



Full wwPDB EM Validation Report ⓘ

Mar 11, 2025 – 03:56 pm GMT

PDB ID : 6ZTN
EMDB ID : EMD-11421
Title : E. coli 70S-RNAP expressome complex in NusG-coupled state (42 nt intervening mRNA)
Authors : Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on : 2020-07-20
Resolution : 3.90 Å (reported)
Based on initial models : 4YBB, 6ALH

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:

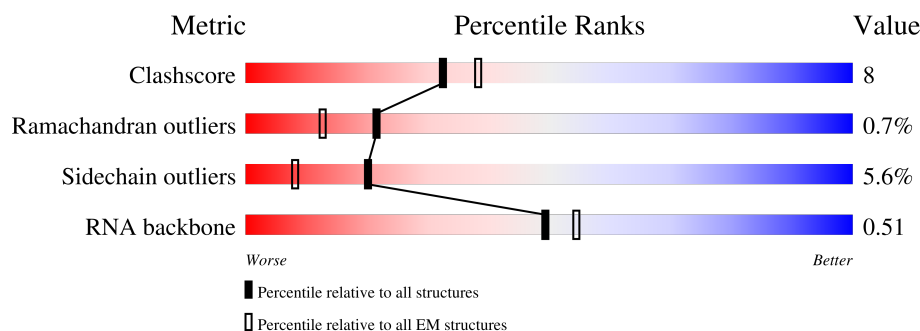
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

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 3.90 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.


















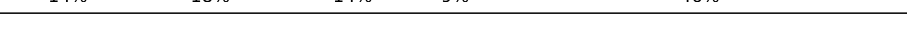









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AA	1542	57% 33% 8% ..
2	AB	241	73% 19% • 6%
3	AC	233	67% 21% • 10%
4	AD	206	74% 24% •
5	AE	167	69% 19% 5% 7%
6	AF	131	44% 31% 5% 21%
7	AG	156	73% 23% ..












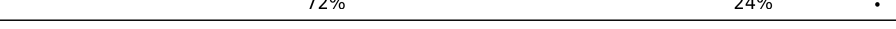













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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	57	
23	AW	77	
24	AX	76	
24	AZ	76	
25	BA	2904	
26	BB	120	
27	BC	273	
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	

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Mol	Chain	Length	Quality of chain
32	BH	149	 66% 30% .
33	BK	142	 85% 14% .
34	BL	123	 81% 18% .
35	BM	144	 77% 21% .
36	BN	136	 79% 21% .
37	BO	127	 73% 18% . 6%
38	BP	117	 72% 26% .
39	BQ	115	 77% 20% ..
40	BR	118	 81% 18% ..
41	BS	103	 72% 28%
42	BT	110	 77% 20% .
43	BU	100	 72% 24% .
44	BV	104	 70% 27% ..
45	BW	94	 76% 23% .
46	BX	85	 76% 12% . 11%
47	BY	78	 67% 31% ..
48	BZ	63	 73% 24% ..
49	B1	59	 73% 25% .
50	B2	57	 68% 28% ..
51	B3	55	 85% 9% . .
52	B4	46	 78% 22%
53	B5	65	 75% 20% ..
54	B6	50	 58% 16% . 24%
55	CA	329	 60% 9% 30%
55	CB	329	 57% 8% . 33%

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Mol	Chain	Length	Quality of chain
56	CC	1342	 78% 17% • •
57	CD	1407	 77% 17% • 5%
58	CE	91	 47% 9% 44%
59	CN	39	 26% 41% 10% 23%
60	CT	39	 8% 51% 18% 23%
61	CF	181	 45% 9% 46%

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
24	7MG	AZ	46	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 174624 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0
			32909	14684	6037	10655	1533		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	209	Total	C	N	O	S	0	0
			1640	1038	308	291	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	156	Total	C	N	O	S	0	0
			1148	715	217	210	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	100	Total	C	N	O	S	0	0
			800	500	153	146	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	57	Total	C	N	O	0	0
			474	298	90	86		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	31	Total	C	N	O	P	0	0
			656	294	117	214	31		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total 1630	C 730	N 290	O 533	P 76	S 1	0	0
24	AZ	76	Total 1630	C 730	N 290	O 533	P 76	S 1	0	0

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2899	Total	C	N	O	P	0	0
			62248	27776	11451	20122	2899		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BO	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BQ	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BR	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BS	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BU	96	Total	C	N	O	S	0	0
			764	484	142	136	2		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BV	103	Total	C	N	O	0	0
			789	498	148	143		

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BY	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BZ	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	B3	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	46	Total	C	N	O	S	0	0
			376	228	89	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 55 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
55	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 56 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CE	51	Total	C	N	O	S	0	0
			399	246	77	75	1		

- Molecule 59 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CN	30	Total	C	N	O	P	0	0
			615	294	114	178	29		

- Molecule 60 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

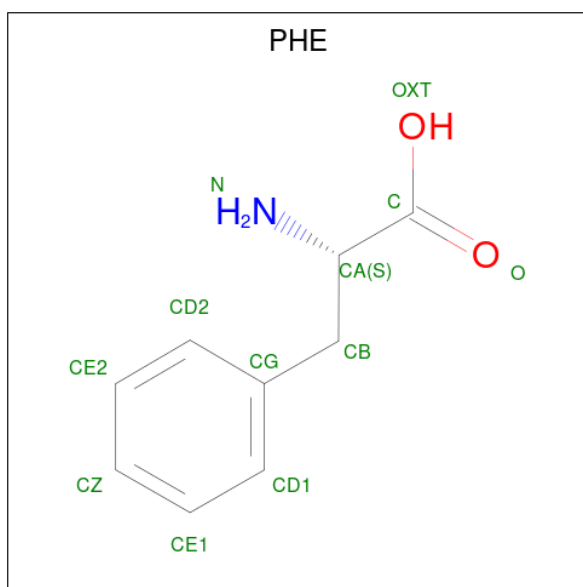
- Molecule 61 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CF	98	Total	C	N	O	S	0	0
			790	505	139	140	6		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	AA	139	Total	Mg	0
			139	139	
62	AL	3	Total	Mg	0
			3	3	
62	AT	1	Total	Mg	0
			1	1	
62	AV	1	Total	Mg	0
			1	1	
62	AW	4	Total	Mg	0
			4	4	
62	AX	1	Total	Mg	0
			1	1	
62	BA	318	Total	Mg	0
			318	318	
62	BB	9	Total	Mg	0
			9	9	
62	BC	3	Total	Mg	0
			3	3	
62	BD	1	Total	Mg	0
			1	1	
62	BN	1	Total	Mg	0
			1	1	
62	BR	1	Total	Mg	0
			1	1	
62	BX	1	Total	Mg	0
			1	1	
62	B2	1	Total	Mg	0
			1	1	
62	B5	1	Total	Mg	0
			1	1	
62	B6	1	Total	Mg	0
			1	1	
62	CD	1	Total	Mg	0
			1	1	

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
63	AX	1	Total	C	N	O	0
			11	9	1	1	

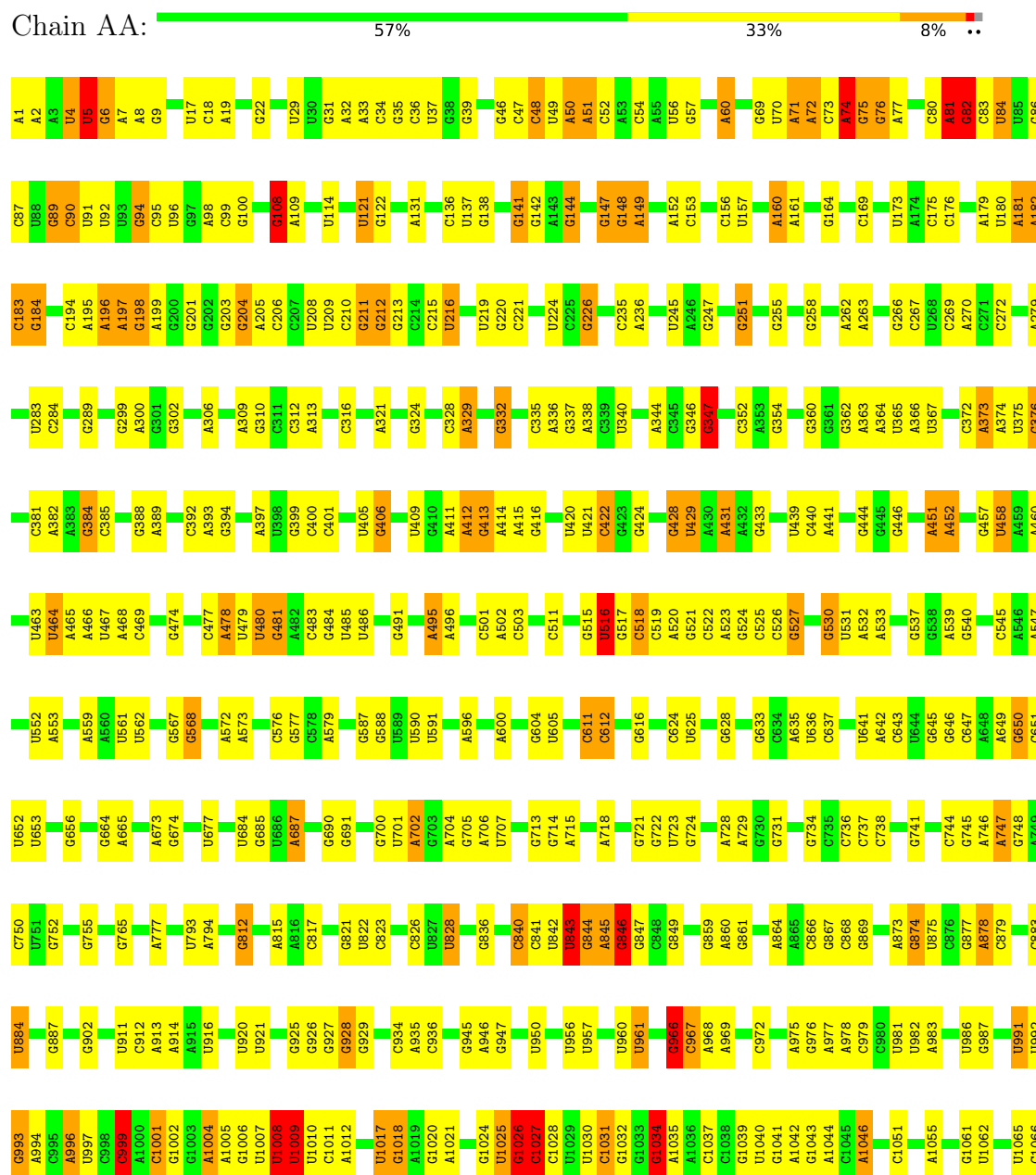
- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

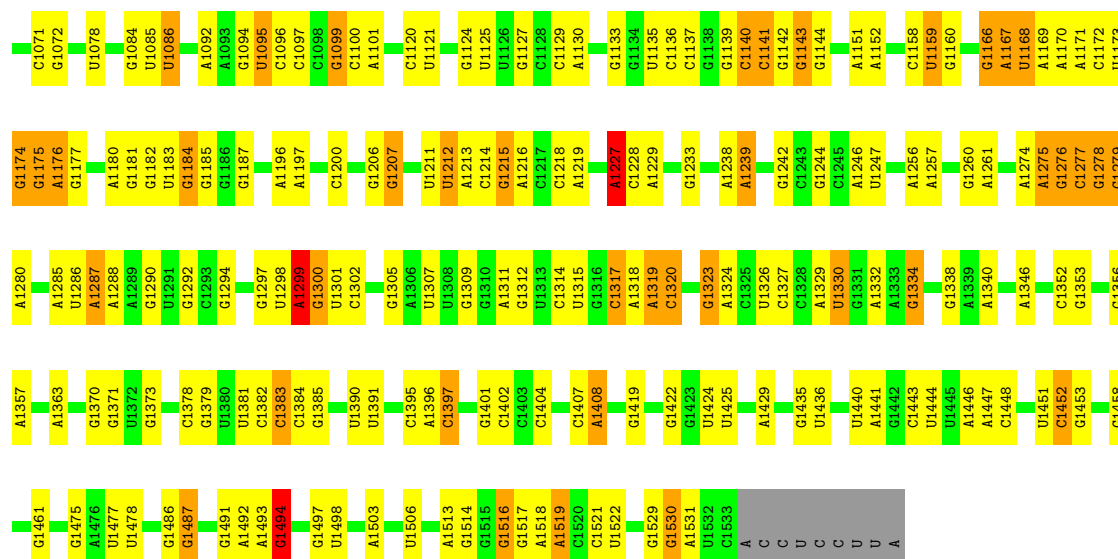
Mol	Chain	Residues	Atoms		AltConf
64	CD	2	Total	Zn	0
			2	2	

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

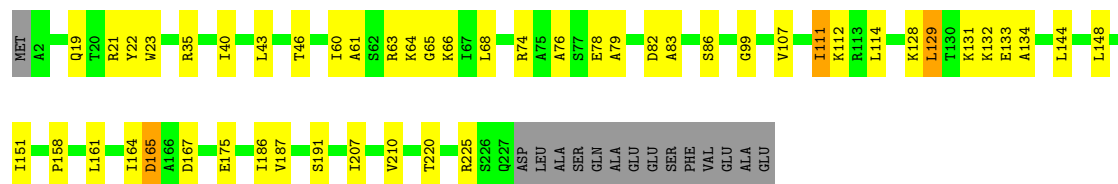
• Molecule 1: 16S ribosomal RNA





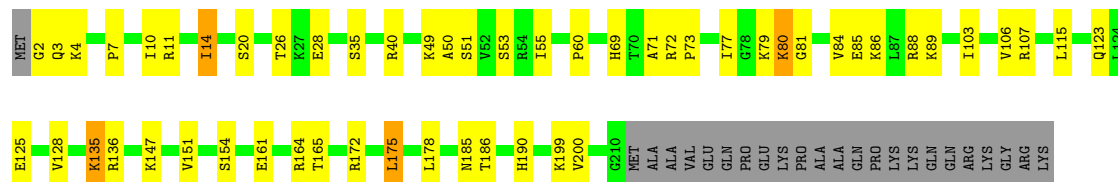
• Molecule 2: 30S ribosomal protein S2

Chain AB: 73% 19% • 6%



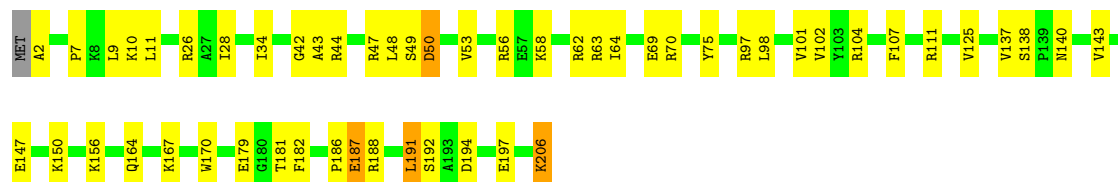
• Molecule 3: 30S ribosomal protein S3

Chain AC: 67% 21% • 10%



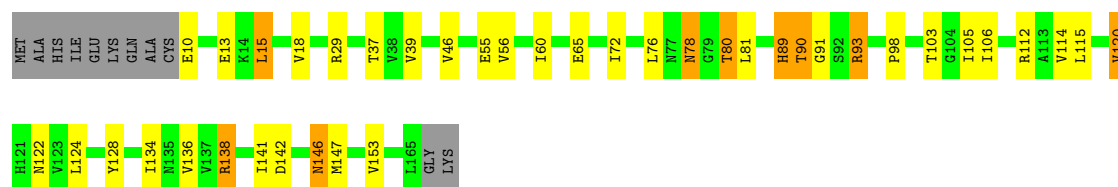
• Molecule 4: 30S ribosomal protein S4

Chain AD: 74% 24% •



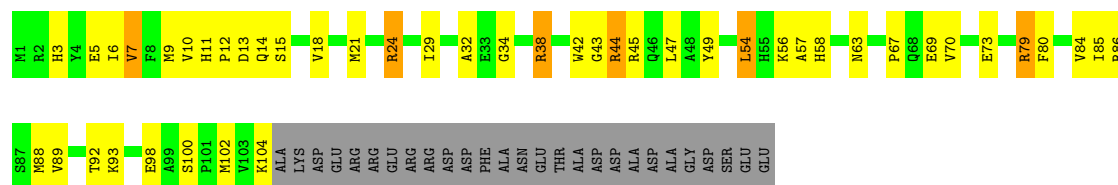
• Molecule 5: 30S ribosomal protein S5

Chain AE: 




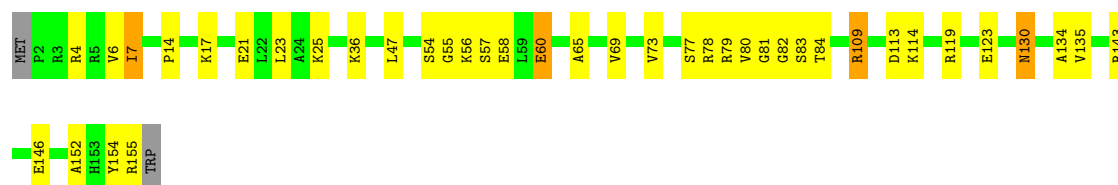
• Molecule 6: 30S ribosomal protein S6

Chain AF: 




• Molecule 7: 30S ribosomal protein S7

Chain AG: 



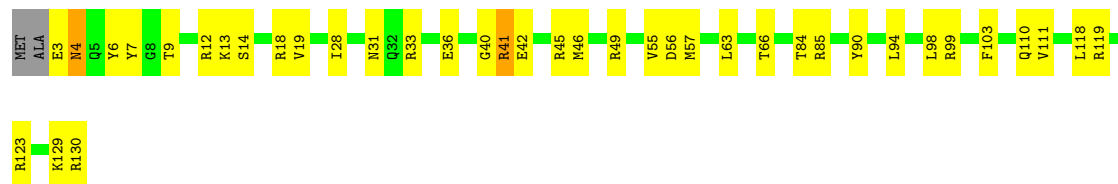
• Molecule 8: 30S ribosomal protein S8

Chain AH: 



• Molecule 9: 30S ribosomal protein S9

Chain AI: 



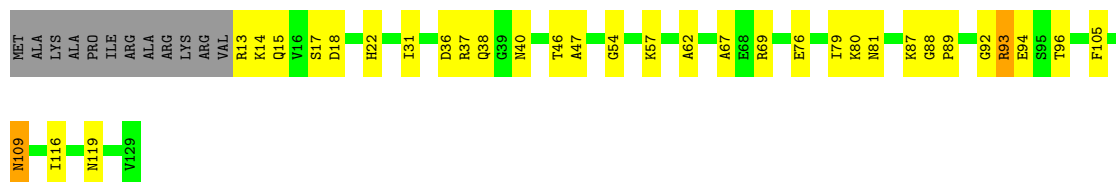
• Molecule 10: 30S ribosomal protein S10

Chain AJ: 



- Molecule 11: 30S ribosomal protein S11

Chain AK: 65% 24% 9%



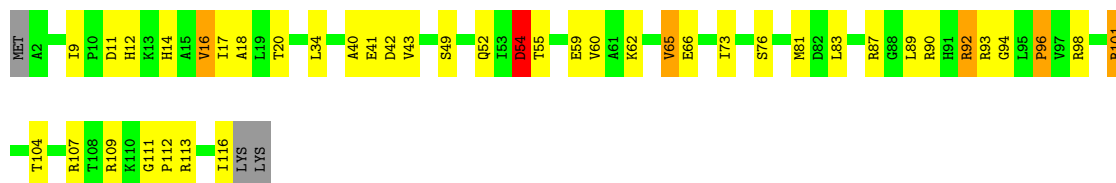
- Molecule 12: 30S ribosomal protein S12

Chain AL: 64% 31% 5%



- Molecule 13: 30S ribosomal protein S13

Chain AM: 62% 31% 7%



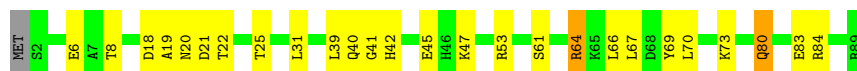
- Molecule 14: 30S ribosomal protein S14

Chain AN: 78% 20% 2%




- Molecule 15: 30S ribosomal protein S15

Chain AO: 70% 27% 3%




- Molecule 16: 30S ribosomal protein S16

Chain AP:  83% 17%



- Molecule 17: 30S ribosomal protein S17

Chain AQ:  75% 20% 5%



- Molecule 18: 30S ribosomal protein S18

Chain AR:  45% 27% 24%




- Molecule 19: 30S ribosomal protein S19

Chain AS:  65% 23% 10%




- Molecule 20: 30S ribosomal protein S20

Chain AT:  80% 15%

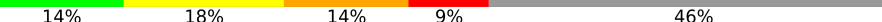


- Molecule 21: 30S ribosomal protein S21

Chain AU:  82% 15%



- Molecule 22: mRNA

Chain AV:  14% 18% 14% 9% 46%



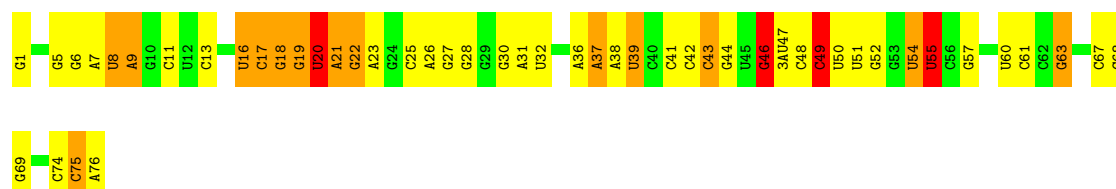
- Molecule 23: tRNA(fmet) P-site

Chain AW: 

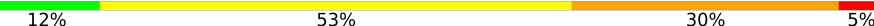


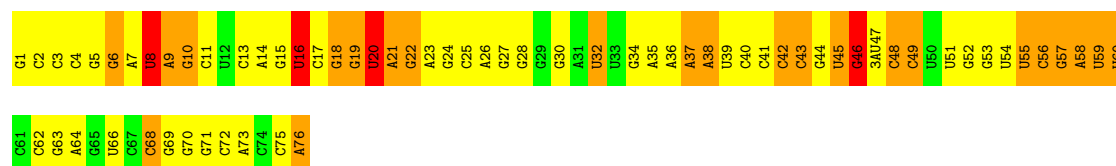
• Molecule 24: Phe-NH-tRNA(Phe) A-site

Chain AX: 



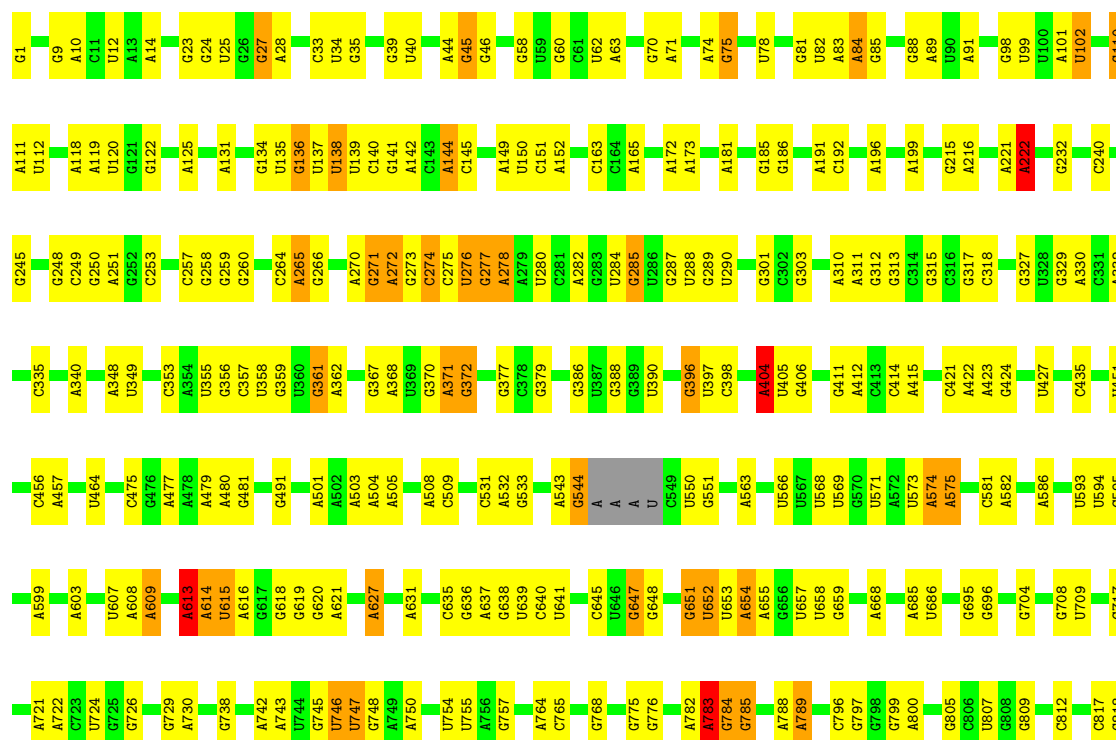
• Molecule 24: Phe-NH-tRNA(Phe) A-site

Chain AZ: 

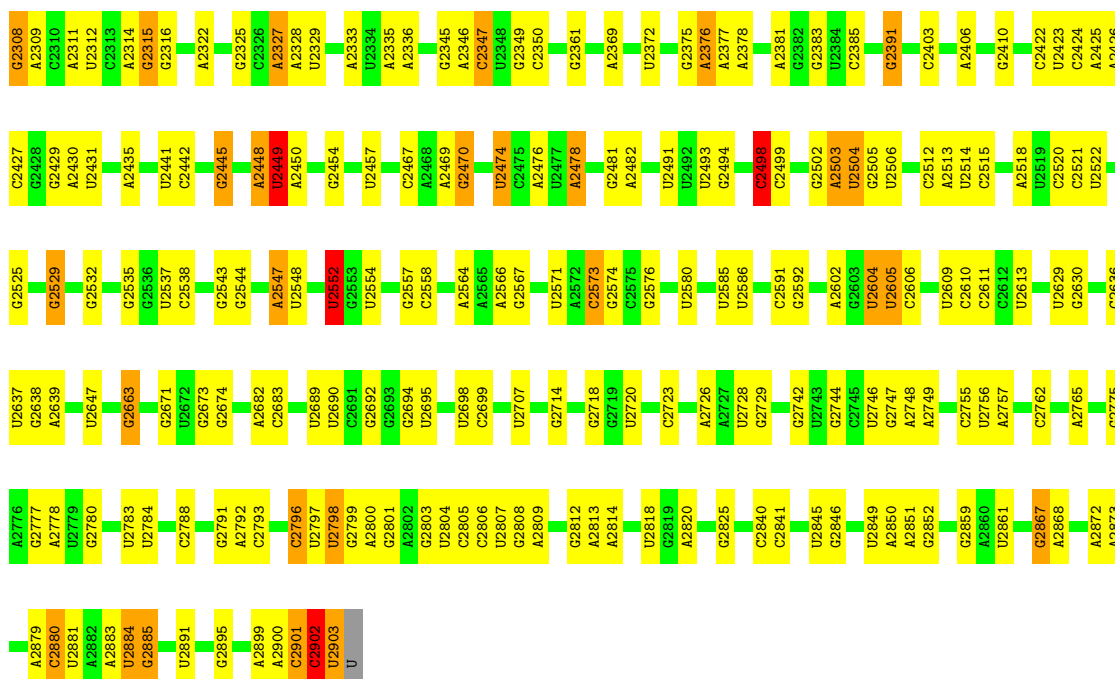


• Molecule 25: 23S ribosomal RNA

Chain BA: 

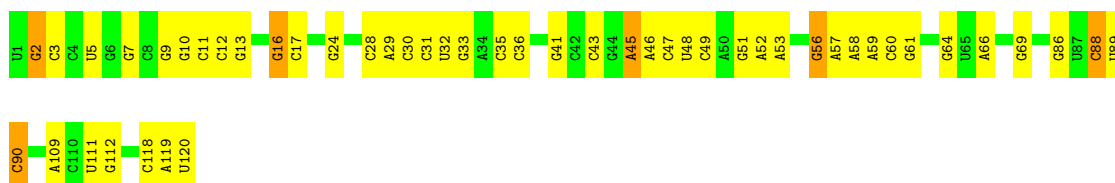


A2212	A2213	U2139	C2065	U1834	U1735	U1599	G1524	G1421	A1322	G1186	A1095	G1026	G924	A819
G2250	G2251	G2140	C2066	G1835	U1736	C1600	A1525	G1422	C1323	G1187	A1096	A1027	A925	U827
G2252	G2253	G2141		A1848	G1737	C1607	C1526	C1428	U1326	C1196	A1103	A1028	A926	U828
G2254	G2255	C2145	G2069	G1857	G1738	A1608	A1529	G1432	G1333	G1197	C1104	U1033	U931	A833
G2256	G2257	A2146	A2070	A1858	G1739	A1609	A1530	A1433	G1334	U1198	U1105	G1034	U932	G834
G2258	G2259	G2147	C2072	U1859	G1741	A1610	C1531	A1434	U1344	U1199	G1107	U1035	U933	U839
G2260	G2261	G2148	G2073	G1860	G1742	G1613	C1532	G1452	C1345	A1204	U1108	G1037	C940	C840
G2262	G2263	U2149	U2074	G1861	G1743	A1614	U1533	G1453	U1346	A1205	C1109	G1038	G940	A845
G2264	G2265	C2150	U2075	G1862	A1744	A1615	U1534	A1454	C1349	G1206	A1110	A1039	A941	U846
G2266	G2267	U2151	U2085	G1863	A1745	A1618	A1535	G1455	C1350	U1211	A1111	A1040	A945	U847
G2268	G2269	C2152	U2086	U1864	G1750	G1619	C1536	G1456	C1351	G1216	U1112	C1043	C946	C848
G2270	G2271	A2154	G2087		U1751	G1622	G1537	U1457	U1352	G1217	U1113	C1045	A947	A849
G2272	G2273	U2155		C1868	G1752	G1623	G1540	U1458	A1354	G1218	G1115	A1046	C948	
G2274	G2275	G1755		C1869		A1630	G1543	G1459	G1360	G1223	U1118	A1043	G953	G855
G2276	G2277	A1756		C1870	G1755	U1647	A1544	U1460	G1361	G1232	U1119	A1050	G954	G856
G2278	G2279	G1757		C1871	A1756	U1648	A1545	U1474	G1362	G1237	G1122	A1051	G955	G857
G2280	G2281	U1758		C1872	U1758	G1649	A1548	G1473	G1365	G1238	U1126	A1052	G956	G858
G2282	G2283	C1761		C1873	U1759	G1650	A1549	U1477	G1366	G1248	A1129	G1056	G957	G859
G2284	G2285	A1762		C1874	G1761	G1651	U1554	U1478	G1367	G1251	U1130	A1057	U963	U870
G2286	G2287	U2172		C1875	C1764	G1656	U1558	G1479	G1368	G1252	U1131	U1058	G969	U871
G2288	G2289	A2173		C1876	A1773	C1657	C1559	G1481	G1371	G1253	A1127	A1054	A960	U872
G2290	G2291	C2174		C1877	C1774	U1657	U1559	U1482	G1378	G1254	A1134	G1060	U970	
G2292	G2293	A2175		C1878	U1775	G1660	U1563	G1483	U1379	G1255	U1135	U1061	C974	G881
G2294	G2295	C2176		C1879	A1779	G1661	C1564	U1486	G1380	G1256	U1140	U1062	C974	G882
G2296	G2297	G2177		C1880	G1791	G1674	C1565	U1487	G1381	G1263	U1141	U1063	A979	U884
G2298	G2299	C2178		C1881	A1794	A1677	C1566	U1498	G1382	G1264	A1142	U1064	C982	C885
G2300	G2301	A2179		C1882	C1795	A1678	G1567	U1499	G1383	G1265	A1143	U1065	C983	A886
G2302	G2303	U2181		C1883	C1796	A1679	C1568	G1500	G1385	G1266	A1144	U1066	U887	C887
G2304	G2305	C2182		C1884	U1798	G1703	A1570	G1506	A1392	G1271	U1163	A1067	C984	C889
G2306	G2307	U2183		C1885	G1799	G1707	U1571	U1507	A1395	A1272	U1174	A1068	C985	C890
G2308	G2309	A2184		C1886	A1800	A1713	U1572	U1508	U1400	G1273	U1175	A1069	C986	G891
G2310	G2311	C2185		C1887	A1801	U1714	C1581	U1509	G1401	A1272	U1176	U1083	C987	A892
G2312	G2313	U2186		C1888	A1802	G1715	C1582	U1510	U1402	U1273	U1177	U1084	A986	U894
G2314	G2315	C2187		C1889	A1803	G1718	A1583	U1511	A1403	G1292	U1178	A1085	U999	A896
G2316	G2317	U2188		C1890	A1804	G1719	U1584	U1512	U1404	G1293	C1170	A1086	C1005	C897
G2318	G2319	C2189		C1891	A1805	U1720	C1585	U1513	U1405	G1294	C1171	U1078	C1006	C898
G2320	G2321	U2190		C1892	A1806	G1721	A1586	U1514	U1406	G1300	U1172	U1079	A1080	C899
G2322	G2323	G2191		C1893	G1812	G1724	U1587	U1515	U1407	A1301	C1173	A1081	A1010	A899
G2324	G2325	C2192		C1894	G1813	U1725	U1588	U1516	G1410	A1302	U1174	U1082	G1011	C908
G2326	G2327	U2193		C1895	C1816	G1728	A1590	U1517	A1413	G1310	U1175	U1083	U1012	C909
G2328	G2329	A2194		C1896	G1826	U1729	C1591	U1518	A1414	G1311	U1176	U1084	A909	A910
G2330	G2331	C2195		C1897	U1827	G1730	U1592	U1519	U1415	U1292	U1177	A1085	U1013	
G2332	G2333	U2196		C1898	G1828	G1731	U1593	U1520	U1416	G1312	C1178	A1086	U1014	G914
G2334	G2335	A2197		C1899	A1829	G1732	C1594	U1521	G1417	C1313	G1179	A1087	G1022	C915
G2336	G2337	C2198		C1900	G1830	G1733	U1595	U1522	G1418	C1314	U1180	A1088	U1023	G923
G2338	G2339	U2199		C1901	C1833	G1734	A1596	U1523	A1420	C1320	U1181	A1089	G1024	
G2340	G2341	C2199		C1902			A1597	U1524		A1321	U1182	A1090		



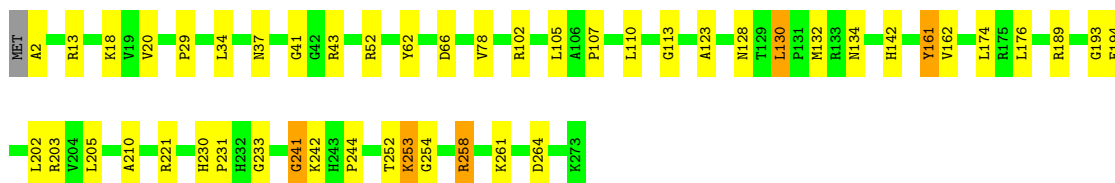
- Molecule 26: 5S ribosomal RNA

Chain BB: 59% 36% 5%



- Molecule 27: 50S ribosomal protein L2

Chain BC: 82% 16% 2%

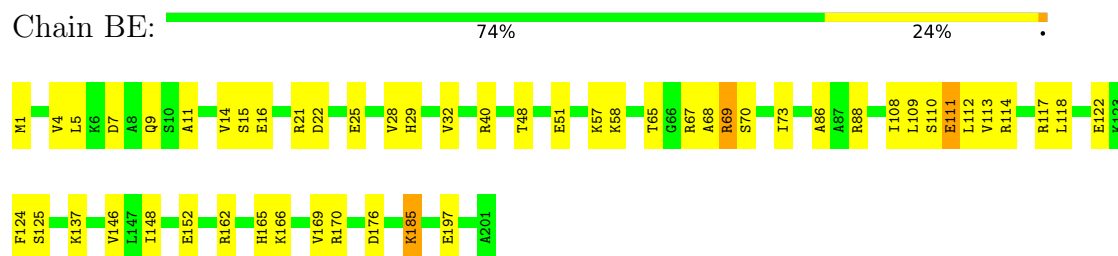


- Molecule 28: 50S ribosomal protein L3

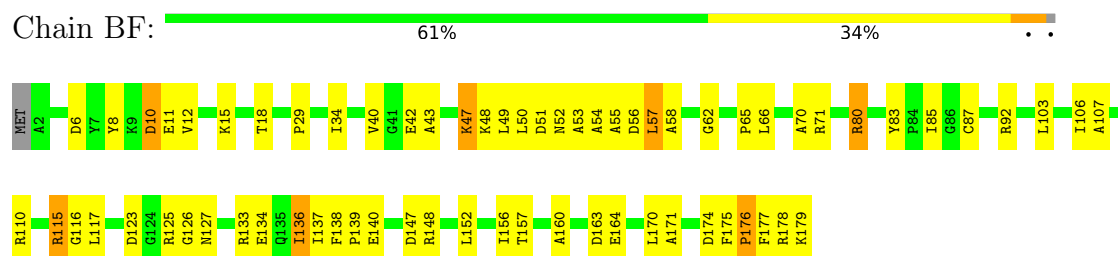
Chain BD: 78% 20% 2%



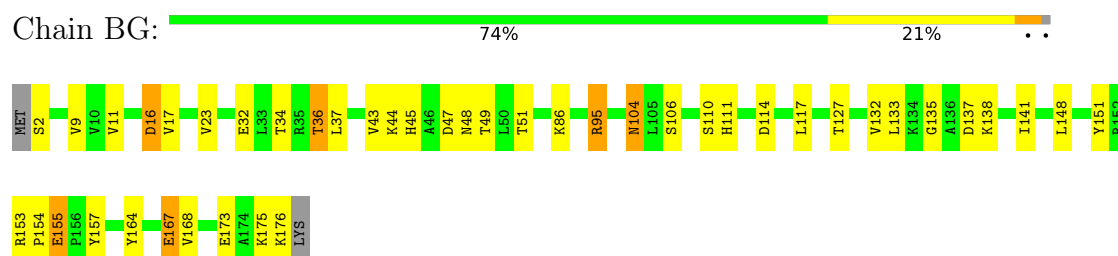
- Molecule 29: 50S ribosomal protein L4



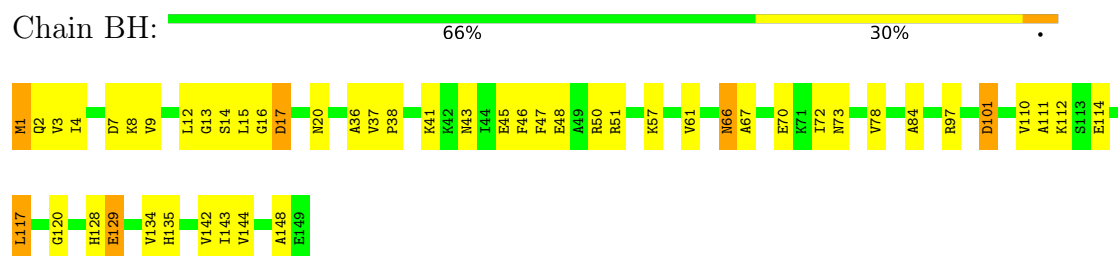
- Molecule 30: 50S ribosomal protein L5



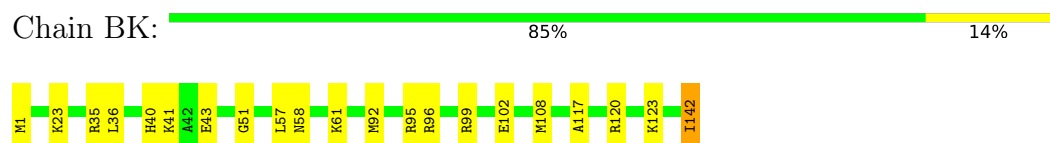
- Molecule 31: 50S ribosomal protein L6




- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13




- Molecule 34: 50S ribosomal protein L14

Chain BL:  81% 18% .




- Molecule 35: 50S ribosomal protein L15

Chain BM:  77% 21% .




- Molecule 36: 50S ribosomal protein L16

Chain BN:  79% 21% .



- Molecule 37: 50S ribosomal protein L17

Chain BO:  73% 18% 6% .




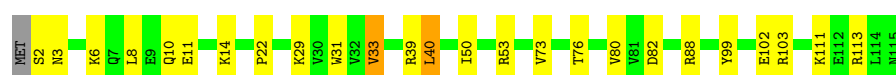
- Molecule 38: 50S ribosomal protein L18

Chain BP:  72% 26% .




- Molecule 39: 50S ribosomal protein L19

Chain BQ:  77% 20% ..



- Molecule 40: 50S ribosomal protein L20

Chain BR:  81% 18% ..




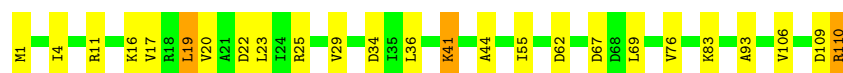
- Molecule 41: 50S ribosomal protein L21

Chain BS:  72% 28%




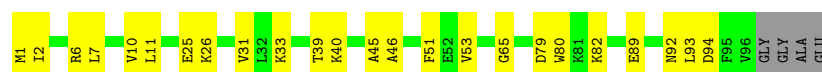
- Molecule 42: 50S ribosomal protein L22

Chain BT:  77% 20%



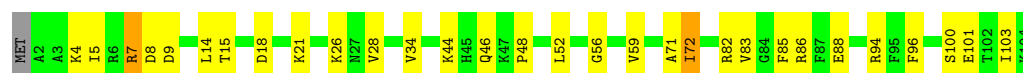
- Molecule 43: 50S ribosomal protein L23

Chain BU:  72% 24%




- Molecule 44: 50S ribosomal protein L24

Chain BV:  70% 27%




- Molecule 45: 50S ribosomal protein L25

Chain BW:  76% 23%



- Molecule 46: 50S ribosomal protein L27

Chain BX:  76% 12% 11%



- Molecule 47: 50S ribosomal protein L28

Chain BY:  67% 31%



- Molecule 48: 50S ribosomal protein L29

Chain BZ:  73% 24% ..



- Molecule 49: 50S ribosomal protein L30

Chain B1:  73% 25% .




- Molecule 50: 50S ribosomal protein L32

Chain B2:  68% 28% ..




- Molecule 51: 50S ribosomal protein L33

Chain B3:  85% 9% . .



- Molecule 52: 50S ribosomal protein L34

Chain B4:  78% 22%



- Molecule 53: 50S ribosomal protein L35

Chain B5:  75% 20% ..



