



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 03:38 PM EDT

PDB ID : 9P7X / pdb_00009p7x
EMDB ID : EMD-71356
Title : In situ human A-P-Z state 80S ribosome
Authors : Zheng, W.; Xiong, Y.
Deposited on : 2025-06-22
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

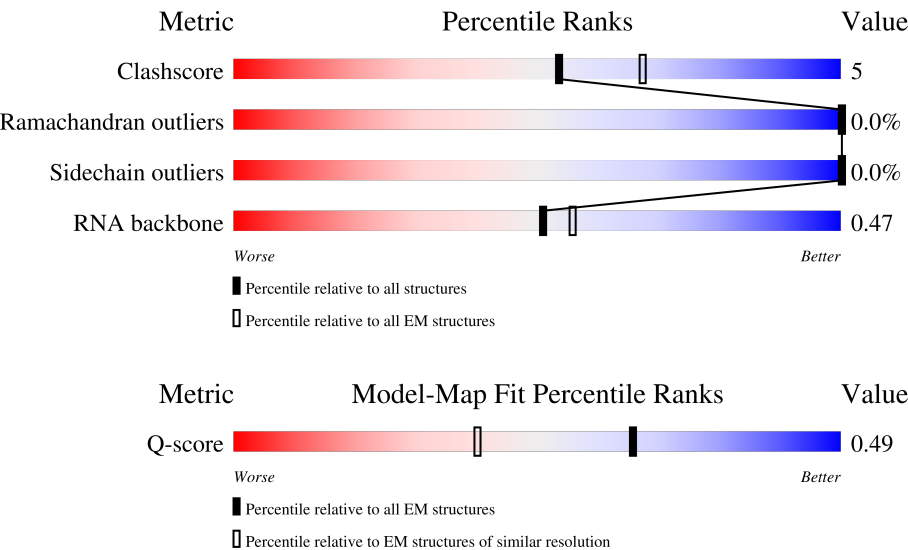
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.83 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.



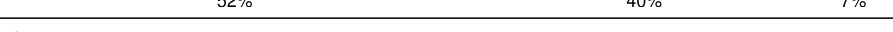
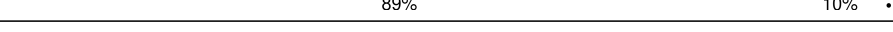
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	SA	221	74% 24%
2	SB	214	78% 22%
3	SC	222	80% 19%

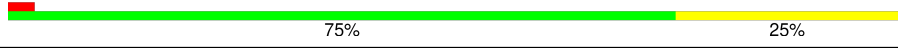
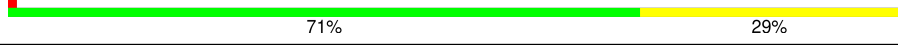
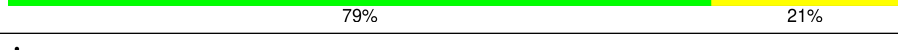
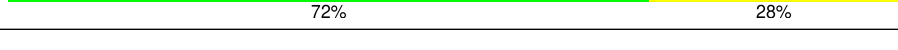
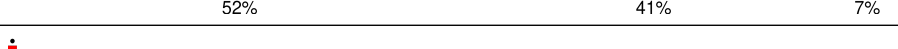
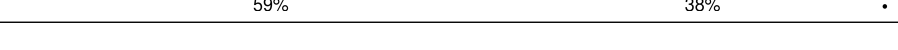
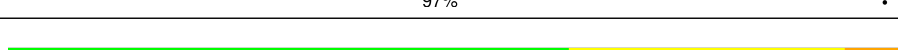
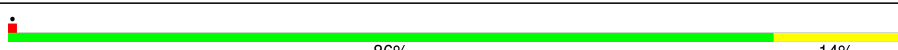
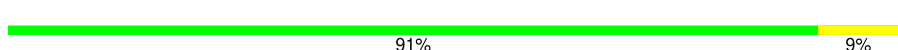
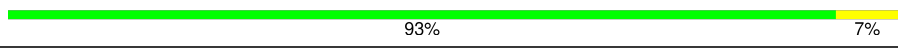
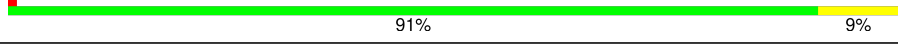
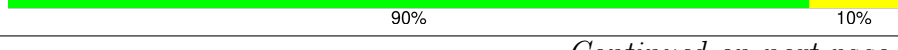
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Mol	Chain	Length	Quality of chain
4	SE	262	
5	SG	237	
6	SH	186	
7	SI	206	
8	SJ	185	
9	SL	153	
10	SN	150	
11	SO	140	
12	SV	83	
13	SW	129	
14	SX	141	
15	SY	131	
16	Sa	102	
17	Sb	83	
18	Se	58	
19	S2	1740	
20	LR	187	
21	LW	118	
22	SR	135	
23	SD	227	
24	SF	189	
25	SK	98	
26	SM	122	
27	SP	121	
28	SQ	144	

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Mol	Chain	Length	Quality of chain
29	SS	145	
30	ST	143	
31	SU	104	
32	SZ	75	
33	Sc	64	
34	Sd	55	
35	Sf	67	
36	Sg	313	
37	At	71	
38	Pt	74	
39	CI	31	
40	L5	3655	
41	L7	120	
42	L8	156	
43	LA	248	
44	LB	402	
45	LC	368	
46	LD	293	
47	LE	250	
48	LF	225	
49	LG	241	
50	LH	190	
51	LI	213	
52	LJ	176	
53	LL	210	

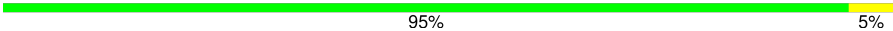
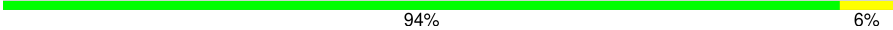
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Mol	Chain	Length	Quality of chain
54	LM	139	
55	LN	203	
56	LO	201	
57	LP	153	
58	LQ	187	
59	LS	175	
60	LT	159	
61	LU	101	
62	LV	131	
63	LX	120	
64	LY	134	
65	LZ	135	
66	La	147	
67	Lb	109	
68	Lc	98	
69	Ld	107	
70	Le	128	
71	Lf	109	
72	Lg	114	
73	Lh	122	
74	Li	102	
75	Lj	86	
76	Lk	69	
77	Ll	50	
78	Lm	52	

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Mol	Chain	Length	Quality of chain
79	Ln	24	 88% 12%
80	Lo	105	 86% 14%
81	Lp	91	 95% 5%
82	Lr	125	 94% 6%
83	Ls	196	 39% 88% 12%
84	Lt	141	 37% 79% 16% 5%
85	Zt	75	 17% 33% 56% 11%

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 221484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 2 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

- Molecule 4 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 5 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 6 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SH	?	-	SER	deletion	UNP P62081
SH	?	-	ARG	deletion	UNP P62081
SH	?	-	THR	deletion	UNP P62081

- Molecule 7 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 8 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 9 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 10 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 12 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 13 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 15 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 16 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 17 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 18 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 19 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S2	1740	Total	C	N	O	P	0	0
			36952	16508	6600	12105	1739		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LW	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	SER	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	ILE	deletion	UNP A0A994J4A5
LW	?	-	GLN	deletion	UNP A0A994J4A5
LW	?	-	LYS	deletion	UNP A0A994J4A5

- Molecule 22 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 23 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 24 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 25 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 26 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 28 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 29 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 30 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 31 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 32 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 34 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 37 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	At	71	Total	C	N	O	P	0	0
			1514	677	275	492	70		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
At	3	C	U	conflict	GB 2583636049
At	?	-	U	deletion	GB 2583636049
At	?	-	U	deletion	GB 2583636049

- Molecule 38 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Pt	74	Total	C	N	O	P	0	0
			1576	705	286	512	73		

- Molecule 39 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	CI	31	Total	C	N	O	S	0	0
			247	153	55	38	1		

- Molecule 40 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L5	3655	Total	C	N	O	P	1	0
			78444	34968	14346	25475	3655		

- Molecule 41 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 42 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 43 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 44 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 45 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 46 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 47 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 48 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 49 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 50 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 51 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 52 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 53 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 54 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 55 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 56 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 57 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 58 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 59 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 61 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 62 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 63 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 64 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 65 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 66 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 67 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLU	deletion	UNP P47914
Lb	?	-	VAL	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	ILE	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLY	deletion	UNP P47914

- Molecule 68 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 69 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 70 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 71 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 72 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 73 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 74 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 75 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 76 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 77 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 78 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 79 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 80 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 81 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 82 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 84 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Lt	134	Total	C	N	O	S	0	0
			998	626	180	189	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	ASP	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050

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Chain	Residue	Modelled	Actual	Comment	Reference
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	GLN	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050
Lt	?	-	ILE	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	HIS	deletion	UNP P30050
Lt	?	-	SER	deletion	UNP P30050
Lt	?	-	GLY	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050

- Molecule 85 is a RNA chain called Z site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Zt	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
86	Sa	1	Total	Zn	0
			1	1	
86	Lg	1	Total	Zn	0
			1	1	
86	Lj	1	Total	Zn	0
			1	1	
86	Lm	1	Total	Zn	0
			1	1	
86	Lo	1	Total	Zn	0
			1	1	
86	Lp	1	Total	Zn	0
			1	1	

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

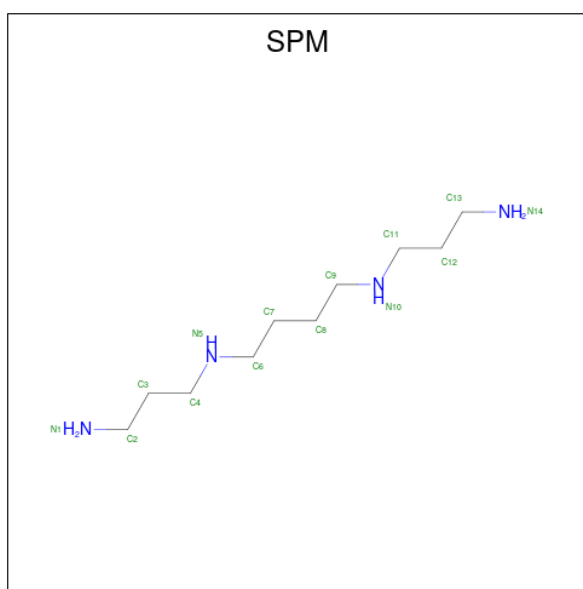
Mol	Chain	Residues	Atoms		AltConf
87	S2	27	Total	Mg	0
			27	27	
87	SS	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	L5	178	Total	Mg	0
			178	178	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	Lj	1	Total	Mg	0
			1	1	

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



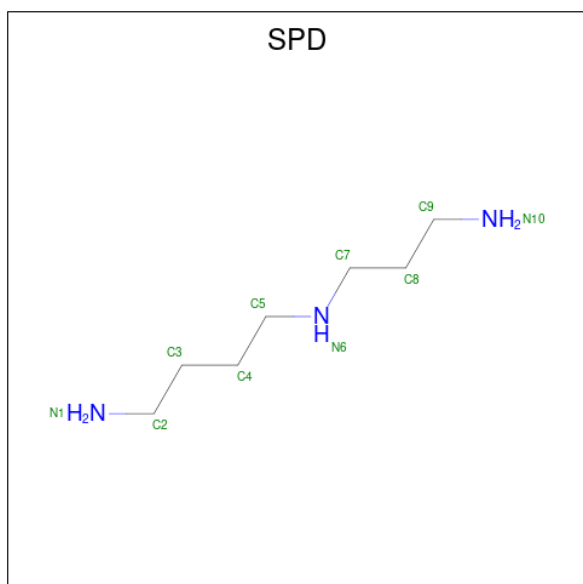
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	

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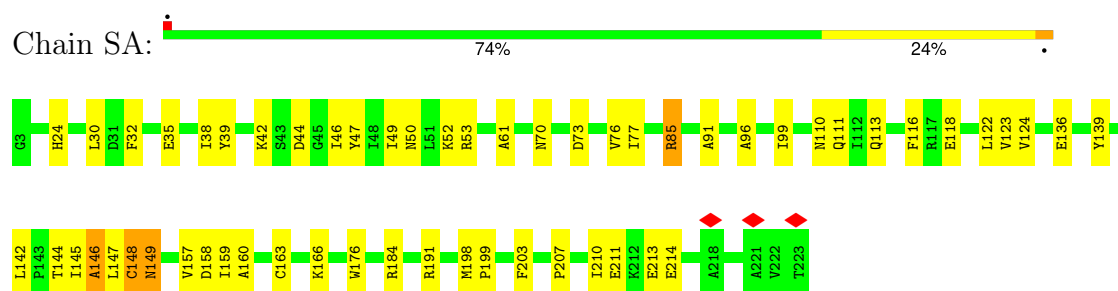
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Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			10	7	3	
89	L8	1	Total	C	N	0
			10	7	3	
89	LN	1	Total	C	N	0
			10	7	3	

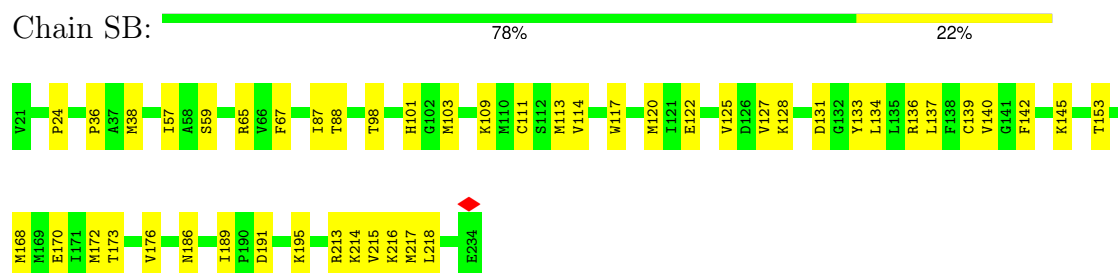
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

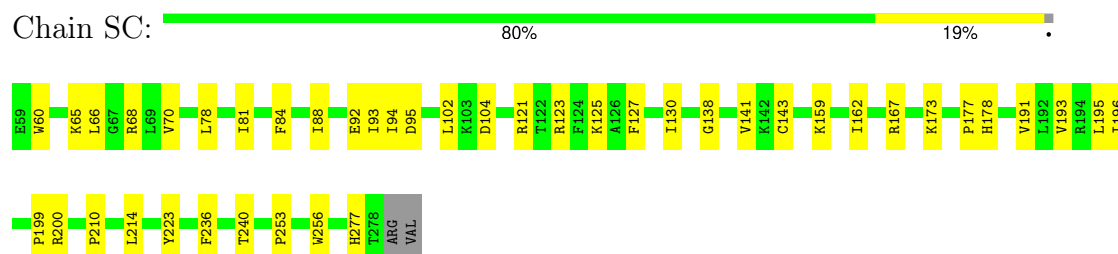
- Molecule 1: 40S ribosomal protein SA



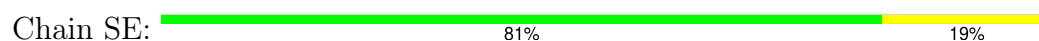
- Molecule 2: 40S ribosomal protein S3a

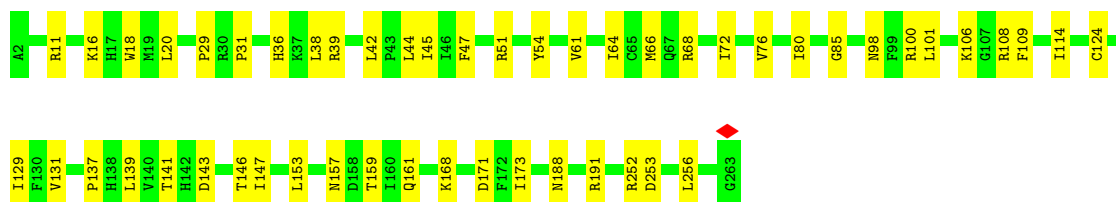


- Molecule 3: 40S ribosomal protein S2



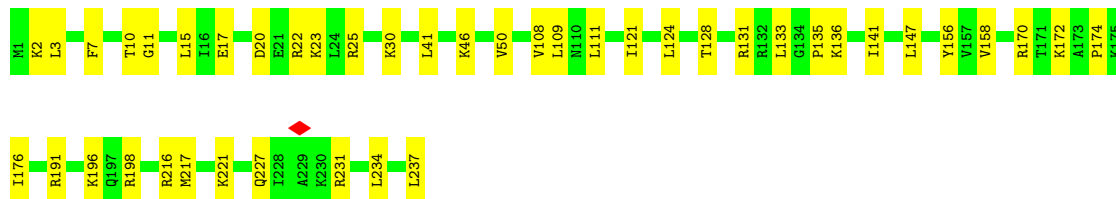
- Molecule 4: Small ribosomal subunit protein eS4, X isoform





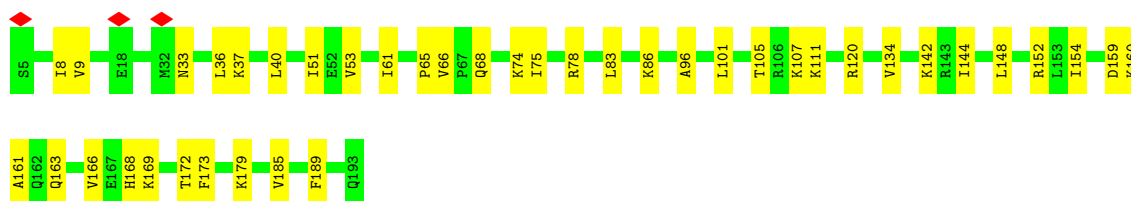
• Molecule 5: 40S ribosomal protein S6

Chain SG: 82% 18%



• Molecule 6: Small ribosomal subunit protein eS7

Chain SH: 78% 22%



• Molecule 7: 40S ribosomal protein S8

Chain SI: 86% 14%



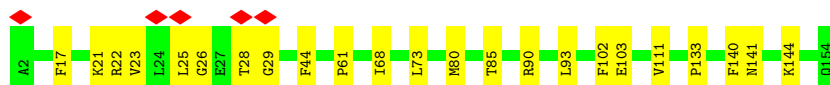
• Molecule 8: 40S ribosomal protein S9

Chain SJ: 84% 16%

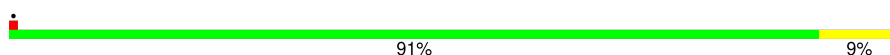


• Molecule 9: 40S ribosomal protein S11

Chain SL: 85% 15%



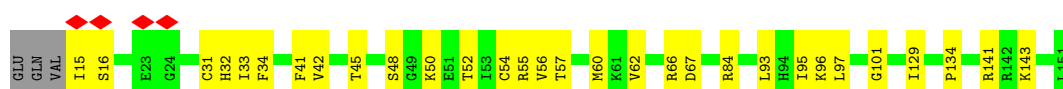
- Molecule 10: 40S ribosomal protein S13

Chain SN:  91% 9%



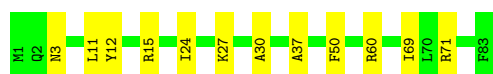
- Molecule 11: Small ribosomal subunit protein uS11

Chain SO:  76% 21%



- Molecule 12: Small ribosomal subunit protein eS21

Chain SV:  86% 14%



- Molecule 13: 40S ribosomal protein S15a

Chain SW:  81% 19%



- Molecule 14: 40S ribosomal protein S23

Chain SX:  90% 10%



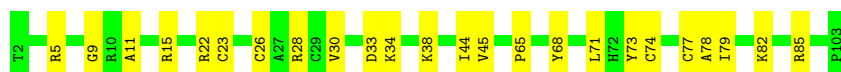
- Molecule 15: 40S ribosomal protein S24

Chain SY:  5% 81% 19%

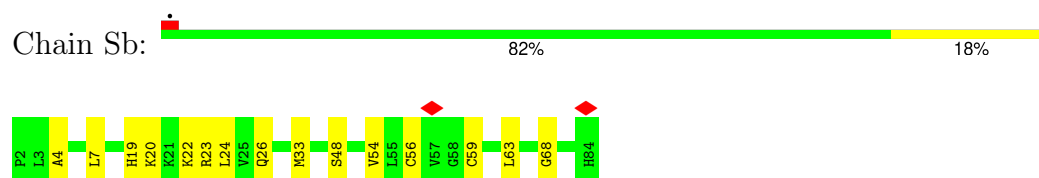


- Molecule 16: 40S ribosomal protein S26

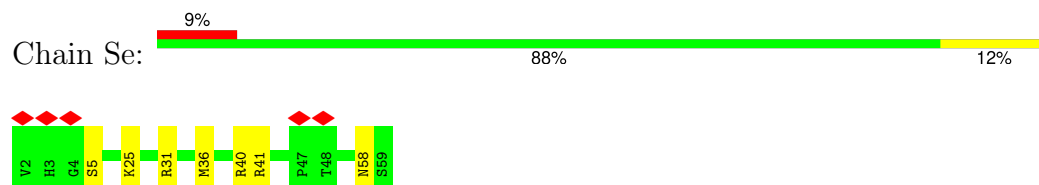
Chain Sa:  76% 24%



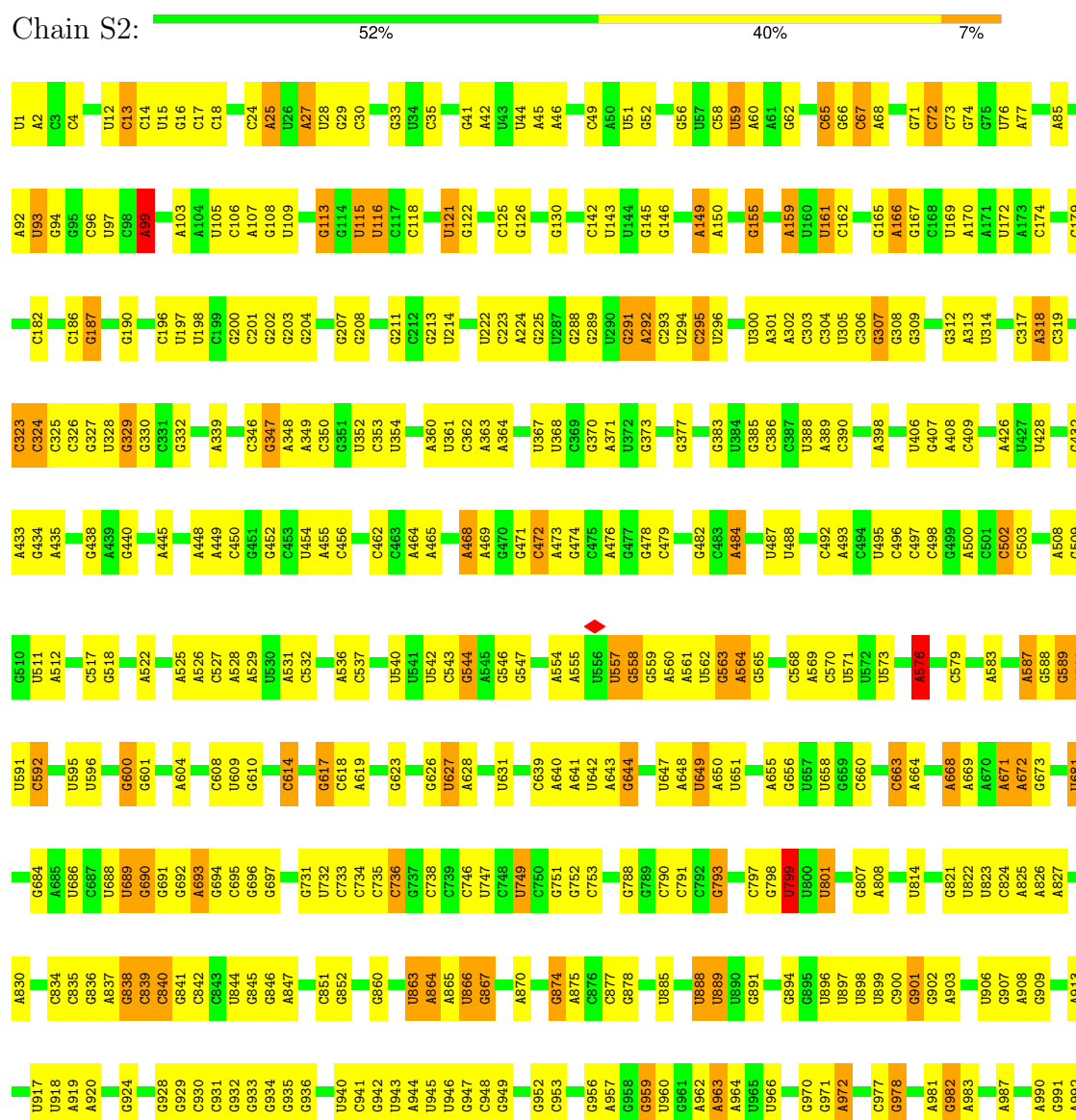
- Molecule 17: Small ribosomal subunit protein eS27

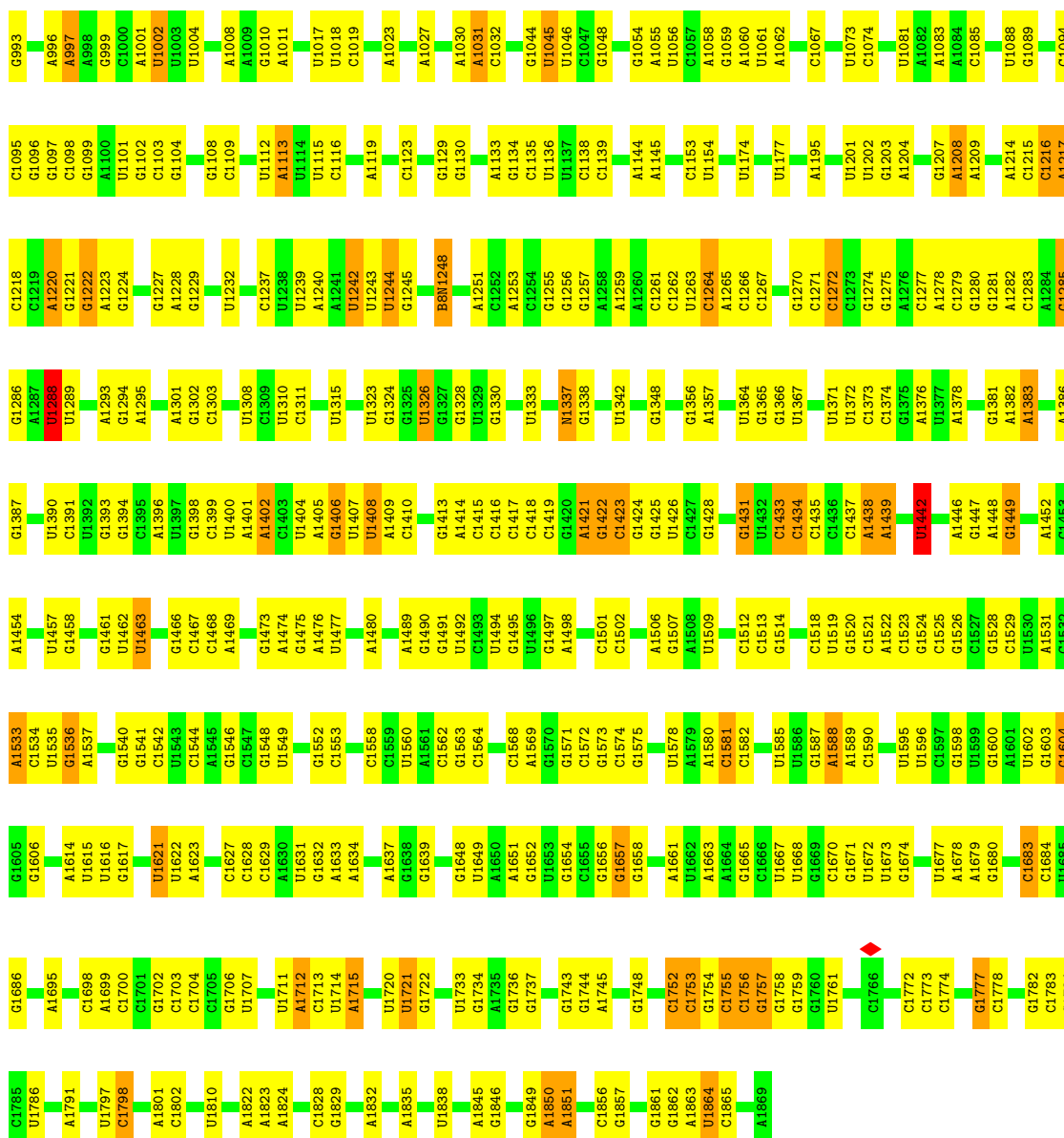


- Molecule 18: Small ribosomal subunit protein eS30



- Molecule 19: 18S rRNA

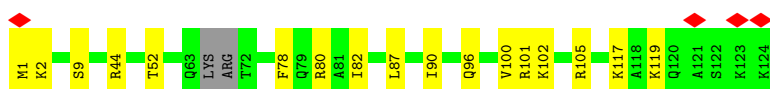
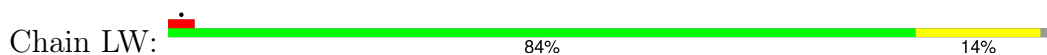




- Molecule 20: 60S ribosomal protein L19



- Molecule 21: Ribosomal protein L24



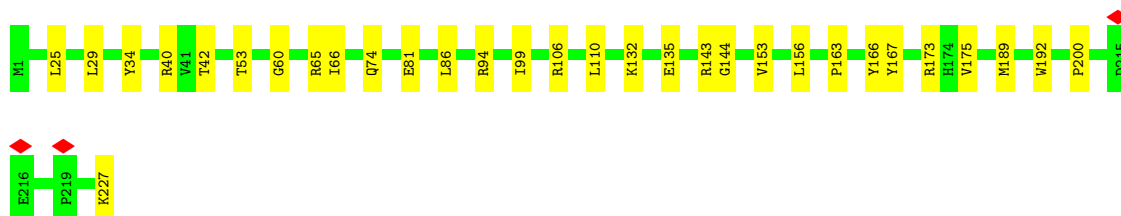
- Molecule 22: Small ribosomal subunit protein eS17

Chain SR:  83% 16%



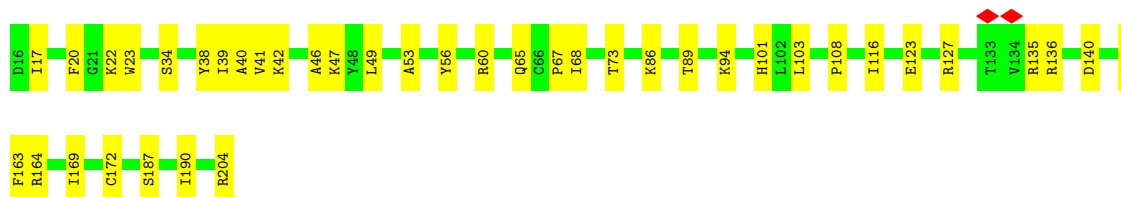
- Molecule 23: Small ribosomal subunit protein uS3

Chain SD:  86% 14%



- Molecule 24: 40S ribosomal protein S5

Chain SF:  79% 21%



- Molecule 25: 40S ribosomal protein S10

Chain SK:  86% 14%



- Molecule 26: Small ribosomal subunit protein eS12

Chain SM:  8% 83% 17%



- Molecule 27: Small ribosomal subunit protein uS19

Chain SP:  86% 14%



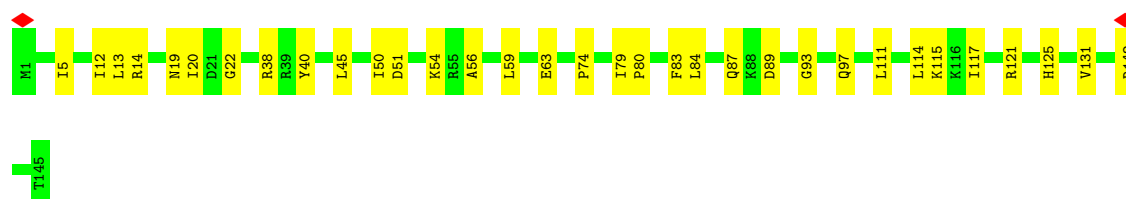
- Molecule 28: Small ribosomal subunit protein uS9

Chain SQ:  81% 19%



- Molecule 29: 40S ribosomal protein S18

Chain SS:  77% 23%



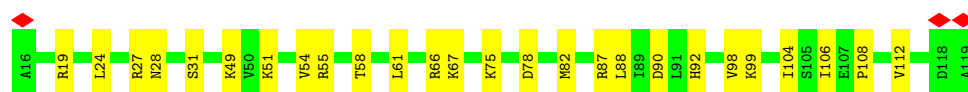
- Molecule 30: 40S ribosomal protein S19

Chain ST:  89% 11%



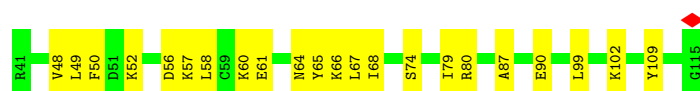
- Molecule 31: 40S ribosomal protein S20

Chain SU:  75% 25%



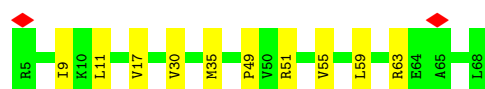
- Molecule 32: Small ribosomal subunit protein eS25

Chain SZ:  71% 29%



- Molecule 33: 40S ribosomal protein S28

Chain Sc:  84% 16%



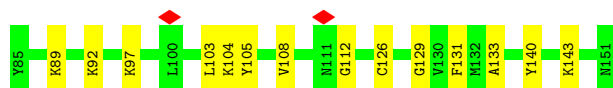
- Molecule 34: 40S ribosomal protein S29

Chain Sd:  89% 11%



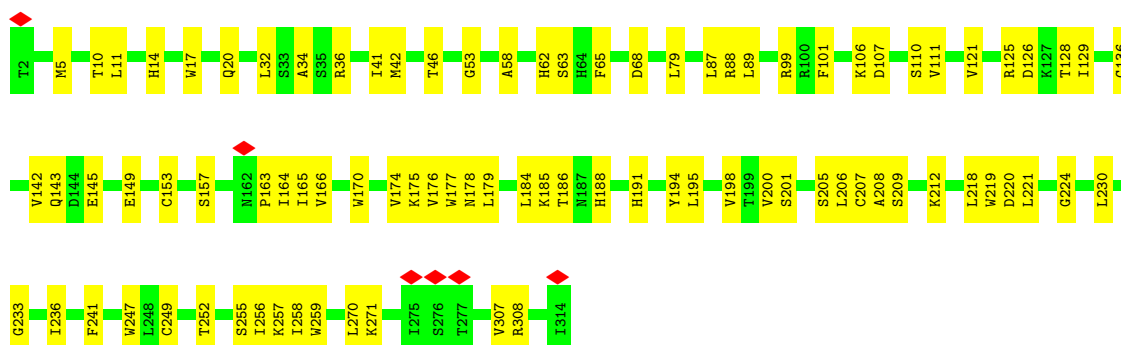
- Molecule 35: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  79% 21%



- Molecule 36: Receptor of activated protein C kinase 1

Chain Sg:  72% 28%



- Molecule 37: A site tRNA

Chain At:  52% 41% 7%

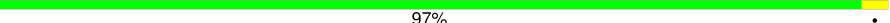


- Molecule 38: P site tRNA

Chain Pt:  59% 38% 3%



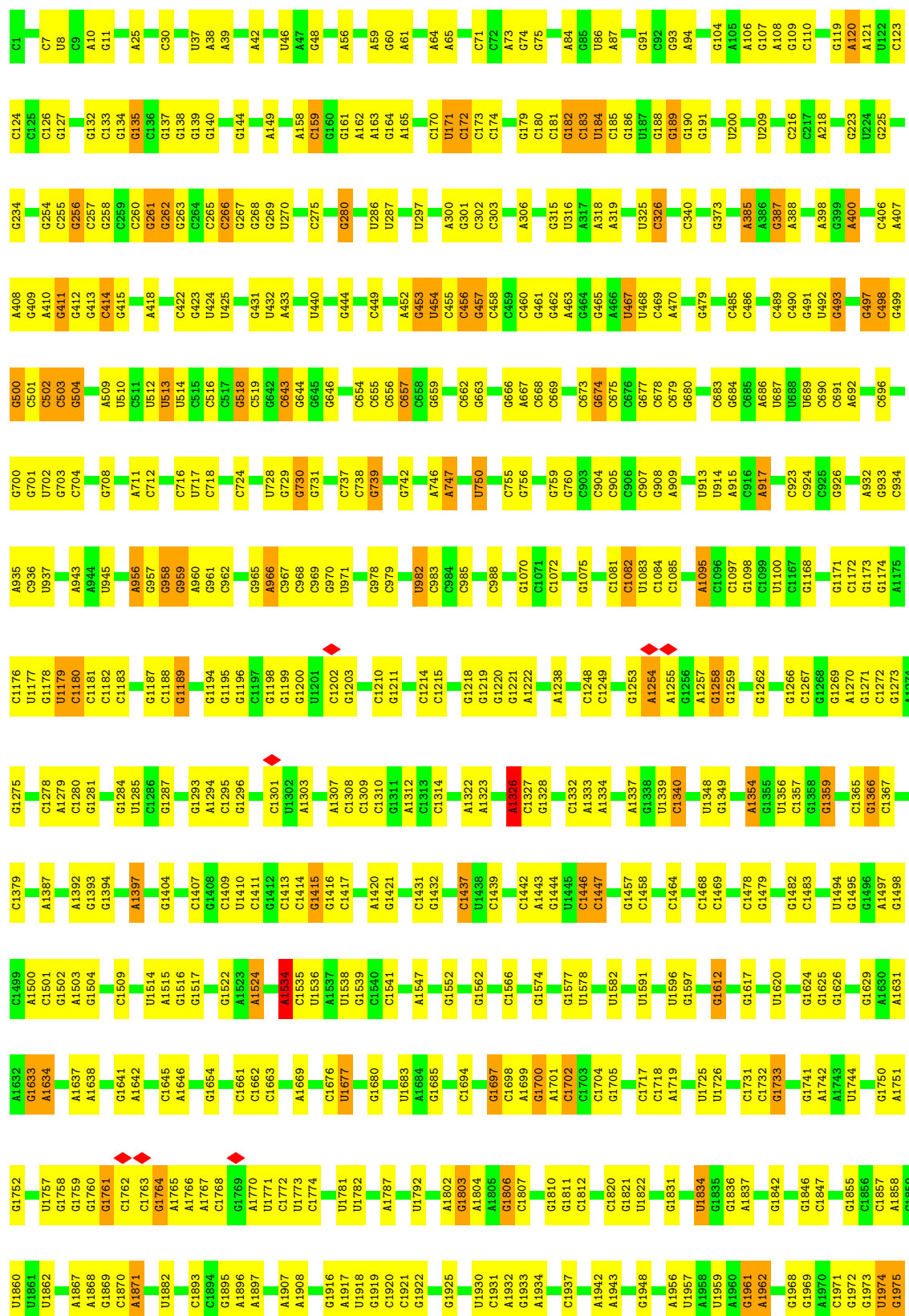
- Molecule 39: Transcription factor BTF3

Chain CI:  97% 3%

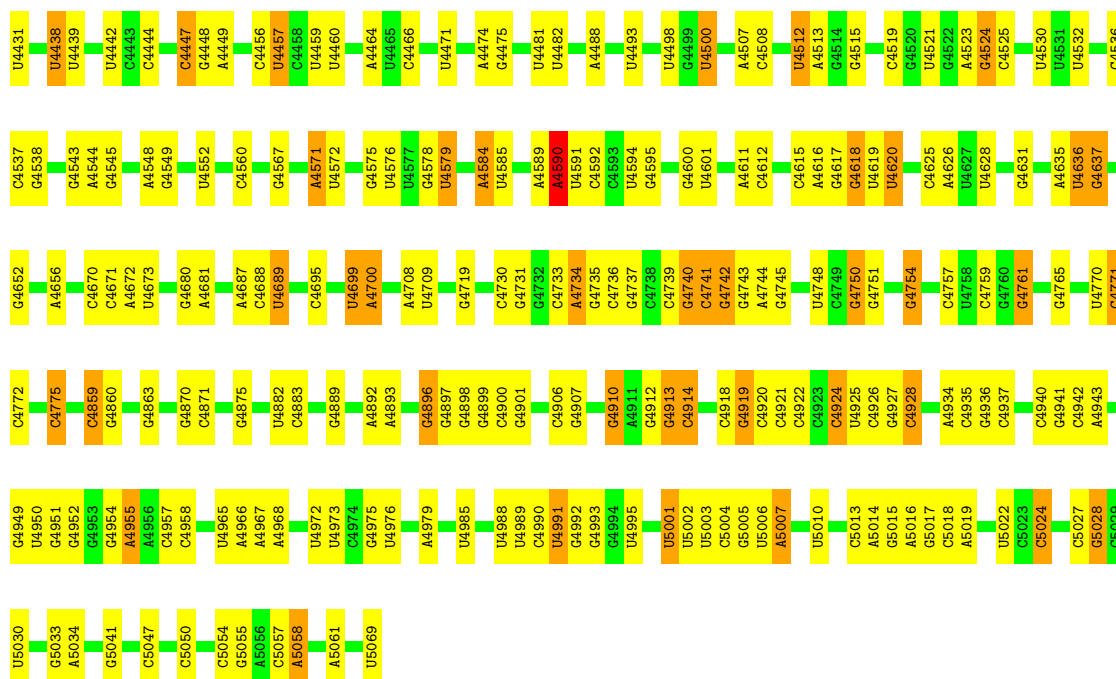


- Molecule 40: 28S rRNA

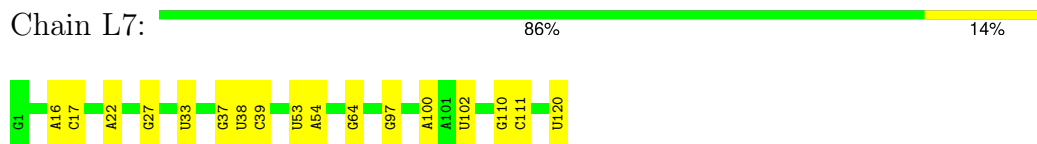
Chain L5:



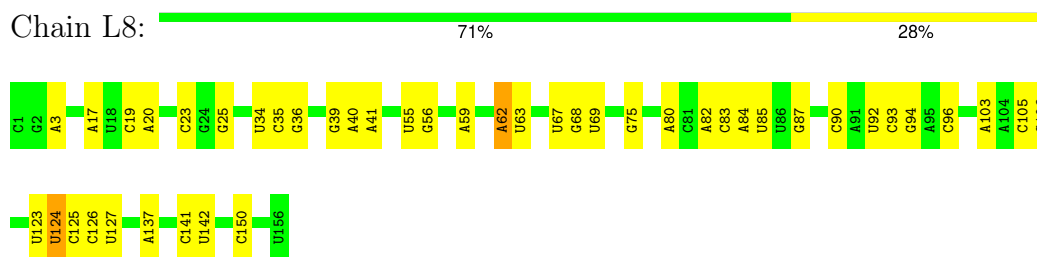
A4304	A4306	U4312	A4313	C4314	C4319	G4329	G4330	G4331	C4332	G4338	U4344	C4345	G4346	G4347	C4348	C4349	C4350	U4353	U4354	U4361	A4362	A4363	A4364	C4365	G4373	A4376	G4377	A4378	A4379	C4386	C4387	G4392	G4393	A4394	G4401	C4402	U4403	U4404	G4405	A4415	C4421	A4422							
G4196	A4203	A4212	A4213	A4214	A4220	A4221	G4222	U4227	G4228	U4229	A4233	A4238	A4239	U4346	C4240	G4241	U4242	C4243	A4244	G4245	A4251	G4254	A4255	A4256	A4257	C4258	U4259	U4260	C4261	U4265	A4268	A4273	A4274	G4275	A4279	A4280	A4281	A4282	G4291	A4292	U4293	C4294	U4295	U4296	U4299				
C4096	G4097	A4098	C4099	C4100	C4101	G4104	A4105	G4106	G4107	G4108	G4109	C4110	U4111	C4112	U4113	U4114	G4115	U4116	U4117	G4121	G4122	A4127	C4133	C4138	G4139	C4140	G4141	C4142	G4143	C4144	C4145	G4146	C4153	G4154	C4155	G4156	A4157	C4162	U4163	G4168	G4169	A4170	G4183	G4184	G4187	U4188	U4189	U4190	G4191
G3906	G3907	A3908	C3909	C3910	C3911	U3912	U3915	C3920	C3923	C3924	U3925	C3928	C3929	C3937	G3938	A3942	A3943	G3944	A3945	G3946	A3947	C3948	A3949	U3950	C3951	A3952	G3953	A3954	A4056	C4057	U4058	C4059	U4060	G4061	A4062	U4063	C4064	G4065	U4068	U4069	U4070	U4071	C4072	G4076	C4088	G4089	G4090	G4094	G4095
U3822	C3823	A3824	C3825	C3826	U3830	C3833	C3834	U3838	G3839	C3840	C3841	U3844	U3848	A3849	C3850	U3851	A3852	U3853	A3856	A3861	A3862	A3867	C3868	C3869	C3870	A3871	A3872	C3873	C3874	A3875	G3876	A3877	C3878	C3879	G3880	G3881	U3884	C3885	A3890	A3891	U3892	G3897	C3898	C3899	A3901				
G3710	A3711	A3712	U3713	A3717	A3718	A3719	U3720	U3721	U3722	A3723	A3724	U3725	A3726	A3727	A3732	A3733	U3734	G3735	A3736	A3737	G3744	A3748	G3753	A3760	U3764	G3765	A3766	U3770	A3774	A3775	G3776	G3777	C3782	A3785	U3786	G3792	U3793	C3808	G3811	U3814	A3817	U3818	G3819						
A3611	G3615	G3619	A3624	G3625	G3626	G3627	A3630	A3635	C3636	U3637	G3638	U3639	U3640	U3641	U3644	U3645	A3646	A3647	A3648	A3652	A3653	A3656	U3657	A3662	A3663	G3664	G3665	C3668	G3669	C3670	C3673	G3674	G3684	C3685	U3690	G3691	A3692	U3695	C3696	U3697	C3698	C3701	U3709						
G2842	U2843	A2844	G2848	G2855	C2856	A2857	A2858	C2861	A2864	U2865	C2866	C2867	C2739	G2742	A2743	A2744	A2745	A2746	U2891	C2892	A2895	U2900	C2901	C2902	G2903	U2904	C2905	U2906	C2907	U2908	G3585	C3588	G3589	C3590	C3591	C3594	U3595	A3596	G3597	C3598	A3599	G3600	C3601	C3605	U3606	U3607	A3610		
C2710	G2711	G2717	U2718	C2719	C2720	G2721	A2725	G2726	C2727	U2730	C2731	G2739	G2742	A2743	A2744	A2745	A2746	U2769	C2770	A2787	U2788	A2789	U2790	U2803	C2804	A2806	C2814	A2815	C2824	A2825	U2826	G2827	U2837	G2838	U2839														
G2557	C2558	G2559	C2560	A2565	C2568	G2569	U2570	A2573	C2583	G2586	A2484	U2485	G2486	G2487	C2488	A2601	G2611	G2612	C2613	G2618	C2627	U2632	U2633	G2640	A2641	C2653	C2654	C2655	G2662	C2669	C2670	G2675	A2676	U2687	G2688	G2694	A2695	A2696	G2706	U2707	U2708	G2709							
G2466	C2469	C2470	G2471	G2474	G2475	C2478	G2479	G2481	C2482	G2483	A2484	U2485	G2486	G2487	C2488	G2490	C2491	C2492	G2493	U2494	U2495	C2497	C2498	C2501	G2502	C2503	C2504	C2505	G2506	A2513	G2514	A2517	G2518	U2519	C2520	G2521	A2537	U2538	C2539	C2540	G2544	U2545	G2546	G2547	U2554	G2555	G2556		
C2301	C2302	C2303	G2306	A2313	A2332	G2333	C2334	C2335	G2336	G2348	C2351	A2360	U2362	G2363	G2364	G2380	C2383	A2389	A2395	A2396	G2397	A2401	C2411	A2412	U2415	G2416	A2417	C2422	A2423	G2424	U2425	A2431	G2448	A2449	G2450	A2453	C2458	C2464	C2465										
C2066	C2067	C2068	A2069	G2076	C2084	U2090	G2091	G2092	A2093	G2094	G2096	U2097	G2098	G2099	A2100	G2101	G2102	G2103	G2104	A2105	G2106	C2107	G2108	G2109	C2110	G2111	G2112	C2249	C2250	G2251	G2252	A2253	G2254	C2255	C2256	C2257	C2258	G2262	A2263	C2264	G2265	G2275	A2276	C2289	U2292	U2293	U2298	G2299	A2300
G1976	C1977	C1978	A1979	U1980	G1981	G1982	A1983	A1984	G1985	U1986	G1989	A1990	A1991	U1992	C1993	C1994	G1995	A1996	U1997	A1998	A1999	G2000	G2001	A2002	G2005	U2006	C2007	U2008	C2011	A2012	C2016	A2017	C2018	C2019	U2020	G2021	G2024	A2025	A2026	A2033	G2034	G2045	G2046	A2047	U2048	G2052	G2055	G2056	G2060



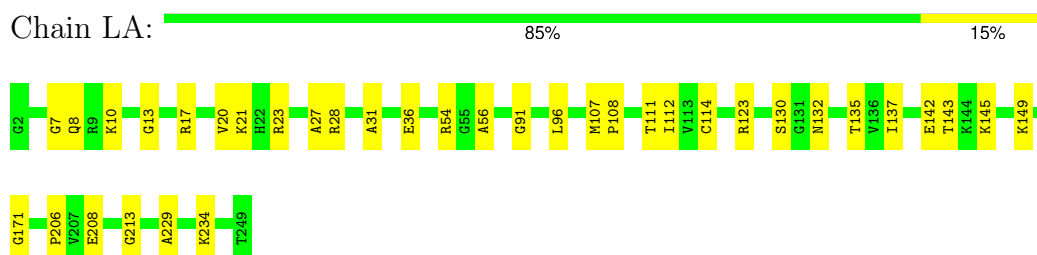
- Molecule 41: 5S rRNA



- Molecule 42: 5.8S rRNA

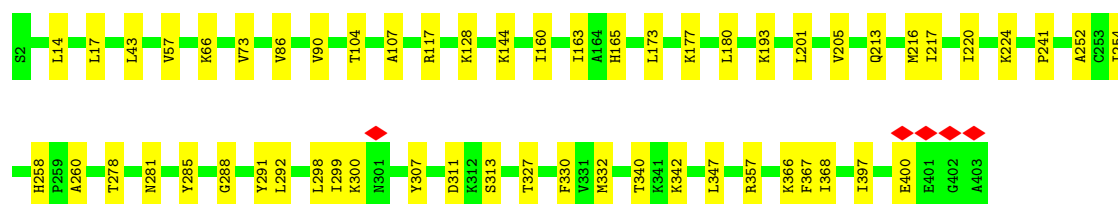


- Molecule 43: 60S ribosomal protein L8

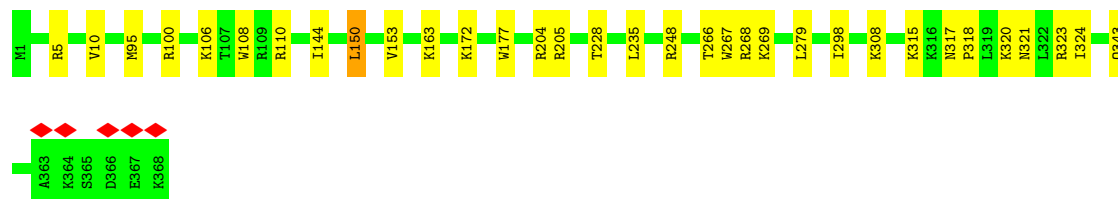


- Molecule 44: Large ribosomal subunit protein uL3





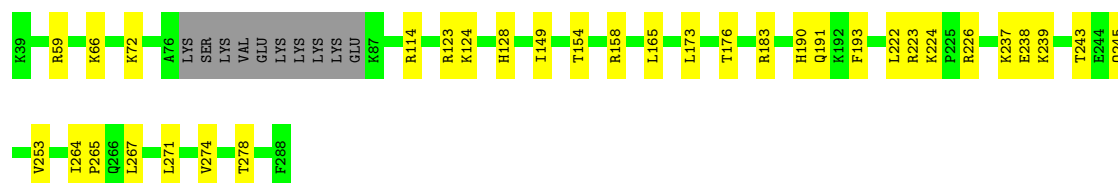
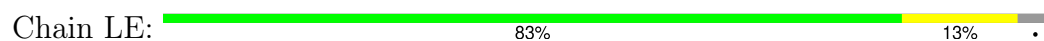
- Molecule 45: 60S ribosomal protein L4



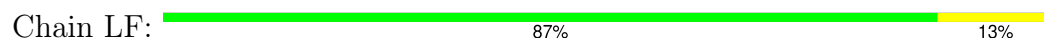
- Molecule 46: Large ribosomal subunit protein uL18



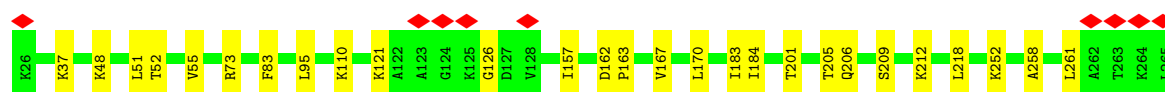
- Molecule 47: Large ribosomal subunit protein eL6



- Molecule 48: 60S ribosomal protein L7



- Molecule 49: 60S ribosomal protein L7a





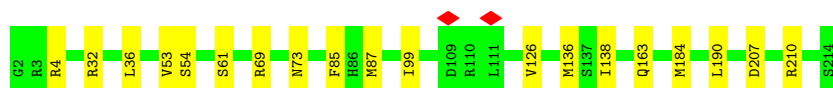
- Molecule 50: 60S ribosomal protein L9

Chain LH: 93% 7%



- Molecule 51: Ribosomal protein uL16-like

Chain LI: 91% 9%



- Molecule 52: 60S ribosomal protein L11

Chain LJ: 86% 10% .



- Molecule 53: Large ribosomal subunit protein eL13

Chain LL: 90% 10%



- Molecule 54: 60S ribosomal protein L14

Chain LM: 84% 16%



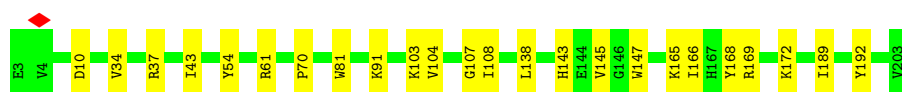
- Molecule 55: 60S ribosomal protein L15

Chain LN: 91% 9%



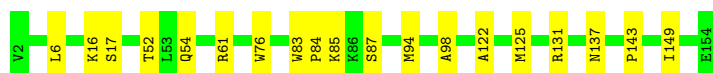
- Molecule 56: 60S ribosomal protein L13a

Chain LO: 88% 12%



- Molecule 57: 60S ribosomal protein L17

Chain LP: 88% 12%



- Molecule 58: 60S ribosomal protein L18

Chain LQ: 96% .



- Molecule 59: 60S ribosomal protein L18a

Chain LS: 93% 7%



- Molecule 60: 60S ribosomal protein L21

Chain LT: 92% 8%



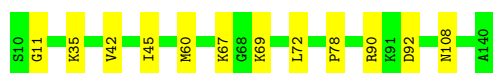
- Molecule 61: Heparin-binding protein HBp15

Chain LU: 88% 12%



- Molecule 62: 60S ribosomal protein L23

Chain LV: 91% 9%



- Molecule 63: 60S ribosomal protein L23a

Chain LX: 89% 11%



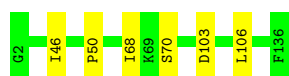
- Molecule 64: 60S ribosomal protein L26

Chain LY: 86% 14%



- Molecule 65: 60S ribosomal protein L27

Chain LZ: 96% .



