



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 11:42 AM EDT

PDB ID : 9P7W / pdb_00009p7w
EMDB ID : EMD-71355
Title : In situ human A-P state 80S ribosome
Authors : Zheng, W.; Xiong, Y.
Deposited on : 2025-06-22
Resolution : 2.93 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.dev132
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) : 2.49

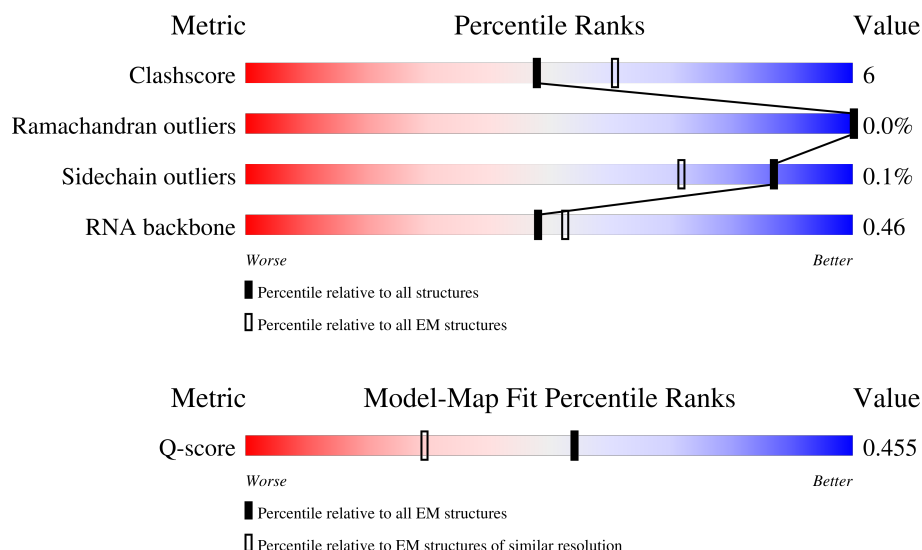
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 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.



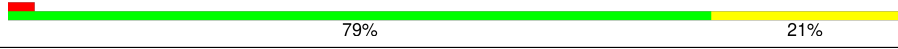
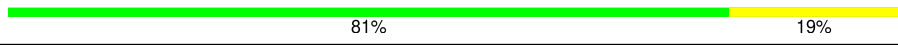
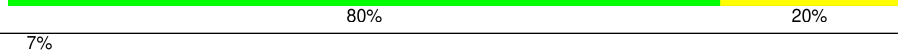
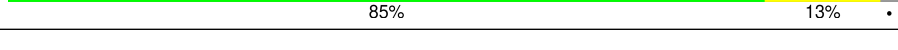
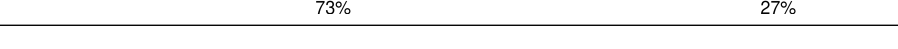
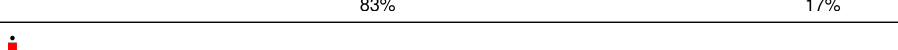
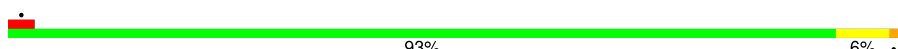
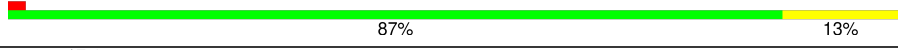
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13037 (2.43 - 3.43)

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	
2	SB	214	
3	SC	222	

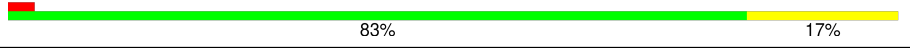
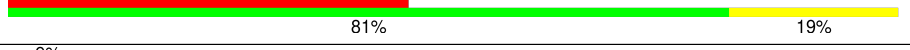
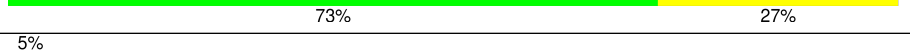
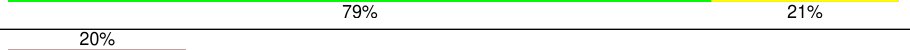
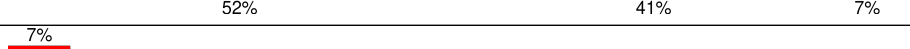
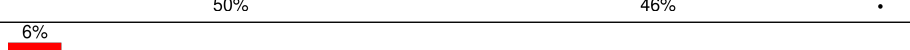
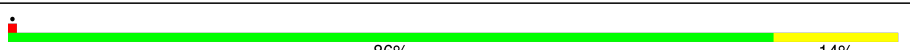
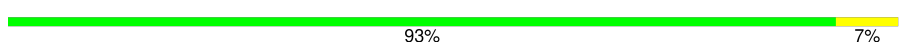
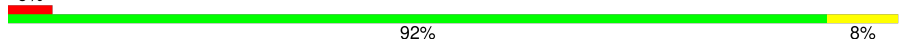
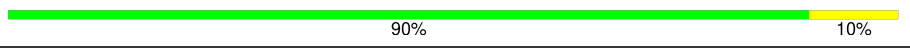
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Mol	Chain	Length	Quality of chain
4	SE	262	
5	SG	237	
6	SH	186	
7	SI	206	
8	SJ	185	
9	SL	153	
10	SN	150	
11	SO	140	
12	SV	83	
13	SW	129	
14	SX	141	
15	SY	131	
16	Sa	102	
17	Sb	83	
18	Se	58	
19	S2	1740	
20	LR	187	
21	LW	118	
22	SR	135	
23	SD	227	
24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

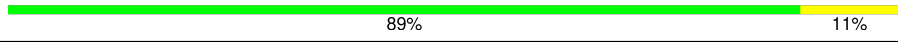
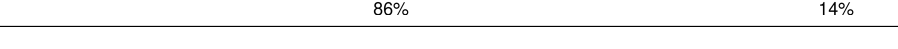
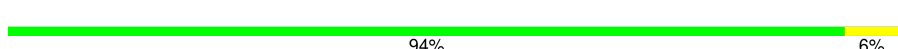
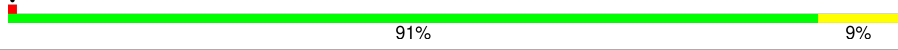
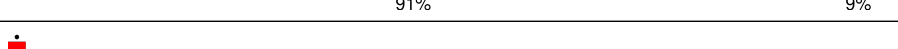
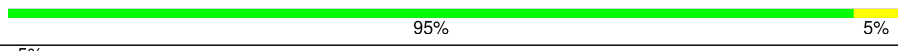
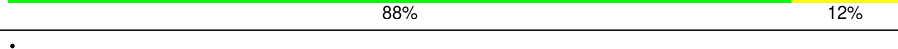
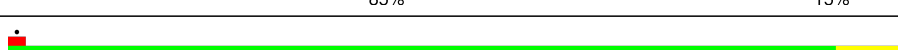
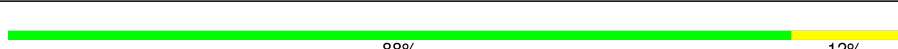
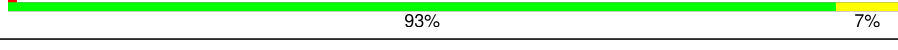
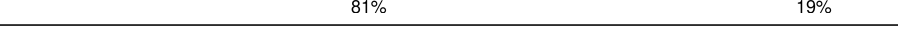
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Mol	Chain	Length	Quality of chain
29	SS	145	
30	ST	143	
31	SU	104	
32	SZ	75	
33	Sc	64	
34	Sd	55	
35	Sf	67	
36	Sg	313	
37	At	71	
38	Pt	74	
39	CI	31	
40	L5	3655	
41	L7	120	
42	L8	156	
43	LA	248	
44	LB	402	
45	LC	368	
46	LD	293	
47	LE	250	
48	LF	225	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

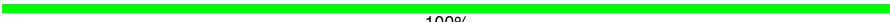
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Mol	Chain	Length	Quality of chain
54	LM	139	
55	LN	203	
56	LO	201	
57	LP	153	
58	LQ	187	
59	LS	175	
60	LT	159	
61	LU	101	
62	LV	131	
63	LX	120	
64	LY	134	
65	LZ	135	
66	La	147	
67	Lb	109	
68	Lc	98	
69	Ld	107	
70	Le	128	
71	Lf	109	
72	Lg	114	
73	Lh	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	 100%
80	Lo	105	 10% 90% 10%
81	Lp	91	 89% 11%
82	Lr	125	 90% 10%
83	Ls	196	 48% 86% 14%
84	Lt	141	 50% 80% 15% 5%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 219891 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 [Homo sapiens].

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		

- 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
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

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
85	SG	1	Total	Mg	0
			1	1	
85	S2	26	Total	Mg	0
			26	26	
85	SS	1	Total	Mg	0
			1	1	
85	L5	178	Total	Mg	0
			178	178	
85	L7	3	Total	Mg	0
			3	3	
85	L8	6	Total	Mg	0
			6	6	
85	LA	1	Total	Mg	0
			1	1	
85	LP	1	Total	Mg	0
			1	1	
85	LV	1	Total	Mg	0
			1	1	
85	Le	1	Total	Mg	0
			1	1	

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

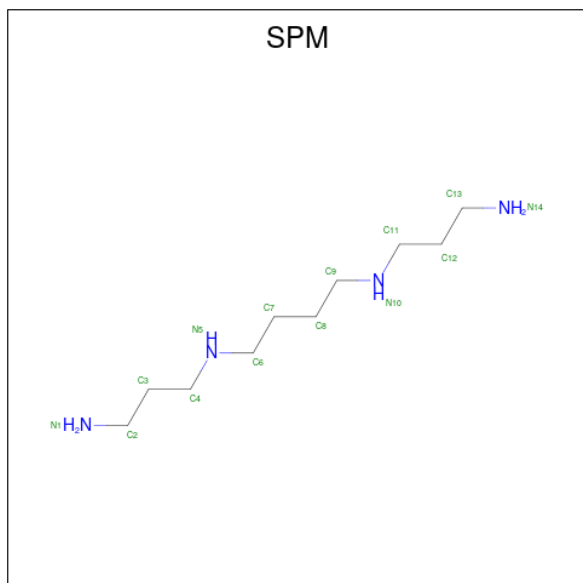
Mol	Chain	Residues	Atoms		AltConf
86	Sa	1	Total	Zn	0
			1	1	
86	Lg	1	Total	Zn	0
			1	1	
86	Lj	1	Total	Zn	0
			1	1	
86	Lm	1	Total	Zn	0
			1	1	

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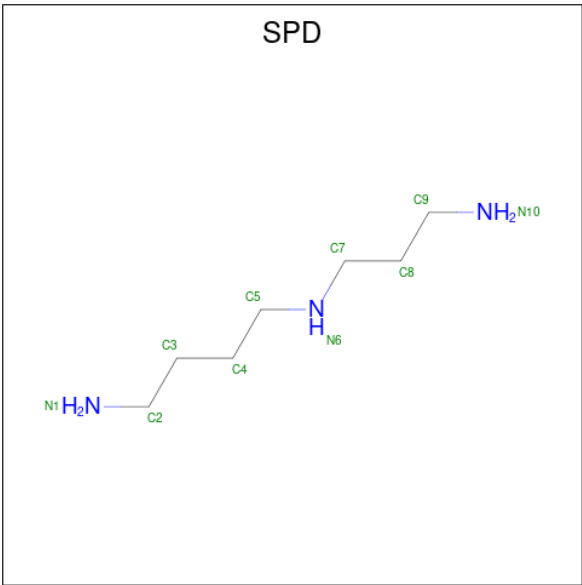
Mol	Chain	Residues	Atoms		AltConf
86	Lo	1	Total	Zn	0
			1	1	
86	Lp	1	Total	Zn	0
			1	1	

- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).

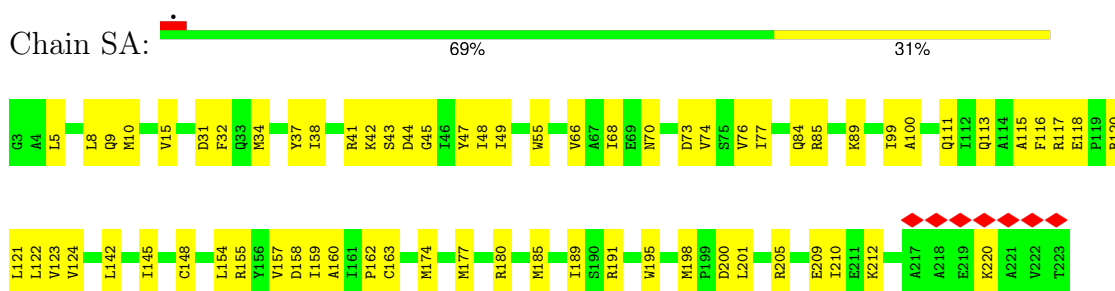


Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L8	1	Total	C	N	0
			10	7	3	
88	LN	1	Total	C	N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

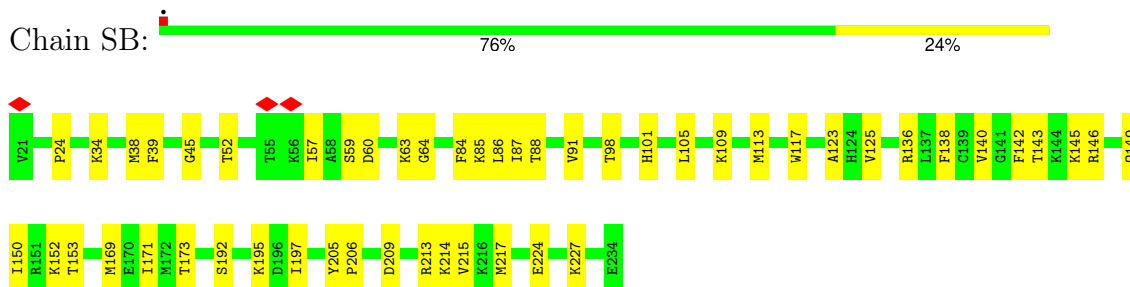
3 Residue-property plots

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.

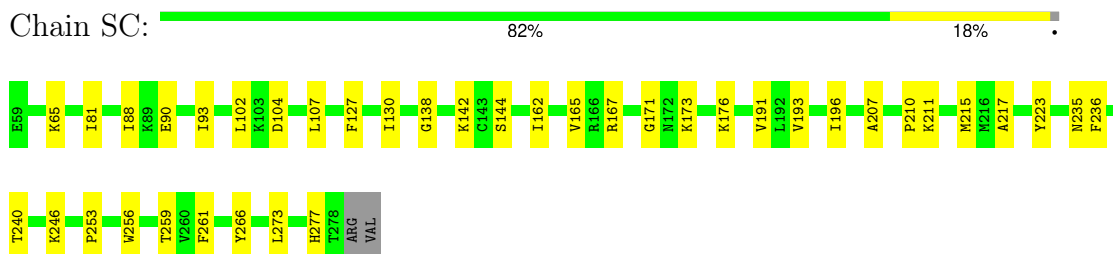
- Molecule 1: 40S ribosomal protein SA



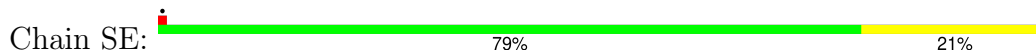
- Molecule 2: 40S ribosomal protein S3a

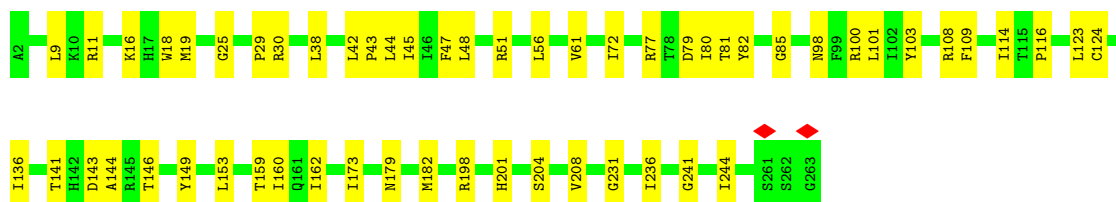


- Molecule 3: 40S ribosomal protein S2

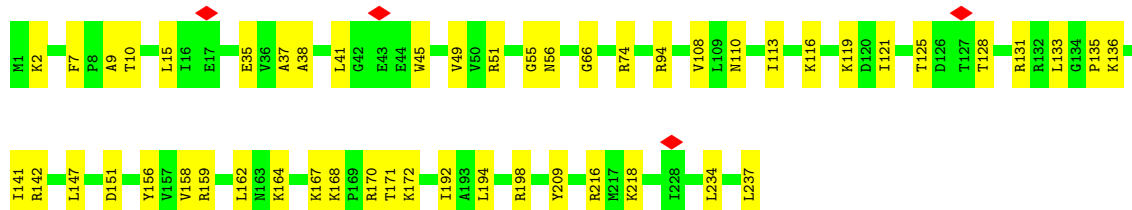
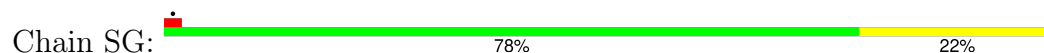


- Molecule 4: Small ribosomal subunit protein eS4, X isoform

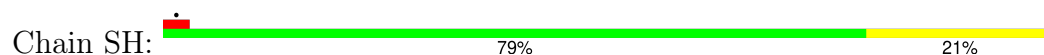




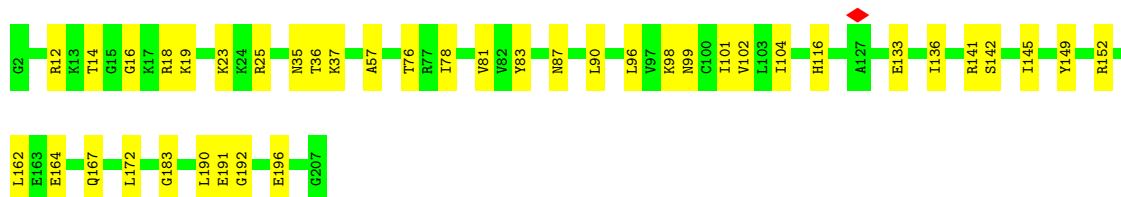
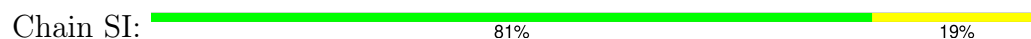
• Molecule 5: 40S ribosomal protein S6



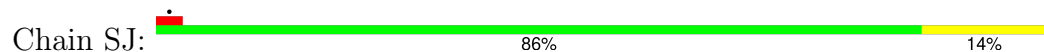
• Molecule 6: Small ribosomal subunit protein eS7



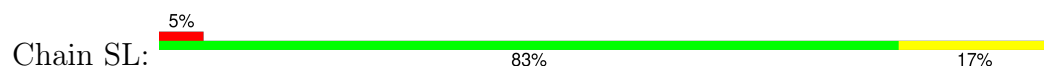
• Molecule 7: 40S ribosomal protein S8



• Molecule 8: 40S ribosomal protein S9

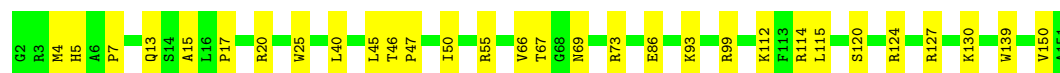
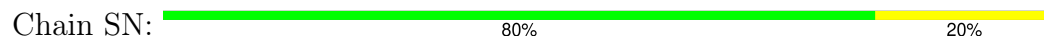


• Molecule 9: 40S ribosomal protein S11

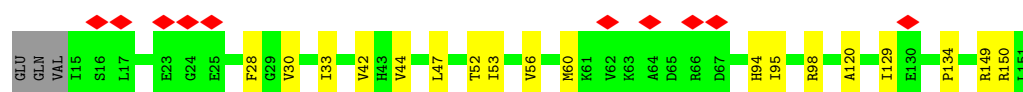
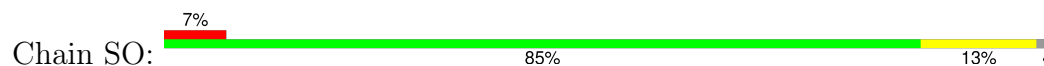




- Molecule 10: 40S ribosomal protein S13



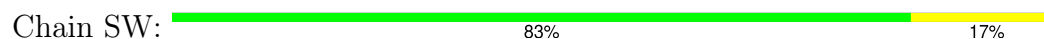
- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein eS21



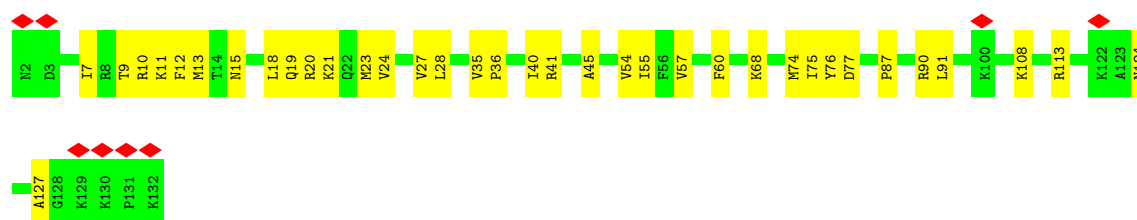
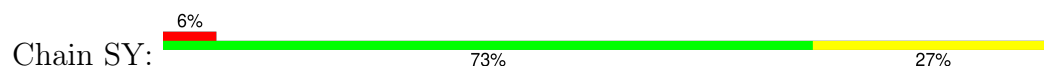
- Molecule 13: 40S ribosomal protein S15a



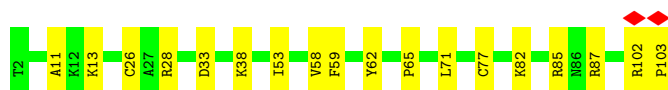
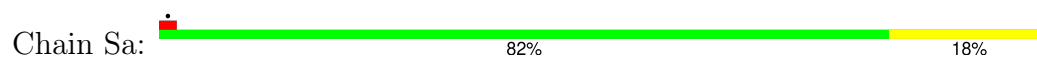
- Molecule 14: 40S ribosomal protein S23



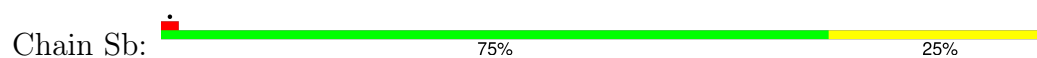
- Molecule 15: 40S ribosomal protein S24



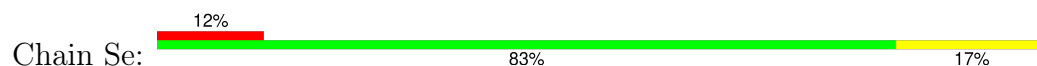
- Molecule 16: 40S ribosomal protein S26



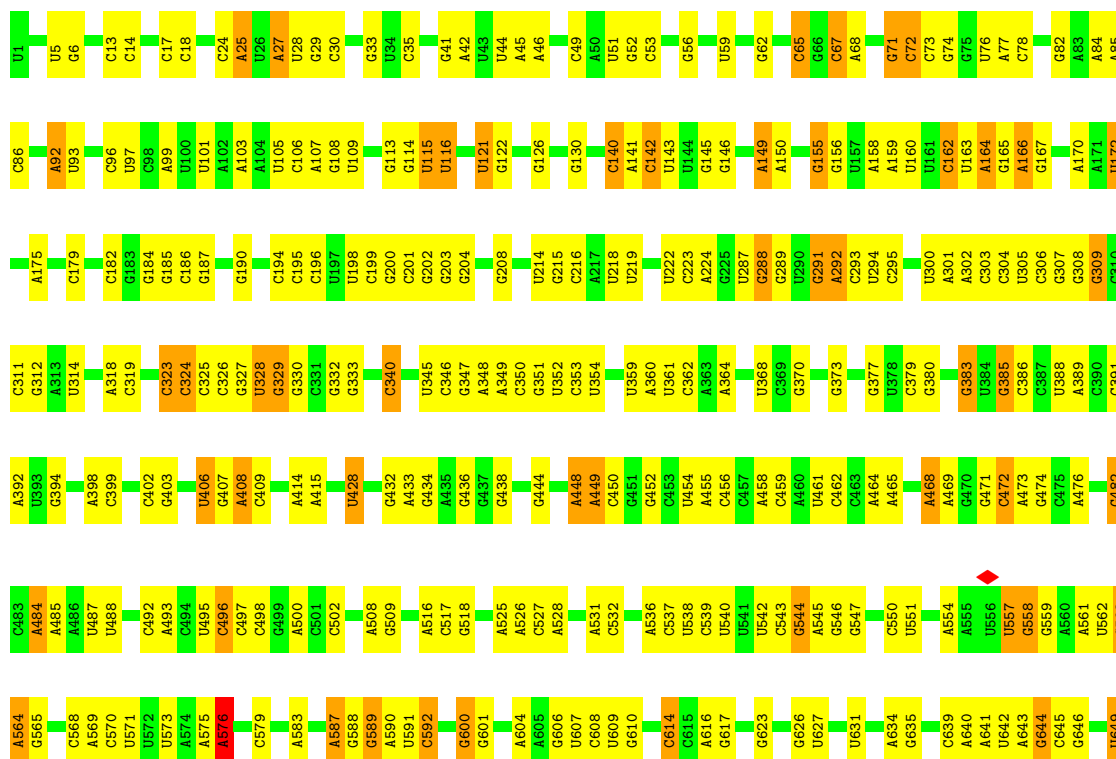
- Molecule 17: Small ribosomal subunit protein eS27



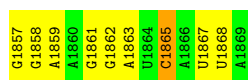
- Molecule 18: Small ribosomal subunit protein eS30



- Molecule 19: 18S rRNA [Homo sapiens]

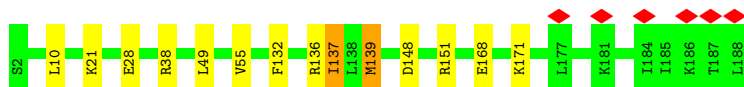


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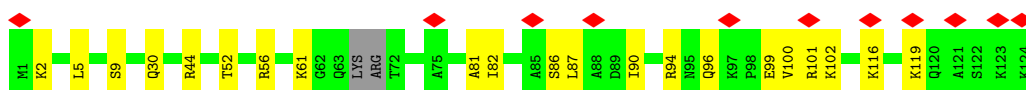
- Molecule 20: 60S ribosomal protein L19

Chain LR: 93% 6%



- Molecule 21: Ribosomal protein L24

Chain LW: 9% 81% 18%



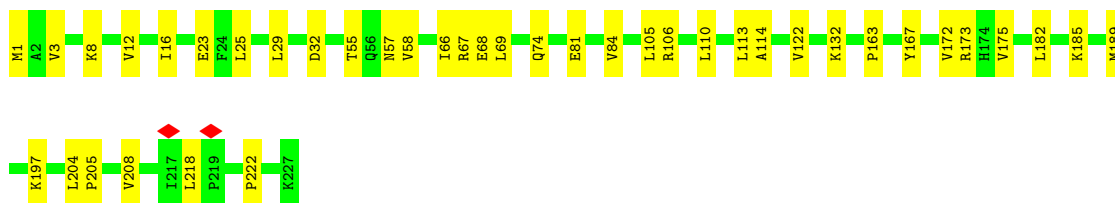
- Molecule 22: Small ribosomal subunit protein eS17

Chain SR: 76% 22%



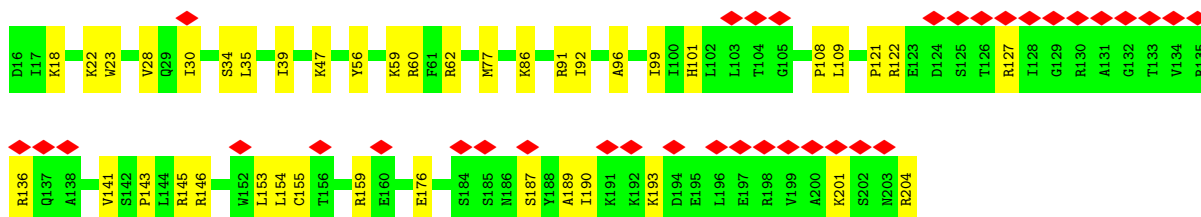
- Molecule 23: Small ribosomal subunit protein uS3

Chain SD: 82% 18%



- Molecule 24: 40S ribosomal protein S5

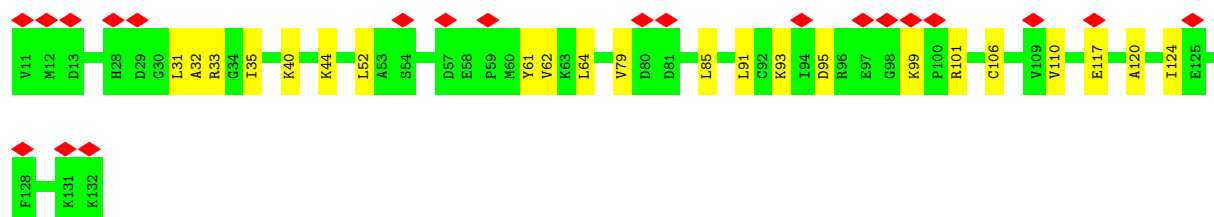
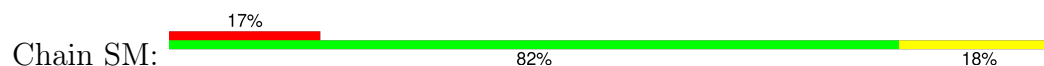
Chain SF: 19% 78% 22%



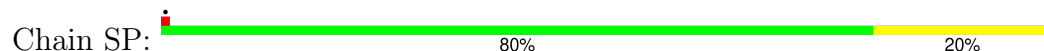
- Molecule 25: 40S ribosomal protein S10



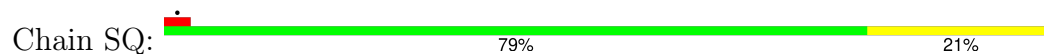
- Molecule 26: Small ribosomal subunit protein eS12



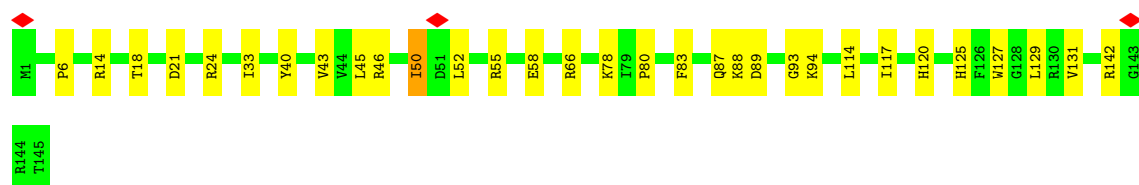
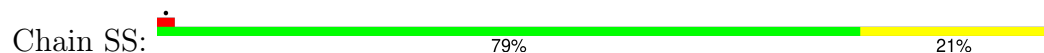
- Molecule 27: Small ribosomal subunit protein uS19



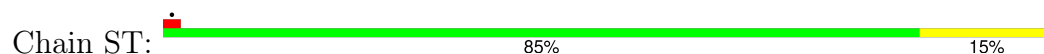
- Molecule 28: Small ribosomal subunit protein uS9



- Molecule 29: 40S ribosomal protein S18



- Molecule 30: 40S ribosomal protein S19



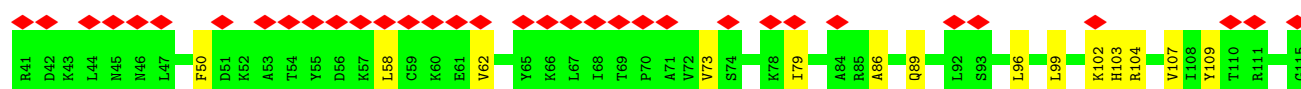
- Molecule 31: 40S ribosomal protein S20

Chain SU:  83% 17%



- Molecule 32: Small ribosomal subunit protein eS25

Chain SZ:  45% 81% 19%



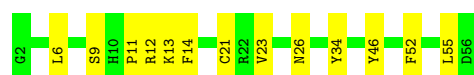
- Molecule 33: 40S ribosomal protein S28

Chain Sc:  9% 72% 28%



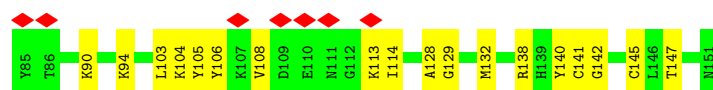
- Molecule 34: 40S ribosomal protein S29

Chain Sd:  76% 24%



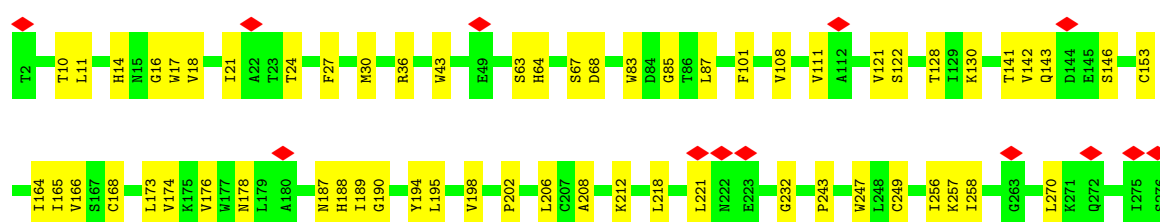
- Molecule 35: Ubiquitin-40S ribosomal protein S27a

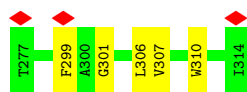
Chain Sf:  10% 73% 27%



- Molecule 36: Receptor of activated protein C kinase 1

Chain Sg:  5% 79% 21%

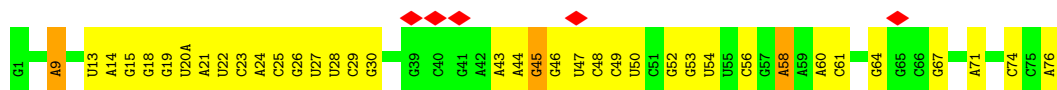




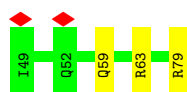
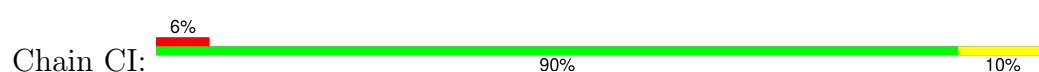
• Molecule 37: A site tRNA



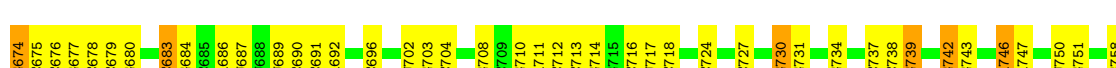
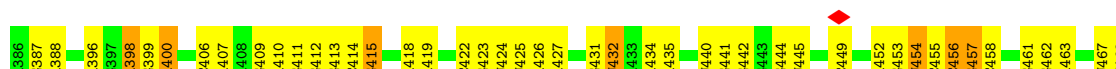
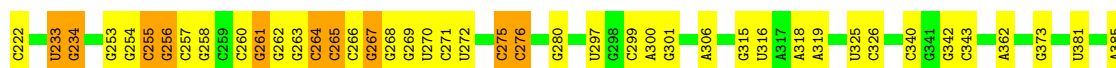
• Molecule 38: P site tRNA



• Molecule 39: Transcription factor BTF3



• Molecule 40: 28S rRNA



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A4708	A4709	G4595	U4512	G4401	A4279	G4184	G4089	U3915	U3838	U3729	A3635	G2855	U2730	U2632
C4402	C4403	A4513	A4510	C4402	A4280	G4185	G4090	G3916	G3839	A3732	G3636	G2861	C2731	U2633
U4404	U4405	C4511	C4511	U4404	A4281	A4186	A4091	A3917	G3840	A3733	U3637	C2861	C2634	U2635
U4406	U4407	C4512	C4512	U4406	A4282	U4187	G4092	G3918	G3841	A3734	G3638	A2864	G2742	U2636
A4415	A4416	C4513	C4513	U4407	A4283	U4188	G4093	G3919	G3842	A3735	U3639	U2865	A2743	A2641
A4417	A4418	C4514	C4514	U4408	A4284	U4189	G4094	G3920	G3843	A3736	U3640	U2866	A2744	G2640
A4419	A4420	C4515	C4515	U4409	A4285	U4190	G4095	G3921	G3844	A3737	U3641	C2867	A2745	A2642
A4421	A4422	C4516	C4516	U4410	A4286	U4191	G4096	U3922	U3845	A3746	U3642	A2870	G2648	G2648
A4423	A4424	C4517	C4517	U4411	A4287	U4192	G4097	U3923	U3846	A3747	U3643	A2871	A2746	G2649
A4425	A4426	C4518	C4518	U4412	A4288	U4193	G4098	U3924	U3847	A3748	U3644	G2872	C2653	C2654
A4427	A4428	C4519	C4519	U4413	A4289	U4194	G4099	U3925	U3848	A3749	U3645	A2873	C2655	U2656
A4429	A4430	C4520	C4520	U4414	A4290	U4195	G4100	U3926	U3849	A3750	U3646	A2874	G2657	G2658
A4431	A4432	C4521	C4521	U4415	A4291	U4196	G4101	U3927	U3850	A3751	U3647	A2875	G2659	G2660
A4433	A4434	C4522	C4522	U4416	A4292	U4197	G4102	U3928	U3851	A3752	U3648	A2876	C2661	C2662
A4435	A4436	C4523	C4523	U4417	A4293	U4198	G4103	U3929	U3852	A3753	U3649	G2877	C2663	C2664
A4437	A4438	C4524	C4524	U4418	A4294	U4199	G4104	U3930	U3853	A3754	U3650	G2878	C2665	U2666
A4439	A4440	C4525	C4525	U4419	A4295	U4200	G4105	U3931	U3854	A3755	U3651	A2879	G2667	G2668
A4441	A4442	C4526	C4526	U4420	A4296	U4201	G4106	U3932	U3855	A3756	U3652	G2880	C2669	C2670
A4443	A4444	C4527	C4527	U4421	A4297	U4202	G4107	U3933	U3856	A3757	U3653	A2881	C2671	C2672
A4445	A4446	C4528	C4528	U4422	A4298	U4203	G4108	U3934	U3857	A3758	U3654	A2882	C2673	C2674
A4447	A4448	C4529	C4529	U4423	A4299	U4204	G4109	U3935	U3858	A3759	U3655	A2883	C2675	C2676
A4449	A4450	C4530	C4530	U4424	A4300	U4205	G4110	U3936	U3859	A3760	U3656	A2884	C2677	C2678
A4451	A4452	C4531	C4531	U4425	A4301	U4206	G4111	U3937	U3860	A3761	U3657	A2885	C2679	C2680
A4453	A4454	C4532	C4532	U4426	A4302	U4207	G4112	U3938	U3861	A3762	U3658	A2886	C2681	C2682
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A4457	A4458	C4534	C4534	U4428	A4304	U4209	G4114	U3940	U3863	A3764	U3660	A2888	C2685	C2686
A4459	A4460	C4535	C4535	U4429	A4305	U4210	G4115	U3941	U3864	A3765	U3661	A2889	C2687	C2688
A4461	A4462	C4536	C4536	U4430	A4306	U4211	G4116	U3942	U3865	A3766	U3662	A2890	C2689	C2690
A4463	A4464	C4537	C4537	U4431	A4307	U4212	G4117	U3943	U3866	A3767	U3663	A2891	C2691	C2692
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A4469	A4470	C4540	C4540	U4434	A4310	U4215	G4120	U3946	U3869	A3770	U3666	A2894	C2697	C2698
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A4473	A4474	C4542	C4542	U4436	A4312	U4217	G4122	U3948	U3871	A3772	U3668	A2896	C2701	C2702
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A4535	A4536	C4573	C4573	U4467	A4343	U4248	G4153	U3979	U3902	A3803	U3699	A2927	C2763	C2764
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A4551	A4552	C4581	C4581	U4475	A4351	U4256	G4161	U3987	U3910	A3811	U3707	A2935	C2779	C2780
A4553	A4554	C4582	C4582	U4476	A4352	U4257	G4162	U3988	U3911	A3812	U3708	A2936	C2781	C2782
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A4559	A4560	C4585	C4585	U4479	A4355	U4260	G4165	U3991	U3914	A3815	U3711	A2939	C2787	C2788
A4561	A4562	C4586	C4586	U4480	A4356	U4261	G4166	U3992	U3915	A3816	U3712	A2940	C2789	C2790
A4563	A4564	C4587	C4587	U4481	A4357	U4262	G4167	U3993	U3916	A3817	U3713	A2941	C2791	C2792
A4565	A4566	C4588	C4588	U4482	A4358	U4263	G4168	U3994	U3917	A3818	U3714	A2942	C2793	C2794
A4567	A4568	C4589	C4589	U4483	A4359	U4264	G4169	U3995	U3918	A3819	U3715	A2943	C2795	C2796
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A4573	A4574	C4592	C4592	U4486	A4362	U4267	G4172	U3998	U3921	A3822	U3718	A2946	C2801	C2802
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A4577														



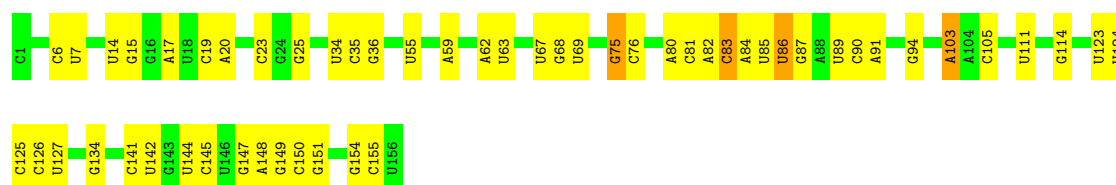
• Molecule 41: 5S rRNA

Chain L7: 76% 22%



• Molecule 42: 5.8S rRNA

Chain L8: 65% 32%



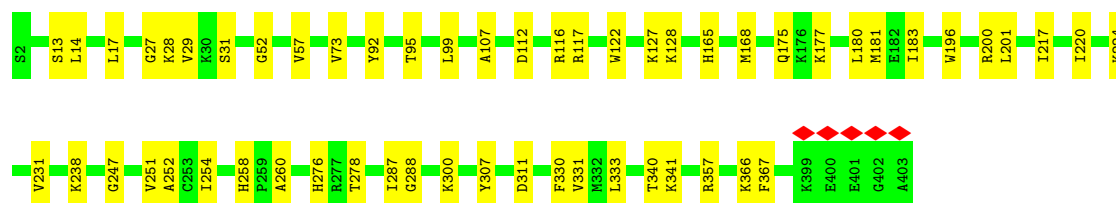
• Molecule 43: 60S ribosomal protein L8

Chain LA: 82% 18%



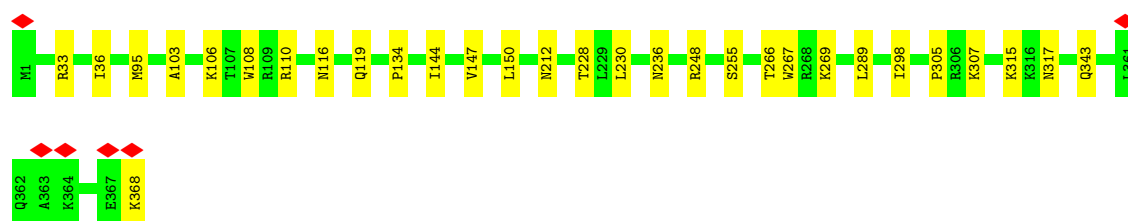
• Molecule 44: Large ribosomal subunit protein uL3

Chain LB: 86% 14%



• Molecule 45: 60S ribosomal protein L4

Chain LC:  92% 8%



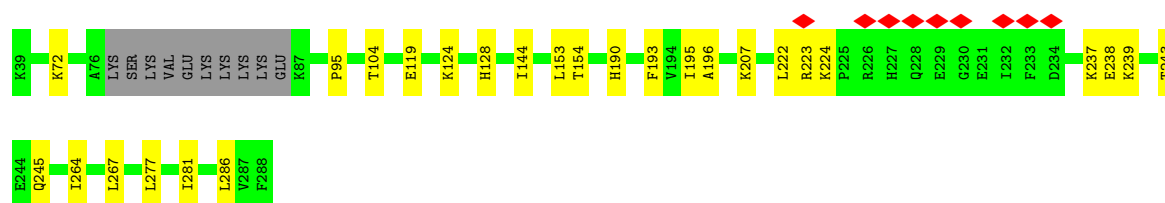
- Molecule 46: Large ribosomal subunit protein uL18

Chain LD:  91% 9%



- Molecule 47: Large ribosomal subunit protein eL6

Chain LE:  85% 11% .

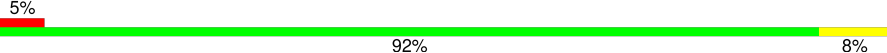


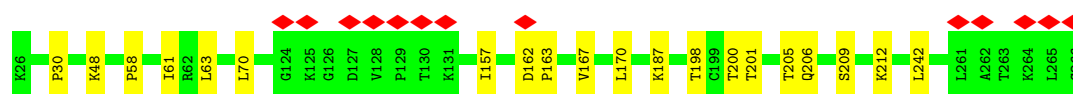
- Molecule 48: 60S ribosomal protein L7

Chain LF:  93% 7%



- Molecule 49: 60S ribosomal protein L7a

Chain LG:  5% 92% 8%



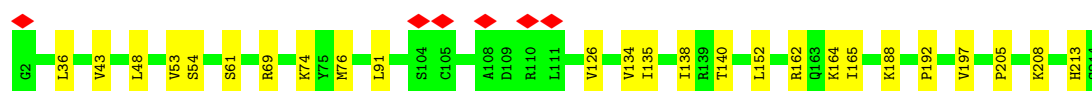
- Molecule 50: 60S ribosomal protein L9

Chain LH:  90% 10%



- Molecule 51: Ribosomal protein uL16-like

Chain LI:  88% 12%



- Molecule 52: 60S ribosomal protein L11

Chain LJ:  89% 7% ..



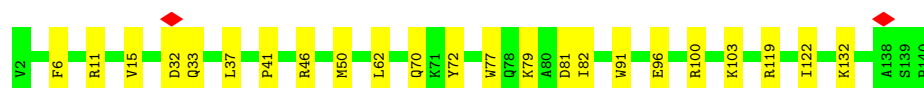
- Molecule 53: Large ribosomal subunit protein eL13

Chain LL:  89% 11%



- Molecule 54: 60S ribosomal protein L14

Chain LM:  83% 17%



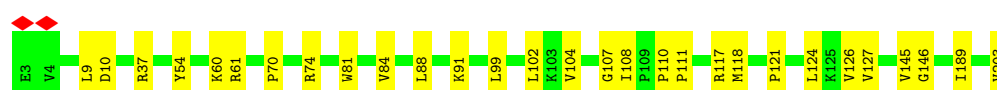
- Molecule 55: 60S ribosomal protein L15

Chain LN:  89% 11%



- Molecule 56: 60S ribosomal protein L13a

Chain LO:  86% 14%



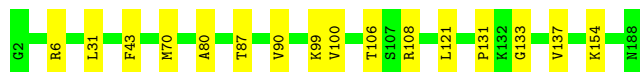
- Molecule 57: 60S ribosomal protein L17

Chain LP:  84% 16%



- Molecule 58: 60S ribosomal protein L18

Chain LQ:  91% 9%



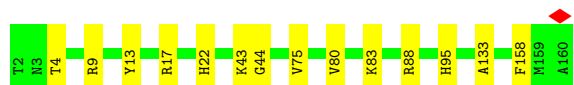
- Molecule 59: 60S ribosomal protein L18a

Chain LS:  94% 6%



- Molecule 60: 60S ribosomal protein L21

Chain LT:  91% 9%



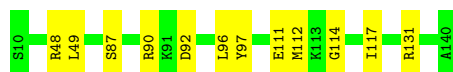
- Molecule 61: Heparin-binding protein HBp15

Chain LU:  77% 23%



- Molecule 62: 60S ribosomal protein L23

Chain LV:  91% 9%



- Molecule 63: 60S ribosomal protein L23a

Chain LX:  91% 9%



- Molecule 64: 60S ribosomal protein L26

Chain LY:  90% 10%

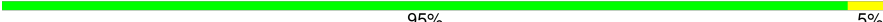


- Molecule 65: 60S ribosomal protein L27

Chain LZ:  91% 9%



- Molecule 66: 60S ribosomal protein L27a

Chain La:  95% 5%



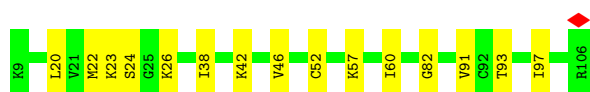
- Molecule 67: Large ribosomal subunit protein eL29

Chain Lb:  5% 88% 12%



- Molecule 68: 60S ribosomal protein L30

Chain Lc:  85% 15%



- Molecule 69: 60S ribosomal protein L31

Chain Ld:  93% 7%



- Molecule 70: 60S ribosomal protein L32

Chain Le:  88% 12%



- Molecule 71: 60S ribosomal protein L35a

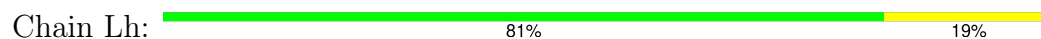
Chain Lf:  90% 10%



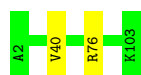
- Molecule 72: 60S ribosomal protein L34



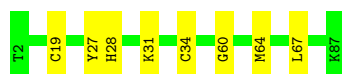
- Molecule 73: 60S ribosomal protein L35



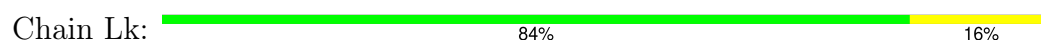
- Molecule 74: 60S ribosomal protein L36



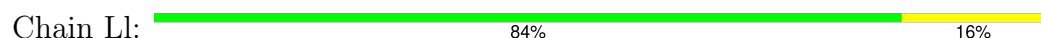
- Molecule 75: 60S ribosomal protein L37



- Molecule 76: 60S ribosomal protein L38



- Molecule 77: 60S ribosomal protein L39



- Molecule 78: Large ribosomal subunit protein eL40



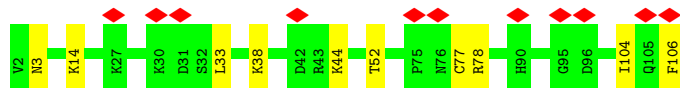
- Molecule 79: 60S ribosomal protein L41

Chain Ln:  100%

There are no outlier residues recorded for this chain.

- Molecule 80: 60S ribosomal protein L36a

Chain Lo:  10% 90% 10%



- Molecule 81: 60S ribosomal protein L37a

Chain Lp:  89% 11%



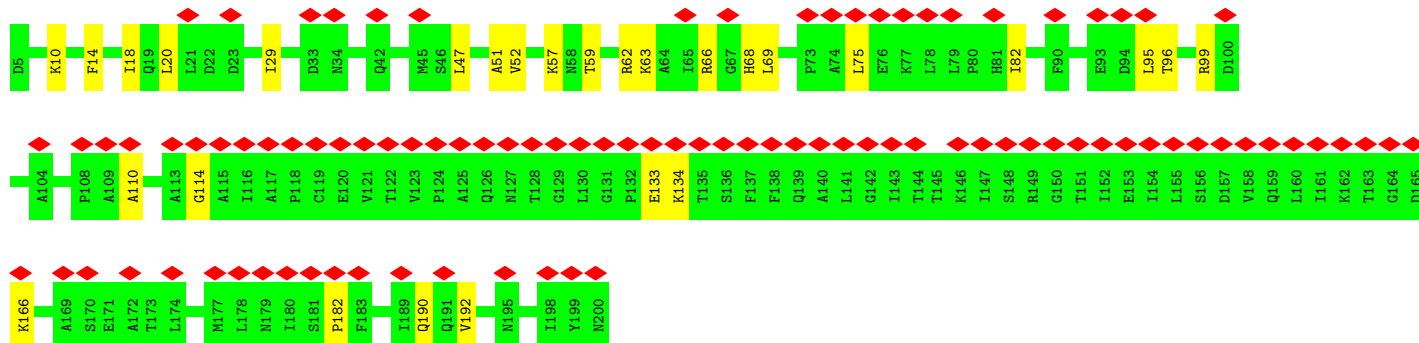
- Molecule 82: 60S ribosomal protein L28

Chain Lr:  90% 10%



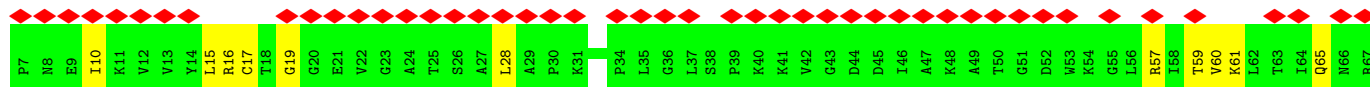
- Molecule 83: 60S acidic ribosomal protein P0

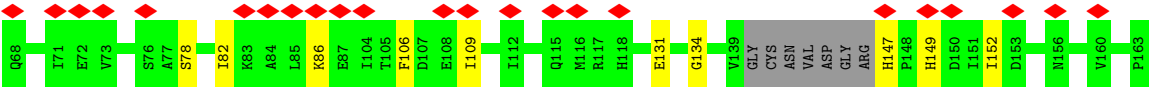
Chain Ls:  48% 86% 14%



- Molecule 84: Large ribosomal subunit protein uL11

Chain Lt:  50% 80% 15% 5%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66380	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	0.121	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0119	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: 1MA, UY1, ZN, UR3, 6MZ, 5MC, OMG, 4AC, G7M, B8N, MA6, OMU, SPM, SPD, MG, PSU, OMC, A2M

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	0.20	0/1778	0.38	0/2416
2	SB	0.16	0/1765	0.32	0/2362
3	SC	0.17	0/1744	0.34	0/2357
4	SE	0.16	0/2118	0.34	0/2849
5	SG	0.15	0/1946	0.33	0/2590
6	SH	0.15	0/1519	0.37	0/2033
7	SI	0.17	0/1715	0.35	0/2287
8	SJ	0.15	0/1550	0.32	0/2069
9	SL	0.18	0/1268	0.31	0/1696
10	SN	0.16	0/1232	0.29	0/1656
11	SO	0.16	0/1037	0.35	0/1391
12	SV	0.15	0/643	0.34	0/860
13	SW	0.17	0/1051	0.32	0/1406
14	SX	0.19	0/1116	0.35	0/1490
15	SY	0.16	0/1083	0.36	0/1438
16	Sa	0.17	0/836	0.34	0/1121
17	Sb	0.15	0/665	0.35	0/891
18	Se	0.14	0/465	0.35	0/612
19	S2	0.22	0/39756	0.31	0/61939
20	LR	0.30	0/1582	0.42	0/2091
21	LW	0.23	0/959	0.34	0/1270
22	SR	0.25	0/1105	0.47	0/1484
23	SD	0.15	0/1793	0.30	0/2414
24	SF	0.14	0/1516	0.32	0/2037
25	SK	0.13	0/851	0.32	0/1147
26	SM	0.14	0/950	0.34	0/1275
27	SP	0.15	0/1003	0.32	0/1342
28	SQ	0.16	0/1160	0.38	0/1553
29	SS	0.18	0/1216	0.40	1/1628 (0.1%)
30	ST	0.14	0/1131	0.32	0/1515
31	SU	0.16	0/831	0.30	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SZ	0.16	0/604	0.42	0/810
33	Sc	0.15	0/508	0.33	0/680
34	Sd	0.19	0/470	0.32	0/623
35	Sf	0.16	0/560	0.51	0/745
36	Sg	0.15	0/2493	0.34	0/3394
37	At	0.14	0/1692	0.25	0/2634
38	Pt	0.15	0/1761	0.28	0/2741
39	CI	0.16	0/247	0.30	0/323
40	L5	0.32	0/85098	0.33	0/132762
41	L7	0.30	0/2861	0.28	0/4459
42	L8	0.32	0/3631	0.31	0/5657
43	LA	0.32	0/1936	0.43	0/2596
44	LB	0.30	0/3306	0.37	0/4424
45	LC	0.31	0/2981	0.38	0/4002
46	LD	0.25	0/2428	0.31	0/3252
47	LE	0.26	0/1973	0.39	0/2645
48	LF	0.31	0/1905	0.31	0/2539
49	LG	0.25	0/1960	0.35	0/2637
50	LH	0.27	0/1537	0.35	0/2066
51	LI	0.26	0/1751	0.31	0/2340
52	LJ	0.21	0/1385	0.35	0/1852
53	LL	0.28	0/1732	0.32	0/2315
54	LM	0.28	0/1161	0.35	0/1554
55	LN	0.32	0/1746	0.33	0/2338
56	LO	0.32	0/1682	0.34	0/2250
57	LP	0.31	0/1268	0.36	0/1701
58	LQ	0.31	0/1537	0.35	0/2052
59	LS	0.31	0/1493	0.34	0/2003
60	LT	0.28	0/1326	0.31	0/1770
61	LU	0.23	0/839	0.39	0/1126
62	LV	0.29	0/993	0.36	0/1332
63	LX	0.27	0/1002	0.33	0/1345
64	LY	0.30	0/1132	0.36	0/1504
65	LZ	0.26	0/1130	0.33	0/1507
66	La	0.31	0/1191	0.33	0/1591
67	Lb	0.24	0/889	0.34	0/1175
68	Lc	0.27	0/774	0.39	0/1038
69	Ld	0.28	0/903	0.35	0/1216
70	Le	0.31	0/1071	0.34	0/1429
71	Lf	0.32	0/895	0.37	0/1198
72	Lg	0.27	0/916	0.31	0/1220
73	Lh	0.26	0/1023	0.34	0/1351
74	Li	0.24	0/843	0.34	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lj	0.33	0/720	0.40	0/952
76	Lk	0.23	0/575	0.32	0/761
77	Ll	0.30	0/454	0.29	0/599
78	Lm	0.26	0/435	0.35	0/575
79	Ln	0.21	0/231	0.24	0/294
80	Lo	0.27	0/876	0.36	0/1156
81	Lp	0.29	0/718	0.35	0/953
82	Lr	0.29	0/1017	0.34	0/1364
83	Ls	0.15	0/1519	0.37	0/2052
84	Lt	0.18	0/1009	0.49	0/1363
All	All	0.27	0/231571	0.33	1/339714 (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
20	LR	0	1
22	SR	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SS	43	VAL	N-CA-C	-5.84	108.16	113.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	LR	136	ARG	Sidechain
22	SR	78	ARG	Sidechain
22	SR	80	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SA	1741	0	1744	57	0
2	SB	1738	0	1809	36	0
3	SC	1707	0	1791	31	0
4	SE	2076	0	2177	40	0
5	SG	1923	0	2089	36	0
6	SH	1497	0	1590	24	0
7	SI	1686	0	1772	27	0
8	SJ	1525	0	1640	18	0
9	SL	1247	0	1323	17	0
10	SN	1208	0	1294	22	0
11	SO	1024	0	1050	14	0
12	SV	636	0	637	18	0
13	SW	1034	0	1080	22	0
14	SX	1098	0	1167	12	0
15	SY	1065	0	1142	24	0
16	Sa	821	0	870	15	0
17	Sb	651	0	670	18	0
18	Se	459	0	503	11	0
19	S2	36952	0	18677	520	0
20	LR	1566	0	1729	7	0
21	LW	945	0	1003	13	0
22	SR	1090	0	1149	26	0
23	SD	1765	0	1865	29	0
24	SF	1495	0	1549	28	0
25	SK	827	0	854	10	0
26	SM	940	0	965	15	0
27	SP	985	0	1031	16	0
28	SQ	1142	0	1213	19	0
29	SS	1198	0	1260	22	0
30	ST	1112	0	1146	14	0
31	SU	821	0	883	10	0
32	SZ	598	0	656	11	0
33	Sc	506	0	536	14	0
34	Sd	459	0	449	10	0
35	Sf	548	0	552	16	0
36	Sg	2436	0	2391	43	0
37	At	1514	0	770	20	0
38	Pt	1576	0	803	21	0
39	CI	247	0	283	3	0
40	L5	78444	0	39718	671	0
41	L7	2561	0	1295	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	L8	3315	0	1685	24	0
43	LA	1898	0	1993	35	0
44	LB	3238	0	3376	39	0
45	LC	2927	0	3104	23	0
46	LD	2382	0	2410	20	0
47	LE	1935	0	2096	19	0
48	LF	1870	0	1996	14	0
49	LG	1927	0	2074	14	0
50	LH	1518	0	1601	12	0
51	LI	1711	0	1749	16	0
52	LJ	1362	0	1399	11	0
53	LL	1701	0	1818	19	0
54	LM	1138	0	1204	18	0
55	LN	1701	0	1749	16	0
56	LO	1650	0	1794	20	0
57	LP	1242	0	1269	16	0
58	LQ	1513	0	1628	11	0
59	LS	1453	0	1490	9	0
60	LT	1298	0	1366	9	0
61	LU	825	0	850	14	0
62	LV	979	0	1039	7	0
63	LX	985	0	1066	9	0
64	LY	1115	0	1205	9	0
65	LZ	1107	0	1182	7	0
66	La	1162	0	1213	5	0
67	Lb	876	0	948	10	0
68	Lc	764	0	804	8	0
69	Ld	888	0	930	4	0
70	Le	1053	0	1147	10	0
71	Lf	876	0	912	7	0
72	Lg	906	0	998	6	0
73	Lh	1015	0	1148	18	0
74	Li	832	0	917	2	0
75	Lj	705	0	737	5	0
76	Lk	569	0	637	6	0
77	Ll	444	0	483	6	0
78	Lm	429	0	465	5	0
79	Ln	230	0	276	0	0
80	Lo	862	0	929	7	0
81	Lp	708	0	756	9	0
82	Lr	1002	0	1068	7	0
83	Ls	1496	0	1540	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Lt	998	0	1032	14	0
85	L5	178	0	0	0	0
85	L7	3	0	0	0	0
85	L8	6	0	0	0	0
85	LA	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Le	1	0	0	0	0
85	S2	26	0	0	0	0
85	SG	1	0	0	0	0
85	SS	1	0	0	0	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	98	0	182	5	0
88	L5	80	0	152	2	0
88	L8	10	0	19	0	0
88	LN	10	0	19	0	0
All	All	219891	0	163580	2241	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 6.

