	A1	2729	OMU	C4'-C5'-O5'-P
37	A3	50	PSU	C3'-C4'-C5'-O5'
36	A1	2197	OMC	O4'-C1'-N1-C6
36	A1	1437	OMC	C3'-C2'-O2'-CM2
36	A1	2922	OMG	C3'-C2'-O2'-CM2
36	A1	807	A2M	C4'-C5'-O5'-P
36	A1	1052	PSU	C3'-C4'-C5'-O5'
35	B5	1428	OMG	C4'-C5'-O5'-P
36	A1	2340	PSU	C4'-C5'-O5'-P
35	B5	1415	PSU	C3'-C4'-C5'-O5'
35	B5	1428	OMG	C3'-C4'-C5'-O5'
35	B5	302	PSU	O4'-C4'-C5'-O5'
35	B5	766	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
35	B5	1639	OMC	O4'-C4'-C5'-O5'
36	A1	1437	OMC	O4'-C4'-C5'-O5'
35	B5	1773	4AC	C5-C4-N4-C7
36	A1	1124	PSU	O4'-C4'-C5'-O5'
36	A1	2347	UY1	O4'-C4'-C5'-O5'
35	B5	1007	OMC	C2'-C1'-N1-C2
36	A1	2197	OMC	O4'-C1'-N1-C2

There are no ring outliers.

18 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B5	1126	OMG	2	0
36	A1	966	PSU	2	0
36	A1	2880	PSU	2	0
36	A1	990	PSU	1	0
35	B5	1280	4AC	1	0
35	B5	28	A2M	1	0
36	A1	1449	A2M	1	0
36	A1	986	PSU	1	0
36	A1	2314	PSU	1	0
35	B5	1290	PSU	1	0
35	B5	1773	4AC	3	0
36	A1	1133	A2M	1	0
36	A1	2349	PSU	1	0
36	A1	807	A2M	1	0
36	A1	649	A2M	1	0
36	A1	876	A2M	1	0
36	A1	2220	A2M	1	0
36	A1	776	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 747 ligands modelled in this entry, 747 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	A1	5
53	AP	1
9	BI	1
35	B5	1
43	AE	1
47	AI	1
32	Bf	1
18	BR	1
22	BV	1
38	A4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	1955:U	O3'	2093:A	P	25.26
1	A1	1253:U	O3'	1260:A	P	24.88
1	AP	155:GLU	C	164:LYS	N	23.99
1	BI	123:LYS	C	135:LYS	N	20.70
1	B5	658:C	O3'	676:G	P	18.22
1	A1	1023:C	O3'	1030:A	P	16.66
1	AE	109:GLU	C	129:GLU	N	14.66
1	A1	2445:A	O3'	2501:U	P	14.44
1	A1	440:A	O3'	494:G	P	10.21
1	AI	101:LYS	C	114:GLY	N	9.90
1	Bf	125:THR	C	129:GLY	N	7.22
1	BR	95:ARG	C	100:LEU	N	5.16
1	BV	11:LEU	C	12:TYR	N	4.99
1	A4	73:PSU	O3'	74:U	P	4.85

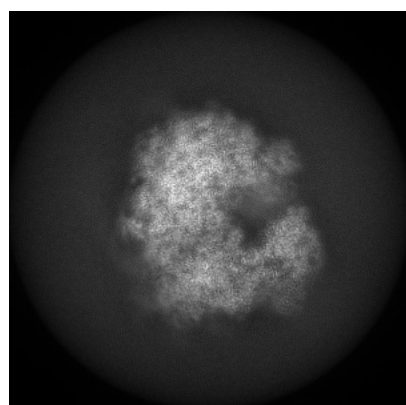
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23935. These allow visual inspection of the internal detail of the map and identification of artifacts.

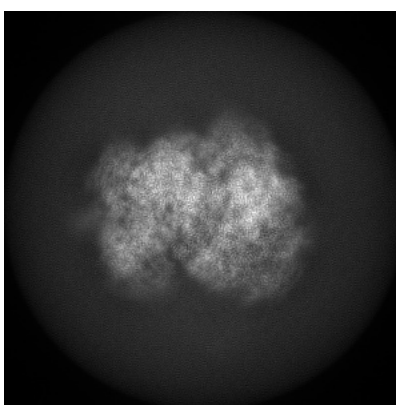
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