- Molecule 54: 50S ribosomal protein L36

Chain B6:  58% 16% . 24%

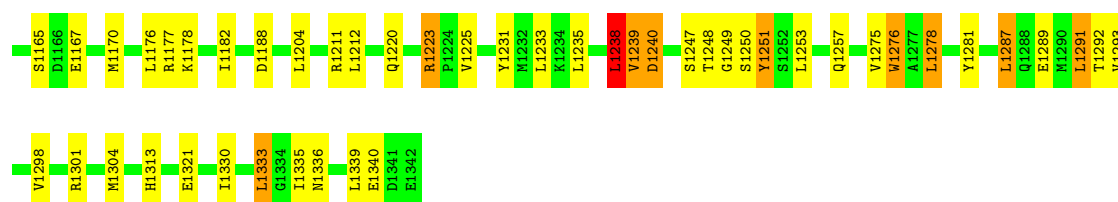


- Molecule 55: DNA-directed RNA polymerase subunit alpha

[illegible]

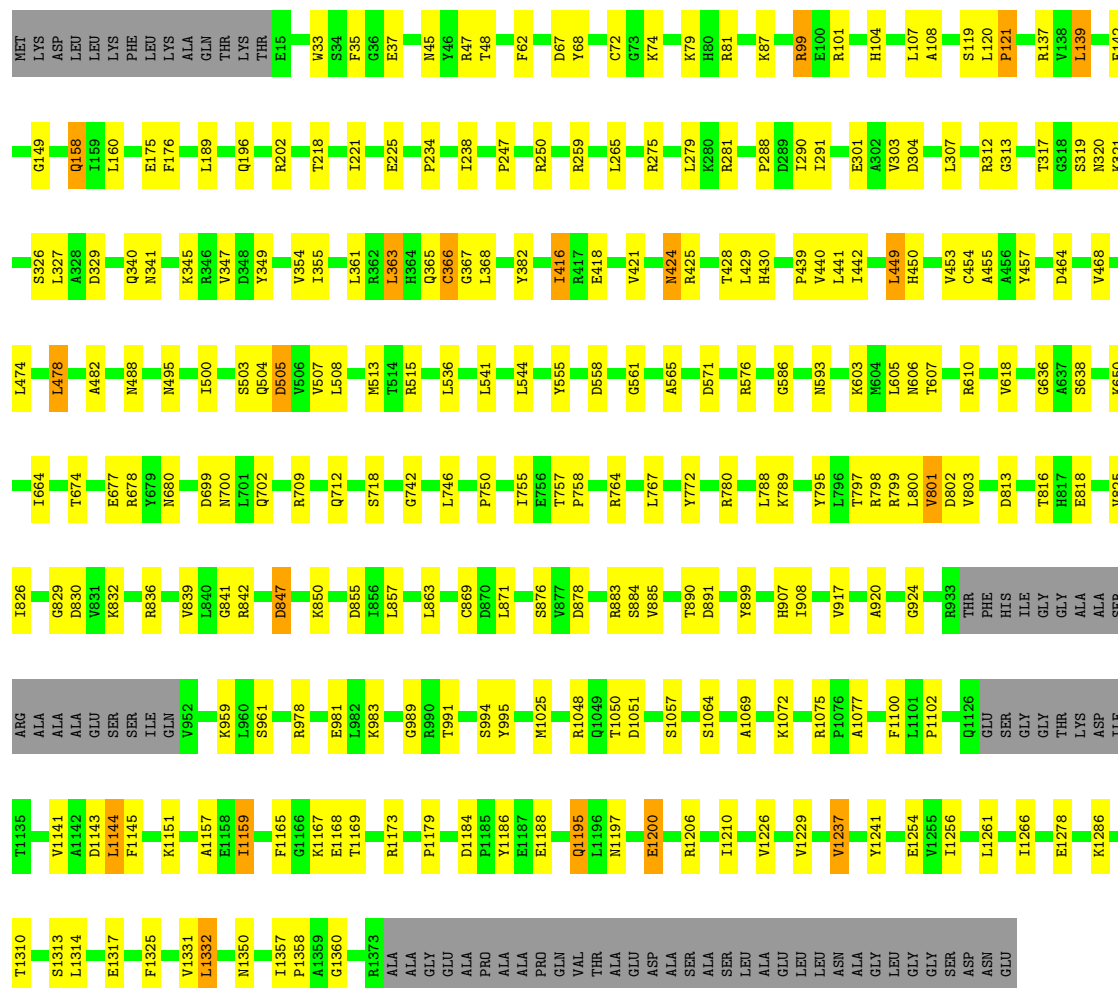
ASP	LEU	VAL	GLN	THR	GLU	VAL	GLU	LEU	LEU	LYS	THR	PRO	ASN	GLY	LYS	LYS	SER	LEU	THR	GLU	ILE	LYS	ASP	GLY	LEU	SER	LEU	GLY	LEU	GLY	MET										
D174	Y185	R191	V192	T196	D199	L228	D233	ARG	ASP	VAL	ARG	GLN	PRO	VAL	GLU	GLY	PHE	ASP	ILE	LEU	LEU	LEU	ARG	PRO	VAL	ASP	ASP	LEU	ASN	TRP	PRO	PRO	THR	ALA	VAL	ARG	ARG	ILE	ALA	ASP	GLU
GLN	GLY	S4	F8	P11	R12	L13	T27	L28	G34	L39	L47	L48	H66	E67	Y68	E72	G73	V74	G75	E76	I81	N84	L102	F103	K104	I130	S139	A155	S156	ARG	ILE	HIS	GLU	GLU	ASP	GLU	ARG	PRO	ILE	G169	R170

L967	V818	H554	E392	P178	H1
L979	V822	G556	Y395	L194	E7
E885	V823	H673	D396	L397	K8
R996	F828	R687	S421	M193	K9
L1002	T829	P691	K422	R197	R10
E1005	E835	D696	D423	R201	I11
L1014	L836	K697	D424	L210	R18
Q1017	T843	L699	K431	L213	D23
K1022	K844	E705	R436	T216	L27
V1052	P855	V708	L448	Q219	L28
K1057	N888	Y726	I453	D234	F38
K1065	T888	V733	R454	Y47	G45
H1070	GLY	E745	F464	D236	Q46
V1075	GLU	A746	L468	L237	Y47
I1076	GLN	Y751	R473	A251	G48
I1079	GLU	N752	E477	E256	L49
I1082	GLU	L753	L481	Y262	V56
V1094	L758	E611	I483	R267	G65
D1095	GLU	S759	N494	R268	Y73
I1096	L760	N760	F506	I269	C85
V1097	LEU	Q761	L511	T270	V90
L1098	ARG	N762	E617	H273	E98
L1101	ALA	N766	D624	I274	K99
R1106	ILE	E625	E625	L277	L100
M1107	PHE	C770	E626	V282	R101
M1108	GLY	V782	G627	N518	E108
E1114	GLU	E793	D632	N519	E121
K1133	LYS	L794	R637	P520	F136
Q1134	ALA	R799	K639	E316	V137
Q1135	ASP	V913	T525	D320	I138
V1138	L918	V802	D651	T336	R143
L1141	Q944	A803	Y652	R528	V144
Y1149	R944	F804	K653	Y346	I145
A1153	E947	N808	D654	I530	V146
L1152	E950	N811	V655	R540	L149
I1153	Q955	E812	V660	E541	H150
	E962	S815	V661	R542	T164
	E962	S815	V662	D549	H165
	I966	I816	V663	V550	S165
	I966	I817	V668	A380	



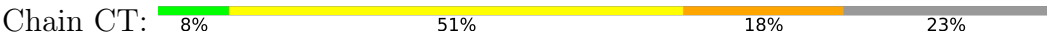
• Molecule 57: DNA-directed RNA polymerase subunit beta'

Chain CD: 77% 17% 5%

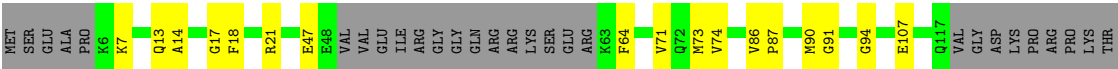




● Molecule 60: Template DNA strand



● Molecule 61: Transcription termination/antitermination protein NusG



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, UR3, 2MA, 6MZ, MA6, 5MC, 1MG, 7MG, 5MU, D2T, PSU, 2MG, 4SU, MG, 4OC, MIA, ZN, 3TD, OMU, MEQ, H2U, 4D4, 3AU, G7M, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.73	1/36569 (0.0%)	1.04	74/57044 (0.1%)
2	AB	0.32	0/1796	0.56	0/2420
3	AC	0.36	0/1667	0.57	0/2246
4	AD	0.34	0/1665	0.53	0/2227
5	AE	0.37	0/1161	0.59	0/1563
6	AF	0.38	0/867	0.55	0/1171
7	AG	0.32	0/1230	0.62	2/1649 (0.1%)
8	AH	0.37	0/989	0.53	0/1326
9	AI	0.36	0/1043	0.62	0/1387
10	AJ	0.35	0/810	0.70	0/1094
11	AK	0.35	0/893	0.57	0/1205
12	AL	0.41	0/954	0.71	0/1279
13	AM	0.33	0/900	0.62	1/1204 (0.1%)
14	AN	0.34	0/817	0.52	0/1088
15	AO	0.36	0/722	0.58	0/964
16	AP	0.32	0/659	0.54	0/884
17	AQ	0.35	0/657	0.58	0/881
18	AR	0.37	0/481	0.65	1/645 (0.2%)
19	AS	0.35	0/680	0.59	0/915
20	AT	0.32	0/676	0.45	0/895
21	AU	0.34	0/598	0.51	0/792
22	AV	1.68	20/731 (2.7%)	1.62	23/1133 (2.0%)
23	AW	0.75	1/1725 (0.1%)	0.98	0/2687
24	AX	0.61	1/1584 (0.1%)	0.87	1/2463 (0.0%)
24	AZ	0.54	1/1584 (0.1%)	0.96	1/2463 (0.0%)
25	BA	0.82	0/69140	1.03	115/107854 (0.1%)
26	BB	0.61	0/2872	0.94	1/4478 (0.0%)
27	BC	0.43	0/2131	0.66	1/2863 (0.0%)
28	BD	0.39	0/1576	0.57	0/2119
29	BE	0.39	0/1571	0.62	2/2113 (0.1%)
30	BF	0.35	0/1444	0.62	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BG	0.33	0/1333	0.57	0/1805
32	BH	0.31	0/1122	0.66	1/1515 (0.1%)
33	BK	0.38	0/1152	0.54	0/1551
34	BL	0.39	0/956	0.60	0/1279
35	BM	0.36	0/1061	0.61	0/1412
36	BN	0.38	0/1081	0.57	0/1443
37	BO	0.38	0/973	0.60	0/1301
38	BP	0.32	0/910	0.58	0/1219
39	BQ	0.38	0/929	0.58	0/1242
40	BR	0.47	0/960	0.54	0/1278
41	BS	0.41	0/829	0.65	0/1107
42	BT	0.38	0/864	0.57	0/1156
43	BU	0.36	0/771	0.58	0/1031
44	BV	0.34	0/797	0.53	0/1062
45	BW	0.36	0/766	0.60	1/1025 (0.1%)
46	BX	0.39	0/589	0.57	0/779
47	BY	0.40	0/635	0.50	0/848
48	BZ	0.31	0/502	0.48	0/667
49	B1	0.34	0/453	0.55	0/605
50	B2	0.40	0/450	0.74	0/599
51	B3	0.33	0/443	0.66	0/587
52	B4	0.37	0/379	0.49	0/496
53	B5	0.39	0/513	0.63	0/676
54	B6	0.35	0/302	0.55	0/397
55	CA	1.02	3/1797 (0.2%)	0.87	0/2436
55	CB	0.74	1/1703 (0.1%)	0.81	4/2308 (0.2%)
56	CC	1.28	79/10581 (0.7%)	0.92	22/14275 (0.2%)
57	CD	1.02	36/10532 (0.3%)	0.87	12/14219 (0.1%)
58	CE	0.48	0/401	0.75	0/540
59	CN	1.55	6/690 (0.9%)	1.17	4/1064 (0.4%)
60	CT	2.23	21/676 (3.1%)	1.25	9/1039 (0.9%)
61	CF	0.41	0/808	0.58	0/1088
All	All	0.78	170/186150 (0.1%)	0.93	275/275038 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	6
5	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	AM	0	1
25	BA	0	2
27	BC	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
57	CD	0	1
All	All	0	15

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	1	G	OP3-P	-10.82	1.48	1.61
23	AW	1	C	OP3-P	-10.78	1.48	1.61
24	AZ	1	G	OP3-P	-10.67	1.48	1.61
60	CT	14	DC	C3'-O3'	-9.25	1.31	1.44
60	CT	18	DC	C3'-O3'	-8.52	1.32	1.44
22	AV	51	G	C6-N1	-8.29	1.33	1.39
22	AV	50	C	N1-C6	-8.22	1.32	1.37
60	CT	12	DT	N1-C2	-8.08	1.31	1.38
56	CC	144	VAL	CB-CG1	-8.06	1.35	1.52
60	CT	16	DC	C3'-O3'	-7.99	1.33	1.44
22	AV	51	G	N3-C4	-7.98	1.29	1.35
57	CD	1357	ILE	C-N	-7.98	1.19	1.34
60	CT	15	DC	C3'-O3'	-7.84	1.33	1.44
56	CC	802	VAL	CB-CG1	-7.75	1.36	1.52
56	CC	146	VAL	CB-CG1	-7.74	1.36	1.52
56	CC	146	VAL	CB-CG2	-7.69	1.36	1.52
57	CD	457	TYR	CE2-CZ	-7.65	1.28	1.38
56	CC	655	VAL	CB-CG1	-7.51	1.37	1.52
57	CD	457	TYR	CD2-CE2	-7.45	1.28	1.39
60	CT	16	DC	N1-C6	-7.39	1.32	1.37
56	CC	558	VAL	CB-CG1	-7.35	1.37	1.52
59	CN	28	DA	N3-C4	-7.12	1.30	1.34
56	CC	591	TYR	CD2-CE2	-7.10	1.28	1.39
56	CC	663	VAL	CB-CG2	-7.07	1.38	1.52
60	CT	22	DC	N1-C6	-7.05	1.32	1.37
56	CC	591	TYR	CG-CD1	-7.03	1.30	1.39
57	CD	421	VAL	CB-CG2	-7.03	1.38	1.52
60	CT	18	DC	N1-C6	-6.94	1.32	1.37
59	CN	26	DG	C3'-O3'	-6.93	1.34	1.44
57	CD	457	TYR	CD1-CE1	-6.93	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	52	C	N1-C6	-6.87	1.33	1.37
60	CT	13	DT	N1-C2	-6.87	1.32	1.38
56	CC	818	VAL	CB-CG2	-6.84	1.38	1.52
56	CC	1239	VAL	CB-CG2	-6.80	1.38	1.52
57	CD	1145	PHE	CB-CG	-6.78	1.39	1.51
22	AV	51	G	N1-C2	-6.74	1.32	1.37
22	AV	53	G	N7-C5	-6.67	1.35	1.39
56	CC	136	PHE	CB-CG	-6.66	1.40	1.51
56	CC	708	VAL	CB-CG2	-6.65	1.38	1.52
22	AV	50	C	N3-C4	-6.64	1.29	1.33
57	CD	453	VAL	CB-CG1	-6.64	1.39	1.52
56	CC	1289	GLU	CB-CG	-6.63	1.39	1.52
59	CN	28	DA	C3'-O3'	-6.59	1.35	1.44
60	CT	16	DC	N1-C2	-6.58	1.33	1.40
56	CC	802	VAL	CB-CG2	-6.54	1.39	1.52
56	CC	578	TYR	CE2-CZ	-6.52	1.30	1.38
56	CC	663	VAL	CB-CG1	-6.47	1.39	1.52
56	CC	591	TYR	CD1-CE1	-6.47	1.29	1.39
56	CC	144	VAL	CB-CG2	-6.39	1.39	1.52
56	CC	708	VAL	CB-CG1	-6.39	1.39	1.52
56	CC	652	TYR	CD1-CE1	-6.37	1.29	1.39
60	CT	14	DC	N1-C6	-6.34	1.33	1.37
22	AV	51	G	C5-C4	-6.33	1.33	1.38
22	AV	50	C	N1-C2	-6.32	1.33	1.40
60	CT	13	DT	C4-C5	-6.30	1.39	1.45
56	CC	591	TYR	CE1-CZ	-6.29	1.30	1.38
56	CC	530	ILE	CB-CG2	-6.25	1.33	1.52
57	CD	801	VAL	CB-CG2	-6.24	1.39	1.52
57	CD	457	TYR	CE1-CZ	-6.22	1.30	1.38
22	AV	47	G	C6-N1	-6.20	1.35	1.39
56	CC	1149	TYR	CD2-CE2	-6.20	1.30	1.39
57	CD	1141	VAL	CB-CG1	-6.20	1.39	1.52
60	CT	19	DG	N7-C5	-6.20	1.35	1.39
56	CC	1094	VAL	CB-CG1	-6.19	1.39	1.52
22	AV	47	G	N7-C5	-6.15	1.35	1.39
56	CC	578	TYR	CD2-CE2	-6.14	1.30	1.39
56	CC	1251	TYR	CE2-CZ	-6.11	1.30	1.38
56	CC	591	TYR	CB-CG	-6.07	1.42	1.51
22	AV	51	G	N7-C5	-6.06	1.35	1.39
57	CD	801	VAL	CB-CG1	-6.03	1.40	1.52
56	CC	464	PHE	CB-CG	-6.02	1.41	1.51
57	CD	803	VAL	CB-CG1	-6.01	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CC	577	VAL	CB-CG1	-5.99	1.40	1.52
57	CD	772	TYR	CD2-CE2	-5.98	1.30	1.39
56	CC	1225	VAL	CB-CG2	-5.95	1.40	1.52
56	CC	519	ASN	CB-CG	-5.85	1.37	1.51
56	CC	727	VAL	CB-CG2	-5.83	1.40	1.52
56	CC	591	TYR	CE2-CZ	-5.83	1.30	1.38
56	CC	818	VAL	CB-CG1	-5.81	1.40	1.52
57	CD	1237	VAL	CB-CG2	-5.79	1.40	1.52
56	CC	822	VAL	CB-CG1	-5.78	1.40	1.52
57	CD	1241	TYR	CE1-CZ	-5.67	1.31	1.38
57	CD	421	VAL	CB-CG1	-5.66	1.41	1.52
56	CC	705	GLU	CG-CD	-5.64	1.43	1.51
56	CC	1251	TYR	CD2-CE2	-5.63	1.30	1.39
55	CA	54	CYS	CB-SG	-5.62	1.72	1.81
56	CC	816	ILE	CB-CG2	-5.62	1.35	1.52
56	CC	137	VAL	CB-CG2	-5.61	1.41	1.52
57	CD	424	ASN	CB-CG	-5.61	1.38	1.51
56	CC	1231	TYR	CE2-CZ	-5.61	1.31	1.38
57	CD	772	TYR	CD1-CE1	-5.59	1.30	1.39
55	CA	68	TYR	CD1-CE1	-5.58	1.30	1.39
57	CD	795	TYR	CE1-CZ	-5.58	1.31	1.38
57	CD	1145	PHE	CD2-CE2	-5.56	1.28	1.39
56	CC	1281	TYR	CE2-CZ	-5.55	1.31	1.38
57	CD	468	VAL	CB-CG2	-5.55	1.41	1.52
60	CT	12	DT	C4-C5	-5.52	1.40	1.45
59	CN	30	DA	N9-C8	-5.51	1.33	1.37
60	CT	17	DG	N3-C4	-5.51	1.31	1.35
22	AV	52	C	N1-C2	-5.50	1.34	1.40
57	CD	1145	PHE	CD1-CE1	-5.50	1.28	1.39
56	CC	652	TYR	CE1-CZ	-5.50	1.31	1.38
56	CC	823	VAL	CB-CG2	-5.46	1.41	1.52
56	CC	448	LEU	CA-C	-5.46	1.38	1.52
56	CC	1052	VAL	CB-CG1	-5.44	1.41	1.52
56	CC	578	TYR	CD1-CE1	-5.44	1.31	1.39
22	AV	51	G	C5-C6	-5.44	1.36	1.42
60	CT	23	DC	N1-C6	-5.41	1.33	1.37
55	CA	68	TYR	CE1-CZ	-5.41	1.31	1.38
57	CD	917	VAL	CB-CG1	-5.41	1.41	1.52
56	CC	1094	VAL	CB-CG2	-5.40	1.41	1.52
56	CC	751	TYR	CE1-CZ	-5.39	1.31	1.38
56	CC	1231	TYR	CD2-CE2	-5.39	1.31	1.39
56	CC	98	VAL	CB-CG2	-5.38	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CT	20	DC	N1-C6	-5.37	1.33	1.37
22	AV	53	G	C6-N1	-5.36	1.35	1.39
56	CC	1097	VAL	CB-CG1	-5.35	1.41	1.52
22	AV	51	G	C2-N3	-5.34	1.28	1.32
56	CC	661	VAL	CB-CG2	-5.34	1.41	1.52
56	CC	877	VAL	CB-CG2	-5.34	1.41	1.52
57	CD	354	VAL	CB-CG1	-5.33	1.41	1.52
57	CD	33	TRP	CB-CG	-5.32	1.40	1.50
22	AV	49	G	N3-C4	-5.31	1.31	1.35
56	CC	835	GLU	CB-CG	-5.31	1.42	1.52
56	CC	1281	TYR	CD2-CE2	-5.30	1.31	1.39
56	CC	660	VAL	CB-CG1	-5.29	1.41	1.52
57	CD	899	TYR	CE2-CZ	-5.29	1.31	1.38
57	CD	303	VAL	CB-CG2	-5.29	1.41	1.52
57	CD	347	VAL	CB-CG2	-5.29	1.41	1.52
60	CT	22	DC	N3-C4	-5.29	1.30	1.33
22	AV	50	C	C4-C5	-5.28	1.38	1.43
56	CC	1096	ILE	CB-CG2	-5.27	1.36	1.52
60	CT	15	DC	C4'-C3'	-5.25	1.47	1.52
57	CD	349	TYR	CE2-CZ	-5.24	1.31	1.38
22	AV	52	C	C4-C5	-5.21	1.38	1.43
56	CC	518	ASN	CB-CG	-5.18	1.39	1.51
56	CC	1149	TYR	CE2-CZ	-5.18	1.31	1.38
56	CC	782	VAL	CB-CG1	-5.18	1.42	1.52
56	CC	1239	VAL	CB-CG1	-5.18	1.42	1.52
56	CC	73	TYR	CE1-CZ	-5.17	1.31	1.38
59	CN	28	DA	C6-N1	-5.17	1.31	1.35
56	CC	799	ASN	CB-CG	-5.17	1.39	1.51
57	CD	795	TYR	CD2-CE2	-5.17	1.31	1.39
1	AA	846	G	N7-C5	-5.16	1.36	1.39
56	CC	578	TYR	CG-CD1	-5.15	1.32	1.39
22	AV	53	G	C5-C6	-5.15	1.37	1.42
56	CC	828	PHE	CE2-CZ	-5.14	1.27	1.37
57	CD	899	TYR	CE1-CZ	-5.13	1.31	1.38
56	CC	591	TYR	CG-CD2	-5.12	1.32	1.39
56	CC	616	ILE	CB-CG2	-5.12	1.36	1.52
55	CB	185	TYR	CB-CG	-5.11	1.44	1.51
56	CC	823	VAL	CB-CG1	-5.11	1.42	1.52
57	CD	382	TYR	CD2-CE2	-5.11	1.31	1.39
57	CD	1331	VAL	CB-CG2	-5.10	1.42	1.52
56	CC	395	TYR	CD2-CE2	-5.09	1.31	1.39
57	CD	899	TYR	CD2-CE2	-5.08	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CD	795	TYR	CD1-CE1	-5.08	1.31	1.39
56	CC	453	ILE	CB-CG2	-5.08	1.37	1.52
56	CC	733	VAL	CB-CG1	-5.08	1.42	1.52
56	CC	1149	TYR	CD1-CE1	-5.07	1.31	1.39
59	CN	29	DG	N7-C5	-5.07	1.36	1.39
57	CD	457	TYR	CG-CD1	-5.06	1.32	1.39
56	CC	1075	VAL	CB-CG2	-5.06	1.42	1.52
60	CT	11	DC	C3'-O3'	-5.05	1.37	1.44
56	CC	1275	VAL	CB-CG1	-5.05	1.42	1.52
60	CT	19	DG	C5-C4	-5.05	1.34	1.38
56	CC	1276	TRP	CB-CG	-5.04	1.41	1.50
56	CC	395	TYR	CD1-CE1	-5.03	1.31	1.39
56	CC	804	PHE	CD1-CE1	-5.01	1.29	1.39
56	CC	506	PHE	CG-CD1	-5.00	1.31	1.38

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1027	C	C6-N1-C2	-27.34	109.36	120.30
1	AA	1027	C	C2-N1-C1'	18.55	139.21	118.80
1	AA	1027	C	C5-C6-N1	16.26	129.13	121.00
1	AA	1027	C	C6-N1-C1'	-15.50	102.20	120.80
1	AA	206	C	C6-N1-C2	-14.18	114.63	120.30
1	AA	82	G	C8-N9-C4	-13.71	100.92	106.40
25	BA	1104	C	C6-N1-C2	-13.35	114.96	120.30
1	AA	206	C	C2-N1-C1'	11.56	131.52	118.80
1	AA	206	C	C5-C6-N1	10.29	126.14	121.00
25	BA	1077	A	O4'-C1'-N9	10.08	116.26	108.20
25	BA	2174	C	N1-C2-O2	9.52	124.61	118.90
60	CT	19	DG	O4'-C1'-N9	9.51	114.66	108.00
25	BA	1170	C	C2-N1-C1'	9.50	129.25	118.80
25	BA	1047	G	O4'-C1'-N9	9.43	115.75	108.20
29	BE	69	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	AA	846	G	C6-C5-N7	-9.06	124.97	130.40
25	BA	2122	U	O5'-P-OP2	-9.03	97.58	105.70
22	AV	52	C	C6-N1-C2	-8.76	116.80	120.30
22	AV	52	C	N1-C2-O2	-8.72	113.67	118.90
25	BA	1104	C	C2-N1-C1'	8.69	128.35	118.80
25	BA	1728	C	C2-N1-C1'	-8.68	109.25	118.80
1	AA	206	C	C6-N1-C1'	-8.36	110.77	120.80
25	BA	652	U	O4'-C1'-N1	-8.09	101.73	108.20
1	AA	82	G	N7-C8-N9	8.05	117.13	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2178	C	C2-N1-C1'	-8.03	109.96	118.80
25	BA	1170	C	C6-N1-C1'	-7.90	111.32	120.80
1	AA	1009	U	N3-C2-O2	-7.88	116.68	122.20
22	AV	49	G	O3'-P-O5'	-7.79	89.19	104.00
55	CB	48	LEU	CA-CB-CG	7.61	132.81	115.30
1	AA	1034	G	C8-N9-C1'	-7.60	117.13	127.00
25	BA	1104	C	C5-C6-N1	7.58	124.79	121.00
1	AA	884	U	C6-N1-C2	-7.54	116.47	121.00
1	AA	1008	U	O4'-C1'-N1	7.53	114.23	108.20
22	AV	53	G	C8-N9-C4	-7.50	103.40	106.40
25	BA	893	C	N1-C2-O2	-7.50	114.40	118.90
1	AA	1034	G	C8-N9-C4	-7.48	103.41	106.40
56	CC	1238	LEU	CB-CG-CD1	-7.47	98.30	111.00
56	CC	571	LEU	CB-CG-CD2	-7.44	98.36	111.00
25	BA	1170	C	C5-C6-N1	7.41	124.71	121.00
25	BA	2164	C	C6-N1-C2	-7.36	117.36	120.30
25	BA	2174	C	N3-C2-O2	-7.35	116.76	121.90
25	BA	1104	C	C6-N1-C1'	-7.32	112.01	120.80
18	AR	55	LEU	CA-CB-CG	7.31	132.11	115.30
1	AA	1026	G	P-O3'-C3'	7.30	128.46	119.70
56	CC	149	LEU	CB-CG-CD1	-7.29	98.60	111.00
60	CT	17	DG	O4'-C1'-N9	7.24	113.07	108.00
25	BA	2124	G	N1-C6-O6	-7.22	115.57	119.90
25	BA	2120	G	C8-N9-C4	-7.19	103.52	106.40
1	AA	60	A	C8-N9-C4	-7.17	102.93	105.80
1	AA	999	C	C6-N1-C2	-7.12	117.45	120.30
25	BA	2164	C	N1-C2-O2	7.11	123.17	118.90
1	AA	1027	C	N3-C4-C5	-7.08	119.07	121.90
25	BA	1728	C	C6-N1-C1'	6.99	129.19	120.80
25	BA	1857	G	O4'-C1'-N9	6.98	113.78	108.20
25	BA	1406	U	C5-C6-N1	6.97	126.18	122.70
25	BA	1869	G	C8-N9-C4	-6.96	103.62	106.40
22	AV	44	A	C8-N9-C4	6.92	108.57	105.80
25	BA	613	A	P-O3'-C3'	-6.90	111.42	119.70
32	BH	13	GLY	N-CA-C	6.88	130.30	113.10
22	AV	50	C	N1-C2-O2	-6.88	114.78	118.90
1	AA	846	G	N3-C4-N9	6.83	130.10	126.00
25	BA	138	U	N1-C1'-C2'	-6.79	104.53	112.00
1	AA	431	A	O4'-C1'-N9	6.77	113.61	108.20
1	AA	812	G	O4'-C1'-N9	6.74	113.59	108.20
1	AA	846	G	C4-N9-C1'	6.74	135.25	126.50
25	BA	783	A	C2-N3-C4	6.67	113.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2808	G	O4'-C1'-N9	6.66	113.53	108.20
22	AV	51	G	N1-C2-N3	6.64	127.88	123.90
1	AA	1009	U	N1-C2-O2	6.62	127.44	122.80
25	BA	1728	C	O4'-C1'-N1	6.61	113.48	108.20
25	BA	887	U	OP2-P-O3'	6.59	119.71	105.20
22	AV	53	G	C6-C5-N7	-6.59	126.44	130.40
25	BA	2124	G	O4'-C1'-N9	6.59	113.47	108.20
25	BA	2125	G	N9-C1'-C2'	6.58	122.55	114.00
25	BA	1266	G	O4'-C1'-N9	6.58	113.46	108.20
1	AA	846	G	C8-N9-C1'	-6.56	118.47	127.00
25	BA	2100	G	C4-N9-C1'	6.55	135.02	126.50
25	BA	2175	C	C2-N1-C1'	-6.54	111.60	118.80
25	BA	2121	G	P-O3'-C3'	6.54	127.55	119.70
25	BA	2902	C	N1-C2-O2	6.51	122.80	118.90
25	BA	1870	C	O5'-P-OP2	6.50	118.50	110.70
25	BA	2124	G	C5-C6-O6	6.47	132.48	128.60
1	AA	82	G	N3-C4-C5	-6.46	125.37	128.60
25	BA	1581	G	C8-N9-C1'	-6.46	118.60	127.00
25	BA	1871	A	P-O3'-C3'	6.45	127.44	119.70
25	BA	138	U	O4'-C1'-N1	6.42	113.33	108.20
56	CC	794	LEU	CB-CG-CD1	-6.42	100.09	111.00
1	AA	1001	C	O4'-C1'-N1	6.42	113.33	108.20
25	BA	2162	G	O5'-P-OP1	6.39	118.37	110.70
56	CC	575	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	AA	846	G	N1-C6-O6	6.38	123.73	119.90
1	AA	846	G	N9-C4-C5	-6.38	102.85	105.40
1	AA	883	C	C6-N1-C2	-6.35	117.76	120.30
25	BA	2120	G	N7-C8-N9	6.34	116.27	113.10
56	CC	213	LEU	CA-CB-CG	-6.34	100.72	115.30
1	AA	108	G	O4'-C1'-N9	-6.32	103.14	108.20
25	BA	2103	C	C2-N1-C1'	-6.32	111.84	118.80
25	BA	370	G	O4'-C1'-N9	-6.32	103.14	108.20
25	BA	2175	C	O4'-C1'-N1	6.30	113.24	108.20
22	AV	51	G	C2-N3-C4	-6.30	108.75	111.90
25	BA	729	G	O4'-C1'-N9	6.28	113.23	108.20
22	AV	44	A	O4'-C1'-N9	6.28	113.22	108.20
1	AA	840	C	C6-N1-C2	6.25	122.80	120.30
22	AV	53	G	N7-C8-N9	6.22	116.21	113.10
56	CC	210	LEU	CA-CB-CG	-6.16	101.13	115.30
1	AA	1330	U	O4'-C1'-N1	6.16	113.13	108.20
25	BA	2168	G	P-O3'-C3'	6.15	127.08	119.70
25	BA	2164	C	C5-C6-N1	6.13	124.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	452	A	O4'-C1'-N9	6.13	113.10	108.20
25	BA	2100	G	C8-N9-C1'	-6.13	119.03	127.00
22	AV	49	G	O5'-P-OP1	-6.11	100.20	105.70
25	BA	2175	C	C6-N1-C1'	6.11	128.13	120.80
22	AV	38	A	P-O3'-C3'	6.10	127.02	119.70
25	BA	2164	C	N3-C2-O2	-6.09	117.64	121.90
1	AA	347	G	N9-C4-C5	-6.08	102.97	105.40
60	CT	16	DC	O4'-C1'-N1	6.08	112.26	108.00
1	AA	5	U	O5'-P-OP1	6.05	117.95	110.70
25	BA	2178	C	C6-N1-C1'	6.05	128.06	120.80
57	CD	307	LEU	CA-CB-CG	-6.03	101.42	115.30
1	AA	347	G	C4-C5-N7	6.01	113.20	110.80
25	BA	2164	C	C2-N1-C1'	6.01	125.41	118.80
25	BA	2573	C	N1-C1'-C2'	-6.00	105.40	112.00
25	BA	2286	G	O4'-C1'-N9	5.97	112.98	108.20
56	CC	1278	LEU	CB-CG-CD2	-5.97	100.85	111.00
25	BA	1068	G	O4'-C1'-N9	5.96	112.97	108.20
25	BA	789	A	C5'-C4'-C3'	-5.95	106.47	116.00
7	AG	55	GLY	N-CA-C	5.95	127.97	113.10
56	CC	1287	LEU	CB-CG-CD1	-5.95	100.89	111.00
25	BA	893	C	O4'-C1'-N1	5.95	112.96	108.20
1	AA	1025	U	P-O3'-C3'	-5.95	112.56	119.70
57	CD	449	LEU	CB-CG-CD1	-5.94	100.90	111.00
25	BA	2391	G	O4'-C1'-N9	5.93	112.94	108.20
25	BA	1494	A	P-O3'-C3'	5.93	126.81	119.70
24	AZ	42	C	C2-N1-C1'	5.92	125.31	118.80
25	BA	885	C	O4'-C1'-N1	5.89	112.91	108.20
25	BA	2146	C	P-O3'-C3'	5.88	126.76	119.70
56	CC	817	LEU	CB-CG-CD1	-5.87	101.02	111.00
1	AA	431	A	N1-C6-N6	-5.86	115.08	118.60
1	AA	347	G	C6-C5-N7	-5.86	126.88	130.40
59	CN	25	DG	C1'-O4'-C4'	-5.85	104.25	110.10
25	BA	1581	G	C4-N9-C1'	5.83	134.09	126.50
25	BA	2901	C	N1-C2-O2	5.83	122.40	118.90
1	AA	840	C	P-O3'-C3'	5.82	126.69	119.70
25	BA	2065	C	C6-N1-C2	-5.82	117.97	120.30
56	CC	184	LEU	CB-CG-CD1	-5.81	101.12	111.00
25	BA	2064	C	C6-N1-C2	-5.81	117.97	120.30
57	CD	363	LEU	CB-CG-CD1	-5.79	101.15	111.00
25	BA	27	G	O4'-C1'-N9	5.78	112.83	108.20
1	AA	530	G	C4-N9-C1'	-5.78	118.98	126.50
25	BA	1452	G	O4'-C1'-N9	5.78	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	53	G	C5-N7-C8	-5.76	101.42	104.30
1	AA	846	G	C4-C5-N7	5.76	113.11	110.80
1	AA	1034	G	C4-N9-C1'	5.75	133.97	126.50
56	CC	1141	LEU	CB-CG-CD1	-5.74	101.25	111.00
25	BA	1936	A	O4'-C1'-N9	-5.73	103.62	108.20
25	BA	1565	C	O4'-C1'-N1	5.71	112.77	108.20
1	AA	878	A	C8-N9-C1'	-5.71	117.42	127.70
25	BA	884	U	N1-C1'-C2'	-5.71	105.72	112.00
25	BA	1349	C	C6-N1-C2	-5.71	118.02	120.30
56	CC	511	LEU	CB-CG-CD1	-5.71	101.30	111.00
1	AA	1494	G	P-O5'-C5'	-5.70	111.78	120.90
56	CC	529	ARG	CA-CB-CG	5.69	125.92	113.40
60	CT	18	DC	O5'-P-OP1	-5.68	100.58	105.70
1	AA	1008	U	C2-N1-C1'	-5.68	110.89	117.70
1	AA	1299	A	O4'-C1'-N9	-5.66	103.67	108.20
25	BA	2138	G	N3-C4-N9	-5.66	122.60	126.00
29	BE	69	ARG	NE-CZ-NH2	-5.66	117.47	120.30
25	BA	894	U	O4'-C1'-N1	5.65	112.72	108.20
57	CD	1332	LEU	CB-CG-CD2	-5.65	101.39	111.00
25	BA	12	U	N3-C2-O2	-5.63	118.26	122.20
25	BA	222	A	O4'-C1'-N9	-5.63	103.69	108.20
57	CD	1144	LEU	CB-CG-CD1	-5.62	101.44	111.00
25	BA	2902	C	N3-C2-O2	-5.62	117.97	121.90
25	BA	2103	C	C6-N1-C1'	5.60	127.53	120.80
25	BA	2159	G	P-O5'-C5'	-5.60	111.94	120.90
1	AA	347	G	N1-C6-O6	5.60	123.26	119.90
1	AA	206	C	O4'-C1'-N1	-5.59	103.73	108.20
57	CD	478	LEU	CA-CB-CG	-5.59	102.44	115.30
45	BW	66	ASP	CB-CG-OD1	5.57	123.31	118.30
1	AA	1494	G	O4'-C1'-N9	-5.55	103.76	108.20
25	BA	828	U	O4'-C1'-N1	-5.55	103.76	108.20
26	BB	17	C	O4'-C1'-N1	5.54	112.63	108.20
25	BA	2103	C	N1-C2-O2	-5.53	115.58	118.90
25	BA	1728	C	N1-C2-O2	-5.49	115.60	118.90
22	AV	47	G	C4-N9-C1'	5.49	133.63	126.50
1	AA	121	U	C5'-C4'-O4'	-5.48	102.52	109.10
1	AA	478	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	1491	G	O3'-P-O5'	5.47	114.39	104.00
22	AV	47	G	C6-C5-N7	-5.46	127.12	130.40
25	BA	1313	U	C2-N1-C1'	5.46	124.25	117.70
25	BA	894	U	C5'-C4'-O4'	5.45	115.64	109.10
1	AA	999	C	C2-N1-C1'	5.44	124.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1774	C	N3-C2-O2	-5.44	118.09	121.90
1	AA	1027	C	N3-C2-O2	-5.44	118.09	121.90
22	AV	53	G	C4-C5-N7	5.43	112.97	110.80
22	AV	52	C	N1-C2-N3	5.41	122.99	119.20
25	BA	613	A	C8-N9-C4	-5.41	103.64	105.80
22	AV	48	C	C6-N1-C2	-5.41	118.14	120.30
25	BA	892	A	O4'-C1'-N9	5.41	112.53	108.20
59	CN	21	DC	O4'-C1'-N1	5.41	111.78	108.00
1	AA	5	U	O5'-C5'-C4'	5.40	121.96	111.70
60	CT	12	DT	N3-C4-O4	5.40	123.14	119.90
59	CN	25	DG	O4'-C1'-N9	5.39	111.77	108.00
24	AX	49	C	C2-N1-C1'	5.38	124.72	118.80
25	BA	1775	U	C5-C4-O4	-5.38	122.67	125.90
1	AA	204	G	C8-N9-C1'	-5.38	120.01	127.00
1	AA	5	U	P-O5'-C5'	5.37	129.50	120.90
25	BA	2103	C	O4'-C1'-N1	5.37	112.50	108.20
25	BA	2901	C	C2-N1-C1'	5.37	124.71	118.80
25	BA	136	G	C8-N9-C1'	-5.37	120.03	127.00
57	CD	139	LEU	CA-CB-CG	-5.37	102.96	115.30
1	AA	612	C	C6-N1-C2	-5.36	118.16	120.30
56	CC	28	LEU	CA-CB-CG	-5.36	102.98	115.30
1	AA	883	C	N3-C2-O2	-5.35	118.16	121.90
57	CD	327	LEU	CB-CG-CD2	-5.33	101.93	111.00
25	BA	2120	G	O4'-C1'-N9	-5.33	103.94	108.20
1	AA	251	G	O4'-C1'-N9	-5.33	103.94	108.20
7	AG	54	SER	C-N-CA	-5.32	111.13	122.30
57	CD	605	LEU	CB-CG-CD2	-5.32	101.96	111.00
60	CT	18	DC	O4'-C1'-N1	5.32	111.72	108.00
1	AA	843	U	P-O3'-C3'	5.30	126.06	119.70
13	AM	54	ASP	CB-CG-OD1	5.30	123.07	118.30
22	AV	46	G	C5-C6-N1	5.30	114.15	111.50
1	AA	611	C	C6-N1-C2	-5.30	118.18	120.30
60	CT	20	DC	O4'-C1'-N1	5.29	111.70	108.00
57	CD	788	LEU	CB-CG-CD1	-5.28	102.03	111.00
25	BA	2158	A	O4'-C1'-N9	-5.27	103.98	108.20
56	CC	1076	ILE	CG1-CB-CG2	-5.27	99.81	111.40
25	BA	2120	G	C4-N9-C1'	5.26	133.34	126.50
25	BA	2101	A	N1-C6-N6	5.26	121.76	118.60
60	CT	13	DT	N3-C4-O4	5.26	123.05	119.90
25	BA	1869	G	N3-C4-N9	-5.25	122.85	126.00
1	AA	611	C	C6-N1-C1'	-5.23	114.53	120.80
1	AA	1227	A	O4'-C1'-N9	-5.23	104.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	CB	47	LEU	CA-CB-CG	-5.23	103.27	115.30
22	AV	53	G	C4-N9-C1'	5.22	133.29	126.50
57	CD	307	LEU	CB-CG-CD2	-5.22	102.12	111.00
56	CC	1233	LEU	CA-CB-CG	5.21	127.28	115.30
1	AA	846	G	C4-C5-C6	5.19	121.92	118.80
60	CT	8	DT	N3-C4-O4	5.19	123.02	119.90
1	AA	74	A	P-O3'-C3'	5.19	125.93	119.70
25	BA	783	A	N1-C6-N6	-5.18	115.49	118.60
1	AA	1066	C	C6-N1-C2	-5.18	118.23	120.30
25	BA	2573	C	C2-N1-C1'	5.18	124.49	118.80
1	AA	999	C	C6-N1-C1'	-5.16	114.61	120.80
25	BA	2162	G	OP1-P-O3'	5.16	116.56	105.20
25	BA	2120	G	C5'-C4'-O4'	-5.16	102.91	109.10
56	CC	1291	LEU	CA-CB-CG	5.14	127.13	115.30
27	BC	241	GLY	N-CA-C	5.13	125.94	113.10
22	AV	51	G	O4'-C1'-N9	5.13	112.30	108.20
25	BA	2185	U	O4'-C1'-N1	5.12	112.30	108.20
25	BA	2159	G	N3-C4-N9	-5.12	122.93	126.00
22	AV	45	C	O5'-P-OP2	-5.11	101.10	105.70
25	BA	274	C	N3-C2-O2	-5.11	118.33	121.90
25	BA	2178	C	N3-C4-N4	-5.10	114.43	118.00
25	BA	2178	C	O4'-C1'-N1	5.10	112.28	108.20
25	BA	887	U	P-O3'-C3'	5.09	125.81	119.70
55	CB	102	LEU	CA-CB-CG	5.09	127.00	115.30
1	AA	1025	U	O4'-C1'-N1	-5.09	104.13	108.20
25	BA	2101	A	N9-C4-C5	-5.08	103.77	105.80
25	BA	2145	C	P-O3'-C3'	-5.08	113.60	119.70
55	CB	228	LEU	CA-CB-CG	-5.07	103.64	115.30
1	AA	878	A	C8-N9-C4	-5.07	103.77	105.80
56	CC	1204	LEU	CA-CB-CG	-5.06	103.66	115.30
25	BA	404	A	P-O3'-C3'	5.05	125.76	119.70
56	CC	1291	LEU	CB-CG-CD2	-5.05	102.41	111.00
25	BA	613	A	C3'-C2'-C1'	-5.05	97.46	101.50
25	BA	2164	C	O4'-C1'-N1	-5.04	104.17	108.20
59	CN	26	DG	O4'-C4'-C3'	-5.04	102.48	104.50
25	BA	2123	G	C5-C6-O6	5.04	131.62	128.60
57	CD	1332	LEU	CB-CG-CD1	-5.02	102.47	111.00
56	CC	521	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	AA	439	U	N1-C2-O2	5.01	126.31	122.80
25	BA	2061	G	O4'-C1'-N9	5.01	112.21	108.20
56	CC	1333	LEU	CB-CG-CD2	-5.00	102.50	111.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1027	C	Sidechain
1	AA	1034	G	Sidechain
1	AA	60	A	Sidechain
1	AA	81	A	Sidechain
1	AA	82	G	Sidechain
1	AA	884	U	Sidechain
5	AE	89	HIS	Peptide
13	AM	65	VAL	Peptide
53	B5	31	HIS	Peptide
25	BA	1104	C	Sidechain
25	BA	1869	G	Sidechain
27	BC	176	LEU	Mainchain
37	BO	100	CYS	Mainchain
46	BX	54	GLY	Mainchain
57	CD	764	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32909	0	16575	402	0
2	AB	1765	0	1792	32	0
3	AC	1640	0	1713	48	0
4	AD	1643	0	1707	31	0
5	AE	1148	0	1195	20	0
6	AF	848	0	846	35	0
7	AG	1214	0	1267	20	0
8	AH	979	0	1031	18	0
9	AI	1031	0	1076	23	0
10	AJ	800	0	839	25	0
11	AK	877	0	887	20	0
12	AL	951	0	1012	26	0
13	AM	891	0	952	27	0
14	AN	805	0	844	15	0
15	AO	714	0	734	17	0
16	AP	649	0	666	8	0
17	AQ	648	0	691	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	AR	474	0	494	16	0
19	AS	663	0	688	20	0
20	AT	670	0	719	11	0
21	AU	590	0	629	6	0
22	AV	656	0	336	24	0
23	AW	1645	0	842	24	0
24	AX	1630	0	838	35	0
24	AZ	1630	0	839	64	0
25	BA	62248	0	31319	678	0
26	BB	2569	0	1300	32	0
27	BC	2092	0	2167	27	0
28	BD	1566	0	1618	28	0
29	BE	1552	0	1618	30	0
30	BF	1420	0	1457	53	0
31	BG	1313	0	1358	24	0
32	BH	1111	0	1148	29	0
33	BK	1129	0	1162	13	0
34	BL	947	0	1023	10	0
35	BM	1052	0	1127	20	0
36	BN	1075	0	1155	17	0
37	BO	960	0	1000	18	0
38	BP	900	0	935	23	0
39	BQ	917	0	962	14	0
40	BR	947	0	1018	18	0
41	BS	816	0	839	18	0
42	BT	857	0	922	14	0
43	BU	764	0	829	15	0
44	BV	789	0	844	17	0
45	BW	753	0	780	12	0
46	BX	582	0	598	6	0
47	BY	625	0	652	17	0
48	BZ	501	0	531	12	0
49	B1	449	0	488	6	0
50	B2	444	0	458	13	0
51	B3	436	0	477	5	0
52	B4	376	0	414	5	0
53	B5	504	0	572	9	0
54	B6	301	0	343	5	0
55	CA	1775	0	1800	17	0
55	CB	1684	0	1713	15	0
56	CC	10415	0	10432	154	0
57	CD	10375	0	10597	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CE	399	0	417	4	0
59	CN	615	0	335	40	0
60	CT	606	0	338	43	0
61	CF	790	0	782	51	0
62	AA	139	0	0	1	0
62	AL	3	0	0	0	0
62	AT	1	0	0	0	0
62	AV	1	0	0	0	0
62	AW	4	0	0	0	0
62	AX	1	0	0	0	0
62	B2	1	0	0	0	0
62	B5	1	0	0	0	0
62	B6	1	0	0	0	0
62	BA	318	0	0	0	0
62	BB	9	0	0	0	0
62	BC	3	0	0	0	0
62	BD	1	0	0	0	0
62	BN	1	0	0	0	0
62	BR	1	0	0	0	0
62	BX	1	0	0	0	0
62	CD	1	0	0	0	0
63	AX	11	0	8	0	0
64	CD	2	0	0	0	0
All	All	174624	0	124748	2410	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 8.