All (2241) 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)
38:Pt:50:U:H3	38:Pt:64:G:H1	1.03	1.01
19:S2:1417:C:H42	19:S2:1422:G:H22	1.01	0.99
19:S2:834:C:H42	19:S2:839:C:H42	1.12	0.96
19:S2:1748:G:H1	19:S2:1786:U:H3	1.09	0.94
40:L5:1100:U:H3	40:L5:1194:G:H1	1.05	0.94
19:S2:1096:G:H1	19:S2:1136:U:H3	1.02	0.93
19:S2:834:C:N4	19:S2:839:C:H42	1.67	0.92
19:S2:1652:G:H1	19:S2:1672:U:H3	0.96	0.91
19:S2:1729:U:H3	19:S2:1805:G:H1	1.06	0.91
40:L5:1177:U:H3	40:L5:1183:C:H42	0.91	0.89
40:L5:3944:G:H1	40:L5:4069:U:H3	0.90	0.89
40:L5:1095:A:H2	40:L5:1200:G:H1	1.18	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LR:132:PHE:HA	20:LR:137:ILE:HD11	1.56	0.88
40:L5:1177:U:H3	40:L5:1183:C:N4	1.73	0.87
40:L5:512:U:H3	40:L5:647:G:H1	1.18	0.86
40:L5:1996:C:N4	40:L5:2000:G:H22	1.78	0.82
40:L5:1974:U:H4'	40:L5:1975:G:H3'	1.64	0.79
40:L5:4887:C:H42	40:L5:4932:U:H3	1.31	0.79
40:L5:1759:G:H1	40:L5:1773:U:H3	1.30	0.78
40:L5:184:U:O2	40:L5:253:G:N2	2.17	0.78
1:SA:70:ASN:HB3	1:SA:73:ASP:HB2	1.65	0.77
19:S2:1417:C:N4	19:S2:1422:G:H22	1.82	0.77
40:L5:3717:A:H2'	40:L5:3718:A2M:H8	1.65	0.77
6:SH:144:ILE:HD11	6:SH:152:ARG:HB3	1.66	0.77
19:S2:1533:A:H62	19:S2:1602:U:H3	1.33	0.77
24:SF:101:HIS:HB2	24:SF:108:PRO:HG3	1.66	0.76
83:Ls:96:THR:HG22	83:Ls:99:ARG:HH21	1.48	0.76
9:SL:133:PRO:HG2	19:S2:383:G:H21	1.51	0.76
17:Sb:65:GLN:HB2	17:Sb:72:ARG:HB3	1.68	0.75
1:SA:148:CYS:HB3	1:SA:163:CYS:H	1.51	0.75
19:S2:1417:C:H42	19:S2:1422:G:N2	1.82	0.75
28:SQ:44:PRO:HG2	28:SQ:81:ILE:HD11	1.68	0.75
84:Lt:16:ARG:HH12	84:Lt:28:LEU:HB3	1.52	0.75
19:S2:304:C:H5''	19:S2:305:U:H5'	1.68	0.75
40:L5:1996:C:H42	40:L5:2000:G:N2	1.84	0.75
2:SB:24:PRO:HG3	19:S2:953:C:H5''	1.69	0.74
2:SB:84:PHE:HB3	2:SB:86:LEU:HD23	1.69	0.74
17:Sb:56:CYS:HB2	17:Sb:59:CYS:H	1.52	0.74
40:L5:1095:A:C2	40:L5:1200:G:N1	2.55	0.74
19:S2:834:C:N3	19:S2:839:C:N3	2.36	0.74
40:L5:3754:G:H1	40:L5:3770:U:H3	1.34	0.74
84:Lt:16:ARG:HE	84:Lt:17:CYS:H	1.35	0.74
35:Sf:132:MET:HG2	35:Sf:141:CYS:HB3	1.68	0.74
87:L5:5292:SPM:H112	56:LO:91:LYS:HD3	1.69	0.74
19:S2:1314:U:H2'	25:SK:2:LEU:HD12	1.70	0.74
16:Sa:59:PHE:HB2	16:Sa:62:TYR:HB2	1.71	0.73
19:S2:834:C:H42	19:S2:839:C:N4	1.85	0.73
18:Se:58:ASN:HB3	19:S2:608:C:H5'	1.69	0.73
71:Lf:46:ARG:HH21	71:Lf:89:ARG:HH22	1.36	0.73
19:S2:834:C:O2	19:S2:839:C:O2	2.06	0.72
7:SI:87:ASN:HB3	7:SI:90:LEU:HD23	1.71	0.72
31:SU:51:LYS:HB2	31:SU:90:ASP:HB2	1.72	0.72
54:LM:15:VAL:HG22	54:LM:50:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1095:A:N1	40:L5:1200:G:O6	2.22	0.72
80:Lo:33:LEU:HA	80:Lo:38:LYS:HG2	1.72	0.72
40:L5:1414:C:H2'	40:L5:1415:G:H8	1.55	0.72
16:Sa:82:LYS:HB3	16:Sa:85:ARG:HH22	1.55	0.71
40:L5:4139:G:H21	40:L5:4140:C:H41	1.38	0.71
19:S2:1513:C:H2'	19:S2:1514:G:H8	1.52	0.71
44:LB:107:ALA:HB2	44:LB:201:LEU:HD22	1.72	0.71
19:S2:1653:U:O2	19:S2:1671:G:N2	2.22	0.71
36:Sg:206:LEU:HD12	36:Sg:218:LEU:HD12	1.71	0.71
3:SC:193:VAL:HG11	3:SC:240:THR:HG22	1.73	0.71
43:LA:54:ARG:HG2	43:LA:56:ALA:H	1.56	0.71
17:Sb:68:GLY:HA2	19:S2:928:G:H21	1.57	0.70
5:SG:170:ARG:HB3	19:S2:72:C:H42	1.56	0.70
19:S2:1352:G:H1	19:S2:1359:U:H3	1.39	0.70
19:S2:1829:G:H1'	19:S2:1850:MA6:H2	1.74	0.70
3:SC:90:GLU:HB2	3:SC:93:ILE:HG13	1.74	0.70
72:Lg:83:CYS:SG	72:Lg:86:CYS:HB2	2.31	0.70
19:S2:1030:A:H2'	19:S2:1031:A2M:H8	1.73	0.69
19:S2:928:G:H2'	19:S2:929:G:C8	2.26	0.69
19:S2:600:G:H2'	19:S2:601:OMG:H8	1.57	0.69
40:L5:3937:C:H1'	55:LN:125:SER:HB3	1.73	0.69
19:S2:1656:G:H1	19:S2:1668:U:H3	1.38	0.69
40:L5:2557:G:H1	40:L5:2570:U:H3	0.77	0.69
40:L5:3701:OMC:H5	40:L5:3748:A:H62	1.40	0.69
66:La:72:THR:HG22	66:La:110:LYS:HB3	1.75	0.69
45:LC:230:LEU:HD21	45:LC:236:ASN:H	1.57	0.69
19:S2:1748:G:O6	19:S2:1786:U:O4	2.10	0.68
87:L5:5288:SPM:H21	88:L5:5289:SPD:H102	1.58	0.68
1:SA:41:ARG:HE	1:SA:45:GLY:HA2	1.57	0.68
43:LA:114:CYS:HB3	43:LA:165:VAL:HB	1.73	0.68
62:LV:111:GLU:HG3	62:LV:131:ARG:HD3	1.76	0.68
8:SJ:164:PRO:HB3	8:SJ:170:PRO:HA	1.76	0.68
19:S2:1362:U:H5''	19:S2:1363:C:H5	1.59	0.68
28:SQ:43:GLU:HG3	28:SQ:44:PRO:HD3	1.75	0.68
19:S2:186:C:H2'	19:S2:187:G:H8	1.58	0.67
40:L5:1095:A:H2	40:L5:1200:G:N1	1.90	0.67
47:LE:72:LYS:HD3	67:Lb:119:CYS:HB3	1.74	0.67
19:S2:1536:G:H2'	19:S2:1537:A:H8	1.59	0.67
15:SY:9:THR:HG22	19:S2:837:A:H61	1.58	0.67
36:Sg:256:ILE:HB	36:Sg:270:LEU:HB2	1.76	0.67
40:L5:4748:U:H3	40:L5:4952:G:H1	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:ST:42:HIS:HB3	30:ST:93:SER:HB3	1.76	0.67
40:L5:1976:G:O6	40:L5:1990:A:N1	2.27	0.67
51:LI:54:SER:HB3	51:LI:135:ILE:HD11	1.77	0.67
8:SJ:63:LEU:HD23	8:SJ:70:ARG:HB2	1.76	0.67
40:L5:262:G:H2'	40:L5:263:G:H8	1.60	0.67
19:S2:1396:A:N7	19:S2:1449:G:O6	2.28	0.66
19:S2:1581:C:H5'	19:S2:1582:C:H5	1.59	0.66
40:L5:4093:G:H1	40:L5:4114:C:H2'	1.60	0.66
19:S2:874:G:H2'	19:S2:875:A:H8	1.59	0.66
57:LP:118:GLN:HE21	57:LP:120:ASN:HD21	1.43	0.66
51:LI:205:PRO:HD2	51:LI:208:LYS:HE2	1.77	0.66
53:LL:64:VAL:HA	53:LL:67:HIS:CD2	2.30	0.66
1:SA:8:LEU:HD21	1:SA:191:ARG:HH22	1.61	0.66
10:SN:13:GLN:HB2	17:Sb:21:LYS:HE3	1.76	0.66
19:S2:1096:G:N2	19:S2:1136:U:O2	2.27	0.66
4:SE:159:THR:HB	4:SE:173:ILE:HB	1.77	0.66
37:At:15:G:H22	37:At:48:C:H42	1.44	0.66
6:SH:37:LYS:HZ3	6:SH:40:LEU:HD22	1.61	0.65
26:SM:99:LYS:HG2	26:SM:101:ARG:H	1.61	0.65
19:S2:1352:G:N2	19:S2:1359:U:O2	2.28	0.65
40:L5:1942:A:H2'	40:L5:1943:A:C8	2.31	0.65
47:LE:222:LEU:H	47:LE:237:LYS:HE2	1.60	0.65
40:L5:3697:U:H5''	40:L5:3698:G:H5'	1.77	0.65
16:Sa:38:LYS:HB2	16:Sa:71:LEU:HB2	1.78	0.65
55:LN:68:ARG:HE	55:LN:128:LYS:HE3	1.61	0.65
4:SE:160:ILE:HD12	4:SE:162:ILE:HD11	1.79	0.65
19:S2:1421:A:H62	19:S2:1424:G:H1'	1.60	0.65
17:Sb:54:VAL:HG23	17:Sb:63:LEU:HB2	1.79	0.65
28:SQ:24:HIS:HB3	28:SQ:69:ARG:HB2	1.77	0.65
11:SO:134:PRO:HB3	19:S2:944:A:H5''	1.79	0.64
19:S2:1612:G:H1'	29:SS:87:GLN:HE21	1.61	0.64
13:SW:111:MET:HE1	13:SW:119:LYS:HD2	1.80	0.64
15:SY:36:PRO:HG3	19:S2:570:C:H4'	1.79	0.64
19:S2:1417:C:N3	19:S2:1422:G:N1	2.43	0.64
35:Sf:140:TYR:HB2	35:Sf:147:THR:HG22	1.80	0.64
40:L5:1629:G:H1	43:LA:208:GLU:HG2	1.62	0.64
46:LD:223:PHE:HB3	46:LD:226:TYR:HB2	1.80	0.64
57:LP:17:SER:HB2	57:LP:98:ALA:HB2	1.79	0.64
47:LE:223:ARG:HH22	47:LE:238:GLU:HG3	1.62	0.64
19:S2:557:U:H2'	19:S2:558:G:C8	2.33	0.64
40:L5:1332:C:H2'	40:L5:1333:A:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:166:A2M:H2'	19:S2:167:G:H8	1.61	0.64
40:L5:3868:G:H22	40:L5:3900:G:H1'	1.62	0.64
51:LI:162:ARG:HH21	51:LI:164:LYS:HE3	1.63	0.64
19:S2:388:U:H2'	19:S2:389:A:H8	1.63	0.64
40:L5:2351:OMC:HM22	45:LC:95:MET:HG3	1.80	0.64
84:Lt:134:GLY:HA3	84:Lt:152:ILE:HD11	1.79	0.64
6:SH:154:ILE:HB	6:SH:185:VAL:HG22	1.80	0.63
19:S2:1650:A:H5''	28:SQ:139:ALA:HB2	1.79	0.63
84:Lt:82:ILE:HG13	84:Lt:86:LYS:HE2	1.80	0.63
4:SE:141:THR:HG23	4:SE:143:ASP:H	1.63	0.63
62:LV:112:MET:HE1	62:LV:117:ILE:HD11	1.80	0.63
1:SA:155:ARG:HH22	19:S2:1137:U:H4'	1.63	0.63
36:Sg:87:LEU:HB2	36:Sg:101:PHE:HB2	1.78	0.63
49:LG:167:VAL:HG12	49:LG:170:LEU:HD12	1.80	0.63
8:SJ:67:ASP:HB3	8:SJ:70:ARG:HB3	1.81	0.63
11:SO:52:THR:HG21	19:S2:952:G:H21	1.62	0.63
29:SS:6:PRO:HG2	29:SS:58:GLU:HB3	1.80	0.63
16:Sa:28:ARG:HH12	19:S2:1839:U:H5	1.46	0.63
19:S2:1228:A:H2'	19:S2:1229:G:C8	2.33	0.63
40:L5:2362:U:H2'	40:L5:2363:A2M:H8	1.81	0.63
40:L5:1444:G:H22	40:L5:2104:G:H21	1.45	0.63
15:SY:11:LYS:HB2	15:SY:24:VAL:HG12	1.81	0.63
24:SF:59:LYS:HB3	24:SF:62:ARG:HD3	1.80	0.63
36:Sg:142:VAL:HG12	36:Sg:146:SER:HB3	1.80	0.63
44:LB:220:ILE:HG23	44:LB:278:THR:HG22	1.80	0.63
40:L5:1175:A:H2	40:L5:1185:G:H22	1.47	0.63
57:LP:131:ARG:HG3	57:LP:137:ASN:OD1	1.98	0.63
3:SC:210:PRO:HD3	3:SC:236:PHE:HE2	1.63	0.63
19:S2:1652:G:O6	19:S2:1672:U:O4	2.17	0.63
40:L5:3944:G:O6	40:L5:4069:U:O4	2.16	0.63
2:SB:224:GLU:HB3	2:SB:227:LYS:HE3	1.80	0.62
19:S2:1657:G:H1	19:S2:1667:U:H3	1.47	0.62
1:SA:201:LEU:HD11	22:SR:82:ASP:HA	1.80	0.62
7:SI:57:ALA:HB2	7:SI:183:GLY:HA2	1.80	0.62
44:LB:117:ARG:HA	44:LB:177:LYS:HD2	1.82	0.62
7:SI:141:ARG:HD3	7:SI:145:ILE:HG21	1.80	0.62
32:SZ:58:LEU:HD12	32:SZ:62:VAL:HG21	1.80	0.62
19:S2:1228:A:H2'	19:S2:1229:G:H8	1.64	0.62
40:L5:381:U:H4'	40:L5:415:G:H5'	1.80	0.62
40:L5:1094:G:O6	40:L5:1201:U:O2	2.17	0.62
1:SA:113:GLN:HG2	1:SA:115:ALA:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:2017:A:HO2'	40:L5:2018:C:H6	1.45	0.62
5:SG:135:PRO:HG2	5:SG:141:ILE:HG22	1.81	0.62
19:S2:1203:G:H2'	19:S2:1204:A:C8	2.35	0.62
40:L5:4910:G:H4'	44:LB:95:THR:HG22	1.81	0.62
12:SV:74:LYS:HG2	12:SV:79:VAL:HB	1.81	0.61
83:Ls:95:LEU:HD11	83:Ls:192:VAL:HG21	1.81	0.61
4:SE:80:ILE:HG23	4:SE:81:THR:HG23	1.80	0.61
19:S2:639:C:H2'	19:S2:640:A:H8	1.65	0.61
6:SH:144:ILE:HD13	6:SH:154:ILE:HG13	1.81	0.61
17:Sb:72:ARG:HH12	19:S2:1120:U:H5'	1.65	0.61
19:S2:508:A:H3'	19:S2:509:OMG:H8	1.65	0.61
23:SD:106:ARG:HH11	23:SD:110:LEU:HD12	1.65	0.61
24:SF:155:CYS:HB3	24:SF:159:ARG:HH22	1.65	0.61
40:L5:1969:G:H21	40:L5:1999:A:H1'	1.65	0.61
7:SI:98:LYS:HB3	19:S2:377:G:H5'	1.82	0.61
19:S2:1101:U:H2'	19:S2:1102:G:H8	1.64	0.61
49:LG:200:THR:HG22	49:LG:201:THR:HG23	1.81	0.61
6:SH:10:LYS:HZ2	6:SH:17:ASP:HB3	1.65	0.61
56:LO:126:VAL:HG13	56:LO:127:VAL:HG13	1.82	0.61
37:At:18:G:O6	37:At:55:U:O2	2.18	0.61
40:L5:497:G:H21	40:L5:498:C:H41	1.47	0.61
84:Lt:10:ILE:HG12	84:Lt:65:GLN:HB3	1.82	0.61
19:S2:609:U:H2'	19:S2:610:G:H8	1.66	0.61
19:S2:1417:C:O2	19:S2:1422:G:O6	2.18	0.61
5:SG:147:LEU:HD12	5:SG:151:ASP:HB2	1.83	0.61
19:S2:835:C:H5'	19:S2:836:G:H5'	1.81	0.61
83:Ls:59:THR:HA	83:Ls:62:ARG:HB2	1.83	0.61
9:SL:136:LYS:HB2	19:S2:385:G:H3'	1.83	0.60
16:Sa:82:LYS:HD3	16:Sa:85:ARG:HH12	1.65	0.60
19:S2:1536:G:H2'	19:S2:1537:A:C8	2.36	0.60
40:L5:1732:C:H5''	60:LT:43:LYS:HE2	1.81	0.60
40:L5:3754:G:O6	40:L5:3770:U:O4	2.19	0.60
83:Ls:114:GLY:HA2	83:Ls:166:LYS:HD2	1.82	0.60
40:L5:662:C:H2'	40:L5:663:G:H8	1.65	0.60
5:SG:142:ARG:HA	5:SG:147:LEU:HD23	1.82	0.60
15:SY:7:ILE:HG23	15:SY:27:VAL:HG12	1.82	0.60
44:LB:287:ILE:HG12	44:LB:331:VAL:HG22	1.84	0.60
19:S2:1753:C:H5'	19:S2:1780:G:H22	1.67	0.60
24:SF:201:LYS:HA	24:SF:204:ARG:HE	1.66	0.60
32:SZ:102:LYS:HA	32:SZ:107:VAL:HG23	1.82	0.60
7:SI:12:ARG:HH21	7:SI:18:ARG:HG3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:145:G:H2'	19:S2:146:G:C8	2.37	0.60
40:L5:2611:A:H5'	40:L5:2688:G:H4'	1.83	0.60
2:SB:192:SER:HA	2:SB:195:LYS:HD2	1.83	0.60
11:SO:30:VAL:HG22	11:SO:94:HIS:HB2	1.82	0.60
40:L5:1870:C:H2'	40:L5:1871:A2M:H8	1.84	0.60
40:L5:4594:U:H2'	40:L5:4595:G:H8	1.67	0.60
42:L8:90:C:H1'	64:LY:24:HIS:HB3	1.84	0.60
2:SB:57:ILE:HG22	2:SB:59:SER:H	1.67	0.60
49:LG:58:PRO:HD2	49:LG:61:ILE:HD12	1.83	0.60
40:L5:37:U:H4'	66:La:32:ARG:HD2	1.84	0.60
40:L5:137:G:H2'	40:L5:138:G:H8	1.67	0.60
40:L5:190:G:H2'	40:L5:191:G:H8	1.67	0.60
40:L5:1100:U:O4	40:L5:1194:G:O6	2.20	0.60
40:L5:4126:C:H5''	40:L5:4127:A:H5''	1.83	0.60
19:S2:49:C:H2'	19:S2:472:C:H41	1.66	0.59
7:SI:19:LYS:HD3	19:S2:101:U:H5''	1.84	0.59
52:LJ:63:ARG:HD3	80:Lo:106:PHE:HB2	1.83	0.59
1:SA:10:MET:HE2	1:SA:15:VAL:HG22	1.84	0.59
22:SR:12:ALA:HB2	23:SD:208:VAL:HG21	1.84	0.59
40:L5:2411:C:H2'	40:L5:2412:A:H8	1.67	0.59
1:SA:42:LYS:HG3	1:SA:44:ASP:H	1.67	0.59
3:SC:191:VAL:HG11	3:SC:236:PHE:HA	1.82	0.59
52:LJ:56:THR:HG23	52:LJ:63:ARG:HA	1.83	0.59
40:L5:2486:G:O6	40:L5:2493:G:O6	2.20	0.59
40:L5:3717:A:H2'	40:L5:3718:A2M:C8	2.32	0.59
4:SE:149:TYR:HB3	5:SG:209:TYR:HB2	1.82	0.59
5:SG:7:PHE:HD1	5:SG:113:ILE:HD13	1.68	0.59
44:LB:165:HIS:HB3	44:LB:180:LEU:HD23	1.84	0.59
47:LE:281:ILE:HD12	47:LE:286:LEU:HD11	1.83	0.59
54:LM:122:ILE:HB	56:LO:189:ILE:HD11	1.85	0.59
32:SZ:99:LEU:HD11	32:SZ:102:LYS:HB2	1.85	0.59
40:L5:1503:A:H62	58:LQ:87:THR:HG21	1.68	0.59
40:L5:3898:G:H5'	44:LB:254:ILE:HG13	1.84	0.59
40:L5:4220:6MZ:H2'	40:L5:4222:G:H5''	1.85	0.59
45:LC:134:PRO:HG3	45:LC:150:LEU:HD12	1.85	0.59
64:LY:10:ASP:HB3	64:LY:13:LYS:HB2	1.85	0.59
5:SG:37:ALA:HA	5:SG:49:VAL:HA	1.84	0.59
19:S2:525:A:H2'	19:S2:526:A:H8	1.68	0.59
69:Ld:22:THR:HG23	69:Ld:122:VAL:HG13	1.84	0.59
3:SC:196:ILE:HB	3:SC:223:TYR:HB2	1.85	0.58
19:S2:468:A2M:H2'	19:S2:469:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:517:OMC:HM22	19:S2:518:G:H5'	1.85	0.58
29:SS:21:ASP:HB3	29:SS:24:ARG:HD2	1.84	0.58
37:At:3:C:H42	37:At:70:A:H61	1.51	0.58
53:LL:80:GLU:HG3	53:LL:110:LEU:HD12	1.85	0.58
40:L5:4274:A:H2'	40:L5:4275:G:C8	2.38	0.58
83:Ls:29:ILE:HG13	83:Ls:190:GLN:HB2	1.85	0.58
24:SF:204:ARG:HG2	33:Sc:63:ARG:HE	1.68	0.58
4:SE:9:LEU:HB2	4:SE:30:ARG:HD3	1.84	0.58
19:S2:1467:C:H5''	22:SR:1:MET:HA	1.85	0.58
40:L5:194:C:H1'	64:LY:121:ARG:HH12	1.68	0.58
58:LQ:80:ALA:HB3	58:LQ:100:VAL:HG22	1.84	0.58
5:SG:133:LEU:HD12	19:S2:65:C:C4	2.38	0.58
15:SY:124:ASN:HD22	19:S2:84:A:H5''	1.68	0.58
19:S2:1031:A2M:H2'	19:S2:1032:C:C6	2.39	0.58
40:L5:4537:C:H2'	40:L5:4538:G:H8	1.67	0.58
56:LO:37:ARG:HD2	56:LO:108:ILE:HD11	1.84	0.58
40:L5:2764:A:H2'	40:L5:2765:A:H8	1.69	0.58
56:LO:81:TRP:HB2	56:LO:104:VAL:HG21	1.86	0.58
2:SB:146:ARG:HB2	2:SB:149:GLN:HB2	1.86	0.58
24:SF:34:SER:HA	33:Sc:55:VAL:HG13	1.84	0.58
33:Sc:17:VAL:HA	33:Sc:30:VAL:HG12	1.84	0.58
58:LQ:106:THR:HG22	58:LQ:108:ARG:H	1.68	0.58
83:Ls:18:ILE:HG12	83:Ls:68:HIS:ND1	2.18	0.58
40:L5:1258:G:H2'	40:L5:1259:G:C8	2.39	0.58
40:L5:3611:A:H2	40:L5:5016:A:H8	1.52	0.58
50:LH:102:ASN:HB2	50:LH:115:ARG:HB2	1.85	0.58
14:SX:124:LYS:HG2	14:SX:129:SER:HA	1.86	0.58
19:S2:1405:A:H2'	19:S2:1406:G:O4'	2.04	0.57
40:L5:190:G:H2'	40:L5:191:G:C8	2.39	0.57
40:L5:4274:A:H2'	40:L5:4275:G:H8	1.69	0.57
76:Lk:14:THR:HA	76:Lk:17:ARG:HD3	1.86	0.57
19:S2:899:U:H3'	19:S2:900:C:H4'	1.85	0.57
40:L5:3732:A:H2'	40:L5:3733:A:H8	1.68	0.57
3:SC:142:LYS:HE3	3:SC:144:SER:HB2	1.87	0.57
23:SD:74:GLN:HE22	23:SD:81:GLU:HA	1.69	0.57
37:At:15:G:N2	37:At:48:C:H42	2.02	0.57
19:S2:642:U:H4'	19:S2:644:OMG:H4'	1.87	0.57
19:S2:1277:C:H2'	19:S2:1278:A:H8	1.68	0.57
28:SQ:58:LEU:HD13	28:SQ:108:ILE:HD11	1.86	0.57
55:LN:143:ARG:HD2	73:Lh:95:LEU:HD23	1.87	0.57
19:S2:388:U:H2'	19:S2:389:A:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1326:A2M:H2'	40:L5:1327:C:C6	2.39	0.57
53:LL:48:PRO:HG3	73:Lh:118:LYS:HE2	1.87	0.57
11:SO:33:ILE:HG22	11:SO:42:VAL:HA	1.87	0.57
19:S2:943:U:H2'	19:S2:944:A:H8	1.69	0.57
19:S2:1743:G:H21	19:S2:1791:A:H62	1.50	0.57
40:L5:4113:U:H4'	40:L5:4115:G:C4	2.40	0.57
40:L5:4887:C:N4	40:L5:4932:U:H3	2.01	0.57
4:SE:19:MET:HE2	4:SE:108:ARG:HD2	1.86	0.57
40:L5:4571:A2M:H2'	40:L5:4572:U:H6	1.69	0.57
43:LA:112:ILE:HD11	81:Lp:79:VAL:HG22	1.85	0.57
19:S2:329:G:H2'	19:S2:330:G:C8	2.40	0.57
40:L5:1177:U:C4	40:L5:1183:C:N4	2.72	0.57
44:LB:57:VAL:HB	44:LB:367:PHE:HB3	1.87	0.57
1:SA:38:ILE:HD11	1:SA:47:TYR:HB3	1.85	0.57
19:S2:1568:C:H2'	19:S2:1569:A:C8	2.39	0.57
33:Sc:16:LYS:HZ1	33:Sc:18:LEU:HD13	1.69	0.57
40:L5:1996:C:N4	40:L5:2000:G:N2	2.44	0.57
1:SA:154:LEU:HB3	1:SA:157:VAL:HB	1.87	0.57
13:SW:69:LEU:HD21	13:SW:72:CYS:HB3	1.85	0.57
19:S2:1103:C:H2'	19:S2:1104:G:C8	2.40	0.56
61:LU:45:GLU:HA	61:LU:54:GLY:HA2	1.87	0.56
1:SA:89:LYS:NZ	22:SR:82:ASP:HB3	2.21	0.56
2:SB:85:LYS:HB2	2:SB:101:HIS:HB3	1.87	0.56
31:SU:26:SER:HB3	31:SU:110:VAL:HG23	1.87	0.56
40:L5:181:C:H2'	40:L5:182:G:C8	2.40	0.56
40:L5:1768:C:H42	40:L5:1772:C:H41	1.51	0.56
40:L5:2335:C:H2'	40:L5:2336:G:H8	1.69	0.56
19:S2:885:U:O2	19:S2:901:G:O6	2.23	0.56
40:L5:1973:G:H3'	40:L5:1974:U:H2'	1.87	0.56
19:S2:1755:C:H2'	19:S2:1756:C:C6	2.41	0.56
23:SD:66:ILE:HA	23:SD:69:LEU:HD12	1.86	0.56
65:LZ:11:VAL:HG12	65:LZ:82:PRO:HA	1.88	0.56
23:SD:106:ARG:HG2	23:SD:175:VAL:HG22	1.87	0.56
35:Sf:140:TYR:HE1	35:Sf:145:CYS:HA	1.70	0.56
45:LC:110:ARG:HB2	55:LN:204:ARG:HH21	1.69	0.56
13:SW:107:SER:HB2	19:S2:860:G:H21	1.70	0.56
19:S2:1560:U:O2	19:S2:1575:G:O6	2.24	0.56
36:Sg:173:LEU:HD11	36:Sg:187:ASN:HB3	1.88	0.56
87:L5:5292:SPM:H132	56:LO:91:LYS:HB3	1.86	0.56
36:Sg:130:LYS:HG2	36:Sg:141:THR:HG22	1.86	0.56
3:SC:173:LYS:HD3	12:SV:3:ASN:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SH:157:HIS:HB3	6:SH:190:PRO:HG3	1.88	0.56
19:S2:1283:C:H4'	19:S2:1286:G:H4'	1.86	0.56
19:S2:1391:OMC:H4'	34:Sd:55:LEU:HD13	1.88	0.56
35:Sf:140:TYR:CZ	35:Sf:142:GLY:HA2	2.41	0.56
69:Ld:64:ILE:HG23	69:Ld:68:LEU:HD23	1.88	0.56
19:S2:527:C:H2'	19:S2:528:A:C8	2.41	0.56
19:S2:1858:G:H2'	19:S2:1859:A:H8	1.71	0.56
28:SQ:68:ILE:HD13	28:SQ:88:ILE:HG23	1.88	0.56
40:L5:4238:G:H2'	40:L5:4239:A:H8	1.71	0.56
42:L8:134:G:H5''	63:LX:63:LYS:HD2	1.88	0.56
46:LD:194:VAL:HA	46:LD:197:LYS:HD2	1.88	0.56
19:S2:186:C:H2'	19:S2:187:G:C8	2.40	0.55
28:SQ:117:ARG:HH21	28:SQ:121:VAL:HG21	1.71	0.55
40:L5:1254:A:H5''	40:L5:1255:A:H5''	1.88	0.55
19:S2:1259:A:H62	19:S2:1518:C:H3'	1.72	0.55
4:SE:44:LEU:HD11	4:SE:72:ILE:HD11	1.88	0.55
40:L5:1332:C:H2'	40:L5:1333:A:C8	2.41	0.55
40:L5:1942:A:H2'	40:L5:1943:A:H8	1.71	0.55
19:S2:1144:A:H2'	19:S2:1145:A:C8	2.41	0.55
40:L5:655:C:H2'	40:L5:656:C:C6	2.42	0.55
40:L5:1306:C:H2'	40:L5:1307:A:H8	1.72	0.55
40:L5:4530:UR3:H2'	40:L5:4531:U:H2'	1.87	0.55
2:SB:109:LYS:HG3	2:SB:113:MET:HE2	1.89	0.55
4:SE:179:ASN:HA	4:SE:231:GLY:HA2	1.89	0.55
19:S2:17:C:H2'	19:S2:18:C:H6	1.72	0.55
23:SD:132:LYS:HB2	23:SD:189:MET:HG2	1.88	0.55
84:Lt:131:GLU:HA	84:Lt:152:ILE:HD12	1.88	0.55
19:S2:874:G:H2'	19:S2:875:A:C8	2.39	0.55
40:L5:1464:C:H5''	67:Lb:32:LEU:HD12	1.89	0.55
68:Lc:22:MET:O	68:Lc:23:LYS:HG3	2.06	0.55
4:SE:48:LEU:HD12	4:SE:61:VAL:HG23	1.89	0.55
19:S2:1850:MA6:H8	19:S2:1850:MA6:O5'	2.07	0.55
35:Sf:108:VAL:HB	35:Sf:113:LYS:H	1.71	0.55
40:L5:444:G:H2'	40:L5:445:U:C6	2.42	0.55
9:SL:120:VAL:HG22	9:SL:145:VAL:HG11	1.89	0.55
19:S2:864:A:H2'	19:S2:865:A:C8	2.41	0.55
25:SK:21:MET:HB3	25:SK:69:TRP:HB2	1.88	0.55
40:L5:3732:A:H2'	40:L5:3733:A:C8	2.42	0.55
41:L7:4:U:H2'	41:L7:5:A:H8	1.72	0.55
41:L7:119:U:C2	46:LD:261:VAL:HG21	2.42	0.55
19:S2:1031:A2M:H2'	19:S2:1032:C:H6	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1205:C:H2'	19:S2:1206:G:H8	1.71	0.55
19:S2:1513:C:H2'	19:S2:1514:G:C8	2.38	0.55
21:LW:116:LYS:HA	21:LW:119:LYS:HE2	1.88	0.55
46:LD:182:GLY:HA2	46:LD:194:VAL:HG23	1.89	0.55
7:SI:35:ASN:HB3	7:SI:37:LYS:HE2	1.89	0.55
19:S2:1018:U:H2'	19:S2:1019:C:H6	1.72	0.55
19:S2:1279:C:H2'	19:S2:1280:G:C8	2.42	0.55
40:L5:662:C:H2'	40:L5:663:G:C8	2.42	0.55
40:L5:2029:A:H2'	40:L5:2030:A:C8	2.42	0.55
40:L5:4279:A:H5'	40:L5:4281:A:H1'	1.88	0.55
49:LG:157:ILE:HA	49:LG:201:THR:HG22	1.89	0.55
50:LH:93:ARG:HD2	50:LH:143:GLU:HG2	1.89	0.55
59:LS:15:ARG:HH12	59:LS:18:PRO:HG3	1.72	0.55
75:Lj:27:TYR:HA	75:Lj:34:CYS:HA	1.87	0.55
9:SL:73:LEU:HD11	9:SL:109:MET:HE1	1.89	0.54
24:SF:187:SER:HB3	24:SF:190:ILE:HG12	1.88	0.54
25:SK:80:ARG:HD3	25:SK:85:LEU:HB2	1.88	0.54
40:L5:153:G:H2'	40:L5:154:G:H8	1.72	0.54
40:L5:964:A:H2'	40:L5:965:G:H4'	1.89	0.54
40:L5:1444:G:H1	40:L5:2104:G:N2	2.04	0.54
40:L5:2744:A:H2'	40:L5:2745:A:C8	2.43	0.54
1:SA:77:ILE:HG22	1:SA:99:ILE:HB	1.89	0.54
2:SB:213:ARG:HD2	2:SB:214:LYS:HB2	1.89	0.54
7:SI:78:ILE:HG13	7:SI:104:ILE:HG22	1.89	0.54
19:S2:1217:A:H2'	19:S2:1218:C:C6	2.41	0.54
19:S2:1605:G:H2'	19:S2:1606:G:C4	2.43	0.54
21:LW:99:GLU:HB3	21:LW:102:LYS:HE3	1.89	0.54
40:L5:1961:G:H21	40:L5:2025:A:H62	1.54	0.54
40:L5:3932:U:H2'	40:L5:3933:G:H8	1.72	0.54
40:L5:184:U:O2	40:L5:253:G:C2	2.60	0.54
40:L5:432:U:H1'	87:L5:5292:SPM:H82	1.90	0.54
40:L5:2019:C:H2'	40:L5:2020:U:C6	2.42	0.54
40:L5:4740:G:O6	40:L5:4959:U:O2	2.26	0.54
42:L8:19:C:H2'	42:L8:20:A:C8	2.43	0.54
51:LI:61:SER:HA	51:LI:126:VAL:HG12	1.89	0.54
53:LL:48:PRO:HB2	73:Lh:120:ALA:HB2	1.89	0.54
2:SB:87:ILE:H	2:SB:101:HIS:HB2	1.73	0.54
2:SB:88:THR:HA	2:SB:98:THR:HA	1.90	0.54
19:S2:379:C:H2'	19:S2:380:G:C8	2.43	0.54
23:SD:67:ARG:HD3	25:SK:96:ARG:HG2	1.89	0.54
40:L5:1994:C:H2'	40:L5:1995:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4474:A:H5''	78:Lm:125:LYS:HG3	1.89	0.54
4:SE:153:LEU:HD12	5:SG:216:ARG:HH11	1.73	0.54
19:S2:1595:U:H2'	19:S2:1596:U:C6	2.42	0.54
36:Sg:208:ALA:HB2	36:Sg:218:LEU:HD13	1.89	0.54
40:L5:1095:A:N1	40:L5:1200:G:C6	2.75	0.54
40:L5:2557:G:O6	40:L5:2570:U:O4	2.26	0.54
76:Lk:13:LEU:HA	76:Lk:16:ARG:HG2	1.89	0.54
16:Sa:102:ARG:HG3	16:Sa:103:PRO:HD3	1.89	0.54
19:S2:1069:U:H5''	43:LA:248:GLY:HA2	1.90	0.54
40:L5:4615:C:H5''	44:LB:357:ARG:HD2	1.90	0.54
1:SA:120:ARG:HD2	3:SC:266:TYR:HB3	1.89	0.54
19:S2:900:C:H5'	19:S2:901:G:N7	2.23	0.54
35:Sf:138:ARG:HG3	35:Sf:147:THR:HB	1.88	0.54
42:L8:75:OMG:H8	42:L8:75:OMG:OP1	1.90	0.54
45:LC:144:ILE:HG22	45:LC:147:VAL:HG21	1.89	0.54
7:SI:142:SER:H	7:SI:145:ILE:HD12	1.73	0.54
9:SL:5:GLN:HE22	9:SL:11:GLN:HB2	1.73	0.54
19:S2:1228:A:H5''	29:SS:142:ARG:HH12	1.73	0.54
19:S2:1597:C:H3'	19:S2:1598:G:H8	1.73	0.54
34:Sd:6:LEU:HA	34:Sd:9:SER:HB3	1.89	0.54
40:L5:2611:A:H2'	40:L5:2612:G:C8	2.43	0.54
48:LF:127:LYS:HB2	60:LT:133:ALA:HB3	1.89	0.54
54:LM:33:GLN:HB3	59:LS:145:PHE:HZ	1.71	0.54
5:SG:194:LEU:HB3	5:SG:198:ARG:HH21	1.72	0.54
19:S2:223:C:H2'	19:S2:224:A:C8	2.43	0.54
40:L5:4068:U:HO2'	40:L5:4069:U:H6	1.56	0.54
40:L5:4184:G:H5'	43:LA:233:ARG:HB2	1.88	0.54
4:SE:103:TYR:HB2	4:SE:182:MET:HE2	1.90	0.53
9:SL:81:LYS:HD3	19:S2:394:G:H5'	1.90	0.53
24:SF:18:LYS:HE2	24:SF:22:LYS:HA	1.89	0.53
40:L5:1972:G:H2'	40:L5:1973:G:C8	2.43	0.53
40:L5:3718:A2M:H2'	40:L5:3719:A:O4'	2.08	0.53
40:L5:4139:G:H1'	40:L5:4146:G:N1	2.23	0.53
40:L5:4745:G:H1	40:L5:4955:A:H61	1.54	0.53
40:L5:4991:U:H2'	40:L5:4992:G:C8	2.43	0.53
1:SA:42:LYS:HZ1	1:SA:48:ILE:HD11	1.72	0.53
9:SL:85:THR:HG21	19:S2:373:G:H4'	1.91	0.53
23:SD:1:MET:HG2	23:SD:3:VAL:H	1.73	0.53
28:SQ:16:LYS:HG3	28:SQ:123:ASP:HB3	1.90	0.53
43:LA:31:ALA:HB2	43:LA:123:ARG:HH21	1.72	0.53
45:LC:116:ASN:HB2	45:LC:119:GLN:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LF:105:VAL:HG13	48:LF:136:VAL:HG12	1.91	0.53
19:S2:17:C:H2'	19:S2:18:C:C6	2.43	0.53
40:L5:1617:G:H1'	40:L5:2513:A:N6	2.23	0.53
61:LU:61:VAL:HG13	61:LU:74:SER:HB2	1.89	0.53
5:SG:159:ARG:HE	5:SG:171:THR:HG23	1.73	0.53
19:S2:1854:U:H2'	19:S2:1855:G:H8	1.74	0.53
23:SD:8:LYS:HB3	34:Sd:34:TYR:HE1	1.73	0.53
40:L5:2491:C:H2'	40:L5:2492:C:C6	2.44	0.53
40:L5:4992:G:H2'	40:L5:4993:G:C8	2.43	0.53
1:SA:44:ASP:HB2	22:SR:123:THR:HG21	1.91	0.53
1:SA:198:MET:HE2	22:SR:85:VAL:HG13	1.91	0.53
2:SB:140:VAL:HG22	2:SB:213:ARG:HB2	1.90	0.53
19:S2:1562:C:H2'	19:S2:1563:G:C8	2.44	0.53
40:L5:4239:A:H2'	40:L5:4240:G:C8	2.44	0.53
40:L5:4260:U:H2'	40:L5:4261:C:C6	2.44	0.53
68:Lc:52:CYS:HB3	68:Lc:57:LYS:HG3	1.90	0.53
19:S2:106:C:H2'	19:S2:107:A:H8	1.73	0.53
38:Pt:52:G:H2'	38:Pt:53:G:H8	1.73	0.53
46:LD:37:VAL:HB	46:LD:67:ALA:HB2	1.91	0.53
48:LF:182:TYR:HB3	48:LF:200:ARG:HG3	1.90	0.53
53:LL:130:LYS:HB3	53:LL:133:ALA:HB3	1.90	0.53
5:SG:38:ALA:HB1	5:SG:41:LEU:HD13	1.90	0.53
5:SG:168:LYS:HE2	5:SG:170:ARG:HH12	1.74	0.53
6:SH:153:LEU:HD23	6:SH:155:LYS:HZ2	1.73	0.53
19:S2:634:A:H2'	19:S2:635:G:H8	1.73	0.53
19:S2:1010:G:H2'	19:S2:1011:A:H8	1.74	0.53
19:S2:1406:G:H2'	19:S2:1407:U:C6	2.44	0.53
19:S2:1466:G:H4'	22:SR:4:VAL:HG22	1.90	0.53
22:SR:70:SER:HB3	22:SR:73:LEU:HB2	1.90	0.53
26:SM:91:LEU:HD12	26:SM:106:CYS:HB2	1.90	0.53
36:Sg:168:CYS:HB2	36:Sg:195:LEU:HD13	1.91	0.53
57:LP:118:GLN:HE21	57:LP:120:ASN:ND2	2.06	0.53
1:SA:85:ARG:HH22	1:SA:205:ARG:HG3	1.74	0.53
1:SA:185:MET:HA	1:SA:191:ARG:HH21	1.74	0.53
2:SB:142:PHE:HB2	2:SB:209:ASP:HB3	1.91	0.53
7:SI:133:GLU:HA	7:SI:136:ILE:HG12	1.90	0.53
13:SW:87:GLU:HA	13:SW:90:GLN:HB2	1.89	0.53
19:S2:1532:C:H3'	19:S2:1637:A:H62	1.74	0.53
19:S2:1777:G:H2'	19:S2:1778:C:H6	1.74	0.53
40:L5:1969:G:N2	40:L5:1999:A:H1'	2.23	0.53
47:LE:277:LEU:HB2	71:Lf:4:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:118:GLU:HG3	3:SC:65:LYS:HG3	1.91	0.53
2:SB:171:ILE:HD11	2:SB:197:ILE:HG12	1.91	0.53
5:SG:234:LEU:HD11	5:SG:237:LEU:HB3	1.90	0.53
19:S2:391:C:H2'	19:S2:392:A:H8	1.74	0.53
26:SM:31:LEU:HB3	26:SM:33:ARG:HG3	1.90	0.53
32:SZ:99:LEU:HA	32:SZ:109:TYR:HD1	1.74	0.53
2:SB:117:TRP:HD1	2:SB:153:THR:HG22	1.74	0.53
19:S2:359:U:H3	19:S2:403:G:H1	1.57	0.53
40:L5:1339:U:H2'	40:L5:1340:OMC:C6	2.44	0.53
40:L5:4426:C:H2'	40:L5:4427:G:H5'	1.90	0.53
40:L5:4967:A:H2'	40:L5:4968:A:H8	1.74	0.53
50:LH:95:VAL:HG12	78:Lm:82:LEU:HD13	1.91	0.53
83:Ls:133:GLU:HG2	83:Ls:134:LYS:HG2	1.91	0.53
24:SF:143:PRO:HD3	33:Sc:56:LEU:HB3	1.90	0.52
44:LB:168:MET:HE2	44:LB:175:GLN:HG2	1.90	0.52
53:LL:130:LYS:HD2	53:LL:131:PRO:HD2	1.90	0.52
19:S2:1679:A:H2'	24:SF:60:ARG:HD2	1.90	0.52
19:S2:640:A:H2'	19:S2:641:A:C8	2.43	0.52
19:S2:991:G:C6	19:S2:1134:G:H4'	2.45	0.52
19:S2:1729:U:O2	19:S2:1805:G:N2	2.32	0.52
40:L5:2745:A:H2'	40:L5:2746:A:C8	2.45	0.52
40:L5:4415:A:H4'	51:LI:74:LYS:HD3	1.90	0.52
40:L5:4594:U:H2'	40:L5:4595:G:C8	2.44	0.52
40:L5:4742:G:H2'	40:L5:4743:G:C8	2.44	0.52
47:LE:144:ILE:HG12	47:LE:196:ALA:HB2	1.91	0.52
1:SA:49:ILE:HD13	1:SA:163:CYS:HA	1.90	0.52
1:SA:158:ASP:HB2	1:SA:159:ILE:HD12	1.92	0.52
19:S2:106:C:H2'	19:S2:107:A:C8	2.45	0.52
29:SS:40:TYR:HA	29:SS:83:PHE:HE2	1.73	0.52
41:L7:112:U:H2'	41:L7:113:G:H8	1.72	0.52
46:LD:51:MET:HE3	46:LD:105:LEU:HD23	1.91	0.52
49:LG:205:THR:HG22	49:LG:206:GLN:H	1.73	0.52
15:SY:10:ARG:HD2	19:S2:833:C:H41	1.74	0.52
19:S2:1240:A:C2	27:SP:100:LYS:HB2	2.45	0.52
40:L5:1281:G:N1	47:LE:128:HIS:HB2	2.25	0.52
40:L5:1933:G:H2'	40:L5:1934:A:C8	2.45	0.52
84:Lt:15:LEU:HD13	84:Lt:60:VAL:HG13	1.90	0.52
19:S2:28:U:H2'	19:S2:29:G:H8	1.74	0.52
19:S2:1201:U:H2'	19:S2:1202:U:C6	2.45	0.52
32:SZ:99:LEU:HD12	32:SZ:109:TYR:HE1	1.74	0.52
40:L5:3726:A:H2'	40:L5:3727:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:77:ILE:HD11	1:SA:124:VAL:HG22	1.91	0.52
9:SL:78:THR:HG22	9:SL:79:LYS:HG3	1.91	0.52
40:L5:1414:C:H2'	40:L5:1415:G:C8	2.42	0.52
40:L5:2411:C:H2'	40:L5:2412:A:C8	2.44	0.52
40:L5:4238:G:H2'	40:L5:4239:A:C8	2.44	0.52
2:SB:138:PHE:HB3	2:SB:213:ARG:HH21	1.75	0.52
8:SJ:124:HIS:CG	18:Se:35:ARG:HE	2.28	0.52
17:Sb:34:ASP:HB2	17:Sb:80:ARG:HB2	1.91	0.52
19:S2:1679:A:H5''	33:Sc:20:ARG:HH22	1.74	0.52
40:L5:2102:G:H1'	40:L5:2103:G:N7	2.25	0.52
40:L5:4106:G:H3'	40:L5:4107:G:H8	1.75	0.52
40:L5:4991:U:H2'	40:L5:4992:G:H8	1.74	0.52
77:Ll:12:PHE:HE2	77:Ll:51:LEU:HD22	1.75	0.52
83:Ls:14:PHE:HZ	83:Ls:63:LYS:HB3	1.74	0.52
1:SA:210:ILE:HG12	22:SR:80:ARG:HG2	1.91	0.52
15:SY:55:ILE:HG23	15:SY:75:ILE:HG22	1.91	0.52
19:S2:1202:U:H2'	19:S2:1203:G:C8	2.45	0.52
40:L5:418:A:C2	42:L8:17:A:H1'	2.45	0.52
40:L5:3599:A:H2'	40:L5:3600:G:C8	2.45	0.52
40:L5:3736:A:H2'	40:L5:3737:A:C8	2.45	0.52
43:LA:140:ASN:HD21	43:LA:143:THR:HG22	1.74	0.52
46:LD:64:ILE:HD13	46:LD:109:LEU:HD22	1.90	0.52
49:LG:30:PRO:HG2	65:LZ:124:THR:HA	1.91	0.52
61:LU:80:LYS:HZ1	61:LU:109:SER:H	1.58	0.52
5:SG:7:PHE:HB3	5:SG:10:THR:HG22	1.92	0.52
10:SN:66:VAL:HG13	10:SN:67:THR:HG23	1.92	0.52
11:SO:98:ARG:HH21	11:SO:134:PRO:HG2	1.75	0.52
19:S2:352:U:H2'	19:S2:353:C:C6	2.45	0.52
19:S2:848:U:H2'	19:S2:849:A:H8	1.74	0.52
19:S2:1205:C:H2'	19:S2:1206:G:C8	2.44	0.52
19:S2:1529:C:H4'	30:ST:89:PRO:HG3	1.92	0.52
19:S2:1550:G:H3'	19:S2:1579:A:H61	1.75	0.52
19:S2:1562:C:H2'	19:S2:1563:G:H8	1.75	0.52
22:SR:81:ARG:C	22:SR:83:ASN:H	2.18	0.52
35:Sf:106:TYR:HD2	35:Sf:114:ILE:HD11	1.75	0.52
37:At:15:G:H22	37:At:48:C:N4	2.07	0.52
38:Pt:43:A:H2'	38:Pt:44:A:C8	2.46	0.52
40:L5:423:G:H5'	57:LP:26:PHE:HZ	1.74	0.52
40:L5:724:C:H1'	45:LC:343:GLN:HG2	1.91	0.52
40:L5:2777:G:H5''	40:L5:2778:G:H5'	1.91	0.52
40:L5:3932:U:H2'	40:L5:3933:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:189:ILE:HG22	1:SA:191:ARG:H	1.74	0.51
19:S2:149:A:H3'	19:S2:150:A:H8	1.74	0.51
24:SF:154:LEU:HD23	24:SF:176:GLU:HG3	1.92	0.51
26:SM:64:LEU:HD22	35:Sf:104:LYS:HZ3	1.75	0.51
58:LQ:90:VAL:HB	66:La:80:THR:HG21	1.92	0.51
4:SE:42:LEU:HG	4:SE:109:PHE:HD2	1.75	0.51
10:SN:15:ALA:HB2	17:Sb:21:LYS:HE2	1.92	0.51
32:SZ:50:PHE:CZ	32:SZ:58:LEU:HD22	2.45	0.51
40:L5:1188:C:H2'	40:L5:1189:G:C8	2.45	0.51
50:LH:92:MET:HE2	50:LH:179:ILE:HG22	1.93	0.51
3:SC:211:LYS:HG2	3:SC:215:MET:HE2	1.91	0.51
3:SC:256:TRP:CD2	13:SW:68:ARG:HD3	2.45	0.51
19:S2:121:OMU:HM22	19:S2:122:G:H5'	1.93	0.51
19:S2:907:G:H2'	19:S2:908:A:C8	2.46	0.51
19:S2:1202:U:H2'	19:S2:1203:G:H8	1.75	0.51
19:S2:1740:C:H2'	19:S2:1741:U:C6	2.46	0.51
22:SR:17:ILE:HD11	22:SR:54:VAL:HA	1.91	0.51
40:L5:909:A:H2'	40:L5:910:G:H8	1.73	0.51
40:L5:1086:C:H2'	40:L5:1087:A:H8	1.74	0.51
40:L5:4967:A:H2'	40:L5:4968:A:C8	2.46	0.51
55:LN:5:LYS:HD3	55:LN:8:GLN:HE21	1.75	0.51
61:LU:24:ASP:HB3	61:LU:111:GLU:HG2	1.90	0.51
1:SA:85:ARG:HD2	22:SR:81:ARG:HA	1.92	0.51
7:SI:25:ARG:HA	19:S2:448:A:H5''	1.93	0.51
9:SL:75:GLY:HA3	9:SL:88:ILE:HD12	1.92	0.51
19:S2:561:A:H2'	19:S2:562:U:C6	2.45	0.51
40:L5:264:C:H2'	40:L5:265:C:C4	2.46	0.51
40:L5:679:C:H2'	40:L5:680:G:H8	1.74	0.51
40:L5:4688:C:H2'	40:L5:4689:PSU:C6	2.46	0.51
3:SC:261:PHE:HB3	12:SV:33:GLN:NE2	2.25	0.51
18:Se:58:ASN:ND2	19:S2:606:G:H1'	2.26	0.51
19:S2:51:U:H2'	19:S2:52:G:H8	1.75	0.51
19:S2:327:G:H5''	19:S2:328:U:C2	2.45	0.51
19:S2:1218:C:H2'	19:S2:1219:C:C6	2.46	0.51
19:S2:1398:G:H22	19:S2:1448:A:H2	1.58	0.51
36:Sg:249:CYS:HB3	36:Sg:258:ILE:HD13	1.93	0.51
38:Pt:52:G:H2'	38:Pt:53:G:C8	2.46	0.51
40:L5:3910:C:H2'	40:L5:3911:C:C6	2.46	0.51
40:L5:4260:U:H2'	40:L5:4261:C:H6	1.75	0.51
40:L5:4537:C:H2'	40:L5:4538:G:C8	2.45	0.51
14:SX:66:ILE:HG13	18:Se:5:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Sb:64:CYS:HB2	17:Sb:71:ALA:HB1	1.93	0.51
19:S2:399:C:H5	19:S2:680:G:H5''	1.76	0.51
19:S2:639:C:H2'	19:S2:640:A:C8	2.45	0.51
19:S2:1203:G:H2'	19:S2:1204:A:H8	1.76	0.51
19:S2:1421:A:H5''	19:S2:1422:G:H2'	1.93	0.51
40:L5:462:G:H2'	40:L5:463:A:C8	2.46	0.51
40:L5:2539:C:H2'	40:L5:2540:C:C6	2.46	0.51
40:L5:3656:A:H5''	43:LA:245:ARG:HH12	1.75	0.51
44:LB:300:LYS:HG3	44:LB:311:ASP:HA	1.92	0.51
55:LN:116:LEU:HD22	55:LN:135:ILE:HD11	1.92	0.51
14:SX:9:THR:HG22	19:S2:681:PSU:H4'	1.92	0.51
15:SY:57:VAL:HB	15:SY:60:PHE:HE2	1.75	0.51
19:S2:201:C:H3'	19:S2:202:G:H21	1.75	0.51
19:S2:1101:U:H2'	19:S2:1102:G:C8	2.46	0.51
21:LW:56:ARG:HE	21:LW:61:LYS:HB2	1.75	0.51
23:SD:8:LYS:HB3	34:Sd:34:TYR:CE1	2.44	0.51
28:SQ:130:LYS:HA	28:SQ:137:ALA:HA	1.92	0.51
40:L5:318:A:H2'	40:L5:319:A:H8	1.75	0.51
40:L5:1500:A:H5''	40:L5:1501:C:H5''	1.92	0.51
40:L5:4121:G:H21	43:LA:46:LYS:HD2	1.74	0.51
40:L5:4591:U:H2'	40:L5:4592:C:C6	2.46	0.51
42:L8:86:U:H5'	73:Lh:7:ARG:NH2	2.25	0.51
61:LU:63:ILE:HD11	61:LU:70:ILE:HG22	1.93	0.51
1:SA:32:PHE:CD1	19:S2:1097:G:H4'	2.46	0.51
11:SO:44:VAL:HG13	11:SO:53:ILE:HB	1.93	0.51
24:SF:56:TYR:HA	24:SF:62:ARG:HH21	1.76	0.51
40:L5:1095:A:H2'	40:L5:1096:C:H6	1.76	0.51
40:L5:1683:PSU:H2'	40:L5:1684:A:C8	2.45	0.51
40:L5:2303:C:H5''	70:Le:104:SER:HB3	1.93	0.51
47:LE:243:THR:HG22	47:LE:245:GLN:H	1.75	0.51
66:La:36:GLY:HA3	66:La:40:HIS:CE1	2.45	0.51
15:SY:21:LYS:HD2	15:SY:75:ILE:HD11	1.92	0.51
19:S2:564:A:H2'	19:S2:565:G:O4'	2.11	0.51
19:S2:929:G:H2'	19:S2:930:C:O4'	2.10	0.51
19:S2:1667:U:H2'	19:S2:1668:U:C6	2.46	0.51
21:LW:5:LEU:HD12	21:LW:30:GLN:NE2	2.26	0.51
40:L5:318:A:H2'	40:L5:319:A:C8	2.46	0.51
40:L5:500:G:H1'	40:L5:504:G:H3'	1.93	0.51
40:L5:2400:G:H21	72:Lg:6:THR:HG22	1.76	0.51
42:L8:141:C:H2'	42:L8:142:U:C6	2.45	0.51
1:SA:157:VAL:HG11	1:SA:160:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SL:111:VAL:HG12	9:SL:140:PHE:HB2	1.93	0.51
19:S2:587:A:H5'	19:S2:592:C:H41	1.76	0.51
19:S2:588:G:H4'	19:S2:589:G:H5'	1.93	0.51
19:S2:689:U:H3'	19:S2:690:G:H21	1.76	0.51
19:S2:1797:U:H2'	19:S2:1798:C:C6	2.46	0.51
22:SR:20:TYR:HD2	22:SR:23:ARG:HD3	1.76	0.51
23:SD:105:LEU:HD13	23:SD:122:VAL:HG21	1.92	0.51
37:At:50:U:H3	37:At:64:G:H1	1.58	0.51
40:L5:1404:G:N7	40:L5:1408:G:N2	2.59	0.51
58:LQ:6:ARG:HH12	67:Lb:18:ARG:HG2	1.74	0.51
1:SA:41:ARG:HD2	1:SA:47:TYR:CZ	2.47	0.50
1:SA:198:MET:HE1	1:SA:200:ASP:HB2	1.91	0.50
7:SI:164:GLU:HA	7:SI:167:GLN:HG2	1.92	0.50
14:SX:60:LYS:HE3	14:SX:116:PRO:HB3	1.92	0.50
19:S2:29:G:H2'	19:S2:30:C:C6	2.46	0.50
19:S2:115:U:H2'	19:S2:116:OMU:C6	2.41	0.50
19:S2:543:C:H3'	19:S2:544:G:C8	2.46	0.50
19:S2:924:G:H1	19:S2:1018:U:H3	1.59	0.50
19:S2:1743:G:N2	19:S2:1791:A:H62	2.09	0.50
21:LW:96:GLN:HB3	21:LW:100:VAL:HB	1.93	0.50
26:SM:52:LEU:HD11	26:SM:62:VAL:HG12	1.91	0.50
29:SS:24:ARG:HA	29:SS:55:ARG:HH11	1.75	0.50
47:LE:95:PRO:HA	47:LE:104:THR:HG22	1.92	0.50
53:LL:140:SER:HA	53:LL:143:GLU:HG2	1.92	0.50
61:LU:56:LEU:HD11	61:LU:63:ILE:HG22	1.94	0.50
73:Lh:12:LYS:HB3	73:Lh:16:GLU:HG3	1.93	0.50
19:S2:543:C:H3'	19:S2:544:G:H8	1.75	0.50
19:S2:927:C:H2'	19:S2:928:G:H8	1.76	0.50
19:S2:1644:C:H4'	28:SQ:140:ARG:HB2	1.92	0.50
36:Sg:232:GLY:HA2	36:Sg:257:LYS:HZ1	1.75	0.50
37:At:21:A:H61	37:At:46:G:H2'	1.76	0.50
40:L5:1095:A:H2'	40:L5:1096:C:C6	2.46	0.50
40:L5:2870:A:H2'	40:L5:2871:A:C8	2.46	0.50
1:SA:84:GLN:HG2	1:SA:100:ALA:HB1	1.93	0.50
2:SB:63:LYS:HZ2	2:SB:91:VAL:H	1.58	0.50
5:SG:7:PHE:HE2	5:SG:9:ALA:HB3	1.76	0.50
10:SN:47:PRO:HA	10:SN:50:ILE:HD12	1.93	0.50
37:At:69:A:H2'	37:At:70:A:C8	2.46	0.50
40:L5:497:G:N2	40:L5:498:C:H41	2.09	0.50
61:LU:65:ARG:HG2	61:LU:67:LYS:H	1.76	0.50
3:SC:81:ILE:HG21	3:SC:88:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SG:158:VAL:HG21	21:LW:82:ILE:HD11	1.93	0.50
15:SY:45:ALA:HB2	15:SY:55:ILE:HG13	1.93	0.50
15:SY:113:ARG:HG3	15:SY:127:ALA:HB1	1.94	0.50
19:S2:329:G:H2'	19:S2:330:G:H8	1.76	0.50
19:S2:484:A2M:H8	19:S2:484:A2M:O5'	2.12	0.50
40:L5:1645:C:H2'	40:L5:1646:A:C8	2.46	0.50
40:L5:2838:G:H5'	44:LB:247:GLY:HA3	1.93	0.50
43:LA:107:MET:HB3	43:LA:111:THR:HG21	1.93	0.50
51:LI:91:LEU:HD12	51:LI:135:ILE:HG23	1.92	0.50
61:LU:60:VAL:HG13	61:LU:61:VAL:HG23	1.94	0.50
19:S2:166:A2M:H2'	19:S2:167:G:C8	2.43	0.50
19:S2:952:G:H2'	19:S2:953:C:C6	2.47	0.50
40:L5:702:U:H2'	40:L5:703:G:O4'	2.12	0.50
40:L5:2484:A:N6	40:L5:2494:U:H3	2.10	0.50
40:L5:2495:U:H2'	40:L5:2496:G:C8	2.46	0.50
40:L5:2789:A:H1'	77:Ll:45:ARG:HH22	1.77	0.50
40:L5:4257:A:H2	52:LJ:27:GLY:HA2	1.76	0.50
40:L5:4619:U:H2'	40:L5:4620:OMU:H6	1.94	0.50
51:LI:76:MET:HE2	51:LI:138:ILE:HG21	1.93	0.50
53:LL:153:PRO:HG2	53:LL:156:PRO:HB3	1.94	0.50
64:LY:34:LEU:HD21	64:LY:47:MET:HB2	1.94	0.50
7:SI:36:THR:HG22	7:SI:96:LEU:HD12	1.92	0.50
19:S2:51:U:H2'	19:S2:52:G:C8	2.47	0.50
19:S2:1010:G:H2'	19:S2:1011:A:C8	2.47	0.50
19:S2:1337:4AC:H2'	19:S2:1338:G:C8	2.47	0.50
19:S2:1692:U:H2'	19:S2:1693:G:C8	2.47	0.50
36:Sg:67:SER:HG	36:Sg:83:TRP:CD1	2.30	0.50
40:L5:121:A:H62	40:L5:152:U:H3	1.59	0.50
55:LN:146:PRO:HB2	73:Lh:104:THR:HG23	1.93	0.50
77:Ll:43:HIS:HB3	77:Ll:46:ARG:HD3	1.93	0.50
11:SO:95:ILE:HB	11:SO:129:ILE:HG22	1.93	0.50
19:S2:5:U:H2'	19:S2:6:G:H8	1.76	0.50
19:S2:349:A:H2'	19:S2:350:C:C6	2.47	0.50
19:S2:1627:C:H2'	19:S2:1628:C:H6	1.76	0.50
29:SS:114:LEU:HD13	29:SS:117:ILE:HD11	1.94	0.50
30:ST:76:THR:HG23	30:ST:94:ARG:HD3	1.93	0.50
30:ST:104:LEU:HD22	30:ST:121:ARG:HD2	1.94	0.50
40:L5:4364:G:H2'	40:L5:4365:C:H6	1.76	0.50
40:L5:4392:OMG:HM21	40:L5:4394:A:H2'	1.94	0.50
40:L5:4459:U:H2'	40:L5:4460:U:C6	2.46	0.50
43:LA:229:ALA:HB3	43:LA:234:LYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:LO:61:ARG:HA	56:LO:70:PRO:HD2	1.92	0.50
5:SG:116:LYS:HE3	5:SG:125:THR:HG21	1.93	0.50
19:S2:300:U:H2'	19:S2:301:A:C8	2.47	0.50
40:L5:135:G:N7	73:Lh:97:LYS:HG2	2.27	0.50
40:L5:2018:C:H2'	40:L5:2019:C:C6	2.46	0.50
47:LE:264:ILE:HD11	47:LE:267:LEU:HD22	1.94	0.50
83:Ls:18:ILE:HG12	83:Ls:68:HIS:CE1	2.46	0.50
84:Lt:16:ARG:HE	84:Lt:17:CYS:N	2.08	0.50
19:S2:414:A:H2'	19:S2:415:A:H8	1.76	0.50
19:S2:1274:G:H4'	25:SK:47:LYS:HD2	1.93	0.50
36:Sg:166:VAL:HG12	36:Sg:176:VAL:HG12	1.93	0.50
36:Sg:247:TRP:HB3	36:Sg:258:ILE:HD11	1.94	0.50
40:L5:730:G:C5	48:LF:73:ARG:HD3	2.47	0.50
40:L5:4113:U:H3'	40:L5:4114:C:H4'	1.93	0.50
40:L5:4743:G:H2'	40:L5:4744:A:C8	2.46	0.50
53:LL:59:VAL:HG21	53:LL:73:GLY:HA3	1.93	0.50
70:Le:89:LEU:HD13	70:Le:118:LEU:HD22	1.93	0.50
77:Ll:12:PHE:CE2	77:Ll:51:LEU:HD22	2.47	0.50
19:S2:1298:G:H1'	27:SP:79:HIS:HB2	1.94	0.49
19:S2:1680:G:H2'	19:S2:1681:U:C6	2.47	0.49
40:L5:179:G:H2'	40:L5:180:C:C6	2.47	0.49
40:L5:1759:G:O6	40:L5:1773:U:O4	2.30	0.49
54:LM:6:PHE:HB3	59:LS:151:LYS:HG3	1.93	0.49
6:SH:31:GLU:HA	6:SH:37:LYS:HD2	1.93	0.49
19:S2:496:C:H2'	19:S2:497:C:H6	1.77	0.49
19:S2:1468:C:H2'	19:S2:1469:A:H8	1.77	0.49
21:LW:44:ARG:HD3	40:L5:3615:G:H1'	1.94	0.49
23:SD:172:VAL:HG22	23:SD:185:LYS:HG2	1.95	0.49
36:Sg:121:VAL:HG11	36:Sg:165:ILE:HD11	1.94	0.49
38:Pt:22:U:H2'	38:Pt:23:C:H6	1.77	0.49
40:L5:10:A:H2'	40:L5:11:G:C8	2.47	0.49
40:L5:455:C:O2'	40:L5:456:C:H5'	2.11	0.49
40:L5:730:G:C4	48:LF:73:ARG:HD3	2.47	0.49
40:L5:3865:A:H61	40:L5:3881:G:H1	1.58	0.49
43:LA:36:GLU:HG3	43:LA:91:GLY:HA2	1.94	0.49
45:LC:266:THR:HG22	45:LC:267:TRP:H	1.78	0.49
64:LY:4:ASN:HB3	64:LY:7:VAL:HG12	1.94	0.49
13:SW:101:PHE:HA	13:SW:113:HIS:CE1	2.46	0.49
19:S2:71:G:H2'	19:S2:72:C:H4'	1.93	0.49
32:SZ:73:VAL:HG13	32:SZ:79:ILE:HD11	1.93	0.49
40:L5:325:U:H2'	40:L5:326:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:2749:C:H2'	40:L5:2750:G:C8	2.48	0.49
40:L5:4347:G:H2'	40:L5:4348:A:C8	2.48	0.49
2:SB:45:GLY:HA3	11:SO:47:LEU:HD11	1.94	0.49
4:SE:123:LEU:HB2	4:SE:236:ILE:HD11	1.93	0.49
5:SG:164:LYS:HB2	5:SG:167:LYS:HG2	1.93	0.49
6:SH:43:LEU:HD11	6:SH:71:SER:HB2	1.94	0.49
18:Se:39:ASN:HB3	19:S2:551:U:H4'	1.93	0.49
27:SP:81:ARG:HB2	27:SP:117:GLY:HA3	1.95	0.49
37:At:51:C:H2'	37:At:52:G:C8	2.47	0.49
40:L5:1241:C:H41	67:Lb:114:LYS:HE3	1.76	0.49
21:LW:2:LYS:HZ3	62:LV:92:ASP:HB2	1.77	0.49
24:SF:127:ARG:HG3	24:SF:136:ARG:HB3	1.94	0.49
19:S2:649:PSU:H2'	19:S2:650:A:C8	2.47	0.49
19:S2:943:U:H2'	19:S2:944:A:C8	2.46	0.49
19:S2:996:A:H2'	19:S2:997:A:C8	2.47	0.49
19:S2:1232:PSU:H2'	19:S2:1233:G:C8	2.47	0.49
34:Sd:21:CYS:HB3	34:Sd:26:ASN:H	1.77	0.49
40:L5:1076:C:H2'	40:L5:1077:C:C6	2.47	0.49
40:L5:1754:U:H2'	40:L5:1755:C:C6	2.48	0.49
40:L5:4723:A:H2'	40:L5:4724:A:C8	2.47	0.49
41:L7:4:U:H2'	41:L7:5:A:C8	2.46	0.49
3:SC:104:ASP:HA	3:SC:130:ILE:HG22	1.94	0.49
9:SL:13:GLN:HB2	9:SL:16:ILE:HD12	1.93	0.49
13:SW:83:LEU:HD12	19:S2:805:U:H5''	1.94	0.49
19:S2:1673:U:H5''	28:SQ:78:VAL:HG12	1.94	0.49
40:L5:1669:A:H4'	40:L5:1685:G:N2	2.27	0.49
40:L5:5062:G:H2'	40:L5:5063:G:H8	1.78	0.49
43:LA:131:GLY:H	43:LA:169:VAL:HG13	1.78	0.49
46:LD:103:LEU:HG	46:LD:247:ILE:HG21	1.93	0.49
53:LL:145:LYS:HG3	53:LL:146:LEU:HD12	1.94	0.49
19:S2:28:U:H2'	19:S2:29:G:C8	2.47	0.49
19:S2:694:G:H2'	19:S2:695:C:O4'	2.13	0.49
19:S2:875:A:H61	19:S2:911:C:H42	1.61	0.49
19:S2:927:C:H2'	19:S2:928:G:C8	2.47	0.49
36:Sg:68:ASP:HB3	36:Sg:111:VAL:HG12	1.95	0.49
40:L5:163:A:H2'	40:L5:164:G:H8	1.77	0.49
40:L5:4457:PSU:H1'	44:LB:252:ALA:HB3	1.95	0.49
60:LT:75:VAL:HG22	60:LT:88:ARG:HG2	1.95	0.49
67:Lb:116:LEU:HG	67:Lb:117:ARG:HH21	1.77	0.49
5:SG:136:LYS:HB2	19:S2:65:C:H41	1.77	0.49
19:S2:1425:G:H2'	19:S2:1426:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LW:9:SER:HA	21:LW:52:THR:HG23	1.94	0.49
40:L5:93:G:H2'	40:L5:94:A:C8	2.48	0.49
40:L5:261:G:H2'	40:L5:262:G:C8	2.47	0.49
40:L5:1333:A:H2'	40:L5:1334:A:H8	1.78	0.49
40:L5:2745:A:H2'	40:L5:2746:A:H8	1.78	0.49
52:LJ:113:ILE:HG12	52:LJ:119:TYR:HD1	1.78	0.49
55:LN:113:LEU:HB2	55:LN:134:LEU:HD12	1.95	0.49
57:LP:109:VAL:HA	57:LP:112:LEU:HD13	1.94	0.49
69:Ld:26:THR:HB	69:Ld:85:ARG:HH11	1.77	0.49
1:SA:111:GLN:HA	1:SA:116:PHE:CG	2.48	0.49
4:SE:201:HIS:HB2	4:SE:204:SER:HB3	1.95	0.49
40:L5:1307:A:H2'	40:L5:1308:C:C6	2.47	0.49
40:L5:1348:U:H2'	40:L5:1349:G:H8	1.78	0.49
53:LL:150:LEU:HD23	53:LL:154:VAL:HG22	1.95	0.49
59:LS:20:PRO:HA	59:LS:23:HIS:HE1	1.78	0.49
2:SB:152:LYS:HD3	22:SR:133:GLY:HA3	1.95	0.48
19:S2:1004:PSU:H2'	19:S2:1005:G:H8	1.78	0.48
19:S2:1432:U:H2'	19:S2:1438:A:C8	2.48	0.48
27:SP:32:GLN:HA	27:SP:35:GLN:HG2	1.95	0.48
40:L5:1308:C:H2'	40:L5:1309:C:C6	2.48	0.48
40:L5:4098:A:H2'	40:L5:4099:G:H4'	1.94	0.48
40:L5:4954:G:H2'	40:L5:4955:A:H8	1.78	0.48
45:LC:106:LYS:HD3	45:LC:108:TRP:CZ2	2.48	0.48
49:LG:63:LEU:HD22	55:LN:33:LEU:HD21	1.94	0.48
11:SO:56:VAL:HG23	11:SO:60:MET:SD	2.53	0.48
19:S2:162:C:H2'	19:S2:163:U:O4'	2.13	0.48
19:S2:644:OMG:HM23	19:S2:644:OMG:H1'	1.63	0.48
31:SU:24:LEU:HD22	31:SU:112:VAL:HG12	1.95	0.48
40:L5:4389:C:H2'	40:L5:4390:A:C8	2.48	0.48
40:L5:4742:G:H2'	40:L5:4743:G:H8	1.77	0.48
42:L8:67:U:H2'	42:L8:68:G:H8	1.78	0.48
50:LH:106:GLN:HB2	50:LH:111:LEU:HB3	1.94	0.48
57:LP:122:ALA:HB3	57:LP:143:PRO:HG2	1.95	0.48
81:Lp:38:THR:HA	81:Lp:45:THR:HA	1.95	0.48
19:S2:1688:C:H2'	19:S2:1689:C:H6	1.77	0.48
40:L5:441:G:H2'	40:L5:442:G:H8	1.79	0.48
40:L5:665:C:H4'	40:L5:666:G:H5'	1.95	0.48
40:L5:2520:C:H2'	40:L5:2521:G:H8	1.78	0.48
40:L5:2608:G:H2'	40:L5:2609:G:H8	1.78	0.48
40:L5:4920:C:H2'	40:L5:4921:C:C6	2.48	0.48
49:LG:48:LYS:HD2	63:LX:42:THR:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:LX:124:VAL:HG22	63:LX:138:VAL:HG13	1.95	0.48
1:SA:148:CYS:CB	1:SA:163:CYS:H	2.22	0.48
13:SW:101:PHE:HA	13:SW:113:HIS:HE1	1.79	0.48
19:S2:1337:4AC:H2'	19:S2:1338:G:H8	1.78	0.48
36:Sg:153:CYS:SG	36:Sg:198:VAL:HG12	2.53	0.48
38:Pt:22:U:H2'	38:Pt:23:C:C6	2.48	0.48
40:L5:1333:A:H2'	40:L5:1334:A:C8	2.48	0.48
40:L5:2764:A:H2'	40:L5:2765:A:C8	2.47	0.48
40:L5:2765:A:H2'	40:L5:2766:A:C8	2.48	0.48
40:L5:2884:G:H2'	40:L5:2885:A:C8	2.48	0.48
40:L5:4251:A:H5''	52:LJ:108:GLY:HA3	1.94	0.48
49:LG:209:SER:HA	49:LG:212:LYS:HG3	1.95	0.48
59:LS:20:PRO:HA	59:LS:23:HIS:CE1	2.49	0.48
83:Ls:47:LEU:HG	83:Ls:51:ALA:HB3	1.95	0.48
8:SJ:2:PRO:O	19:S2:509:OMG:H5''	2.14	0.48
30:ST:62:ARG:HH12	30:ST:66:LEU:HD11	1.78	0.48
38:Pt:27:U:H2'	38:Pt:28:U:H6	1.79	0.48
40:L5:1084:C:H2'	40:L5:1085:C:C6	2.48	0.48
40:L5:4739:C:H2'	40:L5:4740:G:H5'	1.95	0.48
78:Lm:99:CYS:HB2	78:Lm:114:LYS:HE3	1.94	0.48
2:SB:150:ILE:HG12	19:S2:1124:C:H5''	1.96	0.48
19:S2:495:U:H2'	19:S2:496:C:O4'	2.13	0.48
19:S2:1098:C:H2'	19:S2:1099:G:C8	2.49	0.48
20:LR:28:GLU:HG3	20:LR:49:LEU:HD22	1.96	0.48
23:SD:74:GLN:HB2	23:SD:84:VAL:HG11	1.94	0.48
36:Sg:128:THR:HG22	36:Sg:143:GLN:HA	1.95	0.48
38:Pt:18:G:H21	38:Pt:58:A:H5'	1.77	0.48
40:L5:691:C:H2'	40:L5:692:A:C8	2.48	0.48
40:L5:1248:C:H2'	40:L5:1249:C:C6	2.48	0.48
40:L5:1867:A:H2'	40:L5:1868:A:C8	2.49	0.48
40:L5:2568:C:H2'	40:L5:2569:G:H8	1.78	0.48
40:L5:4523:A2M:H2'	40:L5:4559:A:N7	2.29	0.48
56:LO:10:ASP:HB2	56:LO:117:ARG:HB3	1.94	0.48
83:Ls:20:LEU:HD21	83:Ls:52:VAL:HG11	1.94	0.48
3:SC:102:LEU:HD23	3:SC:130:ILE:HB	1.94	0.48
19:S2:348:A:H2'	19:S2:349:A:C8	2.48	0.48
19:S2:432:G:H2'	19:S2:433:A:C8	2.48	0.48
40:L5:1662:C:H2'	40:L5:1663:C:C6	2.48	0.48
40:L5:1806:G:H2'	40:L5:1807:C:C6	2.49	0.48
40:L5:2884:G:H2'	40:L5:2885:A:H8	1.78	0.48
40:L5:3656:A:H2'	40:L5:3657:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:3946:G:N1	40:L5:4067:U:N3	2.61	0.48
54:LM:6:PHE:H	54:LM:11:ARG:NH2	2.11	0.48
60:LT:44:GLY:HA2	60:LT:95:HIS:HB3	1.96	0.48
69:Ld:36:VAL:HG21	69:Ld:44:ARG:HG2	1.96	0.48
1:SA:85:ARG:NH2	1:SA:205:ARG:HG3	2.28	0.48
5:SG:131:ARG:HB2	21:LW:82:ILE:HG22	1.96	0.48
19:S2:634:A:H2'	19:S2:635:G:C8	2.49	0.48
19:S2:1622:U:H3'	19:S2:1623:A:H4'	1.96	0.48
20:LR:148:ASP:HA	20:LR:151:ARG:HB3	1.96	0.48
26:SM:79:VAL:HG11	26:SM:85:LEU:HB2	1.94	0.48
40:L5:1197:C:H2'	40:L5:1198:G:C8	2.48	0.48
40:L5:2448:G:H2'	40:L5:2449:A:C8	2.49	0.48
40:L5:3870:C:H2'	40:L5:3871:A:H8	1.77	0.48
4:SE:85:GLY:O	4:SE:101:LEU:HD23	2.14	0.48
9:SL:126:VAL:HG12	9:SL:145:VAL:HG22	1.96	0.48
19:S2:1128:C:H2'	19:S2:1129:G:C8	2.49	0.48
19:S2:1804:U:H2'	19:S2:1805:G:C8	2.49	0.48
22:SR:79:GLU:HG2	22:SR:80:ARG:HD3	1.95	0.48
39:CI:79:ARG:HH12	40:L5:2708:U:H4'	1.77	0.48
40:L5:426:A:H2'	40:L5:427:A:C8	2.48	0.48
40:L5:1086:C:H2'	40:L5:1087:A:C8	2.48	0.48
40:L5:1332:C:H5''	70:Le:29:VAL:HB	1.96	0.48
40:L5:2019:C:H2'	40:L5:2020:U:H6	1.77	0.48
81:Lp:75:SER:O	81:Lp:79:VAL:HG23	2.14	0.48
19:S2:678:U:H2'	19:S2:679:A:H8	1.78	0.48
19:S2:1108:G:H21	22:SR:126:MET:HE1	1.79	0.48
19:S2:1591:C:H2'	19:S2:1592:C:H6	1.78	0.48
22:SR:128:PHE:HE1	22:SR:129:LYS:HE3	1.78	0.48
24:SF:141:VAL:HA	33:Sc:47:LYS:HG2	1.96	0.48
40:L5:262:G:H2'	40:L5:263:G:C8	2.44	0.48
40:L5:4188:U:H2'	40:L5:4189:U:C6	2.49	0.48
40:L5:4524:G:C2	44:LB:252:ALA:HB1	2.49	0.48
44:LB:224:LYS:HG2	44:LB:340:THR:HG22	1.96	0.48
46:LD:73:MET:HE3	46:LD:73:MET:HB3	1.78	0.48
2:SB:60:ASP:HA	2:SB:63:LYS:HD2	1.96	0.47
5:SG:2:LYS:HB3	5:SG:15:LEU:HD11	1.96	0.47
19:S2:85:A:H2'	19:S2:86:C:H6	1.77	0.47
19:S2:458:A:H2'	19:S2:459:C:C6	2.49	0.47
19:S2:573:U:O2	19:S2:576:A2M:H8	2.14	0.47
19:S2:956:G:H2'	19:S2:957:A:H8	1.78	0.47
19:S2:1330:G:H4'	19:S2:1331:C:H3'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:683:C:H2'	40:L5:684:G:O4'	2.14	0.47
40:L5:3718:A2M:HM'3	40:L5:3718:A2M:H1'	1.53	0.47
2:SB:52:THR:HG23	2:SB:57:ILE:HA	1.96	0.47
19:S2:155:G:H2'	19:S2:156:G:H8	1.79	0.47
19:S2:694:G:H5''	19:S2:730:C:H5	1.79	0.47
19:S2:1468:C:H2'	19:S2:1469:A:C8	2.49	0.47
19:S2:1858:G:H2'	19:S2:1859:A:C8	2.48	0.47
40:L5:1365:C:H2'	40:L5:1366:G:H3'	1.94	0.47
40:L5:2543:A:H2	40:L5:2773:G:H22	1.62	0.47
40:L5:3870:C:H2'	40:L5:3871:A:C8	2.49	0.47
40:L5:3947:A:C6	40:L5:4068:U:H1'	2.49	0.47
50:LH:101:ILE:HG23	50:LH:114:ILE:HG23	1.97	0.47
19:S2:24:C:HO2'	19:S2:25:A:H8	1.62	0.47
19:S2:1079:C:H4'	19:S2:1182:A:H61	1.79	0.47
19:S2:1845:A:H2'	19:S2:1846:G:C8	2.49	0.47
32:SZ:103:HIS:CE1	32:SZ:104:ARG:HG2	2.49	0.47
40:L5:299:C:H2'	40:L5:300:A:C8	2.49	0.47
40:L5:1437:C:H1'	40:L5:2098:G:H3'	1.96	0.47
40:L5:1972:G:C6	40:L5:1973:G:O6	2.67	0.47
40:L5:5006:U:H4'	40:L5:5007:A:H5'	1.95	0.47
43:LA:7:GLY:HA2	43:LA:10:LYS:HG3	1.96	0.47
47:LE:119:GLU:HG3	70:Le:7:LEU:HD22	1.96	0.47
47:LE:190:HIS:HB3	47:LE:193:PHE:HD1	1.78	0.47
50:LH:187:VAL:HG12	50:LH:188:GLN:HG3	1.97	0.47
1:SA:74:VAL:HG23	1:SA:121:LEU:HB3	1.96	0.47
2:SB:125:VAL:HG21	2:SB:173:THR:HB	1.96	0.47
7:SI:81:VAL:HG22	7:SI:102:VAL:HG12	1.96	0.47
19:S2:166:A2M:HM'3	19:S2:166:A2M:H1'	1.46	0.47
19:S2:309:G:H21	19:S2:340:C:H1'	1.80	0.47
19:S2:674:C:H2'	19:S2:675:U:C6	2.50	0.47
19:S2:1801:A:H2'	19:S2:1802:C:C6	2.49	0.47
24:SF:28:VAL:HG11	24:SF:109:LEU:HB2	1.95	0.47
33:Sc:10:LYS:HE2	33:Sc:34:PHE:CE2	2.50	0.47
40:L5:717:U:H2'	40:L5:718:C:C6	2.49	0.47
40:L5:1406:G:C6	40:L5:1408:G:H5'	2.50	0.47
40:L5:1577:G:O2'	40:L5:1612:G:H4'	2.14	0.47
40:L5:1749:A:H2'	40:L5:1750:G:C8	2.50	0.47
40:L5:1806:G:H2'	40:L5:1807:C:H6	1.79	0.47
40:L5:4910:G:H22	56:LO:107:GLY:HA3	1.79	0.47
6:SH:126:HIS:CE1	6:SH:181:THR:HG23	2.49	0.47
19:S2:835:C:H4'	19:S2:836:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Pt:50:U:O4	38:Pt:64:G:O6	2.32	0.47
40:L5:158:A:H5''	40:L5:159:C:H2'	1.95	0.47
40:L5:1733:G:N3	40:L5:4214:A:H2'	2.29	0.47
3:SC:165:VAL:HG21	3:SC:217:ALA:HB1	1.96	0.47
3:SC:207:ALA:O	3:SC:210:PRO:HD2	2.14	0.47
19:S2:433:A:H2'	19:S2:434:G:C8	2.49	0.47
28:SQ:42:ILE:HG23	28:SQ:44:PRO:HD2	1.96	0.47
40:L5:71:C:H1'	53:LL:62:PRO:O	2.15	0.47
40:L5:1802:A:H5''	40:L5:1803:G:H5'	1.96	0.47
40:L5:3880:G:H2'	40:L5:3881:G:C8	2.48	0.47
1:SA:37:TYR:CG	1:SA:162:PRO:HG3	2.49	0.47
4:SE:56:LEU:HD11	15:SY:74:MET:HE3	1.96	0.47
4:SE:124:CYS:HB3	4:SE:141:THR:OG1	2.14	0.47
19:S2:5:U:H2'	19:S2:6:G:C8	2.50	0.47
19:S2:925:G:H2'	19:S2:926:A:H8	1.79	0.47
19:S2:1004:PSU:H2'	19:S2:1005:G:C8	2.50	0.47
19:S2:1431:G:H4'	19:S2:1434:C:H41	1.80	0.47
19:S2:1432:U:H2'	19:S2:1438:A:H8	1.79	0.47
19:S2:1609:C:H5''	29:SS:131:VAL:HG22	1.95	0.47
27:SP:26:LEU:HD23	27:SP:87:PRO:HB2	1.96	0.47
31:SU:66:ARG:HH12	31:SU:75:LYS:HA	1.80	0.47
33:Sc:20:ARG:HD3	33:Sc:28:THR:HG22	1.95	0.47
36:Sg:174:VAL:HB	36:Sg:188:HIS:HB2	1.96	0.47
38:Pt:23:C:H2'	38:Pt:24:A:C8	2.50	0.47
40:L5:256:G:H2'	40:L5:257:C:C6	2.50	0.47
40:L5:512:U:O4	40:L5:647:G:O6	2.33	0.47
40:L5:734:G:H22	40:L5:929:A:H2	1.61	0.47
40:L5:1167:C:H42	40:L5:1195:G:H21	1.63	0.47
40:L5:1309:C:H2'	40:L5:1310:C:C6	2.50	0.47
40:L5:1768:C:H2'	40:L5:1770:A:N7	2.30	0.47
40:L5:2017:A:O2'	40:L5:2018:C:H6	1.97	0.47
40:L5:2743:A:H2'	40:L5:2744:A:C8	2.49	0.47
40:L5:3707:U:H2'	40:L5:3708:C:C6	2.50	0.47
40:L5:3861:A:H2'	40:L5:3862:A:H8	1.78	0.47
40:L5:4612:C:C2	50:LH:120:GLU:HB2	2.49	0.47
44:LB:14:LEU:HD22	44:LB:17:LEU:HD21	1.95	0.47
55:LN:104:GLU:HA	55:LN:160:GLU:HG3	1.97	0.47
82:Lr:16:PHE:HB3	82:Lr:27:THR:H	1.78	0.47
12:SV:32:ILE:HG12	12:SV:60:ARG:HD2	1.97	0.47
19:S2:786:G:H2'	19:S2:787:G:C8	2.50	0.47
19:S2:1487:A:H2'	19:S2:1488:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1540:G:H2'	19:S2:1541:G:H8	1.80	0.47
19:S2:1671:G:H2'	19:S2:1672:U:H6	1.80	0.47
40:L5:1563:A:H2'	40:L5:1564:A:C8	2.49	0.47
40:L5:3917:A:H2'	40:L5:3918:G:H8	1.80	0.47
40:L5:4220:6MZ:H8	40:L5:4220:6MZ:OP2	2.15	0.47
40:L5:4743:G:H2'	40:L5:4744:A:H8	1.80	0.47
40:L5:4913:G:H4'	40:L5:4914:C:O5'	2.13	0.47
50:LH:1:MET:HG3	59:LS:141:ALA:HB2	1.97	0.47
61:LU:46:ARG:HH22	61:LU:89:LYS:HE3	1.80	0.47
83:Ls:63:LYS:HA	83:Ls:66:ARG:HB3	1.97	0.47
2:SB:146:ARG:HE	2:SB:206:PRO:HG2	1.79	0.47
5:SG:119:LYS:HZ1	5:SG:121:ILE:HD13	1.80	0.47
9:SL:17:PHE:CG	19:S2:222:U:H5''	2.49	0.47
19:S2:107:A:H2'	19:S2:108:G:C8	2.50	0.47
19:S2:223:C:H2'	19:S2:224:A:H8	1.79	0.47
19:S2:496:C:H2'	19:S2:497:C:C6	2.50	0.47
20:LR:168:GLU:HA	20:LR:171:LYS:HE3	1.97	0.47
26:SM:40:LYS:HG3	35:Sf:129:GLY:HA3	1.96	0.47
40:L5:654:C:C4	40:L5:655:C:N4	2.83	0.47
40:L5:742:G:H2'	40:L5:743:G:H8	1.80	0.47
40:L5:4088:C:H2'	40:L5:4089:G:C8	2.50	0.47
40:L5:4364:G:H2'	40:L5:4365:C:C6	2.49	0.47
42:L8:19:C:H2'	42:L8:20:A:H8	1.77	0.47
44:LB:288:GLY:HA3	44:LB:330:PHE:CE1	2.50	0.47
65:LZ:29:ILE:HG22	65:LZ:31:ASP:H	1.79	0.47
3:SC:167:ARG:HH22	3:SC:176:LYS:HE2	1.79	0.47
3:SC:273:LEU:HB3	3:SC:277:HIS:HB3	1.97	0.47
6:SH:8:ILE:HG13	6:SH:9:VAL:HG23	1.96	0.47
8:SJ:87:LEU:HD13	8:SJ:100:LEU:HD11	1.97	0.47
19:S2:538:U:H2'	19:S2:539:C:C6	2.50	0.47
19:S2:1688:C:H2'	19:S2:1689:C:C6	2.50	0.47
29:SS:127:TRP:HE3	29:SS:129:LEU:HD12	1.80	0.47
37:At:2:U:H2'	37:At:3:C:H6	1.79	0.47
40:L5:2413:U:H2'	40:L5:2414:G:H8	1.80	0.47
40:L5:4584:A:H2'	40:L5:4585:U:O4'	2.14	0.47
45:LC:212:ASN:HD22	45:LC:255:SER:HB3	1.80	0.47
62:LV:112:MET:HG2	62:LV:114:GLY:H	1.78	0.47
63:LX:114:LYS:HE2	63:LX:114:LYS:HB3	1.63	0.47
70:Le:86:GLU:HG3	70:Le:118:LEU:HD11	1.96	0.47
71:Lf:33:VAL:HG13	71:Lf:38:GLU:HB3	1.97	0.47
4:SE:146:THR:HG21	19:S2:122:G:H21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SH:30:LEU:HD13	6:SH:86:LYS:HE2	1.97	0.46
10:SN:124:ARG:HG2	10:SN:127:ARG:HH21	1.81	0.46
15:SY:28:LEU:HG	15:SY:68:LYS:HG2	1.96	0.46
19:S2:1003:U:H2'	19:S2:1004:PSU:C6	2.49	0.46
19:S2:1303:C:H4'	35:Sf:94:LYS:HZ1	1.79	0.46
36:Sg:10:THR:HB	36:Sg:306:LEU:HD11	1.97	0.46
40:L5:162:A:H2'	40:L5:163:A:C8	2.50	0.46
40:L5:4401:G:H2'	40:L5:4402:C:H6	1.79	0.46
46:LD:156:GLY:HA2	46:LD:181:PRO:HG3	1.97	0.46
19:S2:1115:U:H3	19:S2:1118:C:H41	1.61	0.46
19:S2:1398:G:H1'	36:Sg:63:SER:HB2	1.96	0.46
25:SK:60:GLU:HB2	25:SK:69:TRP:CD1	2.50	0.46
40:L5:267:G:H2'	40:L5:268:G:H8	1.80	0.46
40:L5:2032:U:H2'	40:L5:2033:A:C8	2.50	0.46
40:L5:4770:U:H2'	40:L5:4771:C:C6	2.50	0.46
43:LA:115:CYS:SG	43:LA:124:GLY:HA3	2.54	0.46
57:LP:13:LYS:HB3	57:LP:152:GLU:HB2	1.97	0.46
1:SA:5:LEU:HD21	12:SV:41:LYS:HD2	1.95	0.46
19:S2:194:C:H2'	19:S2:195:C:H6	1.80	0.46
19:S2:1199:A:H2'	19:S2:1200:A:C8	2.50	0.46
19:S2:1802:C:H2'	19:S2:1803:U:H6	1.81	0.46
23:SD:68:GLU:HB3	25:SK:70:TYR:CE1	2.51	0.46
26:SM:93:LYS:HD3	26:SM:95:ASP:HB2	1.97	0.46
37:At:29:C:H2'	37:At:30:G:H8	1.80	0.46
40:L5:172:C:H4'	40:L5:173:C:H5'	1.96	0.46
40:L5:400:A2M:HM'3	40:L5:400:A2M:H1'	1.60	0.46
40:L5:1307:A:H2'	40:L5:1308:C:H6	1.80	0.46
40:L5:3641:U:H5	40:L5:3646:A:N7	2.14	0.46
40:L5:3684:G:H2'	40:L5:3685:C:C6	2.51	0.46
40:L5:3910:C:H2'	40:L5:3911:C:H6	1.79	0.46
40:L5:4523:A2M:HM'3	40:L5:4523:A2M:H1'	1.53	0.46
40:L5:4563:U:H2'	40:L5:4564:A:H8	1.81	0.46
43:LA:177:LYS:HD2	81:Lp:69:TRP:CH2	2.50	0.46
44:LB:307:TYR:HD2	44:LB:366:LYS:HA	1.80	0.46
47:LE:207:LYS:HA	47:LE:207:LYS:HD3	1.71	0.46
58:LQ:43:PHE:CD2	58:LQ:133:GLY:HA3	2.50	0.46
63:LX:81:LEU:HG	63:LX:83:THR:HG23	1.97	0.46
19:S2:29:G:H2'	19:S2:30:C:H6	1.80	0.46
19:S2:1093:A:H2'	19:S2:1094:C:C6	2.50	0.46
19:S2:1317:C:H2'	19:S2:1318:G:C8	2.51	0.46
23:SD:32:ASP:HA	23:SD:57:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:2613:C:H4'	72:Lg:2:VAL:HG23	1.96	0.46
1:SA:99:ILE:HD11	1:SA:117:ARG:HH12	1.80	0.46
8:SJ:101:LYS:HA	8:SJ:101:LYS:HD2	1.71	0.46
19:S2:1222:G:H2'	19:S2:1223:A:C8	2.51	0.46
19:S2:1253:A:H4'	19:S2:1254:C:H5''	1.96	0.46
20:LR:139:MET:HE3	20:LR:139:MET:HB3	1.66	0.46
36:Sg:18:VAL:HB	36:Sg:301:GLY:HA3	1.97	0.46
40:L5:74:G:H1'	53:LL:62:PRO:HG3	1.96	0.46
40:L5:737:C:C5	40:L5:739:G:H5''	2.51	0.46
40:L5:4622:A:H4'	44:LB:13:SER:HB2	1.97	0.46
50:LH:92:MET:HB2	50:LH:144:LEU:HB2	1.97	0.46
51:LI:53:VAL:HG11	60:LT:158:PHE:HZ	1.81	0.46
53:LL:183:ARG:HA	53:LL:183:ARG:HD2	1.78	0.46
2:SB:105:LEU:HG	2:SB:213:ARG:HA	1.98	0.46
3:SC:138:GLY:HA3	3:SC:162:ILE:HD13	1.96	0.46
19:S2:680:G:H2'	19:S2:681:PSU:H6	1.79	0.46
19:S2:835:C:H4'	19:S2:836:G:C8	2.50	0.46
19:S2:1539:U:H2'	19:S2:1540:G:C8	2.50	0.46
19:S2:1713:C:H2'	19:S2:1714:U:H6	1.80	0.46
24:SF:60:ARG:HH21	33:Sc:49:PRO:HA	1.80	0.46
28:SQ:62:ARG:HD3	28:SQ:108:ILE:HD12	1.98	0.46
38:Pt:27:U:H2'	38:Pt:28:U:C6	2.51	0.46
40:L5:254:G:H2'	40:L5:255:C:O4'	2.16	0.46
40:L5:4942:C:H4'	47:LE:154:THR:HB	1.97	0.46
55:LN:47:LYS:HD2	55:LN:50:ARG:HH11	1.81	0.46
19:S2:1384:C:H2'	19:S2:1385:G:H8	1.81	0.46
19:S2:1515:G:H2'	19:S2:1516:G:H8	1.81	0.46
21:LW:94:ARG:HA	21:LW:101:ARG:HH21	1.80	0.46
22:SR:98:VAL:HG21	22:SR:117:LEU:HD22	1.98	0.46
27:SP:41:GLN:HG3	27:SP:84:ILE:HG21	1.97	0.46
29:SS:89:ASP:HB3	29:SS:93:GLY:H	1.80	0.46
40:L5:150:U:H3	49:LG:163:PRO:HD2	1.80	0.46
40:L5:956:A:H1'	40:L5:2076:G:H5''	1.98	0.46
40:L5:1306:C:H2'	40:L5:1307:A:C8	2.49	0.46
40:L5:1461:C:H2'	40:L5:1462:A:C8	2.51	0.46
44:LB:258:HIS:HA	44:LB:260:ALA:N	2.30	0.46
54:LM:77:TRP:O	54:LM:81:ASP:HA	2.15	0.46
76:Lk:15:ALA:HA	76:Lk:36:VAL:HG21	1.97	0.46
7:SI:172:LEU:HD12	7:SI:190:LEU:HD13	1.96	0.46
15:SY:87:PRO:HG2	15:SY:90:ARG:HB2	1.96	0.46
16:Sa:82:LYS:NZ	19:S2:1209:A:H5''	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1522:A:N7	27:SP:128:HIS:HB3	2.31	0.46
19:S2:1540:G:H2'	19:S2:1541:G:C8	2.51	0.46
19:S2:1589:A:N1	19:S2:1672:U:H1'	2.31	0.46
23:SD:218:LEU:HD11	36:Sg:189:ILE:HB	1.97	0.46
38:Pt:50:U:O2	38:Pt:64:G:N2	2.41	0.46
40:L5:690:C:H2'	40:L5:691:C:C6	2.51	0.46
40:L5:2458:C:H5''	55:LN:67:ARG:HD2	1.97	0.46
40:L5:3768:U:H2'	40:L5:3769:C:H6	1.80	0.46
40:L5:4590:A2M:HM'3	40:L5:4590:A2M:H1'	1.71	0.46
42:L8:144:U:H2'	42:L8:145:C:C6	2.51	0.46
44:LB:196:TRP:O	44:LB:200:ARG:HG2	2.16	0.46
2:SB:87:ILE:HG22	2:SB:101:HIS:HB2	1.98	0.46
16:Sa:87:ARG:HH21	19:S2:1865:C:H5''	1.80	0.46