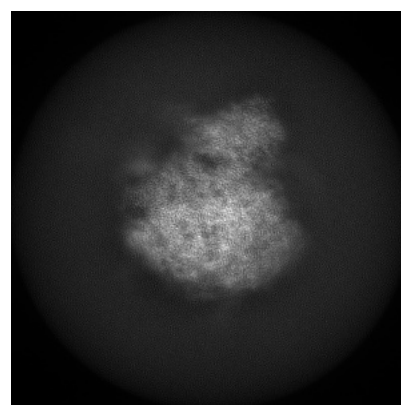
6.1.1 Primary map



X



Y

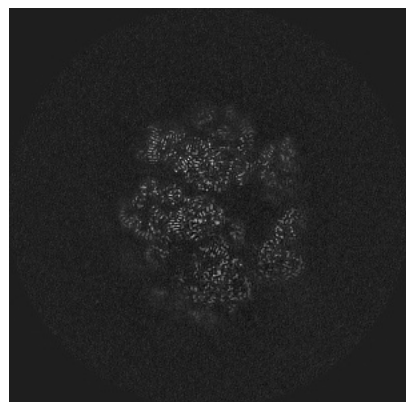


Z

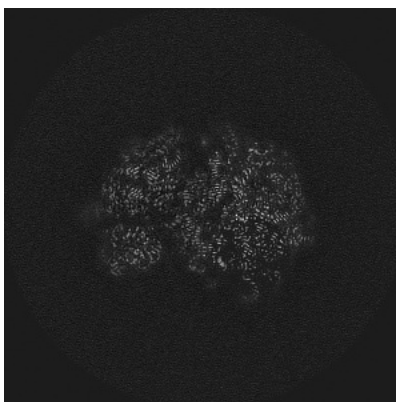
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

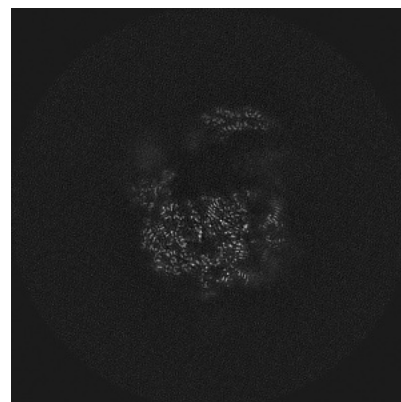
6.2.1 Primary map



X Index: 216



Y Index: 216

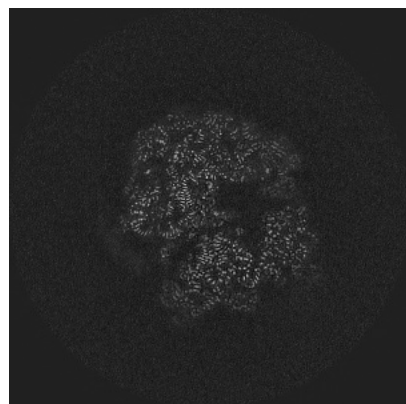


Z Index: 216

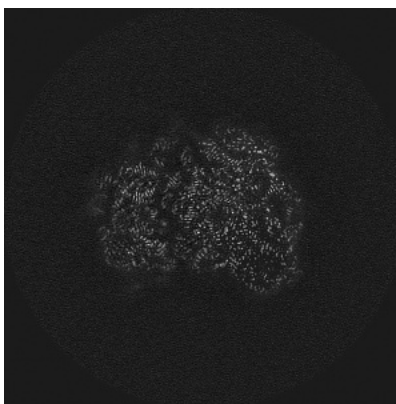
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

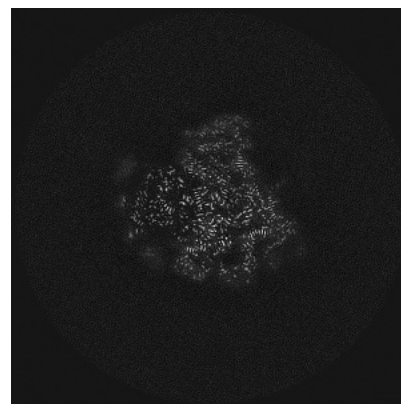
6.3.1 Primary map



X Index: 236



Y Index: 206

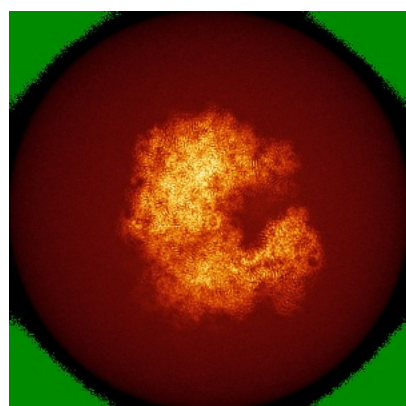


Z Index: 266

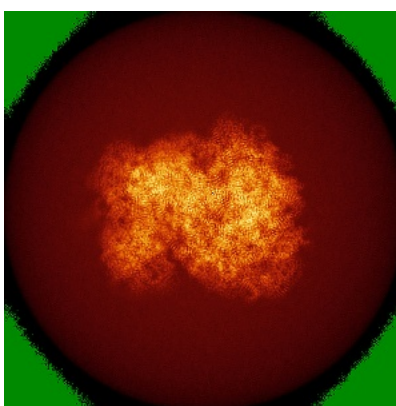
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

