



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 06:29 PM EDT

PDB ID : 9P8H / pdb_00009p8h
EMDB ID : EMD-71377
Title : In situ human A/P-P/E state 80S ribosome
Authors : Zheng, W.; Xiong, Y.
Deposited on : 2025-06-23
Resolution : 2.98 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

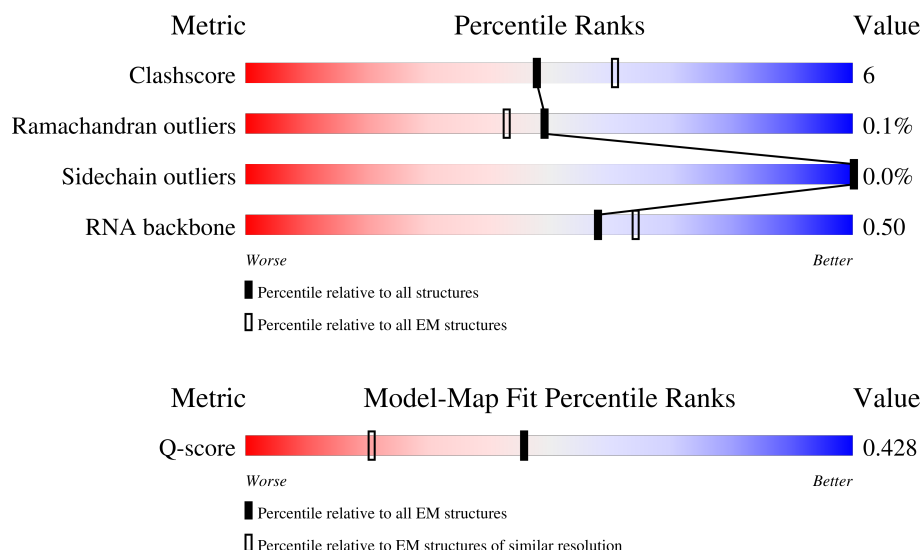
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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.



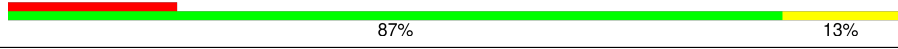
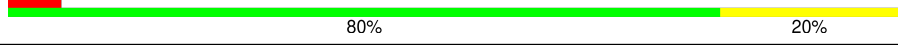
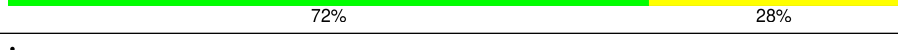
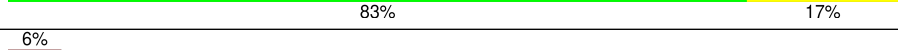
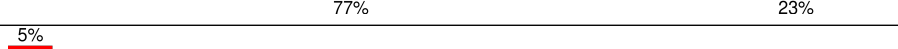
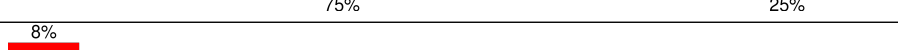
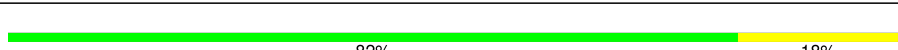
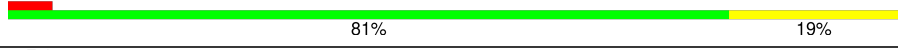
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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	AP	142	
2	PE	150	
3	SD	454	

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Mol	Chain	Length	Quality of chain
4	SF	189	
5	SK	98	
6	SM	122	
7	SP	127	
8	SQ	144	
9	SR	135	
10	SS	145	
11	ST	143	
12	SU	104	
13	SZ	75	
14	Sc	64	
15	Sd	55	
16	Sf	67	
17	Sg	313	
18	SA	221	
19	SB	214	
20	SC	222	
21	SE	262	
22	SG	237	
23	SH	186	
24	SI	206	
25	SJ	185	
26	SL	153	
27	SN	150	
28	SO	140	

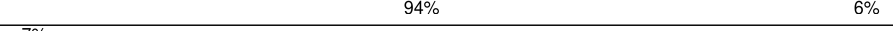
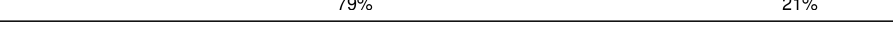
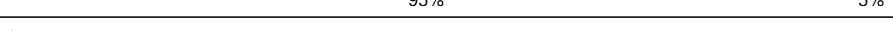
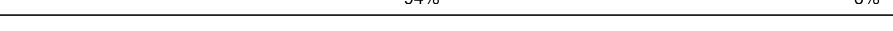
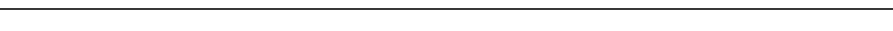
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SW	129	
31	SX	141	
32	SY	131	
33	Sa	102	
34	Sb	83	
35	S2	1740	
36	LR	187	
37	LW	118	
38	CI	31	
39	L5	3655	
40	L7	120	
41	L8	156	
42	LA	248	
43	LB	402	
44	LC	368	
45	LD	293	
46	LE	250	
47	LF	225	
48	LG	241	
49	LH	190	
50	LI	213	
51	LJ	176	
52	LL	210	
53	LM	139	

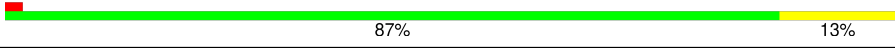
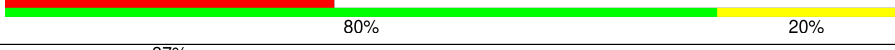
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Mol	Chain	Length	Quality of chain
54	LN	203	
55	LO	201	
56	LP	153	
57	LQ	187	
58	LS	175	
59	LT	159	
60	LU	101	
61	LV	131	
62	LX	120	
63	LY	134	
64	LZ	135	
65	La	147	
66	Lb	109	
67	Lc	98	
68	Ld	107	
69	Le	128	
70	Lf	109	
71	Lg	114	
72	Lh	122	
73	Li	102	
74	Lj	86	
75	Lk	69	
76	Ll	50	
77	Lm	52	
78	Ln	24	

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Mol	Chain	Length	Quality of chain
79	Lo	105	
80	Lp	91	
81	Lr	125	
82	Ls	196	
83	Lt	141	
84	CH	132	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 220526 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called A/P site tRNA.

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

- Molecule 2 is a RNA chain called P/E site tRNA.

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

- Molecule 3 is a protein called 40S ribosomal protein S3.

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

- Molecule 4 is a protein called 40S ribosomal protein S5.

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

- Molecule 5 is a protein called 40S ribosomal protein S10.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 7 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 9 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 10 is a protein called 40S ribosomal protein S18.

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

- Molecule 11 is a protein called 40S ribosomal protein S19.

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

- Molecule 12 is a protein called 40S ribosomal protein S20.

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

- Molecule 13 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 14 is a protein called 40S ribosomal protein S28.

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

- Molecule 15 is a protein called 40S ribosomal protein S29.

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

- Molecule 16 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 17 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 18 is a protein called 40S ribosomal protein SA.

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

- Molecule 19 is a protein called 40S ribosomal protein S3a.

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

- Molecule 20 is a protein called 40S ribosomal protein S2.

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

- Molecule 21 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 22 is a protein called 40S ribosomal protein S6.

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

- Molecule 23 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	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 24 is a protein called 40S ribosomal protein S8.

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

- Molecule 25 is a protein called 40S ribosomal protein S9.

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

- Molecule 26 is a protein called 40S ribosomal protein S11.

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

- Molecule 27 is a protein called 40S ribosomal protein S13.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 29 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 30 is a protein called 40S ribosomal protein S15a.

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

- Molecule 31 is a protein called 40S ribosomal protein S23.

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

- Molecule 32 is a protein called 40S ribosomal protein S24.

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

- Molecule 33 is a protein called 40S ribosomal protein S26.

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

- Molecule 34 is a protein called Small ribosomal subunit protein eS27.

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

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

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

- Molecule 36 is a protein called 60S ribosomal protein L19.

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

- Molecule 37 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	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 38 is a protein called Transcription factor BTF3.

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

- Molecule 39 is a RNA chain called 28S rRNA.

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

- Molecule 40 is a RNA chain called 5S rRNA.

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

- Molecule 41 is a RNA chain called 5.8S rRNA.

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

- Molecule 42 is a protein called 60S ribosomal protein L8.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 44 is a protein called 60S ribosomal protein L4.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 46 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 47 is a protein called 60S ribosomal protein L7.

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

- Molecule 48 is a protein called 60S ribosomal protein L7a.

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

- Molecule 49 is a protein called 60S ribosomal protein L9.

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

- Molecule 50 is a protein called Ribosomal protein uL16-like.

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

- Molecule 51 is a protein called 60S ribosomal protein L11.

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

- Molecule 52 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 53 is a protein called 60S ribosomal protein L14.

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

- Molecule 54 is a protein called 60S ribosomal protein L15.

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

- Molecule 55 is a protein called 60S ribosomal protein L13a.

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

- Molecule 56 is a protein called 60S ribosomal protein L17.

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

- Molecule 57 is a protein called 60S ribosomal protein L18.

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

- Molecule 58 is a protein called 60S ribosomal protein L18a.

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

- Molecule 59 is a protein called 60S ribosomal protein L21.

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

- Molecule 60 is a protein called Heparin-binding protein HBp15.

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

- Molecule 61 is a protein called 60S ribosomal protein L23.

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

- Molecule 62 is a protein called 60S ribosomal protein L23a.

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

- Molecule 63 is a protein called 60S ribosomal protein L26.

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

- Molecule 64 is a protein called 60S ribosomal protein L27.

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

- Molecule 65 is a protein called 60S ribosomal protein L27a.

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

- Molecule 66 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 67 is a protein called 60S ribosomal protein L30.

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

- Molecule 68 is a protein called 60S ribosomal protein L31.

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

- Molecule 69 is a protein called 60S ribosomal protein L32.

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

- Molecule 70 is a protein called 60S ribosomal protein L35a.

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

- Molecule 71 is a protein called 60S ribosomal protein L34.

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

- Molecule 72 is a protein called 60S ribosomal protein L35.

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

- Molecule 73 is a protein called 60S ribosomal protein L36.

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

- Molecule 74 is a protein called 60S ribosomal protein L37.

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

- Molecule 75 is a protein called 60S ribosomal protein L38.

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

- Molecule 76 is a protein called 60S ribosomal protein L39.

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

- Molecule 77 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 78 is a protein called 60S ribosomal protein L41.

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

- Molecule 79 is a protein called 60S ribosomal protein L36a.

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

- Molecule 80 is a protein called 60S ribosomal protein L37a.

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

- Molecule 81 is a protein called 60S ribosomal protein L28.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 83 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	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 84 is a protein called Endothelial differentiation-related factor 1.

Mol	Chain	Residues	Atoms			AltConf	Trace
84	CH	132	Total	C	N	O	
			1018	625	199	194	
						0	0

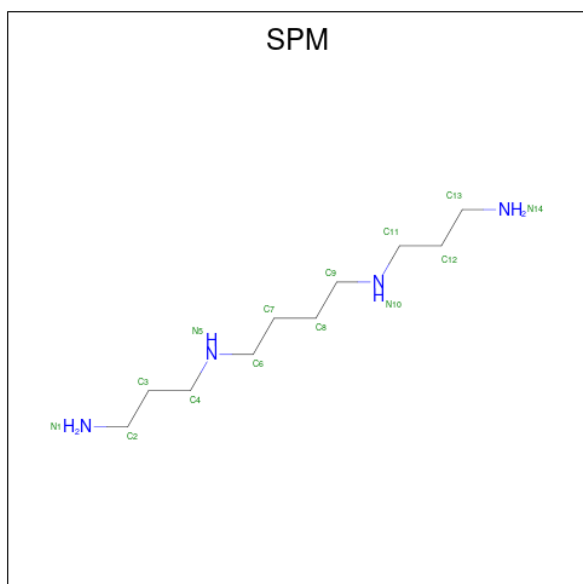
- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
85	SS	1	Total	Mg	0
			1	1	
85	SG	1	Total	Mg	0
			1	1	
85	S2	25	Total	Mg	0
			25	25	
85	L5	178	Total	Mg	0
			178	178	
85	L7	3	Total	Mg	0
			3	3	
85	L8	4	Total	Mg	0
			4	4	
85	LA	1	Total	Mg	0
			1	1	
85	LB	1	Total	Mg	0
			1	1	
85	LI	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	
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).



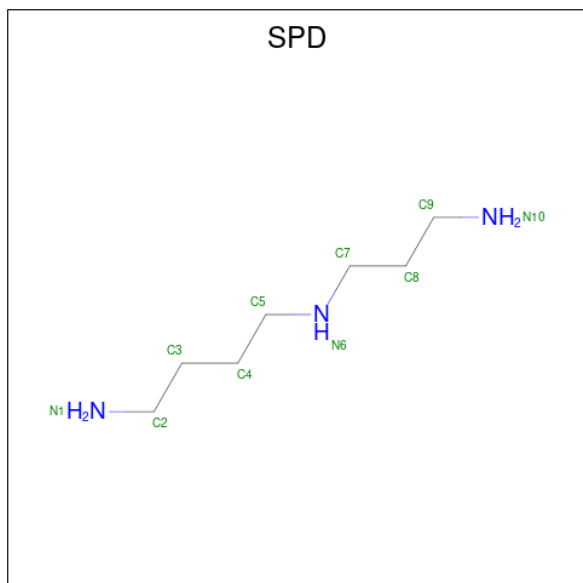
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	

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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	

- 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	

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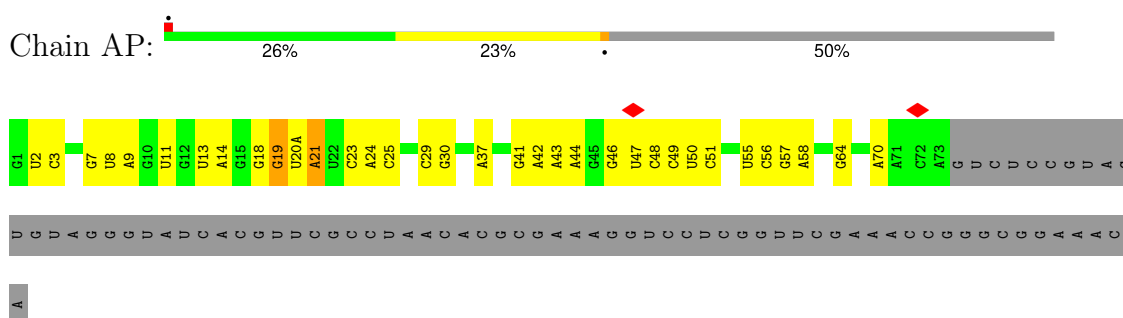
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
88	LN	1	10	7	3	0

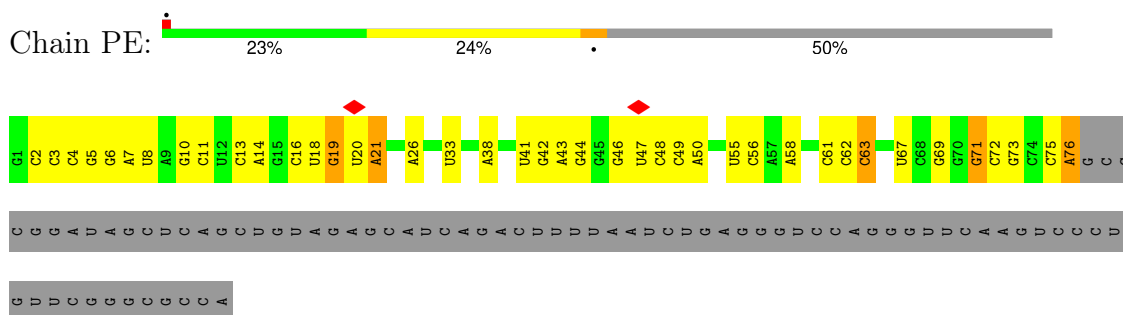
3 Residue-property plots [i](#)

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.

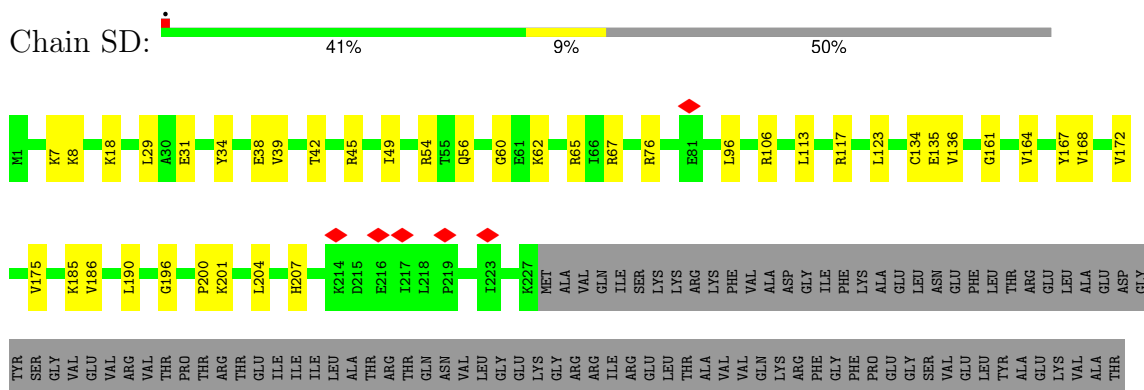
• Molecule 1: A/P site tRNA



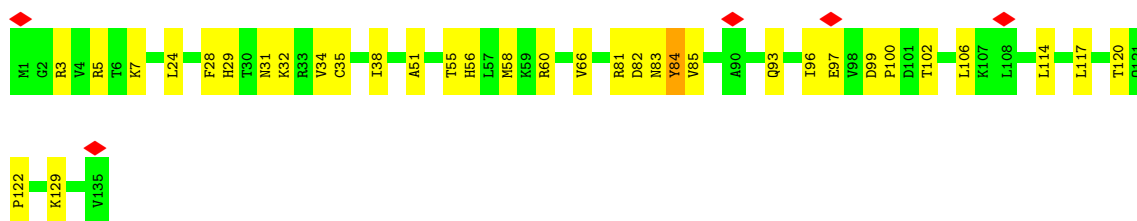
• Molecule 2: P/E site tRNA



• Molecule 3: 40S ribosomal protein S3

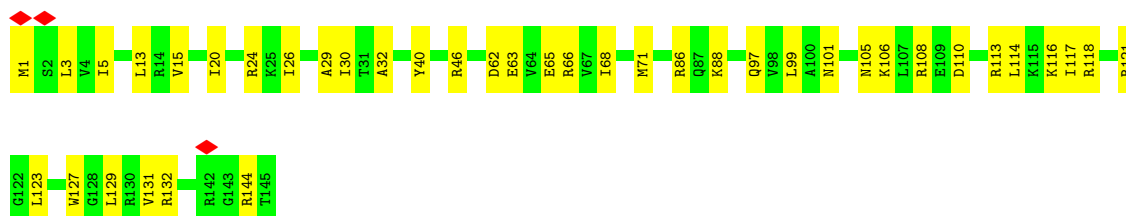


Chain SR:  75% 24%



- Molecule 10: 40S ribosomal protein S18

Chain SS:  72% 28%



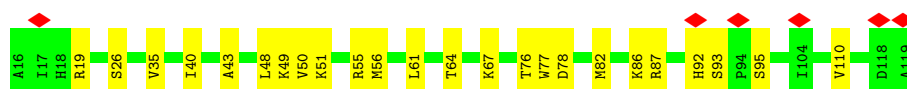
- Molecule 11: 40S ribosomal protein S19

Chain ST:  83% 17%



- Molecule 12: 40S ribosomal protein S20

Chain SU:  6% 77% 23%



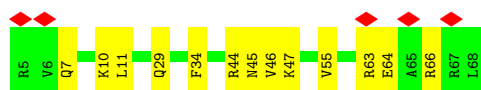
- Molecule 13: Small ribosomal subunit protein eS25

Chain SZ:  5% 75% 25%



- Molecule 14: 40S ribosomal protein S28

Chain Sc:  8% 80% 20%



- Molecule 15: 40S ribosomal protein S29

Chain Sd:  89% 11%



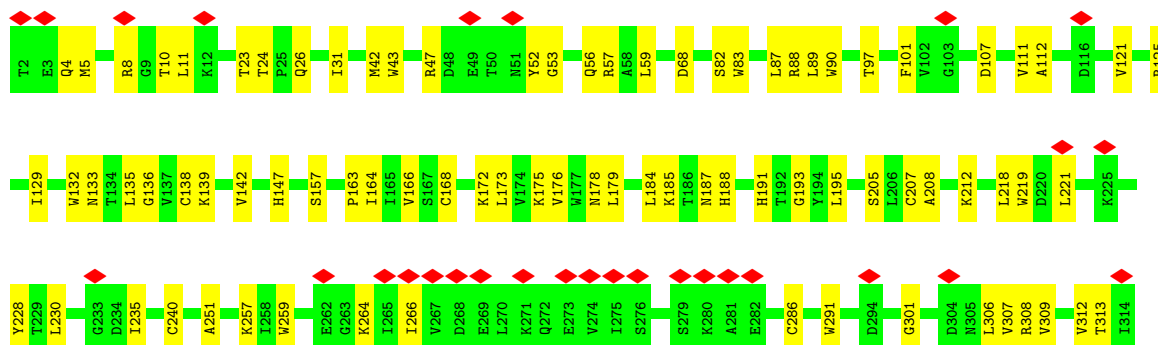
- Molecule 16: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  15% 78% 22%



- Molecule 17: Receptor of activated protein C kinase 1

Chain Sg:  9% 73% 27%



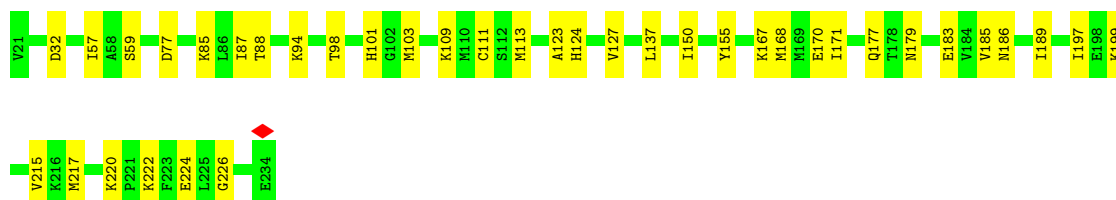
- Molecule 18: 40S ribosomal protein SA

Chain SA:  82% 18%



- Molecule 19: 40S ribosomal protein S3a

Chain SB:  82% 18%



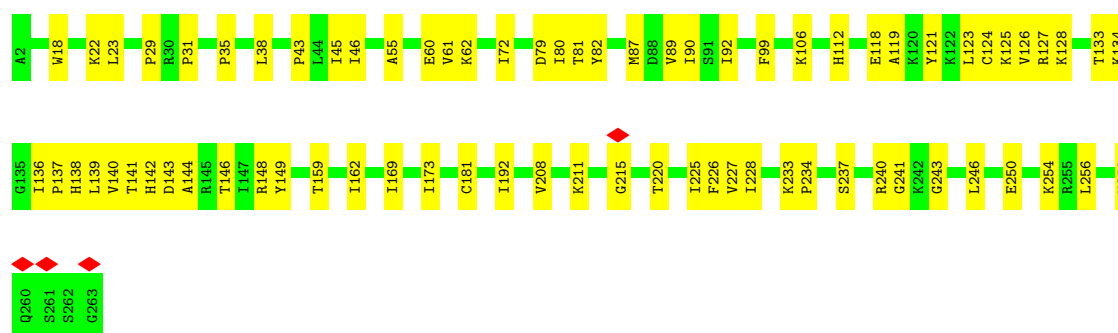
- Molecule 20: 40S ribosomal protein S2

Chain SC:  83% 16%



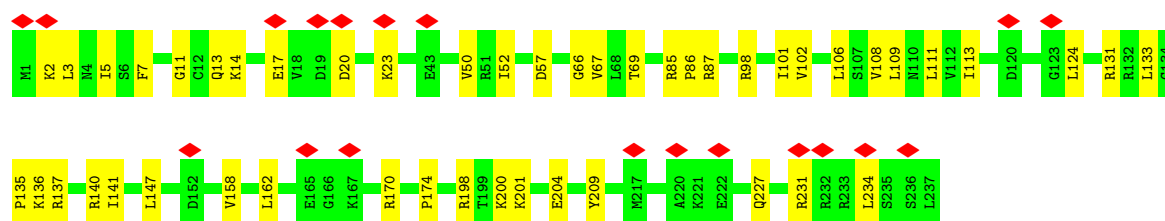
- Molecule 21: Small ribosomal subunit protein eS4, X isoform

Chain SE:  72% 28%



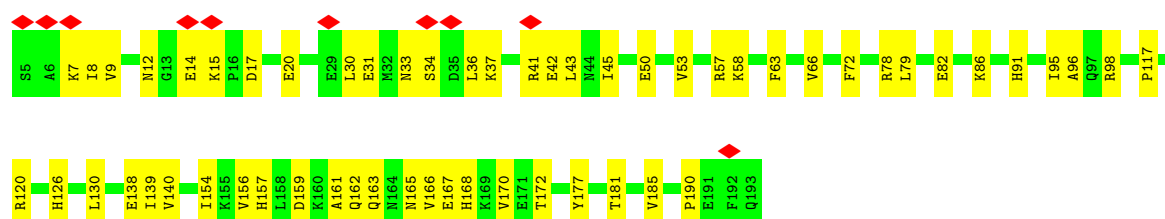
- Molecule 22: 40S ribosomal protein S6

Chain SG:  8% 80% 20%



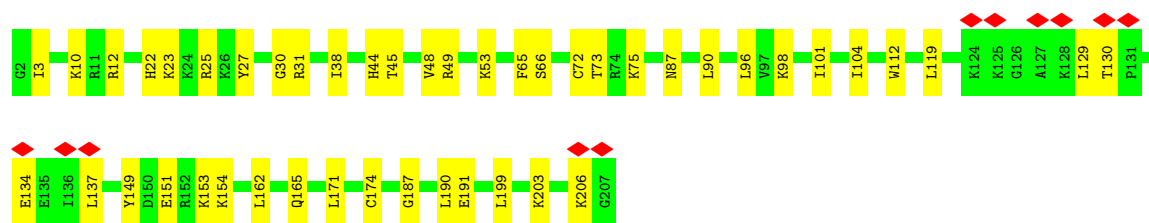
- Molecule 23: Small ribosomal subunit protein eS7

Chain SH:  5% 69% 31%

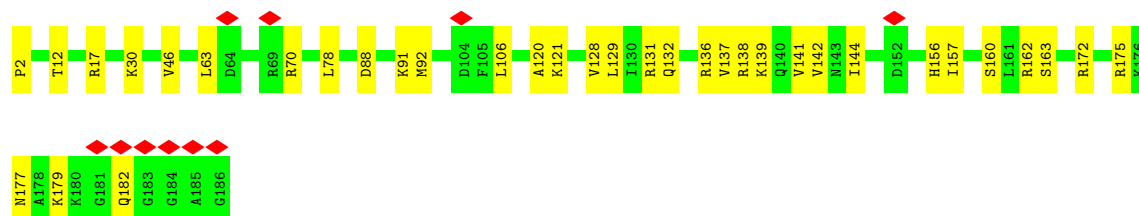
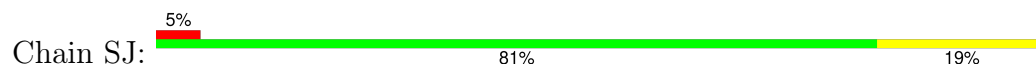


- Molecule 24: 40S ribosomal protein S8

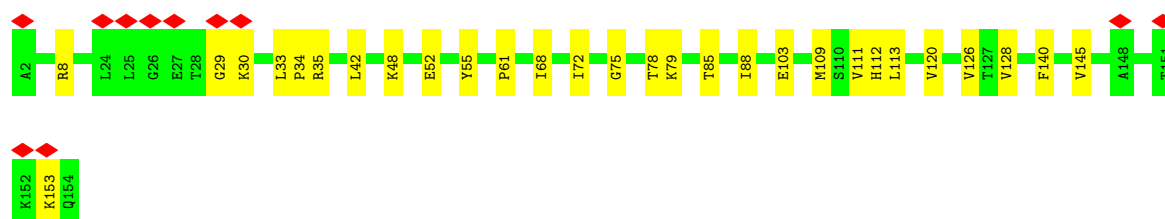
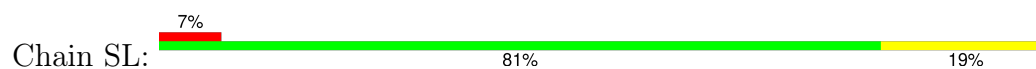
Chain SI:  5% 78% 22%



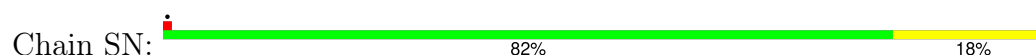
- Molecule 25: 40S ribosomal protein S9



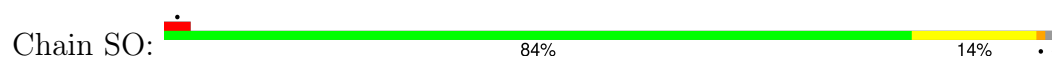
- Molecule 26: 40S ribosomal protein S11



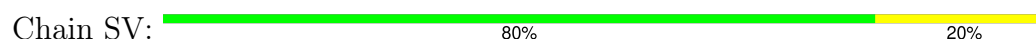
- Molecule 27: 40S ribosomal protein S13



- Molecule 28: Small ribosomal subunit protein uS11



- Molecule 29: Small ribosomal subunit protein eS21





- Molecule 30: 40S ribosomal protein S15a

Chain SW: 81% 19%



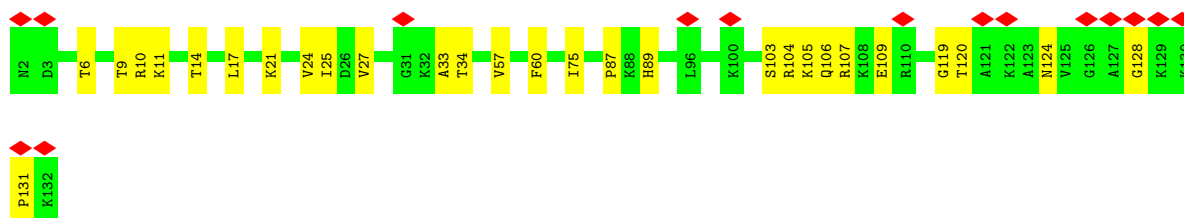
- Molecule 31: 40S ribosomal protein S23

Chain SX: 88% 12%



- Molecule 32: 40S ribosomal protein S24

Chain SY: 11% 79% 21%



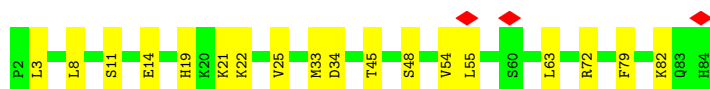
- Molecule 33: 40S ribosomal protein S26

Chain Sa: 82% 18%



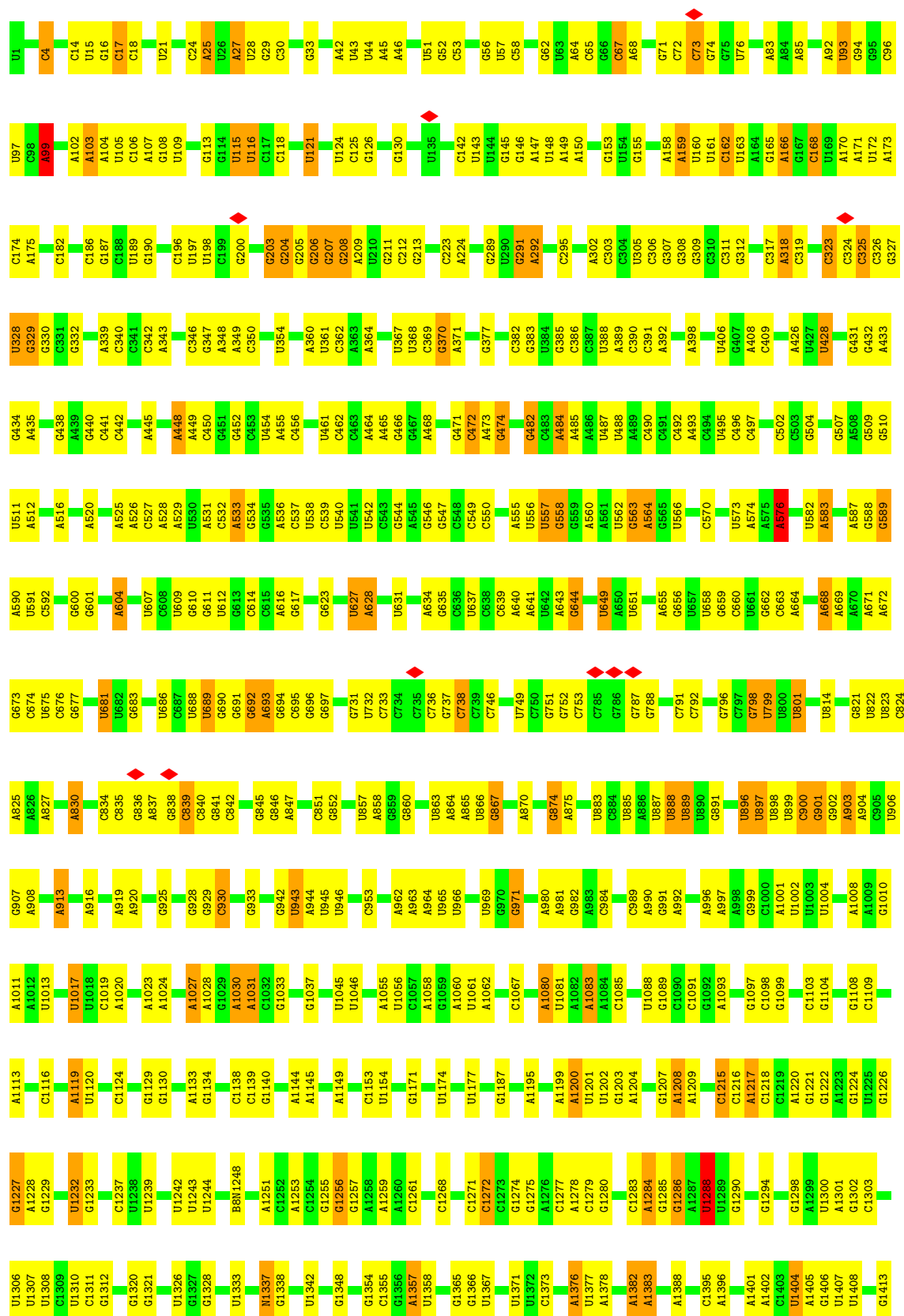
- Molecule 34: Small ribosomal subunit protein eS27

Chain Sb: 78% 22%



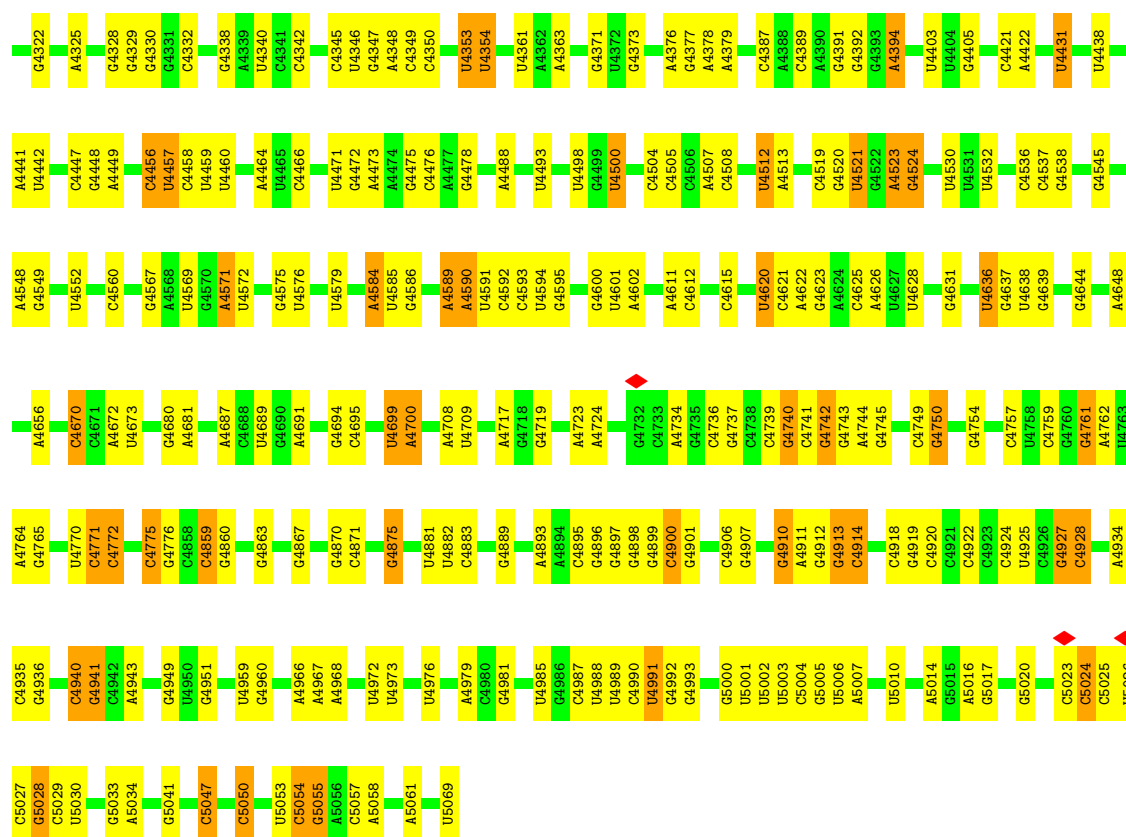
- Molecule 35: 18S rRNA

Chain S2: 55% 37% 7%

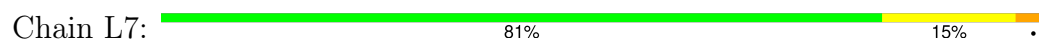




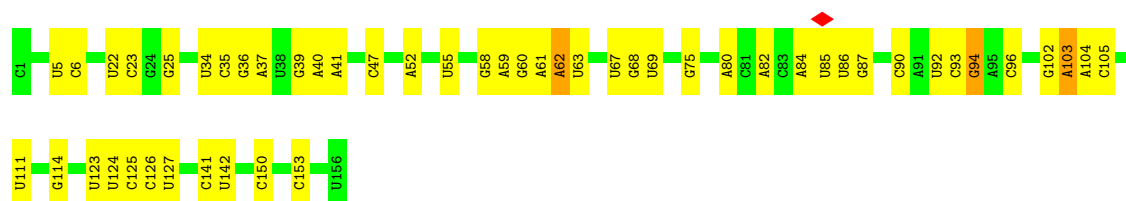
U4227	U4112	U3930	A3852	A3748	A3662	G3877	G2758	C2654	A2529	G2302	C2059	U1974
G4228	U4113	C3931	U3853	G3753	A3663	C2899	G2759	C2655	U2537	C2303	G2060	G1975
U4229	U4114	U3932	A3856	G3754	G3664	U2900	G2760	G2658	U2538	G2306	A2069	G1976
A4233	U4115	G3933	A3857	A3760	G3665	G2901	G2762	G2662	C2540	A2313	C2072	C1977
G4236	U4116	C3937	A3861	C3761	C3670	G2902	A2764	G2663	U2543	G2314	G2076	A1979
G4238	U4117	G3938	A3862	U3762	C3673	G2903	A2765	G2664	A2544	G2318	G2076	U1980
A4239	A4118	A3946	A3865	G3763	G3674	G2904	G2768	U2665	G2544	G2321	G2079	G1981
G4240	U4119	A3947	A3866	U3764	G3675	G2905	U2769	C2666	U2545	G2321	U2080	A1982
U4241	A4120	G3948	A3867	G3765	U3680	G2906	U2769	C2667	G2546	G2321	A1983	
U4242	A4121	A3949	A3868	A3766	G3684	G2907	C2770	C2668	G2547	G2324	G2083	A1984
C4243	A4122	U3950	C3869	C3767	G3685	U2908	G2773	C3669	G2547	C2324	C2083	G1985
A4251	A4123	G3951	C3870	U3770	G3686	C3909	G2773	G2675	A2553	G2331	C2084	U1986
G4254	A4124	A3952	A3871	U3771	G3687	C3588	G2777	A2676	U2554	G2331	G2092	G1987
A4255	A4125	G3953	A3872	U3772	U3688	G3589	G2778	G2677	G2555	G2333	A2093	G1988
U4257	A4126	U4058	A3873	A3773	G3689	G3590	A2783	U2687	G2556	G2333	G2094	A1989
C4258	A4127	C4059	A3874	A3774	U3690	C3591	A2783	G2688	G2557	G2333	A2095	A1991
A4259	A4128	U4060	A3877	A3775	G3691	G3594	A2787	G2688	G2558	G2333	G2096	U1992
U4260	A4129	G4061	A3878	A3776	A3692	U3595	U2788	G2693	G2559	G2333	U2097	C1993
C4261	A4130	A4062	A3879	A3777	U3693	A3596	A2789	G2694	C2561	G2333	C2098	C1994
U4265	A4131	U4063	A3881	C3782	U3694	A3597	U2790	A2695	A2565	G2333	G2098	G1995
U4268	A4132	G4064	C3884	A3785	C3696	C3598	A2806	A2696	G2565	C2351	C2101	C1996
A4269	A4133	G4065	U3884	U3786	U3697	A3599	G2809	G2703	G2566	A2360	G2102	U1997
A4270	A4134	U4066	G3885	U3786	G3698	G3600	G2809	G2706	U2570	A2361	G2103	A1998
A4271	A4135	U4067	G3886	G3792	C3699	G3605	U2810	G2707	C2572	U2362	G2104	G2000
A4272	A4136	A4070	A3890	G3806	C3700	A3611	G2811	U2708	G2573	G2363	C2107	G2001
A4273	A4137	U4071	U3891	A3807	C3701	U3616	G2812	U2709	G2574	G2364	G2108	A2002
A4274	A4138	G4072	U3892	C3808	U3707	U3617	A2813	A2484	U2485	G2364	G2109	G2003
A4275	A4139	A4084	C3893	G3811	C3708	G3618	C2814	U2485	G2486	G2364	G2110	U2004
A4276	A4140	A4085	A3894	G3812	U3709	C3619	G2815	G2487	G2487	G2364	G2111	G2005
A4277	A4141	U4086	G3897	U3813	G3710	G3620	G2816	U2488	G2488	G2364	G2112	U2008
A4278	A4142	C4088	C3898	U3814	A3711	G3621	G2817	U2489	U2489	G2364	G2113	A2009
A4279	A4143	G4089	G3899	U3815	U3712	A3624	G2818	C2490	A2581	G2364	G2114	A2010
A4280	A4144	U4090	C3900	A3817	G3714	G3625	U2826	C2491	G2582	A2382	G2115	C2011
A4281	A4145	G4091	A3901	U3818	U3715	G3626	U2827	C2492	C2492	A2389	G2116	C2016
A4282	A4146	A4092	A3906	G3822	C3716	G3627	U2828	U2493	G2493	A2389	G2117	A2017
A4283	A4147	G4093	A3907	G3823	C3717	A3630	U2829	U2494	G2494	A2389	G2118	C2018
A4284	A4148	A4094	A3908	A3824	U3721	G3633	U2830	U2495	U2495	A2389	G2119	C2019
A4285	A4149	G4095	C3909	A3825	G3722	A3634	U2831	G2496	G2496	G2364	G2120	U2020
A4286	A4150	C4096	C3910	A3826	A3723	U3635	U2832	C2497	G2497	G2364	G2121	G2021
A4287	A4151	U4097	C3911	A3827	A3724	U3636	U2833	C2498	G2498	G2364	G2122	A2024
A4288	A4152	G4098	U3912	A3828	G3725	U3637	U2834	U2499	G2499	G2364	G2123	A2025
A4289	A4153	A4099	U3913	A3829	A3726	U3638	U2835	U2500	G2500	G2364	G2124	A2026
A4290	A4154	C4100	A3914	A3830	A3727	U3639	U2836	C2501	G2501	G2364	G2125	A2027
A4291	A4155	U4101	U3915	U3831	A3728	U3640	U2837	G2502	G2502	G2364	G2126	A2028
A4292	A4156	G4102	G3916	U3832	A3729	U3641	U2838	G2503	G2503	G2364	G2127	A2029
A4293	A4157	C4103	A3917	U3833	A3730	U3642	U2839	C2504	G2504	G2364	G2128	A2030
A4294	A4158	G4104	C3918	U3834	A3731	U3643	U2840	C2505	G2505	G2364	G2129	G2045
A4295	A4159	U4105	C3919	U3835	A3732	U3644	U2841	C2506	G2506	G2364	G2130	G2046
A4296	A4160	G4106	C3920	U3836	A3733	U3645	U2842	G2507	G2507	G2364	G2131	G2047
A4297	A4161	A4107	U3921	U3837	A3734	A3646	U2843	G2508	G2508	G2364	G2132	U2048
A4298	A4162	G4108	G3922	U3838	A3735	A3647	U2844	U2631	G2631	G2364	G2133	G2297
A4299	A4163	U4109	A3923	U3839	A3736	A3648	U2632	G2632	G2632	G2364	G2134	G2298
A4300	A4164	C4110	C3924	U3840	A3737	G3649	U2633	G2633	G2633	G2364	G2135	G2299
A4301	A4165	G4111	U3925	U3841	A3738	G3650	G2634	G2634	G2634	G2364	G2136	A2300
A4302	A4166	U4112	U3926	U3842	A3739	G3651	G2635	G2635	G2635	G2364	G2137	G2055
A4303	A4167	C4113	U3927	U3843	A3740	G3652	G2636	G2636	G2636	G2364	G2138	G2056
A4304	A4168	G4114	U3928	U3844	A3741	G3653	G2637	G2637	G2637	G2364	G2139	
A4305	A4169	U4115	U3929	U3845	A3742	U3654	G2638	G2638	G2638	G2364	G2140	
A4306	A4170	C4116	C3930	U3846	A3743	U3655	U2639	G2639	G2639	G2364	G2141	
A4307	A4171	G4117	U3931	U3847	A3744	U3656	U2640	G2640	G2640	G2364	G2142	
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A4309	A4173	C4119	U3933	U3849	A3746	U3658	U2642	G2642	G2642	G2364	G2144	
A4310	A4174	G4120	U3934	U3850	A3747	U3659	U2643	G2643	G2643	G2364	G2145	
A4311	A4175	U4121	U3935	U3851	A3748	U3660	U2644	G2644	G2644	G2364	G2146	
A4312	A4176	C4122	U3936	U3852	A3749	U3661	U2645	G2645	G2645	G2364	G2147	
A4313	A4177	G4123	U3937	U3853	A3750	U3662	U2646	G2646	G2646	G2364	G2148	
A4314	A4178	U4124	U3938	U3854	A3751	U3663	U2647	G2647	G2647	G2364	G2149	
A4315	A4179	C4125	U3939	U3855	A3752	U3664	U2648	G2648	G2648	G2364	G2150	
A4316	A4180	G4126	U3940	U3856	A3753	U3665	U2649	G2649	G2649	G2364	G2151	
A4317	A4181	U4127	U3941	U3857	A3754	U3666	U2650	G2650	G2650	G2364	G2152	
A4318	A4182	C4128	U3942	U3858	A3755	U3667	U2651	G2651	G2651	G2364	G2153	
A4319	A4183	G4129	U3943	U3859	A3756	U3668	U2652	G2652	G2652	G2364	G2154	
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A4321	A4185	C4131	U3945	U3861	A3758	U3670	U2654	G2654	G2654	G2364	G2156	
A4322	A4186	G4132	U3946	U3862	A3759	U3671	U2655	G2655	G2655	G2364	G2157	
A4323	A4187	U4133	U3947	U3863	A3760	U3672	U2656	G2656	G2656	G2364	G2158	
A4324	A4188	C4134	U3948	U3864	A3761	U3673	U2657	G2657	G2657	G2364	G2159	
A4325	A4189	G4135	U3949	U3865	A3762	U3674	U2658	G2658	G2658	G2364	G2160	
A4326	A4190	U4136	U3950	U3866	A3763	U3675	U2659	G2659	G2659	G2364	G2161	
A4327	A4191	C4137	U3951	U3867	A3764	U3676	U2660	G2660	G2660	G2364	G2162	
A4328	A4192	G4138	U3952	U3868	A3765	U3677	U2661	G2661	G2661	G2364	G2163	
A4329	A4193	U4139	U3953	U3869	A3766	U3678	U2662	G2662	G2662	G2364	G2164	
A4330	A4194	C4140	U3954	U3870	A3767	U3679	U2663	G2663	G2663	G2364	G2165	
A4331	A4195	G4141	U3955	U3871	A3768	U3680	U2664	G2664	G2664	G2364	G2166	
A4332	A4196	U4142	U3956	U3872	A3769	U3681	U2665	G2665	G2665	G2364	G2167	
A4333	A4197	C4143	U3957	U3873	A3770	U3682	U2666	G2666	G2666	G2364	G2168	
A4334	A4198	G4144	U3958	U3874	U3771	U3683	U2667	G2667	G2667	G2364	G2169	
A4335	A4199	U4145	U3959	U3875	U3772	U3684	U2668	G2668	G2668	G2364	G2170	
A4336	A4200	C4146	U3960	U3876	U3773	U3685	U2669	G2669	G2669	G2364	G2171	
A4337	A4201	G4147	U3961	U3877	U3774	U3686	U2670	G2670	G2670	G2364	G2172	
A4338	A4202	U4148	U3962	U3878	U3775	U3687	U2671	G2671	G2671	G2364	G2173	
A4339	A4203	C4149	U3963	U3879	U3776	U3688	U2672	G2672	G2672	G2364	G2174	
A4340	A4204	G4150	U3964	U3880	U3777	U3689	U2673	G2673	G2673	G2364	G2175	
A4341	A4205	U4151	U3965	U3881	U3778	U3690	U2674	G2674	G2674	G2364	G2176	
A4342	A4206	C4152	U3966	U3882	U3779	U3691	U2675	G2675	G2675	G2364	G2177	
A4343	A4207	G4153	U3967	U3883	U3780	U3692	U2676	G2676	G2676	G2364	G2178	
A4344	A4208	U4154	U3968	U3884	U3781	U3693	U2677	G2677	G2677	G2364	G2179	
A4345	A4209	C4155	U3969	U3885	U3782	U3694	U2678	G2678	G2678	G2364	G2180	
A4346	A4210	G4156	U3970	U3886	U3783	U3695	U2679	G2679	G2679	G2364	G2181	
A4347	A4211	U4157	U3971	U3887	U3784	U3696	U2680	G2680	G2680	G2364	G2182	
A4348	A4212	C										