19:S2:1259:A:H1'	19:S2:1264:C:N4	2.31	0.46
24:SF:77:MET:HE1	24:SF:86:LYS:HG3	1.97	0.46
28:SQ:23:ALA:HA	28:SQ:70:VAL:HA	1.97	0.46
33:Sc:46:VAL:HG21	33:Sc:50:VAL:HG21	1.97	0.46
36:Sg:270:LEU:HD13	36:Sg:310:TRP:CD2	2.51	0.46
40:L5:1613:A:H5''	43:LA:183:GLY:HA2	1.98	0.46
40:L5:1989:G:H2'	40:L5:1990:A:C8	2.51	0.46
40:L5:2517:A:H5'	72:Lg:62:LYS:HD3	1.98	0.46
40:L5:2824:OMC:H1'	40:L5:2824:OMC:HM23	1.70	0.46
40:L5:3785:A2M:H2	40:L5:4551:U:O2	2.16	0.46
40:L5:4139:G:N2	40:L5:4140:C:H41	2.10	0.46
40:L5:4906:C:H2'	40:L5:4907:G:H8	1.80	0.46
40:L5:4966:A:H5''	44:LB:128:LYS:HG3	1.97	0.46
40:L5:5018:C:H2'	40:L5:5019:A:H8	1.80	0.46
40:L5:5057:C:H2'	40:L5:5058:A:C8	2.50	0.46
45:LC:150:LEU:HD23	45:LC:150:LEU:HA	1.58	0.46
84:Lt:106:PHE:HB2	84:Lt:109:ILE:HG12	1.96	0.46
2:SB:224:GLU:O	2:SB:227:LYS:HG2	2.16	0.46
8:SJ:2:PRO:HD2	19:S2:428:OMU:H4'	1.98	0.46
8:SJ:31:LEU:HD22	8:SJ:35:TYR:HE2	1.81	0.46
10:SN:130:LYS:HE3	10:SN:139:TRP:HB3	1.98	0.46
15:SY:124:ASN:ND2	19:S2:84:A:H5''	2.31	0.46
18:Se:24:LYS:HB2	18:Se:24:LYS:HE2	1.80	0.46
19:S2:458:A:H2'	19:S2:459:C:H6	1.81	0.46
19:S2:659:G:H2'	19:S2:663:C:C6	2.51	0.46
19:S2:1609:C:H2'	19:S2:1610:G:H8	1.80	0.46
20:LR:10:LEU:HD22	20:LR:38:ARG:HG2	1.97	0.46
29:SS:80:PRO:HG2	30:ST:36:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:457:G:H2'	40:L5:458:C:C6	2.51	0.46
40:L5:518:G:H22	40:L5:643:C:H2'	1.81	0.46
40:L5:3825:A2M:H2'	40:L5:3826:C:O4'	2.17	0.46
40:L5:3873:G:H2'	40:L5:3874:G:C8	2.51	0.46
40:L5:3911:C:H2'	40:L5:3912:U:H6	1.81	0.46
40:L5:4196:OMG:HM23	40:L5:4196:OMG:H1'	1.67	0.46
40:L5:4481:U:H2'	40:L5:4482:U:H6	1.79	0.46
40:L5:4524:G:N3	44:LB:252:ALA:HB1	2.31	0.46
44:LB:29:VAL:HG12	44:LB:31:SER:H	1.81	0.46
47:LE:153:LEU:HD11	47:LE:195:ILE:HG13	1.98	0.46
70:Le:23:HIS:CD2	70:Le:43:ASN:HD21	2.34	0.46
1:SA:76:VAL:HG12	1:SA:123:VAL:HB	1.98	0.45
5:SG:56:ASN:HB2	5:SG:108:VAL:HG22	1.97	0.45
5:SG:66:GLY:HA2	19:S2:1745:A:H1'	1.97	0.45
9:SL:28:THR:HA	9:SL:29:GLY:HA2	1.56	0.45
19:S2:165:G:H2'	19:S2:166:A2M:H8	1.98	0.45
19:S2:172:OMU:H6	19:S2:314:U:H1'	1.98	0.45
19:S2:1414:A:H2'	19:S2:1415:C:C6	2.50	0.45
19:S2:1683:C:H2'	19:S2:1684:C:H6	1.80	0.45
19:S2:1867:U:H4'	19:S2:1868:U:H5'	1.98	0.45
40:L5:138:G:H2'	40:L5:139:G:H8	1.80	0.45
40:L5:1097:C:H2'	40:L5:1098:G:C8	2.51	0.45
40:L5:1278:C:H2'	40:L5:1279:A:O4'	2.17	0.45
49:LG:162:ASP:HB3	49:LG:163:PRO:HD3	1.98	0.45
51:LI:188:LYS:HE2	51:LI:213:HIS:H	1.81	0.45
54:LM:119:ARG:HG3	56:LO:189:ILE:HG23	1.98	0.45
57:LP:39:MET:HG2	57:LP:43:LYS:HD3	1.97	0.45
68:Lc:20:LEU:O	68:Lc:24:SER:HB3	2.15	0.45
73:Lh:87:LYS:HB3	73:Lh:91:MET:HE2	1.98	0.45
82:Lr:47:LYS:HB2	82:Lr:102:TYR:CZ	2.50	0.45
19:S2:568:C:H2'	19:S2:569:A:C8	2.50	0.45
26:SM:44:LYS:HG2	35:Sf:128:ALA:HB3	1.98	0.45
29:SS:18:THR:HG21	29:SS:33:ILE:HA	1.97	0.45
40:L5:162:A:H2'	40:L5:163:A:H8	1.81	0.45
40:L5:270:U:H2'	40:L5:271:C:C6	2.51	0.45
40:L5:711:A:H2'	40:L5:712:C:C6	2.51	0.45
40:L5:1243:C:H2'	40:L5:1244:G:H8	1.81	0.45
40:L5:1982:G:H2'	40:L5:1983:A:O4'	2.15	0.45
40:L5:3867:A2M:H8	40:L5:3867:A2M:H5''	1.97	0.45
40:L5:4965:U:H4'	40:L5:4966:A:H5'	1.98	0.45
58:LQ:154:LYS:HB3	58:LQ:154:LYS:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Lf:45:LYS:HA	71:Lf:107:PRO:HD2	1.98	0.45
73:Lh:89:ARG:O	73:Lh:93:ARG:HG2	2.16	0.45
13:SW:3:ARG:HH22	13:SW:28:ARG:HE	1.63	0.45
14:SX:107:ARG:HG3	14:SX:110:HIS:HB3	1.99	0.45
16:Sa:13:LYS:HD3	16:Sa:13:LYS:HA	1.63	0.45
19:S2:77:A:H2'	19:S2:78:C:C6	2.51	0.45
19:S2:563:G:C2	19:S2:564:A:C8	3.05	0.45
19:S2:1204:A:H2'	19:S2:1205:C:C6	2.51	0.45
19:S2:1438:A:H2'	19:S2:1439:A:C8	2.51	0.45
31:SU:61:LEU:HB2	31:SU:82:MET:HB3	1.99	0.45
36:Sg:202:PRO:HG2	36:Sg:243:PRO:HA	1.98	0.45
40:L5:137:G:H2'	40:L5:138:G:C8	2.49	0.45
40:L5:179:G:H2'	40:L5:180:C:H6	1.81	0.45
40:L5:426:A:H2'	40:L5:427:A:H8	1.81	0.45
40:L5:1317:U:H2'	40:L5:1318:C:C6	2.51	0.45
40:L5:2557:G:N2	40:L5:2570:U:O2	2.25	0.45
40:L5:4600:G:H4'	40:L5:4601:U:O5'	2.16	0.45
42:L8:67:U:H2'	42:L8:68:G:C8	2.52	0.45
44:LB:181:MET:HE3	44:LB:183:ILE:HG12	1.98	0.45
83:Ls:29:ILE:HG21	83:Ls:82:ILE:HD11	1.99	0.45
19:S2:24:C:O2'	19:S2:25:A:H8	2.00	0.45
19:S2:1174:PSU:H2'	19:S2:1175:G:H8	1.80	0.45
19:S2:1671:G:H2'	19:S2:1672:U:C6	2.52	0.45
19:S2:1801:A:H2'	19:S2:1802:C:H6	1.80	0.45
29:SS:46:ARG:HE	29:SS:52:LEU:HD21	1.81	0.45
40:L5:1084:C:H2'	40:L5:1085:C:H6	1.82	0.45
40:L5:4954:G:H2'	40:L5:4955:A:C8	2.51	0.45
51:LI:43:VAL:HG11	51:LI:197:VAL:HG13	1.98	0.45
59:LS:30:MET:HE2	59:LS:30:MET:HB3	1.82	0.45
80:Lo:14:LYS:HB3	80:Lo:77:CYS:SG	2.57	0.45
6:SH:113:LYS:HE3	19:S2:798:G:H4'	1.98	0.45
19:S2:468:A2M:HM'3	19:S2:468:A2M:H1'	1.52	0.45
19:S2:1529:C:H2'	19:S2:1530:U:C6	2.52	0.45
40:L5:184:U:H3	40:L5:253:G:H1	1.63	0.45
40:L5:1190:C:H2'	40:L5:1191:C:C6	2.51	0.45
40:L5:1514:U:H2'	40:L5:1515:A:C8	2.52	0.45
40:L5:1968:G:H2'	40:L5:1969:G:C8	2.52	0.45
40:L5:2267:U:OP1	82:Lr:37:SER:HB2	2.16	0.45
40:L5:2415:U:H2'	40:L5:2416:G:C8	2.50	0.45
40:L5:3664:G:H2'	40:L5:3665:G:H8	1.82	0.45
40:L5:4924:C:H5	40:L5:4925:U:C4	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:LI:53:VAL:HG22	51:LI:134:VAL:HG22	1.97	0.45
65:LZ:75:TYR:CD2	65:LZ:80:LEU:HD21	2.51	0.45
82:Lr:41:ASN:HD22	82:Lr:44:ILE:HD13	1.81	0.45
1:SA:122:LEU:HD13	1:SA:142:LEU:HD21	1.98	0.45
4:SE:19:MET:HE3	4:SE:51:ARG:HH12	1.81	0.45
14:SX:17:ARG:HH12	19:S2:659:G:N2	2.15	0.45
14:SX:54:LYS:HG2	14:SX:91:LEU:HD11	1.98	0.45
19:S2:1393:G:H2'	19:S2:1394:G:C8	2.52	0.45
19:S2:1713:C:H2'	19:S2:1714:U:C6	2.52	0.45
25:SK:58:VAL:HG21	25:SK:69:TRP:HB3	1.99	0.45
31:SU:80:PHE:HB3	34:Sd:52:PHE:HB3	1.98	0.45
38:Pt:26:G:H22	38:Pt:44:A:H2	1.64	0.45
40:L5:1758:G:H2'	40:L5:1759:G:C8	2.52	0.45
40:L5:2490:U:H3'	40:L5:2491:C:C6	2.52	0.45
56:LO:54:TYR:CD1	56:LO:145:VAL:HG21	2.51	0.45
1:SA:145:ILE:HG13	1:SA:159:ILE:HD13	1.99	0.45
19:S2:27:A2M:H1'	19:S2:27:A2M:HM'3	1.67	0.45
19:S2:291:G:H2'	19:S2:292:A:C8	2.51	0.45
19:S2:562:U:H2'	19:S2:563:G:C8	2.51	0.45
19:S2:669:A:H2'	19:S2:670:A:C4	2.52	0.45
28:SQ:86:GLN:HG2	28:SQ:90:LYS:HD3	1.98	0.45
37:At:2:U:H2'	37:At:3:C:C6	2.51	0.45
40:L5:99:A:H2'	40:L5:100:C:O2	2.17	0.45
40:L5:1199:G:H2'	40:L5:1200:G:C8	2.52	0.45
40:L5:1243:C:H2'	40:L5:1244:G:C8	2.52	0.45
40:L5:1494:U:H2'	40:L5:1495:G:H8	1.81	0.45
40:L5:1494:U:H2'	40:L5:1495:G:C8	2.52	0.45
40:L5:2484:A:H62	40:L5:2494:U:H3	1.65	0.45
40:L5:2749:C:H2'	40:L5:2750:G:H8	1.82	0.45
40:L5:3848:U:H2'	40:L5:3849:A:H8	1.82	0.45
41:L7:112:U:H2'	41:L7:113:G:C8	2.52	0.45
45:LC:298:ILE:HD13	58:LQ:131:PRO:HB3	1.98	0.45
48:LF:221:LYS:HA	48:LF:221:LYS:HD3	1.81	0.45
52:LJ:113:ILE:H	52:LJ:113:ILE:HD12	1.82	0.45
54:LM:41:PRO:HB3	54:LM:70:GLN:HG3	1.98	0.45
75:Lj:19:CYS:SG	75:Lj:34:CYS:HB2	2.56	0.45
1:SA:43:SER:HB2	22:SR:126:MET:HG2	1.97	0.45
2:SB:150:ILE:HG23	22:SR:131:PRO:HA	1.98	0.45
3:SC:259:THR:HG23	12:SV:16:LYS:HE2	1.98	0.45
4:SE:47:PHE:O	4:SE:51:ARG:HB2	2.17	0.45
7:SI:14:THR:HG23	7:SI:16:GLY:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:558:G:H1'	19:S2:559:G:C8	2.52	0.45
19:S2:1674:G:H5''	24:SF:86:LYS:HD3	1.98	0.45
23:SD:175:VAL:HB	23:SD:182:LEU:HB3	1.99	0.45
40:L5:1824:G:H2'	40:L5:1825:A:C8	2.52	0.45
40:L5:1921:C:C4	59:LS:161:ARG:HD2	2.51	0.45
40:L5:2293:U:H2'	40:L5:2294:G:C8	2.52	0.45
40:L5:3787:G:H1'	40:L5:3789:C:N4	2.31	0.45
40:L5:4906:C:H2'	40:L5:4907:G:C8	2.52	0.45
40:L5:4921:C:H2'	40:L5:4922:C:C6	2.52	0.45
48:LF:41:MET:HE2	67:Lb:113:ALA:HB2	1.99	0.45
76:Lk:27:LYS:HA	76:Lk:32:VAL:HG22	1.98	0.45
19:S2:649:PSU:H2'	19:S2:650:A:H8	1.81	0.45
19:S2:1515:G:H2'	19:S2:1516:G:C8	2.51	0.45
20:LR:21:LYS:HE3	20:LR:55:VAL:HA	1.98	0.45
36:Sg:24:THR:HG23	36:Sg:27:PHE:H	1.81	0.45
40:L5:123:C:H2'	40:L5:124:C:H6	1.82	0.45
40:L5:678:C:H2'	40:L5:679:C:H6	1.81	0.45
40:L5:1996:C:N3	40:L5:2000:G:N1	2.65	0.45
40:L5:2787:A2M:HM'2	40:L5:2787:A2M:H1'	1.67	0.45
41:L7:58:A:H2'	41:L7:59:G:H8	1.80	0.45
44:LB:92:TYR:HB3	44:LB:99:LEU:HD22	1.98	0.45
47:LE:223:ARG:HB3	47:LE:224:LYS:HB2	1.99	0.45
3:SC:253:PRO:HA	3:SC:256:TRP:CG	2.52	0.45
4:SE:11:ARG:HH12	4:SE:25:GLY:H	1.63	0.45
8:SJ:52:LYS:HB3	8:SJ:52:LYS:HE2	1.69	0.45
10:SN:17:PRO:HG3	19:S2:1016:U:C4	2.52	0.45
10:SN:40:LEU:HD22	10:SN:45:LEU:HD12	1.99	0.45
12:SV:11:LEU:HD23	12:SV:11:LEU:H	1.82	0.45
19:S2:525:A:H2'	19:S2:526:A:C8	2.49	0.45
19:S2:1387:G:H3'	19:S2:1388:A:H8	1.82	0.45
29:SS:50:ILE:HG23	29:SS:66:ARG:NH2	2.32	0.45
29:SS:125:HIS:CD2	29:SS:131:VAL:HG11	2.52	0.45
40:L5:441:G:H2'	40:L5:442:G:C8	2.52	0.45
40:L5:1461:C:H2'	40:L5:1462:A:H8	1.80	0.45
40:L5:1468:C:H2'	40:L5:1469:C:H6	1.82	0.45
40:L5:1577:G:H5'	40:L5:1578:U:H5''	1.99	0.45
40:L5:1976:G:OP1	40:L5:1984:A:H4'	2.17	0.45
40:L5:4088:C:H2'	40:L5:4089:G:H8	1.81	0.45
40:L5:4507:A:H2'	40:L5:4508:C:C6	2.52	0.45
40:L5:4920:C:H2'	40:L5:4921:C:H6	1.81	0.45
40:L5:5015:G:H2'	40:L5:5016:A:C2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:LA:180:LEU:HD11	81:Lp:26:VAL:HG11	1.98	0.45
44:LB:29:VAL:HA	44:LB:220:ILE:HD13	1.99	0.45
73:Lh:71:LYS:HB2	73:Lh:71:LYS:HE3	1.73	0.45
19:S2:142:C:H42	19:S2:329:G:H5''	1.82	0.44
19:S2:825:A:H2'	19:S2:826:A:C8	2.51	0.44
19:S2:864:A:H2'	19:S2:865:A:H8	1.79	0.44
19:S2:1103:C:H2'	19:S2:1104:G:H8	1.80	0.44
19:S2:1198:G:H2'	19:S2:1199:A:C8	2.51	0.44
19:S2:1576:G:H2'	19:S2:1577:G:C8	2.52	0.44
19:S2:1842:4AC:O5'	19:S2:1842:4AC:H6	2.17	0.44
23:SD:163:PRO:HG3	23:SD:205:PRO:HG2	1.99	0.44
27:SP:18:ARG:NH1	29:SS:88:LYS:HG2	2.32	0.44
29:SS:45:LEU:HD22	29:SS:50:ILE:HD11	1.98	0.44
35:Sf:103:LEU:HG	35:Sf:104:LYS:H	1.82	0.44
36:Sg:168:CYS:HB2	36:Sg:195:LEU:HB3	1.99	0.44
40:L5:1179:U:H3'	40:L5:1180:C:H5''	1.99	0.44
40:L5:1976:G:C8	40:L5:2002:A:H2'	2.51	0.44
40:L5:2730:U:H2'	40:L5:2731:C:C6	2.52	0.44
40:L5:4861:G:H2'	40:L5:4862:G:H8	1.82	0.44
45:LC:228:THR:HG23	45:LC:248:ARG:HH22	1.82	0.44
54:LM:96:GLU:O	54:LM:100:ARG:HG2	2.16	0.44
83:Ls:110:ALA:HA	83:Ls:182:PRO:HG2	1.99	0.44
4:SE:42:LEU:HG	4:SE:109:PHE:CD2	2.51	0.44
6:SH:118:ARG:HD3	6:SH:118:ARG:HA	1.70	0.44
7:SI:83:TYR:HB3	7:SI:101:ILE:HG12	1.98	0.44
14:SX:32:LEU:HG	14:SX:34:THR:HG23	1.99	0.44
19:S2:1279:C:H2'	19:S2:1280:G:H8	1.80	0.44
19:S2:1651:A:H2'	19:S2:1652:G:H8	1.81	0.44
36:Sg:173:LEU:HD13	36:Sg:189:ILE:HG22	1.98	0.44
37:At:43:A:H2'	37:At:44:A:C8	2.52	0.44
40:L5:233:U:H4'	40:L5:234:G:OP1	2.17	0.44
40:L5:1346:C:H2'	40:L5:1347:G:H8	1.82	0.44
40:L5:2520:C:H2'	40:L5:2521:G:C8	2.52	0.44
40:L5:2671:C:H2'	40:L5:2672:C:C6	2.52	0.44
40:L5:4638:U:H2'	40:L5:4639:G:N3	2.32	0.44
40:L5:4927:G:H5''	40:L5:4928:C:C5	2.51	0.44
40:L5:5002:U:H2'	40:L5:5003:U:C6	2.52	0.44
40:L5:5004:C:H2'	40:L5:5005:G:O4'	2.16	0.44
61:LU:28:PRO:HB2	61:LU:34:MET:HG3	1.98	0.44
63:LX:152:LYS:HE2	63:LX:152:LYS:HB3	1.83	0.44
68:Lc:82:GLY:HA2	68:Lc:91:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Lj:60:GLY:HA2	75:Lj:64:MET:SD	2.56	0.44
1:SA:209:GLU:HA	1:SA:212:LYS:HG2	1.99	0.44
12:SV:17:CYS:HB3	12:SV:22:ARG:H	1.82	0.44
19:S2:497:C:H2'	19:S2:498:C:C6	2.52	0.44
35:Sf:140:TYR:CE1	35:Sf:145:CYS:HA	2.52	0.44
36:Sg:64:HIS:HB3	36:Sg:83:TRP:HB2	1.97	0.44
40:L5:319:A:H1'	40:L5:3726:A:N3	2.32	0.44
40:L5:4281:A:H2'	40:L5:4282:A:H2'	1.99	0.44
43:LA:143:THR:HG23	43:LA:145:LYS:HG2	1.99	0.44
46:LD:33:ARG:NH1	46:LD:37:VAL:HG11	2.32	0.44
6:SH:176:VAL:HG22	6:SH:180:LEU:HD23	1.99	0.44
12:SV:51:LYS:HE2	12:SV:51:LYS:HB3	1.87	0.44
16:Sa:85:ARG:HD3	19:S2:1209:A:O2'	2.17	0.44
19:S2:1706:G:H2'	19:S2:1707:U:H6	1.82	0.44
19:S2:1736:G:H2'	19:S2:1737:G:H8	1.83	0.44
30:ST:18:LEU:HD22	30:ST:58:ALA:HA	1.99	0.44
38:Pt:25:C:H2'	38:Pt:26:G:O4'	2.17	0.44
40:L5:138:G:H2'	40:L5:139:G:C8	2.53	0.44
40:L5:4089:G:H2'	40:L5:4090:G:C8	2.52	0.44
40:L5:4253:A:H5'	40:L5:4254:G:C8	2.51	0.44
45:LC:289:LEU:HD11	58:LQ:31:LEU:HB2	1.99	0.44
82:Lr:20:ARG:HG2	82:Lr:21:ASN:OD1	2.17	0.44
3:SC:210:PRO:HB3	3:SC:240:THR:HG21	1.98	0.44
5:SG:172:LYS:HD3	19:S2:65:C:H4'	2.00	0.44
7:SI:23:LYS:HG2	19:S2:434:G:OP1	2.17	0.44
10:SN:46:THR:HB	10:SN:86:GLU:HG3	1.99	0.44
11:SO:120:ALA:HB2	16:Sa:53:ILE:HD13	1.99	0.44
11:SO:150:ARG:HB3	19:S2:1838:U:H1'	2.00	0.44
19:S2:92:A:H61	19:S2:444:G:H1'	1.82	0.44
19:S2:656:G:H5'	19:S2:662:G:N2	2.33	0.44
19:S2:1051:G:H2'	19:S2:1052:A:C8	2.52	0.44
19:S2:1447:G:H2'	19:S2:1448:A:C8	2.52	0.44
19:S2:1612:G:H1'	29:SS:87:GLN:NE2	2.31	0.44
19:S2:1733:U:H2'	19:S2:1734:G:O4'	2.18	0.44
27:SP:118:GLU:HG2	29:SS:120:HIS:H	1.81	0.44
30:ST:108:GLU:HG3	30:ST:113:VAL:O	2.17	0.44
35:Sf:103:LEU:HB2	35:Sf:105:TYR:CE1	2.53	0.44
40:L5:468:U:C5	40:L5:469:C:H5	2.35	0.44
40:L5:1504:G:H2'	40:L5:1505:C:C6	2.52	0.44
40:L5:2683:C:H2'	40:L5:2684:C:C6	2.53	0.44
40:L5:2765:A:H2'	40:L5:2766:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:3867:A2M:H2'	40:L5:3868:G:C8	2.53	0.44
40:L5:4146:G:H2'	40:L5:4147:G:C8	2.53	0.44
50:LH:93:ARG:HG2	50:LH:182:SER:HB3	1.99	0.44
53:LL:47:ALA:HB3	53:LL:48:PRO:HD3	1.98	0.44
54:LM:132:LYS:HE3	54:LM:132:LYS:HB3	1.87	0.44
57:LP:37:LYS:HB3	57:LP:37:LYS:HE2	1.72	0.44
66:La:7:LYS:HE2	66:La:7:LYS:HB3	1.75	0.44
1:SA:5:LEU:HD11	12:SV:41:LYS:HB3	1.99	0.44
4:SE:141:THR:HG23	4:SE:143:ASP:N	2.32	0.44
13:SW:22:LYS:HD2	17:Sb:3:LEU:HA	1.98	0.44
14:SX:138:LYS:HE2	14:SX:138:LYS:HB3	1.80	0.44
19:S2:293:C:O2'	19:S2:294:U:H3'	2.17	0.44
19:S2:943:U:C2	19:S2:944:A:C8	3.06	0.44
25:SK:63:ALA:HB2	25:SK:68:TYR:CE2	2.53	0.44
27:SP:72:LYS:HD2	27:SP:72:LYS:HA	1.76	0.44
40:L5:1503:A:H1'	40:L5:1504:G:C8	2.53	0.44
40:L5:1557:C:H2'	40:L5:1558:A:C8	2.53	0.44
40:L5:1725:U:H2'	40:L5:1726:U:H6	1.83	0.44
40:L5:2029:A:H2'	40:L5:2030:A:H8	1.80	0.44
40:L5:2542:G:H2'	40:L5:2543:A:C8	2.53	0.44
43:LA:131:GLY:N	43:LA:169:VAL:HG13	2.33	0.44
3:SC:171:GLY:HA3	13:SW:97:ARG:NH1	2.33	0.44
19:S2:461:U:H2'	19:S2:462:OMC:C6	2.52	0.44
19:S2:601:OMG:H1'	19:S2:601:OMG:HM23	1.65	0.44
26:SM:35:ILE:HD11	26:SM:61:TYR:CZ	2.53	0.44
40:L5:7:C:H2'	40:L5:8:U:C6	2.53	0.44
40:L5:424:U:H2'	40:L5:425:U:C6	2.53	0.44
40:L5:1693:U:H2'	40:L5:1694:C:O4'	2.17	0.44
40:L5:2633:U:H2'	40:L5:2634:C:H6	1.83	0.44
40:L5:4098:A:N7	40:L5:4099:G:H1'	2.33	0.44
40:L5:4611:A:H2'	40:L5:4612:C:H6	1.83	0.44
42:L8:89:U:H2'	42:L8:90:C:C6	2.52	0.44
52:LJ:52:LYS:HB3	52:LJ:65:ASN:HA	2.00	0.44
8:SJ:134:HIS:HA	8:SJ:163:SER:HB3	2.00	0.44
10:SN:55:ARG:NH1	19:S2:1017:U:H5'	2.33	0.44
19:S2:482:G:N2	19:S2:484:A2M:H3'	2.33	0.44
19:S2:807:G:H2'	19:S2:808:A:H8	1.83	0.44
19:S2:1174:PSU:H2'	19:S2:1175:G:C8	2.53	0.44
19:S2:1714:U:H2'	19:S2:1715:A:C8	2.53	0.44
29:SS:78:LYS:HA	29:SS:78:LYS:HD3	1.87	0.44
31:SU:54:VAL:HB	31:SU:88:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1092:G:H2'	40:L5:1093:C:C6	2.53	0.44
40:L5:1772:C:H2'	40:L5:1773:U:H6	1.83	0.44
40:L5:4481:U:H2'	40:L5:4482:U:C6	2.53	0.44
41:L7:63:C:H5'	41:L7:64:G:H5''	2.00	0.44
45:LC:368:LYS:HA	45:LC:368:LYS:HD3	1.76	0.44
47:LE:239:LYS:HD2	47:LE:239:LYS:HA	1.83	0.44
65:LZ:50:PRO:HD3	65:LZ:68:ILE:HG12	2.00	0.44
84:Lt:10:ILE:HG21	84:Lt:65:GLN:HB3	2.00	0.44
5:SG:136:LYS:HB2	19:S2:65:C:N4	2.32	0.44
12:SV:15:ARG:HH21	12:SV:24:ILE:HG21	1.82	0.44
19:S2:1282:A:H2'	19:S2:1283:C:C2	2.53	0.44
19:S2:1323:U:H2'	19:S2:1324:G:C8	2.53	0.44
19:S2:1446:A:H5''	31:SU:58:THR:HG23	2.00	0.44
23:SD:12:VAL:O	23:SD:16:ILE:HG12	2.18	0.44
37:At:51:C:H2'	37:At:52:G:H8	1.82	0.44
37:At:68:G:H2'	37:At:69:A:H8	1.83	0.44
40:L5:37:U:H2'	40:L5:38:A:O4'	2.18	0.44
40:L5:163:A:H2'	40:L5:164:G:C8	2.53	0.44
40:L5:679:C:H2'	40:L5:680:G:C8	2.53	0.44
40:L5:1178:G:H2'	46:LD:286:SER:HB3	1.99	0.44
40:L5:1563:A:H8	40:L5:1563:A:OP1	2.01	0.44
40:L5:2640:G:H2'	40:L5:2641:A:C8	2.52	0.44
40:L5:3599:A:H2'	40:L5:3600:G:H8	1.82	0.44
40:L5:3718:A2M:H2	40:L5:3934:G:O4'	2.17	0.44
40:L5:3848:U:H2'	40:L5:3849:A:C8	2.53	0.44
40:L5:4578:G:H2'	40:L5:4579:PSU:C6	2.52	0.44
40:L5:5018:C:H2'	40:L5:5019:A:C8	2.52	0.44
41:L7:58:A:H2'	41:L7:59:G:C8	2.53	0.44
58:LQ:99:LYS:HE3	58:LQ:121:LEU:HD11	1.99	0.44
5:SG:162:LEU:HD13	19:S2:67:C:C5	2.53	0.43
6:SH:58:LYS:HD3	6:SH:58:LYS:HA	1.89	0.43
17:Sb:64:CYS:HA	17:Sb:73:LEU:HA	1.98	0.43
19:S2:96:C:H2'	19:S2:97:U:C6	2.53	0.43
19:S2:287:U:H2'	19:S2:288:G:C8	2.52	0.43
23:SD:167:TYR:CE2	23:SD:204:LEU:HD23	2.53	0.43
40:L5:1350:C:H5''	45:LC:33:ARG:HH21	1.82	0.43
40:L5:2489:C:H4'	40:L5:2491:C:H42	1.83	0.43
40:L5:2648:G:H2'	40:L5:2649:G:C8	2.53	0.43
40:L5:2844:A:O2'	40:L5:4631:G:H4'	2.18	0.43
40:L5:3690:U:H5'	40:L5:3818:UY1:OP2	2.18	0.43
40:L5:4070:U:H2'	40:L5:4071:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:4299:PSU:H2'	40:L5:4300:U:H6	1.83	0.43
46:LD:62:CYS:HB3	46:LD:105:LEU:HD22	2.00	0.43
48:LF:236:ARG:HB2	48:LF:239:GLN:HB2	2.00	0.43
4:SE:100:ARG:HB2	4:SE:114:ILE:HD13	1.99	0.43
19:S2:163:U:H2'	19:S2:164:A:C8	2.53	0.43
19:S2:185:G:H2'	19:S2:186:C:C6	2.53	0.43
19:S2:680:G:H2'	19:S2:681:PSU:C6	2.54	0.43
19:S2:1518:C:OP1	19:S2:1519:U:H2'	2.18	0.43
19:S2:1616:U:H2'	19:S2:1617:G:C8	2.53	0.43
19:S2:1657:G:H2'	19:S2:1658:G:C8	2.53	0.43
23:SD:218:LEU:HD11	36:Sg:189:ILE:HD12	2.01	0.43
40:L5:2275:G:H2'	40:L5:2276:A:C8	2.53	0.43
51:LI:91:LEU:HD23	51:LI:91:LEU:HA	1.85	0.43
73:Lh:88:THR:HB	73:Lh:91:MET:HB2	2.01	0.43
83:Ls:69:LEU:HG	83:Ls:75:LEU:HB3	2.00	0.43
2:SB:38:MET:HG3	2:SB:39:PHE:CD2	2.53	0.43
5:SG:55:GLY:N	5:SG:110:ASN:HD22	2.15	0.43
5:SG:218:LYS:HA	5:SG:218:LYS:HD2	1.76	0.43
7:SI:116:HIS:CG	7:SI:152:ARG:HH21	2.36	0.43
19:S2:614:C:H5'	19:S2:626:G:O4'	2.18	0.43
19:S2:1112:U:O2	19:S2:1121:G:O6	2.36	0.43
19:S2:1653:U:H3	19:S2:1671:G:H1	1.66	0.43
36:Sg:21:ILE:HG21	36:Sg:299:PHE:HB2	1.99	0.43
40:L5:300:A:H2'	40:L5:301:G:H8	1.83	0.43
40:L5:689:U:H2'	40:L5:690:C:C6	2.54	0.43
40:L5:713:C:H2'	40:L5:714:G:H8	1.82	0.43
40:L5:918:G:H5'	54:LM:72:TYR:CZ	2.54	0.43
40:L5:1847:C:H2'	40:L5:1848:C:C6	2.53	0.43
40:L5:1876:U:O3'	48:LF:103:PRO:HD3	2.18	0.43
40:L5:3832:U:H2'	40:L5:3833:C:H6	1.84	0.43
40:L5:4571:A2M:HM'3	40:L5:4571:A2M:H1'	1.70	0.43
40:L5:4593:C:H2'	40:L5:4594:U:C6	2.54	0.43
41:L7:16:A:H2'	41:L7:17:C:C6	2.53	0.43
46:LD:181:PRO:HD2	46:LD:195:HIS:CD2	2.54	0.43
51:LI:152:LEU:HB3	51:LI:165:ILE:HD12	2.00	0.43
8:SJ:113:GLN:HG3	8:SJ:149:VAL:HG21	2.00	0.43
10:SN:20:ARG:HH21	13:SW:56:HIS:HB3	1.83	0.43
12:SV:30:ALA:O	12:SV:60:ARG:HD3	2.17	0.43
15:SY:18:LEU:HB2	15:SY:20:ARG:HG2	1.99	0.43
19:S2:1392:U:H2'	19:S2:1393:G:C8	2.54	0.43
19:S2:1748:G:O6	19:S2:1786:U:C4	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SP:127:LYS:HB3	27:SP:127:LYS:HE3	1.89	0.43
35:Sf:90:LYS:HA	35:Sf:90:LYS:HD2	1.72	0.43
40:L5:710:G:H2'	40:L5:711:A:H8	1.84	0.43
40:L5:1628:C:H42	43:LA:3:ARG:HD3	1.83	0.43
40:L5:2066:C:H5''	71:Lf:36:ARG:CZ	2.48	0.43
40:L5:2376:A:H2'	40:L5:2377:C:C6	2.53	0.43
40:L5:3597:G:H2'	40:L5:3598:C:H6	1.84	0.43
40:L5:3690:U:H2'	40:L5:3691:G:O4'	2.19	0.43
40:L5:4159:C:H2'	40:L5:4160:C:C6	2.53	0.43
40:L5:4572:U:H1'	40:L5:4720:C:C4	2.54	0.43
40:L5:4593:C:H2'	40:L5:4594:U:H6	1.83	0.43
44:LB:112:ASP:O	44:LB:116:ARG:HG3	2.19	0.43
45:LC:33:ARG:HD3	45:LC:36:ILE:HD12	2.00	0.43
55:LN:75:VAL:HG21	55:LN:80:THR:HG23	2.00	0.43
60:LT:4:THR:OG1	60:LT:9:ARG:HD3	2.19	0.43
1:SA:177:MET:HE3	1:SA:177:MET:HB3	1.81	0.43
2:SB:123:ALA:HB1	2:SB:169:MET:HG3	1.99	0.43
19:S2:345:U:H2'	19:S2:346:C:C6	2.54	0.43
19:S2:455:A:H2'	19:S2:456:C:C6	2.54	0.43
19:S2:576:A2M:HM'3	19:S2:576:A2M:H1'	1.57	0.43
19:S2:1220:A:H2'	19:S2:1221:G:O4'	2.18	0.43
19:S2:1771:G:H2'	19:S2:1772:C:H6	1.83	0.43
19:S2:1777:G:H2'	19:S2:1778:C:C6	2.52	0.43
22:SR:29:HIS:O	22:SR:32:LYS:HG2	2.18	0.43
24:SF:35:LEU:O	24:SF:39:ILE:HG12	2.19	0.43
30:ST:39:LEU:HD11	30:ST:52:TRP:CE3	2.53	0.43
39:CI:59:GLN:HB2	61:LU:99:TRP:HE1	1.84	0.43
40:L5:153:G:H2'	40:L5:154:G:C8	2.51	0.43
40:L5:716:C:OP1	45:LC:317:ASN:HB2	2.18	0.43
40:L5:1545:G:H2'	40:L5:1546:C:C6	2.53	0.43
40:L5:1941:A:C2	40:L5:4434:C:H5'	2.53	0.43
40:L5:2264:C:H2'	40:L5:2265:G:O4'	2.18	0.43
77:Ll:9:ILE:HD12	77:Ll:51:LEU:HD12	2.01	0.43
81:Lp:22:LEU:HD23	81:Lp:22:LEU:HA	1.86	0.43
2:SB:143:THR:HB	2:SB:205:TYR:CE2	2.54	0.43
19:S2:880:G:H3'	19:S2:881:G:H8	1.82	0.43
19:S2:1383:A2M:H1'	19:S2:1383:A2M:HM'3	1.58	0.43
19:S2:1657:G:H2'	19:S2:1658:G:H8	1.84	0.43
19:S2:1856:C:H2'	19:S2:1857:G:H8	1.83	0.43
27:SP:77:LYS:HB3	27:SP:102:PHE:CD1	2.54	0.43
32:SZ:96:LEU:H	32:SZ:96:LEU:HD23	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1503:A:H4'	40:L5:1504:G:H5'	2.01	0.43
40:L5:4299:PSU:H2'	40:L5:4300:U:C6	2.54	0.43
40:L5:4389:C:H2'	40:L5:4390:A:H8	1.84	0.43
40:L5:5002:U:H2'	40:L5:5003:U:H6	1.84	0.43
42:L8:90:C:H2'	42:L8:91:A:C8	2.54	0.43
43:LA:145:LYS:HD3	43:LA:145:LYS:HA	1.72	0.43
44:LB:17:LEU:HA	44:LB:17:LEU:HD23	1.72	0.43
54:LM:62:LEU:HD21	54:LM:82:ILE:HD11	1.99	0.43
67:Lb:65:MET:HG3	67:Lb:68:ARG:HH12	1.84	0.43
72:Lg:41:ALA:O	72:Lg:52:ARG:HD3	2.19	0.43
84:Lt:19:GLY:HA3	84:Lt:57:ARG:O	2.18	0.43
2:SB:217:MET:HE3	2:SB:217:MET:HB2	1.73	0.43
10:SN:4:MET:HE3	19:S2:924:G:H5'	2.01	0.43
19:S2:641:A:H2'	19:S2:642:U:O4'	2.19	0.43
19:S2:872:A:C5	19:S2:874:G:C8	3.06	0.43
19:S2:1112:U:H3	19:S2:1113:A:H62	1.65	0.43
19:S2:1540:G:H5'	30:ST:47:PRO:HB3	1.99	0.43
24:SF:122:ARG:HA	24:SF:146:ARG:HD3	1.99	0.43
40:L5:139:G:H2'	40:L5:140:G:H8	1.84	0.43
40:L5:1541:C:H5''	43:LA:21:LYS:HG2	2.00	0.43
40:L5:2351:OMC:HM23	40:L5:2351:OMC:H1'	1.75	0.43
40:L5:2372:U:H2'	40:L5:2373:C:C6	2.54	0.43
40:L5:3748:A:H5''	43:LA:243:THR:HB	2.01	0.43
42:L8:36:G:C5	73:Lh:89:ARG:HD3	2.53	0.43
44:LB:217:ILE:HD11	44:LB:333:LEU:HD21	1.99	0.43
57:LP:52:THR:HG23	57:LP:85:LYS:HG3	1.99	0.43
71:Lf:18:LEU:HD23	71:Lf:19:ARG:NH1	2.34	0.43
4:SE:123:LEU:HD23	4:SE:123:LEU:HA	1.91	0.43
7:SI:141:ARG:HB3	7:SI:145:ILE:HB	2.00	0.43
11:SO:129:ILE:HG13	16:Sa:65:PRO:HG2	2.01	0.43
16:Sa:26:CYS:HB3	16:Sa:77:CYS:SG	2.58	0.43
19:S2:406:PSU:H2'	19:S2:408:A:H8	1.84	0.43
19:S2:544:G:H2'	19:S2:545:A:C8	2.54	0.43
19:S2:807:G:H2'	19:S2:808:A:C8	2.54	0.43
19:S2:1227:G:C2	19:S2:1228:A:C8	3.07	0.43
19:S2:1241:A:O2'	19:S2:1243:U:H5'	2.19	0.43
19:S2:1320:G:H2'	19:S2:1321:G:O4'	2.18	0.43
19:S2:1802:C:H2'	19:S2:1803:U:C6	2.53	0.43
33:Sc:11:LEU:HB2	33:Sc:35:MET:HE2	2.01	0.43
36:Sg:16:GLY:HA3	36:Sg:36:ARG:HB2	2.01	0.43
40:L5:965:G:N2	40:L5:2092:G:H1'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1094:G:O6	40:L5:1201:U:C2	2.71	0.43
40:L5:1195:G:H2'	40:L5:1196:G:C8	2.53	0.43
40:L5:1609:U:O4	88:L5:5285:SPD:H51	2.17	0.43
40:L5:2573:A:H2'	40:L5:2574:G:O4'	2.19	0.43
40:L5:4472:G:H5''	78:Lm:102:ARG:HH21	1.83	0.43
41:L7:110:G:H2'	41:L7:111:C:C6	2.54	0.43
52:LJ:104:ASN:C	52:LJ:104:ASN:HD22	2.25	0.43
54:LM:32:ASP:O	54:LM:33:GLN:HG2	2.18	0.43
54:LM:37:LEU:HD12	54:LM:37:LEU:HA	1.88	0.43
73:Lh:52:LYS:HA	73:Lh:52:LYS:HD3	1.68	0.43
3:SC:273:LEU:HD22	3:SC:277:HIS:HB2	2.01	0.43
7:SI:116:HIS:CE1	7:SI:152:ARG:HH21	2.37	0.43
15:SY:108:LYS:HD3	19:S2:53:C:H4'	2.00	0.43
23:SD:110:LEU:HD23	23:SD:110:LEU:HA	1.87	0.43
26:SM:93:LYS:HD2	26:SM:99:LYS:HD3	2.00	0.43
40:L5:2401:A2M:H5''	40:L5:2401:A2M:H8	2.00	0.43
40:L5:2538:U:H2'	40:L5:2539:C:C6	2.53	0.43
40:L5:2568:C:H2'	40:L5:2569:G:C8	2.53	0.43
40:L5:3661:G:H4'	40:L5:3662:A:H5'	2.00	0.43
40:L5:3841:OMC:HM23	40:L5:3841:OMC:H1'	1.83	0.43
40:L5:3920:PSU:H2'	40:L5:3921:U:C6	2.53	0.43
40:L5:4069:U:H2'	40:L5:4070:U:C6	2.53	0.43
41:L7:23:A:H2'	41:L7:24:C:C6	2.54	0.43
49:LG:187:LYS:HB2	49:LG:198:THR:HG23	2.01	0.43
56:LO:9:LEU:HD23	56:LO:118:MET:HB2	2.00	0.43
67:Lb:48:LYS:HE3	67:Lb:49:HIS:CE1	2.53	0.43
73:Lh:21:LEU:HD11	73:Lh:25:LYS:HE2	2.01	0.43
1:SA:180:ARG:HG3	1:SA:195:TRP:HB2	2.00	0.43
15:SY:35:VAL:HG13	15:SY:40:ILE:HD11	2.01	0.43
19:S2:1232:PSU:H2'	19:S2:1233:G:H8	1.83	0.43
19:S2:1397:U:OP1	19:S2:1398:G:H8	2.02	0.43
19:S2:1414:A:H2'	19:S2:1415:C:H6	1.83	0.43
19:S2:1705:C:H2'	19:S2:1706:G:C8	2.54	0.43
38:Pt:29:C:H2'	38:Pt:30:G:H8	1.84	0.43
40:L5:419:A:H61	42:L8:15:G:H1'	1.84	0.43
40:L5:1662:C:H2'	40:L5:1663:C:H6	1.84	0.43
40:L5:2390:G:H22	40:L5:2825:A:H2	1.67	0.43
40:L5:5009:G:H2'	40:L5:5010:PSU:H6	1.84	0.43
61:LU:18:VAL:HG13	61:LU:73:THR:HG23	2.01	0.43
2:SB:64:GLY:HA2	2:SB:87:ILE:HD11	2.02	0.42
17:Sb:68:GLY:HA3	19:S2:1105:G:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:614:C:H2'	19:S2:626:G:C8	2.54	0.42
19:S2:795:A:H2'	19:S2:796:G:C8	2.54	0.42
19:S2:811:A:H2'	19:S2:812:A:H8	1.84	0.42
19:S2:1227:G:C6	19:S2:1638:G:C5	3.07	0.42
19:S2:1322:G:H3'	19:S2:1323:U:H6	1.84	0.42
19:S2:1380:C:H2'	19:S2:1381:G:C8	2.53	0.42
19:S2:1391:OMC:HM23	19:S2:1391:OMC:H1'	1.80	0.42
36:Sg:14:HIS:HD2	36:Sg:18:VAL:HG22	1.83	0.42
36:Sg:164:ILE:HD12	36:Sg:178:ASN:HA	2.01	0.42
37:At:3:C:H2'	37:At:4:U:H6	1.84	0.42
40:L5:1405:C:H41	40:L5:1408:G:N2	2.17	0.42
40:L5:4081:G:H2'	40:L5:4082:G:C8	2.54	0.42
40:L5:4227:OMU:HM21	40:L5:4336:A:H1'	2.00	0.42
40:L5:4587:G:O2'	44:LB:17:LEU:HD12	2.19	0.42
45:LC:305:PRO:HB2	45:LC:307:LYS:HG3	2.00	0.42
49:LG:70:LEU:HD23	49:LG:70:LEU:HA	1.81	0.42
52:LJ:115:LEU:HD13	52:LJ:115:LEU:HA	1.87	0.42
52:LJ:146:ARG:HG2	52:LJ:147:ARG:HG3	2.01	0.42
1:SA:68:ILE:HG22	1:SA:70:ASN:H	1.84	0.42
10:SN:93:LYS:HB2	10:SN:150:VAL:HG21	2.01	0.42
10:SN:99:ARG:HE	10:SN:115:LEU:HD21	1.83	0.42
19:S2:1009:A:H2'	19:S2:1010:G:H8	1.84	0.42
19:S2:1233:G:C6	19:S2:1526:G:C6	3.07	0.42
19:S2:1266:C:H2'	19:S2:1267:C:C6	2.54	0.42
19:S2:1277:C:H2'	19:S2:1278:A:C8	2.52	0.42
19:S2:1539:U:H4'	30:ST:47:PRO:HA	2.01	0.42
19:S2:1661:A:H8	34:Sd:14:PHE:HB2	1.85	0.42
22:SR:30:THR:O	22:SR:34:VAL:HG23	2.20	0.42
37:At:27:U:H2'	37:At:28:U:H6	1.84	0.42
40:L5:1444:G:H1	40:L5:2104:G:H22	1.67	0.42
40:L5:2461:G:H2'	40:L5:2462:C:C6	2.53	0.42
40:L5:2676:A:OP2	40:L5:2676:A:H8	2.02	0.42
40:L5:3736:A:H2'	40:L5:3737:A:H8	1.84	0.42
40:L5:4232:U:H5''	80:Lo:3:ASN:O	2.19	0.42
40:L5:4236:G:H2'	40:L5:4237:C:C6	2.54	0.42
40:L5:4618:OMG:HM22	40:L5:4619:U:H5'	2.01	0.42
40:L5:4625:C:O2'	40:L5:4626:A:H5'	2.20	0.42
40:L5:4748:U:OP1	71:Lf:54:LYS:HE2	2.19	0.42
40:L5:4872:G:C2	56:LO:203:VAL:HG23	2.54	0.42
42:L8:75:OMG:H1'	42:L8:75:OMG:HM23	1.71	0.42
43:LA:137:ILE:HD11	43:LA:149:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:LE:223:ARG:HA	47:LE:224:LYS:HA	1.77	0.42
53:LL:42:LYS:HB3	53:LL:42:LYS:HE2	1.75	0.42
54:LM:79:LYS:HE2	54:LM:79:LYS:HB3	1.93	0.42
84:Lt:147:HIS:CE1	84:Lt:149:HIS:HB3	2.54	0.42
4:SE:98:ASN:HD22	4:SE:116:PRO:HA	1.84	0.42
8:SJ:30:LYS:HG2	18:Se:42:PHE:CE2	2.54	0.42
10:SN:25:TRP:CD2	17:Sb:82:LYS:HD3	2.54	0.42
17:Sb:62:VAL:HG23	17:Sb:74:THR:HG21	2.00	0.42
19:S2:929:G:N2	19:S2:1104:G:H4'	2.35	0.42
36:Sg:17:TRP:HB2	36:Sg:36:ARG:HG3	2.00	0.42
40:L5:1167:C:H42	40:L5:1195:G:N2	2.17	0.42
40:L5:3610:A:H2'	40:L5:3611:A:H8	1.83	0.42
40:L5:4426:C:C2'	40:L5:4427:G:H5'	2.50	0.42
41:L7:57:C:H2'	41:L7:58:A:H8	1.85	0.42
51:LI:192:PRO:HA	51:LI:197:VAL:HG12	1.99	0.42
56:LO:121:PRO:HA	56:LO:124:LEU:HD12	2.00	0.42
64:LY:33:PRO:HG2	64:LY:105:VAL:HG12	2.01	0.42
1:SA:89:LYS:HA	1:SA:89:LYS:HD3	1.85	0.42
2:SB:136:ARG:O	2:SB:215:VAL:HA	2.19	0.42
3:SC:107:LEU:HB2	3:SC:127:PHE:HB2	2.01	0.42
12:SV:15:ARG:NH2	12:SV:24:ILE:HG21	2.35	0.42
19:S2:1804:U:H2'	19:S2:1805:G:H8	1.83	0.42
19:S2:1845:A:H2'	19:S2:1846:G:H8	1.84	0.42
21:LW:87:LEU:HA	21:LW:90:ILE:HG12	2.01	0.42
24:SF:91:ARG:HG3	24:SF:92:ILE:N	2.33	0.42
32:SZ:86:ALA:O	32:SZ:89:GLN:HG2	2.20	0.42
38:Pt:76:A:H2'	40:L5:4397:A:H1'	2.00	0.42
40:L5:106:A:H2'	40:L5:107:G:O4'	2.20	0.42
40:L5:123:C:H2'	40:L5:124:C:C6	2.54	0.42
40:L5:674:G:H2'	40:L5:675:C:C6	2.54	0.42
40:L5:1092:G:H2'	40:L5:1093:C:H6	1.84	0.42
40:L5:1202:C:H3'	40:L5:1203:G:H4'	2.00	0.42
40:L5:1298:C:H2'	40:L5:1299:G:C8	2.53	0.42
40:L5:1345:A:H2'	40:L5:1346:C:C6	2.54	0.42
61:LU:65:ARG:HD3	61:LU:70:ILE:HG12	2.01	0.42
1:SA:113:GLN:HE21	1:SA:115:ALA:HB3	1.84	0.42
4:SE:45:ILE:HA	4:SE:61:VAL:HG21	2.02	0.42
4:SE:72:ILE:HD12	4:SE:77:ARG:HG3	2.01	0.42
4:SE:241:GLY:O	4:SE:244:ILE:HG22	2.18	0.42
6:SH:132:ASP:HA	6:SH:135:PHE:HB2	2.01	0.42
7:SI:99:ASN:HB2	19:S2:377:G:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:175:ARG:C	8:SJ:179:LYS:HZ2	2.28	0.42
13:SW:28:ARG:HH21	19:S2:1093:A:H5''	1.84	0.42
19:S2:695:C:H42	19:S2:737:G:H1'	1.84	0.42
19:S2:1547:C:N3	19:S2:1656:G:H1'	2.34	0.42
38:Pt:58:A:H1'	38:Pt:60:A:OP2	2.19	0.42
40:L5:270:U:H2'	40:L5:271:C:H6	1.85	0.42
40:L5:271:C:H2'	40:L5:272:U:C6	2.55	0.42
40:L5:1588:U:H2'	40:L5:1589:C:C6	2.55	0.42
40:L5:2654:C:H2'	40:L5:2655:C:H6	1.85	0.42
40:L5:4186:A:H2'	40:L5:4187:G:C8	2.55	0.42
41:L7:11:A:H4'	41:L7:13:A:C8	2.55	0.42
45:LC:110:ARG:HG3	55:LN:204:ARG:HE	1.83	0.42
1:SA:31:ASP:HB3	1:SA:34:MET:HG2	2.02	0.42
1:SA:220:LYS:HA	1:SA:220:LYS:HD3	1.79	0.42
15:SY:41:ARG:HG3	15:SY:55:ILE:HB	2.01	0.42
19:S2:1852:C:H2'	19:S2:1853:C:C6	2.55	0.42
19:S2:1856:C:H2'	19:S2:1857:G:C8	2.53	0.42
40:L5:21:G:H1'	42:L8:103:A:N3	2.34	0.42
40:L5:2634:C:H2'	40:L5:2635:U:H6	1.85	0.42
40:L5:4585:U:H2'	40:L5:4586:G:C8	2.54	0.42
40:L5:4910:G:H1	56:LO:108:ILE:H	1.67	0.42
40:L5:4957:C:H2'	40:L5:4958:C:C6	2.54	0.42
53:LL:105:LYS:HB3	53:LL:105:LYS:HE2	1.81	0.42
4:SE:144:ALA:HB3	19:S2:121:OMU:HM23	2.02	0.42
10:SN:69:ASN:OD1	10:SN:73:ARG:HD2	2.20	0.42
12:SV:43:THR:HG23	12:SV:45:ARG:H	1.84	0.42
14:SX:130:LEU:HD12	14:SX:133:LEU:HD12	2.01	0.42
19:S2:1088:U:H4'	19:S2:1089:G:OP2	2.19	0.42
19:S2:1514:G:H2'	19:S2:1515:G:C8	2.55	0.42
19:S2:1593:C:H2'	19:S2:1594:A:H8	1.84	0.42
19:S2:1597:C:H4'	19:S2:1603:G:C6	2.54	0.42
19:S2:1653:U:H2'	19:S2:1654:G:C8	2.54	0.42
28:SQ:32:ILE:HG21	28:SQ:39:LEU:HD22	2.02	0.42
36:Sg:30:MET:HE3	36:Sg:30:MET:HB3	1.85	0.42
37:At:29:C:H2'	37:At:30:G:C8	2.54	0.42
40:L5:6:C:H2'	40:L5:7:C:H6	1.84	0.42
40:L5:422:C:H2'	40:L5:423:G:H8	1.85	0.42
40:L5:678:C:H2'	40:L5:679:C:C6	2.55	0.42
40:L5:727:C:H5''	48:LF:73:ARG:NH2	2.34	0.42
40:L5:750:U:C2	40:L5:751:G:C8	3.08	0.42
40:L5:1248:C:H2'	40:L5:1249:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:1564:A:H8	40:L5:1564:A:OP2	2.03	0.42
40:L5:1764:G:H4'	40:L5:1769:G:C6	2.54	0.42
40:L5:2413:U:H2'	40:L5:2414:G:C8	2.55	0.42
40:L5:2656:U:H5''	65:LZ:38:TYR:HB3	2.02	0.42
68:Lc:26:LYS:HB2	68:Lc:97:ILE:HB	2.00	0.42
68:Lc:38:ILE:HD11	68:Lc:46:VAL:HG21	2.01	0.42
72:Lg:33:LEU:HD23	72:Lg:33:LEU:HA	1.87	0.42
84:Lt:59:THR:HG22	84:Lt:61:LYS:HD3	2.02	0.42
1:SA:148:CYS:HB3	1:SA:163:CYS:N	2.27	0.42
5:SG:147:LEU:HD11	5:SG:156:TYR:CD2	2.55	0.42
7:SI:141:ARG:HG3	7:SI:149:TYR:HE2	1.84	0.42
12:SV:2:GLN:H	12:SV:8:PHE:HA	1.84	0.42
19:S2:454:U:H2'	19:S2:455:A:C8	2.54	0.42
19:S2:1488:C:O2'	19:S2:1490:OMG:H8	2.03	0.42
19:S2:1604:G:C5	19:S2:1605:G:C5	3.07	0.42
19:S2:1693:G:H2'	19:S2:1694:U:C6	2.54	0.42
24:SF:30:ILE:HG12	24:SF:39:ILE:HG13	2.01	0.42
26:SM:120:ALA:O	26:SM:124:ILE:HG12	2.20	0.42
29:SS:14:ARG:HD2	29:SS:14:ARG:HA	1.93	0.42
40:L5:257:C:H2'	40:L5:258:G:C8	2.55	0.42
40:L5:454:U:H1'	70:Le:5:ARG:NH1	2.35	0.42
40:L5:1997:U:O2'	40:L5:1998:A:H8	2.03	0.42
40:L5:2293:U:H2'	40:L5:2294:G:H8	1.84	0.42
40:L5:2538:U:H2'	40:L5:2539:C:H6	1.84	0.42
40:L5:3595:U:H5''	40:L5:3597:G:OP2	2.20	0.42
40:L5:3855:C:H2'	40:L5:3856:A:H8	1.85	0.42
40:L5:3866:C:H2'	40:L5:3867:A2M:O4'	2.20	0.42
40:L5:5026:U:H4'	40:L5:5027:C:O4'	2.20	0.42
44:LB:14:LEU:HD22	44:LB:17:LEU:HD11	2.01	0.42
64:LY:117:LYS:HE2	64:LY:117:LYS:HB2	1.88	0.42
4:SE:136:ILE:HD12	4:SE:149:TYR:CE1	2.54	0.42
5:SG:10:THR:HA	5:SG:128:THR:HG23	2.01	0.42
6:SH:66:VAL:HG21	19:S2:913:A:C4	2.55	0.42
6:SH:160:LYS:HD3	6:SH:189:PHE:HB3	2.02	0.42
7:SI:162:LEU:HD21	7:SI:191:GLU:HG3	2.00	0.42
11:SO:149:ARG:HH11	19:S2:1064:C:H4'	1.84	0.42
14:SX:17:ARG:HH22	19:S2:659:G:H21	1.67	0.42
16:Sa:11:ALA:HB3	16:Sa:33:ASP:HB2	2.01	0.42
19:S2:454:U:H2'	19:S2:455:A:H8	1.84	0.42
19:S2:867:OMG:H3'	19:S2:868:G:H21	1.84	0.42
19:S2:895:G:C6	19:S2:896:U:H1'	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1051:G:H2'	19:S2:1052:A:H8	1.85	0.42
19:S2:1139:C:H2'	19:S2:1140:G:O4'	2.20	0.42
24:SF:153:LEU:HB3	24:SF:189:ALA:HA	2.01	0.42
37:At:27:U:H2'	37:At:28:U:C6	2.55	0.42
39:CI:63:ARG:HD2	39:CI:63:ARG:HA	1.85	0.42
40:L5:268:G:H2'	40:L5:269:G:H8	1.84	0.42
40:L5:454:U:H2'	40:L5:455:C:O4'	2.20	0.42
40:L5:907:C:H2'	40:L5:908:G:H8	1.85	0.42
40:L5:2323:C:H2'	40:L5:2324:C:C6	2.54	0.42
40:L5:2610:G:H2'	40:L5:2611:A:C8	2.55	0.42
40:L5:2864:A:H2'	40:L5:2865:U:C6	2.55	0.42
40:L5:3762:U:H3'	40:L5:3763:A:H8	1.85	0.42
40:L5:3832:U:H2'	40:L5:3833:C:C6	2.54	0.42
40:L5:3916:G:H2'	40:L5:3917:A:C8	2.55	0.42
40:L5:4680:G:H2'	40:L5:4681:A:C8	2.55	0.42
40:L5:4699:U:H1'	40:L5:4700:A:H5''	2.01	0.42
45:LC:315:LYS:HD2	48:LF:168:ALA:HB1	2.01	0.42
50:LH:27:VAL:HG12	50:LH:84:VAL:HG21	2.02	0.42
59:LS:157:ARG:HA	59:LS:157:ARG:HD2	1.86	0.42
78:Lm:127:VAL:HG23	78:Lm:128:LYS:HD3	2.01	0.42
81:Lp:61:MET:HE3	81:Lp:61:MET:HB3	1.87	0.42
4:SE:16:LYS:HD2	4:SE:16:LYS:HA	1.76	0.42
4:SE:18:TRP:CZ3	4:SE:29:PRO:HG2	2.55	0.42
6:SH:76:GLN:NE2	6:SH:94:PHE:HB2	2.35	0.42
10:SN:114:ARG:HA	10:SN:114:ARG:HD3	1.91	0.42
18:Se:25:LYS:HE2	18:Se:25:LYS:HB3	1.77	0.42
19:S2:323:C:H5'	19:S2:324:C:OP1	2.20	0.42
19:S2:352:U:H2'	19:S2:353:C:H6	1.82	0.42
19:S2:656:G:N2	19:S2:663:C:H5''	2.35	0.42
19:S2:1736:G:H2'	19:S2:1737:G:C8	2.55	0.42
31:SU:28:ASN:HD21	31:SU:31:SER:HB3	1.85	0.42
40:L5:676:C:H2'	40:L5:677:G:H8	1.85	0.42
40:L5:907:C:H2'	40:L5:908:G:C8	2.55	0.42
40:L5:1309:C:H2'	40:L5:1310:C:H6	1.84	0.42
40:L5:1992:U:H4'	40:L5:1993:C:H5''	2.02	0.42
40:L5:4543:G:H2'	40:L5:4544:A:C8	2.54	0.42
40:L5:4578:G:H2'	40:L5:4579:PSU:H6	1.85	0.42
40:L5:4585:U:H2'	40:L5:4586:G:H8	1.84	0.42
54:LM:100:ARG:HA	54:LM:103:LYS:HG2	2.01	0.42
64:LY:73:VAL:HA	64:LY:80:ILE:HG22	2.01	0.42
3:SC:256:TRP:NE1	13:SW:68:ARG:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SY:13:MET:HE1	15:SY:15:ASN:HB3	2.02	0.41
15:SY:54:VAL:HG22	15:SY:76:TYR:HB2	2.02	0.41
19:S2:215:G:H2'	19:S2:216:C:H6	1.84	0.41
19:S2:218:U:H2'	19:S2:219:U:C6	2.54	0.41
19:S2:323:C:H4'	19:S2:324:C:H5	1.85	0.41
19:S2:1230:C:H2'	19:S2:1231:C:C6	2.56	0.41
19:S2:1453:C:H2'	19:S2:1454:A:H4'	2.02	0.41
19:S2:1501:C:H2'	19:S2:1502:C:H6	1.85	0.41
21:LW:81:ALA:HB1	21:LW:86:SER:HA	2.01	0.41
22:SR:100:PRO:HG2	22:SR:122:PRO:HD3	2.01	0.41
36:Sg:301:GLY:HA2	36:Sg:307:VAL:HA	2.02	0.41
40:L5:2:G:H2'	40:L5:3:C:C6	2.55	0.41
40:L5:677:G:H2'	40:L5:678:C:H6	1.85	0.41
40:L5:1098:G:H2'	40:L5:1099:C:C6	2.55	0.41
40:L5:2674:A:N6	81:Lp:42:CYS:HA	2.35	0.41
40:L5:3722:G:H2'	40:L5:3723:A:H8	1.85	0.41
40:L5:4563:U:H2'	40:L5:4564:A:C8	2.54	0.41
76:Lk:60:LEU:HD23	76:Lk:60:LEU:HA	1.87	0.41
77:Ll:42:ARG:HG3	77:Ll:47:THR:HG23	2.01	0.41
1:SA:66:VAL:HG23	12:SV:37:ALA:HB3	2.02	0.41
6:SH:53:VAL:HG11	6:SH:172:THR:HA	2.02	0.41
6:SH:63:PHE:HA	6:SH:95:ILE:O	2.20	0.41
13:SW:32:LYS:HE3	13:SW:32:LYS:HB2	1.74	0.41
19:S2:107:A:H2'	19:S2:108:G:H8	1.85	0.41
22:SR:97:GLU:HB3	22:SR:120:THR:HG21	2.02	0.41
24:SF:22:LYS:HG3	24:SF:23:TRP:CD2	2.55	0.41
24:SF:47:LYS:HA	24:SF:47:LYS:HD3	1.89	0.41
27:SP:108:LYS:HG2	27:SP:111:MET:HG3	2.01	0.41
36:Sg:85:GLY:HA2	36:Sg:108:VAL:HG23	2.01	0.41
38:Pt:9:A:N3	38:Pt:45:G:H2'	2.35	0.41
40:L5:3727:A:H2'	40:L5:3728:A:C8	2.55	0.41
40:L5:3752:C:O2'	40:L5:3776:G:H1'	2.20	0.41
87:L5:5258:SPM:H32	60:LT:13:TYR:CD1	2.55	0.41
43:LA:133:TYR:HB3	43:LA:168:VAL:HG12	2.03	0.41
58:LQ:70:MET:HE1	58:LQ:137:VAL:HB	2.02	0.41
1:SA:10:MET:HG3	1:SA:55:TRP:CG	2.55	0.41
5:SG:192:ILE:HD11	19:S2:126:G:N2	2.35	0.41
6:SH:62:ILE:HD12	6:SH:94:PHE:HE1	1.84	0.41
9:SL:16:ILE:HD11	9:SL:36:TYR:H	1.85	0.41
19:S2:428:OMU:H6	19:S2:428:OMU:H2'	1.81	0.41
19:S2:550:C:H2'	19:S2:551:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:575:A:H2'	19:S2:576:A2M:O4'	2.20	0.41
19:S2:1702:G:H2'	19:S2:1703:OMC:O4'	2.20	0.41
29:SS:89:ASP:HB2	29:SS:94:LYS:O	2.20	0.41
40:L5:518:G:N2	40:L5:643:C:H2'	2.35	0.41
40:L5:958:G:N2	47:LE:124:LYS:HB3	2.35	0.41
40:L5:1356:U:H2'	40:L5:1357:C:C6	2.55	0.41
40:L5:3867:A2M:HM'3	40:L5:3867:A2M:H1'	1.48	0.41
40:L5:4113:U:H4'	40:L5:4115:G:C5	2.56	0.41
42:L8:154:G:H2'	42:L8:155:C:C6	2.55	0.41
46:LD:61:ILE:HG12	46:LD:79:TYR:CD2	2.55	0.41
57:LP:140:MET:HE3	57:LP:140:MET:HB3	1.87	0.41
67:Lb:73:LYS:HD3	67:Lb:73:LYS:HA	1.74	0.41
70:Le:22:ARG:HB3	70:Le:25:SER:HB3	2.03	0.41
75:Lj:67:LEU:HD23	75:Lj:67:LEU:HA	1.80	0.41
7:SI:14:THR:HG21	19:S2:402:C:OP1	2.20	0.41
13:SW:52:ILE:HG12	13:SW:61:ILE:HG12	2.03	0.41
19:S2:811:A:H2'	19:S2:812:A:C8	2.55	0.41
19:S2:1447:G:H2'	19:S2:1448:A:H8	1.85	0.41
19:S2:1587:G:H21	30:ST:77:LYS:NZ	2.17	0.41
24:SF:121:PRO:HA	24:SF:193:LYS:HG3	2.02	0.41
27:SP:50:ARG:HB2	27:SP:53:GLN:OE1	2.21	0.41
32:SZ:58:LEU:O	32:SZ:62:VAL:HB	2.20	0.41
36:Sg:194:TYR:CZ	36:Sg:212:LYS:HB2	2.56	0.41
40:L5:6:C:H2'	40:L5:7:C:C6	2.56	0.41
40:L5:299:C:H2'	40:L5:300:A:H8	1.85	0.41
40:L5:1207:C:H2'	40:L5:1208:G:H8	1.85	0.41
40:L5:1359:G:H4'	55:LN:203:TYR:HB2	2.01	0.41
40:L5:1517:G:H22	45:LC:103:ALA:HA	1.84	0.41
40:L5:4605:A:H2'	40:L5:4606:G:O4'	2.21	0.41
42:L8:6:C:H2'	42:L8:7:U:C6	2.55	0.41
46:LD:223:PHE:O	46:LD:227:ILE:HG12	2.20	0.41
63:LX:114:LYS:HG2	63:LX:119:ILE:O	2.20	0.41
64:LY:2:LYS:HD2	64:LY:7:VAL:HG13	2.02	0.41
3:SC:246:LYS:HB3	3:SC:246:LYS:HE2	1.78	0.41
4:SE:79:ASP:HB3	4:SE:82:TYR:HB2	2.03	0.41
4:SE:198:ARG:HG3	4:SE:208:VAL:HG12	2.02	0.41
5:SG:38:ALA:O	5:SG:45:TRP:HB3	2.21	0.41
10:SN:20:ARG:NH2	19:S2:918:U:H4'	2.36	0.41
11:SO:28:PHE:HZ	16:Sa:58:VAL:HG21	1.86	0.41
13:SW:57:ARG:NH2	17:Sb:26:GLN:HB2	2.36	0.41
19:S2:484:A2M:HM'2	19:S2:485:A:C4	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:1597:C:H3'	19:S2:1598:G:C8	2.53	0.41
23:SD:55:THR:HA	23:SD:58:VAL:HG22	2.02	0.41
28:SQ:90:LYS:HA	28:SQ:93:VAL:HG22	2.03	0.41
28:SQ:110:ASP:HA	28:SQ:113:ILE:HG22	2.01	0.41
34:Sd:11:PRO:HB3	34:Sd:13:LYS:NZ	2.36	0.41
40:L5:180:C:H2'	40:L5:181:C:C6	2.55	0.41
40:L5:480:C:H2'	40:L5:481:G:H8	1.86	0.41
40:L5:737:C:C4	40:L5:739:G:H5''	2.55	0.41
40:L5:908:G:H2'	40:L5:909:A:H8	1.86	0.41
40:L5:1962:A:H5'	40:L5:1963:C:H5	1.85	0.41
40:L5:2715:G:H2'	40:L5:2716:C:C6	2.55	0.41
40:L5:4961:G:H2'	40:L5:4962:C:C6	2.56	0.41
42:L8:148:A:H2'	42:L8:149:G:C8	2.54	0.41
1:SA:163:CYS:SG	1:SA:174:MET:HG3	2.60	0.41
4:SE:38:LEU:HD22	19:S2:346:C:H5''	2.02	0.41
5:SG:35:GLU:HG2	5:SG:51:ARG:HB2	2.03	0.41
7:SI:76:THR:HG21	7:SI:104:ILE:HD12	2.02	0.41
10:SN:55:ARG:HH22	17:Sb:51:GLN:NE2	2.19	0.41
10:SN:112:LYS:HE3	19:S2:1032:C:H5'	2.02	0.41
19:S2:140:C:H2'	19:S2:141:A:C8	2.55	0.41
19:S2:1143:A:H2'	19:S2:1144:A:C8	2.55	0.41
19:S2:1415:C:H2'	19:S2:1416:C:C6	2.55	0.41
23:SD:23:GLU:HG2	25:SK:64:TRP:HE1	1.86	0.41
34:Sd:23:VAL:HG11	34:Sd:46:TYR:HE2	1.85	0.41
36:Sg:11:LEU:HB3	36:Sg:43:TRP:CH2	2.55	0.41
37:At:40:C:H2'	37:At:41:G:H8	1.85	0.41
40:L5:1266:G:O6	67:Lb:91:ARG:HB2	2.21	0.41
40:L5:2422:OMC:H1'	40:L5:2422:OMC:HM23	1.85	0.41
40:L5:2437:C:H5'	63:LX:127:LEU:HB3	2.02	0.41
40:L5:2561:C:H3'	40:L5:2562:G:H8	1.85	0.41
40:L5:3825:A2M:HM'3	40:L5:3825:A2M:H1'	1.79	0.41
43:LA:109:GLU:OE1	43:LA:138:SER:HA	2.20	0.41
53:LL:64:VAL:HA	53:LL:67:HIS:HD2	1.79	0.41
56:LO:84:VAL:HG11	56:LO:102:LEU:HD22	2.03	0.41
57:LP:54:GLN:HA	57:LP:83:TRP:CD1	2.55	0.41
62:LV:48:ARG:HH11	62:LV:49:LEU:HB3	1.85	0.41
63:LX:64:SER:HB2	73:Lh:69:LEU:HD13	2.02	0.41
80:Lo:78:ARG:HA	80:Lo:78:ARG:HD2	1.89	0.41
3:SC:171:GLY:HA3	13:SW:97:ARG:HH12	1.85	0.41
8:SJ:136:ARG:NH1	8:SJ:158:ASP:HB3	2.36	0.41
10:SN:5:HIS:HE1	10:SN:120:SER:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S2:661:U:H3'	19:S2:662:G:H2'	2.02	0.41
23:SD:113:LEU:HD12	23:SD:114:ALA:H	1.86	0.41
36:Sg:164:ILE:HG21	36:Sg:221:LEU:HD12	2.02	0.41
40:L5:937:U:C6	54:LM:46:ARG:HD2	2.56	0.41
40:L5:2375:A:H2'	40:L5:2376:A:C8	2.56	0.41
40:L5:3861:A:H2'	40:L5:3862:A:C8	2.54	0.41
40:L5:4258:C:H2'	40:L5:4259:C:C6	2.55	0.41
40:L5:4344:U:H2'	40:L5:4345:C:C6	2.56	0.41
40:L5:4581:G:H5'	44:LB:28:LYS:HE2	2.03	0.41
40:L5:4870:G:H5''	54:LM:91:TRP:CD2	2.56	0.41
40:L5:4921:C:H2'	40:L5:4922:C:H6	1.85	0.41
52:LJ:169:LYS:HE3	52:LJ:170:TYR:CZ	2.55	0.41
68:Lc:60:ILE:HD13	68:Lc:93:THR:HG21	2.03	0.41
1:SA:9:GLN:HA	1:SA:55:TRP:HE1	1.85	0.41
4:SE:47:PHE:HA	4:SE:51:ARG:HG3	2.03	0.41
14:SX:46:HIS:CD2	14:SX:103:ALA:HB2	2.56	0.41
15:SY:19:GLN:HB3	15:SY:77:ASP:OD1	2.21	0.41
15:SY:91:LEU:HD23	15:SY:91:LEU:HA	1.90	0.41
19:S2:115:U:H2'	19:S2:116:OMU:H6	2.03	0.41
19:S2:959:G:H2'	19:S2:960:U:C6	2.56	0.41
22:SR:81:ARG:C	22:SR:83:ASN:N	2.79	0.41
23:SD:25:LEU:O	23:SD:29:LEU:HB2	2.21	0.41
40:L5:46:U:H5''	53:LL:16:LYS:HG3	2.01	0.41
40:L5:342:G:H2'	40:L5:343:C:C6	2.56	0.41
40:L5:444:G:H2'	40:L5:445:U:H6	1.85	0.41
40:L5:1081:C:O2'	40:L5:1082:C:H5'	2.21	0.41
40:L5:1539:G:H2'	40:L5:1540:C:H6	1.86	0.41
40:L5:1613:A:H5''	43:LA:183:GLY:CA	2.51	0.41
40:L5:1633:G:H5'	40:L5:1634:A:OP1	2.21	0.41
40:L5:1743:A:O4'	46:LD:15:ARG:HD2	2.21	0.41
40:L5:2046:G:C5	56:LO:60:LYS:HG2	2.56	0.41
40:L5:2621:A:H2'	40:L5:2622:G:C8	2.56	0.41
40:L5:3661:G:C4	43:LA:150:LEU:HD13	2.56	0.41
40:L5:3930:U:H3	40:L5:4180:G:H1	1.67	0.41
40:L5:4685:U:H2'	40:L5:4686:G:C8	2.56	0.41
42:L8:14:U:C4	42:L8:15:G:C6	3.09	0.41
43:LA:171:GLY:O	81:Lp:68:ALA:HB2	2.21	0.41
46:LD:68:ARG:HD3	46:LD:68:ARG:HA	1.86	0.41
74:Li:76:ARG:HD3	74:Li:76:ARG:HA	1.75	0.41
2:SB:34:LYS:HA	2:SB:34:LYS:HD3	1.80	0.41
3:SC:235:ASN:ND2	19:S2:13:C:H5'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SH:79:LEU:HD21	6:SH:94:PHE:HE2	1.85	0.41
8:SJ:116:LYS:HE3	8:SJ:116:LYS:HB3	1.95	0.41
8:SJ:131:ARG:HD2	8:SJ:131:ARG:HA	1.88	0.41
10:SN:7:PRO:HG3	19:S2:996:A:H5''	2.03	0.41
15:SY:12:PHE:HD1	15:SY:23:MET:HE3	1.85	0.41
17:Sb:72:ARG:NH1	19:S2:1120:U:H5'	2.33	0.41
19:S2:645:C:H2'	19:S2:646:G:H8	1.86	0.41
19:S2:956:G:H2'	19:S2:957:A:C8	2.55	0.41
19:S2:1362:U:H5''	19:S2:1363:C:C5	2.47	0.41
19:S2:1415:C:H2'	19:S2:1416:C:H6	1.86	0.41
19:S2:1503:C:H2'	19:S2:1504:U:C6	2.56	0.41
19:S2:1523:C:H2'	19:S2:1524:G:C8	2.56	0.41
19:S2:1595:U:H2'	19:S2:1596:U:H6	1.86	0.41
26:SM:32:ALA:HB3	26:SM:110:VAL:HB	2.02	0.41
27:SP:28:MET:HE2	27:SP:33:LEU:HD23	2.03	0.41
27:SP:72:LYS:HA	27:SP:73:PRO:HD3	1.95	0.41
28:SQ:58:LEU:HD12	28:SQ:63:PHE:HZ	1.85	0.41
33:Sc:58:LEU:HD23	33:Sc:58:LEU:HA	1.88	0.41
35:Sf:103:LEU:HG	35:Sf:104:LYS:N	2.36	0.41
36:Sg:67:SER:HG	36:Sg:83:TRP:HD1	1.68	0.41
40:L5:180:C:H2'	40:L5:181:C:H6	1.86	0.41
40:L5:434:A:H3'	40:L5:435:A:H8	1.85	0.41
40:L5:490:C:H2'	40:L5:491:G:C8	2.56	0.41
40:L5:667:A:H5''	40:L5:668:C:H5''	2.02	0.41
40:L5:750:U:H1'	40:L5:917:A:C8	2.55	0.41
40:L5:1186:U:H2'	40:L5:1187:G:N3	2.35	0.41
40:L5:2021:G:OP1	83:Ls:57:LYS:HA	2.21	0.41
40:L5:2611:A:H2'	40:L5:2612:G:H8	1.85	0.41
40:L5:2624:G:H1	40:L5:2632:PSU:HN3	1.68	0.41
40:L5:3610:A:H2'	40:L5:3611:A:C8	2.56	0.41
40:L5:3656:A:H2'	40:L5:3657:U:C6	2.55	0.41
40:L5:3928:A:H2'	40:L5:3929:G:O4'	2.21	0.41
40:L5:4258:C:H2'	40:L5:4259:C:H6	1.86	0.41
40:L5:4599:A:N1	40:L5:4610:A:H5''	2.36	0.41
42:L8:75:OMG:H2'	42:L8:76:C:C6	2.56	0.41
43:LA:97:ASN:HB2	43:LA:100:ASN:ND2	2.36	0.41
43:LA:245:ARG:HA	43:LA:245:ARG:HD2	1.79	0.41
44:LB:27:GLY:HA2	44:LB:276:HIS:CD2	2.55	0.41
44:LB:238:LYS:HE2	44:LB:238:LYS:HB2	1.82	0.41
56:LO:74:ARG:HG2	56:LO:146:GLY:HA3	2.02	0.41
57:LP:3:ARG:HD2	57:LP:3:ARG:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:LT:17:ARG:HB2	60:LT:22:HIS:CE1	2.56	0.41
61:LU:48:LYS:HG2	61:LU:53:ALA:HB2	2.02	0.41
73:Lh:105:LYS:HG2	73:Lh:108:GLN:HE21	1.86	0.41
12:SV:27:LYS:HA	12:SV:27:LYS:HD3	1.90	0.41
18:Se:12:VAL:HG21	19:S2:616:A:N3	2.36	0.41
19:S2:414:A:H2'	19:S2:415:A:C8	2.55	0.41
19:S2:569:A:H2'	19:S2:570:C:O4'	2.20	0.41
19:S2:666:U:H2'	19:S2:667:U:C6	2.56	0.41
19:S2:942:G:H2'	19:S2:943:U:C6	2.56	0.41
19:S2:1023:A:H2'	19:S2:1024:A:C8	2.55	0.41
19:S2:1588:A:H2'	19:S2:1589:A:C8	2.56	0.41
19:S2:1710:C:H2'	19:S2:1711:U:H6	1.86	0.41
36:Sg:87:LEU:HD21	36:Sg:122:SER:HB3	2.03	0.41
40:L5:10:A:H2'	40:L5:11:G:H8	1.85	0.41
40:L5:654:C:N3	40:L5:655:C:C4	2.88	0.41
40:L5:1176:C:H2'	40:L5:1177:U:H6	1.86	0.41
44:LB:231:VAL:HG21	44:LB:251:VAL:HG23	2.02	0.41
48:LF:184:ILE:HG23	48:LF:189:ASP:HB3	2.01	0.41
51:LI:48:LEU:HD22	51:LI:140:THR:HG22	2.03	0.41
55:LN:6:TYR:CZ	74:Li:40:VAL:HG22	2.55	0.41
56:LO:110:PRO:N	56:LO:111:PRO:HD2	2.35	0.41
57:LP:40:HIS:HE2	57:LP:111:SER:HA	1.85	0.41
2:SB:145:LYS:HE3	2:SB:145:LYS:HB2	1.86	0.40
9:SL:21:LYS:HE3	9:SL:23:VAL:HG11	2.03	0.40
19:S2:85:A:H2'	19:S2:86:C:C6	2.55	0.40
19:S2:398:A:H4'	19:S2:399:C:H5''	2.02	0.40
19:S2:527:C:H2'	19:S2:528:A:H8	1.83	0.40
19:S2:1311:C:H2'	19:S2:1312:G:C8	2.56	0.40
19:S2:1513:C:P	34:Sd:12:ARG:HH22	2.43	0.40
19:S2:1614:A:H2'	19:S2:1615:U:C6	2.57	0.40
19:S2:1631:U:H3'	19:S2:1632:G:H8	1.86	0.40
19:S2:1822:A:H2'	19:S2:1823:A:C8	2.55	0.40
23:SD:173:ARG:HD3	23:SD:173:ARG:HA	1.79	0.40
23:SD:222:PRO:HB3	36:Sg:190:GLY:HA3	2.03	0.40
24:SF:145:ARG:HH12	33:Sc:47:LYS:HE2	1.85	0.40
26:SM:91:LEU:HD23	26:SM:91:LEU:HA	1.94	0.40
38:Pt:53:G:H2'	38:Pt:54:U:H6	1.86	0.40
38:Pt:56:C:C4	80:Lo:104:ILE:HG21	2.56	0.40
40:L5:1942:A:N6	40:L5:2039:G:H2'	2.36	0.40
40:L5:2323:C:H2'	40:L5:2324:C:H6	1.86	0.40
40:L5:2610:G:H2'	40:L5:2611:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:3701:OMC:H5''	40:L5:3746:A:H61	1.86	0.40
40:L5:4130:C:H2'	40:L5:4131:G:H8	1.87	0.40
40:L5:4251:A:H2'	40:L5:4252:C:C6	2.56	0.40
42:L8:81:C:H5'	73:Lh:3:LYS:NZ	2.36	0.40
49:LG:242:LEU:HD23	49:LG:242:LEU:HA	1.89	0.40
70:Le:105:SER:O	70:Le:109:LYS:HG3	2.21	0.40
4:SE:43:PRO:HB2	4:SE:45:ILE:HG22	2.03	0.40
19:S2:35:C:H5''	19:S2:579:C:H5''	2.02	0.40
19:S2:750:C:N4	19:S2:793:G:H1'	2.36	0.40
19:S2:1266:C:H2'	19:S2:1267:C:H6	1.86	0.40
26:SM:117:GLU:HB3	26:SM:120:ALA:HB3	2.03	0.40
40:L5:275:C:H2'	40:L5:276:C:C6	2.56	0.40
40:L5:1088:C:H2'	40:L5:1089:G:C8	2.56	0.40
40:L5:1758:G:H2'	40:L5:1759:G:H8	1.86	0.40
40:L5:1866:U:H2'	40:L5:1867:A:O4'	2.21	0.40
40:L5:2267:U:C6	40:L5:2270:G:H4'	2.56	0.40
40:L5:2439:G:H5'	40:L5:2778:G:OP2	2.20	0.40
40:L5:3718:A2M:H2	40:L5:3934:G:C1'	2.52	0.40
40:L5:4460:U:H2'	40:L5:4461:C:C6	2.56	0.40
40:L5:4508:C:N3	40:L5:4512:U:H5	2.19	0.40
40:L5:4927:G:H5''	40:L5:4928:C:H5	1.85	0.40
44:LB:52:GLY:HA2	44:LB:341:LYS:HE3	2.03	0.40
44:LB:57:VAL:HG22	44:LB:73:VAL:HG12	2.02	0.40
56:LO:88:LEU:HD12	56:LO:99:LEU:HD13	2.02	0.40
68:Lc:42:LYS:HE3	68:Lc:42:LYS:HB3	1.84	0.40
80:Lo:44:LYS:HE3	80:Lo:52:THR:HB	2.03	0.40
1:SA:34:MET:HE3	1:SA:34:MET:HB3	1.97	0.40
3:SC:253:PRO:HA	3:SC:256:TRP:CD2	2.57	0.40
5:SG:74:ARG:HB3	5:SG:94:ARG:HG2	2.03	0.40
8:SJ:127:ARG:HD3	18:Se:31:ARG:HD3	2.03	0.40
12:SV:37:ALA:HB1	12:SV:46:PHE:CE1	2.56	0.40
18:Se:56:ASN:HB3	19:S2:606:G:H5''	2.03	0.40
19:S2:52:G:H2'	19:S2:53:C:H6	1.87	0.40
19:S2:570:C:H2'	19:S2:571:U:O4'	2.22	0.40
19:S2:608:C:H2'	19:S2:609:U:C6	2.56	0.40
19:S2:677:G:H21	19:S2:1028:A:H62	1.67	0.40
19:S2:1514:G:H2'	19:S2:1515:G:H8	1.86	0.40
19:S2:1593:C:H2'	19:S2:1594:A:C8	2.56	0.40
19:S2:1805:G:H2'	19:S2:1806:A:C8	2.56	0.40
23:SD:197:LYS:HA	23:SD:197:LYS:HD3	1.92	0.40
30:ST:45:LEU:HD12	30:ST:45:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Pt:14:A:C2	38:Pt:15:G:H1'	2.57	0.40
40:L5:746:A:H2'	40:L5:747:A:C8	2.56	0.40
40:L5:1392:A:H2'	40:L5:1393:G:C8	2.55	0.40
42:L8:81:C:H2'	42:L8:83:C:OP2	2.21	0.40
43:LA:229:ALA:O	43:LA:234:LYS:HE3	2.22	0.40
45:LC:269:LYS:HA	45:LC:269:LYS:HD2	1.77	0.40
46:LD:61:ILE:HG12	46:LD:79:TYR:HD2	1.86	0.40
48:LF:31:LYS:HE2	48:LF:31:LYS:HB3	1.82	0.40
62:LV:90:ARG:NH2	62:LV:96:LEU:HD23	2.37	0.40
65:LZ:92:ASP:HB3	65:LZ:95:VAL:HB	2.02	0.40
73:Lh:70:ARG:HG2	73:Lh:83:LEU:HD22	2.03	0.40
75:Lj:28:HIS:CD2	75:Lj:31:LYS:HD3	2.56	0.40
82:Lr:95:HIS:O	82:Lr:99:LYS:HB2	2.22	0.40
9:SL:147:LYS:HE2	9:SL:147:LYS:HB2	1.96	0.40
13:SW:23:ARG:HD2	13:SW:23:ARG:HA	1.66	0.40
13:SW:107:SER:HA	19:S2:862:A:C8	2.56	0.40
19:S2:876:C:H2'	19:S2:877:C:C6	2.56	0.40
19:S2:1034:A:H3'	19:S2:1035:A:H8	1.86	0.40
19:S2:1199:A:H2'	19:S2:1200:A:H8	1.86	0.40
22:SR:76:GLU:HA	22:SR:79:GLU:HB3	2.03	0.40
24:SF:96:ALA:HA	24:SF:99:ILE:HD12	2.03	0.40
40:L5:221:C:H2'	40:L5:222:C:C6	2.56	0.40
40:L5:399:G:H2'	40:L5:400:A2M:H8	2.03	0.40
40:L5:425:U:H4'	57:LP:6:LEU:HD21	2.03	0.40
40:L5:1973:G:O2'	84:Lt:78:SER:HB2	2.21	0.40
40:L5:4208:U:H2'	40:L5:4209:G:C8	2.56	0.40
43:LA:130:SER:HB2	43:LA:171:GLY:HA3	2.02	0.40
70:Le:97:ALA:O	70:Le:122:VAL:HA	2.21	0.40
76:Lk:61:PRO:HA	76:Lk:62:PRO:HD3	1.95	0.40
82:Lr:82:ILE:HG23	82:Lr:84:LYS:NZ	2.36	0.40
4:SE:42:LEU:HD12	4:SE:101:LEU:HD11	2.04	0.40
7:SI:192:GLY:O	7:SI:196:GLU:HG3	2.21	0.40
13:SW:45:GLY:O	13:SW:68:ARG:HD2	2.21	0.40
13:SW:52:ILE:HG23	13:SW:61:ILE:HG12	2.04	0.40
17:Sb:33:MET:HB2	17:Sb:79:PHE:HB2	2.03	0.40
19:S2:448:A:H4'	19:S2:449:A:H5''	2.04	0.40
19:S2:1067:C:H3'	19:S2:1068:G:H8	1.85	0.40
19:S2:1805:G:H2'	19:S2:1806:A:H8	1.87	0.40
30:ST:38:LYS:HD2	30:ST:43:LYS:O	2.21	0.40
31:SU:93:SER:H	31:SU:97:ILE:HD11	1.86	0.40
40:L5:173:C:H2'	40:L5:174:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L5:461:G:H2'	40:L5:462:G:H8	1.86	0.40
40:L5:677:G:H2'	40:L5:678:C:C6	2.56	0.40
40:L5:1960:A:N3	83:Ls:10:LYS:HB3	2.37	0.40
40:L5:2495:U:H2'	40:L5:2496:G:H8	1.84	0.40
40:L5:2751:G:H2'	40:L5:2752:G:H8	1.86	0.40
40:L5:2845:A:H61	40:L5:3843:C:H42	1.68	0.40
40:L5:3606:U:H2'	40:L5:3607:U:C6	2.56	0.40
40:L5:4406:U:C2	40:L5:4407:G:C8	3.10	0.40
40:L5:4749:C:H2'	40:L5:4750:G:O4'	2.21	0.40
44:LB:122:TRP:CH2	44:LB:127:LYS:HG2	2.57	0.40
46:LD:256:LYS:H	46:LD:256:LYS:HG2	1.71	0.40
48:LF:69:ILE:O	48:LF:73:ARG:HB2	2.21	0.40
51:LI:36:LEU:HD11	51:LI:69:ARG:HH11	1.86	0.40
60:LT:80:VAL:O	60:LT:83:LYS:HG2	2.21	0.40
62:LV:87:SER:HA	62:LV:97:TYR:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SA	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
2	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	SC	218/222 (98%)	207 (95%)	11 (5%)	0	100	100
4	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
5	SG	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
6	SH	182/186 (98%)	169 (93%)	13 (7%)	0	100	100
7	SI	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
8	SJ	183/185 (99%)	174 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	SL	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
10	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
11	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
12	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
13	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
14	SX	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
15	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
16	Sa	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
17	Sb	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
18	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
20	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
21	LW	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
22	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	36
23	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
24	SF	187/189 (99%)	180 (96%)	7 (4%)	0	100	100
25	SK	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
26	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
27	SP	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
28	SQ	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
29	SS	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
30	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
31	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
32	SZ	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
33	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
35	Sf	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
36	Sg	311/313 (99%)	290 (93%)	21 (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%)	387 (97%)	13 (3%)	0	100	100
45	LC	366/368 (100%)	350 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	LD	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
47	LE	236/250 (94%)	217 (92%)	19 (8%)	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%)	181 (96%)	7 (4%)	0	100	100
51	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
52	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
53	LL	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
54	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
55	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
56	LO	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
57	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
58	LQ	185/187 (99%)	178 (96%)	7 (4%)	0	100	100
59	LS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
60	LT	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
61	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
62	LV	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
63	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
64	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
65	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
66	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
67	Lb	105/109 (96%)	100 (95%)	5 (5%)	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%)	125 (99%)	1 (1%)	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%)	116 (97%)	4 (3%)	0	100	100
74	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
75	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
76	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
78	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
79	Ln	22/24 (92%)	22 (100%)	0	0	100	100
80	Lo	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
81	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
82	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
83	Ls	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
84	Lt	128/141 (91%)	109 (85%)	19 (15%)	0	100	100
All	All	11672/11870 (98%)	11145 (96%)	526 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	224 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	164 (99%)	2 (1%)	63	78
21	LW	95/97 (98%)	95 (100%)	0	100	100
22	SR	122/122 (100%)	120 (98%)	2 (2%)	55	74
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%)	125 (99%)	1 (1%)	73	84
30	ST	113/113 (100%)	113 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	142 (99%)	1 (1%)	76	86
53	LL	176/176 (100%)	176 (100%)	0	100	100
54	LM	118/118 (100%)	118 (100%)	0	100	100
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	10141 (100%)	6 (0%)	87	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	LR	137	ILE
20	LR	139	MET
22	SR	79	GLU
22	SR	80	ARG
29	SS	50	ILE
52	LJ	104	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	SA	141	ASN
2	SB	149	GLN
3	SC	136	HIS
3	SC	235	ASN
4	SE	67	GLN
4	SE	138	HIS
5	SG	4	ASN
5	SG	110	ASN
6	SH	44	ASN
6	SH	126	HIS
7	SI	7	ASN
7	SI	52	ASN
7	SI	146	GLN
9	SL	100	ASN
10	SN	36	GLN
13	SW	90	GLN
13	SW	91	ASN
14	SX	26	GLN