All (2410) 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)
59:CN:18:DG:H3'	61:CF:90:MET:CB	1.24	1.46
59:CN:18:DG:C3'	61:CF:90:MET:HB3	0.99	1.41
3:AC:77:ILE:CD1	57:CD:79:LYS:HG3	1.55	1.36
25:BA:1869:G:N2	25:BA:1872:A:C5	2.05	1.25
57:CD:1100:PHE:CD2	57:CD:1200:GLU:HB3	1.71	1.24
30:BF:48:LYS:O	30:BF:52:ASN:N	1.73	1.21
61:CF:47:GLU:HG3	61:CF:64:PHE:HE1	1.01	1.17
61:CF:47:GLU:HG3	61:CF:64:PHE:CE1	1.80	1.15
59:CN:18:DG:C2'	61:CF:90:MET:HB3	1.77	1.14
59:CN:18:DG:C3'	61:CF:90:MET:CB	1.96	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CD:1072:LYS:O	57:CD:1168:GLU:HG3	1.46	1.12
57:CD:1072:LYS:HG2	57:CD:1168:GLU:HB3	1.13	1.12
60:CT:28:DG:H5''	61:CF:18:PHE:CZ	1.87	1.08
60:CT:28:DG:H5''	61:CF:18:PHE:HZ	1.18	1.06
25:BA:1869:G:C2	25:BA:1872:A:C5	2.45	1.05
32:BH:47:PHE:HA	32:BH:51:ARG:HB2	1.42	1.01
3:AC:77:ILE:HD11	57:CD:79:LYS:HG3	1.42	1.01
3:AC:103:ILE:HB	57:CD:79:LYS:NZ	1.77	0.99
3:AC:80:LYS:HD3	57:CD:81:ARG:NH1	1.78	0.99
57:CD:290:ILE:CG2	61:CF:94:GLY:HA2	1.94	0.98
59:CN:18:DG:H3'	61:CF:90:MET:CG	1.92	0.98
61:CF:47:GLU:CG	61:CF:64:PHE:HE1	1.76	0.97
25:BA:2099:U:H3	25:BA:2190:G:H1	1.00	0.97
25:BA:1827:U:OP2	27:BC:221:ARG:NH1	1.96	0.96
3:AC:103:ILE:HB	57:CD:79:LYS:CE	1.95	0.96
25:BA:1869:G:N3	25:BA:1872:A:C6	2.34	0.95
1:AA:1124:G:H5''	10:AJ:37:ARG:HH12	1.32	0.94
57:CD:1072:LYS:HG2	57:CD:1168:GLU:CB	1.95	0.94
1:AA:1307:U:H3	1:AA:1330:U:H3	0.98	0.94
1:AA:458:U:H3	1:AA:474:G:H1	1.13	0.94
57:CD:290:ILE:HG21	61:CF:94:GLY:HA2	1.46	0.94
1:AA:1009:U:H3	1:AA:1020:G:H1	1.08	0.93
57:CD:1072:LYS:NZ	57:CD:1169:THR:O	2.01	0.92
25:BA:1869:G:N2	25:BA:1872:A:N7	2.18	0.92
25:BA:1869:G:N2	25:BA:1872:A:C4	2.38	0.91
25:BA:2107:G:H1	25:BA:2182:U:H3	1.15	0.90
59:CN:19:DA:N1	61:CF:86:VAL:N	2.00	0.90
57:CD:1100:PHE:CD2	57:CD:1200:GLU:CB	2.54	0.90
3:AC:103:ILE:CG2	57:CD:79:LYS:HE3	2.01	0.89
12:AL:12:ARG:HB3	12:AL:12:ARG:HH11	1.38	0.89
57:CD:1072:LYS:HD3	57:CD:1169:THR:O	1.71	0.89
56:CC:481:LEU:HD11	61:CF:87:PRO:HG3	1.54	0.89
59:CN:18:DG:C2'	61:CF:90:MET:CB	2.41	0.88
3:AC:77:ILE:CD1	57:CD:79:LYS:CG	2.48	0.88
1:AA:1239:A:H62	1:AA:1299:A:H62	1.18	0.88
57:CD:1072:LYS:CG	57:CD:1168:GLU:HB3	2.01	0.87
3:AC:77:ILE:HD13	57:CD:79:LYS:HG3	1.56	0.86
60:CT:28:DG:C5'	61:CF:18:PHE:HZ	1.88	0.86
25:BA:2100:G:H1	25:BA:2189:U:H3	0.87	0.86
25:BA:284:U:H3	25:BA:356:G:H1	1.06	0.86
25:BA:2125:G:O2'	25:BA:2173:A:N6	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:284:U:O2	25:BA:356:G:N2	2.08	0.86
57:CD:1179:PRO:HD2	57:CD:1184:ASP:HA	1.57	0.86
57:CD:826:ILE:HG22	57:CD:994:SER:CB	2.05	0.86
6:AF:45:ARG:O	6:AF:56:LYS:HA	1.77	0.84
25:BA:240:C:O2	25:BA:257:C:N4	2.09	0.84
25:BA:1869:G:C2	25:BA:1872:A:N7	2.44	0.84
25:BA:1936:A:H2	25:BA:1943:U:H3	1.26	0.84
25:BA:1216:G:OP1	40:BR:11:ARG:NH1	2.11	0.83
56:CC:481:LEU:HD21	61:CF:87:PRO:CG	2.07	0.83
25:BA:1869:G:N2	25:BA:1872:A:C8	2.45	0.83
25:BA:1869:G:C4	25:BA:1872:A:N6	2.47	0.83
56:CC:477:GLU:OE1	61:CF:87:PRO:HB2	1.77	0.83
24:AZ:22:G:O6	24:AZ:46:7MG:N2	2.11	0.83
25:BA:881:G:H1	25:BA:895:U:H3	0.87	0.83
30:BF:49:LEU:O	30:BF:53:ALA:N	2.11	0.82
25:BA:1869:G:N3	25:BA:1872:A:N6	2.27	0.82
25:BA:1871:A:O2'	25:BA:1872:A:O4'	1.95	0.82
1:AA:201:G:H1	1:AA:216:U:H3	1.25	0.82
50:B2:30:VAL:HG22	50:B2:37:LYS:HG2	1.61	0.82
23:AW:50:U:H3	23:AW:64:G:H1	1.25	0.81
25:BA:2250:G:OP1	36:BN:84:LYS:NZ	2.12	0.81
1:AA:73:C:N4	1:AA:94:G:O6	2.14	0.81
25:BA:2308:G:O6	25:BA:2311:A:N7	2.13	0.81
29:BE:5:LEU:O	29:BE:9:GLN:HA	1.80	0.81
1:AA:1006:G:H2'	1:AA:1007:U:H6	1.46	0.81
6:AF:3:HIS:HB2	6:AF:92:THR:O	1.80	0.80
25:BA:2227:A:H5''	27:BC:261:LYS:HE2	1.63	0.80
55:CB:74:VAL:HG21	55:CB:81:ILE:HD11	1.62	0.80
25:BA:2880:C:O2'	37:BO:90:ARG:NH1	2.14	0.80
25:BA:475:C:O2	25:BA:479:A:N6	2.15	0.80
25:BA:1869:G:C2	25:BA:1872:A:C6	2.69	0.80
25:BA:1407:G:H2'	25:BA:1408:G:H8	1.47	0.80
3:AC:77:ILE:HD12	57:CD:79:LYS:HG3	1.61	0.79
44:BV:86:ARG:NH1	44:BV:100:SER:OG	2.14	0.79
47:BY:43:GLU:OE1	47:BY:45:ARG:NH1	2.16	0.79
56:CC:481:LEU:HD21	61:CF:87:PRO:HG3	1.63	0.79
59:CN:18:DG:H2'	61:CF:90:MET:CB	2.12	0.79
11:AK:88:GLY:O	11:AK:93:ARG:NH1	2.15	0.79
28:BD:8:LYS:O	28:BD:198:GLY:N	2.15	0.79
25:BA:1998:A:OP2	28:BD:141:ARG:NH2	2.16	0.78
25:BA:568:U:H1'	25:BA:2030:6MZ:H9C1	1.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BK:40:HIS:O	40:BR:71:GLN:NE2	2.17	0.78
13:AM:107:ARG:NH1	13:AM:111:GLY:O	2.17	0.78
1:AA:263:A:OP1	20:AT:74:ARG:NH1	2.16	0.78
34:BL:36:GLY:N	34:BL:62:VAL:O	2.16	0.77
30:BF:8:TYR:OH	30:BF:29:PRO:O	2.03	0.77
25:BA:2139:U:O2	25:BA:2152:G:O6	2.03	0.77
25:BA:2467:C:O2	36:BN:123:LYS:NZ	2.18	0.77
56:CC:18:ARG:NH1	56:CC:1188:ASP:OD1	2.18	0.77
7:AG:57:SER:HB3	7:AG:60:GLU:HG2	1.67	0.77
3:AC:71:ALA:HA	3:AC:106:VAL:HB	1.67	0.76
25:BA:1918:A:O2'	25:BA:1919:A:N7	2.17	0.76
57:CD:826:ILE:CG2	57:CD:994:SER:HB2	2.15	0.76
3:AC:103:ILE:HB	57:CD:79:LYS:HZ3	1.47	0.76
25:BA:575:A:OP2	25:BA:2055:C:N4	2.18	0.76
8:AH:77:ARG:HD2	8:AH:79:SER:O	1.84	0.76
57:CD:826:ILE:HG22	57:CD:994:SER:HB3	1.67	0.76
1:AA:1261:A:N6	1:AA:1274:A:O2'	2.19	0.76
24:AZ:18:G:O2'	24:AZ:57:G:N2	2.16	0.76
25:BA:2200:C:OP2	47:BY:37:ARG:NH2	2.19	0.76
25:BA:1594:U:H2'	25:BA:1595:C:C6	2.22	0.75
25:BA:883:G:N2	25:BA:884:U:O4	2.18	0.75
30:BF:50:LEU:O	30:BF:54:ALA:N	2.19	0.75
57:CD:1100:PHE:CE2	57:CD:1200:GLU:HG3	2.21	0.75
1:AA:346:G:OP1	39:BQ:39:ARG:NH1	2.19	0.75
59:CN:18:DG:O6	61:CF:14:ALA:O	2.05	0.75
60:CT:18:DC:H2'	60:CT:19:DG:C8	2.21	0.75
1:AA:522:C:O2	1:AA:527:G7M:N2	2.19	0.75
25:BA:1494:A:O2'	25:BA:1495:A:OP1	2.05	0.75
25:BA:2901:C:H2'	25:BA:2902:C:C6	2.21	0.75
1:AA:481:G:O2'	1:AA:483:C:N4	2.19	0.75
57:CD:1072:LYS:CD	57:CD:1169:THR:O	2.34	0.75
1:AA:90:C:H2'	1:AA:91:U:H6	1.51	0.74
3:AC:77:ILE:HD11	57:CD:79:LYS:CG	2.13	0.74
1:AA:1397:C:O2	22:AV:23:C:N4	2.19	0.74
25:BA:1590:A:H2'	25:BA:1591:A:C8	2.22	0.74
44:BV:96:PHE:O	44:BV:100:SER:HA	1.86	0.74
1:AA:198:G:H2'	1:AA:199:A:H8	1.52	0.74
1:AA:664:G:H22	1:AA:741:G:H1	1.33	0.74
10:AJ:24:GLU:HG3	10:AJ:90:LEU:HD21	1.68	0.74
6:AF:38:ARG:NH1	6:AF:98:GLU:O	2.20	0.74
13:AM:54:ASP:OD1	13:AM:55:THR:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:51:G:H2'	22:AV:52:C:H6	1.51	0.73
7:AG:143:ARG:NH1	24:AZ:42:C:O5'	2.22	0.73
11:AK:36:ASP:OD1	11:AK:37:ARG:N	2.22	0.73
31:BG:164:TYR:HB2	31:BG:167:GLU:HB3	1.70	0.73
25:BA:783:A:H2'	25:BA:783:A:N3	2.02	0.73
31:BG:16:ASP:N	31:BG:16:ASP:OD1	2.21	0.73
10:AJ:44:THR:HA	10:AJ:69:THR:O	1.89	0.73
44:BV:28:VAL:HG22	44:BV:34:VAL:HG12	1.71	0.73
59:CN:18:DG:H2'	61:CF:90:MET:HB2	1.71	0.73
4:AD:64:ILE:O	4:AD:111:ARG:NH1	2.21	0.73
10:AJ:10:LEU:HB3	10:AJ:18:ILE:HD11	1.71	0.73
25:BA:1063:G:O2'	25:BA:1064:C:O4'	2.07	0.73
25:BA:1406:U:C2'	25:BA:1407:G:H5''	2.19	0.73
25:BA:1916:A:H2'	25:BA:1917:PSU:C6	2.24	0.73
7:AG:79:ARG:NH1	7:AG:82:GLY:O	2.22	0.73
11:AK:109:ASN:OD1	11:AK:109:ASN:N	2.22	0.73
25:BA:265:A:N1	25:BA:427:U:O2'	2.21	0.73
1:AA:1180:A:OP2	9:AI:99:ARG:NH2	2.21	0.72
6:AF:42:TRP:HB3	6:AF:45:ARG:HH11	1.55	0.72
26:BB:7:G:O2'	38:BP:38:GLN:OE1	2.07	0.72
25:BA:1178:C:H2'	25:BA:1179:G:C8	2.23	0.72
56:CC:10:ARG:NH2	56:CC:793:GLU:OE1	2.23	0.72
1:AA:986:U:H2'	1:AA:987:G:C8	2.24	0.72
1:AA:1:A:H2'	1:AA:2:A:C8	2.24	0.72
1:AA:195:A:O2'	1:AA:196:A:H5'	1.90	0.72
25:BA:2121:G:HO2'	25:BA:2168:G:H1	1.38	0.72
24:AZ:6:G:H2'	24:AZ:7:A:C8	2.25	0.72
25:BA:2279:G:N7	46:BX:14:ARG:NH2	2.33	0.72
25:BA:2071:A:H2'	25:BA:2072:C:C6	2.24	0.72
25:BA:2377:A:O2'	38:BP:117:PHE:O	2.07	0.72
47:BY:33:LEU:HD12	47:BY:50:ARG:HG2	1.71	0.71
24:AZ:15:G:H2'	24:AZ:16:H2U:C2	2.20	0.71
24:AZ:51:U:O2	24:AZ:63:G:O6	2.09	0.71
1:AA:1008:U:H2'	1:AA:1009:U:C6	2.24	0.71
22:AV:49:G:H5''	56:CC:540:ARG:NH2	2.05	0.71
22:AV:50:C:H2'	22:AV:51:G:H8	1.55	0.71
25:BA:1870:C:H4'	25:BA:1870:C:OP2	1.90	0.71
1:AA:746:A:H2'	1:AA:747:A:C8	2.25	0.71
6:AF:5:GLU:OE2	6:AF:63:ASN:ND2	2.20	0.71
57:CD:826:ILE:CG2	57:CD:994:SER:CB	2.68	0.71
25:BA:1056:G:H1'	25:BA:1103:A:H61	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2134:A:H61	25:BA:2157:G:H1'	1.56	0.71
57:CD:816:THR:OG1	57:CD:818:GLU:OE1	2.07	0.71
6:AF:14:GLN:OE1	6:AF:14:GLN:N	2.23	0.71
57:CD:1100:PHE:CE2	57:CD:1200:GLU:CG	2.74	0.71
1:AA:845:A:H4'	1:AA:846:G:N7	2.05	0.71
25:BA:1592:C:H2'	25:BA:1593:A:H8	1.56	0.70
27:BC:107:PRO:HD2	27:BC:110:LEU:HD22	1.71	0.70
41:BS:34:GLU:HG2	41:BS:60:LYS:HG2	1.72	0.70
1:AA:1317:C:OP1	14:AN:24:ARG:NH2	2.23	0.70
1:AA:152:A:N6	1:AA:169:C:O2	2.24	0.70
19:AS:31:LEU:HB2	19:AS:49:ILE:HG22	1.72	0.70
25:BA:2792:A:H2'	25:BA:2793:C:C6	2.26	0.70
25:BA:278:A:OP2	25:BA:361:G:N1	2.24	0.70
25:BA:2069:G7M:N2	25:BA:2442:C:O2	2.23	0.70
37:BO:101:GLY:O	37:BO:110:MET:N	2.23	0.70
1:AA:90:C:H2'	1:AA:91:U:C6	2.26	0.70
1:AA:411:A:OP1	4:AD:26:ARG:NH1	2.25	0.70
25:BA:1407:G:H2'	25:BA:1408:G:C8	2.25	0.70
29:BE:111:GLU:OE1	29:BE:114:ARG:NH1	2.19	0.70
50:B2:15:MET:O	50:B2:18:SER:HB3	1.92	0.70
56:CC:481:LEU:HD21	61:CF:87:PRO:HG2	1.74	0.70
1:AA:1422:G:O3'	34:BL:49:ARG:NH2	2.25	0.69
3:AC:86:LYS:HA	3:AC:89:LYS:HE3	1.73	0.69
24:AX:37:MIA:O2'	25:BA:1913:A:N1	2.24	0.69
29:BE:58:LYS:NZ	29:BE:70:SER:O	2.25	0.69
55:CA:62:ASP:OD1	55:CA:63:GLY:N	2.25	0.69
3:AC:103:ILE:CB	57:CD:79:LYS:CE	2.70	0.69
25:BA:927:A:H2'	25:BA:928:A:C8	2.27	0.69
55:CB:191:ARG:NH2	55:CB:192:VAL:O	2.24	0.69
25:BA:285:G:O6	25:BA:355:U:O2	2.10	0.69
25:BA:2243:U:H2'	25:BA:2244:U:C6	2.28	0.69
1:AA:409:U:H3	1:AA:433:G:H1	1.41	0.69
1:AA:1318:A:H5''	19:AS:3:ARG:NH2	2.08	0.69
24:AX:54:5MU:H4'	36:BN:51:ARG:HE	1.58	0.69
1:AA:224:U:OP1	20:AT:69:LYS:NZ	2.26	0.69
1:AA:1061:G:N7	3:AC:3:GLN:NE2	2.40	0.69
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.27	0.69
44:BV:4:LYS:O	44:BV:94:ARG:NH2	2.25	0.69
2:AB:164:ILE:HG23	2:AB:186:ILE:HD11	1.75	0.69
25:BA:2146:C:O2'	25:BA:2147:A:OP2	2.09	0.69
38:BP:1:MET:O	38:BP:5:SER:CB	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:CB:191:ARG:HB3	55:CB:196:THR:HG23	1.73	0.69
57:CD:288:PRO:HB3	61:CF:107:GLU:OE1	1.92	0.69
25:BA:2117:A:H8	25:BA:2165:C:H41	1.39	0.69
31:BG:23:VAL:HG22	31:BG:36:THR:HB	1.75	0.69
48:BZ:18:LEU:HD11	48:BZ:54:LYS:HE3	1.73	0.68
7:AG:152:ALA:O	7:AG:155:ARG:NE	2.25	0.68
25:BA:396:G:OP2	47:BY:10:LYS:NZ	2.27	0.68
25:BA:889:C:H2'	25:BA:890:C:H5'	1.75	0.68
25:BA:2375:G:N2	25:BA:2378:A:OP2	2.24	0.68
22:AV:24:A:H2'	22:AV:25:U:O4'	1.93	0.68
23:AW:20:H2U:H61	23:AW:20:H2U:H5'	1.75	0.68
25:BA:639:U:H2'	25:BA:640:C:C6	2.28	0.68
25:BA:2258:C:O2'	25:BA:2427:C:OP2	2.11	0.68
57:CD:290:ILE:HG23	61:CF:94:GLY:HA2	1.73	0.68
27:BC:78:VAL:O	27:BC:113:GLY:N	2.27	0.68
25:BA:2298:A:OP1	30:BF:71:ARG:NH2	2.27	0.68
28:BD:48:ILE:HG23	28:BD:84:LEU:HD11	1.75	0.68
11:AK:18:ASP:HA	11:AK:81:ASN:O	1.94	0.68
14:AN:47:LYS:O	14:AN:50:THR:OG1	2.12	0.68
25:BA:2100:G:O6	25:BA:2189:U:O4	2.12	0.68
1:AA:523:A:N6	12:AL:89:D2T:OD2	2.24	0.68
22:AV:50:C:H2'	22:AV:51:G:C8	2.28	0.68
25:BA:881:G:O6	25:BA:895:U:O4	2.11	0.68
25:BA:1592:C:H2'	25:BA:1593:A:C8	2.29	0.68
25:BA:1083:U:O2'	25:BA:1085:A:OP2	2.10	0.67
25:BA:1565:C:O2'	25:BA:1567:G:N7	2.25	0.67
38:BP:69:ASP:OD1	38:BP:70:ALA:N	2.27	0.67
13:AM:90:ARG:NH2	13:AM:96:PRO:O	2.27	0.67
30:BF:48:LYS:O	30:BF:52:ASN:HB2	1.94	0.67
1:AA:616:G:O2'	16:AP:47:GLU:OE1	2.12	0.67
1:AA:840:C:N4	1:AA:842:U:H4'	2.09	0.67
2:AB:129:LEU:HD22	2:AB:134:ALA:HB2	1.77	0.67
25:BA:274:C:H2'	25:BA:275:C:O4'	1.94	0.67
25:BA:2111:U:H3	25:BA:2145:C:HO2'	1.38	0.67
25:BA:2134:A:N1	25:BA:2157:G:O2'	2.26	0.67
57:CD:1072:LYS:C	57:CD:1168:GLU:HG3	2.14	0.67
1:AA:1320:C:N3	19:AS:36:ARG:NH1	2.43	0.67
30:BF:51:ASP:O	30:BF:55:ALA:HB3	1.94	0.67
25:BA:550:U:H2'	25:BA:551:G:H8	1.58	0.67
1:AA:198:G:H2'	1:AA:199:A:C8	2.29	0.67
25:BA:1404:C:H2'	25:BA:1405:U:H5'	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2718:G:O4'	25:BA:2718:G:O2'	2.01	0.67
34:BL:5:GLN:N	34:BL:21:CYS:O	2.24	0.67
56:CC:481:LEU:CD1	61:CF:87:PRO:HG3	2.23	0.67
57:CD:429:LEU:H	57:CD:429:LEU:HD22	1.58	0.67
22:AV:51:G:H2'	22:AV:52:C:C6	2.28	0.67
32:BH:38:PRO:O	32:BH:43:ASN:ND2	2.27	0.67
1:AA:966:2MG:HM22	23:AW:34:C:H5'	1.77	0.67
25:BA:1084:A:N3	25:BA:1105:U:O2'	2.26	0.67
25:BA:1177:G:O2'	25:BA:1178:C:O5'	2.10	0.67
14:AN:63:ARG:NH1	14:AN:68:GLY:O	2.23	0.67
44:BV:48:PRO:HG3	44:BV:56:GLY:HA3	1.76	0.67
17:AQ:27:ARG:NH1	17:AQ:42:THR:OG1	2.28	0.67
41:BS:61:ALA:HB2	41:BS:98:ILE:HD13	1.77	0.67
56:CC:234:ASP:O	56:CC:235:ASN:ND2	2.28	0.67
4:AD:140:ASN:N	4:AD:182:PHE:O	2.28	0.66
57:CD:797:THR:HG22	57:CD:924:GLY:HA3	1.77	0.66
1:AA:337:G:H2'	1:AA:338:A:C8	2.29	0.66
4:AD:28:ILE:HD12	4:AD:34:ILE:HG12	1.78	0.66
24:AZ:9:A:H1'	24:AZ:45:U:H2'	1.77	0.66
29:BE:152:GLU:OE2	29:BE:152:GLU:N	2.27	0.66
56:CC:27:LEU:O	56:CC:528:ARG:NH1	2.28	0.66
25:BA:886:A:N7	25:BA:891:G:N2	2.42	0.66
57:CD:801:VAL:HG12	57:CD:920:ALA:HB3	1.77	0.66
4:AD:188:ARG:NH2	4:AD:192:SER:O	2.26	0.66
14:AN:46:LEU:HD22	19:AS:13:LEU:HB2	1.75	0.66
25:BA:819:A:OP2	25:BA:1187:G:N2	2.27	0.66
1:AA:927:G:O2'	1:AA:928:G:H5'	1.96	0.66
32:BH:73:ASN:HD22	32:BH:142:VAL:HG21	1.61	0.66
57:CD:978:ARG:HD3	57:CD:1197:ASN:ND2	2.11	0.66
9:AI:28:ILE:HG13	9:AI:63:LEU:HD13	1.77	0.66
25:BA:543:A:C6	25:BA:551:G:C6	2.83	0.66
25:BA:2161:C:OP2	25:BA:2164:C:N4	2.16	0.66
25:BA:2134:A:N6	25:BA:2157:G:H1'	2.11	0.66
25:BA:2746:U:H5''	31:BG:138:LYS:HE2	1.78	0.66
1:AA:477:C:H2'	1:AA:478:A:C8	2.31	0.65
1:AA:636:U:OP1	17:AQ:6:ARG:NH2	2.29	0.65
8:AH:7:ILE:HB	8:AH:77:ARG:HH22	1.61	0.65
25:BA:1105:U:H2'	25:BA:1106:G:H8	1.60	0.65
56:CC:525:THR:HG21	56:CC:687:ARG:HH11	1.59	0.65
25:BA:1175:A:OP2	25:BA:1176:U:O2'	2.14	0.65
1:AA:1100:C:OP1	21:AU:69:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:53:ILE:HD11	10:AJ:63:ASP:HB2	1.77	0.65
24:AX:51:U:H2'	24:AX:52:G:H8	1.60	0.65
1:AA:203:G:N2	1:AA:205:A:H61	1.93	0.65
3:AC:103:ILE:HG22	57:CD:79:LYS:HE3	1.79	0.65
57:CD:878:ASP:OD2	57:CD:991:THR:OG1	2.08	0.65
25:BA:1481:U:O2	25:BA:1510:G:O6	2.15	0.65
25:BA:2131:U:H5'	25:BA:2133:G:C8	2.31	0.65
25:BA:2139:U:O2	25:BA:2152:G:C6	2.49	0.65
3:AC:49:LYS:O	3:AC:72:ARG:NH2	2.25	0.65
25:BA:956:G:OP2	36:BN:86:LYS:NZ	2.30	0.65
25:BA:1404:C:C2'	25:BA:1405:U:H5'	2.27	0.65
40:BR:94:ILE:HG21	41:BS:4:VAL:HG11	1.78	0.65
25:BA:2728:U:HO2'	25:BA:2729:G:H8	1.45	0.65
30:BF:48:LYS:O	30:BF:52:ASN:CA	2.44	0.65
1:AA:152:A:N6	1:AA:169:C:C2	2.65	0.64
56:CC:696:ASP:CG	56:CC:697:LYS:H	2.01	0.64
57:CD:454:CYS:SG	57:CD:455:ALA:N	2.70	0.64
60:CT:28:DG:H5''	61:CF:18:PHE:CE2	2.31	0.64
1:AA:1276:G:O2'	1:AA:1277:C:H5'	1.97	0.64
17:AQ:11:ARG:HE	17:AQ:56:GLY:HA2	1.62	0.64
25:BA:1528:A:H2'	25:BA:1529:G:O4'	1.98	0.64
32:BH:111:ALA:N	32:BH:114:GLU:OE1	2.27	0.64
1:AA:993:G:O2'	1:AA:994:A:N7	2.30	0.64
60:CT:28:DG:H3'	61:CF:18:PHE:CZ	2.32	0.64
1:AA:1318:A:H5''	19:AS:3:ARG:HH22	1.63	0.64
10:AJ:86:ALA:N	10:AJ:89:ARG:HH11	1.96	0.64
25:BA:1724:G:H1	25:BA:1736:U:H3	1.46	0.64
6:AF:6:ILE:HG12	6:AF:89:VAL:HG22	1.80	0.64
4:AD:7:PRO:HB2	4:AD:10:LYS:HB2	1.78	0.64
13:AM:9:ILE:HG23	13:AM:18:ALA:HB1	1.80	0.64
25:BA:2252:G:H2'	25:BA:2253:G:H8	1.63	0.64
25:BA:2071:A:H2'	25:BA:2072:C:H6	1.62	0.64
11:AK:54:GLY:N	11:AK:57:LYS:HG2	2.13	0.63
43:BU:2:ILE:HD11	43:BU:45:ALA:HB1	1.80	0.63
25:BA:1494:A:H2'	25:BA:1495:A:C8	2.34	0.63
25:BA:2328:A:H2'	25:BA:2329:U:C6	2.33	0.63
60:CT:17:DG:C5	60:CT:18:DC:C5	2.86	0.63
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.32	0.63
1:AA:1395:C:HO2'	1:AA:1401:G:HO2'	1.43	0.63
3:AC:125:GLU:OE2	3:AC:190:HIS:N	2.31	0.63
24:AZ:14:A:H2'	24:AZ:15:G:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:3:VAL:HG22	32:BH:36:ALA:HB1	1.79	0.63
1:AA:843:U:O2'	1:AA:844:G:OP1	2.16	0.63
59:CN:32:DA:H5'	59:CN:32:DA:C8	2.33	0.63
25:BA:1070:A:N7	25:BA:1096:A:O2'	2.31	0.63
25:BA:2099:U:O4	25:BA:2190:G:O6	2.17	0.63
57:CD:576:ARG:NH1	57:CD:593:ASN:OD1	2.29	0.63
1:AA:35:G:N3	12:AL:115:SER:OG	2.31	0.63
1:AA:73:C:C2'	1:AA:74:A:H5'	2.29	0.63
1:AA:1297:G:O2'	7:AG:114:LYS:NZ	2.32	0.63
3:AC:103:ILE:CG2	57:CD:79:LYS:CE	2.75	0.63
7:AG:79:ARG:HD2	7:AG:84:THR:HG22	1.80	0.63
56:CC:582:ASN:OD1	56:CC:583:GLU:N	2.31	0.63
33:BK:99:ARG:NH1	33:BK:102:GLU:OE1	2.32	0.63
42:BT:22:ASP:OD1	42:BT:25:ARG:NH2	2.32	0.62
44:BV:7:ARG:NH1	44:BV:26:LYS:O	2.32	0.62
6:AF:3:HIS:ND1	6:AF:93:LYS:O	2.32	0.62
25:BA:2134:A:O2'	25:BA:2159:G:N3	2.31	0.62
41:BS:30:GLY:N	41:BS:63:VAL:O	2.32	0.62
59:CN:18:DG:C2'	61:CF:90:MET:HB2	2.28	0.62
1:AA:197:A:O2'	1:AA:220:G:N2	2.32	0.62
25:BA:1326:U:HO2'	25:BA:2010:G:HO2'	1.45	0.62
1:AA:714:G:H2'	1:AA:715:A:C8	2.34	0.62
1:AA:1233:G:O5'	9:AI:119:ARG:NH1	2.33	0.62
4:AD:50:ASP:OD1	4:AD:50:ASP:N	2.28	0.62
24:AZ:9:A:N6	24:AZ:22:G:N7	2.48	0.62
57:CD:505:ASP:N	57:CD:505:ASP:OD1	2.31	0.62
60:CT:9:DC:H2'	60:CT:10:DT:C6	2.33	0.62
3:AC:3:GLN:OE1	3:AC:3:GLN:N	2.30	0.62
25:BA:2899:A:N1	25:BA:2900:A:N6	2.48	0.62
27:BC:29:PRO:HG2	27:BC:34:LEU:HD11	1.81	0.62
27:BC:161:TYR:HB3	27:BC:194:GLU:HG2	1.82	0.62
1:AA:950:U:OP2	13:AM:101:ARG:NH1	2.32	0.62
1:AA:1017:U:O2'	1:AA:1018:G:O4'	2.17	0.62
6:AF:102:MET:SD	6:AF:102:MET:N	2.73	0.62
29:BE:165:HIS:HE1	29:BE:166:LYS:HE3	1.64	0.62
43:BU:7:LEU:HD22	43:BU:46:ALA:HB2	1.81	0.62
57:CD:1072:LYS:O	57:CD:1168:GLU:CG	2.37	0.62
24:AZ:3:C:H2'	24:AZ:4:C:H6	1.64	0.62
38:BP:39:VAL:HB	38:BP:49:VAL:HG22	1.82	0.62
6:AF:69:GLU:HG2	6:AF:70:VAL:N	2.14	0.62
25:BA:1996:C:OP2	34:BL:31:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2470:G:OP1	36:BN:55:ARG:NH1	2.32	0.62
38:BP:1:MET:O	38:BP:5:SER:HB3	2.00	0.62
41:BS:77:PHE:HD1	41:BS:84:ARG:HB3	1.65	0.62
1:AA:1229:A:OP2	13:AM:113:ARG:NH1	2.33	0.61
15:AO:47:LYS:O	15:AO:53:ARG:NH2	2.30	0.61
25:BA:1265:A:H4'	25:BA:1266:G:H4'	1.80	0.61
25:BA:1528:A:N6	25:BA:1543:G:O2'	2.33	0.61
29:BE:1:MET:HB3	29:BE:14:VAL:HG23	1.81	0.61
60:CT:29:DA:OP1	61:CF:17:GLY:O	2.18	0.61
1:AA:1174:G:H2'	1:AA:1175:G:H5'	1.82	0.61
1:AA:1383:C:H2'	1:AA:1384:C:H6	1.65	0.61
57:CD:1025:MET:CE	57:CD:1195:GLN:HG3	2.29	0.61
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.35	0.61
40:BR:24:TYR:O	40:BR:29:SER:HB3	1.99	0.61
56:CC:481:LEU:CD2	61:CF:87:PRO:HG3	2.31	0.61
1:AA:31:G:O2'	1:AA:48:C:N4	2.34	0.61
14:AN:46:LEU:HD13	19:AS:13:LEU:HD13	1.83	0.61
27:BC:252:THR:HG23	27:BC:253:LYS:HG2	1.83	0.61
26:BB:5:U:OP1	26:BB:61:G:O2'	2.16	0.61
30:BF:126:GLY:O	30:BF:127:ASN:ND2	2.33	0.61
60:CT:19:DG:C5	60:CT:20:DC:C5	2.88	0.61
25:BA:1108:U:H2'	25:BA:1109:C:C6	2.36	0.61
29:BE:5:LEU:O	29:BE:9:GLN:CA	2.48	0.61
25:BA:2291:U:H2'	25:BA:2292:U:C6	2.36	0.61
48:BZ:5:GLU:OE2	48:BZ:5:GLU:N	2.31	0.61
49:B1:6:LYS:NZ	49:B1:37:GLU:OE1	2.29	0.61
25:BA:2244:U:H2'	25:BA:2245:U:C6	2.36	0.61
25:BA:721:A:H2'	25:BA:722:A:C8	2.36	0.60
30:BF:110:ARG:NH1	30:BF:136:ILE:O	2.34	0.60
36:BN:14:LYS:O	36:BN:71:LYS:NZ	2.28	0.60
2:AB:148:LEU:HD22	2:AB:151:ILE:HD11	1.82	0.60
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.31	0.60
3:AC:103:ILE:HG21	57:CD:79:LYS:HE3	1.81	0.60
25:BA:543:A:H2'	25:BA:544:G:C8	2.36	0.60
42:BT:110:ARG:H	42:BT:110:ARG:NE	1.99	0.60
57:CD:290:ILE:HD12	57:CD:290:ILE:H	1.66	0.60
4:AD:48:LEU:HD23	4:AD:53:VAL:HG12	1.83	0.60
38:BP:1:MET:SD	38:BP:2:ASP:N	2.72	0.60
1:AA:302:G:OP1	12:AL:14:ARG:NH2	2.35	0.60
1:AA:1006:G:H2'	1:AA:1007:U:C6	2.33	0.60
33:BK:43:GLU:OE1	33:BK:43:GLU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:7:ILE:HB	8:AH:77:ARG:NH2	2.16	0.60
25:BA:172:A:H2'	25:BA:173:A:C8	2.37	0.60
25:BA:1529:G:H2'	25:BA:1530:G:H8	1.67	0.60
1:AA:823:C:HO2'	8:AH:2:SER:N	1.98	0.60
1:AA:945:G:C2	1:AA:946:A:C8	2.90	0.60
24:AX:20:H2U:O2	24:AX:20:H2U:H2'	2.02	0.60
56:CC:274:ILE:HA	56:CC:277:LEU:HD12	1.84	0.60
1:AA:1383:C:H2'	1:AA:1384:C:C6	2.36	0.60
25:BA:571:U:OP1	41:BS:80:ARG:NH2	2.35	0.60
56:CC:423:ASP:N	56:CC:423:ASP:OD1	2.34	0.60
15:AO:18:ASP:O	15:AO:21:ASP:N	2.24	0.60
30:BF:147:ASP:OD1	30:BF:148:ARG:N	2.35	0.60
1:AA:1039:G:H2'	1:AA:1040:U:C6	2.37	0.59
3:AC:77:ILE:HD11	57:CD:79:LYS:HE2	1.82	0.59
25:BA:1432:G:H2'	25:BA:1433:A:C8	2.37	0.59
56:CC:251:ALA:HB2	56:CC:269:ILE:HD11	1.82	0.59
1:AA:203:G:H21	1:AA:205:A:H61	1.48	0.59
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.84	0.59
24:AX:75:C:H2'	24:AX:76:A:C8	2.37	0.59
24:AZ:3:C:H2'	24:AZ:4:C:C6	2.37	0.59
56:CC:542:ARG:NH1	59:CN:26:DG:OP2	2.35	0.59
1:AA:337:G:H2'	1:AA:338:A:H8	1.67	0.59
1:AA:451:A:H1'	1:AA:452:A:C2	2.37	0.59
1:AA:496:A:H2'	1:AA:496:A:N3	2.16	0.59
3:AC:80:LYS:HD3	57:CD:81:ARG:CZ	2.31	0.59
11:AK:18:ASP:HB3	11:AK:81:ASN:HB2	1.84	0.59
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.84	0.59
30:BF:117:LEU:HB2	30:BF:176:PRO:O	2.03	0.59
25:BA:652:U:OP2	25:BA:654:A:N6	2.36	0.59
56:CC:525:THR:HG21	56:CC:687:ARG:NH1	2.15	0.59
4:AD:147:GLU:HA	4:AD:150:LYS:HB2	1.85	0.59
11:AK:17:SER:O	11:AK:80:LYS:N	2.35	0.59
57:CD:504:GLN:HG3	57:CD:505:ASP:H	1.66	0.59
60:CT:19:DG:C6	60:CT:20:DC:C4	2.91	0.59
1:AA:181:A:O2'	1:AA:194:C:N4	2.35	0.59
1:AA:183:C:H4'	1:AA:184:G:OP2	2.02	0.59
1:AA:736:C:OP1	18:AR:61:ARG:NH1	2.36	0.59
1:AA:1008:U:H2'	1:AA:1009:U:H6	1.64	0.59
25:BA:627:A:OP1	35:BM:78:ARG:NH2	2.30	0.59
25:BA:1915:3TD:H2'	25:BA:1916:A:C8	2.37	0.59
44:BV:5:ILE:HG13	44:BV:72:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:401:C:OP2	4:AD:70:ARG:NH1	2.36	0.59
2:AB:165:ASP:H	2:AB:186:ILE:HG13	1.68	0.59
13:AM:16:VAL:O	13:AM:20:THR:HG23	2.03	0.59
25:BA:172:A:H2'	25:BA:173:A:H8	1.68	0.59
60:CT:19:DG:H2'	60:CT:20:DC:C6	2.38	0.59
1:AA:429:U:H5'	4:AD:9:LEU:HD12	1.85	0.59
25:BA:1406:U:H2'	25:BA:1407:G:H5''	1.85	0.59
25:BA:1594:U:H2'	25:BA:1595:C:H6	1.66	0.59
51:B3:22:THR:HG23	53:B5:34:THR:HG23	1.85	0.59
1:AA:530:G:N2	1:AA:1492:A:H61	1.99	0.58
1:AA:1492:A:OP1	12:AL:44:LYS:HB2	2.03	0.58
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.85	0.58
5:AE:105:ILE:O	5:AE:112:ARG:NH2	2.36	0.58
25:BA:882:G:O6	25:BA:894:U:O4	2.22	0.58
25:BA:1108:U:H2'	25:BA:1109:C:H6	1.68	0.58
56:CC:1321:GLU:OE2	57:CD:99:ARG:NH1	2.33	0.58
57:CD:826:ILE:HG21	57:CD:994:SER:HB2	1.84	0.58
59:CN:38:DA:H2''	59:CN:39:DG:N7	2.17	0.58
2:AB:107:VAL:O	2:AB:111:ILE:HG23	2.03	0.58
24:AZ:20:H2U:H2'	24:AZ:20:H2U:OP2	2.03	0.58
25:BA:78:U:OP1	48:BZ:7:ARG:NH2	2.36	0.58
25:BA:2146:C:H4'	25:BA:2147:A:C8	2.39	0.58
48:BZ:14:LEU:HD22	48:BZ:53:VAL:HG23	1.83	0.58
1:AA:687:A:N1	1:AA:700:G:O2'	2.35	0.58
1:AA:728:A:H2'	1:AA:729:A:C8	2.39	0.58
24:AZ:2:C:H2'	24:AZ:3:C:C6	2.39	0.58
24:AZ:7:A:O2'	24:AZ:49:C:O4'	2.21	0.58
42:BT:34:ASP:OD2	50:B2:37:LYS:NZ	2.35	0.58
56:CC:591:TYR:OH	56:CC:637:ARG:NH2	2.35	0.58
1:AA:458:U:O4	1:AA:474:G:O6	2.22	0.58
56:CC:726:TYR:HB3	56:CC:733:VAL:CG1	2.34	0.58
26:BB:119:A:H2'	26:BB:120:U:C6	2.39	0.58
25:BA:639:U:H2'	25:BA:640:C:H6	1.68	0.58
9:AI:4:ASN:OD1	9:AI:4:ASN:N	2.34	0.58
24:AX:6:G:H2'	24:AX:7:A:C8	2.38	0.58
25:BA:631:A:OP2	53:B5:23:LYS:NZ	2.30	0.58
38:BP:1:MET:O	38:BP:5:SER:HB2	2.04	0.58
57:CD:1169:THR:OG1	57:CD:1173:ARG:HB3	2.04	0.58
60:CT:28:DG:C3'	61:CF:18:PHE:CZ	2.86	0.58
1:AA:51:A:N7	1:AA:114:U:O2'	2.35	0.58
1:AA:866:C:C4	1:AA:867:G:H1'	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:56:HIS:CE1	10:AJ:57:VAL:HG13	2.39	0.58
25:BA:1595:C:O2'	25:BA:1596:A:H5'	2.04	0.58
25:BA:2591:C:H2'	25:BA:2592:G:C8	2.39	0.58
56:CC:638:SER:OG	56:CC:639:LYS:N	2.37	0.58
56:CC:811:ASN:ND2	56:CC:1097:VAL:O	2.36	0.58
57:CD:1025:MET:HE2	57:CD:1195:GLN:HG3	1.84	0.58
24:AZ:40:C:H2'	24:AZ:41:C:H6	1.69	0.58
1:AA:877:G:C2	1:AA:878:A:N7	2.73	0.57
25:BA:2032:G:H21	28:BD:151:THR:HG23	1.69	0.57
1:AA:1184:G:C2	1:AA:1185:G:C8	2.92	0.57
11:AK:47:ALA:HB1	11:AK:62:ALA:HB1	1.85	0.57
25:BA:2163:A:N7	25:BA:2164:C:H6	2.02	0.57
57:CD:1100:PHE:HD2	57:CD:1200:GLU:HB3	1.56	0.57
8:AH:94:LYS:HZ3	8:AH:117:ARG:HH22	1.52	0.57
12:AL:79:VAL:N	12:AL:103:ASP:OD2	2.34	0.57
25:BA:1069:A:H4'	25:BA:1070:A:C8	2.39	0.57
25:BA:1364:G:N2	25:BA:1367:A:OP2	2.34	0.57
25:BA:1059:G:H2'	25:BA:1060:U:C5	2.39	0.57
46:BX:70:GLU:OE2	46:BX:72:LYS:HD2	2.05	0.57
57:CD:891:ASP:OD1	57:CD:1286:LYS:NZ	2.37	0.57
15:AO:25:THR:HG21	15:AO:70:LEU:HD13	1.86	0.57
24:AX:19:G:H3'	24:AX:20:H2U:C2	2.35	0.57
25:BA:2244:U:O2'	25:BA:2245:U:H5'	2.04	0.57
42:BT:17:VAL:HG12	42:BT:76:VAL:HG21	1.85	0.57
1:AA:413:G:O2'	1:AA:428:G:N2	2.38	0.57
3:AC:86:LYS:O	3:AC:89:LYS:HG2	2.04	0.57
9:AI:46:MET:N	9:AI:49:ARG:HH21	2.02	0.57
25:BA:742:A:H2'	25:BA:743:A:C8	2.39	0.57
25:BA:2723:C:OP1	28:BD:114:LYS:NZ	2.36	0.57
32:BH:129:GLU:HA	32:BH:143:ILE:HA	1.87	0.57
57:CD:290:ILE:CG2	61:CF:94:GLY:CA	2.78	0.57
25:BA:245:G:O6	53:B5:8:ARG:NH1	2.38	0.57
25:BA:2637:U:H5''	28:BD:83:ARG:HH22	1.69	0.57
28:BD:33:ARG:NH2	28:BD:74:GLU:O	2.38	0.57
29:BE:165:HIS:CE1	29:BE:166:LYS:HE3	2.40	0.57
60:CT:28:DG:C5'	61:CF:18:PHE:CZ	2.69	0.57
1:AA:160:A:H1'	1:AA:344:A:C5	2.38	0.57
25:BA:856:G:H2'	25:BA:857:G:C8	2.40	0.57
57:CD:1100:PHE:CE2	57:CD:1200:GLU:HB3	2.35	0.57
1:AA:842:U:O2'	1:AA:846:G:O6	2.12	0.57
5:AE:78:ASN:N	5:AE:78:ASN:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:113:ASP:O	7:AG:119:ARG:NE	2.38	0.57
25:BA:1047:G:N2	25:BA:1111:A:C8	2.71	0.57
57:CD:813:ASP:OD1	57:CD:883:ARG:NH2	2.34	0.57
1:AA:413:G:N2	1:AA:428:G:H1'	2.20	0.57
24:AZ:22:G:O6	24:AZ:23:A:N6	2.38	0.57
25:BA:144:A:H2'	25:BA:145:C:C6	2.40	0.57
25:BA:574:A:N6	25:BA:2034:U:OP1	2.38	0.57
56:CC:12:ARG:NE	56:CC:793:GLU:OE2	2.30	0.57
1:AA:56:U:H2'	1:AA:57:G:H8	1.69	0.56
3:AC:73:PRO:HB3	57:CD:79:LYS:HD2	1.86	0.56
25:BA:284:U:C2	25:BA:356:G:N1	2.68	0.56
25:BA:613:A:H5''	25:BA:613:A:H8	1.69	0.56
31:BG:133:LEU:HD11	31:BG:141:ILE:HG23	1.87	0.56
25:BA:1049:C:C2'	25:BA:1050:A:H5'	2.35	0.56
1:AA:911:U:H2'	1:AA:912:C:C6	2.40	0.56
24:AZ:10:G:H2'	24:AZ:11:C:C6	2.40	0.56
25:BA:125:A:OP2	52:B4:19:ARG:NH2	2.32	0.56
25:BA:284:U:O4	25:BA:356:G:O6	2.23	0.56
25:BA:2059:A:H2'	25:BA:2503:2MA:HM23	1.86	0.56
27:BC:162:VAL:HG11	27:BC:174:LEU:HD23	1.86	0.56
29:BE:1:MET:HB2	29:BE:16:GLU:HA	1.88	0.56
30:BF:47:LYS:O	30:BF:51:ASP:N	2.34	0.56
55:CB:27:THR:C	55:CB:28:LEU:HD22	2.26	0.56
5:AE:90:THR:OG1	5:AE:91:GLY:N	2.38	0.56
24:AZ:8:4SU:N3	24:AZ:15:G:O6	2.39	0.56
60:CT:26:DA:H1'	60:CT:27:DG:C4	2.40	0.56
24:AZ:14:A:H61	24:AZ:46:7MG:HN21	1.53	0.56
25:BA:2140:G:N1	25:BA:2151:U:C2	2.74	0.56
25:BA:2328:A:H2'	25:BA:2329:U:H6	1.71	0.56
53:B5:62:LEU:HB3	53:B5:65:ALA:HB3	1.88	0.56
1:AA:384:G:H2'	1:AA:385:C:C6	2.41	0.56
7:AG:7:ILE:HD13	7:AG:7:ILE:H	1.71	0.56
10:AJ:26:VAL:HG13	10:AJ:30:LYS:NZ	2.20	0.56
31:BG:23:VAL:HA	31:BG:36:THR:HA	1.87	0.56
31:BG:104:ASN:ND2	31:BG:114:ASP:OD1	2.38	0.56
33:BK:40:HIS:CE1	33:BK:41:LYS:HG2	2.41	0.56
45:BW:32:GLY:O	45:BW:93:ARG:NH1	2.34	0.56
57:CD:650:LYS:HE3	57:CD:742:GLY:O	2.04	0.56
10:AJ:56:HIS:ND1	10:AJ:57:VAL:HG22	2.20	0.56
24:AX:21:A:N6	24:AX:46:7MG:H2'	2.21	0.56
56:CC:7:GLU:O	56:CC:9:LYS:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CD:847:ASP:OD1	57:CD:847:ASP:N	2.39	0.56
1:AA:1516:2MG:N2	1:AA:1519:MA6:OP2	2.39	0.56
6:AF:44:ARG:HB2	6:AF:44:ARG:HH11	1.70	0.56
25:BA:1173:U:C2	25:BA:1176:U:O2	2.59	0.56
25:BA:301:G:OP2	44:BV:82:ARG:NH1	2.38	0.56
25:BA:1534:U:O2'	25:BA:1537:G:O6	2.24	0.56
12:AL:27:CYS:SG	12:AL:30:LYS:NZ	2.79	0.55
1:AA:197:A:H4'	1:AA:198:G:O5'	2.07	0.55
57:CD:1072:LYS:HD3	57:CD:1169:THR:C	2.27	0.55
4:AD:98:LEU:O	4:AD:101:VAL:HG22	2.06	0.55
31:BG:148:LEU:HA	31:BG:151:TYR:HD2	1.70	0.55
24:AX:51:U:H2'	24:AX:52:G:C8	2.40	0.55
25:BA:1176:U:H2'	25:BA:1177:G:C5	2.41	0.55
57:CD:1072:LYS:CE	57:CD:1169:THR:O	2.54	0.55
57:CD:1186:TYR:OH	57:CD:1188:GLU:OE1	2.15	0.55
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.41	0.55
24:AX:30:G:H2'	24:AX:31:A:H8	1.71	0.55
30:BF:10:ASP:HB2	30:BF:11:GLU:OE2	2.07	0.55
33:BK:92:MET:SD	33:BK:95:ARG:NH2	2.79	0.55
5:AE:106:ILE:HB	5:AE:124:LEU:HD23	1.88	0.55
25:BA:1177:G:O2'	25:BA:1178:C:H6	1.89	0.55
32:BH:78:VAL:HG23	32:BH:142:VAL:HG11	1.89	0.55
56:CC:267:ARG:HH22	56:CC:273:HIS:CE1	2.24	0.55
1:AA:203:G:O2'	1:AA:204:G:N7	2.30	0.55
6:AF:38:ARG:HG2	6:AF:63:ASN:HB2	1.88	0.55
25:BA:543:A:N6	25:BA:551:G:O6	2.40	0.55
25:BA:2147:A:OP2	25:BA:2147:A:H8	1.89	0.55
56:CC:421:SER:H	56:CC:424:ASP:HB2	1.71	0.55
57:CD:290:ILE:HG23	61:CF:94:GLY:CA	2.37	0.55
57:CD:429:LEU:HD22	57:CD:429:LEU:N	2.20	0.55
57:CD:441:LEU:HD22	57:CD:441:LEU:N	2.22	0.55
1:AA:1009:U:O4	1:AA:1020:G:O6	2.25	0.55
5:AE:76:LEU:HD21	5:AE:120:VAL:HG12	1.88	0.55
25:BA:1056:G:H1'	25:BA:1103:A:N6	2.21	0.55
25:BA:2315:G:O2'	25:BA:2316:G:O4'	2.24	0.55
1:AA:744:C:H2'	1:AA:745:G:H8	1.69	0.55
1:AA:1031:C:H4'	1:AA:1032:G:C2	2.42	0.55
9:AI:42:GLU:OE2	9:AI:45:ARG:NH1	2.39	0.55
13:AM:16:VAL:HG13	13:AM:17:ILE:HD12	1.89	0.55
25:BA:2228:G:H2'	25:BA:2229:U:H6	1.71	0.55
55:CB:76:GLU:H	55:CB:76:GLU:CD	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AZ:19:G:OP1	24:AZ:20:H2U:N3	2.40	0.55
35:BM:81:ASP:HB3	35:BM:100:ILE:HD13	1.88	0.55
57:CD:137:ARG:HG3	57:CD:142:GLU:HB2	1.89	0.55
57:CD:288:PRO:HB3	61:CF:107:GLU:CD	2.27	0.55
57:CD:288:PRO:HD2	57:CD:291:ILE:HD12	1.89	0.55
57:CD:746:LEU:HD23	57:CD:758:PRO:HB3	1.89	0.55
4:AD:11:LEU:HD22	4:AD:63:ARG:HE	1.72	0.54
4:AD:147:GLU:OE2	4:AD:147:GLU:N	2.26	0.54
25:BA:2111:U:N3	25:BA:2145:C:O2'	2.28	0.54
1:AA:72:A:N6	1:AA:98:A:H2	2.06	0.54
1:AA:600:A:OP2	8:AH:88:ARG:NH1	2.40	0.54
13:AM:107:ARG:HH12	13:AM:112:PRO:C	2.10	0.54
25:BA:2110:G:O2'	25:BA:2120:G:OP1	2.24	0.54
36:BN:28:PHE:N	36:BN:104:GLU:OE1	2.39	0.54
57:CD:1157:ALA:HB2	57:CD:1210:ILE:HD11	1.87	0.54
1:AA:451:A:OP1	1:AA:481:G:N1	2.35	0.54
1:AA:966:2MG:H5''	1:AA:967:5MC:OP2	2.08	0.54
25:BA:1789:A:OP1	27:BC:221:ARG:HG3	2.08	0.54
38:BP:57:ALA:O	38:BP:61:GLN:HG2	2.08	0.54
56:CC:1176:LEU:O	56:CC:1178:LYS:N	2.40	0.54
1:AA:946:A:H2'	1:AA:947:G:C8	2.42	0.54
4:AD:187:GLU:O	4:AD:191:LEU:HD22	2.07	0.54
22:AV:44:A:O2'	22:AV:45:C:OP2	2.19	0.54
31:BG:137:ASP:O	31:BG:141:ILE:HD12	2.08	0.54
45:BW:75:GLN:HB2	45:BW:92:VAL:HG13	1.87	0.54
52:B4:24:THR:HG23	52:B4:27:GLY:H	1.72	0.54
8:AH:66:PHE:CD2	8:AH:67:GLN:HG3	2.43	0.54
14:AN:8:ALA:O	14:AN:11:VAL:HG22	2.06	0.54
24:AZ:14:A:H61	24:AZ:46:7MG:N2	2.05	0.54
25:BA:994:C:OP2	40:BR:54:LYS:NZ	2.37	0.54
25:BA:2639:A:H4'	33:BK:96:ARG:NH2	2.22	0.54
45:BW:11:GLU:HG3	45:BW:16:ALA:HB1	1.89	0.54
1:AA:346:G:N2	1:AA:347:G:C8	2.76	0.54
1:AA:1004:A:N7	1:AA:1025:U:H5'	2.23	0.54
4:AD:49:SER:O	4:AD:53:VAL:HG13	2.08	0.54
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.90	0.54
25:BA:1506:U:H2'	25:BA:1507:C:C6	2.42	0.54
28:BD:113:SER:O	28:BD:167:ASN:HA	2.06	0.54
38:BP:52:SER:HB2	38:BP:54:VAL:HG22	1.90	0.54
57:CD:1100:PHE:CD2	57:CD:1200:GLU:CG	2.91	0.54
58:CE:9:ALA:HB1	58:CE:19:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:604:G:H2'	1:AA:605:U:O4'	2.08	0.54
1:AA:643:C:OP1	8:AH:31:LYS:NZ	2.24	0.54
1:AA:1277:C:HO2'	1:AA:1278:G:P	2.30	0.54
22:AV:48:C:H2'	22:AV:49:G:O4'	2.07	0.54
25:BA:2120:G:H5'	25:BA:2120:G:H8	1.73	0.54
36:BN:35:ALA:HB2	36:BN:102:LEU:HD11	1.90	0.54
57:CD:495:ASN:OD1	57:CD:495:ASN:N	2.37	0.54
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.69	0.54
2:AB:61:ALA:HB1	2:AB:225:ARG:HG2	1.90	0.54
24:AX:50:U:H2'	24:AX:51:U:C6	2.42	0.54
25:BA:2107:G:N2	25:BA:2182:U:O2	2.32	0.54
25:BA:2130:U:H5''	25:BA:2133:G:H1'	1.90	0.54
25:BA:2799:G:O2'	25:BA:2800:A:H5''	2.08	0.54
59:CN:27:DA:C4	59:CN:28:DA:C8	2.96	0.54
60:CT:26:DA:H1'	60:CT:27:DG:C5	2.42	0.54
1:AA:842:U:H3'	1:AA:843:U:C5'	2.37	0.54
7:AG:65:ALA:O	7:AG:69:VAL:HG23	2.08	0.54
34:BL:34:GLY:N	34:BL:37:ASP:OD2	2.41	0.54
1:AA:147:G:H2'	1:AA:148:G:C8	2.42	0.54
1:AA:269:C:H2'	1:AA:270:A:H8	1.72	0.54
23:AW:16:C:O2'	23:AW:60:U:O3'	2.26	0.54
25:BA:1494:A:HO2'	25:BA:1495:A:P	2.31	0.54
35:BM:37:GLY:H	35:BM:40:SER:HB3	1.72	0.54
56:CC:660:VAL:HG13	56:CC:661:VAL:HG13	1.90	0.54
1:AA:840:C:C4	1:AA:842:U:H4'	2.43	0.53
13:AM:11:ASP:OD1	13:AM:12:HIS:N	2.40	0.53
24:AZ:34:G:H2'	24:AZ:35:A:C8	2.43	0.53
25:BA:1168:G:H2'	25:BA:1169:A:C8	2.42	0.53
31:BG:95:ARG:HD2	31:BG:106:SER:HB3	1.88	0.53
1:AA:1256:A:H62	1:AA:1279:G:N2	2.06	0.53
16:AP:9:HIS:O	16:AP:16:PHE:N	2.38	0.53
21:AU:61:ALA:O	21:AU:65:ALA:HB3	2.08	0.53
25:BA:1062:G:N7	25:BA:1088:A:O2'	2.42	0.53
25:BA:1173:U:O2	25:BA:1176:U:O2	2.27	0.53
25:BA:1333:G:C2	25:BA:1334:G:C8	2.96	0.53
25:BA:2121:G:O2'	25:BA:2168:G:N1	2.33	0.53
30:BF:48:LYS:O	30:BF:52:ASN:CB	2.56	0.53
56:CC:150:HIS:CE1	56:CC:454:ARG:HG3	2.43	0.53
56:CC:297:VAL:HA	56:CC:335:THR:HG22	1.89	0.53
1:AA:1025:U:H5''	1:AA:1026:G:O5'	2.08	0.53
13:AM:60:VAL:HG13	13:AM:65:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:49:G:H5''	56:CC:540:ARG:HH22	1.73	0.53
25:BA:871:U:H2'	25:BA:872:U:C6	2.44	0.53
25:BA:1060:U:H4'	25:BA:1061:U:O5'	2.09	0.53
25:BA:2796:C:H2'	25:BA:2798:U:C5	2.44	0.53
43:BU:2:ILE:HG12	43:BU:7:LEU:HD11	1.90	0.53
49:B1:9:GLN:O	49:B1:33:GLY:N	2.41	0.53
1:AA:160:A:H1'	1:AA:344:A:C6	2.43	0.53
3:AC:80:LYS:CD	57:CD:81:ARG:CZ	2.86	0.53
50:B2:31:ASP:O	50:B2:35:GLY:HA2	2.09	0.53
56:CC:267:ARG:NE	56:CC:268:ARG:O	2.36	0.53
1:AA:1124:G:H3'	10:AJ:37:ARG:HH22	1.74	0.53
18:AR:55:LEU:HD12	18:AR:56:ALA:N	2.23	0.53
25:BA:2187:U:O2'	25:BA:2188:U:H6	1.92	0.53
32:BH:2:GLN:NE2	32:BH:20:ASN:HB2	2.24	0.53
56:CC:12:ARG:HH21	56:CC:793:GLU:CD	2.11	0.53
25:BA:614:A:OP2	25:BA:614:A:H8	1.91	0.53
25:BA:1720:U:H2'	25:BA:1721:G:O4'	2.09	0.53
37:BO:20:MET:HG3	37:BO:21:PHE:N	2.24	0.53
53:B5:4:ILE:HD13	53:B5:63:PRO:HG3	1.90	0.53
57:CD:857:LEU:HD11	57:CD:871:LEU:HD21	1.90	0.53
11:AK:92:GLY:C	11:AK:94:GLU:H	2.12	0.53
16:AP:6:LEU:HD22	16:AP:17:TYR:HB3	1.90	0.53
24:AZ:76:A:N6	25:BA:2422:C:O4'	2.42	0.53
25:BA:1481:U:C2	25:BA:1510:G:O6	2.62	0.53
25:BA:2796:C:H2'	25:BA:2798:U:H5	1.74	0.53
57:CD:1313:SER:HG	57:CD:1325:PHE:HE2	1.56	0.53
1:AA:56:U:H2'	1:AA:57:G:C8	2.44	0.53
1:AA:182:A:O2'	1:AA:183:C:H3'	2.09	0.53
4:AD:97:ARG:O	4:AD:101:VAL:HG13	2.09	0.53
8:AH:94:LYS:HZ1	8:AH:117:ARG:HH12	1.55	0.53
39:BQ:33:VAL:O	39:BQ:33:VAL:HG12	2.08	0.53
1:AA:212:G:C2	1:AA:213:G:C8	2.97	0.53
12:AL:99:ARG:HA	12:AL:104:CYS:SG	2.49	0.53
24:AZ:27:G:H2'	24:AZ:28:G:H8	1.74	0.53
24:AZ:40:C:H2'	24:AZ:41:C:C6	2.44	0.53
25:BA:833:A:H2'	25:BA:834:G:C8	2.44	0.53
25:BA:1255:U:C5	29:BE:68:ALA:HA	2.44	0.53
25:BA:2287:A:C8	25:BA:2289:G:C8	2.96	0.53
29:BE:170:ARG:NH2	29:BE:176:ASP:OD1	2.38	0.53
57:CD:301:GLU:OE1	57:CD:312:ARG:NE	2.39	0.53
59:CN:18:DG:H2'	61:CF:91:GLY:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.90	0.53
25:BA:1178:C:H2'	25:BA:1179:G:H8	1.71	0.53
25:BA:2102:G:H2'	25:BA:2103:C:C6	2.44	0.53
32:BH:1:MET:O	32:BH:20:ASN:HA	2.09	0.53
38:BP:48:LEU:HD13	38:BP:87:ILE:HD13	1.91	0.53
12:AL:42:PRO:HG3	12:AL:48:ALA:N	2.24	0.52
23:AW:17:C:H2'	23:AW:17(A):U:C6	2.44	0.52
25:BA:893:C:O2'	25:BA:894:U:H6	1.92	0.52
56:CC:549:ASP:OD2	57:CD:750:PRO:HB3	2.09	0.52
60:CT:19:DG:H2'	60:CT:20:DC:H6	1.72	0.52
1:AA:413:G:H21	1:AA:428:G:H1'	1.75	0.52
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.43	0.52
24:AZ:56:C:H2'	24:AZ:57:G:C8	2.44	0.52
24:AZ:56:C:H2'	24:AZ:57:G:H8	1.73	0.52
25:BA:1045:C:H41	25:BA:1111:A:H2'	1.74	0.52
29:BE:29:HIS:O	29:BE:32:VAL:HG22	2.10	0.52
25:BA:2798:U:H1'	25:BA:2799:G:C6	2.44	0.52
55:CB:28:LEU:HD22	55:CB:28:LEU:N	2.24	0.52
4:AD:42:GLY:O	4:AD:44:ARG:N	2.40	0.52
24:AX:38:A:H5'	25:BA:1913:A:N1	2.24	0.52
24:AZ:27:G:H2'	24:AZ:28:G:C8	2.45	0.52
25:BA:144:A:H2'	25:BA:145:C:H6	1.75	0.52
25:BA:799:G:C6	25:BA:800:A:C6	2.97	0.52
25:BA:1068:G:H1	25:BA:1095:A:H2	1.55	0.52
25:BA:1579:A:H2'	25:BA:1580:A:C8	2.45	0.52
25:BA:1802:A:H2'	25:BA:1803:A:C8	2.44	0.52
25:BA:2537:U:H2'	25:BA:2538:C:C6	2.44	0.52
31:BG:86:LYS:HG2	31:BG:132:VAL:HG22	1.92	0.52
38:BP:57:ALA:O	38:BP:60:GLU:HG2	2.08	0.52
1:AA:299:G:H2'	1:AA:300:A:C8	2.45	0.52
3:AC:151:VAL:HG22	3:AC:200:VAL:HG22	1.91	0.52
9:AI:36:GLU:HA	9:AI:45:ARG:HE	1.74	0.52
25:BA:2243:U:H2'	25:BA:2244:U:H6	1.74	0.52
49:B1:12:SER:HB2	49:B1:32:ILE:HD11	1.91	0.52
1:AA:381:C:H2'	1:AA:382:A:O4'	2.09	0.52
1:AA:673:A:H2'	1:AA:674:G:C8	2.45	0.52
14:AN:90:ARG:NE	14:AN:92:GLU:OE2	2.32	0.52
25:BA:1141:U:H4'	25:BA:1142:A:O4'	2.10	0.52
25:BA:2591:C:H2'	25:BA:2592:G:H8	1.74	0.52
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.44	0.52
12:AL:12:ARG:HH11	12:AL:12:ARG:CB	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:74:ARG:NH1	20:AT:74:ARG:HB2	2.25	0.52
25:BA:614:A:O2'	25:BA:615:U:OP2	2.24	0.52
25:BA:1405:U:O2'	25:BA:1406:U:O4'	2.27	0.52
25:BA:1980:G:O2'	25:BA:1982:U:OP2	2.26	0.52
25:BA:2285:C:OP2	51:B3:6:ARG:NE	2.32	0.52
31:BG:11:VAL:N	31:BG:48:ASN:O	2.29	0.52
43:BU:51:PHE:CD2	43:BU:93:LEU:HD11	2.45	0.52
57:CD:664:ILE:HG22	57:CD:678:ARG:HG2	1.91	0.52
60:CT:21:DG:C6	60:CT:22:DC:N4	2.78	0.52
1:AA:269:C:H2'	1:AA:270:A:C8	2.44	0.52
1:AA:530:G:H22	1:AA:1492:A:H61	1.58	0.52
1:AA:925:G:C6	1:AA:927:G:N7	2.78	0.52
24:AZ:4:C:H2'	24:AZ:5:G:C8	2.45	0.52
24:AZ:26:A:H2	24:AZ:44:G:H22	1.58	0.52
35:BM:85:VAL:HG21	35:BM:90:VAL:HG22	1.91	0.52
1:AA:545:C:H5'	4:AD:69:GLU:HB2	1.91	0.52
5:AE:15:LEU:HB2	5:AE:37:THR:HG22	1.91	0.52
19:AS:3:ARG:NH1	19:AS:7:LYS:HD3	2.25	0.52
23:AW:15:G:H22	23:AW:48:C:H42	1.58	0.52
24:AX:5:G:H2'	24:AX:6:G:H8	1.75	0.52
25:BA:807:U:O2	29:BE:69:ARG:NH2	2.43	0.52
25:BA:2850:A:N7	25:BA:2868:A:O2'	2.36	0.52
27:BC:130:LEU:HD12	27:BC:134:ASN:HB2	1.91	0.52
59:CN:28:DA:H2''	59:CN:29:DG:H8	1.74	0.52
1:AA:1055:A:H62	1:AA:1200:C:H42	1.57	0.52
11:AK:54:GLY:H	11:AK:57:LYS:HG2	1.74	0.52
12:AL:50:ARG:HD2	12:AL:90:LEU:HD21	1.91	0.52
25:BA:284:U:N3	25:BA:356:G:N1	2.24	0.52
25:BA:1469:A:H2'	25:BA:1470:A:C8	2.45	0.52
28:BD:149:ASN:OD1	28:BD:150:MEQ:N	2.43	0.52
55:CA:44:ARG:HG3	55:CA:183:ILE:HB	1.91	0.52
59:CN:18:DG:C8	61:CF:13:GLN:NE2	2.45	0.52
3:AC:79:LYS:O	3:AC:81:GLY:N	2.42	0.51
25:BA:276:U:H2'	25:BA:277:G:N3	2.25	0.51
25:BA:908:C:O2'	36:BN:70:ASP:OD2	2.26	0.51
25:BA:1078:U:H5''	25:BA:1079:C:OP1	2.09	0.51
25:BA:1595:C:H2'	25:BA:1596:A:C8	2.45	0.51
25:BA:1730:C:H1'	25:BA:1731:G:C2	2.45	0.51
25:BA:2123:G:OP2	25:BA:2169:A:H5'	2.10	0.51
25:BA:2312:U:H5'	30:BF:85:ILE:HD11	1.91	0.51
25:BA:2000:C:OP1	37:BO:5:LYS:NZ	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BB:52:A:N7	38:BP:64:TYR:OH	2.41	0.51
39:BQ:14:LYS:NZ	39:BQ:76:THR:O	2.44	0.51
56:CC:696:ASP:OD1	56:CC:697:LYS:N	2.43	0.51
57:CD:35:PHE:CD1	57:CD:101:ARG:HB3	2.45	0.51
59:CN:18:DG:H3'	61:CF:90:MET:HB3	0.52	0.51
1:AA:1451:U:OP2	1:AA:1452:C:N4	2.39	0.51
25:BA:1010:A:H5''	40:BR:66:ASN:ND2	2.25	0.51
25:BA:1596:A:O2'	25:BA:1597:A:H5'	2.10	0.51
1:AA:180:U:O2	1:AA:196:A:N6	2.44	0.51
1:AA:362:G:N2	1:AA:365:U:OP2	2.42	0.51
1:AA:874:G:C6	1:AA:875:U:C4	2.99	0.51
19:AS:3:ARG:HE	19:AS:7:LYS:HB3	1.75	0.51
25:BA:581:C:H2'	25:BA:582:A:H8	1.75	0.51
25:BA:1263:U:OP1	50:B2:13:ARG:NH1	2.44	0.51
25:BA:1408:G:H2'	25:BA:1409:U:C6	2.45	0.51
59:CN:18:DG:H5''	61:CF:90:MET:SD	2.50	0.51
3:AC:103:ILE:HB	57:CD:79:LYS:HE2	1.85	0.51
14:AN:23:LYS:HD3	14:AN:51:LEU:HD21	1.93	0.51
25:BA:357:C:H2'	25:BA:358:U:C6	2.46	0.51
25:BA:1371:G:H8	25:BA:1371:G:O5'	1.93	0.51
25:BA:1527:G:N1	25:BA:1544:A:OP2	2.44	0.51
43:BU:93:LEU:HD23	43:BU:94:ASP:O	2.10	0.51
56:CC:605:TYR:C	56:CC:606:LEU:HD12	2.31	0.51
57:CD:1069:ALA:HA	57:CD:1072:LYS:HB3	1.92	0.51
59:CN:26:DG:C6	59:CN:27:DA:N6	2.78	0.51
1:AA:913:A:OP1	12:AL:43:LYS:NZ	2.44	0.51
1:AA:1011:C:H2'	1:AA:1012:A:H8	1.75	0.51
18:AR:73:ARG:NE	18:AR:73:ARG:HA	2.25	0.51
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.92	0.51
25:BA:284:U:O2	25:BA:356:G:C2	2.63	0.51
25:BA:1868:C:H2'	25:BA:1869:G:H8	1.75	0.51
25:BA:2805:C:H2'	25:BA:2806:C:O4'	2.11	0.51
25:BA:2884:U:C2	50:B2:50:ARG:HG2	2.46	0.51
27:BC:123:ALA:O	27:BC:128:ASN:ND2	2.44	0.51
27:BC:142:HIS:HD2	27:BC:193:GLY:O	1.93	0.51
30:BF:43:ALA:HB1	30:BF:50:LEU:HB2	1.92	0.51
61:CF:71:VAL:HG12	61:CF:73:MET:HB2	1.93	0.51
6:AF:79:ARG:HG3	6:AF:80:PHE:N	2.25	0.51
15:AO:25:THR:HG23	15:AO:66:LEU:HD22	1.92	0.51
15:AO:80:GLN:O	15:AO:83:GLU:HG2	2.11	0.51
42:BT:41:LYS:O	42:BT:44:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BV:14:LEU:HD11	44:BV:71:ALA:HB2	1.93	0.51
59:CN:34:DT:H6	59:CN:34:DT:H5'	1.74	0.51
1:AA:312:C:H2'	1:AA:313:A:C8	2.46	0.51
6:AF:10:VAL:HG22	6:AF:84:VAL:HG12	1.93	0.51
9:AI:129:LYS:NZ	23:AW:33:U:OP1	2.43	0.51
15:AO:18:ASP:O	15:AO:20:ASN:N	2.43	0.51
25:BA:2156:G:C6	25:BA:2157:G:N2	2.79	0.51
25:BA:2316:G:H4'	30:BF:125:ARG:NH1	2.24	0.51
25:BA:2788:C:O2'	25:BA:2809:A:N3	2.44	0.51
28:BD:102:ALA:HA	28:BD:180:VAL:HG11	1.91	0.51
57:CD:482:ALA:O	57:CD:488:ASN:ND2	2.44	0.51
25:BA:150:U:H2'	25:BA:151:C:H6	1.76	0.51
25:BA:151:C:H2'	25:BA:152:A:H8	1.76	0.51
25:BA:2547:A:H2'	25:BA:2548:U:C6	2.46	0.51
34:BL:88:ASN:OD1	34:BL:90:ASN:N	2.42	0.51
56:CC:519:ASN:C	56:CC:519:ASN:OD1	2.49	0.51
57:CD:288:PRO:HB3	61:CF:107:GLU:OE2	2.10	0.51
1:AA:1034:G:H2'	1:AA:1035:A:C8	2.46	0.51
2:AB:129:LEU:O	2:AB:133:GLU:HB2	2.11	0.51
11:AK:92:GLY:O	11:AK:94:GLU:N	2.43	0.51
13:AM:92:ARG:NH1	25:BA:888:C:O2'	2.41	0.51
25:BA:276:U:O2'	25:BA:278:A:N6	2.40	0.51
25:BA:340:A:O2'	29:BE:162:ARG:NH1	2.44	0.51
35:BM:23:ILE:HG12	41:BS:82:HIS:CD2	2.45	0.51
56:CC:1079:ILE:HG23	56:CC:1079:ILE:O	2.11	0.51
56:CC:1098:LEU:HD12	56:CC:1098:LEU:N	2.26	0.51
56:CC:1165:SER:O	56:CC:1167:GLU:N	2.40	0.51
1:AA:1096:C:H2'	1:AA:1097:C:H6	1.76	0.50
1:AA:1390:U:H2'	1:AA:1391:U:C6	2.46	0.50
11:AK:79:ILE:HB	11:AK:105:PHE:HE2	1.76	0.50
14:AN:46:LEU:O	14:AN:50:THR:HG23	2.11	0.50
25:BA:1365:A:O2'	47:BY:11:ARG:NH2	2.44	0.50
25:BA:2747:G:O6	25:BA:2755:C:H5''	2.11	0.50
39:BQ:99:TYR:HD1	39:BQ:103:ARG:HD2	1.75	0.50
60:CT:9:DC:H2'	60:CT:10:DT:C5	2.45	0.50
1:AA:147:G:O2'	1:AA:148:G:O4'	2.28	0.50
1:AA:1160:G:H5''	2:AB:131:LYS:NZ	2.26	0.50
25:BA:150:U:H2'	25:BA:151:C:C6	2.46	0.50
37:BO:24:MET:HG2	37:BO:44:LEU:HD22	1.92	0.50
38:BP:7:ARG:HH12	38:BP:95:SER:HB3	1.76	0.50
57:CD:1075:ARG:HH21	57:CD:1102:PRO:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1244:G:C6	1:AA:1294:G:C6	2.99	0.50
2:AB:187:VAL:HG13	2:AB:191:SER:HB2	1.93	0.50
8:AH:96:MET:HB3	8:AH:99:LEU:HB2	1.93	0.50
18:AR:63:ARG:HD3	18:AR:70:TYR:CD1	2.46	0.50
23:AW:19:G:H5''	23:AW:20:H2U:H52	1.92	0.50
25:BA:1413:A:H2'	25:BA:1414:C:O4'	2.11	0.50
57:CD:558:ASP:OD1	57:CD:561:GLY:N	2.43	0.50
57:CD:767:LEU:HD12	57:CD:767:LEU:N	2.27	0.50
1:AA:71:A:C6	1:AA:100:G:C5	2.99	0.50
10:AJ:41:PRO:HA	10:AJ:72:ARG:HD3	1.94	0.50
10:AJ:56:HIS:CG	10:AJ:57:VAL:H	2.29	0.50
25:BA:1421:G:C2	25:BA:1422:G:C8	2.99	0.50
25:BA:2085:U:O2	25:BA:2234:G:O6	2.28	0.50
25:BA:2327:A:H2'	25:BA:2328:A:C8	2.46	0.50
39:BQ:2:SER:OG	39:BQ:3:ASN:N	2.44	0.50
42:BT:4:ILE:HG12	42:BT:106:VAL:HG22	1.92	0.50
56:CC:696:ASP:CG	56:CC:697:LYS:N	2.65	0.50
25:BA:550:U:H2'	25:BA:551:G:C8	2.41	0.50
25:BA:1528:A:OP2	25:BA:1543:G:N2	2.42	0.50
25:BA:2252:G:H2'	25:BA:2253:G:C8	2.46	0.50
33:BK:58:ASN:OD1	33:BK:61:LYS:NZ	2.39	0.50
57:CD:1064:SER:HB3	57:CD:1169:THR:HB	1.93	0.50
1:AA:8:A:C6	4:AD:206:LYS:HA	2.46	0.50
1:AA:420:U:H2'	1:AA:422:C:C5	2.47	0.50
1:AA:1309:G:OP2	13:AM:98:ARG:NE	2.33	0.50
7:AG:69:VAL:HG11	7:AG:134:ALA:HB1	1.94	0.50
22:AV:44:A:O2'	22:AV:44:A:N3	2.45	0.50
22:AV:52:C:H2'	22:AV:53:G:C1'	2.42	0.50
24:AZ:19:G:O2'	24:AZ:20:H2U:H52	2.11	0.50
25:BA:721:A:H2'	25:BA:722:A:H8	1.75	0.50
25:BA:1060:U:C2	25:BA:1062:G:H5'	2.47	0.50
1:AA:979:C:O2	14:AN:59:ARG:NE	2.44	0.50
1:AA:1307:U:O4	1:AA:1330:U:O4	2.29	0.50
9:AI:41:ARG:HH21	9:AI:41:ARG:HG3	1.77	0.50
13:AM:52:GLN:OE1	13:AM:52:GLN:N	2.44	0.50
25:BA:2175:C:H2'	25:BA:2176:A:C8	2.46	0.50
25:BA:2286:G:OP2	51:B3:6:ARG:NH2	2.45	0.50
37:BO:101:GLY:O	37:BO:109:PRO:HA	2.11	0.50
1:AA:84:U:H2'	1:AA:86:G:N2	2.27	0.50
1:AA:946:A:H2'	1:AA:947:G:H8	1.76	0.50
13:AM:83:LEU:HD21	19:AS:65:GLU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:45:THR:HG23	18:AR:47:THR:H	1.77	0.50
23:AW:21:A:O2'	23:AW:46:A:N6	2.41	0.50
24:AZ:55:PSU:HN3	24:AZ:58:A:P	2.35	0.50
25:BA:1086:A:H4'	25:BA:1103:A:C2	2.47	0.50
25:BA:1168:G:H1	25:BA:1181:U:H3	1.58	0.50
25:BA:1607:C:N4	25:BA:1622:G:OP2	2.45	0.50
25:BA:2557:G:H2'	25:BA:2558:C:C6	2.47	0.50
47:BY:68:LEU:HB3	47:BY:72:ARG:HH12	1.76	0.50
57:CD:326:SER:O	57:CD:329:ASP:N	2.45	0.50
57:CD:428:THR:O	57:CD:428:THR:HG23	2.12	0.50
1:AA:99:C:HO2'	1:AA:100:G:H8	1.57	0.50
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.40	0.50
24:AZ:52:G:H2'	24:AZ:53:G:C8	2.46	0.50
25:BA:357:C:H2'	25:BA:358:U:H6	1.76	0.50
25:BA:2228:G:H2'	25:BA:2229:U:C6	2.46	0.50
25:BA:2552:OMU:H6	25:BA:2552:OMU:O5'	2.12	0.50
27:BC:13:ARG:HH12	27:BC:18:LYS:HE3	1.77	0.50
29:BE:28:VAL:HG13	29:BE:108:ILE:HD11	1.94	0.50
30:BF:48:LYS:C	30:BF:52:ASN:HB2	2.31	0.50
56:CC:193:ASN:HD22	56:CC:193:ASN:N	2.10	0.50
56:CC:1070:HIS:NE2	56:CC:1114:GLU:OE1	2.45	0.50
57:CD:149:GLY:HA2	57:CD:176:PHE:HB2	1.93	0.50
60:CT:18:DC:H2'	60:CT:19:DG:H8	1.73	0.50
23:AW:7:G:O2'	23:AW:49:G:O4'	2.30	0.49
23:AW:55:PSU:O5'	23:AW:55:PSU:H6	1.95	0.49
25:BA:404:A:H1'	25:BA:406:G:C5	2.46	0.49
25:BA:1936:A:H2	25:BA:1943:U:N3	2.03	0.49
1:AA:652:U:O4	1:AA:752:G:O2'	2.25	0.49
1:AA:1051:C:H42	1:AA:1207:2MG:HN1	1.60	0.49
25:BA:619:G:P	25:BA:620:G:H22	2.34	0.49
25:BA:1216:G:H5''	40:BR:11:ARG:NH1	2.27	0.49
25:BA:1826:G:O2'	25:BA:1971:U:OP2	2.28	0.49
26:BB:59:A:O2'	38:BP:1:MET:HG3	2.12	0.49
30:BF:171:ALA:O	30:BF:174:ASP:N	2.44	0.49
39:BQ:22:PRO:HD3	39:BQ:50:ILE:HD12	1.93	0.49
57:CD:1360:GLY:HA2	58:CE:17:PHE:CZ	2.47	0.49
1:AA:91:U:H2'	1:AA:92:U:H6	1.76	0.49
1:AA:713:G:H2'	1:AA:714:G:C8	2.47	0.49
3:AC:11:ARG:NH2	3:AC:175:LEU:O	2.40	0.49
9:AI:40:GLY:HA2	9:AI:45:ARG:NH2	2.26	0.49
15:AO:21:ASP:OD1	15:AO:22:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1223:G:OP2	41:BS:90:ARG:NH1	2.46	0.49
25:BA:1808:A:H3'	25:BA:1809:A:C8	2.46	0.49
25:BA:2698:U:H2'	25:BA:2699:C:C6	2.48	0.49
57:CD:1050:THR:C	57:CD:1057:SER:HB3	2.33	0.49
61:CF:47:GLU:CG	61:CF:64:PHE:CE1	2.64	0.49
24:AZ:51:U:H2'	24:AZ:52:G:H8	1.77	0.49
25:BA:464:U:O3'	52:B4:12:ARG:NH1	2.44	0.49
25:BA:1074:G:H2'	25:BA:1075:C:C6	2.48	0.49
33:BK:58:ASN:HB3	33:BK:61:LYS:HD2	1.95	0.49
57:CD:72:CYS:HB2	57:CD:87:LYS:HD3	1.93	0.49
59:CN:31:DG:H2''	59:CN:32:DA:C8	2.48	0.49
60:CT:20:DC:H2'	60:CT:21:DG:H8	1.78	0.49
1:AA:81:A:N6	1:AA:89:G:O6	2.45	0.49
1:AA:376:G:H5'	16:AP:5:ARG:HB2	1.93	0.49
1:AA:1095:U:H2'	1:AA:1096:C:C6	2.48	0.49
1:AA:1227:A:N3	13:AM:116:ILE:HD12	2.26	0.49
25:BA:2780:G:N1	33:BK:102:GLU:OE2	2.44	0.49
25:BA:2900:A:C6	25:BA:2901:C:N4	2.80	0.49
37:BO:33:ILE:HB	37:BO:118:ARG:HD2	1.93	0.49
56:CC:705:GLU:HB3	56:CC:794:LEU:H	1.77	0.49
60:CT:28:DG:H3'	61:CF:18:PHE:CE1	2.47	0.49
1:AA:375:U:OP1	16:AP:70:ARG:NH1	2.45	0.49
1:AA:707:U:OP1	11:AK:87:LYS:NZ	2.31	0.49
1:AA:1055:A:C6	1:AA:1206:G:C5	3.01	0.49
3:AC:2:GLY:O	3:AC:4:LYS:NZ	2.36	0.49
3:AC:123:GLN:O	3:AC:128:VAL:HG23	2.12	0.49
12:AL:88:LYS:HG2	12:AL:89:D2T:H6	1.93	0.49
24:AX:38:A:H2'	24:AX:39:PSU:O4'	2.13	0.49
24:AZ:9:A:H62	24:AZ:23:A:H62	1.61	0.49
24:AZ:72:C:H2'	24:AZ:73:A:H8	1.77	0.49
30:BF:134:GLU:HG2	30:BF:136:ILE:HG23	1.95	0.49
55:CA:8:PHE:O	55:CA:10:LYS:NZ	2.38	0.49
56:CC:514:PHE:CE1	56:CC:760:ASN:HB3	2.48	0.49
57:CD:160:LEU:HD23	57:CD:160:LEU:H	1.78	0.49
2:AB:60:ILE:O	2:AB:63:ARG:HG3	2.13	0.49
2:AB:68:LEU:HB3	2:AB:161:LEU:HD12	1.95	0.49
6:AF:32:ALA:CB	6:AF:70:VAL:HG11	2.42	0.49
25:BA:371:A:H4'	25:BA:372:G:OP1	2.13	0.49
25:BA:887:U:H5'	25:BA:888:C:H5	1.78	0.49
25:BA:1599:U:H2'	25:BA:1600:C:H6	1.78	0.49
25:BA:1739:A:H2'	25:BA:1740:G:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BB:58:A:H2'	26:BB:59:A:O4'	2.12	0.49
1:AA:91:U:H2'	1:AA:92:U:C6	2.48	0.49
1:AA:148:G:N2	1:AA:175:C:O2	2.45	0.49
1:AA:201:G:O6	1:AA:216:U:O4	2.30	0.49
21:AU:30:ALA:HA	21:AU:33:ARG:HE	1.77	0.49
22:AV:38:A:C4	22:AV:39:C:C5	3.01	0.49
25:BA:848:C:H2'	25:BA:849:A:H8	1.77	0.49
25:BA:1019:U:OP1	25:BA:1035:U:O2'	2.21	0.49
25:BA:1038:G:C2	25:BA:1118:C:C2	3.01	0.49
37:BO:100:CYS:O	37:BO:110:MET:HB2	2.12	0.49
45:BW:27:PRO:O	45:BW:88:HIS:HA	2.12	0.49
56:CC:1276:TRP:CE2	57:CD:801:VAL:HG21	2.48	0.49
57:CD:907:HIS:ND1	57:CD:908:ILE:O	2.38	0.49
1:AA:1096:C:H2'	1:AA:1097:C:C6	2.48	0.49
8:AH:88:ARG:HB3	8:AH:88:ARG:HH11	1.78	0.49
22:AV:51:G:C2	22:AV:52:C:C4	3.01	0.49
24:AZ:26:A:C2	24:AZ:44:G:N1	2.69	0.49
25:BA:608:A:H2'	25:BA:609:A:C8	2.48	0.49
25:BA:2346:A:H4'	25:BA:2347:C:OP2	2.13	0.49
27:BC:261:LYS:HA	27:BC:264:ASP:OD2	2.13	0.49
37:BO:2:ARG:NE	37:BO:2:ARG:O	2.45	0.49
57:CD:825:VAL:HG13	57:CD:825:VAL:O	2.13	0.49
1:AA:72:A:C5	1:AA:73:C:C5	3.01	0.49
23:AW:6:G:C2	23:AW:68:C:C2	3.01	0.49
24:AZ:51:U:H2'	24:AZ:52:G:C8	2.48	0.49
25:BA:372:G:OP2	47:BY:62:LYS:HE2	2.13	0.49
25:BA:2130:U:H5''	25:BA:2133:G:C1'	2.42	0.49
38:BP:18:LEU:HD12	38:BP:23:ALA:HB3	1.94	0.49
56:CC:69:GLN:OE1	56:CC:101:ARG:NE	2.44	0.49
56:CC:1133:LYS:O	56:CC:1135:GLN:NE2	2.45	0.49
1:AA:1039:G:H2'	1:AA:1040:U:H6	1.76	0.48
4:AD:75:TYR:OH	4:AD:97:ARG:NH1	2.41	0.48
4:AD:101:VAL:HG21	4:AD:137:VAL:HG21	1.94	0.48
5:AE:13:GLU:HB2	5:AE:39:VAL:HG12	1.95	0.48
25:BA:640:C:H2'	25:BA:641:U:H6	1.79	0.48
56:CC:549:ASP:OD1	56:CC:550:VAL:N	2.46	0.48
57:CD:876:SER:HB2	57:CD:989:GLY:O	2.12	0.48
5:AE:81:LEU:HB2	5:AE:98:PRO:HB3	1.95	0.48
7:AG:109:ARG:CG	7:AG:109:ARG:HH11	2.26	0.48
18:AR:22:ASP:HB2	18:AR:25:ASP:HB2	1.94	0.48
25:BA:81:G:H2'	25:BA:82:U:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1272:A:N7	25:BA:1618:6MZ:H1'	2.28	0.48
30:BF:50:LEU:HD12	30:BF:54:ALA:HB2	1.95	0.48
47:BY:12:PRO:HB3	47:BY:30:LEU:HD23	1.94	0.48
47:BY:59:ILE:HG12	47:BY:67:VAL:HG21	1.96	0.48
61:CF:47:GLU:HG3	61:CF:64:PHE:CD1	2.44	0.48
1:AA:203:G:C2	1:AA:215:C:C2	3.01	0.48
1:AA:1382:C:C2'	1:AA:1383:C:H5'	2.43	0.48
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.47	0.48
25:BA:2291:U:H2'	25:BA:2292:U:H6	1.76	0.48
25:BA:2376:A:N3	38:BP:111:ARG:NH1	2.60	0.48
30:BF:34:ILE:HG12	30:BF:156:ILE:HG12	1.94	0.48
46:BX:33:ALA:N	46:BX:64:ASP:OD1	2.41	0.48
1:AA:1373:G:H5''	7:AG:36:LYS:HE2	1.95	0.48
19:AS:40:ILE:HD13	19:AS:66:MET:HB3	1.95	0.48
22:AV:46:G:C2	60:CT:24:DG:C2	3.01	0.48
25:BA:1167:C:C2	25:BA:1168:G:C8	3.01	0.48
25:BA:2146:C:HO2'	25:BA:2147:A:P	2.35	0.48
30:BF:52:ASN:O	30:BF:56:ASP:HB2	2.13	0.48
56:CC:944:ARG:NE	56:CC:947:GLU:OE1	2.45	0.48
1:AA:524:G:H2'	1:AA:525:C:C6	2.49	0.48
2:AB:78:GLU:OE1	2:AB:78:GLU:N	2.40	0.48
12:AL:100:GLY:HA3	12:AL:118:GLY:HA3	1.96	0.48
19:AS:47:LEU:O	19:AS:61:PHE:HA	2.13	0.48
25:BA:2122:U:OP2	25:BA:2169:A:C4	2.65	0.48
25:BA:2637:U:H5''	28:BD:83:ARG:NH2	2.28	0.48
28:BD:32:ASN:HD22	28:BD:32:ASN:N	2.11	0.48
45:BW:51:GLN:OE1	45:BW:57:TYR:OH	2.29	0.48
57:CD:312:ARG:HG2	57:CD:313:GLY:N	2.28	0.48
60:CT:17:DG:C6	60:CT:18:DC:C4	3.01	0.48
1:AA:181:A:C6	1:AA:195:A:C8	3.01	0.48
1:AA:1181:G:O2'	1:AA:1182:G:N7	2.33	0.48
10:AJ:65:TYR:HB3	14:AN:96:LEU:HD11	1.96	0.48
25:BA:599:A:C6	25:BA:659:G:C6	3.02	0.48
25:BA:2122:U:OP1	25:BA:2168:G:H2'	2.14	0.48
25:BA:2139:U:C2	25:BA:2152:G:O6	2.67	0.48
30:BF:10:ASP:HB2	30:BF:11:GLU:CD	2.34	0.48
37:BO:42:LYS:HG2	37:BO:45:ARG:NH2	2.28	0.48
59:CN:28:DA:H2''	59:CN:29:DG:C8	2.48	0.48
3:AC:77:ILE:HG12	3:AC:84:VAL:HG21	1.96	0.48
12:AL:7:LEU:HD23	12:AL:7:LEU:HA	1.67	0.48
18:AR:71:THR:C	18:AR:73:ARG:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1590:A:C6	25:BA:1591:A:C6	3.01	0.48
30:BF:58:ALA:HB2	30:BF:65:PRO:HD3	1.94	0.48
56:CC:758:ARG:NH2	56:CC:762:ASN:OD1	2.41	0.48
1:AA:6:G:N2	5:AE:103:THR:HG23	2.28	0.48
1:AA:677:U:H3	1:AA:713:G:H22	1.60	0.48
1:AA:1078:U:H4'	5:AE:138:ARG:NH1	2.29	0.48
1:AA:1246:A:C6	1:AA:1292:G:C6	3.01	0.48
1:AA:1277:C:O2'	1:AA:1278:G:P	2.71	0.48
25:BA:945:A:C5	25:BA:2448:A:C2	3.01	0.48
25:BA:2280:G:C2	25:BA:2281:A:C8	3.01	0.48
25:BA:2720:U:OP1	39:BQ:53:ARG:NH2	2.46	0.48
31:BG:155:GLU:OE1	31:BG:157:TYR:N	2.47	0.48
60:CT:9:DC:H2'	60:CT:10:DT:H71	1.95	0.48
1:AA:376:G:H4'	16:AP:5:ARG:HD2	1.96	0.48
1:AA:1215:G:C2	1:AA:1216:A:C8	3.01	0.48
13:AM:34:LEU:HD13	13:AM:41:GLU:HG2	1.94	0.48
27:BC:66:ASP:OD2	27:BC:102:ARG:NH1	2.47	0.48
28:BD:12:THR:OG1	28:BD:13:ARG:N	2.45	0.48
55:CB:11:PRO:O	55:CB:12:ARG:HD2	2.14	0.48
56:CC:746:ALA:HB2	56:CC:967:LEU:HD21	1.95	0.48
57:CD:301:GLU:OE1	57:CD:312:ARG:NH1	2.47	0.48
1:AA:1011:C:H2'	1:AA:1012:A:C8	2.48	0.48
3:AC:50:ALA:HA	3:AC:72:ARG:HE	1.79	0.48
4:AD:192:SER:OG	4:AD:194:ASP:OD2	2.29	0.48
6:AF:21:MET:HG2	6:AF:24:ARG:HH21	1.78	0.48
7:AG:14:PRO:HB3	7:AG:21:GLU:OE1	2.14	0.48
9:AI:6:TYR:CE2	9:AI:90:TYR:HD1	2.31	0.48
23:AW:44:A:H2'	23:AW:45:G:O4'	2.14	0.48
23:AW:74:C:H42	25:BA:2252:G:H1	1.61	0.48
25:BA:1012:U:OP2	40:BR:70:ARG:NH1	2.44	0.48
25:BA:2052:A:O2'	28:BD:148:GLN:O	2.26	0.48
25:BA:2316:G:H4'	30:BF:125:ARG:HH11	1.78	0.48
35:BM:17:LYS:HE2	35:BM:27:LEU:HD11	1.96	0.48
43:BU:10:VAL:HG12	43:BU:11:LEU:HD23	1.95	0.48
57:CD:35:PHE:CZ	57:CD:101:ARG:HD2	2.48	0.48
1:AA:750:C:O2'	15:AO:21:ASP:OD1	2.31	0.47
1:AA:1383:C:O2'	1:AA:1384:C:H5'	2.13	0.47
7:AG:78:ARG:HG3	7:AG:79:ARG:N	2.28	0.47
25:BA:2187:U:O2'	25:BA:2188:U:H5'	2.13	0.47
25:BA:2498:OMC:HM23	25:BA:2498:OMC:H1'	1.60	0.47
29:BE:48:THR:N	29:BE:51:GLU:OE1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BW:55:GLU:H	45:BW:55:GLU:CD	2.17	0.47
59:CN:27:DA:C6	59:CN:28:DA:C6	3.02	0.47
1:AA:567:G:H2'	1:AA:568:G:O4'	2.14	0.47
25:BA:638:G:C5	25:BA:651:G:C2	3.02	0.47
26:BB:16:G:N2	26:BB:69:G:H1'	2.28	0.47
27:BC:37:ASN:HB2	27:BC:62:TYR:HB2	1.97	0.47
57:CD:826:ILE:HG22	57:CD:994:SER:N	2.29	0.47
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.79	0.47
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.50	0.47
12:AL:50:ARG:HB3	12:AL:66:TYR:HE1	1.80	0.47
14:AN:7:LYS:O	14:AN:11:VAL:HG13	2.13	0.47
24:AZ:21:A:O2'	24:AZ:46:7MG:HM71	2.13	0.47
25:BA:833:A:H2'	25:BA:834:G:H8	1.80	0.47
26:BB:118:C:C2	26:BB:119:A:C8	3.03	0.47
56:CC:23:ASP:OD1	56:CC:23:ASP:N	2.47	0.47
1:AA:46:G:H2'	1:AA:366:A:N7	2.29	0.47
1:AA:195:A:C2'	1:AA:196:A:H5'	2.43	0.47
3:AC:28:GLU:OE1	3:AC:28:GLU:N	2.46	0.47
25:BA:250:G:H2'	25:BA:251:A:C8	2.49	0.47
25:BA:2345:G:N3	25:BA:2381:A:H2'	2.29	0.47
31:BG:17:VAL:HB	31:BG:45:HIS:CE1	2.50	0.47
32:BH:97:ARG:HH11	32:BH:112:LYS:HD2	1.79	0.47
41:BS:1:MET:HA	41:BS:42:ALA:O	2.13	0.47
50:B2:31:ASP:O	50:B2:35:GLY:CA	2.61	0.47
57:CD:606:ASN:ND2	57:CD:610:ARG:HH21	2.12	0.47
57:CD:961:SER:HB2	57:CD:981:GLU:HB2	1.97	0.47
60:CT:22:DC:H2''	60:CT:23:DC:C6	2.50	0.47
1:AA:36:C:H2'	1:AA:37:U:O4'	2.14	0.47
1:AA:1175:G:HO2'	1:AA:1176:A:P	2.38	0.47
1:AA:1218:C:H2'	1:AA:1219:A:H8	1.78	0.47
6:AF:47:LEU:HD21	6:AF:57:ALA:HB3	1.96	0.47
13:AM:59:GLU:O	13:AM:62:LYS:HB2	2.15	0.47
24:AX:26:A:H2'	24:AX:27:G:H8	1.79	0.47
25:BA:1406:U:O2'	25:BA:1407:G:H5''	2.14	0.47
25:BA:1580:A:H2'	25:BA:1581:G:O4'	2.14	0.47
25:BA:2303:G:O6	25:BA:2314:A:N6	2.47	0.47
25:BA:2506:U:OP2	25:BA:2576:G:N1	2.33	0.47
30:BF:57:LEU:HD12	30:BF:87:CYS:SG	2.54	0.47
32:BH:67:ALA:O	32:BH:70:GLU:HG2	2.15	0.47
51:B3:5:ILE:H	51:B3:5:ILE:HD13	1.79	0.47
56:CC:28:LEU:HD23	56:CC:28:LEU:HA	1.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:CC:516:ASP:O	56:CC:518:ASN:N	2.45	0.47
57:CD:441:LEU:HD22	57:CD:441:LEU:H	1.79	0.47
2:AB:66:LYS:HB2	2:AB:158:PRO:HA	1.95	0.47
9:AI:18:ARG:NH1	9:AI:66:THR:OG1	2.47	0.47
25:BA:404:A:N6	25:BA:421:C:O2'	2.47	0.47
25:BA:1473:G:C6	25:BA:1519:G:C6	3.02	0.47
25:BA:1588:G:C2	25:BA:1589:U:C4	3.02	0.47
25:BA:1591:A:H2'	25:BA:1592:C:H6	1.78	0.47
25:BA:1614:A:N1	42:BT:93:ALA:HB2	2.30	0.47
25:BA:2104:C:H42	25:BA:2185:U:H3	1.60	0.47
25:BA:2474:U:O4	25:BA:2529:G:N2	2.48	0.47
25:BA:2692:G:C6	25:BA:2718:G:C6	3.02	0.47
25:BA:2707:U:O2	37:BO:71:ARG:NH2	2.47	0.47
26:BB:2:G:C6	26:BB:119:A:N1	2.82	0.47
40:BR:83:LEU:HD22	40:BR:88:VAL:HB	1.96	0.47
1:AA:363:A:N6	12:AL:27:CYS:SG	2.87	0.47
1:AA:611:C:H2'	1:AA:612:C:H6	1.79	0.47
1:AA:745:G:H2'	1:AA:746:A:H8	1.80	0.47
1:AA:978:A:C5	1:AA:1319:A:C2	3.03	0.47
1:AA:996:A:C4	1:AA:997:U:C5	3.03	0.47
1:AA:1026:G:H2'	1:AA:1027:C:C5	2.50	0.47
6:AF:29:ILE:HG23	6:AF:34:GLY:HA3	1.97	0.47
23:AW:20:H2U:H61	23:AW:20:H2U:C5'	2.44	0.47
24:AZ:18:G:C2	24:AZ:58:A:C8	3.03	0.47
24:AZ:21:A:C6	24:AZ:46:7MG:H81	2.50	0.47
25:BA:9:G:N2	25:BA:2895:G:C4	2.83	0.47
25:BA:1045:C:N4	25:BA:1111:A:H2'	2.29	0.47
25:BA:1251:C:OP2	40:BR:6:ARG:NH2	2.48	0.47
25:BA:2104:C:N4	25:BA:2185:U:N3	2.62	0.47
25:BA:2164:C:O2	25:BA:2164:C:H2'	2.14	0.47
25:BA:2806:C:C4	25:BA:2807:U:C4	3.02	0.47
25:BA:2812:G:H2'	25:BA:2813:A:O4'	2.14	0.47
32:BH:8:LYS:NZ	32:BH:9:VAL:O	2.48	0.47
32:BH:46:PHE:O	32:BH:50:ARG:HG3	2.15	0.47
37:BO:86:ARG:NH1	37:BO:117:ASP:O	2.47	0.47