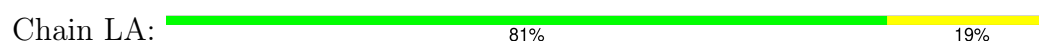
• Molecule 40: 5S rRNA



• Molecule 41: 5.8S rRNA

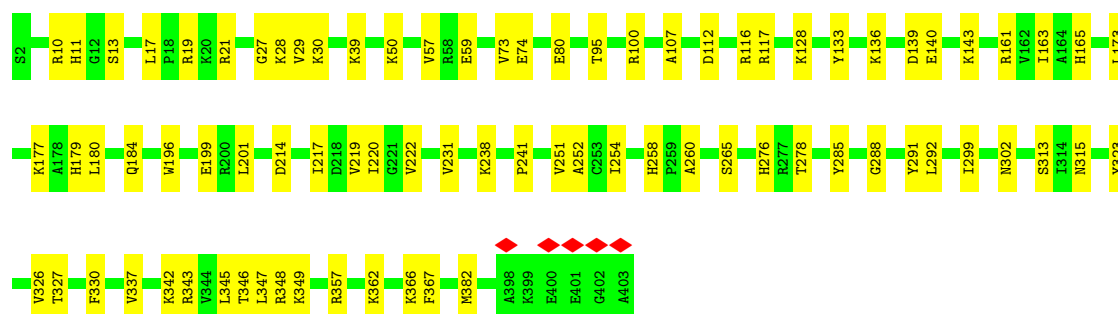
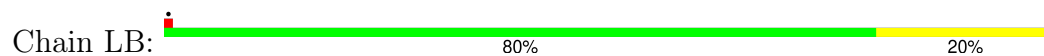


• Molecule 42: 60S ribosomal protein L8

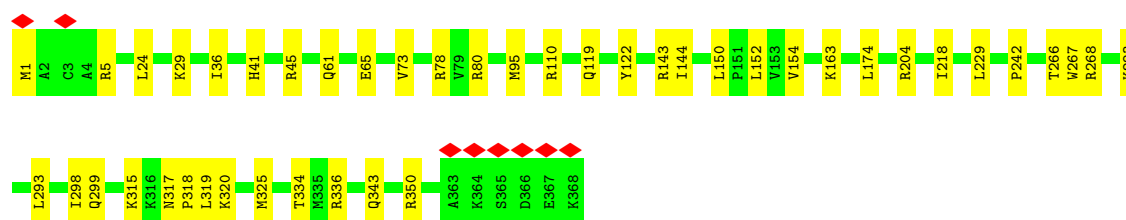
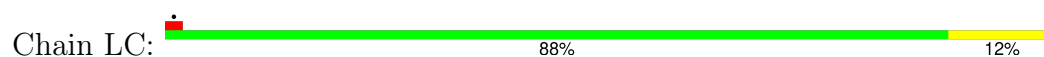




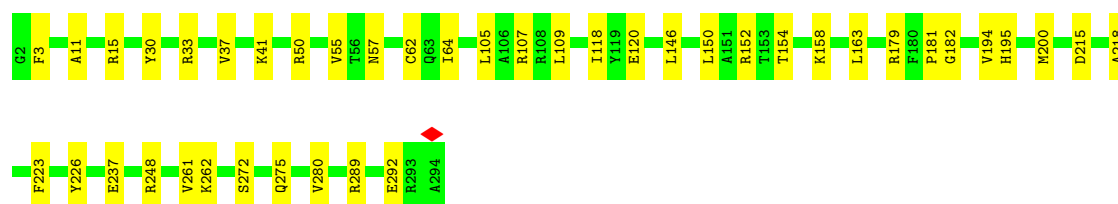
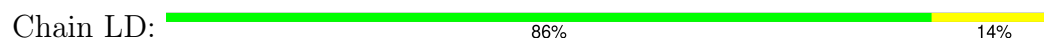
- Molecule 43: Large ribosomal subunit protein uL3



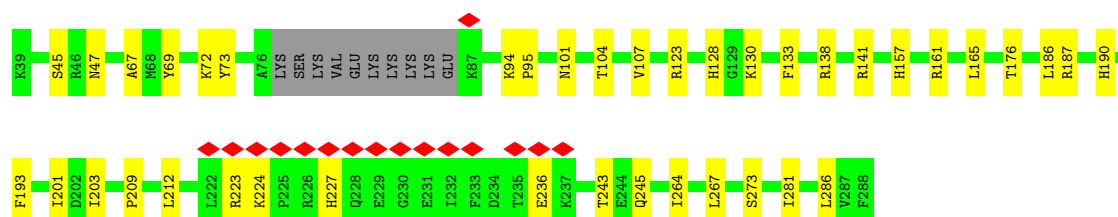
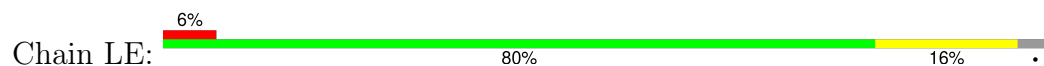
- Molecule 44: 60S ribosomal protein L4



- Molecule 45: Large ribosomal subunit protein uL18



- Molecule 46: Large ribosomal subunit protein eL6



- Molecule 47: 60S ribosomal protein L7

Chain LF:  88% 12%



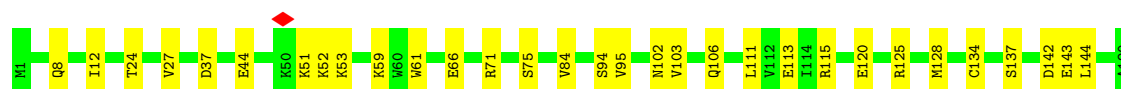
- Molecule 48: 60S ribosomal protein L7a

Chain LG:  6% 88% 12%



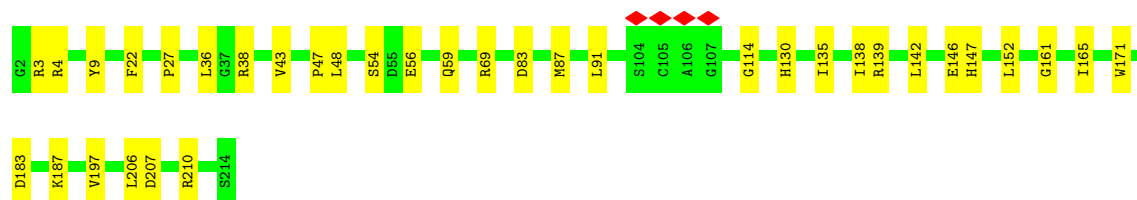
- Molecule 49: 60S ribosomal protein L9

Chain LH:  84% 16%



- Molecule 50: Ribosomal protein uL16-like

Chain LI:  84% 16%



- Molecule 51: 60S ribosomal protein L11

Chain LJ:  82% 15%



- Molecule 52: Large ribosomal subunit protein eL13

Chain LL:  89% 11%



- Molecule 53: 60S ribosomal protein L14

Chain LM:  88% 12%



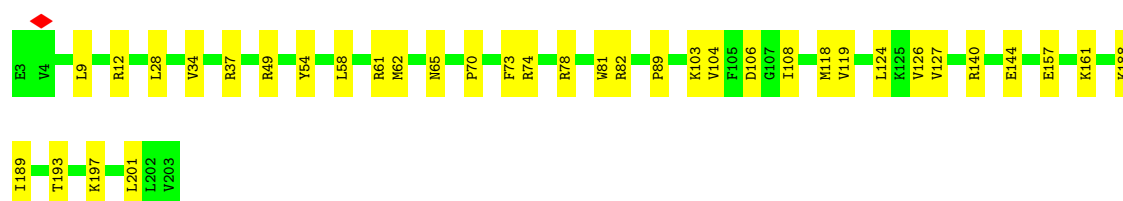
- Molecule 54: 60S ribosomal protein L15

Chain LN:  89% 11%



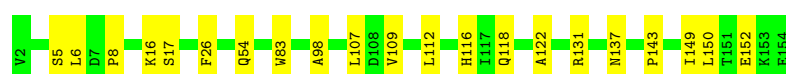
- Molecule 55: 60S ribosomal protein L13a

Chain LO:  82% 18%



- Molecule 56: 60S ribosomal protein L17

Chain LP:  86% 14%



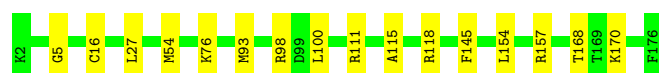
- Molecule 57: 60S ribosomal protein L18

Chain LQ:  91% 9%



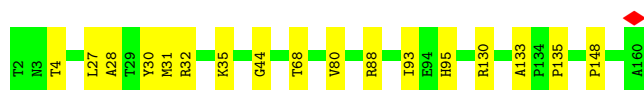
- Molecule 58: 60S ribosomal protein L18a

Chain LS:  91% 9%

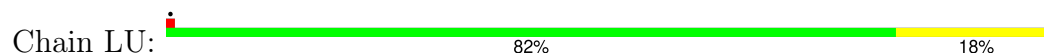


- Molecule 59: 60S ribosomal protein L21

Chain LT:  89% 11%



- Molecule 60: Heparin-binding protein HBp15



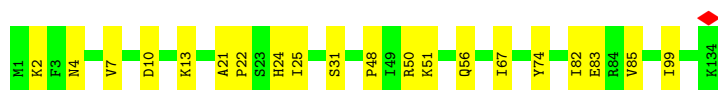
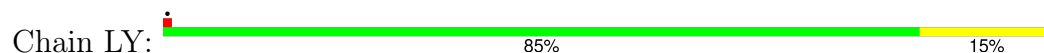
- Molecule 61: 60S ribosomal protein L23



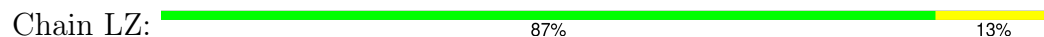
- Molecule 62: 60S ribosomal protein L23a



- Molecule 63: 60S ribosomal protein L26



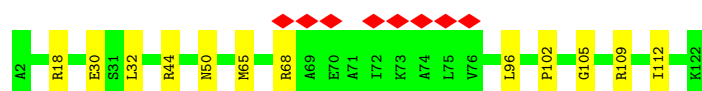
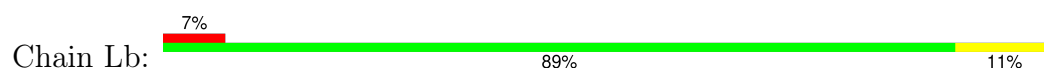
- Molecule 64: 60S ribosomal protein L27



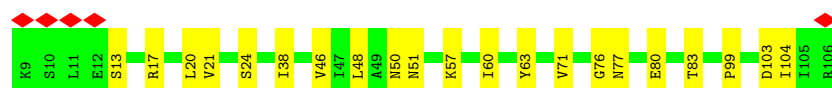
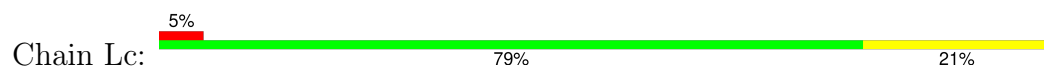
- Molecule 65: 60S ribosomal protein L27a



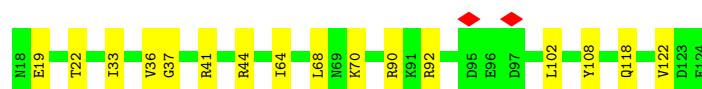
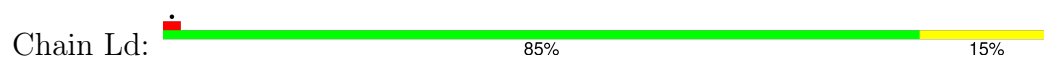
- Molecule 66: Large ribosomal subunit protein eL29



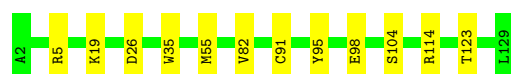
- Molecule 67: 60S ribosomal protein L30



- Molecule 68: 60S ribosomal protein L31



- Molecule 69: 60S ribosomal protein L32



- Molecule 70: 60S ribosomal protein L35a



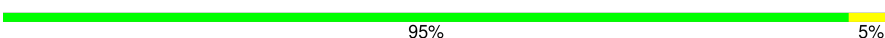
- Molecule 71: 60S ribosomal protein L34



- Molecule 72: 60S ribosomal protein L35



- Molecule 73: 60S ribosomal protein L36

Chain Li:  95% 5%



- Molecule 74: 60S ribosomal protein L37

Chain Lj:  86% 14%



- Molecule 75: 60S ribosomal protein L38

Chain Lk:  86% 14%

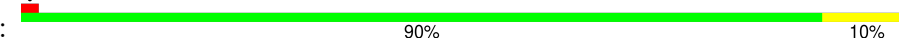


- Molecule 76: 60S ribosomal protein L39

Chain Ll:  80% 20%



- Molecule 77: Large ribosomal subunit protein eL40

Chain Lm:  90% 10%



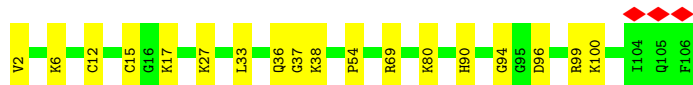
- Molecule 78: 60S ribosomal protein L41

Chain Ln:  79% 21%

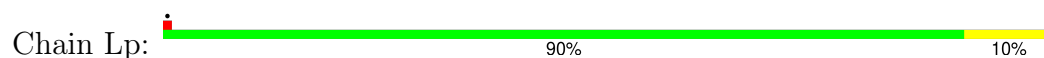


- Molecule 79: 60S ribosomal protein L36a

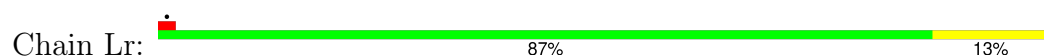
Chain Lo:  83% 17%



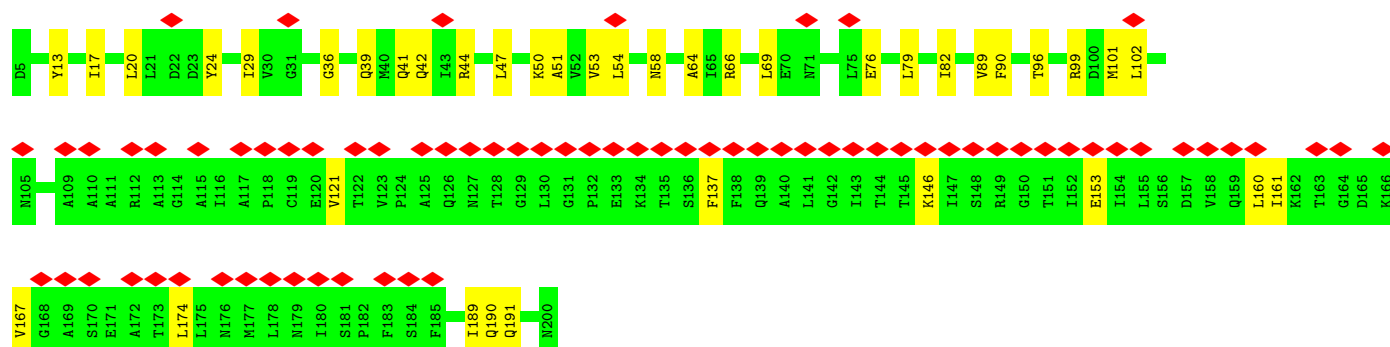
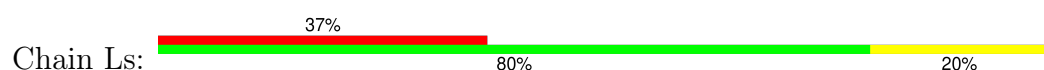
- Molecule 80: 60S ribosomal protein L37a



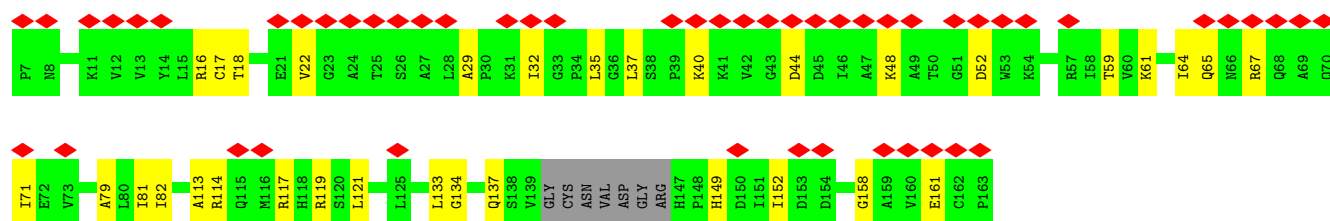
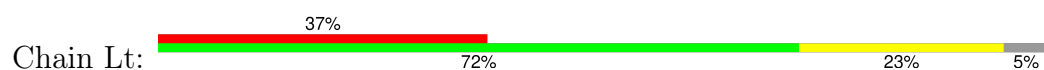
- Molecule 81: 60S ribosomal protein L28



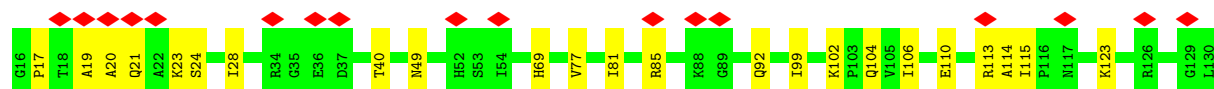
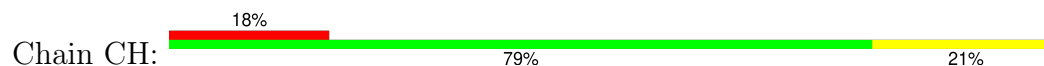
- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: Large ribosomal subunit protein uL11



- Molecule 84: Endothelial differentiation-related factor 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36954	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)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0126	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 [i](#)

5.1 Standard geometry [i](#)

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

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	AP	0.15	0/1692	0.24	0/2634
2	PE	0.21	0/1778	0.31	0/2767
3	SD	0.19	0/1793	0.31	0/2414
4	SF	0.19	0/1516	0.38	0/2037
5	SK	0.20	0/851	0.42	0/1147
6	SM	0.15	0/950	0.39	0/1275
7	SP	0.18	0/1065	0.31	0/1423
8	SQ	0.18	0/1160	0.37	0/1553
9	SR	0.25	0/1105	0.50	0/1484
10	SS	0.19	0/1216	0.36	0/1628
11	ST	0.18	0/1131	0.32	0/1515
12	SU	0.19	0/831	0.40	0/1115
13	SZ	0.19	0/604	0.38	0/810
14	Sc	0.19	0/508	0.34	0/680
15	Sd	0.21	0/470	0.32	0/623
16	Sf	0.19	0/560	0.44	0/745
17	Sg	0.16	0/2493	0.40	0/3394
18	SA	0.22	0/1778	0.36	0/2416
19	SB	0.21	0/1765	0.38	0/2362
20	SC	0.23	0/1744	0.39	0/2357
21	SE	0.18	0/2118	0.36	0/2849
22	SG	0.16	0/1946	0.32	0/2590
23	SH	0.17	0/1519	0.37	0/2033
24	SI	0.19	0/1715	0.36	0/2287
25	SJ	0.16	0/1550	0.32	0/2069
26	SL	0.20	0/1268	0.30	0/1696
27	SN	0.21	0/1232	0.32	0/1656
28	SO	0.24	0/1037	0.41	0/1391
29	SV	0.18	0/643	0.30	0/860
30	SW	0.23	0/1051	0.37	0/1406
31	SX	0.22	0/1116	0.39	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SY	0.17	0/1083	0.36	0/1438
33	Sa	0.25	0/836	0.39	0/1121
34	Sb	0.19	0/665	0.32	0/891
35	S2	0.25	0/39756	0.28	0/61939
36	LR	0.29	0/1582	0.40	0/2091
37	LW	0.23	0/959	0.31	0/1270
38	CI	0.16	0/247	0.27	0/323
39	L5	0.34	0/85098	0.32	0/132762
40	L7	0.33	0/2861	0.27	0/4459
41	L8	0.34	0/3631	0.29	0/5657
42	LA	0.34	0/1936	0.44	0/2596
43	LB	0.31	0/3306	0.40	0/4424
44	LC	0.32	0/2981	0.38	0/4002
45	LD	0.26	0/2428	0.35	0/3252
46	LE	0.25	0/1973	0.40	0/2645
47	LF	0.32	0/1905	0.34	0/2539
48	LG	0.26	0/1960	0.37	0/2637
49	LH	0.27	0/1537	0.38	0/2066
50	LI	0.28	0/1751	0.32	0/2340
51	LJ	0.24	0/1385	0.39	0/1852
52	LL	0.27	0/1732	0.34	0/2315
53	LM	0.29	0/1161	0.39	0/1554
54	LN	0.33	0/1746	0.36	0/2338
55	LO	0.32	0/1682	0.37	0/2250
56	LP	0.33	0/1268	0.43	0/1701
57	LQ	0.32	0/1537	0.37	0/2052
58	LS	0.31	0/1493	0.36	0/2003
59	LT	0.29	0/1326	0.33	0/1770
60	LU	0.25	0/839	0.48	0/1126
61	LV	0.30	0/993	0.39	0/1332
62	LX	0.28	0/1002	0.34	0/1345
63	LY	0.28	0/1132	0.36	0/1504
64	LZ	0.27	0/1130	0.34	0/1507
65	La	0.31	0/1191	0.34	0/1591
66	Lb	0.24	0/889	0.41	0/1175
67	Lc	0.27	0/774	0.39	0/1038
68	Ld	0.30	0/903	0.38	0/1216
69	Le	0.34	0/1071	0.36	0/1429
70	Lf	0.33	0/895	0.37	0/1198
71	Lg	0.30	0/916	0.35	0/1220
72	Lh	0.27	0/1023	0.38	0/1351
73	Li	0.24	0/843	0.32	0/1115
74	Lj	0.34	0/720	0.42	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lk	0.24	0/575	0.34	0/761
76	Ll	0.30	0/454	0.28	0/599
77	Lm	0.27	0/435	0.35	0/575
78	Ln	0.23	0/231	0.32	0/294
79	Lo	0.30	0/876	0.34	0/1156
80	Lp	0.30	0/718	0.38	0/953
81	Lr	0.31	0/1017	0.36	0/1364
82	Ls	0.14	0/1519	0.38	0/2052
83	Lt	0.16	0/1009	0.45	0/1363
84	CH	0.16	0/1028	0.40	0/1376
All	All	0.29	0/232213	0.33	0/340585