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Mol	Chain	Res	Type
15	SY	2	ASN
15	SY	19	GLN
16	Sa	7	ASN
16	Sa	43	ASN
17	Sb	9	HIS
18	Se	58	ASN
20	LR	118	HIS
21	LW	17	HIS
21	LW	48	GLN
22	SR	74	GLN
22	SR	83	ASN
22	SR	116	ASN
24	SF	79	HIS
24	SF	114	ASN
24	SF	137	GLN
24	SF	179	ASN
26	SM	19	GLN
26	SM	119	GLN
28	SQ	24	HIS
29	SS	72	GLN
29	SS	135	HIS
30	ST	42	HIS
34	Sd	26	ASN
36	Sg	4	GLN
36	Sg	56	GLN
36	Sg	76	GLN
36	Sg	222	ASN
44	LB	68	ASN
44	LB	301	ASN
45	LC	38	ASN
45	LC	112	HIS
45	LC	198	ASN
45	LC	215	ASN
45	LC	362	GLN
46	LD	122	GLN
46	LD	131	ASN
46	LD	195	HIS
46	LD	250	ASN
47	LE	266	GLN
49	LG	90	GLN
49	LG	94	GLN
49	LG	112	GLN

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Mol	Chain	Res	Type
50	LH	39	ASN
50	LH	98	HIS
50	LH	138	GLN
50	LH	156	ASN
52	LJ	104	ASN
53	LL	19	GLN
54	LM	34	ASN
55	LN	32	GLN
55	LN	145	ASN
57	LP	25	HIS
57	LP	34	GLN
57	LP	116	HIS
57	LP	118	GLN
57	LP	133	HIS
59	LS	23	HIS
60	LT	22	HIS
60	LT	90	ASN
60	LT	144	ASN
63	LX	111	GLN
64	LY	14	ASN
64	LY	40	GLN
64	LY	72	GLN
66	La	17	HIS
66	La	34	ASN
66	La	67	GLN
67	Lb	6	ASN
70	Le	23	HIS
70	Le	52	GLN
70	Le	107	ASN
71	Lf	20	ASN
71	Lf	21	GLN
72	Lg	100	GLN
74	Li	15	HIS
75	Lj	66	HIS
80	Lo	105	GLN
83	Ls	127	ASN
83	Ls	190	GLN
84	Lt	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S2	1715/1740 (98%)	428 (24%)	5 (0%)
37	At	69/71 (97%)	15 (21%)	0
38	Pt	72/74 (97%)	15 (20%)	0
40	L5	3643/3655 (99%)	829 (22%)	14 (0%)
41	L7	119/120 (99%)	13 (10%)	0
42	L8	155/156 (99%)	28 (18%)	0
All	All	5773/5816 (99%)	1328 (23%)	19 (0%)

