



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:34 pm BST

PDB ID : 6ZTN / pdb_00006ztn
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 : 6ALH, 4YBB

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

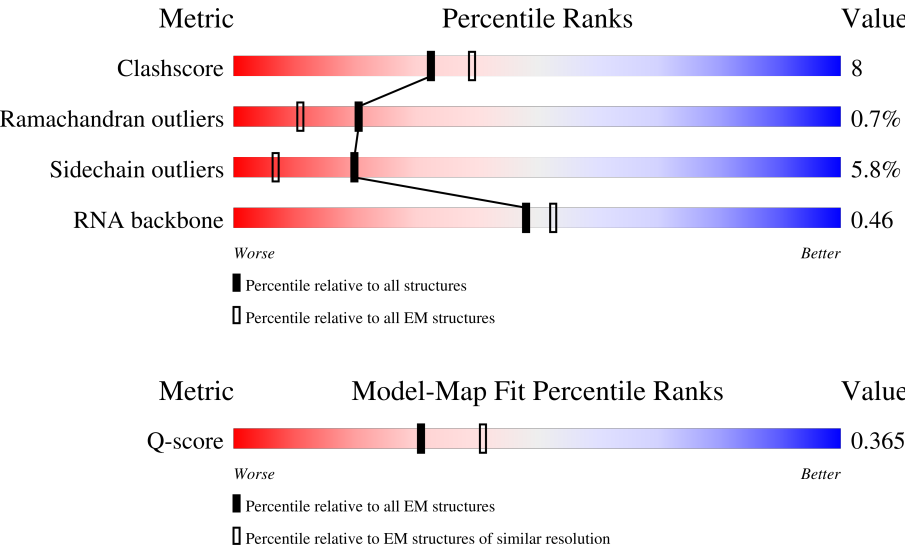
1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	57% 34% 8% ..
2	AB	241	73% 73% 19% 6%
3	AC	233	20% 65% 22% 10%

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Mol	Chain	Length	Quality of chain
4	AD	206	
5	AE	167	
6	AF	131	
7	AG	156	
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	

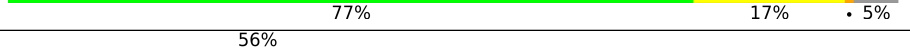
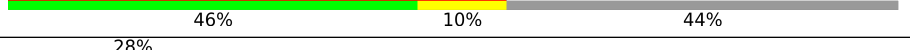
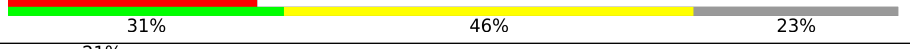
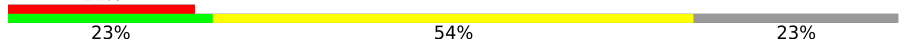
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Mol	Chain	Length	Quality of chain
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	
32	BH	149	
33	BK	142	
34	BL	123	
35	BM	144	
36	BN	136	
37	BO	127	
38	BP	117	
39	BQ	115	
40	BR	118	
41	BS	103	
42	BT	110	
43	BU	100	
44	BV	104	
45	BW	94	
46	BX	85	
47	BY	78	
48	BZ	63	
49	B1	59	
50	B2	57	
51	B3	55	
52	B4	46	

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Mol	Chain	Length	Quality of chain
53	B5	65	
54	B6	50	
55	CA	329	
55	CB	329	
56	CC	1342	
57	CD	1407	
58	CE	91	
59	CN	39	
60	CT	39	
61	CF	181	

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		

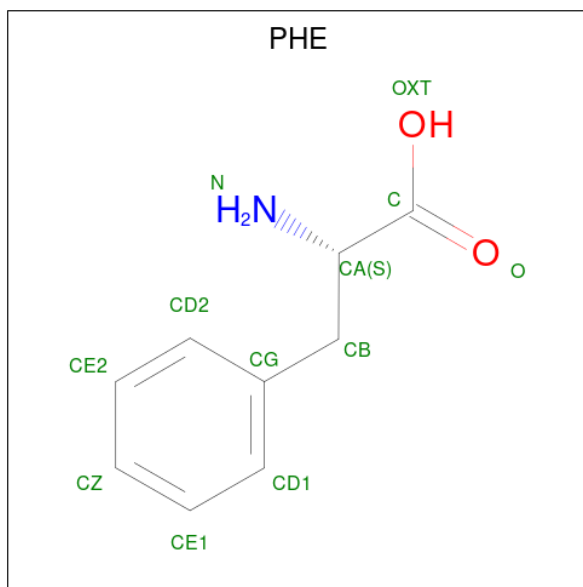
- Molecule 61 is a protein called Transcription termination/antitermination protein NusG.

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 (CCD ID: 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	

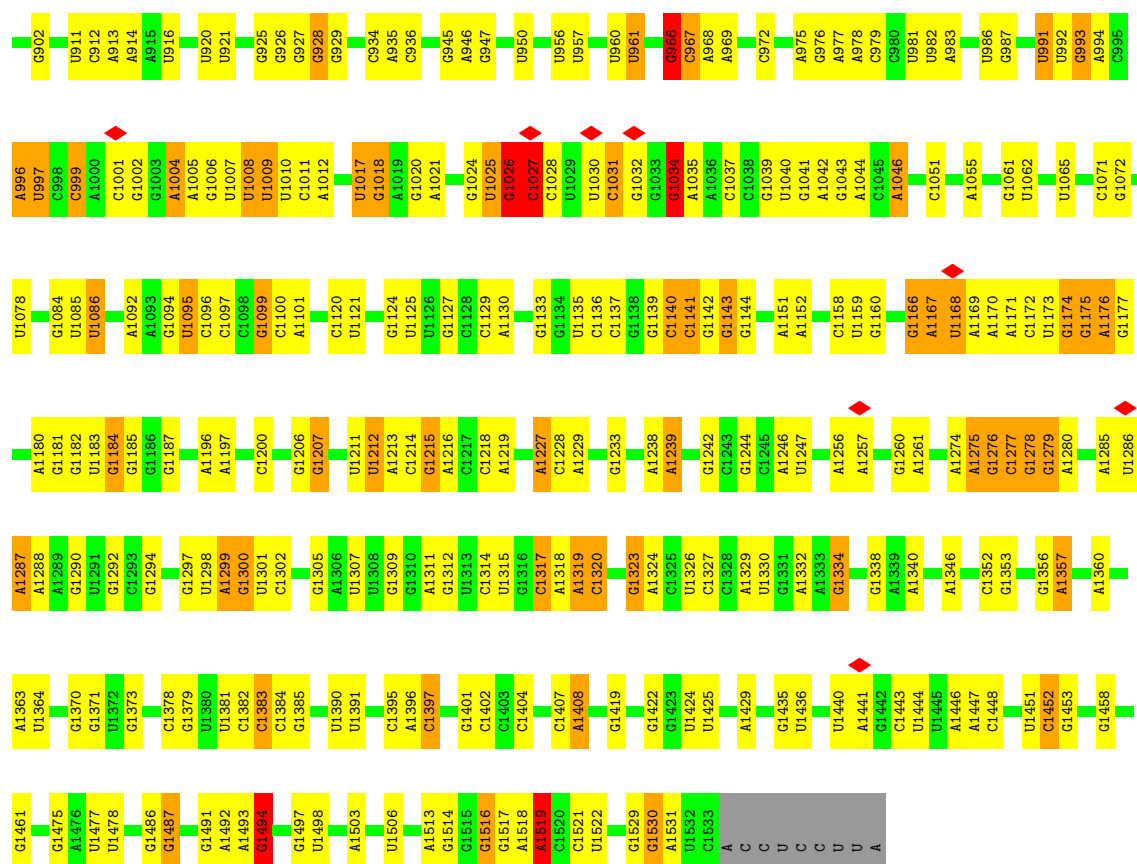
- Molecule 63 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



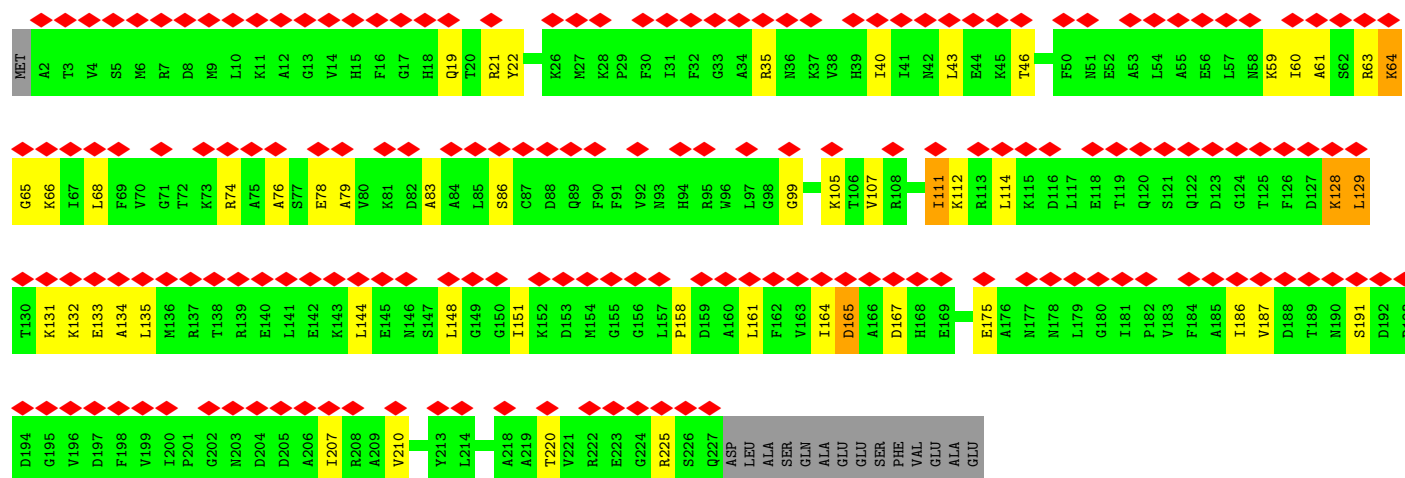
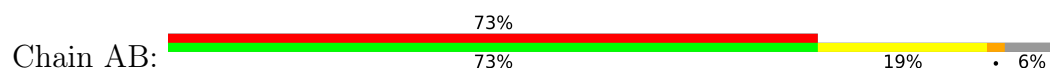
Mol	Chain	Residues	Atoms				AltConf
63	AX	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

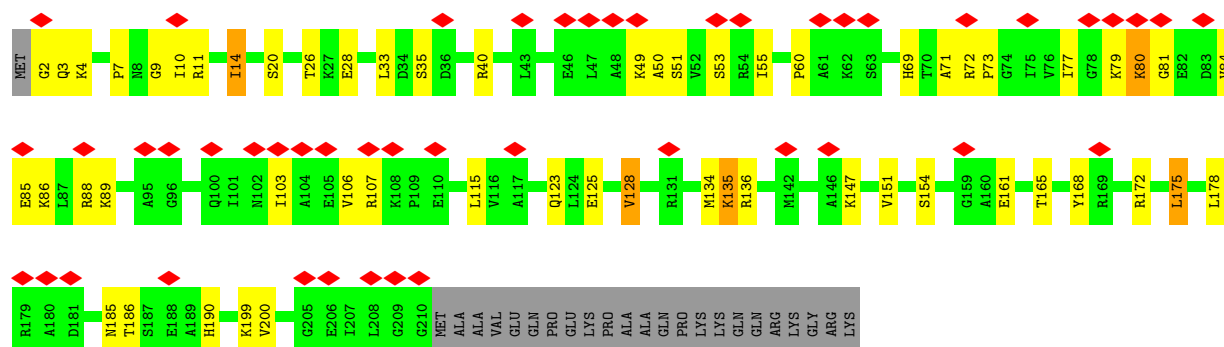


• Molecule 2: 30S ribosomal protein S2

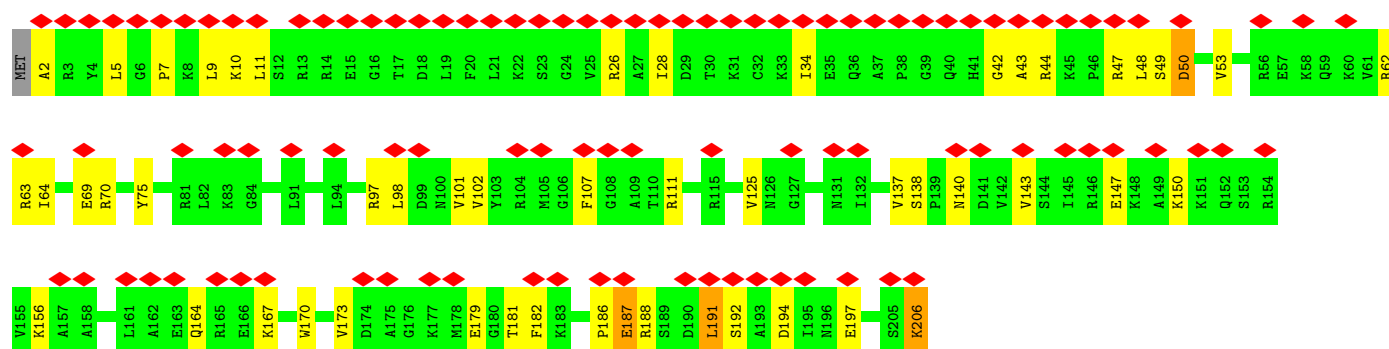
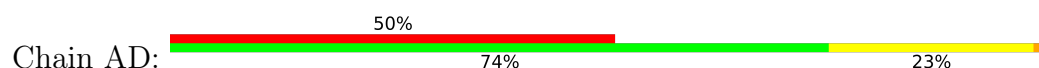


• Molecule 3: 30S ribosomal protein S3

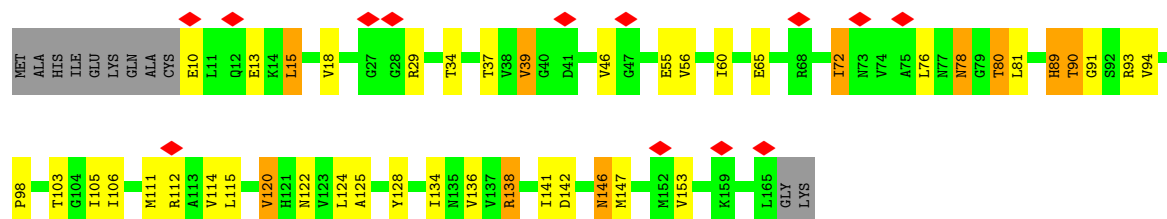




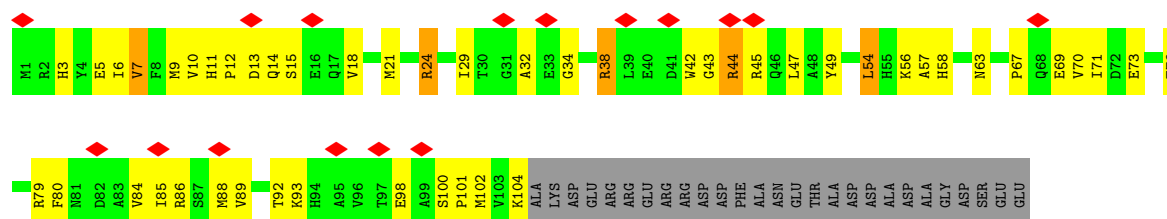
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

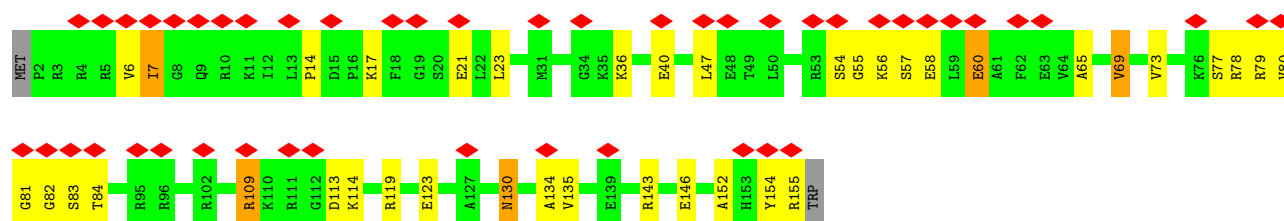


• Molecule 6: 30S ribosomal protein S6



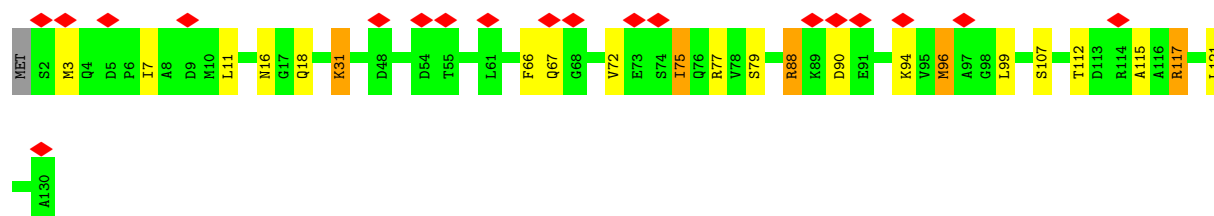
• Molecule 7: 30S ribosomal protein S7

Chain AG: 



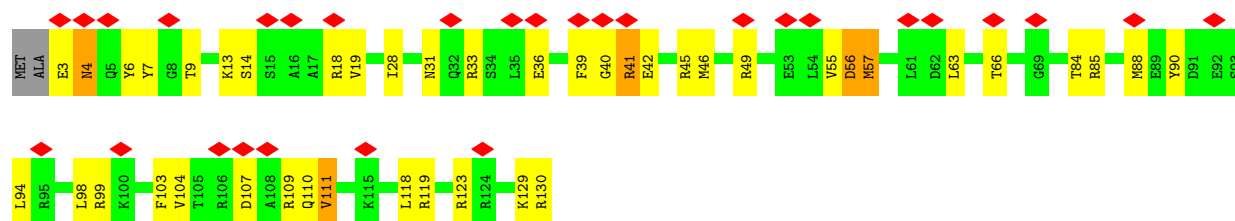
• Molecule 8: 30S ribosomal protein S8

Chain AH: 



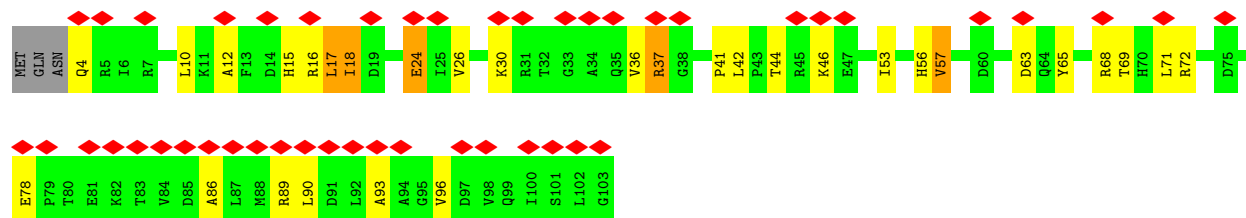
• Molecule 9: 30S ribosomal protein S9

Chain AI: 



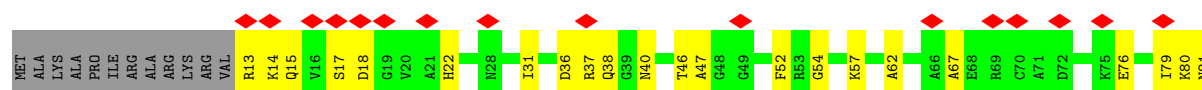
• Molecule 10: 30S ribosomal protein S10

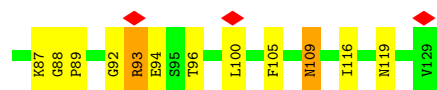
Chain AJ: 



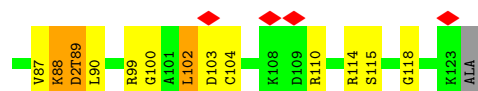
• Molecule 11: 30S ribosomal protein S11

Chain AK: 

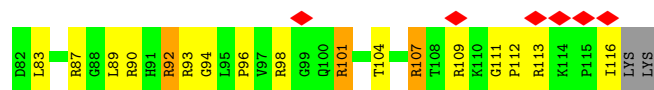
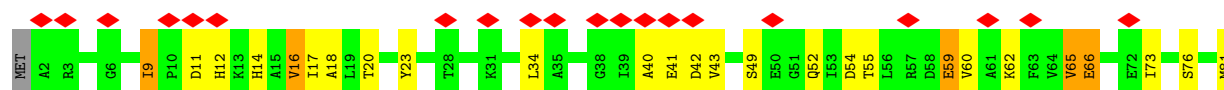




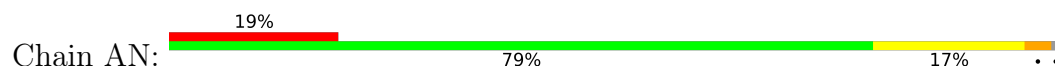
- Molecule 12: 30S ribosomal protein S12



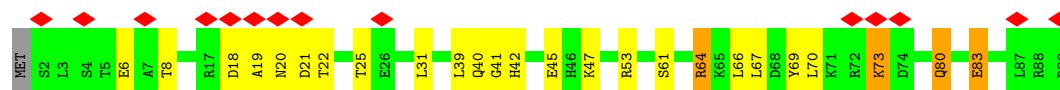
- Molecule 13: 30S ribosomal protein S13



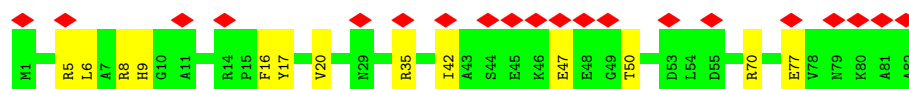
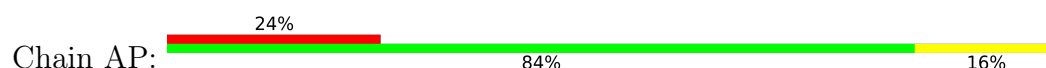
- Molecule 14: 30S ribosomal protein S14



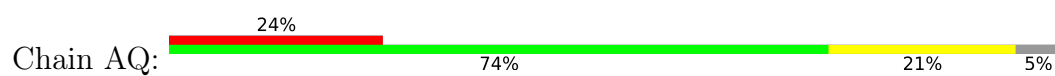
- Molecule 15: 30S ribosomal protein S15



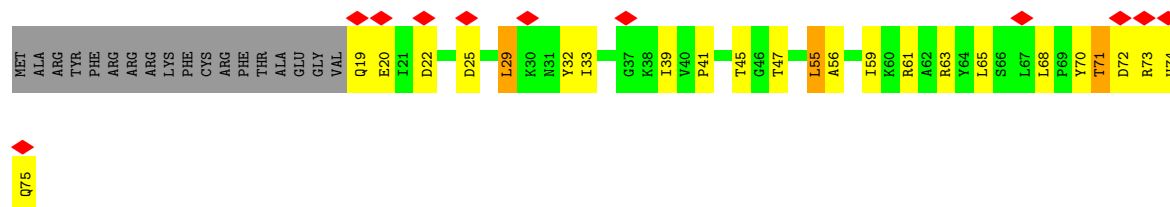
- Molecule 16: 30S ribosomal protein S16



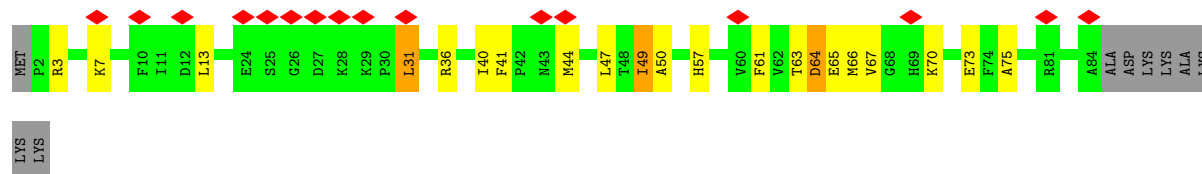
- Molecule 17: 30S ribosomal protein S17



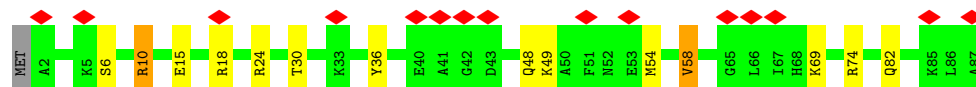
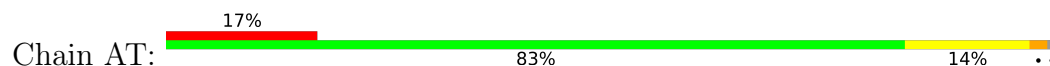
- Molecule 18: 30S ribosomal protein S18



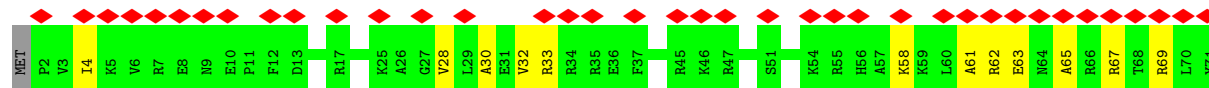
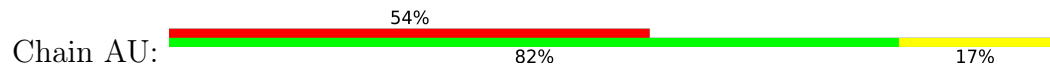
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



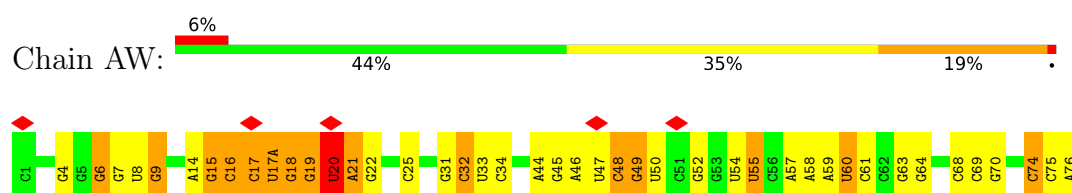
- Molecule 21: 30S ribosomal protein S21