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
9	SR	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	SR	81	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	AP	1514	0	770	22	0
2	PE	1593	0	810	23	0
3	SD	1765	0	1865	28	0
4	SF	1495	0	1549	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	SK	827	0	854	14	0
6	SM	940	0	965	11	0
7	SP	1045	0	1095	20	0
8	SQ	1142	0	1213	21	0
9	SR	1090	0	1149	21	0
10	SS	1198	0	1261	29	0
11	ST	1112	0	1146	18	0
12	SU	821	0	883	18	0
13	SZ	598	0	656	17	0
14	Sc	506	0	536	8	0
15	Sd	459	0	452	5	0
16	Sf	548	0	551	9	0
17	Sg	2436	0	2393	55	0
18	SA	1741	0	1746	26	0
19	SB	1738	0	1809	25	0
20	SC	1707	0	1791	23	0
21	SE	2076	0	2177	52	0
22	SG	1923	0	2089	41	0
23	SH	1497	0	1590	36	0
24	SI	1686	0	1772	31	0
25	SJ	1525	0	1640	25	0
26	SL	1247	0	1323	18	0
27	SN	1208	0	1294	19	0
28	SO	1024	0	1050	16	0
29	SV	636	0	637	11	0
30	SW	1034	0	1080	19	0
31	SX	1098	0	1167	16	0
32	SY	1065	0	1142	20	0
33	Sa	821	0	870	14	0
34	Sb	651	0	672	14	0
35	S2	36952	0	18678	412	0
36	LR	1566	0	1729	13	0
37	LW	945	0	1003	15	0
38	CI	247	0	283	2	0
39	L5	78444	0	39719	673	0
40	L7	2561	0	1295	13	0
41	L8	3315	0	1685	23	0
42	LA	1898	0	1993	41	0
43	LB	3238	0	3376	61	0
44	LC	2927	0	3104	37	0
45	LD	2382	0	2410	33	0
46	LE	1935	0	2096	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	LF	1870	0	1996	19	0
48	LG	1927	0	2074	19	0
49	LH	1518	0	1601	20	0
50	LI	1711	0	1749	22	0
51	LJ	1362	0	1399	15	0
52	LL	1701	0	1818	20	0
53	LM	1138	0	1204	16	0
54	LN	1701	0	1749	19	0
55	LO	1650	0	1794	29	0
56	LP	1242	0	1269	15	0
57	LQ	1513	0	1628	14	0
58	LS	1453	0	1490	12	0
59	LT	1298	0	1366	16	0
60	LU	825	0	850	13	0
61	LV	979	0	1039	9	0
62	LX	985	0	1066	8	0
63	LY	1115	0	1205	14	0
64	LZ	1107	0	1182	11	0
65	La	1162	0	1213	9	0
66	Lb	876	0	948	10	0
67	Lc	764	0	804	13	0
68	Ld	888	0	930	11	0
69	Le	1053	0	1147	9	0
70	Lf	876	0	912	3	0
71	Lg	906	0	998	6	0
72	Lh	1015	0	1148	14	0
73	Li	832	0	917	5	0
74	Lj	705	0	737	9	0
75	Lk	569	0	637	8	0
76	Ll	444	0	483	7	0
77	Lm	429	0	465	4	0
78	Ln	230	0	276	3	0
79	Lo	862	0	929	12	0
80	Lp	708	0	756	7	0
81	Lr	1002	0	1068	10	0
82	Ls	1496	0	1540	26	0
83	Lt	998	0	1032	25	0
84	CH	1018	0	1064	20	0
85	L5	178	0	0	0	0
85	L7	3	0	0	0	0
85	L8	4	0	0	0	0
85	LA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	LB	1	0	0	0	0
85	LI	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	25	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	3	0
88	L8	10	0	19	0	0
88	LN	10	0	19	0	0
All	All	220526	0	164223	2225	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 (2225) 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)
39:L5:1095:A:H2	39:L5:1200:G:N1	1.45	1.15
39:L5:1095:A:C2	39:L5:1200:G:N1	2.19	1.05
2:PE:26:A:H61	2:PE:44:G:H1	1.06	0.91
39:L5:1100:U:H3	39:L5:1194:G:H1	1.23	0.87
35:S2:1815:A:H8	39:L5:3806:G:H21	1.21	0.83
35:S2:1729:U:H3	35:S2:1805:G:H1	1.25	0.83
19:SB:103:MET:HG3	19:SB:215:VAL:HG12	1.60	0.82
35:S2:1033:G:H1	35:S2:1080:A:HO2'	1.26	0.82
1:AP:50:U:H3	1:AP:64:G:H1	1.27	0.81
2:PE:26:A:N6	2:PE:44:G:H1	1.79	0.80
35:S2:1812:U:H2'	35:S2:1813:A:H8	1.47	0.79
4:SF:140:ASP:HB2	14:Sc:46:VAL:HG12	1.64	0.79
35:S2:1722:G:H2'	35:S2:1723:G:H8	1.47	0.79
14:Sc:44:ARG:HH12	14:Sc:63:ARG:HH11	1.31	0.79
39:L5:3773:U:H3	39:L5:3775:A:H62	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1656:G:H1	35:S2:1668:U:H3	1.32	0.77
49:LH:106:GLN:HB2	49:LH:111:LEU:HB3	1.67	0.77
17:Sg:87:LEU:HB2	17:Sg:101:PHE:HB2	1.67	0.77
16:Sf:126:CYS:SG	16:Sf:144:CYS:N	2.57	0.76
83:Lt:65:GLN:HG3	83:Lt:67:ARG:H	1.53	0.74
1:AP:18:G:O2'	1:AP:57:G:N2	2.21	0.73
35:S2:1748:G:H1	35:S2:1786:U:H3	1.37	0.73
50:LI:36:LEU:HD11	50:LI:69:ARG:HH11	1.53	0.73
22:SG:13:GLN:NE2	35:S2:153:G:N3	2.37	0.73
24:SI:98:LYS:HB3	35:S2:377:G:H5'	1.70	0.73
39:L5:4775:C:H41	39:L5:4859:C:H42	1.37	0.72
42:LA:28:ARG:HD2	42:LA:123:ARG:HG3	1.71	0.72
39:L5:1095:A:N1	39:L5:1200:G:O6	2.23	0.72
39:L5:2611:A:H5'	39:L5:2688:G:H4'	1.72	0.72
39:L5:4897:G:N2	39:L5:4924:C:O2	2.22	0.72
35:S2:925:G:H1	35:S2:1017:U:H3	1.37	0.71
17:Sg:107:ASP:HB2	17:Sg:125:ARG:HD2	1.71	0.71
39:L5:2520:C:O2	39:L5:2640:G:N2	2.23	0.71
39:L5:2601:A:N6	39:L5:2744:A:OP2	2.24	0.71
35:S2:1722:G:H2'	35:S2:1723:G:C8	2.26	0.71
57:LQ:68:ARG:HA	57:LQ:71:LYS:HE3	1.72	0.71
34:Sb:11:SER:OG	34:Sb:14:GLU:OE1	2.08	0.71
39:L5:3701:OMC:H5	39:L5:3748:A:H62	1.35	0.71
2:PE:14:A:H61	2:PE:21:A:H2	1.39	0.70
39:L5:387:G:HO2'	39:L5:412:G:H1	1.39	0.70
12:SU:49:LYS:HB3	12:SU:92:HIS:HB2	1.74	0.70
30:SW:2:VAL:N	35:S2:1091:C:HO2'	1.88	0.70
21:SE:211:LYS:HE2	21:SE:215:GLY:HA2	1.74	0.70
39:L5:497:G:H21	39:L5:498:C:H41	1.37	0.69
39:L5:2092:G:O2'	39:L5:2262:G:N2	2.26	0.69
39:L5:1414:C:H2'	39:L5:1415:G:H8	1.56	0.69
39:L5:3773:U:O4	39:L5:3775:A:N7	2.26	0.69
39:L5:1994:C:H2'	39:L5:1995:G:H8	1.58	0.69
42:LA:54:ARG:HH11	42:LA:58:LEU:HD21	1.58	0.69
83:Lt:117:ARG:HH12	83:Lt:121:LEU:HD13	1.56	0.69
22:SG:2:LYS:HB2	22:SG:108:VAL:HG12	1.74	0.69
51:LJ:112:HIS:ND1	51:LJ:125:ILE:O	2.25	0.69
83:Lt:16:ARG:HE	83:Lt:17:CYS:H	1.41	0.68
39:L5:171:U:H4'	52:LL:135:LYS:HG2	1.75	0.68
18:SA:77:ILE:HD11	18:SA:124:VAL:HG22	1.76	0.68
21:SE:173:ILE:HG21	21:SE:227:VAL:HG11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SE:125:LYS:HB3	21:SE:142:HIS:HB3	1.75	0.68
21:SE:127:ARG:HG3	21:SE:142:HIS:HA	1.76	0.68
20:SC:66:LEU:HD11	20:SC:81:ILE:HD12	1.75	0.67
35:S2:1752:C:N3	35:S2:1779:G:N1	2.39	0.67
39:L5:4623:OMG:OP1	43:LB:19:ARG:NH2	2.27	0.67
84:CH:17:PRO:HG2	84:CH:21:GLN:HB2	1.74	0.67
24:SI:31:ARG:HH12	24:SI:48:VAL:HG12	1.58	0.67
39:L5:1997:U:H4'	82:Ls:44:ARG:HH12	1.59	0.67
5:SK:24:LYS:O	5:SK:42:ASN:ND2	2.28	0.67
6:SM:89:VAL:HG21	6:SM:109:VAL:HG11	1.76	0.67
32:SY:10:ARG:HG3	32:SY:24:VAL:HG23	1.77	0.67
21:SE:45:ILE:HA	21:SE:61:VAL:HG11	1.77	0.67
22:SG:162:LEU:HD11	22:SG:170:ARG:HG2	1.77	0.67
35:S2:1658:G:OP2	35:S2:1660:C:N4	2.27	0.67
18:SA:70:ASN:HB3	18:SA:73:ASP:HB2	1.77	0.66
23:SH:31:GLU:HA	23:SH:37:LYS:HG3	1.76	0.66
82:Ls:53:VAL:HG12	82:Ls:89:VAL:HG22	1.77	0.66
18:SA:163:CYS:SG	18:SA:164:ASN:N	2.69	0.66
39:L5:3680:U:OP1	42:LA:54:ARG:NH2	2.29	0.66
35:S2:557:U:H2'	35:S2:558:G:C8	2.31	0.66
39:L5:1932:A:OP1	55:LO:49:ARG:NH2	2.28	0.66
35:S2:928:G:H2'	35:S2:929:G:C8	2.30	0.66
39:L5:1402:C:N3	39:L5:1415:G:N1	2.31	0.66
7:SP:111:MET:HA	10:SS:117:ILE:HD11	1.78	0.65
23:SH:17:ASP:HB2	23:SH:20:GLU:HB3	1.79	0.65
21:SE:31:PRO:HA	21:SE:81:THR:HB	1.77	0.65
23:SH:34:SER:O	23:SH:78:ARG:NH2	2.29	0.65
48:LG:167:VAL:HG12	48:LG:170:LEU:HD12	1.78	0.65
53:LM:15:VAL:HG22	53:LM:50:MET:HE1	1.79	0.65
50:LI:56:GLU:HG3	50:LI:161:GLY:HA3	1.79	0.65
17:Sg:157:SER:HB3	17:Sg:164:ILE:HG22	1.78	0.65
3:SD:67:ARG:HD3	5:SK:96:ARG:HG2	1.79	0.65
25:SJ:177:ASN:ND2	35:S2:560:A:OP2	2.29	0.65
27:SN:103:GLU:O	27:SN:106:ARG:NH1	2.29	0.65
39:L5:2486:G:O6	39:L5:2493:G:O6	2.15	0.65
39:L5:919:C:OP1	53:LM:69:HIS:ND1	2.30	0.65
21:SE:38:LEU:HD22	35:S2:346:C:H5''	1.78	0.65
39:L5:137:G:H2'	39:L5:138:G:H8	1.62	0.65
39:L5:2458:C:H5''	54:LN:67:ARG:HD2	1.79	0.65
1:AP:21:A:H61	1:AP:46:G:H2'	1.61	0.65
10:SS:63:GLU:HG2	10:SS:66:ARG:HH21	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SX:100:VAL:HG12	31:SX:125:VAL:HG22	1.78	0.64
39:L5:2083:C:OP2	57:LQ:14:ARG:NH2	2.31	0.64
39:L5:2557:G:H1	39:L5:2570:U:H3	1.44	0.64
3:SD:42:THR:OG1	3:SD:45:ARG:O	2.15	0.64
35:S2:106:C:H2'	35:S2:107:A:H8	1.61	0.64
18:SA:207:PRO:HA	18:SA:210:ILE:HG22	1.78	0.64
26:SL:35:ARG:NH2	26:SL:55:TYR:O	2.31	0.64
39:L5:1669:A:OP1	66:Lb:18:ARG:NH2	2.30	0.64
21:SE:128:LYS:HG2	21:SE:140:VAL:HB	1.78	0.64
22:SG:137:ARG:HB3	22:SG:140:ARG:HG2	1.78	0.64
35:S2:1228:A:H2'	35:S2:1229:G:C8	2.31	0.64
35:S2:1277:C:H2'	35:S2:1278:A:H8	1.61	0.64
45:LD:272:SER:HB3	45:LD:275:GLN:HG3	1.79	0.64
39:L5:3949:A:OP1	39:L5:4065:G:N2	2.30	0.64
83:Lt:37:LEU:HA	83:Lt:40:LYS:HE3	1.79	0.64
9:SR:100:PRO:HG2	9:SR:122:PRO:HD3	1.80	0.64
49:LH:95:VAL:HG12	77:Lm:82:LEU:HD13	1.79	0.64
39:L5:2351:OMC:HM22	44:LC:95:MET:HG3	1.80	0.64
39:L5:4472:G:O2'	77:Lm:100:TYR:O	2.16	0.64
29:SV:14:PRO:HG2	29:SV:23:ILE:HD12	1.79	0.64
35:S2:885:U:O2	35:S2:901:G:O6	2.15	0.64
36:LR:108:ARG:NH2	39:L5:2899:C:OP1	2.31	0.63
39:L5:268:G:H2'	39:L5:269:G:H8	1.64	0.63
39:L5:3697:U:H5''	39:L5:3698:G:H5'	1.80	0.63
42:LA:29:LEU:O	42:LA:123:ARG:NH1	2.27	0.63
26:SL:42:LEU:HD13	26:SL:72:ILE:HD11	1.80	0.63
44:LC:110:ARG:HB2	54:LN:204:ARG:HH21	1.64	0.63
5:SK:80:ARG:HH11	5:SK:87:PRO:HA	1.63	0.63
39:L5:1974:U:H4'	39:L5:1975:G:H3'	1.81	0.63
55:LO:81:TRP:HB2	55:LO:104:VAL:HG21	1.79	0.63
18:SA:77:ILE:HG22	18:SA:99:ILE:HB	1.81	0.63
39:L5:2695:A:OP1	75:Lk:35:LYS:NZ	2.30	0.63
35:S2:1536:G:H2'	35:S2:1537:A:H8	1.64	0.63
39:L5:1095:A:H2	39:L5:1200:G:H1	0.69	0.63
41:L8:75:OMG:OP2	63:LY:74:TYR:OH	2.17	0.63
21:SE:192:ILE:HG12	21:SE:243:GLY:HA3	1.81	0.62
31:SX:68:LYS:NZ	35:S2:616:A:OP1	2.32	0.62
39:L5:2658:G:N2	39:L5:2676:A:OP2	2.32	0.62
39:L5:4092:G:N7	39:L5:4114:C:N4	2.48	0.62
39:L5:184:U:O2	39:L5:253:G:N2	2.31	0.62
42:LA:147:ARG:HG2	42:LA:157:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SZ:96:LEU:HD12	13:SZ:97:ILE:HG12	1.81	0.62
36:LR:173:ARG:HG2	36:LR:176:ARG:HH12	1.63	0.62
48:LG:106:THR:OG1	48:LG:109:GLU:OE1	2.17	0.62
55:LO:34:VAL:HG22	55:LO:103:LYS:HB2	1.82	0.62
39:L5:513:U:N3	39:L5:516:C:OP2	2.28	0.62
39:L5:3811:G:O2'	39:L5:3814:U:OP2	2.16	0.62
39:L5:4094:G:N2	39:L5:4115:G:OP2	2.31	0.62
46:LE:281:ILE:HD12	46:LE:286:LEU:HD11	1.81	0.62
22:SG:131:ARG:HB2	37:LW:82:ILE:HG22	1.82	0.62
22:SG:133:LEU:HD12	35:S2:65:C:C4	2.35	0.62
25:SJ:121:LYS:HD2	35:S2:527:C:H4'	1.80	0.62
25:SJ:132:GLN:OE1	35:S2:562:U:O2'	2.17	0.62
45:LD:280:VAL:HG23	50:LI:206:LEU:HD11	1.80	0.62
82:Ls:47:LEU:HD23	82:Ls:51:ALA:HB3	1.82	0.62
5:SK:21:MET:HG2	5:SK:49:MET:HE3	1.82	0.62
50:LI:87:MET:HG2	50:LI:138:ILE:HG12	1.82	0.62
39:L5:4927:G:H5''	39:L5:4928:C:H5	1.65	0.62
81:Lr:26:SER:OG	81:Lr:28:GLU:OE1	2.16	0.62
3:SD:172:VAL:HG22	3:SD:185:LYS:HG2	1.81	0.62
35:S2:1228:A:H2'	35:S2:1229:G:H8	1.65	0.62
39:L5:67:C:OP2	39:L5:312:G:N2	2.33	0.62
15:Sd:8:TRP:HZ3	35:S2:1512:C:H5''	1.65	0.62
17:Sg:176:VAL:HG23	17:Sg:185:LYS:HB2	1.82	0.62
35:S2:329:G:H2'	35:S2:330:G:H8	1.64	0.62
39:L5:4281:A:H2'	39:L5:4282:A:H2'	1.81	0.62
55:LO:37:ARG:HD2	55:LO:108:ILE:HD11	1.81	0.61
67:Lc:20:LEU:O	67:Lc:24:SER:OG	2.14	0.61
39:L5:2295:C:O2'	44:LC:45:ARG:NH2	2.32	0.61
39:L5:4251:A:H5''	51:LJ:108:GLY:HA3	1.81	0.61
84:CH:23:LYS:HG3	84:CH:28:ILE:HD11	1.82	0.61
18:SA:30:LEU:HD21	18:SA:35:GLU:HG2	1.81	0.61
21:SE:144:ALA:HB3	35:S2:121:OMU:HM23	1.83	0.61
35:S2:165:G:OP2	35:S2:165:G:N2	2.31	0.61
39:L5:3641:U:OP2	39:L5:3646:A:N6	2.33	0.61
39:L5:4221:C:OP1	87:L5:5263:SPM:N14	2.33	0.61
35:S2:1812:U:H2'	35:S2:1813:A:C8	2.31	0.61
39:L5:1499:C:OP1	57:LQ:150:ARG:NH2	2.34	0.61
42:LA:107:MET:HB3	42:LA:111:THR:HG21	1.82	0.61
20:SC:166:ARG:HD3	20:SC:181:PRO:HG3	1.83	0.61
82:Ls:102:LEU:HD21	82:Ls:189:ILE:HD11	1.83	0.61
17:Sg:4:GLN:H	17:Sg:313:THR:HG22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Sg:208:ALA:HB2	17:Sg:218:LEU:HD13	1.82	0.61
35:S2:1777:G:H2'	35:S2:1778:C:H6	1.65	0.61
66:Lb:102:PRO:HA	66:Lb:109:ARG:HH22	1.66	0.61
76:Ll:9:ILE:HD12	76:Ll:51:LEU:HD11	1.81	0.61
39:L5:3710:G:O2'	39:L5:3712:A:OP2	2.19	0.61
39:L5:4992:G:H2'	39:L5:4993:G:C8	2.36	0.61
20:SC:173:LYS:HD3	29:SV:3:ASN:HA	1.81	0.61
32:SY:9:THR:HG22	32:SY:25:ILE:HG22	1.82	0.61
39:L5:5016:A:C2	39:L5:5033:G:N2	2.66	0.61
37:LW:52:THR:HG22	37:LW:54:LEU:H	1.65	0.60
39:L5:3633:C:OP1	87:L5:5291:SPM:N10	2.30	0.60
39:L5:4100:C:OP2	39:L5:4101:C:N4	2.34	0.60
50:LI:48:LEU:HB2	50:LI:142:LEU:HD23	1.83	0.60
83:Lt:81:ILE:HD12	83:Lt:113:ALA:HB1	1.83	0.60
1:AP:29:C:H2'	1:AP:30:G:H8	1.66	0.60
39:L5:3717:A:H2'	39:L5:3718:A2M:H8	1.83	0.60
67:Lc:99:PRO:HG3	67:Lc:104:ILE:HG12	1.82	0.60
14:Sc:7:GLN:HE22	14:Sc:10:LYS:HD3	1.66	0.60
18:SA:7:VAL:HG13	18:SA:8:LEU:HD12	1.83	0.60
20:SC:210:PRO:HD3	20:SC:236:PHE:CE2	2.37	0.60
35:S2:150:A:N6	35:S2:168:C:O2	2.35	0.60
24:SI:87:ASN:HB3	24:SI:90:LEU:HD23	1.82	0.60
3:SD:38:GLU:HG2	3:SD:49:ILE:HB	1.83	0.60
39:L5:1645:C:OP1	44:LC:80:ARG:NH2	2.30	0.60
39:L5:4076:G:OP1	48:LG:73:ARG:NE	2.35	0.60
63:LY:22:PRO:HD2	63:LY:25:ILE:HD11	1.82	0.60
32:SY:14:THR:HG23	32:SY:21:LYS:HG2	1.84	0.60
39:L5:1269:G:O2'	39:L5:1440:U:O2'	2.20	0.60
39:L5:1975:G:N2	39:L5:1983:A:OP1	2.35	0.60
23:SH:53:VAL:HG11	23:SH:172:THR:HA	1.82	0.60
39:L5:1175:A:H2	39:L5:1185:G:H1	1.49	0.60
57:LQ:70:MET:HE1	57:LQ:137:VAL:HB	1.84	0.60
31:SX:28:LYS:HE2	31:SX:32:LEU:HD11	1.83	0.60
35:S2:981:A:H2'	35:S2:982:G:C8	2.37	0.60
35:S2:1130:G:OP2	35:S2:1130:G:N2	2.32	0.60
39:L5:1095:A:H2	39:L5:1200:G:C2	2.18	0.60
39:L5:1404:G:O6	39:L5:1413:C:N4	2.35	0.60
51:LJ:141:ILE:HA	51:LJ:144:LYS:HG2	1.83	0.60
61:LV:13:LYS:HD3	61:LV:128:LEU:HD22	1.84	0.59
63:LY:4:ASN:HB3	63:LY:7:VAL:HG12	1.82	0.59
3:SD:18:LYS:HE3	3:SD:39:VAL:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:1100:U:O4	39:L5:1194:G:O6	2.20	0.59
39:L5:1402:C:O2	39:L5:1415:G:N2	2.18	0.59
82:Ls:24:TYR:HB2	82:Ls:90:PHE:HB3	1.84	0.59
21:SE:62:LYS:HA	21:SE:80:ILE:HD11	1.84	0.59
39:L5:664:G:N2	39:L5:666:G:O6	2.35	0.59
17:Sg:89:LEU:HB2	17:Sg:101:PHE:HE1	1.65	0.59
39:L5:1697:G:H22	39:L5:2084:C:P	2.26	0.59
39:L5:4910:G:N2	55:LO:106:ASP:O	2.36	0.59
53:LM:119:ARG:HG3	55:LO:189:ILE:HG23	1.85	0.59
82:Ls:20:LEU:HD12	82:Ls:54:LEU:HD22	1.84	0.59
13:SZ:99:LEU:HD11	13:SZ:102:LYS:HB2	1.85	0.59
24:SI:22:HIS:HB3	35:S2:433:A:H5''	1.84	0.59
36:LR:44:LEU:HD22	36:LR:49:LEU:HD12	1.85	0.59
7:SP:130:ARG:HD3	7:SP:131:PRO:HD2	1.85	0.59
39:L5:1700:G:H5''	39:L5:1704:C:H42	1.67	0.59
39:L5:3868:G:H22	39:L5:3900:G:H1'	1.67	0.59
24:SI:10:LYS:NZ	35:S2:370:G:O2'	2.36	0.59
24:SI:149:TYR:HB3	24:SI:153:LYS:HZ3	1.68	0.59
35:S2:1536:G:H2'	35:S2:1537:A:C8	2.38	0.59
43:LB:222:VAL:O	43:LB:343:ARG:NH1	2.36	0.59
31:SX:17:ARG:NH2	35:S2:658:U:O2	2.36	0.59
35:S2:549:C:H4'	84:CH:19:ALA:H	1.67	0.59
39:L5:4615:C:H5''	43:LB:357:ARG:HD2	1.85	0.59
60:LU:46:ARG:HH22	60:LU:89:LYS:HE2	1.67	0.59
17:Sg:132:TRP:CD1	17:Sg:138:CYS:HA	2.38	0.59
20:SC:65:LYS:HD2	20:SC:273:LEU:HD13	1.84	0.58
39:L5:1972:G:H2'	39:L5:1973:G:C8	2.38	0.58
46:LE:223:ARG:NH2	46:LE:236:GLU:O	2.36	0.58
3:SD:54:ARG:HH22	3:SD:56:GLN:HB3	1.68	0.58
17:Sg:24:THR:HG22	17:Sg:26:GLN:H	1.67	0.58
26:SL:75:GLY:HA3	26:SL:88:ILE:HD12	1.84	0.58
40:L7:7:G:OP1	45:LD:33:ARG:NH1	2.36	0.58
42:LA:114:CYS:HB3	42:LA:165:VAL:HB	1.84	0.58
43:LB:107:ALA:HB2	43:LB:201:LEU:HD22	1.85	0.58
2:PE:16:C:O2'	2:PE:19:G:OP2	2.21	0.58
6:SM:33:ARG:HD2	6:SM:91:LEU:HD11	1.85	0.58
19:SB:222:LYS:NZ	19:SB:224:GLU:OE1	2.36	0.58
35:S2:928:G:H1	35:S2:1013:U:H3	1.50	0.58
39:L5:1994:C:H2'	39:L5:1995:G:C8	2.38	0.58
46:LE:243:THR:HG22	46:LE:245:GLN:H	1.68	0.58
52:LL:64:VAL:HA	52:LL:67:HIS:CD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:LN:159:ARG:HB3	54:LN:164:LEU:HB2	1.84	0.58
35:S2:1417:C:H42	35:S2:1422:G:H22	1.51	0.58
41:L8:52:A:H5'	76:L1:21:ARG:HD3	1.86	0.58
45:LD:223:PHE:HB3	45:LD:226:TYR:HB2	1.85	0.58
20:SC:193:VAL:HG11	20:SC:240:THR:HG22	1.85	0.58
35:S2:207:G:H3'	35:S2:208:G:H8	1.68	0.58
39:L5:1095:A:N1	39:L5:1200:G:C6	2.71	0.58
35:S2:1550:G:H3'	35:S2:1579:A:H61	1.68	0.58
39:L5:369:G:N2	39:L5:372:A:OP2	2.33	0.58
39:L5:1176:C:H42	39:L5:1184:A:H61	1.52	0.58
53:LM:36:ALA:HB3	53:LM:55:MET:HE1	1.84	0.58
4:SF:88:MET:HG3	4:SF:91:ARG:HH21	1.69	0.58
39:L5:382:G:N1	39:L5:385:A:OP2	2.36	0.58
39:L5:2108:G:H2'	39:L5:2109:G:H8	1.69	0.58
39:L5:4322:G:N2	39:L5:4325:A:OP2	2.35	0.58
58:LS:76:LYS:NZ	58:LS:100:LEU:O	2.36	0.58
18:SA:141:ASN:ND2	29:SV:31:SER:O	2.29	0.58
27:SN:99:ARG:NH2	27:SN:119:GLU:OE2	2.37	0.58
22:SG:66:GLY:HA2	35:S2:1745:A:H1'	1.85	0.58
39:L5:1281:G:N1	46:LE:128:HIS:HB2	2.19	0.58
5:SK:41:PRO:HG2	5:SK:44:HIS:HD2	1.69	0.57
17:Sg:88:ARG:HH11	17:Sg:97:THR:HG21	1.68	0.57
20:SC:183:LYS:HA	20:SC:195:LEU:O	2.04	0.57
24:SI:75:LYS:HD2	35:S2:303:C:H5'	1.85	0.57
39:L5:4260:U:H2'	39:L5:4261:C:C6	2.39	0.57
84:CH:92:GLN:NE2	84:CH:110:GLU:OE1	2.34	0.57
12:SU:55:ARG:HG2	12:SU:87:ARG:HD2	1.86	0.57
39:L5:2568:C:H2'	39:L5:2569:G:H8	1.68	0.57
43:LB:219:VAL:HG11	43:LB:337:VAL:HG13	1.85	0.57
30:SW:32:LYS:O	30:SW:36:ARG:HG2	2.03	0.57
39:L5:2579:G:N2	39:L5:2582:A:OP2	2.32	0.57
39:L5:3946:G:H1	39:L5:4067:U:H3	1.50	0.57
67:Lc:17:ARG:HD2	67:Lc:103:ASP:HA	1.86	0.57
19:SB:85:LYS:HB2	19:SB:101:HIS:HB3	1.85	0.57
25:SJ:30:LYS:NZ	84:CH:40:THR:OG1	2.38	0.57
39:L5:665:C:H4'	39:L5:666:G:H5'	1.85	0.57
68:Ld:19:GLU:OE2	68:Ld:92:ARG:NH1	2.37	0.57
72:Lh:99:GLU:HA	72:Lh:102:LEU:HD22	1.87	0.57
17:Sg:68:ASP:HB3	17:Sg:111:VAL:HG22	1.86	0.57
34:Sb:33:MET:HE2	34:Sb:48:SER:HA	1.86	0.57
20:SC:191:VAL:HG11	20:SC:236:PHE:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:SC:210:PRO:HB3	20:SC:240:THR:HG21	1.87	0.57
25:SJ:160:SER:O	25:SJ:163:SER:OG	2.21	0.57
35:S2:969:U:O2	35:S2:971:G:N1	2.38	0.57
35:S2:1722:G:H22	35:S2:1813:A:H1'	1.70	0.57
35:S2:1776:G:N2	35:S2:1776:G:OP2	2.38	0.57
35:S2:1811:C:H2'	35:S2:1812:U:O4'	2.05	0.57
39:L5:2407:G:O6	76:Ll:2:SER:N	2.38	0.57
49:LH:44:GLU:HG3	53:LM:2:VAL:HG12	1.86	0.57
52:LL:80:GLU:HG3	52:LL:110:LEU:HD12	1.87	0.57
67:Lc:51:ASN:HB2	67:Lc:77:ASN:HB2	1.87	0.57
35:S2:864:A:H2'	35:S2:865:A:H8	1.69	0.57
39:L5:1489:G:H5'	65:La:131:ARG:HH12	1.69	0.57
82:Ls:29:ILE:HG12	82:Ls:191:GLN:HG2	1.86	0.57
1:AP:18:G:O6	1:AP:55:U:O2	2.22	0.57
35:S2:64:A:N6	35:S2:83:A:OP2	2.38	0.57
39:L5:3599:A:H2'	39:L5:3600:G:C8	2.40	0.57
43:LB:50:LYS:HB2	43:LB:345:LEU:HD11	1.87	0.57
49:LH:106:GLN:HG3	49:LH:111:LEU:HD23	1.85	0.57
79:Lo:33:LEU:HA	79:Lo:38:LYS:HG2	1.85	0.57
82:Ls:76:GLU:HA	82:Ls:79:LEU:HD13	1.85	0.57
35:S2:328:U:H5	37:LW:116:LYS:HG2	1.68	0.57
35:S2:482:G:N2	35:S2:484:A2M:H3'	2.19	0.57
35:S2:628:A:N6	35:S2:1500:G:O2'	2.38	0.57
39:L5:1503:A:H62	57:LQ:87:THR:HG21	1.69	0.57
24:SI:27:TYR:HB3	24:SI:49:ARG:HH12	1.70	0.57
35:S2:186:C:H2'	35:S2:187:G:C8	2.40	0.57
35:S2:1764:G:H5'	35:S2:1765:C:H5''	1.87	0.57
39:L5:24:G:N7	74:Lj:46:LYS:NZ	2.53	0.57
39:L5:662:C:N4	39:L5:663:G:O6	2.38	0.57
46:LE:264:ILE:HD11	46:LE:267:LEU:HD22	1.86	0.57
35:S2:146:G:H1	35:S2:173:A:H61	1.53	0.56
37:LW:9:SER:HA	37:LW:52:THR:HG23	1.86	0.56
39:L5:178:C:N4	39:L5:179:G:O6	2.38	0.56
43:LB:117:ARG:HA	43:LB:177:LYS:HD2	1.87	0.56
51:LJ:29:SER:OG	51:LJ:67:LYS:O	2.22	0.56
35:S2:51:U:H2'	35:S2:52:G:C8	2.40	0.56
39:L5:2845:A:H61	39:L5:3843:C:H42	1.52	0.56
10:SS:129:LEU:HD23	10:SS:144:ARG:HH21	1.70	0.56
19:SB:57:ILE:HG22	19:SB:59:SER:H	1.70	0.56
28:SO:137:SER:O	35:S2:942:G:N2	2.33	0.56
35:S2:588:G:H4'	35:S2:589:G:H5'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:692:G:O6	35:S2:738:C:O2'	2.23	0.56
35:S2:830:A:OP2	35:S2:846:G:N2	2.37	0.56
39:L5:174:C:OP1	52:LL:129:ARG:NH2	2.38	0.56
39:L5:4076:G:H5'	48:LG:73:ARG:HG3	1.88	0.56
39:L5:4742:G:OP1	39:L5:4900:C:N4	2.38	0.56
55:LO:58:LEU:HD21	55:LO:74:ARG:HH21	1.70	0.56
30:SW:107:SER:HB2	35:S2:860:G:H21	1.69	0.56
39:L5:4594:U:H2'	39:L5:4595:G:H8	1.70	0.56
13:SZ:80:ARG:HD2	35:S2:1598:G:H3'	1.87	0.56
9:SR:97:GLU:HG3	9:SR:120:THR:HG21	1.85	0.56
35:S2:1354:G:N2	35:S2:1357:A:OP2	2.36	0.56
37:LW:2:LYS:NZ	61:LV:92:ASP:O	2.38	0.56
39:L5:2491:C:H2'	39:L5:2492:C:C6	2.40	0.56
45:LD:182:GLY:HA2	45:LD:194:VAL:HG23	1.87	0.56
56:LP:131:ARG:HG3	56:LP:137:ASN:OD1	2.06	0.56
82:Ls:17:ILE:HD11	82:Ls:64:ALA:HB3	1.88	0.56
26:SL:61:PRO:HB3	26:SL:68:ILE:HD11	1.88	0.56
39:L5:2484:A:N6	39:L5:2494:U:H3	2.04	0.56
15:Sd:38:MET:HE3	15:Sd:43:PHE:HA	1.88	0.56
20:SC:72:ASP:OD2	20:SC:272:HIS:NE2	2.28	0.56
39:L5:1094:G:O6	39:L5:1201:U:O2	2.24	0.56
39:L5:3774:A:H2'	39:L5:3775:A:C8	2.40	0.56
39:L5:4126:C:OP1	48:LG:37:LYS:NZ	2.39	0.56
44:LC:1:MET:O	44:LC:29:LYS:NZ	2.38	0.56
53:LM:50:MET:HE2	53:LM:55:MET:HG2	1.88	0.56
35:S2:51:U:H2'	35:S2:52:G:H8	1.70	0.56
35:S2:323:C:H2'	35:S2:327:G:H1	1.70	0.56
39:L5:1942:A:H2'	39:L5:1943:A:C8	2.40	0.56
39:L5:4431:PSU:OP2	50:LI:3:ARG:NH2	2.37	0.56
46:LE:190:HIS:HB3	46:LE:193:PHE:HD1	1.70	0.56
81:Lr:47:LYS:HB2	81:Lr:102:TYR:CZ	2.40	0.56
28:SO:134:PRO:HB3	35:S2:944:A:H5''	1.86	0.56
39:L5:1258:G:H2'	39:L5:1259:G:C8	2.41	0.56
39:L5:3717:A:H2'	39:L5:3718:A2M:C8	2.36	0.56
39:L5:3717:A:OP2	39:L5:3735:G:N2	2.38	0.56
39:L5:4279:A:H5'	39:L5:4281:A:H1'	1.88	0.56
3:SD:136:VAL:HG12	3:SD:186:VAL:HG22	1.87	0.55
5:SK:14:LEU:HD22	5:SK:35:LEU:HD23	1.87	0.55
13:SZ:68:ILE:HB	13:SZ:109:TYR:HB2	1.88	0.55
23:SH:42:GLU:HG2	23:SH:43:LEU:HD22	1.88	0.55
39:L5:109:G:OP2	52:LL:74:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:1339:U:H2'	39:L5:1340:OMC:C6	2.40	0.55
39:L5:4967:A:H2'	39:L5:4968:A:H8	1.71	0.55
41:L8:96:C:H5''	72:Lh:66:LYS:HG2	1.88	0.55
35:S2:329:G:H2'	35:S2:330:G:C8	2.40	0.55
35:S2:520:A:O2'	35:S2:825:A:N3	2.37	0.55
35:S2:640:A:H2'	35:S2:641:A:C8	2.41	0.55
39:L5:4340:U:O2	88:L5:5261:SPD:N10	2.39	0.55
39:L5:4478:G:O2'	39:L5:4602:A:N1	2.39	0.55
35:S2:907:G:H2'	35:S2:908:A:C8	2.41	0.55
39:L5:2846:G:O2'	61:LV:19:GLY:O	2.24	0.55
39:L5:3700:C:O2'	39:L5:3774:A:N3	2.38	0.55
39:L5:4967:A:H2'	39:L5:4968:A:C8	2.41	0.55
66:Lb:109:ARG:HA	66:Lb:112:ILE:HG12	1.88	0.55
22:SG:50:VAL:HG11	22:SG:111:LEU:HB3	1.89	0.55
82:Ls:96:THR:HG22	82:Ls:99:ARG:HH21	1.72	0.55
17:Sg:240:CYS:HG	17:Sg:291:TRP:CD1	2.25	0.55
39:L5:1480:C:O2'	39:L5:1482:G:OP2	2.24	0.55
39:L5:3898:G:H5'	43:LB:254:ILE:HG13	1.88	0.55
33:Sa:38:LYS:HD2	33:Sa:83:VAL:HG21	1.88	0.55
37:LW:2:LYS:HZ3	61:LV:92:ASP:HB2	1.71	0.55
39:L5:2489:C:H4'	39:L5:2491:C:H42	1.70	0.55
39:L5:5006:U:H4'	39:L5:5007:A:H5'	1.89	0.55
48:LG:38:ASN:ND2	48:LG:43:GLN:OE1	2.40	0.55
49:LH:12:ILE:HB	49:LH:53:LYS:HB2	1.89	0.55
10:SS:46:ARG:HG2	11:ST:35:ASP:HB2	1.89	0.55
19:SB:32:ASP:OD2	19:SB:94:LYS:NZ	2.38	0.55
35:S2:1030:A:H2'	35:S2:1031:A2M:H8	1.87	0.55
35:S2:1528:G:O2'	35:S2:1666:C:OP1	2.24	0.55
51:LJ:159:LYS:HG2	51:LJ:163:MET:HE2	1.88	0.55
62:LX:124:VAL:HG22	62:LX:138:VAL:HG13	1.89	0.55
32:SY:104:ARG:HG3	32:SY:107:ARG:HH21	1.72	0.55
39:L5:2324:C:O2'	69:Le:98:GLU:OE1	2.24	0.55
82:Ls:29:ILE:HG13	82:Ls:190:GLN:HB2	1.88	0.55
35:S2:1562:C:H2'	35:S2:1563:G:H8	1.72	0.55
35:S2:1588:A:H2'	35:S2:1589:A:C8	2.41	0.55
39:L5:1259:G:H2'	39:L5:1260:G:H8	1.72	0.55
39:L5:4571:A2M:H2'	39:L5:4572:U:H6	1.71	0.55
60:LU:40:GLU:OE1	60:LU:65:ARG:NH1	2.40	0.55
79:Lo:99:ARG:HE	79:Lo:100:LYS:H	1.55	0.55
20:SC:146:GLU:HB3	20:SC:149:THR:HG22	1.89	0.55
39:L5:4274:A:H2'	39:L5:4275:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Ld:90:ARG:HD3	68:Ld:102:LEU:HD13	1.87	0.55
84:CH:85:ARG:NH1	84:CH:110:GLU:OE2	2.38	0.55
35:S2:367:U:H4'	35:S2:371:A:C8	2.43	0.54
35:S2:525:A:H2'	35:S2:526:A:H8	1.71	0.54
35:S2:1171:G:O2'	35:S2:1187:G:O6	2.22	0.54
43:LB:59:GLU:HB2	43:LB:366:LYS:HE2	1.88	0.54
1:AP:19:G:H4'	1:AP:20(A):U:H5'	1.89	0.54
17:Sg:10:THR:HG22	17:Sg:308:ARG:HG2	1.88	0.54
32:SY:104:ARG:HH22	35:S2:507:G:P	2.30	0.54
43:LB:10:ARG:NH1	43:LB:11:HIS:O	2.41	0.54
46:LE:161:ARG:NH1	46:LE:273:SER:OG	2.40	0.54
23:SH:117:PRO:HG2	23:SH:120:ARG:HG2	1.88	0.54
31:SX:17:ARG:HH12	35:S2:659:G:H21	1.54	0.54
39:L5:1328:G:O2'	39:L5:2349:A:OP1	2.25	0.54
39:L5:2809:G:O2'	39:L5:4644:G:OP1	2.22	0.54
39:L5:4242:U:H3	39:L5:4281:A:H2	1.52	0.54
47:LF:105:VAL:HG13	47:LF:136:VAL:HG12	1.88	0.54
71:Lg:42:PRO:HB2	71:Lg:53:LEU:HD12	1.89	0.54
26:SL:126:VAL:HG12	26:SL:145:VAL:HG22	1.89	0.54
39:L5:136:C:N4	72:Lh:77:LYS:O	2.41	0.54
39:L5:1777:C:O2'	45:LD:3:PHE:O	2.25	0.54
39:L5:1971:C:H1'	82:Ls:41:GLN:HE22	1.72	0.54
39:L5:1971:C:O2	82:Ls:41:GLN:NE2	2.41	0.54
39:L5:2362:U:H2'	39:L5:2363:A2M:H8	1.88	0.54
43:LB:57:VAL:HG22	43:LB:73:VAL:HG12	1.89	0.54
30:SW:86:LEU:HD21	30:SW:113:HIS:HB2	1.90	0.54
39:L5:1332:C:H2'	39:L5:1333:A:H8	1.73	0.54
39:L5:4537:C:H2'	39:L5:4538:G:C8	2.42	0.54
62:LX:73:HIS:HB3	62:LX:116:LEU:HD23	1.88	0.54
65:La:72:THR:HG22	65:La:110:LYS:HB3	1.88	0.54
83:Lt:32:ILE:HA	83:Lt:35:LEU:HD13	1.89	0.54
16:Sf:108:VAL:HB	16:Sf:113:LYS:H	1.73	0.54
31:SX:9:THR:HG22	35:S2:681:PSU:H4'	1.89	0.54
36:LR:168:GLU:OE1	36:LR:172:ARG:NH2	2.41	0.54
39:L5:1404:G:N7	39:L5:1408:G:N2	2.55	0.54
39:L5:2568:C:H2'	39:L5:2569:G:C8	2.43	0.54
82:Ls:137:PHE:HB3	82:Ls:174:LEU:HD21	1.90	0.54
35:S2:639:C:H2'	35:S2:640:A:H8	1.73	0.54
39:L5:3937:C:H1'	54:LN:125:SER:HB3	1.90	0.54
83:Lt:117:ARG:NE	83:Lt:119:ARG:H	2.06	0.54
2:PE:3:C:O2'	39:L5:3715:U:OP1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:942:G:H2'	35:S2:943:U:C6	2.43	0.54
39:L5:2484:A:H62	39:L5:2494:U:H3	1.55	0.54
39:L5:2754:G:OP2	64:LZ:133:LYS:NZ	2.39	0.54
39:L5:3910:C:H2'	39:L5:3911:C:C6	2.43	0.54
42:LA:229:ALA:HB3	42:LA:234:LYS:HB3	1.88	0.54
44:LC:154:VAL:HG11	44:LC:174:LEU:HD11	1.89	0.54
32:SY:21:LYS:HD2	32:SY:75:ILE:HD11	1.90	0.54
39:L5:2382:A:N1	39:L5:2829:U:O2'	2.36	0.54
39:L5:3823:G:OP2	39:L5:3823:G:N2	2.32	0.54
43:LB:315:ASN:HD21	43:LB:326:VAL:H	1.56	0.54
2:PE:26:A:N1	2:PE:44:G:N2	2.49	0.53
21:SE:43:PRO:HG2	21:SE:46:ILE:HG12	1.88	0.53
22:SG:20:ASP:HB3	22:SG:23:LYS:HD3	1.90	0.53
22:SG:135:PRO:HG2	22:SG:141:ILE:HG13	1.89	0.53
39:L5:280:G:H5''	54:LN:14:LYS:HE2	1.91	0.53
39:L5:4441:A:H5''	50:LI:114:GLY:HA2	1.89	0.53
51:LJ:112:HIS:HD2	51:LJ:117:ILE:HD11	1.73	0.53
24:SI:119:LEU:HD11	24:SI:153:LYS:HG3	1.90	0.53
35:S2:1422:G:H4'	35:S2:1423:C:H3'	1.90	0.53
39:L5:935:A:O2'	53:LM:44:GLN:O	2.25	0.53
39:L5:2008:U:H1'	39:L5:2011:C:H5	1.72	0.53
48:LG:157:ILE:HA	48:LG:201:THR:HG22	1.90	0.53
61:LV:65:VAL:HG23	61:LV:73:ARG:HA	1.89	0.53
68:Ld:64:ILE:HG23	68:Ld:68:LEU:HD23	1.90	0.53
12:SU:35:VAL:HG11	12:SU:110:VAL:HG21	1.89	0.53
19:SB:109:LYS:O	19:SB:113:MET:HG2	2.09	0.53
25:SJ:63:LEU:HD22	25:SJ:70:ARG:HB2	1.88	0.53
39:L5:2108:G:H2'	39:L5:2109:G:C8	2.43	0.53
39:L5:3953:G:N2	39:L5:4059:C:O2'	2.41	0.53
19:SB:88:THR:HG22	19:SB:98:THR:HG22	1.90	0.53
25:SJ:12:THR:HG23	35:S2:520:A:H5''	1.91	0.53
35:S2:639:C:H2'	35:S2:640:A:C8	2.43	0.53
35:S2:689:U:H3'	35:S2:690:G:H21	1.73	0.53
52:LL:48:PRO:HG3	72:Lh:118:LYS:HE2	1.90	0.53
63:LY:2:LYS:HD2	63:LY:7:VAL:HG13	1.90	0.53
4:SF:113:VAL:O	4:SF:117:ILE:HG12	2.08	0.53
35:S2:118:C:H1'	35:S2:445:A:C5	2.44	0.53
35:S2:350:C:HO2'	35:S2:383:G:H1	1.44	0.53
35:S2:1277:C:H2'	35:S2:1278:A:C8	2.42	0.53
39:L5:2758:G:O2'	39:L5:2765:A:N3	2.34	0.53
39:L5:3736:A:H2'	39:L5:3737:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:LA:101:VAL:HG22	42:LA:165:VAL:HG22	1.90	0.53
12:SU:19:ARG:HH22	12:SU:93:SER:H	1.57	0.53
16:Sf:139:HIS:O	16:Sf:147:THR:HA	2.08	0.53
39:L5:491:G:H2'	39:L5:492:U:C6	2.44	0.53
51:LJ:35:ARG:HD2	51:LJ:123:ILE:HA	1.90	0.53
58:LS:27:LEU:HB3	59:LT:148:PRO:HB3	1.91	0.53
21:SE:208:VAL:HG21	21:SE:225:ILE:HG13	1.91	0.53
21:SE:233:LYS:HD2	21:SE:234:PRO:HD2	1.90	0.53
31:SX:105:PHE:HD1	31:SX:121:LYS:HB3	1.74	0.53
39:L5:3732:A:H2'	39:L5:3733:A:C8	2.44	0.53
62:LX:148:ASP:HA	62:LX:151:ASN:HB2	1.90	0.53
21:SE:148:ARG:NH1	35:S2:124:U:OP1	2.41	0.53
39:L5:4742:G:H2'	39:L5:4743:G:C8	2.43	0.53
1:AP:37:A:O2'	39:L5:3760:A:N1	2.42	0.53
9:SR:114:LEU:HB2	9:SR:117:LEU:HG	1.91	0.53
17:Sg:31:ILE:HG22	17:Sg:43:TRP:HB2	1.90	0.53
39:L5:2296:G:O2'	44:LC:242:PRO:O	2.23	0.53
39:L5:4457:PSU:H1'	43:LB:252:ALA:HB3	1.91	0.53
45:LD:62:CYS:HB3	45:LD:105:LEU:HD22	1.89	0.53
21:SE:79:ASP:HB3	21:SE:82:TYR:HB2	1.91	0.53
24:SI:25:ARG:HA	35:S2:448:A:H5''	1.91	0.53
25:SJ:136:ARG:HD3	25:SJ:160:SER:HA	1.91	0.53
35:S2:106:C:H2'	35:S2:107:A:C8	2.44	0.53
39:L5:158:A:H5''	39:L5:159:C:H2'	1.91	0.53
39:L5:2400:G:H21	71:Lg:6:THR:HG22	1.73	0.53
68:Ld:33:ILE:HD11	68:Ld:44:ARG:HB3	1.91	0.53
21:SE:133:THR:HG22	21:SE:134:LYS:HG2	1.91	0.52
28:SO:43:HIS:CD2	28:SO:55:ARG:HB2	2.43	0.52
33:Sa:41:ILE:HG23	33:Sa:68:TYR:CE1	2.43	0.52
39:L5:1741:G:O2'	39:L5:1781:PSU:OP2	2.26	0.52
48:LG:33:GLU:OE2	48:LG:35:ARG:NH1	2.41	0.52
8:SQ:74:GLY:O	8:SQ:80:GLN:NE2	2.29	0.52
35:S2:145:G:H2'	35:S2:146:G:C8	2.44	0.52
35:S2:885:U:O2	35:S2:901:G:C6	2.63	0.52
39:L5:93:G:H2'	39:L5:94:A:C8	2.45	0.52
39:L5:3732:A:H2'	39:L5:3733:A:H8	1.73	0.52
79:Lo:12:CYS:HB3	79:Lo:15:CYS:HB2	1.91	0.52
21:SE:106:LYS:NZ	35:S2:846:G:OP1	2.43	0.52
22:SG:227:GLN:HB3	22:SG:231:ARG:HH21	1.73	0.52
35:S2:388:U:H2'	35:S2:389:A:C8	2.44	0.52
37:LW:72:THR:OG1	37:LW:74:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:4537:C:H2'	39:L5:4538:G:H8	1.73	0.52
43:LB:80:GLU:OE1	43:LB:323:TYR:OH	2.24	0.52
82:Ls:66:ARG:HA	82:Ls:69:LEU:HD23	1.91	0.52
10:SS:132:ARG:HD3	35:S2:1623:A:C6	2.45	0.52
11:ST:62:ARG:HH22	35:S2:1543:U:P	2.32	0.52
35:S2:186:C:H2'	35:S2:187:G:H8	1.75	0.52
35:S2:888:U:H4'	35:S2:889:U:H5'	1.91	0.52
39:L5:10:A:H2'	39:L5:11:G:C8	2.45	0.52
39:L5:4058:U:H4'	39:L5:4059:C:C5	2.45	0.52
3:SD:123:LEU:HD13	3:SD:136:VAL:HG22	1.92	0.52
28:SO:34:PHE:HB3	28:SO:41:PHE:HB2	1.91	0.52
32:SY:57:VAL:HB	32:SY:60:PHE:HE2	1.73	0.52
39:L5:653:U:H2'	39:L5:654:C:C6	2.44	0.52
39:L5:1188:C:H2'	39:L5:1189:G:C8	2.45	0.52
39:L5:4742:G:H2'	39:L5:4743:G:H8	1.74	0.52
34:Sb:45:THR:HG22	34:Sb:82:LYS:HE3	1.90	0.52
39:L5:1979:A:H2	39:L5:1987:C:H42	1.58	0.52
39:L5:3720:G:H22	39:L5:3733:A:H2	1.57	0.52
39:L5:4363:A:H5''	79:Lo:36:GLN:HG2	1.91	0.52
45:LD:64:ILE:HD13	45:LD:109:LEU:HD22	1.91	0.52
21:SE:29:PRO:HA	35:S2:496:C:H5'	1.90	0.52
30:SW:11:LEU:HD12	30:SW:74:VAL:HB	1.92	0.52
39:L5:1333:A:H2'	39:L5:1334:A:C8	2.45	0.52
39:L5:1933:G:H2'	39:L5:1934:A:C8	2.45	0.52
39:L5:3950:U:H3'	39:L5:3951:G:C8	2.44	0.52
39:L5:4260:U:H2'	39:L5:4261:C:H6	1.74	0.52
18:SA:145:ILE:HG23	18:SA:159:ILE:HB	1.92	0.52
35:S2:388:U:H2'	35:S2:389:A:H8	1.75	0.52
35:S2:1705:C:H2'	35:S2:1706:G:C8	2.45	0.52
39:L5:2017:A:O2'	39:L5:2018:C:O5'	2.28	0.52
54:LN:13:LYS:HE3	73:Li:45:ARG:HH11	1.75	0.52
82:Ls:146:LYS:HE3	82:Ls:153:GLU:HB3	1.92	0.52
3:SD:76:ARG:HG3	5:SK:68:TYR:HE1	1.74	0.52
6:SM:31:LEU:HD22	6:SM:89:VAL:HG13	1.92	0.52
35:S2:796:G:N2	35:S2:798:G:O6	2.43	0.52
42:LA:137:ILE:HD11	42:LA:149:LYS:HB2	1.92	0.52
31:SX:105:PHE:CE2	31:SX:112:VAL:HB	2.44	0.52
39:L5:1866:U:OP1	50:LI:4:ARG:NH1	2.42	0.52
39:L5:1942:A:H2'	39:L5:1943:A:H8	1.73	0.52
39:L5:1969:G:H4'	82:Ls:36:GLY:HA2	1.91	0.52
42:LA:180:LEU:HD21	80:Lp:22:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SM:33:ARG:HG3	35:S2:1284:A:C8	2.45	0.51
7:SP:97:TYR:OH	35:S2:1268:C:O2	2.27	0.51
32:SY:104:ARG:NH2	35:S2:507:G:OP2	2.38	0.51
35:S2:1777:G:H2'	35:S2:1778:C:C6	2.44	0.51
39:L5:261:G:H2'	39:L5:262:G:C8	2.45	0.51
39:L5:330:G:N7	88:L5:5284:SPD:N1	2.58	0.51
3:SD:96:LEU:HD22	3:SD:190:LEU:HD13	1.92	0.51
17:Sg:59:LEU:HD23	17:Sg:90:TRP:CG	2.45	0.51
19:SB:124:HIS:HA	19:SB:137:LEU:O	2.10	0.51
20:SC:113:GLN:HG3	20:SC:120:GLN:HG3	1.92	0.51
35:S2:28:U:H2'	35:S2:29:G:H8	1.75	0.51
35:S2:1779:G:H2'	35:S2:1780:G:C8	2.46	0.51
39:L5:729:G:H5''	47:LF:76:ARG:HD2	1.93	0.51
39:L5:4717:A:OP2	43:LB:30:LYS:NZ	2.30	0.51
43:LB:74:GLU:OE1	43:LB:285:TYR:OH	2.16	0.51
72:Lh:95:LEU:HB3	72:Lh:99:GLU:HG3	1.93	0.51
7:SP:51:ARG:NH1	35:S2:1300:U:O2	2.43	0.51
8:SQ:8:GLN:HG2	8:SQ:27:ARG:HB2	1.91	0.51
11:ST:108:GLU:OE2	11:ST:121:ARG:NE	2.39	0.51
19:SB:150:ILE:HG12	35:S2:1124:C:H5''	1.92	0.51
21:SE:124:CYS:HB3	21:SE:141:THR:OG1	2.11	0.51
22:SG:102:VAL:HG23	22:SG:106:LEU:HD12	1.93	0.51
35:S2:1217:A:H2'	35:S2:1218:C:C6	2.46	0.51
35:S2:1232:PSU:H2'	35:S2:1233:G:H8	1.75	0.51
36:LR:168:GLU:HA	36:LR:171:LYS:HG2	1.93	0.51
39:L5:1326:A2M:H2'	39:L5:1327:C:C6	2.45	0.51
43:LB:315:ASN:ND2	43:LB:326:VAL:H	2.07	0.51
64:LZ:5:MET:O	64:LZ:28:ASN:ND2	2.43	0.51
22:SG:14:LYS:HD3	22:SG:124:LEU:HB2	1.93	0.51
39:L5:62:A:N3	39:L5:77:U:O2'	2.34	0.51
39:L5:1870:C:H2'	39:L5:1871:A2M:H8	1.92	0.51
39:L5:2318:G:N2	39:L5:2321:G:OP2	2.35	0.51
39:L5:4966:A:H5''	43:LB:128:LYS:HG3	1.92	0.51
6:SM:128:PHE:O	6:SM:132:LYS:HG2	2.10	0.51
39:L5:260:C:H2'	39:L5:261:G:C8	2.45	0.51
39:L5:3911:C:H2'	39:L5:3912:U:H6	1.74	0.51
49:LH:103:VAL:HG11	49:LH:144:LEU:HD21	1.92	0.51
59:LT:44:GLY:HA2	59:LT:95:HIS:HB3	1.92	0.51
2:PE:5:G:H2'	2:PE:6:G:H8	1.75	0.51
35:S2:695:C:H41	35:S2:737:G:H21	1.58	0.51
35:S2:1779:G:H2'	35:S2:1780:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:408:A:O2'	39:L5:411:G:OP2	2.25	0.51
39:L5:467:U:C4	39:L5:468:U:H1'	2.45	0.51
39:L5:1548:G:O2'	39:L5:2812:A:N3	2.39	0.51
39:L5:4084:G:O6	42:LA:72:ARG:NH2	2.44	0.51
42:LA:20:VAL:HA	42:LA:23:ARG:HG3	1.91	0.51
60:LU:25:CYS:O	60:LU:68:SER:OG	2.29	0.51
21:SE:126:VAL:HG22	21:SE:139:LEU:HD21	1.91	0.51
23:SH:8:ILE:HG13	23:SH:9:VAL:HG23	1.92	0.51
35:S2:1396:A:N7	35:S2:1449:G:O6	2.42	0.51
35:S2:1724:A:H5''	61:LV:70:PRO:HG3	1.93	0.51
39:L5:121:A:H62	39:L5:152:U:H3	1.59	0.51
39:L5:2666:U:O2'	39:L5:2668:G:N7	2.44	0.51
54:LN:146:PRO:HB2	72:Lh:104:THR:HG23	1.93	0.51
4:SF:134:VAL:H	4:SF:203:ASN:HD21	1.57	0.51
6:SM:91:LEU:HD22	6:SM:106:CYS:HB2	1.92	0.51
24:SI:101:ILE:HD12	24:SI:190:LEU:HD11	1.93	0.51
24:SI:151:GLU:HA	24:SI:154:LYS:HE2	1.93	0.51
39:L5:4524:G:C2	43:LB:252:ALA:HB1	2.46	0.51
55:LO:54:TYR:OH	55:LO:73:PHE:O	2.28	0.51
67:Lc:48:LEU:HD11	67:Lc:60:ILE:HG21	1.91	0.51
13:SZ:73:VAL:HG12	13:SZ:79:ILE:HD11	1.93	0.51
34:Sb:19:HIS:HD2	34:Sb:21:LYS:H	1.59	0.51
35:S2:1203:G:H2'	35:S2:1204:A:C8	2.45	0.51
39:L5:1993:C:H2'	39:L5:1994:C:C6	2.46	0.51
45:LD:200:MET:HB3	45:LD:237:GLU:HG2	1.93	0.51
83:Lt:158:GLY:HA2	83:Lt:161:GLU:HB2	1.93	0.51
12:SU:86:LYS:NZ	35:S2:1404:U:O4	2.37	0.51
16:Sf:103:LEU:HD12	16:Sf:105:TYR:CE1	2.46	0.51
16:Sf:110:GLU:OE2	16:Sf:113:LYS:NZ	2.40	0.51
21:SE:220:THR:HB	21:SE:225:ILE:HD11	1.93	0.51
35:S2:24:C:HO2'	35:S2:25:A:H8	1.58	0.51
35:S2:659:G:O2'	35:S2:662:G:O2'	2.26	0.51
35:S2:692:G:N7	35:S2:693:A:N6	2.59	0.51
35:S2:1748:G:O6	37:LW:73:ARG:NH2	2.39	0.51
45:LD:150:LEU:HD12	51:LJ:146:ARG:HG3	1.93	0.51
60:LU:64:GLU:HG3	60:LU:71:THR:HB	1.93	0.51
63:LY:50:ARG:NH1	63:LY:51:LYS:HB3	2.26	0.51
2:PE:41:U:H2'	2:PE:42:G:H8	1.76	0.50
3:SD:113:LEU:HD11	3:SD:117:ARG:HD2	1.93	0.50
11:ST:104:LEU:HD22	11:ST:121:ARG:HD2	1.92	0.50
22:SG:162:LEU:HD13	35:S2:67:C:C5	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SL:78:THR:HG22	26:SL:79:LYS:HG3	1.93	0.50
32:SY:119:GLY:HA2	35:S2:85:A:H5'	1.93	0.50
35:S2:1405:A:H2'	35:S2:1406:G:O4'	2.11	0.50
39:L5:4987:C:OP2	43:LB:116:ARG:NH2	2.44	0.50
40:L7:23:A:N3	40:L7:118:C:O2'	2.36	0.50
40:L7:120:U:H4'	45:LD:262:LYS:HG2	1.92	0.50
56:LP:54:GLN:HA	56:LP:83:TRP:CD1	2.46	0.50
17:Sg:163:PRO:HB2	17:Sg:179:LEU:HB2	1.92	0.50
21:SE:125:LYS:HB2	21:SE:226:PHE:CD1	2.46	0.50
32:SY:34:THR:O	35:S2:570:C:O2'	2.28	0.50
35:S2:1417:C:O2	35:S2:1422:G:O6	2.29	0.50
36:LR:167:LYS:HG2	36:LR:170:ARG:HH21	1.76	0.50
39:L5:1591:U:OP2	39:L5:2856:C:O2'	2.18	0.50
39:L5:3664:G:H2'	39:L5:3665:G:H8	1.76	0.50
84:CH:113:ARG:O	84:CH:115:ILE:N	2.44	0.50
35:S2:851:C:H5''	35:S2:852:G:H5'	1.93	0.50
39:L5:1175:A:H2	39:L5:1185:G:H22	1.59	0.50
39:L5:2745:A:H2'	39:L5:2746:A:C8	2.47	0.50
43:LB:217:ILE:HD12	43:LB:347:LEU:HB3	1.92	0.50
47:LF:220:MET:HB3	47:LF:232:ASP:OD2	2.10	0.50
11:ST:18:LEU:HD22	11:ST:58:ALA:HA	1.92	0.50
35:S2:1595:U:H2'	35:S2:1596:U:C6	2.46	0.50
39:L5:1466:G:OP2	66:Lb:44:ARG:NH2	2.45	0.50
39:L5:2017:A:O2'	39:L5:2018:C:H6	1.94	0.50
39:L5:2745:A:H2'	39:L5:2746:A:H8	1.77	0.50
39:L5:4473:A:H5''	77:Lm:95:ILE:HD12	1.92	0.50
39:L5:4612:C:C2	49:LH:120:GLU:HB2	2.47	0.50
3:SD:167:TYR:CE2	3:SD:204:LEU:HD23	2.47	0.50
11:ST:4:VAL:HG11	11:ST:136:GLY:HA2	1.94	0.50
18:SA:76:VAL:HG12	18:SA:123:VAL:HB	1.94	0.50
18:SA:212:LYS:O	18:SA:215:GLN:HG3	2.11	0.50
22:SG:5:ILE:HG22	22:SG:113:ILE:HD11	1.93	0.50
27:SN:40:LEU:HB3	27:SN:50:ILE:HG12	1.92	0.50
35:S2:1010:G:H2'	35:S2:1011:A:C8	2.47	0.50
36:LR:62:ARG:NH2	39:L5:4648:A:OP1	2.43	0.50
39:L5:268:G:H2'	39:L5:269:G:C8	2.45	0.50
39:L5:1617:G:H1'	39:L5:2513:A:N6	2.26	0.50
40:L7:6:C:O2'	45:LD:50:ARG:NH2	2.45	0.50
50:LI:9:TYR:O	50:LI:59:GLN:NE2	2.43	0.50
1:AP:43:A:H2'	1:AP:44:A:H8	1.77	0.50
12:SU:93:SER:OG	12:SU:95:SER:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Sc:64:GLU:OE2	14:Sc:66:ARG:HG2	2.12	0.50
19:SB:87:ILE:HG22	19:SB:101:HIS:HB2	1.94	0.50
39:L5:1172:C:O2'	39:L5:1173:G:O5'	2.28	0.50
39:L5:2543:A:H2	39:L5:2773:G:H22	1.59	0.50
39:L5:4278:C:HO2'	39:L5:4281:A:H8	1.58	0.50
39:L5:4611:A:H2	49:LH:120:GLU:HB3	1.75	0.50
73:Li:41:ARG:O	73:Li:45:ARG:HG2	2.11	0.50
3:SD:31:GLU:HG3	84:CH:69:HIS:ND1	2.27	0.50
7:SP:124:LYS:HD3	35:S2:1239:U:H5''	1.93	0.50
25:SJ:162:ARG:NH2	35:S2:583:A:OP2	2.44	0.50
28:SO:55:ARG:NH2	35:S2:953:C:O2	2.44	0.50
35:S2:1736:G:H2'	35:S2:1737:G:C8	2.47	0.50
39:L5:497:G:N2	39:L5:498:C:H41	2.05	0.50
39:L5:1646:A:O2'	74:Lj:49:TRP:O	2.28	0.50
39:L5:2411:C:H2'	39:L5:2412:A:H8	1.76	0.50
39:L5:2848:G:O2'	39:L5:3838:U:O4	2.21	0.50
39:L5:3822:PSU:OP1	87:L5:5291:SPM:N5	2.39	0.50
39:L5:3910:C:H2'	39:L5:3911:C:H6	1.77	0.50
46:LE:94:LYS:HE2	46:LE:107:VAL:HG11	1.93	0.50
35:S2:964:A:H2'	35:S2:965:U:H6	1.77	0.50
39:L5:492:U:H2'	39:L5:493:G:C8	2.47	0.50
7:SP:57:LEU:HD11	7:SP:83:MET:HE2	1.93	0.50
39:L5:3680:U:H5''	42:LA:54:ARG:HH21	1.77	0.50
39:L5:3950:U:H3'	39:L5:3951:G:H8	1.77	0.50
9:SR:35:CYS:HA	9:SR:38:ILE:HG12	1.92	0.49
35:S2:1144:A:H2'	35:S2:1145:A:C8	2.47	0.49
39:L5:1703:C:O2'	39:L5:1704:C:OP1	2.28	0.49
39:L5:3611:A:H2	39:L5:5016:A:H8	1.59	0.49
43:LB:57:VAL:HB	43:LB:367:PHE:HB3	1.93	0.49
44:LC:73:VAL:HB	44:LC:78:ARG:HH12	1.77	0.49
79:Lo:2:VAL:N	79:Lo:90:HIS:O	2.45	0.49
24:SI:130:THR:HG23	24:SI:134:GLU:HG3	1.93	0.49
39:L5:172:C:H4'	39:L5:173:C:H5'	1.94	0.49
40:L7:38:U:N3	40:L7:41:G:OP2	2.34	0.49
12:SU:26:SER:HB3	12:SU:110:VAL:HG23	1.93	0.49
19:SB:171:ILE:HD11	19:SB:197:ILE:HA	1.94	0.49
21:SE:31:PRO:HG2	21:SE:38:LEU:HB2	1.94	0.49
26:SL:113:LEU:HD11	26:SL:120:VAL:HG21	1.94	0.49
31:SX:54:LYS:HG2	31:SX:70:VAL:HG12	1.95	0.49
32:SY:33:ALA:HB2	35:S2:582:U:H1'	1.95	0.49
35:S2:634:A:H2'	35:S2:635:G:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1616:U:O2'	35:S2:1661:A:N3	2.40	0.49
39:L5:2093:A:N3	39:L5:2094:G:N1	2.61	0.49
39:L5:2095:A:O2'	47:LF:32:ARG:NH2	2.45	0.49
39:L5:4188:U:H2'	39:L5:4189:U:C6	2.48	0.49
39:L5:4584:A:H2'	39:L5:4585:U:O4'	2.12	0.49
41:L8:58:G:N7	74:Lj:63:ARG:NH2	2.47	0.49
43:LB:173:LEU:HD22	43:LB:342:LYS:HD2	1.94	0.49
49:LH:128:MET:HE2	49:LH:134:CYS:HB2	1.93	0.49
49:LH:137:SER:OG	49:LH:143:GLU:HB3	2.12	0.49
7:SP:56:LEU:HD22	7:SP:80:LEU:HD11	1.94	0.49
8:SQ:72:VAL:HG11	8:SQ:84:ILE:HD11	1.94	0.49
9:SR:56:HIS:NE2	35:S2:1465:A:OP1	2.43	0.49
26:SL:85:THR:HG22	26:SL:112:HIS:HA	1.94	0.49
35:S2:533:A:H62	35:S2:550:C:H42	1.60	0.49
35:S2:562:U:H2'	35:S2:563:G:C8	2.46	0.49
35:S2:996:A:H2'	35:S2:997:A:C8	2.47	0.49
39:L5:2741:U:H2'	42:LA:50:HIS:CD2	2.48	0.49
39:L5:3861:A:H2'	39:L5:3862:A:C8	2.47	0.49
48:LG:200:THR:HG22	48:LG:201:THR:HG23	1.93	0.49
59:LT:27:LEU:HB3	59:LT:31:MET:HE3	1.94	0.49
67:Lc:38:ILE:HD11	67:Lc:46:VAL:HG21	1.94	0.49
32:SY:10:ARG:HA	35:S2:839:C:H41	1.77	0.49
35:S2:1438:A:H2'	35:S2:1439:A:C8	2.48	0.49
39:L5:652:G:H2'	39:L5:653:U:C6	2.47	0.49
42:LA:13:GLY:O	42:LA:17:ARG:HG3	2.13	0.49
43:LB:288:GLY:HA3	43:LB:330:PHE:CE1	2.47	0.49
46:LE:141:ARG:NH2	70:Lf:110:ILE:O	2.45	0.49
54:LN:200:LEU:HB3	54:LN:204:ARG:NH1	2.28	0.49
2:PE:13:C:H2'	2:PE:14:A:H8	1.78	0.49
3:SD:204:LEU:HB2	3:SD:207:HIS:HB2	1.94	0.49
6:SM:57:ASP:OD1	35:S2:1285:G:N1	2.46	0.49
7:SP:131:PRO:HA	35:S2:1237:C:H5'	1.95	0.49
10:SS:114:LEU:HA	10:SS:117:ILE:HG22	1.94	0.49
10:SS:118:ARG:HE	10:SS:123:LEU:HD21	1.77	0.49
35:S2:690:G:H3'	35:S2:691:G:H21	1.77	0.49
35:S2:1037:G:H4'	35:S2:1845:A:H4'	1.94	0.49
35:S2:1805:G:H2'	35:S2:1806:A:C8	2.46	0.49
39:L5:85:G:O2'	39:L5:97:G:O6	2.24	0.49
39:L5:2521:G:H5'	39:L5:2640:G:H1'	1.94	0.49
39:L5:3880:G:H2'	39:L5:3881:G:C8	2.48	0.49
74:Lj:2:THR:HG22	74:Lj:4:GLY:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Lr:47:LYS:O	81:Lr:103:ARG:HD2	2.13	0.49
83:Lt:59:THR:HG22	83:Lt:61:LYS:HD3	1.94	0.49
9:SR:60:ARG:HH21	9:SR:66:VAL:HG13	1.77	0.49
22:SG:3:LEU:HD23	22:SG:109:LEU:HB3	1.94	0.49
23:SH:63:PHE:HA	23:SH:95:ILE:O	2.12	0.49
27:SN:112:LYS:O	27:SN:116:ILE:HD12	2.13	0.49
35:S2:17:C:H2'	35:S2:18:C:C6	2.47	0.49
35:S2:96:C:H2'	35:S2:97:U:C6	2.47	0.49
38:CI:74:LYS:HA	60:LU:116:GLN:HB2	1.95	0.49
63:LY:10:ASP:HB3	63:LY:13:LYS:HB2	1.95	0.49
10:SS:113:ARG:HA	10:SS:116:LYS:HE2	1.93	0.49
22:SG:57:ASP:HA	22:SG:106:LEU:HD23	1.93	0.49
25:SJ:136:ARG:HA	25:SJ:141:VAL:HA	1.94	0.49
32:SY:6:THR:O	32:SY:27:VAL:HA	2.12	0.49
32:SY:105:LYS:O	32:SY:109:GLU:HG2	2.12	0.49
35:S2:170:A:H2'	35:S2:171:A:C8	2.48	0.49
39:L5:513:U:H3'	39:L5:514:U:H4'	1.94	0.49
39:L5:1326:A2M:HM'3	39:L5:1326:A2M:H1'	1.62	0.49
39:L5:1628:C:OP1	42:LA:14:SER:OG	2.29	0.49
39:L5:2744:A:H2'	39:L5:2745:A:C8	2.48	0.49
39:L5:2763:U:H4'	39:L5:2764:A:H5''	1.95	0.49
44:LC:110:ARG:HG3	54:LN:204:ARG:HE	1.78	0.49
45:LD:41:LYS:NZ	59:LT:32:ARG:O	2.44	0.49
47:LF:127:LYS:HB2	59:LT:133:ALA:HB3	1.94	0.49
75:Lk:5:ILE:HD11	75:Lk:43:TYR:HB3	1.94	0.49
31:SX:17:ARG:HH22	35:S2:659:G:N2	2.11	0.49
35:S2:556:U:OP1	84:CH:146:ARG:NH2	2.45	0.49
39:L5:717:U:H2'	39:L5:718:C:C6	2.47	0.49
39:L5:748:G:O6	58:LS:98:ARG:NH2	2.31	0.49
39:L5:3641:U:H5	39:L5:3646:A:N7	2.10	0.49
39:L5:4459:U:H2'	39:L5:4460:U:C6	2.47	0.49
7:SP:18:ARG:NH1	10:SS:88:LYS:O	2.46	0.49
9:SR:83:ASN:O	9:SR:84:TYR:C	2.56	0.49
20:SC:130:ILE:HG23	20:SC:162:ILE:HD11	1.95	0.49
39:L5:1837:A:OP2	59:LT:130:ARG:NH1	2.39	0.49
39:L5:4070:U:H2'	39:L5:4071:U:C6	2.48	0.49
46:LE:157:HIS:HD2	46:LE:187:ARG:NH1	2.10	0.49
56:LP:8:PRO:HD3	56:LP:149:ILE:HD13	1.94	0.49
67:Lc:38:ILE:HG21	67:Lc:63:TYR:HB3	1.94	0.49
5:SK:80:ARG:NH1	5:SK:87:PRO:HA	2.28	0.48
17:Sg:259:TRP:CD1	17:Sg:266:ILE:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Sg:301:GLY:HA2	17:Sg:307:VAL:HG12	1.95	0.48
35:S2:1083:A:N7	35:S2:1841:C:O2'	2.37	0.48
39:L5:4184:G:H5'	42:LA:233:ARG:HB2	1.95	0.48
70:Lf:29:LYS:HB2	70:Lf:83:MET:HE3	1.95	0.48
14:Sc:11:LEU:HD12	14:Sc:55:VAL:HG12	1.93	0.48
25:SJ:172:ARG:HA	25:SJ:175:ARG:HG2	1.94	0.48
27:SN:55:ARG:HD3	35:S2:1017:U:H5'	1.95	0.48
31:SX:129:SER:HB2	35:S2:29:G:H4'	1.95	0.48
35:S2:609:U:H2'	35:S2:610:G:H8	1.78	0.48
35:S2:677:G:N1	35:S2:1027:A:OP2	2.34	0.48
35:S2:1825:A:O2'	39:L5:3760:A:N1	2.44	0.48
39:L5:3760:A:H4'	39:L5:3761:C:H5''	1.95	0.48
43:LB:133:TYR:O	43:LB:136:LYS:HG2	2.13	0.48
52:LL:111:GLN:HA	52:LL:114:VAL:HG22	1.95	0.48
61:LV:37:LEU:HD23	61:LV:65:VAL:HG12	1.94	0.48
69:Le:26:ASP:OD1	69:Le:26:ASP:N	2.46	0.48
75:Lk:8:ILE:HG23	75:Lk:56:LEU:HD12	1.95	0.48
2:PE:5:G:H2'	2:PE:6:G:C8	2.48	0.48
35:S2:549:C:H5''	84:CH:20:ALA:HB3	1.94	0.48
35:S2:1395:C:H1'	35:S2:1474:A:C5	2.48	0.48
39:L5:2255:C:OP1	47:LF:24:ASN:N	2.46	0.48
66:Lb:65:MET:SD	66:Lb:68:ARG:NH1	2.87	0.48
17:Sg:147:HIS:CD2	17:Sg:175:LYS:HD2	2.48	0.48
23:SH:37:LYS:HB3	23:SH:41:ARG:NH1	2.28	0.48
30:SW:37:PHE:HE1	30:SW:41:MET:HE3	1.77	0.48
30:SW:115:GLU:HB3	30:SW:118:ARG:HH21	1.78	0.48
35:S2:472:C:O2'	35:S2:474:G:OP1	2.22	0.48
35:S2:1457:U:H2'	35:S2:1458:G:H8	1.78	0.48
35:S2:1805:G:H2'	35:S2:1806:A:H8	1.77	0.48
39:L5:982:U:OP1	46:LE:73:TYR:OH	2.21	0.48
39:L5:1332:C:H2'	39:L5:1333:A:C8	2.48	0.48
39:L5:3619:G:H22	39:L5:3624:A:H1'	1.77	0.48
39:L5:3773:U:C4	39:L5:3775:A:N7	2.81	0.48
39:L5:3930:U:H3	39:L5:4180:G:H1	1.62	0.48
39:L5:4239:A:H2'	39:L5:4240:G:C8	2.48	0.48
43:LB:29:VAL:HA	43:LB:220:ILE:HD13	1.94	0.48
43:LB:220:ILE:HG23	43:LB:278:THR:HG22	1.95	0.48
47:LF:50:ILE:HD12	47:LF:186:CYS:HB3	1.95	0.48
51:LJ:30:GLY:O	51:LJ:32:ARG:N	2.47	0.48
4:SF:168:THR:HB	4:SF:171:GLU:HG3	1.95	0.48
17:Sg:257:LYS:HB3	17:Sg:259:TRP:NE1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SJ:142:VAL:HG12	25:SJ:144:ILE:H	1.79	0.48
35:S2:327:G:H5'	35:S2:328:U:C2	2.47	0.48
39:L5:1345:A:H2'	39:L5:1346:C:C6	2.48	0.48
39:L5:1984:A:N7	39:L5:2010:A:O2'	2.35	0.48
42:LA:49:ILE:HD13	42:LA:60:LYS:HE3	1.95	0.48
4:SF:40:ALA:HB1	4:SF:45:TYR:CG	2.49	0.48
10:SS:101:ASN:ND2	51:LJ:119:TYR:O	2.46	0.48
13:SZ:69:THR:H	13:SZ:72:VAL:HG12	1.78	0.48
35:S2:525:A:H2'	35:S2:526:A:C8	2.47	0.48
35:S2:1013:U:OP1	35:S2:1129:G:O2'	2.31	0.48
35:S2:1215:C:O2'	35:S2:1645:C:OP2	2.31	0.48
35:S2:1736:G:H2'	35:S2:1737:G:H8	1.79	0.48
36:LR:127:VAL:HG12	36:LR:132:PHE:HD2	1.79	0.48
39:L5:68:U:OP1	54:LN:178:HIS:ND1	2.42	0.48
39:L5:325:U:H2'	39:L5:326:C:C6	2.48	0.48
39:L5:1187:G:OP2	39:L5:1187:G:N2	2.38	0.48
49:LH:8:GLN:HE22	49:LH:71:ARG:HD3	1.79	0.48
58:LS:154:LEU:HB3	58:LS:157:ARG:HD3	1.96	0.48
64:LZ:11:VAL:HG12	64:LZ:82:PRO:HA	1.95	0.48
9:SR:31:ASN:HA	9:SR:34:VAL:HG22	1.96	0.48
25:SJ:88:ASP:HB3	25:SJ:91:LYS:HB2	1.94	0.48
35:S2:29:G:H2'	35:S2:30:C:C6	2.49	0.48
35:S2:159:A2M:O5'	35:S2:159:A2M:H8	2.13	0.48
35:S2:328:U:O2'	35:S2:329:G:O5'	2.28	0.48
35:S2:538:U:H2'	35:S2:539:C:C6	2.48	0.48
35:S2:1797:U:H2'	35:S2:1798:C:C6	2.49	0.48
35:S2:1812:U:C2	35:S2:1813:A:C8	3.02	0.48
39:L5:663:G:H2'	39:L5:664:G:C8	2.48	0.48
42:LA:131:GLY:H	42:LA:169:VAL:HG13	1.78	0.48
45:LD:181:PRO:HD2	45:LD:195:HIS:CD2	2.48	0.48
5:SK:14:LEU:HD23	5:SK:21:MET:HE1	1.96	0.48
18:SA:4:ALA:HA	29:SV:80:SER:HB3	1.95	0.48
23:SH:157:HIS:HB3	23:SH:190:PRO:HG3	1.96	0.48
39:L5:1662:C:H2'	39:L5:1663:C:C6	2.49	0.48
43:LB:220:ILE:HG12	43:LB:278:THR:HG22	1.96	0.48
43:LB:258:HIS:HA	43:LB:260:ALA:N	2.27	0.48
83:Lt:16:ARG:HD2	83:Lt:32:ILE:HD13	1.95	0.48
8:SQ:19:ALA:HB2	8:SQ:75:GLY:HA3	1.95	0.48
17:Sg:11:LEU:HD21	17:Sg:53:GLY:H	1.79	0.48
17:Sg:184:LEU:HD21	17:Sg:187:ASN:HD21	1.79	0.48
22:SG:147:LEU:HD13	37:LW:101:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:SH:30:LEU:HG	23:SH:33:ASN:HD22	1.78	0.48
35:S2:205:G:H2'	35:S2:206:G:H8	1.78	0.48
39:L5:423:G:H5'	56:LP:26:PHE:HZ	1.78	0.48
39:L5:3923:A:H2'	39:L5:3924:C:C6	2.49	0.48
39:L5:4736:C:H2'	39:L5:4737:G:H8	1.79	0.48
41:L8:141:C:H2'	41:L8:142:U:C6	2.48	0.48
42:LA:180:LEU:HD22	80:Lp:18:TYR:HB3	1.96	0.48
54:LN:157:LYS:O	54:LN:162:ARG:NH1	2.47	0.48
82:Ls:161:ILE:HG12	82:Ls:167:VAL:HG22	1.95	0.48
1:AP:29:C:H2'	1:AP:30:G:C8	2.47	0.48
8:SQ:45:ARG:HH21	35:S2:1593:C:H4'	1.78	0.48
9:SR:99:ASP:HB3	9:SR:102:THR:HG23	1.95	0.48
16:Sf:107:LYS:O	16:Sf:115:SER:OG	2.29	0.48
20:SC:167:ARG:HB3	20:SC:177:PRO:HB2	1.96	0.48
20:SC:259:THR:HG21	29:SV:16:LYS:H	1.79	0.48
35:S2:1217:A:H2'	35:S2:1218:C:H6	1.79	0.48
35:S2:1337:4AC:H2'	35:S2:1338:G:C8	2.48	0.48
39:L5:106:A:H2'	39:L5:107:G:O4'	2.13	0.48
39:L5:1446:C:H2'	39:L5:1447:C:C6	2.49	0.48
39:L5:2588:C:OP1	39:L5:2768:C:O2'	2.28	0.48
39:L5:4196:OMG:HM23	39:L5:4196:OMG:H1'	1.67	0.48
39:L5:4620:OMU:OP2	39:L5:4670:C:N4	2.39	0.48
39:L5:4875:G:H5''	58:LS:170:LYS:HE3	1.95	0.48
43:LB:28:LYS:HG3	43:LB:30:LYS:HG3	1.96	0.48
11:ST:62:ARG:CZ	35:S2:1542:C:H5''	2.44	0.47
17:Sg:47:ARG:HG2	17:Sg:52:TYR:CZ	2.49	0.47
17:Sg:191:HIS:CG	17:Sg:195:LEU:HD21	2.49	0.47
17:Sg:212:LYS:HD2	17:Sg:235:ILE:HG12	1.95	0.47
18:SA:82:THR:HG22	18:SA:171:VAL:HG21	1.96	0.47
23:SH:140:VAL:HG12	27:SN:19:ARG:HD2	1.96	0.47
24:SI:165:GLN:HB3	24:SI:171:LEU:HD23	1.95	0.47
35:S2:929:G:H2'	35:S2:930:C:O4'	2.14	0.47
35:S2:1714:U:H2'	35:S2:1715:A:C8	2.49	0.47
39:L5:210:C:HO2'	39:L5:233:U:HO2'	1.60	0.47
39:L5:934:C:H41	44:LC:350:ARG:HH21	1.62	0.47
39:L5:1352:C:O2'	39:L5:1356:U:OP1	2.29	0.47
39:L5:1464:C:H5''	66:Lb:32:LEU:HD12	1.95	0.47
50:LI:54:SER:OG	50:LI:130:HIS:O	2.32	0.47
55:LO:61:ARG:HA	55:LO:70:PRO:HD2	1.96	0.47
35:S2:1643:U:H2'	35:S2:1644:C:C6	2.49	0.47
39:L5:959:G:C8	46:LE:123:ARG:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:L8:67:U:H2'	41:L8:68:G:H8	1.79	0.47
47:LF:162:ILE:HD12	47:LF:167:ILE:HB	1.96	0.47
3:SD:29:LEU:HB3	3:SD:34:TYR:HB2	1.95	0.47
7:SP:93:MET:SD	7:SP:104:GLN:NE2	2.86	0.47
17:Sg:8:ARG:HB2	17:Sg:309:VAL:HG23	1.96	0.47
17:Sg:107:ASP:OD2	17:Sg:125:ARG:NH1	2.47	0.47
19:SB:155:TYR:OH	35:S2:989:C:OP2	2.27	0.47
28:SO:45:THR:HA	28:SO:52:THR:HA	1.97	0.47
35:S2:604:A:N3	35:S2:639:C:O2'	2.42	0.47
35:S2:1010:G:H2'	35:S2:1011:A:H8	1.79	0.47
35:S2:1201:U:H2'	35:S2:1202:U:C6	2.49	0.47
39:L5:308:G:OP2	39:L5:308:G:N2	2.39	0.47
39:L5:2045:G:O6	39:L5:3870:C:O2'	2.31	0.47
63:LY:50:ARG:HH11	63:LY:51:LYS:HB3	1.79	0.47
68:Ld:92:ARG:HA	68:Ld:102:LEU:HD23	1.96	0.47
22:SG:98:ARG:NH2	22:SG:101:ILE:O	2.30	0.47
39:L5:1298:C:H2'	39:L5:1299:G:C8	2.49	0.47
39:L5:2072:C:OP1	57:LQ:2:GLY:N	2.48	0.47
44:LC:266:THR:HG22	44:LC:267:TRP:H	1.80	0.47
55:LO:193:THR:HG22	55:LO:197:LYS:HE2	1.95	0.47
57:LQ:43:PHE:CD2	57:LQ:133:GLY:HA3	2.49	0.47
1:AP:41:G:H2'	1:AP:42:A:H8	1.79	0.47
5:SK:94:LEU:HD23	5:SK:95:ARG:HG3	1.96	0.47
32:SY:87:PRO:HB2	32:SY:89:HIS:CD2	2.49	0.47
35:S2:16:G:H2'	35:S2:17:C:C6	2.49	0.47
36:LR:105:LEU:HD23	36:LR:138:LEU:HD23	1.95	0.47
39:L5:737:C:C5	39:L5:739:G:H5''	2.49	0.47
39:L5:1254:A:H5''	39:L5:1255:A:H5''	1.96	0.47
39:L5:1733:G:N3	39:L5:4214:A:H2'	2.29	0.47
39:L5:5016:A:H2	39:L5:5033:G:H21	1.55	0.47
42:LA:206:PRO:HG3	42:LA:213:GLY:HA3	1.96	0.47
56:LP:16:LYS:HG2	56:LP:149:ILE:HG12	1.95	0.47
77:Lm:99:CYS:HB2	77:Lm:114:LYS:HE3	1.94	0.47
81:Lr:90:LEU:HD22	81:Lr:111:ILE:HG23	1.97	0.47
6:SM:36:ARG:HE	6:SM:40:LYS:HG3	1.78	0.47
17:Sg:89:LEU:HB2	17:Sg:101:PHE:CE1	2.49	0.47
20:SC:210:PRO:HD3	20:SC:236:PHE:HE2	1.78	0.47
33:Sa:79:ILE:HD13	35:S2:1863:A:H1'	1.97	0.47
35:S2:634:A:H2'	35:S2:635:G:C8	2.49	0.47
39:L5:173:C:H5''	52:LL:129:ARG:HH12	1.79	0.47
39:L5:2611:A:H2'	39:L5:2612:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:2845:A:H61	39:L5:3843:C:N4	2.13	0.47
39:L5:4088:C:H2'	39:L5:4089:G:C8	2.50	0.47
39:L5:4589:A:N1	39:L5:4621:C:O2'	2.46	0.47
53:LM:104:MET:HG3	53:LM:108:ASP:HB2	1.96	0.47
79:Lo:27:LYS:HD3	79:Lo:27:LYS:HA	1.67	0.47
3:SD:161:GLY:HA3	35:S2:1388:A:H61	1.78	0.47
7:SP:81:ARG:NH1	7:SP:98:ASN:HA	2.29	0.47
11:ST:52:TRP:HA	11:ST:55:THR:HG22	1.96	0.47
17:Sg:112:ALA:HB3	17:Sg:121:VAL:HG12	1.96	0.47
28:SO:33:ILE:HB	28:SO:97:LEU:HD23	1.97	0.47
39:L5:956:A:H1'	39:L5:2076:G:H5''	1.96	0.47
39:L5:2539:C:H2'	39:L5:2540:C:C6	2.50	0.47
39:L5:3873:G:H2'	39:L5:3874:G:C8	2.50	0.47
39:L5:3917:A:H2'	39:L5:3918:G:H8	1.79	0.47
39:L5:4238:G:H2'	39:L5:4239:A:C8	2.50	0.47
39:L5:4456:OMC:HM21	43:LB:241:PRO:HD3	1.97	0.47
41:L8:62:A:OP1	72:Lh:52:LYS:NZ	2.44	0.47
62:LX:127:LEU:HD11	62:LX:135:LYS:HE3	1.96	0.47
67:Lc:50:ASN:ND2	67:Lc:76:GLY:O	2.48	0.47
83:Lt:22:VAL:HA	83:Lt:48:LYS:HG2	1.97	0.47
4:SF:81:ARG:HH21	35:S2:1536:G:H5'	1.79	0.47
7:SP:78:THR:HA	35:S2:1298:G:H4'	1.97	0.47
7:SP:92:SER:HB2	7:SP:107:ILE:HD13	1.97	0.47
17:Sg:101:PHE:CD2	17:Sg:136:GLY:HA2	2.50	0.47
23:SH:98:ARG:O	35:S2:913:A:N6	2.34	0.47
39:L5:425:U:H4'	56:LP:6:LEU:HD21	1.97	0.47
39:L5:1359:G:H4'	54:LN:203:TYR:HB2	1.96	0.47
39:L5:4935:C:H2'	39:L5:4936:G:C8	2.49	0.47
41:L8:75:OMG:HM23	41:L8:75:OMG:H1'	1.72	0.47
48:LG:187:LYS:HB2	48:LG:198:THR:HG23	1.96	0.47
13:SZ:56:ASP:OD1	13:SZ:57:LYS:N	2.48	0.47
19:SB:179:ASN:HD21	19:SB:183:GLU:HB3	1.79	0.47
23:SH:126:HIS:CE1	23:SH:181:THR:HG23	2.50	0.47
25:SJ:128:VAL:O	25:SJ:132:GLN:HG2	2.15	0.47
29:SV:73:ALA:HB1	29:SV:78:ILE:HB	1.95	0.47
35:S2:1724:A:H2'	35:S2:1725:U:C6	2.50	0.47
39:L5:10:A:H2'	39:L5:11:G:H8	1.79	0.47
39:L5:137:G:H2'	39:L5:138:G:C8	2.47	0.47
39:L5:433:A:C2	39:L5:3867:A2M:H4'	2.49	0.47
39:L5:1538:U:H2'	39:L5:1539:G:H8	1.80	0.47
46:LE:223:ARG:HA	46:LE:224:LYS:HA	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:LP:5:SER:OG	56:LP:118:GLN:OE1	2.31	0.47
65:La:36:GLY:HA3	65:La:40:HIS:CE1	2.50	0.47
24:SI:134:GLU:HA	24:SI:137:LEU:HG	1.97	0.47
30:SW:14:ILE:HG22	30:SW:25:VAL:HG11	1.96	0.47
35:S2:1139:C:H2'	35:S2:1140:G:O4'	2.14	0.47
35:S2:1589:A:N3	35:S2:1653:U:O2'	2.46	0.47
39:L5:99:A:H5''	54:LN:184:ILE:HD12	1.96	0.47
39:L5:1259:G:H2'	39:L5:1260:G:C8	2.50	0.47
39:L5:1725:U:H2'	39:L5:1726:U:H6	1.80	0.47
39:L5:1824:G:H5''	59:LT:35:LYS:HE2	1.96	0.47
39:L5:1932:A:H8	55:LO:49:ARG:HH22	1.63	0.47
39:L5:4906:C:H2'	39:L5:4907:G:H8	1.79	0.47
52:LL:59:VAL:HG21	52:LL:73:GLY:HA3	1.97	0.47
53:LM:33:GLN:HB2	58:LS:145:PHE:HZ	1.80	0.47
1:AP:50:U:H2'	1:AP:51:C:C6	2.50	0.46
9:SR:28:PHE:HA	9:SR:55:THR:HG21	1.97	0.46
21:SE:87:MET:HE1	21:SE:123:LEU:HB2	1.96	0.46
21:SE:125:LYS:O	21:SE:142:HIS:N	2.48	0.46
23:SH:57:ARG:HD3	23:SH:91:HIS:CD2	2.50	0.46
31:SX:45:SER:HB3	35:S2:649:PSU:H1'	1.98	0.46
33:Sa:11:ALA:HB3	33:Sa:33:ASP:HB2	1.97	0.46
35:S2:43:U:OP2	35:S2:485:A:N6	2.42	0.46
35:S2:857:U:H2'	35:S2:858:A:C8	2.51	0.46
35:S2:1606:G:N2	35:S2:1632:G:H1'	2.30	0.46
39:L5:352:G:O2'	41:L8:22:U:O4	2.32	0.46
39:L5:2059:C:O2	58:LS:118:ARG:NH2	2.48	0.46
39:L5:4723:A:H2'	39:L5:4724:A:C8	2.50	0.46
39:L5:4743:G:H2'	39:L5:4744:A:C8	2.50	0.46
39:L5:5027:C:O2'	39:L5:5028:G:H5''	2.15	0.46
44:LC:218:ILE:HA	44:LC:229:LEU:HD22	1.98	0.46
48:LG:182:CYS:HB3	48:LG:222:ILE:HD12	1.96	0.46
53:LM:132:LYS:HE3	53:LM:132:LYS:HB3	1.81	0.46
12:SU:48:LEU:HD13	12:SU:93:SER:HB3	1.97	0.46
17:Sg:10:THR:HB	17:Sg:306:LEU:HD21	1.97	0.46
17:Sg:56:GLN:HG2	17:Sg:57:ARG:HG2	1.97	0.46
27:SN:64:ARG:HD3	27:SN:70:LYS:HG2	1.97	0.46
28:SO:75:MET:HG3	28:SO:118:ALA:HB2	1.96	0.46
30:SW:62:VAL:HG11	34:Sb:8:LEU:HG	1.97	0.46
34:Sb:22:LYS:HE3	35:S2:1129:G:H5''	1.98	0.46
35:S2:102:A:H4'	35:S2:104:A:C8	2.50	0.46
35:S2:454:U:H2'	35:S2:455:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1144:A:H5'	35:S2:1355:C:H41	1.79	0.46
37:LW:5:LEU:HD12	37:LW:30:GLN:NE2	2.30	0.46
39:L5:305:A:OP2	54:LN:15:GLN:NE2	2.42	0.46
39:L5:1613:A:H5''	42:LA:183:GLY:CA	2.46	0.46
39:L5:3893:C:O2'	39:L5:4979:A:N1	2.48	0.46
40:L7:27:G:H5''	45:LD:57:ASN:ND2	2.30	0.46
44:LC:65:GLU:HG2	44:LC:80:ARG:HH11	1.79	0.46
48:LG:162:ASP:HB3	48:LG:163:PRO:HD3	1.97	0.46
2:PE:6:G:H2'	2:PE:7:A:C8	2.50	0.46
8:SQ:140:ARG:HB2	35:S2:1644:C:H4'	1.98	0.46
11:ST:85:ASN:HB3	11:ST:88:MET:HB2	1.96	0.46
20:SC:108:LYS:HD2	20:SC:233:LEU:HD13	1.97	0.46
33:Sa:7:ASN:HB2	35:S2:1865:C:O2	2.14	0.46
35:S2:204:G:H2'	35:S2:205:G:O4'	2.16	0.46
35:S2:1713:C:H2'	35:S2:1714:U:C6	2.51	0.46
35:S2:1845:A:H2'	35:S2:1846:G:C8	2.51	0.46
39:L5:1982:G:H2'	39:L5:1983:A:O4'	2.16	0.46
39:L5:4088:C:H2'	39:L5:4089:G:H8	1.80	0.46
39:L5:5000:G:O2'	43:LB:382:MET:HE1	2.16	0.46
39:L5:5047:C:O2'	39:L5:5050:C:OP2	2.26	0.46
59:LT:88:ARG:NH1	66:Lb:30:GLU:OE2	2.48	0.46
8:SQ:33:LYS:NZ	35:S2:1425:G:O3'	2.49	0.46
35:S2:106:C:OP1	35:S2:431:G:O2'	2.26	0.46
39:L5:293:G:OP1	87:L5:5264:SPM:N1	2.34	0.46
39:L5:1187:G:H2'	39:L5:1188:C:C6	2.50	0.46
39:L5:1846:G:H2'	39:L5:1847:C:C6	2.50	0.46
39:L5:2351:OMC:HM23	39:L5:2351:OMC:H1'	1.71	0.46
43:LB:140:GLU:HA	43:LB:143:LYS:HE3	1.98	0.46
51:LJ:26:VAL:HG11	51:LJ:32:ARG:HB3	1.97	0.46
54:LN:116:LEU:HD22	54:LN:135:ILE:HD11	1.97	0.46
55:LO:119:VAL:N	58:LS:168:THR:O	2.43	0.46
64:LZ:50:PRO:HD3	64:LZ:68:ILE:HG12	1.95	0.46
72:Lh:73:TYR:HB3	72:Lh:79:LYS:HG2	1.97	0.46
83:Lt:117:ARG:HE	83:Lt:119:ARG:H	1.62	0.46
13:SZ:102:LYS:HA	13:SZ:107:VAL:HG23	1.98	0.46
17:Sg:101:PHE:HB3	17:Sg:132:TRP:CZ3	2.51	0.46
22:SG:11:GLY:HA2	35:S2:166:A2M:HM'1	1.97	0.46
35:S2:391:C:H2'	35:S2:392:A:H8	1.80	0.46
35:S2:695:C:H41	35:S2:737:G:N2	2.12	0.46
35:S2:1724:A:H2'	35:S2:1725:U:H6	1.80	0.46
39:L5:88:A:N7	57:LQ:173:LYS:NZ	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:2696:A:H5'	75:Lk:70:LYS:HE2	1.96	0.46
74:Lj:60:GLY:HA2	74:Lj:64:MET:SD	2.55	0.46
82:Ls:39:GLN:O	82:Ls:42:GLN:HG3	2.16	0.46
4:SF:95:HIS:O	4:SF:99:ILE:HD12	2.16	0.46
19:SB:199:LYS:HB2	19:SB:199:LYS:HE2	1.73	0.46
25:SJ:138:ARG:HD2	25:SJ:156:HIS:HB2	1.98	0.46
26:SL:153:LYS:HA	26:SL:153:LYS:HD3	1.73	0.46
33:Sa:23:CYS:HB3	33:Sa:28:ARG:H	1.80	0.46
35:S2:527:C:H2'	35:S2:528:A:C8	2.50	0.46
35:S2:1226:G:N1	35:S2:1639:G7M:OP2	2.43	0.46