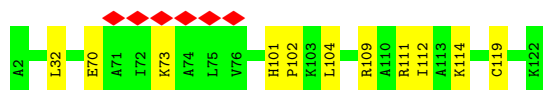
- Molecule 66: 60S ribosomal protein L27a

Chain La: 95% 5%



- Molecule 67: Large ribosomal subunit protein eL29

Chain Lb: 6% 90% 10%



- Molecule 68: 60S ribosomal protein L30

Chain Lc: 90% 10%



- Molecule 69: 60S ribosomal protein L31

Chain Ld: 86% 14%



- Molecule 70: 60S ribosomal protein L32

Chain Le: 94% 6%



- Molecule 71: 60S ribosomal protein L35a

Chain Lf: 89% 11%



- Molecule 72: 60S ribosomal protein L34

Chain Lg: 94% 6%



- Molecule 73: 60S ribosomal protein L35

Chain Lh: 90% 10%



- Molecule 74: 60S ribosomal protein L36

Chain Li: 90% 10%



- Molecule 75: 60S ribosomal protein L37

Chain Lj: 95% 5%



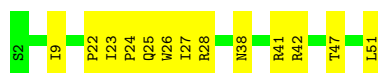
- Molecule 76: 60S ribosomal protein L38

Chain Lk: 78% 22%



- Molecule 77: 60S ribosomal protein L39

Chain Ll: 74% 26%



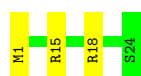
- Molecule 78: Large ribosomal subunit protein eL40

Chain Lm: 90% 10%



- Molecule 79: 60S ribosomal protein L41

Chain Ln: 88% 12%



- Molecule 80: 60S ribosomal protein L36a

Chain Lo: 86% 14%



- Molecule 81: 60S ribosomal protein L37a

Chain Lp: 95% 5%



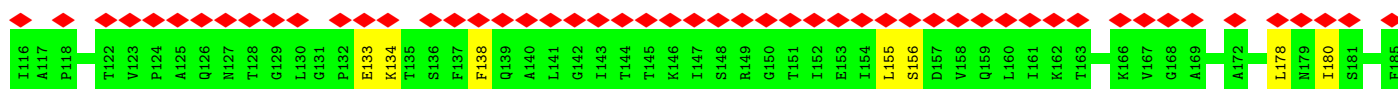
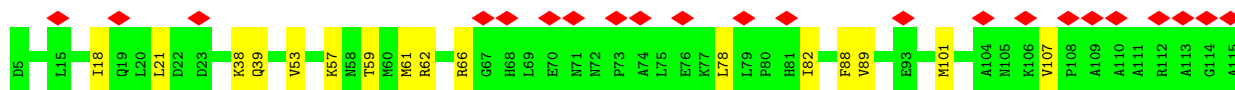
- Molecule 82: 60S ribosomal protein L28

Chain Lr: 94% 6%



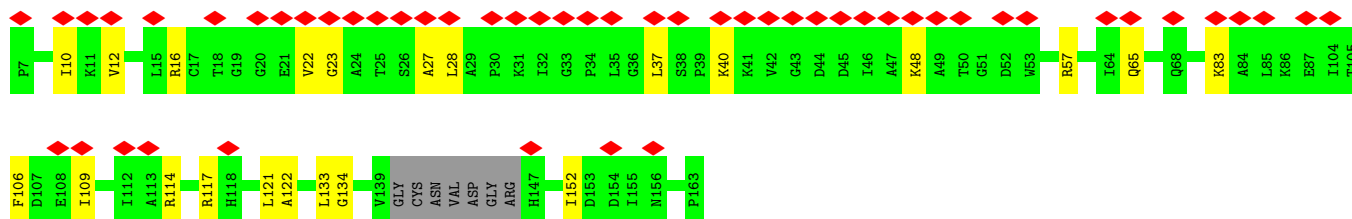
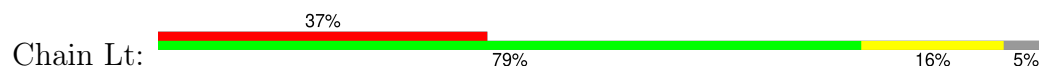
- Molecule 83: 60S acidic ribosomal protein P0

Chain Ls: 39% 88% 12%

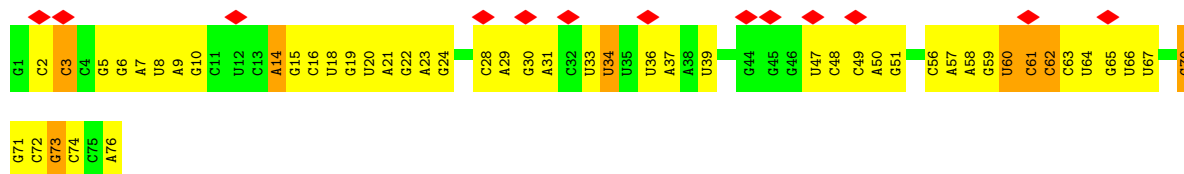




- Molecule 84: Large ribosomal subunit protein uL11



- Molecule 85: Z site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.156	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0125	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, ZN, OMU, 1MA, 5MC, G7M, B8N, OMC, UY1, SPD, OMG, MG, MA6, A2M, SPM, PSU, UR3, 4AC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	SA	0.55	3/1778 (0.2%)	0.63	6/2416 (0.2%)
2	SB	0.17	0/1765	0.33	0/2362
3	SC	0.20	0/1744	0.31	0/2357
4	SE	0.19	0/2118	0.34	0/2849
5	SG	0.17	0/1946	0.32	0/2590
6	SH	0.16	0/1519	0.38	0/2033
7	SI	0.21	0/1715	0.38	0/2287
8	SJ	0.18	0/1550	0.34	0/2069
9	SL	0.22	0/1268	0.31	0/1696
10	SN	0.17	0/1232	0.28	0/1656
11	SO	0.18	0/1037	0.35	0/1391
12	SV	0.16	0/643	0.30	0/860
13	SW	0.22	0/1051	0.33	0/1406
14	SX	0.24	0/1116	0.39	0/1490
15	SY	0.17	0/1083	0.32	0/1438
16	Sa	0.20	0/836	0.35	0/1121
17	Sb	0.17	0/665	0.35	0/891
18	Se	0.16	0/465	0.35	0/612
19	S2	0.25	0/39756	0.30	0/61939
20	LR	0.35	0/1582	0.44	0/2091
21	LW	0.26	0/959	0.33	0/1270
22	SR	0.25	0/1105	0.48	0/1484
23	SD	0.17	0/1793	0.31	0/2414
24	SF	0.16	0/1516	0.32	0/2037
25	SK	0.15	0/851	0.31	0/1147
26	SM	0.12	0/950	0.31	0/1275
27	SP	0.17	0/1003	0.35	0/1342
28	SQ	0.16	0/1160	0.35	0/1553
29	SS	0.16	0/1216	0.35	0/1628
30	ST	0.16	0/1131	0.31	0/1515
31	SU	0.18	0/831	0.34	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SZ	0.17	0/604	0.42	0/810
33	Sc	0.16	0/508	0.33	0/680
34	Sd	0.21	0/470	0.35	0/623
35	Sf	0.17	0/560	0.43	0/745
36	Sg	0.14	0/2493	0.36	0/3394
37	At	0.17	0/1692	0.27	0/2634
38	Pt	0.18	0/1761	0.27	0/2741
39	CI	0.19	0/247	0.30	0/323
40	L5	0.38	0/85098	0.34	0/132762
41	L7	0.36	0/2861	0.30	0/4459
42	L8	0.38	0/3631	0.32	0/5657
43	LA	0.37	0/1936	0.43	0/2596
44	LB	0.35	0/3306	0.39	0/4424
45	LC	0.37	0/2981	0.42	1/4002 (0.0%)
46	LD	0.28	0/2428	0.32	0/3252
47	LE	0.28	0/1973	0.42	0/2645
48	LF	0.35	0/1905	0.33	0/2539
49	LG	0.30	0/1960	0.37	0/2637
50	LH	0.32	0/1537	0.33	0/2066
51	LI	0.31	0/1751	0.33	0/2340
52	LJ	0.24	0/1385	0.35	0/1852
53	LL	0.32	0/1732	0.33	0/2315
54	LM	0.33	0/1161	0.34	0/1554
55	LN	0.39	0/1746	0.36	0/2338
56	LO	0.36	0/1682	0.36	0/2250
57	LP	0.36	0/1268	0.37	0/1701
58	LQ	0.37	0/1537	0.37	0/2052
59	LS	0.36	0/1493	0.32	0/2003
60	LT	0.33	0/1326	0.34	0/1770
61	LU	0.25	0/839	0.39	0/1126
62	LV	0.35	0/993	0.39	0/1332
63	LX	0.31	0/1002	0.33	0/1345
64	LY	0.33	0/1132	0.35	0/1504
65	LZ	0.29	0/1130	0.31	0/1507
66	La	0.36	0/1191	0.31	0/1591
67	Lb	0.27	0/889	0.35	0/1175
68	Lc	0.29	0/774	0.37	0/1038
69	Ld	0.33	0/903	0.35	0/1216
70	Le	0.37	0/1071	0.33	0/1429
71	Lf	0.46	0/895	0.58	0/1198
72	Lg	0.34	0/916	0.34	0/1220
73	Lh	0.31	0/1023	0.34	0/1351
74	Li	0.28	0/843	0.32	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lj	0.37	0/720	0.41	0/952
76	Lk	0.31	0/575	0.39	0/761
77	Ll	0.33	0/454	0.27	0/599
78	Lm	0.31	0/435	0.35	0/575
79	Ln	0.27	0/231	0.29	0/294
80	Lo	0.34	0/876	0.34	0/1156
81	Lp	0.33	0/718	0.33	0/953
82	Lr	0.35	0/1017	0.38	0/1364
83	Ls	0.13	0/1519	0.32	0/2052
84	Lt	0.16	0/1009	0.47	0/1363
85	Zt	0.15	0/1779	0.32	0/2771
All	All	0.32	3/233350 (0.0%)	0.34	7/342485 (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	SA	0	1
20	LR	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	148	CYS	CA-C	-13.81	1.34	1.52
1	SA	148	CYS	CA-CB	13.09	1.75	1.53
1	SA	147	LEU	N-CA	-9.47	1.34	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SA	148	CYS	N-CA-CB	-13.99	86.84	110.49
1	SA	148	CYS	N-CA-C	12.01	136.38	110.80
1	SA	146	ALA	CA-C-N	7.00	132.81	121.74
1	SA	146	ALA	C-N-CA	7.00	132.81	121.74
1	SA	147	LEU	N-CA-C	6.34	119.30	109.60
1	SA	147	LEU	N-CA-CB	6.30	119.90	110.39
45	LC	150	LEU	CA-CB-CG	-5.57	96.81	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	LR	136	ARG	Sidechain
1	SA	85	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	SA	1741	0	1744	43	0
2	SB	1738	0	1809	32	0
3	SC	1707	0	1791	29	0
4	SE	2076	0	2177	38	0
5	SG	1923	0	2089	35	0
6	SH	1497	0	1590	27	0
7	SI	1686	0	1772	20	0
8	SJ	1525	0	1640	22	0
9	SL	1247	0	1323	18	0
10	SN	1208	0	1294	9	0
11	SO	1024	0	1050	21	0
12	SV	636	0	637	9	0
13	SW	1034	0	1080	21	0
14	SX	1098	0	1167	10	0
15	SY	1065	0	1142	19	0
16	Sa	821	0	870	15	0
17	Sb	651	0	670	14	0
18	Se	459	0	503	6	0
19	S2	36952	0	18678	427	0
20	LR	1566	0	1729	12	0
21	LW	945	0	1003	13	0
22	SR	1090	0	1149	19	0
23	SD	1765	0	1865	19	0
24	SF	1495	0	1549	31	0
25	SK	827	0	854	12	0
26	SM	940	0	965	14	0
27	SP	985	0	1031	11	0
28	SQ	1142	0	1213	21	0
29	SS	1198	0	1261	22	0
30	ST	1112	0	1146	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	SU	821	0	883	18	0
32	SZ	598	0	656	17	0
33	Sc	506	0	536	7	0
34	Sd	459	0	449	8	0
35	Sf	548	0	553	9	0
36	Sg	2436	0	2391	58	0
37	At	1514	0	770	21	0
38	Pt	1576	0	803	18	0
39	CI	247	0	283	1	0
40	L5	78444	0	39718	561	0
41	L7	2561	0	1295	5	0
42	L8	3315	0	1685	14	0
43	LA	1898	0	1993	26	0
44	LB	3238	0	3376	39	0
45	LC	2927	0	3104	28	0
46	LD	2382	0	2410	16	0
47	LE	1935	0	2096	27	0
48	LF	1870	0	1996	22	0
49	LG	1927	0	2074	17	0
50	LH	1518	0	1601	10	0
51	LI	1711	0	1749	17	0
52	LJ	1362	0	1399	11	0
53	LL	1701	0	1818	14	0
54	LM	1138	0	1204	15	0
55	LN	1701	0	1749	14	0
56	LO	1650	0	1794	18	0
57	LP	1242	0	1269	14	0
58	LQ	1513	0	1628	8	0
59	LS	1453	0	1490	9	0
60	LT	1298	0	1366	10	0
61	LU	825	0	850	9	0
62	LV	979	0	1039	8	0
63	LX	985	0	1066	8	0
64	LY	1115	0	1205	13	0
65	LZ	1107	0	1182	4	0
66	La	1162	0	1213	5	0
67	Lb	876	0	948	7	0
68	Lc	764	0	804	6	0
69	Ld	888	0	930	8	0
70	Le	1053	0	1147	5	0
71	Lf	876	0	912	9	0
72	Lg	906	0	998	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	Lh	1015	0	1148	11	0
74	Li	832	0	917	8	0
75	Lj	705	0	737	3	0
76	Lk	569	0	637	9	0
77	Ll	444	0	483	9	0
78	Lm	429	0	465	5	0
79	Ln	230	0	276	2	0
80	Lo	862	0	929	11	0
81	Lp	708	0	756	4	0
82	Lr	1002	0	1068	4	0
83	Ls	1496	0	1540	15	0
84	Lt	998	0	1032	20	0
85	Zt	1593	0	809	18	0
86	Lg	1	0	0	0	0
86	Lj	1	0	0	0	0
86	Lm	1	0	0	0	0
86	Lo	1	0	0	0	0
86	Lp	1	0	0	0	0
86	Sa	1	0	0	0	0
87	L5	178	0	0	0	0
87	L7	3	0	0	0	0
87	L8	5	0	0	0	0
87	LA	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lj	1	0	0	0	0
87	S2	27	0	0	0	0
87	SS	1	0	0	0	0
88	L5	98	0	182	2	0
89	L5	80	0	152	1	0
89	L8	10	0	19	0	0
89	LN	10	0	19	0	0
All	All	221484	0	164392	2006	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 5.