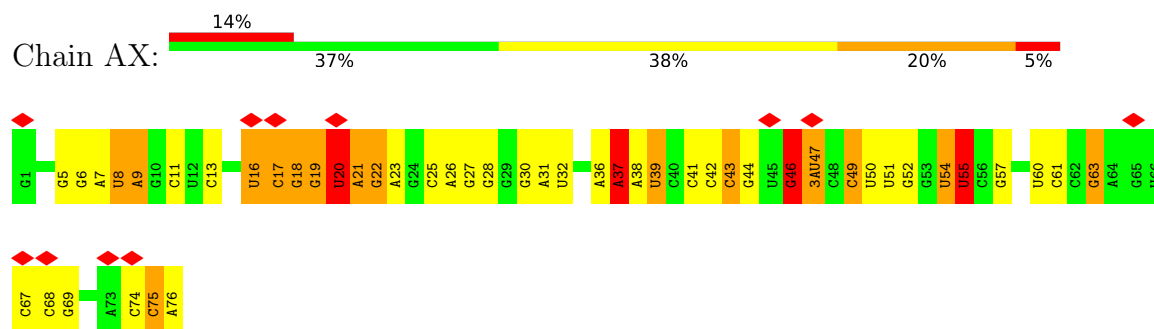
- Molecule 22: mRNA



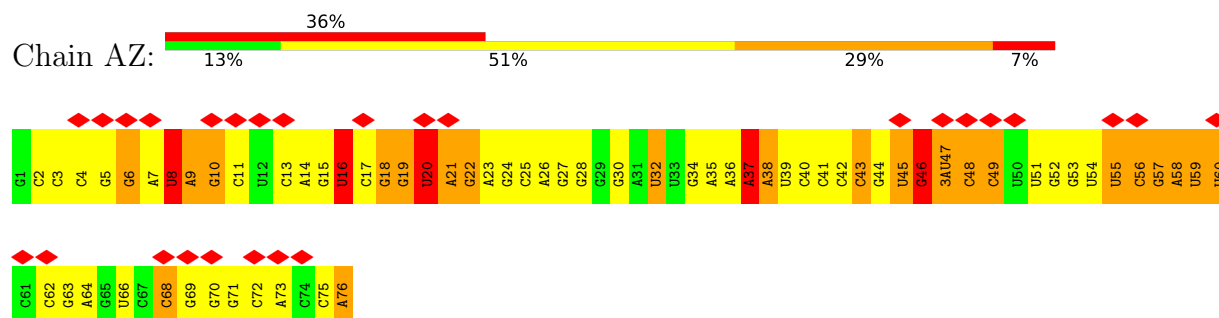
- Molecule 23: tRNA(fmet) P-site



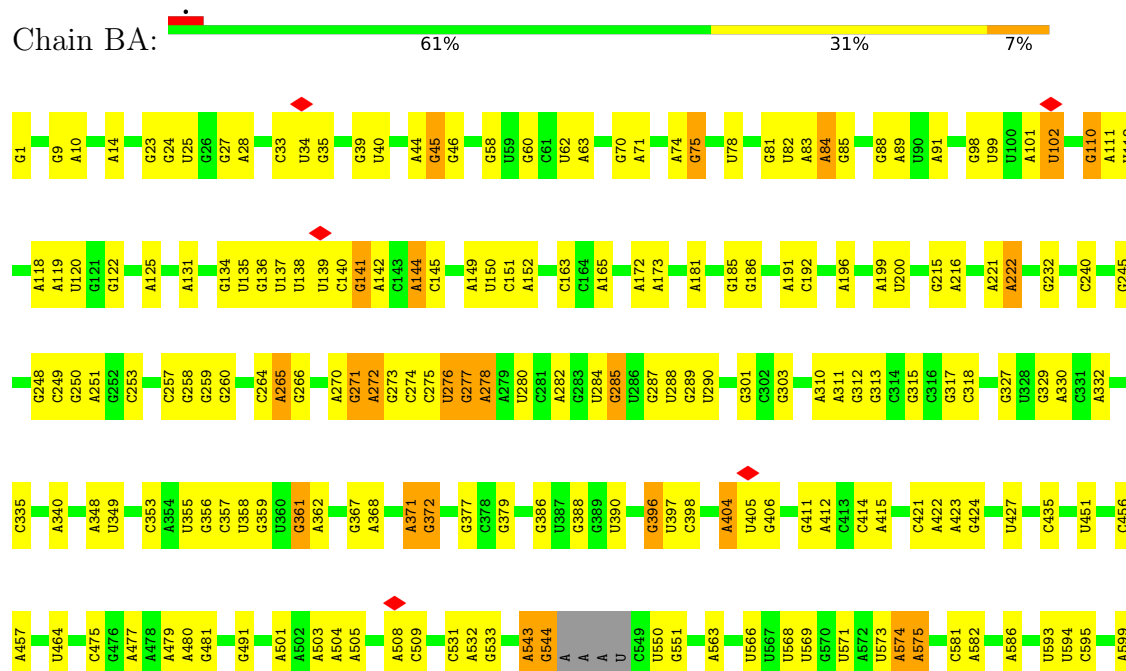
• Molecule 24: Phe-NH-tRNA(Phe) A-site

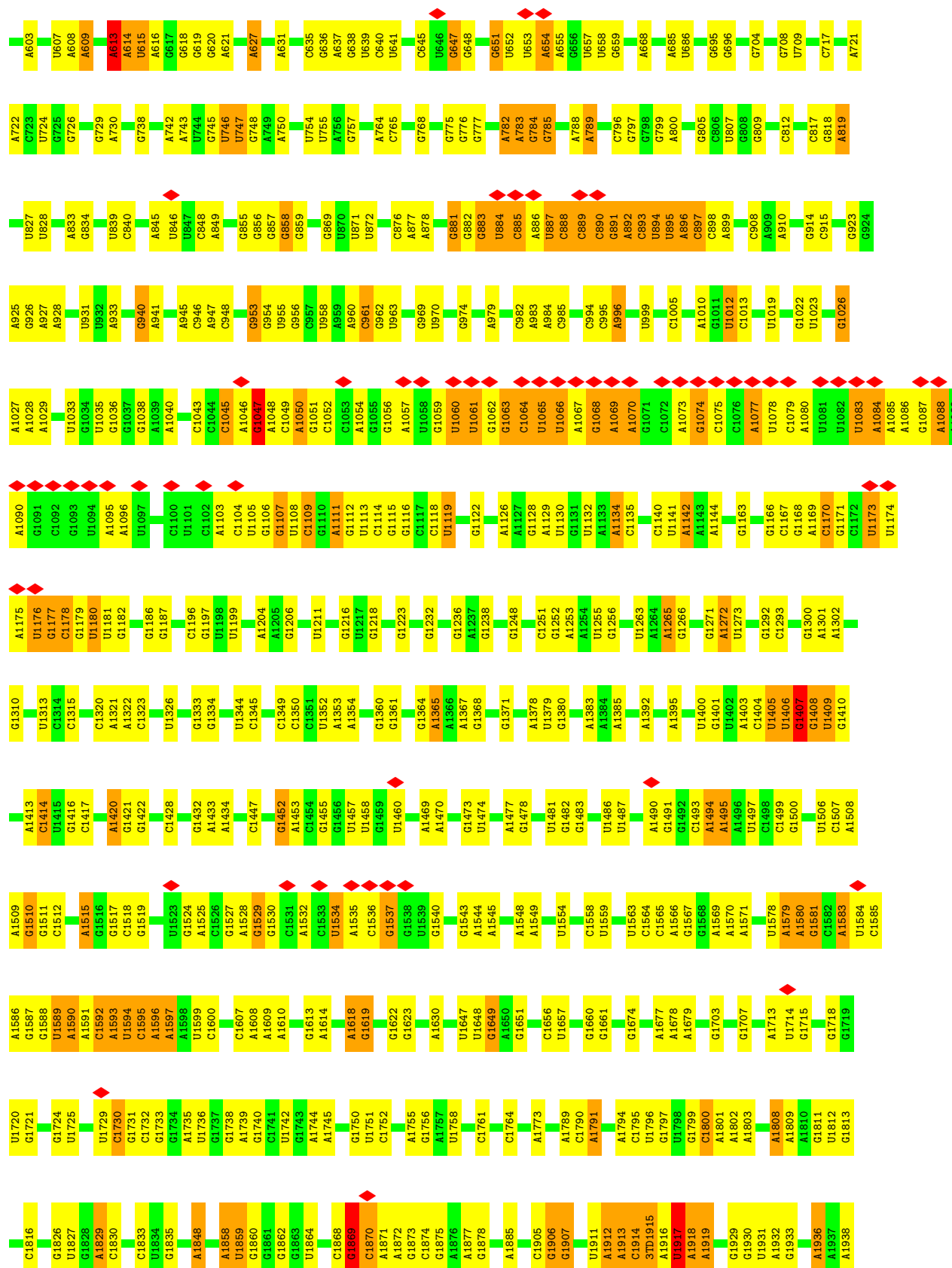


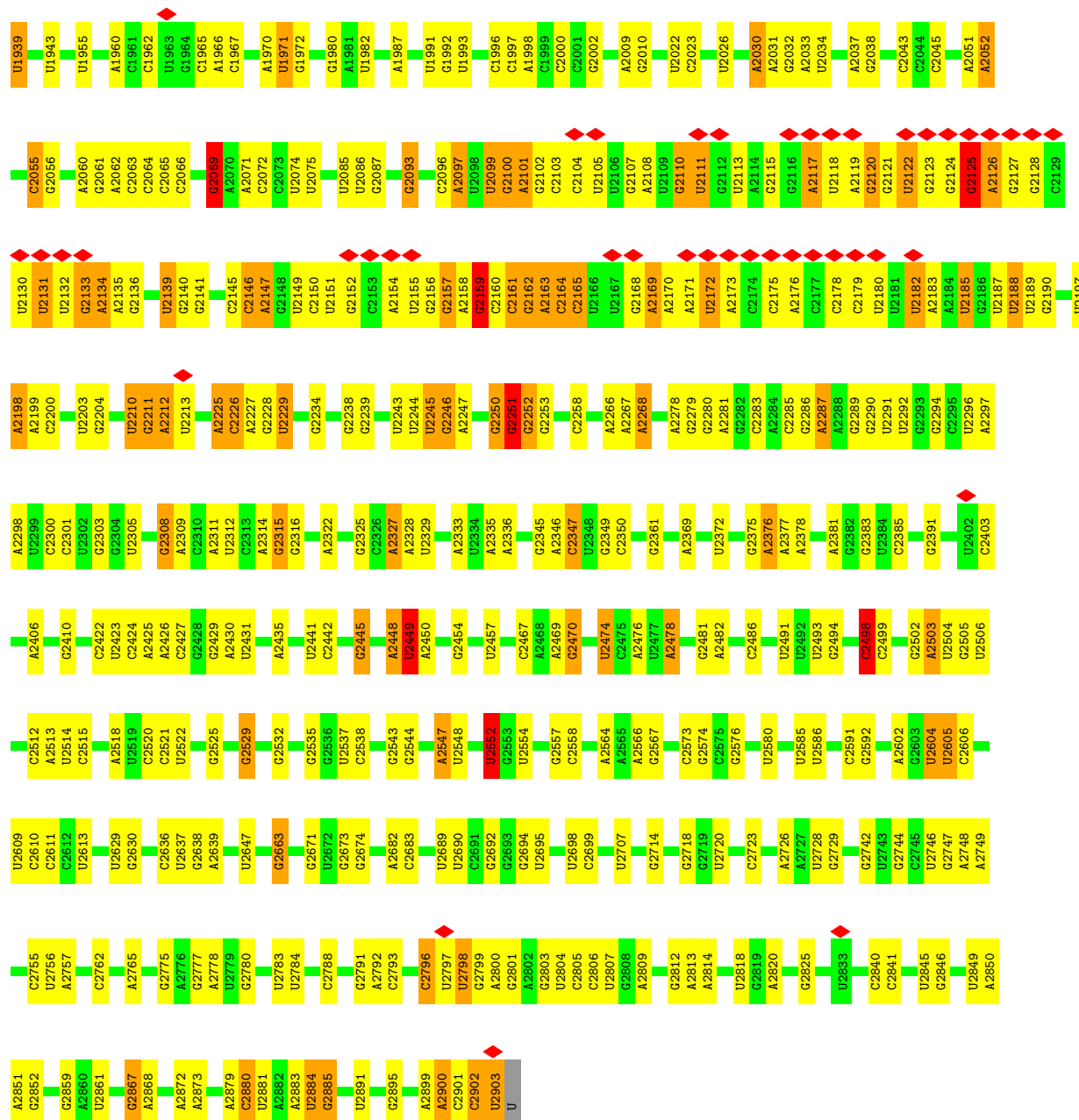
• Molecule 24: Phe-NH-tRNA(Phe) A-site



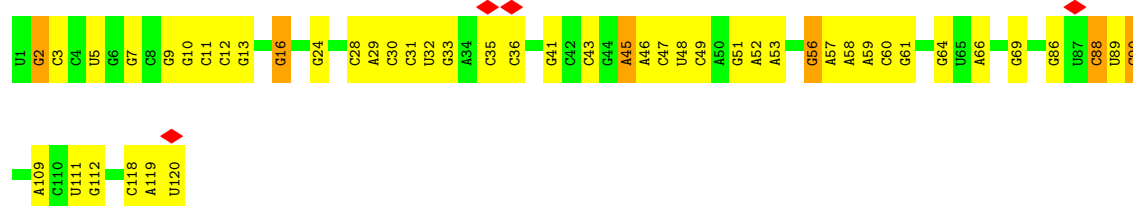
• Molecule 25: 23S ribosomal RNA



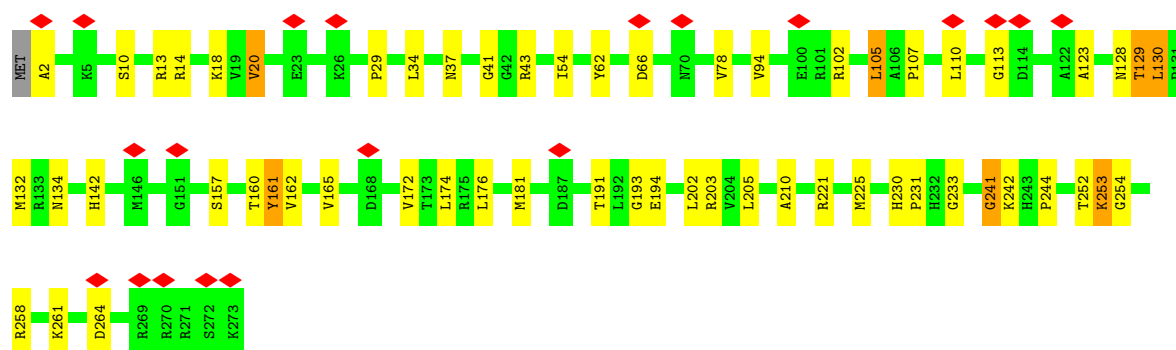
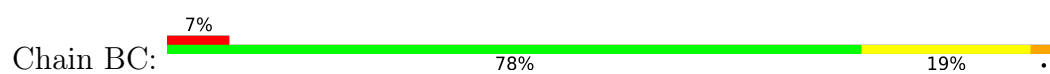




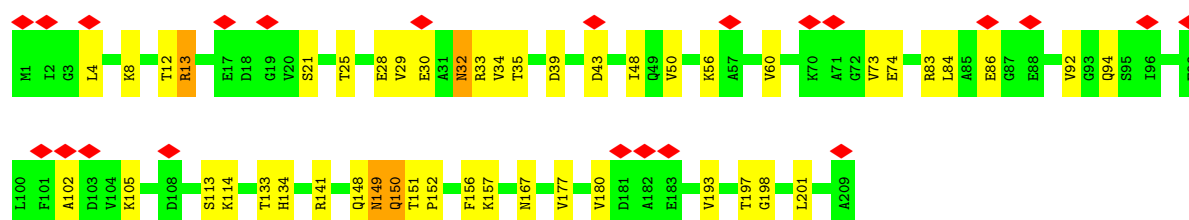
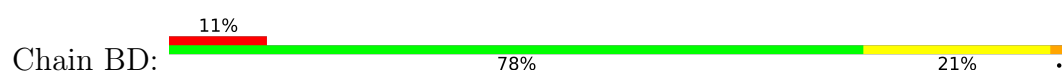
• Molecule 26: 5S ribosomal RNA



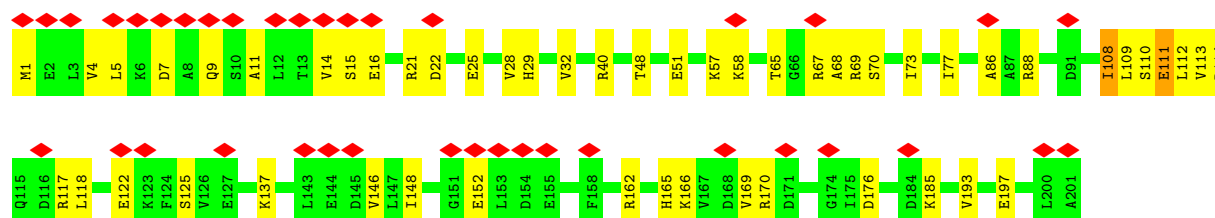
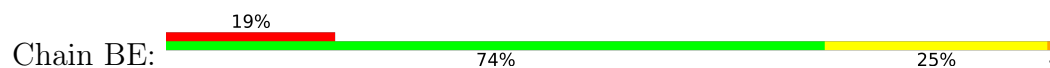
• Molecule 27: 50S ribosomal protein L2



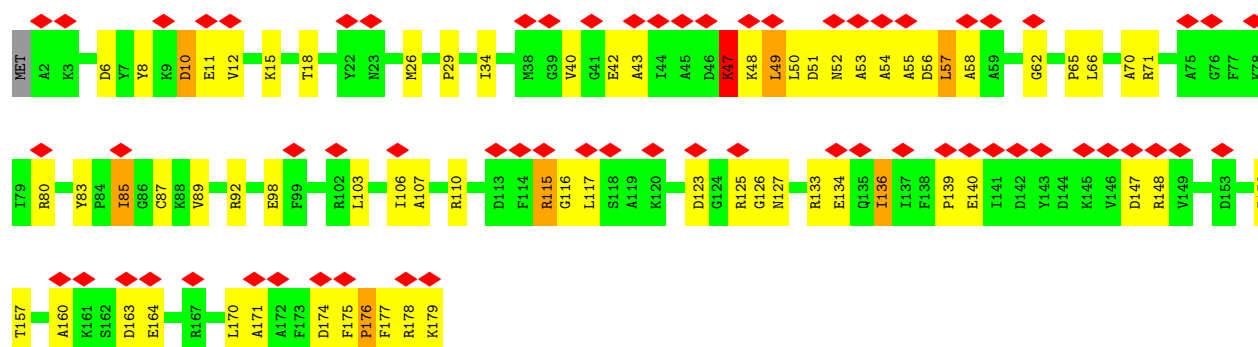
- Molecule 28: 50S ribosomal protein L3



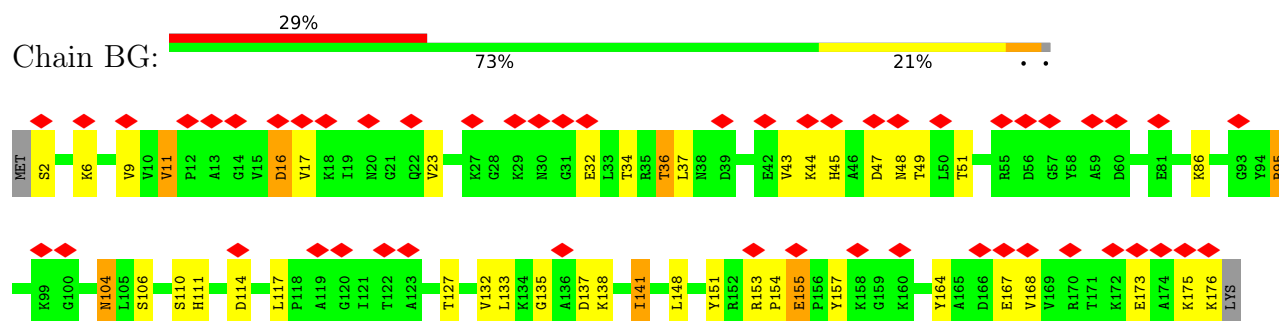
- Molecule 29: 50S ribosomal protein L4



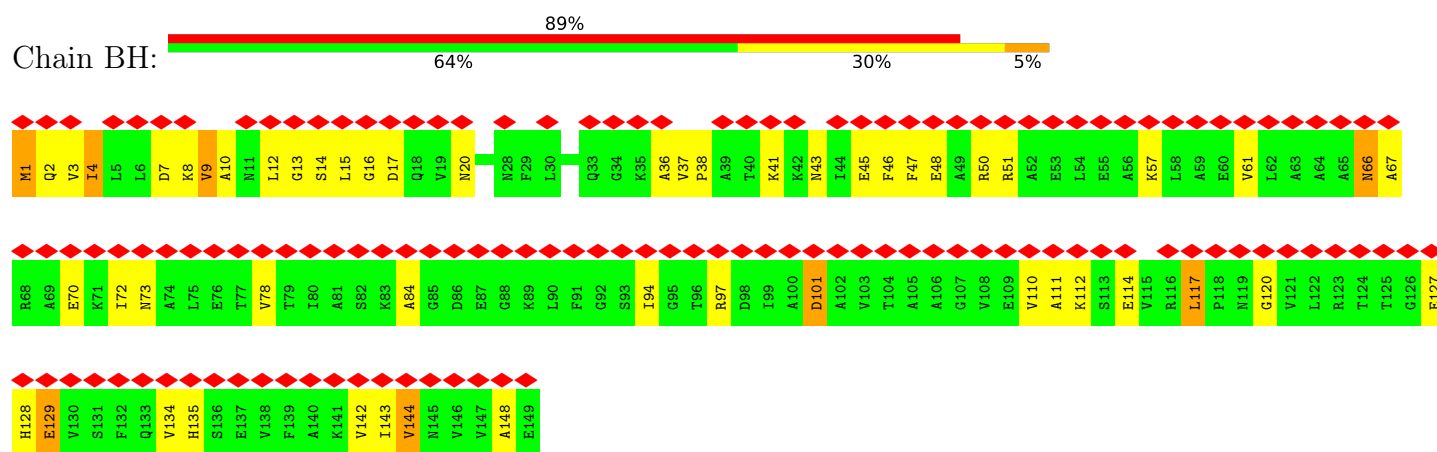
- Molecule 30: 50S ribosomal protein L5



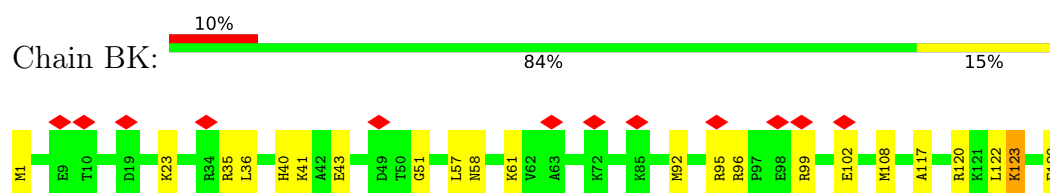
- Molecule 31: 50S ribosomal protein L6



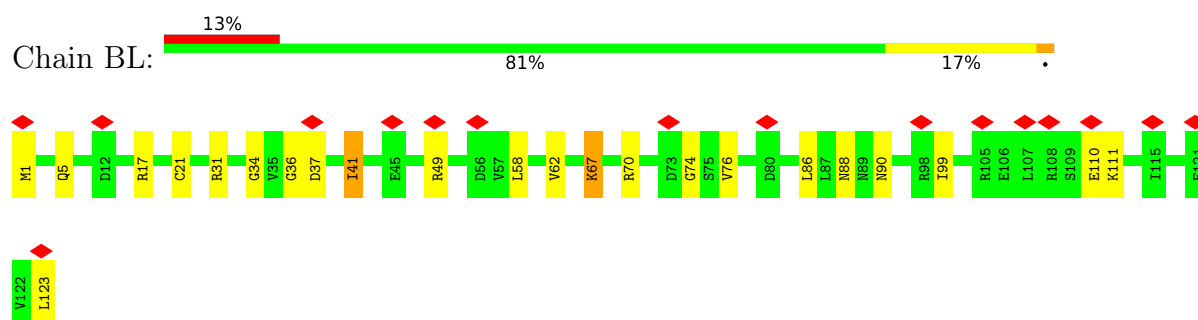
- Molecule 32: 50S ribosomal protein L9



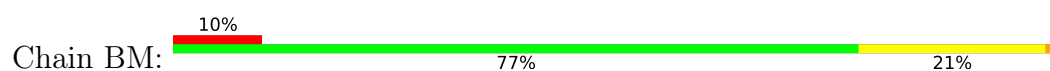
- Molecule 33: 50S ribosomal protein L13

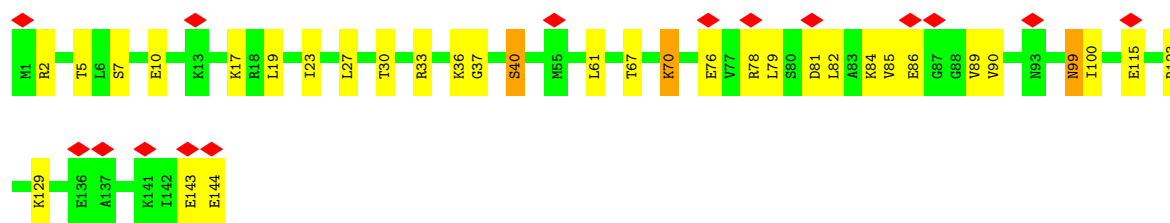


- Molecule 34: 50S ribosomal protein L14

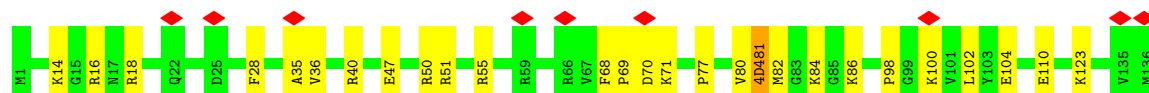
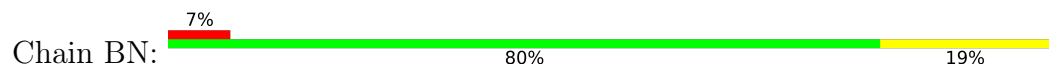


- Molecule 35: 50S ribosomal protein L15

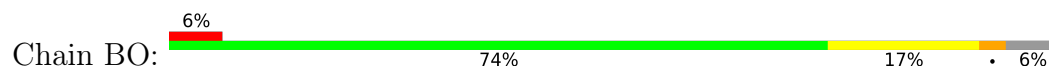




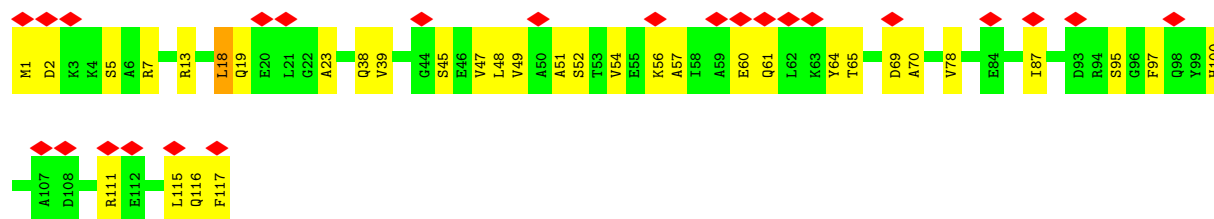
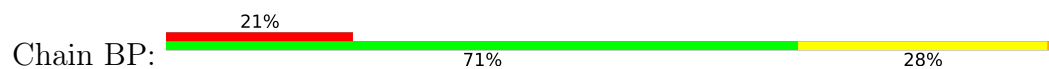
- Molecule 36: 50S ribosomal protein L16



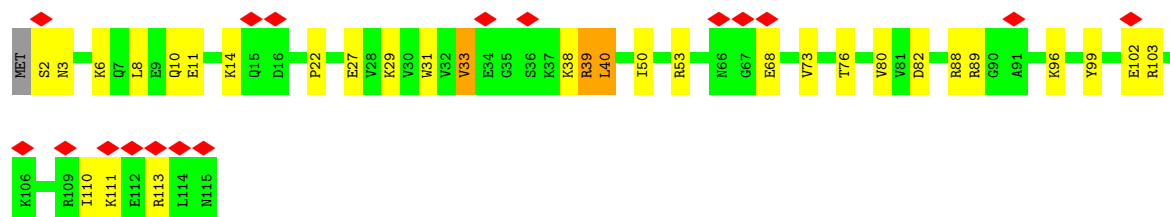
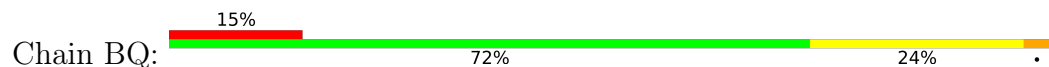
- Molecule 37: 50S ribosomal protein L17



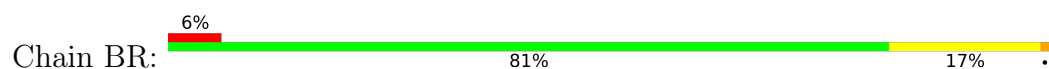
- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

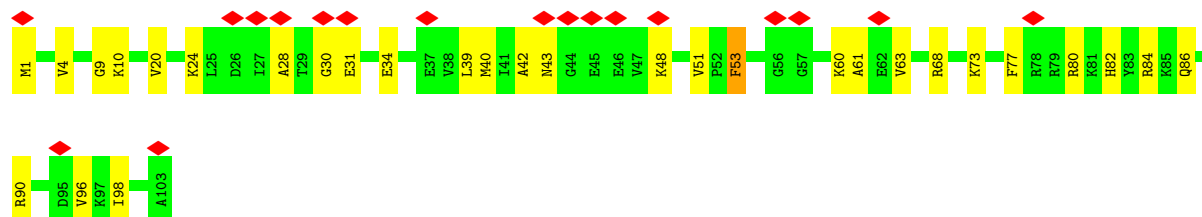
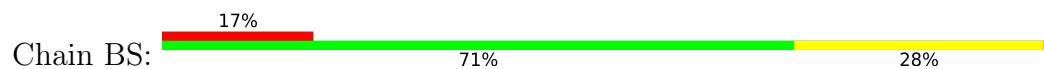


- Molecule 40: 50S ribosomal protein L20

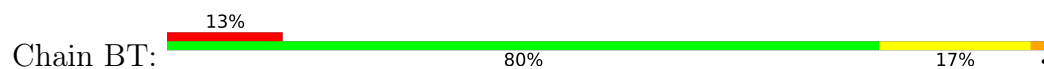




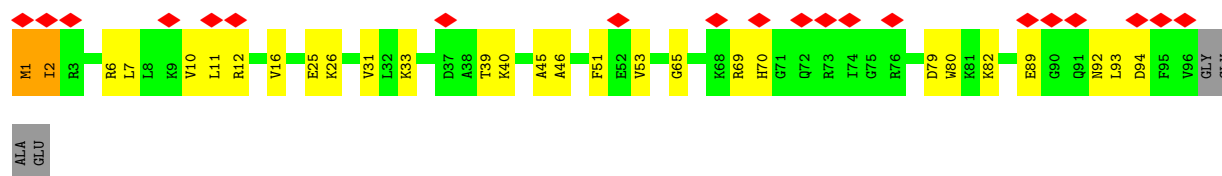
- Molecule 41: 50S ribosomal protein L21