37:LW:96:GLN:HB2	37:LW:101:ARG:HE	1.80	0.46
39:L5:75:G:O2'	52:LL:101:ARG:NH1	2.40	0.46
39:L5:270:U:H2'	39:L5:271:C:C6	2.51	0.46
39:L5:1996:C:N4	39:L5:2000:G:H22	2.14	0.46
39:L5:3664:G:H2'	39:L5:3665:G:C8	2.50	0.46
39:L5:3723:A:H2'	39:L5:3724:A:C8	2.51	0.46
40:L7:4:U:H2'	40:L7:5:A:H8	1.80	0.46
41:L8:37:A:OP2	72:Lh:89:ARG:HD2	2.16	0.46
41:L8:90:C:H1'	63:LY:24:HIS:HB3	1.98	0.46
62:LX:145:ASP:HB3	62:LX:148:ASP:OD1	2.16	0.46
82:Ls:50:LYS:HG3	82:Ls:101:MET:HE1	1.96	0.46
84:CH:99:ILE:HG23	84:CH:123:LYS:HB3	1.97	0.46
4:SF:60:ARG:HD2	35:S2:1679:A:H2'	1.96	0.46
5:SK:24:LYS:HE3	5:SK:65:ARG:HE	1.79	0.46
22:SG:2:LYS:HG2	22:SG:17:GLU:HG2	1.96	0.46
27:SN:16:LEU:HD12	35:S2:919:A:H5''	1.97	0.46
27:SN:124:ARG:NH2	35:S2:1024:A:OP2	2.41	0.46
30:SW:94:LEU:HD21	30:SW:102:ILE:HG13	1.97	0.46
35:S2:907:G:H2'	35:S2:908:A:H8	1.80	0.46
35:S2:964:A:H2'	35:S2:965:U:C6	2.50	0.46
35:S2:1337:4AC:O5'	35:S2:1337:4AC:H6	2.15	0.46
39:L5:1244:G:H2'	39:L5:1245:C:H6	1.79	0.46
39:L5:2553:A:OP2	39:L5:2574:G:O2'	2.29	0.46
39:L5:4591:U:H2'	39:L5:4592:C:C6	2.50	0.46
3:SD:167:TYR:CD1	3:SD:200:PRO:HG2	2.51	0.46
8:SQ:78:VAL:HG22	35:S2:1673:U:H5''	1.98	0.46
11:ST:42:HIS:NE2	11:ST:43:LYS:HE3	2.30	0.46
17:Sg:82:SER:OG	17:Sg:83:TRP:N	2.49	0.46
18:SA:208:GLU:O	18:SA:212:LYS:HG2	2.16	0.46
19:SB:88:THR:HA	19:SB:98:THR:HA	1.98	0.46
35:S2:1841:C:H2'	35:S2:1842:4AC:H6	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:71:C:H1'	52:LL:62:PRO:O	2.15	0.46
39:L5:1390:G:N2	39:L5:1393:G:OP2	2.41	0.46
39:L5:2303:C:H5''	69:Le:104:SER:HB3	1.98	0.46
39:L5:2824:OMC:HM23	39:L5:2824:OMC:H1'	1.75	0.46
83:Lt:29:ALA:HB1	83:Lt:44:ASP:HB2	1.97	0.46
6:SM:62:VAL:HA	6:SM:65:VAL:HG22	1.98	0.46
10:SS:5:ILE:N	13:SZ:50:PHE:O	2.41	0.46
10:SS:15:VAL:HG22	10:SS:68:ILE:HD11	1.98	0.46
14:Sc:10:LYS:HE2	14:Sc:34:PHE:HE2	1.79	0.46
35:S2:1754:G:N7	35:S2:1779:G:N2	2.64	0.46
39:L5:3848:U:H2'	39:L5:3849:A:C8	2.51	0.46
39:L5:3861:A:H2'	39:L5:3862:A:H8	1.81	0.46
67:Lc:80:GLU:HA	67:Lc:83:THR:HB	1.98	0.46
2:PE:62:C:H2'	2:PE:63:C:C6	2.51	0.46
22:SG:158:VAL:HG21	37:LW:82:ILE:HD11	1.98	0.46
23:SH:162:GLN:O	23:SH:163:GLN:NE2	2.48	0.46
25:SJ:78:LEU:HD22	25:SJ:92:MET:HA	1.97	0.46
30:SW:55:ASP:HB3	34:Sb:25:VAL:HG13	1.97	0.46
35:S2:317:C:H2'	35:S2:318:A:C4	2.51	0.46
35:S2:432:G:H2'	35:S2:433:A:C8	2.51	0.46
35:S2:461:U:H2'	35:S2:462:OMC:C6	2.51	0.46
39:L5:1241:C:H5'	46:LE:72:LYS:NZ	2.31	0.46
39:L5:3599:A:H2'	39:L5:3600:G:H8	1.78	0.46
45:LD:152:ARG:HG3	45:LD:154:THR:HG23	1.98	0.46
45:LD:289:ARG:O	45:LD:292:GLU:HG3	2.16	0.46
52:LL:105:LYS:HB3	52:LL:105:LYS:HE2	1.76	0.46
17:Sg:173:LEU:HD11	17:Sg:187:ASN:HB3	1.99	0.45
20:SC:182:CYS:HB2	30:SW:95:PRO:HB2	1.98	0.45
23:SH:177:TYR:O	23:SH:181:THR:HB	2.16	0.45
27:SN:73:ARG:HH21	35:S2:916:A:H1'	1.82	0.45
32:SY:11:LYS:HB2	32:SY:24:VAL:HG22	1.98	0.45
35:S2:867:OMG:HM23	35:S2:867:OMG:H1'	1.77	0.45
35:S2:1651:A:H2'	35:S2:1652:G:H8	1.81	0.45
37:LW:34:ALA:HA	37:LW:37:GLU:HG2	1.98	0.45
39:L5:691:C:H2'	39:L5:692:A:C8	2.51	0.45
39:L5:1743:A:O4'	45:LD:15:ARG:HD2	2.17	0.45
39:L5:3689:G:O2'	39:L5:3818:UY1:OP2	2.31	0.45
39:L5:3953:G:H1'	39:L5:4060:U:H1'	1.97	0.45
43:LB:17:LEU:O	43:LB:19:ARG:N	2.49	0.45
23:SH:7:LYS:NZ	23:SH:15:LYS:O	2.38	0.45
25:SJ:131:ARG:HA	25:SJ:131:ARG:HD2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:455:A:H2'	35:S2:456:C:H6	1.81	0.45
35:S2:1337:4AC:H2'	35:S2:1338:G:H8	1.81	0.45
39:L5:170:C:H42	39:L5:266:C:H42	1.63	0.45
39:L5:1669:A:H4'	39:L5:1685:G:N2	2.31	0.45
39:L5:1867:A:H2'	39:L5:1868:A:C8	2.51	0.45
39:L5:4910:G:H4'	43:LB:95:THR:HG22	1.99	0.45
41:L8:102:G:OP2	41:L8:104:A:O2'	2.29	0.45
84:CH:92:GLN:HE21	84:CH:110:GLU:CD	2.23	0.45
4:SF:129:GLY:O	4:SF:136:ARG:NH1	2.50	0.45
9:SR:99:ASP:OD2	18:SA:42:LYS:HD2	2.16	0.45
17:Sg:188:HIS:HB3	17:Sg:219:TRP:CE2	2.52	0.45
19:SB:123:ALA:HB2	19:SB:168:MET:HE3	1.98	0.45
23:SH:9:VAL:HG12	23:SH:45:ILE:H	1.82	0.45
35:S2:212:C:N4	35:S2:213:G:O6	2.50	0.45
35:S2:348:A:H2'	35:S2:349:A:C8	2.51	0.45
35:S2:440:G:OP1	35:S2:1798:C:O2'	2.32	0.45
35:S2:637:U:O2	84:CH:49:ASN:ND2	2.45	0.45
35:S2:1208:A:H2'	35:S2:1209:A:H8	1.81	0.45
39:L5:468:U:C5	39:L5:469:C:H5	2.35	0.45
39:L5:1308:C:H2'	39:L5:1309:C:C6	2.51	0.45
39:L5:1705:G:H2'	39:L5:1706:A:O4'	2.16	0.45
39:L5:2570:U:H2'	39:L5:2571:C:C6	2.51	0.45
39:L5:2730:U:H2'	39:L5:2731:C:C6	2.51	0.45
39:L5:4940:C:H5'	39:L5:4941:G:H5''	1.97	0.45
39:L5:5004:C:H2'	39:L5:5005:G:O4'	2.16	0.45
47:LF:46:ARG:O	47:LF:50:ILE:HG12	2.16	0.45
63:LY:82:ILE:HG22	63:LY:83:GLU:H	1.81	0.45
1:AP:2:U:H2'	1:AP:3:C:H6	1.80	0.45
21:SE:22:LYS:HG3	21:SE:23:LEU:HD12	1.99	0.45
26:SL:48:LYS:O	26:SL:52:GLU:HG3	2.16	0.45
27:SN:25:TRP:CD2	34:Sb:82:LYS:HD3	2.51	0.45
34:Sb:55:LEU:HD23	34:Sb:55:LEU:HA	1.85	0.45
35:S2:1718:G:C6	35:S2:1813:A:N6	2.85	0.45
36:LR:20:LYS:HD3	39:L5:2823:G:N7	2.31	0.45
39:L5:37:U:H2'	39:L5:38:A:O4'	2.16	0.45
39:L5:1097:C:H2'	39:L5:1098:G:C8	2.52	0.45
39:L5:4504:C:H2'	39:L5:4505:C:C6	2.52	0.45
39:L5:5002:U:H2'	39:L5:5003:U:C6	2.51	0.45
40:L7:4:U:H2'	40:L7:5:A:C8	2.51	0.45
42:LA:114:CYS:N	42:LA:165:VAL:O	2.49	0.45
44:LC:5:ARG:HD2	44:LC:24:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:LC:318:PRO:HB2	44:LC:325:MET:HE2	1.98	0.45
69:Le:19:LYS:HE3	69:Le:19:LYS:HB3	1.85	0.45
4:SF:127:ARG:HB3	4:SF:136:ARG:HB3	1.98	0.45
6:SM:35:ILE:HD11	6:SM:61:TYR:CE2	2.52	0.45
9:SR:24:LEU:HB3	9:SR:58:MET:SD	2.57	0.45
35:S2:349:A:H2'	35:S2:350:C:C6	2.51	0.45
35:S2:1628:C:H2'	35:S2:1629:C:C6	2.51	0.45
35:S2:1692:U:H2'	35:S2:1693:G:C8	2.52	0.45
39:L5:99:A:H2'	39:L5:100:C:O2	2.17	0.45
39:L5:256:G:H2'	39:L5:257:C:C6	2.51	0.45
39:L5:478:G:OP1	81:Lr:66:ARG:NH2	2.42	0.45
39:L5:1534:A2M:HM'3	39:L5:1637:A:C4	2.52	0.45
39:L5:2654:C:H2'	39:L5:2655:C:H6	1.82	0.45
39:L5:3765:G:O2'	39:L5:3767:C:N4	2.49	0.45
43:LB:299:ILE:HB	43:LB:313:SER:HB3	1.98	0.45
46:LE:95:PRO:HA	46:LE:104:THR:HG22	1.98	0.45
63:LY:31:SER:HA	63:LY:48:PRO:HA	1.99	0.45
13:SZ:73:VAL:HG21	13:SZ:88:LEU:HD21	1.99	0.45
24:SI:38:ILE:HD11	24:SI:96:LEU:HD21	1.98	0.45
24:SI:44:HIS:ND1	35:S2:1740:C:OP1	2.47	0.45
31:SX:105:PHE:CD1	31:SX:121:LYS:HB3	2.52	0.45
35:S2:1722:G:N3	35:S2:1723:G:C8	2.84	0.45
39:L5:1340:OMC:HM23	39:L5:1340:OMC:H1'	1.74	0.45
39:L5:1509:C:H5''	65:La:2:PRO:HD3	1.98	0.45
39:L5:2696:A:H62	75:Lk:35:LYS:NZ	2.14	0.45
44:LC:144:ILE:HG13	44:LC:144:ILE:O	2.16	0.45
80:Lp:51:ALA:HB3	80:Lp:54:ILE:HD12	1.98	0.45
9:SR:3:ARG:HG3	35:S2:1454:A:C8	2.52	0.45
15:Sd:3:HIS:H	15:Sd:3:HIS:CD2	2.35	0.45
17:Sg:205:SER:O	17:Sg:221:LEU:N	2.49	0.45
23:SH:91:HIS:CD2	23:SH:172:THR:HG21	2.52	0.45
35:S2:611:G:H2'	35:S2:612:U:H6	1.82	0.45
39:L5:190:G:H2'	39:L5:191:G:H8	1.82	0.45
39:L5:1179:U:H3'	39:L5:1180:C:H5''	1.98	0.45
39:L5:3726:A:H2'	39:L5:3727:A:C8	2.51	0.45
39:L5:4620:OMU:HM23	39:L5:4620:OMU:H1'	1.81	0.45
39:L5:4859:C:H2'	39:L5:4860:G:C8	2.52	0.45
41:L8:67:U:H2'	41:L8:68:G:C8	2.52	0.45
43:LB:165:HIS:HA	43:LB:179:HIS:O	2.16	0.45
44:LC:163:LYS:HE3	44:LC:163:LYS:HB3	1.74	0.45
49:LH:61:TRP:CZ3	53:LM:33:GLN:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LI:47:PRO:HB3	50:LI:171:TRP:CZ2	2.51	0.45
52:LL:103:ARG:H	52:LL:103:ARG:HD3	1.82	0.45
11:ST:18:LEU:HG	11:ST:134:ILE:HD13	1.98	0.45
11:ST:31:PRO:HB3	11:ST:102:ARG:HH11	1.82	0.45
19:SB:185:VAL:O	19:SB:189:ILE:HG13	2.16	0.45
21:SE:55:ALA:HB1	21:SE:60:GLU:HB2	1.99	0.45
21:SE:89:VAL:HA	21:SE:99:PHE:O	2.17	0.45
26:SL:29:GLY:HA3	26:SL:30:LYS:HA	1.57	0.45
35:S2:528:A:H2'	35:S2:529:A:C8	2.52	0.45
35:S2:883:U:N3	35:S2:904:A:C6	2.85	0.45
39:L5:424:U:H2'	39:L5:425:U:C6	2.52	0.45
39:L5:1961:G:N2	39:L5:2024:G:O2'	2.49	0.45
39:L5:3856:A:H5''	56:LP:83:TRP:O	2.17	0.45
39:L5:4749:C:H2'	39:L5:4750:G:O4'	2.16	0.45
44:LC:36:ILE:HD12	44:LC:122:TYR:CE2	2.52	0.45
53:LM:25:VAL:HB	53:LM:38:VAL:HG13	1.98	0.45
57:LQ:9:LYS:HA	57:LQ:9:LYS:HD3	1.78	0.45
59:LT:28:ALA:O	59:LT:32:ARG:HG2	2.17	0.45
9:SR:83:ASN:C	9:SR:85:VAL:N	2.75	0.45
9:SR:106:LEU:HD21	18:SA:19:LEU:HD11	1.98	0.45
15:Sd:10:HIS:NE2	35:S2:1261:C:O2'	2.44	0.45
21:SE:141:THR:HG23	21:SE:143:ASP:N	2.32	0.45
24:SI:162:LEU:HD11	24:SI:191:GLU:HG2	1.99	0.45
35:S2:1031:A2M:H1'	35:S2:1031:A2M:HM'3	1.63	0.45
39:L5:1392:A:H2'	39:L5:1393:G:C8	2.52	0.45
39:L5:1739:G:N3	39:L5:1742:A:N6	2.65	0.45
39:L5:1773:U:H2'	39:L5:1774:C:C6	2.52	0.45
39:L5:3748:A:H5''	42:LA:243:THR:HB	1.99	0.45
39:L5:3867:A2M:HM'3	39:L5:3867:A2M:H1'	1.58	0.45
42:LA:75:LEU:HD12	42:LA:75:LEU:HA	1.84	0.45
2:PE:41:U:H2'	2:PE:42:G:C8	2.52	0.45
8:SQ:43:GLU:HG2	35:S2:1542:C:O2'	2.17	0.45
18:SA:177:MET:HE1	18:SA:180:ARG:HH21	1.81	0.45
21:SE:18:TRP:HH2	21:SE:31:PRO:HD3	1.81	0.45
21:SE:138:HIS:CD2	21:SE:148:ARG:HG2	2.52	0.45
28:SO:150:ARG:NH2	35:S2:1854:U:OP1	2.45	0.45
34:Sb:72:ARG:HH22	35:S2:1119:A:H2'	1.81	0.45
35:S2:1683:C:H2'	35:S2:1684:C:H6	1.81	0.45
39:L5:120:A:H2'	39:L5:149:A:H61	1.82	0.45
39:L5:318:A:H2'	39:L5:319:A:C8	2.52	0.45
39:L5:1084:C:H2'	39:L5:1085:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:1204:C:H2'	39:L5:1205:G:C8	2.52	0.45
39:L5:1444:G:N2	39:L5:2103:G:H1	2.15	0.45
39:L5:4318:C:H4'	79:Lo:17:LYS:HA	1.99	0.45
48:LG:105:GLU:HB2	48:LG:109:GLU:HB3	1.98	0.45
49:LH:24:THR:HA	49:LH:37:ASP:HA	1.99	0.45
49:LH:27:VAL:HG12	49:LH:84:VAL:HG21	1.98	0.45
64:LZ:42:LEU:HD21	64:LZ:96:VAL:HG12	1.99	0.45
81:Lr:28:GLU:OE2	81:Lr:31:ASN:ND2	2.42	0.45
82:Ls:17:ILE:HG22	82:Ls:54:LEU:HD21	1.99	0.45
83:Lt:16:ARG:HE	83:Lt:17:CYS:N	2.09	0.45
9:SR:29:HIS:HA	9:SR:32:LYS:HE3	1.99	0.44
14:Sc:29:GLN:HG2	14:Sc:45:ASN:HB3	1.99	0.44
20:SC:207:ALA:HB2	35:S2:4:C:H4'	1.99	0.44
22:SG:67:VAL:HG12	22:SG:69:THR:HG22	1.97	0.44
35:S2:689:U:H3'	35:S2:690:G:N2	2.32	0.44
35:S2:1288:OMU:HN3	35:S2:1311:C:H42	1.64	0.44
39:L5:1996:C:H42	39:L5:2000:G:N2	2.15	0.44
39:L5:2298:U:H5''	44:LC:204:ARG:HH21	1.81	0.44
39:L5:4208:U:OP2	59:LT:4:THR:OG1	2.27	0.44
43:LB:292:LEU:HD23	43:LB:292:LEU:HA	1.85	0.44
49:LH:94:SER:OG	49:LH:142:ASP:HB3	2.16	0.44
13:SZ:91:LEU:HG	13:SZ:96:LEU:HD11	1.99	0.44
25:SJ:2:PRO:HG2	35:S2:428:OMU:H4'	1.99	0.44
35:S2:461:U:H2'	35:S2:462:OMC:H6	1.82	0.44
35:S2:563:G:O2'	35:S2:564:A:OP1	2.32	0.44
35:S2:1221:G:H2'	35:S2:1222:G:C8	2.52	0.44
39:L5:3654:G:O2'	39:L5:3693:U:OP1	2.30	0.44
39:L5:4106:G:H3'	39:L5:4107:G:H8	1.82	0.44
39:L5:4775:C:H41	39:L5:4859:C:N4	2.11	0.44
39:L5:4906:C:H2'	39:L5:4907:G:C8	2.52	0.44
22:SG:174:PRO:HB3	35:S2:65:C:C6	2.53	0.44
30:SW:28:ARG:HH22	35:S2:1093:A:H5''	1.82	0.44
33:Sa:45:VAL:HG11	33:Sa:53:ILE:HG13	1.99	0.44
35:S2:159:A2M:HM'3	35:S2:159:A2M:H1'	1.53	0.44
35:S2:885:U:C2	35:S2:901:G:O6	2.69	0.44
35:S2:1227:G:C2	35:S2:1228:A:C8	3.06	0.44
39:L5:185:C:O2'	39:L5:187:U:H5'	2.18	0.44
39:L5:1475:G:H2'	39:L5:1476:C:C6	2.53	0.44
39:L5:1516:G:O2'	52:LL:18:TRP:NE1	2.50	0.44
39:L5:3848:U:H2'	39:L5:3849:A:H8	1.82	0.44
45:LD:41:LYS:NZ	59:LT:30:TYR:O	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LI:152:LEU:HB3	50:LI:165:ILE:HD12	1.99	0.44
52:LL:63:THR:HG21	65:La:66:ASN:HB3	1.99	0.44
57:LQ:172:ARG:NH2	65:La:59:LYS:HA	2.32	0.44
75:Lk:47:ILE:HD11	75:Lk:56:LEU:HD13	1.99	0.44
2:PE:43:A:H2'	2:PE:44:G:C8	2.52	0.44
10:SS:24:ARG:HG3	10:SS:29:ALA:HB2	1.99	0.44
19:SB:111:CYS:HB3	33:Sa:68:TYR:HD2	1.83	0.44
26:SL:103:GLU:HG3	31:SX:11:ARG:HB2	1.98	0.44
27:SN:36:GLN:HG2	27:SN:54:LEU:HD11	2.00	0.44
33:Sa:41:ILE:HG23	33:Sa:68:TYR:HE1	1.83	0.44
35:S2:694:G:H2'	35:S2:695:C:O4'	2.17	0.44
35:S2:874:G:H2'	35:S2:875:A:H8	1.82	0.44
39:L5:432:U:H1'	87:L5:5292:SPM:H82	1.99	0.44
39:L5:492:U:H2'	39:L5:493:G:H8	1.83	0.44
39:L5:2632:PSU:H2'	39:L5:2633:U:C6	2.53	0.44
39:L5:3687:A:O2'	42:LA:236:GLY:N	2.50	0.44
39:L5:4301:U:OP2	39:L5:4303:C:N4	2.51	0.44
39:L5:4536:OMC:HM22	39:L5:4537:C:O4'	2.17	0.44
50:LI:48:LEU:O	50:LI:139:ARG:HA	2.17	0.44
76:Ll:23:ILE:HG23	76:Ll:38:ASN:HB2	1.99	0.44
28:SO:33:ILE:HA	28:SO:41:PHE:O	2.18	0.44
35:S2:1473:G:N2	35:S2:1476:A:OP2	2.46	0.44
39:L5:189:G:H2'	39:L5:190:G:H8	1.83	0.44
39:L5:1081:C:O2'	39:L5:1082:C:H5'	2.17	0.44
39:L5:1188:C:H2'	39:L5:1189:G:H8	1.82	0.44
39:L5:1398:A:N1	39:L5:1419:G:O2'	2.48	0.44
39:L5:1952:G:H4'	58:LS:93:MET:HG2	2.00	0.44
39:L5:2364:OMG:HM23	39:L5:2364:OMG:H1'	1.76	0.44
39:L5:2461:G:H2'	39:L5:2462:C:C6	2.52	0.44
39:L5:3690:U:H2'	39:L5:3691:G:O4'	2.18	0.44
39:L5:3782:5MC:OP1	78:Ln:23:ARG:NH2	2.44	0.44
39:L5:3865:A:H61	39:L5:3881:G:H1	1.65	0.44
39:L5:3911:C:H2'	39:L5:3912:U:C6	2.51	0.44
39:L5:4392:OMG:HM21	39:L5:4394:A:H2'	1.99	0.44
39:L5:4508:C:N3	39:L5:4512:U:H5	2.15	0.44
56:LP:17:SER:HB2	56:LP:98:ALA:HB2	1.98	0.44
79:Lo:6:LYS:HG3	79:Lo:94:GLY:HA3	2.00	0.44
83:Lt:64:ILE:HB	83:Lt:71:ILE:HG13	1.99	0.44
1:AP:23:C:H2'	1:AP:24:A:C8	2.53	0.44
10:SS:40:TYR:CZ	10:SS:97:GLN:HG2	2.52	0.44
10:SS:132:ARG:NH1	35:S2:1623:A:N1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Sg:251:ALA:HB1	17:Sg:286:CYS:HB3	1.98	0.44
18:SA:163:CYS:SG	18:SA:174:MET:HG3	2.58	0.44
22:SG:52:ILE:HA	22:SG:111:LEU:HD23	2.00	0.44
23:SH:166:VAL:O	23:SH:170:VAL:HG13	2.16	0.44
25:SJ:46:VAL:HG21	25:SJ:106:LEU:HD21	1.99	0.44
35:S2:223:C:H2'	35:S2:224:A:C8	2.52	0.44
35:S2:1199:A:H2'	35:S2:1200:A:C8	2.52	0.44
36:LR:171:LYS:O	36:LR:174:GLU:HG3	2.17	0.44
39:L5:1700:G:H5''	39:L5:1704:C:N4	2.33	0.44
39:L5:1881:C:H5'	39:L5:2281:U:H1'	1.98	0.44
39:L5:4524:G:N3	43:LB:252:ALA:HB1	2.33	0.44
43:LB:258:HIS:HA	43:LB:260:ALA:H	1.82	0.44
43:LB:348:ARG:HG2	43:LB:349:LYS:O	2.18	0.44
44:LC:298:ILE:HD13	57:LQ:131:PRO:HB3	1.99	0.44
49:LH:113:GLU:OE2	49:LH:125:ARG:NH1	2.51	0.44
58:LS:5:GLY:O	58:LS:111:ARG:NH2	2.50	0.44
69:Le:91:CYS:HB3	69:Le:95:TYR:HD2	1.83	0.44
69:Le:98:GLU:HG3	69:Le:123:THR:OG1	2.17	0.44
78:Ln:12:ARG:HG3	78:Ln:15:ARG:HH12	1.81	0.44
3:SD:7:LYS:HD3	3:SD:7:LYS:HA	1.84	0.44
3:SD:161:GLY:O	3:SD:164:VAL:HG12	2.17	0.44
8:SQ:76:GLY:HA3	35:S2:1672:U:O3'	2.18	0.44
9:SR:93:GLN:HE21	9:SR:96:ILE:HG12	1.82	0.44
12:SU:67:LYS:HG2	12:SU:78:ASP:HB2	1.99	0.44
21:SE:162:ILE:HG22	21:SE:169:ILE:HD13	1.98	0.44
29:SV:30:ALA:O	29:SV:60:ARG:HD3	2.17	0.44
35:S2:495:U:H2'	35:S2:496:C:O4'	2.18	0.44
39:L5:162:A:H2'	39:L5:163:A:H8	1.83	0.44
39:L5:444:G:H2'	39:L5:445:U:C6	2.52	0.44
39:L5:907:C:H2'	39:L5:908:G:H8	1.82	0.44
39:L5:1613:A:H5''	42:LA:183:GLY:HA2	2.00	0.44
39:L5:1802:A:N3	59:LT:130:ARG:NH2	2.62	0.44
39:L5:1857:C:H2'	39:L5:1858:A:H8	1.82	0.44
39:L5:2411:C:H2'	39:L5:2412:A:C8	2.52	0.44
39:L5:4101:C:N3	39:L5:4107:G:N2	2.66	0.44
39:L5:4911:A:OP2	43:LB:100:ARG:HD3	2.16	0.44
40:L7:110:G:H2'	40:L7:111:C:C6	2.52	0.44
42:LA:115:CYS:SG	42:LA:124:GLY:HA3	2.58	0.44
44:LC:293:LEU:O	44:LC:299:GLN:NE2	2.47	0.44
2:PE:2:C:H2'	2:PE:3:C:C6	2.53	0.44
8:SQ:10:VAL:HG12	8:SQ:98:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SE:89:VAL:HG11	21:SE:119:ALA:HB1	2.00	0.44
21:SE:92:ILE:HG21	32:SY:17:LEU:HD21	2.00	0.44
23:SH:154:ILE:HB	23:SH:185:VAL:HG23	1.98	0.44
35:S2:107:A:H2'	35:S2:108:G:C8	2.53	0.44
35:S2:677:G:H21	35:S2:1028:A:H62	1.65	0.44
39:L5:518:G:N1	39:L5:643:C:H2'	2.33	0.44
39:L5:702:U:H2'	39:L5:703:G:O4'	2.18	0.44
39:L5:1414:C:H2'	39:L5:1415:G:C8	2.45	0.44
42:LA:133:TYR:HB3	42:LA:168:VAL:HG12	1.99	0.44
43:LB:163:ILE:HG22	43:LB:180:LEU:HD22	2.00	0.44
45:LD:55:VAL:HG11	45:LD:158:LYS:HE3	2.00	0.44
49:LH:102:ASN:HB2	49:LH:115:ARG:HB2	2.00	0.44
54:LN:149:GLN:NE2	72:Lh:99:GLU:O	2.51	0.44
60:LU:112:LEU:HD23	60:LU:112:LEU:H	1.82	0.44
23:SH:139:ILE:HG23	23:SH:156:VAL:HG13	2.00	0.44
35:S2:382:C:H2'	35:S2:383:G:C8	2.53	0.44
35:S2:455:A:H2'	35:S2:456:C:C6	2.52	0.44
39:L5:188:G:O2'	39:L5:190:G:OP2	2.24	0.44
39:L5:978:G:H2'	39:L5:979:C:C6	2.53	0.44
39:L5:2583:C:OP2	71:Lg:76:ARG:NH1	2.48	0.44
39:L5:2626:U:O2	60:LU:89:LYS:HD2	2.17	0.44
39:L5:4458:C:H2'	39:L5:4459:U:C6	2.52	0.44
40:L7:52:C:O2'	40:L7:54:A:N7	2.49	0.44
40:L7:119:U:C2	45:LD:261:VAL:HG21	2.53	0.44
63:LY:82:ILE:HD11	63:LY:99:ILE:HD11	2.00	0.44
76:Ll:26:TRP:CD1	76:Ll:26:TRP:H	2.36	0.44
84:CH:85:ARG:HH12	84:CH:106:ILE:HG23	1.83	0.44
4:SF:92:ILE:HD13	4:SF:169:ILE:HG21	2.00	0.43
13:SZ:103:HIS:NE2	35:S2:1593:C:OP1	2.36	0.43
19:SB:186:ASN:HA	19:SB:189:ILE:HD12	2.00	0.43
22:SG:87:ARG:HH22	35:S2:162:C:H5''	1.83	0.43
25:SJ:137:VAL:HG22	25:SJ:157:ILE:HD12	2.00	0.43
29:SV:17:CYS:HB2	29:SV:56:CYS:HB3	1.99	0.43
35:S2:945:U:H2'	35:S2:946:U:C6	2.53	0.43
35:S2:991:G:C6	35:S2:1134:G:H4'	2.52	0.43
35:S2:1232:PSU:H2'	35:S2:1233:G:C8	2.51	0.43
35:S2:1328:OMG:HM23	35:S2:1328:OMG:H1'	1.85	0.43
39:L5:148:C:OP2	48:LG:197:LYS:NZ	2.51	0.43
39:L5:1577:G:O2'	39:L5:1612:G:H4'	2.18	0.43
39:L5:3684:G:H2'	39:L5:3685:C:C6	2.53	0.43
39:L5:4347:G:H2'	39:L5:4348:A:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:L8:39:G:H1'	41:L8:103:A:N6	2.33	0.43
53:LM:104:MET:HE1	55:LO:201:LEU:HD11	2.00	0.43
68:Ld:22:THR:HG23	68:Ld:122:VAL:HG23	2.00	0.43
73:Li:76:ARG:HD3	73:Li:76:ARG:HA	1.72	0.43
84:CH:24:SER:H	84:CH:28:ILE:HG13	1.82	0.43
84:CH:102:LYS:HB3	84:CH:104:GLN:HG2	1.99	0.43
2:PE:75:C:O2'	79:Lo:54:PRO:O	2.26	0.43
10:SS:105:ASN:HA	10:SS:108:ARG:HG2	1.98	0.43
32:SY:103:SER:HB3	32:SY:106:GLN:OE1	2.18	0.43
35:S2:906:U:H2'	35:S2:907:G:C8	2.53	0.43
35:S2:1648:G:O2'	35:S2:1674:G:O6	2.31	0.43
39:L5:267:G:H2'	39:L5:268:G:C8	2.53	0.43
39:L5:3722:G:H2'	39:L5:3723:A:H8	1.83	0.43
43:LB:196:TRP:O	43:LB:199:GLU:HG2	2.18	0.43
63:LY:21:ALA:HB1	63:LY:25:ILE:HG13	2.00	0.43
82:Ls:36:GLY:H	82:Ls:39:GLN:HE21	1.65	0.43
18:SA:8:LEU:HD23	18:SA:59:LEU:HD13	2.00	0.43
37:LW:96:GLN:HB2	37:LW:101:ARG:HH21	1.83	0.43
39:L5:1979:A:C6	39:L5:1980:U:H5	2.36	0.43
39:L5:4238:G:H2'	39:L5:4239:A:H8	1.83	0.43
43:LB:27:GLY:HA2	43:LB:276:HIS:CD2	2.53	0.43
47:LF:241:ASN:O	47:LF:245:ARG:HG2	2.18	0.43
56:LP:107:LEU:HD12	56:LP:152:GLU:HG3	2.00	0.43
69:Le:35:TRP:CH2	69:Le:55:MET:HG2	2.52	0.43
83:Lt:16:ARG:HD3	83:Lt:18:THR:HG22	2.00	0.43
83:Lt:48:LYS:HZ2	83:Lt:52:ASP:HA	1.83	0.43
84:CH:131:LYS:HG2	84:CH:142:GLU:HA	1.99	0.43
3:SD:167:TYR:HD1	3:SD:200:PRO:HG2	1.84	0.43
5:SK:64:TRP:CD1	15:Sd:23:VAL:HG13	2.54	0.43
10:SS:20:ILE:HG22	10:SS:32:ALA:HB3	1.99	0.43
19:SB:77:ASP:N	19:SB:77:ASP:OD1	2.52	0.43
21:SE:139:LEU:O	21:SE:146:THR:HA	2.19	0.43
35:S2:512:A:H4'	35:S2:576:A2M:H2	2.01	0.43
35:S2:896:U:C2	35:S2:897:U:H5	2.37	0.43
35:S2:1255:G:OP1	35:S2:1256:G:O2'	2.28	0.43
35:S2:1752:C:H42	35:S2:1778:C:H42	1.67	0.43
38:CI:66:GLY:HA3	68:Ld:70:LYS:NZ	2.34	0.43
39:L5:754:U:H2'	39:L5:755:C:C6	2.54	0.43
39:L5:1344:C:H1'	52:LL:10:LEU:HD11	1.99	0.43
39:L5:1577:G:C8	42:LA:181:LYS:HE3	2.53	0.43
39:L5:1998:A:O2'	39:L5:1999:A:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:2693:G:OP2	75:Lk:33:LYS:NZ	2.48	0.43
46:LE:186:LEU:HD13	46:LE:212:LEU:HD21	1.99	0.43
56:LP:107:LEU:HD23	56:LP:107:LEU:H	1.83	0.43
60:LU:100:LEU:HD13	60:LU:112:LEU:HD12	2.00	0.43
64:LZ:123:LYS:O	64:LZ:124:THR:OG1	2.27	0.43
1:AP:2:U:H2'	1:AP:3:C:C6	2.53	0.43
2:PE:76:A:H62	39:L5:4371:G:H5'	1.84	0.43
30:SW:115:GLU:HA	30:SW:118:ARG:HB2	2.00	0.43
34:Sb:19:HIS:CD2	34:Sb:21:LYS:H	2.35	0.43
35:S2:490:C:O2'	35:S2:574:A:N1	2.50	0.43
35:S2:906:U:H2'	35:S2:907:G:H8	1.84	0.43
35:S2:1748:G:O6	35:S2:1786:U:O4	2.36	0.43
39:L5:1186:U:H2'	39:L5:1187:G:N3	2.34	0.43
39:L5:1281:G:C6	46:LE:128:HIS:HB2	2.53	0.43
39:L5:1914:C:H4'	55:LO:89:PRO:HD3	2.01	0.43
39:L5:2777:G:H5''	39:L5:2778:G:H5'	2.01	0.43
39:L5:4342:C:O3'	79:Lo:37:GLY:HA3	2.18	0.43
41:L8:150:C:N4	48:LG:52:THR:O	2.49	0.43
44:LC:41:HIS:NE2	44:LC:45:ARG:HD2	2.33	0.43
44:LC:334:THR:HG21	47:LF:51:TYR:OH	2.19	0.43
46:LE:45:SER:C	46:LE:47:ASN:H	2.26	0.43
46:LE:201:ILE:HG13	46:LE:203:ILE:HG23	1.99	0.43
55:LO:126:VAL:HG13	55:LO:127:VAL:HG13	2.00	0.43
64:LZ:9:LYS:HD2	64:LZ:83:THR:O	2.18	0.43
72:Lh:52:LYS:HD3	72:Lh:52:LYS:HA	1.74	0.43
7:SP:29:SER:H	7:SP:32:GLN:NE2	2.17	0.43
10:SS:68:ILE:HA	10:SS:71:MET:HE3	2.00	0.43
16:Sf:116:ARG:HG2	16:Sf:131:PHE:HE2	1.84	0.43
24:SI:12:ARG:NH1	35:S2:103:A:H5'	2.34	0.43
24:SI:72:CYS:HG	24:SI:112:TRP:CG	2.36	0.43
26:SL:111:VAL:HG12	26:SL:140:PHE:HB2	2.00	0.43
28:SO:138:ASP:HB3	35:S2:984:C:O2'	2.18	0.43
35:S2:29:G:H2'	35:S2:30:C:H6	1.83	0.43
35:S2:1098:C:H2'	35:S2:1099:G:C8	2.54	0.43
39:L5:262:G:H2'	39:L5:263:G:C8	2.53	0.43
39:L5:400:A2M:HM'3	39:L5:400:A2M:H1'	1.60	0.43
39:L5:4699:U:H1'	39:L5:4700:A:H5''	1.99	0.43
39:L5:4913:G:H4'	39:L5:4914:C:O5'	2.17	0.43
49:LH:51:LYS:HG3	49:LH:52:LYS:N	2.33	0.43
56:LP:116:HIS:HB3	56:LP:149:ILE:HB	2.00	0.43
6:SM:26:LEU:HD23	6:SM:31:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:SB:127:VAL:HG23	19:SB:177:GLN:HG3	1.99	0.43
24:SI:206:LYS:HD2	24:SI:206:LYS:HA	1.79	0.43
28:SO:145:GLY:O	33:Sa:22:ARG:NH2	2.51	0.43
35:S2:27:A2M:H2'	35:S2:28:U:O4'	2.19	0.43
35:S2:115:U:H2'	35:S2:116:OMU:H6	2.00	0.43
35:S2:189:U:H1'	35:S2:211:G:N2	2.33	0.43
35:S2:845:G:H2'	35:S2:846:G:C8	2.54	0.43
35:S2:1491:G:H2'	35:S2:1492:U:C6	2.54	0.43
39:L5:3830:A2M:HM'3	39:L5:3830:A2M:H1'	1.80	0.43
39:L5:4981:G:O6	43:LB:21:ARG:NH2	2.51	0.43
42:LA:108:PRO:HG3	80:Lp:90:LYS:HD2	2.01	0.43
83:Lt:149:HIS:HA	83:Lt:152:ILE:HG12	2.01	0.43
1:AP:3:C:H42	1:AP:70:A:N6	2.16	0.43
3:SD:196:GLY:HA3	3:SD:201:LYS:HE3	2.01	0.43
12:SU:40:ILE:HG12	12:SU:50:VAL:HG11	2.01	0.43
13:SZ:57:LYS:HA	13:SZ:60:LYS:HG2	1.99	0.43
13:SZ:99:LEU:HD21	13:SZ:102:LYS:HB2	1.99	0.43
17:Sg:133:ASN:HB3	17:Sg:139:LYS:HE2	2.00	0.43
35:S2:1550:G:O2'	35:S2:1558:C:O2	2.33	0.43
39:L5:1806:G:H2'	39:L5:1807:C:H6	1.84	0.43
39:L5:4910:G:H1	55:LO:108:ILE:H	1.67	0.43
44:LC:315:LYS:HD2	47:LF:168:ALA:HB1	2.01	0.43
44:LC:318:PRO:C	44:LC:320:LYS:H	2.26	0.43
50:LI:43:VAL:HG21	50:LI:197:VAL:HG13	2.00	0.43
50:LI:183:ASP:O	50:LI:187:LYS:HG2	2.19	0.43
50:LI:207:ASP:HA	50:LI:210:ARG:HG2	2.00	0.43
7:SP:30:TYR:O	7:SP:34:MET:HG2	2.19	0.43
7:SP:44:ARG:HH21	7:SP:53:GLN:NE2	2.16	0.43
10:SS:121:ARG:HG3	10:SS:131:VAL:HB	2.01	0.43
12:SU:56:MET:HB2	12:SU:86:LYS:HB3	2.00	0.43
17:Sg:11:LEU:HB2	17:Sg:307:VAL:HG23	2.00	0.43
17:Sg:133:ASN:HD21	17:Sg:135:LEU:HB2	1.83	0.43
21:SE:137:PRO:HG2	21:SE:149:TYR:HA	2.01	0.43
24:SI:65:PHE:CD2	24:SI:104:ILE:HD13	2.53	0.43
35:S2:962:A:N1	35:S2:1055:A:O2'	2.50	0.43
37:LW:104:GLN:O	37:LW:107:GLN:HG3	2.19	0.43
39:L5:1084:C:H2'	39:L5:1085:C:C6	2.54	0.43
39:L5:3893:C:H2'	39:L5:3894:A:C8	2.54	0.43
39:L5:4881:U:C4	53:LM:113:MET:HG3	2.54	0.43
39:L5:5024:C:C5	39:L5:5025:C:H1'	2.54	0.43
43:LB:117:ARG:HG2	43:LB:180:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:LM:96:GLU:O	53:LM:100:ARG:HG2	2.19	0.43
56:LP:112:LEU:HD23	56:LP:150:LEU:HD12	2.01	0.43
62:LX:80:PRO:HG2	62:LX:155:ILE:HG21	2.01	0.43
83:Lt:114:ARG:CZ	83:Lt:117:ARG:HD2	2.49	0.43
1:AP:7:G:O2'	1:AP:49:C:O4'	2.34	0.43
2:PE:38:A:O2'	35:S2:1058:A:OP1	2.28	0.43
22:SG:201:LYS:NZ	35:S2:124:U:OP1	2.52	0.43
35:S2:1850:MA6:H8	35:S2:1850:MA6:O5'	2.19	0.43
39:L5:1251:C:H2'	39:L5:1252:C:C6	2.54	0.43
39:L5:1444:G:H22	39:L5:2104:G:H21	1.67	0.43
39:L5:1497:A:N6	57:LQ:175:GLU:O	2.52	0.43
39:L5:2495:U:H2'	39:L5:2496:G:H8	1.84	0.43
39:L5:4594:U:H2'	39:L5:4595:G:C8	2.50	0.43
39:L5:5053:U:H5'	39:L5:5054:C:C5	2.54	0.43
48:LG:120:LYS:HA	48:LG:120:LYS:HD3	1.81	0.43
80:Lp:85:ARG:O	80:Lp:88:GLU:HG2	2.19	0.43
1:AP:43:A:H2'	1:AP:44:A:C8	2.54	0.42
3:SD:62:LYS:HE3	3:SD:62:LYS:HB3	1.89	0.42
8:SQ:90:LYS:HA	8:SQ:93:VAL:HG22	2.01	0.42
25:SJ:136:ARG:NH1	25:SJ:139:LYS:HA	2.34	0.42
35:S2:573:U:O2	35:S2:576:A2M:H8	2.19	0.42
35:S2:746:C:O2'	35:S2:798:G:N2	2.41	0.42
35:S2:1279:C:H2'	35:S2:1280:G:H8	1.84	0.42
35:S2:1286:G:N2	35:S2:1312:G:O2'	2.52	0.42
39:L5:170:C:H42	39:L5:266:C:N4	2.17	0.42
39:L5:460:C:H2'	39:L5:461:G:H8	1.84	0.42
39:L5:1333:A:H2'	39:L5:1334:A:H8	1.82	0.42
39:L5:1444:G:N2	39:L5:2104:G:H21	2.16	0.42
39:L5:1743:A:H5'	45:LD:11:ALA:HB1	2.00	0.42
39:L5:2664:G:H4'	39:L5:2677:G:H4'	2.00	0.42
56:LP:122:ALA:HB3	56:LP:143:PRO:HG2	2.00	0.42
60:LU:65:ARG:HG3	60:LU:70:ILE:HG13	2.00	0.42
81:Lr:65:LYS:O	81:Lr:102:TYR:OH	2.29	0.42
82:Ls:13:TYR:O	82:Ls:17:ILE:HG23	2.19	0.42
4:SF:162:ALA:HB3	4:SF:169:ILE:HD13	2.00	0.42
18:SA:53:ARG:HD2	29:SV:83:PHE:CZ	2.54	0.42
22:SG:133:LEU:HD21	35:S2:168:C:O2	2.19	0.42
22:SG:198:ARG:O	22:SG:201:LYS:HG3	2.19	0.42
33:Sa:13:LYS:HD3	33:Sa:13:LYS:HA	1.73	0.42
35:S2:27:A2M:H1'	35:S2:27:A2M:HM'3	1.57	0.42
35:S2:511:U:H2'	35:S2:512:A:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:644:OMG:HM23	35:S2:644:OMG:H1'	1.89	0.42
39:L5:667:A:H5''	39:L5:668:C:H5''	2.01	0.42
39:L5:947:C:OP1	44:LC:336:ARG:NH1	2.50	0.42
39:L5:1503:A:H4'	39:L5:1504:G:H5'	2.00	0.42
39:L5:1514:U:H2'	39:L5:1515:A:C8	2.53	0.42
39:L5:2569:G:H2'	39:L5:2570:U:C6	2.54	0.42
39:L5:4859:C:H2'	39:L5:4860:G:H8	1.84	0.42
40:L7:49:A:N6	45:LD:57:ASN:O	2.53	0.42
43:LB:214:ASP:OD2	43:LB:362:LYS:HA	2.19	0.42
44:LC:150:LEU:O	44:LC:152:LEU:N	2.53	0.42
46:LE:128:HIS:ND1	46:LE:128:HIS:O	2.52	0.42
55:LO:58:LEU:HD23	55:LO:58:LEU:HA	1.85	0.42
55:LO:140:ARG:O	55:LO:144:GLU:HG3	2.19	0.42
72:Lh:89:ARG:O	72:Lh:93:ARG:HG2	2.19	0.42
4:SF:145:ARG:HD3	14:Sc:47:LYS:HG3	2.01	0.42
12:SU:51:LYS:HD3	12:SU:51:LYS:HA	1.74	0.42
12:SU:61:LEU:HB2	12:SU:82:MET:HB3	2.01	0.42
19:SB:137:LEU:HD13	19:SB:215:VAL:HB	2.01	0.42
22:SG:136:LYS:HB2	35:S2:65:C:H41	1.84	0.42
23:SH:50:GLU:OE2	23:SH:58:LYS:HB3	2.20	0.42
23:SH:165:ASN:HA	23:SH:168:HIS:HE2	1.84	0.42
35:S2:115:U:H2'	35:S2:116:OMU:C6	2.48	0.42
35:S2:205:G:H2'	35:S2:206:G:C8	2.54	0.42
35:S2:656:G:H5'	35:S2:662:G:N2	2.34	0.42
39:L5:31:U:H2'	39:L5:32:G:O4'	2.19	0.42
39:L5:1494:U:H2'	39:L5:1495:G:H8	1.84	0.42
39:L5:4680:G:H2'	39:L5:4681:A:C8	2.53	0.42
42:LA:234:LYS:HG3	42:LA:234:LYS:O	2.19	0.42
43:LB:161:ARG:HG2	43:LB:184:GLN:HA	2.01	0.42
43:LB:302:ASN:HB2	43:LB:313:SER:HA	2.02	0.42
57:LQ:19:LYS:HE3	57:LQ:19:LYS:HB3	1.88	0.42
1:AP:18:G:O6	1:AP:55:U:C2	2.72	0.42
8:SQ:51:LEU:HG	8:SQ:81:ILE:HG23	2.02	0.42
17:Sg:172:LYS:HE3	17:Sg:193:GLY:HA2	2.01	0.42
20:SC:253:PRO:HA	20:SC:256:TRP:CE2	2.54	0.42
24:SI:199:LEU:HD23	24:SI:199:LEU:HA	1.93	0.42
34:Sb:54:VAL:HG23	34:Sb:63:LEU:HB2	2.00	0.42
35:S2:150:A:N6	35:S2:168:C:C2	2.88	0.42
35:S2:291:G:H2'	35:S2:292:A:C8	2.54	0.42
35:S2:1824:A:O2'	35:S2:1825:A:O4'	2.30	0.42
39:L5:123:C:H2'	39:L5:124:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:162:A:H2'	39:L5:163:A:C8	2.54	0.42
39:L5:1324:A:O2'	39:L5:1326:A2M:OP1	2.30	0.42
39:L5:1633:G:H5'	39:L5:1634:A:OP1	2.19	0.42
39:L5:1683:PSU:H2'	39:L5:1684:A:C8	2.54	0.42
39:L5:2306:G:H1'	39:L5:2332:A:N6	2.34	0.42
39:L5:2478:C:H2'	39:L5:2479:G:H5'	2.01	0.42
39:L5:2676:A:OP2	39:L5:2676:A:H8	2.02	0.42
39:L5:3723:A:H2'	39:L5:3724:A:H8	1.85	0.42
39:L5:4523:A2M:HM'3	39:L5:4523:A2M:H1'	1.85	0.42
46:LE:209:PRO:HB2	46:LE:212:LEU:HD13	2.02	0.42
63:LY:82:ILE:HD12	63:LY:85:VAL:HG21	2.01	0.42
82:Ls:121:VAL:HG23	82:Ls:160:LEU:HD22	2.01	0.42
83:Lt:134:GLY:HA2	83:Lt:137:GLN:CD	2.43	0.42
1:AP:24:A:H2'	1:AP:25:C:C6	2.54	0.42
3:SD:8:LYS:HG2	12:SU:61:LEU:HD11	2.02	0.42
19:SB:167:LYS:O	19:SB:170:GLU:HG3	2.20	0.42
19:SB:226:GLY:HA2	39:L5:4101:C:OP1	2.19	0.42
35:S2:1376:A:H2'	35:S2:1377:U:O4'	2.20	0.42
35:S2:1560:U:H2'	35:S2:1561:A:H8	1.83	0.42
35:S2:1562:C:H2'	35:S2:1563:G:C8	2.53	0.42
39:L5:270:U:H2'	39:L5:271:C:H6	1.84	0.42
39:L5:907:C:H2'	39:L5:908:G:C8	2.54	0.42
39:L5:1806:G:H2'	39:L5:1807:C:C6	2.55	0.42
39:L5:2020:U:H2'	39:L5:2021:G:H8	1.83	0.42
39:L5:2079:G:H2'	39:L5:2080:U:C6	2.55	0.42
39:L5:2297:G:H4'	44:LC:242:PRO:HB2	2.00	0.42
39:L5:2372:U:H2'	39:L5:2373:C:C6	2.55	0.42
39:L5:3707:U:H2'	39:L5:3708:C:C6	2.54	0.42
42:LA:186:TYR:HB2	42:LA:196:TRP:CZ3	2.54	0.42
45:LD:107:ARG:HD2	45:LD:107:ARG:HA	1.74	0.42
51:LJ:95:ARG:HD2	51:LJ:177:GLY:HA3	2.01	0.42
66:Lb:96:LEU:HD23	66:Lb:96:LEU:HA	1.86	0.42
68:Ld:36:VAL:HG21	68:Ld:44:ARG:HD3	2.01	0.42
74:Lj:67:LEU:HD23	74:Lj:67:LEU:HA	1.84	0.42
21:SE:72:ILE:HD12	21:SE:90:ILE:HD12	2.02	0.42
22:SG:234:LEU:HD21	35:S2:787:G:H3'	2.01	0.42
23:SH:130:LEU:HB2	23:SH:177:TYR:HE2	1.84	0.42
25:SJ:17:ARG:NH1	35:S2:21:U:O2	2.52	0.42
26:SL:120:VAL:HG22	26:SL:145:VAL:HG11	2.01	0.42
27:SN:54:LEU:HD12	27:SN:60:VAL:HG21	2.01	0.42
30:SW:115:GLU:HB3	30:SW:118:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:1869:G:C6	88:L5:5286:SPD:H31	2.54	0.42
39:L5:2284:G:OP1	65:La:7:LYS:NZ	2.47	0.42
39:L5:2375:A:H2'	39:L5:2376:A:C8	2.55	0.42
39:L5:2459:G:N2	39:L5:2462:C:OP2	2.47	0.42
39:L5:5024:C:H41	39:L5:5028:G:H21	1.67	0.42
51:LJ:78:LYS:HE3	51:LJ:82:ILE:HD11	2.02	0.42
51:LJ:165:TRP:CZ2	51:LJ:169:LYS:HD3	2.55	0.42
10:SS:13:LEU:HD22	10:SS:20:ILE:HD11	2.01	0.42
21:SE:159:THR:HB	21:SE:173:ILE:HB	2.01	0.42
22:SG:133:LEU:HB2	35:S2:65:C:N3	2.35	0.42
23:SH:33:ASN:ND2	23:SH:36:LEU:HB3	2.34	0.42
30:SW:22:LYS:HD3	34:Sb:3:LEU:HA	2.01	0.42
34:Sb:34:ASP:O	34:Sb:79:PHE:HA	2.20	0.42
35:S2:323:C:O2'	35:S2:325:C:N4	2.53	0.42
35:S2:674:C:H2'	35:S2:675:U:C6	2.54	0.42
39:L5:138:G:H2'	39:L5:139:G:H8	1.85	0.42
39:L5:1317:U:H2'	39:L5:1318:C:C6	2.55	0.42
39:L5:1788:A:H2'	50:LI:22:PHE:CZ	2.55	0.42
39:L5:2021:G:OP1	82:Ls:58:ASN:N	2.40	0.42
39:L5:4274:A:H2'	39:L5:4275:G:H8	1.81	0.42
39:L5:5055:G:N2	68:Ld:118:GLN:OE1	2.51	0.42
43:LB:337:VAL:HG11	43:LB:345:LEU:HD13	2.01	0.42
55:LO:189:ILE:HG22	55:LO:193:THR:OG1	2.19	0.42
4:SF:49:LEU:HD12	8:SQ:50:LYS:HG2	2.00	0.42
10:SS:99:LEU:HD12	10:SS:99:LEU:O	2.19	0.42
13:SZ:80:ARG:HD3	13:SZ:80:ARG:HA	1.75	0.42
22:SG:200:LYS:O	22:SG:204:GLU:HG2	2.20	0.42
23:SH:163:GLN:O	23:SH:167:GLU:HG2	2.20	0.42
35:S2:434:G:H2'	35:S2:435:A:C8	2.55	0.42
35:S2:496:C:H2'	35:S2:497:C:C6	2.55	0.42
35:S2:1103:C:H2'	35:S2:1104:G:C8	2.54	0.42
35:S2:1829:G:H1'	35:S2:1850:MA6:H2	2.02	0.42
35:S2:1839:U:H2'	35:S2:1840:U:C6	2.55	0.42
39:L5:257:C:H2'	39:L5:258:G:C8	2.55	0.42
39:L5:267:G:H2'	39:L5:268:G:H8	1.84	0.42
39:L5:654:C:OP1	44:LC:268:ARG:NH2	2.53	0.42
39:L5:1662:C:H2'	39:L5:1663:C:H6	1.85	0.42
39:L5:2459:G:H2'	39:L5:2461:G:OP2	2.19	0.42
39:L5:2497:C:H2'	39:L5:2498:C:C6	2.55	0.42
39:L5:4119:C:H42	71:Lg:100:GLN:CD	2.28	0.42
39:L5:4691:A:OP1	49:LH:75:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L5:4739:C:H2'	39:L5:4740:G:H5'	2.01	0.42
43:LB:136:LYS:HA	43:LB:139:ASP:OD1	2.20	0.42
55:LO:62:MET:HG2	55:LO:65:ASN:H	1.85	0.42
67:Lc:13:SER:HB3	67:Lc:17:ARG:NH1	2.35	0.42
74:Lj:52:LYS:O	74:Lj:55:ARG:HG2	2.19	0.42
81:Lr:38:PHE:O	81:Lr:45:HIS:NE2	2.42	0.42
83:Lt:114:ARG:HG3	83:Lt:133:LEU:HD11	2.02	0.42
3:SD:134:CYS:SG	3:SD:135:GLU:N	2.93	0.42
4:SF:84:GLY:O	35:S2:1673:U:O2'	2.35	0.42
5:SK:3:MET:HE1	5:SK:48:ALA:HB2	2.01	0.42
12:SU:64:THR:HG22	12:SU:77:TRP:CE3	2.55	0.42
17:Sg:164:ILE:HD12	17:Sg:178:ASN:HA	2.01	0.42
18:SA:137:ALA:HB1	18:SA:142:LEU:HB3	2.01	0.42
23:SH:82:GLU:O	23:SH:86:LYS:HG2	2.20	0.42
23:SH:130:LEU:HB2	23:SH:177:TYR:CE2	2.55	0.42
28:SO:74:ALA:HB1	28:SO:115:ALA:HB2	2.00	0.42
35:S2:342:C:H2'	35:S2:343:A:H8	1.85	0.42
35:S2:1306:U:H2'	35:S2:1307:U:C6	2.55	0.42
35:S2:1558:C:H2'	35:S2:1559:C:C6	2.55	0.42
35:S2:1681:U:H2'	35:S2:1682:C:C6	2.55	0.42
35:S2:1781:A:H5''	35:S2:1783:C:N4	2.35	0.42
39:L5:716:C:OP1	44:LC:317:ASN:HB2	2.20	0.42
39:L5:964:A:C6	39:L5:966:A:H1'	2.55	0.42
39:L5:1962:A:H2	39:L5:2024:G:H21	1.67	0.42
39:L5:2448:G:H2'	39:L5:2449:A:C8	2.55	0.42
39:L5:2631:U:O4	60:LU:51:GLY:N	2.51	0.42
39:L5:4113:U:H4'	39:L5:4115:G:C6	2.54	0.42
39:L5:4139:G:H1'	39:L5:4146:G:C6	2.54	0.42
39:L5:4622:A:H4'	43:LB:13:SER:HB2	2.01	0.42
45:LD:33:ARG:O	45:LD:37:VAL:HG22	2.20	0.42
55:LO:124:LEU:HD23	55:LO:124:LEU:HA	1.88	0.42
62:LX:65:ALA:HB2	72:Lh:69:LEU:HD11	2.02	0.42
83:Lt:79:ALA:HA	83:Lt:82:ILE:HG12	2.01	0.42
3:SD:106:ARG:HG3	3:SD:175:VAL:HG22	2.01	0.42
11:ST:114:GLU:HB3	11:ST:124:THR:HG22	2.02	0.42
13:SZ:99:LEU:HD12	13:SZ:109:TYR:CE1	2.55	0.42
17:Sg:23:THR:HB	17:Sg:31:ILE:HG13	2.01	0.42
20:SC:121:ARG:NH1	20:SC:123:ARG:HD3	2.35	0.42
21:SE:181:CYS:HA	21:SE:227:VAL:HA	2.02	0.42
21:SE:240:ARG:NE	21:SE:241:GLY:H	2.18	0.42
35:S2:15:U:H2'	35:S2:16:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:887:U:H3	35:S2:900:C:H5	1.68	0.42
35:S2:980:A:H2'	35:S2:981:A:C8	2.54	0.42
35:S2:1279:C:H2'	35:S2:1280:G:C8	2.54	0.42
35:S2:1457:U:H2'	35:S2:1458:G:C8	2.55	0.42
39:L5:163:A:H2'	39:L5:164:G:H8	1.84	0.42
39:L5:481:G:H2'	39:L5:482:G:C8	2.55	0.42
39:L5:1204:C:H2'	39:L5:1205:G:H8	1.85	0.42
39:L5:1283:G:N1	39:L5:2076:G:OP1	2.41	0.42
39:L5:2029:A:H2'	39:L5:2030:A:C8	2.54	0.42
39:L5:3685:C:H5'	42:LA:193:ARG:CZ	2.50	0.42
39:L5:4345:C:H2'	39:L5:4346:U:C6	2.55	0.42
39:L5:4585:U:H2'	39:L5:4586:G:C8	2.55	0.42
45:LD:41:LYS:HD2	59:LT:93:ILE:HD13	2.01	0.42
46:LE:133:PHE:O	46:LE:138:ARG:NH2	2.48	0.42
50:LI:146:GLU:HG2	50:LI:147:HIS:N	2.35	0.42
52:LL:182:LEU:HA	73:LI:7:MET:HE1	2.01	0.42
10:SS:106:LYS:HD2	10:SS:106:LYS:HA	1.83	0.41
17:Sg:207:CYS:SG	17:Sg:219:TRP:HB2	2.60	0.41
21:SE:254:LYS:HE3	21:SE:254:LYS:HB3	1.88	0.41
24:SI:45:THR:HG23	24:SI:53:LYS:HG3	2.02	0.41
25:SJ:179:LYS:HA	25:SJ:182:GLN:HG3	2.02	0.41
30:SW:111:MET:HE2	30:SW:119:LYS:HD2	2.01	0.41
31:SX:67:ARG:HG3	31:SX:115:ILE:HG12	2.02	0.41
35:S2:160:U:O2'	35:S2:161:U:H3'	2.20	0.41
35:S2:1365:G:H2'	35:S2:1366:G:H8	1.85	0.41
35:S2:1709:G:HO2'	39:L5:3763:A:H61	1.67	0.41
39:L5:1248:C:H2'	39:L5:1249:C:H6	1.85	0.41
39:L5:4761:G:P	55:LO:37:ARG:HH22	2.43	0.41
39:L5:4893:A:OP1	55:LO:188:LYS:NZ	2.36	0.41
42:LA:171:GLY:O	80:Lp:68:ALA:HB2	2.21	0.41
43:LB:238:LYS:HE2	43:LB:238:LYS:HB2	1.86	0.41
44:LC:143:ARG:HA	44:LC:143:ARG:HD2	1.93	0.41
45:LD:118:ILE:H	45:LD:118:ILE:HD12	1.85	0.41
46:LE:224:LYS:HD3	46:LE:227:HIS:ND1	2.35	0.41
53:LM:33:GLN:O	53:LM:33:GLN:HG2	2.19	0.41
83:Lt:48:LYS:HA	83:Lt:48:LYS:HD2	1.75	0.41
4:SF:101:HIS:HB2	4:SF:108:PRO:HG3	2.02	0.41
11:ST:84:ARG:NH2	35:S2:1605:G:OP1	2.53	0.41
17:Sg:24:THR:HG22	17:Sg:26:GLN:N	2.34	0.41
23:SH:43:LEU:HD12	23:SH:72:PHE:CD2	2.55	0.41
24:SI:174:CYS:HB2	24:SI:190:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SN:39:LYS:O	27:SN:42:LYS:HG3	2.20	0.41
27:SN:87:ASP:OD1	27:SN:87:ASP:N	2.50	0.41
33:Sa:10:ARG:HH12	35:S2:1859:A:P	2.43	0.41
35:S2:52:G:H2'	35:S2:53:C:H6	1.85	0.41
35:S2:93:PSU:H2'	35:S2:94:G:O4'	2.20	0.41
35:S2:509:OMG:H2'	35:S2:510:G:H8	1.85	0.41
35:S2:1438:A:H2'	35:S2:1439:A:H8	1.86	0.41
35:S2:1813:A:C3'	35:S2:1814:G:H5'	2.50	0.41
39:L5:1195:G:H2'	39:L5:1196:G:C8	2.55	0.41
39:L5:1578:U:H2'	39:L5:1579:C:C6	2.55	0.41
39:L5:3709:U:H2'	39:L5:3710:G:O4'	2.19	0.41
39:L5:4776:G:O6	39:L5:4859:C:N4	2.53	0.41
41:L8:36:G:C5	72:Lh:89:ARG:HD3	2.55	0.41
43:LB:39:LYS:HA	43:LB:39:LYS:HD2	1.89	0.41
51:LJ:94:LEU:O	51:LJ:174:ILE:HA	2.20	0.41
55:LO:28:LEU:HD23	55:LO:28:LEU:HA	1.94	0.41
58:LS:16:CYS:SG	58:LS:54:MET:HG2	2.60	0.41
66:Lb:105:GLY:O	66:Lb:109:ARG:HG2	2.20	0.41
80:Lp:46:LYS:HD2	80:Lp:46:LYS:HA	1.89	0.41
4:SF:134:VAL:HG11	4:SF:199:VAL:HB	2.02	0.41
10:SS:62:ASP:O	10:SS:65:GLU:HG3	2.19	0.41
25:SJ:162:ARG:HH22	35:S2:583:A:P	2.43	0.41
27:SN:60:VAL:HG13	27:SN:66:VAL:HG21	2.02	0.41
29:SV:11:LEU:HD12	29:SV:12:TYR:HD1	1.85	0.41
35:S2:675:U:H2'	35:S2:676:C:H6	1.85	0.41
35:S2:1320:G:H2'	35:S2:1321:G:O4'	2.20	0.41
35:S2:1382:A:H2'	35:S2:1383:A2M:H8	2.02	0.41
35:S2:1568:C:H2'	35:S2:1569:A:C8	2.55	0.41
39:L5:1811:G:H2'	39:L5:1812:C:C6	2.56	0.41
39:L5:2422:OMC:HM23	39:L5:2422:OMC:H1'	1.83	0.41
39:L5:3946:G:H2'	39:L5:3947:A:H8	1.85	0.41
39:L5:4098:A:H2'	39:L5:4099:G:H4'	2.02	0.41
39:L5:5057:C:H2'	39:L5:5058:A:C8	2.55	0.41
44:LC:283:LYS:HB3	44:LC:283:LYS:HE2	1.83	0.41
45:LD:120:GLU:O	45:LD:248:ARG:NH1	2.53	0.41
47:LF:182:TYR:HB3	47:LF:200:ARG:HG3	2.02	0.41
50:LI:54:SER:HB3	50:LI:135:ILE:HD11	2.02	0.41
68:Ld:37:GLY:O	68:Ld:41:ARG:HG3	2.19	0.41
2:PE:61:C:H2'	2:PE:62:C:H6	1.84	0.41
18:SA:57:LYS:HD2	18:SA:57:LYS:HA	1.87	0.41
21:SE:141:THR:HG23	21:SE:143:ASP:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SE:256:LEU:HD13	21:SE:259:LYS:HD3	2.01	0.41
23:SH:138:GLU:HG2	23:SH:159:ASP:OD1	2.21	0.41
30:SW:57:ARG:HD2	35:S2:919:A:H4'	2.03	0.41
35:S2:99:A2M:H8	35:S2:99:A2M:O5'	2.20	0.41
35:S2:116:OMU:H1'	35:S2:116:OMU:HM23	1.83	0.41
35:S2:428:OMU:H6	35:S2:428:OMU:H2'	1.90	0.41
35:S2:656:G:N2	35:S2:663:C:H5''	2.35	0.41
35:S2:1365:G:H2'	35:S2:1366:G:C8	2.55	0.41
35:S2:1597:C:H4'	35:S2:1603:G:O6	2.20	0.41
39:L5:724:C:H1'	44:LC:343:GLN:HG2	2.03	0.41
39:L5:1489:G:C5'	65:La:131:ARG:HH12	2.33	0.41
39:L5:1693:U:H2'	39:L5:1694:C:O4'	2.20	0.41
39:L5:2060:G:N2	58:LS:115:ALA:HB2	2.36	0.41
39:L5:5002:U:H2'	39:L5:5003:U:H6	1.85	0.41
43:LB:10:ARG:NH2	43:LB:265:SER:O	2.46	0.41
55:LO:12:ARG:HD3	55:LO:37:ARG:NH2	2.34	0.41
60:LU:107:LYS:O	60:LU:108:GLU:HG3	2.21	0.41
70:Lf:46:ARG:HH21	70:Lf:89:ARG:NH2	2.18	0.41
4:SF:134:VAL:N	4:SF:203:ASN:HD21	2.18	0.41
18:SA:22:GLY:C	18:SA:24:HIS:H	2.28	0.41
18:SA:51:LEU:HD23	18:SA:51:LEU:HA	1.88	0.41
23:SH:36:LEU:HD21	23:SH:79:LEU:HB3	2.03	0.41
24:SI:23:LYS:HE2	24:SI:23:LYS:HB3	1.79	0.41
24:SI:129:LEU:HD12	24:SI:129:LEU:HA	1.92	0.41
29:SV:43:THR:HG23	29:SV:45:ARG:HB2	2.03	0.41
35:S2:441:C:H2'	35:S2:442:C:C6	2.55	0.41
35:S2:550:C:H5'	84:CH:19:ALA:HB3	2.01	0.41
39:L5:123:C:H2'	39:L5:124:C:C6	2.54	0.41
39:L5:264:C:H2'	39:L5:265:C:C5	2.55	0.41
39:L5:679:C:H2'	39:L5:680:G:H8	1.84	0.41
39:L5:755:C:H2'	39:L5:756:G:H8	1.85	0.41
39:L5:1356:U:H2'	39:L5:1357:C:C6	2.56	0.41
39:L5:1541:C:H5''	42:LA:21:LYS:HG2	2.02	0.41
39:L5:1697:G:H2'	39:L5:1698:C:C6	2.55	0.41
39:L5:2110:C:N4	39:L5:2111:G:O6	2.53	0.41
39:L5:4625:C:O2'	39:L5:4626:A:H5'	2.20	0.41
39:L5:4991:U:H2'	39:L5:4992:G:C8	2.56	0.41
41:L8:40:A:H2'	41:L8:41:A:C8	2.56	0.41
43:LB:112:ASP:O	43:LB:116:ARG:HG3	2.20	0.41
55:LO:78:ARG:HA	55:LO:78:ARG:HD2	1.90	0.41
76:Ll:25:GLN:OE1	76:Ll:28:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Lt:37:LEU:HD23	83:Lt:40:LYS:HZ1	1.86	0.41
4:SF:91:ARG:HD2	13:SZ:103:HIS:CE1	2.56	0.41
8:SQ:39:LEU:HD21	8:SQ:51:LEU:HB3	2.03	0.41
9:SR:83:ASN:HB3	9:SR:84:TYR:H	1.67	0.41
12:SU:67:LYS:HE3	12:SU:76:THR:HG22	2.03	0.41
20:SC:168:GLY:N	20:SC:179:THR:O	2.35	0.41
25:SJ:120:ALA:HB2	25:SJ:129:LEU:HD12	2.03	0.41
35:S2:600:G:H2'	35:S2:601:OMG:H8	1.86	0.41
35:S2:1407:U:H2'	35:S2:1408:U:C6	2.56	0.41
35:S2:1672:U:H2'	35:S2:1673:U:C6	2.55	0.41
35:S2:1775:U:H2'	35:S2:1776:G:C4	2.55	0.41
36:LR:183:GLU:O	36:LR:186:LYS:HG3	2.21	0.41
39:L5:300:A:H2'	39:L5:301:G:H8	1.85	0.41
39:L5:469:C:N4	46:LE:101:ASN:OD1	2.53	0.41
39:L5:1197:C:H2'	39:L5:1198:G:C8	2.54	0.41
39:L5:1244:G:H2'	39:L5:1245:C:C6	2.54	0.41
39:L5:1327:C:H2'	39:L5:1328:G:C8	2.56	0.41
39:L5:1794:A:H5''	39:L5:4214:A:N6	2.35	0.41
39:L5:2000:G:O2'	39:L5:2001:G:N7	2.51	0.41
39:L5:2293:U:H2'	39:L5:2294:G:C8	2.56	0.41
39:L5:4507:A:H2'	39:L5:4508:C:C6	2.55	0.41
39:L5:4638:U:H2'	39:L5:4639:G:N3	2.36	0.41
60:LU:23:LEU:HD13	60:LU:110:TYR:HB2	2.03	0.41
63:LY:56:GLN:HB3	63:LY:67:ILE:HD13	2.03	0.41
65:La:7:LYS:HB3	65:La:7:LYS:HE2	1.82	0.41
4:SF:97:PHE:HA	4:SF:100:ILE:HG12	2.02	0.41
4:SF:126:THR:O	4:SF:136:ARG:HB3	2.20	0.41
8:SQ:42:ILE:HD13	8:SQ:42:ILE:HA	1.89	0.41
11:ST:104:LEU:HB3	11:ST:121:ARG:HD2	2.03	0.41
22:SG:3:LEU:HB3	22:SG:5:ILE:HD11	2.02	0.41
22:SG:137:ARG:O	22:SG:141:ILE:HD12	2.20	0.41
35:S2:1525:C:H2'	35:S2:1526:G:H8	1.86	0.41
39:L5:86:U:H2'	39:L5:87:A:C8	2.56	0.41
39:L5:153:G:H2'	39:L5:154:G:H8	1.85	0.41
39:L5:655:C:P	44:LC:268:ARG:HH12	2.44	0.41
39:L5:1794:A:H5''	39:L5:4214:A:H61	1.85	0.41
39:L5:1824:G:H2'	39:L5:1825:A:C8	2.56	0.41
39:L5:1857:C:H2'	39:L5:1858:A:C8	2.55	0.41
39:L5:1978:C:H2'	39:L5:1979:A:C8	2.55	0.41
39:L5:3822:PSU:H3'	39:L5:3823:G:N2	2.36	0.41
43:LB:291:TYR:CD2	43:LB:327:THR:HG23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LD:179:ARG:HD3	45:LD:179:ARG:HA	1.84	0.41
47:LF:92:VAL:O	47:LF:120:GLY:HA2	2.20	0.41
52:LL:142:GLU:HG3	52:LL:146:LEU:HD12	2.03	0.41
66:Lb:50:ASN:O	66:Lb:50:ASN:ND2	2.50	0.41
75:Lk:54:GLU:O	75:Lk:58:GLN:HG2	2.20	0.41
1:AP:41:G:H2'	1:AP:42:A:C8	2.55	0.41
2:PE:13:C:H2'	2:PE:14:A:C8	2.56	0.41
9:SR:7:LYS:HB2	9:SR:7:LYS:HE3	1.77	0.41
10:SS:123:LEU:HD12	10:SS:127:TRP:CZ2	2.56	0.41
12:SU:64:THR:HG22	12:SU:77:TRP:HE3	1.86	0.41
28:SO:88:LEU:HD23	28:SO:88:LEU:HA	1.88	0.41
32:SY:120:THR:O	32:SY:124:ASN:HB2	2.21	0.41
35:S2:902:G:O2'	35:S2:903:A:O4'	2.39	0.41
35:S2:1531:A:H2'	35:S2:1532:C:C6	2.56	0.41
39:L5:319:A:H1'	39:L5:3726:A:N3	2.36	0.41
39:L5:406:C:O2'	39:L5:407:A:OP1	2.37	0.41
39:L5:705:G:P	69:Le:5:ARG:HH22	2.44	0.41
39:L5:965:G:N2	39:L5:2092:G:H1'	2.36	0.41
39:L5:1097:C:H2'	39:L5:1098:G:H8	1.86	0.41
39:L5:1199:G:H2'	39:L5:1200:G:H8	1.86	0.41
39:L5:2409:U:H5	39:L5:2783:A:N1	2.19	0.41
39:L5:3867:A2M:H2'	39:L5:3868:G:O4'	2.20	0.41
39:L5:4239:A:H2'	39:L5:4240:G:H8	1.86	0.41
39:L5:4520:G:H2'	39:L5:4521:PSU:O4'	2.20	0.41
39:L5:4593:C:H2'	39:L5:4594:U:H6	1.86	0.41
42:LA:132:ASN:O	42:LA:169:VAL:HG12	2.20	0.41
44:LC:318:PRO:O	44:LC:319:LEU:HB2	2.21	0.41
46:LE:165:LEU:HD11	46:LE:176:THR:HG22	2.03	0.41
57:LQ:172:ARG:HA	57:LQ:176:ARG:HD2	2.02	0.41
64:LZ:28:ASN:HB2	64:LZ:77:TYR:OH	2.20	0.41
67:Lc:57:LYS:HB2	67:Lc:57:LYS:HE3	1.84	0.41
79:Lo:69:ARG:NH2	79:Lo:80:LYS:HD3	2.36	0.41
79:Lo:96:ASP:OD1	79:Lo:96:ASP:N	2.53	0.41
84:CH:132:LEU:HA	84:CH:137:ILE:HG23	2.02	0.41
1:AP:64:G:H4'	50:LI:27:PRO:HA	2.02	0.41
2:PE:33:U:OP2	8:SQ:146:ARG:NH1	2.54	0.41
2:PE:42:G:H2'	2:PE:43:A:H8	1.86	0.41
4:SF:47:LYS:NZ	8:SQ:115:TYR:O	2.54	0.41
5:SK:58:VAL:HG21	5:SK:69:TRP:HB3	2.02	0.41
7:SP:111:MET:HG2	10:SS:117:ILE:HD11	2.03	0.41
9:SR:51:ALA:O	9:SR:55:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SS:86:ARG:HH22	10:SS:110:ASP:CG	2.29	0.41
11:ST:39:LEU:HD11	11:ST:52:TRP:CE3	2.55	0.41
17:Sg:129:ILE:O	17:Sg:142:VAL:HG22	2.20	0.41
17:Sg:228:TYR:CE2	17:Sg:264:LYS:HD2	2.56	0.41
17:Sg:228:TYR:HD2	17:Sg:230:LEU:HD22	1.86	0.41
21:SE:87:MET:HE3	21:SE:87:MET:HB2	1.89	0.41
21:SE:112:HIS:NE2	21:SE:237:SER:O	2.52	0.41
21:SE:136:ILE:HG23	21:SE:149:TYR:CE1	2.56	0.41
21:SE:246:LEU:HD13	21:SE:250:GLU:HB2	2.01	0.41
22:SG:5:ILE:HD13	22:SG:111:LEU:HB2	2.02	0.41
22:SG:7:PHE:HB2	22:SG:113:ILE:HD13	2.03	0.41
22:SG:198:ARG:HD2	35:S2:125:C:OP2	2.21	0.41
23:SH:66:VAL:HG22	23:SH:96:ALA:HB1	2.01	0.41
24:SI:3:ILE:O	24:SI:30:GLY:N	2.43	0.41
24:SI:66:SER:HA	24:SI:73:THR:HG22	2.02	0.41
32:SY:128:GLY:C	32:SY:131:PRO:HD2	2.46	0.41
35:S2:99:A2M:HM'3	35:S2:99:A2M:H1'	1.75	0.41
39:L5:466:A:H2'	39:L5:467:U:C6	2.56	0.41
39:L5:1197:C:H2'	39:L5:1198:G:H8	1.86	0.41
39:L5:1304:C:H2'	39:L5:1305:C:C6	2.56	0.41
39:L5:1346:C:H2'	39:L5:1347:G:H8	1.86	0.41
39:L5:1351:G:O4'	44:LC:119:GLN:NE2	2.53	0.41
39:L5:1523:A:N3	39:L5:4389:C:O2'	2.51	0.41
39:L5:1846:G:H2'	39:L5:1847:C:H6	1.85	0.41
39:L5:2500:U:H2'	39:L5:2501:C:H6	1.85	0.41
39:L5:2559:G:H2'	39:L5:2560:C:O4'	2.21	0.41
39:L5:3808:OMC:HM23	39:L5:3808:OMC:H1'	1.83	0.41
39:L5:3920:PSU:H2'	39:L5:3921:U:C6	2.56	0.41
39:L5:4085:A:C5	48:LG:56:LYS:HD3	2.55	0.41
39:L5:4303:C:O2'	39:L5:4304:A:H2'	2.21	0.41
39:L5:4305:G:C6	59:LT:80:VAL:HG21	2.55	0.41
39:L5:4353:PSU:H5'	39:L5:4354:U:H5'	2.02	0.41
39:L5:4771:C:H2'	39:L5:4772:C:C6	2.56	0.41
39:L5:4919:G:H2'	39:L5:4920:C:C6	2.56	0.41
41:L8:94:G:H21	74:Lj:82:THR:HB	1.85	0.41
41:L8:102:G:H5''	74:Lj:39:TYR:HE1	1.84	0.41
43:LB:128:LYS:HD2	43:LB:128:LYS:HA	1.83	0.41
45:LD:41:LYS:HB2	59:LT:68:THR:O	2.21	0.41
45:LD:146:LEU:HB2	45:LD:163:LEU:HD12	2.03	0.41
45:LD:215:ASP:HB3	45:LD:218:ALA:HB3	2.02	0.41
47:LF:124:LYS:HG3	47:LF:197:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:LH:59:LYS:HE2	49:LH:66:GLU:HG3	2.03	0.41
50:LI:38:ARG:HD3	50:LI:83:ASP:HB3	2.03	0.41
54:LN:6:TYR:CZ	73:LI:40:VAL:HG22	2.55	0.41
55:LO:9:LEU:HD23	55:LO:118:MET:HB2	2.03	0.41
67:Lc:48:LEU:HD13	67:Lc:71:VAL:HG13	2.03	0.41
78:Ln:1:MET:HE2	78:Ln:5:TRP:CZ2	2.55	0.41
81:Lr:54:ALA:HA	81:Lr:61:VAL:HG23	2.02	0.41
82:Ls:58:ASN:HD21	82:Ls:82:ILE:C	2.29	0.41
11:ST:12:GLN:NE2	35:S2:1593:C:O2	2.51	0.41
31:SX:105:PHE:HE2	31:SX:112:VAL:HB	1.86	0.41
35:S2:203:G:H3'	35:S2:204:G:C8	2.56	0.41
35:S2:943:U:C2	35:S2:944:A:C8	3.09	0.41
39:L5:457:G:H2'	39:L5:458:C:C6	2.56	0.41
39:L5:2519:U:H1'	39:L5:2520:C:C6	2.56	0.41
39:L5:4740:G:O6	39:L5:4959:U:O2	2.39	0.41
39:L5:4918:C:H2'	39:L5:4919:G:C8	2.56	0.41
48:LG:123:ALA:HA	48:LG:124:GLY:HA2	1.86	0.41
64:LZ:14:LEU:O	71:Lg:88:ARG:HG2	2.20	0.41
4:SF:51:HIS:NE2	35:S2:1674:G:OP1	2.45	0.40
9:SR:5:ARG:HH21	35:S2:1454:A:H3'	1.86	0.40
17:Sg:184:LEU:HD21	17:Sg:187:ASN:ND2	2.36	0.40
17:Sg:235:ILE:H	17:Sg:235:ILE:HD12	1.85	0.40
19:SB:217:MET:HE2	19:SB:220:LYS:HG2	2.04	0.40
20:SC:145:LYS:H	20:SC:145:LYS:HG2	1.65	0.40
21:SE:192:ILE:HD12	21:SE:228:ILE:HD11	2.02	0.40
26:SL:8:ARG:HH21	35:S2:390:C:H4'	1.87	0.40
26:SL:33:LEU:HD12	26:SL:34:PRO:HD2	2.02	0.40
28:SO:66:ARG:HE	35:S2:962:A:H4'	1.86	0.40
35:S2:57:U:OP1	35:S2:504:G:O2'	2.39	0.40
35:S2:1019:C:H2'	35:S2:1020:A:O4'	2.21	0.40
35:S2:1103:C:H2'	35:S2:1104:G:H8	1.85	0.40
35:S2:1310:U:H2'	35:S2:1311:C:C6	2.56	0.40
39:L5:358:C:H5	44:LC:61:GLN:HE22	1.69	0.40
39:L5:473:C:H2'	39:L5:474:C:C6	2.56	0.40
39:L5:1213:G:H5''	39:L5:1214:C:H5'	2.03	0.40
39:L5:1762:C:H5'	39:L5:1764:G:H22	1.86	0.40
39:L5:2421:G:OP2	39:L5:2828:U:H1'	2.21	0.40
39:L5:2741:U:H2'	42:LA:50:HIS:HD2	1.84	0.40
39:L5:2811:G:N1	39:L5:2814:C:OP2	2.47	0.40
40:L7:35:U:O2	40:L7:45:U:O2'	2.38	0.40
41:L8:60:G:OP1	62:LX:68:ARG:NH2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:L8:92:U:H2'	41:L8:93:C:O4'	2.21	0.40
47:LF:222:LYS:HB3	47:LF:231:GLY:HA2	2.02	0.40
3:SD:60:GLY:H	3:SD:65:ARG:HB2	1.86	0.40
8:SQ:90:LYS:HE2	8:SQ:90:LYS:HB3	1.78	0.40
10:SS:105:ASN:OD1	10:SS:106:LYS:N	2.54	0.40
11:ST:127:GLY:O	11:ST:131:LEU:HD23	2.20	0.40
16:Sf:105:TYR:HE2	16:Sf:131:PHE:CG	2.40	0.40
17:Sg:5:MET:SD	17:Sg:312:VAL:HG22	2.61	0.40
21:SE:35:PRO:HB3	21:SE:144:ALA:H	1.86	0.40
21:SE:149:TYR:HB3	22:SG:209:TYR:HB2	2.04	0.40
23:SH:159:ASP:C	23:SH:161:ALA:H	2.27	0.40
24:SI:65:PHE:HA	24:SI:187:GLY:O	2.21	0.40
26:SL:88:ILE:HD11	26:SL:109:MET:HE2	2.03	0.40
27:SN:110:ASP:O	27:SN:114:ARG:HG2	2.21	0.40
33:Sa:37:LYS:HA	33:Sa:71:LEU:O	2.21	0.40
35:S2:52:G:H2'	35:S2:53:C:C6	2.57	0.40
35:S2:1218:C:H1'	35:S2:1683:C:H42	1.86	0.40
35:S2:1523:C:H2'	35:S2:1524:G:H8	1.87	0.40
39:L5:467:U:N3	39:L5:468:U:O2'	2.49	0.40
39:L5:1588:U:H2'	39:L5:1589:C:C6	2.57	0.40
39:L5:2474:G:H2'	39:L5:2502:G:N2	2.36	0.40
39:L5:2844:A:O2'	39:L5:4631:G:H4'	2.21	0.40
39:L5:4927:G:H5''	39:L5:4928:C:C5	2.49	0.40
39:L5:5003:U:H2'	39:L5:5004:C:C6	2.56	0.40
41:L8:47:C:H1'	41:L8:61:A:H2'	2.02	0.40
46:LE:67:ALA:HA	46:LE:69:TYR:CE2	2.56	0.40
50:LI:91:LEU:HD23	50:LI:91:LEU:HA	1.94	0.40
52:LL:42:LYS:HB3	52:LL:42:LYS:HE2	1.74	0.40
61:LV:42:VAL:HB	61:LV:45:ILE:HG13	2.03	0.40
68:Ld:68:LEU:HA	68:Ld:108:TYR:HB2	2.03	0.40
1:AP:3:C:H42	1:AP:70:A:H61	1.70	0.40
3:SD:190:LEU:HB3	3:SD:200:PRO:HD3	2.02	0.40
7:SP:81:ARG:HH12	7:SP:98:ASN:HA	1.85	0.40
7:SP:82:ASP:OD2	35:S2:1619:A:O2'	2.39	0.40
16:Sf:119:ARG:HB3	16:Sf:132:MET:HB2	2.03	0.40
18:SA:88:LEU:HD23	18:SA:88:LEU:HA	1.91	0.40
21:SE:118:GLU:HG2	21:SE:121:TYR:OH	2.21	0.40
24:SI:199:LEU:O	24:SI:203:LYS:HG2	2.21	0.40
27:SN:45:LEU:HD23	27:SN:45:LEU:HA	1.88	0.40
35:S2:71:G:N2	35:S2:73:C:OP1	2.55	0.40
35:S2:1088:U:H4'	35:S2:1089:G:OP2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:1723:G:H2'	35:S2:1724:A:C8	2.56	0.40
36:LR:110:ARG:HE	36:LR:110:ARG:HB3	1.73	0.40
39:L5:302:C:H2'	39:L5:303:C:C6	2.56	0.40
39:L5:302:C:H2'	39:L5:303:C:H6	1.87	0.40
39:L5:1749:A:H2'	39:L5:1750:G:C8	2.57	0.40
39:L5:2640:G:H2'	39:L5:2641:A:C8	2.56	0.40
39:L5:3917:A:H2'	39:L5:3918:G:C8	2.57	0.40
39:L5:4070:U:H2'	39:L5:4071:U:H6	1.85	0.40
39:L5:4236:G:H4'	39:L5:4328:G:O2'	2.22	0.40
39:L5:4476:C:O2'	39:L5:4478:G:OP2	2.31	0.40
42:LA:54:ARG:HG2	42:LA:56:ALA:H	1.85	0.40
42:LA:131:GLY:N	42:LA:169:VAL:HG13	2.35	0.40
43:LB:220:ILE:HB	43:LB:346:THR:HB	2.03	0.40
47:LF:86:GLU:HB3	59:LT:135:PRO:HB3	2.03	0.40
47:LF:125:LEU:HD23	47:LF:125:LEU:HA	1.95	0.40
55:LO:157:GLU:HG3	55:LO:161:LYS:HE3	2.04	0.40
64:LZ:135:ARG:HD2	64:LZ:135:ARG:HA	1.77	0.40
67:Lc:17:ARG:O	67:Lc:21:VAL:HG23	2.22	0.40
71:Lg:43:LYS:HE2	71:Lg:43:LYS:HB2	1.97	0.40
4:SF:51:HIS:HE1	8:SQ:82:TYR:HE2	1.68	0.40
4:SF:100:ILE:HD11	4:SF:108:PRO:HB3	2.02	0.40
4:SF:136:ARG:HA	4:SF:136:ARG:HD2	1.83	0.40
8:SQ:31:LEU:HB3	8:SQ:67:ASP:OD1	2.21	0.40
10:SS:26:ILE:O	10:SS:30:ILE:HG12	2.22	0.40
17:Sg:168:CYS:HB2	17:Sg:195:LEU:HD13	2.03	0.40
22:SG:50:VAL:CG1	22:SG:111:LEU:HB3	2.51	0.40
26:SL:111:VAL:HG11	26:SL:128:VAL:HG11	2.03	0.40
28:SO:113:GLN:OE1	33:Sa:46:GLU:N	2.54	0.40
39:L5:120:A:H2'	39:L5:149:A:N6	2.36	0.40
39:L5:1080:C:H2'	39:L5:1081:C:H6	1.85	0.40
39:L5:1666:C:O2'	39:L5:1688:G:OP1	2.31	0.40
39:L5:1996:C:H42	39:L5:2000:G:H22	1.69	0.40
39:L5:2580:U:P	64:LZ:36:ARG:HH22	2.44	0.40
39:L5:2654:C:H2'	39:L5:2655:C:C6	2.57	0.40
39:L5:2749:C:H2'	39:L5:2750:G:C8	2.57	0.40
39:L5:4770:U:H2'	39:L5:4771:C:C6	2.56	0.40
41:L8:5:U:H2'	41:L8:6:C:H6	1.87	0.40
43:LB:231:VAL:HG21	43:LB:251:VAL:HG23	2.04	0.40
46:LE:130:LYS:HD2	46:LE:130:LYS:N	2.36	0.40
47:LF:200:ARG:HA	47:LF:200:ARG:HD3	1.93	0.40
52:LL:47:ALA:HB3	52:LL:48:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:LN:75:VAL:HG11	54:LN:80:THR:HG22	2.04	0.40
56:LP:109:VAL:HA	56:LP:112:LEU:HD13	2.03	0.40
61:LV:87:SER:HA	61:LV:97:TYR:HB3	2.03	0.40
81:Lr:16:PHE:HB3	81:Lr:27:THR:H	1.86	0.40
83:Lt:29:ALA:HA	83:Lt:32:ILE:HG12	2.04	0.40
2:PE:71:G:H2'	2:PE:72:C:O4'	2.21	0.40
3:SD:164:VAL:O	3:SD:168:VAL:HG22	2.21	0.40
7:SP:29:SER:OG	7:SP:30:TYR:N	2.55	0.40
10:SS:1:MET:SD	10:SS:3:LEU:HB3	2.62	0.40
12:SU:43:ALA:HB1	12:SU:48:LEU:HB2	2.02	0.40
17:Sg:42:MET:HE1	17:Sg:56:GLN:NE2	2.37	0.40
17:Sg:166:VAL:HG12	17:Sg:176:VAL:HG12	2.02	0.40
18:SA:32:PHE:CD1	35:S2:1097:G:H4'	2.57	0.40
22:SG:85:ARG:HA	22:SG:86:PRO:HD3	1.98	0.40
23:SH:12:ASN:ND2	23:SH:14:GLU:HB2	2.35	0.40
27:SN:78:LYS:HD3	27:SN:78:LYS:HA	1.89	0.40
30:SW:41:MET:HE2	30:SW:129:PHE:HB3	2.04	0.40
35:S2:147:A:H2'	35:S2:148:U:C6	2.57	0.40
35:S2:1278:A:H2'	35:S2:1279:C:C6	2.57	0.40
35:S2:1844:U:H2'	35:S2:1845:A:C8	2.57	0.40
39:L5:701:G:H2'	39:L5:702:U:C6	2.56	0.40
39:L5:1195:G:H2'	39:L5:1196:G:H8	1.86	0.40
39:L5:1248:C:H2'	39:L5:1249:C:C6	2.57	0.40
39:L5:1278:C:H2'	39:L5:1279:A:O4'	2.21	0.40
39:L5:2407:G:H2'	76:Ll:13:LEU:HD22	2.03	0.40
39:L5:2465:C:H2'	39:L5:2466:G:O4'	2.22	0.40
39:L5:2560:C:H2'	39:L5:2561:C:C6	2.57	0.40
39:L5:3871:A:H2'	39:L5:3872:A:C8	2.56	0.40
39:L5:3886:G:H5''	55:LO:82:ARG:NH2	2.37	0.40
39:L5:3932:U:H2'	39:L5:3933:G:C8	2.57	0.40
39:L5:4761:G:H2'	39:L5:4762:A:C8	2.56	0.40
45:LD:30:TYR:HA	45:LD:33:ARG:HB3	2.02	0.40
48:LG:149:ASN:HB3	48:LG:151:LYS:HD3	2.02	0.40
54:LN:178:HIS:HA	54:LN:181:HIS:NE2	2.37	0.40
60:LU:35:ASP:N	60:LU:35:ASP:OD1	2.52	0.40
69:Le:82:VAL:HG13	69:Le:114:ARG:HG2	2.04	0.40
84:CH:77:VAL:O	84:CH:81:ILE:HG12	2.21	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	
3	SD	225/454 (50%)	219 (97%)	6 (3%)	0	100	100
4	SF	187/189 (99%)	168 (90%)	18 (10%)	1 (0%)	24	58
5	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
6	SM	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
7	SP	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
8	SQ	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
9	SR	133/135 (98%)	126 (95%)	5 (4%)	2 (2%)	8	33
10	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
11	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
12	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
13	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
14	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
15	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
16	Sf	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
17	Sg	311/313 (99%)	287 (92%)	24 (8%)	0	100	100
18	SA	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
19	SB	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
20	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
21	SE	260/262 (99%)	246 (95%)	14 (5%)	0	100	100
22	SG	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
23	SH	182/186 (98%)	168 (92%)	14 (8%)	0	100	100
24	SI	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
25	SJ	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
26	SL	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
27	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	SO	135/140 (96%)	128 (95%)	6 (4%)	1 (1%)	18	50
29	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
30	SW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
31	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
32	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
33	Sa	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
34	Sb	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
36	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
37	LW	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
38	CI	29/31 (94%)	29 (100%)	0	0	100	100
42	LA	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
43	LB	400/402 (100%)	382 (96%)	18 (4%)	0	100	100
44	LC	366/368 (100%)	350 (96%)	16 (4%)	0	100	100
45	LD	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
46	LE	236/250 (94%)	221 (94%)	15 (6%)	0	100	100
47	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
48	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
49	LH	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
50	LI	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
51	LJ	168/176 (96%)	159 (95%)	8 (5%)	1 (1%)	21	53
52	LL	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
53	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
54	LN	201/203 (99%)	199 (99%)	2 (1%)	0	100	100
55	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
56	LP	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
57	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
58	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
59	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
60	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
61	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
62	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
64	LZ	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
65	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
66	Lb	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
67	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
68	Ld	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
69	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
70	Lf	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
71	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
72	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
73	Li	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
74	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
75	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
76	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
77	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
78	Ln	22/24 (92%)	22 (100%)	0	0	100	100
79	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
80	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
81	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
82	Ls	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
83	Lt	128/141 (91%)	110 (86%)	18 (14%)	0	100	100
84	CH	130/132 (98%)	108 (83%)	21 (16%)	1 (1%)	16	47
All	All	11752/12177 (96%)	11226 (96%)	520 (4%)	6 (0%)	49	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	SF	136	ARG
84	CH	114	ALA
9	SR	84	TYR
51	LJ	31	ASP
9	SR	129	LYS
28	SO	138	ASP