40:BR:100:VAL:O	40:BR:103:LYS:NZ	2.48	0.47
44:BV:44:LYS:N	44:BV:59:VAL:O	2.48	0.47
46:BX:53:CYS:SG	46:BX:57:HIS:HA	2.55	0.47
56:CC:85:CYS:SG	56:CC:90:VAL:HG23	2.55	0.47
57:CD:175:GLU:CD	57:CD:175:GLU:H	2.18	0.47
57:CD:474:LEU:HD21	58:CE:27:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CD:755:ILE:HG22	57:CD:757:THR:H	1.80	0.47
59:CN:13:DC:H2'	59:CN:14:DT:C4	2.49	0.47
60:CT:19:DG:C4	60:CT:20:DC:C5	3.02	0.47
1:AA:160:A:N6	1:AA:346:G:O6	2.48	0.47
18:AR:29:LEU:O	18:AR:32:TYR:N	2.47	0.47
24:AX:6:G:H2'	24:AX:7:A:H8	1.77	0.47
28:BD:28:GLU:HG2	28:BD:30:GLU:OE2	2.14	0.47
56:CC:178:PRO:HB3	56:CC:395:TYR:CZ	2.50	0.47
25:BA:348:A:H2'	25:BA:349:U:O4'	2.15	0.47
25:BA:1199:U:H1'	40:BR:4:VAL:HG22	1.97	0.47
25:BA:1872:A:C8	25:BA:1873:G:C8	3.03	0.47
25:BA:2899:A:H2'	25:BA:2900:A:H8	1.78	0.47
28:BD:8:LYS:HB2	28:BD:201:LEU:HD11	1.97	0.47
43:BU:25:GLU:HG3	43:BU:26:LYS:N	2.30	0.47
56:CC:320:ASP:N	56:CC:320:ASP:OD1	2.48	0.47
56:CC:530:ILE:HD13	56:CC:530:ILE:HA	1.66	0.47
1:AA:198:G:H1	1:AA:219:U:H3	1.63	0.47
2:AB:43:LEU:HA	2:AB:46:THR:HB	1.97	0.47
10:AJ:42:LEU:HB2	10:AJ:71:LEU:CB	2.45	0.47
25:BA:1407:G:C6	25:BA:1596:A:C6	3.03	0.47
25:BA:1529:G:H2'	25:BA:1530:G:C8	2.47	0.47
25:BA:1707:G:C8	25:BA:1756:G:C5	3.02	0.47
25:BA:1794:A:H2'	25:BA:1795:C:C6	2.50	0.47
25:BA:2683:C:O2	34:BL:70:ARG:NH2	2.48	0.47
40:BR:88:VAL:HG22	41:BS:51:VAL:HG12	1.97	0.47
44:BV:18:ASP:HA	44:BV:21:LYS:NZ	2.29	0.47
57:CD:789:LYS:HE2	57:CD:789:LYS:HB3	1.66	0.47
1:AA:312:C:H2'	1:AA:313:A:H8	1.79	0.46
2:AB:111:ILE:HG13	2:AB:112:LYS:N	2.29	0.46
24:AX:17:C:H1'	24:AX:18:G:H5''	1.97	0.46
25:BA:566:U:O2'	25:BA:809:G:OP2	2.28	0.46
25:BA:1168:G:H2'	25:BA:1169:A:H8	1.79	0.46
25:BA:1873:G:C6	25:BA:1874:C:C4	3.04	0.46
38:BP:7:ARG:NH1	38:BP:95:SER:O	2.48	0.46
40:BR:92:ARG:HA	40:BR:95:LEU:HB2	1.96	0.46
1:AA:384:G:H2'	1:AA:385:C:H6	1.78	0.46
1:AA:444:G:C6	1:AA:491:G:C6	3.02	0.46
3:AC:7:PRO:HA	3:AC:10:ILE:HG22	1.96	0.46
10:AJ:37:ARG:NH1	10:AJ:37:ARG:HB3	2.31	0.46
24:AZ:43:C:H2'	24:AZ:44:G:C8	2.51	0.46
25:BA:947:A:H2'	25:BA:948:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1163:G:OP1	41:BS:24:LYS:NZ	2.40	0.46
25:BA:2303:G:C6	25:BA:2314:A:C6	3.04	0.46
38:BP:7:ARG:HD2	38:BP:97:PHE:CZ	2.50	0.46
56:CC:494:ASN:HD22	56:CC:494:ASN:C	2.19	0.46
59:CN:23:DT:H1'	59:CN:24:DC:C4	2.51	0.46
1:AA:35:G:H2'	1:AA:36:C:C6	2.51	0.46
1:AA:399:G:H2'	1:AA:400:C:C6	2.50	0.46
1:AA:728:A:H2'	1:AA:729:A:H8	1.79	0.46
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.80	0.46
20:AT:69:LYS:HE3	20:AT:69:LYS:HB2	1.78	0.46
25:BA:640:C:H2'	25:BA:641:U:C6	2.51	0.46
26:BB:9:G:O2'	38:BP:45:SER:OG	2.22	0.46
44:BV:94:ARG:HB2	44:BV:103:ILE:HD12	1.98	0.46
56:CC:473:ARG:HH11	56:CC:473:ARG:HG3	1.80	0.46
56:CC:962:GLU:O	56:CC:966:ILE:HD13	2.14	0.46
1:AA:451:A:H61	1:AA:481:G:H5'	1.79	0.46
24:AX:49:C:C2	24:AX:50:U:C5	3.03	0.46
25:BA:839:U:H2'	25:BA:840:C:C6	2.51	0.46
25:BA:1385:A:C6	25:BA:1403:A:C5	3.03	0.46
25:BA:2086:U:H2'	25:BA:2087:G:C8	2.51	0.46
25:BA:2391:G:OP2	53:B5:35:LYS:NZ	2.36	0.46
37:BO:119:SER:OG	37:BO:120:GLU:OE2	2.33	0.46
45:BW:78:GLN:O	45:BW:87:GLN:N	2.44	0.46
56:CC:606:LEU:HD12	56:CC:606:LEU:N	2.30	0.46
56:CC:617:ALA:HB2	56:CC:650:VAL:HG21	1.97	0.46
1:AA:148:G:HO2'	1:AA:149:A:P	2.38	0.46
1:AA:842:U:O3'	1:AA:846:G:C6	2.69	0.46
2:AB:19:GLN:HB2	2:AB:22:TYR:HD2	1.79	0.46
24:AZ:6:G:H2'	24:AZ:7:A:H8	1.78	0.46
25:BA:1932:A:H2'	25:BA:1933:G:O4'	2.15	0.46
30:BF:134:GLU:OE1	30:BF:136:ILE:HG12	2.14	0.46
33:BK:23:LYS:NZ	33:BK:142:ILE:O	2.46	0.46
38:BP:51:ALA:HB3	38:BP:78:VAL:HB	1.97	0.46
55:CA:68:TYR:CD1	55:CA:68:TYR:N	2.84	0.46
1:AA:74:A:H2'	1:AA:75:G:O4'	2.15	0.46
1:AA:1167:A:O2'	1:AA:1168:U:P	2.73	0.46
1:AA:1477:U:H2'	1:AA:1478:U:C6	2.50	0.46
3:AC:103:ILE:CB	57:CD:79:LYS:NZ	2.66	0.46
17:AQ:19:LYS:HA	17:AQ:48:ASP:O	2.16	0.46
25:BA:1583:A:H1'	25:BA:1585:C:N4	2.30	0.46
25:BA:1914:C:H2'	25:BA:1915:3TD:O4	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2312:U:H5'	30:BF:85:ILE:CD1	2.44	0.46
25:BA:2469:A:N6	25:BA:2481:G:O2'	2.48	0.46
25:BA:2636:C:H2'	25:BA:2637:U:H6	1.80	0.46
28:BD:4:LEU:HD13	28:BD:4:LEU:HA	1.81	0.46
57:CD:515:ARG:NH2	57:CD:718:SER:O	2.44	0.46
1:AA:1006:G:C5	1:AA:1007:U:C5	3.04	0.46
1:AA:1166:G:O2'	1:AA:1167:A:OP1	2.23	0.46
1:AA:1277:C:O2'	1:AA:1278:G:O5'	2.30	0.46
9:AI:7:TYR:HA	9:AI:19:VAL:O	2.16	0.46
25:BA:748:G:C8	25:BA:750:A:C8	3.04	0.46
56:CC:392:GLU:H	56:CC:392:GLU:CD	2.18	0.46
56:CC:632:ASP:N	56:CC:632:ASP:OD1	2.47	0.46
1:AA:373:A:C2	1:AA:374:A:C8	3.04	0.46
1:AA:946:A:C2	1:AA:947:G:C5	3.04	0.46
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.81	0.46
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.51	0.46
3:AC:53:SER:N	3:AC:69:HIS:O	2.38	0.46
12:AL:74:LEU:HD21	12:AL:104:CYS:HA	1.96	0.46
18:AR:29:LEU:HG	18:AR:59:ILE:HG12	1.97	0.46
25:BA:258:G:C2	25:BA:259:G:C8	3.03	0.46
25:BA:414:C:H2'	25:BA:415:A:C8	2.51	0.46
25:BA:1065:U:O2'	25:BA:1066:U:O5'	2.27	0.46
25:BA:1410:G:C6	25:BA:1593:A:C6	3.03	0.46
25:BA:1494:A:H2'	25:BA:1495:A:H8	1.79	0.46
25:BA:1510:G:H2'	25:BA:1511:G:O4'	2.15	0.46
25:BA:2149:U:H2'	25:BA:2150:C:C6	2.50	0.46
28:BD:152:PRO:HG3	28:BD:156:PHE:CZ	2.51	0.46
34:BL:70:ARG:HH12	34:BL:74:GLY:HA2	1.80	0.46
35:BM:79:LEU:HA	35:BM:82:LEU:HD12	1.98	0.46
35:BM:89:VAL:HG21	35:BM:123:ARG:HH21	1.80	0.46
53:B5:27:ALA:O	53:B5:28:ASN:HB2	2.16	0.46
56:CC:624:ASP:OD1	56:CC:627:GLY:N	2.30	0.46
57:CD:62:PHE:O	57:CD:101:ARG:NH2	2.41	0.46
57:CD:1100:PHE:CZ	57:CD:1200:GLU:HG3	2.51	0.46
1:AA:72:A:N6	1:AA:98:A:C2	2.84	0.46
1:AA:545:C:P	4:AD:62:ARG:HH12	2.38	0.46
1:AA:996:A:C6	1:AA:997:U:C4	3.04	0.46
2:AB:99:GLY:N	2:AB:175:GLU:OE2	2.49	0.46
20:AT:15:GLU:OE2	20:AT:18:ARG:NH2	2.34	0.46
20:AT:59:ASP:OD1	20:AT:76:LYS:NZ	2.42	0.46
24:AZ:68:C:N4	24:AZ:69:G:O6	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:44:A:H2'	25:BA:45:G:O4'	2.15	0.46
25:BA:2300:C:H2'	25:BA:2301:C:C6	2.51	0.46
57:CD:1266:ILE:HB	57:CD:1278:GLU:H	1.80	0.46
1:AA:72:A:C4	1:AA:73:C:C6	3.04	0.46
1:AA:562:U:C2	12:AL:13:ALA:O	2.69	0.46
16:AP:20:VAL:HG12	16:AP:35:ARG:HA	1.98	0.46
18:AR:33:ILE:HD13	18:AR:68:LEU:HD13	1.98	0.46
25:BA:414:C:H2'	25:BA:415:A:H8	1.81	0.46
25:BA:621:A:OP2	35:BM:99:ASN:ND2	2.50	0.46
25:BA:1064:C:O2'	25:BA:1065:U:H5'	2.16	0.46
25:BA:1413:A:N6	25:BA:1590:A:N6	2.63	0.46
25:BA:2189:U:H2'	25:BA:2190:G:O4'	2.15	0.46
25:BA:2478:A:OP2	54:B6:2:LYS:NZ	2.31	0.46
25:BA:2529:G:H4'	31:BG:175:LYS:HE2	1.98	0.46
29:BE:125:SER:O	29:BE:137:LYS:NZ	2.49	0.46
43:BU:6:ARG:O	43:BU:10:VAL:HG23	2.16	0.46
1:AA:1140:C:HO2'	1:AA:1141:C:C5'	2.28	0.45
25:BA:1169:A:H2'	25:BA:1170:C:C6	2.50	0.45
25:BA:2117:A:H8	25:BA:2165:C:N4	2.10	0.45
25:BA:2804:U:HO2'	25:BA:2805:C:H6	1.64	0.45
28:BD:33:ARG:HA	28:BD:94:GLN:O	2.16	0.45
28:BD:34:VAL:HG22	28:BD:50:VAL:HG12	1.97	0.45
29:BE:113:VAL:HG12	29:BE:118:LEU:HD23	1.97	0.45
32:BH:41:LYS:O	32:BH:45:GLU:HG2	2.16	0.45
56:CC:563:THR:OG1	56:CC:564:PRO:HD2	2.16	0.45
60:CT:1:DC:H6	60:CT:1:DC:H2'	1.65	0.45
5:AE:93:ARG:HG3	5:AE:128:TYR:HB2	1.97	0.45
7:AG:58:GLU:OE1	7:AG:58:GLU:N	2.49	0.45
25:BA:543:A:C6	25:BA:544:G:C6	3.04	0.45
25:BA:1292:G:H2'	25:BA:1293:C:C6	2.51	0.45
25:BA:1499:C:C2	25:BA:1500:G:C8	3.03	0.45
25:BA:1796:U:H2'	25:BA:1797:G:H8	1.80	0.45
29:BE:165:HIS:CE1	29:BE:166:LYS:HG3	2.51	0.45
56:CC:524:ILE:HG22	56:CC:525:THR:N	2.30	0.45
1:AA:706:A:C5	1:AA:707:U:C5	3.05	0.45
6:AF:11:HIS:HD2	6:AF:13:ASP:H	1.64	0.45
7:AG:77:SER:HB3	24:AZ:32:PSU:H4'	1.98	0.45
24:AZ:21:A:C2	24:AZ:46:7MG:C4	3.04	0.45
25:BA:1315:C:O2'	25:BA:1392:A:N3	2.41	0.45
25:BA:2102:G:C6	25:BA:2188:U:C4	3.04	0.45
25:BA:2162:G:H3'	25:BA:2162:G:P	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2522:U:O2'	25:BA:2647:U:OP1	2.24	0.45
25:BA:2636:C:H2'	25:BA:2637:U:C6	2.52	0.45
25:BA:2885:G:N2	50:B2:32:LYS:HB3	2.32	0.45
26:BB:9:G:C6	26:BB:112:G:C6	3.04	0.45
29:BE:48:THR:HG23	29:BE:86:ALA:HB3	1.98	0.45
30:BF:42:GLU:HB2	30:BF:49:LEU:HD23	1.97	0.45
47:BY:31:PRO:HG2	47:BY:33:LEU:HD23	1.98	0.45
1:AA:1239:A:H62	1:AA:1299:A:N6	2.00	0.45
1:AA:1435:G:H2'	1:AA:1436:U:H6	1.82	0.45
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.17	0.45
13:AM:81:MET:SD	13:AM:92:ARG:HB3	2.57	0.45
24:AX:42:C:C2'	24:AX:43:C:H5'	2.46	0.45
25:BA:2314:A:H2'	25:BA:2315:G:C8	2.51	0.45
25:BA:2315:G:HO2'	25:BA:2316:G:H8	1.62	0.45
29:BE:28:VAL:O	29:BE:32:VAL:HG13	2.17	0.45
32:BH:4:ILE:HD11	32:BH:37:VAL:HB	1.98	0.45
32:BH:117:LEU:HD21	32:BH:120:GLY:HA2	1.99	0.45
1:AA:17:U:H2'	1:AA:18:C:C6	2.51	0.45
1:AA:412:A:H62	1:AA:431:A:H61	1.64	0.45
1:AA:590:U:H2'	1:AA:591:U:H6	1.82	0.45
1:AA:1239:A:N6	1:AA:1299:A:H62	1.99	0.45
6:AF:69:GLU:HG2	6:AF:70:VAL:H	1.80	0.45
12:AL:35:THR:OG1	12:AL:54:ARG:O	2.22	0.45
17:AQ:25:ILE:O	17:AQ:25:ILE:HG22	2.16	0.45
24:AZ:9:A:H3'	24:AZ:11:C:OP2	2.17	0.45
24:AZ:16:H2U:H3'	24:AZ:60:U:O2	2.17	0.45
25:BA:273:G:H2'	25:BA:274:C:O4'	2.15	0.45
25:BA:301:G:C6	25:BA:317:G:C5	3.04	0.45
25:BA:593:U:H2'	25:BA:594:U:C6	2.51	0.45
25:BA:1106:G:C4	25:BA:1107:G:C8	3.04	0.45
25:BA:1408:G:H2'	25:BA:1409:U:H6	1.80	0.45
25:BA:1744:A:H3'	25:BA:1745:A:H8	1.82	0.45
25:BA:1916:A:H2'	25:BA:1917:PSU:H6	1.79	0.45
25:BA:2104:C:N4	25:BA:2185:U:H3	2.14	0.45
26:BB:30:C:H1'	26:BB:57:A:H61	1.81	0.45
28:BD:39:ASP:N	28:BD:39:ASP:OD1	2.49	0.45
30:BF:50:LEU:O	30:BF:54:ALA:HB3	2.16	0.45
30:BF:127:ASN:ND2	30:BF:157:THR:HG23	2.32	0.45
56:CC:1278:LEU:HD23	56:CC:1278:LEU:HA	1.50	0.45
57:CD:45:ASN:HB3	57:CD:48:THR:O	2.17	0.45
57:CD:108:ALA:HB3	57:CD:279:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CD:247:PRO:HA	57:CD:250:ARG:CZ	2.45	0.45
57:CD:319:SER:O	57:CD:321:LYS:N	2.49	0.45
1:AA:109:A:H62	1:AA:324:G:H21	1.65	0.45
6:AF:49:TYR:HA	18:AR:75:GLN:O	2.17	0.45
6:AF:104:LYS:HE3	6:AF:104:LYS:HB3	1.65	0.45
24:AX:50:U:H2'	24:AX:51:U:H6	1.80	0.45
25:BA:24:G:H2'	25:BA:25:U:C6	2.51	0.45
25:BA:638:G:H2'	25:BA:639:U:O4'	2.17	0.45
25:BA:657:U:H2'	25:BA:658:U:C6	2.52	0.45
25:BA:1800:C:OP1	27:BC:258:ARG:NH2	2.46	0.45
35:BM:123:ARG:NH1	35:BM:143:GLU:OE2	2.50	0.45
38:BP:56:LYS:HE3	38:BP:56:LYS:HB2	1.70	0.45
41:BS:63:VAL:HG22	41:BS:96:VAL:HG12	1.98	0.45
45:BW:61:LEU:O	45:BW:71:LYS:HA	2.17	0.45
55:CB:84:ASN:ND2	55:CB:130:ILE:HA	2.32	0.45
57:CD:366:CYS:O	57:CD:439:PRO:HA	2.15	0.45
1:AA:1140:C:O2'	1:AA:1141:C:H6	1.99	0.45
2:AB:129:LEU:CD2	2:AB:134:ALA:HB2	2.44	0.45
9:AI:18:ARG:HB2	9:AI:66:THR:OG1	2.16	0.45
19:AS:34:TRP:HD1	19:AS:52:HIS:HD1	1.64	0.45
24:AX:20:H2U:O2'	24:AX:21:A:H5''	2.16	0.45
25:BA:379:G:C2	25:BA:396:G:C6	3.04	0.45
29:BE:14:VAL:HG12	29:BE:197:GLU:OE1	2.16	0.45
32:BH:4:ILE:HD12	32:BH:4:ILE:O	2.16	0.45
35:BM:86:GLU:OE1	35:BM:86:GLU:N	2.50	0.45
56:CC:197:ARG:NH1	56:CC:201:ARG:O	2.47	0.45
1:AA:986:U:H2'	1:AA:987:G:H8	1.78	0.45
1:AA:1440:U:H3	1:AA:1461:G:H1	1.65	0.45
18:AR:41:PRO:O	18:AR:45:THR:HG22	2.16	0.45
24:AX:67:C:H2'	24:AX:68:C:C6	2.51	0.45
25:BA:102:U:O4	48:BZ:2:LYS:N	2.49	0.45
25:BA:1051:G:C5	25:BA:1052:C:C5	3.05	0.45
25:BA:1062:G:C2	25:BA:1077:A:N7	2.85	0.45
25:BA:1177:G:O2'	25:BA:1178:C:O4'	2.35	0.45
25:BA:1477:A:C4	25:BA:1515:A:C6	3.04	0.45
42:BT:20:VAL:HG11	42:BT:44:ALA:HA	1.99	0.45
56:CC:56:VAL:HG21	56:CC:468:LEU:HB3	1.99	0.45
57:CD:500:ILE:O	57:CD:500:ILE:HG22	2.16	0.45
57:CD:850:LYS:N	57:CD:855:ASP:O	2.40	0.45
59:CN:32:DA:H5'	59:CN:32:DA:H8	1.78	0.45
1:AA:148:G:O2'	1:AA:149:A:O5'	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:156:C:H2'	1:AA:157:U:O4'	2.16	0.45
1:AA:707:U:H4'	11:AK:22:HIS:ND1	2.32	0.45
1:AA:842:U:H2'	1:AA:845:A:OP1	2.16	0.45
1:AA:864:A:H5''	5:AE:90:THR:HB	1.99	0.45
1:AA:1175:G:O2'	1:AA:1176:A:H8	1.99	0.45
5:AE:72:ILE:HD12	5:AE:72:ILE:O	2.16	0.45
25:BA:39:G:H2'	25:BA:40:U:C6	2.52	0.45
25:BA:882:G:H1	25:BA:894:U:H3	1.64	0.45
26:BB:86:G:C8	26:BB:88:C:N4	2.85	0.45
28:BD:13:ARG:HD3	28:BD:21:SER:OG	2.16	0.45
28:BD:105:LYS:O	28:BD:177:VAL:HG22	2.17	0.45
39:BQ:8:LEU:O	39:BQ:11:GLU:HG2	2.17	0.45
46:BX:37:ILE:HG22	46:BX:38:VAL:HG23	1.99	0.45
57:CD:1064:SER:HB2	57:CD:1173:ARG:HH21	1.81	0.45
6:AF:69:GLU:O	6:AF:73:GLU:HG3	2.17	0.45
25:BA:896:A:O2'	25:BA:897:C:O4'	2.30	0.45
25:BA:1057:A:H61	25:BA:1080:A:N6	2.15	0.45
25:BA:1432:G:H2'	25:BA:1433:A:H8	1.80	0.45
25:BA:2136:G:C2	25:BA:2156:G:H1'	2.52	0.45
41:BS:68:ARG:NH1	41:BS:90:ARG:HB2	2.31	0.45
57:CD:959:LYS:HB3	57:CD:983:LYS:HB2	1.98	0.45
57:CD:1332:LEU:HA	57:CD:1332:LEU:HD12	1.75	0.45
1:AA:81:A:N6	1:AA:89:G:C6	2.85	0.44
1:AA:690:G:H2'	1:AA:691:G:O4'	2.18	0.44
1:AA:868:C:H2'	1:AA:869:G:O4'	2.17	0.44
1:AA:1352:C:C2	1:AA:1371:G:C6	3.05	0.44
3:AC:20:SER:O	14:AN:94:PRO:HB3	2.17	0.44
13:AM:49:SER:HB3	13:AM:52:GLN:OE1	2.17	0.44
25:BA:388:G:N7	25:BA:390:U:H2'	2.32	0.44
25:BA:550:U:C2	25:BA:551:G:N7	2.85	0.44
25:BA:1790:C:H2'	25:BA:1791:A:C5	2.52	0.44
30:BF:106:ILE:HG21	30:BF:139:PRO:HG3	1.98	0.44
55:CA:67:GLU:OE1	56:CC:1057:LYS:NZ	2.41	0.44
57:CD:1075:ARG:NH2	57:CD:1102:PRO:HA	2.32	0.44
1:AA:73:C:O2'	1:AA:74:A:H5'	2.17	0.44
1:AA:451:A:N1	1:AA:480:U:H2'	2.33	0.44
1:AA:636:U:H2'	1:AA:637:C:C6	2.52	0.44
1:AA:1275:A:H3'	1:AA:1276:G:H8	1.83	0.44
1:AA:1424:U:H2'	1:AA:1425:U:O4'	2.16	0.44
8:AH:18:GLN:HE21	8:AH:72:VAL:HG12	1.82	0.44
25:BA:784:G:H5'	25:BA:785:G:OP1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1107:G:C5	25:BA:1108:U:C5	3.04	0.44
25:BA:1589:U:C2	25:BA:1590:A:C8	3.05	0.44
25:BA:1731:G:C2	25:BA:1733:G:C5	3.05	0.44
25:BA:1915:3TD:H2'	25:BA:1916:A:H8	1.80	0.44
25:BA:2314:A:O2'	25:BA:2315:G:H5'	2.17	0.44
25:BA:2885:G:H21	50:B2:32:LYS:HB3	1.82	0.44
41:BS:1:MET:HG3	41:BS:43:ASN:HA	1.98	0.44
50:B2:32:LYS:HG3	50:B2:33:THR:N	2.32	0.44
56:CC:210:LEU:HA	56:CC:210:LEU:HD23	1.66	0.44
56:CC:745:GLU:HG2	56:CC:746:ALA:H	1.82	0.44
56:CC:1339:LEU:HA	56:CC:1339:LEU:HD23	1.76	0.44
1:AA:736:C:H2'	1:AA:737:C:C6	2.52	0.44
1:AA:1140:C:O2'	1:AA:1141:C:O5'	2.34	0.44
25:BA:312:G:C2	25:BA:313:G:C8	3.05	0.44
25:BA:2210:U:O2	25:BA:2212:A:H2'	2.17	0.44
39:BQ:29:LYS:HB3	39:BQ:40:LEU:CD2	2.47	0.44
56:CC:705:GLU:OE1	56:CC:705:GLU:N	2.42	0.44
1:AA:235:C:H2'	1:AA:236:A:H8	1.83	0.44
1:AA:705:G:C5	1:AA:706:A:C8	3.05	0.44
1:AA:1206:G:C6	1:AA:1207:2MG:C5	3.05	0.44
22:AV:51:G:C4	22:AV:52:C:C5	3.06	0.44
23:AW:52:G:C6	23:AW:63:G:C6	3.05	0.44
24:AX:41:C:H2'	24:AX:42:C:H6	1.82	0.44
25:BA:377:G:C6	25:BA:398:C:N3	2.85	0.44
25:BA:848:C:H2'	25:BA:849:A:C8	2.53	0.44
25:BA:958:U:H2'	26:BB:89:U:C2	2.52	0.44
25:BA:1593:A:H2'	25:BA:1594:U:C6	2.52	0.44
25:BA:2187:U:O2'	25:BA:2188:U:C6	2.68	0.44
42:BT:69:LEU:HD23	42:BT:69:LEU:HA	1.82	0.44
45:BW:78:GLN:HB3	45:BW:87:GLN:HB2	2.00	0.44
56:CC:1065:LYS:HD3	56:CC:1235:LEU:HD12	2.00	0.44
56:CC:1239:VAL:HG13	56:CC:1240:ASP:N	2.32	0.44
57:CD:478:LEU:HD23	57:CD:478:LEU:HA	1.71	0.44
1:AA:335:C:H2'	1:AA:336:A:H8	1.82	0.44
1:AA:744:C:H2'	1:AA:745:G:C8	2.50	0.44
1:AA:927:G:H2'	1:AA:928:G:H8	1.82	0.44
2:AB:64:LYS:HA	2:AB:225:ARG:HH11	1.82	0.44
2:AB:83:ALA:O	2:AB:86:SER:OG	2.24	0.44
15:AO:39:LEU:HD23	15:AO:39:LEU:HA	1.68	0.44
23:AW:17:C:H2'	23:AW:17(A):U:H6	1.82	0.44
24:AZ:46:7MG:OP2	24:AZ:46:7MG:H82	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:134:G:H2'	25:BA:135:U:C6	2.52	0.44
25:BA:996:A:H1'	41:BS:9:GLY:O	2.17	0.44
25:BA:1413:A:C6	25:BA:1590:A:C6	3.04	0.44
25:BA:2130:U:H4'	25:BA:2133:G:H1'	1.98	0.44
26:BB:48:U:H2'	26:BB:49:C:C6	2.53	0.44
32:BH:73:ASN:ND2	32:BH:142:VAL:HG21	2.31	0.44
56:CC:270:THR:HG1	56:CC:273:HIS:CE1	2.35	0.44
56:CC:660:VAL:O	56:CC:660:VAL:HG22	2.17	0.44
56:CC:1182:ILE:HG21	56:CC:1182:ILE:HD13	1.72	0.44
56:CC:1211:ARG:NH1	56:CC:1220:GLN:OE1	2.49	0.44
60:CT:19:DG:C5	60:CT:20:DC:C4	3.06	0.44
1:AA:50:A:O2'	1:AA:360:G:N2	2.51	0.44
1:AA:76:G:C4	1:AA:77:A:C8	3.05	0.44
1:AA:1384:C:H2'	1:AA:1385:G:H8	1.83	0.44
13:AM:92:ARG:HG3	25:BA:888:C:O2	2.17	0.44
15:AO:64:ARG:HD2	15:AO:64:ARG:HA	1.42	0.44
20:AT:10:ARG:HA	20:AT:10:ARG:HD3	1.73	0.44
22:AV:52:C:H2'	22:AV:53:G:O4'	2.18	0.44
25:BA:151:C:H2'	25:BA:152:A:C8	2.52	0.44
25:BA:287:G:H2'	25:BA:288:U:C6	2.53	0.44
25:BA:858:G:C2	25:BA:2268:A:C2	3.06	0.44
25:BA:1113:U:H2'	25:BA:1114:C:C6	2.53	0.44
25:BA:1524:G:C4	25:BA:1525:A:C8	3.06	0.44
25:BA:2172:U:OP2	25:BA:2173:A:H5'	2.17	0.44
27:BC:244:PRO:HB2	27:BC:252:THR:HG22	1.99	0.44
56:CC:38:PHE:CZ	56:CC:49:LEU:HD21	2.53	0.44
56:CC:493:ILE:C	56:CC:493:ILE:HD12	2.37	0.44
56:CC:1106:ARG:NH1	56:CC:1108:ASN:HD21	2.16	0.44
57:CD:139:LEU:HD23	57:CD:139:LEU:HA	1.69	0.44
1:AA:518:C:O2'	1:AA:530:G:N2	2.51	0.44
1:AA:1408:A:C6	1:AA:1494:G:C6	3.05	0.44
6:AF:43:GLY:HA2	6:AF:58:HIS:CE1	2.53	0.44
8:AH:18:GLN:OE1	8:AH:18:GLN:HA	2.17	0.44
13:AM:14:HIS:ND1	13:AM:42:ASP:HA	2.33	0.44
15:AO:70:LEU:HD12	15:AO:70:LEU:HA	1.67	0.44
25:BA:958:U:O4	36:BN:40:ARG:NE	2.50	0.44
25:BA:1068:G:C8	25:BA:1069:A:C5	3.06	0.44
25:BA:1721:G:H1'	25:BA:1739:A:H61	1.82	0.44
25:BA:2287:A:N7	25:BA:2289:G:C8	2.86	0.44
31:BG:37:LEU:HD12	31:BG:43:VAL:HG11	2.00	0.44
32:BH:7:ASP:HA	32:BH:15:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BL:76:VAL:HG12	39:BQ:73:VAL:HB	2.00	0.44
49:B1:31:ARG:HG2	49:B1:34:HIS:HB2	2.00	0.44
55:CA:96:ASP:OD1	55:CA:96:ASP:N	2.49	0.44
56:CC:166:SER:OG	57:CD:1151:LYS:HE3	2.18	0.44
56:CC:377:THR:HB	56:CC:380:ALA:HB3	1.99	0.44
57:CD:1314:LEU:HA	57:CD:1314:LEU:HD23	1.79	0.44
1:AA:6:G:O2'	1:AA:7:A:H8	2.01	0.44
1:AA:687:A:C2	1:AA:704:A:C4	3.06	0.44
1:AA:956:U:H2'	1:AA:957:U:O4'	2.18	0.44
1:AA:996:A:N6	1:AA:1046:A:O4'	2.50	0.44
2:AB:60:ILE:CG2	2:AB:65:GLY:HA3	2.48	0.44
3:AC:77:ILE:HG23	3:AC:81:GLY:HA2	2.00	0.44
17:AQ:8:LEU:HD23	17:AQ:8:LEU:HA	1.83	0.44
24:AZ:37:MIA:H121	24:AZ:38:A:C5	2.53	0.44
25:BA:2134:A:N1	25:BA:2135:A:C5	2.86	0.44
39:BQ:31:TRP:CD1	39:BQ:82:ASP:HB2	2.53	0.44
57:CD:355:ILE:HG21	57:CD:355:ILE:HD13	1.74	0.44
1:AA:108:G:C6	20:AT:10:ARG:HG2	2.52	0.44
1:AA:138:G:C6	1:AA:226:G:C6	3.06	0.44
1:AA:362:G:N2	1:AA:364:A:H3'	2.33	0.44
1:AA:590:U:OP1	8:AH:31:LYS:HG2	2.18	0.44
1:AA:706:A:C6	1:AA:707:U:C4	3.06	0.44
1:AA:1130:A:OP1	9:AI:18:ARG:NH2	2.38	0.44
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.53	0.44
6:AF:44:ARG:HG2	6:AF:56:LYS:HB3	2.00	0.44
10:AJ:15:HIS:O	10:AJ:18:ILE:HG22	2.18	0.44
19:AS:70:LYS:O	19:AS:73:GLU:N	2.51	0.44
22:AV:38:A:C5	22:AV:39:C:C5	3.06	0.44
25:BA:1028:A:H2'	25:BA:1029:A:C8	2.53	0.44
25:BA:1168:G:C6	25:BA:1182:G:C6	3.06	0.44
25:BA:1599:U:H2'	25:BA:1600:C:C6	2.53	0.44
25:BA:1789:A:C5	25:BA:1790:C:C4	3.05	0.44
25:BA:2159:G:H2'	25:BA:2160:C:C6	2.53	0.44
25:BA:2179:C:H2'	25:BA:2180:U:C6	2.53	0.44
25:BA:2289:G:C2	25:BA:2290:G:C8	3.06	0.44
25:BA:2449:H2U:H4'	25:BA:2450:A:OP1	2.18	0.44
25:BA:2901:C:N3	25:BA:2902:C:N4	2.65	0.44
27:BC:105:LEU:O	27:BC:107:PRO:HD3	2.18	0.44
31:BG:135:GLY:CA	31:BG:141:ILE:HD11	2.48	0.44
32:BH:14:SER:C	32:BH:16:GLY:H	2.21	0.44
56:CC:668:ILE:HG21	56:CC:668:ILE:HD13	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:CC:1106:ARG:HB2	56:CC:1106:ARG:HH11	1.83	0.44
56:CC:1238:LEU:CD2	56:CC:1238:LEU:H	2.31	0.44
60:CT:5:DG:H2'	60:CT:6:DA:C8	2.52	0.44
1:AA:519:C:H2'	1:AA:520:A:O4'	2.17	0.43
1:AA:765:G:C6	1:AA:812:G:C4	3.06	0.43
1:AA:1382:C:H2'	1:AA:1383:C:H5'	2.00	0.43
1:AA:1458:G:OP1	20:AT:30:THR:OG1	2.29	0.43
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.99	0.43
17:AQ:27:ARG:HH12	17:AQ:41:THR:C	2.20	0.43
23:AW:18:G:C4	23:AW:58:A:C2	3.06	0.43
24:AX:21:A:H62	24:AX:46:7MG:H2'	1.82	0.43
24:AZ:2:C:H2'	24:AZ:3:C:H6	1.82	0.43
24:AZ:9:A:H4'	24:AZ:46:7MG:H4'	2.00	0.43
25:BA:84:A:N1	25:BA:98:G:O2'	2.42	0.43
25:BA:1360:G:N7	25:BA:1361:G:C8	2.86	0.43
25:BA:2901:C:C4	25:BA:2902:C:N4	2.86	0.43
29:BE:4:VAL:HA	29:BE:11:ALA:HA	2.00	0.43
30:BF:47:LYS:O	30:BF:48:LYS:C	2.55	0.43
30:BF:103:LEU:HD12	30:BF:107:ALA:HB3	2.00	0.43
45:BW:36:ALA:O	45:BW:93:ARG:NH2	2.43	0.43
55:CA:79:LEU:HD23	55:CA:79:LEU:O	2.18	0.43
56:CC:138:ILE:HA	56:CC:138:ILE:HD13	1.59	0.43
57:CD:1226:VAL:O	57:CD:1229:VAL:HG12	2.18	0.43
60:CT:4:DT:H2''	60:CT:5:DG:H8	1.83	0.43
60:CT:22:DC:H2''	60:CT:23:DC:H5'	2.00	0.43
24:AZ:36:A:N6	24:AZ:37:MIA:HN6	2.16	0.43
24:AZ:70:G:H2'	24:AZ:71:G:C8	2.52	0.43
25:BA:303:G:C6	25:BA:315:G:C6	3.06	0.43
25:BA:1590:A:H2'	25:BA:1591:A:H8	1.80	0.43
25:BA:1869:G:N2	25:BA:1872:A:N9	2.63	0.43
25:BA:1906:G:C2	25:BA:1907:G:C8	3.06	0.43
32:BH:67:ALA:HA	32:BH:70:GLU:HG2	2.00	0.43
36:BN:68:PHE:HA	36:BN:69:PRO:HD3	1.89	0.43
55:CB:66:HIS:CE1	55:CB:68:TYR:HD1	2.36	0.43
56:CC:363:LEU:HA	56:CC:363:LEU:HD23	1.78	0.43
56:CC:794:LEU:HA	56:CC:794:LEU:HD12	1.73	0.43
57:CD:218:THR:HA	57:CD:221:ILE:HG12	2.00	0.43
57:CD:416:ILE:HD13	57:CD:416:ILE:HG21	1.62	0.43
57:CD:1350:ASN:ND2	57:CD:1358:PRO:HD3	2.32	0.43
1:AA:144:G:C6	1:AA:179:A:C6	3.05	0.43
1:AA:235:C:H2'	1:AA:236:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:561:U:HO2'	1:AA:562:U:P	2.41	0.43
1:AA:1125:U:C4	1:AA:1127:G:C4	3.07	0.43
1:AA:1183:U:H3'	1:AA:1184:G:C5'	2.49	0.43
1:AA:1521:C:H2'	1:AA:1522:U:C6	2.53	0.43
9:AI:9:THR:O	9:AI:85:ARG:HD2	2.17	0.43
25:BA:135:U:C2	25:BA:136:G:C8	3.07	0.43
25:BA:358:U:H2'	25:BA:359:G:C8	2.53	0.43
25:BA:953:G:C2	25:BA:954:G:C8	3.06	0.43
25:BA:1026:G:OP1	25:BA:1134:A:O2'	2.29	0.43
25:BA:1062:G:C2	25:BA:1063:G:C5	3.06	0.43
25:BA:2133:G:N1	25:BA:2157:G:O6	2.51	0.43
25:BA:2537:U:H2'	25:BA:2538:C:H6	1.82	0.43
26:BB:45:A:C4	26:BB:46:A:C8	3.06	0.43
35:BM:33:ARG:NH2	35:BM:40:SER:O	2.51	0.43
36:BN:16:ARG:HD3	36:BN:16:ARG:HA	1.81	0.43
43:BU:92:ASN:OD1	43:BU:92:ASN:N	2.51	0.43
56:CC:7:GLU:C	56:CC:9:LYS:H	2.21	0.43
56:CC:671:LEU:O	56:CC:673:HIS:N	2.52	0.43
57:CD:1100:PHE:CZ	57:CD:1200:GLU:CG	3.01	0.43
1:AA:684:U:O2'	11:AK:40:ASN:HB3	2.19	0.43
1:AA:877:G:C2	1:AA:878:A:C8	3.06	0.43
6:AF:15:SER:HA	6:AF:18:VAL:HG23	2.01	0.43
10:AJ:18:ILE:HD12	10:AJ:18:ILE:HA	1.71	0.43
25:BA:1027:A:C6	25:BA:1126:A:C4	3.06	0.43
25:BA:1107:G:C6	25:BA:1108:U:C4	3.06	0.43
25:BA:1494:A:O2'	25:BA:1495:A:P	2.77	0.43
25:BA:1587:G:H2'	25:BA:1588:G:H8	1.83	0.43
25:BA:1618:6MZ:H4'	25:BA:1619:G:OP2	2.17	0.43
25:BA:2100:G:C6	25:BA:2101:A:C5	3.06	0.43
31:BG:117:LEU:HD23	31:BG:117:LEU:HA	1.87	0.43
37:BO:51:LEU:HA	37:BO:51:LEU:HD13	1.86	0.43
51:B3:32:GLU:OE1	51:B3:32:GLU:N	2.41	0.43
56:CC:269:ILE:HD12	56:CC:269:ILE:N	2.33	0.43
56:CC:753:LEU:HA	56:CC:753:LEU:HD23	1.77	0.43
56:CC:766:ASN:CG	56:CC:766:ASN:O	2.56	0.43
57:CD:158:GLN:O	57:CD:158:GLN:NE2	2.46	0.43
57:CD:363:LEU:HA	57:CD:450:HIS:CD2	2.53	0.43
57:CD:504:GLN:O	57:CD:507:VAL:HG12	2.18	0.43
1:AA:1086:U:H5	1:AA:1099:G:H22	1.67	0.43
5:AE:55:GLU:N	5:AE:55:GLU:OE1	2.52	0.43
5:AE:146:ASN:OD1	5:AE:147:MET:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:41:ARG:HH21	9:AI:41:ARG:CG	2.31	0.43
25:BA:253:C:OP2	53:B5:5:LYS:NZ	2.40	0.43
25:BA:571:U:H3'	41:BS:80:ARG:HH12	1.83	0.43
25:BA:885:C:C2	25:BA:887:U:O4	2.71	0.43
25:BA:1048:A:C8	25:BA:1111:A:C6	3.06	0.43
25:BA:1407:G:O6	25:BA:1596:A:N6	2.52	0.43
25:BA:1544:A:H2'	25:BA:1545:A:C8	2.53	0.43
25:BA:2867:G:O2'	25:BA:2868:A:OP2	2.30	0.43
26:BB:29:A:H2'	26:BB:30:C:O4'	2.19	0.43
26:BB:60:C:C2	26:BB:61:G:C8	3.06	0.43
29:BE:25:GLU:OE2	35:BM:7:SER:OG	2.35	0.43
32:BH:128:HIS:O	32:BH:144:VAL:HG22	2.19	0.43
37:BO:38:LEU:HB3	37:BO:39:PRO:HD3	2.00	0.43
43:BU:33:LYS:HG3	43:BU:80:TRP:CE3	2.54	0.43
55:CB:13:LEU:HA	55:CB:28:LEU:HD13	2.00	0.43
56:CC:1238:LEU:CD2	56:CC:1238:LEU:N	2.82	0.43
57:CD:189:LEU:HD22	57:CD:234:PRO:HB3	1.99	0.43
57:CD:780:ARG:O	57:CD:780:ARG:HG2	2.19	0.43
59:CN:28:DA:C6	59:CN:29:DG:C6	3.06	0.43
1:AA:255:G:C2	1:AA:272:C:C2	3.07	0.43
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.54	0.43
1:AA:1390:U:H2'	1:AA:1391:U:H6	1.82	0.43
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	2.00	0.43
25:BA:695:G:C6	25:BA:768:G:C6	3.07	0.43
25:BA:1794:A:H2'	25:BA:1795:C:H6	1.84	0.43
25:BA:2803:G:H2'	25:BA:2804:U:C6	2.53	0.43
28:BD:8:LYS:NZ	28:BD:195:GLY:O	2.41	0.43
39:BQ:6:LYS:O	39:BQ:10:GLN:HG3	2.19	0.43
48:BZ:57:LEU:HA	48:BZ:57:LEU:HD23	1.79	0.43
56:CC:98:VAL:O	56:CC:121:GLU:HA	2.18	0.43
56:CC:799:ASN:O	56:CC:799:ASN:ND2	2.39	0.43
1:AA:704:A:C4	1:AA:705:G:C8	3.07	0.43
1:AA:1229:A:P	13:AM:113:ARG:HH11	2.42	0.43
1:AA:1443:C:H2'	1:AA:1444:U:O4'	2.19	0.43
2:AB:76:ALA:CB	2:AB:210:VAL:HG11	2.48	0.43
6:AF:7:VAL:HG13	6:AF:88:MET:HB3	1.99	0.43
15:AO:69:TYR:OH	15:AO:73:LYS:HD2	2.19	0.43
19:AS:41:PHE:N	19:AS:44:MET:SD	2.89	0.43
25:BA:110:G:C2	25:BA:111:A:C8	3.06	0.43
25:BA:287:G:H2'	25:BA:288:U:H6	1.83	0.43
25:BA:1054:A:C6	25:BA:1106:G:C6	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2135:A:C2	25:BA:2136:G:H1'	2.54	0.43
25:BA:2469:A:C6	25:BA:2482:A:C8	3.07	0.43
56:CC:530:ILE:HD12	56:CC:530:ILE:HG23	1.66	0.43
56:CC:836:LEU:HA	56:CC:836:LEU:HD23	1.82	0.43
56:CC:855:PRO:HG3	56:CC:913:VAL:HG23	1.99	0.43
56:CC:1098:LEU:N	56:CC:1098:LEU:CD1	2.82	0.43
57:CD:120:LEU:HB3	57:CD:121:PRO:CD	2.48	0.43
1:AA:71:A:C6	1:AA:72:A:N7	2.87	0.43
1:AA:1298:U:C5	7:AG:114:LYS:HE3	2.54	0.43
3:AC:73:PRO:CB	57:CD:79:LYS:HD2	2.49	0.43
12:AL:29:GLN:HB3	12:AL:81:LEU:HG	2.01	0.43
13:AM:73:ILE:O	13:AM:76:SER:OG	2.34	0.43
15:AO:67:LEU:HA	15:AO:67:LEU:HD23	1.61	0.43
22:AV:45:C:OP1	56:CC:1253:LEU:HB2	2.19	0.43
24:AZ:75:C:OP1	47:BY:20:HIS:NE2	2.50	0.43
25:BA:885:C:H2'	25:BA:887:U:O4	2.19	0.43
25:BA:2514:U:H2'	25:BA:2515:C:C6	2.54	0.43
25:BA:2783:U:H2'	25:BA:2784:U:C6	2.53	0.43
26:BB:89:U:O2'	26:BB:90:C:P	2.77	0.43
34:BL:41:ILE:HD11	34:BL:86:LEU:HD22	2.01	0.43
56:CC:1076:ILE:O	56:CC:1076:ILE:HG13	2.17	0.43
56:CC:1096:ILE:HD13	56:CC:1096:ILE:HG21	1.63	0.43
1:AA:1120:C:C2	1:AA:1121:U:C5	3.06	0.43
4:AD:7:PRO:HB2	4:AD:10:LYS:CB	2.47	0.43
10:AJ:26:VAL:HG13	10:AJ:30:LYS:HZ2	1.82	0.43
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	2.00	0.43
15:AO:42:HIS:O	15:AO:45:GLU:HG3	2.18	0.43
19:AS:70:LYS:O	19:AS:73:GLU:HB2	2.19	0.43
22:AV:25:U:H3'	22:AV:26:A:H8	1.84	0.43
24:AX:43:C:H2'	24:AX:44:G:C8	2.54	0.43
25:BA:647:G:C6	25:BA:648:G:C5	3.07	0.43
25:BA:1322:A:C5	25:BA:1323:C:C5	3.07	0.43
26:BB:24:G:N7	26:BB:56:G:H2'	2.33	0.43
28:BD:133:THR:OG1	28:BD:134:HIS:N	2.51	0.43
44:BV:18:ASP:HA	44:BV:21:LYS:HZ3	1.84	0.43
48:BZ:31:GLN:HA	48:BZ:36:GLN:OE1	2.19	0.43
56:CC:1238:LEU:N	56:CC:1238:LEU:HD23	2.33	0.43
57:CD:424:ASN:ND2	57:CD:424:ASN:C	2.72	0.43
1:AA:91:U:C2	1:AA:92:U:C5	3.07	0.43
1:AA:148:G:O2'	1:AA:149:A:C5'	2.67	0.43
1:AA:160:A:H2'	1:AA:161:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:736:C:H2'	1:AA:737:C:H6	1.82	0.43
1:AA:828:U:C4	1:AA:859:G:C4	3.07	0.43
9:AI:31:ASN:O	9:AI:33:ARG:NH2	2.51	0.43
25:BA:278:A:N1	25:BA:361:G:O2'	2.49	0.43
25:BA:1179:G:H2'	25:BA:1180:U:C6	2.53	0.43
25:BA:1735:A:C6	25:BA:1736:U:C4	3.07	0.43
26:BB:46:A:C6	26:BB:47:C:C4	3.07	0.43
27:BC:132:MET:HE1	27:BC:174:LEU:HD11	2.01	0.43
30:BF:15:LYS:O	30:BF:18:THR:OG1	2.29	0.43
30:BF:47:LYS:HG2	30:BF:51:ASP:OD2	2.18	0.43
32:BH:66:ASN:HB2	32:BH:135:HIS:HB2	2.01	0.43
56:CC:149:LEU:HA	56:CC:149:LEU:HD12	1.74	0.43
57:CD:1072:LYS:HG2	57:CD:1168:GLU:CG	2.48	0.43
60:CT:19:DG:C4	60:CT:20:DC:C6	3.07	0.43
1:AA:141:G:C6	1:AA:142:G:C5	3.07	0.42
1:AA:181:A:HO2'	1:AA:182:A:H8	1.60	0.42
1:AA:1309:G:OP2	13:AM:87:ARG:NH2	2.52	0.42
23:AW:53:G:C8	23:AW:54:5MU:H72	2.54	0.42
24:AX:26:A:H2'	24:AX:27:G:C8	2.54	0.42
24:AX:68:C:H2'	24:AX:69:G:C8	2.53	0.42
25:BA:1595:C:H2'	25:BA:1596:A:H8	1.83	0.42
42:BT:1:MET:HG2	42:BT:62:ASP:OD1	2.19	0.42
55:CA:179:PRO:HA	55:CA:208:ASN:ND2	2.34	0.42
57:CD:367:GLY:HA2	57:CD:440:VAL:O	2.19	0.42
57:CD:1100:PHE:CE2	57:CD:1200:GLU:CB	2.97	0.42
59:CN:32:DA:H1'	59:CN:33:DT:O4'	2.18	0.42
1:AA:515:G:H2'	1:AA:516:PSU:H6	1.84	0.42
1:AA:552:U:C2	1:AA:553:A:C8	3.07	0.42
13:AM:94:GLY:HA2	13:AM:109:ARG:NH2	2.34	0.42
24:AZ:36:A:H2'	24:AZ:37:MIA:C8	2.49	0.42
25:BA:1:G:C2	25:BA:2903:U:O2	2.72	0.42
25:BA:1022:G:C6	25:BA:1140:C:C4	3.07	0.42
25:BA:2225:A:H4'	25:BA:2226:C:O5'	2.19	0.42
55:CA:102:LEU:HD23	55:CA:102:LEU:C	2.39	0.42
56:CC:1257:GLN:OE1	57:CD:345:LYS:HB2	2.18	0.42
57:CD:544:LEU:HD12	57:CD:544:LEU:HA	1.79	0.42
1:AA:72:A:N6	1:AA:99:C:H1'	2.34	0.42
1:AA:646:G:C6	1:AA:647:C:C4	3.07	0.42
1:AA:1397:C:OP2	5:AE:29:ARG:NH2	2.41	0.42
2:AB:78:GLU:HG2	2:AB:79:ALA:N	2.34	0.42
9:AI:98:LEU:HD23	9:AI:98:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:40:ALA:O	13:AM:43:VAL:HG22	2.18	0.42
24:AZ:4:C:N4	24:AZ:5:G:O6	2.53	0.42
25:BA:276:U:H2'	25:BA:277:G:C2	2.54	0.42
25:BA:285:G:O6	25:BA:355:U:C2	2.72	0.42
25:BA:355:U:H2'	25:BA:356:G:H8	1.83	0.42
25:BA:636:G:N1	35:BM:76:GLU:OE1	2.51	0.42
25:BA:1799:G:OP1	27:BC:258:ARG:NE	2.47	0.42
25:BA:2074:U:H2'	25:BA:2075:U:C6	2.55	0.42
25:BA:2104:C:N4	25:BA:2185:U:C4	2.87	0.42
25:BA:2813:A:C4	25:BA:2814:A:C8	3.07	0.42
30:BF:163:ASP:OD1	30:BF:164:GLU:N	2.53	0.42
32:BH:97:ARG:NE	32:BH:101:ASP:OD1	2.52	0.42
55:CA:150:ARG:HD2	55:CB:8:PHE:CE2	2.54	0.42
55:CB:34:GLY:N	55:CB:199:ASP:OD2	2.49	0.42
56:CC:477:GLU:OE1	61:CF:87:PRO:CB	2.59	0.42
56:CC:1248:THR:HG22	56:CC:1249:GLY:N	2.34	0.42
57:CD:160:LEU:HD23	57:CD:160:LEU:N	2.33	0.42
57:CD:699:ASP:HA	57:CD:702:GLN:HG2	2.02	0.42
60:CT:10:DT:H2''	60:CT:11:DC:C6	2.55	0.42
61:CF:7:LYS:HG2	61:CF:74:VAL:HG13	2.01	0.42
1:AA:1061:G:C5	1:AA:1062:U:C4	3.08	0.42
1:AA:1172:C:H2'	1:AA:1173:U:H6	1.85	0.42
1:AA:1319:A:C8	1:AA:1323:G:C5	3.07	0.42
6:AF:88:MET:SD	18:AR:65:LEU:HD11	2.59	0.42
10:AJ:17:LEU:HD11	10:AJ:93:ALA:HB3	2.01	0.42
14:AN:48:LEU:HD12	14:AN:51:LEU:HD12	2.01	0.42
25:BA:185:G:C4	25:BA:186:G:C8	3.08	0.42
25:BA:1473:G:C6	25:BA:1474:U:C4	3.07	0.42
25:BA:1548:A:H2'	25:BA:1549:A:C8	2.54	0.42
25:BA:1721:G:H1'	25:BA:1739:A:N6	2.34	0.42
25:BA:1724:G:C6	25:BA:1725:U:C4	3.08	0.42
25:BA:2349:G:C6	25:BA:2369:A:C6	3.07	0.42
25:BA:2543:G:C6	25:BA:2544:G:C5	3.08	0.42
25:BA:2749:A:OP1	31:BG:2:SER:N	2.51	0.42
26:BB:41:G:H8	30:BF:66:LEU:HD11	1.84	0.42
29:BE:110:SER:O	29:BE:113:VAL:HG22	2.19	0.42
30:BF:40:VAL:HG11	30:BF:49:LEU:HB3	2.01	0.42
30:BF:80:ARG:HB3	30:BF:83:TYR:CE1	2.54	0.42
31:BG:44:LYS:HG2	31:BG:51:THR:OG1	2.19	0.42
33:BK:36:LEU:O	33:BK:51:GLY:HA3	2.18	0.42
57:CD:175:GLU:CD	57:CD:175:GLU:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CD:800:LEU:HB3	57:CD:920:ALA:HB1	2.01	0.42
1:AA:590:U:H2'	1:AA:591:U:C6	2.54	0.42
6:AF:9:MET:O	6:AF:85:ILE:N	2.51	0.42
23:AW:4:G:C6	23:AW:70:G:C6	3.06	0.42
23:AW:53:G:C5	23:AW:54:5MU:H72	2.54	0.42
24:AZ:23:A:C6	24:AZ:24:G:C5	3.07	0.42
25:BA:1510:G:C6	25:BA:1511:G:C5	3.08	0.42
26:BB:43:C:O2	30:BF:92:ARG:HD2	2.19	0.42
49:B1:16:ARG:HA	49:B1:16:ARG:HD3	1.85	0.42
54:B6:30:GLU:HG3	54:B6:32:LYS:HB2	2.01	0.42
57:CD:72:CYS:SG	57:CD:74:LYS:HB2	2.60	0.42
57:CD:836:ARG:HG3	57:CD:869:CYS:SG	2.60	0.42
59:CN:27:DA:C2	59:CN:28:DA:C4	3.08	0.42
1:AA:4:U:O2'	1:AA:5:U:H3'	2.19	0.42
1:AA:136:C:H2'	1:AA:137:U:O4'	2.20	0.42
1:AA:1172:C:C2	1:AA:1173:U:C5	3.08	0.42
1:AA:1173:U:C2	1:AA:1174:G:C8	3.08	0.42
7:AG:81:GLY:C	7:AG:83:SER:H	2.23	0.42
16:AP:8:ARG:O	16:AP:9:HIS:ND1	2.53	0.42
17:AQ:39:LYS:HB2	17:AQ:39:LYS:HE3	1.73	0.42
25:BA:271:G:C4	25:BA:272:A:C8	3.08	0.42
25:BA:280:U:O4	25:BA:361:G:N2	2.53	0.42
25:BA:2155:U:H2'	25:BA:2156:G:C8	2.55	0.42
25:BA:2251:OMG:HM23	25:BA:2251:OMG:H1'	1.71	0.42
55:CA:82:LEU:HA	55:CA:82:LEU:HD23	1.71	0.42
57:CD:1159:ILE:O	57:CD:1206:ARG:N	2.48	0.42
60:CT:18:DC:O2	60:CT:19:DG:C8	2.73	0.42
1:AA:429:U:H3'	4:AD:9:LEU:HD12	2.01	0.42
1:AA:451:A:H2'	1:AA:481:G:O6	2.19	0.42
25:BA:282:A:C6	25:BA:359:G:C6	3.08	0.42
25:BA:289:G:H2'	25:BA:290:U:O4'	2.19	0.42
25:BA:636:G:N2	35:BM:76:GLU:OE1	2.49	0.42
25:BA:1874:C:H2'	25:BA:1875:G:O4'	2.20	0.42
25:BA:2065:C:H2'	25:BA:2066:C:H6	1.85	0.42
26:BB:28:C:H2'	26:BB:29:A:O4'	2.19	0.42
28:BD:25:THR:HG21	28:BD:193:VAL:HG22	2.01	0.42
32:BH:78:VAL:HG23	32:BH:142:VAL:CG1	2.49	0.42
56:CC:571:LEU:HD23	56:CC:571:LEU:HA	1.64	0.42
60:CT:10:DT:H2''	60:CT:11:DC:C5	2.54	0.42
1:AA:309:A:H2'	1:AA:310:G:H8	1.85	0.42
1:AA:502:A:H2'	1:AA:503:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:74:ARG:H	2:AB:74:ARG:HG3	1.48	0.42
3:AC:175:LEU:HA	3:AC:175:LEU:HD12	1.82	0.42
6:AF:11:HIS:HA	6:AF:85:ILE:HD11	2.02	0.42
18:AR:73:ARG:HB3	18:AR:74:HIS:H	1.64	0.42
21:AU:58:LYS:HE2	21:AU:62:ARG:NH2	2.34	0.42
25:BA:651:G:C2	25:BA:652:U:O2	2.73	0.42
25:BA:962:G:C5	25:BA:963:U:C5	3.08	0.42
25:BA:1057:A:N7	25:BA:1086:A:H2'	2.35	0.42
25:BA:1142:A:C5	25:BA:1144:A:C8	3.07	0.42
25:BA:1486:U:H2'	25:BA:1487:U:C6	2.54	0.42
25:BA:1532:A:C6	25:BA:1540:G:C6	3.07	0.42
31:BG:9:VAL:O	31:BG:49:THR:HA	2.19	0.42
43:BU:7:LEU:HD13	43:BU:46:ALA:HA	2.00	0.42
48:BZ:14:LEU:HD23	48:BZ:14:LEU:HA	1.91	0.42
56:CC:555:TYR:OH	56:CC:654:ASP:OD2	2.30	0.42
56:CC:1251:TYR:CE2	56:CC:1301:ARG:NH1	2.88	0.42
57:CD:107:LEU:HA	57:CD:107:LEU:HD23	1.84	0.42
57:CD:304:ASP:OD1	57:CD:304:ASP:C	2.58	0.42
57:CD:442:ILE:HG23	57:CD:442:ILE:HD12	1.70	0.42
57:CD:830:ASP:OD1	57:CD:832:LYS:NZ	2.49	0.42
1:AA:49:U:C4	1:AA:364:A:C6	3.08	0.42
1:AA:147:G:C2	1:AA:176:C:C2	3.08	0.42
1:AA:415:A:C4	1:AA:416:G:C8	3.08	0.42
1:AA:826:C:O2	8:AH:16:ASN:ND2	2.53	0.42
1:AA:1026:G:H1	1:AA:1035:A:N6	2.18	0.42
1:AA:1247:U:O2	1:AA:1290:G:O6	2.37	0.42
1:AA:1300:G:C6	1:AA:1334:G:C5	3.07	0.42
2:AB:129:LEU:HD22	2:AB:134:ALA:CB	2.47	0.42
6:AF:11:HIS:CD2	6:AF:12:PRO:HD2	2.55	0.42
8:AH:112:THR:HG23	8:AH:115:ALA:H	1.84	0.42
17:AQ:81:LYS:HE2	17:AQ:81:LYS:HB2	1.84	0.42
18:AR:20:GLU:OE1	18:AR:20:GLU:N	2.53	0.42
22:AV:51:G:C6	22:AV:52:C:N4	2.88	0.42
25:BA:638:G:C5	25:BA:639:U:C4	3.08	0.42
25:BA:704:G:C2	25:BA:726:G:C4	3.08	0.42
25:BA:796:C:H2'	25:BA:797:G:H8	1.85	0.42
25:BA:855:G:C6	25:BA:923:G:C6	3.07	0.42
25:BA:858:G:N2	25:BA:2268:A:C4	2.87	0.42
25:BA:1036:G:H1	25:BA:1119:U:H3	1.67	0.42
25:BA:1420:A:H1'	25:BA:2211:G:C2	2.55	0.42
25:BA:1452:G:H22	25:BA:1457:U:H2'	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1511:G:H2'	25:BA:1512:C:H6	1.85	0.42
25:BA:1586:A:H2'	25:BA:1587:G:C8	2.55	0.42
25:BA:2126:A:C5	25:BA:2162:G:C8	3.08	0.42
25:BA:2266:A:H4'	25:BA:2267:A:N3	2.34	0.42
25:BA:2605:PSU:H2'	25:BA:2606:C:C6	2.55	0.42
26:BB:32:U:C2	26:BB:33:G:C8	3.08	0.42
27:BC:2:ALA:N	27:BC:20:VAL:O	2.53	0.42
28:BD:35:THR:HG22	28:BD:73:VAL:HG21	2.02	0.42
42:BT:36:LEU:HD23	42:BT:36:LEU:HA	1.79	0.42
44:BV:85:PHE:CE1	44:BV:94:ARG:HG2	2.55	0.42
56:CC:524:ILE:HG21	56:CC:524:ILE:HD13	1.77	0.42
56:CC:1292:THR:OG1	56:CC:1293:VAL:N	2.53	0.42
56:CC:1333:LEU:HA	56:CC:1333:LEU:HD23	1.83	0.42
57:CD:365:GLN:OE1	57:CD:440:VAL:HG11	2.19	0.42
57:CD:636:GLY:O	57:CD:638:SER:N	2.52	0.42
59:CN:37:DG:H2''	59:CN:38:DA:OP2	2.20	0.42
60:CT:4:DT:C2	60:CT:5:DG:N7	2.88	0.42
1:AA:650:G:C6	1:AA:651:C:C4	3.08	0.42
2:AB:167:ASP:OD2	2:AB:191:SER:OG	2.25	0.42
5:AE:56:VAL:O	5:AE:60:ILE:HG13	2.20	0.42
8:AH:90:ASP:OD1	8:AH:90:ASP:N	2.48	0.42
24:AX:9:A:C5	24:AX:46:7MG:C2	3.08	0.42
24:AX:28:G:N1	24:AX:43:C:N3	2.68	0.42
24:AX:68:C:H2'	24:AX:69:G:H8	1.85	0.42
24:AZ:22:G:C6	24:AZ:23:A:C6	3.08	0.42
25:BA:136:G:C6	25:BA:137:U:C4	3.08	0.42
25:BA:259:G:C2	25:BA:260:G:C8	3.08	0.42
25:BA:1618:6MZ:O2'	25:BA:1619:G:OP1	2.36	0.42
25:BA:1751:U:H2'	25:BA:1752:C:C6	2.55	0.42
25:BA:2532:G:N2	25:BA:2663:G:O2'	2.53	0.42
26:BB:86:G:N7	26:BB:88:C:N4	2.68	0.42
32:BH:57:LYS:O	32:BH:61:VAL:HG23	2.19	0.42
39:BQ:99:TYR:HA	39:BQ:102:GLU:HG3	2.01	0.42
56:CC:745:GLU:HG2	56:CC:746:ALA:N	2.35	0.42
57:CD:541:LEU:HD23	57:CD:541:LEU:HA	1.85	0.42
59:CN:13:DC:O2	60:CT:28:DG:N2	2.52	0.42
59:CN:19:DA:OP1	61:CF:90:MET:HG2	2.19	0.42
1:AA:604:G:C6	1:AA:635:A:C6	3.07	0.41
10:AJ:37:ARG:HB3	10:AJ:37:ARG:HH11	1.85	0.41
11:AK:36:ASP:OD2	11:AK:38:GLN:HG2	2.20	0.41
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:66:LEU:HD23	15:AO:66:LEU:HA	1.82	0.41
22:AV:45:C:H6	22:AV:45:C:H2'	1.59	0.41
25:BA:111:A:C6	25:BA:112:U:C4	3.08	0.41
25:BA:379:G:N1	25:BA:396:G:C6	2.88	0.41
25:BA:876:C:H2'	25:BA:877:A:O4'	2.19	0.41
25:BA:2290:G:H2'	25:BA:2291:U:C6	2.55	0.41
25:BA:2571:U:HO2'	28:BD:151:THR:HG1	1.66	0.41
25:BA:2639:A:H4'	33:BK:96:ARG:HH22	1.83	0.41
27:BC:230:HIS:ND1	27:BC:231:PRO:HD2	2.35	0.41
40:BR:83:LEU:HD23	40:BR:83:LEU:HA	1.76	0.41
56:CC:554:HIS:O	56:CC:555:TYR:C	2.58	0.41
56:CC:1212:LEU:HD23	56:CC:1212:LEU:HA	1.59	0.41
56:CC:1333:LEU:C	56:CC:1335:ILE:H	2.23	0.41
57:CD:503:SER:OG	57:CD:504:GLN:N	2.50	0.41
59:CN:18:DG:C4	61:CF:90:MET:HB2	2.55	0.41
1:AA:33:A:H2'	1:AA:34:C:C6	2.55	0.41
3:AC:135:LYS:HA	3:AC:135:LYS:HD2	1.83	0.41
5:AE:80:THR:HG22	5:AE:122:ASN:O	2.20	0.41
23:AW:9:G:N3	23:AW:45:G:H2'	2.35	0.41
25:BA:75:G:H4'	48:BZ:48:ARG:NH2	2.34	0.41
25:BA:817:C:H2'	25:BA:818:G:O4'	2.20	0.41
25:BA:960:A:C8	25:BA:962:G:C8	3.08	0.41
25:BA:1010:A:H5''	40:BR:66:ASN:HD22	1.85	0.41
25:BA:1310:G:N2	25:BA:1313:U:C4	2.88	0.41
25:BA:1353:A:H2'	25:BA:1354:A:C8	2.55	0.41
25:BA:1859:U:H2'	25:BA:1860:G:O4'	2.21	0.41
25:BA:2037:A:H2'	25:BA:2038:G:C8	2.55	0.41
25:BA:2131:U:H5'	25:BA:2133:G:N7	2.35	0.41
25:BA:2134:A:O2'	25:BA:2159:G:N2	2.53	0.41
25:BA:2210:U:C2	25:BA:2212:A:C8	3.08	0.41
25:BA:2287:A:C5	25:BA:2289:G:C8	3.07	0.41
25:BA:2638:G:O2'	25:BA:2775:G:N2	2.35	0.41
25:BA:2899:A:H2'	25:BA:2900:A:C8	2.55	0.41
30:BF:170:LEU:HD23	30:BF:170:LEU:HA	1.80	0.41
32:BH:37:VAL:HG12	32:BH:43:ASN:ND2	2.35	0.41
32:BH:117:LEU:HD21	32:BH:120:GLY:CA	2.51	0.41
33:BK:117:ALA:O	33:BK:120:ARG:HB2	2.20	0.41
35:BM:70:LYS:HB2	35:BM:70:LYS:NZ	2.36	0.41
37:BO:86:ARG:HD3	37:BO:117:ASP:CB	2.50	0.41
56:CC:216:THR:N	56:CC:219:GLN:OE1	2.46	0.41
56:CC:616:ILE:HA	56:CC:652:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CN:29:DG:H2''	59:CN:30:DA:O5'	2.20	0.41
60:CT:20:DC:H2'	60:CT:21:DG:C8	2.55	0.41
1:AA:846:G:N1	1:AA:847:G:C5	2.88	0.41
1:AA:846:G:O5'	1:AA:846:G:C8	2.73	0.41
1:AA:860:A:H2'	1:AA:861:G:O4'	2.20	0.41
1:AA:878:A:C2	1:AA:879:C:C2	3.08	0.41
1:AA:1046:A:H4'	62:AA:1738:MG:MG	1.44	0.41
19:AS:63:THR:HG22	19:AS:64:ASP:H	1.86	0.41
24:AX:55:PSU:P	36:BN:50:ARG:HH12	2.43	0.41
25:BA:222:A:N6	25:BA:232:G:H1'	2.35	0.41
25:BA:355:U:C2	25:BA:356:G:N7	2.89	0.41
25:BA:708:G:C6	25:BA:709:U:C4	3.08	0.41
25:BA:754:U:H2'	25:BA:755:U:C6	2.55	0.41
25:BA:1252:G:N2	40:BR:33:ARG:HB3	2.35	0.41
25:BA:1660:G:C2	25:BA:1661:G:C8	3.08	0.41
25:BA:2045:C:HO2'	50:B2:19:HIS:CD2	2.35	0.41
25:BA:2136:G:C6	25:BA:2156:G:N3	2.88	0.41
29:BE:146:VAL:HA	29:BE:185:LYS:O	2.20	0.41
30:BF:48:LYS:O	30:BF:49:LEU:C	2.55	0.41
36:BN:77:PRO:HG2	36:BN:80:VAL:HG11	2.02	0.41
38:BP:18:LEU:HD13	38:BP:18:LEU:HA	1.62	0.41
42:BT:16:LYS:HA	42:BT:19:LEU:HD22	2.02	0.41
55:CA:217:ILE:HD12	55:CA:217:ILE:HA	1.88	0.41
56:CC:164:THR:O	56:CC:166:SER:N	2.48	0.41
56:CC:616:ILE:N	56:CC:616:ILE:HD12	2.36	0.41
56:CC:812:PHE:O	56:CC:814:ASP:N	2.53	0.41
56:CC:1082:ILE:HG21	56:CC:1082:ILE:HD13	1.83	0.41
56:CC:1138:VAL:HG12	56:CC:1170:MET:SD	2.61	0.41
56:CC:1235:LEU:HA	56:CC:1235:LEU:HD23	1.81	0.41
1:AA:611:C:H2'	1:AA:612:C:C6	2.56	0.41
1:AA:624:C:C4	1:AA:625:U:C4	3.09	0.41
1:AA:999:C:N3	1:AA:1042:A:N6	2.68	0.41
1:AA:1120:C:H2'	1:AA:1121:U:C6	2.55	0.41
1:AA:1228:C:H2'	1:AA:1229:A:H8	1.85	0.41
2:AB:21:ARG:HD2	2:AB:22:TYR:CZ	2.54	0.41
19:AS:36:ARG:NH2	19:AS:75:ALA:O	2.50	0.41
24:AX:22:G:H2'	24:AX:23:A:H8	1.85	0.41
24:AZ:6:G:N1	24:AZ:68:C:O2	2.53	0.41
25:BA:1063:G:H2'	25:BA:1064:C:H6	1.86	0.41
25:BA:1599:U:C2	25:BA:1600:C:C5	3.09	0.41
25:BA:2521:C:O2'	25:BA:2564:A:N3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BB:10:G:C8	26:BB:11:C:C5	3.09	0.41
31:BG:153:ARG:HG3	31:BG:154:PRO:HD2	2.02	0.41
52:B4:1:MET:SD	52:B4:3:ARG:NH1	2.93	0.41
55:CA:85:LEU:HD23	55:CA:85:LEU:HA	1.91	0.41
1:AA:393:A:C2	1:AA:394:G:C8	3.09	0.41
1:AA:405:U:O4	4:AD:2:ALA:N	2.54	0.41
1:AA:501:C:H2'	1:AA:502:A:H8	1.84	0.41
1:AA:821:G:C6	1:AA:822:U:C4	3.08	0.41
1:AA:920:U:C2	1:AA:921:U:C5	3.08	0.41
1:AA:981:U:H2'	1:AA:982:U:C5	2.56	0.41
1:AA:1143:G:C2	1:AA:1144:G:C5	3.08	0.41
1:AA:1299:A:O2'	1:AA:1301:U:O4'	2.29	0.41
3:AC:115:LEU:HD23	3:AC:115:LEU:HA	1.73	0.41
7:AG:23:LEU:HD11	7:AG:47:LEU:HD21	2.03	0.41
9:AI:110:GLN:O	9:AI:111:VAL:HG23	2.21	0.41
12:AL:49:LEU:HD23	12:AL:49:LEU:HA	1.78	0.41
25:BA:289:G:H2'	25:BA:290:U:C6	2.56	0.41
25:BA:332:A:C5	25:BA:335:C:C4	3.08	0.41
25:BA:543:A:N1	25:BA:544:G:C6	2.88	0.41
25:BA:1105:U:H2'	25:BA:1106:G:C8	2.47	0.41
25:BA:1166:G:C6	25:BA:1167:C:C4	3.08	0.41
25:BA:1175:A:H3'	25:BA:1176:U:C4'	2.51	0.41
25:BA:1177:G:O2'	25:BA:1178:C:C6	2.72	0.41
43:BU:31:VAL:HG11	43:BU:82:LYS:HE3	2.01	0.41
47:BY:2:SER:O	47:BY:4:VAL:N	2.54	0.41
47:BY:39:TRP:NE1	47:BY:41:GLU:OE1	2.51	0.41
57:CD:508:LEU:HA	57:CD:508:LEU:HD12	1.88	0.41
57:CD:536:LEU:HD23	57:CD:536:LEU:HA	1.85	0.41
59:CN:18:DG:N1	61:CF:14:ALA:N	2.65	0.41
1:AA:961:U:C2	1:AA:983:A:C5	3.09	0.41
1:AA:1256:A:H62	1:AA:1279:G:H21	1.67	0.41
1:AA:1261:A:H62	1:AA:1274:A:H1'	1.85	0.41
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.55	0.41
1:AA:1384:C:H2'	1:AA:1385:G:C8	2.55	0.41
2:AB:35:ARG:NH2	2:AB:40:ILE:HG21	2.36	0.41
12:AL:87:VAL:O	12:AL:87:VAL:HG12	2.21	0.41
15:AO:41:GLY:O	15:AO:45:GLU:HG2	2.20	0.41
19:AS:64:ASP:O	19:AS:67:VAL:HG23	2.20	0.41
25:BA:594:U:H2'	25:BA:595:C:C6	2.56	0.41
25:BA:925:A:H2'	25:BA:926:G:H8	1.86	0.41
25:BA:1063:G:O2'	25:BA:1064:C:O5'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1517:G:C6	25:BA:1518:C:C4	3.09	0.41
25:BA:2187:U:C2	25:BA:2188:U:C5	3.08	0.41
25:BA:2845:U:C2	25:BA:2846:G:C8	3.08	0.41
30:BF:70:ALA:HA	30:BF:85:ILE:HD11	2.03	0.41
35:BM:61:LEU:O	53:B5:13:ARG:NH2	2.51	0.41
42:BT:23:LEU:HD23	42:BT:23:LEU:HA	1.84	0.41
43:BU:39:THR:HG23	43:BU:40:LYS:N	2.35	0.41
43:BU:65:GLY:N	43:BU:79:ASP:OD1	2.54	0.41
54:B6:15:LYS:O	54:B6:26:ILE:HD13	2.21	0.41
56:CC:726:TYR:CD1	56:CC:727:VAL:N	2.89	0.41
56:CC:1251:TYR:CE2	56:CC:1301:ARG:CZ	3.03	0.41
56:CC:1330:ILE:HD13	56:CC:1330:ILE:HG21	1.84	0.41
57:CD:416:ILE:O	57:CD:416:ILE:HG23	2.20	0.41
59:CN:26:DG:C4	59:CN:27:DA:N7	2.89	0.41
1:AA:204:G:C5	1:AA:465:A:N1	2.89	0.41
1:AA:384:G:C4	1:AA:385:C:C5	3.09	0.41
1:AA:440:C:C2	1:AA:441:A:C8	3.08	0.41
2:AB:114:LEU:HA	2:AB:144:LEU:HD13	2.02	0.41
4:AD:102:VAL:HG13	4:AD:107:PHE:HB2	2.02	0.41
5:AE:89:HIS:CE1	5:AE:138:ARG:HH11	2.39	0.41
6:AF:67:PRO:O	6:AF:70:VAL:HG22	2.21	0.41
9:AI:55:VAL:HG11	9:AI:94:LEU:HD13	2.02	0.41
24:AZ:9:A:H5''	24:AZ:46:7MG:O3'	2.19	0.41
24:AZ:41:C:H2'	24:AZ:42:C:H6	1.86	0.41
25:BA:635:C:H2'	25:BA:636:G:O4'	2.21	0.41
25:BA:882:G:O6	25:BA:894:U:C4	2.72	0.41
25:BA:1400:U:H2'	25:BA:1401:G:O4'	2.20	0.41
25:BA:1481:U:O2	25:BA:1510:G:C6	2.73	0.41
25:BA:1874:C:C4	25:BA:1875:G:C5	3.09	0.41
25:BA:2125:G:N2	25:BA:2170:A:H4'	2.36	0.41
25:BA:2901:C:C2	25:BA:2902:C:C4	3.09	0.41
27:BC:142:HIS:CD2	27:BC:193:GLY:O	2.72	0.41
29:BE:15:SER:N	29:BE:197:GLU:OE2	2.54	0.41
30:BF:49:LEU:O	30:BF:53:ALA:HB3	2.21	0.41
30:BF:137:ILE:HG13	30:BF:138:PHE:N	2.36	0.41
32:BH:84:ALA:HB3	32:BH:148:ALA:CB	2.51	0.41
35:BM:27:LEU:HD23	35:BM:27:LEU:HA	1.85	0.41
41:BS:73:LYS:HB3	41:BS:73:LYS:HE3	1.73	0.41
42:BT:29:VAL:CG2	42:BT:55:ILE:HD11	2.51	0.41
43:BU:26:LYS:HB3	43:BU:26:LYS:HE2	1.63	0.41
44:BV:96:PHE:O	44:BV:100:SER:CA	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:B4:5:PHE:O	52:B4:6:GLN:NE2	2.51	0.41
56:CC:213:LEU:HD23	56:CC:213:LEU:HA	1.82	0.41
56:CC:699:LEU:HA	56:CC:699:LEU:HD23	1.68	0.41
56:CC:1014:LEU:HD12	56:CC:1017:GLN:HB3	2.01	0.41
57:CD:555:TYR:CE2	57:CD:565:ALA:HB2	2.56	0.41
60:CT:28:DG:C4'	61:CF:18:PHE:CZ	3.03	0.41
1:AA:684:U:H2'	1:AA:685:G:O4'	2.20	0.41
1:AA:928:G:H2'	1:AA:929:G:H8	1.84	0.41
6:AF:44:ARG:HB2	6:AF:44:ARG:NH1	2.35	0.41
7:AG:60:GLU:OE1	7:AG:60:GLU:N	2.54	0.41
25:BA:748:G:C8	25:BA:750:A:N7	2.88	0.41
25:BA:940:G:H5''	25:BA:941:A:OP2	2.21	0.41
25:BA:1115:G:N3	25:BA:1116:G:C8	2.89	0.41
25:BA:1218:G:C2	25:BA:1232:G:C5	3.09	0.41
25:BA:1656:C:H2'	25:BA:1657:U:H6	1.84	0.41
25:BA:2093:G:H21	25:BA:2198:A:N6	2.19	0.41
26:BB:12:C:O2'	46:BX:74:PRO:HA	2.20	0.41
26:BB:31:C:O2'	26:BB:53:A:N1	2.43	0.41
30:BF:8:TYR:HA	30:BF:12:VAL:HB	2.03	0.41
31:BG:148:LEU:HA	31:BG:148:LEU:HD23	1.84	0.41
31:BG:148:LEU:O	31:BG:151:TYR:HB2	2.20	0.41
45:BW:7:GLU:O	45:BW:40:ILE:HA	2.21	0.41
55:CB:39:LEU:HD23	55:CB:39:LEU:HA	1.85	0.41
56:CC:100:LEU:HA	56:CC:100:LEU:HD23	1.84	0.41
56:CC:431:LYS:HE3	56:CC:431:LYS:HB2	1.87	0.41
56:CC:696:ASP:OD1	56:CC:696:ASP:N	2.49	0.41
57:CD:449:LEU:HD12	57:CD:449:LEU:HA	1.60	0.41
57:CD:571:ASP:OD1	57:CD:571:ASP:N	2.44	0.41
57:CD:1310:THR:O	57:CD:1310:THR:HG22	2.20	0.41
1:AA:300:A:H8	1:AA:300:A:O5'	2.03	0.41
1:AA:1125:U:OP1	10:AJ:37:ARG:NH2	2.54	0.41
4:AD:125:VAL:HG22	4:AD:143:VAL:HG22	2.03	0.41
6:AF:67:PRO:HB2	6:AF:69:GLU:OE1	2.20	0.41
9:AI:130:ARG:NH1	23:AW:33:U:OP2	2.53	0.41
14:AN:46:LEU:HD23	14:AN:46:LEU:HA	1.87	0.41
18:AR:39:ILE:HG12	18:AR:59:ILE:HD13	2.03	0.41
20:AT:36:TYR:HE1	20:AT:82:GLN:HE22	1.67	0.41
21:AU:63:GLU:HG3	21:AU:67:ARG:NH2	2.36	0.41
22:AV:13:U:H2'	22:AV:14:U:H6	1.86	0.41
24:AZ:26:A:H2	24:AZ:44:G:H1	1.54	0.41
24:AZ:48:C:C6	24:AZ:59:U:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:24:G:H2'	25:BA:25:U:H6	1.85	0.41
25:BA:607:U:C5	25:BA:620:G:C5	3.09	0.41
25:BA:1591:A:H2'	25:BA:1592:C:C6	2.56	0.41
25:BA:1678:A:H2'	25:BA:1679:A:O4'	2.21	0.41
25:BA:2064:C:H2'	25:BA:2065:C:C6	2.56	0.41
25:BA:2315:G:O2'	25:BA:2316:G:O5'	2.39	0.41
25:BA:2345:G:C2	25:BA:2381:A:C4	3.09	0.41
25:BA:2742:G:P	54:B6:24:ARG:HH12	2.44	0.41
25:BA:2900:A:C4	25:BA:2901:C:C5	3.08	0.41
27:BC:41:GLY:O	27:BC:43:ARG:NH1	2.43	0.41
29:BE:65:THR:HG23	29:BE:67:ARG:H	1.86	0.41
29:BE:148:ILE:O	29:BE:169:VAL:HA	2.21	0.41
30:BF:175:PHE:HA	30:BF:176:PRO:HD3	1.86	0.41
44:BV:4:LYS:HD3	44:BV:83:VAL:HB	2.03	0.41
45:BW:35:GLU:HB3	45:BW:93:ARG:CZ	2.50	0.41
47:BY:6:GLN:OE1	47:BY:50:ARG:N	2.54	0.41
47:BY:37:ARG:HG2	47:BY:48:THR:HG22	2.02	0.41
56:CC:178:PRO:HA	56:CC:397:LEU:HD23	2.02	0.41
57:CD:265:LEU:HD23	57:CD:265:LEU:HA	1.66	0.41
57:CD:340:GLN:HG3	57:CD:341:ASN:OD1	2.21	0.41
57:CD:424:ASN:ND2	57:CD:425:ARG:O	2.45	0.41
60:CT:2:DT:H2''	60:CT:3:DC:H5	1.86	0.41
60:CT:21:DG:H2'	60:CT:22:DC:C6	2.56	0.41
1:AA:464:U:O2'	1:AA:466:A:N7	2.28	0.41
1:AA:864:A:C5'	5:AE:90:THR:HB	2.51	0.41
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.56	0.41
1:AA:1326:U:C2	1:AA:1327:C:C5	3.09	0.41
2:AB:164:ILE:HA	2:AB:186:ILE:HG12	2.03	0.41
3:AC:186:THR:HG22	3:AC:199:LYS:HG2	2.03	0.41
10:AJ:12:ALA:CB	10:AJ:18:ILE:HD13	2.51	0.41
25:BA:27:G:O2'	25:BA:28:A:OP2	2.34	0.41
25:BA:1563:U:H2'	25:BA:1564:C:C6	2.56	0.41
25:BA:1812:U:H2'	25:BA:1813:G:H8	1.85	0.41
25:BA:2104:C:H2'	25:BA:2105:U:O4'	2.21	0.41
25:BA:2673:G:C2	25:BA:2674:G:C8	3.09	0.41
25:BA:2881:U:H5'	37:BO:90:ARG:HH12	1.86	0.41
36:BN:36:VAL:O	36:BN:98:PRO:HB3	2.21	0.41
37:BO:2:ARG:HG2	37:BO:5:LYS:HB2	2.03	0.41
41:BS:28:ALA:HB3	41:BS:31:GLU:OE1	2.20	0.41
48:BZ:34:SER:OG	48:BZ:36:GLN:OE1	2.28	0.41
56:CC:346:TYR:CZ	56:CC:436:ARG:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CD:238:ILE:HD12	57:CD:238:ILE:HG23	1.74	0.41
57:CD:425:ARG:NE	57:CD:464:ASP:OD2	2.39	0.41
57:CD:884:SER:OG	57:CD:885:VAL:N	2.53	0.41
1:AA:718:A:H5'	11:AK:119:ASN:OD1	2.21	0.40
1:AA:737:C:H2'	1:AA:738:C:H6	1.86	0.40
1:AA:927:G:C2'	1:AA:928:G:H5'	2.51	0.40
1:AA:991:U:C4	1:AA:1212:U:H1'	2.56	0.40
1:AA:996:A:C5	1:AA:997:U:C5	3.09	0.40
1:AA:1159:U:H5	1:AA:1182:G:HO2'	1.68	0.40
2:AB:111:ILE:HG22	2:AB:148:LEU:HD13	2.03	0.40
15:AO:8:THR:HG23	15:AO:31:LEU:HD21	2.03	0.40
24:AX:51:U:H3	24:AX:63:G:H1	1.69	0.40
25:BA:317:G:C6	25:BA:318:C:C4	3.09	0.40
25:BA:422:A:C6	25:BA:423:A:C6	3.09	0.40
25:BA:796:C:H2'	25:BA:797:G:C8	2.56	0.40
25:BA:1622:G:C2	25:BA:1623:G:C8	3.09	0.40
25:BA:1649:G:C6	25:BA:2009:A:N6	2.89	0.40
25:BA:2096:C:C2	25:BA:2097:A:C8	3.08	0.40
25:BA:2121:G:H5''	25:BA:2169:A:N6	2.35	0.40
25:BA:2122:U:H5	25:BA:2169:A:N3	2.19	0.40
25:BA:2493:U:C4	25:BA:2494:G:C8	3.09	0.40
25:BA:2604:PSU:C4	25:BA:2605:PSU:C6	3.09	0.40
25:BA:2694:G:H2'	25:BA:2695:U:O4'	2.21	0.40
26:BB:2:G:C6	26:BB:3:C:C4	3.09	0.40
35:BM:19:LEU:HD23	35:BM:19:LEU:HA	1.83	0.40
44:BV:86:ARG:NH2	44:BV:88:GLU:OE1	2.54	0.40
49:B1:23:THR:HG23	49:B1:47:MET:HG2	2.03	0.40
50:B2:32:LYS:HG3	50:B2:33:THR:HG23	2.04	0.40
55:CA:20:SER:C	55:CA:22:THR:H	2.23	0.40
55:CA:159:ILE:HD12	55:CA:160:HIS:N	2.36	0.40
55:CA:213:PRO:HA	55:CA:216:ALA:HB3	2.03	0.40
55:CB:13:LEU:HA	55:CB:28:LEU:CD1	2.51	0.40
56:CC:918:LEU:HD12	56:CC:918:LEU:HA	1.81	0.40
57:CD:841:GLY:HA2	57:CD:863:LEU:HD11	2.03	0.40
57:CD:890:THR:HG22	57:CD:891:ASP:N	2.36	0.40
58:CE:45:LYS:NZ	58:CE:47:THR:OG1	2.47	0.40
1:AA:645:G:C2	1:AA:646:G:C8	3.09	0.40
1:AA:702:A:C8	25:BA:1848:A:H1'	2.56	0.40
25:BA:191:A:H2'	25:BA:192:C:C6	2.56	0.40
25:BA:367:G:C4	25:BA:368:A:C8	3.10	0.40
25:BA:653:U:H6	25:BA:653:U:H2'	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:969:G:H2'	25:BA:970:U:C6	2.56	0.40
25:BA:1204:A:O4'	25:BA:1206:G:C8	2.73	0.40
25:BA:1570:A:H2'	25:BA:1571:A:C8	2.57	0.40
25:BA:1877:A:H2'	25:BA:1878:G:O4'	2.21	0.40
25:BA:2140:G:N1	25:BA:2151:U:O2	2.54	0.40
25:BA:2454:G:C6	25:BA:2499:C:N4	2.90	0.40
25:BA:2840:C:C2	25:BA:2841:C:C5	3.10	0.40
25:BA:2851:A:C6	25:BA:2852:G:C5	3.10	0.40
26:BB:111:U:H2'	26:BB:112:G:H8	1.86	0.40
36:BN:47:GLU:OE2	36:BN:51:ARG:NH1	2.54	0.40
56:CC:557:ARG:NH2	56:CC:611:GLU:OE1	2.40	0.40
56:CC:1176:LEU:HD23	56:CC:1176:LEU:HA	1.75	0.40
57:CD:37:GLU:HB2	57:CD:104:HIS:CE1	2.55	0.40
57:CD:513:MET:HG3	57:CD:544:LEU:HD21	2.03	0.40
57:CD:674:THR:OG1	57:CD:677:GLU:OE2	2.35	0.40
57:CD:842:ARG:NH2	57:CD:1254:GLU:OE2	2.39	0.40
59:CN:27:DA:H1'	59:CN:28:DA:H5'	2.03	0.40
1:AA:152:A:C8	1:AA:153:C:C5	3.09	0.40
1:AA:211:G:C6	1:AA:212:G:H1'	2.57	0.40
1:AA:329:A:C5	1:AA:332:G:C6	3.10	0.40
1:AA:406:G:C5	1:AA:495:A:C5	3.09	0.40
1:AA:721:G:H4'	1:AA:722:G:O4'	2.21	0.40
1:AA:846:G:O5'	1:AA:846:G:H8	2.04	0.40
1:AA:920:U:H2'	1:AA:921:U:C6	2.57	0.40
1:AA:1181:G:H1'	1:AA:1182:G:C5	2.56	0.40
6:AF:11:HIS:CE1	6:AF:54:LEU:HD13	2.56	0.40
17:AQ:25:ILE:HD12	17:AQ:44:LEU:HD12	2.03	0.40
23:AW:32:OMC:H1'	23:AW:32:OMC:HM23	1.60	0.40
25:BA:543:A:N1	25:BA:551:G:C6	2.89	0.40
25:BA:892:A:H2'	25:BA:893:C:O4'	2.21	0.40
25:BA:979:A:C5	25:BA:982:C:C4	3.10	0.40
25:BA:1045:C:C2	25:BA:1047:G:N2	2.90	0.40
25:BA:1196:C:C2	25:BA:1197:G:C8	3.09	0.40
25:BA:1349:C:C2	25:BA:1350:C:C5	3.09	0.40
25:BA:1405:U:H2'	25:BA:1406:U:C6	2.56	0.40
25:BA:1707:G:C5	25:BA:1756:G:C6	3.09	0.40
25:BA:2121:G:H4'	25:BA:2168:G:O6	2.21	0.40
26:BB:51:G:C6	26:BB:52:A:C6	3.09	0.40
27:BC:205:LEU:HB3	27:BC:210:ALA:HB3	2.03	0.40
29:BE:112:LEU:HD22	29:BE:117:ARG:HB2	2.02	0.40
30:BF:115:ARG:O	30:BF:178:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BM:2:ARG:N	35:BM:5:THR:OG1	2.51	0.40
36:BN:81:4D4:OB	36:BN:82:MET:N	2.49	0.40
47:BY:68:LEU:HB3	47:BY:72:ARG:NH1	2.36	0.40
48:BZ:12:GLU:OE1	48:BZ:12:GLU:N	2.52	0.40
55:CA:183:ILE:HD12	55:CA:183:ILE:HG23	1.75	0.40
56:CC:143:ARG:HH11	56:CC:143:ARG:HD3	1.71	0.40
56:CC:816:ILE:HD13	56:CC:816:ILE:HG21	1.84	0.40
57:CD:361:LEU:HD23	57:CD:361:LEU:HA	1.83	0.40
57:CD:798:ARG:O	57:CD:799:ARG:C	2.60	0.40
57:CD:1256:ILE:HG23	57:CD:1256:ILE:HD12	1.61	0.40
1:AA:215:C:H2'	1:AA:216:U:O4'	2.22	0.40
1:AA:220:G:C2	1:AA:221:C:C6	3.09	0.40
1:AA:283:U:C4	1:AA:284:C:C4	3.10	0.40
1:AA:539:A:H2'	1:AA:540:G:C8	2.56	0.40
1:AA:967:5MC:H3'	1:AA:968:A:C8	2.55	0.40
1:AA:1513:A:H2'	1:AA:1514:G:C8	2.57	0.40
2:AB:76:ALA:HB2	2:AB:210:VAL:HG11	2.03	0.40
4:AD:50:ASP:O	4:AD:53:VAL:HG22	2.21	0.40
24:AX:5:G:H2'	24:AX:6:G:C8	2.55	0.40
25:BA:88:G:C2	25:BA:89:A:C8	3.10	0.40
25:BA:1829:A:C8	25:BA:1830:C:C5	3.10	0.40
25:BA:1869:G:H1	25:BA:1871:A:H3'	1.86	0.40
25:BA:2246:G:H2'	25:BA:2247:A:C8	2.57	0.40
25:BA:2308:G:C6	25:BA:2311:A:N7	2.86	0.40
25:BA:2720:U:H5''	39:BQ:53:ARG:NH2	2.35	0.40
30:BF:116:GLY:O	30:BF:178:ARG:NH1	2.54	0.40
48:BZ:3:ALA:O	48:BZ:7:ARG:HB2	2.21	0.40
50:B2:40:ARG:HA	50:B2:40:ARG:HD3	1.79	0.40
54:B6:18:LYS:CE	54:B6:21:GLY:HA2	2.51	0.40
56:CC:528:ARG:HH11	56:CC:528:ARG:HD2	1.66	0.40
56:CC:603:ILE:HD12	56:CC:603:ILE:O	2.21	0.40
56:CC:979:LEU:HD21	56:CC:985:GLU:H	1.86	0.40
57:CD:67:ASP:N	57:CD:67:ASP:OD1	2.54	0.40
57:CD:603:LYS:O	57:CD:607:THR:HG23	2.22	0.40
57:CD:618:VAL:H	57:CD:618:VAL:HG22	1.70	0.40
57:CD:978:ARG:HD3	57:CD:1197:ASN:HD21	1.81	0.40
57:CD:1143:ASP:OD1	57:CD:1143:ASP:C	2.60	0.40
59:CN:26:DG:H5''	59:CN:26:DG:C8	2.56	0.40
60:CT:4:DT:H2''	60:CT:5:DG:C8	2.56	0.40
1:AA:1025:U:OP1	1:AA:1026:G:H5'	2.21	0.40
1:AA:1494:G:N2	25:BA:1912:A:C2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:85:GLU:OE1	3:AC:88:ARG:NE	2.31	0.40
10:AJ:56:HIS:CG	10:AJ:57:VAL:N	2.88	0.40
19:AS:63:THR:HG22	19:AS:64:ASP:N	2.37	0.40
20:AT:54:MET:O	20:AT:58:VAL:HG22	2.21	0.40
22:AV:20:U:H2'	22:AV:21:C:H6	1.87	0.40
24:AX:19:G:H3'	24:AX:20:H2U:N3	2.36	0.40
25:BA:273:G:C6	25:BA:274:C:C4	3.09	0.40
25:BA:396:G:C6	25:BA:397:U:C4	3.10	0.40
25:BA:960:A:H5''	25:BA:961:C:OP1	2.20	0.40
25:BA:962:G:C6	25:BA:963:U:C4	3.10	0.40
25:BA:1064:C:H2'	25:BA:1065:U:C6	2.57	0.40
25:BA:1407:G:O2'	25:BA:1408:G:O4'	2.25	0.40
25:BA:1596:A:O2'	25:BA:1597:A:C5'	2.70	0.40
25:BA:1796:U:O2'	27:BC:254:GLY:N	2.32	0.40
25:BA:1858:A:C6	25:BA:1885:A:C8	3.10	0.40
30:BF:126:GLY:HA3	30:BF:160:ALA:O	2.22	0.40
40:BR:117:LEU:HA	40:BR:117:LEU:HD23	1.82	0.40
47:BY:32:ASN:OD1	47:BY:34:HIS:NE2	2.55	0.40
55:CB:104:LYS:O	55:CB:139:SER:OG	2.30	0.40
57:CD:202:ARG:HH21	57:CD:225:GLU:HB2	1.86	0.40
57:CD:829:GLY:HA2	57:CD:995:TYR:CZ	2.57	0.40
57:CD:1077:ALA:HA	57:CD:1100:PHE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
2	AB	224/241 (93%)	209 (93%)	14 (6%)	1 (0%)	30	65
3	AC	207/233 (89%)	193 (93%)	10 (5%)	4 (2%)	6	34
4	AD	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	25	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	154/167 (92%)	143 (93%)	10 (6%)	1 (1%)	22	57
6	AF	102/131 (78%)	96 (94%)	6 (6%)	0	100	100
7	AG	152/156 (97%)	139 (91%)	11 (7%)	2 (1%)	10	41
8	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	51
9	AI	126/130 (97%)	110 (87%)	13 (10%)	3 (2%)	5	30
10	AJ	98/103 (95%)	89 (91%)	7 (7%)	2 (2%)	6	33
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	14	48
12	AL	119/124 (96%)	110 (92%)	7 (6%)	2 (2%)	7	36
13	AM	113/118 (96%)	108 (96%)	4 (4%)	1 (1%)	14	48
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	11	43
16	AP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	AQ	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
18	AR	55/75 (73%)	52 (94%)	2 (4%)	1 (2%)	7	35
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	12	45
28	BD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	25	60
29	BE	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
30	BF	176/179 (98%)	165 (94%)	8 (4%)	3 (2%)	7	36
31	BG	173/177 (98%)	159 (92%)	13 (8%)	1 (1%)	22	57
32	BH	147/149 (99%)	128 (87%)	18 (12%)	1 (1%)	19	54
33	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
35	BM	142/144 (99%)	130 (92%)	10 (7%)	2 (1%)	9	39
36	BN	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
37	BO	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
38	BP	115/117 (98%)	107 (93%)	7 (6%)	1 (1%)	14	48
39	BQ	112/115 (97%)	104 (93%)	7 (6%)	1 (1%)	14	48
40	BR	115/118 (98%)	113 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BS	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	13	46
42	BT	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
43	BU	94/100 (94%)	88 (94%)	6 (6%)	0	100	100
44	BV	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	13	46
45	BW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
46	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
47	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	BZ	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	6	34
51	B3	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
52	B4	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
53	B5	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	8	37
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
55	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
55	CB	215/329 (65%)	201 (94%)	13 (6%)	1 (0%)	25	60
56	CC	1316/1342 (98%)	1201 (91%)	100 (8%)	15 (1%)	12	45
57	CD	1327/1407 (94%)	1222 (92%)	96 (7%)	9 (1%)	19	54
58	CE	49/91 (54%)	40 (82%)	8 (16%)	1 (2%)	6	33
61	CF	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
All	All	8773/9507 (92%)	8169 (93%)	540 (6%)	64 (1%)	21	54