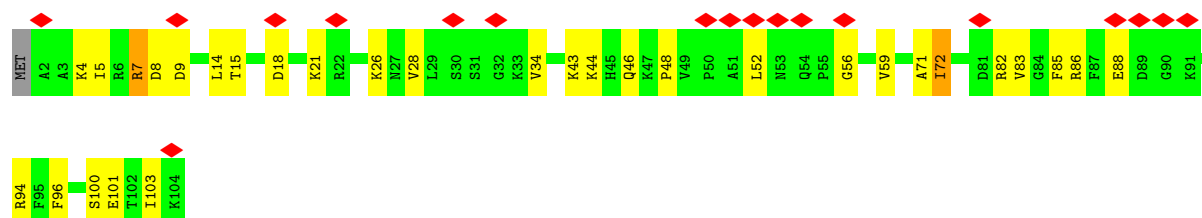
- Molecule 42: 50S ribosomal protein L22



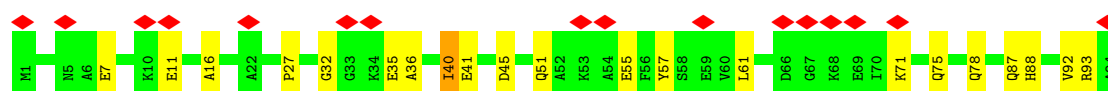
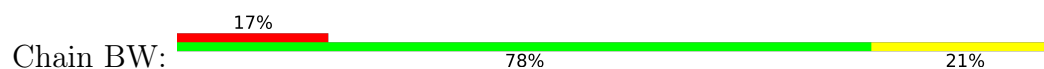
- Molecule 43: 50S ribosomal protein L23



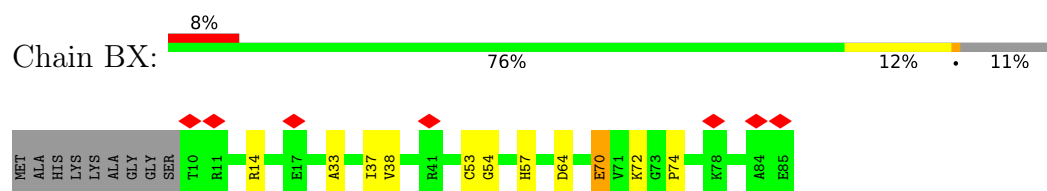
- Molecule 44: 50S ribosomal protein L24



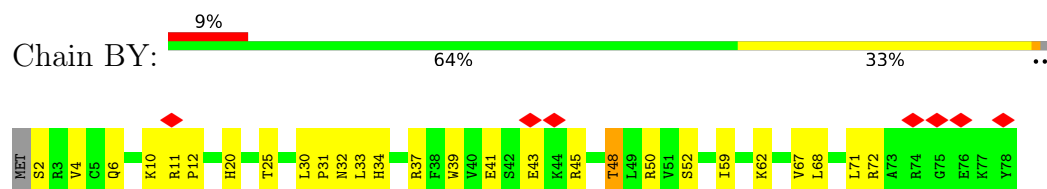
- Molecule 45: 50S ribosomal protein L25



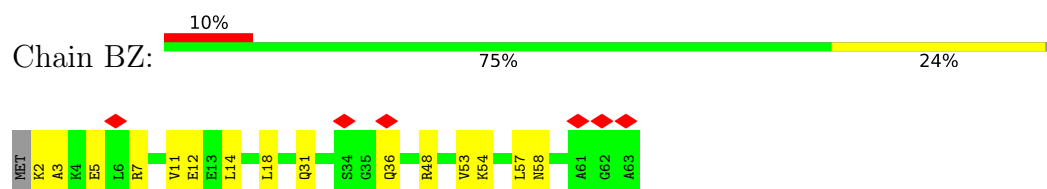
• Molecule 46: 50S ribosomal protein L27



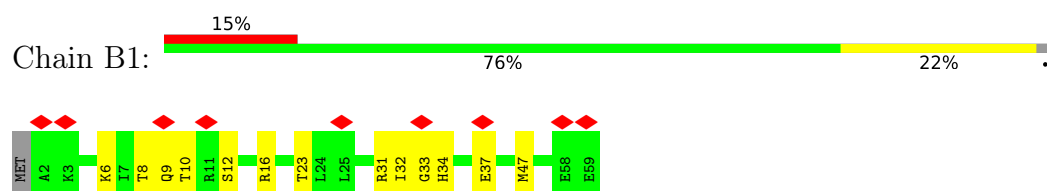
• Molecule 47: 50S ribosomal protein L28



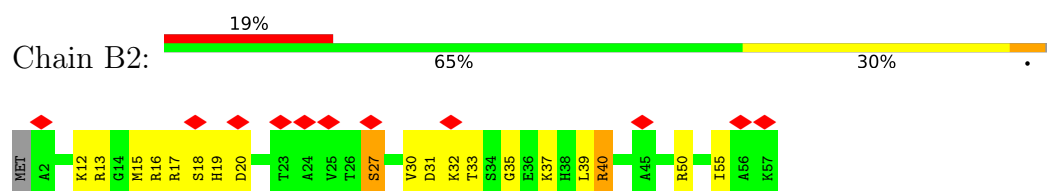
• Molecule 48: 50S ribosomal protein L29



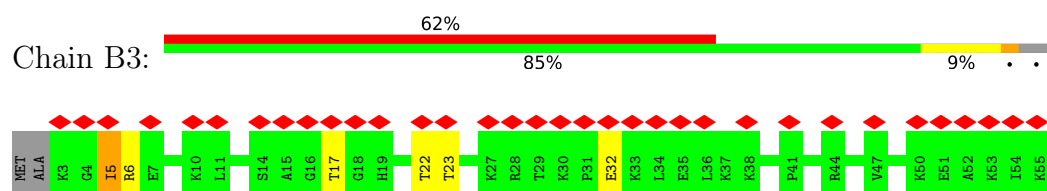
• Molecule 49: 50S ribosomal protein L30



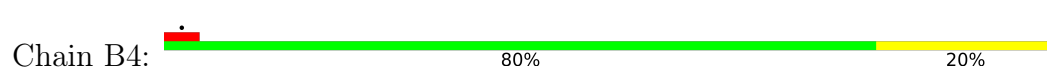
• Molecule 50: 50S ribosomal protein L32



• Molecule 51: 50S ribosomal protein L33

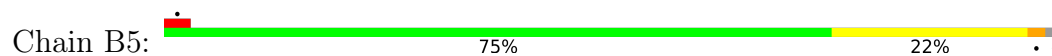


• Molecule 52: 50S ribosomal protein L34

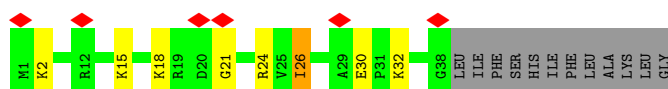




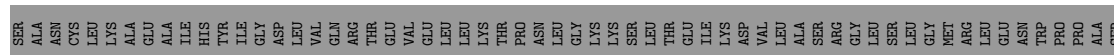
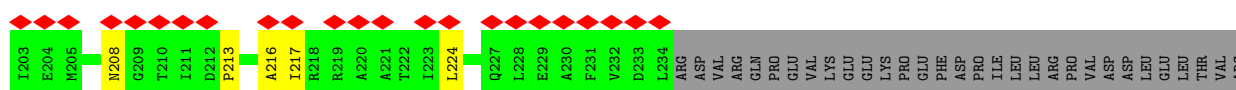
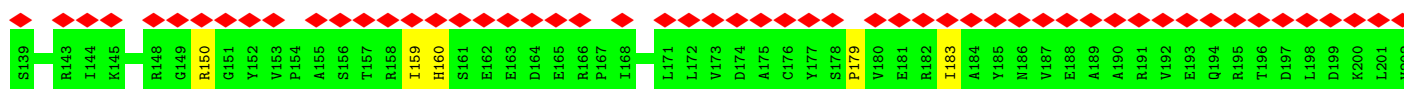
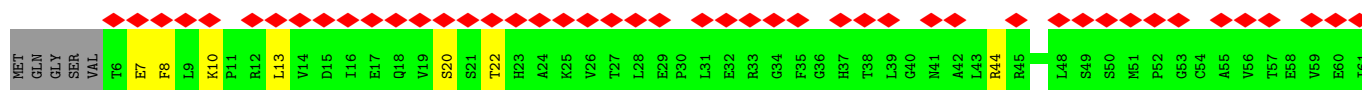
- Molecule 53: 50S ribosomal protein L35



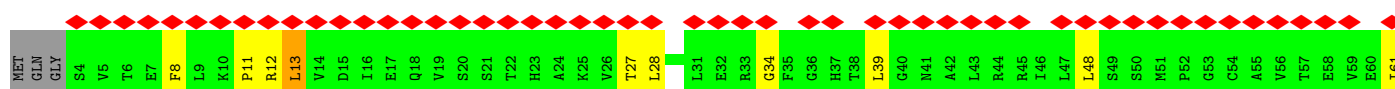
- Molecule 54: 50S ribosomal protein L36

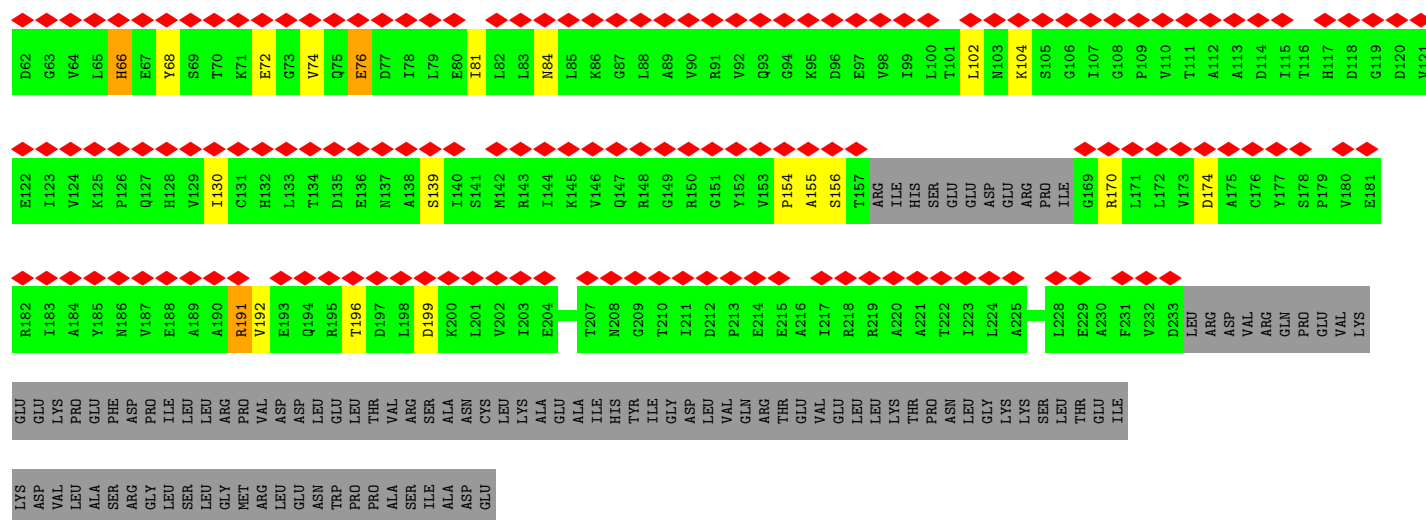


- Molecule 55: DNA-directed RNA polymerase subunit alpha

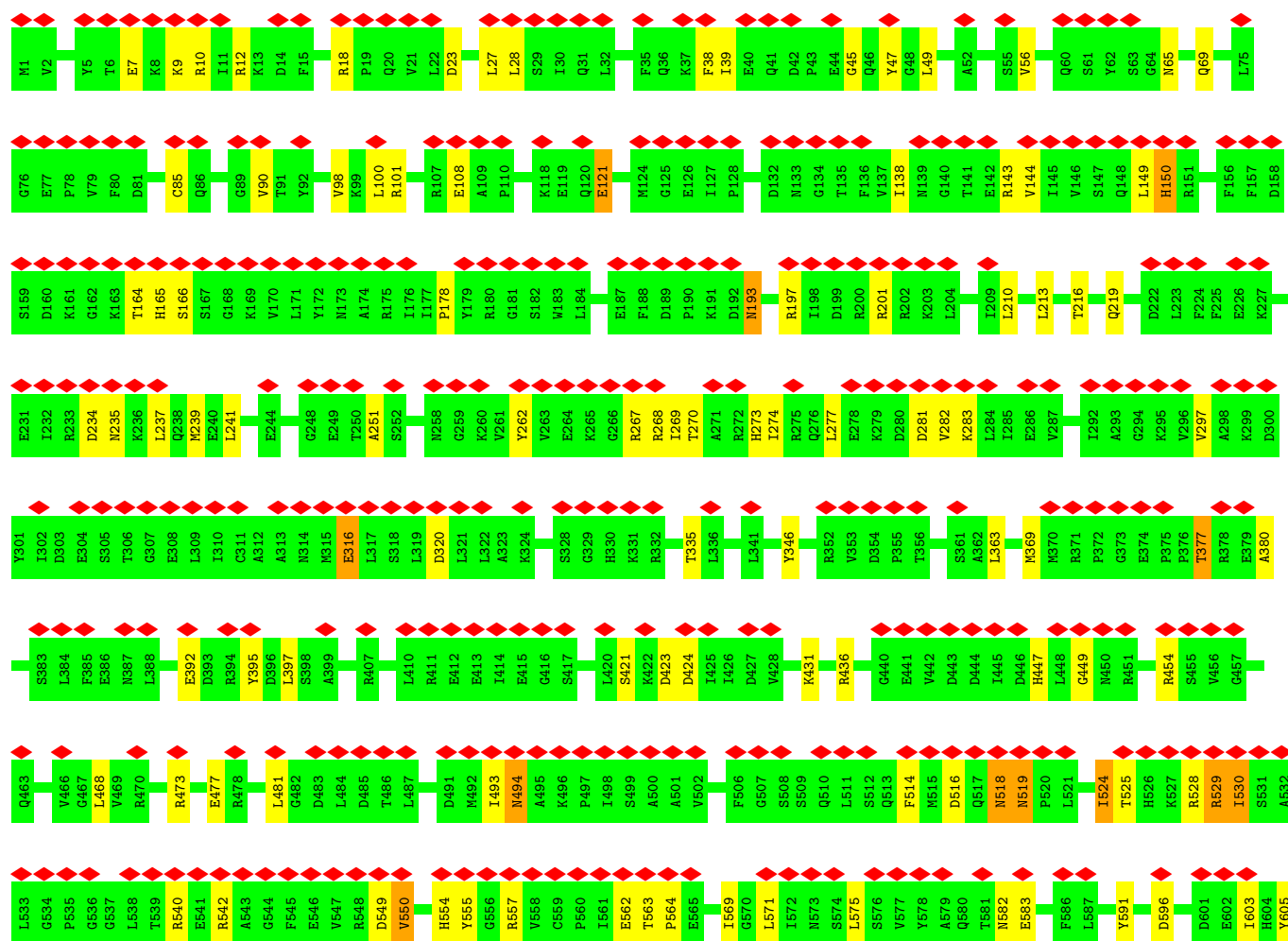


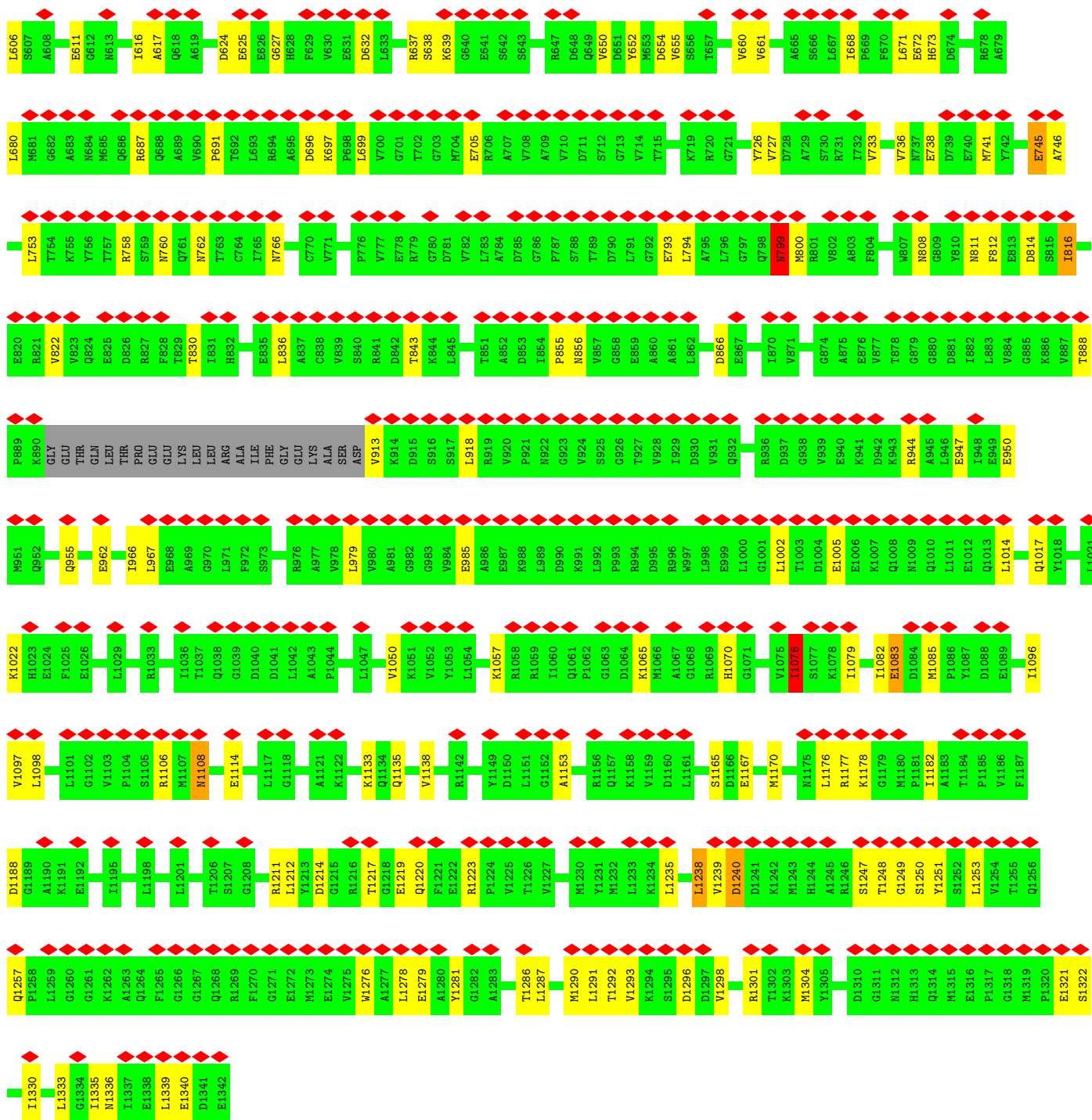
- Molecule 55: DNA-directed RNA polymerase subunit alpha



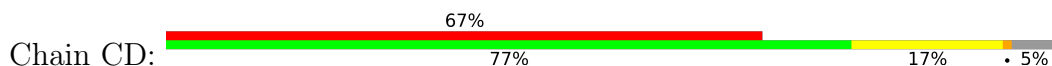


• Molecule 56: DNA-directed RNA polymerase subunit beta

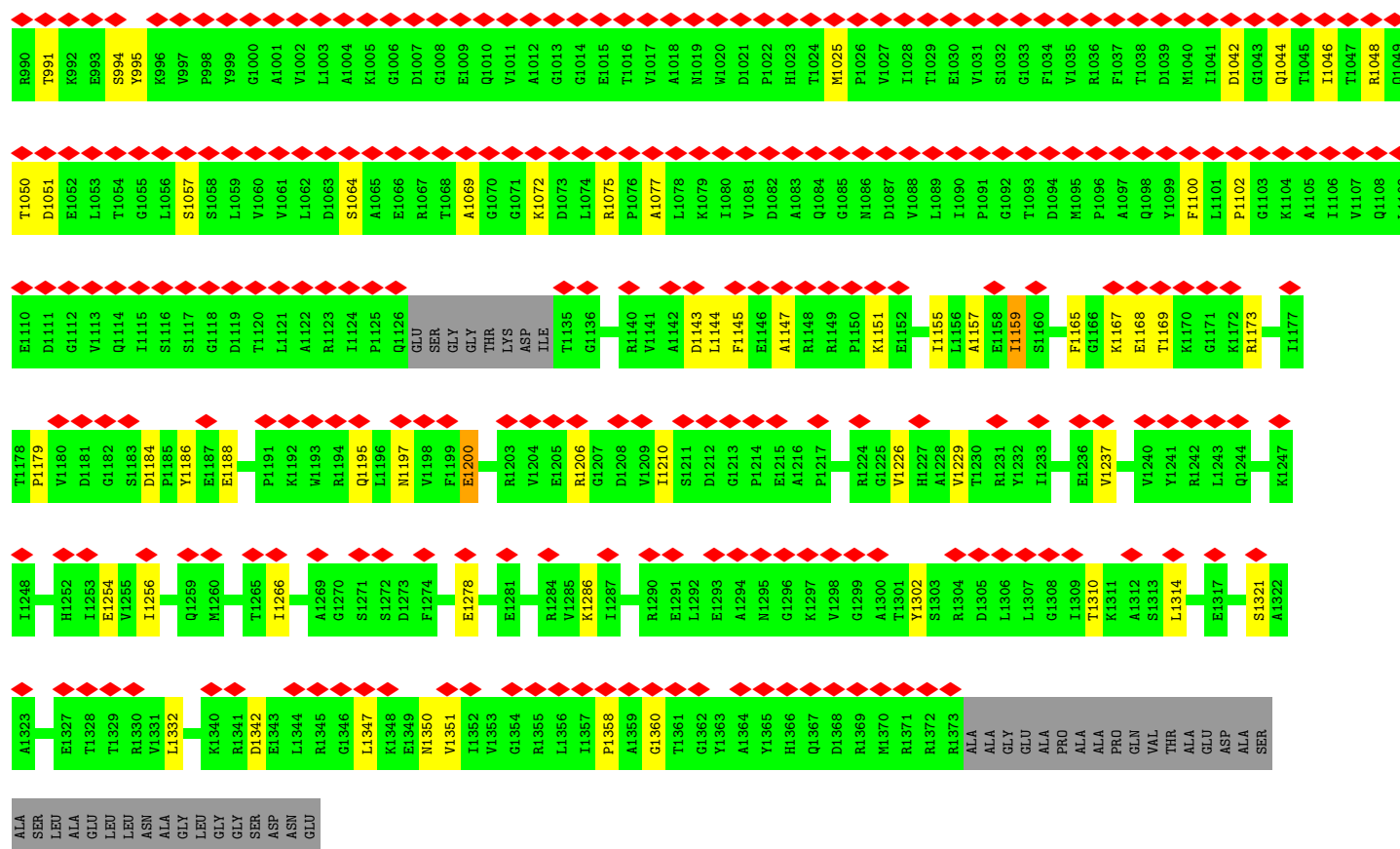




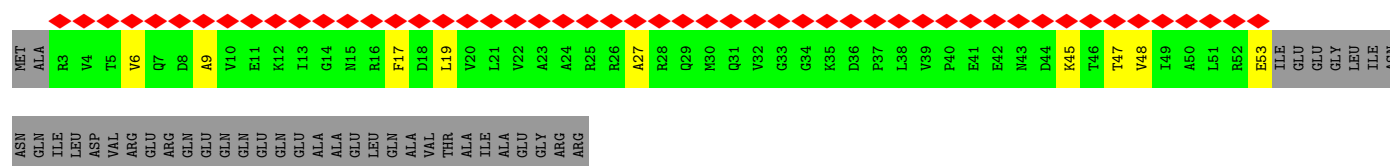
• Molecule 57: DNA-directed RNA polymerase subunit beta'



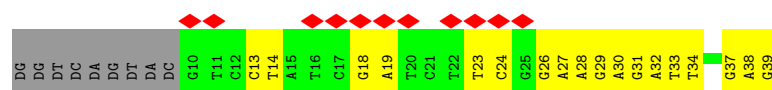
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T931	L856	T788	T722	A662	A533	T473	A406	G344	R281	E211	D134	D67
M932	L857	K789	Y723	E663	E534	L474	V407	K345	L282	K215	I135	E68
R933	T790	M724	M724	T664	R535	E475	V408	R346	L283	T218	V136	L71
THR	N861	A791	M725	Q665	Y537	A476	V409	V347	D284	L219	R137	C70
PHE	T862	A792	A726	E666	R538	Q477	D410	D348	L285	K219	L139	C72
HIS	L863	S793	T727	Q667	S539	E478	I411	Y349	A286	R220	L139	G73
ILE	L864	G794	S728	F668	S539	E479	L412	S350	A287	Y140	Y140	G74
GLY	H865	Y795	G728	Q669	G540	A480	D413	G351	P288	I221	F141	K74
GLY	E866	L796	G729	Q670	L541	A480	D413	R352	A287	I221	F141	K74
ALA	C869	T797	A730	S670	A542	R481	E414	R352	D289	E225	E142	Y75
SER	D870	R798	R731	Q671	S543	A482	V415	S353	I290	K226	S143	K76
ARG	L871	R799	G732	L672	S543	L483	I416	V354	T291	K226	S143	K76
ALA	L800	L800	S733	V673	M611	M484	E418	T227	V292	Y228	Y144	R77
ALA	A734	T674	A734	T674	G613	M485	E418	T227	R293	Q229	V145	L78
A735	A675	A675	A735	A675	G613	S486	H419	T356	K293	Q229	V145	L78
Q736	Q736	Q736	Q736	Q736	K615	T487	P420	V357	S230	S230	E148	K79
T737	T737	T737	T737	T737	F616	M488	V421	G358	Q231	Q231	G149	R81
R738	R738	R738	R738	R738	V551	N488	V421	P359	K232	K232	G149	R81
L739	V679	V679	V679	V679	I552	N489	N424	R362	N233	N233	G150	G82
L740	N680	N680	N680	N680	T553	I490	R425	R362	K233	K233	M151	V83
A741	K681	K681	A741	K681	E554	L491	A426	L363	P234	E235	T152	T84
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V682	V682	V682	V682	V682	E556	A494	T428	Q365	L306	M237	L154	E86
M743	M743	M743	M743	M743	K557	N495	L429	C366	L307	V241	E155	E86
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G745	G745	G745	G745	G745	A559	E497	R431	L368	N309	V244	Q157	C88
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M747	M747	M747	M747	M747	H560	I499	G433	K370	R311	L245	I159	V90
K749	K749	K749	K749	K749	C561	I500	L434	K371	G313	P247	T161	V92
P750	P750	P750	P750	P750	E562	V501	Q435	L374	R314	D248	E162	T93
D751	D751	D751	D751	D751	L563	P502	A436	E375	G310	V244	I159	G89
T823	T823	T823	T823	T823	V564	S503	L376	L376	A315	R250	Q164	V95
R924	R924	R924	R924	R924	A565	Q504	P439	E375	I316	P251	E171	V97
R826	R826	R826	R826	R826	K566	D505	V440	F379	T317	L252	E171	V97
E827	E827	E827	E827	E827	T567	V506	I442	F380	G318	V253	F172	R98
G828	G828	G828	G828	G828	S568	V507	E443	I381	S319	P254	G173	R99
A904	A904	A904	A904	A904	L508	L508	G444	G383	N320	L255	D174	E100
R905	R905	R905	R905	R905	G509	G509	K445	K384	K321	D256	E175	R101
G971	G971	G971	G971	G971	D571	L510	A446	L385	R322	G257	F176	H104
P758	P758	P758	P758	P758	T572	Y511	L641	L395	P323	Q258	I105	I105
L759	L759	L759	L759	L759	R576	Y512	Q448	E386	P323	G258	E106	I105
T760	T760	T760	T760	T760	D642	M513	L449	L324	R259	R259	L107	E106
A761	A761	A761	A761	A761	D643	T514	H450	L387	K325	F260	G181	L107
N702	N702	N702	N702	N702	R515	R515	H450	R388	S326	A261	A182	A108
Q702	Q702	Q702	Q702	Q702	L579	L579	C454	G389	L327	T262	E182	S109
T703	T703	T703	T703	T703	N580	N580	A455	L390	A328	S263	A184	P110
E704	E704	E704	E704	E704	H581	H581	A456	A391	D329	D264	I185	A112
T705	T705	T705	T705	T705	I582	I582	Y457	T392	K332	L268	Q186	H113
V706	V706	V706	V706	V706	V583	V583	E522	T393	L394	L268	Q186	H113
T707	T707	T707	T707	T707	K649	K649	N458	K393	R270	L268	Q186	H113
N708	N708	N708	N708	N708	K650	K650	A459	A396	R271	L268	Q186	H113
R709	R709	R709	R709	R709	H651	H651	D460	A397	K335	L268	Q186	H113
D710	D710	D710	D710	D710	G586	G586	F461	A397	K335	L268	Q186	H113
G711	G711	G711	G711	G711	L587	L587	D462	A397	K335	L268	Q186	H113
Q712	Q712	Q712	Q712	Q712	I591	I591	V526	A397	K335	L268	Q186	H113
T713	T713	T713	T713	T713	V592	V592	D462	A397	K335	L268	Q186	H113
E714	E714	E714	E714	E714	N593	N593	D464	A397	K335	L268	Q186	H113
K715	K715	K715	K715	K715	Q594	Q594	D464	A397	K335	L268	Q186	H113
Q716	Q716	Q716	Q716	Q716	A595	A595	Q465	A397	K335	L268	Q186	H113
V717	V717	V717	V717	V717	L596	L596	M466	A397	K335	L268	Q186	H113
S719	S719	S719	S719	S719	A659	A659	P530	A397	K335	L268	Q186	H113