All (2006) 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)
1:SA:148:CYS:CA	1:SA:148:CYS:CB	1.75	1.61
1:SA:148:CYS:CB	1:SA:148:CYS:N	2.22	1.03
40:L5:1095:A:H2	40:L5:1200:G:H1	1.16	0.92
38:Pt:50:U:H3	38:Pt:64:G:H1	1.17	0.92
40:L5:1996:C:N4	40:L5:2000:G:H22	1.69	0.91
40:L5:3944:G:H1	40:L5:4069:U:H3	1.17	0.88
19:S2:1656:G:H1	19:S2:1668:U:H3	0.91	0.87
1:SA:148:CYS:CB	1:SA:148:CYS:C	2.47	0.87
40:L5:1996:C:H42	40:L5:2000:G:H22	1.22	0.87
19:S2:1533:A:H62	19:S2:1602:U:H3	1.22	0.87
40:L5:1974:U:H4'	40:L5:1975:G:H3'	1.59	0.85
19:S2:1652:G:H1	19:S2:1672:U:H3	0.85	0.84
37:At:50:U:H3	37:At:64:G:H1	0.86	0.84
40:L5:1996:C:H42	40:L5:2000:G:N2	1.75	0.84
7:SI:48:VAL:HG11	7:SI:54:LYS:HD3	1.61	0.82
19:S2:1748:G:H1	19:S2:1786:U:H3	1.23	0.82
40:L5:1095:A:C2	40:L5:1200:G:N1	2.47	0.82
40:L5:2557:G:H1	40:L5:2570:U:H3	0.86	0.80
40:L5:5024:C:H41	40:L5:5028:G:H21	1.28	0.80
19:S2:508:A:H3'	19:S2:509:OMG:H8	1.48	0.77
6:SH:53:VAL:HG11	6:SH:172:THR:HA	1.66	0.77
19:S2:1417:C:H42	19:S2:1422:G:H22	1.32	0.76
40:L5:3701:OMC:H5	40:L5:3748:A:H62	1.33	0.76
2:SB:134:LEU:HB3	2:SB:218:LEU:HB2	1.67	0.75
9:SL:133:PRO:HG2	19:S2:383:G:H21	1.54	0.73
40:L5:1414:C:H2'	40:L5:1415:G:H8	1.51	0.73
40:L5:2484:A:H62	40:L5:2494:U:H3	1.35	0.73
84:Lt:16:ARG:HH12	84:Lt:28:LEU:HB3	1.53	0.73
40:L5:2611:A:H5'	40:L5:2688:G:H4'	1.69	0.73
40:L5:3937:C:H1'	55:LN:125:SER:HB3	1.71	0.72
11:SO:52:THR:HG21	19:S2:952:G:H21	1.52	0.72
40:L5:1095:A:H2	40:L5:1200:G:N1	1.85	0.72
6:SH:144:ILE:HD11	6:SH:152:ARG:HB3	1.71	0.72
11:SO:95:ILE:HB	11:SO:129:ILE:HG22	1.72	0.72
1:SA:42:LYS:HG3	1:SA:44:ASP:H	1.55	0.72
40:L5:2458:C:H5''	55:LN:67:ARG:HD2	1.73	0.71
40:L5:1100:U:H3	40:L5:1194:G:H1	1.36	0.70
4:SE:141:THR:HG23	4:SE:143:ASP:H	1.56	0.70
24:SF:103:LEU:HD13	32:SZ:67:LEU:HB2	1.72	0.70
40:L5:1996:C:N3	40:L5:2000:G:N1	2.40	0.70
20:LR:133:LYS:N	20:LR:137:ILE:HD11	2.06	0.70
47:LE:264:ILE:HD11	47:LE:267:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SO:57:THR:H	11:SO:60:MET:HE3	1.57	0.69
40:L5:502:C:H3'	40:L5:503:C:H3'	1.75	0.69
19:S2:1581:C:H5'	19:S2:1582:C:H5	1.55	0.69
83:Ls:133:GLU:HG2	83:Ls:134:LYS:HG2	1.73	0.69
7:SI:87:ASN:HB3	7:SI:90:LEU:HD23	1.75	0.69
19:S2:1536:G:H2'	19:S2:1537:A:H8	1.58	0.69
44:LB:299:ILE:HG22	44:LB:313:SER:HB3	1.73	0.69
38:Pt:50:U:O2	38:Pt:64:G:N2	2.24	0.69
21:LW:87:LEU:HD12	21:LW:90:ILE:HD11	1.73	0.69
19:S2:928:G:H2'	19:S2:929:G:C8	2.28	0.69
1:SA:70:ASN:HB3	1:SA:73:ASP:HB2	1.74	0.68
33:Sc:17:VAL:HA	33:Sc:30:VAL:HG12	1.74	0.68
19:S2:1030:A:H2'	19:S2:1031:A2M:H8	1.75	0.68
47:LE:222:LEU:HB3	47:LE:237:LYS:HE2	1.74	0.68
23:SD:42:THR:HG22	31:SU:106:ILE:HD11	1.75	0.68
3:SC:196:ILE:HB	3:SC:223:TYR:HB2	1.76	0.68
88:L5:5291:SPM:H112	56:LO:91:LYS:HD3	1.76	0.68
26:SM:60:MET:HE3	26:SM:64:LEU:HB2	1.77	0.67
28:SQ:23:ALA:HB2	28:SQ:87:SER:HB3	1.74	0.67
5:SG:11:GLY:HA2	19:S2:166:A2M:HM'1	1.75	0.67
19:S2:1398:G:H1'	36:Sg:63:SER:HB2	1.75	0.67
19:S2:1096:G:H1	19:S2:1136:U:H3	1.43	0.67
40:L5:2303:C:H5''	70:Le:104:SER:HB3	1.77	0.67
19:S2:1228:A:H2'	19:S2:1229:G:H8	1.60	0.67
54:LM:15:VAL:HG22	54:LM:50:MET:HE1	1.76	0.67
40:L5:1095:A:N1	40:L5:1200:G:O6	2.27	0.67
26:SM:26:LEU:HA	26:SM:31:LEU:HD21	1.76	0.67
83:Ls:18:ILE:HD12	83:Ls:21:LEU:HD21	1.77	0.67
85:Zt:3:C:H41	85:Zt:70:G:H21	1.42	0.67
5:SG:170:ARG:HB3	19:S2:72:C:H42	1.61	0.66
19:S2:1513:C:H2'	19:S2:1514:G:H8	1.59	0.66
40:L5:4594:U:H2'	40:L5:4595:G:H8	1.60	0.66
43:LA:107:MET:HB3	43:LA:111:THR:HG21	1.78	0.66
31:SU:51:LYS:HB2	31:SU:90:ASP:HB2	1.78	0.66
36:Sg:157:SER:HB3	36:Sg:164:ILE:HG22	1.78	0.66
23:SD:29:LEU:HB3	23:SD:34:TYR:HB2	1.78	0.66
40:L5:2486:G:O6	40:L5:2493:G:O6	2.13	0.66
40:L5:3717:A:H2'	40:L5:3718:A2M:H8	1.76	0.65
8:SJ:54:ARG:HH12	19:S2:1:U:H5'	1.60	0.65
19:S2:1417:C:O2	19:S2:1422:G:O6	2.14	0.65
20:LR:168:GLU:HA	20:LR:171:LYS:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SH:37:LYS:HZ3	6:SH:40:LEU:HD22	1.60	0.65
7:SI:98:LYS:HB3	19:S2:377:G:H5'	1.77	0.65
3:SC:193:VAL:HG11	3:SC:240:THR:HG22	1.78	0.65
24:SF:101:HIS:HB2	24:SF:108:PRO:HG3	1.78	0.65
36:Sg:129:ILE:HB	36:Sg:142:VAL:HB	1.78	0.65
48:LF:157:ARG:HE	48:LF:248:ASN:HB2	1.61	0.65
15:SY:55:ILE:HG23	15:SY:75:ILE:HG22	1.78	0.65
2:SB:109:LYS:HG3	2:SB:113:MET:HE2	1.79	0.65
37:At:18:G:O6	37:At:55:U:O2	2.14	0.65
46:LD:208:MET:HB2	46:LD:233:PRO:HG3	1.79	0.65
76:Lk:14:THR:HA	76:Lk:17:ARG:HD3	1.79	0.65
80:Lo:6:LYS:HE2	80:Lo:94:GLY:HA3	1.77	0.65
15:SY:36:PRO:HG3	19:S2:570:C:H4'	1.79	0.64
40:L5:1942:A:H2'	40:L5:1943:A:C8	2.32	0.64
24:SF:103:LEU:HD12	32:SZ:66:LYS:HE2	1.80	0.64
16:Sa:38:LYS:HB2	16:Sa:71:LEU:HB2	1.79	0.64
40:L5:1258:G:H2'	40:L5:1259:G:C8	2.32	0.64
40:L5:2017:A:HO2'	40:L5:2018:C:H6	1.43	0.64
69:Ld:54:MET:HE3	69:Ld:60:PRO:HA	1.77	0.64
28:SQ:72:VAL:HG11	28:SQ:80:GLN:HG3	1.79	0.64
2:SB:128:LYS:HE3	2:SB:134:LEU:HD13	1.79	0.64
20:LR:169:ALA:HA	20:LR:172:ARG:HE	1.63	0.64
21:LW:9:SER:HA	21:LW:52:THR:HG23	1.80	0.63
76:Lk:13:LEU:HA	76:Lk:16:ARG:HG2	1.79	0.63
5:SG:131:ARG:HB2	21:LW:82:ILE:HG22	1.80	0.63
19:S2:1228:A:H2'	19:S2:1229:G:C8	2.33	0.63
19:S2:1396:A:N7	19:S2:1449:G:O6	2.31	0.63
65:LZ:103:ASP:HB3	65:LZ:106:LEU:HB2	1.80	0.63
4:SE:18:TRP:HH2	4:SE:31:PRO:HD3	1.62	0.63
23:SD:106:ARG:HH11	23:SD:110:LEU:HD12	1.63	0.63
19:S2:1461:G:H3'	19:S2:1463:U:H3	1.64	0.63
49:LG:205:THR:HG22	49:LG:206:GLN:H	1.62	0.63
19:S2:116:OMU:HN3	19:S2:347:G:H1	1.47	0.63
40:L5:2362:U:H2'	40:L5:2363:A2M:H8	1.81	0.63
36:Sg:208:ALA:HB2	36:Sg:218:LEU:HD13	1.80	0.63
40:L5:4111:U:H2'	40:L5:4112:C:H5	1.63	0.63
19:S2:1237:C:H5'	27:SP:131:PRO:HA	1.80	0.62
19:S2:1673:U:H5''	28:SQ:78:VAL:HG12	1.81	0.62
23:SD:143:ARG:HG3	23:SD:144:GLY:H	1.64	0.62
44:LB:165:HIS:HB3	44:LB:180:LEU:HD23	1.81	0.62
19:S2:864:A:H2'	19:S2:865:A:H8	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:LA:36:GLU:HG3	43:LA:91:GLY:HA2	1.80	0.62
19:S2:981:A:H2'	19:S2:982:G:C8	2.34	0.62
40:L5:3611:A:H2	40:L5:5016:A:H8	1.47	0.62
19:S2:1337:4AC:H2'	19:S2:1338:G:H8	1.65	0.62
40:L5:137:G:H2'	40:L5:138:G:H8	1.63	0.62
40:L5:444:G:H22	40:L5:1303:A:H2	1.47	0.62
40:L5:2554:U:O2	40:L5:2764:A:N7	2.33	0.62
17:Sb:68:GLY:HA2	19:S2:928:G:H21	1.65	0.62
40:L5:262:G:H2'	40:L5:263:G:H8	1.64	0.62
19:S2:1018:U:H2'	19:S2:1019:C:H6	1.65	0.62
36:Sg:46:THR:H	36:Sg:53:GLY:HA2	1.65	0.62
40:L5:2486:G:N7	40:L5:2493:G:N1	2.43	0.62
11:SO:15:ILE:HG23	11:SO:16:SER:H	1.62	0.62
19:S2:1452:A:C2	19:S2:1473:G:N2	2.68	0.62
69:Ld:64:ILE:HG23	69:Ld:68:LEU:HD23	1.81	0.61
19:S2:874:G:H2'	19:S2:875:A:H8	1.65	0.61
7:SI:98:LYS:HG3	7:SI:178:ARG:HG2	1.82	0.61
25:SK:80:ARG:HD3	25:SK:85:LEU:HB2	1.81	0.61
36:Sg:247:TRP:HB3	36:Sg:258:ILE:HD11	1.81	0.61
5:SG:217:MET:HG2	5:SG:221:LYS:HE2	1.82	0.61
19:S2:1706:G:H5'	79:Ln:1:MET:HG3	1.81	0.61
4:SE:29:PRO:HA	19:S2:496:C:H5'	1.82	0.61
20:LR:133:LYS:H	20:LR:137:ILE:HD11	1.66	0.61
84:Lt:37:LEU:HA	84:Lt:40:LYS:HE3	1.82	0.61
7:SI:57:ALA:HB2	7:SI:183:GLY:HA2	1.83	0.61
19:S2:1203:G:H2'	19:S2:1204:A:C8	2.36	0.61
36:Sg:17:TRP:HB2	36:Sg:36:ARG:HD2	1.83	0.61
36:Sg:106:LYS:HD3	36:Sg:126:ASP:HA	1.83	0.61
68:Lc:29:LEU:HD22	68:Lc:91:VAL:HG21	1.83	0.61
28:SQ:130:LYS:HA	28:SQ:137:ALA:HA	1.81	0.61
40:L5:691:C:H2'	40:L5:692:A:C8	2.35	0.61
45:LC:317:ASN:HD22	45:LC:320:LYS:HD3	1.64	0.61
43:LA:114:CYS:HB3	43:LA:165:VAL:HB	1.83	0.61
77:Ll:9:ILE:HD12	77:Ll:51:LEU:HD12	1.83	0.61
84:Lt:57:ARG:HD2	84:Lt:83:LYS:HB3	1.83	0.61
3:SC:173:LYS:HD3	12:SV:3:ASN:HA	1.81	0.61
10:SN:66:VAL:HG23	10:SN:67:THR:HG23	1.82	0.61
19:S2:1222:G:H2'	19:S2:1223:A:C8	2.36	0.61
40:L5:4279:A:H5'	40:L5:4281:A:H1'	1.83	0.61
43:LA:20:VAL:HA	43:LA:23:ARG:HG3	1.83	0.61
19:S2:329:G:H2'	19:S2:330:G:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1829:G:H1'	19:S2:1850:MA6:H2	1.83	0.61
40:L5:181:C:H2'	40:L5:182:G:C8	2.35	0.61
11:SO:33:ILE:HG22	11:SO:42:VAL:HA	1.83	0.60
36:Sg:206:LEU:HD12	36:Sg:218:LEU:HD12	1.83	0.60
83:Ls:59:THR:HA	83:Ls:62:ARG:HE	1.66	0.60
23:SD:106:ARG:HG2	23:SD:175:VAL:HG22	1.83	0.60
36:Sg:163:PRO:HB2	36:Sg:179:LEU:HD12	1.83	0.60
44:LB:220:ILE:HG23	44:LB:278:THR:HG22	1.84	0.60
40:L5:4615:C:H5''	44:LB:357:ARG:HD2	1.84	0.60
5:SG:22:ARG:HA	5:SG:25:ARG:HE	1.66	0.60
19:S2:956:G:H2'	19:S2:957:A:H8	1.67	0.60
40:L5:4098:A:H2'	40:L5:4099:G:H4'	1.84	0.60
19:S2:1277:C:H2'	19:S2:1278:A:H8	1.65	0.60
19:S2:1542:C:H4'	30:ST:11:GLN:HB2	1.84	0.60
50:LH:106:GLN:HB2	50:LH:111:LEU:HB3	1.83	0.60
6:SH:163:GLN:HA	6:SH:166:VAL:HG12	1.84	0.60
19:S2:323:C:H2'	19:S2:327:G:H22	1.66	0.60
40:L5:3697:U:H5''	40:L5:3698:G:H5'	1.83	0.60
49:LG:167:VAL:HG12	49:LG:170:LEU:HD12	1.84	0.60
19:S2:807:G:H2'	19:S2:808:A:H8	1.65	0.60
19:S2:1560:U:O2	19:S2:1575:G:O6	2.19	0.60
36:Sg:89:LEU:HB3	36:Sg:99:ARG:HB3	1.84	0.60
17:Sb:19:HIS:HB3	17:Sb:22:LYS:HG3	1.83	0.60
37:At:21:A:H61	37:At:46:G:H2'	1.67	0.60
37:At:29:C:H2'	37:At:30:G:H8	1.66	0.60
19:S2:71:G:H2'	19:S2:72:C:H4'	1.84	0.59
50:LH:92:MET:HE2	50:LH:179:ILE:HG22	1.84	0.59
5:SG:227:GLN:HB3	5:SG:231:ARG:HH21	1.67	0.59
6:SH:105:THR:HG23	6:SH:107:LYS:H	1.67	0.59
14:SX:107:ARG:HD3	14:SX:112:VAL:HG22	1.84	0.59
40:L5:2763:U:H4'	40:L5:2764:A:H5''	1.84	0.59
19:S2:1711:U:H2'	19:S2:1712:A:H8	1.68	0.59
21:LW:1:MET:HE2	44:LB:307:TYR:HB3	1.85	0.59
24:SF:34:SER:HA	33:Sc:55:VAL:HG13	1.83	0.59
84:Lt:106:PHE:HB2	84:Lt:109:ILE:HG12	1.84	0.59
3:SC:210:PRO:HD3	3:SC:236:PHE:HE2	1.68	0.59
40:L5:3717:A:H2'	40:L5:3718:A2M:C8	2.32	0.59
40:L5:3868:G:H22	40:L5:3900:G:H1'	1.66	0.59
59:LS:27:LEU:HB3	60:LT:148:PRO:HB3	1.85	0.59
57:LP:131:ARG:HG3	57:LP:137:ASN:OD1	2.02	0.59
83:Ls:53:VAL:HG23	83:Ls:89:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1634:A:H4'	29:SS:142:ARG:HH21	1.67	0.59
40:L5:5016:A:C2	40:L5:5033:G:N2	2.67	0.59
19:S2:166:A2M:H2'	19:S2:167:G:H8	1.68	0.59
19:S2:525:A:H2'	19:S2:526:A:H8	1.68	0.59
68:Lc:38:ILE:HD11	68:Lc:46:VAL:HG21	1.85	0.59
2:SB:57:ILE:HG22	2:SB:59:SER:H	1.67	0.59
64:LY:33:PRO:HG2	64:LY:105:VAL:HG12	1.84	0.59
2:SB:191:ASP:HB3	2:SB:195:LYS:HZ3	1.67	0.59
3:SC:94:ILE:HD11	3:SC:159:LYS:HG2	1.83	0.59
40:L5:3944:G:O6	40:L5:4069:U:O4	2.21	0.58
19:S2:907:G:H2'	19:S2:908:A:H8	1.68	0.58
19:S2:1536:G:H2'	19:S2:1537:A:C8	2.37	0.58
19:S2:1652:G:O6	19:S2:1672:U:O4	2.21	0.58
40:L5:1503:A:H62	58:LQ:87:THR:HG21	1.68	0.58
40:L5:1339:U:H2'	40:L5:1340:OMC:C6	2.38	0.58
40:L5:4967:A:H2'	40:L5:4968:A:H8	1.69	0.58
40:L5:966:A:H5''	40:L5:2092:G:H22	1.66	0.58
19:S2:145:G:H2'	19:S2:146:G:C8	2.39	0.58
19:S2:1433:C:H42	31:SU:92:HIS:HD2	1.50	0.58
38:Pt:62:C:H2'	38:Pt:63:G:H8	1.68	0.58
40:L5:1732:C:H5''	60:LT:43:LYS:HE2	1.85	0.58
46:LD:238:GLU:HG3	46:LD:242:LYS:HE2	1.86	0.58
19:S2:587:A:H5'	19:S2:592:C:H41	1.68	0.58
19:S2:614:C:H2'	19:S2:626:G:C8	2.39	0.58
40:L5:2517:A:H5'	72:Lg:62:LYS:HD3	1.86	0.58
19:S2:907:G:H2'	19:S2:908:A:C8	2.38	0.58
40:L5:4954:G:H2'	40:L5:4955:A:C8	2.38	0.58
54:LM:104:MET:HE3	54:LM:109:ARG:HG2	1.86	0.58
36:Sg:106:LYS:HE2	36:Sg:125:ARG:HB3	1.85	0.58
50:LH:95:VAL:HG12	78:Lm:82:LEU:HD13	1.86	0.58
11:SO:66:ARG:HG2	19:S2:962:A:H5''	1.86	0.57
27:SP:22:LEU:HA	27:SP:25:LEU:HB2	1.86	0.57
38:Pt:29:C:H2'	38:Pt:30:G:H8	1.69	0.57
48:LF:127:LYS:HB2	60:LT:133:ALA:HB3	1.84	0.57
1:SA:145:ILE:HG12	1:SA:159:ILE:HD13	1.86	0.57
36:Sg:107:ASP:HB2	36:Sg:125:ARG:HD2	1.85	0.57
17:Sb:22:LYS:HE3	19:S2:1129:G:H5''	1.85	0.57
19:S2:1337:4AC:H2'	19:S2:1338:G:C8	2.39	0.57
56:LO:37:ARG:HD2	56:LO:108:ILE:HD11	1.87	0.57
19:S2:640:A:H2'	19:S2:641:A:C8	2.39	0.57
40:L5:1959:U:H5''	40:L5:1961:G:H1'	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LH:93:ARG:HD2	50:LH:143:GLU:HG2	1.86	0.57
83:Ls:62:ARG:HB3	83:Ls:66:ARG:HH22	1.68	0.57
40:L5:490:C:H2'	40:L5:491:G:C8	2.40	0.57
40:L5:1994:C:H2'	40:L5:1995:G:C8	2.39	0.57
83:Ls:138:PHE:HZ	83:Ls:178:LEU:HD13	1.70	0.57
37:At:50:U:O4	37:At:64:G:O6	2.22	0.57
26:SM:128:PHE:HA	26:SM:131:LYS:HG2	1.87	0.57
36:Sg:233:GLY:H	36:Sg:257:LYS:HZ1	1.52	0.57
19:S2:1405:A:H2'	19:S2:1406:G:O4'	2.04	0.57
19:S2:1553:C:H41	34:Sd:22:ARG:HH12	1.52	0.57
40:L5:1332:C:H2'	40:L5:1333:A:H8	1.70	0.57
80:Lo:64:LYS:HE2	85:Zt:76:A:H5''	1.87	0.57
19:S2:201:C:H3'	19:S2:202:G:H21	1.70	0.56
40:L5:1961:G:H21	40:L5:2025:A:H62	1.53	0.56
40:L5:4935:C:H2'	40:L5:4936:G:C8	2.40	0.56
12:SV:71:ARG:HH11	17:Sb:4:ALA:HB2	1.70	0.56
27:SP:108:LYS:HD2	29:SS:117:ILE:HG22	1.87	0.56
47:LE:165:LEU:HD11	47:LE:176:THR:HG22	1.86	0.56
6:SH:154:ILE:HB	6:SH:185:VAL:HG22	1.87	0.56
19:S2:573:U:O2	19:S2:576:A2M:H8	2.05	0.56
40:L5:93:G:H2'	40:L5:94:A:C8	2.41	0.56
40:L5:4106:G:H3'	40:L5:4107:G:H8	1.70	0.56
47:LE:149:ILE:HD12	47:LE:271:LEU:HD21	1.86	0.56
56:LO:166:ILE:HG12	56:LO:169:ARG:HH21	1.70	0.56
6:SH:33:ASN:HD21	6:SH:37:LYS:HE3	1.71	0.56
19:S2:690:G:H3'	19:S2:691:G:H21	1.70	0.56
19:S2:1590:C:H42	28:SQ:77:HIS:HE1	1.51	0.56
25:SK:3:MET:HE1	25:SK:48:ALA:HB2	1.86	0.56
8:SJ:54:ARG:HD2	8:SJ:58:ARG:HH12	1.71	0.56
9:SL:61:PRO:HB3	9:SL:68:ILE:HD11	1.88	0.56
13:SW:111:MET:HE1	13:SW:119:LYS:HD2	1.88	0.56
20:LR:170:ARG:HH12	20:LR:174:GLU:HG2	1.70	0.56
22:SR:5:ARG:HB2	22:SR:10:LYS:HE3	1.87	0.56
64:LY:22:PRO:HD2	64:LY:25:ILE:HD11	1.87	0.56
19:S2:671:A:H4'	19:S2:672:A:H5''	1.87	0.56
27:SP:81:ARG:HB2	27:SP:117:GLY:HA3	1.87	0.56
31:SU:61:LEU:HB2	31:SU:82:MET:HB3	1.88	0.56
40:L5:2108:G:H2'	40:L5:2109:G:H8	1.71	0.56
54:LM:119:ARG:HG3	56:LO:189:ILE:HG23	1.88	0.56
19:S2:106:C:H2'	19:S2:107:A:H8	1.71	0.56
19:S2:1711:U:H2'	19:S2:1712:A:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:2483:G:O6	40:L5:2495:U:O2	2.23	0.56
68:Lc:22:MET:O	68:Lc:23:LYS:HG3	2.05	0.56
5:SG:10:THR:HA	5:SG:128:THR:HG23	1.87	0.56
8:SJ:18:ARG:HH21	19:S2:4:C:H1'	1.71	0.56
19:S2:1010:G:H2'	19:S2:1011:A:H8	1.70	0.56
22:SR:79:GLU:HA	22:SR:82:ASP:OD1	2.06	0.56
31:SU:67:LYS:HG2	31:SU:78:ASP:HB2	1.88	0.56
40:L5:280:G:H5''	55:LN:14:LYS:HE2	1.88	0.56
18:Se:36:MET:HE3	18:Se:40:ARG:HH12	1.71	0.56
19:S2:562:U:H2'	19:S2:563:G:C8	2.41	0.56
36:Sg:256:ILE:HB	36:Sg:270:LEU:HB2	1.88	0.56
40:L5:4274:A:H2'	40:L5:4275:G:C8	2.40	0.56
51:LI:207:ASP:HA	51:LI:210:ARG:HG2	1.88	0.56
1:SA:122:LEU:HB3	1:SA:144:THR:HG22	1.87	0.56
6:SH:144:ILE:HD13	6:SH:154:ILE:HG13	1.88	0.56
19:S2:528:A:H2'	19:S2:529:A:C8	2.41	0.56
19:S2:1201:U:H2'	19:S2:1202:U:C6	2.41	0.56
32:SZ:99:LEU:HD21	32:SZ:102:LYS:HB2	1.87	0.56
40:L5:4260:U:H2'	40:L5:4261:C:C6	2.41	0.56
16:Sa:79:ILE:HD11	19:S2:1864:U:H5'	1.87	0.55
26:SM:31:LEU:HB3	26:SM:33:ARG:HG3	1.88	0.55
36:Sg:145:GLU:HB3	36:Sg:177:TRP:HH2	1.70	0.55
40:L5:1996:C:O2	40:L5:2000:G:O6	2.23	0.55
40:L5:3898:G:H5'	44:LB:254:ILE:HG13	1.88	0.55
43:LA:31:ALA:HB2	43:LA:123:ARG:HH21	1.71	0.55
11:SO:129:ILE:HD11	16:Sa:65:PRO:HD2	1.88	0.55
19:S2:639:C:H2'	19:S2:640:A:H8	1.71	0.55
19:S2:885:U:O2	19:S2:901:G:O6	2.24	0.55
19:S2:1203:G:H2'	19:S2:1204:A:H8	1.71	0.55
29:SS:22:GLY:HA2	29:SS:56:ALA:HB3	1.88	0.55
38:Pt:62:C:H2'	38:Pt:63:G:C8	2.40	0.55
40:L5:135:G:H22	73:Lh:94:ARG:HG3	1.70	0.55
8:SJ:176:LYS:HA	8:SJ:179:LYS:HG2	1.89	0.55
11:SO:31:CYS:HB2	11:SO:93:LEU:HD13	1.87	0.55
13:SW:57:ARG:HH21	17:Sb:26:GLN:HB2	1.72	0.55
36:Sg:20:GLN:HB3	36:Sg:34:ALA:HB3	1.88	0.55
40:L5:2108:G:H2'	40:L5:2109:G:C8	2.41	0.55
43:LA:13:GLY:O	43:LA:17:ARG:HG3	2.06	0.55
46:LD:55:VAL:HG11	46:LD:158:LYS:HE3	1.87	0.55
57:LP:52:THR:HG23	57:LP:85:LYS:HG3	1.89	0.55
17:Sb:56:CYS:HB2	17:Sb:59:CYS:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:908:G:H2'	40:L5:909:A:H8	1.71	0.55
5:SG:2:LYS:HB2	5:SG:108:VAL:HG12	1.89	0.55
6:SH:36:LEU:HD21	6:SH:78:ARG:HH21	1.72	0.55
19:S2:1383:A2M:H4'	23:SD:156:LEU:HD22	1.87	0.55
35:Sf:108:VAL:HB	35:Sf:112:GLY:HA2	1.89	0.55
40:L5:1629:G:H1	43:LA:208:GLU:HG2	1.70	0.55
40:L5:4992:G:H2'	40:L5:4993:G:C8	2.41	0.55
3:SC:78:LEU:HD12	3:SC:81:ILE:HD12	1.89	0.55
19:S2:329:G:H2'	19:S2:330:G:H8	1.71	0.55
38:Pt:6:C:H2'	38:Pt:7:G:H8	1.71	0.55
40:L5:268:G:H2'	40:L5:269:G:H8	1.71	0.55
40:L5:4967:A:H2'	40:L5:4968:A:C8	2.42	0.55
61:LU:65:ARG:HG2	61:LU:67:LYS:H	1.72	0.55
3:SC:104:ASP:HA	3:SC:130:ILE:HG22	1.89	0.55
47:LE:72:LYS:HD3	67:Lb:119:CYS:HB3	1.88	0.55
47:LE:223:ARG:HH22	47:LE:238:GLU:HG3	1.71	0.55
40:L5:4363:A:H5''	80:Lo:36:GLN:HG2	1.87	0.55
40:L5:4618:OMG:HM22	40:L5:4619:U:H5'	1.88	0.55
43:LA:112:ILE:HD11	81:Lp:79:VAL:HG22	1.89	0.55
21:LW:78:PHE:HE1	21:LW:80:ARG:HH11	1.54	0.55
28:SQ:19:ALA:HB2	28:SQ:75:GLY:HA3	1.87	0.55
4:SE:252:ARG:HH21	8:SJ:72:PHE:HD1	1.53	0.55
24:SF:103:LEU:HD22	32:SZ:67:LEU:HD22	1.87	0.55
40:L5:2765:A:H2'	40:L5:2766:A:C8	2.41	0.55
19:S2:1512:C:H5''	34:Sd:8:TRP:HZ3	1.72	0.54
40:L5:2557:G:O6	40:L5:2570:U:O4	2.25	0.54
55:LN:124:ASP:HB3	55:LN:127:TYR:H	1.72	0.54
40:L5:1095:A:N1	40:L5:1200:G:C6	2.75	0.54
44:LB:57:VAL:HG22	44:LB:73:VAL:HG12	1.89	0.54
81:Lp:38:THR:HA	81:Lp:45:THR:HA	1.88	0.54
8:SJ:3:VAL:HB	8:SJ:5:ARG:HD3	1.89	0.54
19:S2:557:U:H2'	19:S2:558:G:C8	2.42	0.54
40:L5:171:U:H4'	53:LL:135:LYS:HG2	1.89	0.54
40:L5:4571:A2M:H2'	40:L5:4572:U:H6	1.72	0.54
19:S2:28:U:H2'	19:S2:29:G:H8	1.71	0.54
19:S2:1417:C:N3	19:S2:1422:G:N1	2.51	0.54
40:L5:513:U:H1'	40:L5:516:C:H41	1.72	0.54
40:L5:1942:A:H2'	40:L5:1943:A:H8	1.73	0.54
84:Lt:12:VAL:HG11	84:Lt:65:GLN:H	1.73	0.54
19:S2:527:C:H2'	19:S2:528:A:C8	2.43	0.54
76:Lk:25:ILE:HD13	76:Lk:57:LYS:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SG:7:PHE:HB3	5:SG:10:THR:HG22	1.89	0.54
40:L5:2640:G:H2'	40:L5:2641:A:C8	2.43	0.54
40:L5:3720:G:H22	40:L5:3733:A:H2	1.54	0.54
44:LB:217:ILE:HD12	44:LB:347:LEU:HB3	1.87	0.54
4:SE:159:THR:HB	4:SE:173:ILE:HB	1.89	0.54
15:SY:83:LYS:HA	15:SY:91:LEU:HD11	1.89	0.54
29:SS:84:LEU:HB2	29:SS:87:GLN:HG2	1.89	0.54
40:L5:2018:C:H2'	40:L5:2019:C:C6	2.43	0.54
80:Lo:4:VAL:HG23	80:Lo:93:LEU:HD12	1.90	0.54
38:Pt:23:C:H2'	38:Pt:24:A:C8	2.43	0.54
40:L5:3910:C:H2'	40:L5:3911:C:C6	2.43	0.54
8:SJ:88:ASP:HB3	8:SJ:91:LYS:HB2	1.90	0.54
40:L5:261:G:H2'	40:L5:262:G:C8	2.42	0.54
40:L5:2903:G:H1'	40:L5:2904:U:H5	1.73	0.54
64:LY:10:ASP:HB3	64:LY:13:LYS:HB2	1.90	0.54
4:SE:106:LYS:HB3	4:SE:108:ARG:HH12	1.71	0.54
36:Sg:191:HIS:CE1	36:Sg:195:LEU:HD21	2.43	0.54
40:L5:4274:A:H2'	40:L5:4275:G:H8	1.73	0.54
56:LO:81:TRP:HB2	56:LO:104:VAL:HG21	1.89	0.54
84:Lt:114:ARG:HE	84:Lt:117:ARG:HD2	1.73	0.54
5:SG:133:LEU:HD12	19:S2:65:C:C4	2.42	0.53
11:SO:55:ARG:HH12	19:S2:972:A:H61	1.54	0.53
19:S2:149:A:N7	19:S2:169:U:O2	2.40	0.53
40:L5:2870:A:H2'	40:L5:2871:A:C8	2.43	0.53
56:LO:168:TYR:CE2	56:LO:172:LYS:HD2	2.42	0.53
65:LZ:50:PRO:HD3	65:LZ:68:ILE:HG12	1.89	0.53
3:SC:125:LYS:HG3	3:SC:143:CYS:HB2	1.90	0.53
6:SH:51:ILE:HG21	6:SH:179:LYS:HG2	1.89	0.53
40:L5:461:G:H2'	40:L5:462:G:H8	1.73	0.53
40:L5:746:A:H2'	40:L5:747:A:C8	2.43	0.53
40:L5:4260:U:H2'	40:L5:4261:C:H6	1.74	0.53
82:Lr:90:LEU:HD22	82:Lr:111:ILE:HG23	1.90	0.53
19:S2:996:A:H2'	19:S2:997:A:C8	2.43	0.53
19:S2:1348:G:O6	19:S2:1381:G:N2	2.36	0.53
19:S2:1417:C:H42	19:S2:1422:G:N2	2.04	0.53
40:L5:460:C:H2'	40:L5:461:G:H8	1.73	0.53
40:L5:2744:A:H2'	40:L5:2745:A:C8	2.43	0.53
19:S2:851:C:H5''	19:S2:852:G:H5'	1.91	0.53
19:S2:1468:C:H2'	19:S2:1469:A:H8	1.73	0.53
24:SF:20:PHE:HB3	24:SF:94:LYS:HZ3	1.74	0.53
40:L5:518:G:H1	40:L5:643:C:H2'	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1458:C:H5''	58:LQ:69:LYS:HD2	1.90	0.53
40:L5:1995:G:H21	84:Lt:122:ALA:HB3	1.72	0.53
40:L5:4935:C:H2'	40:L5:4936:G:H8	1.72	0.53
67:Lb:111:ARG:HA	67:Lb:114:LYS:HE2	1.89	0.53
1:SA:76:VAL:HG12	1:SA:123:VAL:HB	1.91	0.53
15:SY:10:ARG:HA	19:S2:839:C:H41	1.74	0.53
19:S2:1850:MA6:H8	19:S2:1850:MA6:O5'	2.09	0.53
40:L5:1437:C:H1'	40:L5:2098:G:H3'	1.90	0.53
40:L5:3910:C:H2'	40:L5:3911:C:H6	1.73	0.53
2:SB:65:ARG:H	2:SB:88:THR:HG22	1.73	0.53
6:SH:160:LYS:HB2	6:SH:189:PHE:HB3	1.90	0.53
19:S2:588:G:H4'	19:S2:589:G:H5'	1.91	0.53
38:Pt:43:A:H2'	38:Pt:44:A:C8	2.44	0.53
40:L5:518:G:N1	40:L5:643:C:H2'	2.24	0.53
40:L5:717:U:H2'	40:L5:718:C:C6	2.43	0.53
40:L5:4748:U:H3	40:L5:4952:G:H1	1.54	0.53
40:L5:4920:C:H2'	40:L5:4921:C:H6	1.73	0.53
57:LP:16:LYS:HG2	57:LP:149:ILE:HG12	1.91	0.53
11:SO:101:GLY:HA3	11:SO:134:PRO:HD2	1.90	0.53
19:S2:49:C:H2'	19:S2:472:C:H41	1.74	0.53
19:S2:1845:A:H2'	19:S2:1846:G:C8	2.43	0.53
22:SR:98:VAL:HG21	22:SR:117:LEU:HB3	1.90	0.53
29:SS:40:TYR:HA	29:SS:83:PHE:HE2	1.74	0.53
31:SU:66:ARG:HH12	31:SU:75:LYS:HD3	1.72	0.53
34:Sd:22:ARG:HG3	34:Sd:23:VAL:HG23	1.90	0.53
40:L5:1972:G:C6	40:L5:1973:G:O6	2.62	0.53
5:SG:23:LYS:HD3	5:SG:41:LEU:HA	1.91	0.53
19:S2:864:A:H2'	19:S2:865:A:C8	2.44	0.53
19:S2:1144:A:H2'	19:S2:1145:A:C8	2.44	0.53
40:L5:1327:C:H2'	40:L5:1328:G:C8	2.44	0.53
40:L5:1617:G:H1'	40:L5:2513:A:N6	2.24	0.53
40:L5:4242:U:H3	40:L5:4281:A:H2	1.55	0.53
3:SC:167:ARG:HB3	3:SC:177:PRO:HB2	1.90	0.53
7:SI:114:GLU:HB3	7:SI:136:ILE:HD12	1.90	0.53
40:L5:4220:6MZ:H2'	40:L5:4222:G:H5''	1.90	0.53
64:LY:56:GLN:HB3	64:LY:67:ILE:HD13	1.90	0.53
14:SX:28:LYS:HD2	14:SX:32:LEU:HD22	1.91	0.53
19:S2:166:A2M:H2'	19:S2:167:G:C8	2.44	0.53
19:S2:1657:G:H1	19:S2:1667:U:H3	1.56	0.53
36:Sg:174:VAL:HB	36:Sg:188:HIS:HB2	1.91	0.53
40:L5:71:C:H1'	53:LL:62:PRO:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1972:G:H2'	40:L5:1973:G:C8	2.44	0.53
2:SB:186:ASN:HA	2:SB:189:ILE:HD12	1.91	0.52
8:SJ:127:ARG:HD3	18:Se:31:ARG:HD3	1.89	0.52
20:LR:127:VAL:HG12	20:LR:132:PHE:HD2	1.74	0.52
40:L5:497:G:H1	40:L5:657:C:H42	1.57	0.52
47:LE:274:VAL:HG21	71:Lf:2:SER:HB2	1.91	0.52
52:LJ:146:ARG:HG2	52:LJ:147:ARG:HG3	1.91	0.52
62:LV:42:VAL:HB	62:LV:45:ILE:HG13	1.89	0.52
1:SA:85:ARG:HD3	1:SA:203:PHE:O	2.08	0.52
2:SB:170:GLU:HA	2:SB:173:THR:HG22	1.92	0.52
19:S2:1310:U:H2'	19:S2:1311:C:H6	1.74	0.52
5:SG:2:LYS:HD3	5:SG:15:LEU:HD21	1.91	0.52
32:SZ:65:TYR:HB3	85:Zt:34:U:H5'	1.89	0.52
36:Sg:175:LYS:HB3	36:Sg:184:LEU:HD11	1.92	0.52
9:SL:93:LEU:HB3	9:SL:102:PHE:HB3	1.91	0.52
14:SX:67:ARG:HG3	14:SX:115:ILE:HG12	1.91	0.52
19:S2:1101:U:H2'	19:S2:1102:G:H8	1.74	0.52
30:ST:64:LEU:HD12	30:ST:122:LYS:HA	1.92	0.52
36:Sg:164:ILE:HD11	36:Sg:185:LYS:HG3	1.91	0.52
40:L5:2696:A:H62	76:Lk:35:LYS:NZ	2.08	0.52
40:L5:4281:A:H2'	40:L5:4282:A:H2'	1.90	0.52
13:SW:107:SER:HB2	19:S2:860:G:H21	1.75	0.52
15:SY:11:LYS:HB2	15:SY:24:VAL:HG12	1.92	0.52
16:Sa:26:CYS:HB3	16:Sa:77:CYS:SG	2.49	0.52
45:LC:110:ARG:HB2	55:LN:204:ARG:HH21	1.73	0.52
48:LF:105:VAL:HG13	48:LF:136:VAL:HG12	1.92	0.52
5:SG:3:LEU:HD23	5:SG:109:LEU:HB3	1.91	0.52
36:Sg:249:CYS:HB3	36:Sg:258:ILE:HD13	1.92	0.52
40:L5:3641:U:H5	40:L5:3646:A:N7	2.08	0.52
5:SG:135:PRO:HG2	5:SG:141:ILE:HG22	1.90	0.52
33:Sc:11:LEU:HB2	33:Sc:35:MET:HE2	1.92	0.52
49:LG:121:LYS:HG2	49:LG:126:GLY:HA2	1.91	0.52
34:Sd:3:HIS:CE1	34:Sd:5:GLN:HB2	2.45	0.52
40:L5:1503:A:H4'	40:L5:1504:G:H5'	1.92	0.52
19:S2:564:A:H2'	19:S2:565:G:O4'	2.09	0.52
19:S2:1394:G:H21	19:S2:1475:G:H1'	1.74	0.52
23:SD:99:ILE:HG23	23:SD:173:ARG:HH21	1.75	0.52
40:L5:1179:U:H3'	40:L5:1180:C:H5''	1.91	0.52
40:L5:1333:A:H2'	40:L5:1334:A:C8	2.45	0.52
40:L5:1933:G:H2'	40:L5:1934:A:C8	2.45	0.52
40:L5:4743:G:H2'	40:L5:4744:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SG:121:ILE:HB	5:SG:124:LEU:HB3	1.91	0.52
9:SL:111:VAL:HG12	9:SL:140:PHE:HB2	1.91	0.52
13:SW:6:VAL:HG12	13:SW:34:ILE:HD11	1.92	0.52
19:S2:149:A:H3'	19:S2:150:A:H8	1.75	0.52
29:SS:114:LEU:HD13	29:SS:117:ILE:HD11	1.92	0.52
40:L5:1100:U:O4	40:L5:1194:G:O6	2.28	0.52
40:L5:2557:G:N2	40:L5:2570:U:O2	2.30	0.52
40:L5:2613:C:H4'	72:Lg:2:VAL:HG23	1.92	0.52
40:L5:4113:U:H4'	40:L5:4115:G:C5	2.45	0.52
6:SH:144:ILE:HG23	13:SW:52:ILE:HB	1.92	0.51
19:S2:656:G:N2	19:S2:663:C:H5''	2.25	0.51
38:Pt:51:C:H2'	38:Pt:52:G:H8	1.76	0.51
40:L5:2745:A:H2'	40:L5:2746:A:C8	2.45	0.51
3:SC:68:ARG:HG2	3:SC:277:HIS:HB2	1.93	0.51
11:SO:62:VAL:HG21	11:SO:67:ASP:HB2	1.92	0.51
40:L5:3732:A:H2'	40:L5:3733:A:H8	1.75	0.51
44:LB:117:ARG:HA	44:LB:177:LYS:HD2	1.92	0.51
66:La:72:THR:HG22	66:La:110:LYS:HB3	1.92	0.51
82:Lr:41:ASN:HB3	82:Lr:44:ILE:HG12	1.92	0.51
84:Lt:134:GLY:HA3	84:Lt:152:ILE:HD11	1.92	0.51
19:S2:349:A:H2'	19:S2:350:C:C6	2.46	0.51
19:S2:484:A2M:H8	19:S2:484:A2M:O5'	2.10	0.51
40:L5:1188:C:H2'	40:L5:1189:G:C8	2.46	0.51
51:LI:85:PHE:HE2	51:LI:87:MET:HE2	1.75	0.51
4:SE:36:HIS:CG	4:SE:85:GLY:HA3	2.46	0.51
6:SH:142:LYS:HB3	13:SW:54:ASP:HB3	1.92	0.51
6:SH:148:LEU:HA	13:SW:42:MET:HE2	1.92	0.51
19:S2:12:U:H2'	19:S2:13:C:C6	2.45	0.51
19:S2:807:G:H2'	19:S2:808:A:C8	2.45	0.51
29:SS:45:LEU:HD13	29:SS:50:ILE:HD11	1.91	0.51
40:L5:418:A:C2	42:L8:17:A:H1'	2.46	0.51
40:L5:683:C:H2'	40:L5:684:G:O4'	2.10	0.51
40:L5:1281:G:N1	47:LE:128:HIS:HB2	2.25	0.51
40:L5:2298:U:H5''	45:LC:204:ARG:HH12	1.75	0.51
48:LF:50:ILE:HD12	48:LF:186:CYS:HB3	1.93	0.51
82:Lr:47:LYS:HB2	82:Lr:102:TYR:CZ	2.45	0.51
5:SG:20:ASP:HB3	5:SG:23:LYS:HG3	1.91	0.51
40:L5:10:A:H2'	40:L5:11:G:C8	2.46	0.51
40:L5:2745:A:H2'	40:L5:2746:A:H8	1.76	0.51
21:LW:96:GLN:HB3	21:LW:100:VAL:HB	1.92	0.51
37:At:3:C:H42	37:At:70:A:H61	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:158:A:H5''	40:L5:159:C:H2'	1.93	0.51
17:Sb:20:LYS:HA	17:Sb:23:ARG:HE	1.76	0.51
19:S2:496:C:H2'	19:S2:497:C:H6	1.76	0.51
40:L5:2481:G:H2'	40:L5:2482:C:C6	2.46	0.51
19:S2:1468:C:H2'	19:S2:1469:A:C8	2.46	0.51
19:S2:1755:C:H2'	19:S2:1756:C:C6	2.46	0.51
38:Pt:6:C:H2'	38:Pt:7:G:C8	2.46	0.51
40:L5:189:G:H2'	40:L5:190:G:H8	1.76	0.51
40:L5:3712:A:C5	40:L5:3713:U:H1'	2.46	0.51
40:L5:4508:C:N3	40:L5:4512:U:H5	2.08	0.51
40:L5:4537:C:H2'	40:L5:4538:G:H8	1.73	0.51
40:L5:711:A:H2'	40:L5:712:C:C6	2.46	0.51
40:L5:1308:C:H2'	40:L5:1309:C:C6	2.46	0.51
40:L5:4594:U:H2'	40:L5:4595:G:C8	2.42	0.51
62:LV:69:LYS:HB2	62:LV:72:LEU:HD12	1.93	0.51
4:SE:129:ILE:HD13	4:SE:139:LEU:HD12	1.93	0.51
18:Se:58:ASN:HB3	19:S2:608:C:H5'	1.93	0.51
19:S2:107:A:H2'	19:S2:108:G:C8	2.45	0.51
19:S2:304:C:H5''	19:S2:305:U:H5'	1.93	0.51
19:S2:874:G:H2'	19:S2:875:A:C8	2.45	0.51
40:L5:2544:G:H22	42:L8:124:U:H4'	1.76	0.51
69:Ld:22:THR:HG23	69:Ld:122:VAL:HG13	1.93	0.51
2:SB:65:ARG:HE	11:SO:50:LYS:HD3	1.76	0.50
19:S2:1822:A:H2'	19:S2:1823:A:C8	2.47	0.50
85:Zt:28:C:H2'	85:Zt:29:A:H8	1.76	0.50
1:SA:148:CYS:N	1:SA:148:CYS:SG	2.85	0.50
19:S2:1396:A:C5	19:S2:1449:G:O6	2.64	0.50
23:SD:227:LYS:H	36:Sg:186:THR:HA	1.75	0.50
40:L5:1258:G:H2'	40:L5:1259:G:H8	1.76	0.50
40:L5:1348:U:H2'	40:L5:1349:G:H8	1.77	0.50
40:L5:4537:C:H2'	40:L5:4538:G:C8	2.46	0.50
40:L5:4954:G:H2'	40:L5:4955:A:H8	1.76	0.50
42:L8:141:C:H2'	42:L8:142:U:C6	2.46	0.50
55:LN:183:THR:HG22	55:LN:188:ARG:HD2	1.93	0.50
5:SG:158:VAL:HG21	21:LW:82:ILE:HD11	1.93	0.50
19:S2:66:G:H2'	19:S2:67:C:H4'	1.92	0.50
19:S2:1748:G:O6	19:S2:1786:U:O4	2.28	0.50
32:SZ:87:ALA:HA	32:SZ:90:GLU:HG2	1.94	0.50
38:Pt:23:C:H2'	38:Pt:24:A:H8	1.76	0.50
40:L5:2007:G:H21	40:L5:2012:A:H62	1.60	0.50
19:S2:434:G:H2'	19:S2:435:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1417:C:N4	19:S2:1422:G:H22	2.05	0.50
24:SF:60:ARG:HH21	33:Sc:49:PRO:HA	1.77	0.50
40:L5:460:C:H2'	40:L5:461:G:C8	2.47	0.50
46:LD:181:PRO:HD2	46:LD:195:HIS:CD2	2.47	0.50
47:LE:222:LEU:HD21	47:LE:226:ARG:HH22	1.75	0.50
7:SI:146:GLN:HA	7:SI:149:TYR:HD2	1.76	0.50
8:SJ:54:ARG:HH11	8:SJ:58:ARG:HH12	1.58	0.50
16:Sa:15:ARG:HG3	19:S2:993:G:O6	2.12	0.50
19:S2:609:U:H2'	19:S2:610:G:H8	1.76	0.50
19:S2:1447:G:H2'	19:S2:1448:A:C8	2.46	0.50
37:At:29:C:H2'	37:At:30:G:C8	2.45	0.50
57:LP:122:ALA:HB3	57:LP:143:PRO:HG2	1.92	0.50
72:Lg:83:CYS:SG	72:Lg:86:CYS:HB2	2.50	0.50
7:SI:22:HIS:HB3	19:S2:433:A:H5''	1.94	0.50
22:SR:78:ARG:O	22:SR:82:ASP:N	2.45	0.50
37:At:43:A:H2'	37:At:44:A:C8	2.46	0.50
40:L5:1697:G:H22	40:L5:2084:C:P	2.34	0.50
16:Sa:11:ALA:HB3	16:Sa:33:ASP:HB2	1.93	0.50
19:S2:647:U:H2'	19:S2:648:A:H8	1.76	0.50
46:LD:197:LYS:HB3	46:LD:202:GLN:HB2	1.94	0.50
56:LO:54:TYR:CD1	56:LO:145:VAL:HG21	2.47	0.50
1:SA:42:LYS:HZ3	1:SA:46:ILE:HB	1.76	0.50
15:SY:12:PHE:HD1	15:SY:23:MET:HB3	1.75	0.50
19:S2:367:U:H4'	19:S2:371:A:C8	2.46	0.50
36:Sg:149:GLU:HB3	36:Sg:170:TRP:HB2	1.93	0.50
40:L5:2568:C:H2'	40:L5:2569:G:H8	1.77	0.50
40:L5:4405:G:H4'	51:LI:4:ARG:HE	1.75	0.50
53:LL:153:PRO:HG2	53:LL:156:PRO:HB3	1.93	0.50
69:Ld:90:ARG:HD3	69:Ld:102:LEU:HD13	1.92	0.50
73:Lh:99:GLU:HA	73:Lh:102:LEU:HD23	1.93	0.50
16:Sa:23:CYS:HB3	16:Sa:28:ARG:H	1.77	0.50
27:SP:130:ARG:HD3	27:SP:131:PRO:HD2	1.93	0.50
36:Sg:220:ASP:HB3	36:Sg:224:GLY:H	1.77	0.50
40:L5:318:A:H2'	40:L5:319:A:C8	2.47	0.50
40:L5:3911:C:H2'	40:L5:3912:U:H6	1.76	0.50
40:L5:4612:C:C2	50:LH:120:GLU:HB2	2.47	0.50
44:LB:43:LEU:HD12	44:LB:205:VAL:HG11	1.94	0.50
44:LB:258:HIS:HA	44:LB:260:ALA:N	2.26	0.50
80:Lo:22:LYS:HG3	80:Lo:73:VAL:HG12	1.93	0.50
83:Ls:39:GLN:HG3	83:Ls:107:VAL:HG21	1.93	0.50
1:SA:30:LEU:HD21	1:SA:35:GLU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1670:C:H2'	19:S2:1671:G:H8	1.77	0.49
23:SD:74:GLN:HE22	23:SD:81:GLU:HA	1.77	0.49
61:LU:24:ASP:HB3	61:LU:111:GLU:HG2	1.93	0.49
83:Ls:155:LEU:HD12	83:Ls:156:SER:HB3	1.94	0.49
19:S2:1217:A:H2'	19:S2:1218:C:C6	2.47	0.49
25:SK:63:ALA:HB2	25:SK:68:TYR:HE2	1.77	0.49
28:SQ:78:VAL:HA	28:SQ:81:ILE:HD12	1.94	0.49
40:L5:1973:G:H3'	40:L5:1974:U:H2'	1.94	0.49
42:L8:96:C:H5''	73:Lh:66:LYS:HG2	1.93	0.49
23:SD:60:GLY:HA3	23:SD:65:ARG:H	1.77	0.49
32:SZ:52:LYS:NZ	32:SZ:56:ASP:HB3	2.27	0.49
35:Sf:89:LYS:HZ3	35:Sf:92:LYS:HE3	1.77	0.49
40:L5:183:C:H1'	40:L5:184:U:H5	1.77	0.49
40:L5:1645:C:H2'	40:L5:1646:A:C8	2.46	0.49
40:L5:1733:G:N3	40:L5:4214:A:H2'	2.27	0.49
40:L5:3880:G:H2'	40:L5:3881:G:C8	2.47	0.49
85:Zt:73:G:H2'	85:Zt:74:C:C6	2.47	0.49
2:SB:88:THR:HA	2:SB:98:THR:HA	1.93	0.49
8:SJ:145:PRO:HD2	19:S2:522:A:H5''	1.94	0.49
15:SY:54:VAL:HG22	15:SY:76:TYR:HB2	1.93	0.49
19:S2:1438:A:H2'	19:S2:1439:A:C8	2.46	0.49
23:SD:53:THR:HB	23:SD:94:ARG:HD2	1.93	0.49
23:SD:132:LYS:HB2	23:SD:189:MET:HG2	1.95	0.49
28:SQ:128:GLU:HG2	28:SQ:137:ALA:HB1	1.93	0.49
40:L5:411:G:H5''	40:L5:414:C:H1'	1.94	0.49
40:L5:1332:C:H2'	40:L5:1333:A:C8	2.47	0.49
40:L5:1857:C:H2'	40:L5:1858:A:H8	1.77	0.49
40:L5:4942:C:H4'	47:LE:154:THR:HB	1.93	0.49
46:LD:41:LYS:HD2	60:LT:93:ILE:HG21	1.95	0.49
28:SQ:97:GLN:HE21	36:Sg:58:ALA:HB3	1.78	0.49
40:L5:1500:A:H5''	40:L5:1501:C:H5''	1.95	0.49
40:L5:4699:U:H1'	40:L5:4700:A:H5''	1.93	0.49
19:S2:1402:A:H5'	31:SU:51:LYS:HE3	1.95	0.49
40:L5:5006:U:H4'	40:L5:5007:A:H5'	1.93	0.49
9:SL:85:THR:HG21	19:S2:373:G:H4'	1.93	0.49
19:S2:291:G:H2'	19:S2:292:A:C8	2.47	0.49
19:S2:906:U:H2'	19:S2:907:G:C8	2.47	0.49
19:S2:940:U:H3	19:S2:1002:U:H3	1.58	0.49
19:S2:963:A:H2'	19:S2:964:A:C8	2.47	0.49
19:S2:1277:C:H2'	19:S2:1278:A:C8	2.46	0.49
40:L5:257:C:H2'	40:L5:258:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4524:G:C2	44:LB:252:ALA:HB1	2.48	0.49
40:L5:4924:C:H2'	40:L5:4925:U:C6	2.48	0.49
42:L8:19:C:H2'	42:L8:20:A:C8	2.48	0.49
19:S2:432:G:H2'	19:S2:433:A:C8	2.48	0.49
19:S2:693:A:H2'	19:S2:694:G:C8	2.48	0.49
19:S2:1217:A:H2'	19:S2:1218:C:H6	1.77	0.49
19:S2:1285:G:N2	26:SM:58:GLU:HB2	2.28	0.49
19:S2:1393:G:H2'	19:S2:1394:G:C8	2.47	0.49
19:S2:1588:A:H2'	19:S2:1589:A:C8	2.48	0.49
24:SF:187:SER:HB3	24:SF:190:ILE:HG12	1.95	0.49
40:L5:3732:A:H2'	40:L5:3733:A:C8	2.48	0.49
60:LT:14:MET:HE1	60:LT:55:LYS:HB2	1.95	0.49
68:Lc:38:ILE:HG21	68:Lc:63:TYR:HB3	1.95	0.49
85:Zt:14:A:H3'	85:Zt:15:G:C8	2.47	0.49
1:SA:184:ARG:HE	1:SA:191:ARG:HA	1.77	0.49
24:SF:17:ILE:HG21	24:SF:46:ALA:HB1	1.94	0.49
31:SU:49:LYS:HZ2	31:SU:92:HIS:HB2	1.78	0.49
36:Sg:153:CYS:SG	36:Sg:198:VAL:HG12	2.53	0.49
40:L5:2102:G:H1'	40:L5:2103:G:N7	2.27	0.49
19:S2:1112:U:H2'	19:S2:1113:A:C8	2.47	0.49
53:LL:48:PRO:HG3	73:Lh:118:LYS:HE2	1.94	0.49
56:LO:54:TYR:HD1	56:LO:145:VAL:HG21	1.78	0.49
56:LO:61:ARG:HA	56:LO:70:PRO:HD2	1.95	0.49
84:Lt:10:ILE:HG21	84:Lt:65:GLN:HB3	1.93	0.49
1:SA:148:CYS:CB	1:SA:148:CYS:H	2.18	0.48
8:SJ:174:LYS:HG3	19:S2:560:A:H5'	1.95	0.48
19:S2:300:U:H2'	19:S2:301:A:H8	1.78	0.48
19:S2:929:G:H2'	19:S2:930:C:O4'	2.13	0.48
19:S2:1323:U:H2'	19:S2:1324:G:C8	2.48	0.48
40:L5:2474:G:H2'	40:L5:2502:G:N2	2.28	0.48
51:LI:4:ARG:HH12	51:LI:99:ILE:HG13	1.78	0.48
6:SH:51:ILE:HG12	6:SH:61:ILE:HD11	1.95	0.48
19:S2:115:U:H2'	19:S2:116:OMU:H6	1.94	0.48
19:S2:388:U:H2'	19:S2:389:A:C8	2.48	0.48
22:SR:31:ASN:HD22	22:SR:55:THR:HG22	1.79	0.48
28:SQ:42:ILE:HG23	28:SQ:44:PRO:HD2	1.94	0.48
40:L5:490:C:H2'	40:L5:491:G:H8	1.78	0.48
40:L5:2351:OMC:HM22	45:LC:95:MET:HG3	1.94	0.48
40:L5:3856:A:H5''	57:LP:83:TRP:O	2.13	0.48
40:L5:4965:U:H4'	40:L5:4966:A:H5'	1.95	0.48
77:Ll:25:GLN:HE22	77:Ll:28:ARG:HH11	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:455:A:H2'	19:S2:456:C:C6	2.48	0.48
19:S2:952:G:H2'	19:S2:953:C:C6	2.47	0.48
19:S2:1452:A:H5''	22:SR:48:ASN:HD22	1.79	0.48
19:S2:1563:G:H5''	30:ST:121:ARG:HH21	1.79	0.48
29:SS:5:ILE:HA	32:SZ:49:LEU:HD13	1.95	0.48
23:SD:132:LYS:HE3	23:SD:192:TRP:H	1.77	0.48
40:L5:1751:A:H2'	40:L5:1752:G:C8	2.48	0.48
40:L5:4578:G:H2'	40:L5:4579:PSU:C6	2.48	0.48
44:LB:292:LEU:HD12	44:LB:298:LEU:HD23	1.96	0.48
51:LI:87:MET:HG2	51:LI:138:ILE:HG12	1.95	0.48
70:Le:35:TRP:CZ2	70:Le:56:PRO:HD2	2.48	0.48
19:S2:888:U:H4'	19:S2:889:U:H5'	1.95	0.48
19:S2:1523:C:H2'	19:S2:1524:G:H8	1.78	0.48
29:SS:13:LEU:HB2	29:SS:20:ILE:HG12	1.95	0.48
40:L5:1509:C:H5''	66:La:2:PRO:HD3	1.94	0.48
40:L5:1577:G:O2'	40:L5:1612:G:H4'	2.14	0.48
45:LC:266:THR:HG22	45:LC:267:TRP:H	1.79	0.48
46:LD:108:ARG:CZ	46:LD:253:TYR:HB2	2.43	0.48
49:LG:83:PHE:HA	49:LG:183:ILE:HD13	1.95	0.48
76:Lk:60:LEU:HD12	76:Lk:66:VAL:HG13	1.95	0.48
19:S2:656:G:H21	19:S2:663:C:H5''	1.78	0.48
29:SS:74:PRO:HA	29:SS:79:ILE:HD12	1.94	0.48
40:L5:4364:G:H2'	40:L5:4365:C:H6	1.78	0.48
1:SA:38:ILE:HD11	1:SA:47:TYR:HB3	1.95	0.48
1:SA:148:CYS:CB	1:SA:149:ASN:N	2.76	0.48
4:SE:161:GLN:HB3	4:SE:171:ASP:H	1.78	0.48
9:SL:21:LYS:HE3	9:SL:23:VAL:HG11	1.95	0.48
32:SZ:61:GLU:O	32:SZ:64:ASN:HB2	2.12	0.48
40:L5:457:G:H2'	40:L5:458:C:C6	2.49	0.48
51:LI:53:VAL:HG11	60:LT:158:PHE:HZ	1.78	0.48
4:SE:42:LEU:HB2	4:SE:101:LEU:HD21	1.95	0.48
19:S2:1845:A:H2'	19:S2:1846:G:H8	1.78	0.48
36:Sg:166:VAL:HG12	36:Sg:176:VAL:HG12	1.95	0.48
46:LD:64:ILE:HG13	46:LD:105:LEU:HD21	1.96	0.48
52:LJ:104:ASN:HD22	52:LJ:133:VAL:HG13	1.79	0.48
57:LP:54:GLN:HA	57:LP:83:TRP:CD1	2.49	0.48
84:Lt:117:ARG:HH11	84:Lt:133:LEU:HD11	1.79	0.48
6:SH:134:VAL:HG23	6:SH:173:PHE:CE2	2.49	0.48
13:SW:26:LEU:HB2	17:Sb:7:LEU:HD23	1.96	0.48
21:LW:44:ARG:HD3	40:L5:3615:G:H1'	1.94	0.48
37:At:50:U:H2'	37:At:51:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:325:U:H2'	40:L5:326:C:C6	2.49	0.48
40:L5:1961:G:N2	40:L5:2025:A:H62	2.11	0.48
40:L5:4474:A:H5''	78:Lm:125:LYS:HG3	1.96	0.48
74:Li:29:ARG:HH22	74:Li:34:THR:HG22	1.78	0.48
77:Ll:23:ILE:HG23	77:Ll:38:ASN:HB2	1.96	0.48
13:SW:52:ILE:HG23	13:SW:61:ILE:HG12	1.96	0.48
19:S2:1221:G:H2'	19:S2:1222:G:C8	2.49	0.48
40:L5:2495:U:H2'	40:L5:2496:G:H8	1.77	0.48
49:LG:162:ASP:HB3	49:LG:163:PRO:HD3	1.96	0.48
58:LQ:43:PHE:CD2	58:LQ:133:GLY:HA3	2.49	0.48
85:Zt:30:G:H2'	85:Zt:31:A:H8	1.78	0.48
85:Zt:64:U:H2'	85:Zt:65:G:H8	1.79	0.48
9:SL:28:THR:HA	9:SL:29:GLY:HA2	1.59	0.47
13:SW:94:LEU:HD21	13:SW:102:ILE:HG13	1.96	0.47
19:S2:186:C:H2'	19:S2:187:G:C8	2.47	0.47
19:S2:1714:U:H2'	19:S2:1715:A:C8	2.49	0.47
21:LW:2:LYS:HZ3	62:LV:92:ASP:HB2	1.79	0.47
29:SS:80:PRO:HG2	30:ST:36:THR:HG21	1.95	0.47
40:L5:4070:U:H2'	40:L5:4071:U:C6	2.49	0.47
44:LB:258:HIS:HA	44:LB:260:ALA:H	1.78	0.47
3:SC:210:PRO:HB3	3:SC:240:THR:HG21	1.95	0.47
40:L5:139:G:H2'	40:L5:140:G:H8	1.79	0.47
40:L5:1307:A:H2'	40:L5:1308:C:C6	2.48	0.47
40:L5:3610:A:H2'	40:L5:3611:A:H8	1.78	0.47
40:L5:4991:U:H2'	40:L5:4992:G:C8	2.49	0.47
84:Lt:10:ILE:HG12	84:Lt:65:GLN:HG2	1.95	0.47
1:SA:77:ILE:HD11	1:SA:124:VAL:HG22	1.96	0.47
15:SY:57:VAL:HB	15:SY:60:PHE:CE1	2.49	0.47
19:S2:1541:G:H2'	19:S2:1542:C:H6	1.79	0.47
19:S2:1571:G:H2'	19:S2:1572:C:C6	2.50	0.47
19:S2:1677:U:H2'	19:S2:1678:A:H8	1.79	0.47
36:Sg:68:ASP:HB3	36:Sg:111:VAL:HG12	1.96	0.47
49:LG:258:ALA:HA	49:LG:261:LEU:HB2	1.96	0.47
54:LM:25:VAL:HB	54:LM:38:VAL:HG22	1.97	0.47
4:SE:45:ILE:HG13	4:SE:61:VAL:HG11	1.95	0.47
19:S2:1279:C:H2'	19:S2:1280:G:H8	1.78	0.47
40:L5:1726:U:H5'	48:LF:135:ILE:HD11	1.95	0.47
40:L5:2485:U:H3	40:L5:2491:C:H42	1.62	0.47
19:S2:543:C:H3'	19:S2:544:G:H8	1.79	0.47
19:S2:600:G:H2'	19:S2:601:OMG:H8	1.79	0.47
19:S2:977:C:H2'	19:S2:978:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1743:G:H21	19:S2:1791:A:H62	1.61	0.47
24:SF:127:ARG:H	24:SF:135:ARG:HD2	1.80	0.47
38:Pt:56:C:N3	80:Lo:104:ILE:HG21	2.30	0.47
40:L5:674:G:H2'	40:L5:675:C:C6	2.49	0.47
40:L5:4280:A:C8	52:LJ:145:LYS:HE3	2.50	0.47
47:LE:158:ARG:HG2	71:Lf:5:LEU:HD22	1.97	0.47
67:Lb:102:PRO:HA	67:Lb:109:ARG:HH22	1.79	0.47
4:SE:139:LEU:HD22	4:SE:147:ILE:HD11	1.96	0.47
11:SO:141:ARG:HG3	16:Sa:22:ARG:HH12	1.79	0.47
19:S2:24:C:HO2'	19:S2:25:A:H8	1.62	0.47
19:S2:838:G:C2	19:S2:840:C:H4'	2.50	0.47
19:S2:991:G:C6	19:S2:1134:G:H4'	2.49	0.47
31:SU:27:ARG:HD3	31:SU:82:MET:HE3	1.96	0.47
40:L5:737:C:C5	40:L5:739:G:H5''	2.49	0.47
40:L5:3848:U:H2'	40:L5:3849:A:C8	2.49	0.47
40:L5:4584:A:H2'	40:L5:4585:U:O4'	2.15	0.47
40:L5:4619:U:H2'	40:L5:4620:OMU:H6	1.97	0.47
40:L5:4775:C:H5	40:L5:4859:C:H42	1.62	0.47
42:L8:67:U:H2'	42:L8:68:G:H8	1.79	0.47
2:SB:24:PRO:HG2	19:S2:953:C:H5''	1.97	0.47
5:SG:174:PRO:HB3	19:S2:65:C:C6	2.49	0.47
8:SJ:86:VAL:HG12	8:SJ:108:ARG:HG3	1.97	0.47
19:S2:1098:C:H2'	19:S2:1099:G:C8	2.50	0.47
19:S2:1407:U:H2'	19:S2:1408:U:C6	2.49	0.47
19:S2:1506:A:H4'	19:S2:1507:G:H3'	1.97	0.47
19:S2:1513:C:H2'	19:S2:1514:G:C8	2.47	0.47
19:S2:1540:G:H2'	19:S2:1541:G:H8	1.79	0.47
19:S2:1733:U:H2'	19:S2:1734:G:O4'	2.15	0.47
38:Pt:29:C:H2'	38:Pt:30:G:C8	2.48	0.47
40:L5:730:G:C5	48:LF:73:ARG:HD3	2.49	0.47
40:L5:4089:G:H2'	40:L5:4090:G:H8	1.80	0.47
40:L5:4392:OMG:HM21	40:L5:4394:A:H2'	1.97	0.47
40:L5:4637:OMG:HM23	40:L5:4637:OMG:H1'	1.68	0.47
45:LC:10:VAL:HG13	45:LC:153:VAL:HG12	1.95	0.47
49:LG:95:LEU:HD23	49:LG:184:ILE:HD12	1.96	0.47
80:Lo:33:LEU:HA	80:Lo:38:LYS:HG2	1.96	0.47
1:SA:77:ILE:HG22	1:SA:99:ILE:HB	1.94	0.47
12:SV:15:ARG:HH21	12:SV:24:ILE:HG21	1.79	0.47
19:S2:113:G:N2	19:S2:292:A:H2'	2.30	0.47
19:S2:348:A:H2'	19:S2:349:A:C8	2.50	0.47
19:S2:1421:A:H3'	19:S2:1422:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1568:C:H2'	19:S2:1569:A:C8	2.49	0.47
19:S2:1828:C:H2'	19:S2:1829:G:C8	2.49	0.47
36:Sg:32:LEU:HA	36:Sg:42:MET:HA	1.96	0.47
40:L5:701:G:H2'	40:L5:702:U:C6	2.50	0.47
40:L5:1278:C:H2'	40:L5:1279:A:O4'	2.14	0.47
40:L5:1534:A2M:N3	75:Lj:11:ARG:HB2	2.30	0.47
47:LE:243:THR:HG22	47:LE:245:GLN:H	1.79	0.47
48:LF:221:LYS:HA	48:LF:221:LYS:HD3	1.72	0.47
49:LG:52:THR:HG22	63:LX:41:ARG:HG3	1.95	0.47
57:LP:125:MET:HE2	57:LP:143:PRO:HG3	1.97	0.47
3:SC:102:LEU:HD23	3:SC:130:ILE:HD12	1.97	0.47
19:S2:649:PSU:H2'	19:S2:650:A:H8	1.79	0.47
36:Sg:236:ILE:HG13	36:Sg:252:THR:HA	1.96	0.47
40:L5:268:G:H2'	40:L5:269:G:C8	2.49	0.47
40:L5:318:A:H2'	40:L5:319:A:H8	1.79	0.47
40:L5:2558:C:H2'	40:L5:2559:G:H8	1.79	0.47
40:L5:3736:A:H2'	40:L5:3737:A:C8	2.49	0.47
40:L5:4162:C:H6	49:LG:73:ARG:HH22	1.63	0.47
51:LI:36:LEU:HD21	51:LI:69:ARG:NH1	2.30	0.47
63:LX:64:SER:HB2	73:Lh:69:LEU:HD13	1.96	0.47
4:SE:42:LEU:HG	4:SE:109:PHE:HD2	1.80	0.47
19:S2:455:A:H2'	19:S2:456:C:H6	1.80	0.47
19:S2:931:C:H2'	19:S2:932:G:C8	2.49	0.47
19:S2:1595:U:H2'	19:S2:1596:U:C6	2.50	0.47
19:S2:1651:A:H2'	19:S2:1652:G:H8	1.80	0.47
25:SK:63:ALA:HB2	25:SK:68:TYR:CE2	2.49	0.47
36:Sg:68:ASP:HB2	36:Sg:110:SER:HA	1.95	0.47
40:L5:400:A2M:HM'3	40:L5:400:A2M:HI'	1.49	0.47
40:L5:455:C:N4	40:L5:456:C:N4	2.63	0.47
40:L5:4742:G:H2'	40:L5:4743:G:H8	1.79	0.47
45:LC:106:LYS:HD3	45:LC:108:TRP:CZ2	2.49	0.47
46:LD:182:GLY:HA2	46:LD:194:VAL:HG23	1.97	0.47
85:Zt:60:U:H5''	85:Zt:61:C:H5	1.79	0.47
9:SL:80:MET:HE3	9:SL:80:MET:HB2	1.81	0.46
19:S2:941:C:H2'	19:S2:942:G:C8	2.50	0.46
22:SR:105:MET:HE2	22:SR:105:MET:HB3	1.78	0.46
29:SS:12:ILE:HD11	52:LJ:121:PRO:HD3	1.96	0.46
40:L5:300:A:H2'	40:L5:301:G:H8	1.80	0.46
40:L5:1857:C:H2'	40:L5:1858:A:C8	2.49	0.46
40:L5:1962:A:H5''	40:L5:2024:G:H22	1.80	0.46
40:L5:4459:U:H2'	40:L5:4460:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4591:U:H2'	40:L5:4592:C:C6	2.50	0.46
43:LA:27:ALA:HB3	43:LA:54:ARG:HH12	1.81	0.46
71:Lf:45:LYS:HE3	71:Lf:108:SER:HA	1.96	0.46
85:Zt:6:G:N2	85:Zt:67:U:O2	2.48	0.46
19:S2:106:C:H2'	19:S2:107:A:C8	2.49	0.46
19:S2:1010:G:H2'	19:S2:1011:A:C8	2.49	0.46
19:S2:1103:C:H2'	19:S2:1104:G:C8	2.51	0.46
19:S2:1103:C:H2'	19:S2:1104:G:H8	1.80	0.46
19:S2:1265:A:H5'	19:S2:1266:C:OP2	2.15	0.46
19:S2:1518:C:H5''	19:S2:1519:U:H5''	1.97	0.46
19:S2:1713:C:H2'	19:S2:1714:U:C6	2.51	0.46
29:SS:121:ARG:HG3	29:SS:131:VAL:HB	1.98	0.46
40:L5:1725:U:H2'	40:L5:1726:U:H6	1.80	0.46
40:L5:4139:G:H1'	40:L5:4146:G:N1	2.30	0.46
43:LA:132:ASN:O	43:LA:169:VAL:HG12	2.16	0.46
52:LJ:95:ARG:H	52:LJ:98:ASN:HD22	1.62	0.46
19:S2:1244:PSU:H2'	19:S2:1245:G:H8	1.79	0.46
24:SF:127:ARG:HG3	24:SF:136:ARG:HB3	1.96	0.46
40:L5:180:C:H2'	40:L5:181:C:H6	1.80	0.46
40:L5:3664:G:H2'	40:L5:3665:G:H8	1.81	0.46
40:L5:3723:A:H2'	40:L5:3724:A:C8	2.50	0.46
40:L5:4239:A:H2'	40:L5:4240:G:C8	2.50	0.46
40:L5:4750:G:H2'	40:L5:4751:G:H8	1.80	0.46
47:LE:190:HIS:HB3	47:LE:193:PHE:HD1	1.81	0.46
54:LM:30:VAL:HG11	59:LS:150:ILE:HD13	1.98	0.46
73:Lh:18:LEU:HD23	73:Lh:18:LEU:HA	1.78	0.46
30:ST:85:ASN:HB3	30:ST:88:MET:HB2	1.96	0.46
36:Sg:128:THR:HG22	36:Sg:143:GLN:HA	1.97	0.46
40:L5:702:U:H2'	40:L5:703:G:O4'	2.16	0.46
43:LA:54:ARG:HG2	43:LA:56:ALA:H	1.80	0.46
43:LA:143:THR:HG23	43:LA:145:LYS:HG2	1.97	0.46
67:Lb:70:GLU:HA	67:Lb:73:LYS:HB2	1.97	0.46
4:SE:54:TYR:HE1	15:SY:13:MET:HE1	1.80	0.46
14:SX:105:PHE:CD2	14:SX:112:VAL:HG21	2.50	0.46
19:S2:1031:A2M:H2'	19:S2:1032:C:C6	2.51	0.46
19:S2:1386:A:H2'	19:S2:1387:G:O4'	2.16	0.46
36:Sg:87:LEU:HB2	36:Sg:101:PHE:HB2	1.97	0.46
40:L5:1248:C:H2'	40:L5:1249:C:H6	1.81	0.46
44:LB:332:MET:HE1	44:LB:368:ILE:HD13	1.97	0.46
19:S2:93:PSU:H2'	19:S2:94:G:O4'	2.15	0.46
19:S2:906:U:H2'	19:S2:907:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1239:U:H3	19:S2:1242:U:H5''	1.81	0.46
40:L5:3722:G:H2'	40:L5:3723:A:H8	1.80	0.46
40:L5:3861:A:H2'	40:L5:3862:A:H8	1.80	0.46
41:L7:27:G:H5''	46:LD:57:ASN:OD1	2.16	0.46
46:LD:223:PHE:HB3	46:LD:226:TYR:HB2	1.96	0.46
80:Lo:6:LYS:HG3	80:Lo:94:GLY:HA3	1.97	0.46
2:SB:127:VAL:HG21	2:SB:176:VAL:HB	1.98	0.46
3:SC:256:TRP:CD2	13:SW:68:ARG:HD3	2.50	0.46
10:SN:4:MET:HG2	10:SN:5:HIS:CD2	2.51	0.46
12:SV:27:LYS:HA	12:SV:27:LYS:HD3	1.73	0.46
13:SW:57:ARG:NH2	17:Sb:26:GLN:HB2	2.31	0.46
19:S2:28:U:H2'	19:S2:29:G:C8	2.51	0.46
19:S2:51:U:H2'	19:S2:52:G:H8	1.80	0.46
19:S2:1222:G:H2'	19:S2:1223:A:H8	1.77	0.46
19:S2:1330:G:N7	19:S2:1492:U:H3'	2.31	0.46
19:S2:1337:4AC:O5'	19:S2:1337:4AC:H6	2.15	0.46
19:S2:1431:G:H4'	19:S2:1434:C:H41	1.79	0.46
40:L5:173:C:H5''	53:LL:129:ARG:HH12	1.80	0.46
40:L5:457:G:H2'	40:L5:458:C:H6	1.81	0.46
40:L5:3792:OMG:HM22	40:L5:3793:U:H5'	1.97	0.46
44:LB:288:GLY:HA3	44:LB:330:PHE:CE1	2.50	0.46
44:LB:397:ILE:HA	44:LB:400:GLU:HB2	1.97	0.46
5:SG:172:LYS:HD3	19:S2:65:C:H4'	1.98	0.46
19:S2:941:C:H2'	19:S2:942:G:H8	1.81	0.46
38:Pt:51:C:H2'	38:Pt:52:G:C8	2.50	0.46
40:L5:2099:G:H2'	40:L5:2100:A:O4'	2.16	0.46
40:L5:2380:G:N2	40:L5:2424:OMG:H5''	2.30	0.46
40:L5:2676:A:OP2	40:L5:2676:A:H8	1.98	0.46
40:L5:2870:A:H2'	40:L5:2871:A:H8	1.78	0.46
60:LT:4:THR:OG1	60:LT:9:ARG:HD3	2.15	0.46
1:SA:110:ASN:HB3	1:SA:113:GLN:HE22	1.80	0.46
1:SA:176:TRP:CD1	1:SA:199:PRO:HA	2.51	0.46
3:SC:60:TRP:CE2	3:SC:92:GLU:HB2	2.51	0.46
7:SI:67:TRP:CD2	7:SI:70:GLU:HG3	2.50	0.46
19:S2:27:A2M:H1'	19:S2:27:A2M:HM'3	1.59	0.46
19:S2:51:U:H2'	19:S2:52:G:C8	2.51	0.46
19:S2:1563:G:H2'	19:S2:1564:C:H6	1.81	0.46
35:Sf:103:LEU:HG	35:Sf:104:LYS:H	1.81	0.46
35:Sf:133:ALA:HB3	35:Sf:140:TYR:H	1.80	0.46
36:Sg:10:THR:HG22	36:Sg:308:ARG:HG2	1.98	0.46
40:L5:730:G:C6	48:LF:73:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:3610:A:H2'	40:L5:3611:A:C8	2.51	0.46
46:LD:156:GLY:HA2	46:LD:181:PRO:HG3	1.98	0.46
51:LI:36:LEU:HD11	51:LI:69:ARG:HH11	1.79	0.46
56:LO:143:HIS:HA	56:LO:147:TRP:HB3	1.98	0.46
85:Zt:62:C:H2'	85:Zt:63:C:H6	1.81	0.46
1:SA:50:ASN:HD22	1:SA:53:ARG:NH1	2.14	0.46
3:SC:178:HIS:CG	3:SC:200:ARG:HE	2.34	0.46
16:Sa:82:LYS:HD3	16:Sa:85:ARG:HH12	1.80	0.46
17:Sb:54:VAL:HG23	17:Sb:63:LEU:HD12	1.97	0.46
19:S2:96:C:H2'	19:S2:97:U:C6	2.51	0.46
19:S2:1446:A:H5''	31:SU:58:THR:HG23	1.98	0.46
24:SF:68:ILE:HD11	24:SF:116:ILE:HG13	1.98	0.46
26:SM:43:ASP:OD1	35:Sf:129:GLY:HA2	2.16	0.46
27:SP:49:LEU:HD23	27:SP:54:HIS:CE1	2.51	0.46
40:L5:907:C:H2'	40:L5:908:G:H8	1.81	0.46
40:L5:979:C:OP2	47:LE:66:LYS:HD3	2.16	0.46
40:L5:1195:G:H2'	40:L5:1196:G:C8	2.51	0.46
43:LA:7:GLY:HA2	43:LA:10:LYS:HG3	1.98	0.46
84:Lt:114:ARG:HH21	84:Lt:117:ARG:NH1	2.14	0.46
1:SA:111:GLN:HA	1:SA:116:PHE:CG	2.51	0.45
5:SG:136:LYS:HB2	19:S2:65:C:H41	1.81	0.45
8:SJ:136:ARG:HD3	8:SJ:160:SER:HA	1.97	0.45
19:S2:118:C:H1'	19:S2:445:A:C5	2.50	0.45
19:S2:587:A:H1'	19:S2:590:A:C8	2.51	0.45
24:SF:56:TYR:HD1	24:SF:65:GLN:HE22	1.63	0.45
36:Sg:5:MET:HB2	36:Sg:270:LEU:HD21	1.97	0.45
40:L5:1198:G:H2'	40:L5:1199:G:C8	2.51	0.45
40:L5:1961:G:H21	40:L5:2025:A:N6	2.14	0.45
40:L5:4457:PSU:H1'	44:LB:252:ALA:HB3	1.99	0.45
42:L8:90:C:H1'	64:LY:24:HIS:HB3	1.97	0.45
53:LL:63:THR:HG22	53:LL:64:VAL:H	1.81	0.45
64:LY:21:ALA:HB1	64:LY:25:ILE:HG13	1.97	0.45
64:LY:72:GLN:NE2	64:LY:74:TYR:HD1	2.14	0.45
66:La:71:PRO:HG2	66:La:108:TYR:HA	1.98	0.45
4:SE:45:ILE:HA	4:SE:61:VAL:HG21	1.98	0.45
17:Sb:20:LYS:HB3	17:Sb:23:ARG:HH21	1.80	0.45
19:S2:746:C:H2'	19:S2:747:U:C6	2.51	0.45
24:SF:22:LYS:HG3	24:SF:23:TRP:CD2	2.51	0.45
29:SS:89:ASP:HB3	29:SS:93:GLY:N	2.32	0.45
33:Sc:9:ILE:HG12	33:Sc:59:LEU:HD22	1.98	0.45
40:L5:422:C:H2'	40:L5:423:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1097:C:H2'	40:L5:1098:G:C8	2.52	0.45
40:L5:1495:G:H4'	58:LQ:187:LYS:HE3	1.97	0.45
40:L5:2632:PSU:H2'	40:L5:2633:U:C6	2.51	0.45
40:L5:4108:G:H2'	40:L5:4109:G:H8	1.81	0.45
40:L5:4353:PSU:H5'	40:L5:4354:U:H5'	1.97	0.45
40:L5:4920:C:H2'	40:L5:4921:C:C6	2.51	0.45
45:LC:5:ARG:HH12	45:LC:268:ARG:NH2	2.13	0.45
64:LY:2:LYS:HD2	64:LY:7:VAL:HG13	1.98	0.45
2:SB:213:ARG:HD2	2:SB:214:LYS:HB2	1.98	0.45
4:SE:100:ARG:HB2	4:SE:114:ILE:HD13	1.97	0.45
4:SE:131:VAL:HA	4:SE:137:PRO:HA	1.99	0.45
6:SH:36:LEU:HD21	6:SH:78:ARG:HE	1.81	0.45
8:SJ:122:SER:H	8:SJ:125:HIS:HB3	1.80	0.45
19:S2:825:A:H2'	19:S2:826:A:C8	2.51	0.45
19:S2:943:U:C2	19:S2:944:A:C8	3.05	0.45
19:S2:1266:C:H2'	19:S2:1267:C:C6	2.51	0.45
40:L5:2611:A:H2'	40:L5:2612:G:C8	2.51	0.45
40:L5:4730:C:H2'	40:L5:4731:G:C8	2.52	0.45
19:S2:35:C:H5''	19:S2:579:C:H5''	1.99	0.45
19:S2:1261:C:H41	19:S2:1661:A:H62	1.64	0.45
22:SR:70:SER:HB3	22:SR:73:LEU:HB2	1.98	0.45
30:ST:41:LYS:HE3	30:ST:41:LYS:HB3	1.79	0.45
31:SU:28:ASN:HD21	31:SU:31:SER:HB3	1.81	0.45
40:L5:2021:G:OP1	83:Ls:57:LYS:HA	2.17	0.45
40:L5:3861:A:H2'	40:L5:3862:A:C8	2.51	0.45
42:L8:36:G:C5	73:Lh:89:ARG:HD3	2.52	0.45
68:Lc:48:LEU:HD13	68:Lc:71:VAL:HG13	1.98	0.45
84:Lt:22:VAL:HG13	84:Lt:48:LYS:HG2	1.98	0.45
3:SC:66:LEU:HD21	3:SC:88:ILE:HD13	1.98	0.45
10:SN:75:LEU:HB3	10:SN:81:ALA:HB2	1.98	0.45
11:SO:54:CYS:HB3	11:SO:84:ARG:HG2	1.97	0.45
19:S2:174:OMC:H1'	19:S2:174:OMC:HM23	1.74	0.45
19:S2:1572:C:H2'	19:S2:1573:G:C8	2.51	0.45
19:S2:1628:C:H2'	19:S2:1629:C:C6	2.50	0.45
24:SF:204:ARG:HG2	33:Sc:63:ARG:HH21	1.81	0.45
32:SZ:57:LYS:HA	32:SZ:60:LYS:HG2	1.99	0.45
37:At:23:C:H2'	37:At:24:A:C8	2.52	0.45
37:At:43:A:H2'	37:At:44:A:H8	1.82	0.45
40:L5:260:C:H2'	40:L5:261:G:C8	2.52	0.45
40:L5:2539:C:H2'	40:L5:2540:C:C6	2.52	0.45
40:L5:3723:A:H2'	40:L5:3724:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4095:G:H2'	40:L5:4096:C:C6	2.50	0.45
40:L5:4347:G:H2'	40:L5:4348:A:C8	2.52	0.45
70:Le:76:LYS:HD3	70:Le:98:GLU:OE2	2.16	0.45
82:Lr:16:PHE:HB3	82:Lr:27:THR:H	1.82	0.45
4:SE:44:LEU:HD11	4:SE:72:ILE:HD11	1.99	0.45
8:SJ:2:PRO:O	19:S2:509:OMG:H5''	2.17	0.45
10:SN:4:MET:HE3	19:S2:924:G:H5'	1.99	0.45
19:S2:300:U:H2'	19:S2:301:A:C8	2.52	0.45
19:S2:1315:U:H4'	25:SK:2:LEU:HD13	1.98	0.45
19:S2:1398:G:H22	19:S2:1448:A:H2	1.65	0.45
19:S2:1474:A:H2'	19:S2:1475:G:O4'	2.16	0.45
19:S2:1797:U:H2'	19:S2:1798:C:C6	2.51	0.45
21:LW:102:LYS:HA	21:LW:105:ARG:HE	1.81	0.45
24:SF:53:ALA:HB1	28:SQ:125:ARG:HH21	1.81	0.45
27:SP:32:GLN:HA	27:SP:35:GLN:HG2	1.98	0.45
28:SQ:39:LEU:HD11	28:SQ:51:LEU:HB3	1.99	0.45
40:L5:3946:G:H2'	40:L5:3947:A:H5''	1.98	0.45
43:LA:130:SER:HB2	43:LA:171:GLY:HA3	1.98	0.45
67:Lb:109:ARG:HA	67:Lb:112:ILE:HG12	1.99	0.45
71:Lf:41:PHE:HE1	71:Lf:110:ILE:HD13	1.81	0.45
6:SH:66:VAL:HG22	6:SH:96:ALA:HB1	1.97	0.45
19:S2:845:G:H2'	19:S2:846:G:C8	2.52	0.45
19:S2:1031:A2M:HM'3	19:S2:1031:A2M:H1'	1.50	0.45
22:SR:128:PHE:HD1	22:SR:129:LYS:HG3	1.82	0.45
40:L5:462:G:H2'	40:L5:463:A:C8	2.52	0.45
40:L5:3597:G:H2'	40:L5:3598:C:H6	1.81	0.45
47:LE:173:LEU:HD21	47:LE:191:GLN:HB3	1.98	0.45
51:LI:73:ASN:HB2	51:LI:87:MET:HE1	1.97	0.45
66:La:36:GLY:HA3	66:La:40:HIS:CE1	2.52	0.45
3:SC:127:PHE:HD1	3:SC:141:VAL:HG22	1.82	0.45
4:SE:153:LEU:HD12	5:SG:216:ARG:HH11	1.81	0.45
7:SI:141:ARG:HG3	7:SI:149:TYR:CE2	2.52	0.45
19:S2:1214:A:H2'	19:S2:1217:A:N7	2.31	0.45
19:S2:1328:OMG:HM23	19:S2:1328:OMG:H1'	1.78	0.45
19:S2:1562:C:H2'	19:S2:1563:G:H8	1.82	0.45
19:S2:1801:A:H2'	19:S2:1802:C:C6	2.52	0.45
30:ST:39:LEU:HD13	30:ST:47:PRO:HG3	1.99	0.45
32:SZ:67:LEU:HD12	32:SZ:67:LEU:HA	1.80	0.45
36:Sg:165:ILE:HB	36:Sg:179:LEU:HD21	1.99	0.45
40:L5:121:A:OP1	49:LG:110:LYS:HE2	2.17	0.45
40:L5:190:G:H2'	40:L5:191:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1220:G:H2'	40:L5:1221:G:C8	2.52	0.45
40:L5:2364:OMG:HM23	40:L5:2364:OMG:H1'	1.71	0.45
40:L5:3923:A:H2'	40:L5:3924:C:C6	2.51	0.45
40:L5:4896:G:H2'	40:L5:4897:G:H8	1.81	0.45
44:LB:128:LYS:HA	44:LB:128:LYS:HD2	1.75	0.45
45:LC:315:LYS:HD2	48:LF:168:ALA:HB1	1.99	0.45
55:LN:68:ARG:HE	55:LN:128:LYS:HE3	1.80	0.45
2:SB:191:ASP:HB3	2:SB:195:LYS:NZ	2.31	0.45
16:Sa:5:ARG:HH21	19:S2:1864:U:H3'	1.82	0.45
23:SD:66:ILE:HD11	23:SD:86:LEU:HB3	1.98	0.45
37:At:10:G:C2	37:At:26:G:H1'	2.52	0.45
40:L5:37:U:H2'	40:L5:38:A:O4'	2.17	0.45
40:L5:1751:A:H2'	40:L5:1752:G:H8	1.81	0.45
40:L5:2696:A:H62	76:Lk:35:LYS:HZ2	1.65	0.45
40:L5:2765:A:H2'	40:L5:2766:A:H8	1.82	0.45
41:L7:39:C:O2'	52:LJ:46:GLN:HG2	2.17	0.45
44:LB:213:GLN:HE22	44:LB:285:TYR:C	2.25	0.45
85:Zt:60:U:H5''	85:Zt:61:C:C5	2.52	0.45
1:SA:157:VAL:HG11	1:SA:160:ALA:HB2	1.99	0.45
5:SG:191:ARG:HH12	19:S2:314:U:H5	1.64	0.45
19:S2:508:A:H3'	19:S2:509:OMG:C8	2.40	0.45
19:S2:1208:A:H2'	19:S2:1209:A:H8	1.82	0.45
19:S2:1266:C:H2'	19:S2:1267:C:H6	1.81	0.45
19:S2:1683:C:H2'	19:S2:1684:C:H6	1.82	0.45
37:At:50:U:H2'	37:At:51:C:H6	1.81	0.45
40:L5:1446:C:H2'	40:L5:1447:C:C6	2.51	0.45
42:L8:67:U:H2'	42:L8:68:G:C8	2.52	0.45
45:LC:318:PRO:C	45:LC:320:LYS:H	2.24	0.45
61:LU:112:LEU:HD23	61:LU:112:LEU:H	1.81	0.45
77:Ll:41:ARG:HA	77:Ll:41:ARG:HD2	1.68	0.45
1:SA:39:TYR:CE2	22:SR:105:MET:HB2	2.52	0.44
2:SB:36:PRO:HB2	2:SB:38:MET:HE3	1.99	0.44
9:SL:23:VAL:HG23	9:SL:25:LEU:HG	1.98	0.44
13:SW:46:TYR:HD2	13:SW:69:LEU:HD13	1.82	0.44
19:S2:317:C:H2'	19:S2:318:A:C4	2.52	0.44
19:S2:388:U:H2'	19:S2:389:A:H8	1.82	0.44
19:S2:468:A2M:H1'	19:S2:468:A2M:HM'3	1.78	0.44
19:S2:468:A2M:H2'	19:S2:469:A:O4'	2.16	0.44
19:S2:644:OMG:HM23	19:S2:644:OMG:H1'	1.66	0.44
19:S2:929:G:N2	19:S2:1104:G:H4'	2.32	0.44
19:S2:1399:C:H2'	19:S2:1400:U:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SQ:145:TYR:C	28:SQ:146:ARG:HD2	2.42	0.44
37:At:34:A:H2'	37:At:35:A:C8	2.52	0.44
37:At:35:A:H2'	37:At:36:C:O4'	2.16	0.44
40:L5:10:A:H2'	40:L5:11:G:H8	1.81	0.44
40:L5:1081:C:O2'	40:L5:1082:C:H5'	2.17	0.44
40:L5:2465:C:H2'	40:L5:2466:G:O4'	2.17	0.44
45:LC:144:ILE:HD12	45:LC:150:LEU:HD11	1.99	0.44
61:LU:63:ILE:HD13	61:LU:72:VAL:HG22	1.99	0.44
74:Li:41:ARG:O	74:Li:45:ARG:HG2	2.18	0.44
1:SA:91:ALA:HA	1:SA:96:ALA:HB3	1.99	0.44
19:S2:29:G:H2'	19:S2:30:C:C6	2.52	0.44
31:SU:19:ARG:HG2	31:SU:92:HIS:HB3	1.98	0.44
40:L5:677:G:H2'	40:L5:678:C:H6	1.82	0.44
40:L5:1238:A:C8	47:LE:59:ARG:HD2	2.53	0.44
40:L5:1340:OMC:HM23	40:L5:1340:OMC:H1'	1.76	0.44
40:L5:1514:U:H2'	40:L5:1515:A:C8	2.53	0.44
40:L5:1662:C:H2'	40:L5:1663:C:C6	2.52	0.44
40:L5:2448:G:H2'	40:L5:2449:A:C8	2.53	0.44
40:L5:4088:C:H2'	40:L5:4089:G:C8	2.52	0.44
40:L5:4742:G:H2'	40:L5:4743:G:C8	2.51	0.44
40:L5:4927:G:H5''	40:L5:4928:C:H5	1.82	0.44
44:LB:57:VAL:HB	44:LB:367:PHE:HB3	1.98	0.44
64:LY:28:LYS:HE3	64:LY:28:LYS:HB3	1.83	0.44
3:SC:199:PRO:HG2	8:SJ:58:ARG:HD2	1.98	0.44
13:SW:53:ILE:HD13	17:Sb:24:LEU:HG	1.98	0.44
13:SW:101:PHE:HA	13:SW:113:HIS:HE1	1.82	0.44
19:S2:1391:OMC:HM23	19:S2:1391:OMC:H1'	1.78	0.44
23:SD:135:GLU:HB2	23:SD:153:VAL:HG23	1.99	0.44
40:L5:491:G:H2'	40:L5:492:U:C6	2.51	0.44
40:L5:2495:U:H2'	40:L5:2496:G:C8	2.53	0.44
40:L5:2824:OMC:H1'	40:L5:2824:OMC:HM23	1.73	0.44
40:L5:4578:G:H2'	40:L5:4579:PSU:H6	1.82	0.44
40:L5:4590:A2M:HM'3	40:L5:4590:A2M:H1'	1.74	0.44
47:LE:223:ARG:HB3	47:LE:224:LYS:HB2	2.00	0.44
61:LU:28:PRO:HB2	61:LU:34:MET:HG3	1.99	0.44
77:Ll:26:TRP:CD1	77:Ll:26:TRP:H	2.35	0.44
3:SC:70:VAL:HG11	3:SC:93:ILE:HG23	2.00	0.44
5:SG:136:LYS:HB2	19:S2:65:C:N4	2.33	0.44
6:SH:168:HIS:CE1	6:SH:169:LYS:HG3	2.52	0.44
11:SO:45:THR:HG22	11:SO:52:THR:HG22	1.98	0.44
19:S2:24:C:O2'	19:S2:25:A:H8	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1528:G:H2'	19:S2:1529:C:C6	2.53	0.44
19:S2:1679:A:H2'	24:SF:60:ARG:HD2	1.99	0.44
23:SD:163:PRO:HA	23:SD:166:TYR:CZ	2.52	0.44
40:L5:1366:G:N7	53:LL:37:LYS:HD2	2.33	0.44
40:L5:2903:G:H1'	40:L5:2904:U:C5	2.53	0.44
40:L5:4734:A:H1'	40:L5:4735:G:C8	2.52	0.44
49:LG:209:SER:HA	49:LG:212:LYS:HG3	1.99	0.44
84:Lt:48:LYS:HD3	84:Lt:48:LYS:HA	1.80	0.44
1:SA:158:ASP:HB2	1:SA:159:ILE:HD12	1.99	0.44
5:SG:147:LEU:HD21	5:SG:156:TYR:HD2	1.83	0.44
14:SX:66:ILE:HG13	18:Se:5:SER:HB2	2.00	0.44
19:S2:1409:A:H2'	19:S2:1410:C:C6	2.52	0.44
19:S2:1457:U:H2'	19:S2:1458:G:C8	2.53	0.44
19:S2:1553:C:N4	34:Sd:22:ARG:HH12	2.16	0.44
19:S2:1563:G:H2'	19:S2:1564:C:C6	2.52	0.44
26:SM:95:ASP:HB3	26:SM:99:LYS:HB3	1.98	0.44
29:SS:59:LEU:HD12	29:SS:63:GLU:HB3	2.00	0.44
40:L5:966:A:C2	40:L5:2093:A:H2	2.35	0.44
40:L5:1534:A2M:HM'3	40:L5:1637:A:C4	2.52	0.44
40:L5:2292:C:H2'	40:L5:2293:U:C6	2.52	0.44
40:L5:3710:G:H1'	40:L5:3711:A:C8	2.52	0.44
40:L5:3848:U:H2'	40:L5:3849:A:H8	1.82	0.44
42:L8:92:U:H2'	42:L8:93:C:O4'	2.17	0.44
56:LO:34:VAL:HG22	56:LO:103:LYS:HB2	2.00	0.44
63:LX:129:ARG:HE	63:LX:133:GLU:HB2	1.82	0.44
19:S2:1525:C:H2'	19:S2:1526:G:H8	1.83	0.44
20:LR:139:MET:HE3	20:LR:139:MET:HB3	1.70	0.44
24:SF:40:ALA:HB3	24:SF:67:PRO:HA	2.00	0.44
40:L5:978:G:H2'	40:L5:979:C:C6	2.52	0.44
40:L5:1359:G:H4'	55:LN:203:TYR:HB2	2.00	0.44
40:L5:4775:C:H41	40:L5:4859:C:N4	2.15	0.44
44:LB:90:VAL:HG23	44:LB:163:ILE:HD11	2.00	0.44
54:LM:104:MET:HE3	54:LM:109:ARG:CG	2.47	0.44
56:LO:165:LYS:HE2	56:LO:165:LYS:HB2	1.83	0.44
6:SH:111:LYS:HZ1	19:S2:747:U:H1'	1.83	0.44
19:S2:352:U:H2'	19:S2:353:C:C6	2.53	0.44
19:S2:885:U:C2	19:S2:901:G:O6	2.71	0.44
19:S2:1562:C:H2'	19:S2:1563:G:C8	2.53	0.44
19:S2:1736:G:H2'	19:S2:1737:G:H8	1.83	0.44
36:Sg:101:PHE:CE2	36:Sg:136:GLY:HA2	2.52	0.44
36:Sg:121:VAL:HG11	36:Sg:165:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:2787:A2M:HM'2	40:L5:2787:A2M:H1'	1.75	0.44
40:L5:4089:G:H2'	40:L5:4090:G:C8	2.52	0.44
40:L5:4153:C:H2'	40:L5:4154:G:H8	1.82	0.44
59:LS:4:SER:HB3	59:LS:111:ARG:HH22	1.82	0.44
69:Ld:29:ILE:O	69:Ld:33:ILE:HG12	2.18	0.44
83:Ls:78:LEU:O	83:Ls:82:ILE:HG12	2.17	0.44
84:Lt:117:ARG:NH1	84:Lt:133:LEU:HD11	2.32	0.44
11:SO:56:VAL:HG23	11:SO:60:MET:SD	2.58	0.44
19:S2:561:A:H2'	19:S2:562:U:C6	2.52	0.44
19:S2:1627:C:H2'	19:S2:1628:C:C6	2.53	0.44
36:Sg:176:VAL:HG23	36:Sg:185:LYS:HB2	2.00	0.44
40:L5:163:A:H2'	40:L5:164:G:H8	1.82	0.44
40:L5:2415:U:H2'	40:L5:2416:G:C8	2.53	0.44
40:L5:3744:OMG:HM23	40:L5:3744:OMG:H1'	1.79	0.44
40:L5:4859:C:H2'	40:L5:4860:G:C8	2.53	0.44
43:LA:142:GLU:O	43:LA:143:THR:HG22	2.18	0.44
43:LA:206:PRO:HG3	43:LA:213:GLY:HA3	1.99	0.44
45:LC:5:ARG:HH12	45:LC:268:ARG:HH21	1.66	0.44
71:Lf:45:LYS:HD2	71:Lf:105:LEU:HA	2.00	0.44
80:Lo:83:LEU:HD23	80:Lo:83:LEU:HA	1.85	0.44
2:SB:145:LYS:HB2	2:SB:145:LYS:HE3	1.76	0.44
5:SG:2:LYS:HG2	5:SG:17:GLU:HG3	1.99	0.44
19:S2:115:U:H2'	19:S2:116:OMU:C6	2.47	0.44
19:S2:1457:U:H2'	19:S2:1458:G:H8	1.83	0.44
19:S2:1541:G:H2'	19:S2:1542:C:C6	2.52	0.44
19:S2:1573:G:H2'	19:S2:1574:C:O4'	2.18	0.44
32:SZ:74:SER:HA	32:SZ:79:ILE:HG13	1.98	0.44
35:Sf:103:LEU:HB2	35:Sf:105:TYR:CE2	2.53	0.44
40:L5:162:A:H2'	40:L5:163:A:C8	2.53	0.44
40:L5:2497:C:H2'	40:L5:2498:C:H6	1.83	0.44
40:L5:2717:G:H5'	61:LU:107:LYS:HE3	1.99	0.44
40:L5:3656:A:H2'	40:L5:3657:U:H6	1.83	0.44
40:L5:3867:A2M:HM'3	40:L5:3867:A2M:H1'	1.51	0.44
44:LB:173:LEU:HD22	44:LB:342:LYS:HD2	1.99	0.44
48:LF:162:ILE:HD12	48:LF:167:ILE:HB	2.00	0.44
51:LI:4:ARG:NH1	51:LI:99:ILE:HG13	2.33	0.44
55:LN:140:LYS:HA	55:LN:143:ARG:HB3	1.99	0.44
71:Lf:104:MET:O	71:Lf:105:LEU:HB2	2.18	0.44
2:SB:103:MET:HB3	2:SB:215:VAL:HG12	1.99	0.43
10:SN:47:PRO:HD2	10:SN:86:GLU:HG3	1.99	0.43
17:Sb:20:LYS:HA	17:Sb:23:ARG:NE	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:618:C:H2'	19:S2:619:A:O4'	2.18	0.43
19:S2:1073:U:H2'	19:S2:1074:C:H6	1.83	0.43
19:S2:1590:C:H42	28:SQ:77:HIS:CE1	2.34	0.43
37:At:27:U:H2'	37:At:28:U:C6	2.52	0.43
39:Cl:63:ARG:HD2	39:Cl:63:ARG:HA	1.87	0.43
40:L5:106:A:H2'	40:L5:107:G:O4'	2.18	0.43
40:L5:286:U:H2'	40:L5:287:U:C6	2.53	0.43
40:L5:1478:C:H2'	40:L5:1479:G:H8	1.82	0.43
40:L5:1669:A:H4'	40:L5:1685:G:N2	2.33	0.43
40:L5:3709:U:H2'	40:L5:3710:G:O4'	2.18	0.43
40:L5:3722:G:H2'	40:L5:3723:A:C8	2.54	0.43
40:L5:5002:U:H2'	40:L5:5003:U:C6	2.52	0.43
44:LB:14:LEU:HD22	44:LB:17:LEU:HD11	1.99	0.43
45:LC:228:THR:HG23	45:LC:248:ARG:HH22	1.83	0.43
53:LL:210:LYS:HE3	53:LL:210:LYS:HB3	1.81	0.43
4:SE:66:MET:HG3	19:S2:502:C:O4'	2.17	0.43
16:Sa:44:ILE:HG23	16:Sa:45:VAL:HG13	2.00	0.43
19:S2:462:OMC:HM23	19:S2:462:OMC:H1'	1.76	0.43
19:S2:601:OMG:HM23	19:S2:601:OMG:H1'	1.69	0.43
19:S2:996:A:H2'	19:S2:997:A:H8	1.83	0.43
19:S2:1670:C:H2'	19:S2:1671:G:C8	2.54	0.43
22:SR:103:LYS:HE2	22:SR:117:LEU:HD12	1.99	0.43
30:ST:42:HIS:CE1	30:ST:43:LYS:HG3	2.53	0.43
38:Pt:3:C:H42	38:Pt:70:A:H61	1.66	0.43
40:L5:385:A:N3	40:L5:387:G:H5''	2.33	0.43
40:L5:982:U:H2'	40:L5:983:C:C6	2.53	0.43
40:L5:1702:C:H5''	45:LC:308:LYS:HD3	1.99	0.43
40:L5:1867:A:H2'	40:L5:1868:A:C8	2.54	0.43
40:L5:2109:G:H2'	40:L5:2110:C:C6	2.53	0.43
40:L5:4064:C:H2'	40:L5:4065:G:C8	2.53	0.43
40:L5:4188:U:H2'	40:L5:4189:U:C6	2.54	0.43
40:L5:4306:OMU:HM23	40:L5:4306:OMU:H1'	1.85	0.43
40:L5:4611:A:H2	50:LH:120:GLU:HB3	1.81	0.43
40:L5:4957:C:H2'	40:L5:4958:C:C6	2.53	0.43
52:LJ:159:LYS:HG2	52:LJ:163:MET:HE3	1.99	0.43
54:LM:24:LEU:HD11	54:LM:86:TRP:CG	2.53	0.43
78:Lm:93:LYS:HD3	78:Lm:102:ARG:HG2	2.00	0.43
19:S2:159:A2M:HM'3	19:S2:159:A2M:H1'	1.48	0.43
19:S2:389:A:H2'	19:S2:390:C:C6	2.53	0.43
19:S2:496:C:H2'	19:S2:497:C:C6	2.53	0.43
19:S2:948:C:H2'	19:S2:949:G:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:179:G:H2'	40:L5:180:C:C6	2.53	0.43
40:L5:1978:C:H2'	40:L5:1979:A:H8	1.84	0.43
40:L5:4344:U:H2'	40:L5:4345:C:C6	2.53	0.43
42:L8:40:A:H2'	42:L8:41:A:C8	2.54	0.43
43:LA:108:PRO:HB2	81:Lp:86:LEU:HD22	1.99	0.43
48:LF:182:TYR:HB3	48:LF:200:ARG:HG3	2.00	0.43
52:LJ:94:LEU:HD23	52:LJ:166:PHE:CZ	2.54	0.43
55:LN:5:LYS:HG3	74:Li:40:VAL:HG11	1.99	0.43
57:LP:125:MET:HE3	57:LP:125:MET:HB2	1.92	0.43
67:Lb:101:HIS:CE1	67:Lb:104:LEU:HD23	2.53	0.43
81:Lp:75:SER:O	81:Lp:79:VAL:HG23	2.18	0.43
15:SY:46:LYS:HE3	15:SY:46:LYS:HB3	1.87	0.43
19:S2:1442:OMU:HM23	19:S2:1442:OMU:H1'	1.87	0.43
19:S2:1501:C:H2'	19:S2:1502:C:H6	1.83	0.43
19:S2:1621:U:O2'	19:S2:1622:U:H2'	2.18	0.43
19:S2:1856:C:H2'	19:S2:1857:G:C8	2.54	0.43
32:SZ:65:TYR:HB3	85:Zt:34:U:O4'	2.18	0.43
36:Sg:36:ARG:HG2	36:Sg:65:PHE:CG	2.53	0.43
40:L5:424:U:H2'	40:L5:425:U:C6	2.53	0.43
40:L5:1326:A2M:H1'	40:L5:1326:A2M:HM'3	1.64	0.43
40:L5:1811:G:H2'	40:L5:1812:C:H6	1.83	0.43
40:L5:1846:G:H2'	40:L5:1847:C:C6	2.53	0.43
40:L5:3606:U:H2'	40:L5:3607:U:C6	2.53	0.43
57:LP:94:MET:HE3	57:LP:94:MET:HB2	1.82	0.43
64:LY:117:LYS:HE3	64:LY:117:LYS:HB2	1.84	0.43
4:SE:47:PHE:O	4:SE:51:ARG:HB2	2.19	0.43
6:SH:83:LEU:HA	6:SH:86:LYS:HD2	2.01	0.43
19:S2:323:C:H4'	19:S2:324:C:C5	2.54	0.43
19:S2:1674:G:H5''	24:SF:86:LYS:HD3	2.00	0.43
32:SZ:68:ILE:HG23	32:SZ:109:TYR:HB2	1.99	0.43
36:Sg:17:TRP:H	36:Sg:36:ARG:HB2	1.81	0.43
36:Sg:79:LEU:HD11	36:Sg:89:LEU:HD12	2.00	0.43
36:Sg:145:GLU:HB3	36:Sg:177:TRP:CH2	2.50	0.43
36:Sg:194:TYR:CZ	36:Sg:212:LYS:HB2	2.54	0.43
36:Sg:230:LEU:HD11	36:Sg:259:TRP:CG	2.52	0.43
40:L5:453:G:H4'	40:L5:454:U:H5'	2.00	0.43
40:L5:467:U:N3	40:L5:468:U:H1'	2.34	0.43
40:L5:728:U:H5''	48:LF:76:ARG:NH1	2.33	0.43
40:L5:1538:U:H2'	40:L5:1539:G:H8	1.84	0.43
40:L5:3599:A:H2'	40:L5:3600:G:C8	2.53	0.43
40:L5:4255:A:H2'	40:L5:4256:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4688:C:H2'	40:L5:4689:PSU:C6	2.54	0.43
49:LG:157:ILE:HA	49:LG:201:THR:HG22	2.01	0.43
84:Lt:10:ILE:HD12	84:Lt:10:ILE:HA	1.88	0.43
2:SB:125:VAL:HG12	2:SB:172:MET:HE3	2.01	0.43
3:SC:253:PRO:HA	3:SC:256:TRP:CD2	2.53	0.43
4:SE:42:LEU:HD12	4:SE:101:LEU:HD11	2.00	0.43
6:SH:8:ILE:HG13	6:SH:9:VAL:HG23	2.01	0.43
10:SN:72:LEU:HD22	19:S2:1019:C:H5''	2.01	0.43
11:SO:33:ILE:HG13	11:SO:97:LEU:HA	2.00	0.43
15:SY:57:VAL:HB	15:SY:60:PHE:HE1	1.83	0.43
19:S2:454:U:H2'	19:S2:455:A:C8	2.54	0.43
19:S2:497:C:H2'	19:S2:498:C:C6	2.53	0.43
19:S2:945:U:H2'	19:S2:946:U:C6	2.53	0.43
24:SF:162:ALA:HB2	24:SF:172:CYS:SG	2.58	0.43
25:SK:41:PRO:HG2	25:SK:44:HIS:CG	2.53	0.43
31:SU:104:ILE:HB	31:SU:106:ILE:HG23	1.99	0.43
36:Sg:164:ILE:HD12	36:Sg:178:ASN:HA	2.00	0.43
40:L5:1333:A:H2'	40:L5:1334:A:H8	1.81	0.43
40:L5:4741:C:H2'	40:L5:4950:U:H3	1.82	0.43
51:LI:54:SER:HA	51:LI:163:GLN:HG3	2.00	0.43
56:LO:10:ASP:OD1	56:LO:37:ARG:HD3	2.19	0.43
4:SE:38:LEU:HD22	19:S2:346:C:H5''	1.99	0.43
4:SE:168:LYS:HA	4:SE:168:LYS:HD3	1.86	0.43
12:SV:30:ALA:O	12:SV:60:ARG:HD3	2.18	0.43
15:SY:8:ARG:HD3	15:SY:8:ARG:HA	1.84	0.43
19:S2:59:U:H5'	19:S2:503:C:N4	2.33	0.43
19:S2:1383:A2M:HM'3	19:S2:1383:A2M:H1'	1.53	0.43
26:SM:42:LEU:HD23	26:SM:42:LEU:HA	1.92	0.43
29:SS:111:LEU:HG	29:SS:115:LYS:HE3	2.00	0.43
37:At:3:C:N4	37:At:70:A:H61	2.16	0.43
40:L5:690:C:H2'	40:L5:691:C:H6	1.84	0.43
40:L5:1501:C:H2'	58:LQ:68:ARG:NH1	2.34	0.43
40:L5:2422:OMC:H1'	40:L5:2422:OMC:HM23	1.84	0.43
40:L5:2640:G:H2'	40:L5:2641:A:H8	1.82	0.43
40:L5:2764:A:H2'	40:L5:2765:A:H8	1.83	0.43
40:L5:2864:A:H2'	40:L5:2865:U:C6	2.53	0.43
40:L5:2876:OMG:HM22	40:L5:2877:G:H5'	2.00	0.43
40:L5:3870:C:H2'	40:L5:3871:A:C8	2.53	0.43
40:L5:4345:C:H2'	40:L5:4346:U:C6	2.54	0.43
44:LB:300:LYS:HG3	44:LB:311:ASP:HA	2.00	0.43
48:LF:66:ARG:HA	48:LF:66:ARG:HD2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:LG:252:LYS:HE2	49:LG:252:LYS:HB2	1.86	0.43
70:Le:19:LYS:HE3	70:Le:19:LYS:HB3	1.79	0.43
6:SH:74:LYS:HG3	6:SH:75:ILE:HG23	2.00	0.43
19:S2:866:PSU:H2'	19:S2:867:OMG:C8	2.54	0.43
19:S2:1244:PSU:HN3	19:S2:1255:G:H1	1.67	0.43
19:S2:1310:U:H2'	19:S2:1311:C:C6	2.54	0.43
20:LR:44:LEU:HD22	20:LR:49:LEU:HD12	2.00	0.43
32:SZ:48:VAL:HG23	32:SZ:80:ARG:HD2	2.01	0.43
35:Sf:126:CYS:SG	35:Sf:143:LYS:HB2	2.58	0.43
40:L5:126:C:H2'	40:L5:127:G:H8	1.84	0.43
40:L5:1084:C:H2'	40:L5:1085:C:H6	1.83	0.43
40:L5:1956:A:H2'	40:L5:1957:U:C6	2.54	0.43
40:L5:3652:A:H2'	40:L5:3653:A:C5	2.53	0.43
40:L5:4088:C:H2'	40:L5:4089:G:H8	1.83	0.43
40:L5:4364:G:H2'	40:L5:4365:C:C6	2.53	0.43
40:L5:4754:G:N7	47:LE:278:THR:HG23	2.34	0.43
44:LB:86:VAL:HG12	44:LB:201:LEU:HD23	2.00	0.43
80:Lo:70:LEU:HD11	80:Lo:83:LEU:HD12	2.01	0.43
1:SA:198:MET:HE3	22:SR:85:VAL:HG12	2.01	0.43
1:SA:207:PRO:O	1:SA:210:ILE:HG22	2.19	0.43
3:SC:195:LEU:HD13	3:SC:214:LEU:HD11	2.00	0.43
12:SV:37:ALA:HA	12:SV:50:PHE:HB3	2.00	0.43
14:SX:63:ASN:HD22	14:SX:114:ASP:HB3	1.84	0.43
19:S2:1018:U:H2'	19:S2:1019:C:C6	2.49	0.43
19:S2:1262:C:H2'	19:S2:1263:U:O4'	2.19	0.43
19:S2:1415:C:H2'	19:S2:1416:C:H6	1.84	0.43
19:S2:1423:C:H5	28:SQ:4:LYS:HG2	1.84	0.43
36:Sg:205:SER:C	36:Sg:221:LEU:HD23	2.44	0.43
36:Sg:207:CYS:SG	36:Sg:219:TRP:HB2	2.59	0.43
37:At:18:G:H2'	37:At:57:G:N2	2.33	0.43
38:Pt:2:U:H2'	38:Pt:3:C:C6	2.53	0.43
40:L5:123:C:H2'	40:L5:124:C:H6	1.84	0.43
40:L5:737:C:C4	40:L5:739:G:H5''	2.54	0.43
40:L5:959:G:C8	47:LE:123:ARG:HG2	2.54	0.43
40:L5:1972:G:H21	84:Lt:121:LEU:HD11	1.84	0.43
40:L5:4196:OMG:HM23	40:L5:4196:OMG:H1'	1.64	0.43
40:L5:4543:G:H2'	40:L5:4544:A:C8	2.54	0.43
40:L5:4892:A:H2'	40:L5:4893:A:O4'	2.18	0.43
40:L5:4991:U:H2'	40:L5:4992:G:H8	1.83	0.43
43:LA:137:ILE:HD11	43:LA:149:LYS:HB2	2.00	0.43
2:SB:67:PHE:CZ	11:SO:48:SER:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SE:68:ARG:NH2	4:SE:76:VAL:HG21	2.34	0.43
4:SE:146:THR:HG21	19:S2:122:G:H21	1.83	0.43
6:SH:159:ASP:C	6:SH:161:ALA:H	2.26	0.43
8:SJ:31:LEU:HD11	8:SJ:102:ILE:HD12	2.01	0.43
16:Sa:30:VAL:HG21	16:Sa:74:CYS:HB3	2.01	0.43
19:S2:495:U:H2'	19:S2:496:C:O4'	2.18	0.43
19:S2:1031:A2M:H2'	19:S2:1032:C:H6	1.84	0.43
19:S2:1533:A:C5	19:S2:1604:G:H1'	2.53	0.43
19:S2:1703:OMC:H2'	19:S2:1704:C:O4'	2.19	0.43
25:SK:22:VAL:HG22	25:SK:68:TYR:HD1	1.83	0.43
29:SS:74:PRO:HG3	29:SS:97:GLN:HB3	2.01	0.43
40:L5:500:G:H1'	40:L5:504:G:H2'	1.99	0.43
40:L5:1907:A:H2'	40:L5:1908:A:C8	2.54	0.43
40:L5:2431:A:OP1	77:Ll:22:PRO:HG3	2.19	0.43
40:L5:2568:C:H2'	40:L5:2569:G:C8	2.54	0.43
40:L5:3690:U:H2'	40:L5:3691:G:O4'	2.19	0.43
40:L5:3870:C:H2'	40:L5:3871:A:H8	1.84	0.43
40:L5:4913:G:H4'	40:L5:4914:C:O5'	2.17	0.43
41:L7:16:A:H2'	41:L7:17:C:C6	2.54	0.43
44:LB:14:LEU:HA	44:LB:17:LEU:HG	2.01	0.43
47:LE:239:LYS:HD2	47:LE:239:LYS:HA	1.78	0.43
48:LF:236:ARG:HB2	48:LF:239:GLN:HB2	2.01	0.43
63:LX:88:LYS:O	63:LX:92:ASP:HB2	2.19	0.43
65:LZ:46:ILE:HA	65:LZ:70:SER:HA	2.01	0.43
2:SB:114:VAL:HG11	19:S2:987:A:H2'	2.01	0.42
19:S2:525:A:H2'	19:S2:526:A:C8	2.51	0.42
19:S2:648:A:H2'	19:S2:649:PSU:H6	1.83	0.42
19:S2:1616:U:H2'	19:S2:1617:G:C8	2.54	0.42
36:Sg:198:VAL:HB	36:Sg:209:SER:HB3	2.01	0.42
40:L5:172:C:H4'	40:L5:173:C:H5'	2.01	0.42
40:L5:689:U:H2'	40:L5:690:C:C6	2.54	0.42
40:L5:1270:A:N7	40:L5:2107:C:H1'	2.34	0.42
40:L5:2485:U:H4'	40:L5:2486:G:N2	2.34	0.42
40:L5:3833:C:H2'	40:L5:3834:C:H6	1.84	0.42
40:L5:4507:A:H2'	40:L5:4508:C:C6	2.54	0.42
40:L5:4739:C:H2'	40:L5:4740:G:H5'	2.00	0.42
59:LS:48:VAL:HG12	60:LT:151:LEU:HD12	2.01	0.42
69:Ld:37:GLY:O	69:Ld:41:ARG:HG3	2.19	0.42
1:SA:24:HIS:HA	1:SA:49:ILE:HG12	2.00	0.42
1:SA:52:LYS:HB2	22:SR:109:LEU:HD13	2.00	0.42
9:SL:17:PHE:CG	19:S2:222:U:H5''	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SO:143:LYS:HG3	19:S2:1048:G:P	2.59	0.42
17:Sb:33:MET:HE2	17:Sb:48:SER:HA	2.01	0.42
19:S2:1129:G:H2'	19:S2:1130:G:N3	2.34	0.42
19:S2:1656:G:O6	19:S2:1668:U:O4	2.37	0.42
19:S2:1752:C:H3'	19:S2:1753:C:O4'	2.19	0.42
27:SP:81:ARG:NH1	27:SP:98:ASN:HA	2.34	0.42
29:SS:89:ASP:HB3	29:SS:93:GLY:H	1.84	0.42
40:L5:161:G:H2'	40:L5:162:A:H8	1.84	0.42
40:L5:455:C:O2'	40:L5:456:C:H5'	2.19	0.42
40:L5:492:U:H2'	40:L5:493:G:O4'	2.18	0.42
40:L5:1248:C:H2'	40:L5:1249:C:C6	2.54	0.42
40:L5:1281:G:H5'	45:LC:323:ARG:HB2	2.01	0.42
40:L5:1811:G:H2'	40:L5:1812:C:C6	2.54	0.42
40:L5:2411:C:H2'	40:L5:2412:A:C8	2.54	0.42
40:L5:2538:U:H2'	40:L5:2539:C:C6	2.54	0.42
40:L5:4238:G:H2'	40:L5:4239:A:H8	1.84	0.42
40:L5:4919:G:H2'	40:L5:4920:C:H6	1.83	0.42
42:L8:106:G:H4'	42:L8:137:A:H5'	2.00	0.42
45:LC:172:LYS:HA	45:LC:177:TRP:HB2	2.00	0.42
48:LF:181:LYS:HE3	48:LF:182:TYR:CZ	2.54	0.42
51:LI:87:MET:HB2	51:LI:87:MET:HE3	1.88	0.42
54:LM:94:LYS:HB2	54:LM:94:LYS:HE3	1.87	0.42
63:LX:124:VAL:HG22	63:LX:138:VAL:HG13	2.01	0.42
73:Lh:89:ARG:O	73:Lh:93:ARG:HG2	2.18	0.42
4:SE:98:ASN:HB2	4:SE:114:ILE:HG13	2.01	0.42
7:SI:116:HIS:ND1	7:SI:152:ARG:HD3	2.34	0.42
7:SI:141:ARG:HG3	7:SI:149:TYR:HE2	1.83	0.42
19:S2:352:U:H2'	19:S2:353:C:H6	1.85	0.42
19:S2:440:G:H5'	19:S2:1798:C:O2'	2.19	0.42
19:S2:689:U:H3'	19:S2:690:G:H21	1.84	0.42
19:S2:1476:A:H4'	19:S2:1477:U:H5''	2.02	0.42
19:S2:1614:A:H2'	19:S2:1615:U:C6	2.54	0.42
19:S2:1777:G:H2'	19:S2:1778:C:C6	2.55	0.42
36:Sg:107:ASP:HB2	36:Sg:125:ARG:HH11	1.84	0.42
40:L5:1307:A:H2'	40:L5:1308:C:H6	1.84	0.42
40:L5:1870:C:H2'	40:L5:1871:A2M:H8	2.02	0.42
40:L5:3668:C:H5'	43:LA:8:GLN:O	2.19	0.42
45:LC:163:LYS:HE3	45:LC:163:LYS:HB3	1.83	0.42
51:LI:61:SER:HA	51:LI:126:VAL:HG12	2.00	0.42
63:LX:81:LEU:HG	63:LX:83:THR:HG23	2.01	0.42
70:Le:85:LEU:HD21	70:Le:115:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SG:198:ARG:HH11	19:S2:125:C:H3'	1.84	0.42
7:SI:148:LYS:HD3	7:SI:152:ARG:NH2	2.35	0.42
19:S2:15:U:H2'	19:S2:16:G:O4'	2.19	0.42
19:S2:642:U:H4'	19:S2:644:OMG:H4'	2.01	0.42
19:S2:1216:C:H5''	19:S2:1217:A:H5'	2.01	0.42
19:S2:1713:C:H2'	19:S2:1714:U:H6	1.83	0.42
19:S2:1801:A:H2'	19:S2:1802:C:H6	1.84	0.42
23:SD:40:ARG:HG2	31:SU:108:PRO:HG3	2.01	0.42
24:SF:123:GLU:HA	24:SF:140:ASP:HA	2.01	0.42
28:SQ:44:PRO:HG2	28:SQ:81:ILE:HD11	2.00	0.42
30:ST:30:VAL:HG13	30:ST:34:VAL:HG11	2.02	0.42
40:L5:679:C:H2'	40:L5:680:G:H8	1.84	0.42
40:L5:2045:G:O2'	40:L5:2046:G:H5''	2.19	0.42
40:L5:4106:G:H3'	40:L5:4107:G:C8	2.52	0.42
89:L5:5289:SPD:HN6	89:L5:5289:SPD:H31	1.71	0.42
46:LD:60:ILE:HB	46:LD:80:ALA:HB2	2.00	0.42
46:LD:68:ARG:HD3	46:LD:68:ARG:HA	1.80	0.42
49:LG:37:LYS:HE2	49:LG:37:LYS:HB3	1.80	0.42
52:LJ:20:LEU:HD21	52:LJ:130:PHE:CD2	2.55	0.42
57:LP:17:SER:HB2	57:LP:98:ALA:HB2	2.02	0.42
64:LY:24:HIS:CE1	64:LY:25:ILE:HG23	2.54	0.42
83:Ls:59:THR:HA	83:Ls:62:ARG:HB2	2.00	0.42
85:Zt:23:A:H2'	85:Zt:24:G:O4'	2.19	0.42
1:SA:146:ALA:HB3	1:SA:157:VAL:HG13	2.01	0.42
4:SE:16:LYS:HA	4:SE:16:LYS:HD2	1.84	0.42
5:SG:3:LEU:HD22	5:SG:111:LEU:HD11	2.01	0.42
9:SL:22:ARG:HH22	9:SL:26:GLY:HA3	1.83	0.42
13:SW:42:MET:HE3	13:SW:49:GLU:HA	2.01	0.42
15:SY:21:LYS:HD2	15:SY:75:ILE:HD11	2.00	0.42
18:Se:41:ARG:HH22	19:S2:639:C:H5''	1.85	0.42
19:S2:749:U:H3	19:S2:793:G:N2	2.18	0.42
19:S2:1657:G:H2'	19:S2:1658:G:H8	1.84	0.42
24:SF:73:THR:O	24:SF:89:THR:HG21	2.19	0.42
40:L5:135:G:H2'	40:L5:135:G:N3	2.35	0.42
40:L5:139:G:H2'	40:L5:140:G:C8	2.54	0.42
40:L5:162:A:H2'	40:L5:163:A:H8	1.85	0.42
40:L5:750:U:H1'	40:L5:917:A:C8	2.54	0.42
40:L5:755:C:H2'	40:L5:756:G:H8	1.84	0.42
40:L5:1431:C:H2'	40:L5:1432:G:O4'	2.20	0.42
40:L5:1978:C:H2'	40:L5:1979:A:C8	2.55	0.42
40:L5:3690:U:H5'	40:L5:3818:UY1:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:LB:66:LYS:HG2	62:LV:11:GLY:HA3	2.02	0.42
51:LI:136:MET:HE3	51:LI:136:MET:HB2	1.78	0.42
56:LO:43:ILE:HD11	56:LO:138:LEU:HD13	2.01	0.42
62:LV:35:LYS:HB2	62:LV:67:LYS:HG3	2.01	0.42
72:Lg:41:ALA:O	72:Lg:52:ARG:HD3	2.20	0.42
5:SG:15:LEU:HD22	19:S2:155:G:H4'	2.01	0.42
5:SG:30:LYS:HD3	5:SG:30:LYS:HA	1.83	0.42
11:SO:34:PHE:HB3	11:SO:41:PHE:HB2	2.01	0.42
13:SW:69:LEU:HD21	13:SW:72:CYS:HB3	2.01	0.42
16:Sa:9:GLY:O	16:Sa:34:LYS:HG3	2.20	0.42
19:S2:568:C:H2'	19:S2:569:A:O4'	2.19	0.42
19:S2:901:G:H2'	19:S2:902:G:C8	2.55	0.42
19:S2:1289:U:H4'	25:SK:2:LEU:HD21	2.01	0.42
19:S2:1706:G:H2'	19:S2:1707:U:H6	1.84	0.42
38:Pt:2:U:H2'	38:Pt:3:C:H6	1.85	0.42
40:L5:180:C:H2'	40:L5:181:C:C6	2.54	0.42
40:L5:2654:C:H2'	40:L5:2655:C:H6	1.85	0.42
40:L5:3600:G:H2'	40:L5:3601:C:C6	2.55	0.42
40:L5:4108:G:H2'	40:L5:4109:G:C8	2.54	0.42
40:L5:4680:G:H2'	40:L5:4681:A:C8	2.54	0.42
40:L5:4906:C:H2'	40:L5:4907:G:H8	1.85	0.42
88:L5:5259:SPM:H32	60:LT:13:TYR:HD1	1.85	0.42
45:LC:100:ARG:H	45:LC:100:ARG:HD3	1.85	0.42
45:LC:317:ASN:ND2	45:LC:320:LYS:HD3	2.33	0.42
50:LH:95:VAL:HG21	78:Lm:86:ALA:HB2	2.01	0.42
55:LN:135:ILE:HG21	55:LN:151:ILE:HG21	2.02	0.42
62:LV:60:MET:HE2	62:LV:78:PRO:HB3	2.00	0.42
83:Ls:101:MET:HE2	83:Ls:101:MET:HB2	1.98	0.42
4:SE:45:ILE:HD12	4:SE:80:ILE:HD11	2.00	0.42
4:SE:101:LEU:HD12	4:SE:101:LEU:HA	1.89	0.42
8:SJ:25:LEU:HD23	8:SJ:25:LEU:HA	1.90	0.42
8:SJ:131:ARG:HD2	8:SJ:131:ARG:HA	1.80	0.42
13:SW:111:MET:HE3	13:SW:116:ALA:HA	2.01	0.42
19:S2:165:G:H2'	19:S2:166:A2M:H8	2.02	0.42
19:S2:1415:C:H2'	19:S2:1416:C:C6	2.55	0.42
24:SF:47:LYS:HD3	28:SQ:115:TYR:CZ	2.55	0.42
26:SM:18:LEU:HA	26:SM:21:VAL:HB	2.01	0.42
27:SP:33:LEU:HD23	27:SP:33:LEU:HA	1.86	0.42
37:At:15:G:H22	37:At:48:C:H42	1.67	0.42
40:L5:262:G:H2'	40:L5:263:G:C8	2.51	0.42
40:L5:425:U:H4'	57:LP:6:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1761:G:H1'	40:L5:1764:G:H22	1.84	0.42
40:L5:3726:A:H2'	40:L5:3727:A:C8	2.53	0.42
40:L5:3928:A:H2'	40:L5:3929:G:O4'	2.19	0.42
44:LB:107:ALA:HB2	44:LB:201:LEU:HD22	2.01	0.42
45:LC:269:LYS:HD2	45:LC:269:LYS:HA	1.90	0.42
47:LE:237:LYS:HE3	47:LE:237:LYS:HB3	1.84	0.42
52:LJ:113:ILE:HG12	52:LJ:119:TYR:CD2	2.54	0.42
59:LS:93:MET:HE1	59:LS:117:HIS:CE1	2.54	0.42
62:LV:60:MET:HE1	62:LV:108:ASN:HA	2.02	0.42
1:SA:122:LEU:HB2	1:SA:142:LEU:HD21	2.02	0.42
1:SA:203:PHE:HZ	22:SR:91:LEU:HD11	1.84	0.42
2:SB:87:ILE:H	2:SB:101:HIS:HB2	1.83	0.42
4:SE:64:ILE:HD12	4:SE:64:ILE:HA	1.81	0.42
4:SE:106:LYS:HB3	4:SE:108:ARG:NH1	2.32	0.42
7:SI:151:GLU:O	7:SI:154:LYS:HG2	2.19	0.42
8:SJ:80:ARG:HA	8:SJ:83:ARG:HB2	2.01	0.42
16:Sa:73:TYR:HB3	16:Sa:78:ALA:HB2	2.02	0.42
19:S2:1094:C:H2'	19:S2:1095:C:C6	2.54	0.42
19:S2:1102:G:H2'	19:S2:1103:C:C6	2.55	0.42
19:S2:1220:A:H2'	19:S2:1221:G:O4'	2.20	0.42
19:S2:1390:U:H2'	19:S2:1391:OMC:C6	2.54	0.42
19:S2:1467:C:H2'	19:S2:1468:C:H6	1.85	0.42
19:S2:1672:U:H2'	19:S2:1673:U:C6	2.55	0.42
26:SM:79:VAL:HG11	26:SM:85:LEU:HB2	2.01	0.42
40:L5:1356:U:H2'	40:L5:1357:C:C6	2.55	0.42
40:L5:1392:A:H2'	40:L5:1393:G:C8	2.55	0.42
40:L5:1968:G:H2'	40:L5:1969:G:C8	2.54	0.42
40:L5:3911:C:H2'	40:L5:3912:U:C6	2.53	0.42
40:L5:4058:U:H4'	40:L5:4059:C:C6	2.55	0.42
40:L5:4238:G:H2'	40:L5:4239:A:C8	2.55	0.42
40:L5:5015:G:H2'	40:L5:5016:A:C2	2.54	0.42
49:LG:48:LYS:HB3	63:LX:42:THR:HB	2.02	0.42
57:LP:76:TRP:CD1	57:LP:76:TRP:H	2.38	0.42
64:LY:4:ASN:HB3	64:LY:7:VAL:HG12	2.01	0.42
74:Li:100:ALA:HA	74:Li:103:LYS:HE2	2.01	0.42
85:Zt:50:A:H2'	85:Zt:51:G:C8	2.54	0.42
1:SA:148:CYS:HB3	1:SA:149:ASN:H	1.85	0.42
2:SB:117:TRP:HB3	2:SB:153:THR:HA	2.02	0.42
3:SC:253:PRO:HA	3:SC:256:TRP:CE2	2.55	0.42
5:SG:196:LYS:HA	5:SG:196:LYS:HD2	1.91	0.42
18:Se:25:LYS:HE2	18:Se:25:LYS:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:799:OMU:HM23	19:S2:799:OMU:H1'	1.91	0.42
19:S2:935:G:H2'	19:S2:936:G:H8	1.85	0.42
19:S2:1058:A:H2'	19:S2:1059:G:C8	2.55	0.42
20:LR:126:LYS:HD3	20:LR:131:VAL:HG21	2.02	0.42
20:LR:176:ARG:NH1	20:LR:177:LEU:HG	2.35	0.42
21:LW:96:GLN:HB2	21:LW:101:ARG:HG3	2.01	0.42
25:SK:64:TRP:HB3	34:Sd:23:VAL:HA	2.02	0.42
40:L5:223:G:H4'	40:L5:225:G:C8	2.54	0.42
40:L5:458:C:OP1	47:LE:114:ARG:HG2	2.20	0.42
40:L5:1468:C:H2'	40:L5:1469:C:C6	2.54	0.42
40:L5:2275:G:H2'	40:L5:2276:A:C8	2.55	0.42
40:L5:2730:U:H2'	40:L5:2731:C:C6	2.54	0.42
40:L5:4094:G:H1	40:L5:4114:C:H2'	1.85	0.42
40:L5:4750:G:H2'	40:L5:4751:G:C8	2.55	0.42
40:L5:4910:G:H22	56:LO:107:GLY:HA3	1.84	0.42
44:LB:224:LYS:HG2	44:LB:340:THR:HG22	2.00	0.42
50:LH:51:LYS:HG3	50:LH:52:LYS:HG2	2.01	0.42
51:LI:184:MET:HE2	51:LI:190:LEU:HG	2.01	0.42
55:LN:38:ARG:HG3	55:LN:62:TYR:CE1	2.53	0.42
84:Lt:12:VAL:HG11	84:Lt:65:GLN:N	2.34	0.42
84:Lt:23:GLY:HA3	84:Lt:27:ALA:HB2	2.00	0.42
84:Lt:114:ARG:HA	84:Lt:114:ARG:HD2	1.88	0.42
5:SG:50:VAL:HG21	5:SG:111:LEU:HB3	2.02	0.42
5:SG:176:ILE:HG12	19:S2:77:A:H1'	2.02	0.42
19:S2:527:C:H2'	19:S2:528:A:H8	1.83	0.42
19:S2:1491:G:H2'	19:S2:1492:U:C6	2.55	0.42
20:LR:19:LYS:HB2	20:LR:19:LYS:HE2	1.79	0.42
21:LW:119:LYS:HB2	21:LW:119:LYS:HE2	1.89	0.42
26:SM:48:HIS:HB3	26:SM:114:TYR:CZ	2.55	0.42
36:Sg:14:HIS:CE1	36:Sg:41:ILE:HD12	2.54	0.42
37:At:27:U:H2'	37:At:28:U:H6	1.85	0.42
40:L5:7:C:H2'	40:L5:8:U:C6	2.55	0.42
40:L5:3873:G:H2'	40:L5:3874:G:C8	2.55	0.42
40:L5:4244:A:H2'	40:L5:4245:G:O4'	2.20	0.42
40:L5:4456:OMC:HM21	44:LB:241:PRO:HD3	2.02	0.42
51:LI:32:ARG:HE	51:LI:32:ARG:HB3	1.56	0.42
53:LL:130:LYS:HD2	53:LL:131:PRO:HD2	2.01	0.42
83:Ls:61:MET:HB3	83:Ls:88:PHE:HE2	1.85	0.42
1:SA:85:ARG:HB2	22:SR:81:ARG:NH1	2.34	0.41
1:SA:166:LYS:HD2	1:SA:166:LYS:HA	1.74	0.41
4:SE:11:ARG:HD2	4:SE:20:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:130:ILE:HG12	8:SJ:135:ILE:HG21	2.02	0.41
19:S2:517:OMC:HM22	19:S2:518:G:H5'	2.02	0.41
19:S2:573:U:H1'	19:S2:576:A2M:N7	2.35	0.41
19:S2:639:C:H2'	19:S2:640:A:C8	2.52	0.41
19:S2:649:PSU:H2'	19:S2:650:A:C8	2.55	0.41
19:S2:735:C:H5''	19:S2:736:C:C2	2.55	0.41
19:S2:1373:C:H2'	19:S2:1374:C:C6	2.55	0.41
22:SR:79:GLU:HG3	22:SR:80:ARG:N	2.35	0.41
36:Sg:11:LEU:HB2	36:Sg:307:VAL:HG13	2.00	0.41
40:L5:46:U:H5''	53:LL:16:LYS:HG3	2.01	0.41
40:L5:170:C:H42	40:L5:266:C:N4	2.18	0.41
40:L5:1254:A:H5''	40:L5:1255:A:H5''	2.02	0.41
40:L5:2335:C:H2'	40:L5:2336:G:H8	1.84	0.41
40:L5:2389:A:H5'	69:Ld:70:LYS:HD3	2.02	0.41
40:L5:2501:C:H2'	40:L5:2502:G:C8	2.55	0.41
40:L5:4187:G:H2'	40:L5:4188:U:O4'	2.20	0.41
41:L7:120:U:H4'	46:LD:261:VAL:HA	2.01	0.41
43:LA:96:LEU:HD11	43:LA:108:PRO:HG2	2.00	0.41
45:LC:150:LEU:HA	45:LC:150:LEU:HD23	1.71	0.41
57:LP:84:PRO:HB2	57:LP:87:SER:HB2	2.02	0.41
76:Lk:49:ASP:HB3	76:Lk:52:LYS:HB2	2.02	0.41
76:Lk:50:LYS:O	76:Lk:54:GLU:HG2	2.19	0.41
1:SA:61:ALA:HB1	1:SA:145:ILE:HD13	2.03	0.41
2:SB:137:LEU:HB3	2:SB:172:MET:SD	2.60	0.41
3:SC:210:PRO:HD3	3:SC:236:PHE:CE2	2.53	0.41
4:SE:124:CYS:HB3	4:SE:141:THR:OG1	2.19	0.41
4:SE:253:ASP:HA	4:SE:256:LEU:HB2	2.02	0.41
5:SG:234:LEU:HD11	5:SG:237:LEU:HB3	2.03	0.41
6:SH:36:LEU:HD11	6:SH:78:ARG:HG2	2.02	0.41
12:SV:69:ILE:HD13	12:SV:69:ILE:HA	1.96	0.41
14:SX:24:ASP:HB3	19:S2:658:U:C4	2.56	0.41
19:S2:17:C:H2'	19:S2:18:C:C6	2.55	0.41
19:S2:99:A2M:H8	19:S2:99:A2M:O5'	2.19	0.41
19:S2:121:OMU:HM23	19:S2:121:OMU:H1'	1.90	0.41
19:S2:511:U:H2'	19:S2:512:A:C8	2.55	0.41
19:S2:1288:OMU:H3'	35:Sf:97:LYS:HZ2	1.85	0.41
19:S2:1452:A:N1	19:S2:1473:G:C2	2.88	0.41
21:LW:117:LYS:HA	21:LW:117:LYS:HD3	1.80	0.41
23:SD:25:LEU:HD23	23:SD:25:LEU:HA	1.89	0.41
25:SK:64:TRP:CD1	34:Sd:23:VAL:HG13	2.54	0.41
29:SS:111:LEU:HD11	29:SS:125:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Sg:201:SER:HA	36:Sg:241:PHE:HD2	1.84	0.41
40:L5:1697:G:H2'	40:L5:1698:C:C6	2.55	0.41
40:L5:3925:OMU:HM23	40:L5:3925:OMU:H1'	1.76	0.41
40:L5:4291:G:H5'	40:L5:4293:PSU:C6	2.56	0.41
40:L5:4401:G:H2'	40:L5:4402:C:H6	1.84	0.41
40:L5:4524:G:N3	44:LB:252:ALA:HB1	2.35	0.41
40:L5:4736:C:H2'	40:L5:4737:G:H8	1.86	0.41
40:L5:5018:C:H2'	40:L5:5019:A:H8	1.85	0.41
43:LA:28:ARG:HB3	43:LA:123:ARG:HD3	2.01	0.41
45:LC:298:ILE:HD13	58:LQ:131:PRO:HB3	2.02	0.41
47:LE:183:ARG:HA	47:LE:183:ARG:HD2	1.83	0.41
50:LH:44:GLU:HG3	54:LM:2:VAL:HG23	2.02	0.41
51:LI:36:LEU:HD11	51:LI:69:ARG:HD2	2.01	0.41
61:LU:34:MET:HB3	61:LU:96:LEU:HD11	2.01	0.41
80:Lo:88:CYS:SG	80:Lo:91:PHE:HB2	2.60	0.41
1:SA:211:GLU:HA	1:SA:214:GLU:OE2	2.20	0.41
6:SH:101:LEU:HG	6:SH:120:ARG:HB3	2.02	0.41
9:SL:17:PHE:CD2	19:S2:222:U:H5''	2.55	0.41
9:SL:103:GLU:HG3	14:SX:11:ARG:HB2	2.02	0.41
19:S2:1631:U:H3'	19:S2:1632:G:H8	1.85	0.41
19:S2:1720:U:H5''	19:S2:1721:U:H5''	2.01	0.41
28:SQ:10:VAL:HG11	28:SQ:98:LYS:HD3	2.02	0.41
31:SU:24:LEU:HD22	31:SU:112:VAL:HG12	2.02	0.41
35:Sf:105:TYR:HE1	35:Sf:131:PHE:HD2	1.68	0.41
40:L5:433:A:C2	40:L5:3867:A2M:H4'	2.55	0.41
40:L5:491:G:H2'	40:L5:492:U:H6	1.86	0.41
40:L5:677:G:H2'	40:L5:678:C:C6	2.55	0.41
40:L5:700:G:O6	40:L5:701:G:O6	2.38	0.41
40:L5:1806:G:H2'	40:L5:1807:C:H6	1.84	0.41
40:L5:1994:C:H2'	40:L5:1995:G:H8	1.84	0.41
40:L5:3595:U:H5''	40:L5:3597:G:OP2	2.21	0.41
40:L5:3947:A:H3'	40:L5:3948:C:O4'	2.21	0.41
40:L5:4438:U:H2'	40:L5:4439:U:O4'	2.20	0.41
42:L8:56:G:H21	42:L8:62:A:H5'	1.85	0.41
44:LB:144:LYS:HB3	44:LB:144:LYS:HE2	1.78	0.41
47:LE:223:ARG:HA	47:LE:224:LYS:HA	1.77	0.41
61:LU:67:LYS:HD3	61:LU:67:LYS:HA	1.79	0.41
72:Lg:33:LEU:HD23	72:Lg:33:LEU:HA	1.80	0.41
74:Li:75:LYS:HA	74:Li:75:LYS:HD2	1.93	0.41
2:SB:111:CYS:HB3	16:Sa:68:TYR:HB2	2.03	0.41
2:SB:122:GLU:HG2	2:SB:140:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:570:C:H2'	19:S2:571:U:O4'	2.20	0.41
19:S2:917:U:H2'	19:S2:918:U:C6	2.55	0.41
20:LR:173:ARG:HG2	20:LR:176:ARG:NH2	2.34	0.41
36:Sg:200:VAL:HG12	36:Sg:207:CYS:HB3	2.02	0.41
40:L5:123:C:H2'	40:L5:124:C:C6	2.54	0.41
40:L5:497:G:H21	40:L5:498:C:H41	1.69	0.41
40:L5:500:G:O2'	40:L5:504:G:H3'	2.21	0.41
40:L5:956:A:H1'	40:L5:2076:G:H5''	2.03	0.41
40:L5:1541:C:H5''	43:LA:21:LYS:HG2	2.01	0.41
40:L5:1633:G:H5'	40:L5:1634:A:OP1	2.21	0.41
40:L5:2844:A:O2'	40:L5:4631:G:H4'	2.21	0.41
40:L5:3867:A2M:H2'	40:L5:3868:G:O4'	2.20	0.41
45:LC:205:ARG:HA	45:LC:205:ARG:HD3	1.78	0.41
45:LC:235:LEU:HD23	45:LC:235:LEU:HA	1.86	0.41
76:Lk:15:ALA:HA	76:Lk:36:VAL:HG21	2.03	0.41
2:SB:139:CYS:HB2	2:SB:172:MET:SD	2.60	0.41
10:SN:89:TYR:CE1	10:SN:150:VAL:HG23	2.56	0.41
12:SV:11:LEU:HG	12:SV:12:TYR:HD1	1.86	0.41
15:SY:119:GLY:HA2	19:S2:85:A:H5'	2.03	0.41
19:S2:946:U:H2'	19:S2:947:G:C8	2.55	0.41
19:S2:1054:G:C2	19:S2:1055:A:H1'	2.55	0.41
19:S2:1535:U:P	24:SF:169:ILE:HG12	2.60	0.41
19:S2:1617:G:H4'	34:Sd:14:PHE:CE2	2.54	0.41
24:SF:38:TYR:HE1	33:Sc:51:ARG:HH21	1.69	0.41
24:SF:39:ILE:HG22	24:SF:41:VAL:HG22	2.03	0.41
40:L5:729:G:H5''	48:LF:76:ARG:HD2	2.02	0.41
40:L5:1620:U:H5''	75:Lj:30:GLN:HE21	1.86	0.41
40:L5:1725:U:H2'	40:L5:1726:U:C6	2.55	0.41
40:L5:1972:G:C6	40:L5:1973:G:C6	3.08	0.41
40:L5:2411:C:H2'	40:L5:2412:A:H8	1.83	0.41
71:Lf:48:ALA:HB2	71:Lf:71:TRP:CZ3	2.55	0.41
74:Li:45:ARG:HA	74:Li:45:ARG:HD2	1.94	0.41
75:Lj:52:LYS:O	75:Lj:55:ARG:HG2	2.21	0.41
78:Lm:82:LEU:HD23	78:Lm:82:LEU:HA	1.86	0.41
85:Zt:29:A:H2'	85:Zt:30:G:H8	1.86	0.41
3:SC:84:PHE:HA	12:SV:15:ARG:CZ	2.50	0.41
6:SH:65:PRO:HG2	6:SH:68:GLN:HB2	2.02	0.41
10:SN:130:LYS:NZ	10:SN:139:TRP:HB3	2.36	0.41
14:SX:9:THR:HG22	19:S2:681:PSU:H4'	2.01	0.41
19:S2:307:G:P	19:S2:307:G:H8	2.43	0.41
19:S2:1134:G:H2'	19:S2:1135:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1281:G:C6	19:S2:1282:A:C6	3.09	0.41
19:S2:1702:G:H2'	19:S2:1703:OMC:O4'	2.21	0.41
22:SR:78:ARG:O	22:SR:79:GLU:C	2.64	0.41
40:L5:86:U:H2'	40:L5:87:A:C8	2.55	0.41
40:L5:662:C:H2'	40:L5:663:G:C8	2.55	0.41
40:L5:716:C:OP1	45:LC:317:ASN:HB2	2.20	0.41
40:L5:908:G:H2'	40:L5:909:A:C8	2.53	0.41
40:L5:1662:C:H2'	40:L5:1663:C:H6	1.86	0.41
59:LS:83:ARG:HG3	59:LS:125:GLN:HB3	2.03	0.41
79:Ln:15:ARG:HG2	79:Ln:18:ARG:NH2	2.36	0.41
5:SG:23:LYS:HB3	5:SG:41:LEU:HG	2.03	0.41
7:SI:10:LYS:HB3	7:SI:10:LYS:HE3	1.85	0.41
9:SL:73:LEU:HD13	9:SL:90:ARG:NE	2.36	0.41
11:SO:32:HIS:CD2	11:SO:96:LYS:HD2	2.56	0.41
13:SW:3:ARG:HD3	13:SW:6:VAL:HG22	2.03	0.41
15:SY:116:LYS:HB3	19:S2:161:U:H5'	2.02	0.41
19:S2:224:A:H2'	19:S2:225:G:C8	2.56	0.41
19:S2:295:C:H2'	19:S2:296:U:H6	1.85	0.41
19:S2:943:U:H2'	19:S2:944:A:H8	1.86	0.41
19:S2:959:G:H2'	19:S2:960:U:C6	2.56	0.41
19:S2:1438:A:H2'	19:S2:1439:A:H8	1.85	0.41
19:S2:1673:U:H2'	19:S2:1674:G:O4'	2.21	0.41
31:SU:55:ARG:HG3	31:SU:87:ARG:CZ	2.51	0.41
40:L5:173:C:H2'	40:L5:174:C:C6	2.55	0.41
40:L5:269:G:H2'	40:L5:270:U:H6	1.86	0.41
40:L5:724:C:H1'	45:LC:343:GLN:HG2	2.02	0.41
40:L5:1771:U:H1'	40:L5:1772:C:C5	2.56	0.41
40:L5:1956:A:H2'	40:L5:1957:U:H6	1.86	0.41
40:L5:2669:C:H2'	40:L5:2670:C:O4'	2.21	0.41
40:L5:4616:A:H2'	40:L5:4617:G:O4'	2.21	0.41
44:LB:160:ILE:HG12	44:LB:193:LYS:HD3	2.03	0.41
44:LB:307:TYR:CE2	44:LB:366:LYS:HE2	2.56	0.41
54:LM:32:ASP:O	54:LM:33:GLN:HG2	2.20	0.41
71:Lf:92:LEU:HD23	71:Lf:92:LEU:HA	1.88	0.41
2:SB:139:CYS:HB3	2:SB:168:MET:HE3	2.03	0.41
7:SI:129:LEU:HD12	7:SI:129:LEU:HA	1.94	0.41
15:SY:79:LEU:HG	15:SY:83:LYS:HE2	2.02	0.41
15:SY:91:LEU:HD22	15:SY:96:LEU:HD22	2.03	0.41
15:SY:111:LYS:HE3	15:SY:111:LYS:HB3	1.90	0.41
24:SF:49:LEU:HD13	28:SQ:49:TYR:HB2	2.02	0.41
26:SM:53:ALA:HA	26:SM:79:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SU:98:VAL:HB	31:SU:99:LYS:HZ2	1.85	0.41
40:L5:958:G:C2	47:LE:124:LYS:HB3	2.55	0.41
40:L5:1348:U:H2'	40:L5:1349:G:C8	2.55	0.41
40:L5:1354:A:OP2	58:LQ:106:THR:HG21	2.21	0.41
40:L5:1503:A:N6	58:LQ:87:THR:HG21	2.33	0.41
40:L5:1700:G:H5'	40:L5:1702:C:OP2	2.20	0.41
40:L5:1834:U:H3	60:LT:128:LEU:HD23	1.86	0.41
40:L5:4153:C:H2'	40:L5:4154:G:C8	2.55	0.41
40:L5:4770:U:H2'	40:L5:4771:C:C6	2.55	0.41
40:L5:5057:C:H2'	40:L5:5058:A:C8	2.55	0.41
48:LF:171:ASP:H	48:LF:174:LEU:HD12	1.85	0.41
53:LL:48:PRO:HB2	73:Lh:120:ALA:HB2	2.01	0.41
55:LN:10:LEU:HD12	74:Li:48:CYS:SG	2.61	0.41
83:Ls:38:LYS:HA	83:Ls:38:LYS:HD3	1.80	0.41
85:Zt:73:G:H2'	85:Zt:74:C:H6	1.83	0.41
1:SA:32:PHE:CG	19:S2:1097:G:H4'	2.55	0.41
1:SA:118:GLU:HG3	3:SC:65:LYS:HE2	2.02	0.41
1:SA:136:GLU:HA	1:SA:139:TYR:HD2	1.86	0.41
1:SA:213:GLU:HB3	22:SR:84:TYR:OH	2.21	0.41
3:SC:121:ARG:CZ	3:SC:123:ARG:HD2	2.51	0.41
9:SL:22:ARG:NH2	9:SL:26:GLY:HA3	2.36	0.41
13:SW:83:LEU:HD23	13:SW:83:LEU:HA	1.86	0.41
13:SW:119:LYS:HG3	13:SW:121:THR:HG22	2.03	0.41
14:SX:88:ASP:HA	19:S2:617:G:H4'	2.02	0.41
19:S2:223:C:H2'	19:S2:224:A:C8	2.56	0.41
19:S2:982:G:H2'	19:S2:983:A:H8	1.86	0.41
19:S2:1406:G:H2'	19:S2:1407:U:C6	2.56	0.41
19:S2:1548:G:H2'	19:S2:1549:U:C6	2.56	0.41
19:S2:1589:A:H2'	19:S2:1590:C:O4'	2.21	0.41
19:S2:1736:G:H2'	19:S2:1737:G:C8	2.56	0.41
23:SD:167:TYR:CD1	23:SD:200:PRO:HG3	2.55	0.41
27:SP:56:LEU:HD22	27:SP:80:LEU:HD11	2.03	0.41
32:SZ:50:PHE:CZ	32:SZ:58:LEU:HD22	2.56	0.41
32:SZ:102:LYS:HA	32:SZ:102:LYS:HD3	1.91	0.41
36:Sg:230:LEU:HD11	36:Sg:259:TRP:CD2	2.55	0.41
40:L5:120:A:H2'	40:L5:149:A:H61	1.86	0.41
40:L5:256:G:H2'	40:L5:257:C:C6	2.56	0.41
40:L5:1464:C:H5''	67:Lb:32:LEU:HD12	2.03	0.41
40:L5:1962:A:H5''	40:L5:2024:G:N2	2.35	0.41
40:L5:2857:A:H2'	40:L5:2858:A:O4'	2.21	0.41
40:L5:2891:U:H2'	40:L5:2892:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:3765:G:H21	40:L5:3766:A:N6	2.19	0.41
40:L5:3841:OMC:HM23	40:L5:3841:OMC:H1'	1.86	0.41
40:L5:5001:PSU:H2'	40:L5:5002:U:O4'	2.21	0.41
40:L5:5002:U:H2'	40:L5:5003:U:H6	1.86	0.41
42:L8:19:C:H2'	42:L8:20:A:H8	1.85	0.41
43:LA:112:ILE:HG22	43:LA:135:THR:HG23	2.03	0.41
44:LB:216:MET:HE3	44:LB:281:ASN:HB3	2.03	0.41
44:LB:291:TYR:CD2	44:LB:327:THR:HG23	2.56	0.41
47:LE:264:ILE:HA	47:LE:265:PRO:HD3	1.91	0.41
48:LF:164:LYS:HB2	48:LF:164:LYS:HE2	1.77	0.41
49:LG:51:LEU:O	49:LG:55:VAL:HG23	2.21	0.41
61:LU:100:LEU:HD13	61:LU:112:LEU:HD12	2.02	0.41
73:Lh:17:LEU:HA	73:Lh:17:LEU:HD23	1.84	0.41
83:Ls:178:LEU:HB3	83:Ls:180:ILE:HG12	2.03	0.41
1:SA:49:ILE:HD13	1:SA:163:CYS:HA	2.02	0.41
2:SB:131:ASP:HB3	2:SB:133:TYR:HD1	1.86	0.41
8:SJ:111:GLN:NE2	8:SJ:127:ARG:HB2	2.36	0.41
15:SY:103:SER:HB3	15:SY:106:GLN:OE1	2.21	0.41
19:S2:99:A2M:HM'3	19:S2:99:A2M:H1'	1.63	0.41
19:S2:648:A:H2'	19:S2:649:PSU:C6	2.56	0.41
24:SF:127:ARG:HD2	24:SF:127:ARG:HA	1.86	0.41
27:SP:62:LYS:HA	27:SP:65:LYS:HD3	2.03	0.41
28:SQ:39:LEU:HD11	28:SQ:51:LEU:HD22	2.03	0.41
31:SU:54:VAL:HB	31:SU:88:LEU:HB2	2.03	0.41
40:L5:1176:C:H2'	40:L5:1177:U:C6	2.55	0.41
40:L5:1198:G:H2'	40:L5:1199:G:H8	1.86	0.41
40:L5:1326:A2M:H2'	40:L5:1327:C:C6	2.56	0.41
40:L5:1700:G:H5''	40:L5:1704:C:N4	2.36	0.41
40:L5:2264:C:H2'	40:L5:2265:G:O4'	2.20	0.41
40:L5:2306:G:H1'	40:L5:2332:A:N6	2.36	0.41
40:L5:4625:C:O2'	40:L5:4626:A:H5'	2.21	0.41
40:L5:4965:U:H5''	44:LB:128:LYS:NZ	2.36	0.41
53:LL:69:LYS:HG3	53:LL:159:ASN:HD21	1.85	0.41
54:LM:100:ARG:HA	54:LM:103:LYS:HG2	2.03	0.41
62:LV:90:ARG:O	62:LV:90:ARG:HG2	2.21	0.41
2:SB:136:ARG:HB2	2:SB:216:LYS:HG3	2.03	0.40
3:SC:138:GLY:HA3	3:SC:162:ILE:HD13	2.02	0.40
7:SI:148:LYS:HD3	7:SI:152:ARG:HH22	1.87	0.40
9:SL:22:ARG:HA	9:SL:22:ARG:NH1	2.36	0.40
19:S2:595:U:H2'	19:S2:596:U:C6	2.55	0.40
30:ST:27:LYS:HE2	30:ST:27:LYS:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Pt:43:A:H2'	38:Pt:44:A:H8	1.85	0.40
40:L5:1494:U:H2'	40:L5:1495:G:H8	1.85	0.40
40:L5:1629:G:N1	43:LA:208:GLU:HG2	2.34	0.40
40:L5:1806:G:H2'	40:L5:1807:C:C6	2.56	0.40
40:L5:2726:G:H2'	40:L5:2727:C:C6	2.56	0.40
40:L5:4156:G:H5''	40:L5:4157:A:H2'	2.03	0.40
40:L5:4761:G:P	56:LO:37:ARG:HH22	2.43	0.40
40:L5:5003:U:H2'	40:L5:5004:C:C6	2.55	0.40
40:L5:5004:C:H2'	40:L5:5005:G:O4'	2.19	0.40
41:L7:120:U:H5'	46:LD:261:VAL:HG23	2.03	0.40
43:LA:229:ALA:HB3	43:LA:234:LYS:HB3	2.04	0.40
68:Lc:65:MET:HB3	68:Lc:65:MET:HE3	1.89	0.40
2:SB:120:MET:HE2	2:SB:142:PHE:HE1	1.87	0.40
2:SB:136:ARG:O	2:SB:215:VAL:HA	2.21	0.40
3:SC:191:VAL:HG11	3:SC:236:PHE:HA	2.03	0.40
4:SE:188:ASN:HB3	4:SE:191:ARG:HD3	2.02	0.40
9:SL:61:PRO:HG3	9:SL:141:ASN:CG	2.46	0.40
19:S2:116:OMU:H6	19:S2:116:OMU:O5'	2.22	0.40
19:S2:554:A:O2'	19:S2:555:A:H8	2.04	0.40
19:S2:1221:G:H2'	19:S2:1222:G:H8	1.84	0.40
19:S2:1264:C:H4'	19:S2:1326:OMU:HM21	2.03	0.40
19:S2:1756:C:H5	19:S2:1757:G:N3	2.20	0.40
24:SF:163:PHE:HD2	24:SF:164:ARG:HG3	1.86	0.40
26:SM:33:ARG:HD2	26:SM:91:LEU:HG	2.03	0.40
26:SM:40:LYS:HB2	26:SM:40:LYS:HE3	1.82	0.40
28:SQ:58:LEU:HD11	28:SQ:112:LEU:HD11	2.02	0.40
29:SS:51:ASP:O	29:SS:54:LYS:HG2	2.21	0.40
40:L5:254:G:O5'	40:L5:254:G:H8	2.05	0.40
40:L5:469:C:H2'	40:L5:470:A:H8	1.85	0.40
40:L5:2066:C:O2'	71:Lf:79:GLY:HA2	2.21	0.40
40:L5:3825:A2M:H2'	40:L5:3826:C:O4'	2.20	0.40
40:L5:4071:U:H2'	40:L5:4072:C:C6	2.55	0.40
40:L5:4536:OMC:HM22	40:L5:4537:C:O4'	2.21	0.40
40:L5:4918:C:H2'	40:L5:4919:G:H8	1.85	0.40
47:LE:176:THR:HG21	47:LE:253:VAL:HG11	2.03	0.40
48:LF:46:ARG:O	48:LF:50:ILE:HG12	2.22	0.40
53:LL:79:GLU:O	53:LL:83:VAL:HG22	2.21	0.40
54:LM:122:ILE:HB	56:LO:189:ILE:HD11	2.03	0.40
59:LS:149:LYS:HB2	59:LS:149:LYS:HE2	1.85	0.40
63:LX:73:HIS:ND1	63:LX:115:LYS:HE2	2.36	0.40
69:Ld:63:ARG:HD3	69:Ld:103:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SB:217:MET:HE3	2:SB:217:MET:HB2	1.81	0.40
10:SN:149:LEU:HD12	10:SN:149:LEU:HA	1.87	0.40
19:S2:166:A2M:H1'	19:S2:166:A2M:HM'3	1.73	0.40
19:S2:1088:U:H4'	19:S2:1089:G:OP2	2.21	0.40
19:S2:1603:G:H4'	29:SS:38:ARG:HH21	1.86	0.40
37:At:9:A:H5'	37:At:11:U:OP2	2.21	0.40
40:L5:60:G:H2'	40:L5:61:A:C8	2.57	0.40
40:L5:302:C:H2'	40:L5:303:C:H6	1.86	0.40
40:L5:469:C:H2'	40:L5:470:A:C8	2.56	0.40
40:L5:691:C:H2'	40:L5:692:A:H8	1.84	0.40
40:L5:1773:U:H2'	40:L5:1774:C:C6	2.56	0.40
40:L5:1895:G:H2'	40:L5:1896:A:O4'	2.22	0.40
40:L5:2060:G:N2	59:LS:115:ALA:HB2	2.36	0.40
40:L5:2478:C:H2'	40:L5:2479:G:H5'	2.03	0.40
40:L5:3619:G:H22	40:L5:3624:A:H1'	1.86	0.40
40:L5:4069:U:H2'	40:L5:4070:U:C6	2.56	0.40
40:L5:4481:U:H2'	40:L5:4482:U:C6	2.56	0.40
43:LA:145:LYS:HD3	43:LA:145:LYS:HA	1.75	0.40
45:LC:279:LEU:HD23	45:LC:279:LEU:HA	1.82	0.40
49:LG:95:LEU:HA	49:LG:218:LEU:HD11	2.03	0.40
59:LS:30:MET:HE2	59:LS:30:MET:HB3	1.95	0.40
85:Zt:14:A:H3'	85:Zt:15:G:H8	1.85	0.40
4:SE:39:ARG:HE	4:SE:39:ARG:HB3	1.71	0.40
5:SG:46:LYS:HD3	5:SG:46:LYS:HA	1.83	0.40
7:SI:12:ARG:HH21	7:SI:18:ARG:HG3	1.87	0.40
7:SI:89:GLU:HA	7:SI:92:ARG:HD3	2.03	0.40
19:S2:29:G:H2'	19:S2:30:C:H6	1.87	0.40
19:S2:149:A:N7	19:S2:169:U:C2	2.90	0.40
19:S2:293:C:O2'	19:S2:294:U:H3'	2.21	0.40
19:S2:1365:G:H2'	19:S2:1366:G:H8	1.86	0.40
19:S2:1425:G:H2'	19:S2:1426:U:C6	2.56	0.40
19:S2:1667:U:H2'	19:S2:1668:U:C6	2.56	0.40
24:SF:42:LYS:HA	24:SF:42:LYS:HD3	1.85	0.40
36:Sg:255:SER:HB3	36:Sg:271:LYS:NZ	2.37	0.40
40:L5:126:C:H2'	40:L5:127:G:C8	2.57	0.40
40:L5:408:A:H1'	40:L5:411:G:OP2	2.21	0.40
40:L5:690:C:H2'	40:L5:691:C:C6	2.57	0.40
40:L5:1802:A:H5''	40:L5:1803:G:H5'	2.04	0.40
40:L5:3648:A:H1'	40:L5:3785:A2M:N6	2.37	0.40
40:L5:3684:G:H2'	40:L5:3685:C:C6	2.57	0.40
44:LB:90:VAL:HG22	44:LB:104:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LC:321:ASN:HB3	45:LC:324:ILE:HB	2.03	0.40
48:LF:242:ARG:O	48:LF:246:ARG:HG3	2.22	0.40
52:LJ:166:PHE:CE2	52:LJ:172:GLY:HA3	2.57	0.40
53:LL:87:HIS:CE1	53:LL:89:LYS:HB2	2.57	0.40
54:LM:27:ILE:HA	54:LM:38:VAL:HG23	2.02	0.40
54:LM:118:MET:HG2	56:LO:192:TYR:CZ	2.56	0.40
64:LY:50:ARG:HG3	64:LY:51:LYS:N	2.36	0.40
74:Li:16:LYS:HA	74:Li:16:LYS:HD3	1.77	0.40
77:Ll:24:PRO:HD2	77:Ll:27:ILE:HG13	2.03	0.40
3:SC:94:ILE:HG13	3:SC:95:ASP:N	2.37	0.40
4:SE:61:VAL:HA	4:SE:64:ILE:HG22	2.04	0.40
7:SI:162:LEU:HD11	7:SI:191:GLU:HG2	2.04	0.40
9:SL:44:PHE:HE1	9:SL:144:LYS:HE2	1.86	0.40
22:SR:75:GLU:HA	22:SR:78:ARG:HB2	2.03	0.40
24:SF:103:LEU:HD12	24:SF:103:LEU:HA	1.92	0.40
25:SK:14:LEU:HD12	25:SK:17:LYS:HE2	2.03	0.40
25:SK:79:LEU:HD23	25:SK:79:LEU:HA	1.90	0.40
29:SS:14:ARG:HH11	29:SS:19:ASN:HB3	1.87	0.40
30:ST:31:PRO:HG2	30:ST:34:VAL:HG13	2.03	0.40
36:Sg:62:HIS:CE1	36:Sg:88:ARG:HB2	2.57	0.40
40:L5:1309:C:H2'	40:L5:1310:C:C6	2.57	0.40
40:L5:1397:A:OP1	66:La:132:ARG:HB2	2.21	0.40
40:L5:1468:C:H2'	40:L5:1469:C:H6	1.86	0.40
40:L5:1893:C:H1'	40:L5:1937:C:O2	2.22	0.40
40:L5:2521:G:H5'	40:L5:2640:G:H1'	2.03	0.40
40:L5:2803:U:H2'	40:L5:2804:OMC:H6	1.87	0.40
40:L5:4919:G:H2'	40:L5:4920:C:C6	2.56	0.40
48:LF:104:LYS:HB2	48:LF:104:LYS:HE2	1.95	0.40
48:LF:213:LEU:HB3	48:LF:247:MET:HG2	2.02	0.40
50:LH:41:ILE:HG21	50:LH:73:ILE:HD11	2.04	0.40
54:LM:77:TRP:O	54:LM:81:ASP:HA	2.20	0.40
55:LN:5:LYS:HA	55:LN:5:LYS:HD3	1.93	0.40
57:LP:61:ARG:NH2	57:LP:76:TRP:HB3	2.37	0.40
65:LZ:106:LEU:HD23	65:LZ:106:LEU:HA	1.91	0.40
73:Lh:3:LYS:HB3	73:Lh:3:LYS:HE2	1.75	0.40
77:Ll:25:GLN:HE22	77:Ll:28:ARG:NH1	2.20	0.40
77:Ll:42:ARG:HG3	77:Ll:47:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SA	219/221 (99%)	206 (94%)	12 (6%)	1 (0%)	24	43
2	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	SC	218/222 (98%)	207 (95%)	11 (5%)	0	100	100
4	SE	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
5	SG	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
6	SH	182/186 (98%)	163 (90%)	19 (10%)	0	100	100
7	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
8	SJ	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
9	SL	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
10	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
11	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
12	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
13	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
14	SX	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
15	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
16	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
17	Sb	81/83 (98%)	71 (88%)	10 (12%)	0	100	100
18	Se	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
20	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
21	LW	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
22	SR	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	31
23	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
24	SF	187/189 (99%)	177 (95%)	10 (5%)	0	100	100
25	SK	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
26	SM	120/122 (98%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	SP	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
28	SQ	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
29	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
30	ST	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
31	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
32	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
33	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
34	Sd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
35	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
36	Sg	311/313 (99%)	288 (93%)	23 (7%)	0	100	100
39	CI	29/31 (94%)	29 (100%)	0	0	100	100
43	LA	246/248 (99%)	233 (95%)	13 (5%)	0	100	100
44	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
45	LC	366/368 (100%)	350 (96%)	16 (4%)	0	100	100
46	LD	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
47	LE	236/250 (94%)	223 (94%)	13 (6%)	0	100	100
48	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
49	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
50	LH	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
51	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
52	LJ	168/176 (96%)	160 (95%)	8 (5%)	0	100	100
53	LL	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
54	LM	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
55	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
56	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
57	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
58	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
59	LS	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
60	LT	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
61	LU	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
62	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
64	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
65	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
66	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
67	Lb	105/109 (96%)	101 (96%)	4 (4%)	0	100	100
68	Lc	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
69	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
70	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
71	Lf	107/109 (98%)	107 (100%)	0	0	100	100
72	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
73	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
74	Li	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
75	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
76	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
77	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
78	Lm	50/52 (96%)	50 (100%)	0	0	100	100
79	Ln	22/24 (92%)	22 (100%)	0	0	100	100
80	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
81	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
82	Lr	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
83	Ls	194/196 (99%)	177 (91%)	17 (9%)	0	100	100
84	Lt	128/141 (91%)	107 (84%)	21 (16%)	0	100	100
All	All	11672/11870 (98%)	11134 (95%)	536 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	SA	149	ASN
22	SR	129	LYS