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	80	LYS
9	AI	56	ASP
10	AJ	57	VAL
11	AK	93	ARG
12	AL	88	LYS
12	AL	102	LEU
15	AO	19	ALA
30	BF	62	GLY
31	BG	47	ASP
56	CC	165	HIS

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Mol	Chain	Res	Type
57	CD	320	ASN
2	AB	165	ASP
3	AC	51	SER
9	AI	13	LYS
27	BC	241	GLY
28	BD	149	ASN
32	BH	17	ASP
35	BM	36	LYS
38	BP	100	HIS
56	CC	47	TYR
56	CC	121	GLU
56	CC	282	VAL
57	CD	1051	ASP
57	CD	1159	ILE
4	AD	43	ALA
7	AG	130	ASN
9	AI	14	SER
18	AR	72	ASP
30	BF	177	PHE
41	BS	53	PHE
53	B5	32	ILE
56	CC	625	GLU
56	CC	672	GLU
56	CC	1153	ALA
56	CC	1177	ARG
58	CE	6	VAL
3	AC	14	ILE
7	AG	56	LYS
13	AM	66	GLU
27	BC	233	GLY
27	BC	253	LYS
30	BF	176	PRO
35	BM	99	ASN
44	BV	8	ASP
50	B2	27	SER
55	CB	155	ALA
56	CC	237	LEU
56	CC	596	ASP
57	CD	586	GLY
57	CD	712	GLN
57	CD	1200	GLU
3	AC	60	PRO