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	
3	SD	190/380 (50%)	190 (100%)	0	100	100
4	SF	159/159 (100%)	159 (100%)	0	100	100
5	SK	89/89 (100%)	89 (100%)	0	100	100
6	SM	102/104 (98%)	102 (100%)	0	100	100
7	SP	113/113 (100%)	113 (100%)	0	100	100
8	SQ	119/119 (100%)	119 (100%)	0	100	100
9	SR	122/122 (100%)	121 (99%)	1 (1%)	73	86
10	SS	126/126 (100%)	126 (100%)	0	100	100
11	ST	113/113 (100%)	113 (100%)	0	100	100
12	SU	94/94 (100%)	94 (100%)	0	100	100
13	SZ	66/66 (100%)	66 (100%)	0	100	100
14	Sc	57/57 (100%)	57 (100%)	0	100	100
15	Sd	48/48 (100%)	48 (100%)	0	100	100
16	Sf	60/60 (100%)	60 (100%)	0	100	100
17	Sg	272/272 (100%)	272 (100%)	0	100	100
18	SA	183/183 (100%)	183 (100%)	0	100	100
19	SB	195/195 (100%)	195 (100%)	0	100	100
20	SC	186/188 (99%)	186 (100%)	0	100	100
21	SE	224/224 (100%)	224 (100%)	0	100	100
22	SG	207/207 (100%)	207 (100%)	0	100	100
23	SH	166/166 (100%)	166 (100%)	0	100	100
24	SI	178/178 (100%)	178 (100%)	0	100	100
25	SJ	161/161 (100%)	161 (100%)	0	100	100
26	SL	137/137 (100%)	137 (100%)	0	100	100
27	SN	130/130 (100%)	130 (100%)	0	100	100
28	SO	107/110 (97%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	SV	67/67 (100%)	67 (100%)	0	100	100
30	SW	112/112 (100%)	112 (100%)	0	100	100
31	SX	113/113 (100%)	113 (100%)	0	100	100
32	SY	113/113 (100%)	113 (100%)	0	100	100
33	Sa	89/89 (100%)	89 (100%)	0	100	100
34	Sb	75/75 (100%)	75 (100%)	0	100	100
36	LR	166/166 (100%)	166 (100%)	0	100	100
37	LW	95/97 (98%)	95 (100%)	0	100	100
38	CI	25/25 (100%)	25 (100%)	0	100	100
42	LA	190/190 (100%)	190 (100%)	0	100	100
43	LB	348/348 (100%)	348 (100%)	0	100	100
44	LC	306/306 (100%)	306 (100%)	0	100	100
45	LD	246/247 (100%)	246 (100%)	0	100	100
46	LE	212/222 (96%)	212 (100%)	0	100	100
47	LF	194/194 (100%)	194 (100%)	0	100	100
48	LG	203/205 (99%)	203 (100%)	0	100	100
49	LH	169/169 (100%)	169 (100%)	0	100	100
50	LI	180/180 (100%)	180 (100%)	0	100	100
51	LJ	143/148 (97%)	143 (100%)	0	100	100
52	LL	176/176 (100%)	176 (100%)	0	100	100
53	LM	118/118 (100%)	118 (100%)	0	100	100
54	LN	171/171 (100%)	171 (100%)	0	100	100
55	LO	173/173 (100%)	173 (100%)	0	100	100
56	LP	134/134 (100%)	134 (100%)	0	100	100
57	LQ	164/164 (100%)	164 (100%)	0	100	100
58	LS	156/156 (100%)	156 (100%)	0	100	100
59	LT	139/139 (100%)	139 (100%)	0	100	100
60	LU	91/91 (100%)	91 (100%)	0	100	100
61	LV	101/101 (100%)	101 (100%)	0	100	100
62	LX	108/108 (100%)	108 (100%)	0	100	100
63	LY	124/124 (100%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	LZ	117/117 (100%)	117 (100%)	0	100	100
65	La	120/120 (100%)	120 (100%)	0	100	100
66	Lb	88/90 (98%)	88 (100%)	0	100	100
67	Lc	83/83 (100%)	83 (100%)	0	100	100
68	Ld	98/98 (100%)	98 (100%)	0	100	100
69	Le	114/114 (100%)	114 (100%)	0	100	100
70	Lf	88/88 (100%)	88 (100%)	0	100	100
71	Lg	98/98 (100%)	98 (100%)	0	100	100
72	Lh	109/109 (100%)	109 (100%)	0	100	100
73	Li	86/86 (100%)	86 (100%)	0	100	100
74	Lj	73/73 (100%)	73 (100%)	0	100	100
75	Lk	64/64 (100%)	64 (100%)	0	100	100
76	Ll	47/47 (100%)	47 (100%)	0	100	100
77	Lm	48/48 (100%)	48 (100%)	0	100	100
78	Ln	23/23 (100%)	23 (100%)	0	100	100
79	Lo	93/93 (100%)	93 (100%)	0	100	100
80	Lp	74/74 (100%)	74 (100%)	0	100	100
81	Lr	109/109 (100%)	109 (100%)	0	100	100
82	Ls	162/164 (99%)	162 (100%)	0	100	100
83	Lt	107/115 (93%)	107 (100%)	0	100	100
84	CH	106/106 (100%)	106 (100%)	0	100	100
All	All	10212/10441 (98%)	10211 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	SR	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
3	SD	165	ASN
4	SF	107	ASN
4	SF	114	ASN