All (1328) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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	59	U
19	S2	62	G
19	S2	65	C
19	S2	67	C
19	S2	68	A
19	S2	71	G
19	S2	72	C
19	S2	73	C
19	S2	74	G
19	S2	76	U
19	S2	82	G
19	S2	92	A
19	S2	103	A
19	S2	113	G
19	S2	114	G
19	S2	115	U
19	S2	130	G
19	S2	140	C
19	S2	142	C
19	S2	143	U
19	S2	149	A
19	S2	155	G
19	S2	158	A

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Mol	Chain	Res	Type
19	S2	160	U
19	S2	162	C
19	S2	164	A
19	S2	170	A
19	S2	175	A
19	S2	179	C
19	S2	182	C
19	S2	184	G
19	S2	190	G
19	S2	196	C
19	S2	198	U
19	S2	199	C
19	S2	200	G
19	S2	203	G
19	S2	204	G
19	S2	208	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	311	C
19	S2	312	G
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
19	S2	333	G
19	S2	340	C
19	S2	347	G

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Mol	Chain	Res	Type
19	S2	351	G
19	S2	360	A
19	S2	361	U
19	S2	362	C
19	S2	364	A
19	S2	368	U
19	S2	370	G
19	S2	383	G
19	S2	385	G
19	S2	386	C
19	S2	407	G
19	S2	408	A
19	S2	409	C
19	S2	436	OMG
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	482	G
19	S2	487	U
19	S2	488	U
19	S2	492	C
19	S2	493	A
19	S2	496	C
19	S2	500	A
19	S2	502	C
19	S2	516	A
19	S2	531	A
19	S2	532	C
19	S2	536	A
19	S2	537	C
19	S2	540	U
19	S2	542	U
19	S2	544	G

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Mol	Chain	Res	Type
19	S2	546	G
19	S2	547	G
19	S2	554	A
19	S2	557	U
19	S2	558	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	607	U
19	S2	614	C
19	S2	617	G
19	S2	623	G
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	670	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
19	S2	696	G
19	S2	697	G

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Mol	Chain	Res	Type
19	S2	698	G
19	S2	732	U
19	S2	733	C
19	S2	734	C
19	S2	735	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	791	C
19	S2	792	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	841	G
19	S2	842	C
19	S2	844	U
19	S2	847	A
19	S2	860	G
19	S2	862	A
19	S2	863	PSU
19	S2	864	A
19	S2	867	OMG
19	S2	870	A
19	S2	871	U
19	S2	874	G
19	S2	877	C

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Mol	Chain	Res	Type
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	913	A
19	S2	917	U
19	S2	918	U
19	S2	919	A
19	S2	920	A
19	S2	922	A
19	S2	930	C
19	S2	933	G
19	S2	934	G
19	S2	954	U
19	S2	955	A
19	S2	956	G
19	S2	963	A
19	S2	970	G
19	S2	971	G
19	S2	978	G
19	S2	985	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	1029	G
19	S2	1030	A
19	S2	1033	G

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Mol	Chain	Res	Type
19	S2	1045	PSU
19	S2	1060	A
19	S2	1061	U
19	S2	1062	A
19	S2	1067	C
19	S2	1083	A
19	S2	1085	C
19	S2	1107	G
19	S2	1108	G
19	S2	1109	C
19	S2	1113	A
19	S2	1116	C
19	S2	1118	C
19	S2	1119	A
19	S2	1121	G
19	S2	1126	G
19	S2	1133	A
19	S2	1138	C
19	S2	1139	C
19	S2	1153	C
19	S2	1154	U
19	S2	1166	G
19	S2	1195	A
19	S2	1207	G
19	S2	1208	A
19	S2	1212	G
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	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	1264	C
19	S2	1270	G

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Mol	Chain	Res	Type
19	S2	1272	OMC
19	S2	1274	G
19	S2	1275	G
19	S2	1281	G
19	S2	1282	A
19	S2	1283	C
19	S2	1284	A
19	S2	1285	G
19	S2	1286	G
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	1304	U
19	S2	1308	U
19	S2	1333	U
19	S2	1342	U
19	S2	1348	G
19	S2	1357	A
19	S2	1364	U
19	S2	1371	U
19	S2	1372	U
19	S2	1373	C
19	S2	1375	G
19	S2	1376	A
19	S2	1378	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	1428	G

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Mol	Chain	Res	Type
19	S2	1433	C
19	S2	1435	C
19	S2	1436	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
19	S2	1463	U
19	S2	1466	G
19	S2	1489	A
19	S2	1490	OMG
19	S2	1492	U
19	S2	1494	U
19	S2	1495	G
19	S2	1497	G
19	S2	1498	A
19	S2	1507	G
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	1544	C
19	S2	1546	G
19	S2	1547	C
19	S2	1552	G
19	S2	1553	C
19	S2	1555	U
19	S2	1558	C
19	S2	1574	C
19	S2	1580	A
19	S2	1581	C
19	S2	1584	G
19	S2	1585	U
19	S2	1587	G
19	S2	1588	A
19	S2	1598	G
19	S2	1600	G

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Mol	Chain	Res	Type
19	S2	1604	G
19	S2	1606	G
19	S2	1614	A
19	S2	1621	U
19	S2	1623	A
19	S2	1631	U
19	S2	1633	A
19	S2	1634	A
19	S2	1637	A
19	S2	1646	C
19	S2	1648	G
19	S2	1654	G
19	S2	1662	U
19	S2	1663	A
19	S2	1665	G
19	S2	1680	G
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	1715	A
19	S2	1721	U
19	S2	1722	G
19	S2	1727	G
19	S2	1744	G
19	S2	1745	A
19	S2	1748	G
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	1759	G
19	S2	1761	U
19	S2	1772	C
19	S2	1773	C
19	S2	1774	C
19	S2	1777	G
19	S2	1780	G

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Mol	Chain	Res	Type
19	S2	1782	G
19	S2	1783	C
19	S2	1784	G
19	S2	1786	U
19	S2	1798	C
19	S2	1810	U
19	S2	1820	G
19	S2	1824	A
19	S2	1829	G
19	S2	1835	A
19	S2	1838	U
19	S2	1849	G
19	S2	1851	MA6
19	S2	1852	C
19	S2	1861	G
19	S2	1862	G
19	S2	1863	A
19	S2	1865	C
37	At	9	A
37	At	13	U
37	At	14	A
37	At	21	A
37	At	26	G
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	64	G
37	At	67	G
37	At	70	A
38	Pt	9	A
38	Pt	13	U
38	Pt	19	G
38	Pt	20(A)	U
38	Pt	21	A
38	Pt	45	G
38	Pt	46	G
38	Pt	47	U
38	Pt	48	C

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Mol	Chain	Res	Type
38	Pt	49	C
38	Pt	58	A
38	Pt	61	C
38	Pt	67	G
38	Pt	71	A
38	Pt	74	C
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	91	G
40	L5	108	A
40	L5	109	G
40	L5	110	C
40	L5	115	C
40	L5	119	G
40	L5	120	A
40	L5	122	U
40	L5	128	C
40	L5	132	G
40	L5	133	C
40	L5	134	G
40	L5	135	G
40	L5	151	G
40	L5	159	C
40	L5	164	G
40	L5	165	A
40	L5	173	C
40	L5	175	C
40	L5	176	G
40	L5	182	G
40	L5	183	C
40	L5	184	U
40	L5	185	C
40	L5	186	G
40	L5	188	G

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Mol	Chain	Res	Type
40	L5	189	G
40	L5	200	U
40	L5	209	U
40	L5	216	C
40	L5	218	A
40	L5	220	C
40	L5	233	U
40	L5	234	G
40	L5	255	C
40	L5	256	G
40	L5	260	C
40	L5	261	G
40	L5	264	C
40	L5	265	C
40	L5	266	C
40	L5	267	G
40	L5	275	C
40	L5	276	C
40	L5	280	G
40	L5	297	U
40	L5	306	A
40	L5	315	G
40	L5	316	U
40	L5	340	C
40	L5	362	A
40	L5	373	G
40	L5	385	A
40	L5	387	G
40	L5	388	A
40	L5	396	A
40	L5	398	A2M
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

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Mol	Chain	Res	Type
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	467	U
40	L5	485	C
40	L5	486	C
40	L5	489	C
40	L5	493	G
40	L5	494	U
40	L5	497	G
40	L5	498	C
40	L5	500	G
40	L5	501	C
40	L5	502	C
40	L5	503	C
40	L5	504	G
40	L5	505	G
40	L5	509	A
40	L5	510	U
40	L5	512	U
40	L5	513	U
40	L5	514	U
40	L5	516	C
40	L5	517	C
40	L5	518	G
40	L5	519	C
40	L5	643	C
40	L5	645	G
40	L5	646	G
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

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Mol	Chain	Res	Type
40	L5	674	G
40	L5	683	C
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	746	A
40	L5	758	G
40	L5	759	G
40	L5	760	G
40	L5	904	C
40	L5	905	C
40	L5	910	G
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	936	C
40	L5	937	U
40	L5	941	C
40	L5	943	A
40	L5	945	U
40	L5	946	C
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

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Mol	Chain	Res	Type
40	L5	966	A
40	L5	967	C
40	L5	969	C
40	L5	970	G
40	L5	982	U
40	L5	985	C
40	L5	1070	G
40	L5	1071	C
40	L5	1072	C
40	L5	1075	G
40	L5	1076	C
40	L5	1082	C
40	L5	1083	U
40	L5	1095	A
40	L5	1168	G
40	L5	1169	G
40	L5	1171	G
40	L5	1172	C
40	L5	1173	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	1200	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
40	L5	1218	G
40	L5	1219	G
40	L5	1221	G
40	L5	1222	A
40	L5	1240	G
40	L5	1246	G
40	L5	1247	U
40	L5	1253	G
40	L5	1254	A
40	L5	1256	G

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Mol	Chain	Res	Type
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	1270	A
40	L5	1271	G
40	L5	1272	C
40	L5	1273	G
40	L5	1275	G
40	L5	1277	G
40	L5	1278	C
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	1302	U
40	L5	1312	A
40	L5	1313	C
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	1370	G
40	L5	1379	C
40	L5	1387	A
40	L5	1394	G
40	L5	1397	A
40	L5	1398	A
40	L5	1404	G
40	L5	1405	C
40	L5	1407	C

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Mol	Chain	Res	Type
40	L5	1408	G
40	L5	1409	C
40	L5	1410	U
40	L5	1411	C
40	L5	1413	C
40	L5	1415	G
40	L5	1416	G
40	L5	1417	C
40	L5	1418	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	1452	A
40	L5	1482	G
40	L5	1483	C
40	L5	1497	A
40	L5	1498	G
40	L5	1502	G
40	L5	1504	G
40	L5	1516	G
40	L5	1517	G
40	L5	1534	A2M
40	L5	1535	C
40	L5	1536	PSU
40	L5	1537	A
40	L5	1547	A
40	L5	1563	A
40	L5	1566	C
40	L5	1574	G
40	L5	1578	U
40	L5	1586	G
40	L5	1591	U
40	L5	1596	U
40	L5	1612	G
40	L5	1624	G
40	L5	1625	OMG

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Mol	Chain	Res	Type
40	L5	1626	G
40	L5	1631	A
40	L5	1633	G
40	L5	1634	A
40	L5	1637	A
40	L5	1638	A
40	L5	1640	C
40	L5	1641	G
40	L5	1642	A
40	L5	1654	G
40	L5	1661	C
40	L5	1676	C
40	L5	1677	PSU
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	1703	C
40	L5	1704	C
40	L5	1705	G
40	L5	1706	A
40	L5	1717	C
40	L5	1718	C
40	L5	1719	A
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	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

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Mol	Chain	Res	Type
40	L5	1772	C
40	L5	1787	A
40	L5	1797	G
40	L5	1803	G
40	L5	1804	A
40	L5	1806	G
40	L5	1810	G
40	L5	1815	G
40	L5	1820	C
40	L5	1821	G
40	L5	1822	U
40	L5	1833	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	1892	A
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	1931	C
40	L5	1932	A
40	L5	1936	C
40	L5	1948	G
40	L5	1961	G
40	L5	1962	A
40	L5	1971	C
40	L5	1972	G
40	L5	1974	U
40	L5	1975	G
40	L5	1976	G
40	L5	1978	C
40	L5	1980	U

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Mol	Chain	Res	Type
40	L5	1981	G
40	L5	1982	G
40	L5	1984	A
40	L5	1985	G
40	L5	1986	U
40	L5	1990	A
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
40	L5	2001	G
40	L5	2002	A
40	L5	2003	G
40	L5	2004	U
40	L5	2005	G
40	L5	2011	C
40	L5	2016	C
40	L5	2017	A
40	L5	2018	C
40	L5	2024	G
40	L5	2025	A
40	L5	2026	A
40	L5	2034	G
40	L5	2046	G
40	L5	2048	U
40	L5	2055	G
40	L5	2056	G
40	L5	2069	A
40	L5	2072	C
40	L5	2084	C
40	L5	2090	U
40	L5	2092	G
40	L5	2093	A
40	L5	2095	A
40	L5	2096	G
40	L5	2097	U
40	L5	2098	G
40	L5	2101	C

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Mol	Chain	Res	Type
40	L5	2102	G
40	L5	2103	G
40	L5	2104	G
40	L5	2106	G
40	L5	2107	C
40	L5	2110	C
40	L5	2112	G
40	L5	2250	C
40	L5	2252	G
40	L5	2253	A
40	L5	2256	C
40	L5	2258	C
40	L5	2259	G
40	L5	2260	C
40	L5	2269	C
40	L5	2289	C
40	L5	2300	A
40	L5	2301	G
40	L5	2310	C
40	L5	2313	A
40	L5	2331	G
40	L5	2332	A
40	L5	2333	G
40	L5	2345	G
40	L5	2348	G
40	L5	2351	OMC
40	L5	2360	A
40	L5	2364	OMG
40	L5	2382	A
40	L5	2383	C
40	L5	2389	A
40	L5	2395	A
40	L5	2397	G
40	L5	2398	U
40	L5	2401	A2M
40	L5	2402	G
40	L5	2408	U
40	L5	2411	C
40	L5	2412	A
40	L5	2417	A
40	L5	2425	U
40	L5	2450	G

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Mol	Chain	Res	Type
40	L5	2453	A
40	L5	2464	C
40	L5	2465	C
40	L5	2469	C
40	L5	2470	C
40	L5	2471	G
40	L5	2474	G
40	L5	2475	G
40	L5	2478	C
40	L5	2479	G
40	L5	2480	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	2505	C
40	L5	2506	G
40	L5	2513	A
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	2606	G
40	L5	2618	G
40	L5	2653	C

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Mol	Chain	Res	Type
40	L5	2658	G
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	2702	C
40	L5	2703	G
40	L5	2706	G
40	L5	2708	U
40	L5	2709	C
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	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	2828	U
40	L5	2829	U
40	L5	2838	G
40	L5	2842	G
40	L5	2848	G
40	L5	2855	G
40	L5	2867	C

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Mol	Chain	Res	Type
40	L5	2876	OMG
40	L5	2877	G
40	L5	2892	C
40	L5	2894	A
40	L5	2899	C
40	L5	2900	U
40	L5	2902	G
40	L5	2903	G
40	L5	2904	U
40	L5	2905	C
40	L5	2907	G
40	L5	2908	U
40	L5	3590	G
40	L5	3591	C
40	L5	3592	G
40	L5	3594	C
40	L5	3595	U
40	L5	3596	A
40	L5	3597	G
40	L5	3599	A
40	L5	3605	C
40	L5	3615	G
40	L5	3616	U
40	L5	3617	G
40	L5	3619	G
40	L5	3626	G
40	L5	3635	A
40	L5	3644	U
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	3696	C
40	L5	3701	OMC
40	L5	3710	G
40	L5	3711	A
40	L5	3713	U
40	L5	3726	A
40	L5	3727	A

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Mol	Chain	Res	Type
40	L5	3729	U
40	L5	3748	A
40	L5	3753	G
40	L5	3760	A
40	L5	3761	C
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	3791	C
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	3881	G
40	L5	3885	G
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	3939	G
40	L5	3942	A

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Mol	Chain	Res	Type
40	L5	3943	A
40	L5	3944	G
40	L5	3946	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	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	4084	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	4109	G
40	L5	4111	U
40	L5	4114	C
40	L5	4115	G
40	L5	4116	C
40	L5	4119	C
40	L5	4122	G
40	L5	4127	A
40	L5	4138	C
40	L5	4140	C
40	L5	4141	G
40	L5	4142	C
40	L5	4143	G
40	L5	4144	C

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Mol	Chain	Res	Type
40	L5	4146	G
40	L5	4162	C
40	L5	4163	U
40	L5	4170	A
40	L5	4183	G
40	L5	4184	G
40	L5	4191	G
40	L5	4201	G
40	L5	4203	A
40	L5	4220	6MZ
40	L5	4222	G
40	L5	4225	G
40	L5	4228	OMG
40	L5	4229	U
40	L5	4233	A
40	L5	4238	G
40	L5	4242	U
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	4282	A
40	L5	4283	G
40	L5	4291	G
40	L5	4305	G
40	L5	4306	OMU
40	L5	4329	G
40	L5	4330	G
40	L5	4332	C
40	L5	4338	G
40	L5	4349	C
40	L5	4350	C
40	L5	4373	G
40	L5	4377	G
40	L5	4378	A
40	L5	4387	C
40	L5	4391	G
40	L5	4394	A

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Mol	Chain	Res	Type
40	L5	4405	G
40	L5	4422	A
40	L5	4427	G
40	L5	4438	U
40	L5	4444	C
40	L5	4449	A
40	L5	4464	A
40	L5	4466	C
40	L5	4475	G
40	L5	4488	A
40	L5	4491	G
40	L5	4500	PSU
40	L5	4512	U
40	L5	4513	A
40	L5	4519	C
40	L5	4524	G
40	L5	4525	C
40	L5	4529	G
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
40	L5	4599	A
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	4657	U
40	L5	4670	C
40	L5	4671	C
40	L5	4672	A
40	L5	4687	A
40	L5	4694	G
40	L5	4695	C

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Mol	Chain	Res	Type
40	L5	4700	A
40	L5	4707	A
40	L5	4708	A
40	L5	4709	U
40	L5	4719	G
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	4776	G
40	L5	4859	C
40	L5	4865	C
40	L5	4867	G
40	L5	4870	G
40	L5	4871	C
40	L5	4875	G
40	L5	4881	U
40	L5	4882	U
40	L5	4883	C
40	L5	4889	G
40	L5	4895	C
40	L5	4896	G
40	L5	4897	G
40	L5	4898	G
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	4923	C
40	L5	4925	U

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Mol	Chain	Res	Type
40	L5	4927	G
40	L5	4928	C
40	L5	4934	A
40	L5	4940	C
40	L5	4941	G
40	L5	4943	A
40	L5	4944	C
40	L5	4949	G
40	L5	4951	G
40	L5	4963	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	5006	U
40	L5	5013	C
40	L5	5014	A
40	L5	5017	G
40	L5	5022	U
40	L5	5023	C
40	L5	5024	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
40	L5	5055	G
40	L5	5060	A
40	L5	5061	A
40	L5	5064	G
40	L5	5069	U
41	L7	22	A
41	L7	33	U
41	L7	37	G
41	L7	38	U
41	L7	39	C

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Mol	Chain	Res	Type
41	L7	49	A
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
42	L8	23	C
42	L8	25	G
42	L8	34	U
42	L8	35	C
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	86	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
42	L8	147	G
42	L8	150	C
42	L8	151	G

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	S2	291	G
19	S2	531	A

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Mol	Chain	Res	Type
19	S2	563	G
19	S2	688	U
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	2416	G
40	L5	2675	G
40	L5	2760	G
40	L5	3673	C
40	L5	3951	G
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$
19	OMU	S2	354	19	19,22,23	3.29	7 (36%)	25,31,34	1.80	5 (20%)
40	OMC	L5	2365	40,85	19,22,23	0.60	0	25,31,34	0.56	0
19	OMU	S2	799	19	19,22,23	3.41	7 (36%)	25,31,34	1.80	4 (16%)
40	PSU	L5	1782	40	18,21,22	1.08	2 (11%)	21,30,33	1.92	4 (19%)
19	PSU	S2	93	19	18,21,22	1.13	1 (5%)	21,30,33	1.74	4 (19%)
19	A2M	S2	468	19	22,25,26	1.26	2 (9%)	30,36,39	1.57	6 (20%)
40	A2M	L5	1534	40,85	22,25,26	1.20	2 (9%)	30,36,39	1.46	8 (26%)
40	PSU	L5	4296	40	18,21,22	1.11	2 (11%)	21,30,33	1.89	4 (19%)
19	PSU	S2	105	19	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PSU	S2	801	19	18,21,22	1.12	1 (5%)	21,30,33	1.73	4 (19%)
19	OMG	S2	683	19	23,26,27	0.50	0	32,38,41	0.51	0
40	OMG	L5	3792	40	23,26,27	0.57	0	32,38,41	0.54	0
19	OMU	S2	1442	19	19,22,23	3.42	7 (36%)	25,31,34	1.86	5 (20%)
40	PSU	L5	3884	40	18,21,22	1.10	2 (11%)	21,30,33	1.91	5 (23%)
42	OMG	L8	75	42	23,26,27	0.58	0	32,38,41	0.49	0
40	OMC	L5	2351	40,85	19,22,23	0.76	1 (5%)	25,31,34	1.07	2 (8%)
19	PSU	S2	814	19	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
40	PSU	L5	1582	40	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
40	OMG	L5	4392	40	23,26,27	0.62	0	32,38,41	0.56	0
19	PSU	S2	109	19	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
40	A2M	L5	1524	40	22,25,26	1.30	2 (9%)	30,36,39	1.50	6 (20%)
40	PSU	L5	1744	40	18,21,22	1.12	2 (11%)	21,30,33	2.04	6 (28%)
19	PSU	S2	1004	19	18,21,22	1.24	1 (5%)	21,30,33	1.77	4 (19%)
19	OMC	S2	462	19	19,22,23	0.52	0	25,31,34	0.74	0
40	PSU	L5	4500	40	18,21,22	1.15	2 (11%)	21,30,33	2.05	5 (23%)
19	PSU	S2	1232	19	18,21,22	1.17	1 (5%)	21,30,33	1.88	4 (19%)
19	4AC	S2	1337	19	21,24,25	0.40	0	28,34,37	0.81	2 (7%)
40	OMG	L5	1625	40	23,26,27	0.57	0	32,38,41	0.44	0
40	A2M	L5	3830	40	22,25,26	1.20	1 (4%)	30,36,39	1.53	6 (20%)
19	A2M	S2	99	85,19	22,25,26	1.16	1 (4%)	30,36,39	1.55	7 (23%)
19	OMU	S2	116	19	19,22,23	3.26	7 (36%)	25,31,34	1.69	4 (16%)
40	PSU	L5	4353	40	18,21,22	1.06	2 (11%)	21,30,33	1.90	4 (19%)
19	OMC	S2	1391	19	19,22,23	0.56	0	25,31,34	0.72	0
40	PSU	L5	3853	40,85	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)
40	6MZ	L5	4220	40	22,25,26	2.91	5 (22%)	29,36,39	2.51	10 (34%)
40	A2M	L5	1871	40,85	22,25,26	1.35	3 (13%)	30,36,39	1.64	7 (23%)
40	PSU	L5	1683	40	18,21,22	1.09	1 (5%)	21,30,33	1.99	4 (19%)
40	PSU	L5	4299	40	18,21,22	1.08	2 (11%)	21,30,33	1.83	4 (19%)
40	OMU	L5	2837	40	19,22,23	3.30	7 (36%)	25,31,34	1.89	4 (16%)
40	PSU	L5	3920	40,85	18,21,22	1.08	2 (11%)	21,30,33	1.94	5 (23%)
40	PSU	L5	4576	40	18,21,22	1.09	1 (5%)	21,30,33	2.04	5 (23%)
19	6MZ	S2	1832	85,19	22,25,26	3.99	11 (50%)	29,36,39	2.32	11 (37%)
40	OMU	L5	4620	40	19,22,23	3.20	7 (36%)	25,31,34	1.84	5 (20%)
40	OMC	L5	2824	40	19,22,23	0.64	0	25,31,34	0.68	0
40	OMU	L5	4227	40	19,22,23	3.26	7 (36%)	25,31,34	1.76	5 (20%)