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Mol	Chain	Res	Type
5	AE	90	THR
10	AJ	78	GLU
56	CC	108	GLU
56	CC	691	PRO
56	CC	808	ASN
57	CD	1048	ARG
56	CC	45	GLY
56	CC	1223	ARG
57	CD	119	SER
8	AH	75	ILE
57	CD	121	PRO
39	BQ	33	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	
2	AB	187/199 (94%)	179 (96%)	8 (4%)	25	49
3	AC	171/190 (90%)	156 (91%)	15 (9%)	8	29
4	AD	172/173 (99%)	157 (91%)	15 (9%)	8	30
5	AE	118/126 (94%)	100 (85%)	18 (15%)	2	13
6	AF	91/112 (81%)	83 (91%)	8 (9%)	8	29
7	AG	127/129 (98%)	113 (89%)	14 (11%)	5	21
8	AH	104/105 (99%)	97 (93%)	7 (7%)	13	38
9	AI	106/107 (99%)	99 (93%)	7 (7%)	14	38
10	AJ	87/90 (97%)	81 (93%)	6 (7%)	13	37
11	AK	90/99 (91%)	83 (92%)	7 (8%)	10	33
12	AL	102/103 (99%)	90 (88%)	12 (12%)	4	20
13	AM	93/96 (97%)	85 (91%)	8 (9%)	8	31
14	AN	83/84 (99%)	78 (94%)	5 (6%)	16	41
15	AO	76/77 (99%)	70 (92%)	6 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AP	65/65 (100%)	61 (94%)	4 (6%)	15	40
17	AQ	74/78 (95%)	70 (95%)	4 (5%)	18	44
18	AR	50/65 (77%)	47 (94%)	3 (6%)	16	41
19	AS	72/79 (91%)	70 (97%)	2 (3%)	38	59
20	AT	65/66 (98%)	58 (89%)	7 (11%)	5	22
21	AU	60/61 (98%)	57 (95%)	3 (5%)	20	45
27	BC	217/218 (100%)	209 (96%)	8 (4%)	29	53
28	BD	163/163 (100%)	155 (95%)	8 (5%)	21	46
29	BE	165/165 (100%)	153 (93%)	12 (7%)	11	35
30	BF	149/150 (99%)	137 (92%)	12 (8%)	9	33
31	BG	136/138 (99%)	122 (90%)	14 (10%)	6	23
32	BH	114/114 (100%)	103 (90%)	11 (10%)	7	25
33	BK	116/116 (100%)	110 (95%)	6 (5%)	19	45
34	BL	104/104 (100%)	95 (91%)	9 (9%)	8	30
35	BM	103/103 (100%)	94 (91%)	9 (9%)	8	30
36	BN	108/108 (100%)	103 (95%)	5 (5%)	23	47
37	BO	100/103 (97%)	93 (93%)	7 (7%)	12	36
38	BP	87/87 (100%)	80 (92%)	7 (8%)	10	33
39	BQ	99/100 (99%)	94 (95%)	5 (5%)	20	45
40	BR	89/90 (99%)	84 (94%)	5 (6%)	17	43
41	BS	84/84 (100%)	79 (94%)	5 (6%)	16	41
42	BT	93/93 (100%)	86 (92%)	7 (8%)	11	34
43	BU	83/84 (99%)	80 (96%)	3 (4%)	30	54
44	BV	84/85 (99%)	77 (92%)	7 (8%)	9	32
45	BW	78/78 (100%)	74 (95%)	4 (5%)	20	45
46	BX	58/63 (92%)	57 (98%)	1 (2%)	56	72
47	BY	67/68 (98%)	65 (97%)	2 (3%)	36	58
48	BZ	54/55 (98%)	51 (94%)	3 (6%)	17	43
49	B1	48/49 (98%)	44 (92%)	4 (8%)	9	32
50	B2	47/48 (98%)	42 (89%)	5 (11%)	5	22
51	B3	48/49 (98%)	45 (94%)	3 (6%)	15	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	B4	37/38 (97%)	35 (95%)	2 (5%)	18	44
53	B5	51/52 (98%)	48 (94%)	3 (6%)	16	41
54	B6	34/44 (77%)	32 (94%)	2 (6%)	16	41
55	CA	197/286 (69%)	191 (97%)	6 (3%)	36	58
55	CB	187/286 (65%)	180 (96%)	7 (4%)	29	53
56	CC	1139/1157 (98%)	1099 (96%)	40 (4%)	31	54
57	CD	1118/1168 (96%)	1090 (98%)	28 (2%)	42	62
58	CE	43/75 (57%)	42 (98%)	1 (2%)	45	64
61	CF	86/158 (54%)	85 (99%)	1 (1%)	67	78
All	All	7379/7883 (94%)	6968 (94%)	411 (6%)	20	43