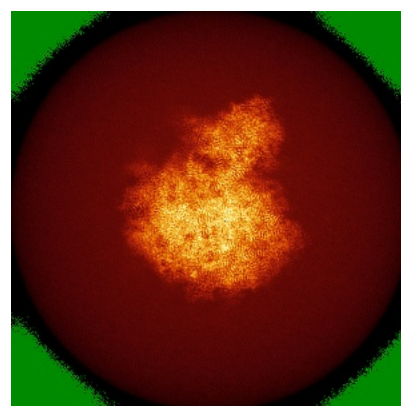
6.4.1 Primary map



X



Y

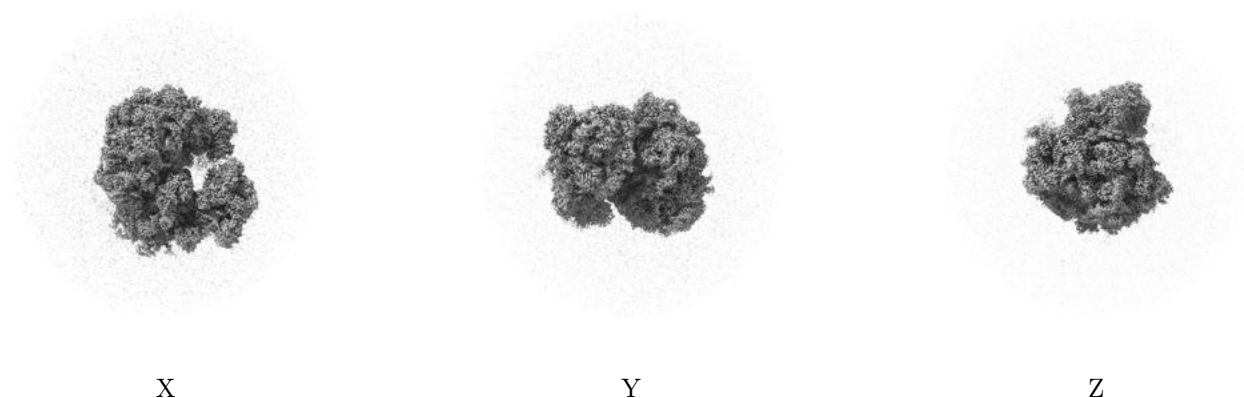


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