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Mol	Chain	Res	Type
4	SF	118	ASN
4	SF	203	ASN
5	SK	28	HIS
5	SK	44	HIS
6	SM	19	GLN
8	SQ	11	GLN
8	SQ	142	GLN
9	SR	93	GLN
10	SS	72	GLN
11	ST	126	GLN
14	Sc	29	GLN
16	Sf	91	ASN
16	Sf	151	ASN
17	Sg	20	GLN
17	Sg	26	GLN
17	Sg	56	GLN
17	Sg	272	GLN
19	SB	101	HIS
20	SC	113	GLN
21	SE	98	ASN
21	SE	138	HIS
21	SE	214	ASN
22	SG	105	ASN
22	SG	225	GLN
23	SH	44	ASN
23	SH	91	HIS
24	SI	116	HIS
25	SJ	140	GLN
25	SJ	156	HIS
31	SX	46	HIS
31	SX	92	ASN
32	SY	2	ASN
36	LR	40	GLN
37	LW	17	HIS
42	LA	8	GLN
42	LA	50	HIS
42	LA	215	ASN
43	LB	121	ASN
43	LB	167	GLN
43	LB	209	GLN
43	LB	315	ASN
44	LC	112	HIS

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Mol	Chain	Res	Type
44	LC	178	ASN
44	LC	215	ASN
44	LC	329	ASN
45	LD	131	ASN
45	LD	202	GLN
45	LD	282	GLN
47	LF	63	GLN
47	LF	80	ASN
47	LF	119	ASN
48	LG	225	ASN
49	LH	138	GLN
49	LH	189	GLN
50	LI	92	HIS
52	LL	19	GLN
53	LM	34	ASN
55	LO	26	GLN
55	LO	42	ASN
55	LO	50	ASN
55	LO	167	HIS
55	LO	180	GLN
56	LP	97	ASN
56	LP	133	HIS
58	LS	125	GLN
62	LX	57	GLN
62	LX	93	ASN
63	LY	20	ASN
65	La	60	HIS
65	La	67	GLN
65	La	120	GLN
66	Lb	27	GLN
67	Lc	72	HIS
69	Le	23	HIS
69	Le	52	GLN
69	Le	117	GLN
70	Lf	21	GLN
70	Lf	99	HIS
72	Lh	30	GLN
72	Lh	65	GLN
73	Li	92	ASN
77	Lm	87	GLN
79	Lo	102	GLN
81	Lr	21	ASN

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Mol	Chain	Res	Type
82	Ls	39	GLN
82	Ls	41	GLN
83	Lt	68	GLN
84	CH	51	GLN
84	CH	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AP	69/142 (48%)	11 (15%)	0
2	PE	74/150 (49%)	21 (28%)	1 (1%)
35	S2	1715/1740 (98%)	374 (21%)	3 (0%)
39	L5	3643/3655 (99%)	729 (20%)	15 (0%)
40	L7	119/120 (99%)	10 (8%)	0
41	L8	155/156 (99%)	24 (15%)	0
All	All	5775/5963 (96%)	1169 (20%)	19 (0%)

All (1169) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AP	8	U
1	AP	9	A
1	AP	11	U
1	AP	13	U
1	AP	14	A
1	AP	19	G
1	AP	21	A
1	AP	47	U
1	AP	48	C
1	AP	56	C
1	AP	58	A
2	PE	4	C
2	PE	8	U
2	PE	10	G
2	PE	11	C
2	PE	19	G
2	PE	20	U
2	PE	21	A
2	PE	46	G
2	PE	47	U
2	PE	48	C

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Mol	Chain	Res	Type
2	PE	49	C
2	PE	50	A
2	PE	55	U
2	PE	56	C
2	PE	58	A
2	PE	63	C
2	PE	67	U
2	PE	69	G
2	PE	71	G
2	PE	73	G
2	PE	76	A
35	S2	4	C
35	S2	14	C
35	S2	17	C
35	S2	25	A
35	S2	33	G
35	S2	42	A
35	S2	44	U
35	S2	45	A
35	S2	46	A
35	S2	56	G
35	S2	58	C
35	S2	62	G
35	S2	67	C
35	S2	68	A
35	S2	72	C
35	S2	73	C
35	S2	74	G
35	S2	76	U
35	S2	92	A
35	S2	99	A2M
35	S2	103	A
35	S2	113	G
35	S2	115	U
35	S2	126	G
35	S2	130	G
35	S2	142	C
35	S2	143	U
35	S2	149	A
35	S2	155	G
35	S2	158	A
35	S2	162	C

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Mol	Chain	Res	Type
35	S2	163	U
35	S2	168	C
35	S2	175	A
35	S2	182	C
35	S2	190	G
35	S2	196	C
35	S2	197	U
35	S2	198	U
35	S2	200	G
35	S2	203	G
35	S2	204	G
35	S2	206	G
35	S2	207	G
35	S2	208	G
35	S2	209	A
35	S2	289	G
35	S2	291	G
35	S2	292	A
35	S2	295	C
35	S2	302	A
35	S2	305	U
35	S2	306	C
35	S2	307	G
35	S2	308	G
35	S2	309	G
35	S2	311	C
35	S2	312	G
35	S2	318	A
35	S2	319	C
35	S2	323	C
35	S2	324	C
35	S2	325	C
35	S2	326	C
35	S2	328	U
35	S2	329	G
35	S2	332	G
35	S2	339	A
35	S2	340	C
35	S2	347	G
35	S2	360	A
35	S2	361	U
35	S2	362	C

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Mol	Chain	Res	Type
35	S2	364	A
35	S2	368	U
35	S2	369	C
35	S2	370	G
35	S2	385	G
35	S2	386	C
35	S2	398	A
35	S2	408	A
35	S2	409	C
35	S2	426	A
35	S2	438	G
35	S2	448	A
35	S2	449	A
35	S2	450	C
35	S2	452	G
35	S2	464	A
35	S2	465	A
35	S2	466	G
35	S2	471	G
35	S2	472	C
35	S2	473	A
35	S2	474	G
35	S2	482	G
35	S2	487	U
35	S2	488	U
35	S2	492	C
35	S2	493	A
35	S2	502	C
35	S2	516	A
35	S2	531	A
35	S2	532	C
35	S2	533	A
35	S2	534	G
35	S2	536	A
35	S2	537	C
35	S2	540	U
35	S2	542	U
35	S2	544	G
35	S2	546	G
35	S2	547	G
35	S2	555	A
35	S2	557	U

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Mol	Chain	Res	Type
35	S2	558	G
35	S2	563	G
35	S2	564	A
35	S2	566	U
35	S2	576	A2M
35	S2	583	A
35	S2	587	A
35	S2	589	G
35	S2	590	A
35	S2	591	U
35	S2	592	C
35	S2	604	A
35	S2	607	U
35	S2	614	C
35	S2	617	G
35	S2	623	G
35	S2	627	OMU
35	S2	628	A
35	S2	631	U
35	S2	643	A
35	S2	644	OMG
35	S2	655	A
35	S2	660	C
35	S2	664	A
35	S2	668	A2M
35	S2	669	A
35	S2	671	A
35	S2	672	A
35	S2	673	G
35	S2	683	OMG
35	S2	688	U
35	S2	689	U
35	S2	692	G
35	S2	693	A
35	S2	696	G
35	S2	697	G
35	S2	731	G
35	S2	732	U
35	S2	733	C
35	S2	736	C
35	S2	738	C
35	S2	749	U

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Mol	Chain	Res	Type
35	S2	751	G
35	S2	752	G
35	S2	753	C
35	S2	788	G
35	S2	791	C
35	S2	792	C
35	S2	798	G
35	S2	799	OMU
35	S2	801	PSU
35	S2	821	G
35	S2	822	U
35	S2	823	U
35	S2	824	C
35	S2	827	A
35	S2	830	A
35	S2	834	C
35	S2	835	C
35	S2	836	G
35	S2	837	A
35	S2	838	G
35	S2	839	C
35	S2	840	C
35	S2	841	G
35	S2	842	C
35	S2	847	A
35	S2	867	OMG
35	S2	870	A
35	S2	874	G
35	S2	888	U
35	S2	889	U
35	S2	891	G
35	S2	896	U
35	S2	897	U
35	S2	898	U
35	S2	899	U
35	S2	900	C
35	S2	901	G
35	S2	903	A
35	S2	913	A
35	S2	920	A
35	S2	930	C
35	S2	933	G

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Mol	Chain	Res	Type
35	S2	943	U
35	S2	963	A
35	S2	971	G
35	S2	990	A
35	S2	992	A
35	S2	999	G
35	S2	1001	A
35	S2	1002	U
35	S2	1008	A
35	S2	1017	U
35	S2	1023	A
35	S2	1027	A
35	S2	1030	A
35	S2	1060	A
35	S2	1061	U
35	S2	1062	A
35	S2	1067	C
35	S2	1080	A
35	S2	1083	A
35	S2	1085	C
35	S2	1108	G
35	S2	1109	C
35	S2	1113	A
35	S2	1116	C
35	S2	1119	A
35	S2	1120	U
35	S2	1133	A
35	S2	1138	C
35	S2	1149	A
35	S2	1153	C
35	S2	1154	U
35	S2	1195	A
35	S2	1200	A
35	S2	1207	G
35	S2	1208	A
35	S2	1215	C
35	S2	1216	C
35	S2	1217	A
35	S2	1220	A
35	S2	1224	G
35	S2	1227	G
35	S2	1242	U

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Mol	Chain	Res	Type
35	S2	1243	U
35	S2	1251	A
35	S2	1253	A
35	S2	1256	G
35	S2	1257	G
35	S2	1259	A
35	S2	1271	C
35	S2	1272	OMC
35	S2	1274	G
35	S2	1275	G
35	S2	1283	C
35	S2	1284	A
35	S2	1286	G
35	S2	1288	OMU
35	S2	1290	G
35	S2	1294	G
35	S2	1301	A
35	S2	1302	G
35	S2	1303	C
35	S2	1308	U
35	S2	1333	U
35	S2	1342	U
35	S2	1348	G
35	S2	1357	A
35	S2	1358	U
35	S2	1371	U
35	S2	1373	C
35	S2	1376	A
35	S2	1378	A
35	S2	1382	A
35	S2	1401	A
35	S2	1402	A
35	S2	1404	U
35	S2	1413	G
35	S2	1414	A
35	S2	1418	C
35	S2	1419	C
35	S2	1420	G
35	S2	1421	A
35	S2	1422	G
35	S2	1423	C
35	S2	1433	C

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Mol	Chain	Res	Type
35	S2	1435	C
35	S2	1436	C
35	S2	1437	C
35	S2	1439	A
35	S2	1442	OMU
35	S2	1449	G
35	S2	1452	A
35	S2	1454	A
35	S2	1462	U
35	S2	1463	U
35	S2	1480	A
35	S2	1484	A
35	S2	1489	A
35	S2	1490	OMG
35	S2	1492	U
35	S2	1494	U
35	S2	1495	G
35	S2	1497	G
35	S2	1498	A
35	S2	1521	C
35	S2	1522	A
35	S2	1531	A
35	S2	1533	A
35	S2	1536	G
35	S2	1544	C
35	S2	1546	G
35	S2	1556	A
35	S2	1574	C
35	S2	1580	A
35	S2	1581	C
35	S2	1582	C
35	S2	1587	G
35	S2	1588	A
35	S2	1600	G
35	S2	1604	G
35	S2	1606	G
35	S2	1621	U
35	S2	1623	A
35	S2	1633	A
35	S2	1634	A
35	S2	1637	A
35	S2	1648	G

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Mol	Chain	Res	Type
35	S2	1654	G
35	S2	1663	A
35	S2	1665	G
35	S2	1683	C
35	S2	1686	G
35	S2	1698	C
35	S2	1715	A
35	S2	1721	U
35	S2	1722	G
35	S2	1726	G
35	S2	1727	G
35	S2	1728	U
35	S2	1744	G
35	S2	1745	A
35	S2	1752	C
35	S2	1753	C
35	S2	1754	G
35	S2	1756	C
35	S2	1757	G
35	S2	1758	G
35	S2	1759	G
35	S2	1761	U
35	S2	1772	C
35	S2	1773	C
35	S2	1774	C
35	S2	1775	U
35	S2	1777	G
35	S2	1782	G
35	S2	1783	C
35	S2	1784	G
35	S2	1786	U
35	S2	1798	C
35	S2	1807	C
35	S2	1809	A
35	S2	1813	A
35	S2	1814	G
35	S2	1815	A
35	S2	1821	U
35	S2	1823	A
35	S2	1824	A
35	S2	1831	A
35	S2	1835	A

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Mol	Chain	Res	Type
35	S2	1838	U
35	S2	1849	G
35	S2	1851	MA6
35	S2	1861	G
35	S2	1862	G
35	S2	1863	A
35	S2	1865	C
39	L5	25	A
39	L5	30	C
39	L5	39	A
39	L5	42	A
39	L5	48	G
39	L5	56	A
39	L5	59	A
39	L5	64	A
39	L5	65	A
39	L5	73	A
39	L5	74	G
39	L5	91	G
39	L5	104	G
39	L5	108	A
39	L5	109	G
39	L5	110	C
39	L5	119	G
39	L5	120	A
39	L5	132	G
39	L5	133	C
39	L5	134	G
39	L5	144	G
39	L5	151	G
39	L5	159	C
39	L5	165	A
39	L5	172	C
39	L5	182	G
39	L5	183	C
39	L5	185	C
39	L5	186	G
39	L5	188	G
39	L5	200	U
39	L5	209	U
39	L5	216	C
39	L5	218	A

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Mol	Chain	Res	Type
39	L5	234	G
39	L5	254	G
39	L5	255	C
39	L5	256	G
39	L5	261	G
39	L5	263	G
39	L5	264	C
39	L5	265	C
39	L5	266	C
39	L5	267	G
39	L5	275	C
39	L5	276	C
39	L5	280	G
39	L5	297	U
39	L5	306	A
39	L5	315	G
39	L5	316	U
39	L5	340	C
39	L5	373	G
39	L5	385	A
39	L5	387	G
39	L5	396	A
39	L5	407	A
39	L5	409	G
39	L5	410	A
39	L5	411	G
39	L5	412	G
39	L5	413	G
39	L5	415	G
39	L5	431	G
39	L5	432	U
39	L5	449	C
39	L5	452	A
39	L5	453	G
39	L5	454	U
39	L5	455	C
39	L5	456	C
39	L5	457	G
39	L5	467	U
39	L5	485	C
39	L5	486	C
39	L5	489	C

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Mol	Chain	Res	Type
39	L5	493	G
39	L5	494	U
39	L5	495	C
39	L5	497	G
39	L5	498	C
39	L5	499	G
39	L5	500	G
39	L5	501	C
39	L5	502	C
39	L5	503	C
39	L5	504	G
39	L5	509	A
39	L5	510	U
39	L5	513	U
39	L5	514	U
39	L5	516	C
39	L5	517	C
39	L5	518	G
39	L5	643	C
39	L5	644	G
39	L5	646	G
39	L5	653	U
39	L5	654	C
39	L5	656	C
39	L5	657	C
39	L5	659	G
39	L5	666	G
39	L5	667	A
39	L5	668	C
39	L5	669	C
39	L5	673	C
39	L5	686	A
39	L5	687	U
39	L5	696	C
39	L5	704	C
39	L5	708	G
39	L5	730	G
39	L5	731	G
39	L5	738	C
39	L5	739	G
39	L5	742	G
39	L5	746	A

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Mol	Chain	Res	Type
39	L5	904	C
39	L5	905	C
39	L5	906	C
39	L5	910	G
39	L5	913	U
39	L5	914	U
39	L5	915	A
39	L5	917	A
39	L5	923	C
39	L5	924	C
39	L5	926	G
39	L5	932	A
39	L5	933	G
39	L5	934	C
39	L5	936	C
39	L5	944	A
39	L5	945	U
39	L5	946	C
39	L5	958	G
39	L5	959	G
39	L5	960	A
39	L5	961	G
39	L5	962	C
39	L5	963	G
39	L5	965	G
39	L5	966	A
39	L5	967	C
39	L5	969	C
39	L5	970	G
39	L5	982	U
39	L5	985	C
39	L5	989	U
39	L5	1070	G
39	L5	1072	C
39	L5	1075	G
39	L5	1082	C
39	L5	1083	U
39	L5	1095	A
39	L5	1168	G
39	L5	1171	G
39	L5	1172	C
39	L5	1173	G

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Mol	Chain	Res	Type
39	L5	1179	U
39	L5	1180	C
39	L5	1181	C
39	L5	1182	C
39	L5	1183	C
39	L5	1200	G
39	L5	1202	C
39	L5	1203	G
39	L5	1210	C
39	L5	1211	G
39	L5	1214	C
39	L5	1215	C
39	L5	1216	C
39	L5	1218	G
39	L5	1219	G
39	L5	1222	A
39	L5	1246	G
39	L5	1253	G
39	L5	1254	A
39	L5	1257	A
39	L5	1262	G
39	L5	1266	G
39	L5	1267	C
39	L5	1269	G
39	L5	1270	A
39	L5	1271	G
39	L5	1272	C
39	L5	1273	G
39	L5	1275	G
39	L5	1277	G
39	L5	1280	C
39	L5	1284	G
39	L5	1285	U
39	L5	1287	G
39	L5	1293	G
39	L5	1294	A
39	L5	1295	C
39	L5	1296	G
39	L5	1301	C
39	L5	1314	C
39	L5	1326	A2M
39	L5	1337	A

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Mol	Chain	Res	Type
39	L5	1354	A
39	L5	1359	G
39	L5	1365	C
39	L5	1366	G
39	L5	1379	C
39	L5	1387	A
39	L5	1394	G
39	L5	1397	A
39	L5	1398	A
39	L5	1401	C
39	L5	1404	G
39	L5	1405	C
39	L5	1407	C
39	L5	1409	C
39	L5	1410	U
39	L5	1415	G
39	L5	1416	G
39	L5	1417	C
39	L5	1420	A
39	L5	1437	C
39	L5	1439	C
39	L5	1442	C
39	L5	1443	A
39	L5	1444	G
39	L5	1446	C
39	L5	1482	G
39	L5	1483	C
39	L5	1489	G
39	L5	1497	A
39	L5	1498	G
39	L5	1502	G
39	L5	1517	G
39	L5	1534	A2M
39	L5	1535	C
39	L5	1537	A
39	L5	1547	A
39	L5	1562	G
39	L5	1564	A
39	L5	1566	C
39	L5	1578	U
39	L5	1591	U
39	L5	1596	U

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Mol	Chain	Res	Type
39	L5	1624	G
39	L5	1625	OMG
39	L5	1626	G
39	L5	1631	A
39	L5	1633	G
39	L5	1634	A
39	L5	1638	A
39	L5	1640	C
39	L5	1641	G
39	L5	1642	A
39	L5	1654	G
39	L5	1661	C
39	L5	1676	C
39	L5	1677	PSU
39	L5	1691	G
39	L5	1694	C
39	L5	1697	G
39	L5	1699	A
39	L5	1700	G
39	L5	1702	C
39	L5	1704	C
39	L5	1705	G
39	L5	1717	C
39	L5	1718	C
39	L5	1719	A
39	L5	1721	G
39	L5	1731	C
39	L5	1734	G
39	L5	1740	C
39	L5	1741	G
39	L5	1742	A
39	L5	1750	G
39	L5	1757	U
39	L5	1758	G
39	L5	1760	G
39	L5	1761	G
39	L5	1762	C
39	L5	1763	C
39	L5	1764	G
39	L5	1765	A
39	L5	1766	A
39	L5	1767	A

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Mol	Chain	Res	Type
39	L5	1768	C
39	L5	1770	A
39	L5	1785	C
39	L5	1787	A
39	L5	1797	G
39	L5	1803	G
39	L5	1804	A
39	L5	1806	G
39	L5	1810	G
39	L5	1815	G
39	L5	1820	C
39	L5	1821	G
39	L5	1822	U
39	L5	1834	U
39	L5	1836	G
39	L5	1837	A
39	L5	1842	G
39	L5	1855	G
39	L5	1869	G
39	L5	1882	U
39	L5	1892	A
39	L5	1897	A
39	L5	1917	A
39	L5	1918	U
39	L5	1919	G
39	L5	1920	C
39	L5	1921	C
39	L5	1922	G
39	L5	1925	G
39	L5	1931	C
39	L5	1932	A
39	L5	1936	C
39	L5	1940	G
39	L5	1948	G
39	L5	1951	G
39	L5	1960	A
39	L5	1961	G
39	L5	1962	A
39	L5	1965	G
39	L5	1971	C
39	L5	1974	U
39	L5	1975	G

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Mol	Chain	Res	Type
39	L5	1978	C
39	L5	1980	U
39	L5	1981	G
39	L5	1982	G
39	L5	1983	A
39	L5	1984	A
39	L5	1985	G
39	L5	1986	U
39	L5	1989	G
39	L5	1991	A
39	L5	1992	U
39	L5	1993	C
39	L5	1997	U
39	L5	1999	A
39	L5	2002	A
39	L5	2004	U
39	L5	2005	G
39	L5	2011	C
39	L5	2016	C
39	L5	2017	A
39	L5	2018	C
39	L5	2024	G
39	L5	2026	A
39	L5	2046	G
39	L5	2048	U
39	L5	2055	G
39	L5	2056	G
39	L5	2069	A
39	L5	2084	C
39	L5	2092	G
39	L5	2093	A
39	L5	2095	A
39	L5	2096	G
39	L5	2097	U
39	L5	2098	G
39	L5	2101	C
39	L5	2102	G
39	L5	2103	G
39	L5	2107	C
39	L5	2108	G
39	L5	2111	G
39	L5	2112	G

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Mol	Chain	Res	Type
39	L5	2250	C
39	L5	2252	G
39	L5	2256	C
39	L5	2261	G
39	L5	2289	C
39	L5	2300	A
39	L5	2301	G
39	L5	2313	A
39	L5	2314	G
39	L5	2331	G
39	L5	2333	G
39	L5	2345	G
39	L5	2348	G
39	L5	2351	OMC
39	L5	2360	A
39	L5	2364	OMG
39	L5	2389	A
39	L5	2395	A
39	L5	2397	G
39	L5	2411	C
39	L5	2412	A
39	L5	2417	A
39	L5	2425	U
39	L5	2447	U
39	L5	2450	G
39	L5	2453	A
39	L5	2464	C
39	L5	2465	C
39	L5	2469	C
39	L5	2471	G
39	L5	2474	G
39	L5	2475	G
39	L5	2478	C
39	L5	2479	G
39	L5	2484	A
39	L5	2485	U
39	L5	2486	G
39	L5	2487	G
39	L5	2488	C
39	L5	2489	C
39	L5	2490	U
39	L5	2491	C

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Mol	Chain	Res	Type
39	L5	2494	U
39	L5	2504	C
39	L5	2505	C
39	L5	2506	G
39	L5	2513	A
39	L5	2519	U
39	L5	2529	A
39	L5	2537	A
39	L5	2544	G
39	L5	2546	G
39	L5	2547	G
39	L5	2554	U
39	L5	2555	G
39	L5	2559	G
39	L5	2560	C
39	L5	2565	A
39	L5	2573	A
39	L5	2583	C
39	L5	2586	G
39	L5	2587	A
39	L5	2589	C
39	L5	2601	A
39	L5	2627	C
39	L5	2653	C
39	L5	2662	G
39	L5	2669	C
39	L5	2675	G
39	L5	2676	A
39	L5	2687	U
39	L5	2694	G
39	L5	2695	A
39	L5	2696	A
39	L5	2703	G
39	L5	2706	G
39	L5	2708	U
39	L5	2710	C
39	L5	2711	G
39	L5	2712	G
39	L5	2721	G
39	L5	2724	G
39	L5	2726	G
39	L5	2739	C

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Mol	Chain	Res	Type
39	L5	2742	G
39	L5	2743	A
39	L5	2757	A
39	L5	2761	U
39	L5	2763	U
39	L5	2769	U
39	L5	2770	C
39	L5	2788	U
39	L5	2790	U
39	L5	2806	A
39	L5	2814	C
39	L5	2815	A2M
39	L5	2826	U
39	L5	2827	G
39	L5	2838	G
39	L5	2855	G
39	L5	2867	C
39	L5	2877	G
39	L5	2900	U
39	L5	2902	G
39	L5	2903	G
39	L5	2904	U
39	L5	2905	C
39	L5	2907	G
39	L5	2908	U
39	L5	3588	C
39	L5	3590	G
39	L5	3591	C
39	L5	3594	C
39	L5	3595	U
39	L5	3596	A
39	L5	3597	G
39	L5	3599	A
39	L5	3605	C
39	L5	3616	U
39	L5	3617	G
39	L5	3626	G
39	L5	3630	A
39	L5	3635	A
39	L5	3644	U
39	L5	3646	A
39	L5	3648	A

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Mol	Chain	Res	Type
39	L5	3662	A
39	L5	3664	G
39	L5	3670	C
39	L5	3673	C
39	L5	3674	G
39	L5	3701	OMC
39	L5	3710	G
39	L5	3711	A
39	L5	3713	U
39	L5	3727	A
39	L5	3748	A
39	L5	3753	G
39	L5	3754	G
39	L5	3760	A
39	L5	3764	U
39	L5	3770	U
39	L5	3773	U
39	L5	3774	A
39	L5	3775	A
39	L5	3776	G
39	L5	3777	G
39	L5	3785	A2M
39	L5	3786	U
39	L5	3792	OMG
39	L5	3811	G
39	L5	3812	C
39	L5	3814	U
39	L5	3817	A
39	L5	3819	G
39	L5	3824	A
39	L5	3838	U
39	L5	3839	G
39	L5	3840	U
39	L5	3877	A
39	L5	3878	C
39	L5	3879	G
39	L5	3885	G
39	L5	3890	A
39	L5	3892	U
39	L5	3897	G
39	L5	3901	A
39	L5	3906	A

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Mol	Chain	Res	Type
39	L5	3907	G
39	L5	3908	A
39	L5	3915	U
39	L5	3938	G
39	L5	3947	A
39	L5	3948	C
39	L5	3949	A
39	L5	3950	U
39	L5	3951	G
39	L5	3953	G
39	L5	4059	C
39	L5	4060	U
39	L5	4061	G
39	L5	4062	A
39	L5	4064	C
39	L5	4076	G
39	L5	4084	G
39	L5	4093	G
39	L5	4095	G
39	L5	4097	G
39	L5	4099	G
39	L5	4101	C
39	L5	4103	C
39	L5	4104	G
39	L5	4106	G
39	L5	4108	G
39	L5	4111	U
39	L5	4114	C
39	L5	4115	G
39	L5	4116	C
39	L5	4117	U
39	L5	4122	G
39	L5	4127	A
39	L5	4139	G
39	L5	4140	C
39	L5	4141	G
39	L5	4142	C
39	L5	4143	G
39	L5	4144	C
39	L5	4146	G
39	L5	4150	G
39	L5	4162	C

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Mol	Chain	Res	Type
39	L5	4163	U
39	L5	4166	G
39	L5	4168	G
39	L5	4170	A
39	L5	4183	G
39	L5	4184	G
39	L5	4191	G
39	L5	4203	A
39	L5	4212	A
39	L5	4222	G
39	L5	4225	G
39	L5	4228	OMG
39	L5	4229	U
39	L5	4233	A
39	L5	4243	C
39	L5	4251	A
39	L5	4254	G
39	L5	4257	A
39	L5	4258	C
39	L5	4265	U
39	L5	4268	A
39	L5	4273	A
39	L5	4291	G
39	L5	4304	A
39	L5	4305	G
39	L5	4314	C
39	L5	4319	C
39	L5	4329	G
39	L5	4330	G
39	L5	4332	C
39	L5	4338	G
39	L5	4349	C
39	L5	4350	C
39	L5	4354	U
39	L5	4373	G
39	L5	4376	A
39	L5	4377	G
39	L5	4378	A
39	L5	4379	A
39	L5	4387	C
39	L5	4391	G
39	L5	4394	A

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Mol	Chain	Res	Type
39	L5	4405	G
39	L5	4421	C
39	L5	4422	A
39	L5	4438	U
39	L5	4448	G
39	L5	4449	A
39	L5	4464	A
39	L5	4466	C
39	L5	4475	G
39	L5	4488	A
39	L5	4500	PSU
39	L5	4512	U
39	L5	4513	A
39	L5	4519	C
39	L5	4524	G
39	L5	4545	G
39	L5	4548	A
39	L5	4549	G
39	L5	4560	C
39	L5	4567	G
39	L5	4569	U
39	L5	4575	G
39	L5	4584	A
39	L5	4589	A
39	L5	4590	A2M
39	L5	4600	G
39	L5	4601	U
39	L5	4636	PSU
39	L5	4637	OMG
39	L5	4656	A
39	L5	4670	C
39	L5	4672	A
39	L5	4687	A
39	L5	4694	G
39	L5	4695	C
39	L5	4700	A
39	L5	4708	A
39	L5	4709	U
39	L5	4719	G
39	L5	4734	A
39	L5	4740	G
39	L5	4741	C