All (411) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	82	ASP
2	AB	111	ILE
2	AB	128	LYS
2	AB	129	LEU
2	AB	132	LYS
2	AB	207	ILE
2	AB	220	THR
3	AC	14	ILE
3	AC	26	THR
3	AC	35	SER
3	AC	107	ARG
3	AC	135	LYS
3	AC	136	ARG
3	AC	147	LYS
3	AC	154	SER
3	AC	161	GLU
3	AC	164	ARG
3	AC	165	THR
3	AC	172	ARG
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
4	AD	47	ARG
4	AD	50	ASP

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Mol	Chain	Res	Type
4	AD	56	ARG
4	AD	58	LYS
4	AD	104	ARG
4	AD	138	SER
4	AD	156	LYS
4	AD	164	GLN
4	AD	167	LYS
4	AD	179	GLU
4	AD	181	THR
4	AD	187	GLU
4	AD	191	LEU
4	AD	197	GLU
4	AD	206	LYS
5	AE	10	GLU
5	AE	15	LEU
5	AE	18	VAL
5	AE	46	VAL
5	AE	65	GLU
5	AE	78	ASN
5	AE	80	THR
5	AE	93	ARG
5	AE	114	VAL
5	AE	115	LEU
5	AE	120	VAL
5	AE	134	ILE
5	AE	136	VAL
5	AE	138	ARG
5	AE	141	ILE
5	AE	142	ASP
5	AE	146	ASN
5	AE	153	VAL
6	AF	7	VAL
6	AF	24	ARG
6	AF	38	ARG
6	AF	44	ARG
6	AF	54	LEU
6	AF	79	ARG
6	AF	86	ARG
6	AF	100	SER
7	AG	4	ARG
7	AG	6	VAL
7	AG	7	ILE

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Mol	Chain	Res	Type
7	AG	17	LYS
7	AG	25	LYS
7	AG	60	GLU
7	AG	73	VAL
7	AG	80	VAL
7	AG	109	ARG
7	AG	123	GLU
7	AG	130	ASN
7	AG	135	VAL
7	AG	146	GLU
7	AG	154	TYR
8	AH	3	MET
8	AH	31	LYS
8	AH	87	LYS
8	AH	88	ARG
8	AH	96	MET
8	AH	117	ARG
8	AH	121	LEU
9	AI	3	GLU
9	AI	4	ASN
9	AI	12	ARG
9	AI	41	ARG
9	AI	57	MET
9	AI	118	LEU
9	AI	123	ARG
10	AJ	4	GLN
10	AJ	5	ARG
10	AJ	17	LEU
10	AJ	18	ILE
10	AJ	36	VAL
10	AJ	37	ARG
11	AK	13	ARG
11	AK	14	LYS
11	AK	15	GLN
11	AK	69	ARG
11	AK	76	GLU
11	AK	109	ASN
11	AK	116	ILE
12	AL	4	VAL
12	AL	5	ASN
12	AL	12	ARG
12	AL	24	LEU

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Mol	Chain	Res	Type
12	AL	40	THR
12	AL	47	SER
12	AL	52	VAL
12	AL	55	VAL
12	AL	58	THR
12	AL	62	GLU
12	AL	64	THR
12	AL	102	LEU
13	AM	16	VAL
13	AM	54	ASP
13	AM	89	LEU
13	AM	92	ARG
13	AM	93	ARG
13	AM	96	PRO
13	AM	101	ARG
13	AM	104	THR
14	AN	10	GLU
14	AN	52	PRO
14	AN	89	MET
14	AN	92	GLU
14	AN	100	SER
15	AO	6	GLU
15	AO	40	GLN
15	AO	61	SER
15	AO	64	ARG
15	AO	80	GLN
15	AO	84	ARG
16	AP	1	MET
16	AP	42	ILE
16	AP	50	THR
16	AP	77	GLU
17	AQ	4	LYS
17	AQ	22	VAL
17	AQ	53	CYS
17	AQ	75	LEU
18	AR	55	LEU
18	AR	71	THR
18	AR	74	HIS
19	AS	49	ILE
19	AS	64	ASP
20	AT	6	SER
20	AT	10	ARG

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Mol	Chain	Res	Type
20	AT	24	ARG
20	AT	43	ASP
20	AT	48	GLN
20	AT	54	MET
20	AT	58	VAL
21	AU	4	ILE
21	AU	28	VAL
21	AU	67	ARG
27	BC	52	ARG
27	BC	130	LEU
27	BC	161	TYR
27	BC	189	ARG
27	BC	202	LEU
27	BC	203	ARG
27	BC	242	LYS
27	BC	258	ARG
28	BD	13	ARG
28	BD	32	ASN
28	BD	43	ASP
28	BD	77	ARG
28	BD	86	GLU
28	BD	92	VAL
28	BD	118	PHE
28	BD	197	THR
29	BE	7	ASP
29	BE	21	ARG
29	BE	22	ASP
29	BE	40	ARG
29	BE	57	LYS
29	BE	73	ILE
29	BE	88	ARG
29	BE	109	LEU
29	BE	111	GLU
29	BE	122	GLU
29	BE	124	PHE
29	BE	185	LYS
30	BF	6	ASP
30	BF	10	ASP
30	BF	47	LYS
30	BF	57	LEU
30	BF	80	ARG
30	BF	115	ARG

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Mol	Chain	Res	Type
30	BF	123	ASP
30	BF	133	ARG
30	BF	136	ILE
30	BF	140	GLU
30	BF	152	LEU
30	BF	179	LYS
31	BG	16	ASP
31	BG	32	GLU
31	BG	34	THR
31	BG	36	THR
31	BG	95	ARG
31	BG	104	ASN
31	BG	110	SER
31	BG	111	HIS
31	BG	127	THR
31	BG	155	GLU
31	BG	167	GLU
31	BG	168	VAL
31	BG	173	GLU
31	BG	176	LYS
32	BH	1	MET
32	BH	12	LEU
32	BH	17	ASP
32	BH	48	GLU
32	BH	66	ASN
32	BH	72	ILE
32	BH	101	ASP
32	BH	110	VAL
32	BH	117	LEU
32	BH	129	GLU
32	BH	134	VAL
33	BK	1	MET
33	BK	35	ARG
33	BK	57	LEU
33	BK	108	MET
33	BK	123	LYS
33	BK	142	ILE
34	BL	17	ARG
34	BL	18	ARG
34	BL	41	ILE
34	BL	58	LEU
34	BL	67	LYS

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Mol	Chain	Res	Type
34	BL	99	ILE
34	BL	110	GLU
34	BL	111	LYS
34	BL	123	LEU
35	BM	10	GLU
35	BM	30	THR
35	BM	33	ARG
35	BM	40	SER
35	BM	48	ARG
35	BM	67	THR
35	BM	84	LYS
35	BM	115	GLU
35	BM	144	GLU
36	BN	18	ARG
36	BN	100	LYS
36	BN	106	ASP
36	BN	110	GLU
36	BN	115	GLU
37	BO	2	ARG
37	BO	13	ASN
37	BO	20	MET
37	BO	51	LEU
37	BO	63	ARG
37	BO	65	LEU
37	BO	69	ARG
38	BP	2	ASP
38	BP	13	ARG
38	BP	18	LEU
38	BP	19	GLN
38	BP	47	VAL
38	BP	115	LEU
38	BP	116	GLN
39	BQ	40	LEU
39	BQ	80	VAL
39	BQ	88	ARG
39	BQ	111	LYS
39	BQ	113	ARG
40	BR	11	ARG
40	BR	51	ARG
40	BR	52	GLN
40	BR	59	GLN
40	BR	91	ASP

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Mol	Chain	Res	Type
41	BS	10	LYS
41	BS	39	LEU
41	BS	48	LYS
41	BS	79	ARG
41	BS	86	GLN
42	BT	11	ARG
42	BT	19	LEU
42	BT	41	LYS
42	BT	67	ASP
42	BT	83	LYS
42	BT	109	ASP
42	BT	110	ARG
43	BU	1	MET
43	BU	53	VAL
43	BU	89	GLU
44	BV	7	ARG
44	BV	9	ASP
44	BV	15	THR
44	BV	46	GLN
44	BV	52	LEU
44	BV	72	ILE
44	BV	101	GLU
45	BW	34	LYS
45	BW	40	ILE
45	BW	41	GLU
45	BW	45	ASP
46	BX	70	GLU
47	BY	48	THR
47	BY	60	ASP
48	BZ	7	ARG
48	BZ	11	VAL
48	BZ	58	ASN
49	B1	8	THR
49	B1	10	THR
49	B1	19	LYS
49	B1	45	ARG
50	B2	12	LYS
50	B2	39	LEU
50	B2	40	ARG
50	B2	42	HIS
50	B2	55	ILE
51	B3	5	ILE

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Mol	Chain	Res	Type
51	B3	17	THR
51	B3	23	THR
52	B4	22	MET
52	B4	25	LYS
53	B5	31	HIS
53	B5	32	ILE
53	B5	55	LEU
54	B6	26	ILE
54	B6	37	GLN
55	CA	13	LEU
55	CA	74	VAL
55	CA	100	LEU
55	CA	166	ARG
55	CA	185	TYR
55	CA	224	LEU
55	CB	13	LEU
55	CB	48	LEU
55	CB	66	HIS
55	CB	72	GLU
55	CB	170	ARG
55	CB	174	ASP
55	CB	191	ARG
56	CC	65	ASN
56	CC	193	ASN
56	CC	256	GLU
56	CC	262	TYR
56	CC	316	GLU
56	CC	369	MET
56	CC	494	ASN
56	CC	524	ILE
56	CC	529	ARG
56	CC	562	GLU
56	CC	568	ASN
56	CC	575	LEU
56	CC	770	CYS
56	CC	799	ASN
56	CC	830	THR
56	CC	843	THR
56	CC	844	LYS
56	CC	856	ASN
56	CC	888	THR
56	CC	950	GLU

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Mol	Chain	Res	Type
56	CC	955	GLN
56	CC	996	ARG
56	CC	1002	LEU
56	CC	1005	GLU
56	CC	1022	LYS
56	CC	1101	LEU
56	CC	1108	ASN
56	CC	1158	LYS
56	CC	1223	ARG
56	CC	1238	LEU
56	CC	1240	ASP
56	CC	1247	SER
56	CC	1250	SER
56	CC	1287	LEU
56	CC	1291	LEU
56	CC	1298	VAL
56	CC	1304	MET
56	CC	1313	HIS
56	CC	1336	ASN
56	CC	1340	GLU
57	CD	47	ARG
57	CD	68	TYR
57	CD	99	ARG
57	CD	158	GLN
57	CD	196	GLN
57	CD	259	ARG
57	CD	275	ARG
57	CD	281	ARG
57	CD	317	THR
57	CD	366	CYS
57	CD	368	LEU
57	CD	416	ILE
57	CD	418	GLU
57	CD	430	HIS
57	CD	505	ASP
57	CD	680	ASN
57	CD	700	ASN
57	CD	709	ARG
57	CD	802	ASP
57	CD	839	VAL
57	CD	847	ASP
57	CD	1144	LEU

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Mol	Chain	Res	Type
57	CD	1165	PHE
57	CD	1167	LYS
57	CD	1195	GLN
57	CD	1237	VAL
57	CD	1261	LEU
57	CD	1317	GLU
58	CE	53	GLU
61	CF	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
5	AE	77	ASN
6	AF	11	HIS
6	AF	46	GLN
27	BC	142	HIS
29	BE	165	HIS
30	BF	127	ASN
31	BG	104	ASN
36	BN	13	HIS
56	CC	235	ASN
57	CD	1197	ASN
57	CD	1367	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	294 (19%)	32 (2%)
22	AV	29/57 (50%)	10 (34%)	1 (3%)
23	AW	76/77 (98%)	22 (28%)	8 (10%)
24	AX	73/76 (96%)	24 (32%)	2 (2%)
24	AZ	73/76 (96%)	30 (41%)	0
25	BA	2893/2904 (99%)	544 (18%)	66 (2%)
26	BB	119/120 (99%)	12 (10%)	0
All	All	4792/4852 (98%)	936 (19%)	109 (2%)

All (936) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U

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Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	19	A
1	AA	22	G
1	AA	29	U
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	54	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	75	G
1	AA	76	G
1	AA	80	C
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	87	C
1	AA	89	G
1	AA	90	C
1	AA	94	G
1	AA	95	C
1	AA	96	U
1	AA	108	G
1	AA	121	U
1	AA	122	G
1	AA	131	A
1	AA	141	G
1	AA	144	G
1	AA	148	G
1	AA	149	A
1	AA	160	A
1	AA	164	G

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Mol	Chain	Res	Type
1	AA	173	U
1	AA	181	A
1	AA	182	A
1	AA	183	C
1	AA	184	G
1	AA	196	A
1	AA	197	A
1	AA	198	G
1	AA	208	U
1	AA	209	U
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	216	U
1	AA	226	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	258	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	289	G
1	AA	306	A
1	AA	316	C
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	340	U
1	AA	347	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	376	G
1	AA	384	G
1	AA	388	G
1	AA	389	A
1	AA	392	C

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Mol	Chain	Res	Type
1	AA	397	A
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	446	G
1	AA	451	A
1	AA	457	G
1	AA	458	U
1	AA	460	A
1	AA	463	U
1	AA	464	U
1	AA	467	U
1	AA	468	A
1	AA	469	C
1	AA	479	U
1	AA	480	U
1	AA	481	G
1	AA	484	G
1	AA	485	U
1	AA	486	U
1	AA	495	A
1	AA	511	C
1	AA	516	PSU
1	AA	517	G
1	AA	518	C
1	AA	521	G
1	AA	526	C
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G

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Mol	Chain	Res	Type
1	AA	579	A
1	AA	588	G
1	AA	596	A
1	AA	628	G
1	AA	633	G
1	AA	642	A
1	AA	649	A
1	AA	650	G
1	AA	653	U
1	AA	656	G
1	AA	665	A
1	AA	687	A
1	AA	702	A
1	AA	723	U
1	AA	724	G
1	AA	731	G
1	AA	734	G
1	AA	747	A
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	836	G
1	AA	841	C
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	849	G
1	AA	874	G
1	AA	887	G
1	AA	902	G
1	AA	914	A
1	AA	916	U
1	AA	926	G
1	AA	928	G
1	AA	934	C
1	AA	935	A
1	AA	936	C

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Mol	Chain	Res	Type
1	AA	960	U
1	AA	961	U
1	AA	966	2MG
1	AA	969	A
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	999	C
1	AA	1004	A
1	AA	1005	A
1	AA	1008	U
1	AA	1009	U
1	AA	1017	U
1	AA	1018	G
1	AA	1021	A
1	AA	1024	G
1	AA	1026	G
1	AA	1028	C
1	AA	1030	U
1	AA	1031	C
1	AA	1037	C
1	AA	1043	G
1	AA	1044	A
1	AA	1046	A
1	AA	1065	U
1	AA	1084	G
1	AA	1085	U
1	AA	1086	U
1	AA	1092	A
1	AA	1094	G
1	AA	1095	U
1	AA	1099	G
1	AA	1101	A
1	AA	1133	G
1	AA	1135	U
1	AA	1136	C
1	AA	1137	C

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Mol	Chain	Res	Type
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1151	A
1	AA	1152	A
1	AA	1158	C
1	AA	1159	U
1	AA	1167	A
1	AA	1168	U
1	AA	1171	A
1	AA	1174	G
1	AA	1175	G
1	AA	1176	A
1	AA	1184	G
1	AA	1187	G
1	AA	1196	A
1	AA	1197	A
1	AA	1211	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1227	A
1	AA	1238	A
1	AA	1239	A
1	AA	1242	G
1	AA	1257	A
1	AA	1260	G
1	AA	1275	A
1	AA	1276	G
1	AA	1277	C
1	AA	1278	G
1	AA	1279	G
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C

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Mol	Chain	Res	Type
1	AA	1305	G
1	AA	1311	A
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1323	G
1	AA	1329	A
1	AA	1332	A
1	AA	1334	G
1	AA	1338	G
1	AA	1340	A
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1378	C
1	AA	1379	G
1	AA	1381	U
1	AA	1383	C
1	AA	1396	A
1	AA	1397	C
1	AA	1404	C
1	AA	1408	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1487	G
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
22	AV	16	A

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Mol	Chain	Res	Type
22	AV	24	A
22	AV	25	U
22	AV	26	A
22	AV	27	C
22	AV	44	A
22	AV	45	C
22	AV	46	G
22	AV	49	G
22	AV	53	G
23	AW	6	G
23	AW	9	G
23	AW	14	A
23	AW	16	C
23	AW	17	C
23	AW	17(A)	U
23	AW	18	G
23	AW	19	G
23	AW	20	H2U
23	AW	21	A
23	AW	22	G
23	AW	25	C
23	AW	31	G
23	AW	47	U
23	AW	48	C
23	AW	49	G
23	AW	57	A
23	AW	59	A
23	AW	69	C
23	AW	74	C
23	AW	75	C
23	AW	76	A
24	AX	8	4SU
24	AX	9	A
24	AX	11	C
24	AX	13	C
24	AX	16	H2U
24	AX	17	C
24	AX	18	G
24	AX	19	G
24	AX	20	H2U
24	AX	21	A
24	AX	22	G

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Mol	Chain	Res	Type
24	AX	25	C
24	AX	36	A
24	AX	43	C
24	AX	46	7MG
24	AX	48	C
24	AX	49	C
24	AX	55	PSU
24	AX	57	G
24	AX	60	U
24	AX	61	C
24	AX	63	G
24	AX	74	C
24	AX	75	C
24	AZ	6	G
24	AZ	8	4SU
24	AZ	9	A
24	AZ	10	G
24	AZ	13	C
24	AZ	16	H2U
24	AZ	17	C
24	AZ	18	G
24	AZ	19	G
24	AZ	20	H2U
24	AZ	21	A
24	AZ	22	G
24	AZ	25	C
24	AZ	30	G
24	AZ	38	A
24	AZ	43	C
24	AZ	45	U
24	AZ	46	7MG
24	AZ	48	C
24	AZ	49	C
24	AZ	56	C
24	AZ	57	G
24	AZ	58	A
24	AZ	59	U
24	AZ	60	U
24	AZ	62	C
24	AZ	64	A
24	AZ	66	U
24	AZ	68	C

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Mol	Chain	Res	Type
24	AZ	76	A
25	BA	10	A
25	BA	14	A
25	BA	23	G
25	BA	34	U
25	BA	35	G
25	BA	45	G
25	BA	46	G
25	BA	58	G
25	BA	60	G
25	BA	62	U
25	BA	63	A
25	BA	71	A
25	BA	74	A
25	BA	75	G
25	BA	83	A
25	BA	84	A
25	BA	85	G
25	BA	91	A
25	BA	99	U
25	BA	101	A
25	BA	102	U
25	BA	110	G
25	BA	118	A
25	BA	119	A
25	BA	120	U
25	BA	122	G
25	BA	131	A
25	BA	138	U
25	BA	139	U
25	BA	140	C
25	BA	141	G
25	BA	142	A
25	BA	144	A
25	BA	149	A
25	BA	163	C
25	BA	165	A
25	BA	181	A
25	BA	196	A
25	BA	215	G
25	BA	216	A
25	BA	221	A

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Mol	Chain	Res	Type
25	BA	222	A
25	BA	248	G
25	BA	249	C
25	BA	264	C
25	BA	265	A
25	BA	266	G
25	BA	270	A
25	BA	271	G
25	BA	272	A
25	BA	276	U
25	BA	277	G
25	BA	278	A
25	BA	285	G
25	BA	311	A
25	BA	327	G
25	BA	329	G
25	BA	330	A
25	BA	353	C
25	BA	361	G
25	BA	362	A
25	BA	371	A
25	BA	372	G
25	BA	386	G
25	BA	396	G
25	BA	405	U
25	BA	411	G
25	BA	412	A
25	BA	424	G
25	BA	435	C
25	BA	451	U
25	BA	456	C
25	BA	457	A
25	BA	477	A
25	BA	480	A
25	BA	481	G
25	BA	491	G
25	BA	501	A
25	BA	503	A
25	BA	504	A
25	BA	505	A
25	BA	508	A
25	BA	509	C

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Mol	Chain	Res	Type
25	BA	531	C
25	BA	532	A
25	BA	533	G
25	BA	544	G
25	BA	563	A
25	BA	569	U
25	BA	573	U
25	BA	574	A
25	BA	575	A
25	BA	586	A
25	BA	603	A
25	BA	609	A
25	BA	613	A
25	BA	614	A
25	BA	615	U
25	BA	616	A
25	BA	618	G
25	BA	627	A
25	BA	637	A
25	BA	645	C
25	BA	647	G
25	BA	651	G
25	BA	654	A
25	BA	655	A
25	BA	668	A
25	BA	686	U
25	BA	696	G
25	BA	717	C
25	BA	724	U
25	BA	730	A
25	BA	738	G
25	BA	746	PSU
25	BA	747	5MU
25	BA	757	G
25	BA	764	A
25	BA	765	C
25	BA	775	G
25	BA	776	G
25	BA	782	A
25	BA	783	A
25	BA	784	G
25	BA	785	G

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Mol	Chain	Res	Type
25	BA	788	A
25	BA	789	A
25	BA	805	G
25	BA	812	C
25	BA	819	A
25	BA	827	U
25	BA	828	U
25	BA	845	A
25	BA	846	U
25	BA	858	G
25	BA	859	G
25	BA	869	G
25	BA	878	A
25	BA	881	G
25	BA	883	G
25	BA	884	U
25	BA	885	C
25	BA	887	U
25	BA	888	C
25	BA	889	C
25	BA	890	C
25	BA	891	G
25	BA	892	A
25	BA	893	C
25	BA	895	U
25	BA	896	A
25	BA	897	C
25	BA	898	C
25	BA	899	A
25	BA	910	A
25	BA	914	G
25	BA	915	C
25	BA	931	U
25	BA	933	A
25	BA	940	G
25	BA	946	C
25	BA	953	G
25	BA	961	C
25	BA	974	G
25	BA	983	A
25	BA	984	A
25	BA	985	C

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Mol	Chain	Res	Type
25	BA	995	C
25	BA	996	A
25	BA	999	U
25	BA	1005	C
25	BA	1012	U
25	BA	1013	C
25	BA	1023	U
25	BA	1026	G
25	BA	1033	U
25	BA	1040	A
25	BA	1043	C
25	BA	1045	C
25	BA	1046	A
25	BA	1047	G
25	BA	1050	A
25	BA	1060	U
25	BA	1061	U
25	BA	1063	G
25	BA	1064	C
25	BA	1065	U
25	BA	1066	U
25	BA	1067	A
25	BA	1068	G
25	BA	1069	A
25	BA	1070	A
25	BA	1073	A
25	BA	1074	G
25	BA	1083	U
25	BA	1084	A
25	BA	1087	G
25	BA	1088	A
25	BA	1090	A
25	BA	1107	G
25	BA	1111	A
25	BA	1112	G
25	BA	1119	U
25	BA	1122	G
25	BA	1130	U
25	BA	1132	U
25	BA	1134	A
25	BA	1135	C
25	BA	1142	A

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Mol	Chain	Res	Type
25	BA	1170	C
25	BA	1171	G
25	BA	1173	U
25	BA	1174	U
25	BA	1176	U
25	BA	1177	G
25	BA	1178	C
25	BA	1180	U
25	BA	1186	G
25	BA	1211	U
25	BA	1236	G
25	BA	1238	G
25	BA	1248	G
25	BA	1253	A
25	BA	1256	G
25	BA	1265	A
25	BA	1271	G
25	BA	1272	A
25	BA	1273	U
25	BA	1301	A
25	BA	1302	A
25	BA	1321	A
25	BA	1345	C
25	BA	1352	U
25	BA	1365	A
25	BA	1368	G
25	BA	1378	A
25	BA	1379	U
25	BA	1380	G
25	BA	1383	A
25	BA	1395	A
25	BA	1405	U
25	BA	1406	U
25	BA	1407	G
25	BA	1408	G
25	BA	1409	U
25	BA	1414	C
25	BA	1416	G
25	BA	1417	C
25	BA	1420	A
25	BA	1428	C
25	BA	1434	A

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Mol	Chain	Res	Type
25	BA	1452	G
25	BA	1453	A
25	BA	1455	G
25	BA	1458	U
25	BA	1460	U
25	BA	1478	G
25	BA	1482	G
25	BA	1483	G
25	BA	1490	A
25	BA	1493	C
25	BA	1495	A
25	BA	1497	U
25	BA	1508	A
25	BA	1509	A
25	BA	1510	G
25	BA	1515	A
25	BA	1529	G
25	BA	1534	U
25	BA	1535	A
25	BA	1536	C
25	BA	1537	G
25	BA	1554	U
25	BA	1558	C
25	BA	1559	U
25	BA	1566	A
25	BA	1569	A
25	BA	1578	U
25	BA	1580	A
25	BA	1581	G
25	BA	1583	A
25	BA	1584	U
25	BA	1589	U
25	BA	1590	A
25	BA	1592	C
25	BA	1593	A
25	BA	1594	U
25	BA	1595	C
25	BA	1596	A
25	BA	1597	A
25	BA	1608	A
25	BA	1609	A
25	BA	1610	A

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Mol	Chain	Res	Type
25	BA	1613	G
25	BA	1630	A
25	BA	1647	U
25	BA	1648	U
25	BA	1649	G
25	BA	1651	G
25	BA	1674	G
25	BA	1677	A
25	BA	1703	G
25	BA	1713	A
25	BA	1714	U
25	BA	1715	G
25	BA	1718	G
25	BA	1729	U
25	BA	1730	C
25	BA	1732	C
25	BA	1738	G
25	BA	1742	U
25	BA	1750	G
25	BA	1755	A
25	BA	1758	U
25	BA	1761	C
25	BA	1764	C
25	BA	1773	A
25	BA	1791	A
25	BA	1800	C
25	BA	1801	A
25	BA	1808	A
25	BA	1811	G
25	BA	1816	C
25	BA	1829	A
25	BA	1833	C
25	BA	1848	A
25	BA	1858	A
25	BA	1859	U
25	BA	1862	G
25	BA	1864	U
25	BA	1869	G
25	BA	1870	C
25	BA	1905	C
25	BA	1906	G
25	BA	1907	G

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Mol	Chain	Res	Type
25	BA	1912	A
25	BA	1913	A
25	BA	1914	C
25	BA	1917	PSU
25	BA	1918	A
25	BA	1919	A
25	BA	1929	G
25	BA	1930	G
25	BA	1931	U
25	BA	1936	A
25	BA	1938	A
25	BA	1939	5MU
25	BA	1955	U
25	BA	1960	A
25	BA	1965	C
25	BA	1966	A
25	BA	1967	C
25	BA	1970	A
25	BA	1971	U
25	BA	1972	G
25	BA	1987	A
25	BA	1991	U
25	BA	1992	G
25	BA	1993	U
25	BA	1997	C
25	BA	2002	G
25	BA	2022	U
25	BA	2023	C
25	BA	2026	U
25	BA	2031	A
25	BA	2033	A
25	BA	2043	C
25	BA	2051	A
25	BA	2052	A
25	BA	2055	C
25	BA	2056	G
25	BA	2060	A
25	BA	2061	G
25	BA	2062	A
25	BA	2063	C
25	BA	2069	G7M
25	BA	2093	G

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Mol	Chain	Res	Type
25	BA	2097	A
25	BA	2099	U
25	BA	2100	G
25	BA	2101	A
25	BA	2108	A
25	BA	2110	G
25	BA	2111	U
25	BA	2113	U
25	BA	2115	G
25	BA	2117	A
25	BA	2118	U
25	BA	2119	A
25	BA	2120	G
25	BA	2122	U
25	BA	2124	G
25	BA	2125	G
25	BA	2126	A
25	BA	2127	G
25	BA	2128	G
25	BA	2131	U
25	BA	2132	U
25	BA	2133	G
25	BA	2134	A
25	BA	2139	U
25	BA	2141	G
25	BA	2146	C
25	BA	2147	A
25	BA	2154	A
25	BA	2157	G
25	BA	2158	A
25	BA	2159	G
25	BA	2161	C
25	BA	2162	G
25	BA	2163	A
25	BA	2164	C
25	BA	2165	C
25	BA	2169	A
25	BA	2171	A
25	BA	2172	U
25	BA	2178	C
25	BA	2182	U
25	BA	2183	A

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Mol	Chain	Res	Type
25	BA	2185	U
25	BA	2188	U
25	BA	2197	U
25	BA	2198	A
25	BA	2199	A
25	BA	2203	U
25	BA	2204	G
25	BA	2211	G
25	BA	2212	A
25	BA	2213	U
25	BA	2225	A
25	BA	2226	C
25	BA	2229	U
25	BA	2238	G
25	BA	2239	G
25	BA	2245	U
25	BA	2246	G
25	BA	2250	G
25	BA	2251	OMG
25	BA	2252	G
25	BA	2268	A
25	BA	2278	A
25	BA	2283	C
25	BA	2287	A
25	BA	2294	G
25	BA	2297	A
25	BA	2305	U
25	BA	2308	G
25	BA	2309	A
25	BA	2315	G
25	BA	2322	A
25	BA	2325	G
25	BA	2327	A
25	BA	2333	A
25	BA	2335	A
25	BA	2336	A
25	BA	2347	C
25	BA	2350	C
25	BA	2361	G
25	BA	2372	U
25	BA	2376	A
25	BA	2383	G

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Mol	Chain	Res	Type
25	BA	2385	C
25	BA	2403	C
25	BA	2406	A
25	BA	2410	G
25	BA	2423	U
25	BA	2424	C
25	BA	2425	A
25	BA	2426	A
25	BA	2429	G
25	BA	2430	A
25	BA	2431	U
25	BA	2435	A
25	BA	2441	U
25	BA	2445	2MG
25	BA	2448	A
25	BA	2449	H2U
25	BA	2470	G
25	BA	2474	U
25	BA	2476	A
25	BA	2478	A
25	BA	2491	U
25	BA	2498	OMC
25	BA	2502	G
25	BA	2504	PSU
25	BA	2505	G
25	BA	2512	C
25	BA	2513	A
25	BA	2518	A
25	BA	2520	C
25	BA	2525	G
25	BA	2529	G
25	BA	2535	G
25	BA	2547	A
25	BA	2552	OMU
25	BA	2554	U
25	BA	2566	A
25	BA	2567	G
25	BA	2573	C
25	BA	2574	G
25	BA	2585	U
25	BA	2586	U
25	BA	2602	A

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Mol	Chain	Res	Type
25	BA	2609	U
25	BA	2610	C
25	BA	2611	C
25	BA	2613	U
25	BA	2629	U
25	BA	2630	G
25	BA	2663	G
25	BA	2671	G
25	BA	2682	A
25	BA	2689	U
25	BA	2690	U
25	BA	2714	G
25	BA	2726	A
25	BA	2744	G
25	BA	2748	A
25	BA	2757	A
25	BA	2762	C
25	BA	2765	A
25	BA	2777	G
25	BA	2778	A
25	BA	2791	G
25	BA	2796	C
25	BA	2797	U
25	BA	2798	U
25	BA	2801	G
25	BA	2818	U
25	BA	2820	A
25	BA	2825	G
25	BA	2849	U
25	BA	2859	G
25	BA	2861	U
25	BA	2867	G
25	BA	2872	A
25	BA	2879	A
25	BA	2880	C
25	BA	2883	A
25	BA	2884	U
25	BA	2885	G
25	BA	2891	U
25	BA	2902	C
25	BA	2903	U
26	BB	2	G

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Mol	Chain	Res	Type
26	BB	13	G
26	BB	16	G
26	BB	35	C
26	BB	36	C
26	BB	45	A
26	BB	56	G
26	BB	64	G
26	BB	66	A
26	BB	88	C
26	BB	90	C
26	BB	109	A

All (109) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	70	U
1	AA	147	G
1	AA	148	G
1	AA	181	A
1	AA	183	C
1	AA	197	A
1	AA	209	U
1	AA	428	G
1	AA	481	G
1	AA	587	G
1	AA	641	U
1	AA	701	U
1	AA	793	U
1	AA	843	U
1	AA	873	A
1	AA	961	U
1	AA	991	U
1	AA	992	U
1	AA	1129	C
1	AA	1166	G
1	AA	1167	A
1	AA	1196	A
1	AA	1211	U
1	AA	1213	A
1	AA	1214	C
1	AA	1277	C

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Mol	Chain	Res	Type
1	AA	1299	A
1	AA	1319	A
1	AA	1363	A
1	AA	1396	A
1	AA	1447	A
22	AV	43	A
23	AW	15	G
23	AW	16	C
23	AW	18	G
23	AW	19	G
23	AW	20	H2U
23	AW	21	A
23	AW	47	U
23	AW	60	U
24	AX	19	G
24	AX	20	H2U
25	BA	33	C
25	BA	62	U
25	BA	70	G
25	BA	71	A
25	BA	101	A
25	BA	138	U
25	BA	140	C
25	BA	196	A
25	BA	199	A
25	BA	271	G
25	BA	310	A
25	BA	404	A
25	BA	503	A
25	BA	685	A
25	BA	764	A
25	BA	776	G
25	BA	784	G
25	BA	883	G
25	BA	884	U
25	BA	887	U
25	BA	892	A
25	BA	894	U
25	BA	984	A
25	BA	1045	C
25	BA	1060	U
25	BA	1064	C

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Mol	Chain	Res	Type
25	BA	1067	A
25	BA	1069	A
25	BA	1109	C
25	BA	1111	A
25	BA	1128	G
25	BA	1173	U
25	BA	1300	G
25	BA	1320	C
25	BA	1344	U
25	BA	1379	U
25	BA	1405	U
25	BA	1407	G
25	BA	1490	A
25	BA	1494	A
25	BA	1509	A
25	BA	1584	U
25	BA	1596	A
25	BA	1608	A
25	BA	1913	A
25	BA	1918	A
25	BA	2062	A
25	BA	2099	U
25	BA	2146	C
25	BA	2162	G
25	BA	2197	U
25	BA	2198	A
25	BA	2210	U
25	BA	2212	A
25	BA	2225	A
25	BA	2250	G
25	BA	2296	U
25	BA	2308	G
25	BA	2425	A
25	BA	2573	C
25	BA	2585	U
25	BA	2610	C
25	BA	2756	U
25	BA	2797	U
25	BA	2798	U
25	BA	2873	A

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

63 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$
1	G7M	AA	527	1	20,26,27	2.29	7 (35%)	17,39,42	1.20	2 (11%)
28	MEQ	BD	150	28	8,9,10	0.91	0	5,10,12	1.07	1 (20%)
24	5MU	AX	54	24	19,22,23	1.36	3 (15%)	28,32,35	2.16	8 (28%)
24	3AU	AX	47	24	18,21,29	3.38	8 (44%)	26,30,43	1.67	5 (19%)
25	2MA	BA	2503	62,25	19,25,26	3.41	8 (42%)	21,37,40	2.37	3 (14%)
25	PSU	BA	2604	62,25	18,21,22	1.04	3 (16%)	22,30,33	1.84	4 (18%)
1	MA6	AA	1519	1	18,26,27	1.40	3 (16%)	19,38,41	3.85	2 (10%)
1	2MG	AA	966	1	18,26,27	2.31	7 (38%)	16,38,41	1.60	4 (25%)
24	PSU	AX	39	24	18,21,22	1.01	1 (5%)	22,30,33	1.90	5 (22%)
24	PSU	AX	55	24	18,21,22	1.04	1 (5%)	22,30,33	1.82	5 (22%)
25	OMG	BA	2251	23,25	18,26,27	2.59	8 (44%)	19,38,41	1.61	4 (21%)
25	PSU	BA	2605	62,25	18,21,22	1.00	2 (11%)	22,30,33	2.03	5 (22%)
1	2MG	AA	1516	1	18,26,27	2.19	7 (38%)	16,38,41	1.62	4 (25%)
24	PSU	AX	32	24	18,21,22	1.04	1 (5%)	22,30,33	1.58	3 (13%)
12	D2T	AL	89	12	7,9,10	1.08	0	6,11,13	2.06	2 (33%)
24	7MG	AZ	46	24	22,26,27	3.74	10 (45%)	29,39,42	1.96	8 (27%)
24	H2U	AZ	16	24	18,21,22	3.01	5 (27%)	21,30,33	2.01	5 (23%)
25	PSU	BA	2457	25	18,21,22	1.09	2 (11%)	22,30,33	2.16	6 (27%)
24	H2U	AX	20	24	18,21,22	3.19	5 (27%)	21,30,33	2.00	5 (23%)
25	6MZ	BA	1618	25	18,25,26	1.91	3 (16%)	16,36,39	2.35	4 (25%)
25	H2U	BA	2449	25	18,21,22	2.89	5 (27%)	21,30,33	2.31	5 (23%)
25	3TD	BA	1915	25	18,22,23	4.46	10 (55%)	22,32,35	1.98	4 (18%)
24	4SU	AZ	8	24	18,21,22	4.17	8 (44%)	26,30,33	2.14	5 (19%)
1	PSU	AA	516	1	18,21,22	1.02	1 (5%)	22,30,33	2.10	6 (27%)
23	H2U	AW	20	23	18,21,22	3.07	5 (27%)	21,30,33	2.28	5 (23%)
25	PSU	BA	2580	25	18,21,22	1.04	3 (16%)	22,30,33	2.25	7 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MU	BA	747	25	19,22,23	1.39	4 (21%)	28,32,35	2.23	6 (21%)
24	7MG	AX	46	24	22,26,27	3.79	10 (45%)	29,39,42	2.08	9 (31%)
24	H2U	AX	16	24	18,21,22	3.04	5 (27%)	21,30,33	2.05	5 (23%)
24	4SU	AX	8	24	18,21,22	4.05	8 (44%)	26,30,33	2.32	5 (19%)
24	MIA	AX	37	24	22,29,32	2.82	4 (18%)	22,41,47	3.01	7 (31%)
23	5MU	AW	54	23	19,22,23	1.41	5 (26%)	28,32,35	2.27	10 (35%)
25	1MG	BA	745	25	18,26,27	2.61	6 (33%)	19,39,42	1.45	4 (21%)
25	OMC	BA	2498	25	19,22,23	2.84	7 (36%)	26,31,34	0.75	1 (3%)
1	2MG	AA	1207	1,62	18,26,27	2.29	7 (38%)	16,38,41	1.65	4 (25%)
24	PSU	AZ	55	24	18,21,22	1.10	1 (5%)	22,30,33	1.83	4 (18%)
25	PSU	BA	746	62,25	18,21,22	1.02	2 (11%)	22,30,33	2.03	6 (27%)
36	4D4	BN	81	36	9,11,12	2.49	3 (33%)	8,13,15	0.74	0
1	5MC	AA	967	1	18,22,23	3.96	7 (38%)	26,32,35	1.13	2 (7%)
25	2MG	BA	2445	25	18,26,27	2.24	7 (38%)	16,38,41	1.61	4 (25%)
24	H2U	AZ	20	24	18,21,22	3.05	5 (27%)	21,30,33	2.04	5 (23%)
23	4SU	AW	8	23	18,21,22	4.04	8 (44%)	26,30,33	2.50	4 (15%)
24	PSU	AZ	32	24	18,21,22	1.00	1 (5%)	22,30,33	1.72	4 (18%)
25	PSU	BA	1911	25	18,21,22	1.07	2 (11%)	22,30,33	1.94	5 (22%)
1	MA6	AA	1518	1	18,26,27	1.39	3 (16%)	19,38,41	4.32	3 (15%)
25	5MC	BA	1962	25	18,22,23	3.83	7 (38%)	26,32,35	1.17	1 (3%)
25	6MZ	BA	2030	25	18,25,26	1.86	3 (16%)	16,36,39	2.65	3 (18%)
24	MIA	AZ	37	24	22,29,32	2.81	4 (18%)	22,41,47	2.97	6 (27%)
23	OMC	AW	32	23	19,22,23	2.90	8 (42%)	26,31,34	0.79	0
24	5MU	AZ	54	24	19,22,23	1.41	6 (31%)	28,32,35	2.04	6 (21%)
1	5MC	AA	1407	1	18,22,23	3.81	7 (38%)	26,32,35	1.02	1 (3%)
25	PSU	BA	2504	25	18,21,22	1.10	3 (16%)	22,30,33	2.16	5 (22%)
24	3AU	AZ	47	24	18,21,29	3.42	8 (44%)	26,30,43	1.64	5 (19%)
1	4OC	AA	1402	1,62	20,23,24	3.35	9 (45%)	26,32,35	1.00	2 (7%)
1	UR3	AA	1498	1	19,22,23	2.50	6 (31%)	26,32,35	1.40	1 (3%)
23	PSU	AW	55	23	18,21,22	1.01	1 (5%)	22,30,33	1.91	6 (27%)
25	PSU	BA	955	62,25	18,21,22	1.14	2 (11%)	22,30,33	1.82	4 (18%)
24	PSU	AZ	39	24	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
25	2MG	BA	1835	25	18,26,27	2.28	7 (38%)	16,38,41	1.65	4 (25%)
25	PSU	BA	1917	25	18,21,22	0.99	2 (11%)	22,30,33	1.91	5 (22%)
25	5MU	BA	1939	62,25	19,22,23	1.44	4 (21%)	28,32,35	2.39	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	G7M	BA	2069	25	20,26,27	2.25	8 (40%)	17,39,42	1.18	1 (5%)
25	OMU	BA	2552	25	19,22,23	2.90	7 (36%)	26,31,34	1.79	5 (19%)

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
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
28	MEQ	BD	150	28	-	3/8/9/11	-
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	3/7/25/35	0/2/2/2
25	2MA	BA	2503	62,25	-	2/3/25/26	0/3/3/3
25	PSU	BA	2604	62,25	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	6/7/29/30	0/3/3/3
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	2/7/25/26	0/2/2/2
25	OMG	BA	2251	23,25	-	1/5/27/28	0/3/3/3
25	PSU	BA	2605	62,25	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/7/12/14	-
24	7MG	AZ	46	24	-	3/7/37/38	0/3/3/3
24	H2U	AZ	16	24	-	3/7/38/39	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
24	H2U	AX	20	24	-	5/7/38/39	0/2/2/2
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
25	3TD	BA	1915	25	-	3/7/25/26	0/2/2/2
24	4SU	AZ	8	24	-	7/7/25/26	0/2/2/2
1	PSU	AA	516	1	-	1/7/25/26	0/2/2/2
23	H2U	AW	20	23	-	4/7/38/39	0/2/2/2
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	1/7/37/38	0/3/3/3
24	H2U	AX	16	24	-	2/7/38/39	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	MIA	AX	37	24	-	6/9/31/34	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
25	OMC	BA	2498	25	-	3/9/27/28	0/2/2/2
1	2MG	AA	1207	1,62	-	1/5/27/28	0/3/3/3
24	PSU	AZ	55	24	-	1/7/25/26	0/2/2/2
25	PSU	BA	746	62,25	-	2/7/25/26	0/2/2/2
36	4D4	BN	81	36	-	4/11/12/14	-
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
25	2MG	BA	2445	25	-	2/5/27/28	0/3/3/3
24	H2U	AZ	20	24	-	5/7/38/39	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
24	PSU	AZ	32	24	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	3/7/29/30	0/3/3/3
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
24	MIA	AZ	37	24	-	8/9/31/34	0/3/3/3
23	OMC	AW	32	23	-	1/9/27/28	0/2/2/2
24	5MU	AZ	54	24	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	PSU	BA	2504	25	-	0/7/25/26	0/2/2/2
24	3AU	AZ	47	24	-	1/7/25/35	0/2/2/2
1	4OC	AA	1402	1,62	-	1/9/29/30	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	3/7/25/26	0/2/2/2
25	PSU	BA	955	62,25	-	0/7/25/26	0/2/2/2
24	PSU	AZ	39	24	-	0/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
25	5MU	BA	1939	62,25	-	2/7/25/26	0/2/2/2
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2