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SA	183/183 (100%)	183 (100%)	0	100	100
2	SB	195/195 (100%)	195 (100%)	0	100	100
3	SC	186/188 (99%)	186 (100%)	0	100	100
4	SE	224/224 (100%)	223 (100%)	1 (0%)	84	92
5	SG	207/207 (100%)	207 (100%)	0	100	100
6	SH	166/166 (100%)	166 (100%)	0	100	100
7	SI	178/178 (100%)	178 (100%)	0	100	100
8	SJ	161/161 (100%)	161 (100%)	0	100	100
9	SL	137/137 (100%)	137 (100%)	0	100	100
10	SN	130/130 (100%)	130 (100%)	0	100	100
11	SO	107/110 (97%)	107 (100%)	0	100	100
12	SV	67/67 (100%)	67 (100%)	0	100	100
13	SW	112/112 (100%)	112 (100%)	0	100	100
14	SX	113/113 (100%)	113 (100%)	0	100	100
15	SY	113/113 (100%)	113 (100%)	0	100	100
16	Sa	89/89 (100%)	89 (100%)	0	100	100
17	Sb	75/75 (100%)	75 (100%)	0	100	100
18	Se	47/47 (100%)	47 (100%)	0	100	100
20	LR	166/166 (100%)	165 (99%)	1 (1%)	78	89
21	LW	95/97 (98%)	95 (100%)	0	100	100
22	SR	122/122 (100%)	122 (100%)	0	100	100
23	SD	190/190 (100%)	190 (100%)	0	100	100
24	SF	159/159 (100%)	159 (100%)	0	100	100
25	SK	89/89 (100%)	89 (100%)	0	100	100
26	SM	102/104 (98%)	102 (100%)	0	100	100
27	SP	107/107 (100%)	107 (100%)	0	100	100
28	SQ	119/119 (100%)	119 (100%)	0	100	100
29	SS	126/126 (100%)	126 (100%)	0	100	100
30	ST	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	SU	94/94 (100%)	94 (100%)	0	100	100
32	SZ	66/66 (100%)	66 (100%)	0	100	100
33	Sc	57/57 (100%)	57 (100%)	0	100	100
34	Sd	48/48 (100%)	48 (100%)	0	100	100
35	Sf	60/60 (100%)	60 (100%)	0	100	100
36	Sg	272/272 (100%)	272 (100%)	0	100	100
39	CI	25/25 (100%)	25 (100%)	0	100	100
43	LA	190/190 (100%)	190 (100%)	0	100	100
44	LB	348/348 (100%)	348 (100%)	0	100	100
45	LC	306/306 (100%)	306 (100%)	0	100	100
46	LD	246/247 (100%)	246 (100%)	0	100	100
47	LE	212/222 (96%)	212 (100%)	0	100	100
48	LF	194/194 (100%)	194 (100%)	0	100	100
49	LG	203/205 (99%)	203 (100%)	0	100	100
50	LH	169/169 (100%)	169 (100%)	0	100	100
51	LI	180/180 (100%)	180 (100%)	0	100	100
52	LJ	143/148 (97%)	143 (100%)	0	100	100
53	LL	176/176 (100%)	175 (99%)	1 (1%)	78	89
54	LM	118/118 (100%)	117 (99%)	1 (1%)	73	86
55	LN	171/171 (100%)	171 (100%)	0	100	100
56	LO	173/173 (100%)	173 (100%)	0	100	100
57	LP	134/134 (100%)	134 (100%)	0	100	100
58	LQ	164/164 (100%)	164 (100%)	0	100	100
59	LS	156/156 (100%)	156 (100%)	0	100	100
60	LT	139/139 (100%)	139 (100%)	0	100	100
61	LU	91/91 (100%)	91 (100%)	0	100	100
62	LV	101/101 (100%)	101 (100%)	0	100	100
63	LX	108/108 (100%)	108 (100%)	0	100	100
64	LY	124/124 (100%)	124 (100%)	0	100	100
65	LZ	117/117 (100%)	117 (100%)	0	100	100
66	La	120/120 (100%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	Lb	88/90 (98%)	88 (100%)	0	100	100
68	Lc	83/83 (100%)	83 (100%)	0	100	100
69	Ld	98/98 (100%)	98 (100%)	0	100	100
70	Le	114/114 (100%)	114 (100%)	0	100	100
71	Lf	88/88 (100%)	88 (100%)	0	100	100
72	Lg	98/98 (100%)	98 (100%)	0	100	100
73	Lh	109/109 (100%)	109 (100%)	0	100	100
74	Li	86/86 (100%)	86 (100%)	0	100	100
75	Lj	73/73 (100%)	73 (100%)	0	100	100
76	Lk	64/64 (100%)	64 (100%)	0	100	100
77	Ll	47/47 (100%)	47 (100%)	0	100	100
78	Lm	48/48 (100%)	48 (100%)	0	100	100
79	Ln	23/23 (100%)	23 (100%)	0	100	100
80	Lo	93/93 (100%)	93 (100%)	0	100	100
81	Lp	74/74 (100%)	74 (100%)	0	100	100
82	Lr	109/109 (100%)	109 (100%)	0	100	100
83	Ls	162/164 (99%)	162 (100%)	0	100	100
84	Lt	107/115 (93%)	107 (100%)	0	100	100
All	All	10147/10186 (100%)	10143 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SE	157	ASN
20	LR	139	MET
53	LL	59	VAL
54	LM	31	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	SA	50	ASN
2	SB	177	GLN
4	SE	138	HIS
4	SE	201	HIS