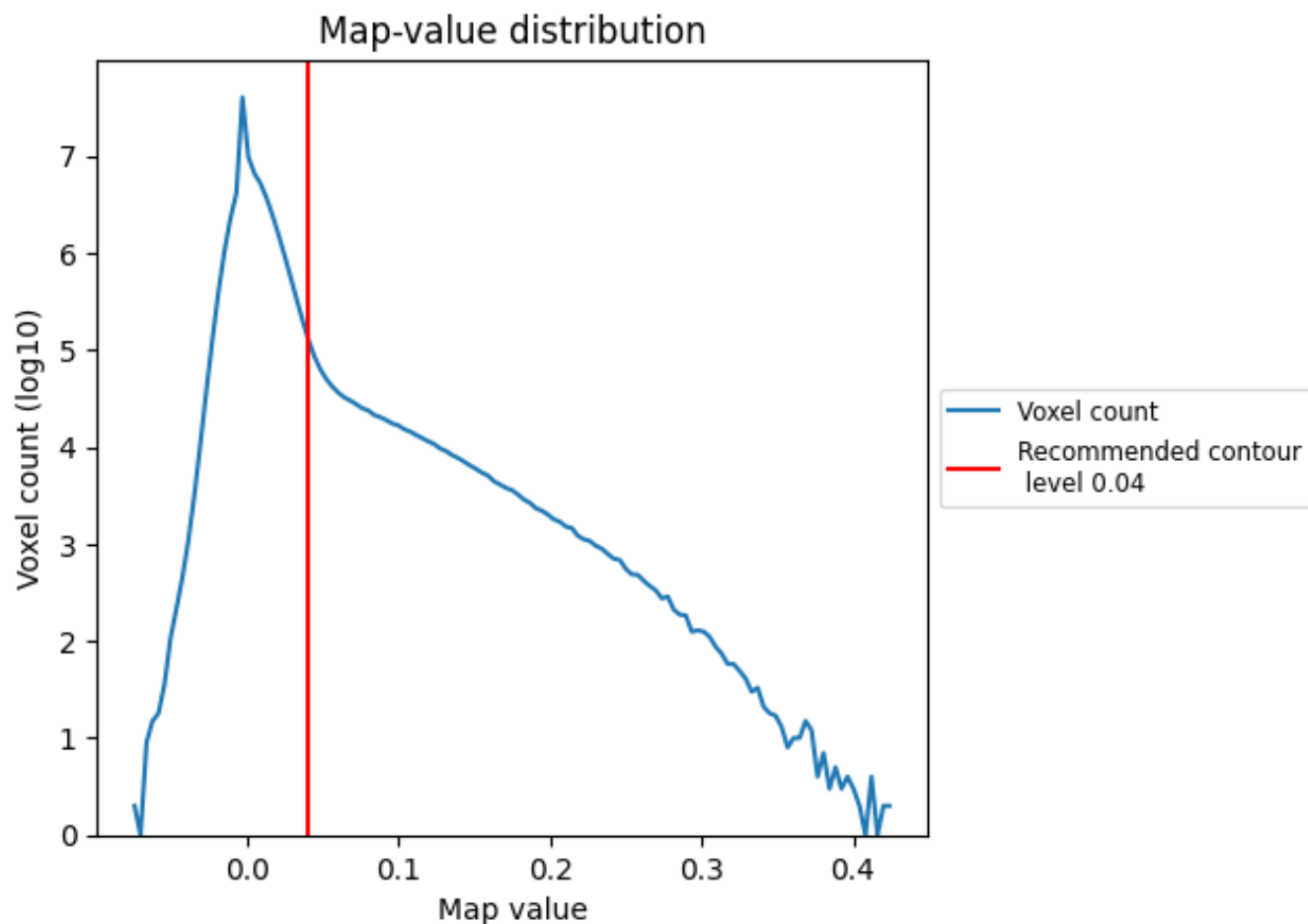
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

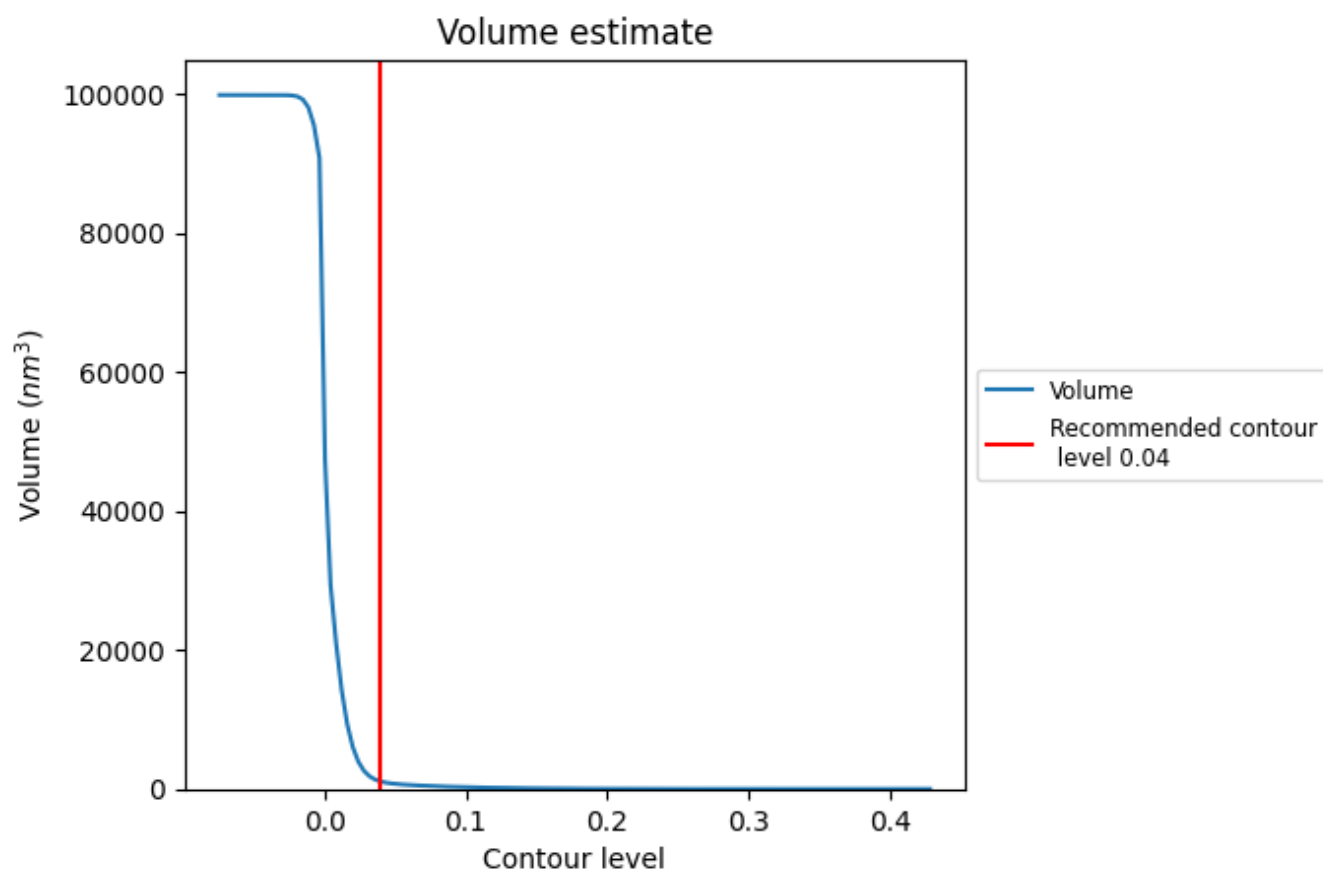
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