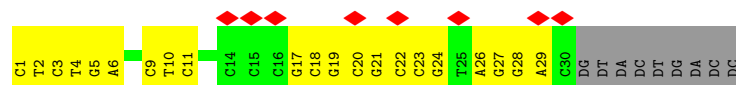
- Molecule 58: DNA-directed RNA polymerase subunit omega



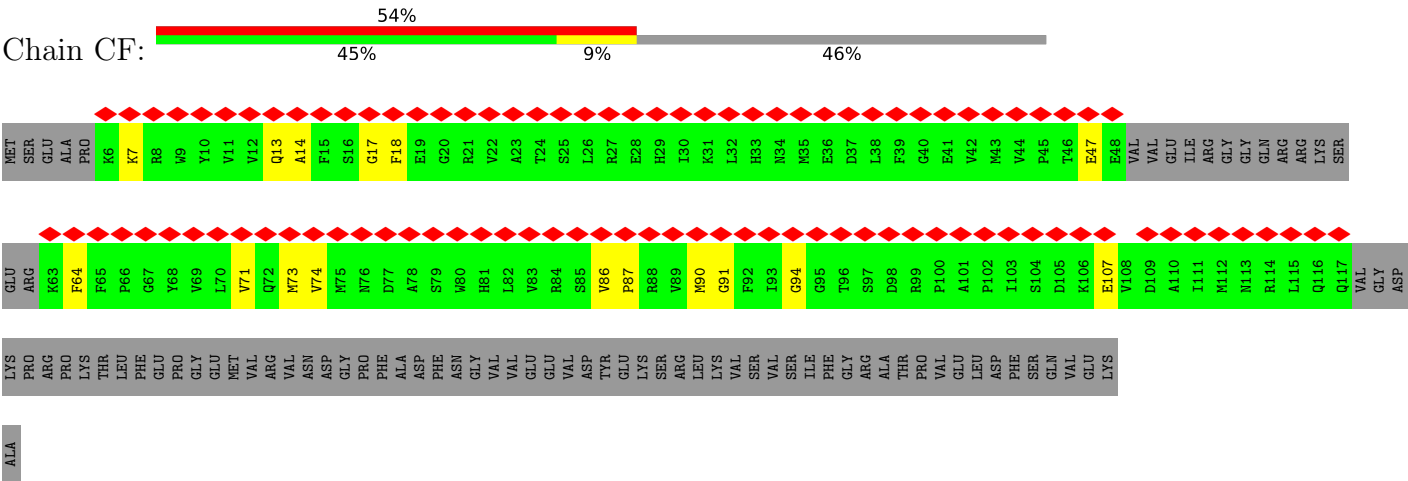
- Molecule 59: Non-template DNA strand



- 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
Maximum map value	2.131	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	723.84, 723.84, 723.84	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.74, 1.74, 1.74	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.36	0/36569	0.59	14/57044 (0.0%)
2	AB	0.26	0/1796	0.64	0/2420
3	AC	0.31	0/1667	0.64	0/2246
4	AD	0.27	0/1665	0.63	0/2227
5	AE	0.30	0/1161	0.67	0/1563
6	AF	0.31	0/867	0.68	0/1171
7	AG	0.28	0/1230	0.76	3/1649 (0.2%)
8	AH	0.29	0/989	0.57	0/1326
9	AI	0.29	0/1043	0.76	0/1387
10	AJ	0.31	0/810	0.82	0/1094
11	AK	0.29	0/893	0.64	0/1205
12	AL	0.34	0/954	0.81	1/1279 (0.1%)
13	AM	0.27	0/900	0.70	0/1204
14	AN	0.28	0/817	0.57	0/1088
15	AO	0.30	0/722	0.63	0/964
16	AP	0.25	0/659	0.59	0/884
17	AQ	0.26	0/657	0.59	0/881
18	AR	0.30	0/481	0.71	0/645
19	AS	0.29	0/680	0.71	0/915
20	AT	0.28	0/676	0.55	0/895
21	AU	0.26	0/598	0.60	0/792
22	AV	0.82	0/731	0.86	1/1133 (0.1%)
23	AW	0.38	0/1725	0.60	0/2687
24	AX	0.27	0/1584	0.31	0/2463
24	AZ	0.25	0/1584	0.34	0/2463
25	BA	0.39	1/69140 (0.0%)	0.59	11/107854 (0.0%)
26	BB	0.31	0/2872	0.50	0/4478
27	BC	0.37	0/2131	0.79	1/2863 (0.0%)
28	BD	0.33	0/1576	0.63	0/2119
29	BE	0.33	0/1571	0.65	0/2113
30	BF	0.29	0/1444	0.80	2/1937 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BG	0.25	0/1333	0.63	0/1805
32	BH	0.25	0/1122	0.82	3/1515 (0.2%)
33	BK	0.31	0/1152	0.61	0/1551
34	BL	0.36	0/956	0.66	0/1279
35	BM	0.32	0/1061	0.69	0/1412
36	BN	0.33	0/1081	0.62	0/1443
37	BO	0.34	0/973	0.66	0/1301
38	BP	0.26	0/910	0.69	0/1219
39	BQ	0.31	0/929	0.68	0/1242
40	BR	0.41	0/960	0.64	0/1278
41	BS	0.35	0/829	0.85	1/1107 (0.1%)
42	BT	0.36	0/864	0.69	0/1156
43	BU	0.30	0/771	0.65	0/1031
44	BV	0.26	0/797	0.62	0/1062
45	BW	0.30	0/766	0.66	0/1025
46	BX	0.34	0/589	0.68	0/779
47	BY	0.35	0/635	0.54	0/848
48	BZ	0.27	0/502	0.57	0/667
49	B1	0.33	0/453	0.67	0/605
50	B2	0.39	0/450	0.94	3/599 (0.5%)
51	B3	0.26	0/443	0.78	0/587
52	B4	0.36	0/379	0.56	0/496
53	B5	0.34	0/513	0.73	0/676
54	B6	0.30	0/302	0.61	0/397
55	CA	0.99	0/1797	0.91	0/2436
55	CB	0.74	0/1703	0.85	0/2308
56	CC	1.22	7/10581 (0.1%)	1.00	1/14275 (0.0%)
57	CD	1.00	1/10532 (0.0%)	0.93	0/14219
58	CE	0.44	0/401	0.83	0/540
59	CN	0.69	0/690	0.72	0/1064
60	CT	1.04	0/676	0.78	0/1039
61	CF	0.31	0/808	0.64	0/1088
All	All	0.52	9/186150 (0.0%)	0.66	41/275038 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CC	519	ASN	CB-CG	-5.78	1.37	1.52
56	CC	530	ILE	CB-CG2	-5.78	1.33	1.52
57	CD	424	ASN	CB-CG	-5.56	1.38	1.52
56	CC	1076	ILE	CB-CG1	-5.49	1.42	1.53
56	CC	816	ILE	CB-CG2	-5.18	1.35	1.52
56	CC	518	ASN	CB-CG	-5.17	1.39	1.52
25	BA	543	A	C1'-N9	-5.16	1.40	1.48
56	CC	799	ASN	CB-CG	-5.16	1.39	1.52
56	CC	144	VAL	CB-CG1	-5.04	1.35	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	49	G	O3'-P-O5'	-9.87	89.19	104.00
32	BH	13	GLY	N-CA-C	7.22	130.30	113.18
25	BA	2125	G	N9-C1'-C2'	7.04	122.55	112.00
1	AA	1491	G	O3'-P-O5'	6.92	114.39	104.00
1	AA	5	U	O5'-C5'-C4'	6.85	121.98	111.70
1	AA	1027	C	C2-N1-C1'	6.80	139.21	118.80
1	AA	1026	G	C4'-C3'-O3'	-6.65	103.02	113.00
30	BF	47	LYS	CA-C-N	-6.30	111.21	120.28
30	BF	47	LYS	C-N-CA	-6.30	111.21	120.28
7	AG	55	GLY	N-CA-C	6.24	127.97	113.18
1	AA	1027	C	C6-N1-C1'	-6.20	102.20	120.80
1	AA	1034	G	O3'-P-O5'	-6.17	94.75	104.00
1	AA	1494	G	P-O5'-C5'	-6.08	111.78	120.90
25	BA	2159	G	P-O5'-C5'	-5.97	111.94	120.90
56	CC	529	ARG	CA-CB-CG	5.91	125.92	114.10
25	BA	613	A	P-O3'-C3'	-5.85	111.42	120.20
25	BA	789	A	C5'-C4'-C3'	-5.82	106.47	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	5	U	P-O5'-C5'	5.69	129.44	120.90
25	BA	2900	A	O3'-P-O5'	5.52	112.28	104.00
25	BA	1579	A	O3'-P-O5'	-5.51	95.73	104.00
1	AA	1026	G	P-O3'-C3'	5.51	128.46	120.20
1	AA	1027	C	O3'-P-O5'	-5.49	95.76	104.00
32	BH	10	ALA	CA-C-N	-5.48	112.56	122.54
32	BH	10	ALA	C-N-CA	-5.48	112.56	122.54
27	BC	241	GLY	N-CA-C	5.38	125.94	113.18
25	BA	789	A	C4'-C3'-O3'	5.37	117.45	109.40
1	AA	1357	A	N9-C1'-C2'	5.31	119.96	112.00
1	AA	997	U	N1-C1'-C2'	5.30	119.95	112.00
50	B2	27	SER	N-CA-C	5.30	122.09	110.80
41	BS	53	PHE	N-CA-C	5.27	122.02	110.80
7	AG	54	SER	CA-C-N	-5.25	111.13	121.41
7	AG	54	SER	C-N-CA	-5.25	111.13	121.41
25	BA	2125	G	P-O5'-C5'	5.24	128.75	120.90
50	B2	16	ARG	CA-C-N	-5.21	110.87	121.18
50	B2	16	ARG	C-N-CA	-5.21	110.87	121.18
25	BA	1077	A	O4'-C1'-N9	5.17	116.26	108.50
1	AA	1025	U	P-O3'-C3'	-5.09	112.56	120.20
1	AA	843	U	C2'-C3'-O3'	5.05	117.07	109.50
25	BA	1047	G	O4'-C1'-N9	5.03	115.75	108.20
12	AL	44	LYS	N-CA-C	5.02	120.90	109.81
25	BA	1407	G	C4'-C3'-O3'	5.01	120.51	113.00

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

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Mol	Chain	Res	Type	Group
46	BX	54	GLY	Mainchain
57	CD	764	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32909	0	16575	401	0
2	AB	1765	0	1792	33	0
3	AC	1640	0	1713	51	0
4	AD	1643	0	1707	32	0
5	AE	1148	0	1195	22	0
6	AF	848	0	846	36	0
7	AG	1214	0	1267	20	0
8	AH	979	0	1031	16	0
9	AI	1031	0	1076	27	0
10	AJ	800	0	839	25	0
11	AK	877	0	887	23	0
12	AL	951	0	1012	26	0
13	AM	891	0	952	31	0
14	AN	805	0	844	17	0
15	AO	714	0	734	17	0
16	AP	649	0	666	8	0
17	AQ	648	0	691	11	0
18	AR	474	0	494	16	0
19	AS	663	0	688	19	0
20	AT	670	0	719	10	0
21	AU	590	0	629	6	0
22	AV	656	0	336	23	0
23	AW	1645	0	842	22	0
24	AX	1630	0	838	35	0
24	AZ	1630	0	839	64	0
25	BA	62248	0	31319	681	0
26	BB	2569	0	1300	32	0
27	BC	2092	0	2167	34	0
28	BD	1566	0	1618	26	0
29	BE	1552	0	1618	31	0
30	BF	1420	0	1457	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BG	1313	0	1358	24	0
32	BH	1111	0	1148	29	0
33	BK	1129	0	1162	14	0
34	BL	947	0	1023	11	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	19	0
42	BT	857	0	922	15	0
43	BU	764	0	829	17	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	15	0
51	B3	436	0	477	6	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	17	0
56	CC	10415	0	10432	175	0
57	CD	10375	0	10597	218	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2481	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 (2481) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
57:CD:1025:MET:HE1	57:CD:1195:GLN:HG3	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1916:A:H2'	25:BA:1917:PSU:C6	2.24	0.73
25:BA:2121:G:HO2'	25:BA:2168:G:H1	1.37	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
57:CD:1072:LYS:C	57:CD:1168:GLU:HG3	2.14	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
57:CD:1025:MET:HE1	57:CD:1195:GLN:CG	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
56:CC:696:ASP:CG	56:CC:697:LYS:H	2.01	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
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
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
36:BN:14:LYS:O	36:BN:71:LYS:NZ	2.28	0.67
14:AN:63:ARG:NH1	14:AN:68:GLY:O	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:AA:842:U:O2'	1:AA:846:G:O6	2.12	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
49:B1:6:LYS:NZ	49:B1:37:GLU:OE1	2.29	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
8:AH:94:LYS:HZ3	8:AH:117:ARG:HH22	1.44	0.65
25:BA:1175:A:OP2	25:BA:1176:U:O2'	2.14	0.65
57:CD:878:ASP:OD2	57:CD:991:THR:OG1	2.08	0.65
1:AA:1100:C:OP1	21:AU:69:ARG:NH1	2.30	0.65
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:AC:9:GLY:HA3	14:AN:89:MET:HE3	1.79	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
27:BC:157:SER:O	27:BC:160:THR:OG1	2.16	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
25:BA:1996:C:OP2	34:BL:31:ARG:NH2	2.33	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:464:U:O2'	1:AA:466:A:N7	2.28	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
22:AV:44:A:O2'	22:AV:45:C:OP2	2.19	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
25:BA:2244:U:H2'	25:BA:2245:U:C6	2.36	0.61
6:AF:69:GLU:HG2	6:AF:70:VAL:N	2.14	0.60
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
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
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
55:CB:27:THR:C	55:CB:28:LEU:HD22	2.26	0.60
57:CD:1072:LYS:HD3	57:CD:1169:THR:C	2.27	0.60
25:BA:2478:A:OP2	54:B6:2:LYS:NZ	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
25:BA:1326:U:HO2'	25:BA:2010:G:HO2'	1.46	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
56:CC:423:ASP:N	56:CC:423:ASP:OD1	2.34	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
25:BA:1796:U:HO2'	27:BC:254:GLY:H	1.47	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
55:CB:76:GLU:H	55:CB:76:GLU:CD	2.09	0.59
13:AM:107:ARG:HH12	13:AM:112:PRO:C	2.10	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:288:PRO:HB3	61:CF:107:GLU:CD	2.27	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
1:AA:401:C:OP2	4:AD:70:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:687:A:N1	1:AA:700:G:O2'	2.35	0.58
1:AA:866:C:C4	1:AA:867:G:H1'	2.39	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2591:C:H2'	25:BA:2592:G:C8	2.39	0.58
56:CC:12:ARG:HH21	56:CC:793:GLU:CD	2.11	0.58
56:CC:811:ASN:ND2	56:CC:1097:VAL:O	2.36	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
11:AK:92:GLY:C	11:AK:94:GLU:H	2.12	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
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
5:AE:78:ASN:N	5:AE:78:ASN:OD1	2.38	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
25:BA:782:A:C6	27:BC:225:MET:HE2	2.40	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
34:BL:1:MET:HE3	34:BL:67:LYS:HG3	1.87	0.56
25:BA:1019:U:OP1	25:BA:1035:U:O2'	2.21	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
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
5:AE:90:THR:OG1	5:AE:91:GLY:N	2.38	0.56
13:AM:17:ILE:O	13:AM:20:THR:OG1	2.20	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:893:C:HO2'	25:BA:894:U:H6	1.52	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
56:CC:605:TYR:C	56:CC:606:LEU:HD12	2.31	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
56:CC:519:ASN:C	56:CC:519:ASN:OD1	2.49	0.55
56:CC:696:ASP:CG	56:CC:697:LYS:N	2.65	0.55
1:AA:197:A:H4'	1:AA:198:G:O5'	2.07	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
2:AB:167:ASP:OD2	2:AB:191:SER:OG	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
30:BF:48:LYS:C	30:BF:52:ASN:HB2	2.31	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
1:AA:1181:G:O2'	1:AA:1182:G:N7	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
26:BB:9:G:O2'	38:BP:45:SER:OG	2.22	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
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
57:CD:1050:THR:C	57:CD:1057:SER:HB3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:AA:604:G:H2'	1:AA:605:U:O4'	2.08	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
45:BW:55:GLU:H	45:BW:55:GLU:CD	2.17	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
3:AC:134:MET:HE3	3:AC:168:TYR:CE2	2.44	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
56:CC:638:SER:OG	56:CC:639:LYS:N	2.37	0.53
57:CD:857:LEU:HD11	57:CD:871:LEU:HD21	1.90	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
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
30:BF:10:ASP:HB2	30:BF:11:GLU:CD	2.34	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
18:AR:71:THR:C	18:AR:73:ARG:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CN:18:DG:H2'	61:CF:91:GLY:N	2.24	0.53
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
57:CD:693:VAL:HG21	57:CD:743:MET:HE3	1.92	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
57:CD:227:PHE:CZ	57:CD:237:MET:HE3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:175:GLU:CD	57:CD:175:GLU:H	2.18	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:84:A:N1	25:BA:98:G:O2'	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:652:U:O4	1:AA:752:G:O2'	2.25	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
56:CC:494:ASN:C	56:CC:494:ASN:HD22	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BF:43:ALA:HB1	30:BF:50:LEU:HB2	1.92	0.51
56:CC:392:GLU:CD	56:CC:392:GLU:H	2.18	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
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
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
25:BA:1826:G:O2'	25:BA:1971:U:OP2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
24:AZ:21:A:O2'	24:AZ:46:7MG:HM73	2.11	0.50
25:BA:1315:C:O2'	25:BA:1392:A:N3	2.41	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
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:1277:C:O2'	1:AA:1278:G:O5'	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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:729:G:OP1	27:BC:10:SER:OG	2.29	0.49
25:BA:1216:G:H5''	40:BR:11:ARG:NH1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2146:C:HO2'	25:BA:2147:A:P	2.34	0.49
25:BA:2698:U:H2'	25:BA:2699:C:C6	2.48	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
1:AA:1395:C:HO2'	1:AA:1401:G:HO2'	1.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
17:AQ:17:MET:HE3	17:AQ:20:SER:HB3	1.95	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: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
17:AQ:27:ARG:HH12	17:AQ:41:THR:C	2.20	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
1:AA:72:A:C5	1:AA:73:C:C5	3.01	0.49
1:AA:1395:C:O2'	1:AA:1401:G:O2'	2.25	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:493:ILE:C	56:CC:493:ILE:HD12	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:640:C:H2'	25:BA:641:U:H6	1.79	0.48
44:BV:18:ASP:HA	44:BV:21:LYS:HZ3	1.78	0.48
56:CC:549:ASP:OD1	56:CC:550:VAL:N	2.46	0.48
57:CD:825:VAL:HG13	57:CD:825:VAL:O	2.13	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
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
30:BF:52:ASN:O	30:BF:56:ASP:HB2	2.13	0.48
32:BH:14:SER:C	32:BH:16:GLY:H	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
37:BO:42:LYS:HG2	37:BO:45:ARG:NH2	2.28	0.48
56:CC:7:GLU:C	56:CC:9:LYS:H	2.21	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
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
56:CC:766:ASN:O	56:CC:766:ASN:CG	2.56	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
6:AF:101:PRO:HD2	6:AF:102:MET:HE1	1.96	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
27:BC:132:MET:HE1	27:BC:174:LEU:HD11	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
42:BT:34:ASP:OD2	50:B2:37:LYS:NZ	2.35	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
2:AB:128:LYS:HZ2	2:AB:128:LYS:HB3	1.79	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
55:CA:102:LEU:HD23	55:CA:102:LEU:C	2.39	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
7:AG:81:GLY:C	7:AG:83:SER:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
56:CC:738:GLU:HA	56:CC:741:MET:HE2	1.96	0.47
57:CD:175:GLU:CD	57:CD:175:GLU:N	2.72	0.47
57:CD:474:LEU:HD21	58:CE:27:ALA:HB3	1.96	0.47
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:OD1	56:CC:320:ASP:N	2.48	0.47
56:CC:530:ILE:HD13	56:CC:530:ILE:HA	1.66	0.47
56:CC:1085:MET:HE2	56:CC:1085:MET:HA	1.96	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:304:ASP:C	57:CD:304:ASP:OD1	2.58	0.47
57:CD:747:MET:HE2	57:CD:775:SER:HA	1.97	0.47
57:CD:789:LYS:HE2	57:CD:789:LYS:HB3	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
25:BA:2391:G:OP2	53:B5:35:LYS:NZ	2.36	0.46
38:BP:7:ARG:HD2	38:BP:97:PHE:CZ	2.50	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
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
56:CC:1333:LEU:C	56:CC:1335:ILE:H	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1447:C:O2'	25:BA:1544:A:N3	2.43	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
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
51:B3:32:GLU:H	51:B3:32:GLU:CD	2.15	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
3:AC:134:MET:HE3	3:AC:168:TYR:HE2	1.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BF:47:LYS:O	30:BF:48:LYS:C	2.55	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
12:AL:88:LYS:NZ	12:AL:89:D2T:H6	2.31	0.46
20:AT:15:GLU:OE2	20:AT:18:ARG:NH2	2.34	0.46
24:AZ:68:C:N4	24:AZ:69:G:O6	2.48	0.46
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
27:BC:132:MET:HE2	27:BC:172:VAL:HG21	1.98	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
30:BF:26:MET:HE2	30:BF:26:MET:HA	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
57:CD:466:MET:HE3	57:CD:466:MET:HB2	1.78	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:CA:20:SER:C	55:CA:22:THR:H	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:CC:270:THR:HG1	56:CC:273:HIS:CE1	2.34	0.45
57:CD:1143:ASP:OD1	57:CD:1143:ASP:C	2.60	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
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
56:CC:1296:ASP:OD2	56:CC:1322:SER:OG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:352:C:O2'	1:AA:354:G:OP1	2.30	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:1026:G:OP1	25:BA:1134:A:O2'	2.29	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
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:141:G:N7	43:BU:1:MET:HE3	2.32	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:680:LEU:HD23	56:CC:680:LEU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:253:C:OP2	53:B5:5:LYS:NZ	2.40	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
13:AM:23:TYR:HB3	13:AM:66:GLU:CD	2.42	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
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
27:BC:165:VAL:HG11	27:BC:181:MET:HE1	2.00	0.44
32:BH:73:ASN:ND2	32:BH:142:VAL:HG21	2.31	0.44
56:CC:554:HIS:O	56:CC:555:TYR:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1028:A:N3	25:BA:2486:C:O2'	2.44	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: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
30:BF:48:LYS:O	30:BF:49:LEU:C	2.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:CC:726:TYR:CD1	56:CC:726:TYR:C	2.96	0.44
57:CD:355:ILE:HG21	57:CD:355:ILE:HD13	1.74	0.44
57:CD:424:ASN:ND2	57:CD:424:ASN:C	2.72	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
56:CC:668:ILE:HG21	56:CC:668:ILE:HD13	1.79	0.44
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
56:CC:1083:GLU:CD	56:CC:1083:GLU:H	2.26	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:798:ARG:O	57:CD:799:ARG:C	2.60	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
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
9:AI:107:ASP:CG	9:AI:109:ARG:HE	2.26	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: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
27:BC:129:THR:OG1	27:BC:191:THR:OG1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
55:CB:154:PRO:C	55:CB:156:SER:H	2.26	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
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
4:AD:147:GLU:H	4:AD:147:GLU:CD	2.23	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
9:AI:41:ARG:HH21	9:AI:41:ARG:CG	2.31	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:738:GLU:CD	56:CC:738:GLU:H	2.26	0.43
56:CC:1238:LEU:CD2	56:CC:1238:LEU:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:AH:94:LYS:HZ3	8:AH:117:ARG:NH2	2.12	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
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
56:CC:800:MET:HA	56:CC:800:MET:HE2	2.00	0.43
57:CD:1302:TYR:CD1	57:CD:1302:TYR:C	2.97	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
13:AM:49:SER:HB3	13:AM:52:GLN:CD	2.44	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
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
30:BF:40:VAL:C	30:BF:42:GLU:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:ASP:OD1	56:CC:23:ASP:N	2.47	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
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
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
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
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:925:GLU:C	57:CD:925:GLU:CD	2.87	0.43
57:CD:1072:LYS:HG2	57:CD:1168:GLU:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CD:1342:ASP:C	57:CD:1342:ASP:OD1	2.59	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:718:A:H5'	11:AK:119:ASN:CG	2.44	0.42
1:AA:1309:G:OP2	13:AM:87:ARG:NH2	2.52	0.42
14:AN:89:MET:HE3	14:AN:89:MET:HA	2.01	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:674:THR:HG1	57:CD:677:GLU:CD	2.22	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
56:CC:705:GLU:H	56:CC:705:GLU:CD	2.25	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
57:CD:603:LYS:O	57:CD:604:MET:C	2.61	0.42
57:CD:700:ASN:HD22	57:CD:700:ASN:C	2.27	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:1315:U:O2'	1:AA:1360:A:N3	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:374:LEU:HD23	57:CD:374:LEU:C	2.44	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
56:CC:316:GLU:CD	56:CC:316:GLU:H	2.26	0.42
56:CC:1286:THR:HG22	56:CC:1290:MET:HE2	2.01	0.42
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
1:AA:981:U:OP2	1:AA:982:U:O2'	2.37	0.42
2:AB:83:ALA:O	2:AB:86:SER:OG	2.24	0.42
6:AF:9:MET:O	6:AF:85:ILE:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:56:ASP:C	9:AI:57:MET:HE3	2.45	0.42
23:AW:4:G:C6	23:AW:70:G:C6	3.06	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
56:CC:392:GLU:CD	56:CC:392:GLU:N	2.77	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
55:CB:34:GLY:H	55:CB:199:ASP:CG	2.28	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: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
57:CD:1145:PHE:C	57:CD:1147:ALA:H	2.27	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
11:AK:92:GLY:C	11:AK:94:GLU:N	2.78	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
25:BA:1511:G:H2'	25:BA:1512:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:MET:HE2	56:CC:241:LEU:HA	2.02	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:430:HIS:O	57:CD:431:ARG:C	2.63	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
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
11:AK:52:PHE:C	11:AK:57:LYS:HB3	2.44	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
29:BE:152:GLU:H	29:BE:152:GLU:CD	2.24	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:281:ASP:C	56:CC:283:LYS:H	2.28	0.42
56:CC:745:GLU:HG2	56:CC:746:ALA:N	2.35	0.42
56:CC:1281:TYR:CE2	57:CD:484:MET:HE3	2.54	0.42
57:CD:336:GLY:O	57:CD:337:ARG:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1212:LEU:HD23	56:CC:1212:LEU:HA	1.59	0.41
57:CD:503:SER:OG	57:CD:504:GLN:N	2.50	0.41
57:CD:504:GLN:O	57:CD:505:ASP:C	2.62	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
9:AI:39:PHE:C	9:AI:41:ARG:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:HIS:C	56:CC:449:GLY:N	2.78	0.41
56:CC:616:ILE:HA	56:CC:652:TYR:O	2.20	0.41
57:CD:475:GLU:H	57:CD:475:GLU:CD	2.27	0.41
57:CD:953:LYS:C	57:CD:954:ASN:HD22	2.27	0.41
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
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:866:ASP:OD1	56:CC:866:ASP:C	2.62	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
57:CD:1042:ASP:C	57:CD:1044:GLN:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
33:BK:122:LEU:C	33:BK:123:LYS:HG2	2.45	0.41
50:B2:17:ARG:C	50:B2:20:ASP:H	2.28	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:88:MET:HE1	9:AI:104:VAL:HG13	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
56:CC:1214:ASP:OD1	56:CC:1214:ASP:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
57:CD:416:ILE:O	57:CD:417:ARG:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
43:BU:69:ARG:O	43:BU:70:HIS:C	2.63	0.41
44:BV:96:PHE:O	44:BV:100:SER:CA	2.63	0.41
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
5:AE:111:MET:HE2	5:AE:125:ALA:HB1	2.02	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
42:BT:34:ASP:CG	50:B2:37:LYS:HZ2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1175:G:HO2'	1:AA:1176:A:H8	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:AE:146:ASN:OD1	5:AE:146:ASN:C	2.63	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
56:CC:346:TYR:CZ	56:CC:436:ARG:HG3	2.56	0.41
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:HIS:C	56:CC:449:GLY:H	2.29	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:884:SER:OG	57:CD:885:VAL:N	2.53	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
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
56:CC:1217:THR:HG1	56:CC:1219:GLU:CD	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
56:CC:1279:GLU:CD	57:CD:1347:LEU:HD23	2.47	0.40
57:CD:361:LEU:HD23	57:CD:361:LEU:HA	1.83	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
13:AM:54:ASP:OD1	13:AM:54:ASP:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BS:40:MET:HE2	41:BS:40:MET:HB3	1.98	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:871:LEU:HD23	57:CD:871:LEU:C	2.46	0.40
57:CD:978:ARG:HD3	57:CD:1197:ASN:HD21	1.81	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
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: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
48:BZ:5:GLU:H	48:BZ:5:GLU:CD	2.22	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	224/241 (93%)	209 (93%)	14 (6%)	1 (0%)	30	64
3	AC	207/233 (89%)	193 (93%)	10 (5%)	4 (2%)	6	33
4	AD	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	24	59
5	AE	154/167 (92%)	143 (93%)	10 (6%)	1 (1%)	21	55
6	AF	102/131 (78%)	96 (94%)	6 (6%)	0	100	100
7	AG	152/156 (97%)	139 (91%)	11 (7%)	2 (1%)	9	40
8	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	50
9	AI	126/130 (97%)	110 (87%)	13 (10%)	3 (2%)	4	29
10	AJ	98/103 (95%)	89 (91%)	7 (7%)	2 (2%)	6	32
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	14	47
12	AL	119/124 (96%)	110 (92%)	7 (6%)	2 (2%)	7	35
13	AM	113/118 (96%)	108 (96%)	4 (4%)	1 (1%)	14	47
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	41
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%)	6	34
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%)	11	43
28	BD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24	59
29	BE	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
30	BF	176/179 (98%)	165 (94%)	8 (4%)	3 (2%)	7	35
31	BG	173/177 (98%)	159 (92%)	13 (8%)	1 (1%)	21	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	147/149 (99%)	128 (87%)	18 (12%)	1 (1%)	18	53
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	38
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	47
39	BQ	112/115 (97%)	104 (93%)	7 (6%)	1 (1%)	14	47
40	BR	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
41	BS	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	12	45
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%)	12	45
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	33
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%)	7	36
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%)	24	59
56	CC	1316/1342 (98%)	1201 (91%)	100 (8%)	15 (1%)	11	43
57	CD	1327/1407 (94%)	1222 (92%)	96 (7%)	9 (1%)	18	53
58	CE	49/91 (54%)	40 (82%)	8 (16%)	1 (2%)	6	32
61	CF	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
All	All	8773/9507 (92%)	8169 (93%)	540 (6%)	64 (1%)	20	53