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Mol	Chain	Res	Type
5	SG	65	GLN
5	SG	81	HIS
5	SG	105	ASN
5	SG	197	GLN
6	SH	163	GLN
7	SI	52	ASN
9	SL	11	GLN
10	SN	5	HIS
10	SN	123	HIS
14	SX	31	HIS
15	SY	94	HIS
21	LW	104	GLN
23	SD	226	GLN
24	SF	36	GLN
24	SF	82	ASN
24	SF	137	GLN
26	SM	28	HIS
28	SQ	48	GLN
28	SQ	77	HIS
30	ST	85	ASN
34	Sd	37	ASN
36	Sg	4	GLN
36	Sg	62	HIS
36	Sg	191	HIS
43	LA	97	ASN
43	LA	132	ASN
44	LB	121	ASN
44	LB	184	GLN
44	LB	289	GLN
45	LC	21	ASN
45	LC	187	GLN
45	LC	203	GLN
45	LC	317	ASN
45	LC	329	ASN
46	LD	81	HIS
46	LD	195	HIS
46	LD	202	GLN
46	LD	250	ASN
46	LD	282	GLN
47	LE	43	HIS
47	LE	266	GLN
48	LF	80	ASN

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Mol	Chain	Res	Type
49	LG	90	GLN
49	LG	94	GLN
50	LH	169	ASN
50	LH	189	GLN
51	LI	73	ASN
51	LI	166	HIS
54	LM	34	ASN
54	LM	44	GLN
54	LM	69	HIS
55	LN	32	GLN
55	LN	109	HIS
55	LN	145	ASN
57	LP	10	ASN
58	LQ	44	ASN
58	LQ	93	GLN
58	LQ	162	HIS
63	LX	93	ASN
63	LX	107	HIS
64	LY	14	ASN
64	LY	56	GLN
65	LZ	132	GLN
66	La	34	ASN
66	La	60	HIS
68	Lc	33	GLN
69	Ld	28	ASN
70	Le	23	HIS
70	Le	52	GLN
70	Le	107	ASN
71	Lf	21	GLN
72	Lg	100	GLN
75	Lj	13	ASN
80	Lo	105	GLN
83	Ls	127	ASN
83	Ls	190	GLN
84	Lt	68	GLN
84	Lt	149	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S2	1715/1740 (98%)	407 (23%)	4 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	At	69/71 (97%)	12 (17%)	0
38	Pt	72/74 (97%)	14 (19%)	0
40	L5	3644/3655 (99%)	778 (21%)	16 (0%)
41	L7	119/120 (99%)	12 (10%)	0
42	L8	155/156 (99%)	27 (17%)	0
85	Zt	74/75 (98%)	34 (45%)	0
All	All	5848/5891 (99%)	1284 (21%)	20 (0%)

All (1284) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S2	2	A
19	S2	13	C
19	S2	14	C
19	S2	25	A
19	S2	33	G
19	S2	41	G
19	S2	42	A
19	S2	44	U
19	S2	45	A
19	S2	46	A
19	S2	56	G
19	S2	58	C
19	S2	59	U
19	S2	60	A
19	S2	62	G
19	S2	65	C
19	S2	67	C
19	S2	68	A
19	S2	72	C
19	S2	73	C
19	S2	74	G
19	S2	76	U
19	S2	92	A
19	S2	99	A2M
19	S2	103	A
19	S2	113	G
19	S2	115	U
19	S2	126	G
19	S2	130	G
19	S2	142	C
19	S2	143	U

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Mol	Chain	Res	Type
19	S2	149	A
19	S2	155	G
19	S2	161	U
19	S2	162	C
19	S2	170	A
19	S2	179	C
19	S2	182	C
19	S2	187	G
19	S2	190	G
19	S2	196	C
19	S2	197	U
19	S2	198	U
19	S2	200	G
19	S2	203	G
19	S2	204	G
19	S2	207	G
19	S2	208	G
19	S2	211	G
19	S2	213	G
19	S2	214	U
19	S2	288	G
19	S2	289	G
19	S2	291	G
19	S2	292	A
19	S2	295	C
19	S2	302	A
19	S2	303	C
19	S2	306	C
19	S2	307	G
19	S2	308	G
19	S2	309	G
19	S2	312	G
19	S2	313	A
19	S2	318	A
19	S2	319	C
19	S2	323	C
19	S2	324	C
19	S2	325	C
19	S2	326	C
19	S2	328	U
19	S2	329	G
19	S2	332	G

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Mol	Chain	Res	Type
19	S2	339	A
19	S2	347	G
19	S2	360	A
19	S2	361	U
19	S2	362	C
19	S2	363	A
19	S2	364	A
19	S2	368	U
19	S2	370	G
19	S2	385	G
19	S2	386	C
19	S2	398	A
19	S2	407	G
19	S2	408	A
19	S2	409	C
19	S2	426	A
19	S2	438	G
19	S2	448	A
19	S2	449	A
19	S2	450	C
19	S2	452	G
19	S2	464	A
19	S2	465	A
19	S2	471	G
19	S2	472	C
19	S2	473	A
19	S2	474	G
19	S2	476	A
19	S2	478	G
19	S2	479	C
19	S2	482	G
19	S2	487	U
19	S2	488	U
19	S2	492	C
19	S2	493	A
19	S2	500	A
19	S2	502	C
19	S2	531	A
19	S2	532	C
19	S2	536	A
19	S2	537	C
19	S2	540	U

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Mol	Chain	Res	Type
19	S2	542	U
19	S2	544	G
19	S2	546	G
19	S2	547	G
19	S2	557	U
19	S2	558	G
19	S2	559	G
19	S2	563	G
19	S2	564	A
19	S2	576	A2M
19	S2	583	A
19	S2	587	A
19	S2	589	G
19	S2	590	A
19	S2	591	U
19	S2	592	C
19	S2	600	G
19	S2	604	A
19	S2	614	C
19	S2	617	G
19	S2	623	G
19	S2	627	OMU
19	S2	628	A
19	S2	631	U
19	S2	643	A
19	S2	644	OMG
19	S2	655	A
19	S2	660	C
19	S2	663	C
19	S2	664	A
19	S2	668	A2M
19	S2	669	A
19	S2	671	A
19	S2	672	A
19	S2	673	G
19	S2	684	G
19	S2	688	U
19	S2	689	U
19	S2	690	G
19	S2	692	G
19	S2	693	A
19	S2	695	C

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Mol	Chain	Res	Type
19	S2	696	G
19	S2	697	G
19	S2	731	G
19	S2	732	U
19	S2	733	C
19	S2	734	C
19	S2	736	C
19	S2	738	C
19	S2	749	U
19	S2	751	G
19	S2	752	G
19	S2	753	C
19	S2	788	G
19	S2	790	C
19	S2	791	C
19	S2	793	G
19	S2	797	C
19	S2	798	G
19	S2	799	OMU
19	S2	801	PSU
19	S2	821	G
19	S2	822	U
19	S2	823	U
19	S2	824	C
19	S2	827	A
19	S2	830	A
19	S2	834	C
19	S2	835	C
19	S2	836	G
19	S2	837	A
19	S2	838	G
19	S2	839	C
19	S2	840	C
19	S2	841	G
19	S2	842	C
19	S2	844	U
19	S2	847	A
19	S2	863	PSU
19	S2	864	A
19	S2	867	OMG
19	S2	870	A
19	S2	874	G

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Mol	Chain	Res	Type
19	S2	877	C
19	S2	878	G
19	S2	888	U
19	S2	889	U
19	S2	891	G
19	S2	894	G
19	S2	896	U
19	S2	897	U
19	S2	898	U
19	S2	899	U
19	S2	900	C
19	S2	901	G
19	S2	903	A
19	S2	909	G
19	S2	913	A
19	S2	919	A
19	S2	920	A
19	S2	933	G
19	S2	934	G
19	S2	959	G
19	S2	963	A
19	S2	970	G
19	S2	971	G
19	S2	972	A
19	S2	978	G
19	S2	982	G
19	S2	990	A
19	S2	992	A
19	S2	997	A
19	S2	999	G
19	S2	1001	A
19	S2	1002	U
19	S2	1008	A
19	S2	1017	U
19	S2	1023	A
19	S2	1027	A
19	S2	1044	G
19	S2	1045	PSU
19	S2	1060	A
19	S2	1061	U
19	S2	1062	A
19	S2	1067	C

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Mol	Chain	Res	Type
19	S2	1083	A
19	S2	1085	C
19	S2	1108	G
19	S2	1109	C
19	S2	1113	A
19	S2	1115	U
19	S2	1116	C
19	S2	1119	A
19	S2	1123	C
19	S2	1133	A
19	S2	1138	C
19	S2	1139	C
19	S2	1153	C
19	S2	1154	U
19	S2	1195	A
19	S2	1207	G
19	S2	1208	A
19	S2	1215	C
19	S2	1216	C
19	S2	1217	A
19	S2	1220	A
19	S2	1222	G
19	S2	1224	G
19	S2	1227	G
19	S2	1240	A
19	S2	1242	U
19	S2	1243	U
19	S2	1248	B8N
19	S2	1251	A
19	S2	1253	A
19	S2	1256	G
19	S2	1257	G
19	S2	1259	A
19	S2	1264	C
19	S2	1270	G
19	S2	1271	C
19	S2	1272	OMC
19	S2	1274	G
19	S2	1275	G
19	S2	1283	C
19	S2	1285	G
19	S2	1286	G

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Mol	Chain	Res	Type
19	S2	1288	OMU
19	S2	1293	A
19	S2	1294	G
19	S2	1295	A
19	S2	1301	A
19	S2	1302	G
19	S2	1303	C
19	S2	1308	U
19	S2	1333	U
19	S2	1342	U
19	S2	1356	G
19	S2	1357	A
19	S2	1364	U
19	S2	1371	U
19	S2	1372	U
19	S2	1376	A
19	S2	1378	A
19	S2	1382	A
19	S2	1401	A
19	S2	1402	A
19	S2	1404	U
19	S2	1406	G
19	S2	1408	U
19	S2	1413	G
19	S2	1414	A
19	S2	1418	C
19	S2	1419	C
19	S2	1421	A
19	S2	1422	G
19	S2	1423	C
19	S2	1424	G
19	S2	1428	G
19	S2	1431	G
19	S2	1433	C
19	S2	1435	C
19	S2	1437	C
19	S2	1438	A
19	S2	1439	A
19	S2	1442	OMU
19	S2	1449	G
19	S2	1454	A
19	S2	1462	U

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Mol	Chain	Res	Type
19	S2	1463	U
19	S2	1466	G
19	S2	1480	A
19	S2	1489	A
19	S2	1490	OMG
19	S2	1494	U
19	S2	1495	G
19	S2	1497	G
19	S2	1498	A
19	S2	1509	U
19	S2	1520	G
19	S2	1521	C
19	S2	1522	A
19	S2	1531	A
19	S2	1533	A
19	S2	1534	C
19	S2	1536	G
19	S2	1544	C
19	S2	1546	G
19	S2	1552	G
19	S2	1558	C
19	S2	1578	U
19	S2	1580	A
19	S2	1581	C
19	S2	1585	U
19	S2	1587	G
19	S2	1588	A
19	S2	1598	G
19	S2	1600	G
19	S2	1604	G
19	S2	1606	G
19	S2	1621	U
19	S2	1623	A
19	S2	1633	A
19	S2	1637	A
19	S2	1648	G
19	S2	1649	U
19	S2	1654	G
19	S2	1657	G
19	S2	1663	A
19	S2	1665	G
19	S2	1680	G

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Mol	Chain	Res	Type
19	S2	1683	C
19	S2	1686	G
19	S2	1695	A
19	S2	1698	C
19	S2	1699	A
19	S2	1700	C
19	S2	1712	A
19	S2	1715	A
19	S2	1721	U
19	S2	1722	G
19	S2	1744	G
19	S2	1745	A
19	S2	1752	C
19	S2	1753	C
19	S2	1754	G
19	S2	1755	C
19	S2	1756	C
19	S2	1757	G
19	S2	1758	G
19	S2	1759	G
19	S2	1761	U
19	S2	1772	C
19	S2	1773	C
19	S2	1774	C
19	S2	1777	G
19	S2	1782	G
19	S2	1783	C
19	S2	1784	G
19	S2	1798	C
19	S2	1810	U
19	S2	1824	A
19	S2	1835	A
19	S2	1838	U
19	S2	1849	G
19	S2	1851	MA6
19	S2	1861	G
19	S2	1862	G
19	S2	1863	A
19	S2	1864	U
19	S2	1865	C
37	At	9	A
37	At	13	U

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Mol	Chain	Res	Type
37	At	14	A
37	At	21	A
37	At	36	C
37	At	46	G
37	At	47	U
37	At	48	C
37	At	49	C
37	At	58	A
37	At	63	G
37	At	67	G
38	Pt	9	A
38	Pt	13	U
38	Pt	19	G
38	Pt	21	A
38	Pt	46	G
38	Pt	47	U
38	Pt	48	C
38	Pt	49	C
38	Pt	58	A
38	Pt	63	G
38	Pt	67	G
38	Pt	70	A
38	Pt	74	C
38	Pt	76	A
40	L5	25	A
40	L5	30	C
40	L5	39	A
40	L5	42	A
40	L5	48	G
40	L5	56	A
40	L5	59	A
40	L5	64	A
40	L5	65	A
40	L5	73	A
40	L5	74	G
40	L5	75	G
40	L5	84	A
40	L5	91	G
40	L5	104	G
40	L5	108	A
40	L5	109	G
40	L5	110	C

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Mol	Chain	Res	Type
40	L5	119	G
40	L5	120	A
40	L5	132	G
40	L5	133	C
40	L5	134	G
40	L5	135	G
40	L5	144	G
40	L5	159	C
40	L5	165	A
40	L5	171	U
40	L5	172	C
40	L5	182	G
40	L5	183	C
40	L5	184	U
40	L5	185	C
40	L5	186	G
40	L5	188	G
40	L5	189	G
40	L5	200	U
40	L5	209	U
40	L5	216	C
40	L5	218	A
40	L5	234	G
40	L5	255	C
40	L5	256	G
40	L5	261	G
40	L5	262	G
40	L5	265	C
40	L5	266	C
40	L5	267	G
40	L5	275	C
40	L5	280	G
40	L5	297	U
40	L5	306	A
40	L5	315	G
40	L5	316	U
40	L5	326	C
40	L5	340	C
40	L5	373	G
40	L5	385	A
40	L5	387	G
40	L5	388	A

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Mol	Chain	Res	Type
40	L5	407	A
40	L5	409	G
40	L5	410	A
40	L5	411	G
40	L5	412	G
40	L5	413	G
40	L5	414	C
40	L5	415	G
40	L5	431	G
40	L5	432	U
40	L5	440	U
40	L5	449	C
40	L5	452	A
40	L5	453	G
40	L5	454	U
40	L5	456	C
40	L5	457	G
40	L5	465	G
40	L5	467	U
40	L5	479	G
40	L5	485	C
40	L5	486	C
40	L5	489	C
40	L5	493	G
40	L5	497	G
40	L5	498	C
40	L5	499	G
40	L5	500	G
40	L5	501	C
40	L5	502	C
40	L5	503	C
40	L5	504	G
40	L5	509	A
40	L5	510	U
40	L5	512	U
40	L5	513	U
40	L5	514	U
40	L5	518	G
40	L5	519	C
40	L5	643	C
40	L5	644	G
40	L5	646	G

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Mol	Chain	Res	Type
40	L5	654	C
40	L5	655	C
40	L5	656	C
40	L5	657	C
40	L5	659	G
40	L5	666	G
40	L5	667	A
40	L5	668	C
40	L5	669	C
40	L5	673	C
40	L5	674	G
40	L5	686	A
40	L5	687	U
40	L5	696	C
40	L5	704	C
40	L5	708	G
40	L5	730	G
40	L5	731	G
40	L5	738	C
40	L5	739	G
40	L5	742	G
40	L5	747	A
40	L5	750	U
40	L5	759	G
40	L5	760	G
40	L5	904	C
40	L5	905	C
40	L5	913	U
40	L5	914	U
40	L5	915	A
40	L5	917	A
40	L5	923	C
40	L5	924	C
40	L5	926	G
40	L5	932	A
40	L5	933	G
40	L5	934	C
40	L5	935	A
40	L5	936	C
40	L5	937	U
40	L5	943	A
40	L5	945	U

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Mol	Chain	Res	Type
40	L5	956	A
40	L5	957	G
40	L5	958	G
40	L5	959	G
40	L5	960	A
40	L5	961	G
40	L5	962	C
40	L5	965	G
40	L5	966	A
40	L5	967	C
40	L5	968	C
40	L5	969	C
40	L5	970	G
40	L5	971	U
40	L5	982	U
40	L5	985	C
40	L5	988	C
40	L5	1070	G
40	L5	1072	C
40	L5	1075	G
40	L5	1082	C
40	L5	1083	U
40	L5	1095	A
40	L5	1168	G
40	L5	1171	G
40	L5	1172	C
40	L5	1173	G
40	L5	1174	G
40	L5	1178	G
40	L5	1179	U
40	L5	1180	C
40	L5	1181	C
40	L5	1182	C
40	L5	1183	C
40	L5	1187	G
40	L5	1189	G
40	L5	1202	C
40	L5	1203	G
40	L5	1210	C
40	L5	1211	G
40	L5	1214	C
40	L5	1215	C

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Mol	Chain	Res	Type
40	L5	1218	G
40	L5	1219	G
40	L5	1222	A
40	L5	1253	G
40	L5	1254	A
40	L5	1257	A
40	L5	1258	G
40	L5	1262	G
40	L5	1266	G
40	L5	1267	C
40	L5	1269	G
40	L5	1271	G
40	L5	1272	C
40	L5	1273	G
40	L5	1275	G
40	L5	1280	C
40	L5	1284	G
40	L5	1285	U
40	L5	1287	G
40	L5	1293	G
40	L5	1294	A
40	L5	1295	C
40	L5	1296	G
40	L5	1301	C
40	L5	1312	A
40	L5	1314	C
40	L5	1326	A2M
40	L5	1337	A
40	L5	1354	A
40	L5	1359	G
40	L5	1365	C
40	L5	1366	G
40	L5	1367	C
40	L5	1379	C
40	L5	1387	A
40	L5	1394	G
40	L5	1397	A
40	L5	1404	G
40	L5	1407	C
40	L5	1409	C
40	L5	1410	U
40	L5	1411	C

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Mol	Chain	Res	Type
40	L5	1413	C
40	L5	1415	G
40	L5	1416	G
40	L5	1417	C
40	L5	1420	A
40	L5	1421	G
40	L5	1437	C
40	L5	1439	C
40	L5	1442	C
40	L5	1443	A
40	L5	1444	G
40	L5	1446	C
40	L5	1447	C
40	L5	1457	G
40	L5	1482	G
40	L5	1483	C
40	L5	1497	A
40	L5	1498	G
40	L5	1502	G
40	L5	1516	G
40	L5	1517	G
40	L5	1524	A2M
40	L5	1534	A2M
40	L5	1535	C
40	L5	1547	A
40	L5	1552	G
40	L5	1562	G
40	L5	1566	C
40	L5	1574	G
40	L5	1578	U
40	L5	1591	U
40	L5	1596	U
40	L5	1597	G
40	L5	1612	G
40	L5	1624	G
40	L5	1625	OMG
40	L5	1626	G
40	L5	1631	A
40	L5	1633	G
40	L5	1634	A
40	L5	1638	A
40	L5	1641	G

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Mol	Chain	Res	Type
40	L5	1642	A
40	L5	1654	G
40	L5	1661	C
40	L5	1676	C
40	L5	1677	PSU
40	L5	1680	G
40	L5	1694	C
40	L5	1697	G
40	L5	1699	A
40	L5	1700	G
40	L5	1701	A
40	L5	1702	C
40	L5	1705	G
40	L5	1717	C
40	L5	1718	C
40	L5	1719	A
40	L5	1731	C
40	L5	1733	G
40	L5	1741	G
40	L5	1742	A
40	L5	1750	G
40	L5	1757	U
40	L5	1758	G
40	L5	1759	G
40	L5	1760	G
40	L5	1761	G
40	L5	1762	C
40	L5	1763	C
40	L5	1764	G
40	L5	1765	A
40	L5	1766	A
40	L5	1767	A
40	L5	1768	C
40	L5	1770	A
40	L5	1787	A
40	L5	1803	G
40	L5	1804	A
40	L5	1806	G
40	L5	1810	G
40	L5	1820	C
40	L5	1821	G
40	L5	1822	U

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Mol	Chain	Res	Type
40	L5	1831	G
40	L5	1834	U
40	L5	1836	G
40	L5	1837	A
40	L5	1842	G
40	L5	1855	G
40	L5	1869	G
40	L5	1882	U
40	L5	1897	A
40	L5	1916	G
40	L5	1917	A
40	L5	1918	U
40	L5	1919	G
40	L5	1920	C
40	L5	1921	C
40	L5	1922	G
40	L5	1925	G
40	L5	1930	U
40	L5	1931	C
40	L5	1932	A
40	L5	1948	G
40	L5	1961	G
40	L5	1962	A
40	L5	1971	C
40	L5	1974	U
40	L5	1975	G
40	L5	1978	C
40	L5	1980	U
40	L5	1981	G
40	L5	1982	G
40	L5	1984	A
40	L5	1985	G
40	L5	1986	U
40	L5	1989	G
40	L5	1991	A
40	L5	1992	U
40	L5	1993	C
40	L5	1995	G
40	L5	1997	U
40	L5	1998	A
40	L5	1999	A
40	L5	2000	G

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Mol	Chain	Res	Type
40	L5	2001	G
40	L5	2002	A
40	L5	2005	G
40	L5	2011	C
40	L5	2016	C
40	L5	2017	A
40	L5	2018	C
40	L5	2019	C
40	L5	2024	G
40	L5	2025	A
40	L5	2026	A
40	L5	2033	A
40	L5	2034	G
40	L5	2046	G
40	L5	2048	U
40	L5	2052	G
40	L5	2055	G
40	L5	2056	G
40	L5	2068	C
40	L5	2069	A
40	L5	2084	C
40	L5	2090	U
40	L5	2092	G
40	L5	2093	A
40	L5	2095	A
40	L5	2097	U
40	L5	2098	G
40	L5	2101	C
40	L5	2102	G
40	L5	2103	G
40	L5	2104	G
40	L5	2105	A
40	L5	2107	C
40	L5	2108	G
40	L5	2110	C
40	L5	2112	G
40	L5	2250	C
40	L5	2252	G
40	L5	2253	A
40	L5	2254	G
40	L5	2256	C
40	L5	2258	C

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Mol	Chain	Res	Type
40	L5	2262	G
40	L5	2289	C
40	L5	2300	A
40	L5	2301	G
40	L5	2306	G
40	L5	2313	A
40	L5	2333	G
40	L5	2348	G
40	L5	2351	OMC
40	L5	2360	A
40	L5	2364	OMG
40	L5	2383	C
40	L5	2395	A
40	L5	2397	G
40	L5	2411	C
40	L5	2412	A
40	L5	2417	A
40	L5	2425	U
40	L5	2450	G
40	L5	2453	A
40	L5	2464	C
40	L5	2465	C
40	L5	2469	C
40	L5	2471	G
40	L5	2474	G
40	L5	2475	G
40	L5	2478	C
40	L5	2479	G
40	L5	2483	G
40	L5	2484	A
40	L5	2485	U
40	L5	2487	G
40	L5	2488	C
40	L5	2489	C
40	L5	2490	U
40	L5	2491	C
40	L5	2494	U
40	L5	2504	C
40	L5	2506	G
40	L5	2513	A
40	L5	2514	G
40	L5	2518	G

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Mol	Chain	Res	Type
40	L5	2519	U
40	L5	2537	A
40	L5	2544	G
40	L5	2546	G
40	L5	2547	G
40	L5	2554	U
40	L5	2555	G
40	L5	2559	G
40	L5	2560	C
40	L5	2565	A
40	L5	2573	A
40	L5	2583	C
40	L5	2586	G
40	L5	2587	A
40	L5	2589	C
40	L5	2601	A
40	L5	2602	G
40	L5	2618	G
40	L5	2627	C
40	L5	2653	C
40	L5	2662	G
40	L5	2669	C
40	L5	2675	G
40	L5	2676	A
40	L5	2687	U
40	L5	2694	G
40	L5	2695	A
40	L5	2696	A
40	L5	2706	G
40	L5	2707	U
40	L5	2708	U
40	L5	2710	C
40	L5	2711	G
40	L5	2719	C
40	L5	2721	G
40	L5	2724	G
40	L5	2726	G
40	L5	2739	C
40	L5	2742	G
40	L5	2743	A
40	L5	2746	A
40	L5	2754	G

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Mol	Chain	Res	Type
40	L5	2761	U
40	L5	2763	U
40	L5	2769	U
40	L5	2770	C
40	L5	2788	U
40	L5	2790	U
40	L5	2806	A
40	L5	2814	C
40	L5	2815	A2M
40	L5	2826	U
40	L5	2827	G
40	L5	2838	G
40	L5	2842	G
40	L5	2848	G
40	L5	2855	G
40	L5	2867	C
40	L5	2877	G
40	L5	2895	A
40	L5	2900	U
40	L5	2901	G
40	L5	2902	G
40	L5	2903	G
40	L5	2904	U
40	L5	2905	C
40	L5	2906	G
40	L5	2907	G
40	L5	2908	U
40	L5	3585	G
40	L5	3588	C
40	L5	3590	G
40	L5	3591	C
40	L5	3594	C
40	L5	3595	U
40	L5	3596	A
40	L5	3597	G
40	L5	3600	G
40	L5	3605	C
40	L5	3615	G
40	L5	3626	G
40	L5	3630	A
40	L5	3635	A
40	L5	3644	U

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Mol	Chain	Res	Type
40	L5	3646	A
40	L5	3648	A
40	L5	3662	A
40	L5	3664	G
40	L5	3670	C
40	L5	3673	C
40	L5	3674	G
40	L5	3692	A
40	L5	3701	OMC
40	L5	3710	G
40	L5	3711	A
40	L5	3713	U
40	L5	3727	A
40	L5	3735	G
40	L5	3736	A
40	L5	3748	A
40	L5	3753	G
40	L5	3760	A
40	L5	3764	U
40	L5	3770	U
40	L5	3774	A
40	L5	3775	A
40	L5	3776	G
40	L5	3777	G
40	L5	3785	A2M
40	L5	3786	U
40	L5	3792	OMG
40	L5	3811	G
40	L5	3814	U
40	L5	3817	A
40	L5	3819	G
40	L5	3824	A
40	L5	3838	U
40	L5	3839	G
40	L5	3840	U
40	L5	3867	A2M
40	L5	3876	A
40	L5	3877	A
40	L5	3878	C
40	L5	3879	G
40	L5	3880	G
40	L5	3885	G

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Mol	Chain	Res	Type
40	L5	3890	A
40	L5	3892	U
40	L5	3897	G
40	L5	3901	A
40	L5	3906	A
40	L5	3907	G
40	L5	3908	A
40	L5	3915	U
40	L5	3938	G
40	L5	3942	A
40	L5	3943	A
40	L5	3944	G
40	L5	3947	A
40	L5	3948	C
40	L5	3949	A
40	L5	3950	U
40	L5	3952	A
40	L5	3953	G
40	L5	4057	C
40	L5	4058	U
40	L5	4059	C
40	L5	4060	U
40	L5	4061	G
40	L5	4062	A
40	L5	4064	C
40	L5	4068	U
40	L5	4069	U
40	L5	4076	G
40	L5	4094	G
40	L5	4095	G
40	L5	4097	G
40	L5	4099	G
40	L5	4101	C
40	L5	4104	G
40	L5	4105	A
40	L5	4106	G
40	L5	4107	G
40	L5	4108	G
40	L5	4111	U
40	L5	4112	C
40	L5	4114	C
40	L5	4115	G

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Mol	Chain	Res	Type
40	L5	4116	C
40	L5	4117	U
40	L5	4121	G
40	L5	4122	G
40	L5	4127	A
40	L5	4133	C
40	L5	4138	C
40	L5	4141	G
40	L5	4142	C
40	L5	4143	G
40	L5	4144	C
40	L5	4146	G
40	L5	4162	C
40	L5	4163	U
40	L5	4168	G
40	L5	4170	A
40	L5	4183	G
40	L5	4184	G
40	L5	4191	G
40	L5	4203	A
40	L5	4212	A
40	L5	4220	6MZ
40	L5	4222	G
40	L5	4228	OMG
40	L5	4229	U
40	L5	4233	A
40	L5	4251	A
40	L5	4254	G
40	L5	4257	A
40	L5	4258	C
40	L5	4265	U
40	L5	4268	A
40	L5	4273	A
40	L5	4281	A
40	L5	4291	G
40	L5	4295	U
40	L5	4304	A
40	L5	4305	G
40	L5	4314	C
40	L5	4319	C
40	L5	4329	G
40	L5	4330	G

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Mol	Chain	Res	Type
40	L5	4332	C
40	L5	4338	G
40	L5	4349	C
40	L5	4350	C
40	L5	4354	U
40	L5	4373	G
40	L5	4376	A
40	L5	4377	G
40	L5	4378	A
40	L5	4379	A
40	L5	4386	C
40	L5	4387	C
40	L5	4394	A
40	L5	4405	G
40	L5	4415	A
40	L5	4421	C
40	L5	4422	A
40	L5	4438	U
40	L5	4444	C
40	L5	4447	5MC
40	L5	4448	G
40	L5	4449	A
40	L5	4464	A
40	L5	4466	C
40	L5	4475	G
40	L5	4488	A
40	L5	4500	PSU
40	L5	4512	U
40	L5	4513	A
40	L5	4515	G
40	L5	4519	C
40	L5	4524	G
40	L5	4525	C
40	L5	4545	G
40	L5	4548	A
40	L5	4549	G
40	L5	4560	C
40	L5	4567	G
40	L5	4575	G
40	L5	4584	A
40	L5	4589	A
40	L5	4590	A2M

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Mol	Chain	Res	Type
40	L5	4600	G
40	L5	4601	U
40	L5	4618	OMG
40	L5	4635	A
40	L5	4636	PSU
40	L5	4637	OMG
40	L5	4652	G
40	L5	4656	A
40	L5	4670	C
40	L5	4671	C
40	L5	4672	A
40	L5	4687	A
40	L5	4695	C
40	L5	4700	A
40	L5	4708	A
40	L5	4709	U
40	L5	4719	G
40	L5	4733	C
40	L5	4734	A
40	L5	4740	G
40	L5	4741	C
40	L5	4742	G
40	L5	4745	G
40	L5	4750	G
40	L5	4754	G
40	L5	4757	C
40	L5	4759	C
40	L5	4761	G
40	L5	4765	G
40	L5	4771	C
40	L5	4772	C
40	L5	4775	C
40	L5	4859	C
40	L5	4863	G
40	L5	4870	G
40	L5	4871	C
40	L5	4875	G
40	L5	4882	U
40	L5	4883	C
40	L5	4889	G
40	L5	4896	G
40	L5	4898	G

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Mol	Chain	Res	Type
40	L5	4899	G
40	L5	4900	C
40	L5	4901	G
40	L5	4910	G
40	L5	4912	G
40	L5	4914	C
40	L5	4919	G
40	L5	4922	C
40	L5	4924	C
40	L5	4926	C
40	L5	4928	C
40	L5	4934	A
40	L5	4937	C
40	L5	4940	C
40	L5	4941	G
40	L5	4943	A
40	L5	4949	G
40	L5	4951	G
40	L5	4955	A
40	L5	4975	G
40	L5	4976	U
40	L5	4979	A
40	L5	4985	U
40	L5	4988	U
40	L5	4989	U
40	L5	4990	C
40	L5	4991	U
40	L5	4995	U
40	L5	5007	A
40	L5	5013	C
40	L5	5014	A
40	L5	5017	G
40	L5	5022	U
40	L5	5024	C
40	L5	5027	C
40	L5	5028	G
40	L5	5030	U
40	L5	5034	A
40	L5	5041	G
40	L5	5047	C
40	L5	5050	C
40	L5	5054	C

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Mol	Chain	Res	Type
40	L5	5055	G
40	L5	5058	A
40	L5	5061	A
40	L5	5069	U
41	L7	22	A
41	L7	33	U
41	L7	37	G
41	L7	38	U
41	L7	53	U
41	L7	54	A
41	L7	64	G
41	L7	97	G
41	L7	100	A
41	L7	102	U
41	L7	110	G
41	L7	111	C
42	L8	3	A
42	L8	23	C
42	L8	25	G
42	L8	34	U
42	L8	35	C
42	L8	39	G
42	L8	59	A
42	L8	62	A
42	L8	63	U
42	L8	75	OMG
42	L8	80	A
42	L8	82	A
42	L8	83	C
42	L8	84	A
42	L8	85	U
42	L8	87	G
42	L8	94	G
42	L8	103	A
42	L8	105	C
42	L8	111	U
42	L8	114	G
42	L8	123	U
42	L8	124	U
42	L8	125	C
42	L8	126	C
42	L8	127	U

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Mol	Chain	Res	Type
42	L8	150	C
85	Zt	2	C
85	Zt	3	C
85	Zt	5	G
85	Zt	7	A
85	Zt	8	U
85	Zt	9	A
85	Zt	10	G
85	Zt	14	A
85	Zt	16	C
85	Zt	18	U
85	Zt	19	G
85	Zt	20	U
85	Zt	21	A
85	Zt	22	G
85	Zt	33	U
85	Zt	34	U
85	Zt	36	U
85	Zt	37	A
85	Zt	39	U
85	Zt	47	U
85	Zt	48	C
85	Zt	49	C
85	Zt	56	C
85	Zt	57	A
85	Zt	58	A
85	Zt	59	G
85	Zt	60	U
85	Zt	61	C
85	Zt	62	C
85	Zt	66	U
85	Zt	70	G
85	Zt	71	G
85	Zt	72	C
85	Zt	73	G

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	S2	291	G
19	S2	563	G
19	S2	688	U

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Mol	Chain	Res	Type
19	S2	1434	C
40	L5	406	C
40	L5	914	U
40	L5	1082	C
40	L5	1366	G
40	L5	1633	G
40	L5	1977	C
40	L5	2252	G
40	L5	2416	G
40	L5	2675	G
40	L5	2760	G
40	L5	3673	C
40	L5	4056	A
40	L5	4447	5MC
40	L5	4600	G
40	L5	4699	U
40	L5	4913	G

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

178 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	$\# Z > 2$
40	OMU	L5	4227	40	19,22,23	3.19	7 (36%)	25,31,34	1.92	5 (20%)
40	OMG	L5	4196	38,40	23,26,27	0.61	0	32,38,41	0.48	0
19	MA6	S2	1850	19	23,26,27	2.62	8 (34%)	33,38,41	3.50	13 (39%)
40	PSU	L5	4493	40	18,21,22	1.02	1 (5%)	21,30,33	1.91	4 (19%)
40	PSU	L5	3884	40	18,21,22	1.10	2 (11%)	21,30,33	2.02	5 (23%)
40	OMG	L5	2424	40	23,26,27	0.65	0	32,38,41	0.44	0
40	PSU	L5	4636	40	18,21,22	1.11	3 (16%)	21,30,33	2.19	7 (33%)
19	OMU	S2	1288	19	19,22,23	3.42	7 (36%)	25,31,34	1.75	4 (16%)
40	PSU	L5	1792	40	18,21,22	1.06	2 (11%)	21,30,33	1.98	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	OMC	S2	1272	19	19,22,23	0.55	0	25,31,34	0.78	1 (4%)
42	OMG	L8	75	42	23,26,27	0.59	0	32,38,41	0.46	0
40	PSU	L5	3639	40	18,21,22	1.11	3 (16%)	21,30,33	1.92	5 (23%)
19	OMG	S2	1490	19	23,26,27	0.60	0	32,38,41	0.54	0
40	A2M	L5	2401	40	22,25,26	1.27	2 (9%)	30,36,39	1.63	8 (26%)
40	PSU	L5	3637	40	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)
19	PSU	S2	1177	19	18,21,22	1.06	2 (11%)	21,30,33	1.83	4 (19%)
40	A2M	L5	1871	40,87	22,25,26	1.39	3 (13%)	30,36,39	1.64	7 (23%)
19	PSU	S2	1081	19	18,21,22	1.09	2 (11%)	21,30,33	2.10	7 (33%)
19	OMU	S2	1326	19	19,22,23	3.29	7 (36%)	25,31,34	1.83	5 (20%)
40	PSU	L5	4471	40	18,21,22	1.10	2 (11%)	21,30,33	1.95	5 (23%)
40	PSU	L5	4299	40	18,21,22	1.05	2 (11%)	21,30,33	1.80	4 (19%)
40	A2M	L5	4523	40,87	22,25,26	1.33	3 (13%)	30,36,39	1.65	9 (30%)
40	PSU	L5	4431	40	18,21,22	1.05	2 (11%)	21,30,33	1.87	4 (19%)
40	OMC	L5	1340	40	19,22,23	0.67	0	25,31,34	0.84	1 (4%)
19	PSU	S2	1045	19	18,21,22	1.12	1 (5%)	21,30,33	1.96	4 (19%)
40	PSU	L5	2632	40	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
19	OMU	S2	116	19	19,22,23	3.28	7 (36%)	25,31,34	1.69	4 (16%)
40	OMG	L5	4499	40	23,26,27	0.59	0	32,38,41	0.49	0
19	PSU	S2	681	19	18,21,22	1.05	1 (5%)	21,30,33	1.92	4 (19%)
40	OMC	L5	3887	40	19,22,23	0.71	0	25,31,34	0.72	0
40	UR3	L5	4530	40	19,22,23	2.57	5 (26%)	26,32,35	1.58	3 (11%)
40	OMC	L5	3841	40	19,22,23	0.76	1 (5%)	25,31,34	0.54	0
19	OMC	S2	174	19	19,22,23	0.58	0	25,31,34	0.67	0
40	A2M	L5	1326	40	22,25,26	1.26	2 (9%)	30,36,39	1.47	8 (26%)
40	PSU	L5	5001	40	18,21,22	1.14	2 (11%)	21,30,33	1.92	4 (19%)
19	A2M	S2	484	19	22,25,26	1.16	1 (4%)	30,36,39	1.44	7 (23%)
40	A2M	L5	1534	40,87	22,25,26	1.19	2 (9%)	30,36,39	1.45	9 (30%)
40	OMG	L5	1625	40	23,26,27	0.63	0	32,38,41	0.48	0
40	OMG	L5	4623	40	23,26,27	0.68	0	32,38,41	0.60	0
19	OMU	S2	121	19	19,22,23	3.26	7 (36%)	25,31,34	1.77	5 (20%)
19	OMU	S2	1442	19	19,22,23	3.33	7 (36%)	25,31,34	1.84	5 (20%)
40	PSU	L5	1582	40	18,21,22	1.06	2 (11%)	21,30,33	1.96	4 (19%)
40	A2M	L5	1323	40	22,25,26	1.37	3 (13%)	30,36,39	1.64	9 (30%)
19	OMU	S2	354	19	19,22,23	3.22	7 (36%)	25,31,34	1.81	5 (20%)
40	OMG	L5	1316	40	23,26,27	0.73	0	32,38,41	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PSU	L5	1781	40	18,21,22	1.06	1 (5%)	21,30,33	1.84	4 (19%)
40	PSU	L5	3844	40	18,21,22	1.12	2 (11%)	21,30,33	1.81	4 (19%)
40	PSU	L5	4353	40	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)
19	OMC	S2	1391	19	19,22,23	0.58	0	25,31,34	0.69	0
40	PSU	L5	4500	40	18,21,22	1.13	3 (16%)	21,30,33	2.10	5 (23%)
19	PSU	S2	651	19	18,21,22	1.04	1 (5%)	21,30,33	2.00	5 (23%)
19	OMU	S2	799	19	19,22,23	3.38	7 (36%)	25,31,34	1.85	5 (20%)
40	OMG	L5	3627	40	23,26,27	0.64	0	32,38,41	0.68	1 (3%)
19	PSU	S2	109	19	18,21,22	1.13	2 (11%)	21,30,33	1.94	5 (23%)
40	PSU	L5	1677	40	18,21,22	1.10	3 (16%)	21,30,33	1.99	5 (23%)
40	PSU	L5	3695	40	18,21,22	1.07	2 (11%)	21,30,33	1.97	6 (28%)
19	PSU	S2	966	19	18,21,22	1.13	1 (5%)	21,30,33	2.04	5 (23%)
19	A2M	S2	576	19	22,25,26	1.20	1 (4%)	30,36,39	1.51	5 (16%)
19	PSU	S2	1174	19	18,21,22	1.08	2 (11%)	21,30,33	1.97	4 (19%)
40	PSU	L5	4972	40	18,21,22	1.05	2 (11%)	21,30,33	1.92	4 (19%)
40	OMU	L5	4498	40	19,22,23	3.18	7 (36%)	25,31,34	1.91	5 (20%)
40	OMC	L5	2861	40	19,22,23	0.72	1 (5%)	25,31,34	0.81	1 (4%)
40	PSU	L5	4361	40	18,21,22	1.06	2 (11%)	21,30,33	1.85	4 (19%)
42	PSU	L8	55	42	18,21,22	1.01	2 (11%)	21,30,33	1.91	4 (19%)
19	OMG	S2	436	19	23,26,27	0.55	0	32,38,41	0.51	0
19	OMU	S2	428	19	19,22,23	3.33	7 (36%)	25,31,34	1.82	5 (20%)
19	G7M	S2	1639	19	23,26,27	2.67	9 (39%)	34,39,42	2.51	11 (32%)
19	6MZ	S2	1832	19,87	22,25,26	4.02	11 (50%)	29,36,39	2.33	11 (37%)
40	OMU	L5	4306	40	19,22,23	3.13	7 (36%)	25,31,34	1.79	4 (16%)
40	PSU	L5	3851	40	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
40	OMG	L5	1522	40	23,26,27	0.66	0	32,38,41	0.75	1 (3%)
40	OMC	L5	2804	40	19,22,23	0.73	0	25,31,34	0.75	1 (4%)
40	A2M	L5	400	40	22,25,26	1.33	3 (13%)	30,36,39	1.62	9 (30%)
40	PSU	L5	2839	40	18,21,22	1.13	2 (11%)	21,30,33	1.98	4 (19%)
40	OMG	L5	2876	40	23,26,27	0.61	0	32,38,41	0.52	0
19	MA6	S2	1851	19	23,26,27	1.29	4 (17%)	33,38,41	3.24	12 (36%)
40	PSU	L5	4689	40	18,21,22	1.14	2 (11%)	21,30,33	1.99	4 (19%)
40	OMG	L5	3744	40	23,26,27	0.63	0	32,38,41	0.46	0
40	A2M	L5	3830	40	22,25,26	1.26	3 (13%)	30,36,39	1.58	8 (26%)
19	OMU	S2	627	19	19,22,23	3.30	7 (36%)	25,31,34	1.83	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PSU	S2	1056	19	18,21,22	1.04	1 (5%)	21,30,33	1.85	4 (19%)
40	OMG	L5	4494	40	23,26,27	0.63	0	32,38,41	0.52	0
40	PSU	L5	4532	40	18,21,22	1.09	2 (11%)	21,30,33	1.88	4 (19%)
40	PSU	L5	1683	40	18,21,22	1.08	2 (11%)	21,30,33	2.02	4 (19%)
40	PSU	L5	4403	40	18,21,22	1.08	2 (11%)	21,30,33	1.98	6 (28%)
19	OMG	S2	644	19	23,26,27	0.48	0	32,38,41	0.47	0
40	A2M	L5	2787	40,87	22,25,26	1.23	1 (4%)	30,36,39	1.54	7 (23%)
19	OMG	S2	509	19	23,26,27	0.53	0	32,38,41	0.49	0
19	PSU	S2	649	19	18,21,22	1.05	2 (11%)	21,30,33	1.73	4 (19%)
40	PSU	L5	4312	40	18,21,22	1.06	2 (11%)	21,30,33	1.86	4 (19%)
19	4AC	S2	1337	19	21,24,25	0.41	0	28,34,37	0.82	2 (7%)
40	OMG	L5	4637	40	23,26,27	0.60	0	32,38,41	0.53	0
40	OMC	L5	2824	40	19,22,23	0.68	0	25,31,34	0.58	0
40	A2M	L5	3718	40	22,25,26	1.18	1 (4%)	30,36,39	1.54	7 (23%)
19	A2M	S2	159	19	22,25,26	1.19	1 (4%)	30,36,39	1.56	8 (26%)
19	B8N	S2	1248	19	25,29,30	3.26	7 (28%)	28,42,45	1.97	8 (28%)
40	A2M	L5	1524	40	22,25,26	1.39	3 (13%)	30,36,39	1.51	8 (26%)
19	A2M	S2	468	19	22,25,26	1.30	1 (4%)	30,36,39	1.65	7 (23%)
19	OMC	S2	517	19	19,22,23	0.58	0	25,31,34	0.68	0
40	OMC	L5	2351	40	19,22,23	0.74	1 (5%)	25,31,34	1.13	2 (8%)
42	PSU	L8	69	42	18,21,22	1.06	2 (11%)	21,30,33	2.09	6 (28%)
40	PSU	L5	4457	40	18,21,22	1.06	3 (16%)	21,30,33	2.03	4 (19%)
19	OMC	S2	1703	19	19,22,23	0.58	0	25,31,34	0.65	0
40	6MZ	L5	4220	40	22,25,26	2.93	6 (27%)	29,36,39	2.52	10 (34%)
40	OMU	L5	2837	40	19,22,23	3.20	7 (36%)	25,31,34	1.94	5 (20%)
19	A2M	S2	668	19,87	22,25,26	1.36	2 (9%)	30,36,39	1.58	6 (20%)
19	A2M	S2	27	19	22,25,26	1.22	1 (4%)	30,36,39	1.51	8 (26%)
40	PSU	L5	4296	40	18,21,22	1.10	2 (11%)	21,30,33	1.92	4 (19%)
40	OMG	L5	3899	40	23,26,27	0.68	0	32,38,41	0.59	0
40	PSU	L5	4628	40	18,21,22	1.12	2 (11%)	21,30,33	2.13	5 (23%)
40	OMC	L5	3701	40	19,22,23	0.80	1 (5%)	25,31,34	1.73	4 (16%)
40	PSU	L5	4576	40	18,21,22	1.09	2 (11%)	21,30,33	1.92	4 (19%)
40	OMC	L5	3808	40,87	19,22,23	0.73	0	25,31,34	0.81	2 (8%)
40	A2M	L5	3867	40	22,25,26	1.28	2 (9%)	30,36,39	1.53	7 (23%)
19	A2M	S2	166	19	22,25,26	1.23	1 (4%)	30,36,39	1.63	7 (23%)
19	A2M	S2	1383	19	22,25,26	1.19	1 (4%)	30,36,39	1.68	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PSU	S2	863	19	18,21,22	1.05	1 (5%)	21,30,33	2.02	4 (19%)
40	PSU	L5	1782	40	18,21,22	1.10	2 (11%)	21,30,33	1.92	5 (23%)
40	OMC	L5	2365	40	19,22,23	0.68	0	25,31,34	0.56	0
40	A2M	L5	3825	40	22,25,26	1.30	2 (9%)	30,36,39	1.64	8 (26%)
40	OMG	L5	4392	40	23,26,27	0.66	0	32,38,41	0.53	0
40	A2M	L5	398	40	22,25,26	1.26	3 (13%)	30,36,39	1.66	7 (23%)
19	PSU	S2	801	19	18,21,22	1.12	1 (5%)	21,30,33	1.76	4 (19%)
40	A2M	L5	2363	40,87	22,25,26	1.38	3 (13%)	30,36,39	1.56	9 (30%)
19	OMG	S2	867	19	23,26,27	0.50	0	32,38,41	0.48	0
19	4AC	S2	1842	19	21,24,25	0.40	0	28,34,37	0.46	0
19	PSU	S2	1244	19	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
40	OMC	L5	4536	40	19,22,23	0.74	0	25,31,34	0.62	0
40	OMG	L5	4228	40	23,26,27	0.64	0	32,38,41	0.69	0
19	PSU	S2	814	19	18,21,22	1.15	1 (5%)	21,30,33	1.88	4 (19%)
40	OMG	L5	4618	40	23,26,27	0.65	0	32,38,41	0.51	0
19	PSU	S2	1232	19	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
40	PSU	L5	1536	40	18,21,22	1.08	2 (11%)	21,30,33	1.89	4 (19%)
40	PSU	L5	4293	40	18,21,22	1.09	2 (11%)	21,30,33	2.11	5 (23%)
19	PSU	S2	866	19	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
19	OMU	S2	172	19	19,22,23	3.29	7 (36%)	25,31,34	1.85	5 (20%)
40	A2M	L5	2815	40	22,25,26	1.21	2 (9%)	30,36,39	1.54	9 (30%)
40	OMG	L5	4370	40	23,26,27	0.60	0	32,38,41	0.54	0
19	PSU	S2	93	19	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
19	OMC	S2	462	19	19,22,23	0.59	0	25,31,34	0.53	0
19	OMG	S2	1328	19	23,26,27	0.52	0	32,38,41	0.51	0
40	OMC	L5	4456	40	19,22,23	0.75	0	25,31,34	0.65	0
40	OMG	L5	3792	40	23,26,27	0.63	0	32,38,41	0.50	0
40	A2M	L5	4590	40	22,25,26	1.33	3 (13%)	30,36,39	1.57	6 (20%)
40	PSU	L5	1860	40	18,21,22	1.06	2 (11%)	21,30,33	1.81	4 (19%)
40	PSU	L5	1744	40,87	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
19	PSU	S2	105	19	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
19	PSU	S2	686	19	18,21,22	1.08	1 (5%)	21,30,33	1.90	5 (23%)
40	PSU	L5	1862	40	18,21,22	1.07	2 (11%)	21,30,33	2.03	5 (23%)
40	PSU	L5	5010	40	18,21,22	1.12	2 (11%)	21,30,33	1.95	4 (19%)
40	A2M	L5	4571	40	22,25,26	1.38	2 (9%)	30,36,39	1.60	8 (26%)
19	A2M	S2	99	19,87	22,25,26	1.23	1 (4%)	30,36,39	1.61	8 (26%)
19	PSU	S2	1004	19	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	A2M	S2	1031	19	22,25,26	1.18	1 (4%)	30,36,39	1.53	8 (26%)
40	PSU	L5	4579	40	18,21,22	1.09	2 (11%)	21,30,33	1.91	4 (19%)
40	OMU	L5	3925	40	19,22,23	3.13	7 (36%)	25,31,34	1.87	5 (20%)
19	PSU	S2	1367	19	18,21,22	1.09	1 (5%)	21,30,33	1.92	5 (23%)
40	PSU	L5	3853	40,87	18,21,22	1.04	1 (5%)	21,30,33	1.96	4 (19%)
40	PSU	L5	4552	40	18,21,22	1.12	2 (11%)	21,30,33	1.98	4 (19%)
19	OMG	S2	683	19	23,26,27	0.53	0	32,38,41	0.57	0
40	UY1	L5	3818	40	19,22,23	4.73	9 (47%)	21,31,34	1.96	6 (28%)
40	A2M	L5	3785	40,87	22,25,26	1.16	1 (4%)	30,36,39	1.55	9 (30%)
40	1MA	L5	1322	40,87	21,25,26	0.76	0	30,37,40	0.83	2 (6%)
40	5MC	L5	3782	40,87	19,22,23	0.81	0	26,32,35	0.81	1 (3%)
40	5MC	L5	4447	40	19,22,23	0.98	1 (5%)	26,32,35	0.63	0
40	OMU	L5	4620	40	19,22,23	3.10	7 (36%)	25,31,34	1.78	5 (20%)
40	OMC	L5	3869	40	19,22,23	0.72	0	25,31,34	0.60	0
40	PSU	L5	4973	40	18,21,22	1.05	2 (11%)	21,30,33	2.07	5 (23%)
19	OMG	S2	601	19	23,26,27	0.55	0	32,38,41	0.41	0
19	PSU	S2	406	19	18,21,22	1.10	2 (11%)	21,30,33	1.99	5 (23%)
40	OMG	L5	2364	40,87	23,26,27	0.66	0	32,38,41	0.42	0
40	PSU	L5	4673	40,87	18,21,22	1.06	2 (11%)	21,30,33	1.94	5 (23%)
40	PSU	L5	3920	40,87	18,21,22	1.10	3 (16%)	21,30,33	2.08	6 (28%)
40	PSU	L5	3822	40	18,21,22	1.08	2 (11%)	21,30,33	1.87	5 (23%)
19	PSU	S2	1046	19	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)
40	OMC	L5	2422	40,87	19,22,23	0.70	0	25,31,34	0.69	0
40	PSU	L5	4442	40	18,21,22	1.09	1 (5%)	21,30,33	2.07	6 (28%)
40	PSU	L5	4521	40,87	18,21,22	1.11	3 (16%)	21,30,33	1.98	5 (23%)