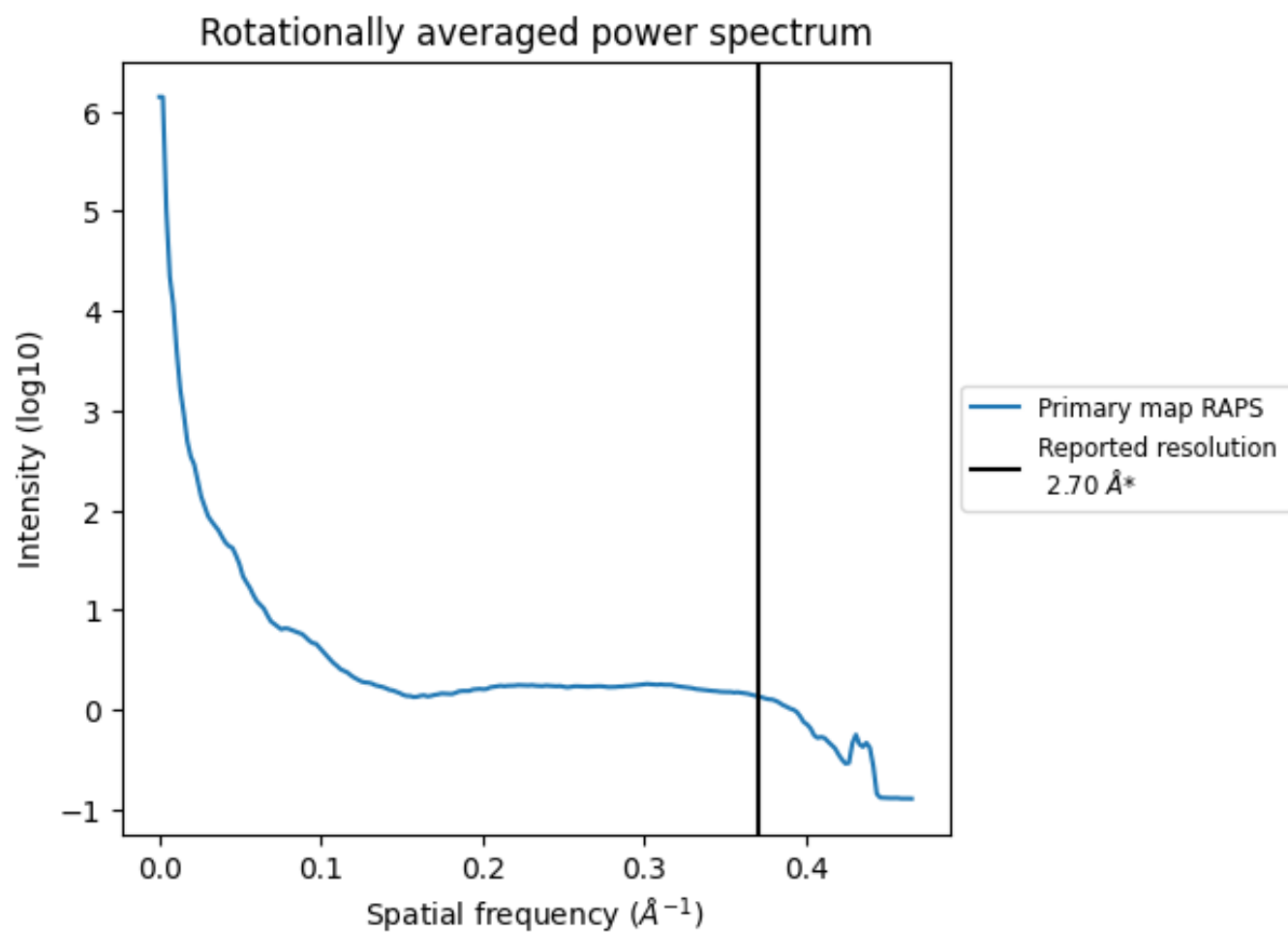
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1070 nm^3 ; this corresponds to an approximate mass of 967 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