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
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

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Mol	Chain	Res	Type
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
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%)	177 (95%)	10 (5%)	20	46
3	AC	171/190 (90%)	155 (91%)	16 (9%)	8	29
4	AD	172/173 (99%)	158 (92%)	14 (8%)	11	35
5	AE	118/126 (94%)	97 (82%)	21 (18%)	2	12
6	AF	91/112 (81%)	82 (90%)	9 (10%)	7	28
7	AG	127/129 (98%)	113 (89%)	14 (11%)	6	24
8	AH	104/105 (99%)	97 (93%)	7 (7%)	15	41
9	AI	106/107 (99%)	99 (93%)	7 (7%)	15	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	87/90 (97%)	79 (91%)	8 (9%)	8	30
11	AK	90/99 (91%)	83 (92%)	7 (8%)	11	36
12	AL	102/103 (99%)	91 (89%)	11 (11%)	6	24
13	AM	93/96 (97%)	84 (90%)	9 (10%)	8	28
14	AN	83/84 (99%)	78 (94%)	5 (6%)	17	44
15	AO	76/77 (99%)	69 (91%)	7 (9%)	8	30
16	AP	65/65 (100%)	62 (95%)	3 (5%)	24	48
17	AQ	74/78 (95%)	71 (96%)	3 (4%)	27	51
18	AR	50/65 (77%)	46 (92%)	4 (8%)	11	35
19	AS	72/79 (91%)	69 (96%)	3 (4%)	26	50
20	AT	65/66 (98%)	59 (91%)	6 (9%)	8	30
21	AU	60/61 (98%)	58 (97%)	2 (3%)	33	56
27	BC	217/218 (100%)	206 (95%)	11 (5%)	21	46
28	BD	163/163 (100%)	153 (94%)	10 (6%)	17	43
29	BE	165/165 (100%)	152 (92%)	13 (8%)	11	36
30	BF	149/150 (99%)	135 (91%)	14 (9%)	8	29
31	BG	136/138 (99%)	120 (88%)	16 (12%)	5	21
32	BH	114/114 (100%)	99 (87%)	15 (13%)	4	19
33	BK	116/116 (100%)	109 (94%)	7 (6%)	17	44
34	BL	104/104 (100%)	96 (92%)	8 (8%)	12	37
35	BM	103/103 (100%)	94 (91%)	9 (9%)	9	33
36	BN	108/108 (100%)	105 (97%)	3 (3%)	38	59
37	BO	100/103 (97%)	94 (94%)	6 (6%)	17	44
38	BP	87/87 (100%)	80 (92%)	7 (8%)	11	35
39	BQ	99/100 (99%)	87 (88%)	12 (12%)	5	21
40	BR	89/90 (99%)	85 (96%)	4 (4%)	24	49
41	BS	84/84 (100%)	79 (94%)	5 (6%)	17	44
42	BT	93/93 (100%)	89 (96%)	4 (4%)	26	49
43	BU	83/84 (99%)	77 (93%)	6 (7%)	13	39
44	BV	84/85 (99%)	76 (90%)	8 (10%)	8	29
45	BW	78/78 (100%)	75 (96%)	3 (4%)	29	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BX	58/63 (92%)	57 (98%)	1 (2%)	53	68
47	BY	67/68 (98%)	63 (94%)	4 (6%)	17	44
48	BZ	54/55 (98%)	52 (96%)	2 (4%)	30	53
49	B1	48/49 (98%)	46 (96%)	2 (4%)	26	50
50	B2	47/48 (98%)	43 (92%)	4 (8%)	10	33
51	B3	48/49 (98%)	45 (94%)	3 (6%)	16	42
52	B4	37/38 (97%)	36 (97%)	1 (3%)	39	60
53	B5	51/52 (98%)	49 (96%)	2 (4%)	28	52
54	B6	34/44 (77%)	33 (97%)	1 (3%)	37	58
55	CA	197/286 (69%)	192 (98%)	5 (2%)	42	62
55	CB	187/286 (65%)	177 (95%)	10 (5%)	20	46
56	CC	1139/1157 (98%)	1096 (96%)	43 (4%)	29	52
57	CD	1118/1168 (96%)	1094 (98%)	24 (2%)	47	65
58	CE	43/75 (57%)	41 (95%)	2 (5%)	23	48
61	CF	86/158 (54%)	86 (100%)	0	100	100
All	All	7379/7883 (94%)	6948 (94%)	431 (6%)	20	44

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	59	LYS
2	AB	64	LYS
2	AB	105	LYS
2	AB	111	ILE
2	AB	128	LYS
2	AB	129	LEU
2	AB	132	LYS
2	AB	135	LEU
2	AB	207	ILE
2	AB	220	THR
3	AC	14	ILE
3	AC	26	THR
3	AC	33	LEU
3	AC	35	SER
3	AC	107	ARG
3	AC	128	VAL
3	AC	135	LYS

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Mol	Chain	Res	Type
3	AC	136	ARG
3	AC	147	LYS
3	AC	154	SER
3	AC	161	GLU
3	AC	165	THR
3	AC	172	ARG
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
4	AD	5	LEU
4	AD	47	ARG
4	AD	50	ASP
4	AD	138	SER
4	AD	156	LYS
4	AD	164	GLN
4	AD	167	LYS
4	AD	173	VAL
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	34	THR
5	AE	39	VAL
5	AE	46	VAL
5	AE	65	GLU
5	AE	72	ILE
5	AE	78	ASN
5	AE	80	THR
5	AE	94	VAL
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

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Mol	Chain	Res	Type
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	71	ILE
6	AF	76	THR
6	AF	86	ARG
6	AF	100	SER
7	AG	6	VAL
7	AG	7	ILE
7	AG	17	LYS
7	AG	40	GLU
7	AG	60	GLU
7	AG	69	VAL
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	88	ARG
8	AH	96	MET
8	AH	107	SER
8	AH	117	ARG
8	AH	121	LEU
9	AI	3	GLU
9	AI	4	ASN
9	AI	41	ARG
9	AI	57	MET
9	AI	111	VAL
9	AI	118	LEU
9	AI	123	ARG
10	AJ	4	GLN
10	AJ	16	ARG
10	AJ	17	LEU

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Mol	Chain	Res	Type
10	AJ	18	ILE
10	AJ	24	GLU
10	AJ	36	VAL
10	AJ	37	ARG
10	AJ	96	VAL
11	AK	13	ARG
11	AK	14	LYS
11	AK	15	GLN
11	AK	76	GLU
11	AK	100	LEU
11	AK	109	ASN
11	AK	116	ILE
12	AL	4	VAL
12	AL	5	ASN
12	AL	12	ARG
12	AL	16	VAL
12	AL	24	LEU
12	AL	40	THR
12	AL	52	VAL
12	AL	55	VAL
12	AL	58	THR
12	AL	64	THR
12	AL	102	LEU
13	AM	9	ILE
13	AM	16	VAL
13	AM	59	GLU
13	AM	89	LEU
13	AM	92	ARG
13	AM	93	ARG
13	AM	101	ARG
13	AM	104	THR
13	AM	107	ARG
14	AN	10	GLU
14	AN	11	VAL
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	73	LYS

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Mol	Chain	Res	Type
15	AO	80	GLN
15	AO	83	GLU
16	AP	42	ILE
16	AP	50	THR
16	AP	77	GLU
17	AQ	22	VAL
17	AQ	53	CYS
17	AQ	75	LEU
18	AR	19	GLN
18	AR	29	LEU
18	AR	55	LEU
18	AR	71	THR
19	AS	31	LEU
19	AS	49	ILE
19	AS	64	ASP
20	AT	6	SER
20	AT	10	ARG
20	AT	24	ARG
20	AT	48	GLN
20	AT	49	LYS
20	AT	58	VAL
21	AU	4	ILE
21	AU	28	VAL
27	BC	14	ARG
27	BC	20	VAL
27	BC	54	ILE
27	BC	94	VAL
27	BC	105	LEU
27	BC	129	THR
27	BC	130	LEU
27	BC	161	TYR
27	BC	202	LEU
27	BC	203	ARG
27	BC	242	LYS
28	BD	13	ARG
28	BD	29	VAL
28	BD	32	ASN
28	BD	43	ASP
28	BD	56	LYS
28	BD	60	VAL
28	BD	86	GLU
28	BD	92	VAL

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Mol	Chain	Res	Type
28	BD	157	LYS
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	77	ILE
29	BE	88	ARG
29	BE	108	ILE
29	BE	109	LEU
29	BE	111	GLU
29	BE	122	GLU
29	BE	193	VAL
30	BF	6	ASP
30	BF	10	ASP
30	BF	47	LYS
30	BF	49	LEU
30	BF	57	LEU
30	BF	85	ILE
30	BF	89	VAL
30	BF	98	GLU
30	BF	115	ARG
30	BF	123	ASP
30	BF	133	ARG
30	BF	136	ILE
30	BF	140	GLU
30	BF	179	LYS
31	BG	6	LYS
31	BG	11	VAL
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	141	ILE
31	BG	155	GLU

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Mol	Chain	Res	Type
31	BG	168	VAL
31	BG	173	GLU
31	BG	176	LYS
32	BH	1	MET
32	BH	4	ILE
32	BH	9	VAL
32	BH	12	LEU
32	BH	48	GLU
32	BH	66	ASN
32	BH	72	ILE
32	BH	94	ILE
32	BH	101	ASP
32	BH	110	VAL
32	BH	117	LEU
32	BH	127	GLU
32	BH	129	GLU
32	BH	134	VAL
32	BH	144	VAL
33	BK	1	MET
33	BK	35	ARG
33	BK	57	LEU
33	BK	108	MET
33	BK	123	LYS
33	BK	129	GLU
33	BK	142	ILE
34	BL	17	ARG
34	BL	41	ILE
34	BL	58	LEU
34	BL	67	LYS
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	40	SER
35	BM	67	THR
35	BM	70	LYS
35	BM	84	LYS
35	BM	115	GLU
35	BM	129	LYS
35	BM	144	GLU

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Mol	Chain	Res	Type
36	BN	18	ARG
36	BN	100	LYS
36	BN	110	GLU
37	BO	2	ARG
37	BO	13	ASN
37	BO	20	MET
37	BO	51	LEU
37	BO	65	LEU
37	BO	69	ARG
38	BP	13	ARG
38	BP	18	LEU
38	BP	19	GLN
38	BP	47	VAL
38	BP	65	THR
38	BP	115	LEU
38	BP	116	GLN
39	BQ	27	GLU
39	BQ	38	LYS
39	BQ	39	ARG
39	BQ	40	LEU
39	BQ	68	GLU
39	BQ	80	VAL
39	BQ	88	ARG
39	BQ	89	ARG
39	BQ	96	LYS
39	BQ	110	ILE
39	BQ	111	LYS
39	BQ	113	ARG
40	BR	11	ARG
40	BR	51	ARG
40	BR	59	GLN
40	BR	91	ASP
41	BS	10	LYS
41	BS	20	VAL
41	BS	39	LEU
41	BS	48	LYS
41	BS	86	GLN
42	BT	11	ARG
42	BT	19	LEU
42	BT	41	LYS
42	BT	110	ARG
43	BU	1	MET

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Mol	Chain	Res	Type
43	BU	2	ILE
43	BU	12	ARG
43	BU	16	VAL
43	BU	53	VAL
43	BU	89	GLU
44	BV	7	ARG
44	BV	9	ASP
44	BV	15	THR
44	BV	43	LYS
44	BV	46	GLN
44	BV	52	LEU
44	BV	72	ILE
44	BV	101	GLU
45	BW	40	ILE
45	BW	41	GLU
45	BW	45	ASP
46	BX	70	GLU
47	BY	25	THR
47	BY	48	THR
47	BY	52	SER
47	BY	71	LEU
48	BZ	11	VAL
48	BZ	58	ASN
49	B1	8	THR
49	B1	10	THR
50	B2	12	LYS
50	B2	39	LEU
50	B2	40	ARG
50	B2	55	ILE
51	B3	5	ILE
51	B3	17	THR
51	B3	23	THR
52	B4	22	MET
53	B5	32	ILE
53	B5	55	LEU
54	B6	26	ILE
55	CA	7	GLU
55	CA	13	LEU
55	CA	74	VAL
55	CA	100	LEU
55	CA	224	LEU
55	CB	13	LEU

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Mol	Chain	Res	Type
55	CB	48	LEU
55	CB	61	ILE
55	CB	66	HIS
55	CB	72	GLU
55	CB	76	GLU
55	CB	102	LEU
55	CB	170	ARG
55	CB	174	ASP
55	CB	191	ARG
56	CC	39	ILE
56	CC	65	ASN
56	CC	150	HIS
56	CC	193	ASN
56	CC	262	TYR
56	CC	316	GLU
56	CC	369	MET
56	CC	377	THR
56	CC	494	ASN
56	CC	524	ILE
56	CC	529	ARG
56	CC	550	VAL
56	CC	562	GLU
56	CC	569	ILE
56	CC	575	LEU
56	CC	655	VAL
56	CC	736	VAL
56	CC	745	GLU
56	CC	799	ASN
56	CC	822	VAL
56	CC	830	THR
56	CC	843	THR
56	CC	856	ASN
56	CC	888	THR
56	CC	950	GLU
56	CC	955	GLN
56	CC	1002	LEU
56	CC	1005	GLU
56	CC	1022	LYS
56	CC	1050	VAL
56	CC	1076	ILE
56	CC	1083	GLU
56	CC	1108	ASN

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Mol	Chain	Res	Type
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	1336	ASN
56	CC	1340	GLU
57	CD	68	TYR
57	CD	158	GLN
57	CD	244	VAL
57	CD	317	THR
57	CD	414	GLU
57	CD	416	ILE
57	CD	418	GLU
57	CD	490	ILE
57	CD	505	ASP
57	CD	592	VAL
57	CD	680	ASN
57	CD	802	ASP
57	CD	839	VAL
57	CD	847	ASP
57	CD	856	ILE
57	CD	871	LEU
57	CD	1046	ILE
57	CD	1144	LEU
57	CD	1155	ILE
57	CD	1165	PHE
57	CD	1167	LYS
57	CD	1237	VAL
57	CD	1321	SER
57	CD	1351	VAL
58	CE	48	VAL
58	CE	53	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	39	HIS
2	AB	58	ASN

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Mol	Chain	Res	Type
3	AC	190	HIS
4	AD	36	GLN
4	AD	71	GLN
4	AD	164	GLN
5	AE	77	ASN
5	AE	135	ASN
6	AF	11	HIS
6	AF	94	HIS
7	AG	52	GLN
7	AG	97	ASN
7	AG	130	ASN
10	AJ	4	GLN
11	AK	22	HIS
12	AL	5	ASN
14	AN	4	GLN
15	AO	80	GLN
20	AT	48	GLN
27	BC	142	HIS
27	BC	143	ASN
27	BC	197	ASN
27	BC	260	ASN
28	BD	94	GLN
28	BD	148	GLN
29	BE	92	HIS
29	BE	115	GLN
29	BE	136	GLN
29	BE	165	HIS
30	BF	63	GLN
30	BF	127	ASN
31	BG	22	GLN
31	BG	104	ASN
32	BH	66	ASN
32	BH	73	ASN
33	BK	130	HIS
34	BL	9	ASN
36	BN	13	HIS
37	BO	18	GLN
39	BQ	75	GLN
39	BQ	77	HIS
40	BR	44	GLN
40	BR	66	ASN
40	BR	81	ASN

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Mol	Chain	Res	Type
41	BS	43	ASN
48	BZ	58	ASN
55	CA	160	HIS
56	CC	150	HIS
56	CC	173	ASN
56	CC	235	ASN
56	CC	673	HIS
56	CC	677	ASN
56	CC	832	HIS
56	CC	1008	GLN
56	CC	1111	GLN
57	CD	206	ASN
57	CD	294	ASN
57	CD	469	HIS
57	CD	545	HIS
57	CD	736	GLN
57	CD	861	ASN
57	CD	910	ASN
57	CD	1227	HIS
57	CD	1326	GLN
57	CD	1350	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1542 (99%)	298 (19%)	32 (2%)
22	AV	29/57 (50%)	10 (34%)	1 (3%)
23	AW	76/77 (98%)	25 (32%)	8 (10%)
24	AX	75/76 (98%)	25 (33%)	2 (2%)
24	AZ	75/76 (98%)	32 (42%)	0
25	BA	2897/2904 (99%)	555 (19%)	66 (2%)
26	BB	119/120 (99%)	12 (10%)	0
All	All	4803/4852 (98%)	957 (19%)	109 (2%)

All (957) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G

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Mol	Chain	Res	Type
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
1	AA	173	U
1	AA	181	A
1	AA	182	A

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Mol	Chain	Res	Type
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
1	AA	397	A
1	AA	406	G
1	AA	412	A

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Mol	Chain	Res	Type
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	482	A
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
1	AA	579	A
1	AA	587	G

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Mol	Chain	Res	Type
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
1	AA	960	U

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Mol	Chain	Res	Type
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
1	AA	1139	G

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Mol	Chain	Res	Type
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
1	AA	1305	G

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Mol	Chain	Res	Type
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	1364	U
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	1519	MA6
1	AA	1529	G
1	AA	1530	G

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Mol	Chain	Res	Type
22	AV	16	A
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	15	G
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	60	U
23	AW	61	C
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

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Mol	Chain	Res	Type
24	AX	19	G
24	AX	20	H2U
24	AX	21	A
24	AX	22	G
24	AX	25	C
24	AX	36	A
24	AX	37	MIA
24	AX	43	C
24	AX	46	7MG
24	AX	47	3AU
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	37	MIA
24	AZ	38	A
24	AZ	43	C
24	AZ	45	U
24	AZ	46	7MG
24	AZ	47	3AU
24	AZ	48	C
24	AZ	49	C
24	AZ	56	C
24	AZ	57	G

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
25	BA	163	C
25	BA	165	A
25	BA	181	A
25	BA	196	A
25	BA	199	A
25	BA	200	U
25	BA	215	G
25	BA	216	A
25	BA	221	A
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	310	A
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

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Mol	Chain	Res	Type
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
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	685	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

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Mol	Chain	Res	Type
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	777	G
25	BA	782	A
25	BA	783	A
25	BA	784	G
25	BA	785	G
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1128	G
25	BA	1129	A
25	BA	1130	U
25	BA	1132	U
25	BA	1134	A
25	BA	1135	C
25	BA	1142	A
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	1320	C
25	BA	1321	A
25	BA	1345	C
25	BA	1352	U
25	BA	1365	A
25	BA	1368	G
25	BA	1378	A

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Mol	Chain	Res	Type
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
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	1491	G
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

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Mol	Chain	Res	Type
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
25	BA	1613	G
25	BA	1619	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	2210	U
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

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Mol	Chain	Res	Type
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
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	2503	2MA

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
25	6MZ	BA	2030	25	22,25,26	2.54	5 (22%)	30,36,39	2.64	11 (36%)
23	H2U	AW	20	23	18,21,22	3.07	5 (27%)	21,30,33	2.28	5 (23%)
24	3AU	AZ	47	24	18,21,29	3.43	8 (44%)	26,30,43	1.64	5 (19%)
1	PSU	AA	516	1	18,21,22	1.02	1 (5%)	22,30,33	2.10	6 (27%)
25	3TD	BA	1915	25	18,22,23	4.46	10 (55%)	22,32,35	1.98	4 (18%)
1	UR3	AA	1498	1	19,22,23	2.50	6 (31%)	26,32,35	1.40	1 (3%)
24	4SU	AX	8	24	18,21,22	4.05	8 (44%)	26,30,33	2.32	5 (19%)
25	5MC	BA	1962	25	18,22,23	3.83	7 (38%)	26,32,35	1.17	1 (3%)
25	PSU	BA	2457	25	18,21,22	1.09	2 (11%)	22,30,33	2.16	6 (27%)
1	2MG	AA	1207	1,62	23,26,27	2.76	9 (39%)	32,38,41	2.93	13 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	AX	32	24	18,21,22	1.04	1 (5%)	22,30,33	1.58	3 (13%)
24	7MG	AX	46	24	22,26,27	3.79	10 (45%)	29,39,42	2.08	9 (31%)
24	PSU	AX	55	24	18,21,22	1.04	1 (5%)	22,30,33	1.82	5 (22%)
1	MA6	AA	1518	1	23,26,27	1.62	6 (26%)	34,38,41	3.94	11 (32%)
1	5MC	AA	1407	1	18,22,23	3.81	7 (38%)	26,32,35	1.02	1 (3%)
23	5MU	AW	54	23	19,22,23	1.41	5 (26%)	28,32,35	2.27	10 (35%)
25	OMG	BA	2251	25,23	23,26,27	2.49	9 (39%)	33,38,41	2.20	11 (33%)
24	H2U	AX	20	24	18,21,22	3.19	5 (27%)	21,30,33	2.00	5 (23%)
25	PSU	BA	746	25,62	18,21,22	1.02	2 (11%)	22,30,33	2.03	6 (27%)
24	4SU	AZ	8	24	18,21,22	4.17	8 (44%)	26,30,33	2.14	5 (19%)
25	OMC	BA	2498	25	19,22,23	2.84	7 (36%)	26,31,34	0.75	1 (3%)
1	2MG	AA	966	1	23,26,27	2.81	9 (39%)	32,38,41	2.94	12 (37%)
24	H2U	AX	16	24	18,21,22	3.04	5 (27%)	21,30,33	2.05	5 (23%)
24	PSU	AZ	39	24	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
1	MA6	AA	1519	1	23,26,27	1.63	5 (21%)	34,38,41	3.67	11 (32%)
1	G7M	AA	527	1	23,26,27	2.58	9 (39%)	35,39,42	2.60	12 (34%)
24	7MG	AZ	46	24	22,26,27	3.74	10 (45%)	29,39,42	1.96	8 (27%)
24	PSU	AZ	55	24	18,21,22	1.10	1 (5%)	22,30,33	1.83	4 (18%)
28	MEQ	BD	150	28	8,9,10	0.91	0	5,10,12	1.07	1 (20%)
25	PSU	BA	2604	25,62	18,21,22	1.04	3 (16%)	22,30,33	1.84	4 (18%)
24	5MU	AX	54	24	19,22,23	1.36	3 (15%)	28,32,35	2.16	8 (28%)
25	PSU	BA	955	25,62	18,21,22	1.14	2 (11%)	22,30,33	1.82	4 (18%)
24	PSU	AZ	32	24	18,21,22	1.00	1 (5%)	22,30,33	1.72	4 (18%)
25	5MU	BA	747	25	19,22,23	1.39	4 (21%)	28,32,35	2.23	6 (21%)
24	PSU	AX	39	24	18,21,22	1.01	1 (5%)	22,30,33	1.90	5 (22%)
25	2MG	BA	2445	25	23,26,27	2.81	9 (39%)	32,38,41	2.97	11 (34%)
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%)
25	PSU	BA	1911	25	18,21,22	1.07	2 (11%)	22,30,33	1.94	5 (22%)
25	PSU	BA	1917	25	18,21,22	0.99	2 (11%)	22,30,33	1.91	5 (22%)
25	PSU	BA	2504	25	18,21,22	1.10	3 (16%)	22,30,33	2.16	5 (22%)
25	OMU	BA	2552	25	19,22,23	2.90	7 (36%)	26,31,34	1.79	5 (19%)
1	2MG	AA	1516	1	23,26,27	2.75	9 (39%)	32,38,41	2.94	11 (34%)
24	3AU	AX	47	24	18,21,29	3.38	8 (44%)	26,30,43	1.67	5 (19%)
25	2MA	BA	2503	25,62	22,25,26	3.89	10 (45%)	33,37,40	2.79	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	BA	2580	25	18,21,22	1.04	3 (16%)	22,30,33	2.25	7 (31%)
1	4OC	AA	1402	1,62	20,23,24	3.35	9 (45%)	26,32,35	1.00	2 (7%)
25	1MG	BA	745	25	22,26,27	2.70	5 (22%)	33,39,42	1.78	6 (18%)
25	H2U	BA	2449	25	18,21,22	2.89	5 (27%)	21,30,33	2.31	5 (23%)
24	H2U	AZ	16	24	18,21,22	3.01	5 (27%)	21,30,33	2.01	5 (23%)
24	MIA	AX	37	24	26,29,32	2.84	5 (19%)	37,41,47	2.84	15 (40%)
25	G7M	BA	2069	25	23,26,27	2.58	9 (39%)	35,39,42	2.53	11 (31%)
23	PSU	AW	55	23	18,21,22	1.01	1 (5%)	22,30,33	1.92	6 (27%)
25	PSU	BA	2605	25,62	18,21,22	1.00	2 (11%)	22,30,33	2.03	5 (22%)
12	D2T	AL	89	12	7,9,10	1.08	0	6,11,13	2.06	2 (33%)
25	6MZ	BA	1618	25	22,25,26	2.59	5 (22%)	30,36,39	2.73	11 (36%)
24	5MU	AZ	54	24	19,22,23	1.41	6 (31%)	28,32,35	2.04	6 (21%)
36	4D4	BN	81	36	9,11,12	2.49	3 (33%)	8,13,15	0.74	0
23	OMC	AW	32	23	19,22,23	2.90	8 (42%)	26,31,34	0.79	0
25	5MU	BA	1939	25,62	19,22,23	1.44	4 (21%)	28,32,35	2.39	6 (21%)
25	2MG	BA	1835	25	23,26,27	2.85	9 (39%)	32,38,41	2.88	12 (37%)
24	MIA	AZ	37	24	26,29,32	2.80	5 (19%)	37,41,47	2.82	13 (35%)
1	5MC	AA	967	1	18,22,23	3.96	7 (38%)	26,32,35	1.13	2 (7%)