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	1.17	1 (4%)	30,36,39	1.48	8 (26%)
40	OMG	L5	2364	40,85	23,26,27	0.59	0	32,38,41	0.45	0
40	UR3	L5	4530	40	19,22,23	2.60	7 (36%)	26,32,35	1.58	2 (7%)
40	OMG	L5	2424	40	23,26,27	0.58	0	32,38,41	0.49	0
40	A2M	L5	4590	40	22,25,26	1.18	1 (4%)	30,36,39	1.52	5 (16%)
19	OMC	S2	174	19	19,22,23	0.55	0	25,31,34	0.69	0
19	OMG	S2	1490	19	23,26,27	0.56	0	32,38,41	0.48	0
19	PSU	S2	1367	19	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
40	PSU	L5	1781	40	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
40	PSU	L5	3639	40	18,21,22	1.10	2 (11%)	21,30,33	1.89	4 (19%)
40	PSU	L5	5010	40	18,21,22	1.03	1 (5%)	21,30,33	1.87	4 (19%)
40	OMU	L5	3925	40	19,22,23	3.15	7 (36%)	25,31,34	1.82	5 (20%)
40	PSU	L5	4403	40	18,21,22	1.10	3 (16%)	21,30,33	1.93	6 (28%)
19	PSU	S2	406	19	18,21,22	1.15	2 (11%)	21,30,33	1.93	4 (19%)
40	OMC	L5	2861	40	19,22,23	0.64	0	25,31,34	0.79	1 (4%)
19	PSU	S2	686	19	18,21,22	1.10	1 (5%)	21,30,33	1.87	3 (14%)
40	OMG	L5	4196	40,38	23,26,27	0.53	0	32,38,41	0.45	0
19	PSU	S2	866	19	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
40	PSU	L5	3695	40	18,21,22	1.09	2 (11%)	21,30,33	2.02	4 (19%)
40	PSU	L5	4673	40,85	18,21,22	1.06	2 (11%)	21,30,33	1.88	4 (19%)
40	1MA	L5	1322	40,85	21,25,26	0.69	0	30,37,40	0.79	2 (6%)
19	PSU	S2	651	19	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
40	OMG	L5	3627	40	23,26,27	0.59	0	32,38,41	0.68	0
40	PSU	L5	1862	40	18,21,22	1.08	1 (5%)	21,30,33	1.97	4 (19%)
19	4AC	S2	1842	19	21,24,25	0.41	0	28,34,37	0.48	0
19	PSU	S2	649	19	18,21,22	1.09	2 (11%)	21,30,33	1.77	4 (19%)
19	B8N	S2	1248	19	25,29,30	3.24	7 (28%)	28,42,45	2.00	7 (25%)
19	A2M	S2	1383	19	22,25,26	1.22	1 (4%)	30,36,39	1.66	8 (26%)
40	OMC	L5	4536	40	19,22,23	0.63	0	25,31,34	0.64	0
40	PSU	L5	1536	40	18,21,22	1.10	2 (11%)	21,30,33	1.95	4 (19%)
19	OMG	S2	509	19	23,26,27	0.52	0	32,38,41	0.55	0
40	PSU	L5	4471	40	18,21,22	1.06	2 (11%)	21,30,33	1.94	4 (19%)
40	PSU	L5	4628	40	18,21,22	1.04	1 (5%)	21,30,33	1.88	5 (23%)
19	PSU	S2	1056	19	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
19	OMU	S2	627	19	19,22,23	3.29	7 (36%)	25,31,34	1.83	5 (20%)
40	OMU	L5	4498	40	19,22,23	3.22	7 (36%)	25,31,34	1.91	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	PSU	L8	55	42	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)
19	OMU	S2	172	19	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
40	OMG	L5	4637	40	23,26,27	0.61	0	32,38,41	0.47	0
40	OMC	L5	4456	40	19,22,23	0.69	0	25,31,34	0.61	0
40	OMG	L5	1522	40	23,26,27	0.59	0	32,38,41	0.62	0
40	OMC	L5	3887	40	19,22,23	0.62	0	25,31,34	0.79	0
40	A2M	L5	2787	40	22,25,26	1.17	1 (4%)	30,36,39	1.49	7 (23%)
19	A2M	S2	484	19	22,25,26	1.17	1 (4%)	30,36,39	1.47	6 (20%)
19	OMG	S2	644	19	23,26,27	0.51	0	32,38,41	0.57	0
19	G7M	S2	1639	19	23,26,27	2.67	8 (34%)	34,39,42	2.64	11 (32%)
19	OMG	S2	601	19	23,26,27	0.50	0	32,38,41	0.53	0
40	PSU	L5	4532	40	18,21,22	1.05	1 (5%)	21,30,33	1.98	4 (19%)
40	A2M	L5	2363	40,85	22,25,26	1.23	2 (9%)	30,36,39	1.54	8 (26%)
40	A2M	L5	3867	40	22,25,26	1.23	2 (9%)	30,36,39	1.49	7 (23%)
19	OMC	S2	1703	19	19,22,23	0.58	0	25,31,34	0.74	0
40	PSU	L5	4312	40	18,21,22	1.06	1 (5%)	21,30,33	1.93	4 (19%)
19	OMG	S2	867	19	23,26,27	0.48	0	32,38,41	0.52	0
19	PSU	S2	1177	19	18,21,22	1.07	1 (5%)	21,30,33	1.79	4 (19%)
19	PSU	S2	1244	19	18,21,22	1.13	1 (5%)	21,30,33	1.85	4 (19%)
40	PSU	L5	4493	40	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
40	PSU	L5	4457	40	18,21,22	1.06	2 (11%)	21,30,33	1.94	4 (19%)
40	A2M	L5	3718	40	22,25,26	1.19	1 (4%)	30,36,39	1.50	5 (16%)
40	A2M	L5	4523	40,85	22,25,26	1.30	3 (13%)	30,36,39	1.51	8 (26%)
40	OMC	L5	2422	40,85	19,22,23	0.68	0	25,31,34	0.78	1 (4%)
40	OMG	L5	4228	40	23,26,27	0.61	0	32,38,41	0.61	0
40	OMG	L5	1316	40	23,26,27	0.67	0	32,38,41	0.63	0
19	OMC	S2	1272	19	19,22,23	0.57	0	25,31,34	1.05	2 (8%)
19	A2M	S2	668	85,19	22,25,26	1.30	2 (9%)	30,36,39	1.51	6 (20%)
40	OMC	L5	3841	40	19,22,23	0.67	0	25,31,34	0.50	0
19	PSU	S2	681	19	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
40	OMC	L5	2804	40	19,22,23	0.63	0	25,31,34	0.60	0
40	PSU	L5	3851	40	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
19	PSU	S2	1046	19	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
40	OMG	L5	3899	40	23,26,27	0.66	0	32,38,41	0.53	0
40	PSU	L5	1677	40	18,21,22	1.07	2 (11%)	21,30,33	2.03	5 (23%)
42	PSU	L8	69	42	18,21,22	1.11	3 (16%)	21,30,33	2.03	5 (23%)
19	A2M	S2	159	19	22,25,26	1.30	2 (9%)	30,36,39	1.53	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	OMU	S2	121	19	19,22,23	3.33	7 (36%)	25,31,34	1.87	4 (16%)
40	PSU	L5	4442	40	18,21,22	1.07	1 (5%)	21,30,33	2.04	6 (28%)
40	A2M	L5	1323	40	22,25,26	1.32	3 (13%)	30,36,39	1.55	8 (26%)
40	PSU	L5	3822	40	18,21,22	1.08	2 (11%)	21,30,33	1.97	6 (28%)
19	MA6	S2	1851	19	23,26,27	1.29	2 (8%)	33,38,41	3.37	12 (36%)
40	A2M	L5	3825	40	22,25,26	1.22	2 (9%)	30,36,39	1.55	7 (23%)
19	OMC	S2	517	19	19,22,23	0.55	0	25,31,34	0.67	0
40	A2M	L5	400	40	22,25,26	1.26	3 (13%)	30,36,39	1.53	7 (23%)
40	OMG	L5	4370	40	23,26,27	0.52	0	32,38,41	0.48	0
40	PSU	L5	4431	40	18,21,22	1.09	2 (11%)	21,30,33	1.81	4 (19%)
40	A2M	L5	2815	40	22,25,26	1.23	2 (9%)	30,36,39	1.54	9 (30%)
40	5MC	L5	4447	40	19,22,23	0.99	1 (5%)	26,32,35	0.76	1 (3%)
40	PSU	L5	1860	40	18,21,22	1.03	1 (5%)	21,30,33	1.76	4 (19%)
19	PSU	S2	966	19	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
40	A2M	L5	1326	40	22,25,26	1.24	2 (9%)	30,36,39	1.49	9 (30%)
19	OMG	S2	436	19	23,26,27	0.50	0	32,38,41	0.63	0
40	OMG	L5	4494	40	23,26,27	0.61	0	32,38,41	0.57	0
40	A2M	L5	398	40	22,25,26	1.24	1 (4%)	30,36,39	1.55	7 (23%)
40	A2M	L5	4571	40	22,25,26	1.27	2 (9%)	30,36,39	1.61	8 (26%)
40	UY1	L5	3818	40	19,22,23	4.82	9 (47%)	21,31,34	2.04	5 (23%)
40	OMG	L5	4499	40	23,26,27	0.58	0	32,38,41	0.49	0
40	PSU	L5	4552	40	18,21,22	1.13	2 (11%)	21,30,33	2.05	4 (19%)
19	PSU	S2	863	19	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	4293	40	18,21,22	1.12	2 (11%)	21,30,33	2.13	5 (23%)
19	OMG	S2	1328	19	23,26,27	0.48	0	32,38,41	0.46	0
19	OMU	S2	1326	19	19,22,23	3.34	7 (36%)	25,31,34	1.81	5 (20%)
40	OMU	L5	4306	40	19,22,23	3.16	7 (36%)	25,31,34	1.74	4 (16%)
40	PSU	L5	4579	40	18,21,22	1.04	2 (11%)	21,30,33	1.88	4 (19%)
40	OMC	L5	1340	40	19,22,23	0.68	0	25,31,34	0.67	0
40	OMG	L5	2876	40	23,26,27	0.55	0	32,38,41	0.57	0
40	PSU	L5	4361	40	18,21,22	1.01	2 (11%)	21,30,33	1.84	4 (19%)
40	PSU	L5	4972	40	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
19	PSU	S2	1081	19	18,21,22	1.04	1 (5%)	21,30,33	2.06	5 (23%)
40	OMC	L5	3701	40	19,22,23	0.70	0	25,31,34	1.75	4 (16%)
40	OMG	L5	4623	40	23,26,27	0.58	0	32,38,41	0.55	0
40	OMG	L5	4618	40	23,26,27	0.60	0	32,38,41	0.48	0
40	OMC	L5	3869	40	19,22,23	0.65	0	25,31,34	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	OMC	L5	3808	40	19,22,23	0.69	0	25,31,34	0.78	1 (4%)
19	A2M	S2	166	19	22,25,26	1.28	1 (4%)	30,36,39	1.52	10 (33%)
19	A2M	S2	576	19	22,25,26	1.22	1 (4%)	30,36,39	1.49	5 (16%)
19	OMU	S2	1288	19	19,22,23	3.38	7 (36%)	25,31,34	1.86	5 (20%)
40	PSU	L5	4973	40	18,21,22	1.08	2 (11%)	21,30,33	1.97	5 (23%)
40	PSU	L5	4636	40	18,21,22	1.06	1 (5%)	21,30,33	2.25	7 (33%)
40	A2M	L5	3785	40	22,25,26	1.12	1 (4%)	30,36,39	1.64	8 (26%)
40	PSU	L5	5001	40	18,21,22	1.05	2 (11%)	21,30,33	2.02	4 (19%)
19	PSU	S2	1045	19	18,21,22	1.10	1 (5%)	21,30,33	2.00	5 (23%)
19	OMU	S2	428	19	19,22,23	3.38	7 (36%)	25,31,34	1.78	5 (20%)
40	PSU	L5	4521	40,85	18,21,22	1.11	2 (11%)	21,30,33	2.05	6 (28%)
19	PSU	S2	1174	19	18,21,22	1.12	2 (11%)	21,30,33	1.99	4 (19%)
19	A2M	S2	27	19	22,25,26	1.19	1 (4%)	30,36,39	1.55	8 (26%)
40	PSU	L5	2632	40	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	1792	40	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
19	MA6	S2	1850	19	23,26,27	2.65	9 (39%)	33,38,41	3.23	13 (39%)
40	PSU	L5	2839	40	18,21,22	1.16	2 (11%)	21,30,33	1.85	4 (19%)
40	PSU	L5	3844	40	18,21,22	1.12	2 (11%)	21,30,33	1.83	4 (19%)
40	PSU	L5	4689	40	18,21,22	1.08	2 (11%)	21,30,33	1.89	4 (19%)
40	PSU	L5	3637	40	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)
40	A2M	L5	2401	40	22,25,26	1.21	1 (4%)	30,36,39	1.55	7 (23%)
40	OMG	L5	3744	40	23,26,27	0.58	0	32,38,41	0.51	0
40	5MC	L5	3782	40,85	19,22,23	0.81	0	26,32,35	0.74	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
19	OMU	S2	354	19	-	0/9/27/28	0/2/2/2
40	OMC	L5	2365	40,85	-	0/9/27/28	0/2/2/2
19	OMU	S2	799	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	1782	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	93	19	-	0/7/25/26	0/2/2/2
19	A2M	S2	468	19	-	1/9/27/28	0/3/3/3
40	A2M	L5	1534	40,85	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	PSU	L5	4296	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	105	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	801	19	-	3/7/25/26	0/2/2/2
19	OMG	S2	683	19	-	0/9/27/28	0/3/3/3
40	OMG	L5	3792	40	-	2/9/27/28	0/3/3/3
19	OMU	S2	1442	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	3884	40	-	0/7/25/26	0/2/2/2
42	OMG	L8	75	42	-	2/9/27/28	0/3/3/3
40	OMC	L5	2351	40,85	-	3/9/27/28	0/2/2/2
19	PSU	S2	814	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1582	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	4392	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	109	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	1524	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	1744	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1004	19	-	1/7/25/26	0/2/2/2
19	OMC	S2	462	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	1232	19	-	0/7/25/26	0/2/2/2
19	4AC	S2	1337	19	-	1/11/29/30	0/2/2/2
40	OMG	L5	1625	40	-	2/9/27/28	0/3/3/3
40	A2M	L5	3830	40	-	2/9/27/28	0/3/3/3
19	A2M	S2	99	85,19	-	1/9/27/28	0/3/3/3
19	OMU	S2	116	19	-	0/9/27/28	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	3853	40,85	-	0/7/25/26	0/2/2/2
40	6MZ	L5	4220	40	-	2/9/27/28	0/3/3/3
40	A2M	L5	1871	40,85	-	0/9/27/28	0/3/3/3
40	PSU	L5	1683	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4299	40	-	0/7/25/26	0/2/2/2
40	OMU	L5	2837	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3920	40,85	-	0/7/25/26	0/2/2/2
40	PSU	L5	4576	40	-	0/7/25/26	0/2/2/2
19	6MZ	S2	1832	85,19	-	2/9/27/28	0/3/3/3
40	OMU	L5	4620	40	-	0/9/27/28	0/2/2/2
40	OMC	L5	2824	40	-	1/9/27/28	0/2/2/2
40	OMU	L5	4227	40	-	0/9/27/28	0/2/2/2
19	A2M	S2	1031	19	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	L5	2364	40,85	-	2/9/27/28	0/3/3/3
40	UR3	L5	4530	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	2424	40	-	0/9/27/28	0/3/3/3
40	A2M	L5	4590	40	-	3/9/27/28	0/3/3/3
19	OMC	S2	174	19	-	0/9/27/28	0/2/2/2
19	OMG	S2	1490	19	-	1/9/27/28	0/3/3/3
19	PSU	S2	1367	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1781	40	-	1/7/25/26	0/2/2/2
40	PSU	L5	3639	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	5010	40	-	0/7/25/26	0/2/2/2
40	OMU	L5	3925	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	4403	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	406	19	-	2/7/25/26	0/2/2/2
40	OMC	L5	2861	40	-	1/9/27/28	0/2/2/2
19	PSU	S2	686	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	4196	40,38	-	1/9/27/28	0/3/3/3
19	PSU	S2	866	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	3695	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4673	40,85	-	0/7/25/26	0/2/2/2
40	1MA	L5	1322	40,85	-	2/7/25/26	0/3/3/3
19	PSU	S2	651	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	3627	40	-	0/9/27/28	0/3/3/3
40	PSU	L5	1862	40	-	0/7/25/26	0/2/2/2
19	4AC	S2	1842	19	-	0/11/29/30	0/2/2/2
19	PSU	S2	649	19	-	0/7/25/26	0/2/2/2
19	B8N	S2	1248	19	-	5/16/34/35	0/2/2/2
19	A2M	S2	1383	19	-	3/9/27/28	0/3/3/3
40	OMC	L5	4536	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	1536	40	-	2/7/25/26	0/2/2/2
19	OMG	S2	509	19	-	0/9/27/28	0/3/3/3
40	PSU	L5	4471	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4628	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1056	19	-	0/7/25/26	0/2/2/2
19	OMU	S2	627	19	-	0/9/27/28	0/2/2/2
40	OMU	L5	4498	40	-	0/9/27/28	0/2/2/2
42	PSU	L8	55	42	-	0/7/25/26	0/2/2/2
19	OMU	S2	172	19	-	0/9/27/28	0/2/2/2
40	OMG	L5	4637	40	-	3/9/27/28	0/3/3/3
40	OMC	L5	4456	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	1522	40	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMC	L5	3887	40	-	1/9/27/28	0/2/2/2
40	A2M	L5	2787	40	-	5/9/27/28	0/3/3/3
19	A2M	S2	484	19	-	0/9/27/28	0/3/3/3
19	OMG	S2	644	19	-	4/9/27/28	0/3/3/3
19	G7M	S2	1639	19	-	0/7/25/26	0/3/3/3
19	OMG	S2	601	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	4532	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	2363	40,85	-	0/9/27/28	0/3/3/3
40	A2M	L5	3867	40	-	3/9/27/28	0/3/3/3
19	OMC	S2	1703	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	4312	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	867	19	-	2/9/27/28	0/3/3/3
19	PSU	S2	1177	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	1244	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	4493	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4457	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	3718	40	-	1/9/27/28	0/3/3/3
40	A2M	L5	4523	40,85	-	1/9/27/28	0/3/3/3
40	OMC	L5	2422	40,85	-	2/9/27/28	0/2/2/2
40	OMG	L5	4228	40	-	2/9/27/28	0/3/3/3
40	OMG	L5	1316	40	-	0/9/27/28	0/3/3/3
19	OMC	S2	1272	19	-	2/9/27/28	0/2/2/2
19	A2M	S2	668	85,19	-	4/9/27/28	0/3/3/3
40	OMC	L5	3841	40	-	0/9/27/28	0/2/2/2
19	PSU	S2	681	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	2804	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3851	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1046	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	3899	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	1677	40	-	1/7/25/26	0/2/2/2
42	PSU	L8	69	42	-	0/7/25/26	0/2/2/2
19	A2M	S2	159	19	-	0/9/27/28	0/3/3/3
19	OMU	S2	121	19	-	0/9/27/28	0/2/2/2
40	PSU	L5	4442	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	1323	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	3822	40	-	0/7/25/26	0/2/2/2
19	MA6	S2	1851	19	-	1/11/29/30	0/3/3/3
40	A2M	L5	3825	40	-	0/9/27/28	0/3/3/3
19	OMC	S2	517	19	-	1/9/27/28	0/2/2/2
40	A2M	L5	400	40	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	L5	4370	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	4431	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	2815	40	-	2/9/27/28	0/3/3/3
40	5MC	L5	4447	40	-	6/7/25/26	0/2/2/2
40	PSU	L5	1860	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	966	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	1326	40	-	4/9/27/28	0/3/3/3
19	OMG	S2	436	19	-	1/9/27/28	0/3/3/3
40	OMG	L5	4494	40	-	1/9/27/28	0/3/3/3
40	A2M	L5	398	40	-	2/9/27/28	0/3/3/3
40	A2M	L5	4571	40	-	2/9/27/28	0/3/3/3
40	UY1	L5	3818	40	-	3/9/27/28	0/2/2/2
40	OMG	L5	4499	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	4552	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	863	19	-	2/7/25/26	0/2/2/2
40	PSU	L5	4293	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	1328	19	-	0/9/27/28	0/3/3/3
19	OMU	S2	1326	19	-	0/9/27/28	0/2/2/2
40	OMU	L5	4306	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	4579	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	1340	40	-	1/9/27/28	0/2/2/2
40	OMG	L5	2876	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	4361	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4972	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1081	19	-	1/7/25/26	0/2/2/2
40	OMC	L5	3701	40	-	6/9/27/28	0/2/2/2
40	OMG	L5	4623	40	-	0/9/27/28	0/3/3/3
40	OMG	L5	4618	40	-	2/9/27/28	0/3/3/3
40	OMC	L5	3869	40	-	0/9/27/28	0/2/2/2
40	OMC	L5	3808	40	-	0/9/27/28	0/2/2/2
19	A2M	S2	166	19	-	1/9/27/28	0/3/3/3
19	A2M	S2	576	19	-	4/9/27/28	0/3/3/3
19	OMU	S2	1288	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	4973	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4636	40	-	2/7/25/26	0/2/2/2
40	A2M	L5	3785	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	5001	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1045	19	-	2/7/25/26	0/2/2/2
19	OMU	S2	428	19	-	5/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	PSU	L5	4521	40,85	-	0/7/25/26	0/2/2/2
19	PSU	S2	1174	19	-	0/7/25/26	0/2/2/2
19	A2M	S2	27	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	2632	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1792	40	-	0/7/25/26	0/2/2/2
19	MA6	S2	1850	19	-	0/11/29/30	0/3/3/3
40	PSU	L5	2839	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3844	40	-	1/7/25/26	0/2/2/2
40	PSU	L5	4689	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3637	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	2401	40	-	2/9/27/28	0/3/3/3
40	OMG	L5	3744	40	-	0/9/27/28	0/3/3/3
40	5MC	L5	3782	40,85	-	1/7/25/26	0/2/2/2

All (327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	3818	UY1	C6-C5	12.54	1.49	1.35
19	S2	1832	6MZ	C6-N6	12.49	1.48	1.34
40	L5	4220	6MZ	C6-N6	11.65	1.47	1.34
40	L5	3818	UY1	C2-N1	11.64	1.51	1.36
19	S2	1442	OMU	C2-N1	8.73	1.52	1.38
19	S2	799	OMU	C2-N1	8.51	1.51	1.38
19	S2	1288	OMU	C2-N1	8.35	1.51	1.38
19	S2	1832	6MZ	C3'-C2'	-8.28	1.30	1.53
40	L5	2837	OMU	C2-N1	8.24	1.51	1.38
19	S2	121	OMU	C2-N1	8.21	1.51	1.38
19	S2	428	OMU	C2-N1	8.20	1.51	1.38
19	S2	172	OMU	C2-N1	8.19	1.51	1.38
19	S2	1326	OMU	C2-N1	8.13	1.51	1.38
19	S2	1850	MA6	C3'-C2'	-7.94	1.31	1.53
19	S2	1248	B8N	C4-N3	-7.93	1.26	1.40
19	S2	627	OMU	C2-N1	7.92	1.50	1.38
19	S2	354	OMU	C2-N1	7.90	1.50	1.38
19	S2	116	OMU	C2-N1	7.89	1.50	1.38
40	L5	4227	OMU	C2-N1	7.85	1.50	1.38
19	S2	1248	B8N	C6-N1	7.78	1.55	1.36
40	L5	4498	OMU	C2-N1	7.72	1.50	1.38
40	L5	3818	UY1	C2-N3	7.64	1.50	1.37
40	L5	4620	OMU	C2-N1	7.61	1.50	1.38
40	L5	4306	OMU	C2-N1	7.60	1.50	1.38
40	L5	3925	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	428	OMU	C2-N3	6.99	1.50	1.38
19	S2	172	OMU	C2-N3	6.96	1.50	1.38
19	S2	799	OMU	C2-N3	6.90	1.50	1.38
19	S2	1288	OMU	C2-N3	6.86	1.49	1.38
19	S2	1248	B8N	C4-C5	6.85	1.63	1.47
19	S2	1442	OMU	C2-N3	6.85	1.49	1.38
19	S2	1326	OMU	C2-N3	6.84	1.49	1.38
19	S2	354	OMU	C2-N3	6.79	1.49	1.38
19	S2	627	OMU	C2-N3	6.75	1.49	1.38
19	S2	121	OMU	C2-N3	6.74	1.49	1.38
19	S2	1639	G7M	C4-N3	6.67	1.49	1.34
19	S2	116	OMU	C2-N3	6.65	1.49	1.38
40	L5	4227	OMU	C2-N3	6.63	1.49	1.38
40	L5	2837	OMU	C2-N3	6.58	1.49	1.38
40	L5	4620	OMU	C2-N3	6.58	1.49	1.38
40	L5	4498	OMU	C2-N3	6.57	1.49	1.38
40	L5	3925	OMU	C2-N3	6.44	1.49	1.38
40	L5	4306	OMU	C2-N3	6.31	1.49	1.38
40	L5	4530	UR3	C6-C5	6.10	1.49	1.35
40	L5	4530	UR3	C2-N1	5.95	1.46	1.38
19	S2	799	OMU	C6-C5	5.88	1.48	1.35
19	S2	1288	OMU	C6-C5	5.87	1.48	1.35
19	S2	1248	B8N	C2-N1	5.87	1.56	1.39
19	S2	428	OMU	C6-C5	5.86	1.48	1.35
19	S2	1326	OMU	C6-C5	5.86	1.48	1.35
19	S2	354	OMU	C6-C5	5.83	1.48	1.35
19	S2	172	OMU	C6-C5	5.83	1.48	1.35
19	S2	121	OMU	C6-C5	5.80	1.48	1.35
40	L5	4227	OMU	C6-C5	5.77	1.48	1.35
19	S2	627	OMU	C6-C5	5.76	1.48	1.35
19	S2	116	OMU	C6-C5	5.74	1.48	1.35
40	L5	2837	OMU	C6-C5	5.72	1.48	1.35
19	S2	1442	OMU	C6-C5	5.72	1.48	1.35
40	L5	4620	OMU	O4-C4	-5.70	1.13	1.24
40	L5	3925	OMU	C6-C5	5.68	1.48	1.35
40	L5	4498	OMU	C6-C5	5.67	1.48	1.35
40	L5	4227	OMU	O4-C4	-5.65	1.13	1.24
19	S2	1639	G7M	C2-N3	5.65	1.46	1.33
40	L5	3925	OMU	O4-C4	-5.63	1.13	1.24
40	L5	4620	OMU	C6-C5	5.59	1.48	1.35
40	L5	4306	OMU	C6-C5	5.59	1.48	1.35
19	S2	1442	OMU	O4-C4	-5.58	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	2837	OMU	O4-C4	-5.58	1.13	1.24
40	L5	4306	OMU	O4-C4	-5.57	1.13	1.24
40	L5	4498	OMU	O4-C4	-5.54	1.13	1.24
19	S2	627	OMU	O4-C4	-5.53	1.13	1.24
19	S2	799	OMU	O4-C4	-5.48	1.13	1.24
19	S2	428	OMU	O4-C4	-5.46	1.13	1.24
40	L5	4530	UR3	C2-N3	5.46	1.49	1.39
19	S2	1326	OMU	O4-C4	-5.46	1.13	1.24
19	S2	354	OMU	O4-C4	-5.46	1.13	1.24
19	S2	116	OMU	O4-C4	-5.44	1.13	1.24
19	S2	172	OMU	O4-C4	-5.42	1.13	1.24
19	S2	1288	OMU	O4-C4	-5.41	1.13	1.24
19	S2	121	OMU	O4-C4	-5.39	1.14	1.24
40	L5	3818	UY1	C6-N1	5.31	1.45	1.36
19	S2	1248	B8N	C6-C5	5.23	1.42	1.35
19	S2	1639	G7M	C2-N2	4.90	1.45	1.34
19	S2	1639	G7M	C5-N7	-4.73	1.33	1.39
19	S2	1832	6MZ	O4'-C1'	-4.72	1.31	1.42
19	S2	1832	6MZ	O4'-C4'	4.67	1.55	1.45
19	S2	428	OMU	C4-N3	4.51	1.46	1.38
19	S2	1832	6MZ	C5'-C4'	-4.49	1.38	1.51
19	S2	172	OMU	C4-N3	4.43	1.46	1.38
19	S2	799	OMU	C4-N3	4.43	1.46	1.38
19	S2	1326	OMU	C4-N3	4.40	1.46	1.38
40	L5	3818	UY1	C4-N3	4.38	1.47	1.38
19	S2	1442	OMU	C4-N3	4.35	1.46	1.38
19	S2	1288	OMU	C4-N3	4.33	1.46	1.38
19	S2	627	OMU	C4-N3	4.31	1.46	1.38
19	S2	1004	PSU	C6-C5	4.21	1.39	1.35
19	S2	116	OMU	C4-N3	4.19	1.45	1.38
19	S2	354	OMU	C4-N3	4.19	1.45	1.38
19	S2	121	OMU	C4-N3	4.18	1.45	1.38
19	S2	1850	MA6	C5'-C4'	-4.17	1.39	1.51
40	L5	4498	OMU	C4-N3	4.04	1.45	1.38
40	L5	4227	OMU	C4-N3	4.02	1.45	1.38
19	S2	1850	MA6	O4'-C4'	4.00	1.53	1.45
40	L5	2837	OMU	C4-N3	4.00	1.45	1.38
19	S2	1232	PSU	C6-C5	3.93	1.39	1.35
40	L5	4306	OMU	C4-N3	3.91	1.45	1.38
40	L5	3925	OMU	C4-N3	3.89	1.45	1.38
19	S2	1639	G7M	C5-C6	3.86	1.54	1.43
40	L5	4620	OMU	C4-N3	3.85	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	801	PSU	C6-C5	3.84	1.39	1.35
19	S2	93	PSU	C6-C5	3.80	1.39	1.35
19	S2	1850	MA6	O4'-C1'	-3.80	1.33	1.42
40	L5	3818	UY1	O4-C4	-3.79	1.16	1.23
19	S2	105	PSU	C6-C5	3.77	1.39	1.35
40	L5	2815	A2M	O5'-C5'	-3.69	1.33	1.44
19	S2	1244	PSU	C6-C5	3.66	1.39	1.35
19	S2	814	PSU	C6-C5	3.64	1.39	1.35
19	S2	1367	PSU	C6-C5	3.64	1.39	1.35
40	L5	4220	6MZ	C5-C4	-3.59	1.32	1.39
40	L5	3830	A2M	O5'-C5'	-3.59	1.33	1.44
19	S2	406	PSU	C6-C5	3.58	1.39	1.35
19	S2	1056	PSU	C6-C5	3.57	1.39	1.35
19	S2	651	PSU	C6-C5	3.57	1.39	1.35
40	L5	1323	A2M	O5'-C5'	-3.57	1.33	1.44
40	L5	1871	A2M	O5'-C5'	-3.57	1.33	1.44
19	S2	966	PSU	C6-C5	3.56	1.39	1.35
19	S2	109	PSU	C6-C5	3.55	1.39	1.35
40	L5	1524	A2M	O5'-C5'	-3.53	1.33	1.44
19	S2	686	PSU	C6-C5	3.52	1.39	1.35
19	S2	1045	PSU	C6-C5	3.52	1.39	1.35
19	S2	1046	PSU	C6-C5	3.50	1.39	1.35
40	L5	4500	PSU	C6-C5	3.50	1.39	1.35
19	S2	1174	PSU	C6-C5	3.46	1.39	1.35
40	L5	3825	A2M	O5'-C5'	-3.46	1.34	1.44
40	L5	400	A2M	O5'-C5'	-3.45	1.34	1.44
40	L5	2839	PSU	C6-C5	3.45	1.39	1.35
19	S2	1248	B8N	C1'-C5	3.44	1.58	1.50
19	S2	649	PSU	C6-C5	3.43	1.39	1.35
40	L5	4571	A2M	O5'-C5'	-3.43	1.34	1.44
40	L5	398	A2M	O5'-C5'	-3.42	1.34	1.44
40	L5	2787	A2M	O5'-C5'	-3.42	1.34	1.44
40	L5	4493	PSU	C6-C5	3.41	1.39	1.35
19	S2	1177	PSU	C6-C5	3.41	1.39	1.35
40	L5	1744	PSU	C6-C5	3.41	1.39	1.35
40	L5	4296	PSU	C6-C5	3.39	1.39	1.35
40	L5	2363	A2M	O5'-C5'	-3.39	1.34	1.44
40	L5	1862	PSU	C6-C5	3.38	1.39	1.35
19	S2	668	A2M	O5'-C5'	-3.37	1.34	1.44
40	L5	1781	PSU	C6-C5	3.36	1.39	1.35
19	S2	99	A2M	O5'-C5'	-3.36	1.34	1.44
40	L5	4220	6MZ	C5-N7	-3.35	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	468	A2M	O5'-C5'	-3.35	1.34	1.44
40	L5	1792	PSU	C6-C5	3.34	1.39	1.35
40	L5	2401	A2M	O5'-C5'	-3.34	1.34	1.44
19	S2	866	PSU	C6-C5	3.32	1.39	1.35
40	L5	1326	A2M	O5'-C5'	-3.32	1.34	1.44
40	L5	4523	A2M	O5'-C5'	-3.32	1.34	1.44
19	S2	27	A2M	O5'-C5'	-3.31	1.34	1.44
40	L5	4552	PSU	C6-C5	3.31	1.39	1.35
40	L5	3718	A2M	O5'-C5'	-3.31	1.34	1.44
19	S2	166	A2M	O5'-C5'	-3.31	1.34	1.44
40	L5	3785	A2M	O5'-C5'	-3.30	1.34	1.44
19	S2	1081	PSU	C6-C5	3.30	1.38	1.35
19	S2	1383	A2M	O5'-C5'	-3.29	1.34	1.44
40	L5	3844	PSU	C6-C5	3.29	1.38	1.35
40	L5	3867	A2M	O5'-C5'	-3.28	1.34	1.44
19	S2	1031	A2M	O5'-C5'	-3.27	1.34	1.44
19	S2	863	PSU	C6-C5	3.27	1.38	1.35
40	L5	4972	PSU	C6-C5	3.24	1.38	1.35
40	L5	2632	PSU	C6-C5	3.24	1.38	1.35
40	L5	4590	A2M	O5'-C5'	-3.23	1.34	1.44
19	S2	576	A2M	O5'-C5'	-3.23	1.34	1.44
19	S2	1832	6MZ	C5-C4	-3.22	1.33	1.39
40	L5	3818	UY1	O2-C2	-3.22	1.16	1.23
19	S2	681	PSU	C6-C5	3.22	1.38	1.35
42	L8	55	PSU	C6-C5	3.22	1.38	1.35
40	L5	4431	PSU	C6-C5	3.21	1.38	1.35
40	L5	1683	PSU	C6-C5	3.21	1.38	1.35
40	L5	4299	PSU	C6-C5	3.20	1.38	1.35
40	L5	1534	A2M	O5'-C5'	-3.19	1.34	1.44
19	S2	1832	6MZ	C5-N7	-3.19	1.33	1.39
40	L5	1536	PSU	C6-C5	3.19	1.38	1.35
40	L5	4293	PSU	C6-C5	3.17	1.38	1.35
19	S2	484	A2M	O5'-C5'	-3.17	1.34	1.44
40	L5	4220	6MZ	C8-N9	-3.17	1.32	1.37
40	L5	4576	PSU	C6-C5	3.16	1.38	1.35
42	L8	69	PSU	C6-C5	3.15	1.38	1.35
40	L5	3822	PSU	C6-C5	3.14	1.38	1.35
40	L5	4353	PSU	C6-C5	3.13	1.38	1.35
19	S2	159	A2M	O5'-C5'	-3.12	1.35	1.44
40	L5	4312	PSU	C6-C5	3.12	1.38	1.35
40	L5	1782	PSU	C6-C5	3.12	1.38	1.35
40	L5	4442	PSU	C6-C5	3.12	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	4579	PSU	C6-C5	3.10	1.38	1.35
40	L5	3695	PSU	C6-C5	3.10	1.38	1.35
40	L5	5010	PSU	C6-C5	3.10	1.38	1.35
40	L5	4521	PSU	C6-C5	3.09	1.38	1.35
40	L5	1582	PSU	C6-C5	3.09	1.38	1.35
40	L5	3639	PSU	C6-C5	3.08	1.38	1.35
40	L5	1860	PSU	C6-C5	3.08	1.38	1.35
40	L5	4532	PSU	C6-C5	3.08	1.38	1.35
19	S2	1832	6MZ	C2'-C1'	3.06	1.63	1.53
19	S2	1851	MA6	C6-N6	3.05	1.45	1.36
40	L5	3851	PSU	C6-C5	3.05	1.38	1.35
40	L5	3637	PSU	C6-C5	3.03	1.38	1.35
19	S2	1850	MA6	C6-N6	3.03	1.45	1.36
40	L5	3884	PSU	C6-C5	3.01	1.38	1.35
40	L5	4973	PSU	C6-C5	3.00	1.38	1.35
40	L5	4403	PSU	C6-C5	3.00	1.38	1.35
40	L5	3853	PSU	C6-C5	2.99	1.38	1.35
40	L5	5001	PSU	C6-C5	2.99	1.38	1.35
40	L5	4628	PSU	C6-C5	2.98	1.38	1.35
40	L5	4471	PSU	C6-C5	2.97	1.38	1.35
40	L5	4673	PSU	C6-C5	2.96	1.38	1.35
40	L5	3818	UY1	C1'-C5	2.96	1.56	1.50
40	L5	4689	PSU	C6-C5	2.95	1.38	1.35
19	S2	1288	OMU	C5-C4	2.93	1.50	1.43
40	L5	3920	PSU	C6-C5	2.92	1.38	1.35
40	L5	4457	PSU	C6-C5	2.92	1.38	1.35
40	L5	4447	5MC	C5-C4	-2.90	1.41	1.44
40	L5	4636	PSU	C6-C5	2.88	1.38	1.35
19	S2	1832	6MZ	C8-N9	-2.86	1.32	1.37
19	S2	799	OMU	C5-C4	2.83	1.49	1.43
19	S2	172	OMU	C5-C4	2.80	1.49	1.43
40	L5	4361	PSU	C6-C5	2.79	1.38	1.35
19	S2	354	OMU	C5-C4	2.77	1.49	1.43
19	S2	1326	OMU	C5-C4	2.77	1.49	1.43
19	S2	428	OMU	C6-N1	2.77	1.44	1.38
19	S2	121	OMU	C5-C4	2.77	1.49	1.43
40	L5	1677	PSU	C6-C5	2.76	1.38	1.35
19	S2	1442	OMU	C5-C4	2.76	1.49	1.43
40	L5	1323	A2M	O4'-C4'	-2.75	1.38	1.45
19	S2	121	OMU	C6-N1	2.73	1.44	1.38
40	L5	4530	UR3	O2-C2	-2.73	1.17	1.22
19	S2	1639	G7M	C2-N1	2.73	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	428	OMU	C5-C4	2.72	1.49	1.43
40	L5	1524	A2M	O4'-C4'	-2.68	1.39	1.45
19	S2	1850	MA6	O3'-C3'	2.68	1.49	1.43
19	S2	1288	OMU	C6-N1	2.67	1.44	1.38
40	L5	4227	OMU	C5-C4	2.67	1.49	1.43
19	S2	1832	6MZ	O3'-C3'	2.66	1.49	1.43
19	S2	1326	OMU	C6-N1	2.65	1.44	1.38
19	S2	799	OMU	C6-N1	2.63	1.44	1.38
19	S2	116	OMU	C5-C4	2.63	1.49	1.43
19	S2	1442	OMU	C6-N1	2.63	1.44	1.38
19	S2	627	OMU	C5-C4	2.63	1.49	1.43
40	L5	4498	OMU	C5-C4	2.62	1.49	1.43
40	L5	3925	OMU	C5-C4	2.59	1.49	1.43
19	S2	1851	MA6	C5-C4	-2.57	1.34	1.39
40	L5	2837	OMU	C6-N1	2.57	1.44	1.38
19	S2	627	OMU	C6-N1	2.56	1.44	1.38
40	L5	2363	A2M	O4'-C4'	-2.55	1.39	1.45
40	L5	4306	OMU	C5-C4	2.54	1.49	1.43
40	L5	2837	OMU	C5-C4	2.54	1.49	1.43
19	S2	1639	G7M	O6-C6	-2.54	1.18	1.23
40	L5	4227	OMU	C6-N1	2.51	1.44	1.38
19	S2	354	OMU	C6-N1	2.51	1.44	1.38
19	S2	116	OMU	C6-N1	2.51	1.44	1.38
40	L5	1871	A2M	O4'-C4'	-2.50	1.39	1.45
40	L5	4523	A2M	O4'-C4'	-2.48	1.39	1.45
40	L5	1534	A2M	O4'-C4'	-2.47	1.39	1.45
19	S2	172	OMU	C6-N1	2.47	1.44	1.38
40	L5	1326	A2M	O4'-C4'	-2.45	1.39	1.45
40	L5	1871	A2M	O3'-C3'	-2.45	1.36	1.43
40	L5	4620	OMU	C5-C4	2.44	1.49	1.43
40	L5	4620	OMU	C6-N1	2.42	1.43	1.38
40	L5	4306	OMU	C6-N1	2.40	1.43	1.38
40	L5	4498	OMU	C6-N1	2.40	1.43	1.38
19	S2	1850	MA6	C5-C4	-2.40	1.34	1.39
40	L5	3925	OMU	C6-N1	2.37	1.43	1.38
19	S2	1639	G7M	C6-N1	2.35	1.43	1.38
40	L5	4530	UR3	C6-N1	2.34	1.43	1.38
19	S2	1832	6MZ	C6-N1	-2.33	1.31	1.35
40	L5	4220	6MZ	C6-N1	-2.30	1.31	1.35
40	L5	1677	PSU	O4'-C1'	-2.30	1.40	1.43
40	L5	4571	A2M	O4'-C4'	-2.28	1.39	1.45
19	S2	668	A2M	O4'-C4'	-2.27	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	4973	PSU	C4-C5	-2.24	1.38	1.44
40	L5	3920	PSU	C4-C5	-2.23	1.38	1.44
40	L5	2839	PSU	C4-C5	-2.23	1.38	1.44
40	L5	3695	PSU	C4-C5	-2.21	1.38	1.44
40	L5	3867	A2M	O4'-C4'	-2.20	1.40	1.45
40	L5	4523	A2M	O3'-C3'	-2.18	1.37	1.43
40	L5	4521	PSU	C4-C5	-2.17	1.38	1.44
40	L5	4689	PSU	C4-C5	-2.16	1.38	1.44
40	L5	2815	A2M	O4'-C4'	-2.15	1.40	1.45
40	L5	2351	OMC	C4-N3	-2.15	1.30	1.34
40	L5	3884	PSU	C4-C5	-2.15	1.38	1.44
42	L8	69	PSU	O4'-C1'	-2.15	1.40	1.43
40	L5	1744	PSU	C4-C5	-2.14	1.38	1.44
19	S2	1850	MA6	C2'-C1'	2.14	1.60	1.53
40	L5	1323	A2M	O3'-C3'	-2.13	1.37	1.43
19	S2	159	A2M	C5-C4	2.13	1.42	1.39
40	L5	4293	PSU	C4-C5	-2.13	1.38	1.44
40	L5	1782	PSU	C4-C5	-2.12	1.38	1.44
40	L5	400	A2M	O3'-C3'	-2.12	1.37	1.43
40	L5	1536	PSU	C4-C5	-2.11	1.38	1.44
40	L5	4457	PSU	C4-C5	-2.11	1.38	1.44
40	L5	3639	PSU	C4-C5	-2.11	1.38	1.44
40	L5	4530	UR3	C5-C4	2.09	1.49	1.43
19	S2	1248	B8N	O4'-C1'	-2.09	1.41	1.43
19	S2	406	PSU	C4-C5	-2.09	1.38	1.44
40	L5	4361	PSU	C4-C5	-2.09	1.38	1.44
40	L5	4530	UR3	C3U-N3	2.09	1.50	1.47
40	L5	4552	PSU	C4-C5	-2.08	1.38	1.44
19	S2	468	A2M	O4'-C4'	-2.08	1.40	1.45
40	L5	1582	PSU	C4-C5	-2.08	1.38	1.44
40	L5	4353	PSU	C4-C5	-2.08	1.38	1.44
40	L5	4471	PSU	C4-C5	-2.08	1.38	1.44
40	L5	4431	PSU	C4-C5	-2.08	1.38	1.44
40	L5	3825	A2M	O4'-C4'	-2.08	1.40	1.45
40	L5	4673	PSU	C4-C5	-2.07	1.38	1.44
40	L5	4500	PSU	C4-C5	-2.06	1.38	1.44
40	L5	4296	PSU	C4-C5	-2.06	1.38	1.44
40	L5	4403	PSU	C4-C5	-2.05	1.38	1.44
19	S2	649	PSU	C4-C5	-2.04	1.38	1.44
42	L8	69	PSU	C4-C5	-2.04	1.38	1.44
40	L5	3818	UY1	O4'-C1'	-2.03	1.41	1.43
40	L5	4299	PSU	C4-C5	-2.03	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	3844	PSU	C4-C5	-2.03	1.38	1.44
40	L5	4403	PSU	O4'-C1'	-2.03	1.41	1.43
19	S2	1174	PSU	C4-C5	-2.02	1.38	1.44
40	L5	3822	PSU	O4'-C1'	-2.02	1.41	1.43
40	L5	5001	PSU	C4-C5	-2.02	1.38	1.44
40	L5	400	A2M	O4'-C4'	-2.01	1.40	1.45
19	S2	1850	MA6	C4-N9	-2.00	1.33	1.37
40	L5	4579	PSU	C4-C5	-2.00	1.38	1.44