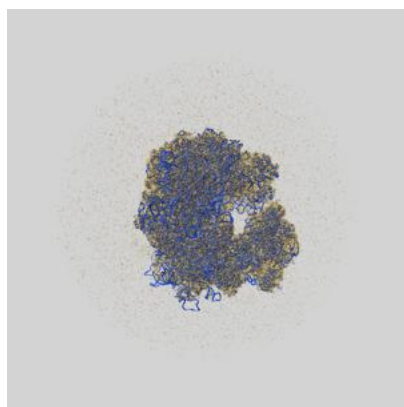
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

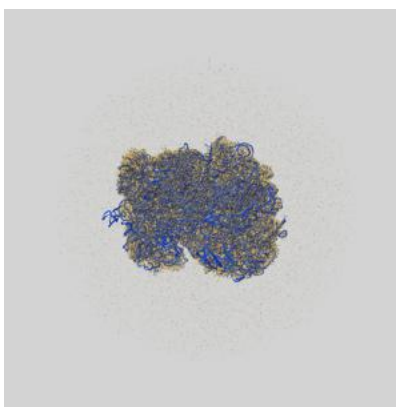
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23935 and PDB model 7MPJ. Per-residue inclusion information can be found in section 3 on page 22.

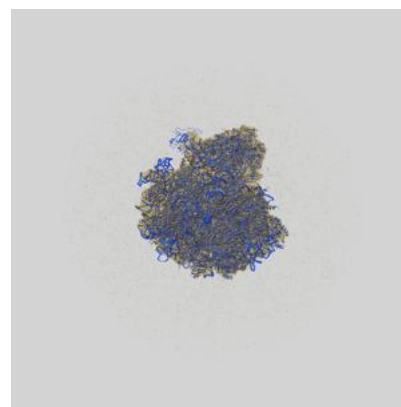
9.1 Map-model overlay [i](#)