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
25	6MZ	BA	2030	25	-	2/9/27/28	0/3/3/3
23	H2U	AW	20	23	-	4/7/38/39	0/2/2/2
24	3AU	AZ	47	24	-	1/7/25/35	0/2/2/2
1	PSU	AA	516	1	-	1/7/25/26	0/2/2/2
25	3TD	BA	1915	25	-	3/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1,62	-	1/9/27/28	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	1/7/37/38	0/3/3/3
24	PSU	AX	55	24	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1518	1	-	3/11/29/30	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
25	OMG	BA	2251	25,23	-	1/9/27/28	0/3/3/3
24	H2U	AX	20	24	-	5/7/38/39	0/2/2/2
25	PSU	BA	746	25,62	-	2/7/25/26	0/2/2/2
24	4SU	AZ	8	24	-	7/7/25/26	0/2/2/2
25	OMC	BA	2498	25	-	3/9/27/28	0/2/2/2
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
24	H2U	AX	16	24	-	2/7/38/39	0/2/2/2
24	PSU	AZ	39	24	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	6/11/29/30	0/3/3/3
1	G7M	AA	527	1	-	1/7/25/26	0/3/3/3
24	7MG	AZ	46	24	-	3/7/37/38	0/3/3/3
24	PSU	AZ	55	24	-	1/7/25/26	0/2/2/2
28	MEQ	BD	150	28	-	3/8/9/11	-
25	PSU	BA	2604	25,62	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
25	PSU	BA	955	25,62	-	0/7/25/26	0/2/2/2
24	PSU	AZ	32	24	-	0/7/25/26	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
25	2MG	BA	2445	25	-	2/9/27/28	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
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
25	PSU	BA	2504	25	-	0/7/25/26	0/2/2/2
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
24	3AU	AX	47	24	-	3/7/25/35	0/2/2/2
25	2MA	BA	2503	25,62	-	2/7/25/26	0/3/3/3
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1,62	-	1/9/29/30	0/2/2/2
25	1MG	BA	745	25	-	0/7/25/26	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
24	H2U	AZ	16	24	-	3/7/38/39	0/2/2/2
24	MIA	AX	37	24	-	6/13/31/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	G7M	BA	2069	25	-	2/7/25/26	0/3/3/3
23	PSU	AW	55	23	-	3/7/25/26	0/2/2/2
25	PSU	BA	2605	25,62	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/7/12/14	-
25	6MZ	BA	1618	25	-	4/9/27/28	0/3/3/3
24	5MU	AZ	54	24	-	0/7/25/26	0/2/2/2
36	4D4	BN	81	36	-	4/11/12/14	-
23	OMC	AW	32	23	-	1/9/27/28	0/2/2/2
25	5MU	BA	1939	25,62	-	2/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/9/27/28	0/3/3/3
24	MIA	AZ	37	24	-	8/13/31/34	0/3/3/3
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2

All (330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2503	2MA	C4-N3	12.12	1.49	1.34
25	BA	1915	3TD	C6-C5	11.84	1.49	1.35
25	BA	1618	6MZ	C6-N6	10.40	1.45	1.34
24	AX	20	H2U	C2-N1	10.31	1.50	1.35
1	AA	967	5MC	C6-C5	9.94	1.50	1.34
25	BA	2030	6MZ	C6-N6	9.81	1.44	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	9.55	1.49	1.35
24	AZ	37	MIA	C13-C14	9.50	1.59	1.32
25	BA	1962	5MC	C6-C5	9.45	1.50	1.34
24	AZ	8	4SU	C4-N3	9.39	1.47	1.37
24	AZ	20	H2U	C2-N1	9.34	1.49	1.35
24	AX	16	H2U	C2-N1	9.30	1.48	1.35
24	AX	8	4SU	C4-N3	9.10	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
24	AZ	37	MIA	C6-N6	8.90	1.48	1.34
24	AX	37	MIA	C6-N6	8.85	1.48	1.34
24	AZ	46	7MG	C8-N9	8.83	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
25	BA	1835	2MG	C2-N3	8.36	1.47	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	966	2MG	C2-N3	8.32	1.47	1.31
24	AZ	46	7MG	C5-N7	8.20	1.45	1.35
25	BA	2445	2MG	C2-N3	8.17	1.47	1.31
1	AA	1516	2MG	C2-N3	8.04	1.47	1.31
1	AA	1207	2MG	C2-N3	8.00	1.47	1.31
24	AZ	8	4SU	C2-N1	7.91	1.51	1.38
25	BA	745	1MG	C2-N3	7.62	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	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	7.21	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
25	BA	2503	2MA	C6-N1	6.46	1.44	1.35
1	AA	1407	5MC	C2-N3	6.44	1.49	1.36
24	AZ	20	H2U	C2-N3	6.43	1.49	1.38
1	AA	1402	4OC	C6-C5	6.42	1.50	1.35
24	AX	47	3AU	C2-N3	6.40	1.49	1.38
23	AW	20	H2U	C2-N3	6.34	1.49	1.38
25	BA	2251	OMG	C4-N3	6.31	1.49	1.34
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	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
1	AA	527	G7M	C4-N3	5.85	1.48	1.34
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	745	1MG	C4-N3	5.79	1.48	1.34
25	BA	2069	G7M	C5-N7	-5.79	1.32	1.39
25	BA	2069	G7M	C4-N3	5.77	1.48	1.34
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	5.58	1.49	1.42
1	AA	527	G7M	C5-N7	-5.49	1.32	1.39
24	AZ	8	4SU	C4-S4	-5.48	1.58	1.68
24	AX	8	4SU	C5-C4	5.45	1.49	1.42
1	AA	966	2MG	C4-N3	5.43	1.47	1.34
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	1835	2MG	C4-N3	5.38	1.47	1.34
25	BA	745	1MG	C2-N2	5.35	1.43	1.34
25	BA	2251	OMG	C2-N3	5.32	1.46	1.33
25	BA	2251	OMG	C2-N2	5.28	1.46	1.34
25	BA	2445	2MG	C4-N3	5.27	1.46	1.34
25	BA	2552	OMU	C2-N1	5.27	1.46	1.38
1	AA	967	5MC	C4-N4	5.27	1.47	1.34
24	AZ	47	3AU	C4-N3	5.26	1.48	1.38
25	BA	1962	5MC	C4-N4	5.26	1.47	1.34
25	BA	2503	2MA	C2-N1	5.21	1.43	1.34
1	AA	1516	2MG	C4-N3	5.19	1.46	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	5.10	1.46	1.38
1	AA	1402	4OC	O2-C2	-4.96	1.14	1.23
1	AA	1207	2MG	C4-N3	4.96	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	G7M	C2-N3	4.96	1.45	1.33
1	AA	1407	5MC	C6-N1	4.93	1.46	1.38
24	AZ	16	H2U	C4-N3	4.93	1.46	1.37
25	BA	2069	G7M	C2-N3	4.92	1.45	1.33
24	AX	16	H2U	C4-N3	4.92	1.46	1.37
23	AW	32	OMC	C4-N3	4.92	1.44	1.34
24	AZ	20	H2U	C4-N3	4.88	1.45	1.37
24	AX	46	7MG	C2-N2	4.85	1.45	1.34
1	AA	1402	4OC	C4-N4	4.81	1.45	1.35
25	BA	1962	5MC	C6-N1	4.79	1.46	1.38
23	AW	20	H2U	C4-N3	4.78	1.45	1.37
23	AW	32	OMC	C4-N4	4.77	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
1	AA	967	5MC	C2-N1	4.49	1.49	1.40
24	AZ	46	7MG	C2-N2	4.49	1.44	1.34
25	BA	2449	H2U	C4-N3	4.45	1.45	1.37
24	AZ	46	7MG	C4-N9	4.43	1.42	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	4.16	1.48	1.37
25	BA	2503	2MA	C5-C6	4.16	1.52	1.41
25	BA	1915	3TD	C2-N3	4.13	1.47	1.38
25	BA	1835	2MG	O6-C6	-4.13	1.15	1.23
25	BA	2445	2MG	O6-C6	-4.09	1.15	1.23
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	1516	2MG	O6-C6	-4.02	1.15	1.23
25	BA	2552	OMU	O4-C4	-3.99	1.16	1.24
1	AA	966	2MG	C2-N1	3.94	1.43	1.36
1	AA	1402	4OC	C2-N1	3.92	1.48	1.40
1	AA	1207	2MG	C2-N1	3.91	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AZ	46	7MG	C5-C6	3.90	1.53	1.43
25	BA	2445	2MG	C5-N7	-3.89	1.31	1.39
25	BA	745	1MG	C5-N7	-3.87	1.31	1.39
25	BA	2552	OMU	C4-N3	3.82	1.45	1.38
24	AZ	46	7MG	C6-N1	3.76	1.45	1.38
1	AA	966	2MG	O6-C6	-3.74	1.16	1.23
1	AA	1516	2MG	C5-N7	-3.70	1.31	1.39
1	AA	1207	2MG	O6-C6	-3.69	1.16	1.23
25	BA	1835	2MG	C5-N7	-3.69	1.31	1.39
24	AX	46	7MG	C5-C6	3.69	1.53	1.43
1	AA	1519	MA6	C6-N6	3.62	1.47	1.36
25	BA	1835	2MG	C2-N1	3.59	1.42	1.36
25	BA	2498	OMC	C2-N1	3.57	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
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	1207	2MG	C5-N7	-3.43	1.32	1.39
1	AA	1518	MA6	C6-N6	3.42	1.46	1.36
24	AX	46	7MG	C6-N1	3.38	1.45	1.38
24	AZ	47	3AU	C6-N1	3.36	1.46	1.38
25	BA	2030	6MZ	C5-C4	-3.35	1.32	1.39
25	BA	2251	OMG	C5-N7	-3.34	1.32	1.39
1	AA	1518	MA6	C5-C4	-3.33	1.32	1.39
1	AA	527	G7M	C5-C6	3.31	1.52	1.43
25	BA	745	1MG	C5-C6	3.29	1.53	1.45
25	BA	1939	5MU	C6-N1	-3.28	1.32	1.38
25	BA	2503	2MA	C8-N7	3.27	1.37	1.31
1	AA	966	2MG	C5-N7	-3.25	1.32	1.39
24	AZ	8	4SU	C6-N1	3.23	1.45	1.38
24	AX	32	PSU	C6-C5	3.22	1.39	1.35
36	BN	81	4D4	CZ-NH2	3.20	1.45	1.32
25	BA	2552	OMU	O2-C2	-3.19	1.17	1.23
23	AW	8	4SU	O2-C2	-3.19	1.17	1.23
25	BA	1618	6MZ	C5-N7	-3.19	1.33	1.39
25	BA	2069	G7M	C5-C6	3.18	1.52	1.43
25	BA	747	5MU	C4-N3	-3.16	1.33	1.38
24	AX	8	4SU	O2-C2	-3.16	1.17	1.23
25	BA	1939	5MU	C4-N3	-3.13	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AZ	39	PSU	C6-C5	3.12	1.39	1.35
25	BA	1915	3TD	O2-C2	-3.12	1.17	1.23
25	BA	2498	OMC	O2-C2	-3.11	1.17	1.23
25	BA	2498	OMC	C6-N1	3.10	1.45	1.38
24	AX	55	PSU	C6-C5	3.10	1.38	1.35
1	AA	1519	MA6	C5-C4	-3.09	1.33	1.39
25	BA	2503	2MA	C6-N6	-3.08	1.26	1.34
24	AZ	8	4SU	O2-C2	-3.08	1.17	1.23
1	AA	1519	MA6	C8-N9	-3.06	1.32	1.37
25	BA	2503	2MA	C5-N7	-3.04	1.33	1.39
25	BA	2030	6MZ	C5-N7	-2.96	1.33	1.39
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
25	BA	1618	6MZ	C5-C4	-2.93	1.33	1.39
24	AZ	32	PSU	C6-C5	2.93	1.38	1.35
24	AX	39	PSU	C6-C5	2.92	1.38	1.35
23	AW	32	OMC	O2-C2	-2.92	1.18	1.23
25	BA	1915	3TD	C4-N3	2.92	1.46	1.40
24	AZ	47	3AU	O4-C4	-2.91	1.18	1.24
25	BA	747	5MU	C6-N1	-2.91	1.33	1.38
25	BA	1915	3TD	O4-C4	-2.91	1.17	1.23
25	BA	746	PSU	C6-C5	2.90	1.38	1.35
24	AX	54	5MU	C4-N3	-2.89	1.33	1.38
24	AX	47	3AU	O4-C4	-2.89	1.18	1.24
1	AA	1402	4OC	C6-N1	2.86	1.44	1.38
24	AX	37	MIA	C4-N9	-2.86	1.31	1.37
24	AX	37	MIA	C5-N7	-2.85	1.33	1.39
1	AA	1519	MA6	C10-N6	2.85	1.52	1.45
1	AA	516	PSU	C6-C5	2.85	1.38	1.35
25	BA	955	PSU	C6-C5	2.84	1.38	1.35
24	AZ	47	3AU	C5-C4	2.84	1.49	1.43
23	AW	55	PSU	C6-C5	2.83	1.38	1.35
24	AZ	54	5MU	C4-N3	-2.81	1.33	1.38
1	AA	527	G7M	O6-C6	-2.81	1.18	1.23
1	AA	1518	MA6	C10-N6	2.80	1.52	1.45
23	AW	54	5MU	C4-N3	-2.77	1.33	1.38
25	BA	2069	G7M	O6-C6	-2.76	1.18	1.23
1	AA	1518	MA6	C8-N9	-2.76	1.32	1.37
25	BA	2251	OMG	O6-C6	-2.73	1.18	1.23
25	BA	1911	PSU	C6-C5	2.73	1.38	1.35
25	BA	2457	PSU	C6-C5	2.70	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	47	3AU	C5-C4	2.69	1.49	1.43
24	AZ	37	MIA	C5-N7	-2.69	1.33	1.39
25	BA	2069	G7M	C4-N9	-2.68	1.31	1.38
1	AA	1207	2MG	C6-N1	2.67	1.43	1.38
25	BA	2030	6MZ	C8-N9	-2.67	1.32	1.37
24	AZ	54	5MU	C6-C5	2.66	1.39	1.34
1	AA	527	G7M	C4-N9	-2.66	1.31	1.38
25	BA	1915	3TD	C10-N3	2.65	1.51	1.47
24	AX	54	5MU	C6-N1	-2.63	1.33	1.38
24	AX	37	MIA	C5-C4	-2.60	1.34	1.39
24	AZ	37	MIA	C4-N9	-2.60	1.31	1.37
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
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
1	AA	1498	UR3	O2-C2	-2.57	1.17	1.22
1	AA	966	2MG	C6-N1	2.57	1.43	1.38
1	AA	527	G7M	C2-N1	2.56	1.44	1.37
24	AX	47	3AU	O2-C2	-2.54	1.18	1.23
1	AA	1207	2MG	C4-N9	-2.54	1.31	1.38
25	BA	2503	2MA	C8-N9	-2.53	1.33	1.37
25	BA	747	5MU	C2-N3	-2.52	1.33	1.38
24	AZ	20	H2U	O2-C2	-2.52	1.18	1.23
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
1	AA	1207	2MG	C5-C6	2.49	1.53	1.44
25	BA	2604	PSU	C6-C5	2.48	1.38	1.35
1	AA	1519	MA6	C5-N7	-2.47	1.34	1.39
25	BA	2580	PSU	C6-C5	2.46	1.38	1.35
24	AX	16	H2U	O2-C2	-2.46	1.18	1.23
23	AW	20	H2U	O2-C2	-2.45	1.18	1.23
25	BA	1835	2MG	C4-N9	-2.45	1.31	1.38
1	AA	1518	MA6	C5-N7	-2.45	1.34	1.39
24	AZ	47	3AU	O2-C2	-2.44	1.18	1.23
25	BA	2605	PSU	C6-C5	2.44	1.38	1.35
25	BA	1618	6MZ	C8-N9	-2.43	1.33	1.37
1	AA	1498	UR3	O4-C4	-2.43	1.18	1.23
25	BA	2445	2MG	C4-N9	-2.42	1.31	1.38
1	AA	1516	2MG	C4-N9	-2.40	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1962	5MC	O2-C2	-2.40	1.19	1.23
24	AX	20	H2U	O2-C2	-2.40	1.18	1.23
36	BN	81	4D4	CZ-NH1	-2.40	1.25	1.34
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	16	H2U	O4-C4	-2.36	1.18	1.23
24	AZ	54	5MU	C6-N1	-2.36	1.34	1.38
24	AX	54	5MU	C2-N3	-2.36	1.33	1.38
24	AZ	16	H2U	O2-C2	-2.35	1.18	1.23
25	BA	2251	OMG	C2-N1	2.35	1.43	1.37
23	AW	54	5MU	C4-C5	2.30	1.48	1.44
25	BA	955	PSU	C4-C5	-2.29	1.37	1.44
25	BA	1618	6MZ	C6-N1	-2.29	1.31	1.35
23	AW	54	5MU	C2-N3	-2.29	1.33	1.38
1	AA	966	2MG	C5-C6	2.29	1.52	1.44
24	AZ	37	MIA	C5-C4	-2.29	1.34	1.39
25	BA	2030	6MZ	C6-N1	-2.28	1.31	1.35
25	BA	2445	2MG	C6-N1	2.28	1.43	1.38
1	AA	966	2MG	C4-N9	-2.25	1.32	1.38
1	AA	527	G7M	C6-N1	2.25	1.43	1.38
25	BA	1835	2MG	C6-N1	2.25	1.43	1.38
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	AX	16	H2U	O4-C4	-2.22	1.18	1.23
24	AZ	54	5MU	C4-C5	2.21	1.48	1.44
25	BA	2552	OMU	C6-N1	2.21	1.43	1.38
25	BA	2251	OMG	C6-N1	2.19	1.42	1.38
25	BA	2251	OMG	C4-N9	-2.19	1.32	1.38
23	AW	32	OMC	C5-C4	2.18	1.47	1.42
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	2.14	1.38	1.34
1	AA	1516	2MG	C6-N1	2.14	1.42	1.38
25	BA	2251	OMG	C5-C6	2.14	1.52	1.44
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
1	AA	1518	MA6	C8-N7	2.09	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1516	2MG	C5-C6	2.09	1.52	1.44
25	BA	2580	PSU	C4-C5	-2.08	1.38	1.44
25	BA	1835	2MG	C5-C6	2.07	1.52	1.44
25	BA	2069	G7M	C6-N1	2.05	1.42	1.38
25	BA	2445	2MG	C5-C6	2.05	1.52	1.44
25	BA	1911	PSU	O4'-C1'	-2.04	1.41	1.43
25	BA	2604	PSU	C4-C5	-2.04	1.38	1.44
25	BA	1917	PSU	C4-C5	-2.04	1.38	1.44
25	BA	746	PSU	C4-C5	-2.03	1.38	1.44
25	BA	2605	PSU	C4-C5	-2.02	1.38	1.44
25	BA	747	5MU	C6-C5	2.01	1.37	1.34
24	AZ	54	5MU	C2-N1	2.01	1.41	1.38