All (684) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1851	MA6	N1-C6-N6	-12.02	102.21	116.86
19	S2	1850	MA6	N1-C6-N6	-11.13	103.29	116.86
19	S2	1851	MA6	C5-C6-N6	7.87	137.79	125.33
19	S2	1639	G7M	C1'-N9-C4	7.77	149.43	126.49
19	S2	1639	G7M	C1'-N9-C8	-7.62	101.03	126.74
19	S2	1850	MA6	C5-C6-N6	7.43	137.09	125.33
40	L5	4498	OMU	C4-N3-C2	-5.97	119.20	126.61
19	S2	1288	OMU	C4-N3-C2	-5.86	119.34	126.61
40	L5	4220	6MZ	N1-C2-N3	-5.83	119.76	128.58
19	S2	627	OMU	C4-N3-C2	-5.73	119.50	126.61
19	S2	1851	MA6	N1-C2-N3	-5.73	119.91	128.58
40	L5	2837	OMU	C4-N3-C2	-5.66	119.59	126.61
19	S2	1326	OMU	C4-N3-C2	-5.65	119.60	126.61
19	S2	172	OMU	C4-N3-C2	-5.61	119.65	126.61
40	L5	4530	UR3	C4-N3-C2	-5.60	120.07	124.58
40	L5	4636	PSU	N1-C2-N3	5.58	121.06	115.17
40	L5	4636	PSU	C4-N3-C2	-5.58	118.69	126.37
40	L5	4220	6MZ	C9-N6-C6	-5.55	117.70	122.85
19	S2	1442	OMU	C4-N3-C2	-5.54	119.73	126.61
40	L5	3925	OMU	C4-N3-C2	-5.53	119.75	126.61
19	S2	1850	MA6	N1-C2-N3	-5.52	120.23	128.58
19	S2	121	OMU	C4-N3-C2	-5.50	119.78	126.61
40	L5	4227	OMU	C4-N3-C2	-5.48	119.81	126.61
19	S2	799	OMU	C4-N3-C2	-5.47	119.82	126.61
19	S2	1832	6MZ	N1-C2-N3	-5.46	120.32	128.58
19	S2	354	OMU	C4-N3-C2	-5.46	119.84	126.61
40	L5	4293	PSU	N1-C2-N3	5.45	120.92	115.17
40	L5	4620	OMU	C4-N3-C2	-5.43	119.87	126.61
19	S2	1851	MA6	N9-C8-N7	-5.42	106.25	113.94
19	S2	428	OMU	C4-N3-C2	-5.39	119.92	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	1677	PSU	C4-N3-C2	-5.37	118.97	126.37
40	L5	4552	PSU	N1-C2-N3	5.35	120.81	115.17
40	L5	4306	OMU	C4-N3-C2	-5.33	120.00	126.61
40	L5	4293	PSU	C4-N3-C2	-5.30	119.06	126.37
40	L5	3637	PSU	N1-C2-N3	5.28	120.74	115.17
40	L5	3701	OMC	C1'-N1-C2	5.28	130.10	118.44
19	S2	1081	PSU	C4-N3-C2	-5.25	119.14	126.37
19	S2	1248	B8N	C5-C4-N3	5.25	125.68	116.15
40	L5	3818	UY1	C4-N3-C2	-5.18	119.24	126.37
40	L5	4576	PSU	N1-C2-N3	5.17	120.62	115.17
40	L5	4521	PSU	C4-N3-C2	-5.16	119.27	126.37
19	S2	1081	PSU	N1-C2-N3	5.15	120.60	115.17
40	L5	1744	PSU	N1-C2-N3	5.14	120.59	115.17
40	L5	4500	PSU	N1-C2-N3	5.13	120.58	115.17
42	L8	69	PSU	N1-C2-N3	5.12	120.56	115.17
19	S2	1850	MA6	N9-C8-N7	-5.10	106.70	113.94
40	L5	5001	PSU	C4-N3-C2	-5.10	119.35	126.37
40	L5	1683	PSU	N1-C2-N3	5.10	120.54	115.17
19	S2	116	OMU	C4-N3-C2	-5.09	120.29	126.61
40	L5	4532	PSU	N1-C2-N3	5.09	120.54	115.17
40	L5	1862	PSU	N1-C2-N3	5.09	120.54	115.17
40	L5	4442	PSU	N1-C2-N3	5.09	120.53	115.17
40	L5	3695	PSU	N1-C2-N3	5.08	120.53	115.17
40	L5	1582	PSU	C4-N3-C2	-5.06	119.41	126.37
40	L5	5001	PSU	N1-C2-N3	5.05	120.50	115.17
40	L5	4552	PSU	C4-N3-C2	-5.04	119.42	126.37
19	S2	105	PSU	N1-C2-N3	5.04	120.49	115.17
19	S2	1367	PSU	N1-C2-N3	5.04	120.48	115.17
40	L5	1862	PSU	C4-N3-C2	-5.03	119.45	126.37
19	S2	1046	PSU	N1-C2-N3	5.02	120.46	115.17
40	L5	4471	PSU	N1-C2-N3	5.01	120.46	115.17
19	S2	1045	PSU	N1-C2-N3	5.01	120.45	115.17
40	L5	4442	PSU	C4-N3-C2	-5.00	119.49	126.37
19	S2	686	PSU	C4-N3-C2	-5.00	119.49	126.37
40	L5	4521	PSU	N1-C2-N3	4.99	120.44	115.17
19	S2	1045	PSU	C4-N3-C2	-4.99	119.49	126.37
40	L5	1744	PSU	C4-N3-C2	-4.99	119.50	126.37
19	S2	1174	PSU	N1-C2-N3	4.98	120.42	115.17
40	L5	3637	PSU	C4-N3-C2	-4.98	119.52	126.37
40	L5	4973	PSU	C4-N3-C2	-4.97	119.52	126.37
40	L5	4220	6MZ	N9-C8-N7	-4.97	106.88	113.94
40	L5	1536	PSU	N1-C2-N3	4.96	120.39	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4312	PSU	N1-C2-N3	4.95	120.39	115.17
40	L5	3920	PSU	C4-N3-C2	-4.94	119.56	126.37
40	L5	3695	PSU	C4-N3-C2	-4.94	119.57	126.37
40	L5	3822	PSU	N1-C2-N3	4.93	120.37	115.17
40	L5	3851	PSU	C4-N3-C2	-4.93	119.58	126.37
40	L5	4457	PSU	C4-N3-C2	-4.93	119.59	126.37
19	S2	866	PSU	C4-N3-C2	-4.92	119.59	126.37
19	S2	966	PSU	C4-N3-C2	-4.92	119.60	126.37
40	L5	1536	PSU	C4-N3-C2	-4.90	119.62	126.37
40	L5	4296	PSU	C4-N3-C2	-4.90	119.62	126.37
19	S2	1174	PSU	C4-N3-C2	-4.90	119.62	126.37
40	L5	4457	PSU	N1-C2-N3	4.89	120.33	115.17
19	S2	1367	PSU	C4-N3-C2	-4.89	119.63	126.37
40	L5	4576	PSU	C4-N3-C2	-4.89	119.63	126.37
40	L5	1792	PSU	N1-C2-N3	4.89	120.33	115.17
40	L5	4353	PSU	C4-N3-C2	-4.89	119.64	126.37
40	L5	1683	PSU	C4-N3-C2	-4.88	119.65	126.37
40	L5	1582	PSU	N1-C2-N3	4.87	120.31	115.17
19	S2	814	PSU	N1-C2-N3	4.87	120.31	115.17
19	S2	109	PSU	C4-N3-C2	-4.86	119.67	126.37
19	S2	105	PSU	C4-N3-C2	-4.86	119.68	126.37
40	L5	3884	PSU	C4-N3-C2	-4.86	119.68	126.37
40	L5	3853	PSU	N1-C2-N3	4.85	120.29	115.17
40	L5	4532	PSU	C4-N3-C2	-4.85	119.69	126.37
40	L5	4689	PSU	N1-C2-N3	4.85	120.28	115.17
40	L5	4973	PSU	N1-C2-N3	4.85	120.28	115.17
19	S2	109	PSU	N1-C2-N3	4.84	120.28	115.17
40	L5	3920	PSU	N1-C2-N3	4.84	120.27	115.17
40	L5	1782	PSU	C4-N3-C2	-4.83	119.72	126.37
40	L5	4403	PSU	N1-C2-N3	4.82	120.25	115.17
40	L5	1792	PSU	C4-N3-C2	-4.82	119.73	126.37
40	L5	4361	PSU	C4-N3-C2	-4.82	119.74	126.37
40	L5	3851	PSU	N1-C2-N3	4.82	120.25	115.17
42	L8	69	PSU	C4-N3-C2	-4.80	119.75	126.37
40	L5	3822	PSU	C4-N3-C2	-4.80	119.76	126.37
40	L5	1677	PSU	N1-C2-N3	4.80	120.23	115.17
40	L5	4403	PSU	C4-N3-C2	-4.80	119.76	126.37
19	S2	651	PSU	C4-N3-C2	-4.80	119.77	126.37
19	S2	866	PSU	N1-C2-N3	4.79	120.22	115.17
40	L5	4673	PSU	N1-C2-N3	4.79	120.22	115.17
19	S2	1248	B8N	C4-N3-C2	-4.77	119.75	125.62
40	L5	4673	PSU	C4-N3-C2	-4.77	119.81	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	863	PSU	C4-N3-C2	-4.76	119.81	126.37
40	L5	5010	PSU	N1-C2-N3	4.76	120.19	115.17
40	L5	1781	PSU	N1-C2-N3	4.76	120.19	115.17
19	S2	966	PSU	N1-C2-N3	4.75	120.18	115.17
40	L5	3853	PSU	C4-N3-C2	-4.75	119.82	126.37
40	L5	2632	PSU	C4-N3-C2	-4.75	119.82	126.37
19	S2	406	PSU	C4-N3-C2	-4.75	119.83	126.37
19	S2	406	PSU	N1-C2-N3	4.75	120.18	115.17
40	L5	4500	PSU	C4-N3-C2	-4.74	119.84	126.37
40	L5	4471	PSU	C4-N3-C2	-4.74	119.84	126.37
40	L5	3639	PSU	N1-C2-N3	4.74	120.17	115.17
40	L5	1782	PSU	N1-C2-N3	4.74	120.17	115.17
19	S2	814	PSU	C4-N3-C2	-4.74	119.84	126.37
40	L5	4579	PSU	N1-C2-N3	4.74	120.16	115.17
40	L5	4493	PSU	N1-C2-N3	4.73	120.16	115.17
40	L5	4353	PSU	N1-C2-N3	4.73	120.16	115.17
40	L5	3884	PSU	N1-C2-N3	4.73	120.16	115.17
19	S2	1046	PSU	C4-N3-C2	-4.73	119.86	126.37
19	S2	1232	PSU	N1-C2-N3	4.72	120.15	115.17
40	L5	4628	PSU	C4-N3-C2	-4.72	119.87	126.37
40	L5	4312	PSU	C4-N3-C2	-4.70	119.89	126.37
40	L5	4579	PSU	C4-N3-C2	-4.70	119.89	126.37
19	S2	1832	6MZ	N9-C8-N7	-4.70	107.26	113.94
40	L5	4431	PSU	C4-N3-C2	-4.70	119.90	126.37
40	L5	4220	6MZ	C5-C4-N3	-4.69	120.25	126.72
40	L5	4972	PSU	C4-N3-C2	-4.69	119.91	126.37
19	S2	1832	6MZ	C5-C4-N3	-4.69	120.26	126.72
40	L5	2632	PSU	N1-C2-N3	4.69	120.11	115.17
19	S2	686	PSU	N1-C2-N3	4.68	120.11	115.17
19	S2	863	PSU	N1-C2-N3	4.68	120.11	115.17
40	L5	4299	PSU	C4-N3-C2	-4.68	119.92	126.37
40	L5	4628	PSU	N1-C2-N3	4.68	120.10	115.17
40	L5	4296	PSU	N1-C2-N3	4.67	120.10	115.17
19	S2	1056	PSU	C4-N3-C2	-4.67	119.94	126.37
40	L5	3844	PSU	N1-C2-N3	4.67	120.09	115.17
42	L8	55	PSU	C4-N3-C2	-4.66	119.95	126.37
19	S2	681	PSU	N1-C2-N3	4.66	120.08	115.17
19	S2	1244	PSU	C4-N3-C2	-4.65	119.96	126.37
19	S2	1244	PSU	N1-C2-N3	4.65	120.07	115.17
40	L5	2839	PSU	N1-C2-N3	4.64	120.06	115.17
19	S2	1232	PSU	C4-N3-C2	-4.64	119.98	126.37
40	L5	5010	PSU	C4-N3-C2	-4.62	120.00	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	L8	55	PSU	N1-C2-N3	4.62	120.04	115.17
40	L5	3639	PSU	C4-N3-C2	-4.60	120.03	126.37
40	L5	4493	PSU	C4-N3-C2	-4.59	120.05	126.37
19	S2	651	PSU	N1-C2-N3	4.59	120.01	115.17
40	L5	1781	PSU	C4-N3-C2	-4.58	120.06	126.37
19	S2	1056	PSU	N1-C2-N3	4.58	120.00	115.17
40	L5	4299	PSU	N1-C2-N3	4.58	120.00	115.17
40	L5	4361	PSU	N1-C2-N3	4.55	119.97	115.17
40	L5	1860	PSU	C4-N3-C2	-4.54	120.11	126.37
19	S2	1639	G7M	C2-N3-C4	4.54	120.12	112.30
40	L5	4972	PSU	N1-C2-N3	4.52	119.93	115.17
19	S2	93	PSU	C4-N3-C2	-4.52	120.15	126.37
19	S2	801	PSU	N1-C2-N3	4.52	119.93	115.17
19	S2	1177	PSU	C4-N3-C2	-4.51	120.16	126.37
19	S2	681	PSU	C4-N3-C2	-4.50	120.17	126.37
19	S2	1177	PSU	N1-C2-N3	4.50	119.91	115.17
19	S2	1004	PSU	N1-C2-N3	4.48	119.89	115.17
40	L5	4431	PSU	N1-C2-N3	4.45	119.86	115.17
19	S2	1851	MA6	C5-C4-N3	-4.44	120.60	126.72
19	S2	649	PSU	N1-C2-N3	4.44	119.86	115.17
40	L5	2839	PSU	C4-N3-C2	-4.40	120.32	126.37
40	L5	3701	OMC	C1'-N1-C6	-4.39	111.39	120.78
19	S2	93	PSU	N1-C2-N3	4.39	119.80	115.17
40	L5	1860	PSU	N1-C2-N3	4.38	119.79	115.17
40	L5	3818	UY1	N1-C2-N3	4.38	119.79	115.17
19	S2	649	PSU	C4-N3-C2	-4.36	120.37	126.37
40	L5	1871	A2M	C3'-C2'-C1'	-4.35	94.48	102.81
40	L5	3844	PSU	C4-N3-C2	-4.34	120.39	126.37
19	S2	1639	G7M	C5-C4-N3	-4.33	119.97	128.15
19	S2	121	OMU	N3-C2-N1	4.29	120.47	114.89
19	S2	1004	PSU	C4-N3-C2	-4.24	120.52	126.37
19	S2	1850	MA6	C4-N9-C8	4.20	110.15	105.74
19	S2	1851	MA6	C4-N9-C8	4.19	110.14	105.74
19	S2	1383	A2M	C3'-C2'-C1'	-4.17	94.82	102.81
40	L5	4498	OMU	N3-C2-N1	4.14	120.28	114.89
40	L5	4689	PSU	C4-N3-C2	-4.11	120.70	126.37
40	L5	3830	A2M	C3'-C2'-C1'	-4.09	94.98	102.81
40	L5	4620	OMU	N3-C2-N1	4.07	120.19	114.89
40	L5	2837	OMU	N3-C2-N1	4.07	120.19	114.89
19	S2	1850	MA6	C5-C4-N3	-4.06	121.12	126.72
19	S2	1639	G7M	C5-C6-N1	3.99	120.08	111.84
19	S2	1288	OMU	N3-C2-N1	3.98	120.08	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	801	PSU	C4-N3-C2	-3.95	120.93	126.37
40	L5	3925	OMU	N3-C2-N1	3.93	120.00	114.89
40	L5	4689	PSU	C6-N1-C2	-3.88	119.09	122.69
19	S2	354	OMU	N3-C2-N1	3.87	119.92	114.89
19	S2	172	OMU	N3-C2-N1	3.84	119.89	114.89
19	S2	1442	OMU	C5-C4-N3	3.80	120.13	114.80
19	S2	1326	OMU	C5-C4-N3	3.80	120.12	114.80
19	S2	627	OMU	C5-C4-N3	3.80	120.12	114.80
19	S2	799	OMU	N3-C2-N1	3.79	119.82	114.89
40	L5	4227	OMU	C5-C4-N3	3.74	120.04	114.80
40	L5	4498	OMU	C5-C4-N3	3.73	120.03	114.80
40	L5	2837	OMU	C5-C4-N3	3.72	120.02	114.80
40	L5	4530	UR3	C5-C4-N3	3.70	119.91	115.04
19	S2	1288	OMU	C5-C4-N3	3.68	119.96	114.80
40	L5	4571	A2M	C3'-C2'-C1'	-3.68	95.77	102.81
19	S2	627	OMU	N3-C2-N1	3.66	119.66	114.89
19	S2	428	OMU	N3-C2-N1	3.65	119.65	114.89
40	L5	4306	OMU	N3-C2-N1	3.65	119.64	114.89
19	S2	1326	OMU	N3-C2-N1	3.64	119.63	114.89
40	L5	4227	OMU	N3-C2-N1	3.63	119.62	114.89
19	S2	428	OMU	C5-C4-N3	3.62	119.87	114.80
19	S2	1442	OMU	N3-C2-N1	3.61	119.59	114.89
40	L5	4306	OMU	C5-C4-N3	3.61	119.86	114.80
19	S2	116	OMU	N3-C2-N1	3.60	119.58	114.89
19	S2	1850	MA6	C2-N1-C6	3.59	120.59	111.83
40	L5	3925	OMU	C5-C4-N3	3.58	119.81	114.80
40	L5	4590	A2M	C3'-C2'-C1'	-3.57	95.97	102.81
19	S2	799	OMU	C5-C4-N3	3.56	119.79	114.80
19	S2	1248	B8N	C1'-C5-C4	3.56	123.00	117.61
19	S2	1639	G7M	N9-C4-N3	3.51	132.97	125.95
19	S2	1248	B8N	N3-C2-N1	3.51	121.00	116.72
19	S2	1851	MA6	C2-N1-C6	3.50	120.39	111.83
40	L5	3825	A2M	C3'-C2'-C1'	-3.50	96.11	102.81
40	L5	4220	6MZ	C4-N9-C8	3.50	109.41	105.74
19	S2	116	OMU	C5-C4-N3	3.47	119.67	114.80
19	S2	172	OMU	C5-C4-N3	3.47	119.66	114.80
19	S2	121	OMU	C5-C4-N3	3.46	119.64	114.80
40	L5	4220	6MZ	C2-N3-C4	3.45	120.26	111.83
40	L5	3867	A2M	C2'-C1'-N9	3.45	119.43	113.75
40	L5	3818	UY1	C6-C5-C4	3.42	120.48	118.17
40	L5	4620	OMU	C5-C4-N3	3.40	119.57	114.80
19	S2	1850	MA6	C4-C5-C6	3.40	119.43	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4636	PSU	C6-C5-C4	3.40	120.47	118.17
19	S2	354	OMU	C5-C4-N3	3.39	119.54	114.80
19	S2	1851	MA6	C4-C5-C6	3.37	119.39	115.91
40	L5	2401	A2M	C3'-C2'-C1'	-3.37	96.36	102.81
40	L5	3785	A2M	O3'-C3'-C2'	3.36	120.60	111.19
40	L5	4571	A2M	O3'-C3'-C2'	3.36	120.58	111.19
40	L5	400	A2M	C3'-C2'-C1'	-3.33	96.42	102.81
40	L5	2351	OMC	C1'-N1-C2	3.31	125.75	118.44
40	L5	4220	6MZ	N3-C4-N9	3.29	132.77	127.17
19	S2	1832	6MZ	C2-N3-C4	3.29	119.87	111.83
40	L5	4500	PSU	O2-C2-N1	-3.29	119.39	122.79
40	L5	3718	A2M	C3'-C2'-C1'	-3.29	96.50	102.81
19	S2	576	A2M	C3'-C2'-C1'	-3.28	96.53	102.81
19	S2	159	A2M	C3'-C2'-C1'	-3.27	96.55	102.81
40	L5	2787	A2M	O3'-C3'-C2'	3.27	120.34	111.19
42	L8	69	PSU	O2-C2-N1	-3.27	119.42	122.79
40	L5	1524	A2M	O3'-C3'-C2'	3.26	120.32	111.19
40	L5	4532	PSU	O2-C2-N1	-3.26	119.42	122.79
19	S2	99	A2M	C3'-C2'-C1'	-3.25	96.59	102.81
19	S2	468	A2M	C3'-C2'-C1'	-3.24	96.60	102.81
19	S2	1851	MA6	N3-C4-N9	3.24	132.68	127.17
40	L5	4523	A2M	C3'-C2'-C1'	-3.24	96.60	102.81
40	L5	398	A2M	O3'-C3'-C2'	3.24	120.25	111.19
19	S2	1851	MA6	C2-N3-C4	3.23	119.71	111.83
19	S2	1639	G7M	O6-C6-C5	-3.22	120.81	128.01
40	L5	3785	A2M	C4'-O4'-C1'	-3.22	102.36	109.47
19	S2	1832	6MZ	C4-C5-C6	3.21	119.45	116.78
40	L5	3718	A2M	O3'-C3'-C2'	3.21	120.16	111.19
40	L5	1323	A2M	C2'-C1'-N9	3.19	119.00	113.75
40	L5	3830	A2M	O3'-C3'-C2'	3.18	120.09	111.19
40	L5	398	A2M	C3'-C2'-C1'	-3.18	96.72	102.81
19	S2	1832	6MZ	N3-C4-N9	3.17	132.55	127.17
19	S2	801	PSU	C6-N1-C2	-3.16	119.76	122.69
40	L5	5001	PSU	O2-C2-N1	-3.14	119.55	122.79
19	S2	1850	MA6	N3-C4-N9	3.14	132.51	127.17
19	S2	1832	6MZ	C4-N9-C8	3.14	109.03	105.74
40	L5	3695	PSU	O2-C2-N1	-3.14	119.56	122.79
19	S2	27	A2M	O3'-C3'-C2'	3.13	119.95	111.19
19	S2	1174	PSU	O2-C2-N1	-3.13	119.56	122.79
40	L5	1683	PSU	O2-C2-N1	-3.13	119.56	122.79
19	S2	1851	MA6	C5-N7-C8	3.12	108.36	103.45
40	L5	1871	A2M	O3'-C3'-C2'	3.12	119.92	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	27	A2M	C3'-C2'-C1'	-3.11	96.85	102.81
19	S2	468	A2M	O3'-C3'-C2'	3.10	119.87	111.19
19	S2	576	A2M	O3'-C3'-C2'	3.10	119.87	111.19
19	S2	627	OMU	O4-C4-C5	-3.10	119.82	125.16
40	L5	4579	PSU	O2-C2-N1	-3.09	119.60	122.79
19	S2	1442	OMU	O4-C4-C5	-3.09	119.84	125.16
19	S2	428	OMU	O4-C4-C5	-3.08	119.86	125.16
19	S2	99	A2M	O3'-C3'-C2'	3.07	119.79	111.19
19	S2	1272	OMC	C1'-N1-C2	3.07	125.22	118.44
19	S2	1639	G7M	C2-N1-C6	-3.07	119.54	125.11
19	S2	1046	PSU	O2-C2-N1	-3.07	119.63	122.79
40	L5	1323	A2M	C3'-C2'-C1'	-3.07	96.94	102.81
40	L5	1536	PSU	O2-C2-N1	-3.06	119.63	122.79
19	S2	1326	OMU	O4-C4-C5	-3.06	119.88	125.16
19	S2	1004	PSU	C6-N1-C2	-3.06	119.85	122.69
40	L5	4220	6MZ	C5-N7-C8	3.05	108.24	103.45
40	L5	4498	OMU	O4-C4-C5	-3.05	119.90	125.16
19	S2	1383	A2M	O3'-C3'-C2'	3.03	119.68	111.19
19	S2	484	A2M	O3'-C3'-C2'	3.02	119.65	111.19
40	L5	2837	OMU	O4-C4-C5	-3.02	119.95	125.16
40	L5	3844	PSU	C6-N1-C2	-3.02	119.89	122.69
19	S2	668	A2M	O3'-C3'-C2'	3.02	119.63	111.19
40	L5	2401	A2M	O3'-C3'-C2'	3.01	119.61	111.19
42	L8	69	PSU	C6-N1-C2	-3.00	119.90	122.69
19	S2	1232	PSU	O2-C2-N1	-3.00	119.69	122.79
40	L5	2363	A2M	C2'-C1'-N9	2.99	118.67	113.75
40	L5	2839	PSU	C6-N1-C2	-2.98	119.92	122.69
40	L5	1323	A2M	O3'-C3'-C2'	2.98	119.53	111.19
19	S2	1639	G7M	CN7-N7-C5	2.98	130.51	126.80
19	S2	99	A2M	C4-N9-C1'	-2.97	119.69	126.63
19	S2	166	A2M	O3'-C3'-C2'	2.97	119.49	111.19
19	S2	1383	A2M	C4-N9-C1'	-2.95	119.73	126.63
40	L5	4293	PSU	O2-C2-N1	-2.95	119.75	122.79
19	S2	1832	6MZ	C5-N7-C8	2.94	108.08	103.45
40	L5	2363	A2M	C3'-C2'-C1'	-2.94	97.17	102.81
19	S2	681	PSU	C6-N1-C2	-2.94	119.96	122.69
19	S2	1850	MA6	C2-N3-C4	2.94	119.01	111.83
19	S2	468	A2M	C4-N9-C1'	-2.94	119.76	126.63
19	S2	1367	PSU	O2-C2-N1	-2.94	119.76	122.79
19	S2	1337	4AC	N4-C4-N3	2.94	118.63	113.87
19	S2	651	PSU	O2-C2-N1	-2.93	119.76	122.79
19	S2	799	OMU	O4-C4-C5	-2.93	120.11	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	116	OMU	O4-C4-C5	-2.93	120.11	125.16
40	L5	1781	PSU	O2-C2-N1	-2.92	119.78	122.79
40	L5	4500	PSU	C6-N1-C2	-2.92	119.98	122.69
40	L5	4442	PSU	O2-C2-N1	-2.92	119.78	122.79
19	S2	172	OMU	O4-C4-C5	-2.91	120.14	125.16
40	L5	3825	A2M	O3'-C3'-C2'	2.91	119.32	111.19
19	S2	1288	OMU	O4-C4-C5	-2.91	120.15	125.16
40	L5	2815	A2M	O3'-C3'-C2'	2.91	119.32	111.19
40	L5	4552	PSU	C6-N1-C2	-2.90	120.00	122.69
19	S2	1046	PSU	C6-N1-C2	-2.89	120.01	122.69
40	L5	1582	PSU	O2-C2-N1	-2.89	119.81	122.79
40	L5	1871	A2M	C4-N9-C1'	-2.88	119.89	126.63
40	L5	4457	PSU	O2-C2-N1	-2.88	119.81	122.79
40	L5	3925	OMU	O4-C4-C5	-2.88	120.19	125.16
40	L5	4220	6MZ	C4-C5-C6	2.87	119.17	116.78
40	L5	3701	OMC	O2-C2-N3	-2.87	117.81	122.33
19	S2	159	A2M	O3'-C3'-C2'	2.86	119.20	111.19
40	L5	3701	OMC	O2-C2-N1	2.86	124.51	118.90
40	L5	4620	OMU	O4-C4-C5	-2.85	120.24	125.16
40	L5	3695	PSU	C6-N1-C2	-2.85	120.04	122.69
40	L5	4471	PSU	O2-C2-N1	-2.85	119.85	122.79
19	S2	159	A2M	C4-N9-C1'	-2.85	119.98	126.63
19	S2	1045	PSU	O2-C2-N1	-2.84	119.86	122.79
40	L5	2401	A2M	C4-N9-C1'	-2.84	119.98	126.63
40	L5	1683	PSU	C6-N1-C2	-2.84	120.05	122.69
40	L5	4636	PSU	O2-C2-N1	-2.84	119.86	122.79
40	L5	1744	PSU	O2-C2-N1	-2.84	119.86	122.79
19	S2	1442	OMU	C1'-N1-C2	2.83	122.68	117.59
40	L5	5010	PSU	O2-C2-N1	-2.83	119.87	122.79
19	S2	1850	MA6	C5-N7-C8	2.83	107.89	103.45
40	L5	4471	PSU	C6-N1-C2	-2.83	120.07	122.69
40	L5	4628	PSU	O2-C2-N1	-2.82	119.88	122.79
40	L5	4552	PSU	O2-C2-N1	-2.82	119.88	122.79
40	L5	4523	A2M	C4-N9-C1'	-2.82	120.03	126.63
19	S2	27	A2M	C4-N9-C1'	-2.82	120.03	126.63
40	L5	1534	A2M	C3'-C2'-C1'	-2.82	97.41	102.81
40	L5	2815	A2M	C2'-C1'-N9	2.81	118.38	113.75
19	S2	1031	A2M	O3'-C3'-C2'	2.81	119.05	111.19
40	L5	400	A2M	O3'-C3'-C2'	2.81	119.04	111.19
40	L5	2787	A2M	O4'-C1'-C2'	2.80	111.41	106.59
40	L5	1792	PSU	O2-C2-N1	-2.80	119.90	122.79
40	L5	2632	PSU	O2-C2-N1	-2.80	119.90	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4306	OMU	O4-C4-C5	-2.80	120.34	125.16
40	L5	4973	PSU	O2-C2-N1	-2.80	119.90	122.79
40	L5	1536	PSU	C6-N1-C2	-2.80	120.09	122.69
19	S2	121	OMU	O4-C4-C5	-2.79	120.35	125.16
40	L5	4312	PSU	C6-N1-C2	-2.79	120.10	122.69
19	S2	668	A2M	C4-N9-C1'	-2.79	120.11	126.63
19	S2	863	PSU	O2-C2-N1	-2.79	119.92	122.79
40	L5	1524	A2M	C4'-O4'-C1'	-2.78	103.32	109.47
19	S2	406	PSU	O2-C2-N1	-2.78	119.92	122.79
40	L5	3822	PSU	O2-C2-N1	-2.78	119.92	122.79
40	L5	4312	PSU	O2-C2-N1	-2.78	119.93	122.79
40	L5	4590	A2M	C4-N9-C1'	-2.77	120.15	126.63
40	L5	4576	PSU	C6-N1-C2	-2.77	120.12	122.69
19	S2	1244	PSU	O2-C2-N1	-2.77	119.93	122.79
40	L5	3637	PSU	C6-N1-C2	-2.77	120.12	122.69
40	L5	2363	A2M	O3'-C3'-C2'	2.76	118.90	111.19
19	S2	1244	PSU	C6-N1-C2	-2.75	120.14	122.69
40	L5	3785	A2M	C3'-C2'-C1'	-2.75	97.54	102.81
19	S2	1081	PSU	O2-C2-N1	-2.75	119.95	122.79
40	L5	3639	PSU	C6-N1-C2	-2.75	120.14	122.69
40	L5	1677	PSU	O2-C2-N1	-2.75	119.95	122.79
40	L5	4532	PSU	C6-N1-C2	-2.74	120.14	122.69
40	L5	3639	PSU	O2-C2-N1	-2.74	119.97	122.79
19	S2	99	A2M	C1'-N9-C8	2.73	133.16	127.09
19	S2	801	PSU	O2-C2-N1	-2.73	119.97	122.79
40	L5	1871	A2M	C1'-N9-C8	2.72	133.14	127.09
40	L5	4220	6MZ	C5-C6-N1	2.72	121.07	118.15
40	L5	3851	PSU	O2-C2-N1	-2.72	119.98	122.79
40	L5	4227	OMU	O4-C4-C5	-2.72	120.47	125.16
40	L5	1781	PSU	C6-N1-C2	-2.72	120.17	122.69
40	L5	1862	PSU	O2-C2-N1	-2.72	119.99	122.79
19	S2	1383	A2M	C1'-N9-C8	2.72	133.12	127.09
40	L5	4493	PSU	C6-N1-C2	-2.71	120.17	122.69
40	L5	2401	A2M	C1'-N9-C8	2.71	133.11	127.09
19	S2	1177	PSU	O2-C2-N1	-2.71	119.99	122.79
40	L5	3785	A2M	C4-N9-C1'	-2.71	120.30	126.63
40	L5	4579	PSU	C6-N1-C2	-2.71	120.18	122.69
40	L5	3825	A2M	C4-N9-C1'	-2.70	120.32	126.63
19	S2	159	A2M	C1'-N9-C8	2.70	133.09	127.09
40	L5	4521	PSU	C6-C5-C4	2.70	120.00	118.17
19	S2	468	A2M	C1'-N9-C8	2.69	133.07	127.09
19	S2	966	PSU	O2-C2-N1	-2.69	120.01	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	649	PSU	C6-N1-C2	-2.69	120.19	122.69
40	L5	4500	PSU	C6-C5-C4	2.69	119.99	118.17
40	L5	1524	A2M	O4'-C1'-C2'	2.68	111.20	106.59
19	S2	354	OMU	O4-C4-C5	-2.68	120.54	125.16
40	L5	4576	PSU	O2-C2-N1	-2.68	120.02	122.79
19	S2	1031	A2M	C4-N9-C1'	-2.68	120.38	126.63
19	S2	814	PSU	O2-C2-N1	-2.68	120.03	122.79
40	L5	4689	PSU	O2-C2-N1	-2.67	120.03	122.79
19	S2	484	A2M	C4-N9-C1'	-2.67	120.39	126.63
19	S2	27	A2M	C1'-N9-C8	2.67	133.01	127.09
40	L5	4576	PSU	C6-C5-C4	2.66	119.97	118.17
40	L5	4457	PSU	C6-N1-C2	-2.66	120.23	122.69
19	S2	484	A2M	C1'-N9-C8	2.65	132.98	127.09
19	S2	1174	PSU	C6-N1-C2	-2.65	120.23	122.69
40	L5	4293	PSU	C6-N1-C2	-2.65	120.23	122.69
40	L5	4571	A2M	C4-N9-C1'	-2.65	120.44	126.63
19	S2	468	A2M	O4'-C1'-C2'	2.64	111.14	106.59
19	S2	1232	PSU	C6-N1-C2	-2.64	120.24	122.69
19	S2	1177	PSU	C6-N1-C2	-2.64	120.25	122.69
19	S2	406	PSU	C6-N1-C2	-2.63	120.25	122.69
40	L5	1744	PSU	C6-N1-C2	-2.63	120.25	122.69
40	L5	4296	PSU	O2-C2-N1	-2.63	120.07	122.79
40	L5	4590	A2M	O3'-C3'-C2'	2.63	118.56	111.19
40	L5	3844	PSU	O2-C2-N1	-2.63	120.08	122.79
40	L5	5010	PSU	C6-N1-C2	-2.63	120.25	122.69
40	L5	3853	PSU	O2-C2-N1	-2.63	120.08	122.79
40	L5	4442	PSU	C6-N1-C2	-2.63	120.25	122.69
40	L5	4973	PSU	C6-N1-C2	-2.63	120.25	122.69
19	S2	1031	A2M	C3'-C2'-C1'	-2.62	97.79	102.81
19	S2	668	A2M	C1'-N9-C8	2.62	132.91	127.09
40	L5	4523	A2M	O3'-C3'-C2'	2.61	118.49	111.19
40	L5	3925	OMU	O2-C2-N1	-2.61	119.40	122.80
19	S2	1081	PSU	C6-C5-C4	2.61	119.93	118.17
19	S2	1031	A2M	C1'-N9-C8	2.60	132.88	127.09
40	L5	3920	PSU	O2-C2-N1	-2.60	120.11	122.79
19	S2	1639	G7M	CN7-N7-C8	-2.60	120.86	124.79
40	L5	3718	A2M	C1'-N9-C8	2.60	132.86	127.09
40	L5	1782	PSU	O2-C2-N1	-2.59	120.11	122.79
40	L5	4521	PSU	O2-C2-N1	-2.59	120.11	122.79
40	L5	3818	UY1	C6-N1-C2	-2.59	120.29	122.69
19	S2	863	PSU	C6-N1-C2	-2.59	120.29	122.69
40	L5	4493	PSU	O2-C2-N1	-2.58	120.13	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	668	A2M	O4'-C1'-C2'	2.58	111.03	106.59
40	L5	3818	UY1	O2-C2-N1	-2.57	120.13	122.79
40	L5	3830	A2M	C4-N9-C1'	-2.57	120.63	126.63
40	L5	4673	PSU	C6-N1-C2	-2.57	120.31	122.69
40	L5	4673	PSU	O2-C2-N1	-2.57	120.14	122.79
19	S2	166	A2M	C4-N9-C1'	-2.56	120.63	126.63
40	L5	4590	A2M	C1'-N9-C8	2.56	132.78	127.09
40	L5	1326	A2M	O3'-C3'-C2'	2.56	118.36	111.19
40	L5	1862	PSU	C6-N1-C2	-2.56	120.31	122.69
40	L5	398	A2M	C4-N9-C1'	-2.56	120.65	126.63
40	L5	3822	PSU	C6-N1-C2	-2.56	120.32	122.69
19	S2	814	PSU	C6-N1-C2	-2.55	120.32	122.69
40	L5	3825	A2M	C1'-N9-C8	2.55	132.76	127.09
40	L5	4403	PSU	C6-N1-C2	-2.55	120.33	122.69
40	L5	4447	5MC	C5-C4-N4	-2.54	117.81	121.39
40	L5	4361	PSU	O2-C2-N1	-2.54	120.17	122.79
40	L5	1326	A2M	C4-N9-C1'	-2.53	120.71	126.63
19	S2	1248	B8N	O4-C4-N3	-2.53	115.88	119.99
40	L5	3785	A2M	C1'-N9-C8	2.52	132.69	127.09
40	L5	3920	PSU	C6-N1-C2	-2.52	120.35	122.69
40	L5	4628	PSU	C6-N1-C2	-2.50	120.37	122.69
40	L5	4571	A2M	C1'-N9-C8	2.49	132.63	127.09
19	S2	1367	PSU	C6-N1-C2	-2.49	120.38	122.69
40	L5	1782	PSU	C6-N1-C2	-2.49	120.38	122.69
19	S2	1004	PSU	O2-C2-N1	-2.49	120.22	122.79
19	S2	1045	PSU	C6-C5-C4	2.48	119.85	118.17
19	S2	109	PSU	O2-C2-N1	-2.48	120.23	122.79
19	S2	93	PSU	O2-C2-N1	-2.47	120.24	122.79
19	S2	1272	OMC	C1'-N1-C6	-2.47	115.50	120.78
19	S2	1056	PSU	O2-C2-N1	-2.47	120.24	122.79
40	L5	1792	PSU	C6-N1-C2	-2.47	120.40	122.69
40	L5	5001	PSU	C6-N1-C2	-2.46	120.41	122.69
19	S2	966	PSU	C6-C5-C4	2.46	119.83	118.17
40	L5	2787	A2M	C4-N9-C1'	-2.46	120.88	126.63
40	L5	398	A2M	C1'-N9-C8	2.46	132.56	127.09
19	S2	866	PSU	C6-C5-C4	2.46	119.83	118.17
40	L5	1582	PSU	C6-N1-C2	-2.45	120.41	122.69
40	L5	4353	PSU	O2-C2-N1	-2.45	120.26	122.79
19	S2	105	PSU	C6-N1-C2	-2.45	120.41	122.69
40	L5	4299	PSU	C6-N1-C2	-2.45	120.42	122.69
19	S2	105	PSU	O2-C2-N1	-2.45	120.26	122.79
40	L5	2815	A2M	C3'-C2'-C1'	-2.45	98.12	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	400	A2M	C4-N9-C1'	-2.45	120.90	126.63
19	S2	1832	6MZ	C9-N6-C6	-2.45	120.58	122.85
19	S2	109	PSU	C6-N1-C2	-2.44	120.43	122.69
40	L5	2363	A2M	C4-N9-C1'	-2.43	120.94	126.63
40	L5	400	A2M	C1'-N9-C8	2.43	132.50	127.09
19	S2	166	A2M	C1'-N9-C8	2.43	132.50	127.09
19	S2	576	A2M	C4-N9-C1'	-2.43	120.94	126.63
40	L5	1860	PSU	O2-C2-N1	-2.43	120.28	122.79
19	S2	1850	MA6	C3'-C2'-C1'	2.43	106.06	101.46
42	L8	55	PSU	C6-N1-C2	-2.43	120.44	122.69
19	S2	354	OMU	O2-C2-N1	-2.42	119.64	122.80
40	L5	4523	A2M	C1'-N9-C8	2.42	132.47	127.09
40	L5	3808	OMC	C1'-N1-C2	2.42	123.78	118.44
40	L5	3867	A2M	C4-N9-C1'	-2.42	120.98	126.63
40	L5	1326	A2M	C3'-C2'-C1'	-2.41	98.19	102.81
40	L5	4299	PSU	O2-C2-N1	-2.41	120.30	122.79
40	L5	1326	A2M	C1'-N9-C8	2.40	132.43	127.09
40	L5	3867	A2M	O3'-C3'-C2'	2.40	117.92	111.19
40	L5	3822	PSU	C6-C5-C4	2.40	119.80	118.17
40	L5	1534	A2M	C1'-N9-C8	2.40	132.43	127.09
42	L8	55	PSU	O2-C2-N1	-2.40	120.31	122.79
19	S2	1248	B8N	O4-C4-C5	-2.39	118.44	122.58
40	L5	3884	PSU	O2-C2-N1	-2.39	120.32	122.79
40	L5	3830	A2M	C1'-N9-C8	2.39	132.40	127.09
40	L5	2839	PSU	O2-C2-N1	-2.39	120.33	122.79
19	S2	1056	PSU	C6-N1-C2	-2.38	120.48	122.69
40	L5	3718	A2M	C4-N9-C1'	-2.38	121.07	126.63
40	L5	3867	A2M	C1'-N9-C8	2.37	132.36	127.09
19	S2	93	PSU	C6-N1-C2	-2.37	120.49	122.69
40	L5	3637	PSU	O2-C2-N1	-2.36	120.35	122.79
40	L5	1534	A2M	C4-N9-C1'	-2.36	121.10	126.63
40	L5	4293	PSU	C6-C5-C4	2.36	119.77	118.17
19	S2	166	A2M	O4'-C1'-C2'	2.36	110.65	106.59
40	L5	2363	A2M	O4'-C1'-C2'	2.36	110.65	106.59
40	L5	2815	A2M	C4-N9-C1'	-2.36	121.11	126.63
40	L5	3884	PSU	C6-N1-C2	-2.36	120.50	122.69
40	L5	2351	OMC	C1'-N1-C6	-2.35	115.75	120.78
19	S2	866	PSU	O2-C2-N1	-2.35	120.36	122.79
40	L5	4972	PSU	O2-C2-N1	-2.35	120.36	122.79
40	L5	2363	A2M	C1'-N9-C8	2.35	132.31	127.09
19	S2	484	A2M	O4'-C1'-C2'	2.34	110.61	106.59
19	S2	1248	B8N	O4'-C1'-C2'	2.33	108.38	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4431	PSU	C6-N1-C2	-2.33	120.53	122.69
40	L5	4523	A2M	O4'-C1'-C2'	2.33	110.60	106.59
40	L5	4972	PSU	C6-N1-C2	-2.32	120.54	122.69
40	L5	2787	A2M	C1'-N9-C8	2.32	132.24	127.09
19	S2	651	PSU	C6-N1-C2	-2.31	120.54	122.69
40	L5	3853	PSU	C6-N1-C2	-2.31	120.55	122.69
40	L5	1860	PSU	C6-N1-C2	-2.31	120.55	122.69
19	S2	1639	G7M	N9-C8-N7	-2.31	106.88	112.48
19	S2	576	A2M	C1'-N9-C8	2.31	132.22	127.09
40	L5	2815	A2M	C1'-N9-C8	2.31	132.21	127.09
40	L5	1871	A2M	C6-C5-C4	-2.30	114.03	117.18
40	L5	1744	PSU	C6-C5-C4	2.30	119.73	118.17
19	S2	468	A2M	C6-C5-C4	-2.30	114.04	117.18
40	L5	4498	OMU	O2-C2-N1	-2.30	119.81	122.80
19	S2	1045	PSU	C6-N1-C2	-2.30	120.56	122.69
40	L5	2422	OMC	C1'-N1-C2	2.29	123.49	118.44
40	L5	1326	A2M	O4'-C1'-C2'	2.28	110.52	106.59
40	L5	2632	PSU	C6-N1-C2	-2.28	120.57	122.69
40	L5	4442	PSU	O4'-C1'-C2'	2.28	108.30	105.15
19	S2	1367	PSU	C6-C5-C4	2.27	119.71	118.17
40	L5	4296	PSU	C6-N1-C2	-2.27	120.58	122.69
40	L5	1534	A2M	O4'-C1'-C2'	2.27	110.50	106.59
40	L5	4431	PSU	O2-C2-N1	-2.27	120.45	122.79
40	L5	4361	PSU	C6-N1-C2	-2.27	120.59	122.69
40	L5	3785	A2M	C2-N1-C6	-2.27	115.01	118.73
19	S2	649	PSU	O2-C2-N1	-2.27	120.45	122.79
40	L5	4620	OMU	O2-C2-N1	-2.27	119.85	122.80
19	S2	1851	MA6	C1'-N9-C8	-2.26	122.08	127.09
40	L5	4403	PSU	O4'-C1'-C2'	2.25	108.27	105.15
40	L5	4442	PSU	C6-C5-C4	2.25	119.69	118.17
40	L5	1326	A2M	C2'-C1'-N9	2.25	117.45	113.75
40	L5	4353	PSU	C6-N1-C2	-2.25	120.61	122.69
40	L5	400	A2M	C2'-C1'-N9	2.24	117.44	113.75
19	S2	627	OMU	O2-C2-N1	-2.24	119.89	122.80
19	S2	1326	OMU	O2-C2-N1	-2.23	119.89	122.80
40	L5	3851	PSU	C6-N1-C2	-2.23	120.62	122.69
19	S2	1383	A2M	C6-C5-C4	-2.22	114.14	117.18
40	L5	4403	PSU	O2-C2-N1	-2.22	120.50	122.79
19	S2	1337	4AC	C5-C4-N4	-2.22	119.20	122.94
40	L5	2787	A2M	O4'-C4'-C3'	2.22	109.55	105.15
40	L5	2815	A2M	O4'-C1'-C2'	2.21	110.40	106.59
19	S2	159	A2M	C6-C5-C4	-2.21	114.16	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	L8	69	PSU	O4'-C1'-C2'	2.21	108.21	105.15
19	S2	99	A2M	C2-N1-C6	-2.21	115.10	118.73
40	L5	4636	PSU	O4'-C1'-C2'	2.20	108.20	105.15
40	L5	4636	PSU	C6-N1-C2	-2.20	120.65	122.69
19	S2	166	A2M	C3'-C2'-C1'	-2.20	98.60	102.81
40	L5	4521	PSU	C6-N1-C2	-2.20	120.65	122.69
40	L5	2861	OMC	C1'-N1-C2	2.20	123.29	118.44
19	S2	1832	6MZ	C3'-C2'-C1'	2.19	105.61	101.46
19	S2	866	PSU	C6-N1-C2	-2.19	120.66	122.69
40	L5	1323	A2M	C2-N1-C6	-2.19	115.14	118.73
40	L5	1322	1MA	CM1-N1-C6	-2.19	116.76	120.15
19	S2	428	OMU	O2-C2-N1	-2.19	119.95	122.80
40	L5	1534	A2M	O3'-C3'-C2'	2.19	117.30	111.19
40	L5	1323	A2M	C4-N9-C1'	-2.18	121.53	126.63
40	L5	1323	A2M	O4'-C1'-C2'	2.17	110.33	106.59
40	L5	3822	PSU	O4'-C1'-C2'	2.17	108.16	105.15
19	S2	966	PSU	C6-N1-C2	-2.17	120.68	122.69
40	L5	3825	A2M	C2-N1-C6	-2.17	115.17	118.73
19	S2	166	A2M	C6-C5-C4	-2.17	114.22	117.18
40	L5	2401	A2M	C6-C5-C4	-2.17	114.22	117.18
40	L5	3785	A2M	C5-C6-N1	2.17	123.01	117.51
19	S2	681	PSU	O2-C2-N1	-2.16	120.56	122.79
40	L5	4636	PSU	C5-C6-N1	-2.16	119.15	122.14
19	S2	1031	A2M	O4'-C1'-C2'	2.15	110.29	106.59
19	S2	166	A2M	C2'-C1'-N9	2.14	117.28	113.75
19	S2	27	A2M	C6-C5-C4	-2.14	114.26	117.18
40	L5	1534	A2M	C2-N1-C6	-2.14	115.22	118.73
19	S2	99	A2M	C5-C6-N1	2.14	122.94	117.51
40	L5	4590	A2M	C6-C5-C4	-2.13	114.27	117.18
40	L5	4523	A2M	C6-C5-C4	-2.13	114.27	117.18
19	S2	686	PSU	O2-C2-N1	-2.13	120.59	122.79
40	L5	398	A2M	C2-N1-C6	-2.13	115.23	118.73
40	L5	2815	A2M	C6-C5-C4	-2.13	114.27	117.18
40	L5	2815	A2M	C5-C6-N1	2.13	122.91	117.51
40	L5	3867	A2M	C2-N1-C6	-2.13	115.24	118.73
19	S2	1081	PSU	C6-N1-C2	-2.12	120.72	122.69
19	S2	576	A2M	C6-C5-C4	-2.12	114.28	117.18
19	S2	1832	6MZ	C5-C6-N1	2.12	120.43	118.15
40	L5	1326	A2M	C6-C5-C4	-2.12	114.29	117.18
40	L5	400	A2M	C6-C5-C4	-2.12	114.29	117.18
40	L5	1322	1MA	N1-C6-N6	2.12	125.02	119.71
19	S2	1031	A2M	C6-C5-C4	-2.11	114.29	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	4523	A2M	C5-C6-N1	2.11	122.87	117.51
40	L5	1534	A2M	C5-C6-N1	2.11	122.87	117.51
40	L5	4571	A2M	C6-C5-C4	-2.11	114.30	117.18
40	L5	1534	A2M	C2'-C1'-N9	2.11	117.22	113.75
40	L5	1677	PSU	O4'-C1'-C2'	2.10	108.06	105.15
40	L5	1524	A2M	C2-N1-C6	-2.10	115.27	118.73
19	S2	668	A2M	C6-C5-C4	-2.10	114.31	117.18
40	L5	2363	A2M	C2-N1-C6	-2.10	115.29	118.73
40	L5	4403	PSU	C6-C5-C4	2.09	119.59	118.17
40	L5	398	A2M	C5-C6-N1	2.09	122.83	117.51
40	L5	1326	A2M	C2-N1-C6	-2.09	115.30	118.73
19	S2	1031	A2M	C5-C6-N1	2.09	122.81	117.51
40	L5	1323	A2M	C1'-N9-C8	2.09	131.73	127.09
40	L5	3825	A2M	C5-C6-N1	2.09	122.81	117.51
19	S2	484	A2M	O4'-C4'-C3'	2.09	109.29	105.15
40	L5	2363	A2M	C5-C6-N1	2.08	122.81	117.51
40	L5	2815	A2M	C2-N1-C6	-2.08	115.31	118.73
40	L5	4523	A2M	C2-N1-C6	-2.08	115.31	118.73
40	L5	4571	A2M	C2-N1-C6	-2.08	115.31	118.73
40	L5	3825	A2M	C6-C5-C4	-2.08	114.34	117.18
19	S2	1288	OMU	O2-C2-N1	-2.08	120.09	122.80
19	S2	166	A2M	C5-C6-N1	2.07	122.77	117.51
40	L5	1326	A2M	C5-C6-N1	2.07	122.76	117.51
40	L5	1524	A2M	C4-N9-C1'	-2.07	121.80	126.63
19	S2	1850	MA6	C1'-N9-C8	-2.07	122.51	127.09
19	S2	99	A2M	C6-C5-C4	-2.06	114.36	117.18
40	L5	4571	A2M	O3'-C3'-C4'	-2.06	105.16	111.08
40	L5	3718	A2M	C2-N1-C6	-2.06	115.35	118.73
40	L5	2787	A2M	C2-N1-C6	-2.06	115.35	118.73
40	L5	2787	A2M	C5-C6-N1	2.06	122.74	117.51
40	L5	400	A2M	C5-C6-N1	2.06	122.73	117.51
19	S2	27	A2M	O4'-C1'-C2'	2.05	110.12	106.59
40	L5	1323	A2M	C5-C6-N1	2.05	122.72	117.51
19	S2	166	A2M	O3'-C3'-C4'	-2.05	105.19	111.08
19	S2	172	OMU	O2-C2-N1	-2.05	120.13	122.80
40	L5	3867	A2M	C6-C5-C4	-2.05	114.38	117.18
40	L5	4227	OMU	O2-C2-N1	-2.05	120.13	122.80
40	L5	1871	A2M	C4'-O4'-C1'	-2.05	104.95	109.47
19	S2	1031	A2M	C2-N1-C6	-2.05	115.37	118.73
40	L5	4973	PSU	C6-C5-C4	2.04	119.55	118.17
19	S2	1383	A2M	C2-N1-C6	-2.04	115.38	118.73
19	S2	1383	A2M	C4'-O4'-C1'	-2.03	104.97	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L5	3884	PSU	C6-C5-C4	2.03	119.55	118.17
40	L5	4628	PSU	O4'-C1'-C2'	2.03	107.96	105.15
40	L5	3830	A2M	C2-N1-C6	-2.03	115.40	118.73
19	S2	105	PSU	C6-C5-C4	2.03	119.54	118.17
40	L5	2401	A2M	C5-C6-N1	2.02	122.65	117.51
40	L5	4571	A2M	C5-C6-N1	2.02	122.65	117.51
40	L5	3785	A2M	C6-C5-C4	-2.02	114.42	117.18
40	L5	1677	PSU	C6-C5-C4	2.02	119.54	118.17
19	S2	1383	A2M	C5-C6-N1	2.02	122.64	117.51
40	L5	1524	A2M	C1'-N9-C8	2.02	131.58	127.09
19	S2	166	A2M	C2-N1-C6	-2.02	115.41	118.73
40	L5	3637	PSU	C6-C5-C4	2.02	119.54	118.17
19	S2	27	A2M	C5-C6-N1	2.01	122.62	117.51
19	S2	27	A2M	C2-N1-C6	-2.01	115.42	118.73
19	S2	668	A2M	C2-N1-C6	-2.01	115.42	118.73
40	L5	3830	A2M	C6-C5-C4	-2.01	114.43	117.18
40	L5	1871	A2M	C5-C6-N1	2.01	122.61	117.51
40	L5	398	A2M	C6-C5-C4	-2.01	114.44	117.18
40	L5	3867	A2M	O4'-C4'-C3'	2.01	109.14	105.15
19	S2	484	A2M	C6-C5-C4	-2.01	114.44	117.18
40	L5	1744	PSU	O4'-C1'-C2'	2.01	107.93	105.15
40	L5	2401	A2M	C2-N1-C6	-2.01	115.44	118.73
40	L5	3920	PSU	O4'-C1'-C2'	2.00	107.92	105.15
40	L5	4521	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	S2	27	A2M	C1'-C2'-O2'-CM'
19	S2	166	A2M	C1'-C2'-O2'-CM'
19	S2	468	A2M	C1'-C2'-O2'-CM'
19	S2	576	A2M	C1'-C2'-O2'-CM'
19	S2	601	OMG	C1'-C2'-O2'-CM2
19	S2	644	OMG	C1'-C2'-O2'-CM2
19	S2	799	OMU	C3'-C4'-C5'-O5'
19	S2	799	OMU	O4'-C4'-C5'-O5'
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	1248	B8N	O4'-C4'-C5'-O5'
19	S2	1272	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
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	1326	A2M	C1'-C2'-O2'-CM'
40	L5	1340	OMC	C1'-C2'-O2'-CM2
40	L5	1625	OMG	O4'-C4'-C5'-O5'
40	L5	2351	OMC	C1'-C2'-O2'-CM2
40	L5	2787	A2M	C1'-C2'-O2'-CM'
40	L5	2824	OMC	C1'-C2'-O2'-CM2
40	L5	2861	OMC	C1'-C2'-O2'-CM2
40	L5	2876	OMG	O4'-C4'-C5'-O5'
40	L5	2876	OMG	C3'-C4'-C5'-O5'
40	L5	3701	OMC	O4'-C4'-C5'-O5'
40	L5	3718	A2M	C1'-C2'-O2'-CM'
40	L5	3792	OMG	O4'-C4'-C5'-O5'
40	L5	3867	A2M	C3'-C4'-C5'-O5'
40	L5	3867	A2M	C1'-C2'-O2'-CM'
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	4523	A2M	C1'-C2'-O2'-CM'
40	L5	4590	A2M	O4'-C4'-C5'-O5'
40	L5	4636	PSU	C2'-C1'-C5-C4
40	L5	4637	OMG	O4'-C4'-C5'-O5'
40	L5	4637	OMG	C1'-C2'-O2'-CM2
42	L8	75	OMG	C1'-C2'-O2'-CM2
19	S2	428	OMU	C2'-C1'-N1-C6
40	L5	3701	OMC	C2'-C1'-N1-C2
19	S2	576	A2M	O4'-C4'-C5'-O5'
19	S2	644	OMG	O4'-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	2401	A2M	C3'-C4'-C5'-O5'
40	L5	2815	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	L5	4590	A2M	C3'-C4'-C5'-O5'
40	L5	4618	OMG	C3'-C4'-C5'-O5'
40	L5	3701	OMC	C2'-C1'-N1-C6
19	S2	576	A2M	C3'-C4'-C5'-O5'
19	S2	801	PSU	C3'-C4'-C5'-O5'
19	S2	1288	OMU	C3'-C4'-C5'-O5'
19	S2	1442	OMU	O4'-C4'-C5'-O5'
19	S2	1703	OMC	O4'-C4'-C5'-O5'
40	L5	398	A2M	O4'-C4'-C5'-O5'
40	L5	1625	OMG	C3'-C4'-C5'-O5'
40	L5	3701	OMC	C3'-C4'-C5'-O5'
40	L5	3867	A2M	O4'-C4'-C5'-O5'
40	L5	4500	PSU	O4'-C4'-C5'-O5'
19	S2	428	OMU	C2'-C1'-N1-C2
40	L5	3818	UY1	C1'-C2'-O2'-CM2
40	L5	3792	OMG	C3'-C4'-C5'-O5'
40	L5	4500	PSU	C3'-C4'-C5'-O5'
19	S2	644	OMG	C3'-C4'-C5'-O5'
19	S2	1045	PSU	C3'-C4'-C5'-O5'
19	S2	1248	B8N	C3'-C4'-C5'-O5'
40	L5	3899	OMG	C3'-C4'-C5'-O5'
40	L5	4220	6MZ	C3'-C4'-C5'-O5'
40	L5	4637	OMG	C3'-C4'-C5'-O5'
19	S2	801	PSU	O4'-C4'-C5'-O5'
19	S2	1045	PSU	O4'-C4'-C5'-O5'
40	L5	2401	A2M	O4'-C4'-C5'-O5'
40	L5	2815	A2M	C3'-C4'-C5'-O5'
40	L5	3830	A2M	O4'-C4'-C5'-O5'
40	L5	4228	OMG	O4'-C4'-C5'-O5'
40	L5	4571	A2M	O4'-C4'-C5'-O5'
40	L5	4618	OMG	O4'-C4'-C5'-O5'
19	S2	436	OMG	O4'-C4'-C5'-O5'
19	S2	1248	B8N	N34-C33-C34-O36
40	L5	2364	OMG	C3'-C4'-C5'-O5'
40	L5	3830	A2M	C3'-C4'-C5'-O5'
40	L5	3899	OMG	O4'-C4'-C5'-O5'
40	L5	4228	OMG	C3'-C4'-C5'-O5'
40	L5	4571	A2M	C3'-C4'-C5'-O5'
40	L5	3818	UY1	C4'-C5'-O5'-P
40	L5	4590	A2M	C4'-C5'-O5'-P
40	L5	398	A2M	C3'-C4'-C5'-O5'
40	L5	3782	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
40	L5	4447	5MC	O4'-C4'-C5'-O5'
19	S2	1383	A2M	O4'-C4'-C5'-O5'
19	S2	1442	OMU	C3'-C4'-C5'-O5'
40	L5	1524	A2M	O4'-C4'-C5'-O5'
40	L5	1524	A2M	C3'-C4'-C5'-O5'
40	L5	2787	A2M	C2'-C1'-N9-C8
19	S2	668	A2M	O4'-C4'-C5'-O5'
40	L5	1781	PSU	C3'-C4'-C5'-O5'
40	L5	2787	A2M	C3'-C4'-C5'-O5'
19	S2	867	OMG	C3'-C4'-C5'-O5'
19	S2	1383	A2M	C3'-C4'-C5'-O5'
40	L5	2422	OMC	C3'-C4'-C5'-O5'
19	S2	428	OMU	O4'-C1'-N1-C6
19	S2	867	OMG	C4'-C5'-O5'-P
19	S2	428	OMU	O4'-C1'-N1-C2
40	L5	4370	OMG	C3'-C2'-O2'-CM2
19	S2	1490	OMG	C4'-C5'-O5'-P
42	L8	75	OMG	C4'-C5'-O5'-P
19	S2	406	PSU	O4'-C1'-C5-C4
19	S2	1004	PSU	O4'-C1'-C5-C4
19	S2	1248	B8N	O4'-C1'-C5-C4
40	L5	1677	PSU	O4'-C1'-C5-C4
40	L5	2787	A2M	C2'-C1'-N9-C4
19	S2	668	A2M	C3'-C4'-C5'-O5'
40	L5	2422	OMC	O4'-C4'-C5'-O5'
40	L5	4447	5MC	C3'-C4'-C5'-O5'
19	S2	644	OMG	C4'-C5'-O5'-P
19	S2	801	PSU	C4'-C5'-O5'-P
40	L5	1534	A2M	C4'-C5'-O5'-P
40	L5	4447	5MC	O4'-C1'-N1-C6
40	L5	1322	1MA	C2'-C1'-N9-C8
19	S2	1703	OMC	C3'-C4'-C5'-O5'
40	L5	4494	OMG	C3'-C2'-O2'-CM2
40	L5	1322	1MA	C2'-C1'-N9-C4
19	S2	576	A2M	C4'-C5'-O5'-P
19	S2	1081	PSU	C4'-C5'-O5'-P
40	L5	3701	OMC	O4'-C1'-N1-C6
19	S2	1851	MA6	C4'-C5'-O5'-P
40	L5	4500	PSU	C4'-C5'-O5'-P
40	L5	1326	A2M	C4'-C5'-O5'-P
40	L5	3844	PSU	C4'-C5'-O5'-P
19	S2	406	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
19	S2	1248	B8N	O4'-C1'-C5-C6
40	L5	3818	UY1	O4'-C1'-C5-C6
19	S2	517	OMC	C3'-C2'-O2'-CM2
40	L5	4499	OMG	C3'-C2'-O2'-CM2
19	S2	99	A2M	O4'-C4'-C5'-O5'
40	L5	1323	A2M	O4'-C4'-C5'-O5'
40	L5	2351	OMC	C2'-C1'-N1-C6
19	S2	668	A2M	O4'-C1'-N9-C8
40	L5	2787	A2M	O4'-C1'-N9-C8
40	L5	4447	5MC	O4'-C1'-N1-C2
40	L5	3785	A2M	C3'-C2'-O2'-CM'
40	L5	3887	OMC	C4'-C5'-O5'-P
40	L5	3701	OMC	O4'-C1'-N1-C2
19	S2	668	A2M	C2'-C1'-N9-C8
40	L5	4636	PSU	O4'-C4'-C5'-O5'
40	L5	2351	OMC	C2'-C1'-N1-C2
19	S2	428	OMU	O4'-C4'-C5'-O5'

There are no ring outliers.

65 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	468	A2M	2	0
42	L8	75	OMG	3	0
40	L5	2351	OMC	2	0
40	L5	4392	OMG	1	0
19	S2	1004	PSU	3	0
19	S2	462	OMC	1	0
19	S2	1232	PSU	2	0
19	S2	1337	4AC	2	0
19	S2	116	OMU	2	0
19	S2	1391	OMC	2	0
40	L5	4220	6MZ	2	0
40	L5	1871	A2M	1	0
40	L5	1683	PSU	1	0
40	L5	4299	PSU	2	0
40	L5	3920	PSU	1	0
40	L5	4620	OMU	1	0
40	L5	2824	OMC	1	0
40	L5	4227	OMU	1	0
19	S2	1031	A2M	3	0
40	L5	4530	UR3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L5	4590	A2M	1	0
19	S2	1490	OMG	1	0
40	L5	5010	PSU	1	0
19	S2	406	PSU	1	0
40	L5	4196	OMG	1	0
19	S2	1842	4AC	1	0
19	S2	649	PSU	2	0
19	S2	1383	A2M	1	0
19	S2	509	OMG	2	0
19	S2	172	OMU	1	0
40	L5	2787	A2M	1	0
19	S2	484	A2M	3	0
19	S2	644	OMG	2	0
19	S2	601	OMG	2	0
40	L5	2363	A2M	1	0
40	L5	3867	A2M	4	0
19	S2	1703	OMC	1	0
19	S2	867	OMG	1	0
40	L5	4457	PSU	1	0
40	L5	3718	A2M	6	0
40	L5	4523	A2M	2	0
40	L5	2422	OMC	1	0
40	L5	3841	OMC	1	0
19	S2	681	PSU	3	0
19	S2	121	OMU	2	0
40	L5	3825	A2M	2	0
19	S2	517	OMC	1	0
40	L5	400	A2M	2	0
40	L5	1326	A2M	1	0
40	L5	4571	A2M	2	0
40	L5	3818	UY1	1	0
40	L5	4579	PSU	2	0
40	L5	1340	OMC	1	0
40	L5	3701	OMC	2	0
40	L5	4618	OMG	1	0
19	S2	166	A2M	4	0
19	S2	576	A2M	3	0
40	L5	3785	A2M	1	0
19	S2	428	OMU	2	0
19	S2	1174	PSU	2	0
19	S2	27	A2M	1	0
40	L5	2632	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	1850	MA6	2	0
40	L5	4689	PSU	1	0
40	L5	2401	A2M	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	$\# Z > 2$
87	SPM	L5	5264	-	13,13,13	0.37	0	12,12,12	1.06	0
88	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.94	0
88	SPD	L8	202	-	9,9,9	0.32	0	8,8,8	0.92	0
88	SPD	L5	5261	-	9,9,9	0.31	0	8,8,8	1.15	0
88	SPD	L5	5285	-	9,9,9	0.34	0	8,8,8	0.87	0
88	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.87	0
87	SPM	L5	5288	-	13,13,13	0.37	0	12,12,12	0.93	0
87	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.82	0
88	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.90	0
87	SPM	L5	5267	-	13,13,13	0.37	0	12,12,12	0.99	0
88	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.90	0
87	SPM	L5	5291	-	13,13,13	0.34	0	12,12,12	0.98	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.95	0
87	SPM	L5	5263	-	13,13,13	0.36	0	12,12,12	0.93	0
88	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.88	0
88	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.87	0
88	SPD	L5	5290	-	9,9,9	0.33	0	8,8,8	0.91	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
87	SPM	L5	5264	-	-	4/11/11/11	-
88	SPD	L5	5289	-	-	1/7/7/7	-
88	SPD	L8	202	-	-	3/7/7/7	-
88	SPD	L5	5261	-	-	3/7/7/7	-
88	SPD	L5	5285	-	-	2/7/7/7	-
88	SPD	L5	5284	-	-	1/7/7/7	-
87	SPM	L5	5288	-	-	4/11/11/11	-
87	SPM	L5	5292	-	-	1/11/11/11	-
88	SPD	L5	5286	-	-	1/7/7/7	-
87	SPM	L5	5267	-	-	5/11/11/11	-
88	SPD	L5	5287	-	-	2/7/7/7	-
87	SPM	L5	5291	-	-	7/11/11/11	-
87	SPM	L5	5258	-	-	4/11/11/11	-
87	SPM	L5	5263	-	-	5/11/11/11	-
88	SPD	LN	301	-	-	3/7/7/7	-
88	SPD	L5	5283	-	-	0/7/7/7	-
88	SPD	L5	5290	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5263	SPM	C7-C8-C9-N10
88	L5	5287	SPD	N6-C7-C8-C9
87	L5	5263	SPM	N10-C11-C12-C13
88	L8	202	SPD	C8-C7-N6-C5
88	L5	5285	SPD	C3-C4-C5-N6
87	L5	5291	SPM	C8-C9-N10-C11
87	L5	5292	SPM	C8-C9-N10-C11
87	L5	5288	SPM	C12-C11-N10-C9
88	LN	301	SPD	C4-C5-N6-C7
88	L5	5284	SPD	C3-C4-C5-N6
87	L5	5264	SPM	N5-C6-C7-C8
87	L5	5264	SPM	N1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
87	L5	5267	SPM	N5-C6-C7-C8
87	L5	5291	SPM	C6-C7-C8-C9
88	L8	202	SPD	N6-C7-C8-C9
88	L5	5285	SPD	C2-C3-C4-C5
88	L8	202	SPD	C2-C3-C4-C5
87	L5	5291	SPM	C3-C4-N5-C6
87	L5	5267	SPM	C6-C7-C8-C9
87	L5	5258	SPM	N5-C6-C7-C8
87	L5	5288	SPM	N1-C2-C3-C4
87	L5	5288	SPM	C3-C4-N5-C6
88	LN	301	SPD	C2-C3-C4-C5
87	L5	5291	SPM	N10-C11-C12-C13
87	L5	5264	SPM	C6-C7-C8-C9
87	L5	5267	SPM	C8-C9-N10-C11
87	L5	5288	SPM	C8-C9-N10-C11
87	L5	5291	SPM	C7-C6-N5-C4
88	L5	5289	SPD	C3-C4-C5-N6
87	L5	5258	SPM	C7-C6-N5-C4
87	L5	5263	SPM	C6-C7-C8-C9
88	L5	5286	SPD	N6-C7-C8-C9
87	L5	5263	SPM	C11-C12-C13-N14
88	L5	5261	SPD	C7-C8-C9-N10
88	L5	5287	SPD	C8-C7-N6-C5
88	L5	5290	SPD	C7-C8-C9-N10
88	LN	301	SPD	C7-C8-C9-N10
88	L5	5261	SPD	N6-C7-C8-C9
87	L5	5258	SPM	C6-C7-C8-C9
87	L5	5267	SPM	C3-C4-N5-C6
87	L5	5291	SPM	C2-C3-C4-N5
87	L5	5258	SPM	C3-C4-N5-C6
88	L5	5290	SPD	C8-C7-N6-C5
88	L5	5261	SPD	C8-C7-N6-C5
87	L5	5263	SPM	C3-C4-N5-C6
87	L5	5264	SPM	C3-C4-N5-C6
87	L5	5267	SPM	N1-C2-C3-C4
87	L5	5291	SPM	N1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

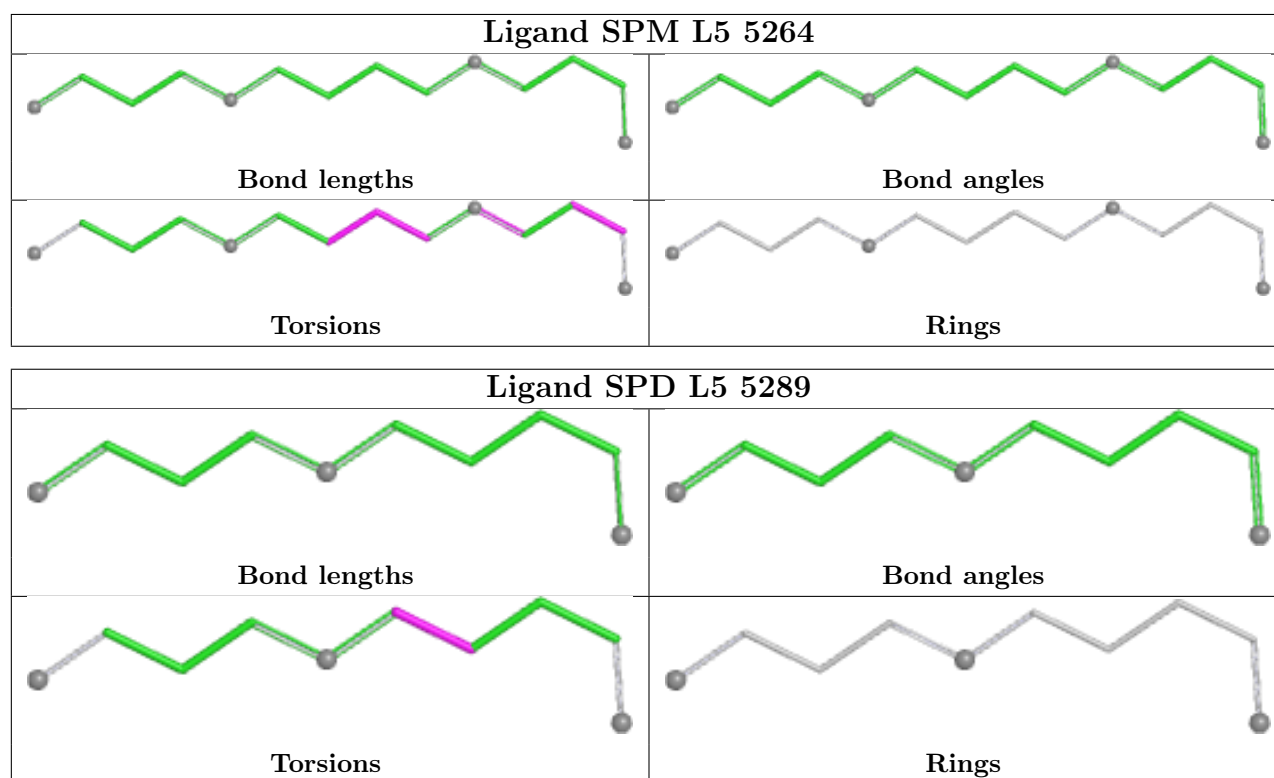
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5289	SPD	1	0

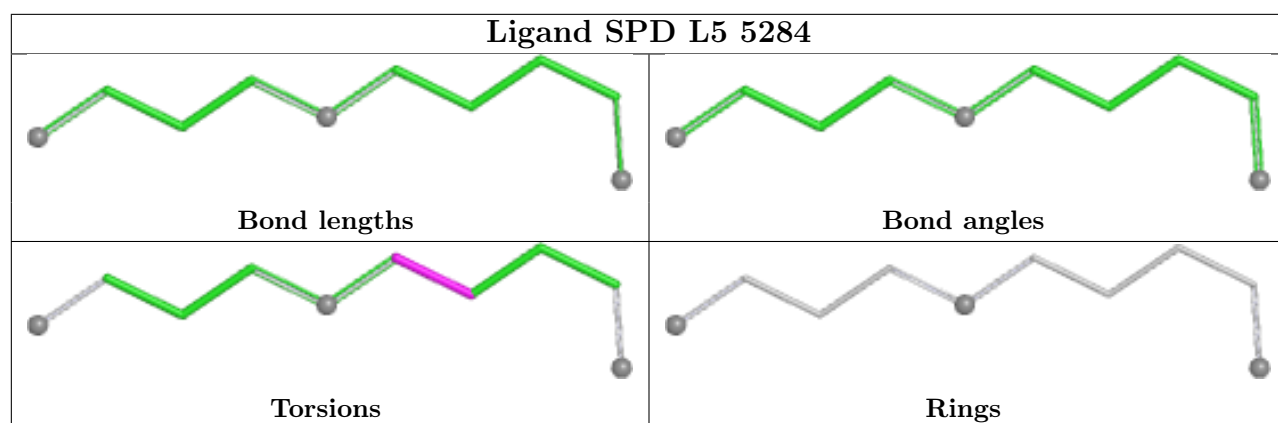
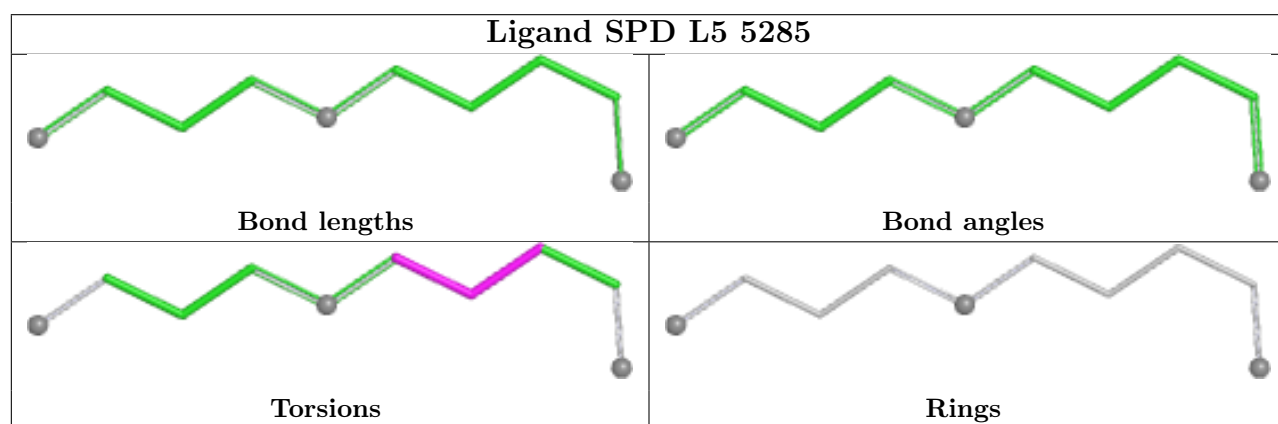
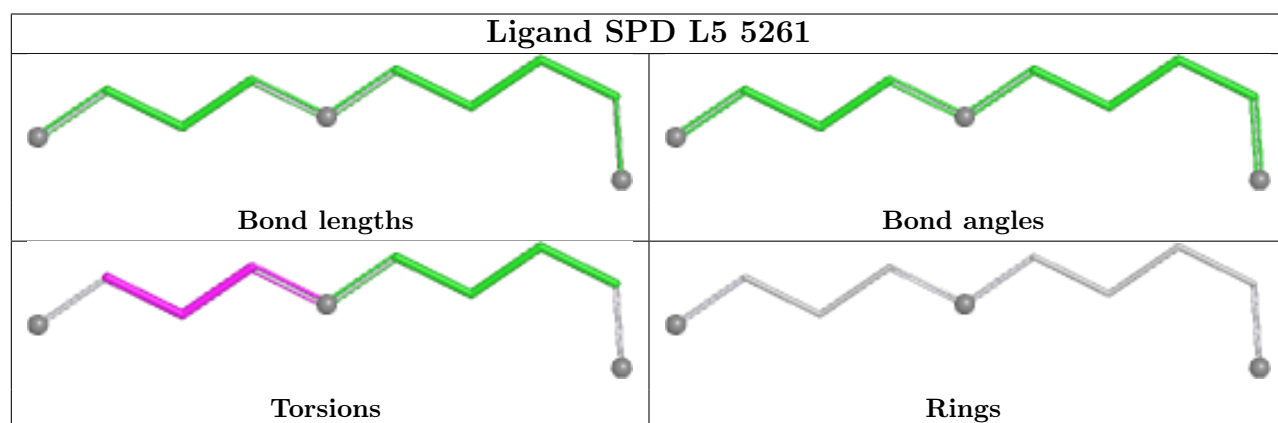
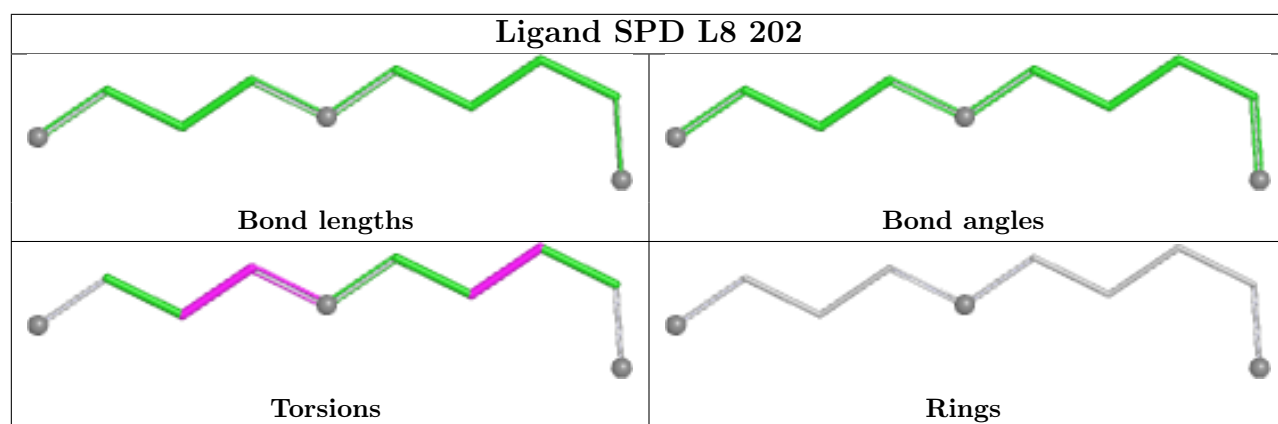
Continued on next page...