X



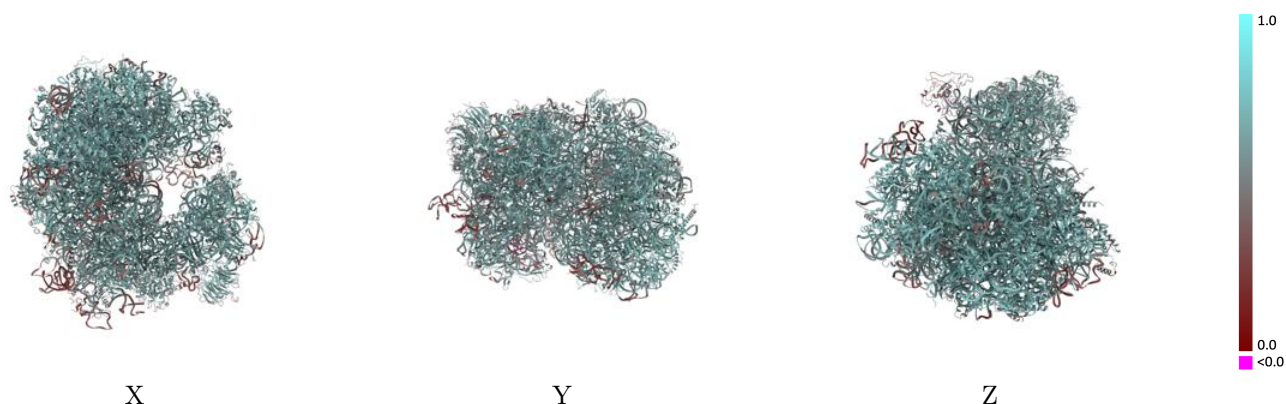
Y



Z

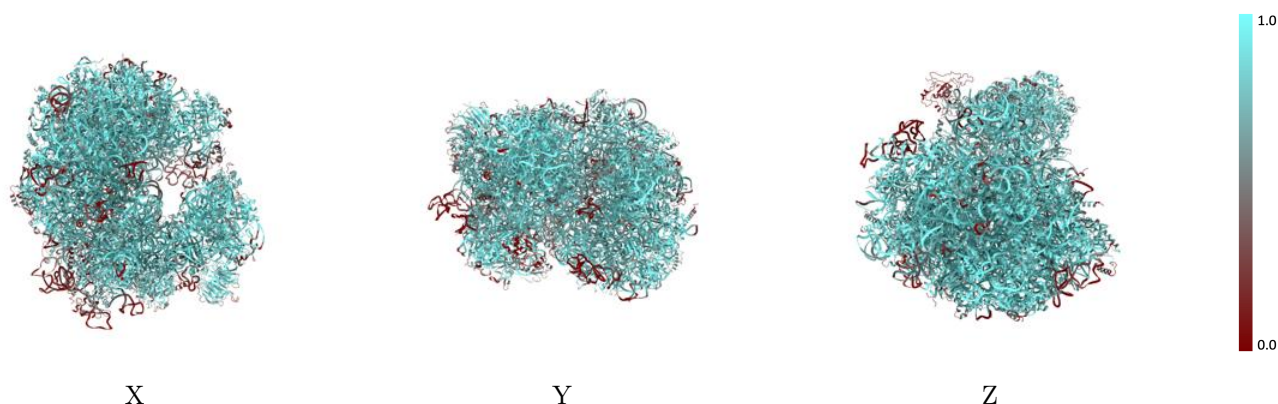
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