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Mol	Chain	Res	Type
39	L5	4742	G
39	L5	4745	G
39	L5	4750	G
39	L5	4754	G
39	L5	4757	C
39	L5	4759	C
39	L5	4761	G
39	L5	4764	A
39	L5	4765	G
39	L5	4771	C
39	L5	4772	C
39	L5	4775	C
39	L5	4859	C
39	L5	4863	G
39	L5	4867	G
39	L5	4870	G
39	L5	4871	C
39	L5	4875	G
39	L5	4882	U
39	L5	4883	C
39	L5	4889	G
39	L5	4895	C
39	L5	4896	G
39	L5	4898	G
39	L5	4899	G
39	L5	4900	C
39	L5	4901	G
39	L5	4910	G
39	L5	4912	G
39	L5	4914	C
39	L5	4922	C
39	L5	4925	U
39	L5	4927	G
39	L5	4928	C
39	L5	4934	A
39	L5	4940	C
39	L5	4941	G
39	L5	4943	A
39	L5	4949	G
39	L5	4951	G
39	L5	4960	G
39	L5	4976	U

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Mol	Chain	Res	Type
39	L5	4985	U
39	L5	4988	U
39	L5	4989	U
39	L5	4990	C
39	L5	4991	U
39	L5	5014	A
39	L5	5017	G
39	L5	5020	G
39	L5	5023	C
39	L5	5024	C
39	L5	5026	U
39	L5	5028	G
39	L5	5029	C
39	L5	5030	U
39	L5	5034	A
39	L5	5041	G
39	L5	5047	C
39	L5	5050	C
39	L5	5054	C
39	L5	5055	G
39	L5	5061	A
39	L5	5069	U
40	L7	7	G
40	L7	33	U
40	L7	38	U
40	L7	53	U
40	L7	54	A
40	L7	64	G
40	L7	97	G
40	L7	100	A
40	L7	110	G
40	L7	111	C
41	L8	23	C
41	L8	25	G
41	L8	34	U
41	L8	35	C
41	L8	59	A
41	L8	62	A
41	L8	63	U
41	L8	80	A
41	L8	82	A
41	L8	84	A

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Mol	Chain	Res	Type
41	L8	85	U
41	L8	86	U
41	L8	87	G
41	L8	94	G
41	L8	103	A
41	L8	105	C
41	L8	111	U
41	L8	114	G
41	L8	123	U
41	L8	124	U
41	L8	125	C
41	L8	126	C
41	L8	127	U
41	L8	153	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	PE	18	U
35	S2	291	G
35	S2	563	G
35	S2	688	U
39	L5	406	C
39	L5	914	U
39	L5	1082	C
39	L5	1590	C
39	L5	1633	G
39	L5	1703	C
39	L5	1977	C
39	L5	2416	G
39	L5	2485	U
39	L5	2675	G
39	L5	2760	G
39	L5	3673	C
39	L5	4600	G
39	L5	4699	U
39	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$
35	PSU	S2	681	35	18,21,22	1.04	1 (5%)	21,30,33	1.94	4 (19%)
41	PSU	L8	55	41	18,21,22	1.04	1 (5%)	21,30,33	1.86	4 (19%)
35	OMC	S2	517	35	19,22,23	0.56	0	25,31,34	0.67	0
35	OMU	S2	116	35	19,22,23	3.30	7 (36%)	25,31,34	1.68	4 (16%)
39	PSU	L5	3920	39,85	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
35	OMG	S2	867	35	23,26,27	0.51	0	32,38,41	0.47	0
39	PSU	L5	3639	39	18,21,22	1.13	2 (11%)	21,30,33	2.05	4 (19%)
39	OMG	L5	4370	39	23,26,27	0.61	0	32,38,41	0.54	0
35	PSU	S2	1367	35	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
39	OMG	L5	1316	39	23,26,27	0.69	0	32,38,41	0.56	0
39	A2M	L5	398	39	22,25,26	1.18	1 (4%)	30,36,39	1.67	7 (23%)
39	A2M	L5	1534	39,85	22,25,26	1.20	2 (9%)	30,36,39	1.42	7 (23%)
39	PSU	L5	1744	39,85	18,21,22	1.06	2 (11%)	21,30,33	1.95	4 (19%)
39	PSU	L5	4296	39	18,21,22	1.09	1 (5%)	21,30,33	1.98	4 (19%)
35	OMC	S2	1391	35	19,22,23	0.58	0	25,31,34	0.63	0
39	PSU	L5	3637	39	18,21,22	1.06	2 (11%)	21,30,33	2.00	5 (23%)
39	OMG	L5	3744	39	23,26,27	0.60	0	32,38,41	0.47	0
39	OMC	L5	4536	39	19,22,23	0.69	0	25,31,34	0.72	0
39	OMC	L5	3869	39	19,22,23	0.67	0	25,31,34	0.70	0
39	OMC	L5	4456	39	19,22,23	0.76	1 (5%)	25,31,34	0.77	0
35	A2M	S2	27	35	22,25,26	1.21	1 (4%)	30,36,39	1.52	8 (26%)
39	PSU	L5	1677	39	18,21,22	1.13	3 (16%)	21,30,33	2.13	5 (23%)
35	OMU	S2	428	35	19,22,23	3.31	7 (36%)	25,31,34	1.84	5 (20%)
39	PSU	L5	1781	39	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)
39	A2M	L5	2815	39	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
35	OMG	S2	601	35	23,26,27	0.52	0	32,38,41	0.41	0
35	PSU	S2	814	35	18,21,22	1.07	1 (5%)	21,30,33	1.81	4 (19%)
39	PSU	L5	3822	39	18,21,22	1.01	1 (5%)	21,30,33	1.98	5 (23%)
39	PSU	L5	3844	39	18,21,22	1.08	2 (11%)	21,30,33	1.91	4 (19%)
39	A2M	L5	3867	39	22,25,26	1.37	3 (13%)	30,36,39	1.52	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	L5	4493	39	18,21,22	1.04	1 (5%)	21,30,33	1.91	4 (19%)
39	PSU	L5	1683	39	18,21,22	1.06	2 (11%)	21,30,33	2.00	4 (19%)
39	PSU	L5	4579	39	18,21,22	1.06	2 (11%)	21,30,33	1.91	4 (19%)
39	PSU	L5	4471	39	18,21,22	1.05	2 (11%)	21,30,33	1.95	4 (19%)
35	PSU	S2	93	35	18,21,22	1.05	1 (5%)	21,30,33	1.76	4 (19%)
39	OMC	L5	2351	39,85	19,22,23	0.74	1 (5%)	25,31,34	0.88	1 (4%)
39	PSU	L5	4299	39	18,21,22	1.04	1 (5%)	21,30,33	1.94	4 (19%)
39	A2M	L5	4523	39,85	22,25,26	1.27	3 (13%)	30,36,39	1.57	8 (26%)
39	A2M	L5	1524	39	22,25,26	1.31	3 (13%)	30,36,39	1.52	6 (20%)
39	OMG	L5	4196	39	23,26,27	0.60	0	32,38,41	0.42	0
35	PSU	S2	1232	35	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
35	MA6	S2	1850	35	23,26,27	2.68	9 (39%)	33,38,41	3.34	13 (39%)
39	6MZ	L5	4220	39	22,25,26	2.89	6 (27%)	29,36,39	2.46	10 (34%)
39	PSU	L5	4500	39	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)
35	A2M	S2	576	35	22,25,26	1.20	1 (4%)	30,36,39	1.54	5 (16%)
35	PSU	S2	863	35	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
35	PSU	S2	1056	35	18,21,22	1.06	2 (11%)	21,30,33	2.01	5 (23%)
39	OMG	L5	4623	39	23,26,27	0.61	0	32,38,41	0.60	0
39	PSU	L5	4552	39	18,21,22	1.08	2 (11%)	21,30,33	2.01	4 (19%)
39	PSU	L5	4442	39	18,21,22	1.04	2 (11%)	21,30,33	2.07	6 (28%)
39	OMG	L5	4637	39	23,26,27	0.60	0	32,38,41	0.48	0
39	PSU	L5	4689	39	18,21,22	1.03	2 (11%)	21,30,33	1.97	4 (19%)
35	OMC	S2	174	35	19,22,23	0.57	0	25,31,34	0.79	1 (4%)
35	PSU	S2	1045	35	18,21,22	1.07	1 (5%)	21,30,33	1.95	4 (19%)
39	A2M	L5	3830	39	22,25,26	1.21	2 (9%)	30,36,39	1.58	6 (20%)
39	OMC	L5	3841	39	19,22,23	0.67	0	25,31,34	0.67	0
39	PSU	L5	4532	39	18,21,22	1.09	2 (11%)	21,30,33	1.95	4 (19%)
35	PSU	S2	109	35	18,21,22	1.11	2 (11%)	21,30,33	2.04	6 (28%)
39	PSU	L5	4636	39	18,21,22	1.08	2 (11%)	21,30,33	2.10	6 (28%)
39	UR3	L5	4530	39	19,22,23	2.61	7 (36%)	26,32,35	1.66	3 (11%)
35	OMU	S2	172	35	19,22,23	3.31	7 (36%)	25,31,34	1.83	5 (20%)
39	OMG	L5	3899	39	23,26,27	0.66	0	32,38,41	0.54	0
39	5MC	L5	3782	39,85	19,22,23	0.77	0	26,32,35	0.77	1 (3%)
35	PSU	S2	105	35	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
39	PSU	L5	4293	39	18,21,22	1.08	2 (11%)	21,30,33	2.07	4 (19%)
39	PSU	L5	4353	39	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	PSU	S2	801	35	18,21,22	1.12	1 (5%)	21,30,33	1.79	4 (19%)
39	OMC	L5	2365	39,85	19,22,23	0.66	0	25,31,34	0.59	0
39	1MA	L5	1322	39,85	21,25,26	0.67	0	30,37,40	0.83	2 (6%)
35	OMU	S2	1288	35	19,22,23	3.35	7 (36%)	25,31,34	1.76	5 (20%)
39	A2M	L5	1323	39	22,25,26	1.27	2 (9%)	30,36,39	1.60	9 (30%)
39	A2M	L5	2401	39	22,25,26	1.24	2 (9%)	30,36,39	1.61	8 (26%)
35	PSU	S2	1046	35	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
39	PSU	L5	5001	39	18,21,22	1.05	1 (5%)	21,30,33	1.92	4 (19%)
35	OMC	S2	462	35	19,22,23	0.60	0	25,31,34	0.78	0
39	PSU	L5	1782	39	18,21,22	1.07	1 (5%)	21,30,33	1.97	4 (19%)
39	OMG	L5	4228	39	23,26,27	0.59	0	32,38,41	0.60	0
39	OMG	L5	3792	39	23,26,27	0.60	0	32,38,41	0.49	0
39	PSU	L5	3884	39	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
35	PSU	S2	1081	35	18,21,22	1.03	1 (5%)	21,30,33	1.81	4 (19%)
39	A2M	L5	2787	39	22,25,26	1.19	1 (4%)	30,36,39	1.53	8 (26%)
39	OMG	L5	3627	39	23,26,27	0.59	0	32,38,41	0.59	0
35	OMG	S2	1328	35	23,26,27	0.51	0	32,38,41	0.45	0
35	OMG	S2	509	35	23,26,27	0.51	0	32,38,41	0.51	0
39	PSU	L5	1862	39	18,21,22	1.08	1 (5%)	21,30,33	2.01	4 (19%)
39	PSU	L5	1792	39	18,21,22	1.07	2 (11%)	21,30,33	1.92	4 (19%)
35	MA6	S2	1851	35	23,26,27	1.30	2 (8%)	33,38,41	3.41	12 (36%)
39	OMC	L5	3701	39	19,22,23	0.75	1 (5%)	25,31,34	1.83	4 (16%)
39	OMU	L5	4306	39	19,22,23	3.22	7 (36%)	25,31,34	1.89	4 (16%)
39	PSU	L5	4361	39	18,21,22	1.01	1 (5%)	21,30,33	1.81	4 (19%)
39	PSU	L5	3853	39,85	18,21,22	1.02	1 (5%)	21,30,33	1.90	4 (19%)
39	OMU	L5	4498	39	19,22,23	3.21	7 (36%)	25,31,34	1.93	5 (20%)
39	A2M	L5	4571	39	22,25,26	1.32	3 (13%)	30,36,39	1.60	8 (26%)
39	PSU	L5	4576	39	18,21,22	1.02	1 (5%)	21,30,33	1.93	4 (19%)
39	PSU	L5	4673	39,85	18,21,22	1.08	2 (11%)	21,30,33	1.97	4 (19%)
39	PSU	L5	4972	39	18,21,22	1.07	2 (11%)	21,30,33	1.92	4 (19%)
35	OMG	S2	1490	35	23,26,27	0.56	0	32,38,41	0.47	0
39	OMG	L5	1625	39	23,26,27	0.59	0	32,38,41	0.46	0
35	PSU	S2	1177	35	18,21,22	1.03	2 (11%)	21,30,33	1.97	4 (19%)
35	OMU	S2	1442	35	19,22,23	3.31	7 (36%)	25,31,34	1.80	5 (20%)
39	A2M	L5	1871	39,85	22,25,26	1.35	3 (13%)	30,36,39	1.64	7 (23%)
39	A2M	L5	400	39	22,25,26	1.30	3 (13%)	30,36,39	1.55	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A2M	S2	166	35	22,25,26	1.24	1 (4%)	30,36,39	1.62	7 (23%)
39	OMC	L5	2824	39	19,22,23	0.63	0	25,31,34	0.66	0
39	PSU	L5	4628	39	18,21,22	1.05	2 (11%)	21,30,33	2.03	4 (19%)
35	OMU	S2	354	35	19,22,23	3.27	7 (36%)	25,31,34	1.92	5 (20%)
41	PSU	L8	69	41	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)
35	A2M	S2	99	35,85	22,25,26	1.17	1 (4%)	30,36,39	1.57	7 (23%)
39	A2M	L5	3825	39	22,25,26	1.20	2 (9%)	30,36,39	1.59	8 (26%)
39	A2M	L5	3785	39,85	22,25,26	1.23	1 (4%)	30,36,39	1.65	10 (33%)
39	OMG	L5	2876	39	23,26,27	0.58	0	32,38,41	0.52	0
39	A2M	L5	3718	39	22,25,26	1.18	2 (9%)	30,36,39	1.57	8 (26%)
39	OMC	L5	2422	39,85	19,22,23	0.66	0	25,31,34	0.73	1 (4%)
39	A2M	L5	4590	39	22,25,26	1.24	2 (9%)	30,36,39	1.58	5 (16%)
39	OMG	L5	4618	39	23,26,27	0.61	0	32,38,41	0.52	0
39	PSU	L5	4973	39	18,21,22	1.04	2 (11%)	21,30,33	1.99	5 (23%)
35	6MZ	S2	1832	35,85	22,25,26	4.04	11 (50%)	29,36,39	2.33	9 (31%)
35	A2M	S2	484	35	22,25,26	1.18	1 (4%)	30,36,39	1.47	8 (26%)
39	PSU	L5	3851	39	18,21,22	1.08	1 (5%)	21,30,33	1.97	4 (19%)
39	PSU	L5	4457	39	18,21,22	1.03	2 (11%)	21,30,33	2.03	5 (23%)
35	OMG	S2	683	35	23,26,27	0.55	0	32,38,41	0.46	0
39	OMC	L5	3808	39	19,22,23	0.72	0	25,31,34	0.88	2 (8%)
35	PSU	S2	686	35	18,21,22	1.07	1 (5%)	21,30,33	1.97	5 (23%)
41	OMG	L8	75	41	23,26,27	0.56	0	32,38,41	0.53	0
39	UY1	L5	3818	39	19,22,23	4.79	9 (47%)	21,31,34	2.00	5 (23%)
39	OMU	L5	2837	39	19,22,23	3.26	7 (36%)	25,31,34	1.91	5 (20%)
39	PSU	L5	4431	39	18,21,22	1.04	2 (11%)	21,30,33	1.95	4 (19%)
35	OMG	S2	644	35	23,26,27	0.50	0	32,38,41	0.46	0
39	PSU	L5	4312	39	18,21,22	1.08	2 (11%)	21,30,33	1.91	4 (19%)
35	A2M	S2	1383	35	22,25,26	1.16	1 (4%)	30,36,39	1.64	8 (26%)
39	OMG	L5	4499	39	23,26,27	0.58	0	32,38,41	0.47	0
35	B8N	S2	1248	35	25,29,30	3.24	7 (28%)	28,42,45	2.01	8 (28%)
39	PSU	L5	1536	39	18,21,22	1.06	2 (11%)	21,30,33	1.93	4 (19%)
35	PSU	S2	1244	35	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
39	OMC	L5	2861	39	19,22,23	0.68	0	25,31,34	0.81	1 (4%)
39	PSU	L5	3695	39	18,21,22	1.04	2 (11%)	21,30,33	1.97	4 (19%)
39	PSU	L5	4521	39,85	18,21,22	1.08	2 (11%)	21,30,33	1.99	5 (23%)
39	5MC	L5	4447	39	19,22,23	0.97	1 (5%)	26,32,35	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	OMU	S2	627	35	19,22,23	3.36	7 (36%)	25,31,34	1.79	4 (16%)
35	PSU	S2	406	35	18,21,22	1.07	2 (11%)	21,30,33	2.02	5 (23%)
39	OMU	L5	4620	39	19,22,23	3.13	7 (36%)	25,31,34	1.72	5 (20%)
35	4AC	S2	1337	35	21,24,25	0.42	0	28,34,37	0.79	2 (7%)
35	PSU	S2	1004	35	18,21,22	1.09	2 (11%)	21,30,33	1.95	4 (19%)
39	OMC	L5	3887	39	19,22,23	0.67	0	25,31,34	0.66	0
35	PSU	S2	649	35	18,21,22	1.10	1 (5%)	21,30,33	1.96	4 (19%)
39	PSU	L5	1860	39	18,21,22	1.07	2 (11%)	21,30,33	1.96	4 (19%)
39	PSU	L5	2839	39	18,21,22	1.07	2 (11%)	21,30,33	2.01	4 (19%)
35	G7M	S2	1639	35,2	23,26,27	2.63	9 (39%)	34,39,42	2.58	11 (32%)
35	PSU	S2	1174	35	18,21,22	1.07	2 (11%)	21,30,33	1.90	4 (19%)
39	OMG	L5	4392	39	23,26,27	0.64	0	32,38,41	0.48	0
35	OMU	S2	799	35	19,22,23	3.39	7 (36%)	25,31,34	1.83	5 (20%)
39	OMG	L5	2364	39,85	23,26,27	0.62	0	32,38,41	0.45	0
35	OMG	S2	436	35	23,26,27	0.53	0	32,38,41	0.55	0
39	OMC	L5	2804	39	19,22,23	0.68	0	25,31,34	0.64	0
39	OMG	L5	4494	39	23,26,27	0.60	0	32,38,41	0.48	0
35	OMC	S2	1703	35	19,22,23	0.64	0	25,31,34	0.69	0
35	PSU	S2	966	35,85	18,21,22	1.07	1 (5%)	21,30,33	1.98	4 (19%)
39	OMG	L5	2424	39	23,26,27	0.61	0	32,38,41	0.41	0
39	OMC	L5	1340	39	19,22,23	0.71	0	25,31,34	0.78	0
35	OMU	S2	121	35	19,22,23	3.32	7 (36%)	25,31,34	1.85	5 (20%)
35	A2M	S2	668	35,85	22,25,26	1.31	2 (9%)	30,36,39	1.67	8 (26%)
35	OMC	S2	1272	35	19,22,23	0.62	0	25,31,34	0.84	1 (4%)
35	OMU	S2	1326	35	19,22,23	3.28	7 (36%)	25,31,34	1.88	5 (20%)
35	PSU	S2	651	35	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
39	OMU	L5	3925	39	19,22,23	3.19	7 (36%)	25,31,34	1.92	5 (20%)
35	A2M	S2	1031	35	22,25,26	1.15	1 (4%)	30,36,39	1.56	7 (23%)
39	OMU	L5	4227	39	19,22,23	3.20	7 (36%)	25,31,34	1.85	4 (16%)
35	A2M	S2	159	35	22,25,26	1.18	1 (4%)	30,36,39	1.51	8 (26%)
39	PSU	L5	4403	39	18,21,22	1.05	2 (11%)	21,30,33	2.09	6 (28%)
39	A2M	L5	2363	39,85	22,25,26	1.25	2 (9%)	30,36,39	1.56	9 (30%)
39	PSU	L5	5010	39	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
35	A2M	S2	468	35	22,25,26	1.24	1 (4%)	30,36,39	1.58	7 (23%)
35	4AC	S2	1842	35	21,24,25	0.40	0	28,34,37	0.46	0
39	PSU	L5	1582	39	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
39	OMG	L5	1522	39	23,26,27	0.63	0	32,38,41	0.65	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	L5	2632	39	18,21,22	1.06	2 (11%)	21,30,33	2.03	5 (23%)
39	A2M	L5	1326	39	22,25,26	1.26	2 (9%)	30,36,39	1.52	9 (30%)
35	PSU	S2	866	35	18,21,22	1.09	2 (11%)	21,30,33	2.01	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	S2	681	35	-	0/7/25/26	0/2/2/2
41	PSU	L8	55	41	-	0/7/25/26	0/2/2/2
35	OMC	S2	517	35	-	0/9/27/28	0/2/2/2
35	OMU	S2	116	35	-	0/9/27/28	0/2/2/2
39	PSU	L5	3920	39,85	-	0/7/25/26	0/2/2/2
35	OMG	S2	867	35	-	2/9/27/28	0/3/3/3
39	PSU	L5	3639	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	4370	39	-	0/9/27/28	0/3/3/3
35	PSU	S2	1367	35	-	0/7/25/26	0/2/2/2
39	OMG	L5	1316	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	398	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	1534	39,85	-	1/9/27/28	0/3/3/3
39	PSU	L5	1744	39,85	-	0/7/25/26	0/2/2/2
39	PSU	L5	4296	39	-	2/7/25/26	0/2/2/2
35	OMC	S2	1391	35	-	0/9/27/28	0/2/2/2
39	PSU	L5	3637	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	3744	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	4536	39	-	0/9/27/28	0/2/2/2
39	OMC	L5	3869	39	-	0/9/27/28	0/2/2/2
39	OMC	L5	4456	39	-	0/9/27/28	0/2/2/2
35	A2M	S2	27	35	-	1/9/27/28	0/3/3/3
39	PSU	L5	1677	39	-	1/7/25/26	0/2/2/2
35	OMU	S2	428	35	-	4/9/27/28	0/2/2/2
39	PSU	L5	1781	39	-	1/7/25/26	0/2/2/2
39	A2M	L5	2815	39	-	2/9/27/28	0/3/3/3
35	OMG	S2	601	35	-	1/9/27/28	0/3/3/3
35	PSU	S2	814	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	3822	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	3844	39	-	1/7/25/26	0/2/2/2
39	A2M	L5	3867	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	4493	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	L5	1683	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4579	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4471	39	-	0/7/25/26	0/2/2/2
35	PSU	S2	93	35	-	0/7/25/26	0/2/2/2
39	OMC	L5	2351	39,85	-	1/9/27/28	0/2/2/2
39	PSU	L5	4299	39	-	0/7/25/26	0/2/2/2
39	A2M	L5	4523	39,85	-	0/9/27/28	0/3/3/3
39	A2M	L5	1524	39	-	3/9/27/28	0/3/3/3
39	OMG	L5	4196	39	-	1/9/27/28	0/3/3/3
35	PSU	S2	1232	35	-	0/7/25/26	0/2/2/2
35	MA6	S2	1850	35	-	0/11/29/30	0/3/3/3
39	6MZ	L5	4220	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	4500	39	-	3/7/25/26	0/2/2/2
35	A2M	S2	576	35	-	3/9/27/28	0/3/3/3
35	PSU	S2	863	35	-	0/7/25/26	0/2/2/2
35	PSU	S2	1056	35	-	0/7/25/26	0/2/2/2
39	OMG	L5	4623	39	-	0/9/27/28	0/3/3/3
39	PSU	L5	4552	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4442	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	4637	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	4689	39	-	0/7/25/26	0/2/2/2
35	OMC	S2	174	35	-	0/9/27/28	0/2/2/2
35	PSU	S2	1045	35	-	2/7/25/26	0/2/2/2
39	A2M	L5	3830	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	3841	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	4532	39	-	0/7/25/26	0/2/2/2
35	PSU	S2	109	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	4636	39	-	2/7/25/26	0/2/2/2
39	UR3	L5	4530	39	-	0/7/25/26	0/2/2/2
35	OMU	S2	172	35	-	0/9/27/28	0/2/2/2
39	OMG	L5	3899	39	-	3/9/27/28	0/3/3/3
39	5MC	L5	3782	39,85	-	1/7/25/26	0/2/2/2
35	PSU	S2	105	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	4293	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4353	39	-	0/7/25/26	0/2/2/2
35	PSU	S2	801	35	-	2/7/25/26	0/2/2/2
39	OMC	L5	2365	39,85	-	0/9/27/28	0/2/2/2
39	1MA	L5	1322	39,85	-	2/7/25/26	0/3/3/3
35	OMU	S2	1288	35	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	A2M	L5	1323	39	-	2/9/27/28	0/3/3/3
39	A2M	L5	2401	39	-	1/9/27/28	0/3/3/3
35	PSU	S2	1046	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	5001	39	-	0/7/25/26	0/2/2/2
35	OMC	S2	462	35	-	1/9/27/28	0/2/2/2
39	PSU	L5	1782	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	4228	39	-	2/9/27/28	0/3/3/3
39	OMG	L5	3792	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	3884	39	-	0/7/25/26	0/2/2/2
35	PSU	S2	1081	35	-	1/7/25/26	0/2/2/2
39	A2M	L5	2787	39	-	5/9/27/28	0/3/3/3
39	OMG	L5	3627	39	-	0/9/27/28	0/3/3/3
35	OMG	S2	1328	35	-	0/9/27/28	0/3/3/3
35	OMG	S2	509	35	-	0/9/27/28	0/3/3/3
39	PSU	L5	1862	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	1792	39	-	0/7/25/26	0/2/2/2
35	MA6	S2	1851	35	-	1/11/29/30	0/3/3/3
39	OMC	L5	3701	39	-	5/9/27/28	0/2/2/2
39	OMU	L5	4306	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	4361	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	3853	39,85	-	0/7/25/26	0/2/2/2
39	OMU	L5	4498	39	-	0/9/27/28	0/2/2/2
39	A2M	L5	4571	39	-	0/9/27/28	0/3/3/3
39	PSU	L5	4576	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4673	39,85	-	0/7/25/26	0/2/2/2
39	PSU	L5	4972	39	-	0/7/25/26	0/2/2/2
35	OMG	S2	1490	35	-	1/9/27/28	0/3/3/3
39	OMG	L5	1625	39	-	2/9/27/28	0/3/3/3
35	PSU	S2	1177	35	-	0/7/25/26	0/2/2/2
35	OMU	S2	1442	35	-	2/9/27/28	0/2/2/2
39	A2M	L5	1871	39,85	-	0/9/27/28	0/3/3/3
39	A2M	L5	400	39	-	1/9/27/28	0/3/3/3
35	A2M	S2	166	35	-	0/9/27/28	0/3/3/3
39	OMC	L5	2824	39	-	1/9/27/28	0/2/2/2
39	PSU	L5	4628	39	-	0/7/25/26	0/2/2/2
35	OMU	S2	354	35	-	0/9/27/28	0/2/2/2
41	PSU	L8	69	41	-	0/7/25/26	0/2/2/2
35	A2M	S2	99	35,85	-	2/9/27/28	0/3/3/3
39	A2M	L5	3825	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	3785	39,85	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OMG	L5	2876	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	3718	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	2422	39,85	-	2/9/27/28	0/2/2/2
39	A2M	L5	4590	39	-	3/9/27/28	0/3/3/3
39	OMG	L5	4618	39	-	1/9/27/28	0/3/3/3
39	PSU	L5	4973	39	-	0/7/25/26	0/2/2/2
35	6MZ	S2	1832	35,85	-	2/9/27/28	0/3/3/3
35	A2M	S2	484	35	-	0/9/27/28	0/3/3/3
39	PSU	L5	3851	39	-	1/7/25/26	0/2/2/2
39	PSU	L5	4457	39	-	0/7/25/26	0/2/2/2
35	OMG	S2	683	35	-	2/9/27/28	0/3/3/3
39	OMC	L5	3808	39	-	1/9/27/28	0/2/2/2
35	PSU	S2	686	35	-	0/7/25/26	0/2/2/2
41	OMG	L8	75	41	-	1/9/27/28	0/3/3/3
39	UY1	L5	3818	39	-	3/9/27/28	0/2/2/2
39	OMU	L5	2837	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	4431	39	-	0/7/25/26	0/2/2/2
35	OMG	S2	644	35	-	3/9/27/28	0/3/3/3
39	PSU	L5	4312	39	-	0/7/25/26	0/2/2/2
35	A2M	S2	1383	35	-	3/9/27/28	0/3/3/3
39	OMG	L5	4499	39	-	0/9/27/28	0/3/3/3
35	B8N	S2	1248	35	-	1/16/34/35	0/2/2/2
39	PSU	L5	1536	39	-	2/7/25/26	0/2/2/2
35	PSU	S2	1244	35	-	0/7/25/26	0/2/2/2
39	OMC	L5	2861	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	3695	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4521	39,85	-	0/7/25/26	0/2/2/2
39	5MC	L5	4447	39	-	4/7/25/26	0/2/2/2
35	OMU	S2	627	35	-	6/9/27/28	0/2/2/2
35	PSU	S2	406	35	-	0/7/25/26	0/2/2/2
39	OMU	L5	4620	39	-	0/9/27/28	0/2/2/2
35	4AC	S2	1337	35	-	1/11/29/30	0/2/2/2
35	PSU	S2	1004	35	-	0/7/25/26	0/2/2/2
39	OMC	L5	3887	39	-	1/9/27/28	0/2/2/2
35	PSU	S2	649	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	1860	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	2839	39	-	0/7/25/26	0/2/2/2
35	G7M	S2	1639	35,2	-	1/7/25/26	0/3/3/3
35	PSU	S2	1174	35	-	0/7/25/26	0/2/2/2
39	OMG	L5	4392	39	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	OMU	S2	799	35	-	2/9/27/28	0/2/2/2
39	OMG	L5	2364	39,85	-	3/9/27/28	0/3/3/3
35	OMG	S2	436	35	-	0/9/27/28	0/3/3/3
39	OMC	L5	2804	39	-	0/9/27/28	0/2/2/2
39	OMG	L5	4494	39	-	1/9/27/28	0/3/3/3
35	OMC	S2	1703	35	-	1/9/27/28	0/2/2/2
35	PSU	S2	966	35,85	-	0/7/25/26	0/2/2/2
39	OMG	L5	2424	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	1340	39	-	1/9/27/28	0/2/2/2
35	OMU	S2	121	35	-	0/9/27/28	0/2/2/2
35	A2M	S2	668	35,85	-	3/9/27/28	0/3/3/3
35	OMC	S2	1272	35	-	2/9/27/28	0/2/2/2
35	OMU	S2	1326	35	-	0/9/27/28	0/2/2/2
35	PSU	S2	651	35	-	0/7/25/26	0/2/2/2
39	OMU	L5	3925	39	-	1/9/27/28	0/2/2/2
35	A2M	S2	1031	35	-	1/9/27/28	0/3/3/3
39	OMU	L5	4227	39	-	0/9/27/28	0/2/2/2
35	A2M	S2	159	35	-	1/9/27/28	0/3/3/3
39	PSU	L5	4403	39	-	0/7/25/26	0/2/2/2
39	A2M	L5	2363	39,85	-	0/9/27/28	0/3/3/3
39	PSU	L5	5010	39	-	0/7/25/26	0/2/2/2
35	A2M	S2	468	35	-	0/9/27/28	0/3/3/3
35	4AC	S2	1842	35	-	0/11/29/30	0/2/2/2
39	PSU	L5	1582	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	1522	39	-	0/9/27/28	0/3/3/3
39	PSU	L5	2632	39	-	0/7/25/26	0/2/2/2
39	A2M	L5	1326	39	-	4/9/27/28	0/3/3/3
35	PSU	S2	866	35	-	0/7/25/26	0/2/2/2

All (342) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	1832	6MZ	C6-N6	12.85	1.48	1.34
39	L5	3818	UY1	C6-C5	12.42	1.49	1.35
39	L5	4220	6MZ	C6-N6	11.50	1.47	1.34
39	L5	3818	UY1	C2-N1	11.43	1.51	1.36
35	S2	799	OMU	C2-N1	8.53	1.51	1.38
35	S2	1832	6MZ	C3'-C2'	-8.48	1.30	1.53
35	S2	1288	OMU	C2-N1	8.33	1.51	1.38
35	S2	627	OMU	C2-N1	8.14	1.51	1.38
35	S2	172	OMU	C2-N1	8.13	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	116	OMU	C2-N1	8.06	1.51	1.38
35	S2	121	OMU	C2-N1	8.01	1.51	1.38
35	S2	1850	MA6	C3'-C2'	-8.01	1.31	1.53
35	S2	428	OMU	C2-N1	8.00	1.51	1.38
35	S2	1442	OMU	C2-N1	7.99	1.51	1.38
35	S2	1326	OMU	C2-N1	7.97	1.50	1.38
35	S2	1248	B8N	C4-N3	-7.96	1.26	1.40
35	S2	354	OMU	C2-N1	7.88	1.50	1.38
39	L5	4306	OMU	C2-N1	7.82	1.50	1.38
39	L5	2837	OMU	C2-N1	7.77	1.50	1.38
35	S2	1248	B8N	C6-N1	7.75	1.55	1.36
39	L5	3925	OMU	C2-N1	7.66	1.50	1.38
39	L5	4227	OMU	C2-N1	7.65	1.50	1.38
39	L5	4498	OMU	C2-N1	7.64	1.50	1.38
39	L5	3818	UY1	C2-N3	7.56	1.49	1.37
39	L5	4620	OMU	C2-N1	7.45	1.50	1.38
35	S2	627	OMU	C2-N3	6.89	1.50	1.38
35	S2	799	OMU	C2-N3	6.87	1.49	1.38
35	S2	1288	OMU	C2-N3	6.85	1.49	1.38
35	S2	428	OMU	C2-N3	6.84	1.49	1.38
35	S2	121	OMU	C2-N3	6.84	1.49	1.38
35	S2	1248	B8N	C4-C5	6.83	1.63	1.47
35	S2	116	OMU	C2-N3	6.78	1.49	1.38
35	S2	172	OMU	C2-N3	6.76	1.49	1.38
35	S2	1442	OMU	C2-N3	6.76	1.49	1.38
39	L5	2837	OMU	C2-N3	6.68	1.49	1.38
35	S2	354	OMU	C2-N3	6.63	1.49	1.38
35	S2	1326	OMU	C2-N3	6.56	1.49	1.38
35	S2	1639	G7M	C4-N3	6.52	1.49	1.34
39	L5	4306	OMU	C2-N3	6.49	1.49	1.38
39	L5	4498	OMU	C2-N3	6.46	1.49	1.38
39	L5	4227	OMU	C2-N3	6.46	1.49	1.38
39	L5	3925	OMU	C2-N3	6.45	1.49	1.38
39	L5	4620	OMU	C2-N3	6.24	1.48	1.38
39	L5	4530	UR3	C6-C5	6.13	1.49	1.35
39	L5	4530	UR3	C2-N1	5.89	1.46	1.38
35	S2	428	OMU	C6-C5	5.83	1.48	1.35
35	S2	799	OMU	C6-C5	5.83	1.48	1.35
35	S2	627	OMU	C6-C5	5.82	1.48	1.35
35	S2	172	OMU	C6-C5	5.80	1.48	1.35
35	S2	1442	OMU	C6-C5	5.79	1.48	1.35
35	S2	121	OMU	C6-C5	5.78	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	1248	B8N	C2-N1	5.78	1.56	1.39
39	L5	3925	OMU	O4-C4	-5.77	1.13	1.24
35	S2	1288	OMU	C6-C5	5.77	1.48	1.35
35	S2	116	OMU	C6-C5	5.74	1.48	1.35
35	S2	354	OMU	C6-C5	5.73	1.48	1.35
39	L5	4620	OMU	O4-C4	-5.73	1.13	1.24
39	L5	2837	OMU	O4-C4	-5.72	1.13	1.24
35	S2	1326	OMU	C6-C5	5.71	1.48	1.35
39	L5	4306	OMU	O4-C4	-5.70	1.13	1.24
39	L5	2837	OMU	C6-C5	5.68	1.48	1.35
39	L5	4498	OMU	C6-C5	5.64	1.48	1.35
39	L5	4227	OMU	O4-C4	-5.63	1.13	1.24
39	L5	4620	OMU	C6-C5	5.62	1.48	1.35
39	L5	4498	OMU	O4-C4	-5.61	1.13	1.24
39	L5	4306	OMU	C6-C5	5.59	1.48	1.35
35	S2	354	OMU	O4-C4	-5.58	1.13	1.24
35	S2	1442	OMU	O4-C4	-5.56	1.13	1.24
39	L5	4227	OMU	C6-C5	5.55	1.47	1.35
35	S2	1326	OMU	O4-C4	-5.54	1.13	1.24
35	S2	121	OMU	O4-C4	-5.53	1.13	1.24
39	L5	3925	OMU	C6-C5	5.52	1.47	1.35
39	L5	4530	UR3	C2-N3	5.51	1.49	1.39
35	S2	428	OMU	O4-C4	-5.49	1.13	1.24
35	S2	116	OMU	O4-C4	-5.47	1.13	1.24
35	S2	1288	OMU	O4-C4	-5.46	1.13	1.24
35	S2	627	OMU	O4-C4	-5.46	1.13	1.24
35	S2	799	OMU	O4-C4	-5.42	1.13	1.24
35	S2	172	OMU	O4-C4	-5.38	1.14	1.24
35	S2	1639	G7M	C2-N3	5.34	1.46	1.33
35	S2	1248	B8N	C6-C5	5.29	1.42	1.35
39	L5	3818	UY1	C6-N1	5.24	1.44	1.36
35	S2	1639	G7M	C2-N2	4.88	1.45	1.34
35	S2	1639	G7M	C5-N7	-4.86	1.33	1.39
35	S2	1832	6MZ	O4'-C4'	4.77	1.55	1.45
35	S2	1832	6MZ	O4'-C1'	-4.71	1.31	1.42
35	S2	627	OMU	C4-N3	4.53	1.46	1.38
35	S2	1832	6MZ	C5'-C4'	-4.45	1.38	1.51
39	L5	3818	UY1	C4-N3	4.37	1.47	1.38
35	S2	1326	OMU	C4-N3	4.35	1.46	1.38
35	S2	799	OMU	C4-N3	4.32	1.46	1.38
35	S2	1288	OMU	C4-N3	4.32	1.46	1.38
35	S2	1442	OMU	C4-N3	4.27	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	121	OMU	C4-N3	4.25	1.45	1.38
35	S2	116	OMU	C4-N3	4.25	1.45	1.38
35	S2	1850	MA6	C5'-C4'	-4.24	1.38	1.51
35	S2	172	OMU	C4-N3	4.19	1.45	1.38
35	S2	428	OMU	C4-N3	4.15	1.45	1.38
35	S2	354	OMU	C4-N3	4.13	1.45	1.38
35	S2	1850	MA6	O4'-C4'	4.07	1.54	1.45
39	L5	4227	OMU	C4-N3	4.00	1.45	1.38
39	L5	2837	OMU	C4-N3	3.99	1.45	1.38
39	L5	4498	OMU	C4-N3	3.99	1.45	1.38
39	L5	3925	OMU	C4-N3	3.84	1.45	1.38
39	L5	4306	OMU	C4-N3	3.83	1.45	1.38
35	S2	1850	MA6	O4'-C1'	-3.83	1.33	1.42
39	L5	3818	UY1	O4-C4	-3.77	1.16	1.23
35	S2	1639	G7M	C5-C6	3.75	1.53	1.43
39	L5	4620	OMU	C4-N3	3.73	1.45	1.38
39	L5	2401	A2M	O5'-C5'	-3.68	1.33	1.44
39	L5	400	A2M	O5'-C5'	-3.67	1.33	1.44
35	S2	801	PSU	C6-C5	3.66	1.39	1.35
39	L5	3785	A2M	O5'-C5'	-3.62	1.33	1.44
35	S2	863	PSU	C6-C5	3.62	1.39	1.35
39	L5	2787	A2M	O5'-C5'	-3.61	1.33	1.44
39	L5	1871	A2M	O5'-C5'	-3.61	1.33	1.44
35	S2	1248	B8N	C1'-C5	3.58	1.58	1.50
39	L5	3825	A2M	O5'-C5'	-3.57	1.33	1.44
39	L5	1326	A2M	O5'-C5'	-3.56	1.33	1.44
39	L5	1524	A2M	O5'-C5'	-3.53	1.33	1.44
39	L5	4220	6MZ	C5-C4	-3.53	1.32	1.39
39	L5	1323	A2M	O5'-C5'	-3.53	1.33	1.44
39	L5	3867	A2M	O5'-C5'	-3.52	1.33	1.44
35	S2	468	A2M	O5'-C5'	-3.52	1.33	1.44
35	S2	649	PSU	C6-C5	3.48	1.39	1.35
39	L5	5010	PSU	C6-C5	3.47	1.39	1.35
35	S2	99	A2M	O5'-C5'	-3.47	1.34	1.44
35	S2	576	A2M	O5'-C5'	-3.47	1.34	1.44
39	L5	4590	A2M	O5'-C5'	-3.47	1.34	1.44
39	L5	4571	A2M	O5'-C5'	-3.46	1.34	1.44
39	L5	2363	A2M	O5'-C5'	-3.46	1.34	1.44
39	L5	3718	A2M	O5'-C5'	-3.44	1.34	1.44
39	L5	4220	6MZ	C5-N7	-3.44	1.32	1.39
35	S2	668	A2M	O5'-C5'	-3.44	1.34	1.44
39	L5	2815	A2M	O5'-C5'	-3.43	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	1383	A2M	O5'-C5'	-3.43	1.34	1.44
39	L5	3830	A2M	O5'-C5'	-3.43	1.34	1.44
35	S2	27	A2M	O5'-C5'	-3.43	1.34	1.44
35	S2	1031	A2M	O5'-C5'	-3.42	1.34	1.44
35	S2	166	A2M	O5'-C5'	-3.42	1.34	1.44
35	S2	814	PSU	C6-C5	3.41	1.39	1.35
35	S2	484	A2M	O5'-C5'	-3.40	1.34	1.44
35	S2	1244	PSU	C6-C5	3.39	1.39	1.35
35	S2	1232	PSU	C6-C5	3.37	1.39	1.35
39	L5	398	A2M	O5'-C5'	-3.37	1.34	1.44
35	S2	966	PSU	C6-C5	3.36	1.39	1.35
35	S2	109	PSU	C6-C5	3.35	1.39	1.35
35	S2	651	PSU	C6-C5	3.33	1.39	1.35
35	S2	1004	PSU	C6-C5	3.32	1.39	1.35
35	S2	105	PSU	C6-C5	3.31	1.39	1.35
35	S2	93	PSU	C6-C5	3.29	1.38	1.35
35	S2	406	PSU	C6-C5	3.29	1.38	1.35
35	S2	1367	PSU	C6-C5	3.29	1.38	1.35
39	L5	4523	A2M	O5'-C5'	-3.28	1.34	1.44
35	S2	159	A2M	O5'-C5'	-3.27	1.34	1.44
39	L5	1862	PSU	C6-C5	3.27	1.38	1.35
35	S2	686	PSU	C6-C5	3.26	1.38	1.35
39	L5	4296	PSU	C6-C5	3.25	1.38	1.35
39	L5	3818	UY1	O2-C2	-3.25	1.16	1.23
35	S2	1045	PSU	C6-C5	3.25	1.38	1.35
35	S2	1174	PSU	C6-C5	3.25	1.38	1.35
35	S2	866	PSU	C6-C5	3.24	1.38	1.35
39	L5	1860	PSU	C6-C5	3.22	1.38	1.35
39	L5	3818	UY1	C1'-C5	3.20	1.57	1.50
39	L5	1782	PSU	C6-C5	3.20	1.38	1.35
35	S2	1046	PSU	C6-C5	3.19	1.38	1.35
39	L5	1781	PSU	C6-C5	3.19	1.38	1.35
35	S2	1081	PSU	C6-C5	3.18	1.38	1.35
39	L5	4532	PSU	C6-C5	3.18	1.38	1.35
39	L5	4972	PSU	C6-C5	3.18	1.38	1.35
39	L5	4552	PSU	C6-C5	3.15	1.38	1.35
39	L5	4312	PSU	C6-C5	3.15	1.38	1.35
35	S2	1850	MA6	C6-N6	3.14	1.45	1.36
39	L5	1744	PSU	C6-C5	3.14	1.38	1.35
39	L5	4293	PSU	C6-C5	3.12	1.38	1.35
35	S2	1832	6MZ	C5-N7	-3.11	1.33	1.39
39	L5	4353	PSU	C6-C5	3.09	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	L5	3851	PSU	C6-C5	3.09	1.38	1.35
35	S2	1851	MA6	C6-N6	3.09	1.45	1.36
39	L5	3639	PSU	C6-C5	3.08	1.38	1.35
35	S2	1177	PSU	C6-C5	3.08	1.38	1.35
39	L5	5001	PSU	C6-C5	3.08	1.38	1.35
39	L5	1534	A2M	O5'-C5'	-3.07	1.35	1.44
35	S2	1056	PSU	C6-C5	3.07	1.38	1.35
41	L8	69	PSU	C6-C5	3.07	1.38	1.35
35	S2	1832	6MZ	C8-N9	-3.07	1.32	1.37
39	L5	4673	PSU	C6-C5	3.06	1.38	1.35
39	L5	2632	PSU	C6-C5	3.06	1.38	1.35
39	L5	3844	PSU	C6-C5	3.06	1.38	1.35
39	L5	4500	PSU	C6-C5	3.06	1.38	1.35
39	L5	1792	PSU	C6-C5	3.04	1.38	1.35
41	L8	55	PSU	C6-C5	3.04	1.38	1.35
39	L5	4493	PSU	C6-C5	3.04	1.38	1.35
35	S2	668	A2M	O4'-C4'	-3.04	1.38	1.45
35	S2	1832	6MZ	C5-C4	-3.03	1.33	1.39
39	L5	2839	PSU	C6-C5	3.03	1.38	1.35
39	L5	4220	6MZ	C8-N9	-3.03	1.32	1.37
39	L5	4636	PSU	C6-C5	3.02	1.38	1.35
39	L5	4299	PSU	C6-C5	3.01	1.38	1.35
39	L5	4579	PSU	C6-C5	3.01	1.38	1.35
39	L5	3695	PSU	C6-C5	2.98	1.38	1.35
39	L5	4431	PSU	C6-C5	2.98	1.38	1.35
39	L5	4521	PSU	C6-C5	2.97	1.38	1.35
39	L5	4973	PSU	C6-C5	2.97	1.38	1.35
39	L5	4471	PSU	C6-C5	2.96	1.38	1.35
39	L5	3920	PSU	C6-C5	2.95	1.38	1.35
35	S2	1832	6MZ	C2'-C1'	2.95	1.62	1.53
39	L5	4576	PSU	C6-C5	2.94	1.38	1.35
35	S2	681	PSU	C6-C5	2.92	1.38	1.35
39	L5	3884	PSU	C6-C5	2.91	1.38	1.35
39	L5	4628	PSU	C6-C5	2.88	1.38	1.35
39	L5	3637	PSU	C6-C5	2.88	1.38	1.35
39	L5	3822	PSU	C6-C5	2.86	1.38	1.35
39	L5	4361	PSU	C6-C5	2.85	1.38	1.35
35	S2	627	OMU	C5-C4	2.85	1.49	1.43
39	L5	1582	PSU	C6-C5	2.84	1.38	1.35
35	S2	1850	MA6	O3'-C3'	2.84	1.50	1.43
39	L5	4530	UR3	O2-C2	-2.84	1.17	1.22
39	L5	1536	PSU	C6-C5	2.83	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	172	OMU	C5-C4	2.82	1.49	1.43
39	L5	1683	PSU	C6-C5	2.81	1.38	1.35
39	L5	2363	A2M	O4'-C4'	-2.81	1.38	1.45
39	L5	4689	PSU	C6-C5	2.81	1.38	1.35
39	L5	1323	A2M	O4'-C4'	-2.80	1.38	1.45
35	S2	121	OMU	C5-C4	2.79	1.49	1.43
39	L5	1677	PSU	C6-C5	2.79	1.38	1.35
35	S2	428	OMU	C5-C4	2.79	1.49	1.43
35	S2	1326	OMU	C5-C4	2.78	1.49	1.43
35	S2	1442	OMU	C5-C4	2.78	1.49	1.43
35	S2	799	OMU	C5-C4	2.77	1.49	1.43
39	L5	1871	A2M	O4'-C4'	-2.77	1.38	1.45
35	S2	354	OMU	C5-C4	2.77	1.49	1.43
39	L5	3867	A2M	O4'-C4'	-2.76	1.38	1.45
39	L5	4403	PSU	C6-C5	2.75	1.38	1.35
39	L5	4442	PSU	C6-C5	2.74	1.38	1.35
39	L5	1524	A2M	O4'-C4'	-2.74	1.38	1.45
35	S2	1288	OMU	C5-C4	2.72	1.49	1.43
35	S2	1639	G7M	C2-N1	2.72	1.44	1.37
39	L5	4571	A2M	O4'-C4'	-2.69	1.39	1.45
39	L5	3853	PSU	C6-C5	2.68	1.38	1.35
39	L5	1534	A2M	O4'-C4'	-2.67	1.39	1.45
35	S2	121	OMU	C6-N1	2.65	1.44	1.38
35	S2	627	OMU	C6-N1	2.64	1.44	1.38
35	S2	799	OMU	C6-N1	2.64	1.44	1.38
39	L5	4227	OMU	C5-C4	2.63	1.49	1.43
35	S2	1442	OMU	C6-N1	2.63	1.44	1.38
39	L5	4457	PSU	C6-C5	2.63	1.38	1.35
39	L5	4498	OMU	C5-C4	2.62	1.49	1.43
35	S2	1288	OMU	C6-N1	2.62	1.44	1.38
35	S2	116	OMU	C5-C4	2.61	1.49	1.43
35	S2	1832	6MZ	O3'-C3'	2.57	1.49	1.43
35	S2	1851	MA6	C5-C4	-2.57	1.34	1.39
35	S2	428	OMU	C6-N1	2.56	1.44	1.38
39	L5	2837	OMU	C5-C4	2.55	1.49	1.43
35	S2	1639	G7M	O6-C6	-2.55	1.18	1.23
39	L5	4306	OMU	C5-C4	2.54	1.49	1.43
39	L5	1326	A2M	O4'-C4'	-2.54	1.39	1.45
35	S2	1326	OMU	C6-N1	2.52	1.44	1.38
39	L5	4523	A2M	O4'-C4'	-2.52	1.39	1.45
35	S2	172	OMU	C6-N1	2.52	1.44	1.38
39	L5	4498	OMU	C6-N1	2.51	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	L5	3925	OMU	C5-C4	2.50	1.49	1.43
35	S2	116	OMU	C6-N1	2.50	1.44	1.38
35	S2	1850	MA6	C5-C4	-2.47	1.34	1.39
35	S2	354	OMU	C6-N1	2.45	1.43	1.38
39	L5	1677	PSU	O4'-C1'	-2.45	1.40	1.43
39	L5	2837	OMU	C6-N1	2.44	1.43	1.38
39	L5	4220	6MZ	C6-N1	-2.44	1.31	1.35
39	L5	4620	OMU	C6-N1	2.43	1.43	1.38
35	S2	1832	6MZ	C6-N1	-2.41	1.31	1.35
39	L5	4227	OMU	C6-N1	2.39	1.43	1.38
39	L5	4530	UR3	C6-N1	2.39	1.43	1.38
39	L5	4306	OMU	C6-N1	2.36	1.43	1.38
39	L5	4447	5MC	C5-C4	-2.34	1.42	1.44
39	L5	3925	OMU	C6-N1	2.34	1.43	1.38
35	S2	1639	G7M	C6-N1	2.33	1.43	1.38
39	L5	3884	PSU	C4-C5	-2.32	1.37	1.44
39	L5	2815	A2M	O4'-C4'	-2.30	1.39	1.45
39	L5	4620	OMU	C5-C4	2.29	1.48	1.43
39	L5	4353	PSU	C4-C5	-2.28	1.38	1.44
39	L5	400	A2M	O4'-C4'	-2.28	1.39	1.45
39	L5	1871	A2M	O3'-C3'	-2.24	1.37	1.43
39	L5	3818	UY1	O4'-C1'	-2.20	1.40	1.43
39	L5	3825	A2M	O4'-C4'	-2.20	1.40	1.45
39	L5	3639	PSU	C4-C5	-2.20	1.38	1.44
39	L5	4293	PSU	C4-C5	-2.19	1.38	1.44
39	L5	2839	PSU	C4-C5	-2.18	1.38	1.44
39	L5	1683	PSU	C4-C5	-2.17	1.38	1.44
39	L5	1677	PSU	C4-C5	-2.17	1.38	1.44
39	L5	4523	A2M	O3'-C3'	-2.17	1.37	1.43
35	S2	1639	G7M	C4-N9	-2.16	1.32	1.38
39	L5	3830	A2M	O4'-C4'	-2.16	1.40	1.45
39	L5	3695	PSU	C4-C5	-2.16	1.38	1.44
35	S2	1850	MA6	C2'-C1'	2.16	1.60	1.53
39	L5	4312	PSU	C4-C5	-2.14	1.38	1.44
39	L5	4456	OMC	C4-N3	-2.14	1.30	1.34
39	L5	2401	A2M	O4'-C4'	-2.14	1.40	1.45
39	L5	4457	PSU	C4-C5	-2.13	1.38	1.44
39	L5	4973	PSU	C4-C5	-2.13	1.38	1.44
39	L5	3718	A2M	O4'-C4'	-2.13	1.40	1.45
39	L5	4220	6MZ	C4-N9	-2.12	1.33	1.37
39	L5	3844	PSU	C4-C5	-2.12	1.38	1.44
39	L5	3867	A2M	O3'-C3'	-2.12	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	L5	4521	PSU	C4-C5	-2.11	1.38	1.44
39	L5	4689	PSU	C4-C5	-2.11	1.38	1.44
39	L5	4673	PSU	C4-C5	-2.11	1.38	1.44
35	S2	1248	B8N	O4'-C1'	-2.11	1.40	1.43
39	L5	4500	PSU	C4-C5	-2.10	1.38	1.44
39	L5	3920	PSU	C4-C5	-2.10	1.38	1.44
39	L5	1536	PSU	C4-C5	-2.09	1.38	1.44
35	S2	1174	PSU	C4-C5	-2.09	1.38	1.44
35	S2	1056	PSU	C4-C5	-2.08	1.38	1.44
39	L5	1524	A2M	O3'-C3'	-2.08	1.37	1.43
39	L5	4530	UR3	C5-C4	2.08	1.49	1.43
41	L8	69	PSU	C4-C5	-2.07	1.38	1.44
39	L5	1744	PSU	C4-C5	-2.07	1.38	1.44
35	S2	1004	PSU	C4-C5	-2.07	1.38	1.44
39	L5	4590	A2M	O4'-C4'	-2.07	1.40	1.45
39	L5	4471	PSU	C4-C5	-2.06	1.38	1.44
39	L5	2351	OMC	C4-N3	-2.06	1.30	1.34
39	L5	4628	PSU	C4-C5	-2.06	1.38	1.44
35	S2	1850	MA6	C5-N7	-2.05	1.35	1.39
39	L5	400	A2M	O3'-C3'	-2.05	1.37	1.43
39	L5	4972	PSU	C4-C5	-2.05	1.38	1.44
39	L5	3701	OMC	C4-N3	-2.05	1.30	1.34
39	L5	4636	PSU	C4-C5	-2.05	1.38	1.44
39	L5	4403	PSU	C4-C5	-2.04	1.38	1.44
35	S2	406	PSU	C4-C5	-2.04	1.38	1.44
35	S2	866	PSU	C4-C5	-2.04	1.38	1.44
39	L5	4431	PSU	C4-C5	-2.04	1.38	1.44
39	L5	4579	PSU	C4-C5	-2.03	1.38	1.44
39	L5	4442	PSU	O4'-C1'	-2.03	1.41	1.43
39	L5	4571	A2M	O3'-C3'	-2.02	1.37	1.43
39	L5	1860	PSU	C4-C5	-2.02	1.38	1.44
39	L5	1792	PSU	C4-C5	-2.02	1.38	1.44
39	L5	4530	UR3	C3U-N3	2.02	1.50	1.47
39	L5	4532	PSU	C4-C5	-2.02	1.38	1.44
39	L5	2632	PSU	C4-C5	-2.01	1.38	1.44
35	S2	1177	PSU	C4-C5	-2.01	1.38	1.44
39	L5	4552	PSU	C4-C5	-2.01	1.38	1.44
35	S2	109	PSU	C4-C5	-2.00	1.38	1.44
39	L5	3637	PSU	C4-C5	-2.00	1.38	1.44