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
40	OMU	L5	4227	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4196	38,40	-	1/9/27/28	0/3/3/3
19	MA6	S2	1850	19	-	0/11/29/30	0/3/3/3
40	PSU	L5	4493	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3884	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	2424	40	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	PSU	L5	4636	40	-	1/7/25/26	0/2/2/2
19	OMU	S2	1288	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	1792	40	-	1/7/25/26	0/2/2/2
19	OMC	S2	1272	19	-	2/9/27/28	0/2/2/2
42	OMG	L8	75	42	-	2/9/27/28	0/3/3/3
40	PSU	L5	3639	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	1490	19	-	1/9/27/28	0/3/3/3
40	A2M	L5	2401	40	-	0/9/27/28	0/3/3/3
40	PSU	L5	3637	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1177	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	1871	40,87	-	0/9/27/28	0/3/3/3
19	PSU	S2	1081	19	-	1/7/25/26	0/2/2/2
19	OMU	S2	1326	19	-	0/9/27/28	0/2/2/2
40	PSU	L5	4471	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4299	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	4523	40,87	-	0/9/27/28	0/3/3/3
40	PSU	L5	4431	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	1340	40	-	1/9/27/28	0/2/2/2
19	PSU	S2	1045	19	-	2/7/25/26	0/2/2/2
40	PSU	L5	2632	40	-	2/7/25/26	0/2/2/2
19	OMU	S2	116	19	-	1/9/27/28	0/2/2/2
40	OMG	L5	4499	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	681	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	3887	40	-	1/9/27/28	0/2/2/2
40	UR3	L5	4530	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3841	40	-	0/9/27/28	0/2/2/2
19	OMC	S2	174	19	-	1/9/27/28	0/2/2/2
40	A2M	L5	1326	40	-	4/9/27/28	0/3/3/3
40	PSU	L5	5001	40	-	0/7/25/26	0/2/2/2
19	A2M	S2	484	19	-	0/9/27/28	0/3/3/3
40	A2M	L5	1534	40,87	-	1/9/27/28	0/3/3/3
40	OMG	L5	1625	40	-	2/9/27/28	0/3/3/3
40	OMG	L5	4623	40	-	0/9/27/28	0/3/3/3
19	OMU	S2	121	19	-	0/9/27/28	0/2/2/2
19	OMU	S2	1442	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	1582	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	1323	40	-	2/9/27/28	0/3/3/3
19	OMU	S2	354	19	-	0/9/27/28	0/2/2/2
40	OMG	L5	1316	40	-	0/9/27/28	0/3/3/3
40	PSU	L5	1781	40	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	PSU	L5	3844	40	-	1/7/25/26	0/2/2/2
40	PSU	L5	4353	40	-	0/7/25/26	0/2/2/2
19	OMC	S2	1391	19	-	0/9/27/28	0/2/2/2
40	PSU	L5	4500	40	-	3/7/25/26	0/2/2/2
19	PSU	S2	651	19	-	0/7/25/26	0/2/2/2
19	OMU	S2	799	19	-	2/9/27/28	0/2/2/2
40	OMG	L5	3627	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	109	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1677	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3695	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	966	19	-	1/7/25/26	0/2/2/2
19	A2M	S2	576	19	-	3/9/27/28	0/3/3/3
19	PSU	S2	1174	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	4972	40	-	0/7/25/26	0/2/2/2
40	OMU	L5	4498	40	-	0/9/27/28	0/2/2/2
40	OMC	L5	2861	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	4361	40	-	0/7/25/26	0/2/2/2
42	PSU	L8	55	42	-	0/7/25/26	0/2/2/2
19	OMG	S2	436	19	-	0/9/27/28	0/3/3/3
19	OMU	S2	428	19	-	6/9/27/28	0/2/2/2
19	G7M	S2	1639	19	-	0/7/25/26	0/3/3/3
19	6MZ	S2	1832	19,87	-	2/9/27/28	0/3/3/3
40	OMU	L5	4306	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3851	40	-	1/7/25/26	0/2/2/2
40	OMG	L5	1522	40	-	0/9/27/28	0/3/3/3
40	OMC	L5	2804	40	-	0/9/27/28	0/2/2/2
40	A2M	L5	400	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	2839	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	2876	40	-	0/9/27/28	0/3/3/3
19	MA6	S2	1851	19	-	1/11/29/30	0/3/3/3
40	PSU	L5	4689	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3744	40	-	1/9/27/28	0/3/3/3
40	A2M	L5	3830	40	-	0/9/27/28	0/3/3/3
19	OMU	S2	627	19	-	2/9/27/28	0/2/2/2
19	PSU	S2	1056	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	4494	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	4532	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1683	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4403	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	644	19	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	A2M	L5	2787	40,87	-	5/9/27/28	0/3/3/3
19	OMG	S2	509	19	-	0/9/27/28	0/3/3/3
19	PSU	S2	649	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	4312	40	-	0/7/25/26	0/2/2/2
19	4AC	S2	1337	19	-	1/11/29/30	0/2/2/2
40	OMG	L5	4637	40	-	3/9/27/28	0/3/3/3
40	OMC	L5	2824	40	-	1/9/27/28	0/2/2/2
40	A2M	L5	3718	40	-	0/9/27/28	0/3/3/3
19	A2M	S2	159	19	-	1/9/27/28	0/3/3/3
19	B8N	S2	1248	19	-	4/16/34/35	0/2/2/2
40	A2M	L5	1524	40	-	2/9/27/28	0/3/3/3
19	A2M	S2	468	19	-	0/9/27/28	0/3/3/3
19	OMC	S2	517	19	-	0/9/27/28	0/2/2/2
40	OMC	L5	2351	40	-	1/9/27/28	0/2/2/2
42	PSU	L8	69	42	-	0/7/25/26	0/2/2/2
40	PSU	L5	4457	40	-	0/7/25/26	0/2/2/2
19	OMC	S2	1703	19	-	1/9/27/28	0/2/2/2
40	6MZ	L5	4220	40	-	2/9/27/28	0/3/3/3
40	OMU	L5	2837	40	-	0/9/27/28	0/2/2/2
19	A2M	S2	668	19,87	-	2/9/27/28	0/3/3/3
19	A2M	S2	27	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	4296	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3899	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	4628	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3701	40	-	6/9/27/28	0/2/2/2
40	PSU	L5	4576	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3808	40,87	-	0/9/27/28	0/2/2/2
40	A2M	L5	3867	40	-	3/9/27/28	0/3/3/3
19	A2M	S2	166	19	-	2/9/27/28	0/3/3/3
19	A2M	S2	1383	19	-	3/9/27/28	0/3/3/3
19	PSU	S2	863	19	-	2/7/25/26	0/2/2/2
40	PSU	L5	1782	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	2365	40	-	0/9/27/28	0/2/2/2
40	A2M	L5	3825	40	-	0/9/27/28	0/3/3/3
40	OMG	L5	4392	40	-	0/9/27/28	0/3/3/3
40	A2M	L5	398	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	801	19	-	2/7/25/26	0/2/2/2
40	A2M	L5	2363	40,87	-	0/9/27/28	0/3/3/3
19	OMG	S2	867	19	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	4AC	S2	1842	19	-	0/11/29/30	0/2/2/2
19	PSU	S2	1244	19	-	1/7/25/26	0/2/2/2
40	OMC	L5	4536	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4228	40	-	2/9/27/28	0/3/3/3
19	PSU	S2	814	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	4618	40	-	2/9/27/28	0/3/3/3
19	PSU	S2	1232	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1536	40	-	2/7/25/26	0/2/2/2
40	PSU	L5	4293	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	866	19	-	0/7/25/26	0/2/2/2
19	OMU	S2	172	19	-	0/9/27/28	0/2/2/2
40	A2M	L5	2815	40	-	2/9/27/28	0/3/3/3
40	OMG	L5	4370	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	93	19	-	0/7/25/26	0/2/2/2
19	OMC	S2	462	19	-	1/9/27/28	0/2/2/2
19	OMG	S2	1328	19	-	1/9/27/28	0/3/3/3
40	OMC	L5	4456	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	3792	40	-	2/9/27/28	0/3/3/3
40	A2M	L5	4590	40	-	3/9/27/28	0/3/3/3
40	PSU	L5	1860	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1744	40,87	-	0/7/25/26	0/2/2/2
19	PSU	S2	105	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	686	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1862	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	5010	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	4571	40	-	0/9/27/28	0/3/3/3
19	A2M	S2	99	19,87	-	3/9/27/28	0/3/3/3
19	PSU	S2	1004	19	-	0/7/25/26	0/2/2/2
19	A2M	S2	1031	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	4579	40	-	0/7/25/26	0/2/2/2
40	OMU	L5	3925	40	-	0/9/27/28	0/2/2/2
19	PSU	S2	1367	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	3853	40,87	-	0/7/25/26	0/2/2/2
40	PSU	L5	4552	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	683	19	-	0/9/27/28	0/3/3/3
40	UY1	L5	3818	40	-	2/9/27/28	0/2/2/2
40	A2M	L5	3785	40,87	-	3/9/27/28	0/3/3/3
40	1MA	L5	1322	40,87	-	2/7/25/26	0/3/3/3
40	5MC	L5	3782	40,87	-	1/7/25/26	0/2/2/2
40	5MC	L5	4447	40	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMU	L5	4620	40	-	1/9/27/28	0/2/2/2
40	OMC	L5	3869	40	-	1/9/27/28	0/2/2/2
40	PSU	L5	4973	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	601	19	-	1/9/27/28	0/3/3/3
19	PSU	S2	406	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	2364	40,87	-	3/9/27/28	0/3/3/3
40	PSU	L5	4673	40,87	-	0/7/25/26	0/2/2/2
40	PSU	L5	3920	40,87	-	0/7/25/26	0/2/2/2
40	PSU	L5	3822	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1046	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	2422	40,87	-	2/9/27/28	0/2/2/2
40	PSU	L5	4442	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4521	40,87	-	0/7/25/26	0/2/2/2

All (359) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1832	6MZ	C6-N6	12.64	1.48	1.34
40	L5	3818	UY1	C6-C5	12.29	1.48	1.35
40	L5	4220	6MZ	C6-N6	11.57	1.47	1.34
40	L5	3818	UY1	C2-N1	11.48	1.51	1.36
19	S2	1288	OMU	C2-N1	8.66	1.52	1.38
19	S2	1832	6MZ	C3'-C2'	-8.54	1.30	1.53
19	S2	799	OMU	C2-N1	8.39	1.51	1.38
19	S2	428	OMU	C2-N1	8.19	1.51	1.38
19	S2	1248	B8N	C4-N3	-8.17	1.26	1.40
19	S2	1850	MA6	C3'-C2'	-8.13	1.31	1.53
19	S2	116	OMU	C2-N1	8.06	1.51	1.38
19	S2	1442	OMU	C2-N1	8.03	1.51	1.38
19	S2	172	OMU	C2-N1	8.02	1.51	1.38
19	S2	1326	OMU	C2-N1	8.02	1.51	1.38
19	S2	121	OMU	C2-N1	7.91	1.50	1.38
19	S2	627	OMU	C2-N1	7.90	1.50	1.38
40	L5	4227	OMU	C2-N1	7.79	1.50	1.38
19	S2	1248	B8N	C6-N1	7.76	1.55	1.36
40	L5	2837	OMU	C2-N1	7.64	1.50	1.38
19	S2	354	OMU	C2-N1	7.63	1.50	1.38
40	L5	4498	OMU	C2-N1	7.61	1.50	1.38
40	L5	4306	OMU	C2-N1	7.51	1.50	1.38
40	L5	3925	OMU	C2-N1	7.43	1.50	1.38
40	L5	3818	UY1	C2-N3	7.37	1.49	1.37
40	L5	4620	OMU	C2-N1	7.36	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1288	OMU	C2-N3	6.91	1.50	1.38
19	S2	627	OMU	C2-N3	6.87	1.49	1.38
19	S2	1248	B8N	C4-C5	6.85	1.63	1.47
19	S2	799	OMU	C2-N3	6.84	1.49	1.38
19	S2	1442	OMU	C2-N3	6.84	1.49	1.38
19	S2	428	OMU	C2-N3	6.84	1.49	1.38
19	S2	172	OMU	C2-N3	6.74	1.49	1.38
19	S2	116	OMU	C2-N3	6.73	1.49	1.38
19	S2	1326	OMU	C2-N3	6.71	1.49	1.38
19	S2	354	OMU	C2-N3	6.63	1.49	1.38
19	S2	1639	G7M	C4-N3	6.62	1.49	1.34
19	S2	121	OMU	C2-N3	6.57	1.49	1.38
40	L5	2837	OMU	C2-N3	6.56	1.49	1.38
40	L5	4227	OMU	C2-N3	6.41	1.49	1.38
40	L5	4498	OMU	C2-N3	6.37	1.49	1.38
40	L5	3925	OMU	C2-N3	6.30	1.48	1.38
40	L5	4620	OMU	C2-N3	6.22	1.48	1.38
40	L5	4306	OMU	C2-N3	6.19	1.48	1.38
40	L5	4530	UR3	C6-C5	5.99	1.49	1.35
19	S2	627	OMU	C6-C5	5.84	1.48	1.35
19	S2	1288	OMU	C6-C5	5.84	1.48	1.35
40	L5	4530	UR3	C2-N1	5.84	1.46	1.38
19	S2	1248	B8N	C2-N1	5.81	1.56	1.39
19	S2	1442	OMU	C6-C5	5.79	1.48	1.35
19	S2	799	OMU	C6-C5	5.78	1.48	1.35
19	S2	1326	OMU	C6-C5	5.77	1.48	1.35
19	S2	121	OMU	C6-C5	5.76	1.48	1.35
40	L5	4306	OMU	O4-C4	-5.75	1.13	1.24
19	S2	428	OMU	C6-C5	5.73	1.48	1.35
19	S2	172	OMU	C6-C5	5.72	1.48	1.35
40	L5	4620	OMU	O4-C4	-5.69	1.13	1.24
19	S2	354	OMU	C6-C5	5.68	1.48	1.35
40	L5	4498	OMU	O4-C4	-5.66	1.13	1.24
40	L5	4227	OMU	C6-C5	5.66	1.48	1.35
19	S2	116	OMU	C6-C5	5.66	1.48	1.35
40	L5	2837	OMU	O4-C4	-5.66	1.13	1.24
40	L5	4530	UR3	C2-N3	5.66	1.50	1.39
40	L5	3925	OMU	O4-C4	-5.61	1.13	1.24
40	L5	2837	OMU	C6-C5	5.59	1.48	1.35
40	L5	3925	OMU	C6-C5	5.59	1.48	1.35
19	S2	799	OMU	O4-C4	-5.58	1.13	1.24
40	L5	4498	OMU	C6-C5	5.54	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	4620	OMU	C6-C5	5.52	1.47	1.35
19	S2	116	OMU	O4-C4	-5.51	1.13	1.24
19	S2	354	OMU	O4-C4	-5.49	1.13	1.24
40	L5	4227	OMU	O4-C4	-5.49	1.13	1.24
40	L5	4306	OMU	C6-C5	5.49	1.47	1.35
19	S2	172	OMU	O4-C4	-5.48	1.13	1.24
19	S2	1639	G7M	C2-N3	5.47	1.46	1.33
19	S2	627	OMU	O4-C4	-5.45	1.13	1.24
19	S2	428	OMU	O4-C4	-5.43	1.13	1.24
19	S2	1326	OMU	O4-C4	-5.43	1.13	1.24
19	S2	121	OMU	O4-C4	-5.42	1.13	1.24
19	S2	1288	OMU	O4-C4	-5.35	1.14	1.24
19	S2	1442	OMU	O4-C4	-5.34	1.14	1.24
19	S2	1248	B8N	C6-C5	5.22	1.42	1.35
40	L5	3818	UY1	C6-N1	5.06	1.44	1.36
19	S2	1639	G7M	C2-N2	4.95	1.45	1.34
19	S2	1832	6MZ	O4'-C4'	4.67	1.55	1.45
19	S2	1639	G7M	C5-N7	-4.64	1.33	1.39
19	S2	1832	6MZ	O4'-C1'	-4.62	1.31	1.42
19	S2	1832	6MZ	C5'-C4'	-4.52	1.38	1.51
19	S2	1442	OMU	C4-N3	4.51	1.46	1.38
19	S2	428	OMU	C4-N3	4.38	1.46	1.38
19	S2	799	OMU	C4-N3	4.37	1.46	1.38
19	S2	1288	OMU	C4-N3	4.36	1.46	1.38
19	S2	1326	OMU	C4-N3	4.27	1.45	1.38
19	S2	172	OMU	C4-N3	4.23	1.45	1.38
19	S2	627	OMU	C4-N3	4.23	1.45	1.38
19	S2	1850	MA6	C5'-C4'	-4.21	1.38	1.51
19	S2	116	OMU	C4-N3	4.20	1.45	1.38
19	S2	121	OMU	C4-N3	4.18	1.45	1.38
40	L5	3818	UY1	C4-N3	4.13	1.46	1.38
19	S2	354	OMU	C4-N3	4.11	1.45	1.38
40	L5	2837	OMU	C4-N3	3.95	1.45	1.38
19	S2	1850	MA6	O4'-C4'	3.93	1.53	1.45
40	L5	4498	OMU	C4-N3	3.90	1.45	1.38
40	L5	4227	OMU	C4-N3	3.88	1.45	1.38
40	L5	3925	OMU	C4-N3	3.81	1.45	1.38
19	S2	1639	G7M	C5-C6	3.79	1.53	1.43
40	L5	4220	6MZ	C5-C4	-3.77	1.32	1.39
40	L5	3818	UY1	O4-C4	-3.76	1.16	1.23
40	L5	400	A2M	O5'-C5'	-3.76	1.33	1.44
40	L5	2401	A2M	O5'-C5'	-3.73	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	814	PSU	C6-C5	3.73	1.39	1.35
40	L5	4620	OMU	C4-N3	3.69	1.44	1.38
40	L5	3830	A2M	O5'-C5'	-3.69	1.33	1.44
40	L5	1871	A2M	O5'-C5'	-3.68	1.33	1.44
19	S2	801	PSU	C6-C5	3.68	1.39	1.35
40	L5	4306	OMU	C4-N3	3.68	1.44	1.38
40	L5	2787	A2M	O5'-C5'	-3.66	1.33	1.44
40	L5	1323	A2M	O5'-C5'	-3.65	1.33	1.44
19	S2	99	A2M	O5'-C5'	-3.62	1.33	1.44
40	L5	4590	A2M	O5'-C5'	-3.61	1.33	1.44
40	L5	3825	A2M	O5'-C5'	-3.59	1.33	1.44
19	S2	966	PSU	C6-C5	3.54	1.39	1.35
19	S2	1045	PSU	C6-C5	3.51	1.39	1.35
40	L5	4571	A2M	O5'-C5'	-3.50	1.34	1.44
40	L5	2363	A2M	O5'-C5'	-3.50	1.34	1.44
19	S2	468	A2M	O5'-C5'	-3.49	1.34	1.44
40	L5	1524	A2M	O5'-C5'	-3.49	1.34	1.44
19	S2	1244	PSU	C6-C5	3.48	1.39	1.35
19	S2	93	PSU	C6-C5	3.48	1.39	1.35
40	L5	4523	A2M	O5'-C5'	-3.48	1.34	1.44
19	S2	1232	PSU	C6-C5	3.48	1.39	1.35
19	S2	866	PSU	C6-C5	3.47	1.39	1.35
19	S2	668	A2M	O5'-C5'	-3.47	1.34	1.44
19	S2	105	PSU	C6-C5	3.47	1.39	1.35
40	L5	5010	PSU	C6-C5	3.47	1.39	1.35
19	S2	1850	MA6	O4'-C1'	-3.47	1.34	1.42
40	L5	3867	A2M	O5'-C5'	-3.47	1.34	1.44
19	S2	576	A2M	O5'-C5'	-3.46	1.34	1.44
40	L5	4220	6MZ	C5-N7	-3.46	1.32	1.39
40	L5	3785	A2M	O5'-C5'	-3.46	1.34	1.44
19	S2	1004	PSU	C6-C5	3.46	1.39	1.35
19	S2	159	A2M	O5'-C5'	-3.44	1.34	1.44
19	S2	1367	PSU	C6-C5	3.44	1.39	1.35
40	L5	2815	A2M	O5'-C5'	-3.44	1.34	1.44
19	S2	109	PSU	C6-C5	3.44	1.39	1.35
40	L5	3718	A2M	O5'-C5'	-3.43	1.34	1.44
19	S2	27	A2M	O5'-C5'	-3.43	1.34	1.44
19	S2	1031	A2M	O5'-C5'	-3.39	1.34	1.44
19	S2	686	PSU	C6-C5	3.37	1.39	1.35
40	L5	1326	A2M	O5'-C5'	-3.36	1.34	1.44
19	S2	1046	PSU	C6-C5	3.35	1.39	1.35
19	S2	1383	A2M	O5'-C5'	-3.33	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	484	A2M	O5'-C5'	-3.31	1.34	1.44
19	S2	406	PSU	C6-C5	3.31	1.39	1.35
40	L5	398	A2M	O5'-C5'	-3.30	1.34	1.44
40	L5	5001	PSU	C6-C5	3.28	1.38	1.35
40	L5	2839	PSU	C6-C5	3.27	1.38	1.35
19	S2	1248	B8N	C1'-C5	3.27	1.57	1.50
19	S2	1081	PSU	C6-C5	3.26	1.38	1.35
19	S2	1832	6MZ	C5-N7	-3.25	1.33	1.39
40	L5	4220	6MZ	C8-N9	-3.24	1.32	1.37
40	L5	2632	PSU	C6-C5	3.23	1.38	1.35
40	L5	4296	PSU	C6-C5	3.22	1.38	1.35
40	L5	1323	A2M	O4'-C4'	-3.21	1.37	1.45
40	L5	1744	PSU	C6-C5	3.19	1.38	1.35
19	S2	651	PSU	C6-C5	3.19	1.38	1.35
40	L5	1862	PSU	C6-C5	3.19	1.38	1.35
40	L5	1534	A2M	O5'-C5'	-3.19	1.34	1.44
40	L5	1782	PSU	C6-C5	3.16	1.38	1.35
40	L5	3844	PSU	C6-C5	3.16	1.38	1.35
40	L5	4628	PSU	C6-C5	3.16	1.38	1.35
19	S2	1832	6MZ	C5-C4	-3.16	1.33	1.39
40	L5	3818	UY1	C1'-C5	3.16	1.57	1.50
19	S2	166	A2M	O5'-C5'	-3.15	1.35	1.44
40	L5	4500	PSU	C6-C5	3.15	1.38	1.35
40	L5	1781	PSU	C6-C5	3.15	1.38	1.35
40	L5	4312	PSU	C6-C5	3.14	1.38	1.35
19	S2	863	PSU	C6-C5	3.14	1.38	1.35
40	L5	4442	PSU	C6-C5	3.13	1.38	1.35
19	S2	1174	PSU	C6-C5	3.13	1.38	1.35
40	L5	4576	PSU	C6-C5	3.12	1.38	1.35
40	L5	3851	PSU	C6-C5	3.09	1.38	1.35
19	S2	1850	MA6	C6-N6	3.08	1.45	1.36
19	S2	649	PSU	C6-C5	3.08	1.38	1.35
40	L5	1524	A2M	O4'-C4'	-3.08	1.38	1.45
40	L5	2363	A2M	O4'-C4'	-3.08	1.38	1.45
40	L5	3818	UY1	O2-C2	-3.07	1.16	1.23
40	L5	4571	A2M	O4'-C4'	-3.07	1.38	1.45
19	S2	1832	6MZ	C2'-C1'	3.06	1.63	1.53
40	L5	4636	PSU	C6-C5	3.05	1.38	1.35
40	L5	3822	PSU	C6-C5	3.05	1.38	1.35
19	S2	668	A2M	O4'-C4'	-3.05	1.38	1.45
19	S2	1056	PSU	C6-C5	3.04	1.38	1.35
40	L5	4579	PSU	C6-C5	3.04	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1177	PSU	C6-C5	3.04	1.38	1.35
40	L5	4689	PSU	C6-C5	3.04	1.38	1.35
40	L5	4493	PSU	C6-C5	3.03	1.38	1.35
40	L5	4293	PSU	C6-C5	3.00	1.38	1.35
40	L5	1860	PSU	C6-C5	2.98	1.38	1.35
40	L5	4972	PSU	C6-C5	2.98	1.38	1.35
40	L5	4521	PSU	C6-C5	2.97	1.38	1.35
40	L5	1536	PSU	C6-C5	2.96	1.38	1.35
19	S2	681	PSU	C6-C5	2.96	1.38	1.35
40	L5	4361	PSU	C6-C5	2.96	1.38	1.35
40	L5	4471	PSU	C6-C5	2.96	1.38	1.35
40	L5	1792	PSU	C6-C5	2.95	1.38	1.35
40	L5	4552	PSU	C6-C5	2.95	1.38	1.35
40	L5	4431	PSU	C6-C5	2.93	1.38	1.35
40	L5	4299	PSU	C6-C5	2.93	1.38	1.35
19	S2	1832	6MZ	C8-N9	-2.93	1.32	1.37
40	L5	1683	PSU	C6-C5	2.92	1.38	1.35
40	L5	4532	PSU	C6-C5	2.91	1.38	1.35
19	S2	1851	MA6	C6-N6	2.90	1.44	1.36
40	L5	4353	PSU	C6-C5	2.90	1.38	1.35
42	L8	69	PSU	C6-C5	2.89	1.38	1.35
19	S2	1288	OMU	C5-C4	2.88	1.50	1.43
40	L5	4973	PSU	C6-C5	2.87	1.38	1.35
40	L5	3637	PSU	C6-C5	2.87	1.38	1.35
19	S2	1442	OMU	C5-C4	2.85	1.49	1.43
19	S2	1639	G7M	C2-N1	2.84	1.44	1.37
40	L5	4403	PSU	C6-C5	2.81	1.38	1.35
42	L8	55	PSU	C6-C5	2.81	1.38	1.35
19	S2	121	OMU	C5-C4	2.80	1.49	1.43
19	S2	172	OMU	C5-C4	2.79	1.49	1.43
40	L5	3884	PSU	C6-C5	2.79	1.38	1.35
19	S2	1326	OMU	C5-C4	2.78	1.49	1.43
40	L5	3695	PSU	C6-C5	2.74	1.38	1.35
40	L5	3853	PSU	C6-C5	2.74	1.38	1.35
19	S2	1851	MA6	C5-C4	-2.71	1.34	1.39
19	S2	627	OMU	C5-C4	2.69	1.49	1.43
19	S2	1288	OMU	C6-N1	2.69	1.44	1.38
19	S2	799	OMU	C5-C4	2.69	1.49	1.43
40	L5	1677	PSU	O4'-C1'	-2.69	1.40	1.43
19	S2	428	OMU	C5-C4	2.68	1.49	1.43
40	L5	1582	PSU	C6-C5	2.67	1.38	1.35
40	L5	1871	A2M	O4'-C4'	-2.66	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1442	OMU	C6-N1	2.66	1.44	1.38
40	L5	3639	PSU	C6-C5	2.65	1.38	1.35
19	S2	799	OMU	C6-N1	2.64	1.44	1.38
40	L5	4530	UR3	O2-C2	-2.64	1.17	1.22
40	L5	4457	PSU	C6-C5	2.63	1.38	1.35
19	S2	354	OMU	C5-C4	2.62	1.49	1.43
40	L5	4673	PSU	C6-C5	2.62	1.38	1.35
40	L5	4227	OMU	C5-C4	2.61	1.49	1.43
40	L5	4498	OMU	C5-C4	2.59	1.49	1.43
40	L5	1326	A2M	O4'-C4'	-2.57	1.39	1.45
19	S2	1248	B8N	O4'-C1'	-2.57	1.40	1.43
19	S2	428	OMU	C6-N1	2.56	1.44	1.38
40	L5	4447	5MC	C5-C4	-2.56	1.42	1.44
19	S2	1639	G7M	C6-N1	2.56	1.43	1.38
19	S2	1326	OMU	C6-N1	2.55	1.44	1.38
40	L5	3920	PSU	C6-C5	2.55	1.38	1.35
19	S2	354	OMU	C6-N1	2.54	1.44	1.38
40	L5	1534	A2M	O4'-C4'	-2.53	1.39	1.45
40	L5	4523	A2M	O4'-C4'	-2.52	1.39	1.45
40	L5	4306	OMU	C6-N1	2.52	1.44	1.38
19	S2	116	OMU	C6-N1	2.52	1.44	1.38
40	L5	4220	6MZ	C6-N1	-2.51	1.31	1.35
19	S2	1832	6MZ	O3'-C3'	2.51	1.49	1.43
19	S2	1639	G7M	O6-C6	-2.51	1.18	1.23
19	S2	627	OMU	C6-N1	2.50	1.44	1.38
40	L5	3925	OMU	C5-C4	2.49	1.49	1.43
19	S2	121	OMU	C6-N1	2.49	1.44	1.38
19	S2	116	OMU	C5-C4	2.48	1.49	1.43
40	L5	400	A2M	O4'-C4'	-2.48	1.39	1.45
19	S2	1850	MA6	C5-C4	-2.48	1.34	1.39
19	S2	172	OMU	C6-N1	2.48	1.44	1.38
40	L5	2837	OMU	C5-C4	2.47	1.49	1.43
40	L5	2837	OMU	C6-N1	2.45	1.43	1.38
19	S2	1850	MA6	O3'-C3'	2.43	1.49	1.43
40	L5	4498	OMU	C6-N1	2.42	1.43	1.38
40	L5	4552	PSU	C4-C5	-2.41	1.37	1.44
40	L5	2815	A2M	O4'-C4'	-2.41	1.39	1.45
40	L5	3884	PSU	C4-C5	-2.39	1.37	1.44
40	L5	3825	A2M	O4'-C4'	-2.38	1.39	1.45
40	L5	4306	OMU	C5-C4	2.38	1.48	1.43
40	L5	4590	A2M	O4'-C4'	-2.37	1.39	1.45
40	L5	1871	A2M	O3'-C3'	-2.37	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	1832	6MZ	C6-N1	-2.37	1.31	1.35
40	L5	3639	PSU	C4-C5	-2.36	1.37	1.44
40	L5	4689	PSU	C4-C5	-2.36	1.37	1.44
40	L5	4620	OMU	C5-C4	2.35	1.48	1.43
40	L5	3925	OMU	C6-N1	2.34	1.43	1.38
40	L5	1677	PSU	C6-C5	2.33	1.37	1.35
40	L5	3695	PSU	C4-C5	-2.32	1.37	1.44
40	L5	4673	PSU	C4-C5	-2.30	1.38	1.44
40	L5	4227	OMU	C6-N1	2.30	1.43	1.38
40	L5	2363	A2M	O3'-C3'	-2.29	1.37	1.43
40	L5	1323	A2M	O3'-C3'	-2.29	1.37	1.43
40	L5	4620	OMU	C6-N1	2.29	1.43	1.38
40	L5	4530	UR3	C6-N1	2.29	1.43	1.38
40	L5	3920	PSU	C4-C5	-2.27	1.38	1.44
40	L5	400	A2M	O3'-C3'	-2.27	1.37	1.43
40	L5	2839	PSU	C4-C5	-2.27	1.38	1.44
40	L5	3818	UY1	O4'-C1'	-2.27	1.40	1.43
40	L5	1524	A2M	O3'-C3'	-2.27	1.37	1.43
40	L5	3701	OMC	C4-N3	-2.26	1.30	1.34
40	L5	1582	PSU	C4-C5	-2.25	1.38	1.44
40	L5	3867	A2M	O4'-C4'	-2.25	1.40	1.45
40	L5	4403	PSU	C4-C5	-2.24	1.38	1.44
40	L5	3844	PSU	C4-C5	-2.23	1.38	1.44
40	L5	1744	PSU	C4-C5	-2.22	1.38	1.44
40	L5	4353	PSU	C4-C5	-2.21	1.38	1.44
40	L5	4457	PSU	C4-C5	-2.21	1.38	1.44
40	L5	4973	PSU	C4-C5	-2.21	1.38	1.44
40	L5	4532	PSU	C4-C5	-2.20	1.38	1.44
40	L5	1677	PSU	C4-C5	-2.20	1.38	1.44
40	L5	4500	PSU	C4-C5	-2.19	1.38	1.44
19	S2	1639	G7M	C4-N9	-2.18	1.32	1.38
40	L5	4521	PSU	C4-C5	-2.17	1.38	1.44
19	S2	1081	PSU	C4-C5	-2.17	1.38	1.44
40	L5	1683	PSU	C4-C5	-2.17	1.38	1.44
40	L5	4471	PSU	C4-C5	-2.16	1.38	1.44
40	L5	398	A2M	O3'-C3'	-2.16	1.37	1.43
40	L5	1860	PSU	C4-C5	-2.16	1.38	1.44
40	L5	4579	PSU	C4-C5	-2.15	1.38	1.44
40	L5	4293	PSU	C4-C5	-2.15	1.38	1.44
19	S2	406	PSU	C4-C5	-2.15	1.38	1.44
40	L5	4521	PSU	O4'-C1'	-2.14	1.40	1.43
19	S2	1177	PSU	C4-C5	-2.14	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	1782	PSU	C4-C5	-2.14	1.38	1.44
40	L5	4636	PSU	C4-C5	-2.13	1.38	1.44
40	L5	3830	A2M	O4'-C4'	-2.13	1.40	1.45
40	L5	4523	A2M	O3'-C3'	-2.13	1.37	1.43
40	L5	4576	PSU	C4-C5	-2.11	1.38	1.44
19	S2	1174	PSU	C4-C5	-2.10	1.38	1.44
19	S2	109	PSU	C4-C5	-2.09	1.38	1.44
40	L5	1536	PSU	C4-C5	-2.09	1.38	1.44
40	L5	4590	A2M	O3'-C3'	-2.09	1.37	1.43
40	L5	4628	PSU	C4-C5	-2.09	1.38	1.44
40	L5	4312	PSU	C4-C5	-2.08	1.38	1.44
40	L5	4296	PSU	C4-C5	-2.08	1.38	1.44
40	L5	2401	A2M	O4'-C4'	-2.07	1.40	1.45
40	L5	3822	PSU	C4-C5	-2.07	1.38	1.44
42	L8	55	PSU	C4-C5	-2.07	1.38	1.44
40	L5	5001	PSU	C4-C5	-2.07	1.38	1.44
40	L5	4972	PSU	C4-C5	-2.06	1.38	1.44
40	L5	5010	PSU	C4-C5	-2.06	1.38	1.44
40	L5	2861	OMC	C4-N3	-2.06	1.30	1.34
19	S2	1851	MA6	C5-N7	-2.06	1.35	1.39
19	S2	649	PSU	C4-C5	-2.06	1.38	1.44
40	L5	4299	PSU	C4-C5	-2.06	1.38	1.44
42	L8	69	PSU	C4-C5	-2.05	1.38	1.44
40	L5	3637	PSU	C4-C5	-2.05	1.38	1.44
40	L5	4431	PSU	C4-C5	-2.05	1.38	1.44
40	L5	3920	PSU	O4'-C1'	-2.05	1.41	1.43
40	L5	1792	PSU	C4-C5	-2.05	1.38	1.44
40	L5	4636	PSU	O4'-C1'	-2.04	1.41	1.43
40	L5	4500	PSU	O4'-C1'	-2.04	1.41	1.43
40	L5	4220	6MZ	C4-N9	-2.03	1.33	1.37
40	L5	3830	A2M	O3'-C3'	-2.03	1.37	1.43
40	L5	1862	PSU	C4-C5	-2.02	1.38	1.44
40	L5	3639	PSU	O4'-C1'	-2.02	1.41	1.43
40	L5	4361	PSU	C4-C5	-2.02	1.38	1.44
40	L5	398	A2M	O4'-C4'	-2.02	1.40	1.45
40	L5	3841	OMC	C4-N3	-2.01	1.30	1.34
19	S2	1851	MA6	C4-N9	-2.01	1.33	1.37
40	L5	2351	OMC	C4-N3	-2.01	1.30	1.34
40	L5	4457	PSU	O4'-C1'	-2.00	1.41	1.43
19	S2	1850	MA6	C5-N7	-2.00	1.35	1.39