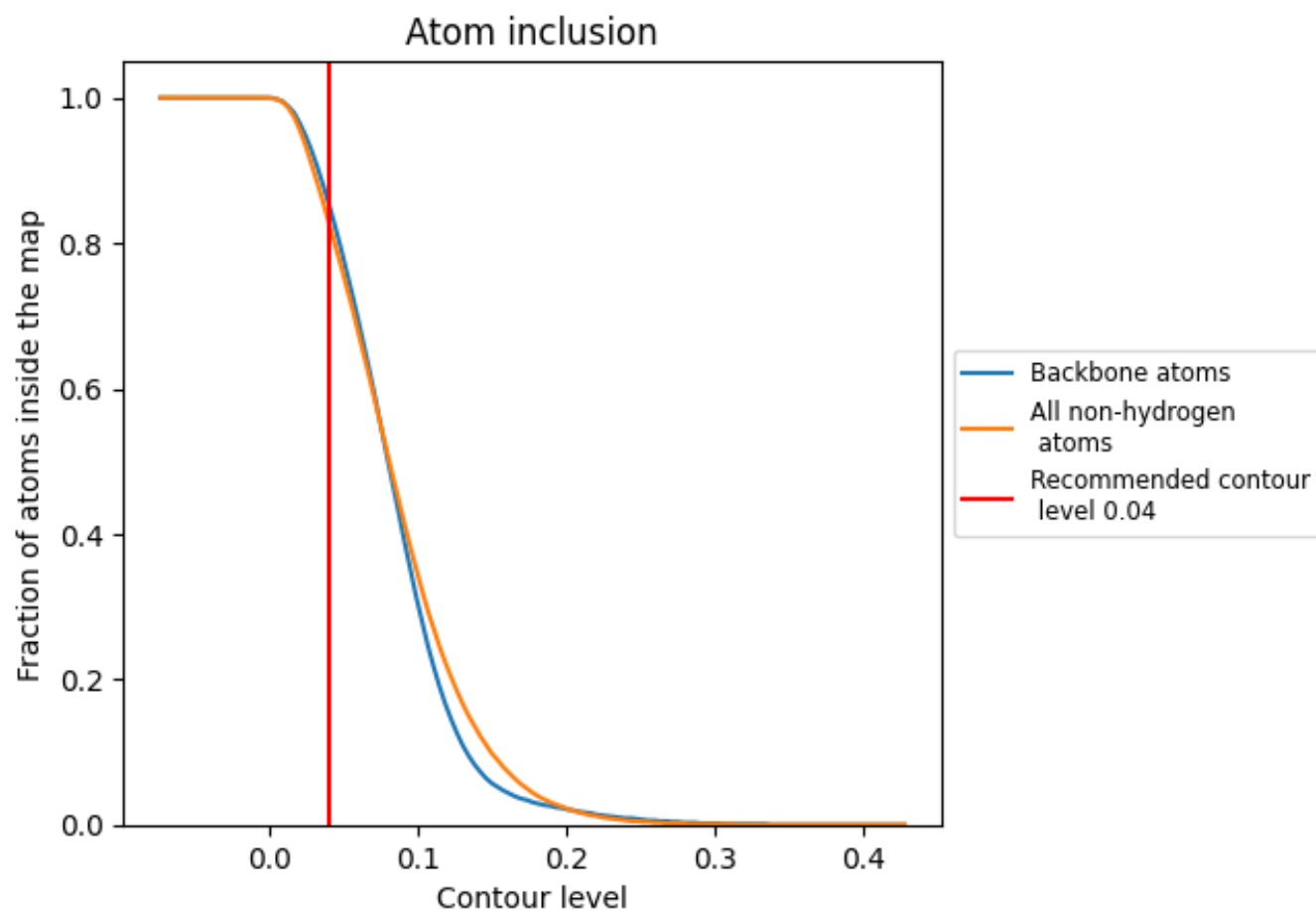
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.6130
A1	 0.8730	 0.6280
A3	 0.9310	 0.6380
A4	 0.9270	 0.6530
AA	 0.9060	 0.6730
AB	 0.8890	 0.6730
AC	 0.8710	 0.6580
AD	 0.7290	 0.5920
AE	 0.7460	 0.6180
AF	 0.8780	 0.6680
AG	 0.7570	 0.6170
AH	 0.8040	 0.6440
AI	 0.7560	 0.6150
AJ	 0.5280	 0.5080
AL	 0.8330	 0.6550
AM	 0.8350	 0.6630
AN	 0.9520	 0.6790
AO	 0.9070	 0.6800
AP	 0.8480	 0.6560
AQ	 0.9080	 0.6730
AR	 0.7230	 0.5860
AS	 0.8750	 0.6700
AT	 0.8330	 0.6390
AU	 0.6380	 0.5700
AV	 0.8480	 0.6520
AW	 0.8440	 0.6570
AX	 0.8360	 0.6490
AY	 0.8460	 0.6490
AZ	 0.7370	 0.6050
Aa	 0.8980	 0.6630
Ab	 0.7410	 0.5910
Ac	 0.7200	 0.5870
Ad	 0.7940	 0.6310
Ae	 0.8820	 0.6690
Af	 0.9260	 0.6940









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Chain	Atom inclusion	Q-score
Ag	 0.8390	 0.6390
Ah	 0.8240	 0.6340
Ai	 0.7650	 0.6030
Aj	 0.9330	 0.6870
Ak	 0.5640	 0.5270
Al	 0.9040	 0.6620
Am	 0.8190	 0.6530
An	 0.6180	 0.5650
Ao	 0.7690	 0.6180
Ap	 0.8210	 0.6440
B5	 0.8240	 0.5850
BA	 0.7650	 0.5780
BB	 0.7100	 0.5630
BC	 0.8260	 0.6080
BD	 0.7580	 0.5820
BE	 0.8250	 0.6130
BF	 0.8140	 0.6000
BG	 0.6500	 0.5590
BH	 0.5360	 0.5090
BI	 0.7810	 0.5920
BJ	 0.8000	 0.5980
BK	 0.7110	 0.5390
BL	 0.7440	 0.5970
BM	 0.0470	 0.3070
BN	 0.7920	 0.6020
BO	 0.7850	 0.5780
BP	 0.7220	 0.5690
BQ	 0.8840	 0.6360
BR	 0.6380	 0.5330
BS	 0.7950	 0.5900
BT	 0.8820	 0.6260
BU	 0.6380	 0.5420
BV	 0.8000	 0.5950
BW	 0.8980	 0.6380
BX	 0.8360	 0.6150
BY	 0.7770	 0.5970
BZ	 0.7580	 0.5740
Ba	 0.8320	 0.5940
Bb	 0.7110	 0.5690
Bc	 0.7340	 0.5710
Bd	 0.9120	 0.6510
Be	 0.6500	 0.5650

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Chain	Atom inclusion	Q-score
Bf	 0.0880	 0.2970
Bg	 0.7720	 0.5850
Bh	 0.3310	 0.4820