All (390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	N1-C6-N6	-17.07	98.41	117.08
1	AA	1519	MA6	N1-C6-N6	-15.19	100.48	117.08
24	AZ	37	MIA	C12-C13-C14	-9.97	107.73	127.14
24	AX	37	MIA	C12-C13-C14	-9.48	108.69	127.14
1	AA	1518	MA6	C5-C6-N6	9.19	141.30	125.30
23	AW	8	4SU	C4-N3-C2	-8.72	118.87	127.34
1	AA	966	2MG	C1'-N9-C8	-8.61	102.19	126.70
25	BA	2503	2MA	C1'-N9-C8	-8.52	107.91	127.14
1	AA	1516	2MG	C1'-N9-C8	-8.44	102.68	126.70
24	AX	8	4SU	C4-N3-C2	-8.31	119.27	127.34
1	AA	1519	MA6	C5-C6-N6	8.29	139.75	125.30
25	BA	2445	2MG	C1'-N9-C8	-8.28	103.14	126.70
25	BA	2449	H2U	C4-N3-C2	-8.24	118.96	125.79
1	AA	1207	2MG	C1'-N9-C8	-8.02	103.88	126.70
25	BA	1835	2MG	C1'-N9-C8	-7.90	104.22	126.70
1	AA	1516	2MG	C1'-N9-C4	7.77	149.58	126.50
25	BA	2445	2MG	C1'-N9-C4	7.67	149.30	126.50
25	BA	2030	6MZ	C9-N6-C6	-7.57	116.35	122.87
1	AA	966	2MG	C1'-N9-C4	7.55	148.94	126.50
23	AW	20	H2U	C4-N3-C2	-7.50	119.57	125.79
1	AA	1207	2MG	C1'-N9-C4	7.34	148.32	126.50
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
25	BA	1835	2MG	C1'-N9-C4	6.93	147.10	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	20	H2U	C4-N3-C2	-6.82	120.13	125.79
25	BA	2069	G7M	C1'-N9-C8	-6.67	104.21	126.74
23	AW	8	4SU	C5-C4-N3	6.61	120.81	114.69
1	AA	527	G7M	C1'-N9-C8	-6.60	104.46	126.74
25	BA	2445	2MG	C2-N3-C4	6.56	120.17	112.04
25	BA	1618	6MZ	C5-C4-N3	-6.50	118.27	126.75
25	BA	2069	G7M	C1'-N9-C4	6.48	145.74	126.50
25	BA	2503	2MA	C4-N9-C1'	6.42	141.89	126.59
1	AA	1207	2MG	C2-N3-C4	6.37	119.94	112.04
1	AA	527	G7M	C1'-N9-C4	6.32	145.29	126.50
25	BA	1835	2MG	C2-N3-C4	6.19	119.71	112.04
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
1	AA	966	2MG	C2-N3-C4	6.08	119.58	112.04
25	BA	1618	6MZ	C9-N6-C6	-6.04	117.67	122.87
1	AA	1516	2MG	C2-N3-C4	5.97	119.44	112.04
25	BA	2503	2MA	C5-C4-N3	-5.85	120.61	127.19
25	BA	2030	6MZ	N1-C2-N3	-5.83	119.49	128.60
1	AA	527	G7M	CN7-N7-C5	5.64	133.78	126.77
25	BA	2503	2MA	N9-C8-N7	-5.62	106.22	113.91
1	AA	1519	MA6	C5-C4-N3	-5.59	119.46	126.75
24	AX	37	MIA	N3-C2-N1	-5.55	119.92	128.60
25	BA	2552	OMU	C4-N3-C2	-5.55	119.26	126.58
25	BA	745	1MG	C5-C4-N3	-5.54	119.47	128.46
25	BA	1618	6MZ	N1-C2-N3	-5.48	120.03	128.60
25	BA	747	5MU	C4-N3-C2	-5.47	120.27	127.35
23	AW	54	5MU	C4-N3-C2	-5.46	120.28	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
1	AA	1518	MA6	N1-C2-N3	-5.43	120.11	128.60
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
24	AZ	37	MIA	C5-C4-N3	-5.22	119.95	126.75
24	AZ	37	MIA	N3-C2-N1	-5.20	120.47	128.60
25	BA	2504	PSU	C4-N3-C2	-5.16	118.90	126.34
25	BA	1618	6MZ	C4-C5-C6	5.15	120.80	116.81
25	BA	2069	G7M	CN7-N7-C5	5.15	133.16	126.77
25	BA	2580	PSU	C4-N3-C2	-5.14	118.94	126.34
1	AA	1498	UR3	C4-N3-C2	-5.13	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1207	2MG	C2-N1-C6	-5.08	118.64	124.48
25	BA	2445	2MG	C2-N1-C6	-5.07	118.64	124.48
24	AZ	54	5MU	N3-C2-N1	5.07	121.62	114.89
24	AX	37	MIA	C5-C4-N3	-5.06	120.14	126.75
25	BA	2030	6MZ	N9-C8-N7	-5.06	106.99	113.91
25	BA	2251	OMG	C5-C4-N3	-5.05	120.26	128.46
24	AZ	54	5MU	C4-N3-C2	-5.05	120.82	127.35
24	AX	46	7MG	C5-C6-N1	5.03	119.85	110.99
25	BA	2580	PSU	N1-C2-N3	5.02	120.82	115.13
25	BA	2605	PSU	N1-C2-N3	5.02	120.82	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
1	AA	1516	2MG	C2-N1-C6	-4.96	118.77	124.48
25	BA	2445	2MG	C5-C4-N3	-4.96	120.41	128.46
25	BA	2457	PSU	C4-N3-C2	-4.95	119.21	126.34
25	BA	2251	OMG	C1'-N9-C8	-4.95	112.62	126.70
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	119.27	126.34
25	BA	747	5MU	C5-C4-N3	4.90	119.49	115.31
25	BA	747	5MU	N3-C2-N1	4.89	121.38	114.89
25	BA	1911	PSU	C4-N3-C2	-4.89	119.30	126.34
1	AA	1519	MA6	N1-C2-N3	-4.87	120.98	128.60
23	AW	54	5MU	N3-C2-N1	4.86	121.34	114.89
24	AX	37	MIA	C16-C14-C13	-4.85	108.63	122.65
1	AA	1516	2MG	C5-C4-N3	-4.84	120.61	128.46
25	BA	2604	PSU	C4-N3-C2	-4.84	119.37	126.34
25	BA	1835	2MG	C2-N1-C6	-4.82	118.93	124.48
24	AX	47	3AU	C4-N3-C2	-4.82	120.22	126.58
25	BA	2030	6MZ	C5-C4-N3	-4.81	120.47	126.75
24	AZ	39	PSU	C4-N3-C2	-4.80	119.42	126.34
24	AX	54	5MU	N3-C2-N1	4.80	121.26	114.89
25	BA	747	5MU	O4-C4-C5	-4.78	119.36	124.90
24	AX	39	PSU	N1-C2-N3	4.78	120.54	115.13
1	AA	1518	MA6	C5-C4-N3	-4.77	120.52	126.75
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
1	AA	1519	MA6	C4-C5-C6	4.71	121.15	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	N9-C8-N7	-4.71	107.47	113.91
25	BA	1835	2MG	C5-C4-N3	-4.70	120.84	128.46
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
1	AA	527	G7M	CN7-N7-C8	-4.66	117.65	124.84
25	BA	1917	PSU	N1-C2-N3	4.62	120.36	115.13
25	BA	1917	PSU	C4-N3-C2	-4.62	119.69	126.34
1	AA	1207	2MG	C5-C4-N3	-4.61	120.97	128.46
1	AA	966	2MG	C5-C4-N3	-4.58	121.02	128.46
24	AX	55	PSU	N1-C2-N3	4.58	120.32	115.13
24	AX	37	MIA	N9-C8-N7	-4.53	107.72	113.91
24	AZ	37	MIA	C16-C14-C13	-4.52	109.57	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	4.35	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	119.99	112.30
1	AA	966	2MG	C2-N1-C6	-4.31	119.52	124.48
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
25	BA	1618	6MZ	N3-C4-N9	4.22	134.04	127.08
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
1	AA	527	G7M	C2-N3-C4	4.18	119.74	112.30
25	BA	746	PSU	N1-C2-N3	4.17	119.86	115.13
24	AZ	37	MIA	N9-C8-N7	-4.17	108.20	113.91
25	BA	1962	5MC	C5-C6-N1	-4.17	119.05	123.34
25	BA	2069	G7M	CN7-N7-C8	-4.15	118.43	124.84
24	AZ	37	MIA	C4-C5-C6	4.14	120.02	116.81
25	BA	2503	2MA	C4-N9-C8	4.11	110.18	105.73
25	BA	1939	5MU	O4-C4-C5	-4.10	120.14	124.90
1	AA	527	G7M	C5-C6-N1	4.10	120.36	111.79
25	BA	2251	OMG	C2-N3-C4	4.10	119.60	112.30
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
1	AA	1519	MA6	N9-C8-N7	-4.07	108.34	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	8	4SU	N3-C2-N1	4.05	120.26	114.89
23	AW	55	PSU	N1-C2-N3	4.03	119.70	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
25	BA	2069	G7M	C5-C6-N1	3.96	120.07	111.79
25	BA	2503	2MA	N3-C4-N9	3.95	132.47	126.99
24	AZ	46	7MG	C2-N3-C4	3.94	119.32	112.30
25	BA	1618	6MZ	C2-N3-C4	3.89	120.95	111.75
25	BA	745	1MG	N9-C4-N3	3.89	133.76	125.94
25	BA	2069	G7M	C2-N3-C4	3.87	119.20	112.30
25	BA	2251	OMG	N9-C8-N7	-3.85	106.13	113.39
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
1	AA	1519	MA6	N3-C4-N9	3.79	133.34	127.08
1	AA	527	G7M	O6-C6-C5	-3.79	119.51	128.06
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
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
25	BA	2069	G7M	O6-C6-C5	-3.73	119.64	128.06
24	AZ	47	3AU	N3-C2-N1	3.71	119.82	114.89
24	AZ	54	5MU	O4-C4-C5	-3.70	120.62	124.90
24	AZ	46	7MG	C5-C4-N9	3.70	111.14	106.35
25	BA	1618	6MZ	N9-C8-N7	-3.67	108.89	113.91
24	AZ	54	5MU	C5-C6-N1	-3.66	119.57	123.34
25	BA	2251	OMG	N9-C4-N3	3.64	133.24	125.94
1	AA	1518	MA6	C4-C5-C6	3.59	119.90	115.88
24	AX	37	MIA	C4-C5-C6	3.59	119.59	116.81
1	AA	967	5MC	C5-C6-N1	-3.58	119.65	123.34
25	BA	745	1MG	C2-N3-C4	3.56	119.97	111.98
24	AX	37	MIA	C2-N3-C4	3.53	120.10	111.75
25	BA	2069	G7M	C5-C4-N3	-3.52	121.41	128.15
25	BA	2251	OMG	C1'-N9-C4	3.50	136.91	126.50
25	BA	2251	OMG	C2-N1-C6	-3.48	118.75	125.10
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	2030	6MZ	C2-N3-C4	3.47	119.94	111.75
1	AA	527	G7M	C5-C4-N3	-3.45	121.53	128.15
25	BA	2503	2MA	C5-N7-C8	3.44	108.39	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AZ	47	3AU	C5-C4-N3	3.44	119.98	114.84
25	BA	2552	OMU	C5-C4-N3	3.43	119.97	114.84
24	AX	16	H2U	N3-C2-N1	3.42	120.27	116.65
24	AX	54	5MU	C5-C6-N1	-3.42	119.82	123.34
1	AA	1518	MA6	C2-N1-C6	3.40	119.78	111.75
25	BA	1835	2MG	N9-C8-N7	-3.39	107.00	113.39
1	AA	966	2MG	N9-C8-N7	-3.36	107.07	113.39
25	BA	1917	PSU	O2-C2-N1	-3.34	119.11	122.79
24	AZ	37	MIA	C2-N3-C4	3.34	119.64	111.75
25	BA	2030	6MZ	C4-C5-C6	3.32	119.38	116.81
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
25	BA	2030	6MZ	C5-N7-C8	3.30	108.19	103.51
25	BA	2449	H2U	C5-C4-N3	3.28	120.33	116.65
24	AZ	20	H2U	N3-C2-N1	3.27	120.11	116.65
1	AA	1519	MA6	C2-N3-C4	3.26	119.44	111.75
1	AA	1518	MA6	C2-N3-C4	3.24	119.41	111.75
1	AA	516	PSU	O4'-C1'-C2'	3.23	109.70	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
25	BA	2069	G7M	C2-N1-C6	-3.17	119.31	125.10
24	AZ	46	7MG	C5-C4-N3	-3.16	122.11	128.13
24	AX	37	MIA	C5-N7-C8	3.15	107.98	103.51
1	AA	1207	2MG	N9-C8-N7	-3.15	107.47	113.39
1	AA	1519	MA6	C2-N1-C6	3.15	119.18	111.75
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	2445	2MG	C5-C6-N1	3.10	121.07	113.19
24	AZ	37	MIA	N3-C4-N9	3.10	132.20	127.08
1	AA	527	G7M	C2-N1-C6	-3.10	119.45	125.10
25	BA	2449	H2U	O2-C2-N1	-3.10	119.22	123.11
25	BA	1911	PSU	O2-C2-N1	-3.09	119.39	122.79
25	BA	2504	PSU	C6-C5-C4	3.05	120.33	118.20
12	AL	89	D2T	OD2-CG-CB	3.05	119.73	113.15
25	BA	2030	6MZ	C4-N9-C8	3.05	109.03	105.73
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	1835	2MG	C5-C6-N1	3.03	120.88	113.19
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
1	AA	1518	MA6	N3-C4-N9	3.01	132.05	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	745	1MG	N9-C8-N7	-3.00	107.74	113.39
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
24	AX	37	MIA	N3-C4-N9	2.93	131.91	127.08
25	BA	2457	PSU	O2-C2-N1	-2.92	119.57	122.79
24	AZ	8	4SU	C5-C4-S4	-2.92	120.71	124.47
1	AA	1518	MA6	C5-N7-C8	2.91	107.65	103.51
24	AZ	46	7MG	O6-C6-C5	-2.91	120.39	127.54
25	BA	2251	OMG	C5-C6-N1	2.91	120.59	113.19
25	BA	2580	PSU	O2-C2-N1	-2.91	119.58	122.79
24	AX	46	7MG	O6-C6-C5	-2.90	120.42	127.54
24	AZ	37	MIA	C5-N7-C8	2.89	107.61	103.51
25	BA	2030	6MZ	N3-C4-N9	2.88	131.84	127.08
1	AA	1518	MA6	C4-N9-C8	2.88	108.84	105.73
1	AA	1516	2MG	N9-C8-N7	-2.87	107.98	113.39
24	AX	47	3AU	O4-C4-C5	-2.87	120.11	125.16
1	AA	1516	2MG	C5-C6-N1	2.85	120.43	113.19
24	AX	16	H2U	C5-C4-N3	2.85	119.85	116.65
25	BA	2580	PSU	O4'-C1'-C2'	2.85	109.16	105.14
25	BA	1618	6MZ	C5-N7-C8	2.84	107.55	103.51
24	AX	20	H2U	C5-C4-N3	2.83	119.83	116.65
25	BA	2552	OMU	O4-C4-C5	-2.83	120.19	125.16
12	AL	89	D2T	CB1-SB-CB	2.82	107.54	102.44
25	BA	2445	2MG	N9-C8-N7	-2.80	108.11	113.39
24	AX	46	7MG	C5-C4-N9	2.80	109.98	106.35
24	AZ	32	PSU	O2-C2-N1	-2.80	119.71	122.79
25	BA	1917	PSU	C6-N1-C2	-2.79	119.83	122.68
25	BA	2503	2MA	N3-C2-N1	-2.79	120.58	125.72
25	BA	2445	2MG	O6-C6-C5	-2.79	119.20	126.60
1	AA	1207	2MG	C5-C6-N1	2.76	120.20	113.19
24	AX	20	H2U	C5-C6-N1	2.76	120.70	111.61
24	AZ	20	H2U	C5-C4-N3	2.76	119.74	116.65
24	AX	16	H2U	C5-C6-N1	2.75	120.69	111.61
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
25	BA	1618	6MZ	C1'-N9-C8	-2.74	120.96	127.14
1	AA	516	PSU	O2-C2-N1	-2.71	119.80	122.79
1	AA	527	G7M	N9-C4-N3	2.71	131.37	125.94
25	BA	2069	G7M	N9-C4-N3	2.70	131.36	125.94
23	AW	20	H2U	C5-C4-N3	2.69	119.67	116.65
24	AZ	46	7MG	N2-C2-N1	2.69	122.44	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	966	2MG	C5-C6-N1	2.68	120.00	113.19
25	BA	2251	OMG	O6-C6-C5	-2.67	119.52	126.60
1	AA	1519	MA6	C5-N7-C8	2.67	107.30	103.51
1	AA	1516	2MG	O6-C6-C5	-2.67	119.53	126.60
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
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	2.59	120.16	111.61
25	BA	2457	PSU	C6-C5-C4	2.59	120.01	118.20
25	BA	1835	2MG	O6-C6-C5	-2.59	119.72	126.60
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
23	AW	55	PSU	O2-C2-N1	-2.56	119.97	122.79
25	BA	2604	PSU	O2-C2-N1	-2.56	119.97	122.79
25	BA	2605	PSU	C6-N1-C2	-2.56	120.07	122.68
24	AZ	16	H2U	O2-C2-N1	-2.56	119.89	123.11
23	AW	20	H2U	O2-C2-N1	-2.55	119.90	123.11
24	AZ	20	H2U	C5-C6-N1	2.53	119.97	111.61
24	AX	55	PSU	O2-C2-N1	-2.53	120.00	122.79
25	BA	2445	2MG	N9-C4-N3	2.53	131.01	125.94
1	AA	966	2MG	N9-C4-N3	2.50	130.97	125.94
1	AA	966	2MG	O6-C6-C5	-2.50	119.98	126.60
24	AX	16	H2U	O2-C2-N1	-2.49	119.98	123.11
1	AA	527	G7M	N9-C8-N7	-2.49	106.06	112.21
25	BA	1835	2MG	N1-C2-N3	-2.48	120.12	123.95
25	BA	2445	2MG	N1-C2-N3	-2.46	120.14	123.95
1	AA	1519	MA6	C4-N9-C8	2.46	108.39	105.73
25	BA	2069	G7M	N9-C8-N7	-2.46	106.12	112.21
25	BA	2457	PSU	O4'-C1'-C2'	2.46	108.61	105.14
1	AA	966	2MG	N1-C2-N3	-2.45	120.16	123.95
24	AX	20	H2U	O2-C2-N3	-2.45	116.94	121.50
25	BA	746	PSU	C3'-C2'-C1'	2.45	104.48	101.64
25	BA	1835	2MG	N9-C4-N3	2.45	130.85	125.94
25	BA	745	1MG	C5-C6-N1	2.43	119.60	114.91
25	BA	2449	H2U	C5-C6-N1	2.42	119.60	111.61
24	AX	39	PSU	C6-C5-C4	2.42	119.89	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1516	2MG	N9-C4-N3	2.42	130.79	125.94
24	AZ	46	7MG	C4-C5-N7	2.41	108.88	105.53
1	AA	1207	2MG	O6-C6-C5	-2.41	120.21	126.60
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	AX	39	PSU	O2-C2-N1	-2.39	120.16	122.79
24	AZ	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	1618	6MZ	C5-C6-N1	2.39	120.75	118.20
25	BA	2445	2MG	CM2-N2-C2	-2.37	118.62	123.86
25	BA	1911	PSU	C6-C5-C4	2.37	119.86	118.20
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	-2.35	120.28	122.68
24	AX	54	5MU	O2-C2-N1	-2.35	119.66	122.79
24	AZ	20	H2U	O2-C2-N1	-2.34	120.17	123.11
24	AX	47	3AU	O2-C2-N1	-2.34	119.68	122.79
24	AX	37	MIA	C4-N9-C8	2.33	108.26	105.73
1	AA	1207	2MG	C4-C5-N7	-2.32	107.04	110.72
25	BA	747	5MU	O2-C2-N1	-2.32	119.70	122.79
23	AW	54	5MU	O2-C2-N1	-2.31	119.71	122.79
25	BA	2251	OMG	C8-N9-C4	2.31	110.45	106.05
25	BA	2030	6MZ	C5-C6-N1	2.31	120.67	118.20
25	BA	2251	OMG	C8-N7-C5	2.31	108.42	104.24
1	AA	1402	4OC	CM4-N4-C4	-2.30	117.95	122.45
1	AA	967	5MC	CM5-C5-C6	-2.28	119.80	122.85
24	AX	37	MIA	C5-C6-N1	2.27	120.62	118.20
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
25	BA	2498	OMC	O3'-C3'-C2'	2.25	117.55	111.17
25	BA	1835	2MG	C8-N7-C5	2.24	108.30	104.24
1	AA	1207	2MG	C8-N7-C5	2.23	108.28	104.24
23	AW	55	PSU	C6-N1-C2	-2.23	120.41	122.68
1	AA	966	2MG	C8-N7-C5	2.22	108.26	104.24
25	BA	2552	OMU	O2-C2-N1	-2.22	119.83	122.79
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
24	AZ	37	MIA	C5-C6-N1	2.19	120.54	118.20
25	BA	1618	6MZ	C4-N9-C1'	2.18	131.78	126.59
1	AA	516	PSU	C6-N1-C2	-2.16	120.47	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AZ	32	PSU	C6-N1-C2	-2.15	120.48	122.68
24	AZ	8	4SU	C1'-N1-C2	2.15	121.46	117.57
25	BA	1835	2MG	CM2-N2-C2	-2.15	119.12	123.86
25	BA	2605	PSU	O4'-C1'-C2'	2.14	108.16	105.14
23	AW	54	5MU	C5M-C5-C6	-2.14	119.99	122.85
24	AZ	37	MIA	C1'-N9-C8	-2.14	122.31	127.14
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	N1-C2-N3	-2.11	120.68	123.95
24	AX	55	PSU	C6-C5-C4	2.11	119.67	118.20
25	BA	745	1MG	C1'-N9-C4	-2.11	120.23	126.50
24	AZ	39	PSU	C6-N1-C2	-2.11	120.53	122.68
25	BA	2580	PSU	C6-N1-C2	-2.11	120.53	122.68
24	AZ	37	MIA	C16-C14-C15	-2.10	109.97	114.60
1	AA	1207	2MG	C5-C4-N9	2.08	109.41	105.63
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	37	MIA	C4-C5-N7	-2.07	108.09	110.62
25	BA	2030	6MZ	C4-C5-N7	-2.07	108.09	110.62
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	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	1516	2MG	N1-C2-N3	-2.01	120.84	123.95
24	AX	37	MIA	C16-C14-C15	-2.00	110.18	114.60

There are no chirality outliers.

All (111) 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
1	AA	1519	MA6	C5-C6-N6-C10
12	AL	89	D2T	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
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	C2'-C1'-N9-C4
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'
24	AZ	46	7MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
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
25	BA	1618	6MZ	C2'-C1'-N9-C8
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
24	AX	37	MIA	N1-C6-N6-C12
25	BA	2445	2MG	C3'-C4'-C5'-O5'
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
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	1518	MA6	C5-C6-N6-C9
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.

37 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	BA	2030	6MZ	1	0
23	AW	20	H2U	3	0
1	AA	516	PSU	1	0
25	BA	1915	3TD	3	0
1	AA	1207	2MG	2	0
24	AX	46	7MG	3	0
24	AX	55	PSU	1	0
25	BA	2251	OMG	1	0
24	AX	20	H2U	4	0
24	AZ	8	4SU	1	0
25	BA	2498	OMC	1	0
1	AA	966	2MG	2	0
1	AA	1519	MA6	1	0
1	AA	527	G7M	1	0
24	AZ	46	7MG	9	0
24	AZ	55	PSU	1	0
28	BD	150	MEQ	1	0
25	BA	2604	PSU	1	0
24	AX	54	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AZ	32	PSU	1	0
24	AX	39	PSU	1	0
24	AZ	20	H2U	3	0
25	BA	1917	PSU	2	0
25	BA	2552	OMU	1	0
1	AA	1516	2MG	1	0
25	BA	2449	H2U	1	0
24	AZ	16	H2U	2	0
24	AX	37	MIA	1	0
25	BA	2069	G7M	1	0
23	AW	55	PSU	1	0
25	BA	2605	PSU	2	0
12	AL	89	D2T	2	0
25	BA	1618	6MZ	3	0
36	BN	81	4D4	1	0
23	AW	32	OMC	1	0
24	AZ	37	MIA	3	0
1	AA	967	5MC	2	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

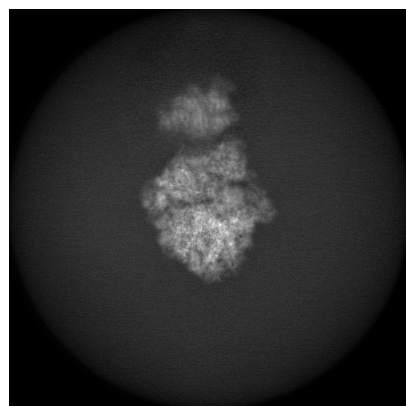
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11421. These allow visual inspection of the internal detail of the map and identification of artifacts.

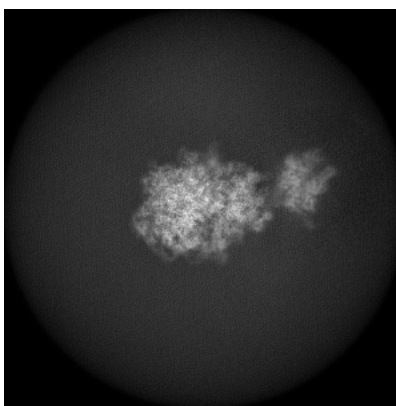
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

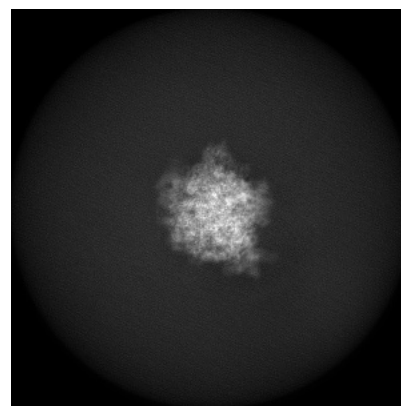
6.1.1 Primary map



X

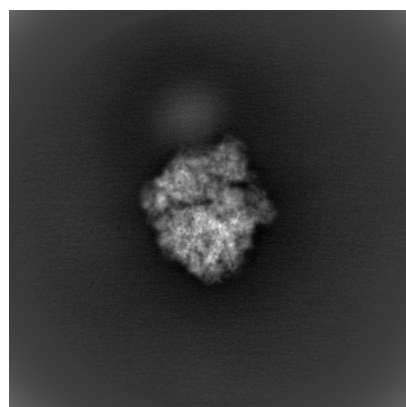


Y

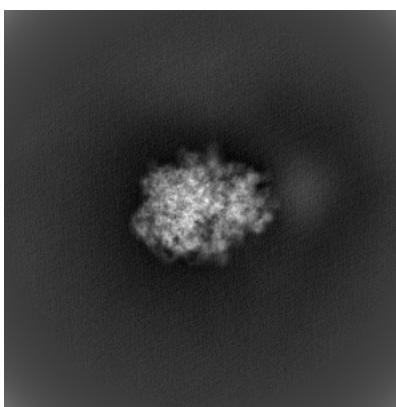


Z

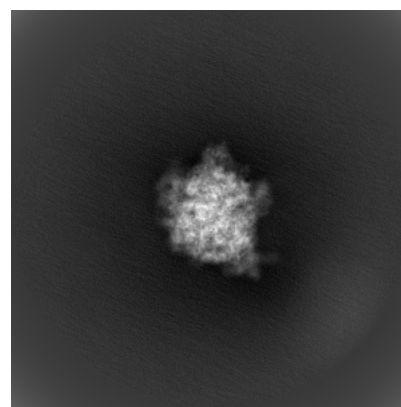
6.1.2 Raw map



X



Y

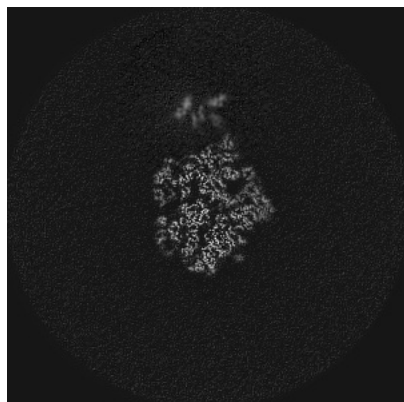


Z

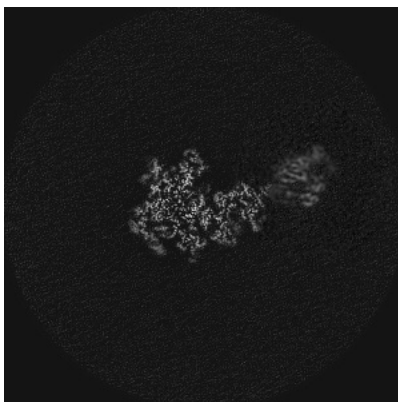
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

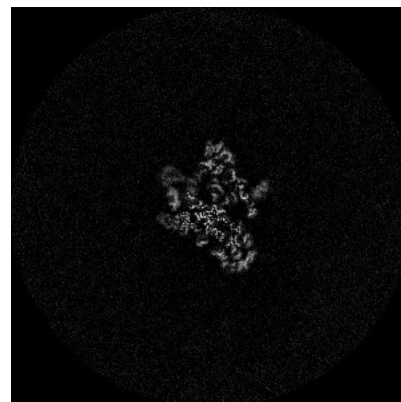
6.2.1 Primary map



X Index: 208

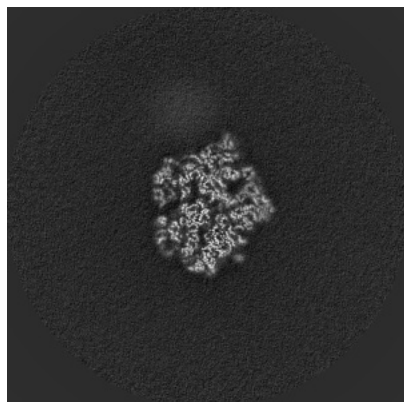


Y Index: 208

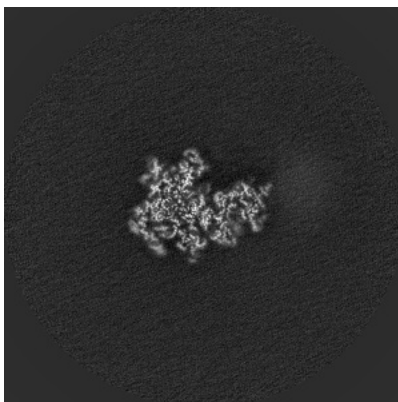


Z Index: 208

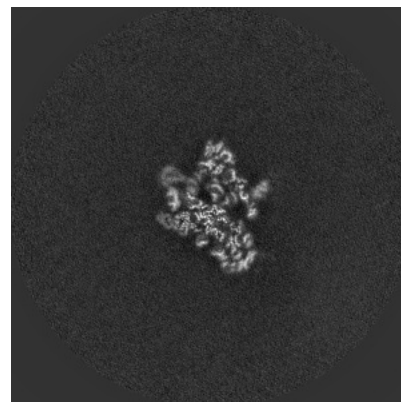
6.2.2 Raw map



X Index: 208



Y Index: 208

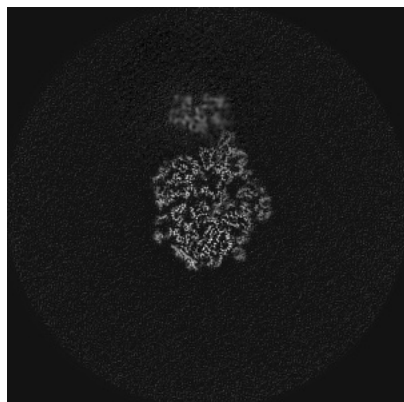


Z Index: 208

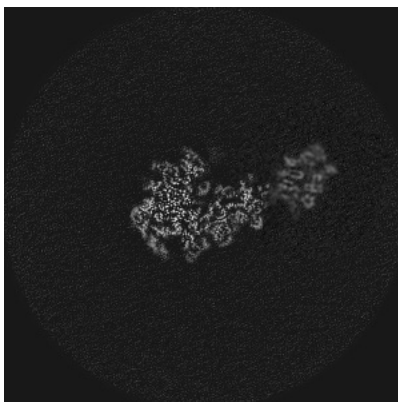
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

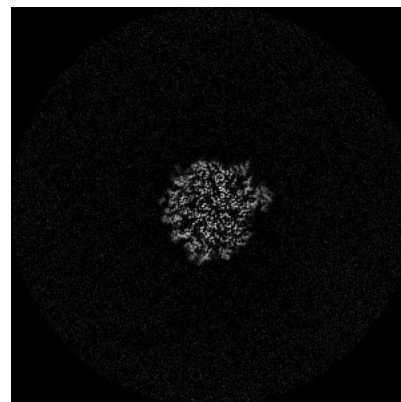
6.3.1 Primary map



X Index: 213

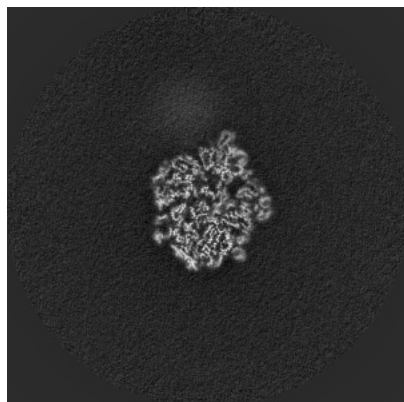


Y Index: 212

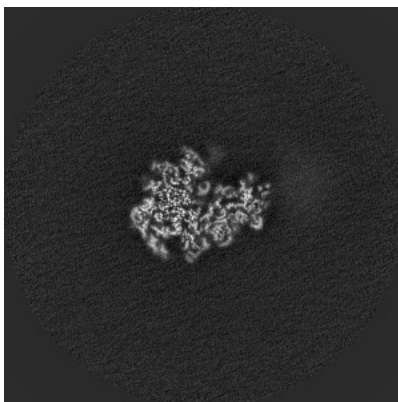


Z Index: 189

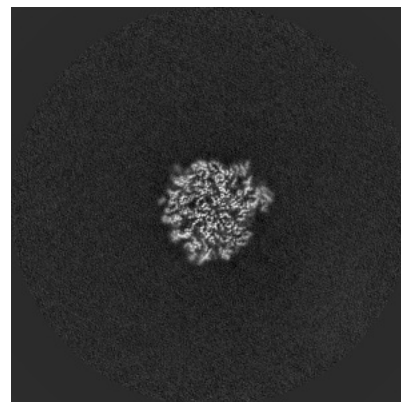
6.3.2 Raw map



X Index: 213



Y Index: 212

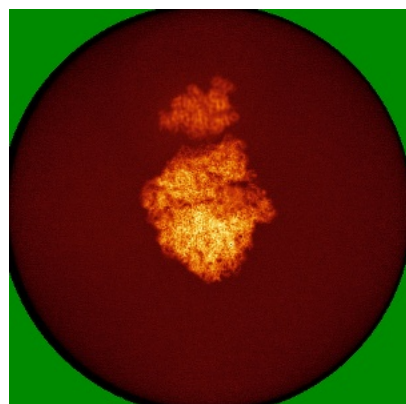


Z Index: 189

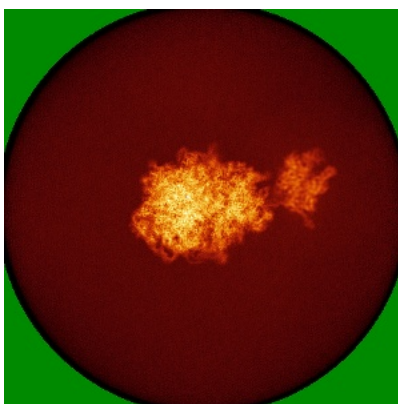
The images above show the largest variance slices of the map in three orthogonal directions.