All (723) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1850	MA6	N1-C6-N6	-12.22	101.97	116.86
19	S2	1851	MA6	N1-C6-N6	-11.21	103.19	116.86
19	S2	1850	MA6	C5-C6-N6	8.26	138.41	125.33
19	S2	1639	G7M	C1'-N9-C8	-7.29	102.11	126.74
19	S2	1639	G7M	C1'-N9-C4	7.24	147.87	126.49
19	S2	1851	MA6	C5-C6-N6	7.11	136.59	125.33
40	L5	4220	6MZ	C9-N6-C6	-6.21	117.09	122.85
40	L5	4227	OMU	C4-N3-C2	-6.01	119.15	126.61
40	L5	4498	OMU	C4-N3-C2	-6.00	119.16	126.61
40	L5	4220	6MZ	N1-C2-N3	-5.87	119.70	128.58
40	L5	2837	OMU	C4-N3-C2	-5.83	119.38	126.61
19	S2	172	OMU	C4-N3-C2	-5.81	119.39	126.61
40	L5	3925	OMU	C4-N3-C2	-5.80	119.41	126.61
19	S2	1326	OMU	C4-N3-C2	-5.75	119.47	126.61
19	S2	1442	OMU	C4-N3-C2	-5.74	119.49	126.61
19	S2	799	OMU	C4-N3-C2	-5.66	119.59	126.61
19	S2	1832	6MZ	N1-C2-N3	-5.58	120.13	128.58
19	S2	1851	MA6	N1-C2-N3	-5.56	120.16	128.58
40	L5	4628	PSU	N1-C2-N3	5.56	121.04	115.17
19	S2	627	OMU	C4-N3-C2	-5.56	119.71	126.61
40	L5	4636	PSU	C4-N3-C2	-5.56	118.72	126.37
19	S2	428	OMU	C4-N3-C2	-5.54	119.74	126.61
19	S2	354	OMU	C4-N3-C2	-5.50	119.79	126.61
40	L5	4530	UR3	C4-N3-C2	-5.48	120.17	124.58
19	S2	1851	MA6	N9-C8-N7	-5.43	106.23	113.94
40	L5	4306	OMU	C4-N3-C2	-5.40	119.90	126.61
19	S2	121	OMU	C4-N3-C2	-5.40	119.91	126.61
40	L5	4636	PSU	N1-C2-N3	5.38	120.85	115.17
40	L5	3637	PSU	N1-C2-N3	5.34	120.80	115.17
19	S2	1850	MA6	N9-C8-N7	-5.32	106.39	113.94
19	S2	1288	OMU	C4-N3-C2	-5.32	120.01	126.61
40	L5	3920	PSU	N1-C2-N3	5.31	120.77	115.17
40	L5	4293	PSU	C4-N3-C2	-5.29	119.08	126.37
40	L5	4442	PSU	N1-C2-N3	5.27	120.72	115.17
40	L5	4293	PSU	N1-C2-N3	5.26	120.72	115.17
42	L8	69	PSU	N1-C2-N3	5.25	120.70	115.17
40	L5	1582	PSU	C4-N3-C2	-5.24	119.15	126.37
40	L5	4500	PSU	N1-C2-N3	5.23	120.68	115.17
40	L5	3701	OMC	C1'-N1-C2	5.21	129.95	118.44
19	S2	1850	MA6	N1-C2-N3	-5.21	120.69	128.58
40	L5	4620	OMU	C4-N3-C2	-5.21	120.14	126.61
40	L5	1683	PSU	N1-C2-N3	5.21	120.66	115.17
40	L5	4457	PSU	C4-N3-C2	-5.20	119.21	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	1862	PSU	N1-C2-N3	5.20	120.65	115.17
40	L5	4973	PSU	N1-C2-N3	5.19	120.64	115.17
19	S2	1081	PSU	C4-N3-C2	-5.17	119.25	126.37
40	L5	4689	PSU	N1-C2-N3	5.17	120.62	115.17
40	L5	1677	PSU	C4-N3-C2	-5.16	119.26	126.37
40	L5	4973	PSU	C4-N3-C2	-5.15	119.27	126.37
19	S2	1248	B8N	C5-C4-N3	5.13	125.48	116.15
19	S2	651	PSU	C4-N3-C2	-5.12	119.32	126.37
19	S2	966	PSU	N1-C2-N3	5.11	120.56	115.17
40	L5	4457	PSU	N1-C2-N3	5.10	120.55	115.17
40	L5	1792	PSU	N1-C2-N3	5.09	120.54	115.17
40	L5	3920	PSU	C4-N3-C2	-5.08	119.38	126.37
40	L5	4353	PSU	C4-N3-C2	-5.08	119.38	126.37
40	L5	3884	PSU	N1-C2-N3	5.07	120.52	115.17
19	S2	966	PSU	C4-N3-C2	-5.07	119.39	126.37
40	L5	4552	PSU	C4-N3-C2	-5.07	119.39	126.37
40	L5	3851	PSU	N1-C2-N3	5.06	120.50	115.17
40	L5	3884	PSU	C4-N3-C2	-5.05	119.41	126.37
19	S2	863	PSU	N1-C2-N3	5.04	120.48	115.17
40	L5	4220	6MZ	N9-C8-N7	-5.03	106.80	113.94
19	S2	1081	PSU	N1-C2-N3	5.03	120.48	115.17
42	L8	69	PSU	C4-N3-C2	-5.03	119.44	126.37
40	L5	1862	PSU	C4-N3-C2	-5.02	119.45	126.37
40	L5	3637	PSU	C4-N3-C2	-5.02	119.46	126.37
19	S2	863	PSU	C4-N3-C2	-5.02	119.46	126.37
40	L5	2839	PSU	N1-C2-N3	5.02	120.46	115.17
19	S2	651	PSU	N1-C2-N3	5.01	120.46	115.17
40	L5	3853	PSU	N1-C2-N3	5.01	120.45	115.17
40	L5	4353	PSU	N1-C2-N3	5.01	120.45	115.17
40	L5	4471	PSU	N1-C2-N3	5.00	120.44	115.17
40	L5	3853	PSU	C4-N3-C2	-5.00	119.49	126.37
19	S2	1244	PSU	C4-N3-C2	-4.99	119.50	126.37
19	S2	1045	PSU	C4-N3-C2	-4.98	119.51	126.37
40	L5	4521	PSU	C4-N3-C2	-4.98	119.52	126.37
19	S2	686	PSU	C4-N3-C2	-4.97	119.52	126.37
19	S2	109	PSU	C4-N3-C2	-4.97	119.52	126.37
19	S2	105	PSU	N1-C2-N3	4.97	120.41	115.17
19	S2	1174	PSU	C4-N3-C2	-4.96	119.54	126.37
40	L5	4628	PSU	C4-N3-C2	-4.96	119.54	126.37
40	L5	5010	PSU	N1-C2-N3	4.95	120.39	115.17
40	L5	4442	PSU	C4-N3-C2	-4.94	119.56	126.37
19	S2	866	PSU	C4-N3-C2	-4.94	119.57	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4972	PSU	N1-C2-N3	4.93	120.37	115.17
19	S2	406	PSU	C4-N3-C2	-4.93	119.58	126.37
40	L5	1792	PSU	C4-N3-C2	-4.93	119.58	126.37
40	L5	4521	PSU	N1-C2-N3	4.92	120.36	115.17
19	S2	116	OMU	C4-N3-C2	-4.91	120.51	126.61
40	L5	4403	PSU	C4-N3-C2	-4.91	119.61	126.37
40	L5	4493	PSU	C4-N3-C2	-4.91	119.61	126.37
40	L5	4500	PSU	C4-N3-C2	-4.90	119.61	126.37
19	S2	1045	PSU	N1-C2-N3	4.90	120.34	115.17
19	S2	681	PSU	N1-C2-N3	4.90	120.33	115.17
19	S2	1174	PSU	N1-C2-N3	4.88	120.32	115.17
40	L5	1744	PSU	N1-C2-N3	4.88	120.31	115.17
40	L5	4552	PSU	N1-C2-N3	4.88	120.31	115.17
19	S2	406	PSU	N1-C2-N3	4.88	120.31	115.17
40	L5	3695	PSU	C4-N3-C2	-4.87	119.67	126.37
19	S2	681	PSU	C4-N3-C2	-4.86	119.67	126.37
19	S2	866	PSU	N1-C2-N3	4.86	120.30	115.17
40	L5	4493	PSU	N1-C2-N3	4.86	120.30	115.17
40	L5	3695	PSU	N1-C2-N3	4.86	120.29	115.17
42	L8	55	PSU	C4-N3-C2	-4.86	119.68	126.37
40	L5	4296	PSU	C4-N3-C2	-4.86	119.68	126.37
40	L5	4403	PSU	N1-C2-N3	4.85	120.28	115.17
19	S2	1244	PSU	N1-C2-N3	4.85	120.28	115.17
40	L5	1536	PSU	N1-C2-N3	4.84	120.27	115.17
40	L5	4471	PSU	C4-N3-C2	-4.84	119.70	126.37
40	L5	3818	UY1	C4-N3-C2	-4.84	119.70	126.37
19	S2	1177	PSU	C4-N3-C2	-4.84	119.70	126.37
19	S2	93	PSU	N1-C2-N3	4.84	120.27	115.17
19	S2	1056	PSU	C4-N3-C2	-4.84	119.71	126.37
40	L5	5001	PSU	N1-C2-N3	4.84	120.27	115.17
40	L5	1683	PSU	C4-N3-C2	-4.83	119.71	126.37
40	L5	4576	PSU	N1-C2-N3	4.83	120.26	115.17
40	L5	1782	PSU	N1-C2-N3	4.83	120.26	115.17
19	S2	93	PSU	C4-N3-C2	-4.83	119.72	126.37
40	L5	5001	PSU	C4-N3-C2	-4.82	119.73	126.37
19	S2	1832	6MZ	C5-C4-N3	-4.82	120.08	126.72
40	L5	2632	PSU	N1-C2-N3	4.82	120.25	115.17
40	L5	4296	PSU	N1-C2-N3	4.81	120.24	115.17
19	S2	1367	PSU	N1-C2-N3	4.81	120.24	115.17
19	S2	1046	PSU	N1-C2-N3	4.80	120.23	115.17
40	L5	4673	PSU	C4-N3-C2	-4.80	119.76	126.37
42	L8	55	PSU	N1-C2-N3	4.79	120.22	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4673	PSU	N1-C2-N3	4.79	120.22	115.17
40	L5	4431	PSU	C4-N3-C2	-4.78	119.78	126.37
40	L5	1582	PSU	N1-C2-N3	4.78	120.21	115.17
40	L5	4579	PSU	N1-C2-N3	4.76	120.19	115.17
40	L5	3851	PSU	C4-N3-C2	-4.76	119.82	126.37
19	S2	1367	PSU	C4-N3-C2	-4.75	119.82	126.37
40	L5	4532	PSU	C4-N3-C2	-4.75	119.83	126.37
40	L5	1781	PSU	N1-C2-N3	4.75	120.18	115.17
40	L5	4972	PSU	C4-N3-C2	-4.75	119.83	126.37
40	L5	3639	PSU	C4-N3-C2	-4.74	119.83	126.37
40	L5	2632	PSU	C4-N3-C2	-4.73	119.86	126.37
40	L5	1536	PSU	C4-N3-C2	-4.73	119.86	126.37
19	S2	814	PSU	C4-N3-C2	-4.73	119.86	126.37
40	L5	4361	PSU	N1-C2-N3	4.72	120.15	115.17
19	S2	1832	6MZ	N9-C8-N7	-4.72	107.24	113.94
40	L5	3822	PSU	N1-C2-N3	4.71	120.14	115.17
40	L5	4532	PSU	N1-C2-N3	4.71	120.14	115.17
40	L5	4576	PSU	C4-N3-C2	-4.70	119.90	126.37
19	S2	814	PSU	N1-C2-N3	4.70	120.12	115.17
19	S2	109	PSU	N1-C2-N3	4.69	120.12	115.17
40	L5	5010	PSU	C4-N3-C2	-4.69	119.91	126.37
19	S2	686	PSU	N1-C2-N3	4.69	120.11	115.17
40	L5	2839	PSU	C4-N3-C2	-4.69	119.91	126.37
19	S2	1232	PSU	N1-C2-N3	4.69	120.11	115.17
19	S2	105	PSU	C4-N3-C2	-4.67	119.94	126.37
40	L5	3639	PSU	N1-C2-N3	4.67	120.09	115.17
19	S2	1046	PSU	C4-N3-C2	-4.67	119.94	126.37
40	L5	1782	PSU	C4-N3-C2	-4.66	119.95	126.37
19	S2	1248	B8N	C4-N3-C2	-4.66	119.89	125.62
40	L5	1744	PSU	C4-N3-C2	-4.65	119.96	126.37
40	L5	4312	PSU	N1-C2-N3	4.64	120.06	115.17
19	S2	1850	MA6	C5-C4-N3	-4.64	120.33	126.72
40	L5	4361	PSU	C4-N3-C2	-4.63	120.00	126.37
40	L5	4312	PSU	C4-N3-C2	-4.63	120.00	126.37
19	S2	1004	PSU	N1-C2-N3	4.62	120.04	115.17
40	L5	4431	PSU	N1-C2-N3	4.62	120.04	115.17
40	L5	4579	PSU	C4-N3-C2	-4.61	120.01	126.37
40	L5	1677	PSU	N1-C2-N3	4.61	120.03	115.17
19	S2	1232	PSU	C4-N3-C2	-4.60	120.03	126.37
40	L5	1781	PSU	C4-N3-C2	-4.58	120.07	126.37
40	L5	1860	PSU	N1-C2-N3	4.57	119.98	115.17
40	L5	3822	PSU	C4-N3-C2	-4.56	120.08	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	3844	PSU	N1-C2-N3	4.55	119.97	115.17
40	L5	4299	PSU	C4-N3-C2	-4.55	120.10	126.37
19	S2	1056	PSU	N1-C2-N3	4.52	119.94	115.17
40	L5	4299	PSU	N1-C2-N3	4.51	119.93	115.17
19	S2	801	PSU	N1-C2-N3	4.50	119.92	115.17
40	L5	4220	6MZ	C5-C4-N3	-4.48	120.55	126.72
19	S2	1177	PSU	N1-C2-N3	4.48	119.89	115.17
40	L5	1860	PSU	C4-N3-C2	-4.44	120.25	126.37
19	S2	1004	PSU	C4-N3-C2	-4.44	120.26	126.37
19	S2	1851	MA6	C4-N9-C8	4.39	110.35	105.74
19	S2	1851	MA6	C5-C4-N3	-4.37	120.70	126.72
40	L5	4689	PSU	C4-N3-C2	-4.36	120.36	126.37
40	L5	1871	A2M	C3'-C2'-C1'	-4.36	94.47	102.81
40	L5	3844	PSU	C4-N3-C2	-4.35	120.38	126.37
40	L5	3701	OMC	C1'-N1-C6	-4.28	111.63	120.78
40	L5	3830	A2M	C3'-C2'-C1'	-4.27	94.63	102.81
19	S2	1639	G7M	C2-N3-C4	4.26	119.64	112.30
19	S2	649	PSU	N1-C2-N3	4.26	119.66	115.17
19	S2	649	PSU	C4-N3-C2	-4.24	120.53	126.37
19	S2	801	PSU	C4-N3-C2	-4.23	120.55	126.37
40	L5	4227	OMU	N3-C2-N1	4.23	120.39	114.89
19	S2	1850	MA6	C4-N9-C8	4.21	110.16	105.74
40	L5	3818	UY1	N1-C2-N3	4.20	119.60	115.17
40	L5	3925	OMU	N3-C2-N1	4.13	120.27	114.89
40	L5	2837	OMU	N3-C2-N1	4.13	120.27	114.89
19	S2	1383	A2M	C3'-C2'-C1'	-4.09	94.97	102.81
40	L5	4523	A2M	C3'-C2'-C1'	-4.02	95.11	102.81
40	L5	4498	OMU	N3-C2-N1	4.02	120.12	114.89
40	L5	4498	OMU	C5-C4-N3	4.01	120.42	114.80
40	L5	3825	A2M	C3'-C2'-C1'	-3.97	95.20	102.81
19	S2	354	OMU	N3-C2-N1	3.93	120.00	114.89
19	S2	627	OMU	N3-C2-N1	3.91	119.98	114.89
19	S2	1639	G7M	C5-C6-N1	3.89	119.87	111.84
40	L5	4620	OMU	N3-C2-N1	3.88	119.94	114.89
40	L5	398	A2M	C3'-C2'-C1'	-3.88	95.38	102.81
19	S2	1850	MA6	C4-C5-C6	3.88	119.92	115.91
40	L5	4689	PSU	C6-N1-C2	-3.85	119.12	122.69
19	S2	121	OMU	N3-C2-N1	3.82	119.87	114.89
19	S2	799	OMU	C5-C4-N3	3.81	120.14	114.80
19	S2	1326	OMU	N3-C2-N1	3.81	119.85	114.89
19	S2	1442	OMU	N3-C2-N1	3.81	119.85	114.89
40	L5	4306	OMU	N3-C2-N1	3.79	119.82	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4227	OMU	C5-C4-N3	3.77	120.08	114.80
19	S2	172	OMU	C5-C4-N3	3.76	120.07	114.80
40	L5	4530	UR3	C5-C4-N3	3.75	119.98	115.04
40	L5	4306	OMU	C5-C4-N3	3.73	120.03	114.80
19	S2	1639	G7M	C5-C4-N3	-3.73	121.11	128.15
19	S2	799	OMU	N3-C2-N1	3.73	119.74	114.89
19	S2	172	OMU	N3-C2-N1	3.72	119.73	114.89
19	S2	1326	OMU	C5-C4-N3	3.71	119.99	114.80
19	S2	1442	OMU	C5-C4-N3	3.70	119.98	114.80
19	S2	99	A2M	C3'-C2'-C1'	-3.69	95.74	102.81
19	S2	1288	OMU	N3-C2-N1	3.69	119.69	114.89
19	S2	468	A2M	C3'-C2'-C1'	-3.68	95.77	102.81
19	S2	428	OMU	C5-C4-N3	3.67	119.94	114.80
40	L5	3925	OMU	C5-C4-N3	3.67	119.94	114.80
40	L5	2837	OMU	C5-C4-N3	3.67	119.94	114.80
19	S2	428	OMU	N3-C2-N1	3.67	119.67	114.89
40	L5	398	A2M	O3'-C3'-C2'	3.60	121.27	111.19
19	S2	1383	A2M	O3'-C3'-C2'	3.60	121.26	111.19
40	L5	3718	A2M	C3'-C2'-C1'	-3.60	95.92	102.81
19	S2	1248	B8N	N3-C2-N1	3.58	121.10	116.72
40	L5	2351	OMC	C1'-N1-C2	3.58	126.35	118.44
40	L5	1323	A2M	C2'-C1'-N9	3.56	119.61	113.75
40	L5	4220	6MZ	C4-N9-C8	3.56	109.48	105.74
19	S2	1850	MA6	N3-C4-N9	3.52	133.15	127.17
19	S2	354	OMU	C5-C4-N3	3.51	119.72	114.80
40	L5	4590	A2M	C3'-C2'-C1'	-3.51	96.09	102.81
19	S2	1248	B8N	C1'-C5-C4	3.49	122.90	117.61
19	S2	1851	MA6	C4-C5-C6	3.49	119.52	115.91
40	L5	4620	OMU	C5-C4-N3	3.48	119.68	114.80
19	S2	121	OMU	C5-C4-N3	3.48	119.67	114.80
19	S2	1851	MA6	N3-C4-N9	3.47	133.07	127.17
40	L5	2401	A2M	O3'-C3'-C2'	3.46	120.88	111.19
19	S2	116	OMU	C5-C4-N3	3.46	119.64	114.80
19	S2	99	A2M	O3'-C3'-C2'	3.45	120.85	111.19
40	L5	4220	6MZ	C2-N3-C4	3.45	120.25	111.83
19	S2	627	OMU	C5-C4-N3	3.44	119.62	114.80
19	S2	116	OMU	N3-C2-N1	3.44	119.37	114.89
19	S2	1850	MA6	C2-N1-C6	3.44	120.22	111.83
19	S2	1288	OMU	C5-C4-N3	3.43	119.61	114.80
19	S2	468	A2M	O3'-C3'-C2'	3.42	120.77	111.19
19	S2	1832	6MZ	C2-N3-C4	3.42	120.18	111.83
40	L5	4628	PSU	C6-N1-C2	-3.39	119.55	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1639	G7M	O6-C6-C5	-3.38	120.47	128.01
40	L5	4500	PSU	O2-C2-N1	-3.35	119.34	122.79
40	L5	4579	PSU	O2-C2-N1	-3.35	119.34	122.79
19	S2	159	A2M	O3'-C3'-C2'	3.34	120.54	111.19
19	S2	1851	MA6	C2-N1-C6	3.34	119.98	111.83
42	L8	69	PSU	O2-C2-N1	-3.34	119.35	122.79
40	L5	4293	PSU	O2-C2-N1	-3.33	119.35	122.79
19	S2	576	A2M	O3'-C3'-C2'	3.33	120.51	111.19
19	S2	166	A2M	C3'-C2'-C1'	-3.33	96.43	102.81
40	L5	4628	PSU	O2-C2-N1	-3.33	119.36	122.79
19	S2	166	A2M	O3'-C3'-C2'	3.32	120.49	111.19
40	L5	2787	A2M	O3'-C3'-C2'	3.31	120.45	111.19
19	S2	1850	MA6	C5-N7-C8	3.29	108.62	103.45
40	L5	4571	A2M	C3'-C2'-C1'	-3.28	96.53	102.81
19	S2	863	PSU	O2-C2-N1	-3.28	119.41	122.79
40	L5	2363	A2M	C2'-C1'-N9	3.25	119.09	113.75
40	L5	1683	PSU	O2-C2-N1	-3.23	119.45	122.79
40	L5	3818	UY1	C6-C5-C4	3.23	120.35	118.17
40	L5	1871	A2M	O3'-C3'-C2'	3.22	120.20	111.19
19	S2	1832	6MZ	C5-N7-C8	3.21	108.49	103.45
19	S2	1832	6MZ	C4-C5-C6	3.21	119.44	116.78
19	S2	668	A2M	O3'-C3'-C2'	3.18	120.08	111.19
40	L5	2839	PSU	C6-N1-C2	-3.17	119.75	122.69
40	L5	2401	A2M	C3'-C2'-C1'	-3.17	96.73	102.81
19	S2	799	OMU	O4-C4-C5	-3.16	119.71	125.16
40	L5	5010	PSU	O2-C2-N1	-3.16	119.53	122.79
19	S2	428	OMU	O4-C4-C5	-3.15	119.72	125.16
19	S2	1232	PSU	O2-C2-N1	-3.14	119.55	122.79
19	S2	1832	6MZ	N3-C4-N9	3.14	132.50	127.17
40	L5	2837	OMU	O4-C4-C5	-3.13	119.76	125.16
40	L5	1323	A2M	C3'-C2'-C1'	-3.13	96.81	102.81
19	S2	468	A2M	C4-N9-C1'	-3.13	119.31	126.63
40	L5	4220	6MZ	N3-C4-N9	3.13	132.49	127.17
40	L5	3718	A2M	O3'-C3'-C2'	3.12	119.93	111.19
19	S2	166	A2M	C4-N9-C1'	-3.12	119.33	126.63
19	S2	1081	PSU	O2-C2-N1	-3.12	119.58	122.79
40	L5	2401	A2M	C4-N9-C1'	-3.11	119.35	126.63
40	L5	3701	OMC	O2-C2-N3	-3.11	117.42	122.33
40	L5	4498	OMU	O4-C4-C5	-3.11	119.80	125.16
19	S2	1851	MA6	C2-N3-C4	3.11	119.42	111.83
40	L5	1323	A2M	O3'-C3'-C2'	3.10	119.86	111.19
40	L5	3830	A2M	O3'-C3'-C2'	3.09	119.84	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	400	A2M	O3'-C3'-C2'	3.09	119.83	111.19
19	S2	1383	A2M	C4-N9-C1'	-3.09	119.41	126.63
40	L5	4523	A2M	C4-N9-C1'	-3.09	119.41	126.63
40	L5	4571	A2M	O3'-C3'-C2'	3.08	119.81	111.19
19	S2	1442	OMU	O4-C4-C5	-3.08	119.86	125.16
19	S2	1639	G7M	N9-C4-N3	3.07	132.10	125.95
40	L5	3825	A2M	O3'-C3'-C2'	3.06	119.76	111.19
19	S2	116	OMU	O4-C4-C5	-3.06	119.88	125.16
40	L5	4500	PSU	C6-N1-C2	-3.06	119.85	122.69
19	S2	1174	PSU	O2-C2-N1	-3.06	119.64	122.79
40	L5	400	A2M	C3'-C2'-C1'	-3.03	97.01	102.81
40	L5	4973	PSU	O2-C2-N1	-3.03	119.67	122.79
19	S2	1850	MA6	C2-N3-C4	3.03	119.22	111.83
19	S2	1851	MA6	C5-N7-C8	3.02	108.19	103.45
40	L5	4227	OMU	O4-C4-C5	-3.01	119.96	125.16
40	L5	1683	PSU	C6-N1-C2	-3.01	119.90	122.69
19	S2	1337	4AC	N4-C4-N3	3.01	118.75	113.87
40	L5	4523	A2M	O3'-C3'-C2'	3.01	119.61	111.19
19	S2	1639	G7M	CN7-N7-C5	3.00	130.53	126.80
19	S2	27	A2M	C3'-C2'-C1'	-3.00	97.07	102.81
40	L5	4220	6MZ	C5-N7-C8	2.99	108.15	103.45
40	L5	5010	PSU	C6-N1-C2	-2.98	119.92	122.69
42	L8	55	PSU	O2-C2-N1	-2.98	119.72	122.79
19	S2	966	PSU	O2-C2-N1	-2.97	119.72	122.79
40	L5	4579	PSU	C6-N1-C2	-2.97	119.93	122.69
40	L5	2815	A2M	O3'-C3'-C2'	2.96	119.47	111.19
19	S2	1031	A2M	O3'-C3'-C2'	2.96	119.46	111.19
19	S2	814	PSU	O2-C2-N1	-2.95	119.75	122.79
40	L5	400	A2M	C2'-C1'-N9	2.95	118.60	113.75
19	S2	121	OMU	O4-C4-C5	-2.94	120.09	125.16
19	S2	1832	6MZ	C4-N9-C8	2.94	108.82	105.74
19	S2	1046	PSU	C6-N1-C2	-2.93	119.97	122.69
19	S2	668	A2M	C4-N9-C1'	-2.93	119.78	126.63
40	L5	3825	A2M	C4-N9-C1'	-2.93	119.78	126.63
40	L5	3701	OMC	O2-C2-N1	2.93	124.64	118.90
40	L5	1524	A2M	C4'-O4'-C1'	-2.93	103.00	109.47
40	L5	4636	PSU	C6-C5-C4	2.92	120.15	118.17
40	L5	1744	PSU	O2-C2-N1	-2.92	119.78	122.79
19	S2	1326	OMU	O4-C4-C5	-2.92	120.13	125.16
19	S2	27	A2M	C4-N9-C1'	-2.92	119.81	126.63
19	S2	627	OMU	O4-C4-C5	-2.91	120.15	125.16
40	L5	3785	A2M	O3'-C3'-C2'	2.91	119.32	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	1536	PSU	O2-C2-N1	-2.91	119.79	122.79
19	S2	99	A2M	C4-N9-C1'	-2.90	119.84	126.63
40	L5	4306	OMU	O4-C4-C5	-2.90	120.16	125.16
40	L5	4442	PSU	O2-C2-N1	-2.90	119.80	122.79
19	S2	1046	PSU	O2-C2-N1	-2.90	119.80	122.79
19	S2	105	PSU	C6-N1-C2	-2.89	120.01	122.69
40	L5	1862	PSU	O2-C2-N1	-2.89	119.81	122.79
40	L5	1524	A2M	O3'-C3'-C2'	2.89	119.27	111.19
40	L5	2401	A2M	C1'-N9-C8	2.88	133.50	127.09
40	L5	4689	PSU	O2-C2-N1	-2.88	119.81	122.79
40	L5	2815	A2M	C2'-C1'-N9	2.88	118.50	113.75
40	L5	3925	OMU	O4-C4-C5	-2.88	120.20	125.16
40	L5	1744	PSU	C6-N1-C2	-2.88	120.02	122.69
40	L5	2839	PSU	O2-C2-N1	-2.88	119.82	122.79
19	S2	1850	MA6	C1'-N9-C8	-2.87	120.72	127.09
19	S2	354	OMU	O4-C4-C5	-2.87	120.21	125.16
40	L5	2351	OMC	C1'-N1-C6	-2.87	114.65	120.78
19	S2	159	A2M	C3'-C2'-C1'	-2.87	97.32	102.81
19	S2	468	A2M	C1'-N9-C8	2.86	133.45	127.09
19	S2	801	PSU	C6-N1-C2	-2.86	120.04	122.69
19	S2	172	OMU	O4-C4-C5	-2.86	120.23	125.16
40	L5	398	A2M	C4-N9-C1'	-2.86	119.95	126.63
42	L8	69	PSU	C6-N1-C2	-2.85	120.04	122.69
40	L5	1871	A2M	C4-N9-C1'	-2.85	119.96	126.63
40	L5	3851	PSU	O2-C2-N1	-2.85	119.85	122.79
40	L5	3844	PSU	C6-N1-C2	-2.85	120.05	122.69
19	S2	109	PSU	O2-C2-N1	-2.85	119.85	122.79
19	S2	1045	PSU	O2-C2-N1	-2.84	119.86	122.79
19	S2	1288	OMU	O4-C4-C5	-2.83	120.28	125.16
40	L5	3853	PSU	O2-C2-N1	-2.83	119.87	122.79
40	L5	4220	6MZ	C5-C6-N1	2.83	121.19	118.15
40	L5	1860	PSU	C6-N1-C2	-2.82	120.07	122.69
19	S2	105	PSU	O2-C2-N1	-2.82	119.88	122.79
40	L5	4576	PSU	O2-C2-N1	-2.82	119.88	122.79
19	S2	1639	G7M	C2-N1-C6	-2.81	120.01	125.11
19	S2	1004	PSU	O2-C2-N1	-2.81	119.89	122.79
40	L5	4403	PSU	O2-C2-N1	-2.81	119.89	122.79
40	L5	4590	A2M	O3'-C3'-C2'	2.81	119.06	111.19
40	L5	4493	PSU	O2-C2-N1	-2.81	119.89	122.79
40	L5	3867	A2M	C4-N9-C1'	-2.81	120.06	126.63
40	L5	4636	PSU	O2-C2-N1	-2.80	119.90	122.79
40	L5	2363	A2M	C3'-C2'-C1'	-2.80	97.44	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4972	PSU	C6-N1-C2	-2.80	120.09	122.69
40	L5	3818	UY1	C6-N1-C2	-2.80	120.09	122.69
19	S2	406	PSU	O2-C2-N1	-2.80	119.90	122.79
19	S2	166	A2M	C1'-N9-C8	2.80	133.30	127.09
19	S2	1244	PSU	O2-C2-N1	-2.79	119.91	122.79
40	L5	4673	PSU	O2-C2-N1	-2.79	119.91	122.79
40	L5	4620	OMU	O4-C4-C5	-2.79	120.35	125.16
40	L5	3825	A2M	C1'-N9-C8	2.78	133.27	127.09
40	L5	3884	PSU	O2-C2-N1	-2.78	119.92	122.79
40	L5	4431	PSU	O2-C2-N1	-2.78	119.93	122.79
19	S2	863	PSU	C6-N1-C2	-2.77	120.12	122.69
19	S2	484	A2M	O3'-C3'-C2'	2.77	118.94	111.19
40	L5	4457	PSU	O2-C2-N1	-2.76	119.94	122.79
40	L5	3920	PSU	C6-N1-C2	-2.76	120.13	122.69
40	L5	3844	PSU	O2-C2-N1	-2.76	119.94	122.79
40	L5	3639	PSU	O2-C2-N1	-2.75	119.96	122.79
40	L5	4590	A2M	C4-N9-C1'	-2.74	120.22	126.63
19	S2	27	A2M	C1'-N9-C8	2.74	133.18	127.09
19	S2	27	A2M	O3'-C3'-C2'	2.74	118.86	111.19
40	L5	2787	A2M	C4-N9-C1'	-2.74	120.23	126.63
40	L5	4571	A2M	C4-N9-C1'	-2.73	120.24	126.63
40	L5	5001	PSU	O2-C2-N1	-2.73	119.97	122.79
40	L5	3867	A2M	C1'-N9-C8	2.73	133.15	127.09
19	S2	649	PSU	C6-N1-C2	-2.73	120.16	122.69
40	L5	2787	A2M	O4'-C1'-C2'	2.72	111.27	106.59
19	S2	93	PSU	O2-C2-N1	-2.72	119.98	122.79
40	L5	1536	PSU	C6-N1-C2	-2.72	120.17	122.69
40	L5	4973	PSU	C6-N1-C2	-2.71	120.17	122.69
40	L5	398	A2M	C1'-N9-C8	2.71	133.12	127.09
40	L5	3920	PSU	O2-C2-N1	-2.71	119.99	122.79
40	L5	1326	A2M	C4-N9-C1'	-2.71	120.29	126.63
40	L5	4442	PSU	C6-C5-C4	2.71	120.00	118.17
40	L5	1871	A2M	C1'-N9-C8	2.70	133.09	127.09
40	L5	4500	PSU	C6-C5-C4	2.70	120.00	118.17
40	L5	3822	PSU	C6-N1-C2	-2.70	120.19	122.69
19	S2	1004	PSU	C6-N1-C2	-2.70	120.19	122.69
19	S2	681	PSU	C6-N1-C2	-2.69	120.19	122.69
40	L5	1781	PSU	C6-N1-C2	-2.69	120.19	122.69
40	L5	4552	PSU	O2-C2-N1	-2.69	120.02	122.79
19	S2	1232	PSU	C6-N1-C2	-2.69	120.20	122.69
19	S2	576	A2M	C3'-C2'-C1'	-2.69	97.66	102.81
40	L5	4523	A2M	C1'-N9-C8	2.69	133.06	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	1782	PSU	C6-N1-C2	-2.69	120.20	122.69
40	L5	1534	A2M	C3'-C2'-C1'	-2.69	97.66	102.81
19	S2	1383	A2M	C1'-N9-C8	2.68	133.05	127.09
40	L5	5001	PSU	C6-N1-C2	-2.68	120.20	122.69
40	L5	4361	PSU	O2-C2-N1	-2.68	120.03	122.79
40	L5	1677	PSU	O2-C2-N1	-2.68	120.03	122.79
40	L5	3830	A2M	C4-N9-C1'	-2.68	120.37	126.63
19	S2	1031	A2M	C4-N9-C1'	-2.67	120.38	126.63
19	S2	159	A2M	C4-N9-C1'	-2.67	120.39	126.63
40	L5	1781	PSU	O2-C2-N1	-2.67	120.04	122.79
19	S2	668	A2M	C1'-N9-C8	2.67	133.01	127.09
19	S2	99	A2M	C1'-N9-C8	2.66	133.00	127.09
40	L5	1782	PSU	O2-C2-N1	-2.66	120.04	122.79
40	L5	4442	PSU	C6-N1-C2	-2.66	120.22	122.69
40	L5	3884	PSU	C6-N1-C2	-2.66	120.23	122.69
19	S2	1031	A2M	C3'-C2'-C1'	-2.65	97.74	102.81
19	S2	686	PSU	O2-C2-N1	-2.64	120.06	122.79
40	L5	1862	PSU	C6-N1-C2	-2.64	120.24	122.69
19	S2	801	PSU	O2-C2-N1	-2.64	120.07	122.79
19	S2	651	PSU	O2-C2-N1	-2.64	120.07	122.79
19	S2	866	PSU	O2-C2-N1	-2.64	120.07	122.79
40	L5	2632	PSU	O2-C2-N1	-2.64	120.07	122.79
40	L5	4296	PSU	O2-C2-N1	-2.63	120.07	122.79
40	L5	4521	PSU	O2-C2-N1	-2.63	120.07	122.79
40	L5	3867	A2M	C2'-C1'-N9	2.63	118.08	113.75
40	L5	4361	PSU	C6-N1-C2	-2.63	120.25	122.69
19	S2	1248	B8N	O4-C4-N3	-2.62	115.73	119.99
40	L5	3822	PSU	O2-C2-N1	-2.62	120.09	122.79
40	L5	1792	PSU	C6-N1-C2	-2.61	120.27	122.69
19	S2	1367	PSU	O2-C2-N1	-2.61	120.10	122.79
40	L5	4576	PSU	C6-N1-C2	-2.61	120.27	122.69
40	L5	3851	PSU	C6-N1-C2	-2.60	120.28	122.69
40	L5	3637	PSU	C6-N1-C2	-2.60	120.28	122.69
40	L5	4590	A2M	C1'-N9-C8	2.60	132.87	127.09
40	L5	4972	PSU	O2-C2-N1	-2.60	120.11	122.79
19	S2	814	PSU	C6-N1-C2	-2.59	120.29	122.69
40	L5	3639	PSU	C6-N1-C2	-2.59	120.29	122.69
40	L5	3695	PSU	O2-C2-N1	-2.59	120.12	122.79
40	L5	4673	PSU	C6-N1-C2	-2.59	120.29	122.69
19	S2	1851	MA6	C1'-N9-C8	-2.58	121.38	127.09
40	L5	4353	PSU	C6-C5-C4	2.57	119.91	118.17
19	S2	576	A2M	C4-N9-C1'	-2.57	120.61	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	3695	PSU	C6-N1-C2	-2.57	120.31	122.69
40	L5	1792	PSU	O2-C2-N1	-2.57	120.14	122.79
40	L5	4471	PSU	C6-N1-C2	-2.57	120.31	122.69
40	L5	3808	OMC	C1'-N1-C2	2.57	124.11	118.44
40	L5	4312	PSU	O2-C2-N1	-2.57	120.14	122.79
40	L5	1524	A2M	O4'-C1'-C2'	2.56	111.00	106.59
19	S2	966	PSU	C6-N1-C2	-2.56	120.31	122.69
40	L5	1860	PSU	O2-C2-N1	-2.56	120.15	122.79
40	L5	3925	OMU	O2-C2-N1	-2.55	119.47	122.80
19	S2	484	A2M	C4-N9-C1'	-2.55	120.66	126.63
40	L5	2815	A2M	C3'-C2'-C1'	-2.55	97.92	102.81
40	L5	2632	PSU	C6-N1-C2	-2.55	120.33	122.69
40	L5	3830	A2M	C1'-N9-C8	2.54	132.73	127.09
40	L5	4532	PSU	O2-C2-N1	-2.54	120.17	122.79
40	L5	4532	PSU	C6-N1-C2	-2.53	120.34	122.69
40	L5	1326	A2M	C1'-N9-C8	2.53	132.71	127.09
40	L5	2363	A2M	O3'-C3'-C2'	2.53	118.26	111.19
40	L5	400	A2M	C4-N9-C1'	-2.53	120.72	126.63
40	L5	3718	A2M	C1'-N9-C8	2.52	132.70	127.09
19	S2	668	A2M	O4'-C1'-C2'	2.51	110.92	106.59
19	S2	484	A2M	C1'-N9-C8	2.51	132.66	127.09
19	S2	1850	MA6	O4'-C4'-C3'	-2.50	100.18	105.15
19	S2	406	PSU	C6-N1-C2	-2.50	120.37	122.69
40	L5	4299	PSU	C6-N1-C2	-2.49	120.38	122.69
40	L5	4431	PSU	C6-N1-C2	-2.49	120.38	122.69
40	L5	1323	A2M	O4'-C1'-C2'	2.49	110.87	106.59
40	L5	2815	A2M	C4-N9-C1'	-2.49	120.82	126.63
40	L5	4403	PSU	C6-N1-C2	-2.49	120.38	122.69
40	L5	2861	OMC	C1'-N1-C2	2.48	123.93	118.44
19	S2	1174	PSU	C6-N1-C2	-2.48	120.39	122.69
40	L5	3920	PSU	C6-C5-C4	2.48	119.85	118.17
19	S2	1081	PSU	C6-C5-C4	2.48	119.85	118.17
40	L5	2787	A2M	C1'-N9-C8	2.47	132.58	127.09
40	L5	4312	PSU	C6-N1-C2	-2.47	120.40	122.69
40	L5	4457	PSU	C6-N1-C2	-2.47	120.40	122.69
19	S2	1031	A2M	C1'-N9-C8	2.47	132.57	127.09
19	S2	576	A2M	C1'-N9-C8	2.46	132.56	127.09
40	L5	3785	A2M	C2-N1-C6	-2.46	114.68	118.73
40	L5	4552	PSU	C6-N1-C2	-2.46	120.41	122.69
40	L5	1326	A2M	O3'-C3'-C2'	2.46	118.07	111.19
40	L5	4571	A2M	C1'-N9-C8	2.46	132.55	127.09
19	S2	159	A2M	C1'-N9-C8	2.46	132.55	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	2363	A2M	C1'-N9-C8	2.46	132.54	127.09
40	L5	3818	UY1	O2-C2-N1	-2.45	120.26	122.79
19	S2	1056	PSU	O2-C2-N1	-2.45	120.26	122.79
40	L5	3718	A2M	C2'-C1'-N9	2.45	117.78	113.75
40	L5	2363	A2M	C4-N9-C1'	-2.45	120.91	126.63
42	L8	55	PSU	C6-N1-C2	-2.45	120.42	122.69
19	S2	1639	G7M	CN7-N7-C8	-2.44	121.09	124.79
40	L5	4521	PSU	C6-N1-C2	-2.44	120.43	122.69
19	S2	93	PSU	C6-N1-C2	-2.43	120.44	122.69
19	S2	1244	PSU	C6-N1-C2	-2.42	120.44	122.69
19	S2	1367	PSU	C6-N1-C2	-2.42	120.44	122.69
40	L5	2815	A2M	C1'-N9-C8	2.41	132.45	127.09
19	S2	354	OMU	O2-C2-N1	-2.41	119.66	122.80
42	L8	69	PSU	C6-C5-C4	2.41	119.80	118.17
40	L5	3867	A2M	O3'-C3'-C2'	2.41	117.93	111.19
40	L5	4296	PSU	C6-N1-C2	-2.40	120.47	122.69
19	S2	1639	G7M	N9-C8-N7	-2.40	106.66	112.48
40	L5	1326	A2M	O4'-C1'-C2'	2.39	110.70	106.59
19	S2	406	PSU	C6-C5-C4	2.39	119.79	118.17
40	L5	3637	PSU	C6-C5-C4	2.39	119.79	118.17
19	S2	1056	PSU	C6-N1-C2	-2.38	120.48	122.69
19	S2	1045	PSU	C6-N1-C2	-2.38	120.49	122.69
40	L5	3853	PSU	C6-N1-C2	-2.37	120.49	122.69
19	S2	681	PSU	O2-C2-N1	-2.37	120.34	122.79
40	L5	2363	A2M	O4'-C1'-C2'	2.37	110.67	106.59
19	S2	468	A2M	C6-C5-C4	-2.37	113.94	117.18
40	L5	4523	A2M	C6-C5-C4	-2.36	113.95	117.18
40	L5	3718	A2M	C4-N9-C1'	-2.36	121.12	126.63
19	S2	166	A2M	C6-C5-C4	-2.36	113.96	117.18
40	L5	4220	6MZ	C4-C5-C6	2.35	118.73	116.78
40	L5	4471	PSU	O2-C2-N1	-2.35	120.37	122.79
40	L5	4293	PSU	C6-N1-C2	-2.35	120.51	122.69
19	S2	649	PSU	O2-C2-N1	-2.35	120.37	122.79
19	S2	1081	PSU	C6-N1-C2	-2.34	120.52	122.69
19	S2	1442	OMU	O2-C2-N1	-2.34	119.75	122.80
40	L5	400	A2M	C1'-N9-C8	2.34	132.28	127.09
40	L5	3825	A2M	C6-C5-C4	-2.33	113.99	117.18
19	S2	484	A2M	O4'-C1'-C2'	2.33	110.60	106.59
19	S2	627	OMU	O2-C2-N1	-2.33	119.77	122.80
40	L5	4530	UR3	C6-N1-C2	-2.32	119.90	121.80
19	S2	966	PSU	C6-C5-C4	2.32	119.74	118.17
40	L5	3785	A2M	C5-C6-N1	2.32	123.41	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	3867	A2M	C6-C5-C4	-2.32	114.01	117.18
40	L5	4590	A2M	C6-C5-C4	-2.32	114.02	117.18
40	L5	1534	A2M	C1'-N9-C8	2.32	132.23	127.09
19	S2	166	A2M	O4'-C1'-C2'	2.31	110.57	106.59
40	L5	1322	1MA	N1-C6-N6	2.31	125.52	119.71
40	L5	4353	PSU	C6-N1-C2	-2.31	120.55	122.69
40	L5	1326	A2M	C6-C5-C4	-2.31	114.02	117.18
40	L5	4293	PSU	C6-C5-C4	2.31	119.73	118.17
19	S2	866	PSU	C6-N1-C2	-2.31	120.55	122.69
40	L5	2837	OMU	O2-C2-N1	-2.31	119.80	122.80
19	S2	1337	4AC	C5-C4-N4	-2.30	119.06	122.94
40	L5	4493	PSU	C6-N1-C2	-2.30	120.55	122.69
40	L5	1534	A2M	C2'-C1'-N9	2.30	117.54	113.75
19	S2	109	PSU	C6-N1-C2	-2.30	120.56	122.69
40	L5	1871	A2M	C6-C5-C4	-2.30	114.04	117.18
40	L5	1522	OMG	C2'-C1'-N9	-2.30	109.88	114.24
40	L5	1524	A2M	C4-N9-C1'	-2.29	121.28	126.63
19	S2	1248	B8N	O4'-C1'-C2'	2.28	108.31	105.15
40	L5	2401	A2M	C6-C5-C4	-2.28	114.06	117.18
19	S2	1383	A2M	C6-C5-C4	-2.28	114.06	117.18
40	L5	1582	PSU	O2-C2-N1	-2.28	120.44	122.79
19	S2	1177	PSU	O2-C2-N1	-2.28	120.44	122.79
40	L5	4353	PSU	O2-C2-N1	-2.27	120.44	122.79
19	S2	651	PSU	C6-C5-C4	2.27	119.71	118.17
40	L5	1534	A2M	C4-N9-C1'	-2.27	121.32	126.63
19	S2	686	PSU	C6-N1-C2	-2.26	120.59	122.69
19	S2	1367	PSU	C6-C5-C4	2.26	119.70	118.17
19	S2	1177	PSU	C6-N1-C2	-2.26	120.59	122.69
40	L5	1323	A2M	C4-N9-C1'	-2.26	121.35	126.63
40	L5	1322	1MA	CM1-N1-C6	-2.25	116.66	120.15
40	L5	3785	A2M	C3'-C2'-C1'	-2.25	98.50	102.81
19	S2	1248	B8N	C31-N3-C2	2.25	120.96	117.64
40	L5	1534	A2M	O4'-C1'-C2'	2.25	110.46	106.59
40	L5	1534	A2M	C2-N1-C6	-2.25	115.04	118.73
40	L5	3867	A2M	C2-N1-C6	-2.25	115.04	118.73
40	L5	398	A2M	C6-C5-C4	-2.24	114.12	117.18
19	S2	1832	6MZ	C4-C5-N7	-2.24	108.02	110.58
40	L5	2804	OMC	C1'-N1-C2	2.24	123.38	118.44
19	S2	651	PSU	C6-N1-C2	-2.23	120.62	122.69
40	L5	1677	PSU	C6-C5-C4	2.23	119.68	118.17
19	S2	668	A2M	C2'-C1'-N9	2.23	117.42	113.75
19	S2	1081	PSU	O4'-C1'-C2'	2.23	108.23	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	866	PSU	C6-C5-C4	2.22	119.67	118.17
40	L5	2787	A2M	C6-C5-C4	-2.22	114.14	117.18
40	L5	1323	A2M	C1'-N9-C8	2.22	132.02	127.09
40	L5	1677	PSU	O4'-C1'-C2'	2.22	108.22	105.15
19	S2	159	A2M	O4'-C1'-C2'	2.22	110.40	106.59
40	L5	3695	PSU	C6-C5-C4	2.21	119.67	118.17
40	L5	4571	A2M	C6-C5-C4	-2.21	114.16	117.18
40	L5	1326	A2M	C3'-C2'-C1'	-2.21	98.58	102.81
40	L5	2815	A2M	O4'-C1'-C2'	2.21	110.39	106.59
40	L5	4403	PSU	O4'-C1'-C2'	2.21	108.20	105.15
19	S2	1031	A2M	C2-N1-C6	-2.20	115.11	118.73
40	L5	1323	A2M	C2-N1-C6	-2.20	115.11	118.73
40	L5	3830	A2M	C6-C5-C4	-2.20	114.17	117.18
40	L5	1534	A2M	O3'-C3'-C2'	2.20	117.34	111.19
40	L5	4299	PSU	O2-C2-N1	-2.19	120.53	122.79
19	S2	1248	B8N	O4-C4-C5	-2.19	118.79	122.58
40	L5	3785	A2M	C4-N9-C1'	-2.19	121.52	126.63
19	S2	1031	A2M	O4'-C1'-C2'	2.18	110.34	106.59
19	S2	172	OMU	O2-C2-N1	-2.18	119.96	122.80
19	S2	484	A2M	O4'-C4'-C3'	2.18	109.48	105.15
40	L5	4227	OMU	O2-C2-N1	-2.18	119.96	122.80
40	L5	400	A2M	O4'-C1'-C2'	2.18	110.34	106.59
40	L5	4636	PSU	O4'-C1'-C2'	2.18	108.16	105.15
19	S2	27	A2M	O4'-C1'-C2'	2.17	110.32	106.59
40	L5	1524	A2M	C1'-N9-C8	2.16	131.90	127.09
19	S2	27	A2M	C2-N1-C6	-2.16	115.18	118.73
40	L5	1534	A2M	C5-C6-N1	2.16	123.00	117.51
40	L5	1323	A2M	C5-C6-N1	2.16	123.00	117.51
19	S2	1031	A2M	C5-C6-N1	2.16	122.99	117.51
40	L5	3782	5MC	C1'-N1-C6	-2.15	117.61	121.15
40	L5	3785	A2M	O4'-C4'-C3'	2.14	109.40	105.15
40	L5	4620	OMU	O2-C2-N1	-2.14	120.01	122.80
40	L5	4523	A2M	C5-C6-N1	2.14	122.95	117.51
40	L5	4636	PSU	C6-N1-C2	-2.14	120.71	122.69
40	L5	1326	A2M	C5-C6-N1	2.14	122.94	117.51
40	L5	4403	PSU	C6-C5-C4	2.13	119.61	118.17
40	L5	2401	A2M	O4'-C1'-C2'	2.13	110.26	106.59
40	L5	4571	A2M	C2'-C1'-N9	2.13	117.26	113.75
19	S2	99	A2M	C2-N1-C6	-2.13	115.23	118.73
40	L5	2815	A2M	C6-C5-C4	-2.13	114.27	117.18
19	S2	99	A2M	C5-C6-N1	2.13	122.91	117.51
40	L5	1871	A2M	C4'-O4'-C1'	-2.13	104.77	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4498	OMU	O2-C2-N1	-2.13	120.03	122.80
40	L5	3822	PSU	O4'-C1'-C2'	2.12	108.09	105.15
19	S2	1031	A2M	C6-C5-C4	-2.12	114.28	117.18
40	L5	2401	A2M	C5-C6-N1	2.12	122.90	117.51
40	L5	2787	A2M	C5-C6-N1	2.12	122.90	117.51
40	L5	4523	A2M	C2-N1-C6	-2.12	115.25	118.73
19	S2	105	PSU	C6-C5-C4	2.12	119.60	118.17
19	S2	799	OMU	C1'-N1-C2	2.12	121.39	117.59
40	L5	400	A2M	C6-C5-C4	-2.11	114.29	117.18
19	S2	1272	OMC	C1'-N1-C2	2.11	123.11	118.44
40	L5	3785	A2M	O4'-C1'-N9	2.11	112.14	108.09
40	L5	2815	A2M	C5-C6-N1	2.11	122.87	117.51
40	L5	3867	A2M	C5-C6-N1	2.11	122.87	117.51
40	L5	1792	PSU	C6-C5-C4	2.11	119.60	118.17
19	S2	159	A2M	C2-N1-C6	-2.11	115.27	118.73
40	L5	4523	A2M	C4'-O4'-C1'	-2.11	104.81	109.47
19	S2	668	A2M	C6-C5-C4	-2.11	114.30	117.18
40	L5	2363	A2M	C5-C6-N1	2.10	122.85	117.51
40	L5	3825	A2M	C5-C6-N1	2.10	122.85	117.51
40	L5	1524	A2M	C6-C5-C4	-2.10	114.31	117.18
19	S2	1832	6MZ	C5'-C4'-C3'	-2.10	107.66	115.21
40	L5	2401	A2M	C2-N1-C6	-2.10	115.28	118.73
19	S2	27	A2M	C6-C5-C4	-2.10	114.31	117.18
40	L5	3718	A2M	C2-N1-C6	-2.10	115.28	118.73
40	L5	4471	PSU	C6-C5-C4	2.10	119.59	118.17
19	S2	1326	OMU	O2-C2-N1	-2.10	120.07	122.80
42	L8	69	PSU	O4'-C1'-C2'	2.10	108.05	105.15
40	L5	1323	A2M	C6-C5-C4	-2.09	114.32	117.18
40	L5	4973	PSU	C6-C5-C4	2.09	119.59	118.17
40	L5	4442	PSU	O4'-C1'-C2'	2.09	108.05	105.15
19	S2	27	A2M	C5-C6-N1	2.09	122.82	117.51
40	L5	1326	A2M	C2-N1-C6	-2.09	115.30	118.73
40	L5	398	A2M	C5-C6-N1	2.09	122.82	117.51
40	L5	4673	PSU	C6-C5-C4	2.09	119.58	118.17
19	S2	121	OMU	O2-C2-N1	-2.09	120.08	122.80
19	S2	484	A2M	C2-N1-C6	-2.09	115.30	118.73
19	S2	428	OMU	C1'-N1-C2	2.09	121.34	117.59
40	L5	3884	PSU	C6-C5-C4	2.08	119.58	118.17
40	L5	3830	A2M	C5-C6-N1	2.08	122.80	117.51
19	S2	1383	A2M	O4'-C1'-C2'	2.08	110.17	106.59
40	L5	4521	PSU	C6-C5-C4	2.08	119.58	118.17
40	L5	1582	PSU	C6-C5-C4	2.08	119.58	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	3695	PSU	O4'-C1'-C2'	2.08	108.03	105.15
40	L5	1524	A2M	C2-N1-C6	-2.08	115.31	118.73
40	L5	400	A2M	O3'-C3'-C4'	-2.08	105.11	111.08
19	S2	159	A2M	C5-C6-N1	2.08	122.78	117.51
40	L5	3920	PSU	O4'-C1'-C2'	2.07	108.02	105.15
19	S2	468	A2M	C4'-O4'-C1'	-2.07	104.89	109.47
40	L5	3808	OMC	C1'-N1-C6	-2.07	116.36	120.78
40	L5	1862	PSU	C6-C5-C4	2.07	119.57	118.17
40	L5	4628	PSU	C6-C5-C4	2.07	119.57	118.17
19	S2	576	A2M	O4'-C4'-C3'	2.07	109.25	105.15
40	L5	3851	PSU	C6-C5-C4	2.06	119.57	118.17
19	S2	99	A2M	C6-C5-C4	-2.06	114.37	117.18
40	L5	2363	A2M	C2-N1-C6	-2.05	115.36	118.73
40	L5	3627	OMG	C2'-C1'-N9	-2.05	110.35	114.24
19	S2	159	A2M	C6-C5-C4	-2.05	114.38	117.18
40	L5	3825	A2M	C2-N1-C6	-2.05	115.37	118.73
40	L5	4571	A2M	C5-C6-N1	2.04	122.70	117.51
40	L5	3825	A2M	C2'-C1'-N9	2.04	117.11	113.75
40	L5	3637	PSU	O2-C2-N3	-2.04	118.23	121.86
40	L5	4590	A2M	C5-C6-N1	2.04	122.70	117.51
40	L5	4523	A2M	O4'-C1'-C2'	2.04	110.10	106.59
19	S2	468	A2M	C5-C6-N1	2.04	122.68	117.51
19	S2	484	A2M	C5-C6-N1	2.04	122.68	117.51
40	L5	4636	PSU	C5-C6-N1	-2.03	119.32	122.14
19	S2	1081	PSU	O4-C4-C5	-2.03	118.95	124.01
19	S2	1383	A2M	C2-N1-C6	-2.03	115.39	118.73
40	L5	3818	UY1	O4'-C1'-C2'	2.03	108.12	104.56
40	L5	3785	A2M	C4'-O4'-C1'	-2.03	104.98	109.47
40	L5	400	A2M	C5-C6-N1	2.03	122.67	117.51
19	S2	166	A2M	C5-C6-N1	2.03	122.67	117.51
40	L5	1782	PSU	C6-C5-C4	2.03	119.54	118.17
19	S2	1832	6MZ	C5-C6-N1	2.03	120.33	118.15
40	L5	398	A2M	C2-N1-C6	-2.02	115.41	118.73
40	L5	1871	A2M	C5-C6-N1	2.02	122.65	117.51
40	L5	4571	A2M	O3'-C3'-C4'	-2.02	105.27	111.08
40	L5	1340	OMC	C1'-N1-C2	2.02	122.90	118.44
19	S2	1383	A2M	C5-C6-N1	2.02	122.64	117.51
40	L5	1524	A2M	C5-C6-N1	2.02	122.64	117.51
19	S2	99	A2M	O4'-C1'-C2'	2.02	110.06	106.59
40	L5	2363	A2M	C6-C5-C4	-2.02	114.42	117.18
40	L5	3830	A2M	C4'-O4'-C1'	-2.01	105.02	109.47
19	S2	686	PSU	O4'-C1'-C2'	2.01	107.94	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	109	PSU	O4'-C1'-C2'	2.01	107.93	105.15
40	L5	3830	A2M	C2-N1-C6	-2.00	115.44	118.73
40	L5	3718	A2M	C5-C6-N1	2.00	122.60	117.51
40	L5	3639	PSU	C6-C5-C4	2.00	119.53	118.17
40	L5	2815	A2M	C2-N1-C6	-2.00	115.44	118.73
40	L5	3785	A2M	C1'-N9-C8	2.00	131.54	127.09
40	L5	2787	A2M	C2-N1-C6	-2.00	115.44	118.73
40	L5	1534	A2M	C6-C5-C4	-2.00	114.45	117.18

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	L8	75	OMG	C1'-C2'-O2'-CM2
19	S2	27	A2M	C1'-C2'-O2'-CM'
19	S2	159	A2M	C1'-C2'-O2'-CM'
19	S2	174	OMC	C1'-C2'-O2'-CM2
19	S2	462	OMC	C1'-C2'-O2'-CM2
19	S2	601	OMG	C1'-C2'-O2'-CM2
19	S2	644	OMG	O4'-C4'-C5'-O5'
19	S2	644	OMG	C1'-C2'-O2'-CM2
19	S2	863	PSU	C3'-C4'-C5'-O5'
19	S2	863	PSU	O4'-C4'-C5'-O5'
19	S2	1031	A2M	C1'-C2'-O2'-CM'
19	S2	1045	PSU	O4'-C4'-C5'-O5'
19	S2	1248	B8N	O4'-C4'-C5'-O5'
19	S2	1248	B8N	C3'-C4'-C5'-O5'
19	S2	1272	OMC	O4'-C4'-C5'-O5'
19	S2	1288	OMU	O4'-C4'-C5'-O5'
19	S2	1337	4AC	N3-C4-N4-C7
19	S2	1383	A2M	C1'-C2'-O2'-CM'
19	S2	1832	6MZ	C5-C6-N6-C9
19	S2	1832	6MZ	N1-C6-N6-C9
40	L5	400	A2M	C1'-C2'-O2'-CM'
40	L5	1326	A2M	O4'-C4'-C5'-O5'
40	L5	1625	OMG	O4'-C4'-C5'-O5'
40	L5	2364	OMG	C1'-C2'-O2'-CM2
40	L5	2787	A2M	C1'-C2'-O2'-CM'
40	L5	2815	A2M	O4'-C4'-C5'-O5'
40	L5	2824	OMC	C1'-C2'-O2'-CM2
40	L5	3792	OMG	O4'-C4'-C5'-O5'
40	L5	3867	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
40	L5	4196	OMG	C1'-C2'-O2'-CM2
40	L5	4220	6MZ	O4'-C4'-C5'-O5'
40	L5	4447	5MC	C2'-C1'-N1-C2
40	L5	4447	5MC	C2'-C1'-N1-C6
40	L5	4620	OMU	C1'-C2'-O2'-CM2
40	L5	4637	OMG	O4'-C4'-C5'-O5'
40	L5	4637	OMG	C1'-C2'-O2'-CM2
40	L5	3701	OMC	C2'-C1'-N1-C2
19	S2	99	A2M	O4'-C4'-C5'-O5'
19	S2	801	PSU	C3'-C4'-C5'-O5'
19	S2	1272	OMC	C3'-C4'-C5'-O5'
19	S2	1288	OMU	C3'-C4'-C5'-O5'
40	L5	1326	A2M	C3'-C4'-C5'-O5'
40	L5	1536	PSU	C3'-C4'-C5'-O5'
40	L5	1536	PSU	O4'-C4'-C5'-O5'
40	L5	2364	OMG	O4'-C4'-C5'-O5'
40	L5	3785	A2M	O4'-C4'-C5'-O5'
40	L5	3792	OMG	C3'-C4'-C5'-O5'
40	L5	3867	A2M	C3'-C4'-C5'-O5'
40	L5	4500	PSU	C3'-C4'-C5'-O5'
40	L5	4500	PSU	O4'-C4'-C5'-O5'
40	L5	4590	A2M	O4'-C4'-C5'-O5'
40	L5	4590	A2M	C3'-C4'-C5'-O5'
40	L5	4618	OMG	C3'-C4'-C5'-O5'
19	S2	801	PSU	O4'-C4'-C5'-O5'
19	S2	1045	PSU	C3'-C4'-C5'-O5'
40	L5	1323	A2M	O4'-C4'-C5'-O5'
40	L5	1625	OMG	C3'-C4'-C5'-O5'
40	L5	3701	OMC	C3'-C4'-C5'-O5'
40	L5	3701	OMC	O4'-C4'-C5'-O5'
40	L5	3785	A2M	C3'-C4'-C5'-O5'
40	L5	3867	A2M	O4'-C4'-C5'-O5'
40	L5	3899	OMG	O4'-C4'-C5'-O5'
40	L5	3899	OMG	C3'-C4'-C5'-O5'
40	L5	3701	OMC	C2'-C1'-N1-C6
40	L5	2815	A2M	C3'-C4'-C5'-O5'
40	L5	4637	OMG	C3'-C4'-C5'-O5'
19	S2	428	OMU	C2'-C1'-N1-C6
19	S2	644	OMG	C3'-C4'-C5'-O5'
19	S2	1442	OMU	O4'-C4'-C5'-O5'
40	L5	4228	OMG	C3'-C4'-C5'-O5'
19	S2	428	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	L5	1524	A2M	O4'-C4'-C5'-O5'
40	L5	4220	6MZ	C3'-C4'-C5'-O5'
40	L5	4228	OMG	O4'-C4'-C5'-O5'
40	L5	4618	OMG	O4'-C4'-C5'-O5'
19	S2	99	A2M	C3'-C4'-C5'-O5'
19	S2	428	OMU	C3'-C4'-C5'-O5'
19	S2	627	OMU	O4'-C4'-C5'-O5'
40	L5	1524	A2M	C3'-C4'-C5'-O5'
40	L5	2364	OMG	C3'-C4'-C5'-O5'
19	S2	668	A2M	O4'-C4'-C5'-O5'
19	S2	799	OMU	C3'-C4'-C5'-O5'
40	L5	3818	UY1	C4'-C5'-O5'-P
19	S2	668	A2M	C3'-C4'-C5'-O5'
40	L5	1323	A2M	C3'-C4'-C5'-O5'
19	S2	1248	B8N	N34-C33-C34-O36
40	L5	2787	A2M	C2'-C1'-N9-C8
19	S2	99	A2M	C1'-C2'-O2'-CM'
40	L5	1340	OMC	C1'-C2'-O2'-CM2
40	L5	2424	OMG	C1'-C2'-O2'-CM2
40	L5	3744	OMG	C1'-C2'-O2'-CM2
19	S2	627	OMU	C3'-C4'-C5'-O5'
40	L5	1781	PSU	C3'-C4'-C5'-O5'
19	S2	1248	B8N	C31-C32-C33-C34
19	S2	1703	OMC	O4'-C4'-C5'-O5'
40	L5	2422	OMC	C3'-C4'-C5'-O5'
40	L5	3818	UY1	C1'-C2'-O2'-CM2
19	S2	428	OMU	O4'-C1'-N1-C6
19	S2	576	A2M	O4'-C4'-C5'-O5'
40	L5	3701	OMC	O4'-C1'-N1-C6
19	S2	428	OMU	C2'-C1'-N1-C2
19	S2	576	A2M	C3'-C4'-C5'-O5'
40	L5	2422	OMC	O4'-C4'-C5'-O5'
40	L5	3782	5MC	O4'-C4'-C5'-O5'
40	L5	4499	OMG	C3'-C2'-O2'-CM2
19	S2	576	A2M	C4'-C5'-O5'-P
19	S2	867	OMG	C4'-C5'-O5'-P
40	L5	4500	PSU	C4'-C5'-O5'-P
40	L5	4590	A2M	C4'-C5'-O5'-P
40	L5	2787	A2M	C2'-C1'-N9-C4
19	S2	166	A2M	O4'-C4'-C5'-O5'
19	S2	166	A2M	C3'-C4'-C5'-O5'
19	S2	1383	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	L5	2632	PSU	C3'-C4'-C5'-O5'
19	S2	1081	PSU	C4'-C5'-O5'-P
19	S2	799	OMU	O4'-C4'-C5'-O5'
19	S2	1383	A2M	O4'-C4'-C5'-O5'
40	L5	4447	5MC	O4'-C1'-N1-C6
42	L8	75	OMG	C4'-C5'-O5'-P
40	L5	1792	PSU	O4'-C4'-C5'-O5'
40	L5	2632	PSU	O4'-C4'-C5'-O5'
40	L5	4494	OMG	C3'-C2'-O2'-CM2
19	S2	1851	MA6	C4'-C5'-O5'-P
40	L5	1534	A2M	C4'-C5'-O5'-P
19	S2	428	OMU	O4'-C1'-N1-C2
19	S2	644	OMG	C4'-C5'-O5'-P
40	L5	3844	PSU	C4'-C5'-O5'-P
40	L5	3887	OMC	C4'-C5'-O5'-P
19	S2	1244	PSU	O4'-C4'-C5'-O5'
40	L5	2351	OMC	C2'-C1'-N1-C6
40	L5	1322	1MA	C2'-C1'-N9-C8
19	S2	116	OMU	C1'-C2'-O2'-CM2
19	S2	1328	OMG	C1'-C2'-O2'-CM2
40	L5	1326	A2M	C1'-C2'-O2'-CM'
19	S2	1490	OMG	C4'-C5'-O5'-P
40	L5	1326	A2M	C4'-C5'-O5'-P
19	S2	1442	OMU	C3'-C4'-C5'-O5'
40	L5	4636	PSU	O4'-C1'-C5-C6
40	L5	3869	OMC	C3'-C2'-O2'-CM2
40	L5	3701	OMC	O4'-C1'-N1-C2
40	L5	398	A2M	O4'-C4'-C5'-O5'
40	L5	2787	A2M	C3'-C4'-C5'-O5'
40	L5	3851	PSU	C3'-C4'-C5'-O5'
40	L5	1322	1MA	C2'-C1'-N9-C4
40	L5	2787	A2M	O4'-C1'-N9-C8
40	L5	3785	A2M	O4'-C1'-N9-C8
40	L5	4447	5MC	O4'-C1'-N1-C2
19	S2	966	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

74 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L5	4196	OMG	1	0
19	S2	1850	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L5	2424	OMG	1	0
19	S2	1288	OMU	1	0
40	L5	1871	A2M	1	0
19	S2	1326	OMU	1	0
40	L5	1340	OMC	2	0
40	L5	2632	PSU	1	0
19	S2	116	OMU	4	0
19	S2	681	PSU	1	0
40	L5	3841	OMC	1	0
19	S2	174	OMC	1	0
40	L5	1326	A2M	2	0
40	L5	5001	PSU	1	0
19	S2	484	A2M	1	0
40	L5	1534	A2M	2	0
19	S2	121	OMU	1	0
19	S2	1442	OMU	1	0
40	L5	4353	PSU	1	0
19	S2	1391	OMC	2	0
19	S2	799	OMU	1	0
19	S2	576	A2M	2	0
40	L5	4306	OMU	1	0
40	L5	2804	OMC	1	0
40	L5	400	A2M	1	0
40	L5	2876	OMG	1	0
40	L5	4689	PSU	1	0
40	L5	3744	OMG	1	0
19	S2	644	OMG	2	0
40	L5	2787	A2M	1	0
19	S2	509	OMG	3	0
19	S2	649	PSU	4	0
19	S2	1337	4AC	3	0
40	L5	4637	OMG	1	0
40	L5	2824	OMC	1	0
40	L5	3718	A2M	2	0
19	S2	159	A2M	1	0
19	S2	468	A2M	2	0
19	S2	517	OMC	1	0
40	L5	2351	OMC	1	0
40	L5	4457	PSU	1	0
19	S2	1703	OMC	2	0
40	L5	4220	6MZ	1	0
19	S2	27	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L5	3701	OMC	1	0
40	L5	3867	A2M	3	0
19	S2	166	A2M	5	0
19	S2	1383	A2M	2	0
40	L5	3825	A2M	1	0
40	L5	4392	OMG	1	0
40	L5	2363	A2M	1	0
19	S2	867	OMG	1	0
19	S2	1244	PSU	2	0
40	L5	4536	OMC	1	0
40	L5	4618	OMG	1	0
40	L5	4293	PSU	1	0
19	S2	866	PSU	1	0
19	S2	93	PSU	1	0
19	S2	462	OMC	1	0
19	S2	1328	OMG	1	0
40	L5	4456	OMC	1	0
40	L5	3792	OMG	1	0
40	L5	4590	A2M	1	0
40	L5	4571	A2M	1	0
19	S2	99	A2M	2	0
19	S2	1031	A2M	4	0
40	L5	4579	PSU	2	0
40	L5	3925	OMU	1	0
40	L5	3818	UY1	1	0
40	L5	3785	A2M	1	0
40	L5	4620	OMU	1	0
19	S2	601	OMG	2	0
40	L5	2364	OMG	1	0
40	L5	2422	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 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	$\# Z > 2$
88	SPM	L5	5291	-	13,13,13	0.38	0	12,12,12	0.83	0
89	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.94	0
89	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.81	0
88	SPM	L5	5267	-	13,13,13	0.38	0	12,12,12	1.11	0
89	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.78	0
89	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.90	0
89	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.91	0
89	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.81	0
89	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.84	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.98	0
88	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.98	0
89	SPD	LN	301	-	9,9,9	0.35	0	8,8,8	0.71	0
89	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.91	0
88	SPM	L5	5264	-	13,13,13	0.36	0	12,12,12	0.97	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.96	0
88	SPM	L5	5287	-	13,13,13	0.36	0	12,12,12	0.96	0
88	SPM	L5	5290	-	13,13,13	0.34	0	12,12,12	0.84	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
88	SPM	L5	5291	-	-	2/11/11/11	-
89	SPD	L5	5261	-	-	1/7/7/7	-
89	SPD	L5	5284	-	-	2/7/7/7	-
88	SPM	L5	5267	-	-	4/11/11/11	-
89	SPD	L8	202	-	-	1/7/7/7	-
89	SPD	L5	5289	-	-	3/7/7/7	-
89	SPD	L5	5283	-	-	2/7/7/7	-
89	SPD	L5	5285	-	-	2/7/7/7	-
89	SPD	L5	5286	-	-	3/7/7/7	-
89	SPD	L5	5288	-	-	0/7/7/7	-
88	SPM	L5	5259	-	-	2/11/11/11	-
89	SPD	LN	301	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5282	-	-	1/7/7/7	-
88	SPM	L5	5264	-	-	4/11/11/11	-
88	SPM	L5	5263	-	-	3/11/11/11	-
88	SPM	L5	5287	-	-	4/11/11/11	-
88	SPM	L5	5290	-	-	6/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5267	SPM	N5-C6-C7-C8
88	L5	5263	SPM	N10-C11-C12-C13
88	L5	5267	SPM	C7-C8-C9-N10
88	L5	5267	SPM	N10-C11-C12-C13
88	L5	5287	SPM	N10-C11-C12-C13
88	L5	5290	SPM	C2-C3-C4-N5
89	L5	5283	SPD	N6-C7-C8-C9
88	L5	5290	SPM	C7-C6-N5-C4
89	L5	5286	SPD	C8-C7-N6-C5
89	L5	5285	SPD	C3-C4-C5-N6
88	L5	5264	SPM	N5-C6-C7-C8
89	L5	5289	SPD	N6-C7-C8-C9
89	L5	5286	SPD	N1-C2-C3-C4
89	L5	5289	SPD	C3-C4-C5-N6
88	L5	5264	SPM	C6-C7-C8-C9
88	L5	5290	SPM	C6-C7-C8-C9
89	L5	5285	SPD	C2-C3-C4-C5
88	L5	5264	SPM	C8-C9-N10-C11
88	L5	5267	SPM	C6-C7-C8-C9
88	L5	5291	SPM	N5-C6-C7-C8
88	L5	5259	SPM	C6-C7-C8-C9
88	L5	5287	SPM	N1-C2-C3-C4
88	L5	5290	SPM	N1-C2-C3-C4
88	L5	5287	SPM	C8-C9-N10-C11
88	L5	5287	SPM	C12-C11-N10-C9
88	L5	5291	SPM	C2-C3-C4-N5
88	L5	5264	SPM	C12-C11-N10-C9
88	L5	5290	SPM	C8-C9-N10-C11

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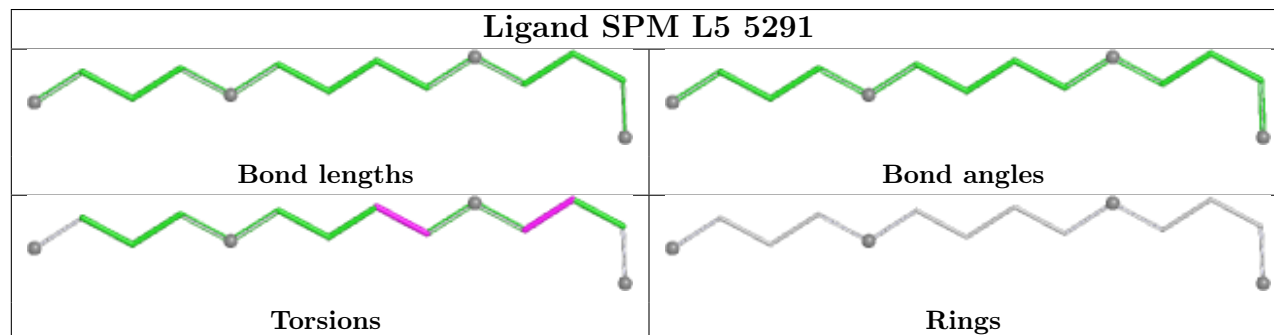
Mol	Chain	Res	Type	Atoms
89	L5	5284	SPD	C2-C3-C4-C5
88	L5	5263	SPM	C2-C3-C4-N5
88	L5	5263	SPM	C7-C6-N5-C4
89	L5	5286	SPD	N6-C7-C8-C9
89	L5	5283	SPD	N1-C2-C3-C4
89	L5	5282	SPD	C2-C3-C4-C5
88	L5	5259	SPM	C3-C4-N5-C6
89	LN	301	SPD	C2-C3-C4-C5
89	L5	5289	SPD	C8-C7-N6-C5
89	L5	5284	SPD	N6-C7-C8-C9
89	L5	5261	SPD	C2-C3-C4-C5
88	L5	5290	SPM	C3-C4-N5-C6
89	L8	202	SPD	N6-C7-C8-C9

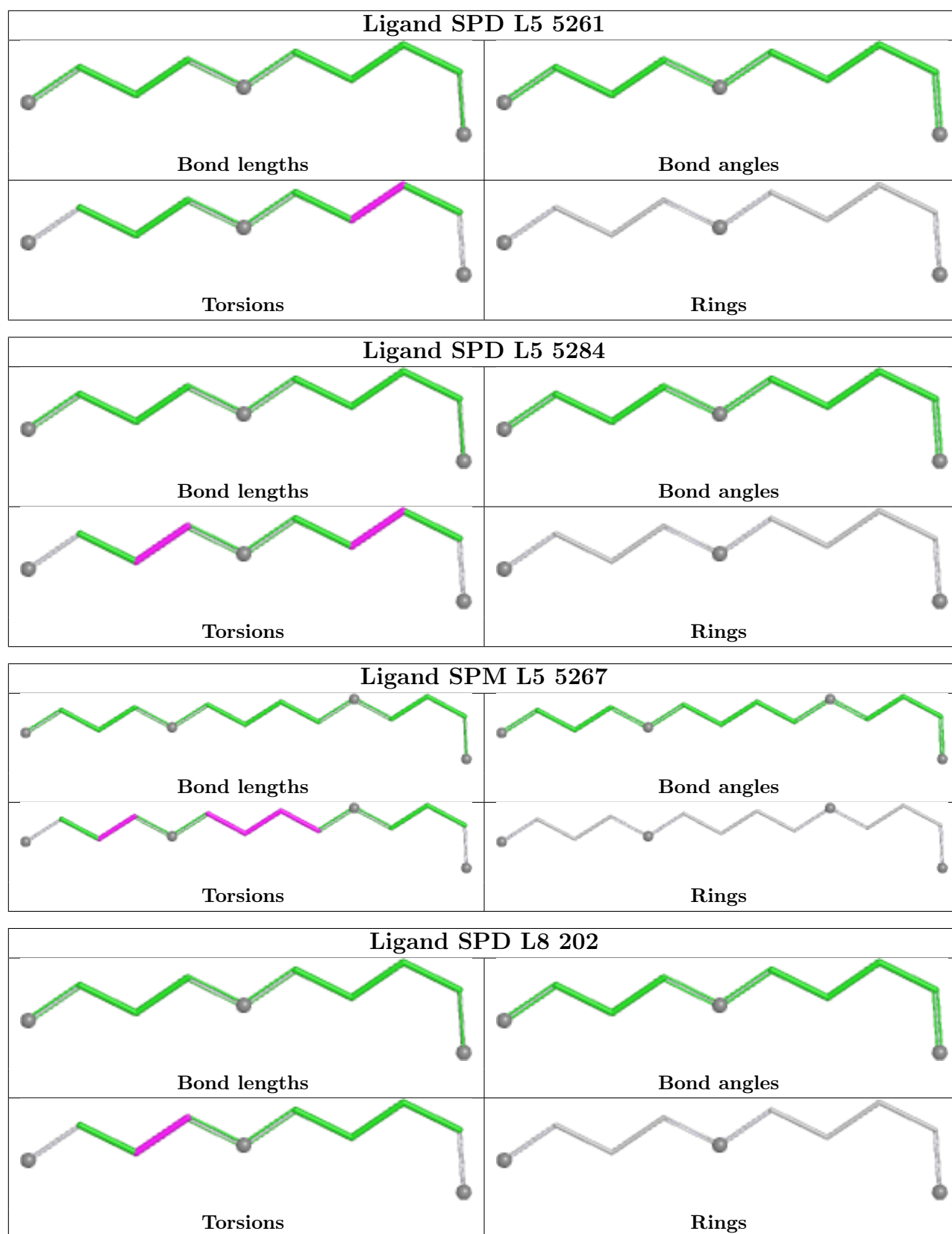
There are no ring outliers.