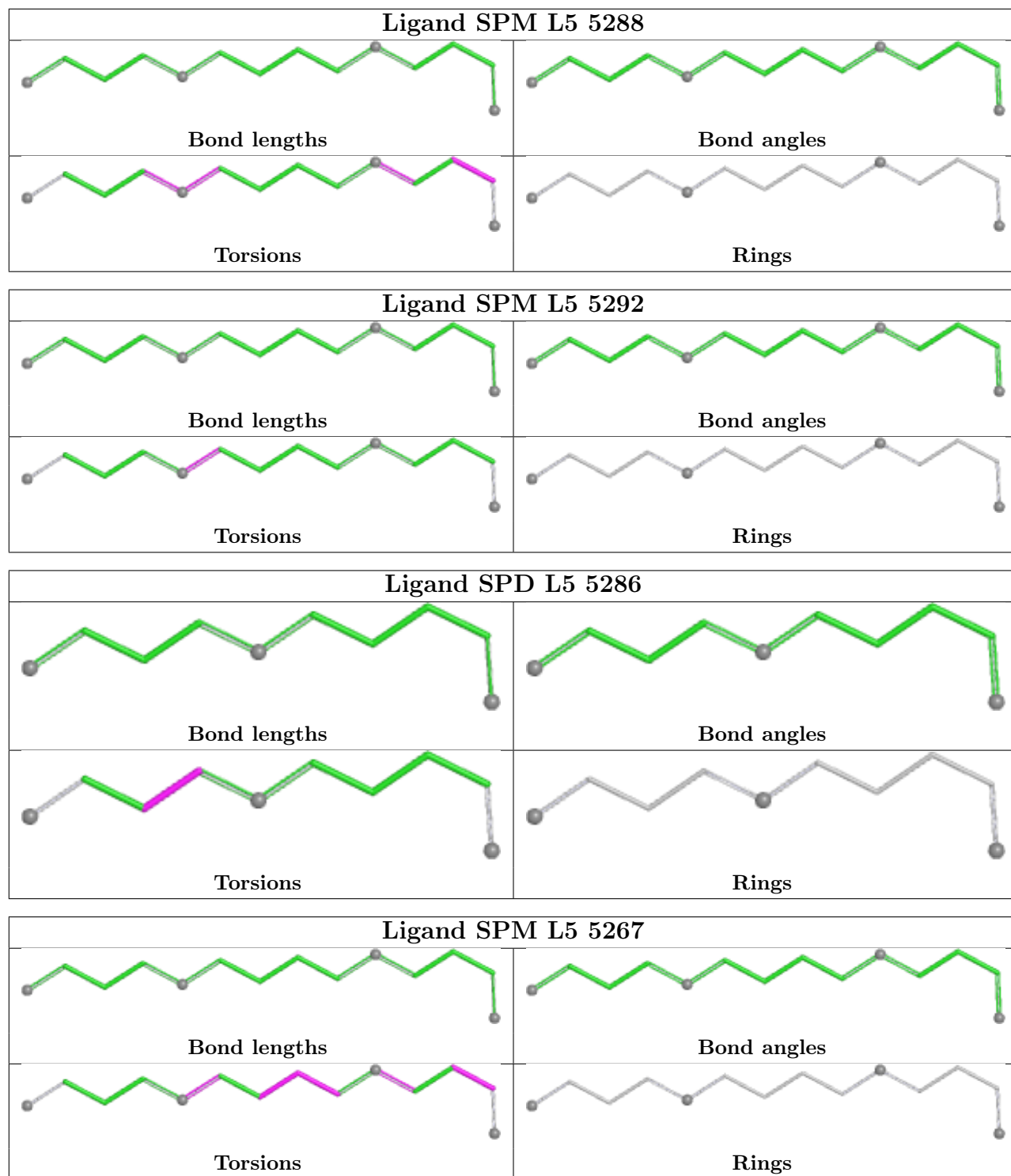
Continued from previous page...

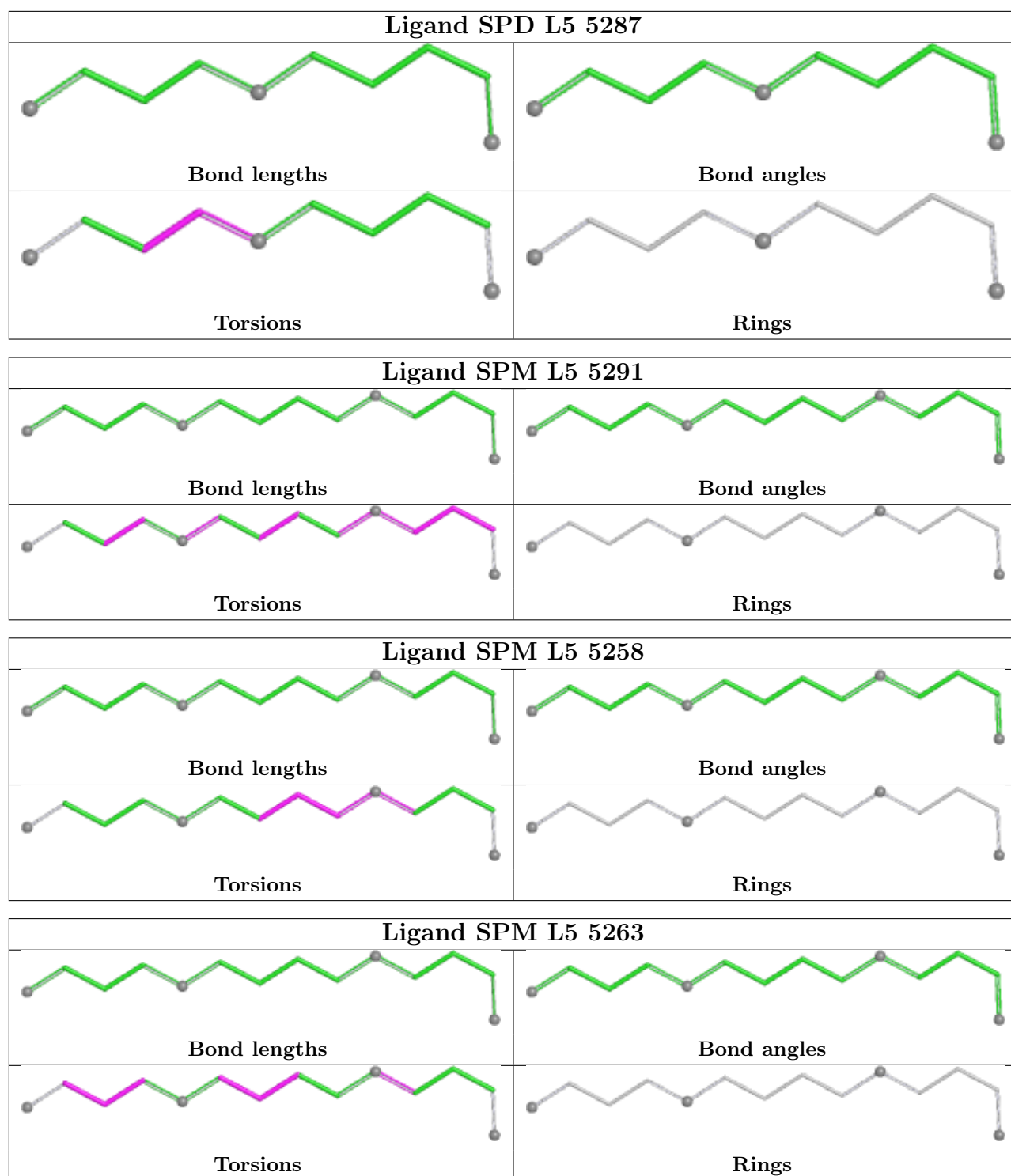
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5285	SPD	1	0
87	L5	5288	SPM	1	0
87	L5	5292	SPM	3	0
87	L5	5258	SPM	1	0

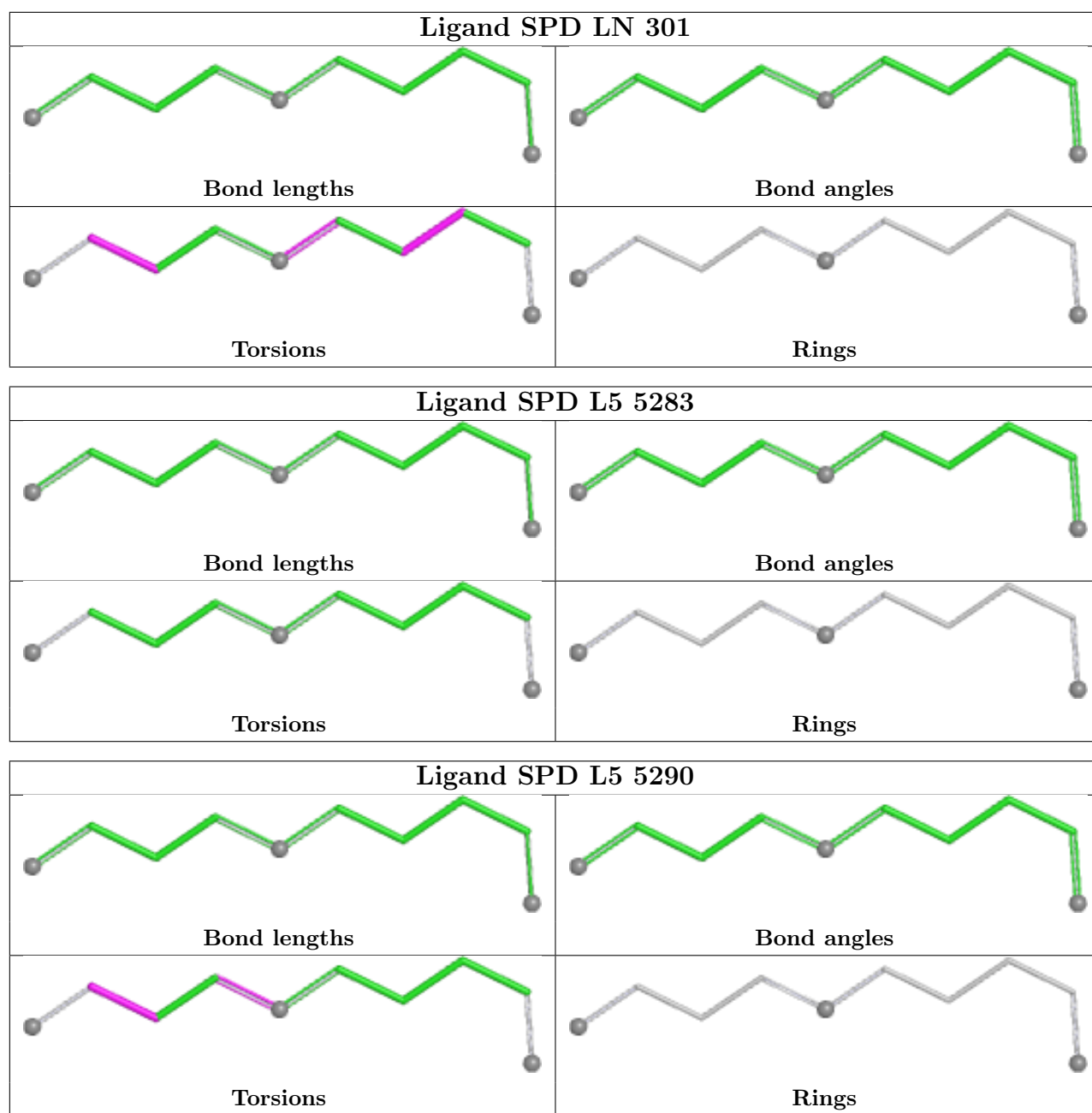
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
19	S2	4
67	Lb	1
84	Lt	1
6	SH	1
37	At	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	35.48
1	S2	753:C	O3'	785:C	P	26.99
1	L5	1706:A	O3'	1716:G	P	20.59
1	L5	2910:G	O3'	3584:C	P	20.30
1	L5	760:G	O3'	903:C	P	16.91
1	L5	3954:A	O3'	4056:A	P	16.30
1	Lt	87:GLU	C	104:ILE	N	15.73
1	S2	698:G	O3'	730:C	P	14.13
1	L5	2112:G	O3'	2249:C	P	13.90
1	S2	739:C	O3'	746:C	P	13.77
1	L5	4776:G	O3'	4858:C	P	13.39
1	L5	519:C	O3'	642:G	P	13.30
1	L5	990:C	O3'	1064:G	P	12.83
1	L5	1222:A	O3'	1234:G	P	12.83
1	SH	107:LYS	C	111:LYS	N	11.97
1	At	15:G	O3'	18:G	P	11.80
1	Pt	15:G	O3'	18:G	P	9.36
1	S2	225:G	O3'	287:U	P	7.30
1	L5	1100:U	O3'	1167:C	P	7.07

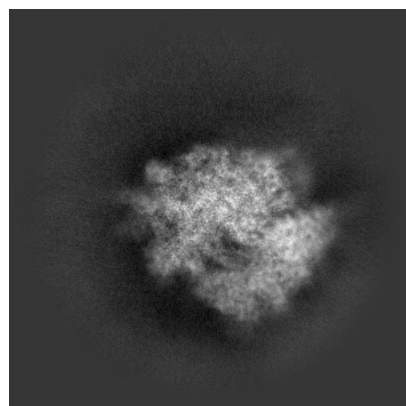
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71355. These allow visual inspection of the internal detail of the map and identification of artifacts.

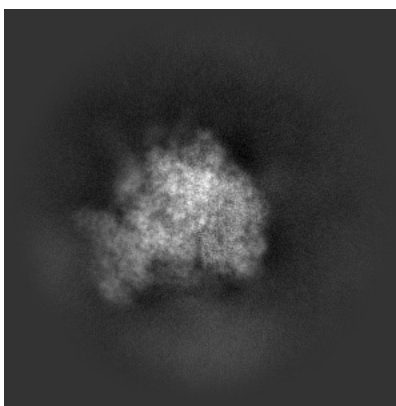
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

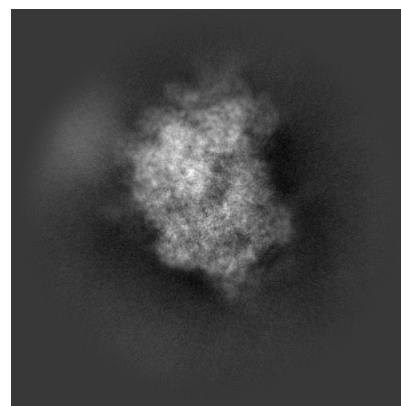
6.1.1 Primary map



X

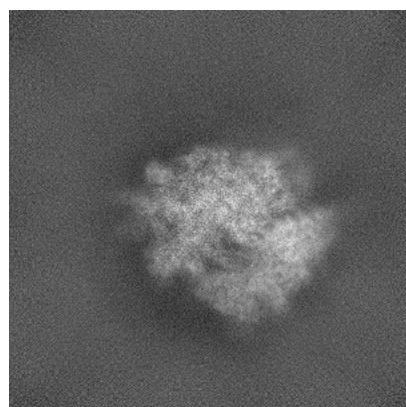


Y

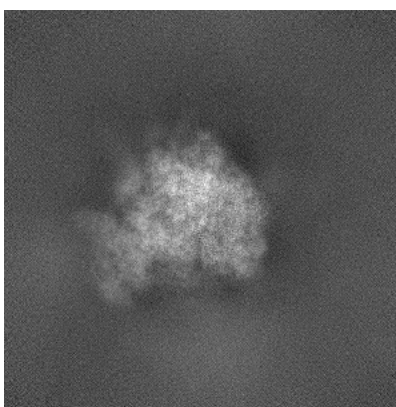


Z

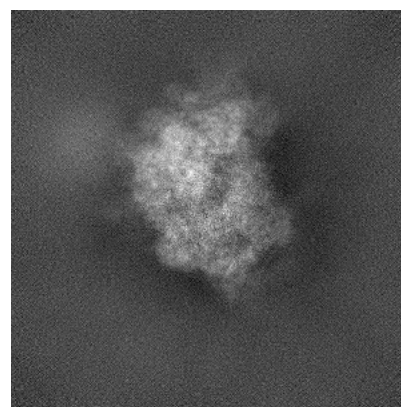
6.1.2 Raw map



X



Y

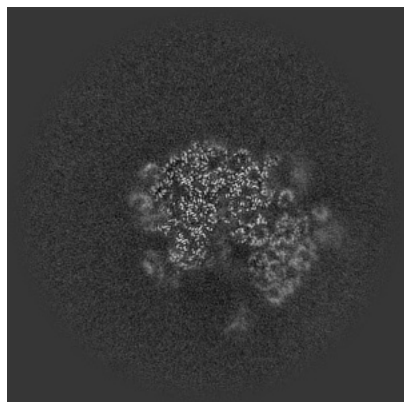


Z

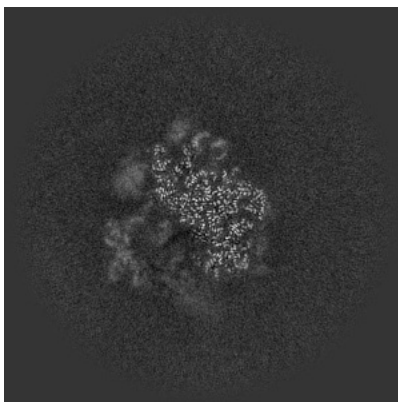
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

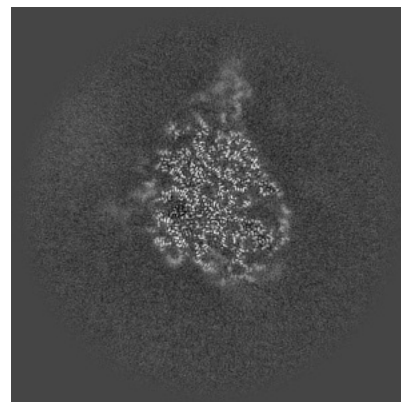
6.2.1 Primary map



X Index: 256

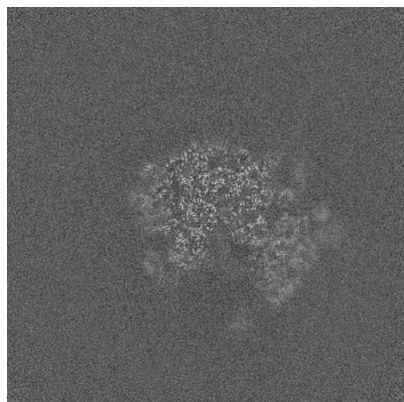


Y Index: 256

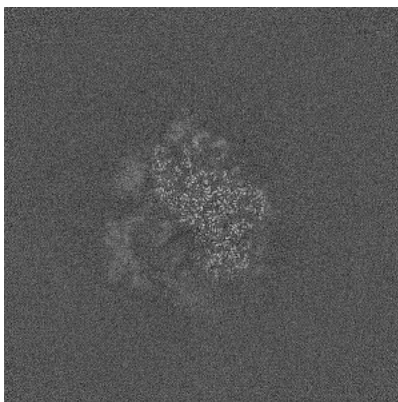


Z Index: 256

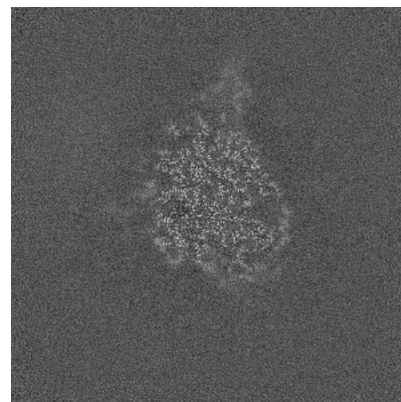
6.2.2 Raw map



X Index: 256



Y Index: 256

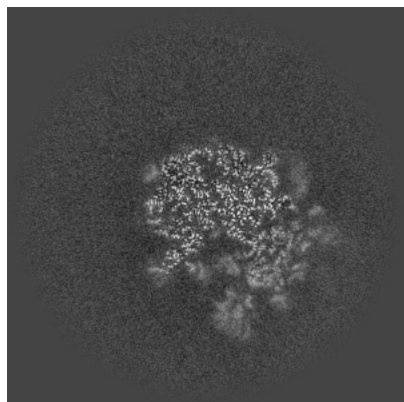


Z Index: 256

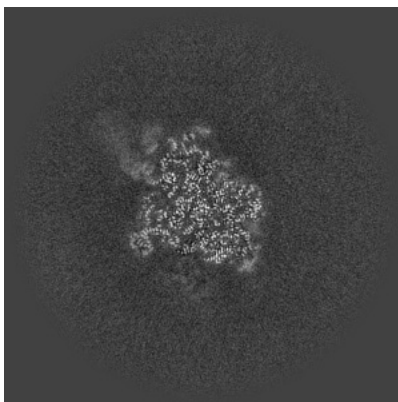
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

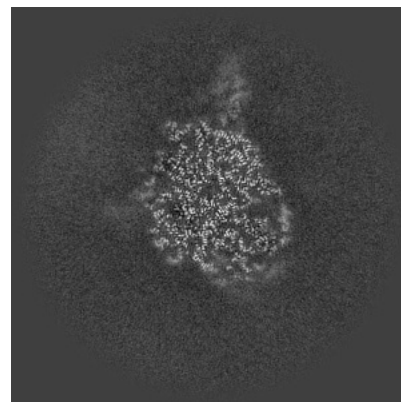
6.3.1 Primary map



X Index: 243

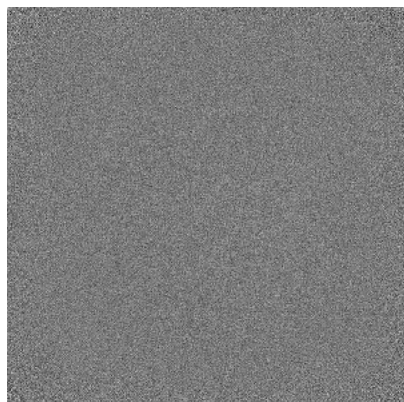


Y Index: 233

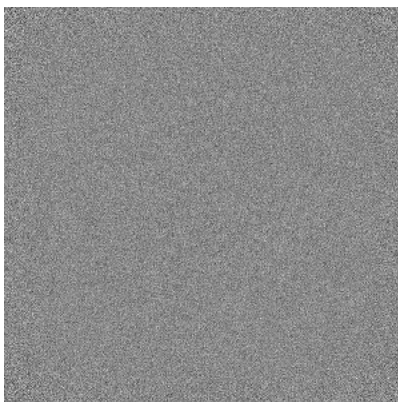


Z Index: 258

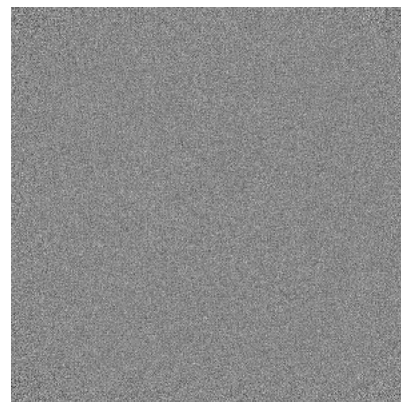
6.3.2 Raw map



X Index: 0



Y Index: 0

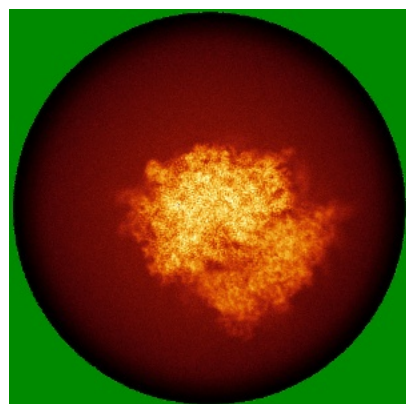


Z Index: 0

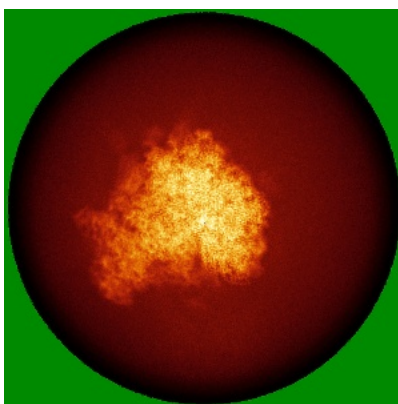
The images above show the largest variance slices of the map in three orthogonal directions.

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

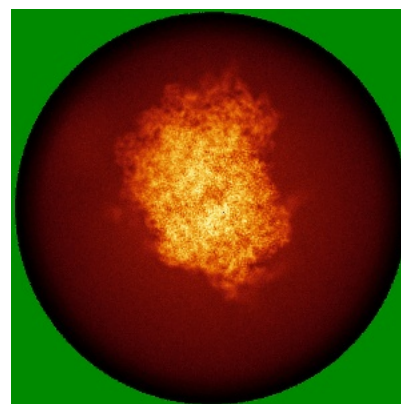
6.4.1 Primary map



X

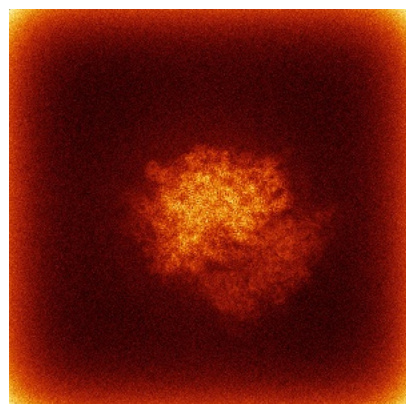


Y

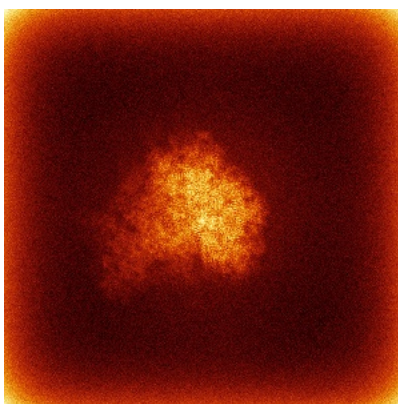


Z

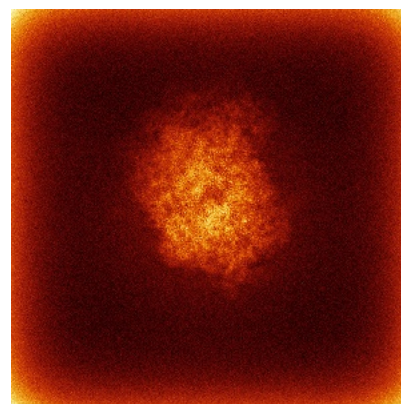
6.4.2 Raw map



X



Y

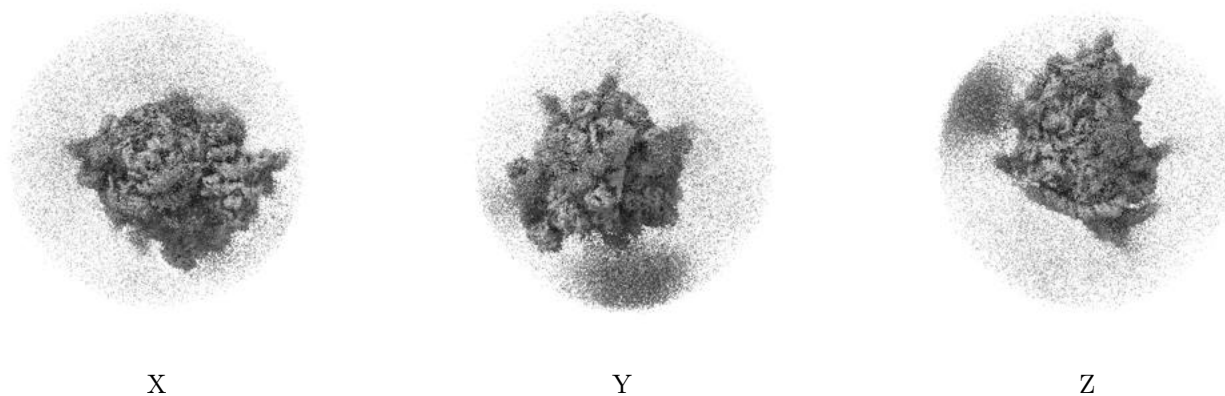


Z

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.

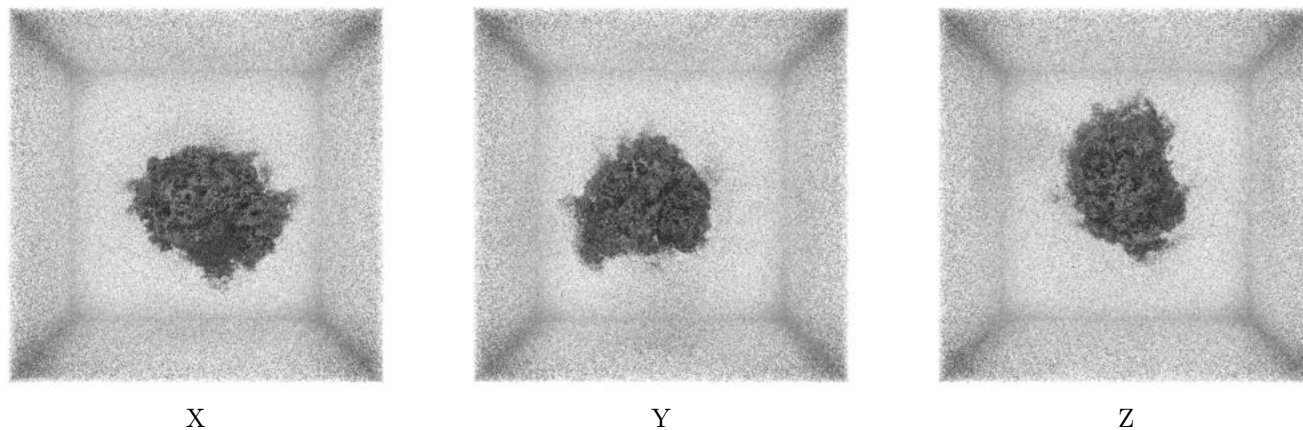
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0119. 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.

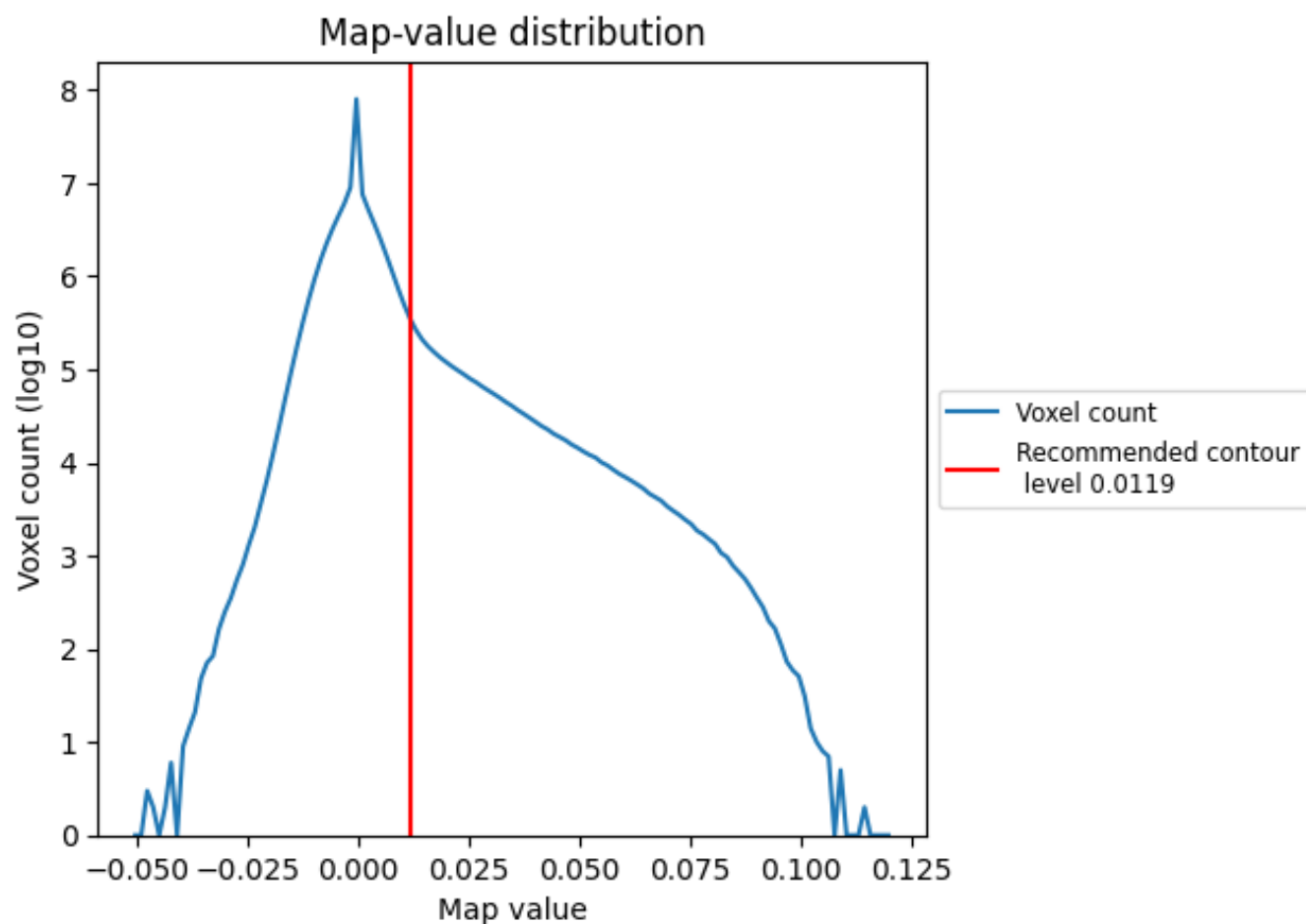
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

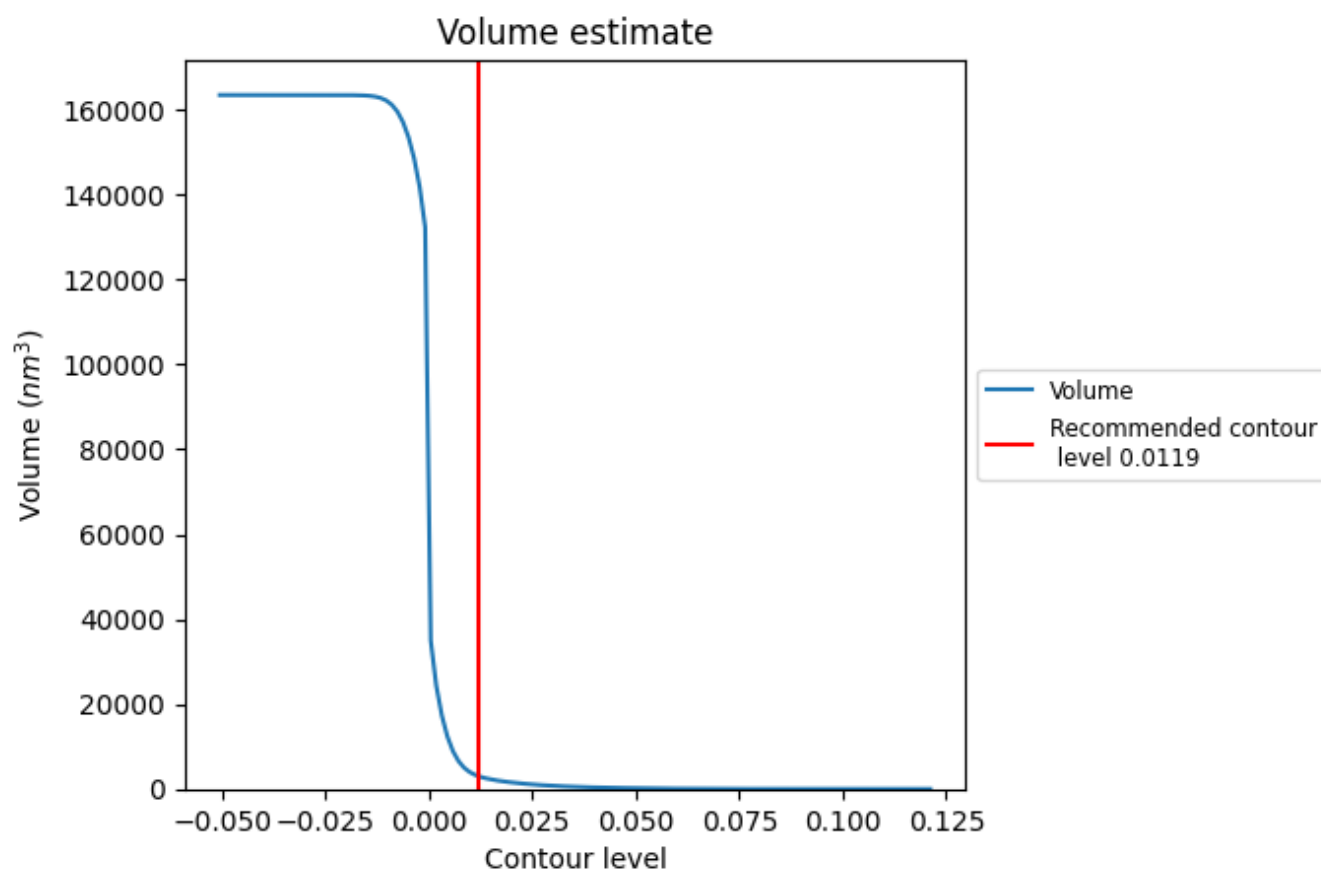
This section contains the results of statistical analysis of the map.

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.

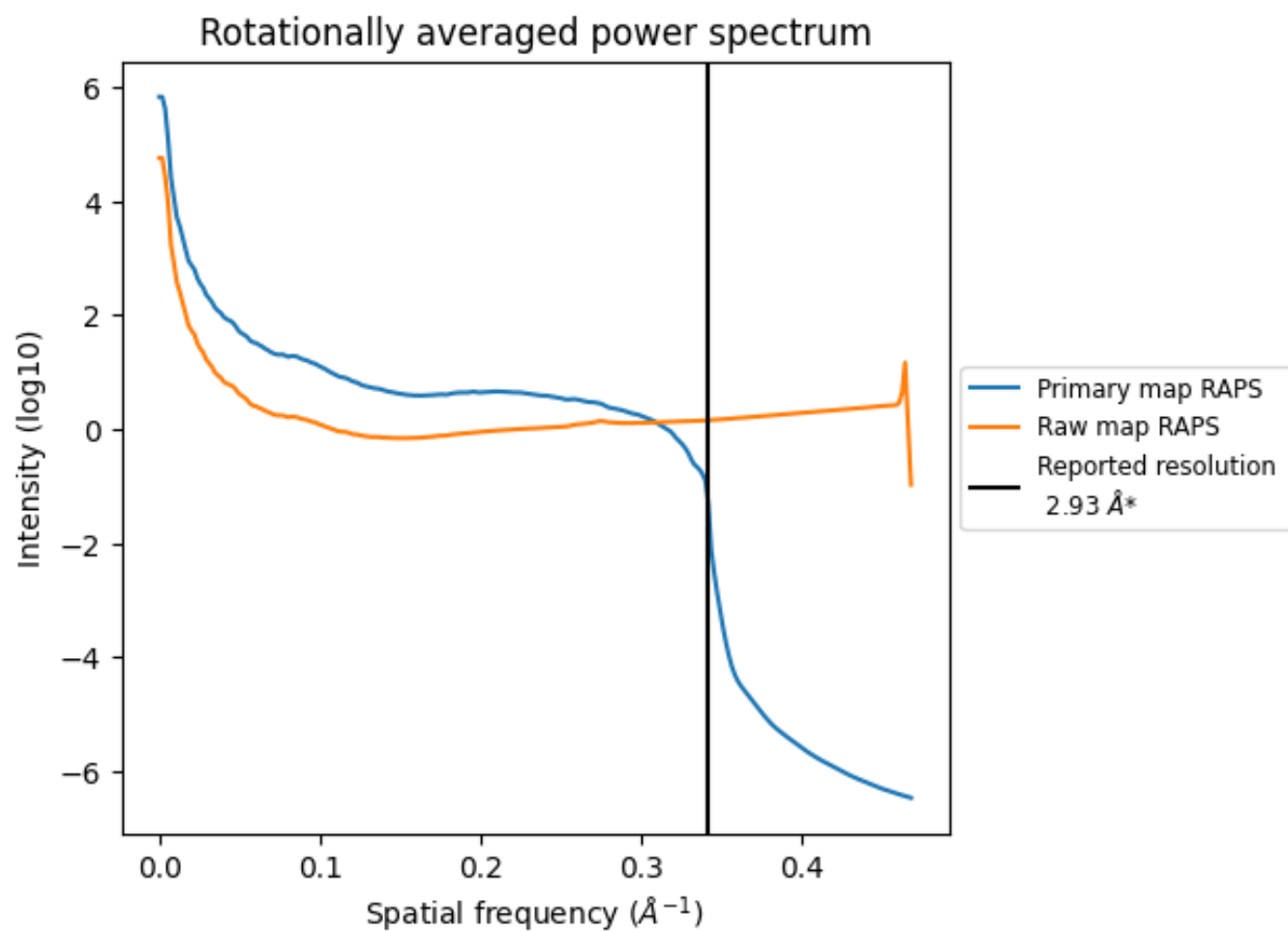
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3076 nm^3 ; this corresponds to an approximate mass of 2778 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 [i](#)

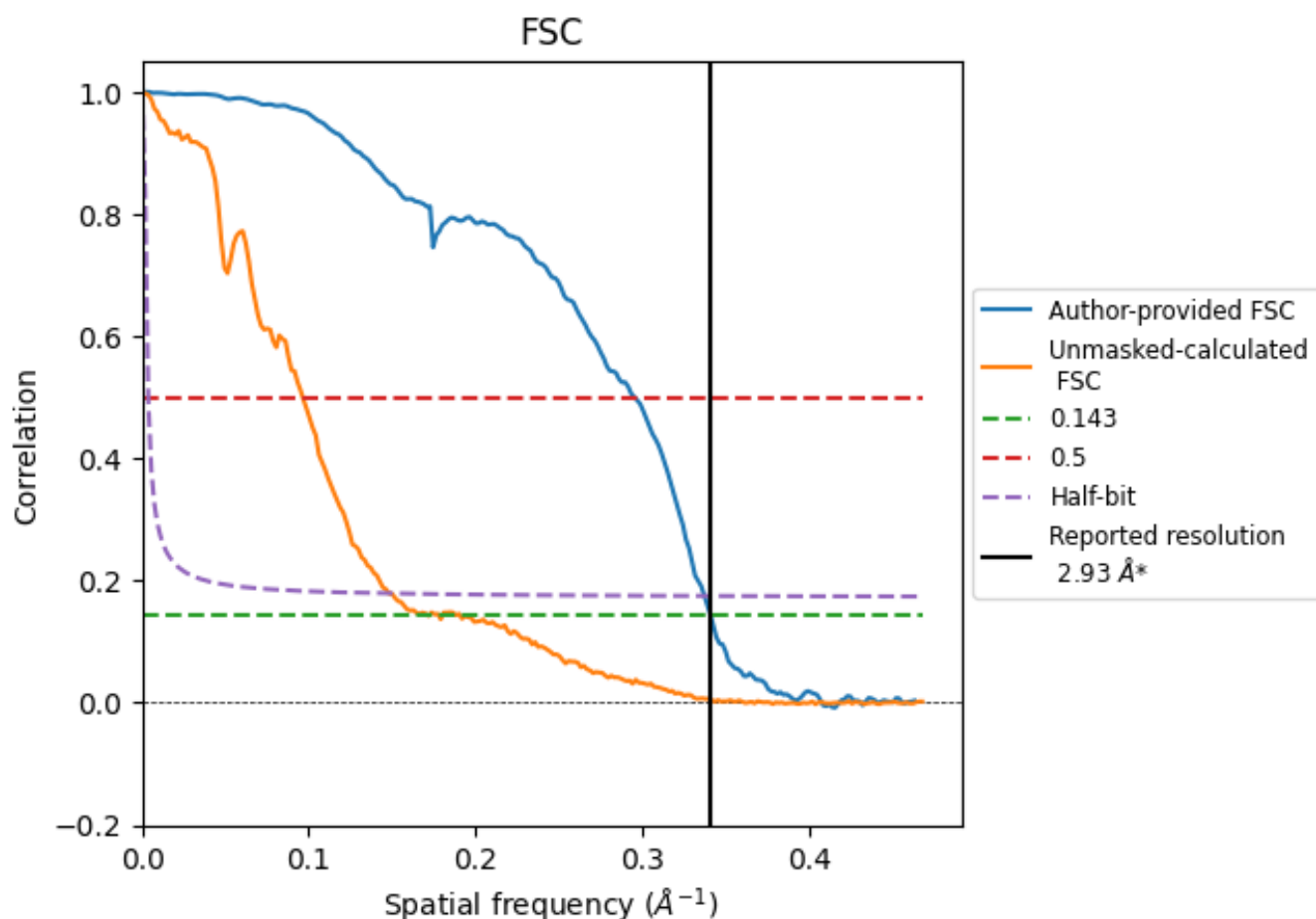


*Reported resolution corresponds to spatial frequency of 0.341 $\text{\AA}^{-1}$

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 0.341 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

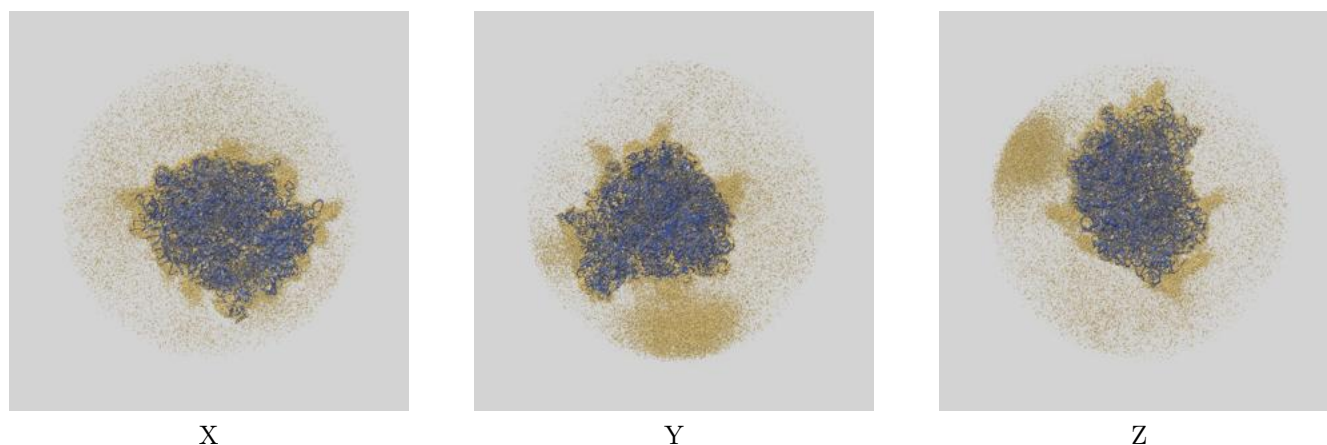
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.93	3.38	2.96
Unmasked-calculated*	5.83	10.37	6.75

*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 5.83 differs from the reported value 2.93 by more than 10 %

9 Map-model fit [i](#)

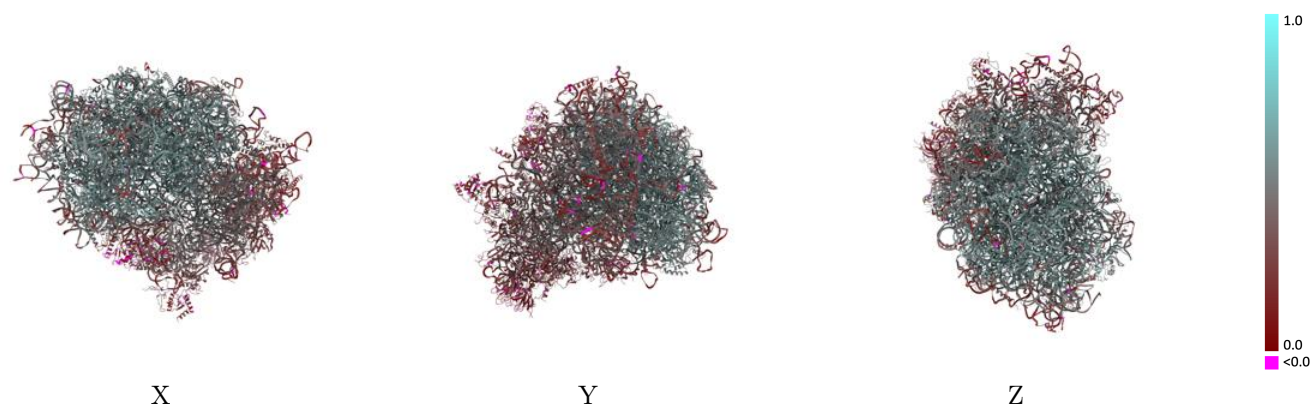
This section contains information regarding the fit between EMDB map EMD-71355 and PDB model 9P7W. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



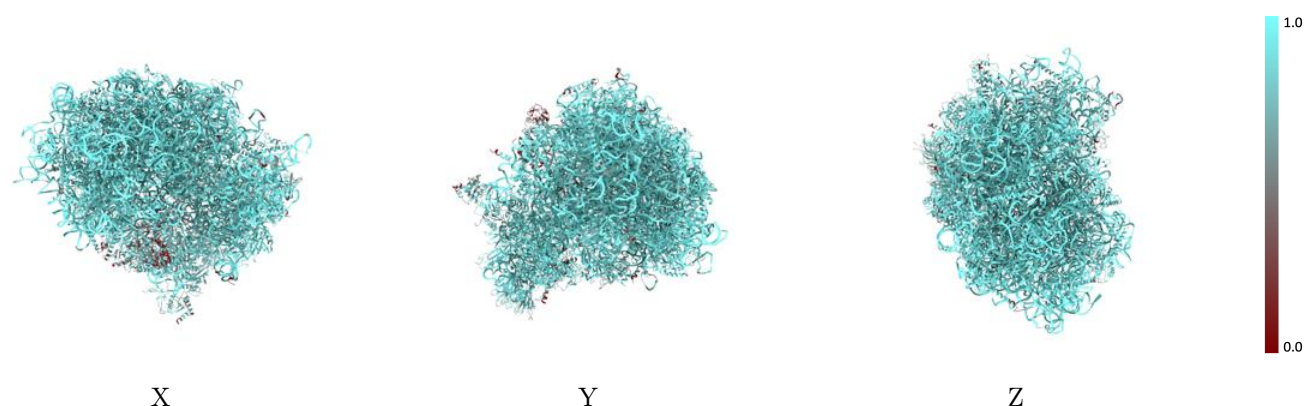
The images above show the 3D surface view of the map at the recommended contour level 0.0119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



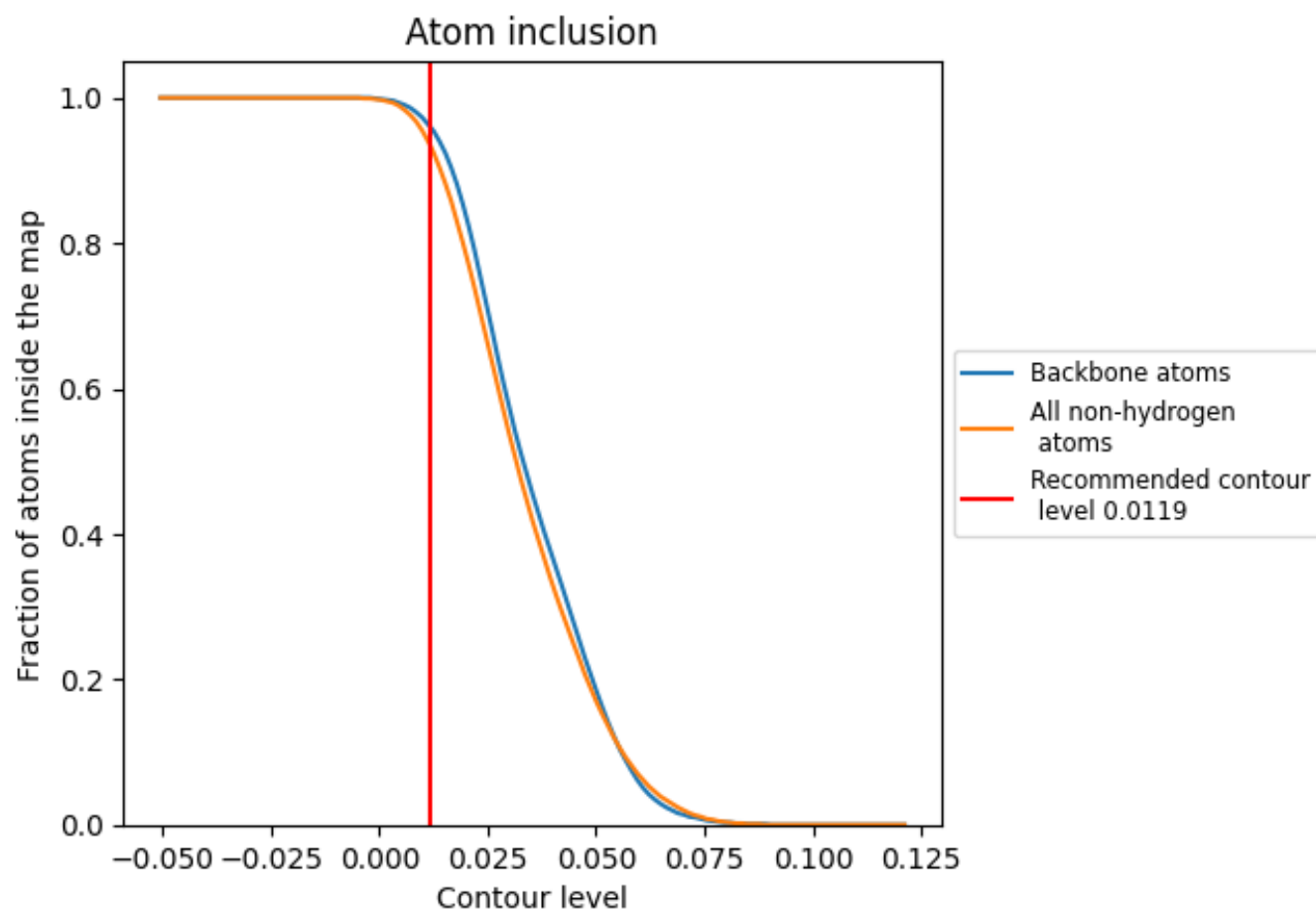
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0119).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.4550
At	 0.6910	 0.3050
CI	 0.7610	 0.4460
L5	 0.9750	 0.5090
L7	 0.9970	 0.5450
L8	 0.9840	 0.5340
LA	 0.9600	 0.5690
LB	 0.9420	 0.5600
LC	 0.9440	 0.5570
LD	 0.9570	 0.5100
LE	 0.9120	 0.4880
LF	 0.9510	 0.5590
LG	 0.8890	 0.4960
LH	 0.9330	 0.5390
LI	 0.9210	 0.5460
LJ	 0.9090	 0.4640
LL	 0.9060	 0.5260
LM	 0.9470	 0.5380
LN	 0.9770	 0.5870
LO	 0.9590	 0.5620
LP	 0.9630	 0.5680
LQ	 0.9640	 0.5820
LR	 0.9100	 0.4910
LS	 0.9710	 0.5730
LT	 0.9400	 0.5420
LU	 0.9220	 0.4630
LV	 0.9480	 0.5600
LW	 0.8190	 0.3940
LX	 0.9320	 0.5380
LY	 0.9560	 0.5460
LZ	 0.9550	 0.5260
La	 0.9680	 0.5820
Lb	 0.9030	 0.4910
Lc	 0.9370	 0.5190
Ld	 0.9230	 0.5380



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Chain	Atom inclusion	Q-score
Le	 0.9670	 0.5800
Lf	 0.9750	 0.5840
Lg	 0.9370	 0.5500
Lh	 0.9360	 0.5410
Li	 0.9250	 0.5280
Lj	 0.9720	 0.5800
Lk	 0.8990	 0.4790
Ll	 0.9480	 0.5600
Lm	 0.9400	 0.5490
Ln	 0.9140	 0.5170
Lo	 0.7610	 0.5440
Lp	 0.9270	 0.5530
Lr	 0.9660	 0.5610
Ls	 0.4580	 0.1590
Lt	 0.4780	 0.1560
Pt	 0.7750	 0.3420
S2	 0.9760	 0.3810
SA	 0.8620	 0.3050
SB	 0.8250	 0.3110
SC	 0.9070	 0.3730
SD	 0.8510	 0.3110
SE	 0.9170	 0.3670
SF	 0.6830	 0.2780
SG	 0.8420	 0.3300
SH	 0.8290	 0.2830
SI	 0.8890	 0.3960
SJ	 0.8950	 0.3300
SK	 0.8480	 0.2780
SL	 0.8500	 0.4100
SM	 0.6420	 0.1570
SN	 0.8920	 0.3780
SO	 0.8200	 0.3430
SP	 0.8400	 0.3060
SQ	 0.8480	 0.2750
SR	 0.8290	 0.2720
SS	 0.8530	 0.3150
ST	 0.8600	 0.2660
SU	 0.8870	 0.3130
SV	 0.8910	 0.3380
SW	 0.9100	 0.3970
SX	 0.8680	 0.4520
SY	 0.8260	 0.3020

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Chain	Atom inclusion	Q-score
SZ	 0.4750	 0.2460
Sa	 0.8810	 0.3550
Sb	 0.8890	 0.3240
Sc	 0.7630	 0.2990
Sd	 0.9210	 0.3600
Se	 0.7630	 0.3270
Sf	 0.7560	 0.2380
Sg	 0.8180	 0.1980