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

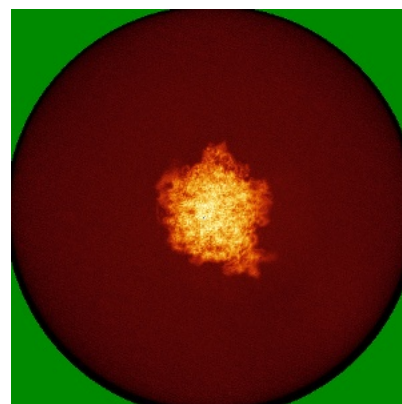
6.4.1 Primary map



X

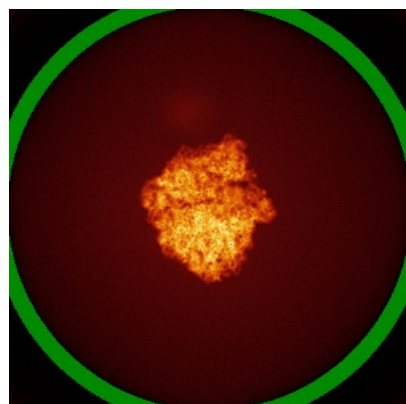


Y

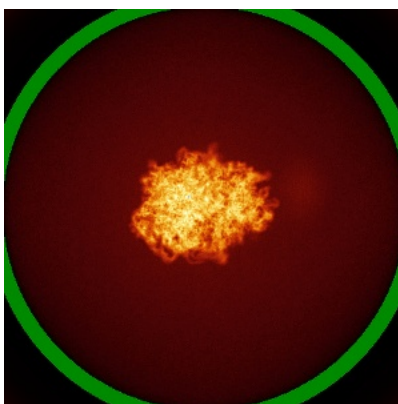


Z

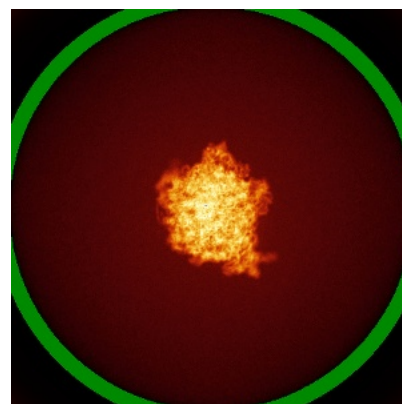
6.4.2 Raw map



X



Y

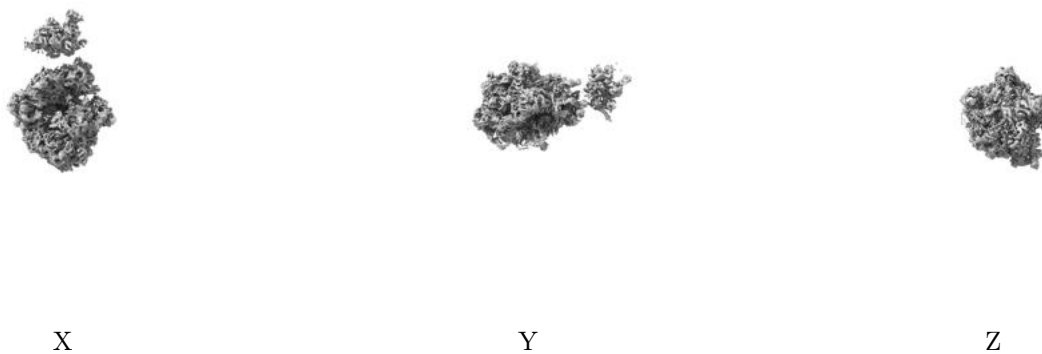


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

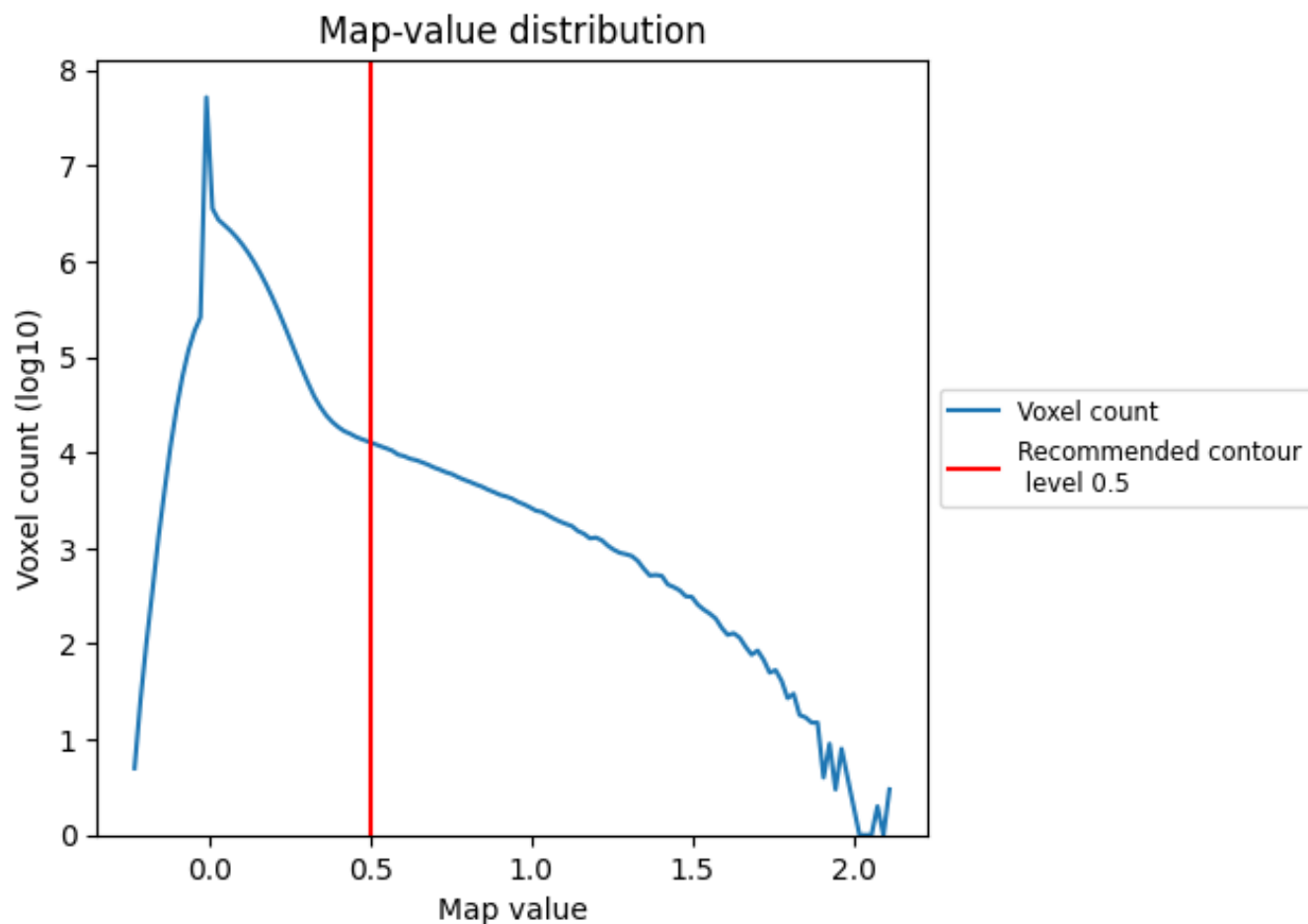
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

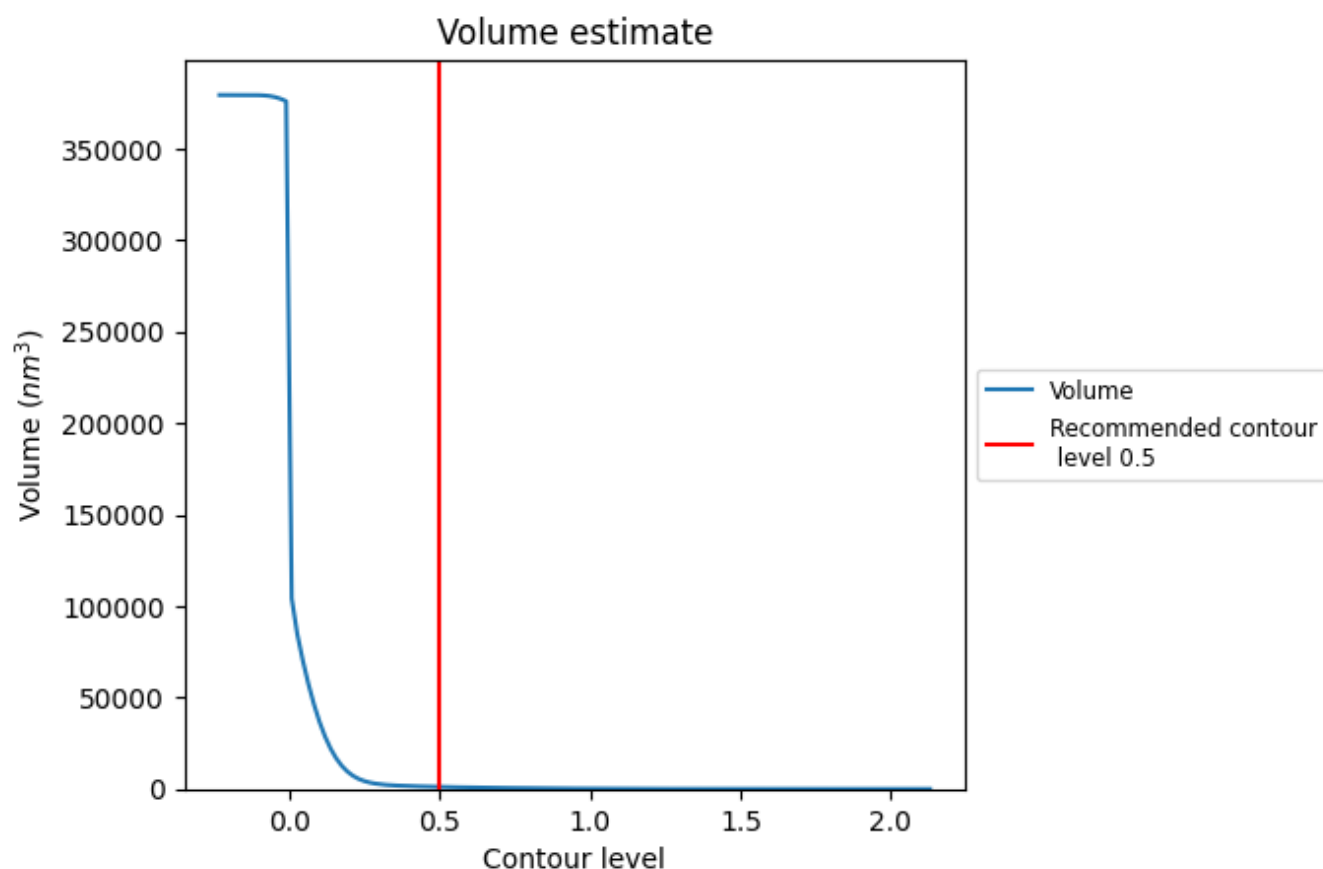
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

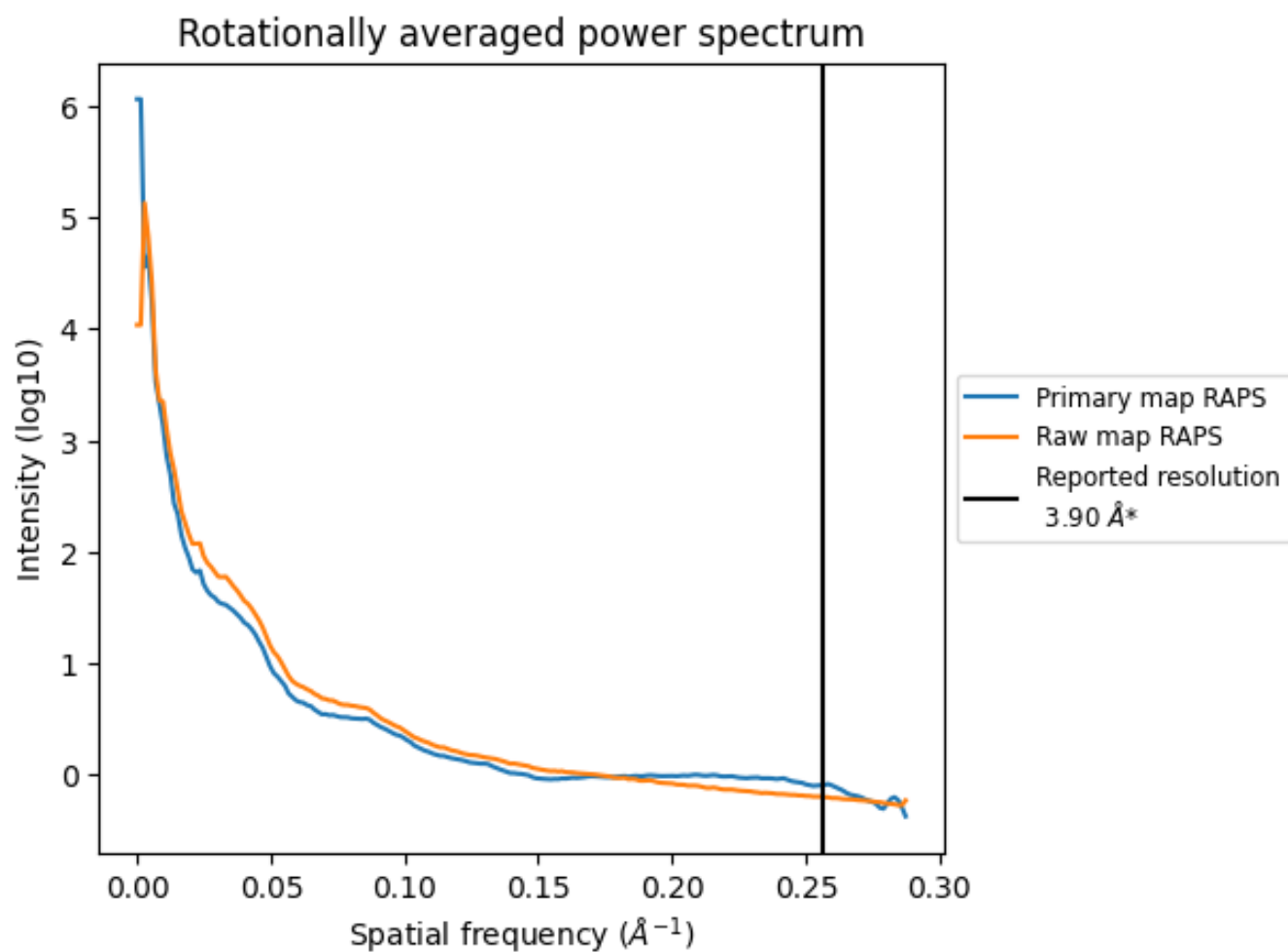
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1135 nm^3 ; this corresponds to an approximate mass of 1025 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

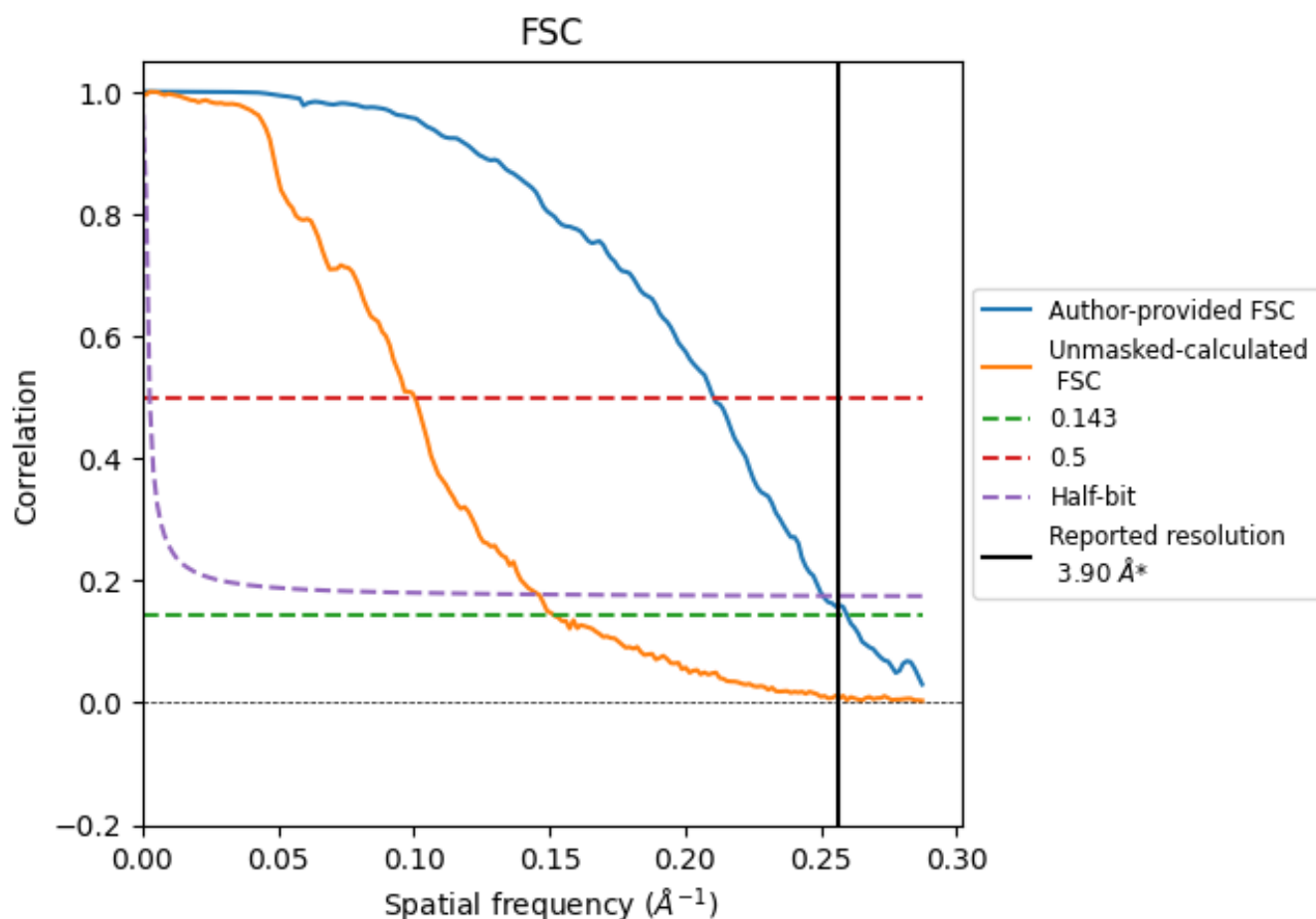


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

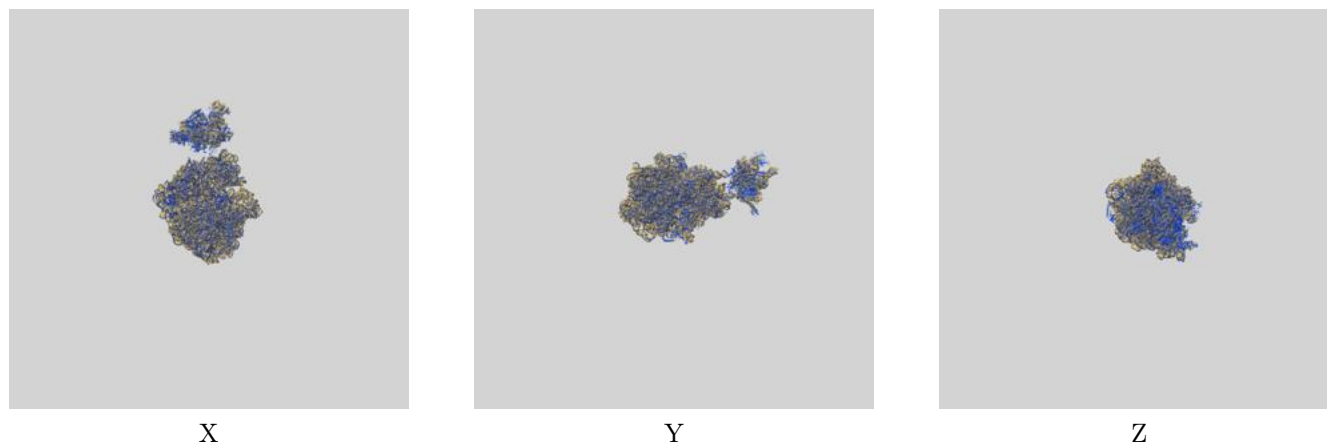
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	4.75	3.99
Unmasked-calculated*	6.59	9.97	6.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.59 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

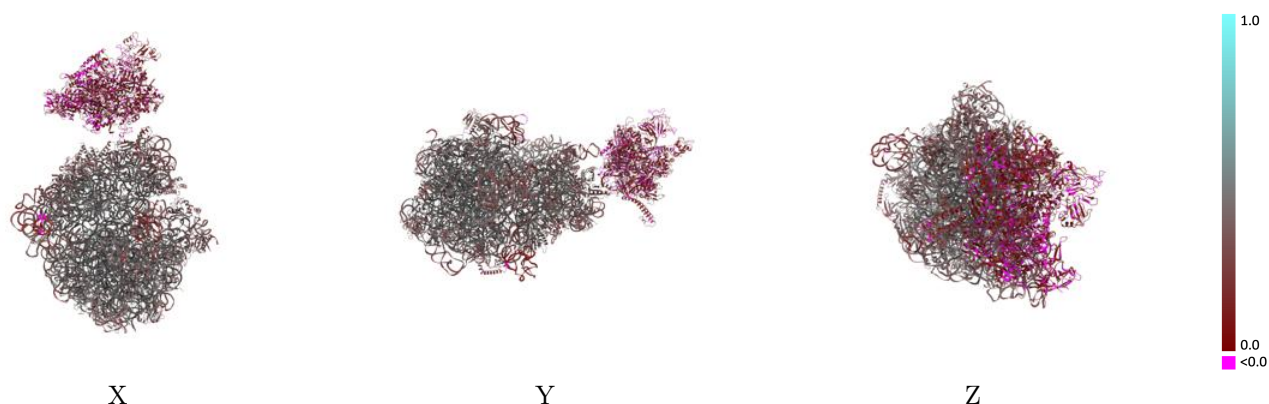
This section contains information regarding the fit between EMDB map EMD-11421 and PDB model 6ZTN. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



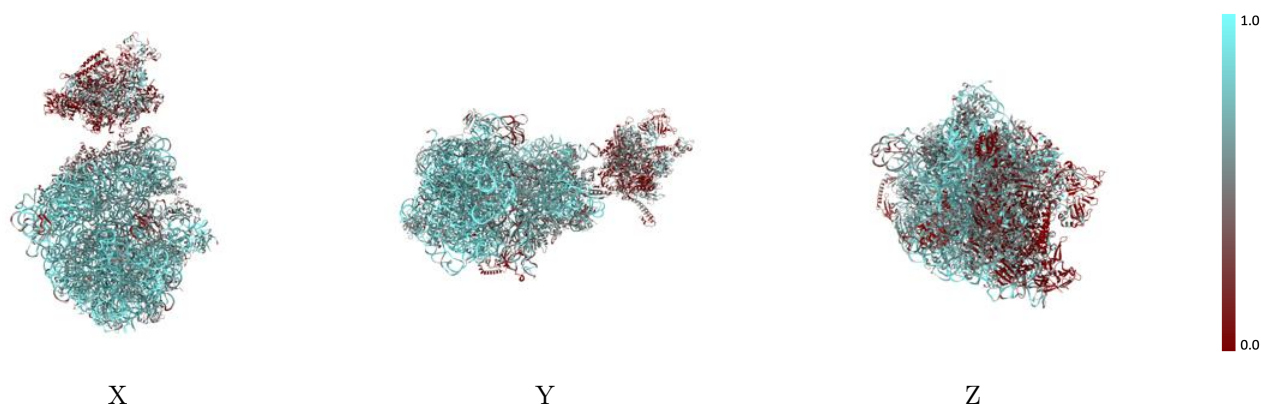
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



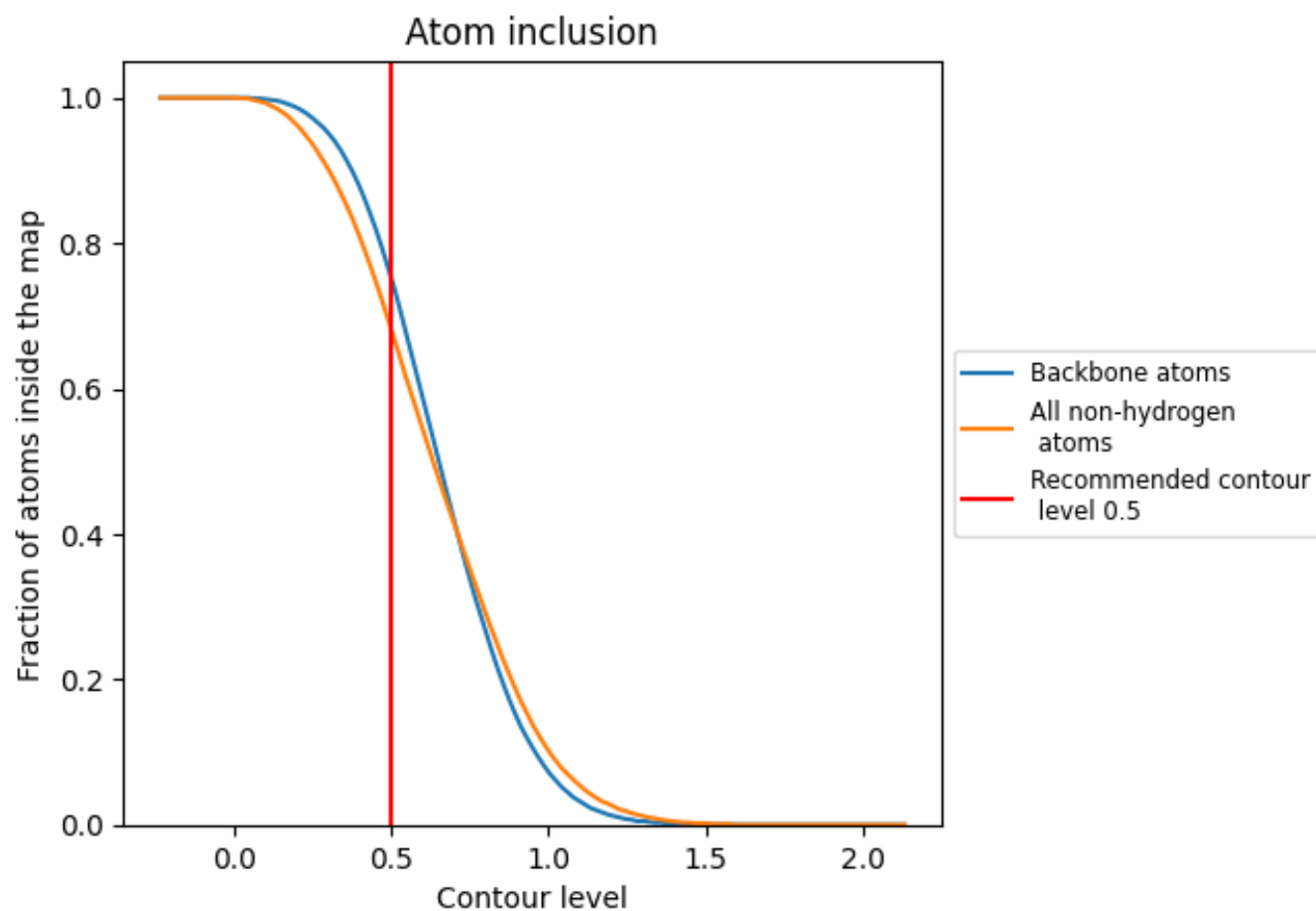
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.3650
AA	 0.8470	 0.4080
AB	 0.2730	 0.3290
AC	 0.5320	 0.3950
AD	 0.3870	 0.3460
AE	 0.6090	 0.4190
AF	 0.5830	 0.3670
AG	 0.4890	 0.3630
AH	 0.5800	 0.4030
AI	 0.5250	 0.3630
AJ	 0.4390	 0.3530
AK	 0.6030	 0.4100
AL	 0.6070	 0.4430
AM	 0.5320	 0.3430
AN	 0.5620	 0.3830
AO	 0.6220	 0.3940
AP	 0.5180	 0.3680
AQ	 0.5470	 0.3970
AR	 0.5650	 0.3970
AS	 0.5530	 0.3750
AT	 0.5580	 0.3550
AU	 0.3550	 0.3510
AV	 0.4720	 0.3150
AW	 0.7390	 0.3920
AX	 0.6280	 0.4120
AZ	 0.4890	 0.3280
B1	 0.5970	 0.4170
B2	 0.6200	 0.4190
B3	 0.3620	 0.3820
B4	 0.7060	 0.4710
B5	 0.6750	 0.4810
B6	 0.6130	 0.4240
BA	 0.8590	 0.4250
BB	 0.8510	 0.3850
BC	 0.6750	 0.4590



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Chain	Atom inclusion	Q-score
BD	 0.6360	 0.4340
BE	 0.5800	 0.3970
BF	 0.4790	 0.3350
BG	 0.4920	 0.3580
BH	 0.1370	 0.2820
BK	 0.6280	 0.4240
BL	 0.5920	 0.4300
BM	 0.6140	 0.4270
BN	 0.6330	 0.4460
BO	 0.6550	 0.4230
BP	 0.5700	 0.3570
BQ	 0.5890	 0.4150
BR	 0.6980	 0.4350
BS	 0.6000	 0.4120
BT	 0.6160	 0.4220
BU	 0.5320	 0.3930
BV	 0.5510	 0.3920
BW	 0.5540	 0.3860
BX	 0.6330	 0.4390
BY	 0.6410	 0.4390
BZ	 0.5930	 0.3550
CA	 0.2260	 0.1180
CB	 0.0770	 0.0990
CC	 0.3520	 0.1340
CD	 0.2460	 0.1130
CE	 0.0000	 -0.0180
CF	 0.0250	 0.1160
CN	 0.4850	 0.1970
CT	 0.5590	 0.2000