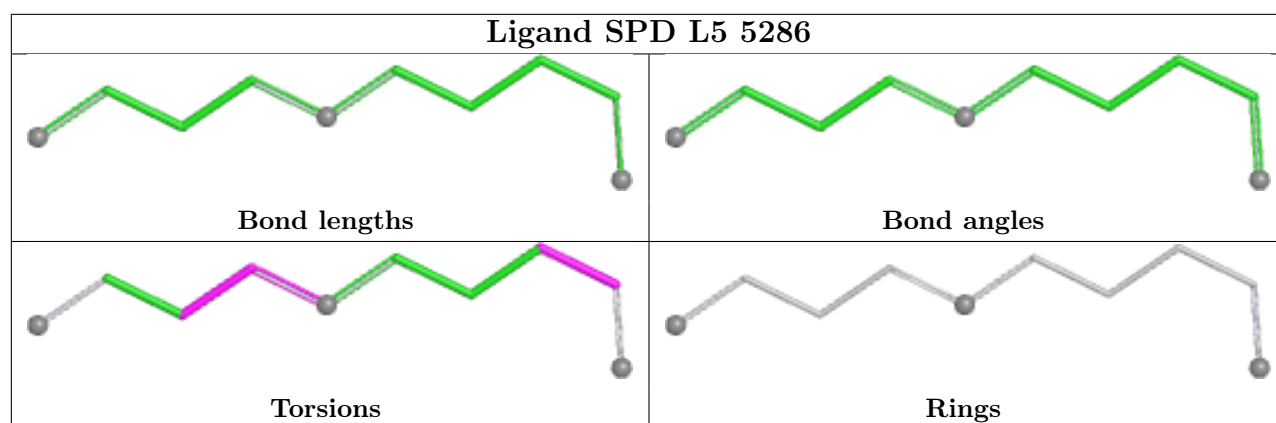
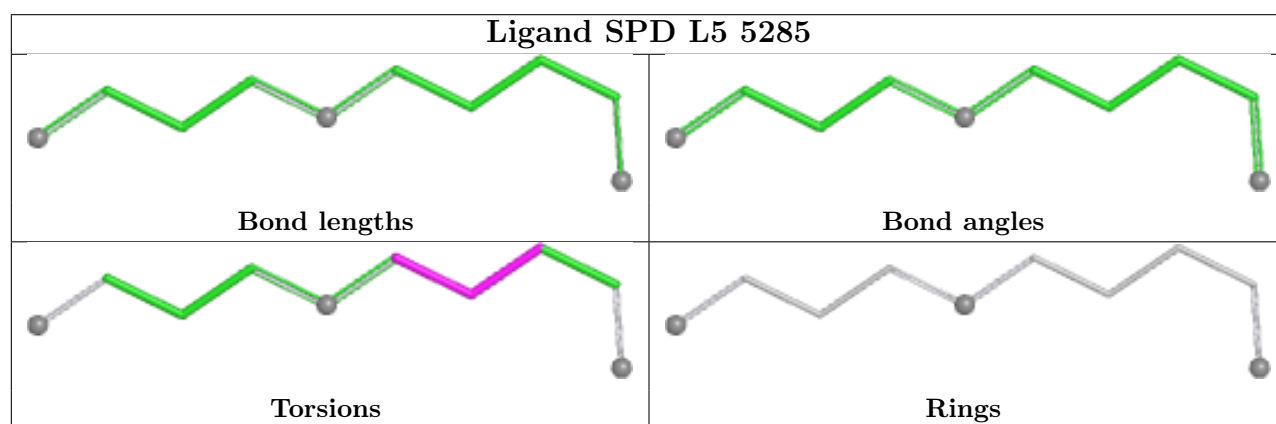
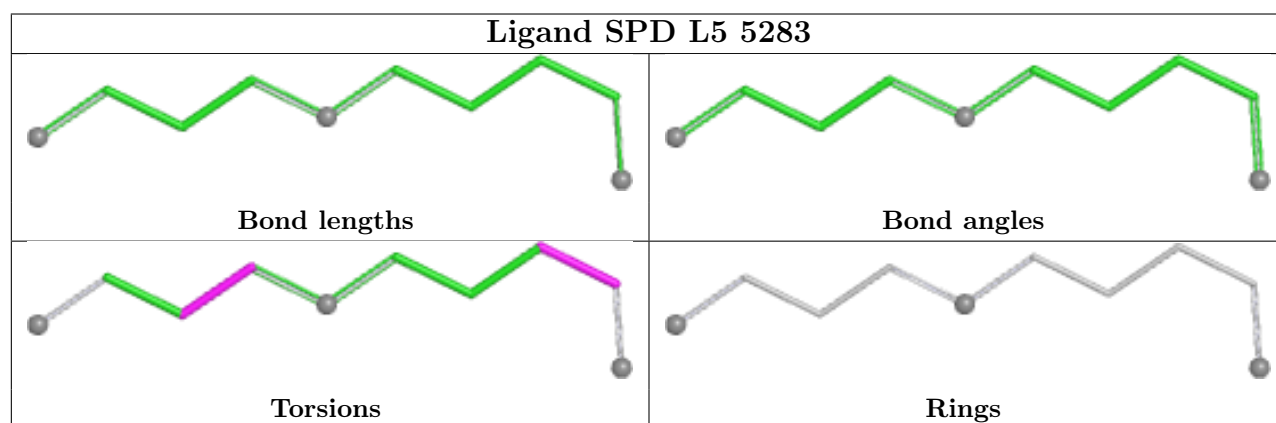
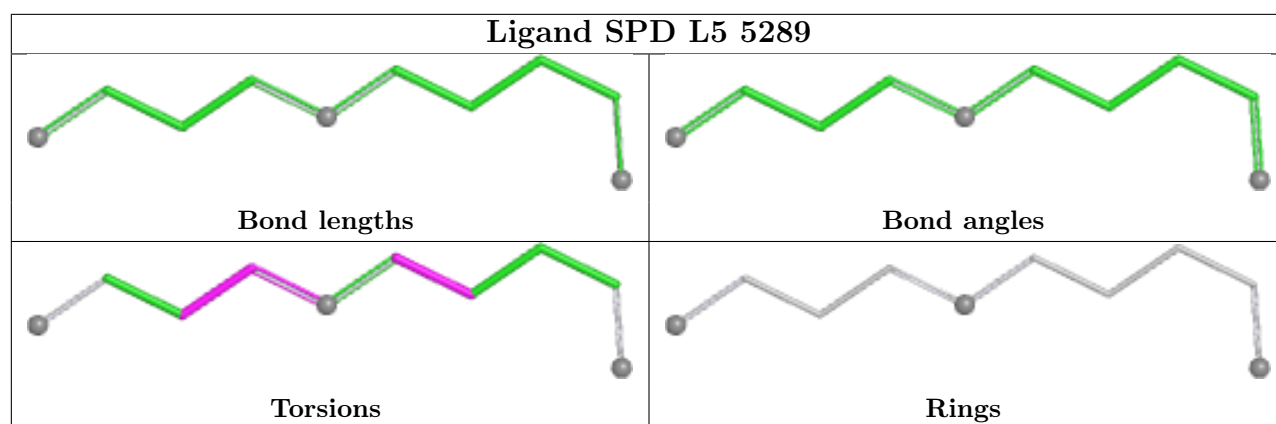
3 monomers are involved in 3 short contacts:

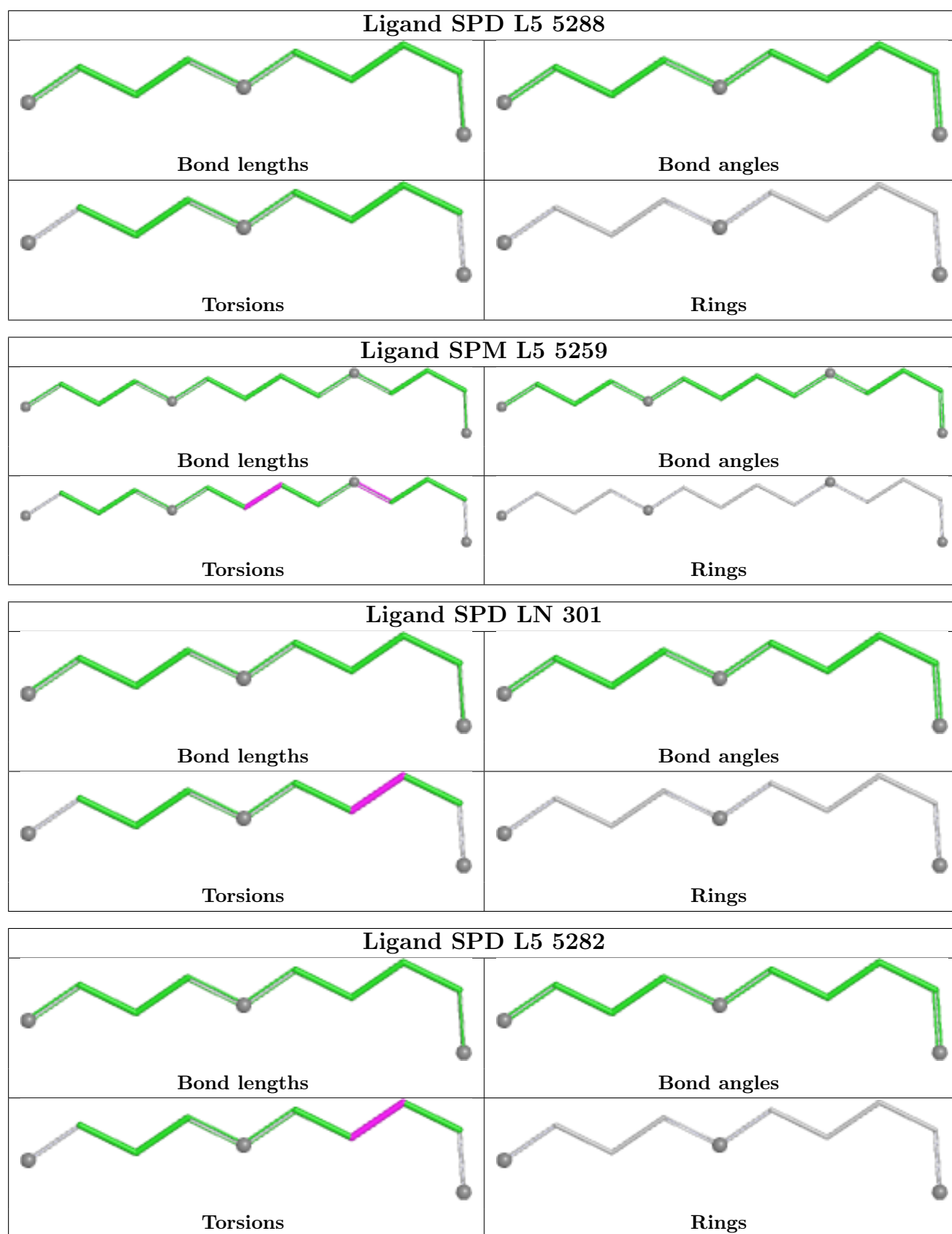
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5291	SPM	1	0
89	L5	5289	SPD	1	0
88	L5	5259	SPM	1	0

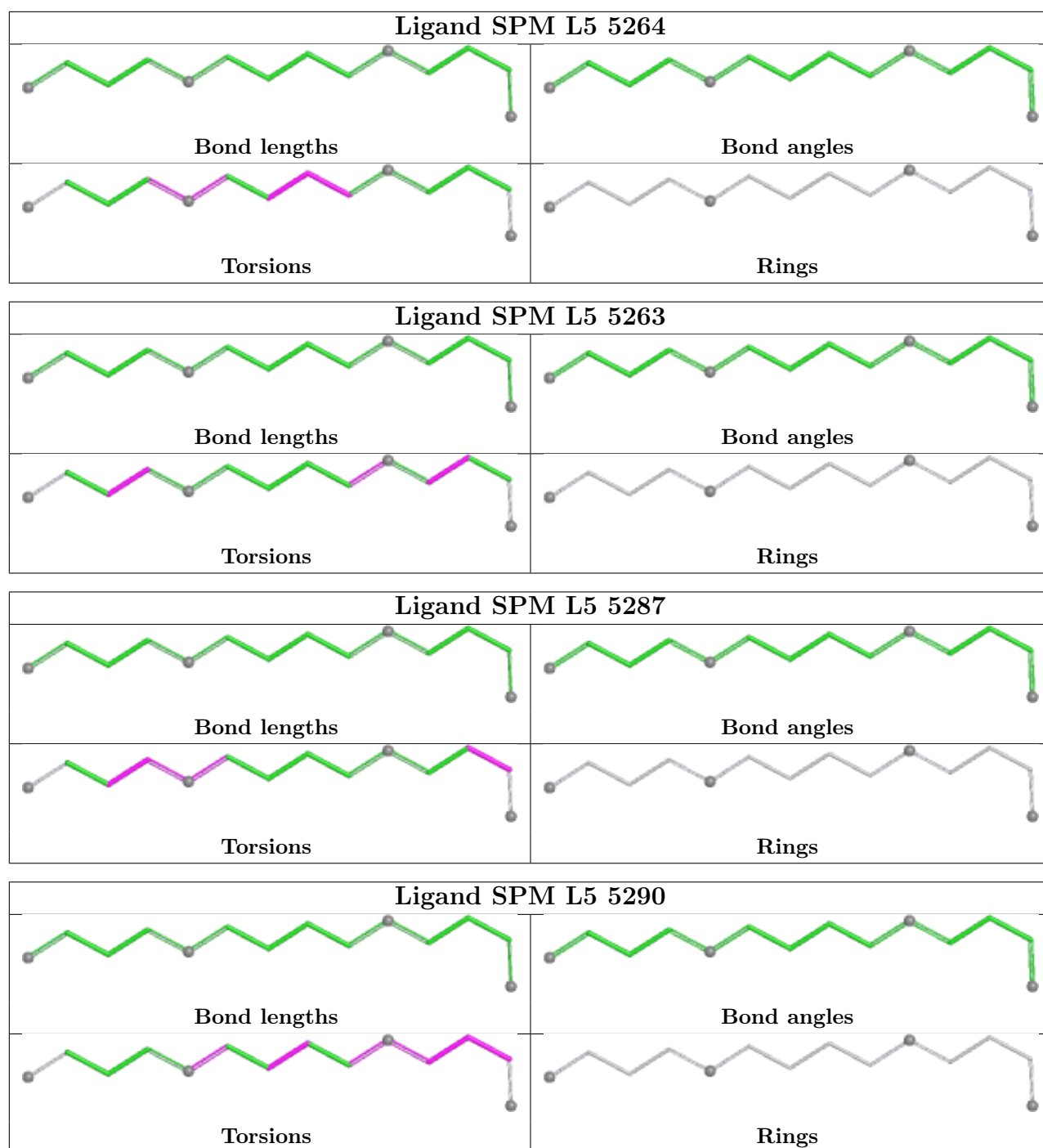
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	L5	10
19	S2	4
67	Lb	1
84	Lt	1
37	At	1
6	SH	1
38	Pt	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	33.76
1	S2	753:C	O3'	785:C	P	28.75
1	L5	1706:A	O3'	1716:G	P	21.42
1	L5	2910:G	O3'	3584:C	P	20.77
1	L5	760:G	O3'	903:C	P	16.71
1	Lt	87:GLU	C	104:ILE	N	15.64
1	L5	519:C	O3'	642:G	P	14.53
1	L5	2112:G	O3'	2249:C	P	13.88
1	S2	698:G	O3'	730:C	P	13.80
1	S2	739:C	O3'	746:C	P	13.79
1	L5	1222:A	O3'	1234:G	P	12.89
1	L5	3954:A	O3'	4056:A	P	12.32
1	L5	4776:G	O3'	4858:C	P	12.22
1	L5	990:C	O3'	1064:G	P	11.82
1	At	15:G	O3'	18:G	P	11.80
1	SH	107:LYS	C	111:LYS	N	10.67
1	Pt	15:G	O3'	18:G	P	9.70
1	S2	225:G	O3'	287:U	P	7.94
1	L5	1100:U	O3'	1167:C	P	6.10

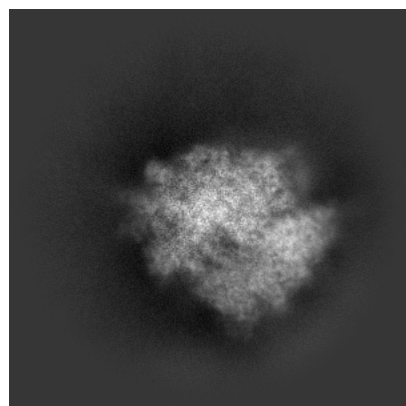
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71356. These allow visual inspection of the internal detail of the map and identification of artifacts.

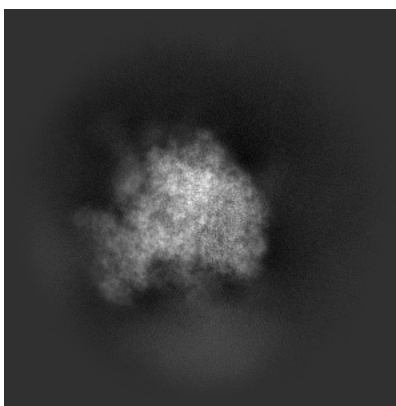
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

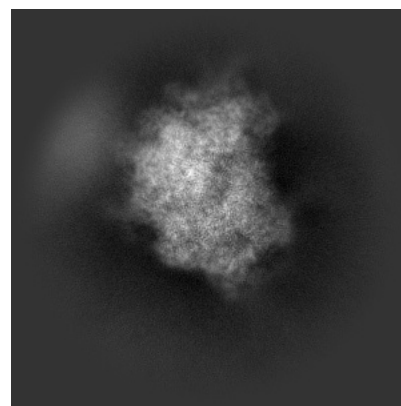
6.1.1 Primary map



X

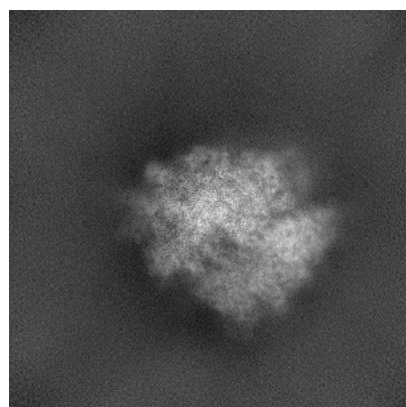


Y

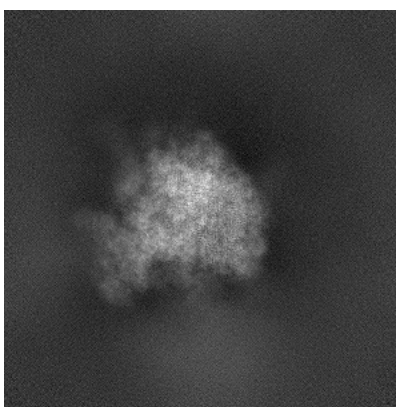


Z

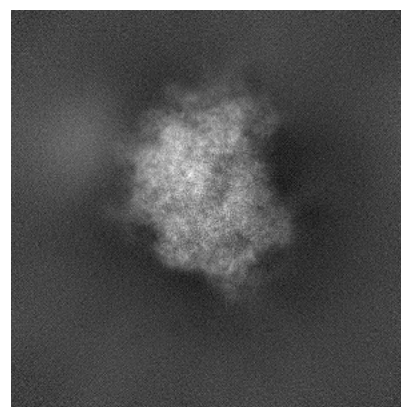
6.1.2 Raw map



X



Y

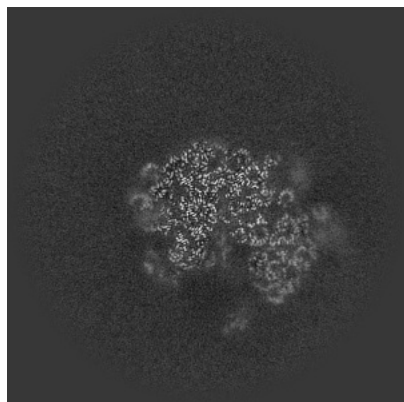


Z

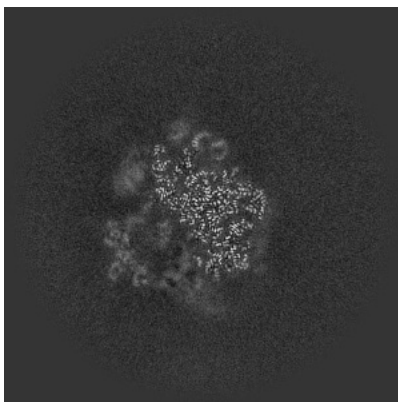
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

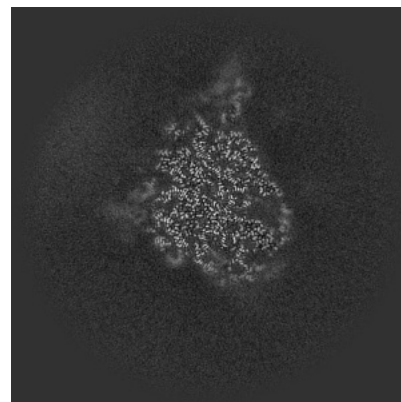
6.2.1 Primary map



X Index: 256

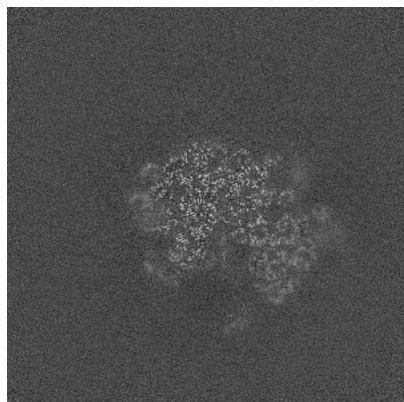


Y Index: 256

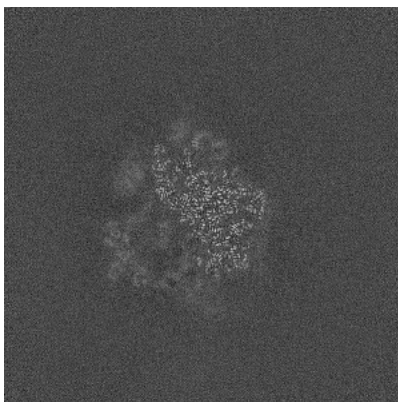


Z Index: 256

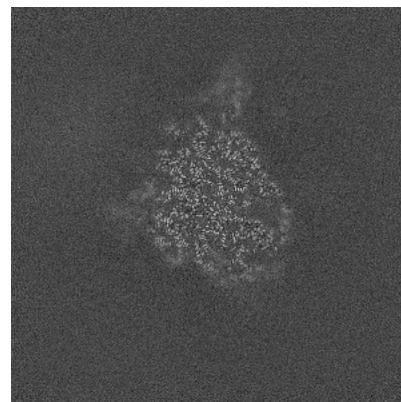
6.2.2 Raw map



X Index: 256



Y Index: 256

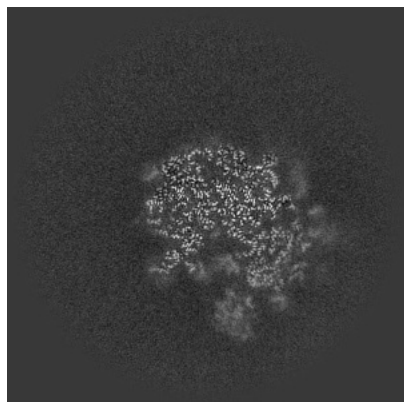


Z Index: 256

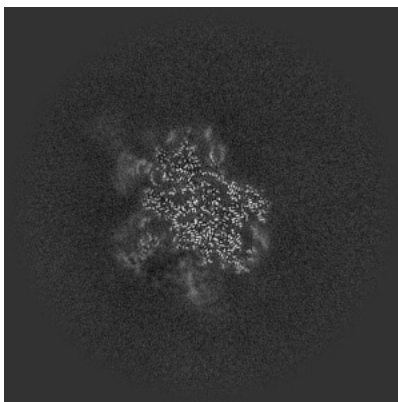
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

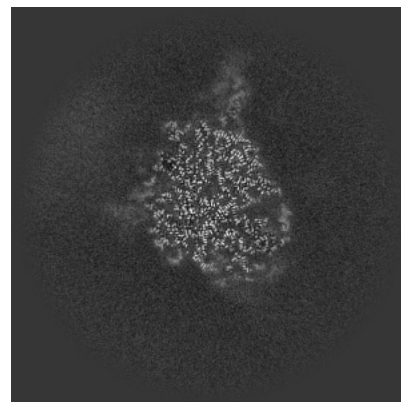
6.3.1 Primary map



X Index: 243

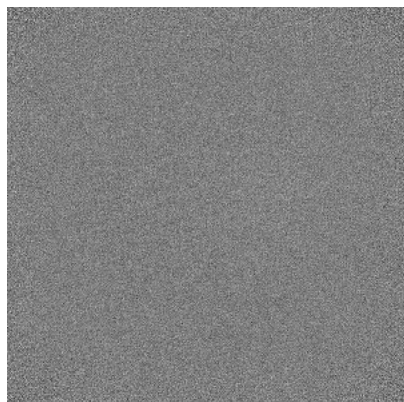


Y Index: 243

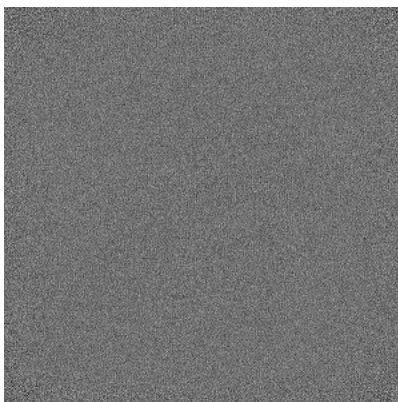


Z Index: 258

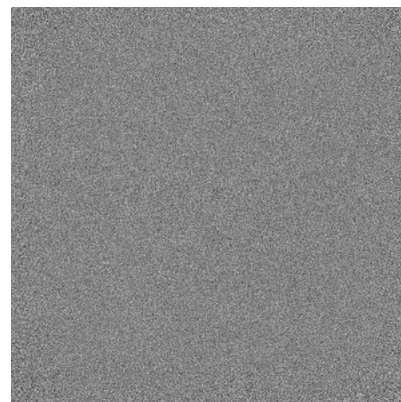
6.3.2 Raw map



X Index: 0



Y Index: 0

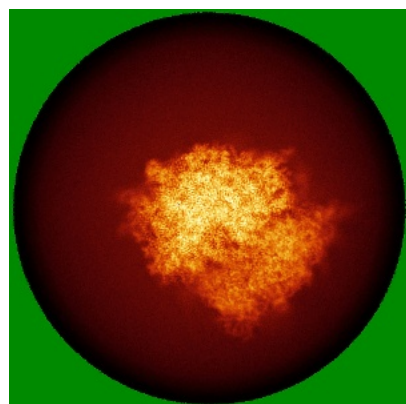


Z Index: 0

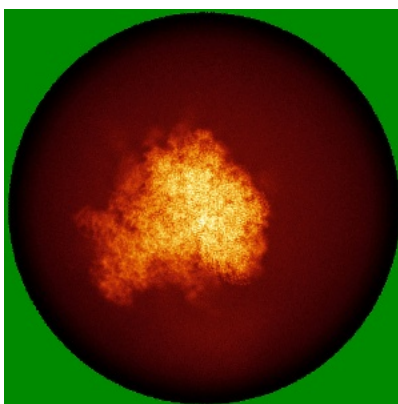
The images above show the largest variance slices of the map in three orthogonal directions.

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

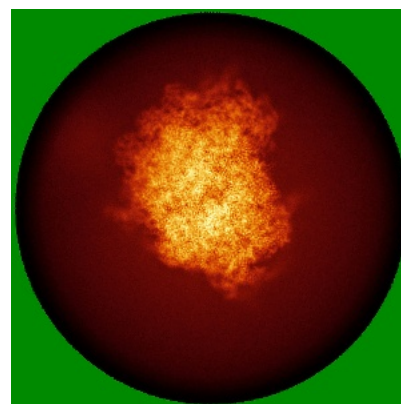
6.4.1 Primary map



X

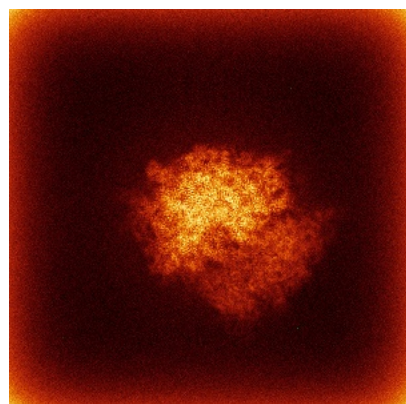


Y

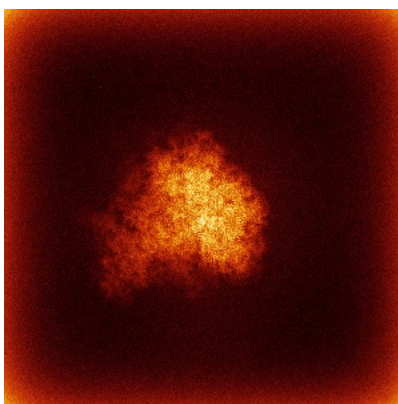


Z

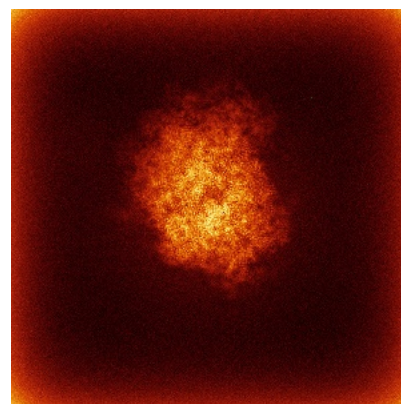
6.4.2 Raw map



X



Y

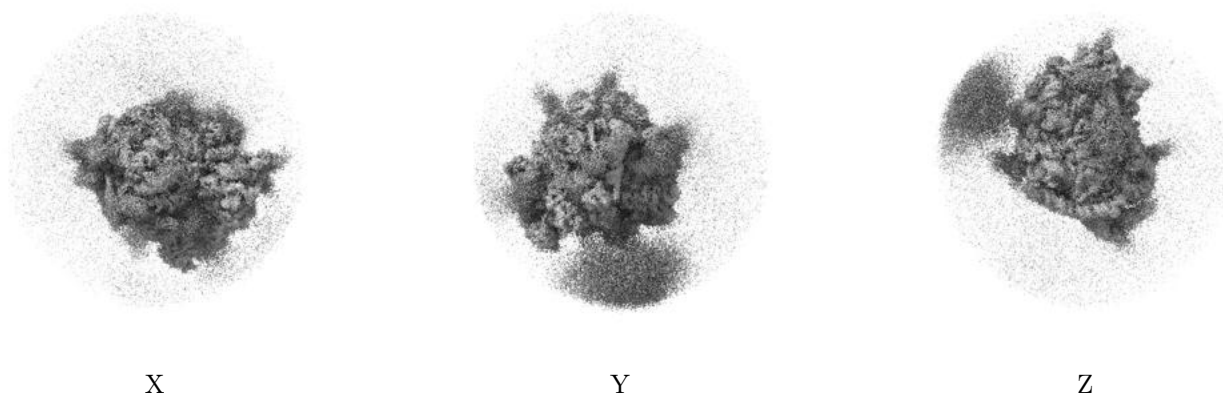


Z

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.

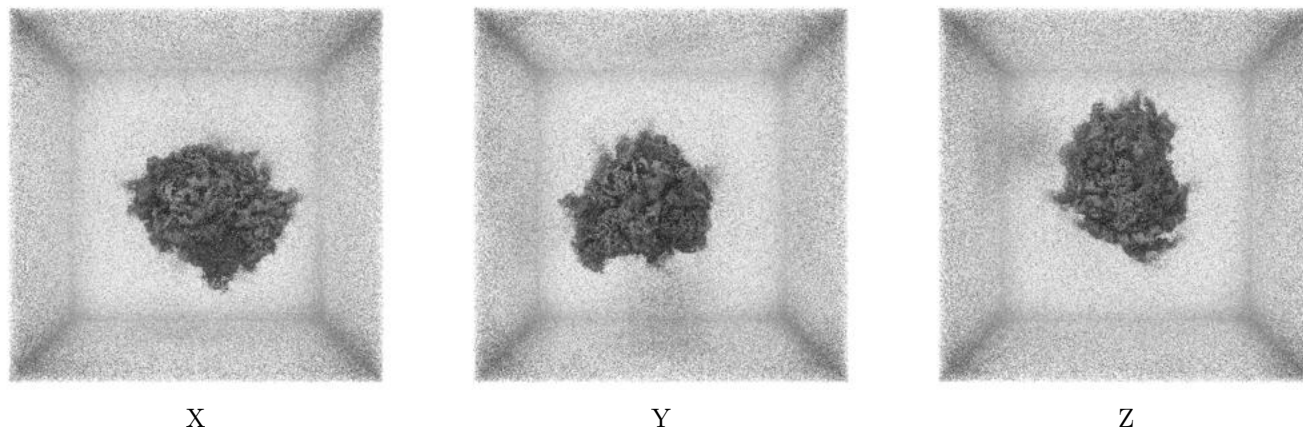
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. 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.

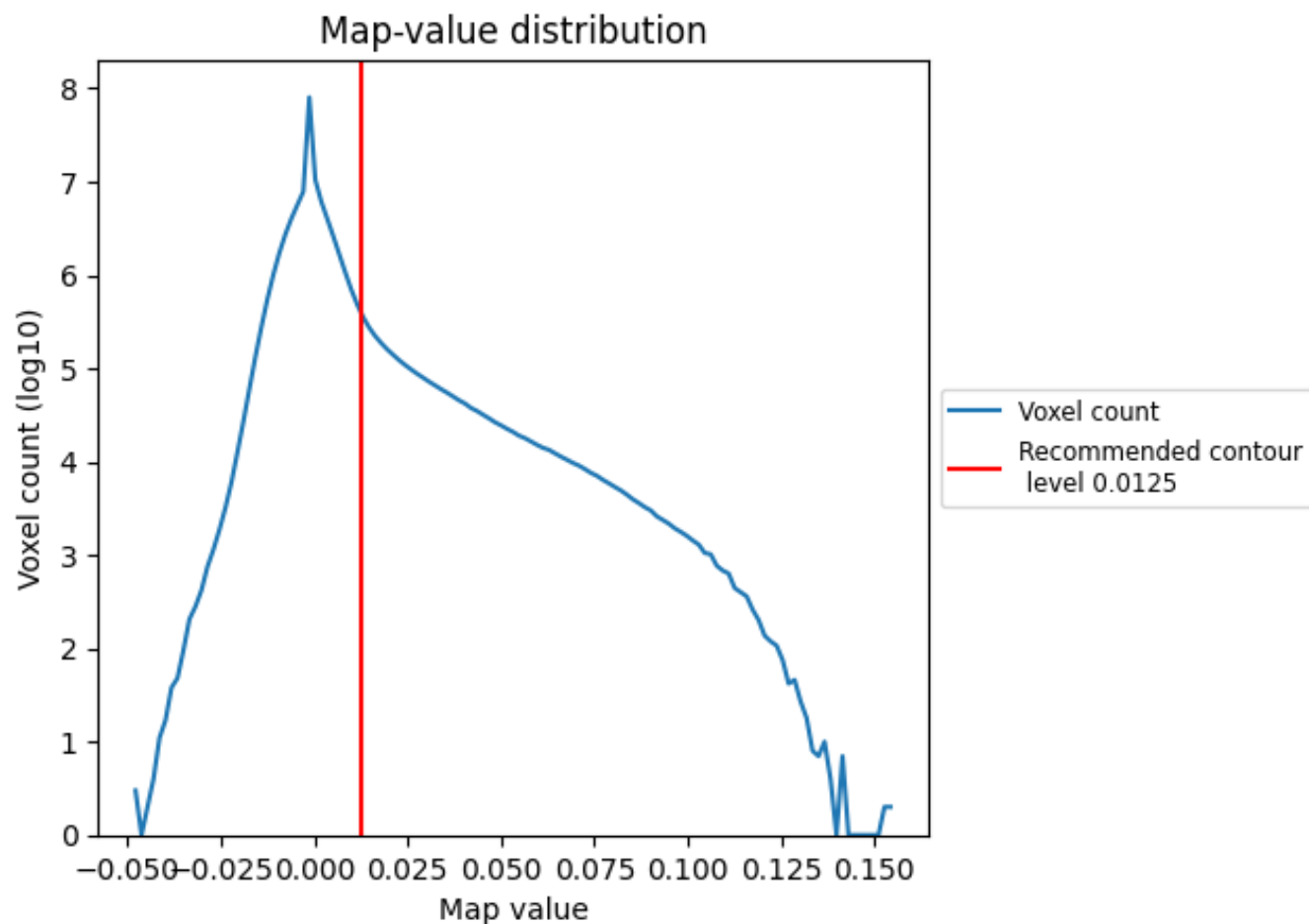
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

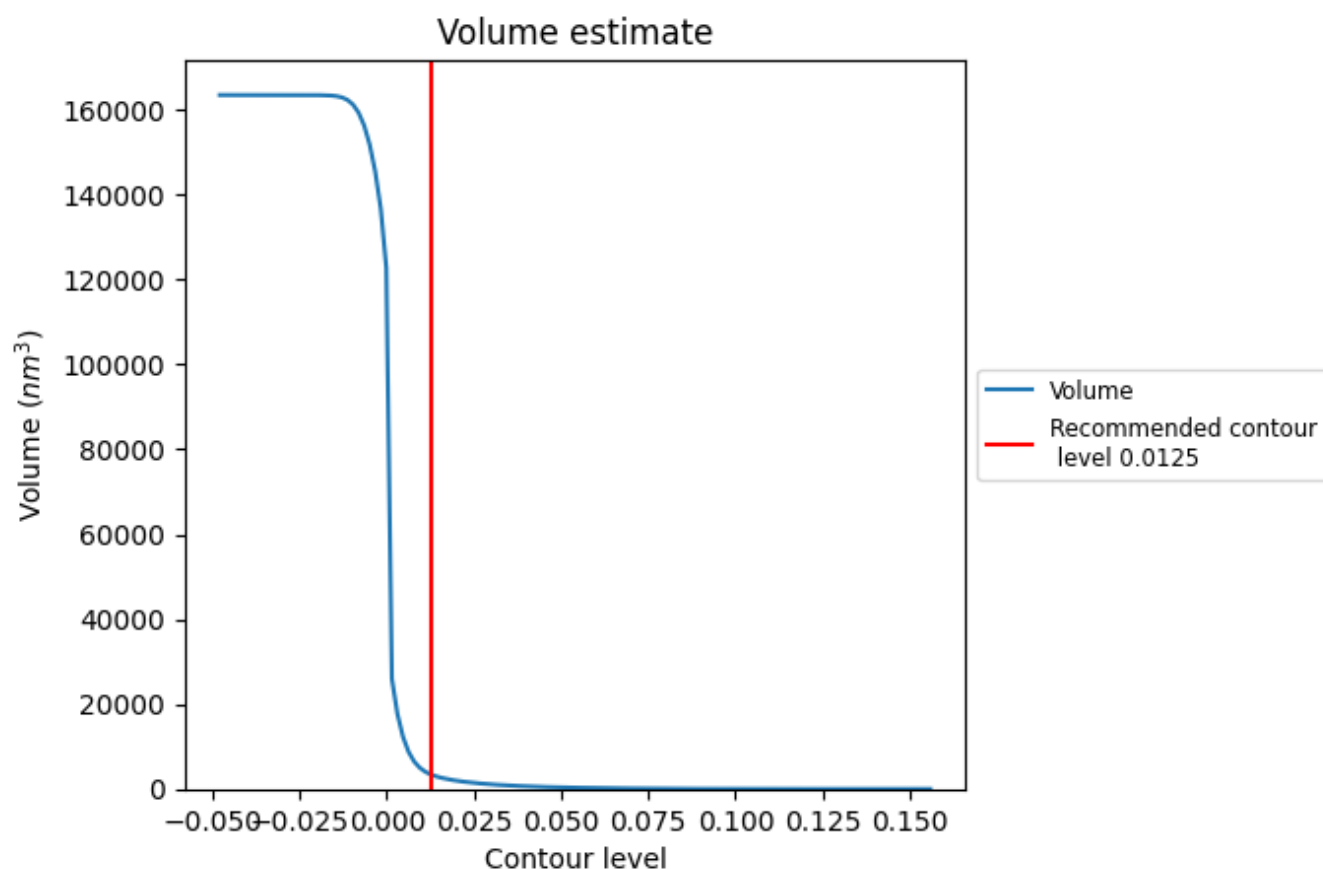
This section contains the results of statistical analysis of the map.

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.

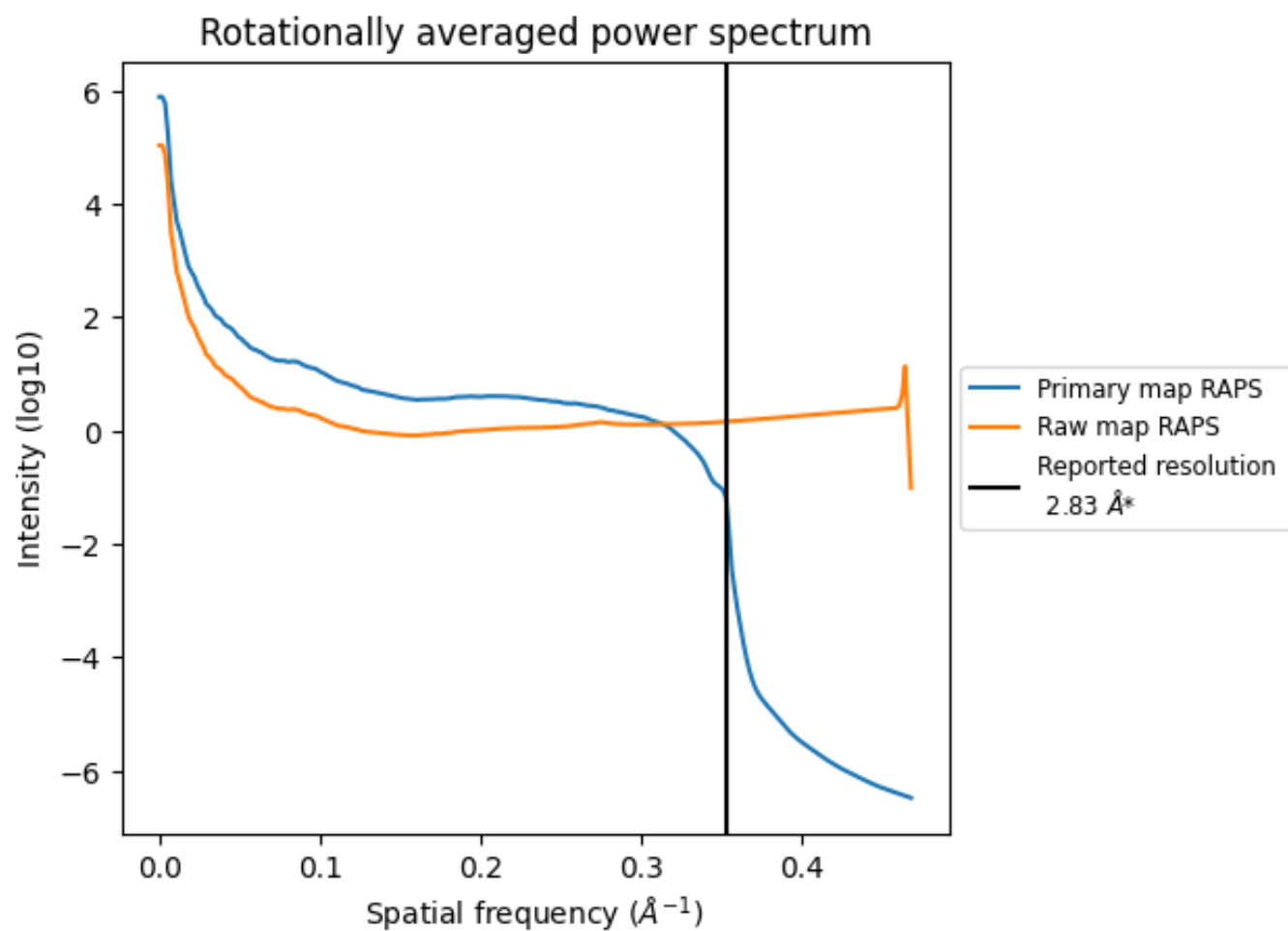
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3462 nm^3 ; this corresponds to an approximate mass of 3127 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 ⓘ

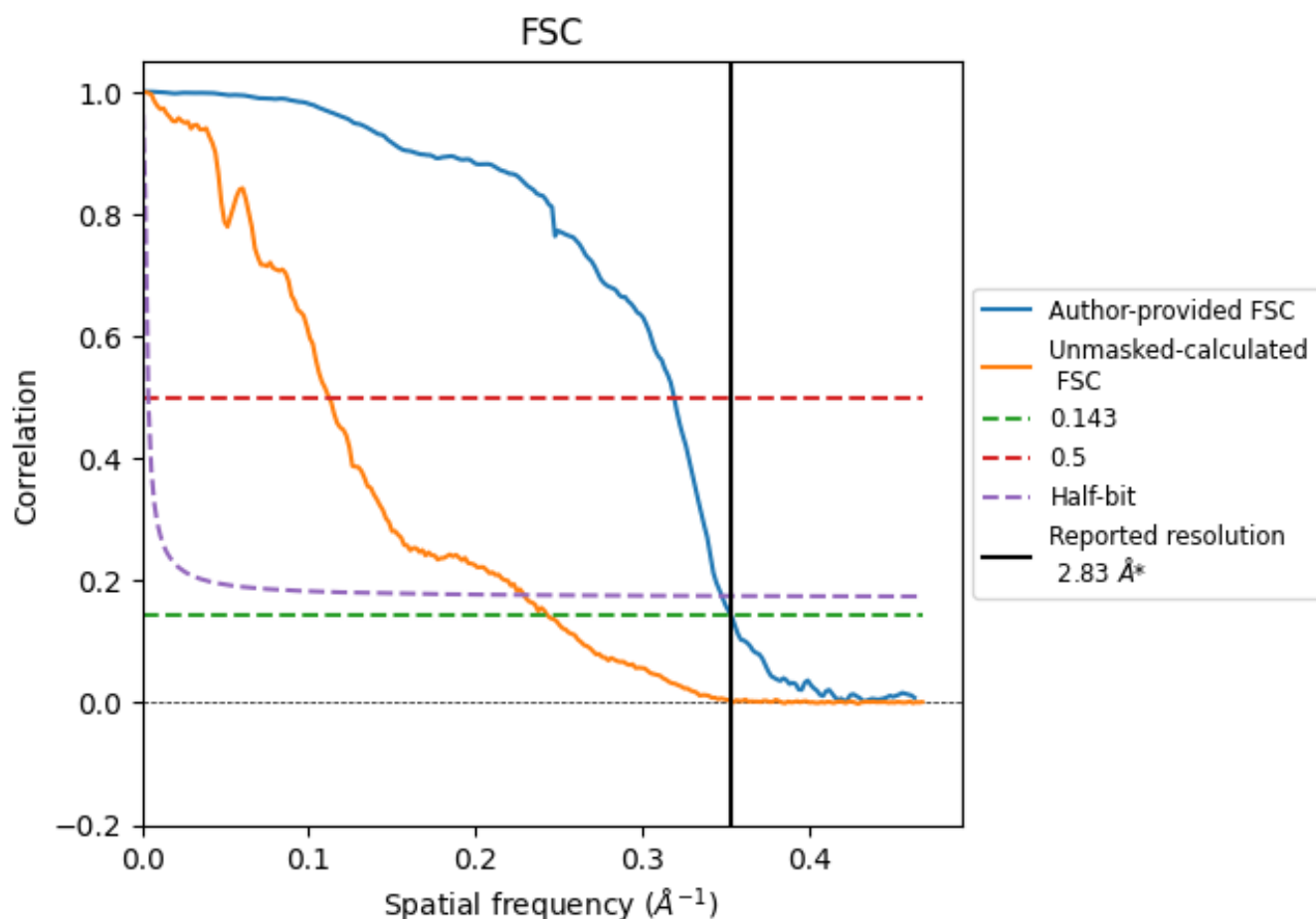


*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

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 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

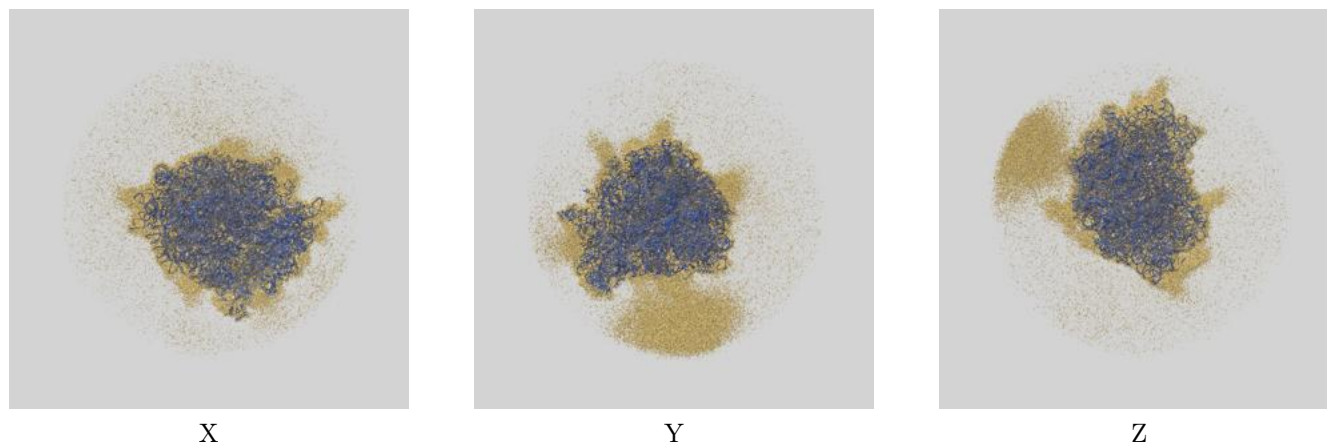
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.13	2.87
Unmasked-calculated*	4.11	8.93	4.36

*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 4.11 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

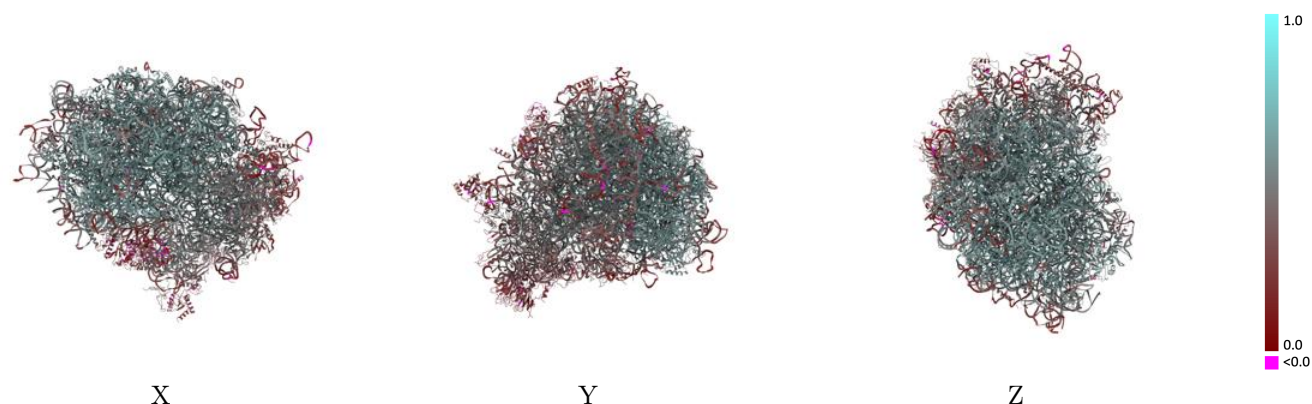
This section contains information regarding the fit between EMDB map EMD-71356 and PDB model 9P7X. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



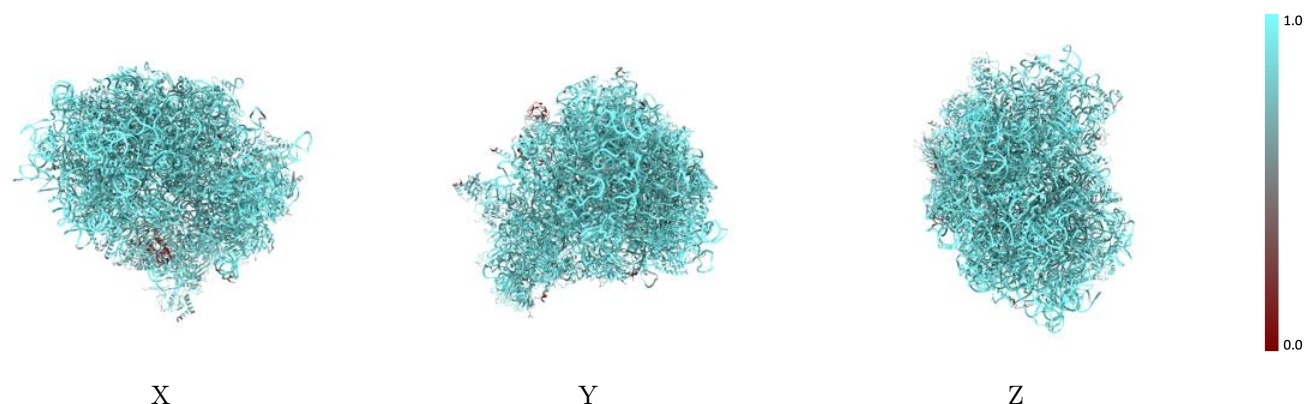
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



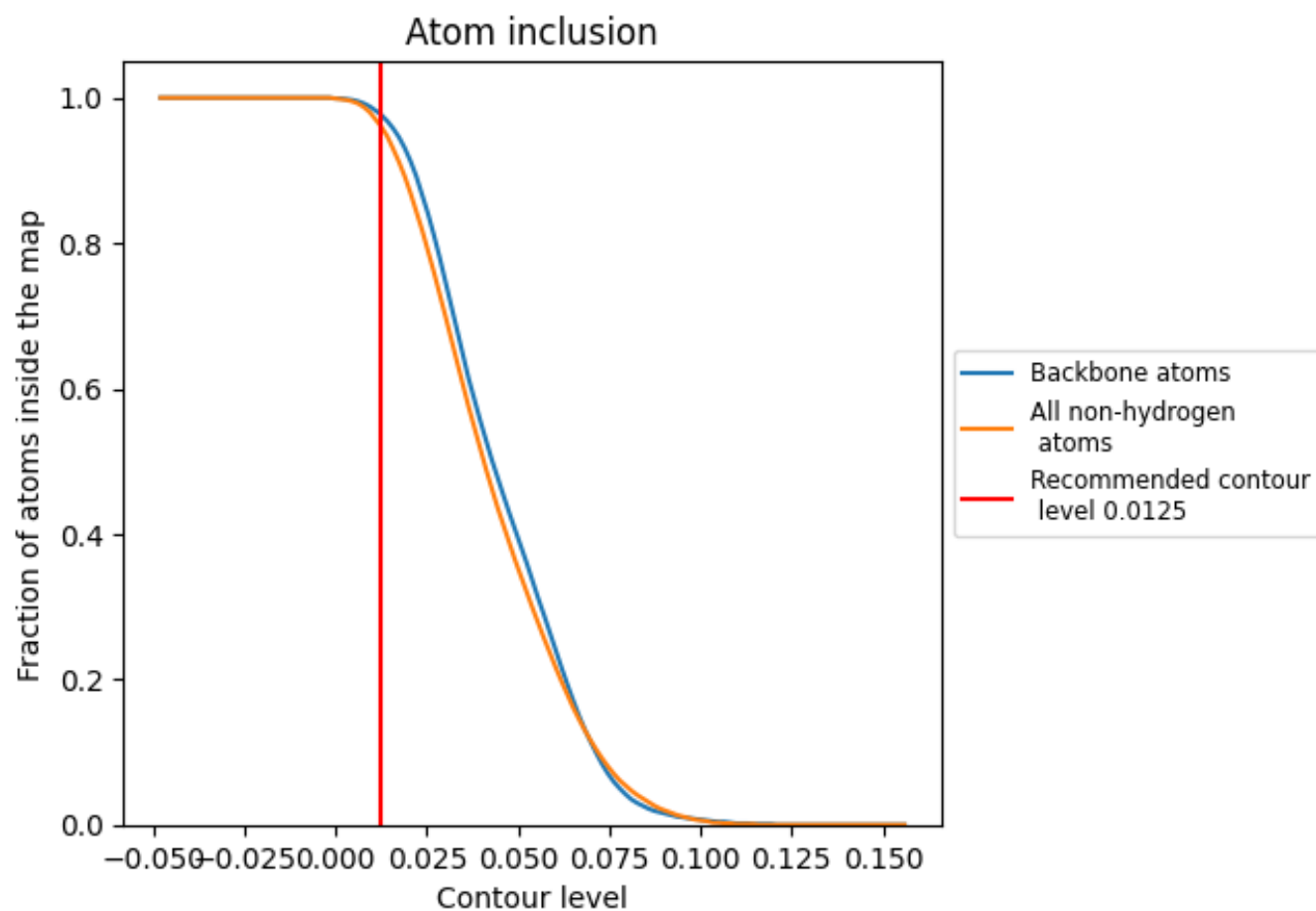
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9610	 0.4900
At	 0.9370	 0.3690
CI	 0.9000	 0.4630
L5	 0.9860	 0.5330
L7	 0.9990	 0.5740
L8	 0.9890	 0.5590
LA	 0.9880	 0.5950
LB	 0.9660	 0.5800
LC	 0.9670	 0.5780
LD	 0.9660	 0.5340
LE	 0.9540	 0.5270
LF	 0.9850	 0.5830
LG	 0.9250	 0.5230
LH	 0.9720	 0.5660
LI	 0.9600	 0.5690
LJ	 0.9370	 0.4870
LL	 0.9460	 0.5580
LM	 0.9740	 0.5620
LN	 0.9960	 0.6090
LO	 0.9790	 0.5860
LP	 0.9790	 0.5900
LQ	 0.9890	 0.6060
LR	 0.9350	 0.5210
LS	 0.9890	 0.5960
LT	 0.9730	 0.5630
LU	 0.9650	 0.5040
LV	 0.9820	 0.5860
LW	 0.8890	 0.4320
LX	 0.9590	 0.5680
LY	 0.9760	 0.5680
LZ	 0.9790	 0.5570
La	 0.9840	 0.6050
Lb	 0.9220	 0.5100
Lc	 0.9560	 0.5350
Ld	 0.9580	 0.5640



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Chain	Atom inclusion	Q-score
Le	 0.9870	 0.5950
Lf	 0.9880	 0.6030
Lg	 0.9770	 0.5720
Lh	 0.9700	 0.5620
Li	 0.9650	 0.5570
Lj	 0.9930	 0.5970
Lk	 0.9230	 0.4980
Ll	 0.9790	 0.5830
Lm	 0.9760	 0.5820
Ln	 0.9810	 0.5640
Lo	 0.9830	 0.5660
Lp	 0.9720	 0.5770
Lr	 0.9780	 0.5760
Ls	 0.5640	 0.1930
Lt	 0.5350	 0.1470
Pt	 0.9580	 0.4180
S2	 0.9890	 0.4410
SA	 0.8990	 0.3660
SB	 0.8920	 0.3760
SC	 0.9520	 0.4410
SD	 0.9190	 0.3820
SE	 0.9520	 0.4360
SF	 0.8840	 0.3380
SG	 0.9060	 0.3960
SH	 0.8980	 0.3470
SI	 0.9320	 0.4540
SJ	 0.9270	 0.4100
SK	 0.9180	 0.3550
SL	 0.9300	 0.4670
SM	 0.7660	 0.2290
SN	 0.9480	 0.4480
SO	 0.9140	 0.4190
SP	 0.8810	 0.3740
SQ	 0.9100	 0.3360
SR	 0.8840	 0.3360
SS	 0.8840	 0.3610
ST	 0.9230	 0.3270
SU	 0.9060	 0.3580
SV	 0.9410	 0.3950
SW	 0.9630	 0.4690
SX	 0.9480	 0.5080
SY	 0.8880	 0.3750

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Chain	Atom inclusion	Q-score
SZ	 0.8490	 0.3260
Sa	 0.9540	 0.4330
Sb	 0.9140	 0.3850
Sc	 0.8850	 0.3560
Sd	 0.9570	 0.4290
Se	 0.8490	 0.3910
Sf	 0.8440	 0.2590
Sg	 0.8750	 0.2400
Zt	 0.6530	 0.1560