All (304) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.84	1.49	1.35
24	AX	20	H2U	C2-N1	10.31	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	967	5MC	C6-C5	9.94	1.50	1.34
25	BA	1915	3TD	C2-N1	9.79	1.49	1.37
1	AA	1407	5MC	C6-C5	9.77	1.50	1.34
24	AX	37	MIA	C13-C14	9.63	1.60	1.32
23	AW	20	H2U	C2-N1	9.54	1.49	1.35
24	AZ	37	MIA	C13-C14	9.51	1.59	1.32
25	BA	1962	5MC	C6-C5	9.45	1.50	1.34
24	AZ	8	4SU	C4-N3	9.40	1.47	1.37
24	AZ	20	H2U	C2-N1	9.35	1.49	1.35
24	AX	16	H2U	C2-N1	9.30	1.48	1.35
24	AX	8	4SU	C4-N3	9.09	1.47	1.37
24	AZ	16	H2U	C2-N1	9.02	1.48	1.35
23	AW	8	4SU	C4-N3	8.99	1.47	1.37
25	BA	2503	2MA	C4-N3	8.93	1.49	1.35
24	AZ	46	7MG	C8-N9	8.82	1.50	1.46
24	AX	46	7MG	C8-N9	8.64	1.50	1.46
25	BA	2449	H2U	C2-N1	8.48	1.47	1.35
24	AZ	46	7MG	C5-N7	8.20	1.45	1.35
24	AZ	8	4SU	C2-N1	7.91	1.51	1.38
24	AZ	37	MIA	C6-N6	7.57	1.48	1.34
23	AW	8	4SU	C2-N1	7.57	1.50	1.38
24	AZ	47	3AU	C2-N1	7.54	1.50	1.38
24	AX	37	MIA	C6-N6	7.53	1.48	1.34
25	BA	745	1MG	C2-N3	7.48	1.48	1.34
24	AX	8	4SU	C2-N1	7.41	1.50	1.38
24	AX	47	3AU	C2-N1	7.37	1.50	1.38
24	AX	46	7MG	C5-N7	7.35	1.44	1.35
1	AA	967	5MC	C4-N3	7.25	1.46	1.34
25	BA	2503	2MA	C2-N3	7.22	1.46	1.34
25	BA	1962	5MC	C4-N3	7.21	1.46	1.34
24	AX	47	3AU	C6-C5	6.99	1.51	1.35
24	AZ	47	3AU	C6-C5	6.99	1.51	1.35
1	AA	1402	4OC	C4-N3	6.90	1.44	1.32
1	AA	967	5MC	C2-N3	6.83	1.50	1.36
1	AA	1407	5MC	C4-N3	6.79	1.45	1.34
25	BA	2552	OMU	C2-N3	6.69	1.49	1.38
25	BA	1962	5MC	C2-N3	6.60	1.49	1.36
24	AZ	8	4SU	C2-N3	6.51	1.49	1.38
24	AZ	47	3AU	C2-N3	6.49	1.49	1.38
24	AZ	16	H2U	C2-N3	6.49	1.49	1.38
24	AX	8	4SU	C2-N3	6.47	1.49	1.38
1	AA	1407	5MC	C2-N3	6.44	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1402	4OC	C6-C5	6.42	1.50	1.35
24	AZ	20	H2U	C2-N3	6.42	1.49	1.38
24	AX	47	3AU	C2-N3	6.40	1.49	1.38
25	BA	1618	6MZ	C6-N6	6.36	1.45	1.35
23	AW	20	H2U	C2-N3	6.34	1.49	1.38
24	AX	16	H2U	C2-N3	6.29	1.49	1.38
24	AX	20	H2U	C2-N3	6.27	1.49	1.38
23	AW	32	OMC	C2-N3	6.17	1.48	1.36
1	AA	1498	UR3	C2-N1	6.16	1.47	1.38
23	AW	8	4SU	C2-N3	6.14	1.48	1.38
25	BA	2449	H2U	C2-N3	6.12	1.48	1.38
24	AX	46	7MG	C2-N3	6.09	1.47	1.33
24	AZ	8	4SU	C6-C5	6.06	1.49	1.35
25	BA	1915	3TD	C6-N1	6.04	1.46	1.36
24	AX	8	4SU	C6-C5	6.03	1.49	1.35
25	BA	2552	OMU	C6-C5	6.00	1.49	1.35
25	BA	2030	6MZ	C6-N6	5.96	1.44	1.35
25	BA	2498	OMC	C2-N3	5.95	1.48	1.36
24	AX	46	7MG	C4-N3	5.93	1.48	1.34
1	AA	1498	UR3	C6-C5	5.88	1.48	1.35
25	BA	2498	OMC	C6-C5	5.87	1.48	1.35
23	AW	8	4SU	C6-C5	5.86	1.48	1.35
23	AW	8	4SU	C4-S4	-5.85	1.57	1.68
23	AW	32	OMC	C6-C5	5.82	1.48	1.35
36	BN	81	4D4	CZ-NE	5.80	1.44	1.33
25	BA	2503	2MA	C6-N1	5.75	1.44	1.33
1	AA	1402	4OC	C2-N3	5.75	1.48	1.36
24	AX	46	7MG	C4-N9	5.72	1.44	1.37
24	AZ	8	4SU	C5-C4	5.57	1.49	1.42
24	AZ	8	4SU	C4-S4	-5.48	1.58	1.68
24	AX	8	4SU	C5-C4	5.45	1.49	1.42
24	AZ	46	7MG	C4-N3	5.42	1.47	1.34
24	AX	8	4SU	C4-S4	-5.42	1.58	1.68
23	AW	8	4SU	C5-C4	5.41	1.49	1.42
24	AZ	46	7MG	C2-N3	5.40	1.46	1.33
25	BA	745	1MG	C2-N2	5.35	1.43	1.34
25	BA	2251	OMG	C2-N2	5.28	1.46	1.34
25	BA	2552	OMU	C2-N1	5.28	1.46	1.38
1	AA	967	5MC	C4-N4	5.27	1.47	1.34
25	BA	2251	OMG	C2-N3	5.27	1.46	1.33
24	AZ	47	3AU	C4-N3	5.26	1.48	1.38
25	BA	1962	5MC	C4-N4	5.26	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2503	2MA	C2-N1	5.21	1.43	1.34
25	BA	1915	3TD	C1'-C5	-5.15	1.38	1.50
1	AA	1407	5MC	C4-N4	5.15	1.47	1.34
24	AX	47	3AU	C4-N3	5.13	1.47	1.38
1	AA	967	5MC	C6-N1	5.11	1.46	1.38
1	AA	1402	4OC	O2-C2	-4.96	1.14	1.23
1	AA	1407	5MC	C6-N1	4.93	1.46	1.38
24	AZ	16	H2U	C4-N3	4.93	1.46	1.37
23	AW	32	OMC	C4-N3	4.92	1.44	1.34
24	AX	16	H2U	C4-N3	4.92	1.46	1.37
1	AA	527	G7M	C2-N3	4.91	1.45	1.33
25	BA	2251	OMG	C4-N3	4.90	1.49	1.37
25	BA	2069	G7M	C2-N3	4.88	1.45	1.33
24	AZ	20	H2U	C4-N3	4.87	1.45	1.37
24	AX	46	7MG	C2-N2	4.84	1.45	1.34
1	AA	1402	4OC	C4-N4	4.81	1.45	1.35
25	BA	1962	5MC	C6-N1	4.80	1.46	1.38
23	AW	20	H2U	C4-N3	4.78	1.45	1.37
23	AW	32	OMC	C4-N4	4.76	1.45	1.33
24	AX	20	H2U	C4-N3	4.70	1.45	1.37
25	BA	2498	OMC	C4-N3	4.70	1.44	1.34
25	BA	2498	OMC	C4-N4	4.64	1.44	1.33
1	AA	966	2MG	C2-N2	4.63	1.43	1.33
25	BA	2445	2MG	C2-N2	4.59	1.43	1.33
25	BA	1835	2MG	C2-N2	4.58	1.43	1.33
25	BA	2069	G7M	C2-N2	4.51	1.44	1.34
25	BA	1962	5MC	C2-N1	4.51	1.49	1.40
1	AA	527	G7M	C2-N2	4.49	1.44	1.34
24	AZ	46	7MG	C2-N2	4.49	1.44	1.34
1	AA	967	5MC	C2-N1	4.49	1.49	1.40
25	BA	2449	H2U	C4-N3	4.45	1.45	1.37
1	AA	527	G7M	C4-N3	4.45	1.48	1.37
24	AZ	46	7MG	C4-N9	4.43	1.42	1.37
25	BA	745	1MG	C4-N3	4.40	1.48	1.37
25	BA	2069	G7M	C4-N3	4.38	1.48	1.37
1	AA	1516	2MG	C2-N2	4.36	1.43	1.33
1	AA	1498	UR3	C2-N3	4.34	1.47	1.39
24	AZ	46	7MG	C2-N1	4.34	1.48	1.37
1	AA	1207	2MG	C2-N2	4.33	1.43	1.33
1	AA	1407	5MC	C2-N1	4.30	1.49	1.40
24	AX	46	7MG	C2-N1	4.17	1.48	1.37
25	BA	1915	3TD	C2-N3	4.13	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	32	OMC	C2-N1	4.08	1.48	1.40
1	AA	1402	4OC	C5-C4	4.06	1.49	1.40
1	AA	966	2MG	C4-N3	4.04	1.47	1.37
25	BA	2552	OMU	O4-C4	-3.99	1.16	1.24
25	BA	1835	2MG	C4-N3	3.99	1.47	1.37
1	AA	1207	2MG	C6-N1	3.98	1.43	1.37
1	AA	966	2MG	C2-N1	3.94	1.43	1.36
1	AA	1402	4OC	C2-N1	3.93	1.48	1.40
1	AA	1207	2MG	C2-N1	3.91	1.43	1.36
24	AZ	46	7MG	C5-C6	3.90	1.53	1.43
25	BA	2445	2MG	C4-N3	3.89	1.46	1.37
1	AA	966	2MG	C6-N1	3.85	1.43	1.37
25	BA	2552	OMU	C4-N3	3.82	1.45	1.38
1	AA	1516	2MG	C4-N3	3.81	1.46	1.37
24	AZ	46	7MG	C6-N1	3.76	1.45	1.38
25	BA	1835	2MG	O6-C6	-3.72	1.15	1.23
25	BA	2445	2MG	O6-C6	-3.69	1.15	1.23
24	AX	46	7MG	C5-C6	3.68	1.53	1.43
1	AA	1516	2MG	O6-C6	-3.62	1.15	1.23
25	BA	1835	2MG	C2-N1	3.59	1.42	1.36
1	AA	1207	2MG	C4-N3	3.58	1.46	1.37
25	BA	2498	OMC	C2-N1	3.58	1.47	1.40
25	BA	2445	2MG	C2-N1	3.56	1.42	1.36
24	AZ	55	PSU	C6-C5	3.52	1.39	1.35
24	AZ	46	7MG	O6-C6	-3.51	1.16	1.23
1	AA	1402	4OC	CM4-N4	3.50	1.51	1.45
1	AA	1516	2MG	C2-N1	3.49	1.42	1.36
25	BA	2445	2MG	C6-N1	3.48	1.43	1.37
24	AX	46	7MG	O6-C6	-3.48	1.17	1.23
24	AX	47	3AU	C6-N1	3.45	1.46	1.38
1	AA	527	G7M	C6-N1	3.45	1.43	1.37
25	BA	1835	2MG	C6-N1	3.45	1.43	1.37
24	AX	46	7MG	C6-N1	3.38	1.45	1.38
25	BA	2251	OMG	C6-N1	3.38	1.42	1.37
24	AZ	47	3AU	C6-N1	3.36	1.46	1.38
1	AA	966	2MG	O6-C6	-3.36	1.16	1.23
1	AA	1516	2MG	C6-N1	3.32	1.42	1.37
1	AA	1207	2MG	O6-C6	-3.31	1.16	1.23
25	BA	1939	5MU	C6-N1	-3.28	1.32	1.38
25	BA	2251	OMG	C5-C4	-3.23	1.34	1.43
24	AZ	8	4SU	C6-N1	3.23	1.45	1.38
24	AX	32	PSU	C6-C5	3.21	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BN	81	4D4	CZ-NH2	3.20	1.45	1.32
25	BA	2069	G7M	C6-N1	3.20	1.42	1.37
25	BA	2552	OMU	O2-C2	-3.19	1.17	1.23
23	AW	8	4SU	O2-C2	-3.19	1.17	1.23
24	AX	8	4SU	O2-C2	-3.17	1.17	1.23
25	BA	747	5MU	C4-N3	-3.16	1.33	1.38
25	BA	1939	5MU	C4-N3	-3.13	1.33	1.38
24	AZ	39	PSU	C6-C5	3.12	1.39	1.35
25	BA	1915	3TD	O2-C2	-3.11	1.17	1.23
25	BA	2498	OMC	O2-C2	-3.11	1.18	1.23
24	AX	55	PSU	C6-C5	3.10	1.38	1.35
25	BA	2498	OMC	C6-N1	3.10	1.45	1.38
25	BA	2030	6MZ	C5-C4	-3.09	1.32	1.40
24	AZ	8	4SU	O2-C2	-3.08	1.17	1.23
1	AA	1518	MA6	C5-C4	-3.07	1.32	1.40
1	AA	1519	MA6	C2-N3	3.07	1.37	1.32
1	AA	1207	2MG	C5-C6	3.06	1.53	1.47
25	BA	1835	2MG	C5-C4	-2.98	1.35	1.43
23	AW	8	4SU	C6-N1	2.95	1.45	1.38
23	AW	32	OMC	C6-N1	2.95	1.45	1.38
24	AX	8	4SU	C6-N1	2.94	1.45	1.38
24	AZ	32	PSU	C6-C5	2.93	1.38	1.35
25	BA	1915	3TD	C4-N3	2.92	1.46	1.40
23	AW	32	OMC	O2-C2	-2.92	1.18	1.23
24	AX	39	PSU	C6-C5	2.91	1.38	1.35
24	AZ	47	3AU	O4-C4	-2.91	1.18	1.24
25	BA	1915	3TD	O4-C4	-2.91	1.17	1.23
25	BA	747	5MU	C6-N1	-2.91	1.33	1.38
1	AA	1519	MA6	C5-C4	-2.90	1.33	1.40
24	AX	54	5MU	C4-N3	-2.89	1.33	1.38
24	AX	47	3AU	O4-C4	-2.89	1.18	1.24
25	BA	746	PSU	C6-C5	2.89	1.38	1.35
25	BA	2445	2MG	C5-C4	-2.88	1.35	1.43
1	AA	1402	4OC	C6-N1	2.86	1.44	1.38
1	AA	1518	MA6	C2-N3	2.86	1.36	1.32
1	AA	1519	MA6	C10-N6	2.85	1.52	1.45
25	BA	955	PSU	C6-C5	2.84	1.38	1.35
24	AZ	47	3AU	C5-C4	2.84	1.49	1.43
1	AA	516	PSU	C6-C5	2.84	1.38	1.35
23	AW	55	PSU	C6-C5	2.84	1.38	1.35
24	AZ	54	5MU	C4-N3	-2.81	1.33	1.38
1	AA	1518	MA6	C10-N6	2.80	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1207	2MG	C5-C4	-2.80	1.35	1.43
25	BA	1618	6MZ	C5-C4	-2.79	1.33	1.40
1	AA	1516	2MG	C5-C4	-2.78	1.36	1.43
23	AW	54	5MU	C4-N3	-2.77	1.33	1.38
1	AA	527	G7M	C5-C6	2.76	1.52	1.45
25	BA	1911	PSU	C6-C5	2.71	1.38	1.35
1	AA	966	2MG	C5-C6	2.71	1.52	1.47
25	BA	2457	PSU	C6-C5	2.70	1.38	1.35
24	AX	47	3AU	C5-C4	2.69	1.49	1.43
24	AZ	54	5MU	C6-C5	2.66	1.39	1.34
1	AA	966	2MG	C5-C4	-2.65	1.36	1.43
25	BA	1915	3TD	C10-N3	2.65	1.51	1.47
24	AX	54	5MU	C6-N1	-2.63	1.33	1.38
25	BA	2069	G7M	C5-C6	2.61	1.52	1.45
25	BA	2504	PSU	C6-C5	2.59	1.38	1.35
25	BA	2449	H2U	O2-C2	-2.59	1.18	1.23
1	AA	1407	5MC	O2-C2	-2.59	1.18	1.23
24	AZ	37	MIA	C2-N3	2.58	1.36	1.32
1	AA	1498	UR3	O2-C2	-2.58	1.17	1.22
25	BA	1917	PSU	C6-C5	2.58	1.38	1.35
1	AA	967	5MC	O2-C2	-2.58	1.18	1.23
25	BA	1915	3TD	O4'-C1'	-2.58	1.40	1.43
24	AX	37	MIA	C5-C4	-2.56	1.34	1.40
1	AA	527	G7M	C2-N1	2.56	1.44	1.37
24	AX	47	3AU	O2-C2	-2.54	1.18	1.23
25	BA	747	5MU	C2-N3	-2.52	1.33	1.38
24	AZ	20	H2U	O2-C2	-2.51	1.18	1.23
25	BA	2503	2MA	C6-C5	2.51	1.52	1.43
25	BA	1939	5MU	C2-N3	-2.51	1.33	1.38
23	AW	54	5MU	C6-N1	-2.51	1.33	1.38
25	BA	2449	H2U	O4-C4	-2.50	1.18	1.23
25	BA	2604	PSU	C6-C5	2.48	1.38	1.35
1	AA	527	G7M	O6-C6	-2.48	1.18	1.23
24	AX	16	H2U	O2-C2	-2.45	1.18	1.23
23	AW	20	H2U	O2-C2	-2.45	1.18	1.23
25	BA	2580	PSU	C6-C5	2.45	1.38	1.35
25	BA	2069	G7M	O6-C6	-2.44	1.18	1.23
24	AZ	47	3AU	O2-C2	-2.44	1.18	1.23
25	BA	2251	OMG	C5-C6	2.44	1.52	1.47
25	BA	2605	PSU	C6-C5	2.44	1.38	1.35
1	AA	1498	UR3	O4-C4	-2.43	1.18	1.23
25	BA	2251	OMG	O6-C6	-2.41	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BN	81	4D4	CZ-NH1	-2.40	1.25	1.34
24	AX	20	H2U	O2-C2	-2.40	1.18	1.23
25	BA	1962	5MC	O2-C2	-2.39	1.19	1.23
25	BA	2069	G7M	C2-N1	2.37	1.43	1.37
23	AW	54	5MU	C6-C5	2.37	1.38	1.34
1	AA	1498	UR3	C6-N1	2.37	1.43	1.38
24	AZ	54	5MU	C6-N1	-2.37	1.34	1.38
24	AZ	16	H2U	O4-C4	-2.36	1.18	1.23
24	AX	54	5MU	C2-N3	-2.36	1.33	1.38
24	AZ	16	H2U	O2-C2	-2.35	1.18	1.23
1	AA	1516	2MG	C5-C6	2.35	1.52	1.47
25	BA	2251	OMG	C2-N1	2.35	1.43	1.37
25	BA	1618	6MZ	C2-N3	2.34	1.35	1.32
24	AZ	37	MIA	C5-C4	-2.34	1.34	1.40
24	AX	37	MIA	C2-N3	2.33	1.35	1.32
25	BA	1835	2MG	C5-C6	2.31	1.52	1.47
23	AW	54	5MU	C4-C5	2.30	1.48	1.44
25	BA	955	PSU	C4-C5	-2.29	1.37	1.44
23	AW	54	5MU	C2-N3	-2.29	1.33	1.38
25	BA	2445	2MG	C5-C6	2.27	1.52	1.47
25	BA	2457	PSU	C4-C5	-2.24	1.37	1.44
25	BA	2503	2MA	CM2-C2	2.22	1.56	1.49
24	AX	20	H2U	O4-C4	-2.22	1.18	1.23
24	AZ	54	5MU	C4-C5	2.22	1.48	1.44
24	AX	16	H2U	O4-C4	-2.22	1.18	1.23
25	BA	2552	OMU	C6-N1	2.21	1.43	1.38
25	BA	745	1MG	C5-C4	-2.20	1.37	1.43
23	AW	32	OMC	C5-C4	2.18	1.47	1.42
25	BA	2030	6MZ	C2-N3	2.17	1.35	1.32
24	AZ	20	H2U	O4-C4	-2.17	1.18	1.23
25	BA	2580	PSU	O4'-C1'	-2.16	1.40	1.43
23	AW	20	H2U	O4-C4	-2.16	1.18	1.23
25	BA	2504	PSU	O4'-C1'	-2.15	1.40	1.43
25	BA	1939	5MU	C6-C5	2.15	1.38	1.34
25	BA	745	1MG	C5-C6	2.14	1.53	1.47
24	AZ	54	5MU	C2-N3	-2.13	1.34	1.38
25	BA	2604	PSU	O4'-C1'	-2.11	1.40	1.43
25	BA	2504	PSU	C4-C5	-2.11	1.38	1.44
25	BA	2580	PSU	C4-C5	-2.08	1.38	1.44
25	BA	2069	G7M	C5-C4	-2.06	1.34	1.39
25	BA	2503	2MA	C6-N6	-2.05	1.26	1.34
25	BA	2604	PSU	C4-C5	-2.04	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1917	PSU	C4-C5	-2.04	1.38	1.44
25	BA	1911	PSU	O4'-C1'	-2.04	1.41	1.43
25	BA	746	PSU	C4-C5	-2.03	1.38	1.44
25	BA	2605	PSU	C4-C5	-2.02	1.38	1.44
24	AZ	54	5MU	C2-N1	2.02	1.41	1.38
25	BA	747	5MU	C6-C5	2.01	1.37	1.34
25	BA	2503	2MA	C5-C4	-2.01	1.35	1.40
25	BA	745	1MG	C6-N1	2.01	1.43	1.39

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	N1-C6-N6	-17.72	98.41	117.06
1	AA	1519	MA6	N1-C6-N6	-15.75	100.48	117.06
24	AZ	37	MIA	C12-C13-C14	-9.98	107.73	127.14
24	AX	37	MIA	C12-C13-C14	-9.48	108.69	127.14
23	AW	8	4SU	C4-N3-C2	-8.72	118.87	127.34
25	BA	2503	2MA	C1'-N9-C4	8.68	141.89	126.64
24	AX	8	4SU	C4-N3-C2	-8.31	119.27	127.34
25	BA	2449	H2U	C4-N3-C2	-8.24	118.96	125.79
25	BA	2030	6MZ	C9-N6-C6	-7.57	116.35	122.87
23	AW	20	H2U	C4-N3-C2	-7.50	119.57	125.79
24	AZ	8	4SU	C4-N3-C2	-7.33	120.22	127.34
24	AZ	20	H2U	C4-N3-C2	-7.16	119.85	125.79
24	AX	16	H2U	C4-N3-C2	-7.03	119.96	125.79
24	AZ	16	H2U	C4-N3-C2	-7.00	119.99	125.79
24	AX	20	H2U	C4-N3-C2	-6.82	120.14	125.79
23	AW	8	4SU	C5-C4-N3	6.60	120.81	114.69
25	BA	1939	5MU	C4-N3-C2	-6.11	119.44	127.35
25	BA	1915	3TD	N1-C2-N3	6.09	120.94	116.14
25	BA	1618	6MZ	C9-N6-C6	-6.04	117.67	122.87
25	BA	2030	6MZ	N3-C2-N1	-5.88	119.49	128.68
24	AX	37	MIA	N3-C2-N1	-5.61	119.92	128.68
25	BA	2552	OMU	C4-N3-C2	-5.55	119.26	126.58
25	BA	1618	6MZ	N3-C2-N1	-5.54	120.03	128.68
1	AA	1518	MA6	N3-C2-N1	-5.48	120.11	128.68
25	BA	747	5MU	C4-N3-C2	-5.47	120.27	127.35
23	AW	54	5MU	C4-N3-C2	-5.47	120.27	127.35
24	AX	8	4SU	C5-C4-N3	5.46	119.75	114.69
24	AZ	8	4SU	C5-C4-N3	5.45	119.75	114.69
25	BA	1939	5MU	N3-C2-N1	5.36	122.00	114.89
24	AX	54	5MU	C4-N3-C2	-5.29	120.51	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AZ	37	MIA	N3-C2-N1	-5.25	120.47	128.68
25	BA	2504	PSU	C4-N3-C2	-5.16	118.90	126.34
25	BA	2580	PSU	C4-N3-C2	-5.14	118.93	126.34
1	AA	1498	UR3	C4-N3-C2	-5.14	119.73	124.56
25	BA	1939	5MU	C5-C6-N1	-5.10	118.09	123.34
25	BA	2504	PSU	N1-C2-N3	5.10	120.91	115.13
25	BA	2605	PSU	C4-N3-C2	-5.08	119.02	126.34
24	AZ	54	5MU	N3-C2-N1	5.06	121.61	114.89
24	AZ	54	5MU	C4-N3-C2	-5.04	120.82	127.35
24	AX	46	7MG	C5-C6-N1	5.03	119.86	110.99
25	BA	2605	PSU	N1-C2-N3	5.02	120.82	115.13
25	BA	2580	PSU	N1-C2-N3	5.02	120.81	115.13
23	AW	54	5MU	C5-C4-N3	5.00	119.58	115.31
25	BA	2457	PSU	N1-C2-N3	4.98	120.77	115.13
25	BA	2457	PSU	C4-N3-C2	-4.95	119.21	126.34
1	AA	1519	MA6	N3-C2-N1	-4.92	120.98	128.68
24	AZ	46	7MG	C5-C6-N1	4.91	119.65	110.99
24	AZ	47	3AU	C4-N3-C2	-4.91	120.10	126.58
25	BA	1911	PSU	N1-C2-N3	4.91	120.69	115.13
24	AX	39	PSU	C4-N3-C2	-4.90	119.28	126.34
25	BA	747	5MU	C5-C4-N3	4.90	119.49	115.31
25	BA	2503	2MA	C2-N3-C4	4.89	119.50	115.52
25	BA	747	5MU	N3-C2-N1	4.89	121.38	114.89
25	BA	1911	PSU	C4-N3-C2	-4.88	119.31	126.34
23	AW	54	5MU	N3-C2-N1	4.86	121.34	114.89
24	AX	37	MIA	C16-C14-C13	-4.85	108.62	122.65
25	BA	2604	PSU	C4-N3-C2	-4.84	119.37	126.34
24	AX	47	3AU	C4-N3-C2	-4.82	120.22	126.58
24	AX	54	5MU	N3-C2-N1	4.80	121.26	114.89
24	AZ	39	PSU	C4-N3-C2	-4.80	119.42	126.34
25	BA	747	5MU	O4-C4-C5	-4.78	119.36	124.90
24	AX	39	PSU	N1-C2-N3	4.77	120.54	115.13
1	AA	516	PSU	C4-N3-C2	-4.77	119.47	126.34
24	AX	55	PSU	C4-N3-C2	-4.76	119.49	126.34
25	BA	746	PSU	C4-N3-C2	-4.74	119.51	126.34
25	BA	1939	5MU	C5-C4-N3	4.73	119.34	115.31
24	AX	54	5MU	C5-C4-N3	4.71	119.33	115.31
24	AZ	55	PSU	N1-C2-N3	4.70	120.45	115.13
24	AZ	39	PSU	N1-C2-N3	4.68	120.43	115.13
25	BA	955	PSU	C4-N3-C2	-4.68	119.60	126.34
25	BA	2604	PSU	N1-C2-N3	4.66	120.41	115.13
25	BA	1917	PSU	C4-N3-C2	-4.62	119.68	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1917	PSU	N1-C2-N3	4.62	120.36	115.13
24	AX	55	PSU	N1-C2-N3	4.58	120.32	115.13
24	AZ	37	MIA	C16-C14-C13	-4.52	109.58	122.65
24	AZ	37	MIA	C15-C14-C13	-4.46	109.76	122.65
24	AZ	55	PSU	C4-N3-C2	-4.44	119.94	126.34
24	AZ	32	PSU	C4-N3-C2	-4.42	119.97	126.34
25	BA	955	PSU	N1-C2-N3	4.40	120.12	115.13
23	AW	55	PSU	C4-N3-C2	-4.40	120.00	126.34
1	AA	516	PSU	N1-C2-N3	4.36	120.06	115.13
25	BA	1915	3TD	C4-N3-C2	-4.35	119.89	124.61
24	AX	46	7MG	C2-N3-C4	4.32	120.00	112.30
24	AX	54	5MU	O4-C4-C5	-4.25	119.98	124.90
24	AZ	32	PSU	N1-C2-N3	4.24	119.94	115.13
24	AX	46	7MG	C5-C4-N3	-4.22	120.08	128.13
24	AX	37	MIA	C15-C14-C13	-4.20	110.51	122.65
24	AX	32	PSU	C4-N3-C2	-4.19	120.31	126.34
25	BA	746	PSU	N1-C2-N3	4.17	119.86	115.13
25	BA	1962	5MC	C5-C6-N1	-4.17	119.05	123.34
25	BA	1939	5MU	O4-C4-C5	-4.11	120.14	124.90
24	AZ	54	5MU	C5-C4-N3	4.09	118.80	115.31
24	AX	47	3AU	N3-C2-N1	4.08	120.31	114.89
24	AX	8	4SU	N3-C2-N1	4.05	120.26	114.89
25	BA	2445	2MG	C5-C6-N1	4.03	121.07	113.95
25	BA	2030	6MZ	C2-N1-C6	4.03	120.05	116.59
23	AW	55	PSU	N1-C2-N3	4.03	119.69	115.13
23	AW	20	H2U	N3-C2-N1	4.02	120.90	116.65
24	AX	32	PSU	N1-C2-N3	3.99	119.65	115.13
25	BA	2552	OMU	N3-C2-N1	3.97	120.16	114.89
23	AW	54	5MU	O4-C4-C5	-3.97	120.30	124.90
24	AZ	46	7MG	C2-N3-C4	3.94	119.32	112.30
25	BA	1835	2MG	C5-C6-N1	3.92	120.87	113.95
23	AW	54	5MU	C5-C6-N1	-3.85	119.38	123.34
23	AW	8	4SU	N3-C2-N1	3.85	120.00	114.89
1	AA	1207	2MG	CM2-N2-C2	-3.84	115.39	123.86
25	BA	745	1MG	C5-C6-N1	3.79	119.59	113.90
25	BA	1939	5MU	O2-C2-N1	-3.78	117.75	122.79
25	BA	747	5MU	C5-C6-N1	-3.78	119.45	123.34
25	BA	2251	OMG	C5-C6-N1	3.76	120.59	113.95
23	AW	8	4SU	C5-C4-S4	-3.74	119.65	124.47
1	AA	1407	5MC	C5-C6-N1	-3.73	119.50	123.34
24	AZ	47	3AU	N3-C2-N1	3.71	119.82	114.89
24	AZ	54	5MU	O4-C4-C5	-3.70	120.61	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AZ	46	7MG	C5-C4-N9	3.70	111.14	106.35
1	AA	1516	2MG	C5-C6-N1	3.67	120.43	113.95
24	AZ	54	5MU	C5-C6-N1	-3.66	119.57	123.34
1	AA	967	5MC	C5-C6-N1	-3.59	119.65	123.34
24	AX	37	MIA	C2-N1-C6	3.56	119.64	116.59
1	AA	1207	2MG	C5-C6-N1	3.54	120.20	113.95
25	BA	2449	H2U	N3-C2-N1	3.48	120.33	116.65
24	AZ	8	4SU	N3-C2-N1	3.47	119.50	114.89
25	BA	2251	OMG	C2-N1-C6	-3.45	118.75	125.10
24	AZ	47	3AU	C5-C4-N3	3.44	119.98	114.84
25	BA	2552	OMU	C5-C4-N3	3.43	119.98	114.84
1	AA	966	2MG	C5-C6-N1	3.43	120.00	113.95
24	AX	16	H2U	N3-C2-N1	3.42	120.27	116.65
24	AX	54	5MU	C5-C6-N1	-3.41	119.83	123.34
25	BA	1917	PSU	O2-C2-N1	-3.34	119.12	122.79
24	AX	47	3AU	C5-C4-N3	3.31	119.80	114.84
24	AX	46	7MG	C4-C5-N7	3.30	110.11	105.53
24	AZ	20	H2U	N3-C2-N1	3.28	120.12	116.65
25	BA	2449	H2U	C5-C4-N3	3.28	120.33	116.65
24	AZ	37	MIA	C2-N1-C6	3.28	119.40	116.59
1	AA	516	PSU	O4'-C1'-C2'	3.23	109.69	105.14
24	AZ	55	PSU	O2-C2-N1	-3.20	119.27	122.79
24	AX	8	4SU	C5-C4-S4	-3.18	120.37	124.47
24	AZ	46	7MG	C5-C4-N3	-3.16	122.11	128.13
25	BA	2069	G7M	C2-N1-C6	-3.14	119.31	125.10
1	AA	1516	2MG	CM2-N2-C2	-3.14	116.92	123.86
24	AX	20	H2U	N3-C2-N1	3.14	119.97	116.65
24	AX	37	MIA	C12-N6-C6	-3.12	117.92	122.55
25	BA	2449	H2U	O2-C2-N1	-3.10	119.22	123.11
25	BA	1911	PSU	O2-C2-N1	-3.09	119.38	122.79
1	AA	527	G7M	C2-N1-C6	-3.07	119.45	125.10
25	BA	2504	PSU	C6-C5-C4	3.05	120.33	118.20
25	BA	1618	6MZ	C2-N1-C6	3.05	119.20	116.59
12	AL	89	D2T	OD2-CG-CB	3.05	119.73	113.15
24	AZ	16	H2U	C5-C4-N3	3.03	120.06	116.65
24	AZ	46	7MG	C2-N1-C6	-3.03	119.57	125.10
25	BA	746	PSU	O2'-C2'-C3'	3.02	121.60	111.82
24	AX	46	7MG	C2-N1-C6	-3.02	119.59	125.10
24	AX	46	7MG	N9-C4-N3	2.99	129.94	125.47
24	AZ	47	3AU	O4-C4-C5	-2.97	119.94	125.16
25	BA	2457	PSU	O2-C2-N1	-2.93	119.57	122.79
25	BA	1618	6MZ	C1'-N9-C4	2.92	131.78	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AZ	46	7MG	O6-C6-C5	-2.91	120.39	127.54
24	AZ	8	4SU	C5-C4-S4	-2.91	120.72	124.47
25	BA	2580	PSU	O2-C2-N1	-2.91	119.59	122.79
24	AX	46	7MG	O6-C6-C5	-2.90	120.42	127.54
24	AX	47	3AU	O4-C4-C5	-2.87	120.12	125.16
24	AX	16	H2U	C5-C4-N3	2.85	119.85	116.65
25	BA	2251	OMG	C8-N7-C5	2.85	108.42	102.99
25	BA	2580	PSU	O4'-C1'-C2'	2.85	109.16	105.14
25	BA	2552	OMU	O4-C4-C5	-2.83	120.18	125.16
24	AX	20	H2U	C5-C4-N3	2.83	119.83	116.65
12	AL	89	D2T	CB1-SB-CB	2.82	107.54	102.44
25	BA	2503	2MA	N3-C2-N1	-2.82	120.58	125.73
24	AZ	32	PSU	O2-C2-N1	-2.80	119.71	122.79
24	AX	46	7MG	C5-C4-N9	2.80	109.98	106.35
25	BA	1917	PSU	C6-N1-C2	-2.79	119.83	122.68
25	BA	1835	2MG	C8-N7-C5	2.79	108.30	102.99
1	AA	1207	2MG	C8-N7-C5	2.78	108.28	102.99
1	AA	966	2MG	C8-N7-C5	2.77	108.26	102.99
24	AX	20	H2U	C5-C6-N1	2.76	120.70	111.61
24	AX	16	H2U	C5-C6-N1	2.75	120.69	111.61
24	AZ	20	H2U	C5-C4-N3	2.75	119.74	116.65
24	AZ	16	H2U	N3-C2-N1	2.75	119.56	116.65
25	BA	2580	PSU	C3'-C2'-C1'	2.75	104.84	101.64
24	AZ	55	PSU	C6-N1-C2	-2.74	119.88	122.68
1	AA	516	PSU	O2-C2-N1	-2.71	119.80	122.79
23	AW	20	H2U	C5-C4-N3	2.69	119.67	116.65
24	AZ	46	7MG	N2-C2-N1	2.69	122.43	116.71
24	AZ	16	H2U	C5-C6-N1	2.66	120.38	111.61
25	BA	1915	3TD	C6-C5-C4	2.65	120.05	118.22
23	AW	54	5MU	C5M-C5-C4	2.65	121.68	118.77
25	BA	2445	2MG	O6-C6-C5	-2.65	119.20	124.37
1	AA	516	PSU	C3'-C2'-C1'	2.64	104.71	101.64
24	AX	8	4SU	O2-C2-N1	-2.61	119.32	122.79
25	BA	2605	PSU	O2-C2-N1	-2.60	119.92	122.79
25	BA	2504	PSU	O2-C2-N1	-2.60	119.93	122.79
23	AW	20	H2U	C5-C6-N1	2.60	120.17	111.61
25	BA	2457	PSU	C6-C5-C4	2.59	120.01	118.20
24	AX	54	5MU	C5M-C5-C4	2.59	121.62	118.77
25	BA	2580	PSU	C6-C5-C4	2.59	120.01	118.20
23	AW	55	PSU	C3'-C2'-C1'	2.58	104.64	101.64
25	BA	2457	PSU	C6-N1-C2	-2.58	120.05	122.68
25	BA	2604	PSU	O2-C2-N1	-2.56	119.97	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2605	PSU	C6-N1-C2	-2.56	120.07	122.68
23	AW	55	PSU	O2-C2-N1	-2.56	119.97	122.79
24	AZ	16	H2U	O2-C2-N1	-2.56	119.89	123.11
23	AW	20	H2U	O2-C2-N1	-2.56	119.90	123.11
25	BA	745	1MG	C8-N7-C5	2.54	107.84	102.99
24	AZ	20	H2U	C5-C6-N1	2.54	119.97	111.61
24	AX	55	PSU	O2-C2-N1	-2.53	120.01	122.79
1	AA	1516	2MG	C8-N7-C5	2.52	107.80	102.99
24	AX	16	H2U	O2-C2-N1	-2.49	119.98	123.11
25	BA	2251	OMG	O6-C6-C5	-2.49	119.52	124.37
1	AA	1516	2MG	O6-C6-C5	-2.48	119.53	124.37
25	BA	2457	PSU	O4'-C1'-C2'	2.46	108.61	105.14
24	AX	20	H2U	O2-C2-N3	-2.45	116.94	121.50
25	BA	746	PSU	C3'-C2'-C1'	2.44	104.48	101.64
24	AX	39	PSU	C6-C5-C4	2.43	119.90	118.20
25	BA	2449	H2U	C5-C6-N1	2.42	119.60	111.61
25	BA	2445	2MG	C8-N7-C5	2.42	107.59	102.99
24	AZ	46	7MG	C4-C5-N7	2.41	108.88	105.53
23	AW	55	PSU	O2'-C2'-C3'	2.41	119.60	111.82
25	BA	746	PSU	O2-C2-N1	-2.40	120.15	122.79
24	AZ	39	PSU	O2-C2-N1	-2.39	120.16	122.79
24	AX	39	PSU	O2-C2-N1	-2.39	120.16	122.79
1	AA	1402	4OC	C6-C5-C4	2.39	119.88	116.96
25	BA	1911	PSU	C6-C5-C4	2.39	119.87	118.20
25	BA	1835	2MG	O6-C6-C5	-2.38	119.72	124.37
25	BA	2445	2MG	CM2-N2-C2	-2.37	118.62	123.86
24	AX	46	7MG	N9-C8-N7	2.37	106.77	103.38
28	BD	150	MEQ	CB-CG-CD	-2.37	107.74	113.04
25	BA	1911	PSU	C6-N1-C2	-2.36	120.27	122.68
24	AX	54	5MU	O2-C2-N1	-2.35	119.66	122.79
24	AZ	20	H2U	O2-C2-N1	-2.35	120.16	123.11
24	AX	47	3AU	O2-C2-N1	-2.34	119.68	122.79
23	AW	54	5MU	O2-C2-N1	-2.32	119.71	122.79
25	BA	747	5MU	O2-C2-N1	-2.32	119.71	122.79
1	AA	1402	4OC	CM4-N4-C4	-2.31	117.94	122.45
1	AA	967	5MC	CM5-C5-C6	-2.29	119.80	122.85
25	BA	1917	PSU	O4'-C1'-C2'	2.26	108.33	105.14
25	BA	2604	PSU	C6-N1-C2	-2.26	120.37	122.68
25	BA	955	PSU	C6-N1-C2	-2.25	120.38	122.68
1	AA	966	2MG	O6-C6-C5	-2.25	119.98	124.37
25	BA	2498	OMC	O3'-C3'-C2'	2.25	117.55	111.17
25	BA	745	1MG	O6-C6-C5	-2.24	120.23	124.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2552	OMU	O2-C2-N1	-2.22	119.83	122.79
23	AW	55	PSU	C6-N1-C2	-2.22	120.41	122.68
25	BA	955	PSU	O2-C2-N1	-2.21	120.36	122.79
24	AZ	54	5MU	O2-C2-N1	-2.20	119.86	122.79
1	AA	966	2MG	O3'-C3'-C4'	2.20	117.41	111.05
1	AA	516	PSU	C6-N1-C2	-2.17	120.47	122.68
24	AZ	32	PSU	C6-N1-C2	-2.15	120.48	122.68
25	BA	1835	2MG	CM2-N2-C2	-2.15	119.12	123.86
24	AZ	8	4SU	C1'-N1-C2	2.15	121.46	117.57
23	AW	54	5MU	C5M-C5-C6	-2.14	119.99	122.85
25	BA	2605	PSU	O4'-C1'-C2'	2.14	108.16	105.14
23	AW	54	5MU	C1'-N1-C6	-2.14	117.57	121.12
24	AX	54	5MU	C5M-C5-C6	-2.13	120.00	122.85
25	BA	2504	PSU	C6-N1-C2	-2.13	120.50	122.68
1	AA	1207	2MG	O6-C6-C5	-2.13	120.21	124.37
24	AX	55	PSU	C6-C5-C4	2.12	119.68	118.20
24	AZ	39	PSU	C6-N1-C2	-2.11	120.53	122.68
25	BA	2580	PSU	C6-N1-C2	-2.10	120.54	122.68
24	AZ	37	MIA	C16-C14-C15	-2.10	109.97	114.60
24	AX	55	PSU	C6-N1-C2	-2.08	120.55	122.68
24	AX	32	PSU	C6-N1-C2	-2.08	120.56	122.68
24	AX	39	PSU	C6-N1-C2	-2.07	120.57	122.68
25	BA	746	PSU	C6-C5-C4	2.07	119.64	118.20
23	AW	54	5MU	C1'-N1-C2	2.06	121.31	117.57
1	AA	527	G7M	N2-C2-N1	2.06	121.09	116.71
25	BA	745	1MG	CM1-N1-C6	2.05	120.36	117.55
25	BA	1915	3TD	O4'-C1'-C2'	2.05	108.04	105.14
24	AZ	47	3AU	O2-C2-N1	-2.05	120.06	122.79
1	AA	1518	MA6	C1'-N9-C4	-2.01	123.10	126.64
24	AX	37	MIA	C16-C14-C15	-2.00	110.18	114.60

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1402	4OC	C1'-C2'-O2'-CM2
1	AA	1518	MA6	C5-C6-N6-C10
1	AA	1518	MA6	N1-C6-N6-C10
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
1	AA	1519	MA6	C5-C6-N6-C10
12	AL	89	D2T	SB-CB-CG-OD2
24	AX	20	H2U	O4'-C4'-C5'-O5'
24	AX	20	H2U	C3'-C4'-C5'-O5'
24	AX	20	H2U	C2'-C1'-N1-C2
24	AX	37	MIA	O4'-C4'-C5'-O5'
24	AX	37	MIA	C5-C6-N6-C12
24	AX	37	MIA	C12-C13-C14-C15
24	AX	37	MIA	C12-C13-C14-C16
24	AX	47	3AU	C3'-C4'-C5'-O5'
24	AX	47	3AU	O4'-C4'-C5'-O5'
24	AX	55	PSU	C3'-C4'-C5'-O5'
24	AX	55	PSU	O4'-C4'-C5'-O5'
24	AZ	8	4SU	O4'-C1'-N1-C2
24	AZ	8	4SU	O4'-C1'-N1-C6
24	AZ	16	H2U	O4'-C4'-C5'-O5'
24	AZ	20	H2U	O4'-C4'-C5'-O5'
24	AZ	37	MIA	O4'-C4'-C5'-O5'
24	AZ	37	MIA	C3'-C4'-C5'-O5'
24	AZ	37	MIA	C5-C6-N6-C12
24	AZ	37	MIA	N1-C6-N6-C12
24	AZ	37	MIA	N6-C12-C13-C14
24	AZ	37	MIA	C12-C13-C14-C15
24	AZ	37	MIA	C12-C13-C14-C16
36	BN	81	4D4	N-CA-CB-CG
23	AW	32	OMC	C1'-C2'-O2'-CM2
25	BA	746	PSU	C2'-C1'-C5-C6
25	BA	1618	6MZ	C5-C6-N6-C9
25	BA	1618	6MZ	N1-C6-N6-C9
25	BA	1915	3TD	O4'-C1'-C5-C4
25	BA	1915	3TD	C2'-C1'-C5-C6
25	BA	1915	3TD	O4'-C1'-C5-C6
25	BA	2030	6MZ	O4'-C4'-C5'-O5'
25	BA	2498	OMC	C1'-C2'-O2'-CM2
25	BA	2552	OMU	O4'-C4'-C5'-O5'
1	AA	967	5MC	O4'-C4'-C5'-O5'
1	AA	967	5MC	C3'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
24	AX	37	MIA	C3'-C4'-C5'-O5'
24	AZ	8	4SU	O4'-C4'-C5'-O5'
24	AZ	16	H2U	C3'-C4'-C5'-O5'
24	AZ	20	H2U	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
24	AZ	46	7MG	O4'-C4'-C5'-O5'
24	AZ	46	7MG	C3'-C4'-C5'-O5'
25	BA	1917	PSU	O4'-C4'-C5'-O5'
25	BA	2030	6MZ	C3'-C4'-C5'-O5'
25	BA	2503	2MA	O4'-C4'-C5'-O5'
25	BA	2552	OMU	C3'-C4'-C5'-O5'
28	BD	150	MEQ	CA-CB-CG-CD
24	AX	20	H2U	C2'-C1'-N1-C6
1	AA	516	PSU	C3'-C4'-C5'-O5'
24	AX	16	H2U	O4'-C4'-C5'-O5'
23	AW	20	H2U	O4'-C4'-C5'-O5'
23	AW	20	H2U	C3'-C4'-C5'-O5'
23	AW	55	PSU	C3'-C4'-C5'-O5'
25	BA	1917	PSU	C3'-C4'-C5'-O5'
25	BA	2498	OMC	C3'-C4'-C5'-O5'
1	AA	1519	MA6	N1-C6-N6-C10
24	AZ	8	4SU	C2'-C1'-N1-C6
25	BA	2445	2MG	C3'-C4'-C5'-O5'
24	AX	37	MIA	N1-C6-N6-C12
25	BA	2498	OMC	O4'-C4'-C5'-O5'
28	BD	150	MEQ	OE1-CD-CG-CB
25	BA	2503	2MA	C3'-C4'-C5'-O5'
28	BD	150	MEQ	NE2-CD-CG-CB
24	AZ	8	4SU	C4'-C5'-O5'-P
24	AZ	37	MIA	C4'-C5'-O5'-P
24	AX	16	H2U	C3'-C4'-C5'-O5'
36	BN	81	4D4	C-CA-CB-OB
24	AX	20	H2U	C4'-C5'-O5'-P
12	AL	89	D2T	CG-CB-SB-CB1
36	BN	81	4D4	NE-CD-CG-CB
25	BA	2445	2MG	O4'-C4'-C5'-O5'
12	AL	89	D2T	CA-CB-CG-OD1
1	AA	1518	MA6	C5-C6-N6-C9
24	AX	46	7MG	C4'-C5'-O5'-P
24	AZ	16	H2U	C4'-C5'-O5'-P
24	AZ	8	4SU	C3'-C4'-C5'-O5'
25	BA	1911	PSU	O4'-C4'-C5'-O5'
25	BA	1939	5MU	O4'-C4'-C5'-O5'
1	AA	527	G7M	C4'-C5'-O5'-P
25	BA	2069	G7M	C4'-C5'-O5'-P
24	AZ	8	4SU	C2'-C1'-N1-C2
24	AZ	55	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
24	AZ	20	H2U	C4'-C5'-O5'-P
1	AA	1207	2MG	O4'-C4'-C5'-O5'
25	BA	2069	G7M	O4'-C4'-C5'-O5'
23	AW	55	PSU	O4'-C4'-C5'-O5'
25	BA	2251	OMG	C1'-C2'-O2'-CM2
25	BA	1939	5MU	C3'-C4'-C5'-O5'
24	AZ	20	H2U	O4'-C1'-N1-C6
23	AW	20	H2U	O4'-C1'-N1-C6
25	BA	746	PSU	O4'-C1'-C5-C6
1	AA	1519	MA6	C4'-C5'-O5'-P
23	AW	55	PSU	C4'-C5'-O5'-P
36	BN	81	4D4	C-CA-CB-CG
24	AX	47	3AU	O4'-C1'-N1-C6
1	AA	967	5MC	C4'-C5'-O5'-P
24	AZ	47	3AU	O4'-C4'-C5'-O5'
24	AZ	20	H2U	C2'-C1'-N1-C2
23	AW	20	H2U	C2'-C1'-N1-C2
24	AZ	46	7MG	C2'-C1'-N9-C8

There are no ring outliers.

39 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	527	G7M	1	0
28	BD	150	MEQ	1	0
24	AX	54	5MU	1	0
25	BA	2503	2MA	1	0
25	BA	2604	PSU	1	0
1	AA	1519	MA6	1	0
1	AA	966	2MG	2	0
24	AX	39	PSU	1	0
24	AX	55	PSU	1	0
25	BA	2251	OMG	1	0
25	BA	2605	PSU	2	0
1	AA	1516	2MG	1	0
12	AL	89	D2T	2	0
24	AZ	46	7MG	9	0
24	AZ	16	H2U	2	0
24	AX	20	H2U	4	0
25	BA	1618	6MZ	3	0
25	BA	2449	H2U	1	0
25	BA	1915	3TD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AZ	8	4SU	1	0
1	AA	516	PSU	1	0
23	AW	20	H2U	3	0
24	AX	46	7MG	3	0
24	AX	37	MIA	1	0
23	AW	54	5MU	2	0
25	BA	2498	OMC	1	0
1	AA	1207	2MG	2	0
24	AZ	55	PSU	1	0
36	BN	81	4D4	1	0
1	AA	967	5MC	2	0
24	AZ	20	H2U	3	0
24	AZ	32	PSU	1	0
25	BA	2030	6MZ	1	0
24	AZ	37	MIA	3	0
23	AW	32	OMC	1	0
23	AW	55	PSU	1	0
25	BA	1917	PSU	2	0
25	BA	2069	G7M	1	0
25	BA	2552	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 490 ligands modelled in this entry, 489 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
63	PHE	AX	102	24	10,11,12	0.59	0	10,13,15	0.27	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
63	PHE	AX	102	24	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	AX	102	PHE	CA-CB-CG-CD1
63	AX	102	PHE	CA-CB-CG-CD2

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
57	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.19