All (700) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S2	1851	MA6	N1-C6-N6	-12.19	102.00	116.86
35	S2	1850	MA6	N1-C6-N6	-11.44	102.91	116.86
35	S2	1851	MA6	C5-C6-N6	8.08	138.12	125.33
35	S2	1850	MA6	C5-C6-N6	7.74	137.59	125.33
35	S2	1639	G7M	C1'-N9-C4	7.42	148.40	126.49
35	S2	1639	G7M	C1'-N9-C8	-7.37	101.86	126.74
39	L5	4498	OMU	C4-N3-C2	-6.04	119.11	126.61
39	L5	3925	OMU	C4-N3-C2	-5.99	119.18	126.61
35	S2	354	OMU	C4-N3-C2	-5.93	119.24	126.61
39	L5	4530	UR3	C4-N3-C2	-5.93	119.81	124.58
39	L5	4220	6MZ	C9-N6-C6	-5.92	117.36	122.85
35	S2	1326	OMU	C4-N3-C2	-5.86	119.34	126.61
39	L5	4220	6MZ	N1-C2-N3	-5.85	119.72	128.58
39	L5	4227	OMU	C4-N3-C2	-5.82	119.38	126.61
39	L5	4306	OMU	C4-N3-C2	-5.77	119.45	126.61
39	L5	2837	OMU	C4-N3-C2	-5.74	119.48	126.61
35	S2	428	OMU	C4-N3-C2	-5.73	119.50	126.61
35	S2	1832	6MZ	N1-C2-N3	-5.73	119.91	128.58
35	S2	1851	MA6	N1-C2-N3	-5.72	119.92	128.58
35	S2	121	OMU	C4-N3-C2	-5.70	119.53	126.61
39	L5	3701	OMC	C1'-N1-C2	5.69	131.02	118.44
35	S2	172	OMU	C4-N3-C2	-5.68	119.56	126.61
35	S2	627	OMU	C4-N3-C2	-5.57	119.69	126.61
35	S2	1442	OMU	C4-N3-C2	-5.54	119.73	126.61
35	S2	799	OMU	C4-N3-C2	-5.49	119.80	126.61
39	L5	1677	PSU	C4-N3-C2	-5.47	118.84	126.37
35	S2	1850	MA6	N1-C2-N3	-5.44	120.35	128.58
39	L5	4636	PSU	C4-N3-C2	-5.41	118.92	126.37
35	S2	1851	MA6	N9-C8-N7	-5.39	106.29	113.94
35	S2	1288	OMU	C4-N3-C2	-5.35	119.97	126.61
39	L5	4403	PSU	C4-N3-C2	-5.26	119.13	126.37
35	S2	1248	B8N	C5-C4-N3	5.25	125.69	116.15
39	L5	4293	PSU	N1-C2-N3	5.24	120.70	115.17
39	L5	3637	PSU	N1-C2-N3	5.24	120.70	115.17
39	L5	4457	PSU	C4-N3-C2	-5.24	119.16	126.37
39	L5	3639	PSU	N1-C2-N3	5.23	120.69	115.17
39	L5	4628	PSU	N1-C2-N3	5.21	120.66	115.17
39	L5	4293	PSU	C4-N3-C2	-5.19	119.22	126.37
39	L5	4552	PSU	N1-C2-N3	5.17	120.62	115.17
35	S2	1850	MA6	N9-C8-N7	-5.15	106.62	113.94
39	L5	4636	PSU	N1-C2-N3	5.15	120.60	115.17
41	L8	69	PSU	N1-C2-N3	5.14	120.59	115.17
39	L5	2632	PSU	N1-C2-N3	5.12	120.57	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	1862	PSU	N1-C2-N3	5.12	120.56	115.17
39	L5	4442	PSU	C4-N3-C2	-5.10	119.34	126.37
35	S2	1177	PSU	C4-N3-C2	-5.09	119.36	126.37
39	L5	4403	PSU	N1-C2-N3	5.08	120.53	115.17
35	S2	109	PSU	N1-C2-N3	5.08	120.52	115.17
39	L5	1683	PSU	C4-N3-C2	-5.08	119.38	126.37
35	S2	406	PSU	N1-C2-N3	5.07	120.51	115.17
39	L5	4442	PSU	N1-C2-N3	5.07	120.51	115.17
39	L5	4457	PSU	N1-C2-N3	5.07	120.51	115.17
39	L5	3637	PSU	C4-N3-C2	-5.07	119.39	126.37
35	S2	1244	PSU	N1-C2-N3	5.06	120.51	115.17
39	L5	1677	PSU	N1-C2-N3	5.06	120.50	115.17
39	L5	2839	PSU	N1-C2-N3	5.06	120.50	115.17
39	L5	4353	PSU	N1-C2-N3	5.06	120.50	115.17
35	S2	406	PSU	C4-N3-C2	-5.05	119.41	126.37
39	L5	4500	PSU	C4-N3-C2	-5.05	119.41	126.37
39	L5	3851	PSU	N1-C2-N3	5.05	120.49	115.17
35	S2	1056	PSU	C4-N3-C2	-5.05	119.42	126.37
39	L5	4521	PSU	C4-N3-C2	-5.05	119.42	126.37
39	L5	4973	PSU	C4-N3-C2	-5.04	119.43	126.37
39	L5	2632	PSU	C4-N3-C2	-5.04	119.43	126.37
39	L5	4500	PSU	N1-C2-N3	5.02	120.47	115.17
39	L5	1862	PSU	C4-N3-C2	-5.02	119.46	126.37
39	L5	1683	PSU	N1-C2-N3	5.02	120.46	115.17
39	L5	4296	PSU	N1-C2-N3	5.02	120.46	115.17
35	S2	966	PSU	N1-C2-N3	5.01	120.46	115.17
39	L5	3695	PSU	C4-N3-C2	-5.01	119.47	126.37
39	L5	4353	PSU	C4-N3-C2	-5.01	119.48	126.37
35	S2	109	PSU	C4-N3-C2	-5.00	119.48	126.37
39	L5	4689	PSU	N1-C2-N3	5.00	120.44	115.17
39	L5	4552	PSU	C4-N3-C2	-5.00	119.48	126.37
39	L5	3639	PSU	C4-N3-C2	-5.00	119.49	126.37
39	L5	4471	PSU	N1-C2-N3	4.99	120.44	115.17
39	L5	1792	PSU	C4-N3-C2	-4.99	119.49	126.37
39	L5	4296	PSU	C4-N3-C2	-4.99	119.49	126.37
39	L5	4673	PSU	N1-C2-N3	4.99	120.43	115.17
39	L5	4620	OMU	C4-N3-C2	-4.99	120.42	126.61
39	L5	1744	PSU	C4-N3-C2	-4.98	119.51	126.37
39	L5	4299	PSU	N1-C2-N3	4.98	120.42	115.17
39	L5	1860	PSU	C4-N3-C2	-4.98	119.51	126.37
39	L5	1782	PSU	C4-N3-C2	-4.98	119.52	126.37
39	L5	1782	PSU	N1-C2-N3	4.98	120.42	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	4576	PSU	C4-N3-C2	-4.97	119.53	126.37
39	L5	4471	PSU	C4-N3-C2	-4.97	119.53	126.37
35	S2	966	PSU	C4-N3-C2	-4.97	119.53	126.37
39	L5	4521	PSU	N1-C2-N3	4.97	120.41	115.17
35	S2	116	OMU	C4-N3-C2	-4.97	120.45	126.61
39	L5	4532	PSU	C4-N3-C2	-4.96	119.54	126.37
39	L5	4431	PSU	C4-N3-C2	-4.96	119.54	126.37
39	L5	3884	PSU	C4-N3-C2	-4.96	119.54	126.37
39	L5	4973	PSU	N1-C2-N3	4.95	120.39	115.17
39	L5	3695	PSU	N1-C2-N3	4.95	120.39	115.17
35	S2	681	PSU	C4-N3-C2	-4.95	119.55	126.37
39	L5	3822	PSU	N1-C2-N3	4.95	120.39	115.17
35	S2	1056	PSU	N1-C2-N3	4.95	120.39	115.17
39	L5	4493	PSU	C4-N3-C2	-4.95	119.55	126.37
39	L5	3920	PSU	N1-C2-N3	4.94	120.38	115.17
39	L5	3818	UY1	C4-N3-C2	-4.94	119.57	126.37
35	S2	866	PSU	C4-N3-C2	-4.94	119.57	126.37
41	L8	69	PSU	C4-N3-C2	-4.94	119.57	126.37
35	S2	1232	PSU	C4-N3-C2	-4.94	119.57	126.37
39	L5	4299	PSU	C4-N3-C2	-4.94	119.57	126.37
39	L5	1860	PSU	N1-C2-N3	4.93	120.37	115.17
39	L5	4689	PSU	C4-N3-C2	-4.93	119.58	126.37
39	L5	3884	PSU	N1-C2-N3	4.92	120.36	115.17
39	L5	4220	6MZ	N9-C8-N7	-4.91	106.97	113.94
39	L5	4431	PSU	N1-C2-N3	4.91	120.35	115.17
35	S2	649	PSU	C4-N3-C2	-4.91	119.61	126.37
35	S2	866	PSU	N1-C2-N3	4.91	120.34	115.17
39	L5	2839	PSU	C4-N3-C2	-4.90	119.62	126.37
35	S2	1367	PSU	C4-N3-C2	-4.90	119.62	126.37
35	S2	686	PSU	C4-N3-C2	-4.90	119.62	126.37
35	S2	1244	PSU	C4-N3-C2	-4.90	119.62	126.37
35	S2	686	PSU	N1-C2-N3	4.89	120.33	115.17
39	L5	3853	PSU	C4-N3-C2	-4.89	119.63	126.37
39	L5	4628	PSU	C4-N3-C2	-4.89	119.63	126.37
35	S2	681	PSU	N1-C2-N3	4.89	120.33	115.17
35	S2	1045	PSU	N1-C2-N3	4.89	120.32	115.17
39	L5	4673	PSU	C4-N3-C2	-4.89	119.64	126.37
39	L5	3920	PSU	C4-N3-C2	-4.88	119.64	126.37
35	S2	649	PSU	N1-C2-N3	4.88	120.32	115.17
35	S2	1177	PSU	N1-C2-N3	4.88	120.31	115.17
39	L5	5001	PSU	N1-C2-N3	4.88	120.31	115.17
39	L5	1536	PSU	N1-C2-N3	4.87	120.31	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	4532	PSU	N1-C2-N3	4.87	120.30	115.17
39	L5	3844	PSU	C4-N3-C2	-4.86	119.67	126.37
39	L5	1536	PSU	C4-N3-C2	-4.86	119.67	126.37
39	L5	4312	PSU	C4-N3-C2	-4.86	119.67	126.37
39	L5	4579	PSU	N1-C2-N3	4.86	120.30	115.17
39	L5	1792	PSU	N1-C2-N3	4.86	120.29	115.17
39	L5	5001	PSU	C4-N3-C2	-4.85	119.69	126.37
39	L5	1744	PSU	N1-C2-N3	4.85	120.29	115.17
39	L5	4972	PSU	N1-C2-N3	4.85	120.28	115.17
39	L5	3851	PSU	C4-N3-C2	-4.84	119.70	126.37
35	S2	1832	6MZ	N9-C8-N7	-4.83	107.09	113.94
35	S2	651	PSU	C4-N3-C2	-4.82	119.73	126.37
35	S2	1045	PSU	C4-N3-C2	-4.82	119.73	126.37
35	S2	1232	PSU	N1-C2-N3	4.82	120.25	115.17
39	L5	5010	PSU	N1-C2-N3	4.82	120.25	115.17
35	S2	1004	PSU	C4-N3-C2	-4.81	119.75	126.37
35	S2	863	PSU	C4-N3-C2	-4.81	119.75	126.37
39	L5	4493	PSU	N1-C2-N3	4.80	120.23	115.17
39	L5	3822	PSU	C4-N3-C2	-4.80	119.76	126.37
35	S2	651	PSU	N1-C2-N3	4.80	120.23	115.17
35	S2	1004	PSU	N1-C2-N3	4.80	120.23	115.17
39	L5	4576	PSU	N1-C2-N3	4.80	120.23	115.17
35	S2	1174	PSU	C4-N3-C2	-4.79	119.78	126.37
39	L5	4361	PSU	C4-N3-C2	-4.79	119.78	126.37
39	L5	1781	PSU	N1-C2-N3	4.79	120.22	115.17
39	L5	3844	PSU	N1-C2-N3	4.79	120.22	115.17
39	L5	3853	PSU	N1-C2-N3	4.78	120.21	115.17
39	L5	4312	PSU	N1-C2-N3	4.77	120.19	115.17
41	L8	55	PSU	C4-N3-C2	-4.76	119.82	126.37
39	L5	1781	PSU	C4-N3-C2	-4.75	119.83	126.37
35	S2	863	PSU	N1-C2-N3	4.74	120.17	115.17
35	S2	105	PSU	N1-C2-N3	4.74	120.17	115.17
35	S2	1367	PSU	N1-C2-N3	4.74	120.17	115.17
35	S2	105	PSU	C4-N3-C2	-4.74	119.84	126.37
39	L5	4972	PSU	C4-N3-C2	-4.73	119.86	126.37
35	S2	1174	PSU	N1-C2-N3	4.72	120.15	115.17
39	L5	1582	PSU	C4-N3-C2	-4.70	119.90	126.37
39	L5	4579	PSU	C4-N3-C2	-4.69	119.91	126.37
41	L8	55	PSU	N1-C2-N3	4.69	120.11	115.17
35	S2	1046	PSU	N1-C2-N3	4.69	120.11	115.17
35	S2	1081	PSU	C4-N3-C2	-4.68	119.92	126.37
39	L5	5010	PSU	C4-N3-C2	-4.68	119.93	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S2	814	PSU	C4-N3-C2	-4.67	119.94	126.37
35	S2	1383	A2M	C3'-C2'-C1'	-4.66	93.88	102.81
35	S2	1046	PSU	C4-N3-C2	-4.65	119.96	126.37
39	L5	1582	PSU	N1-C2-N3	4.64	120.06	115.17
35	S2	801	PSU	N1-C2-N3	4.60	120.02	115.17
35	S2	93	PSU	C4-N3-C2	-4.59	120.05	126.37
35	S2	1248	B8N	C4-N3-C2	-4.55	120.02	125.62
35	S2	814	PSU	N1-C2-N3	4.55	119.96	115.17
35	S2	1639	G7M	C2-N3-C4	4.54	120.13	112.30
35	S2	1081	PSU	N1-C2-N3	4.53	119.95	115.17
39	L5	3701	OMC	C1'-N1-C6	-4.50	111.16	120.78
39	L5	4361	PSU	N1-C2-N3	4.50	119.91	115.17
35	S2	1851	MA6	C5-C4-N3	-4.46	120.57	126.72
35	S2	1850	MA6	C5-C4-N3	-4.46	120.58	126.72
35	S2	801	PSU	C4-N3-C2	-4.45	120.24	126.37
35	S2	93	PSU	N1-C2-N3	4.44	119.86	115.17
35	S2	1832	6MZ	C5-C4-N3	-4.44	120.60	126.72
39	L5	3818	UY1	N1-C2-N3	4.40	119.81	115.17
39	L5	4220	6MZ	C5-C4-N3	-4.39	120.67	126.72
39	L5	3830	A2M	C3'-C2'-C1'	-4.30	94.57	102.81
39	L5	4306	OMU	N3-C2-N1	4.25	120.42	114.89
39	L5	398	A2M	C3'-C2'-C1'	-4.23	94.70	102.81
39	L5	1871	A2M	C3'-C2'-C1'	-4.23	94.71	102.81
35	S2	1851	MA6	C4-N9-C8	4.21	110.16	105.74
39	L5	3925	OMU	N3-C2-N1	4.20	120.36	114.89
39	L5	4498	OMU	N3-C2-N1	4.17	120.32	114.89
35	S2	354	OMU	N3-C2-N1	4.13	120.27	114.89
39	L5	2837	OMU	N3-C2-N1	4.11	120.24	114.89
35	S2	121	OMU	N3-C2-N1	4.05	120.16	114.89
35	S2	1639	G7M	C5-C6-N1	4.03	120.17	111.84
39	L5	4523	A2M	C3'-C2'-C1'	-4.03	95.09	102.81
35	S2	1850	MA6	C4-N9-C8	3.99	109.93	105.74
39	L5	4498	OMU	C5-C4-N3	3.99	120.39	114.80
35	S2	1248	B8N	C1'-C5-C4	3.98	123.65	117.61
35	S2	1639	G7M	C5-C4-N3	-3.97	120.64	128.15
39	L5	398	A2M	O3'-C3'-C2'	3.91	122.14	111.19
35	S2	172	OMU	N3-C2-N1	3.90	119.97	114.89
39	L5	4227	OMU	C5-C4-N3	3.90	120.27	114.80
35	S2	1326	OMU	C5-C4-N3	3.89	120.24	114.80
35	S2	1850	MA6	C4-C5-C6	3.87	119.91	115.91
35	S2	1442	OMU	N3-C2-N1	3.87	119.92	114.89
35	S2	428	OMU	N3-C2-N1	3.87	119.92	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	3718	A2M	C3'-C2'-C1'	-3.86	95.42	102.81
39	L5	4530	UR3	C5-C4-N3	3.85	120.11	115.04
35	S2	99	A2M	C3'-C2'-C1'	-3.84	95.45	102.81
39	L5	4620	OMU	N3-C2-N1	3.83	119.88	114.89
39	L5	4590	A2M	C3'-C2'-C1'	-3.83	95.48	102.81
35	S2	1326	OMU	N3-C2-N1	3.77	119.80	114.89
39	L5	3925	OMU	C5-C4-N3	3.76	120.07	114.80
39	L5	4227	OMU	N3-C2-N1	3.75	119.77	114.89
35	S2	799	OMU	N3-C2-N1	3.74	119.76	114.89
35	S2	627	OMU	C5-C4-N3	3.72	120.01	114.80
35	S2	428	OMU	C5-C4-N3	3.68	119.96	114.80
35	S2	354	OMU	C5-C4-N3	3.67	119.93	114.80
39	L5	1323	A2M	C2'-C1'-N9	3.62	119.71	113.75
35	S2	121	OMU	C5-C4-N3	3.60	119.84	114.80
39	L5	2837	OMU	C5-C4-N3	3.58	119.81	114.80
35	S2	1288	OMU	N3-C2-N1	3.58	119.55	114.89
35	S2	1288	OMU	C5-C4-N3	3.57	119.81	114.80
35	S2	627	OMU	N3-C2-N1	3.57	119.54	114.89
35	S2	1442	OMU	C5-C4-N3	3.56	119.79	114.80
35	S2	799	OMU	C5-C4-N3	3.56	119.79	114.80
39	L5	4306	OMU	C5-C4-N3	3.56	119.78	114.80
35	S2	1851	MA6	C2-N1-C6	3.56	120.51	111.83
39	L5	2401	A2M	O3'-C3'-C2'	3.53	121.07	111.19
35	S2	172	OMU	C5-C4-N3	3.53	119.74	114.80
35	S2	166	A2M	O3'-C3'-C2'	3.52	121.04	111.19
35	S2	1850	MA6	C2-N1-C6	3.51	120.41	111.83
35	S2	116	OMU	N3-C2-N1	3.47	119.41	114.89
35	S2	1832	6MZ	C5-N7-C8	3.46	108.89	103.45
35	S2	1248	B8N	N3-C2-N1	3.44	120.92	116.72
35	S2	116	OMU	C5-C4-N3	3.44	119.62	114.80
35	S2	166	A2M	C3'-C2'-C1'	-3.42	96.27	102.81
39	L5	2787	A2M	O3'-C3'-C2'	3.40	120.69	111.19
35	S2	576	A2M	O3'-C3'-C2'	3.39	120.69	111.19
35	S2	1851	MA6	C4-C5-C6	3.38	119.41	115.91
35	S2	468	A2M	C3'-C2'-C1'	-3.38	96.33	102.81
35	S2	1383	A2M	O3'-C3'-C2'	3.38	120.65	111.19
35	S2	1639	G7M	O6-C6-C5	-3.37	120.48	128.01
35	S2	1850	MA6	N3-C4-N9	3.37	132.90	127.17
39	L5	4620	OMU	C5-C4-N3	3.36	119.51	114.80
39	L5	4220	6MZ	C4-N9-C8	3.36	109.26	105.74
35	S2	1832	6MZ	C2-N3-C4	3.35	120.00	111.83
35	S2	668	A2M	C4-N9-C1'	-3.34	118.81	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	3825	A2M	C3'-C2'-C1'	-3.34	96.41	102.81
39	L5	4220	6MZ	C2-N3-C4	3.31	119.93	111.83
39	L5	4571	A2M	C3'-C2'-C1'	-3.28	96.52	102.81
35	S2	1851	MA6	N3-C4-N9	3.27	132.73	127.17
39	L5	2401	A2M	C3'-C2'-C1'	-3.27	96.55	102.81
39	L5	4628	PSU	O2-C2-N1	-3.26	119.43	122.79
35	S2	1851	MA6	C2-N3-C4	3.22	119.70	111.83
39	L5	4403	PSU	O2-C2-N1	-3.22	119.47	122.79
35	S2	1031	A2M	C3'-C2'-C1'	-3.22	96.65	102.81
39	L5	2839	PSU	O2-C2-N1	-3.20	119.49	122.79
35	S2	1639	G7M	N9-C4-N3	3.20	132.35	125.95
39	L5	1536	PSU	O2-C2-N1	-3.19	119.50	122.79
35	S2	1851	MA6	C5-N7-C8	3.16	108.42	103.45
39	L5	4353	PSU	O2-C2-N1	-3.16	119.53	122.79
39	L5	2632	PSU	O2-C2-N1	-3.16	119.53	122.79
39	L5	3853	PSU	O2-C2-N1	-3.16	119.53	122.79
35	S2	99	A2M	O3'-C3'-C2'	3.15	120.00	111.19
39	L5	4442	PSU	O2-C2-N1	-3.15	119.54	122.79
35	S2	1326	OMU	O4-C4-C5	-3.15	119.74	125.16
35	S2	1031	A2M	O3'-C3'-C2'	3.14	119.97	111.19
39	L5	3785	A2M	C4'-O4'-C1'	-3.13	102.55	109.47
39	L5	1860	PSU	O2-C2-N1	-3.13	119.56	122.79
39	L5	4227	OMU	O4-C4-C5	-3.12	119.78	125.16
39	L5	3718	A2M	O3'-C3'-C2'	3.12	119.91	111.19
39	L5	3851	PSU	O2-C2-N1	-3.11	119.58	122.79
35	S2	1639	G7M	CN7-N7-C5	3.11	130.67	126.80
39	L5	4532	PSU	O2-C2-N1	-3.11	119.58	122.79
39	L5	1871	A2M	C4-N9-C1'	-3.11	119.37	126.63
39	L5	4628	PSU	C6-N1-C2	-3.11	119.81	122.69
35	S2	686	PSU	O2-C2-N1	-3.10	119.59	122.79
35	S2	1850	MA6	C5-N7-C8	3.10	108.32	103.45
35	S2	1045	PSU	O2-C2-N1	-3.10	119.59	122.79
39	L5	3867	A2M	C2'-C1'-N9	3.10	118.85	113.75
39	L5	1524	A2M	O3'-C3'-C2'	3.10	119.86	111.19
35	S2	668	A2M	O3'-C3'-C2'	3.10	119.85	111.19
39	L5	5010	PSU	O2-C2-N1	-3.10	119.60	122.79
39	L5	3822	PSU	O2-C2-N1	-3.09	119.60	122.79
39	L5	3701	OMC	O2-C2-N3	-3.08	117.47	122.33
35	S2	1177	PSU	O2-C2-N1	-3.06	119.63	122.79
35	S2	1832	6MZ	C4-N9-C8	3.06	108.95	105.74
39	L5	4293	PSU	O2-C2-N1	-3.06	119.63	122.79
35	S2	159	A2M	O3'-C3'-C2'	3.06	119.74	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	3920	PSU	O2-C2-N1	-3.06	119.64	122.79
39	L5	1323	A2M	O3'-C3'-C2'	3.06	119.74	111.19
39	L5	4689	PSU	O2-C2-N1	-3.05	119.64	122.79
35	S2	627	OMU	O4-C4-C5	-3.05	119.90	125.16
39	L5	2837	OMU	O4-C4-C5	-3.04	119.91	125.16
35	S2	576	A2M	C3'-C2'-C1'	-3.04	96.98	102.81
35	S2	1850	MA6	C2-N3-C4	3.04	119.26	111.83
35	S2	668	A2M	C1'-N9-C8	3.04	133.84	127.09
39	L5	4576	PSU	O2-C2-N1	-3.03	119.66	122.79
39	L5	400	A2M	C3'-C2'-C1'	-3.03	97.01	102.81
35	S2	468	A2M	C4-N9-C1'	-3.02	119.56	126.63
39	L5	3639	PSU	O2-C2-N1	-3.02	119.67	122.79
39	L5	3818	UY1	C6-N1-C2	-3.02	119.89	122.69
39	L5	3818	UY1	C6-C5-C4	3.01	120.21	118.17
39	L5	5001	PSU	O2-C2-N1	-3.01	119.68	122.79
39	L5	3825	A2M	O3'-C3'-C2'	3.00	119.60	111.19
35	S2	468	A2M	O3'-C3'-C2'	3.00	119.57	111.19
39	L5	4571	A2M	O3'-C3'-C2'	2.99	119.56	111.19
39	L5	4220	6MZ	C5-N7-C8	2.99	108.15	103.45
35	S2	109	PSU	O2-C2-N1	-2.99	119.71	122.79
39	L5	4296	PSU	O2-C2-N1	-2.98	119.71	122.79
39	L5	1871	A2M	O3'-C3'-C2'	2.98	119.53	111.19
35	S2	428	OMU	O4-C4-C5	-2.98	120.02	125.16
39	L5	4552	PSU	O2-C2-N1	-2.98	119.72	122.79
39	L5	4500	PSU	O2-C2-N1	-2.98	119.72	122.79
35	S2	1288	OMU	O4-C4-C5	-2.97	120.03	125.16
35	S2	1442	OMU	O4-C4-C5	-2.97	120.04	125.16
35	S2	1639	G7M	C2-N1-C6	-2.96	119.74	125.11
39	L5	1683	PSU	O2-C2-N1	-2.96	119.74	122.79
39	L5	4431	PSU	O2-C2-N1	-2.96	119.74	122.79
39	L5	3830	A2M	O3'-C3'-C2'	2.96	119.46	111.19
35	S2	406	PSU	O2-C2-N1	-2.96	119.74	122.79
39	L5	4590	A2M	O3'-C3'-C2'	2.95	119.44	111.19
35	S2	966	PSU	O2-C2-N1	-2.95	119.75	122.79
39	L5	3695	PSU	O2-C2-N1	-2.95	119.75	122.79
39	L5	4220	6MZ	N3-C4-N9	2.95	132.18	127.17
39	L5	4498	OMU	O4-C4-C5	-2.95	120.08	125.16
39	L5	1534	A2M	C3'-C2'-C1'	-2.94	97.17	102.81
35	S2	1004	PSU	O2-C2-N1	-2.94	119.76	122.79
35	S2	116	OMU	O4-C4-C5	-2.94	120.10	125.16
35	S2	799	OMU	O4-C4-C5	-2.94	120.10	125.16
35	S2	27	A2M	C3'-C2'-C1'	-2.93	97.20	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	3825	A2M	C4-N9-C1'	-2.92	119.79	126.63
39	L5	2363	A2M	C3'-C2'-C1'	-2.92	97.21	102.81
39	L5	1744	PSU	O2-C2-N1	-2.92	119.77	122.79
35	S2	649	PSU	O2-C2-N1	-2.91	119.79	122.79
39	L5	4590	A2M	C4-N9-C1'	-2.91	119.83	126.63
39	L5	2401	A2M	C4-N9-C1'	-2.91	119.83	126.63
39	L5	2839	PSU	C6-N1-C2	-2.91	120.00	122.69
39	L5	3925	OMU	O4-C4-C5	-2.90	120.16	125.16
39	L5	3844	PSU	O2-C2-N1	-2.90	119.80	122.79
39	L5	3639	PSU	C6-N1-C2	-2.90	120.00	122.69
35	S2	166	A2M	C4-N9-C1'	-2.90	119.85	126.63
41	L8	69	PSU	O2-C2-N1	-2.90	119.80	122.79
39	L5	1862	PSU	O2-C2-N1	-2.90	119.80	122.79
35	S2	1056	PSU	O2-C2-N1	-2.89	119.80	122.79
39	L5	400	A2M	O3'-C3'-C2'	2.89	119.28	111.19
35	S2	866	PSU	O2-C2-N1	-2.89	119.81	122.79
39	L5	4571	A2M	C4-N9-C1'	-2.88	119.89	126.63
35	S2	1174	PSU	O2-C2-N1	-2.88	119.82	122.79
35	S2	1337	4AC	N4-C4-N3	2.87	118.53	113.87
39	L5	2363	A2M	C2'-C1'-N9	2.87	118.48	113.75
39	L5	4306	OMU	O4-C4-C5	-2.87	120.21	125.16
35	S2	354	OMU	O4-C4-C5	-2.87	120.21	125.16
39	L5	4457	PSU	O2-C2-N1	-2.87	119.83	122.79
39	L5	4689	PSU	C6-N1-C2	-2.87	120.03	122.69
35	S2	1244	PSU	O2-C2-N1	-2.86	119.83	122.79
39	L5	2815	A2M	C2'-C1'-N9	2.86	118.46	113.75
41	L8	69	PSU	C6-N1-C2	-2.86	120.04	122.69
35	S2	121	OMU	O4-C4-C5	-2.86	120.23	125.16
39	L5	3884	PSU	O2-C2-N1	-2.86	119.84	122.79
35	S2	484	A2M	O3'-C3'-C2'	2.86	119.18	111.19
35	S2	172	OMU	O4-C4-C5	-2.86	120.24	125.16
39	L5	1677	PSU	O2-C2-N1	-2.85	119.85	122.79
35	S2	99	A2M	C4-N9-C1'	-2.85	119.96	126.63
39	L5	4673	PSU	O2-C2-N1	-2.85	119.85	122.79
35	S2	681	PSU	O2-C2-N1	-2.85	119.85	122.79
39	L5	1871	A2M	C1'-N9-C8	2.84	133.40	127.09
35	S2	1248	B8N	O4-C4-N3	-2.82	115.40	119.99
35	S2	668	A2M	O4'-C1'-C2'	2.82	111.45	106.59
39	L5	5010	PSU	C6-N1-C2	-2.82	120.08	122.69
39	L5	2815	A2M	O3'-C3'-C2'	2.81	119.04	111.19
39	L5	3785	A2M	C3'-C2'-C1'	-2.81	97.44	102.81
39	L5	1524	A2M	C4'-O4'-C1'	-2.80	103.28	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S2	863	PSU	O2-C2-N1	-2.79	119.91	122.79
35	S2	1850	MA6	C3'-C2'-C1'	2.79	106.73	101.46
39	L5	398	A2M	C4-N9-C1'	-2.78	120.13	126.63
35	S2	1046	PSU	C6-N1-C2	-2.78	120.11	122.69
39	L5	3830	A2M	C4-N9-C1'	-2.77	120.15	126.63
35	S2	1832	6MZ	C4-C5-N7	-2.77	107.41	110.58
39	L5	1582	PSU	O2-C2-N1	-2.77	119.93	122.79
35	S2	27	A2M	O3'-C3'-C2'	2.77	118.93	111.19
39	L5	4521	PSU	O2-C2-N1	-2.77	119.94	122.79
39	L5	3825	A2M	C1'-N9-C8	2.76	133.23	127.09
39	L5	4972	PSU	O2-C2-N1	-2.76	119.94	122.79
39	L5	4673	PSU	C6-N1-C2	-2.76	120.13	122.69
39	L5	4523	A2M	O3'-C3'-C2'	2.76	118.90	111.19
35	S2	1383	A2M	C4-N9-C1'	-2.75	120.19	126.63
39	L5	2363	A2M	O3'-C3'-C2'	2.75	118.88	111.19
39	L5	3808	OMC	C1'-N1-C2	2.75	124.51	118.44
39	L5	1782	PSU	O2-C2-N1	-2.75	119.95	122.79
35	S2	1046	PSU	O2-C2-N1	-2.75	119.96	122.79
39	L5	4590	A2M	C1'-N9-C8	2.74	133.19	127.09
39	L5	1326	A2M	O3'-C3'-C2'	2.74	118.87	111.19
35	S2	651	PSU	O2-C2-N1	-2.74	119.96	122.79
39	L5	3822	PSU	C6-N1-C2	-2.73	120.16	122.69
39	L5	4973	PSU	O2-C2-N1	-2.73	119.98	122.79
39	L5	4579	PSU	O2-C2-N1	-2.72	119.98	122.79
35	S2	27	A2M	C4-N9-C1'	-2.72	120.28	126.63
35	S2	468	A2M	C1'-N9-C8	2.71	133.12	127.09
35	S2	1031	A2M	C4-N9-C1'	-2.71	120.29	126.63
39	L5	3867	A2M	C4-N9-C1'	-2.71	120.29	126.63
39	L5	3818	UY1	O2-C2-N1	-2.71	119.99	122.79
39	L5	4972	PSU	C6-N1-C2	-2.71	120.18	122.69
39	L5	1326	A2M	C4-N9-C1'	-2.70	120.32	126.63
39	L5	2401	A2M	C1'-N9-C8	2.70	133.09	127.09
35	S2	105	PSU	O2-C2-N1	-2.70	120.01	122.79
39	L5	4299	PSU	O2-C2-N1	-2.70	120.01	122.79
35	S2	1244	PSU	C6-N1-C2	-2.69	120.19	122.69
39	L5	3701	OMC	O2-C2-N1	2.69	124.17	118.90
39	L5	2351	OMC	C1'-N1-C2	2.69	124.38	118.44
35	S2	1832	6MZ	N3-C4-N9	2.69	131.74	127.17
39	L5	4293	PSU	C6-N1-C2	-2.69	120.19	122.69
41	L8	55	PSU	O2-C2-N1	-2.69	120.02	122.79
39	L5	400	A2M	C4-N9-C1'	-2.68	120.36	126.63
39	L5	1792	PSU	O2-C2-N1	-2.68	120.03	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	1677	PSU	C6-C5-C4	2.68	119.98	118.17
39	L5	398	A2M	C1'-N9-C8	2.67	133.03	127.09
39	L5	3785	A2M	O3'-C3'-C2'	2.67	118.67	111.19
39	L5	4523	A2M	C4-N9-C1'	-2.67	120.38	126.63
35	S2	99	A2M	C1'-N9-C8	2.66	133.00	127.09
35	S2	1232	PSU	O2-C2-N1	-2.66	120.04	122.79
35	S2	166	A2M	C1'-N9-C8	2.66	133.00	127.09
35	S2	1367	PSU	O2-C2-N1	-2.66	120.05	122.79
35	S2	801	PSU	C6-N1-C2	-2.66	120.23	122.69
39	L5	4552	PSU	C6-N1-C2	-2.66	120.23	122.69
39	L5	2787	A2M	O4'-C1'-C2'	2.65	111.14	106.59
39	L5	4579	PSU	C6-N1-C2	-2.65	120.24	122.69
39	L5	4500	PSU	C6-N1-C2	-2.64	120.24	122.69
39	L5	4471	PSU	O2-C2-N1	-2.64	120.07	122.79
39	L5	4493	PSU	O2-C2-N1	-2.64	120.07	122.79
35	S2	801	PSU	O2-C2-N1	-2.63	120.07	122.79
39	L5	4571	A2M	C1'-N9-C8	2.63	132.94	127.09
35	S2	1639	G7M	CN7-N7-C8	-2.63	120.81	124.79
35	S2	1004	PSU	C6-N1-C2	-2.63	120.25	122.69
35	S2	1832	6MZ	C4-C5-C6	2.63	118.96	116.78
35	S2	668	A2M	C2'-C1'-N9	2.62	118.07	113.75
35	S2	406	PSU	C6-N1-C2	-2.62	120.26	122.69
39	L5	4312	PSU	O2-C2-N1	-2.62	120.09	122.79
39	L5	4220	6MZ	C4-C5-C6	2.61	118.95	116.78
35	S2	109	PSU	C6-N1-C2	-2.61	120.27	122.69
35	S2	1174	PSU	C6-N1-C2	-2.61	120.27	122.69
35	S2	576	A2M	C4-N9-C1'	-2.61	120.52	126.63
39	L5	3830	A2M	C1'-N9-C8	2.61	132.88	127.09
39	L5	3884	PSU	C6-N1-C2	-2.61	120.27	122.69
35	S2	814	PSU	O2-C2-N1	-2.60	120.11	122.79
39	L5	1326	A2M	C3'-C2'-C1'	-2.59	97.84	102.81
39	L5	1323	A2M	C3'-C2'-C1'	-2.58	97.86	102.81
39	L5	3851	PSU	C6-N1-C2	-2.58	120.30	122.69
35	S2	681	PSU	C6-N1-C2	-2.58	120.30	122.69
39	L5	2632	PSU	C6-N1-C2	-2.58	120.30	122.69
35	S2	1383	A2M	C1'-N9-C8	2.58	132.82	127.09
39	L5	3785	A2M	C4-N9-C1'	-2.57	120.61	126.63
39	L5	2787	A2M	C4-N9-C1'	-2.57	120.61	126.63
35	S2	354	OMU	O2-C2-N1	-2.57	119.45	122.80
39	L5	1326	A2M	C1'-N9-C8	2.57	132.79	127.09
39	L5	3718	A2M	C1'-N9-C8	2.57	132.79	127.09
39	L5	4296	PSU	C6-N1-C2	-2.56	120.31	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	4442	PSU	C6-C5-C4	2.56	119.90	118.17
35	S2	484	A2M	C1'-N9-C8	2.56	132.78	127.09
35	S2	866	PSU	C6-C5-C4	2.56	119.90	118.17
39	L5	4353	PSU	C6-N1-C2	-2.56	120.32	122.69
39	L5	4636	PSU	O2-C2-N1	-2.55	120.16	122.79
39	L5	2363	A2M	C4-N9-C1'	-2.55	120.67	126.63
35	S2	799	OMU	C1'-N1-C2	2.55	122.17	117.59
35	S2	27	A2M	C1'-N9-C8	2.54	132.74	127.09
39	L5	1862	PSU	C6-N1-C2	-2.54	120.33	122.69
39	L5	4620	OMU	O4-C4-C5	-2.54	120.78	125.16
35	S2	966	PSU	C6-N1-C2	-2.54	120.34	122.69
39	L5	2861	OMC	C1'-N1-C2	2.54	124.04	118.44
39	L5	3867	A2M	C1'-N9-C8	2.54	132.72	127.09
39	L5	2363	A2M	C1'-N9-C8	2.53	132.70	127.09
39	L5	1683	PSU	C6-N1-C2	-2.52	120.35	122.69
39	L5	400	A2M	C1'-N9-C8	2.52	132.69	127.09
35	S2	1031	A2M	C1'-N9-C8	2.52	132.69	127.09
39	L5	1524	A2M	O4'-C1'-C2'	2.52	110.92	106.59
41	L8	55	PSU	C6-N1-C2	-2.51	120.36	122.69
35	S2	863	PSU	C6-N1-C2	-2.51	120.36	122.69
35	S2	484	A2M	C4-N9-C1'	-2.51	120.76	126.63
39	L5	1782	PSU	C6-N1-C2	-2.51	120.36	122.69
39	L5	4523	A2M	C1'-N9-C8	2.51	132.67	127.09
35	S2	159	A2M	C4-N9-C1'	-2.51	120.76	126.63
39	L5	4220	6MZ	C5-C6-N1	2.51	120.84	118.15
39	L5	3637	PSU	C6-N1-C2	-2.51	120.36	122.69
39	L5	1322	1MA	CM1-N1-C6	-2.51	116.26	120.15
35	S2	576	A2M	C1'-N9-C8	2.51	132.66	127.09
39	L5	4636	PSU	C6-C5-C4	2.51	119.86	118.17
39	L5	4431	PSU	C6-N1-C2	-2.51	120.37	122.69
39	L5	3844	PSU	C6-N1-C2	-2.50	120.37	122.69
39	L5	3925	OMU	O2-C2-N1	-2.50	119.54	122.80
39	L5	3695	PSU	C6-N1-C2	-2.50	120.37	122.69
39	L5	4299	PSU	C6-N1-C2	-2.49	120.38	122.69
39	L5	1536	PSU	C6-N1-C2	-2.49	120.38	122.69
39	L5	2837	OMU	O2-C2-N1	-2.49	119.56	122.80
39	L5	1860	PSU	C6-N1-C2	-2.49	120.38	122.69
35	S2	686	PSU	C6-N1-C2	-2.49	120.38	122.69
39	L5	5001	PSU	C6-N1-C2	-2.49	120.38	122.69
35	S2	651	PSU	C6-N1-C2	-2.48	120.39	122.69
39	L5	1781	PSU	O2-C2-N1	-2.48	120.23	122.79
35	S2	1850	MA6	C1'-N9-C8	-2.48	121.59	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	4312	PSU	C6-N1-C2	-2.46	120.41	122.69
35	S2	649	PSU	C6-N1-C2	-2.46	120.41	122.69
39	L5	3920	PSU	C6-N1-C2	-2.46	120.41	122.69
39	L5	4973	PSU	C6-N1-C2	-2.45	120.42	122.69
39	L5	3718	A2M	C2'-C1'-N9	2.45	117.78	113.75
39	L5	1323	A2M	O4'-C1'-C2'	2.45	110.80	106.59
35	S2	1045	PSU	C6-N1-C2	-2.45	120.42	122.69
35	S2	159	A2M	C1'-N9-C8	2.44	132.52	127.09
39	L5	3718	A2M	C4-N9-C1'	-2.44	120.92	126.63
39	L5	2787	A2M	C1'-N9-C8	2.44	132.51	127.09
39	L5	3785	A2M	C2-N1-C6	-2.42	114.75	118.73
39	L5	4521	PSU	C6-N1-C2	-2.42	120.44	122.69
39	L5	4442	PSU	C6-N1-C2	-2.42	120.44	122.69
35	S2	1272	OMC	C1'-N1-C2	2.42	123.78	118.44
35	S2	174	OMC	C1'-N1-C2	2.42	123.78	118.44
35	S2	105	PSU	C6-N1-C2	-2.42	120.45	122.69
35	S2	1851	MA6	C1'-N9-C8	-2.41	121.74	127.09
39	L5	4500	PSU	C6-C5-C4	2.41	119.80	118.17
39	L5	2363	A2M	O4'-C1'-C2'	2.41	110.74	106.59
35	S2	159	A2M	C3'-C2'-C1'	-2.40	98.21	102.81
39	L5	4471	PSU	C6-N1-C2	-2.40	120.46	122.69
35	S2	1367	PSU	C6-N1-C2	-2.39	120.47	122.69
35	S2	93	PSU	O2-C2-N1	-2.39	120.33	122.79
35	S2	1056	PSU	C6-N1-C2	-2.38	120.48	122.69
39	L5	1524	A2M	C4-N9-C1'	-2.38	121.06	126.63
39	L5	4498	OMU	O2-C2-N1	-2.38	119.70	122.80
39	L5	1871	A2M	C6-C5-C4	-2.38	113.93	117.18
39	L5	2815	A2M	C3'-C2'-C1'	-2.38	98.26	102.81
39	L5	4361	PSU	O2-C2-N1	-2.38	120.34	122.79
35	S2	109	PSU	C6-C5-C4	2.37	119.78	118.17
39	L5	4403	PSU	C6-C5-C4	2.37	119.77	118.17
39	L5	2815	A2M	C4-N9-C1'	-2.37	121.09	126.63
39	L5	4576	PSU	C6-N1-C2	-2.37	120.50	122.69
35	S2	1639	G7M	N9-C8-N7	-2.36	106.75	112.48
39	L5	1582	PSU	C6-N1-C2	-2.36	120.50	122.69
35	S2	1177	PSU	C6-N1-C2	-2.35	120.51	122.69
39	L5	1534	A2M	O4'-C1'-C2'	2.35	110.64	106.59
35	S2	1248	B8N	O4'-C1'-C2'	2.35	108.41	105.15
39	L5	4590	A2M	C6-C5-C4	-2.35	113.97	117.18
35	S2	1326	OMU	O2-C2-N1	-2.34	119.75	122.80
39	L5	1326	A2M	O4'-C1'-C2'	2.34	110.61	106.59
35	S2	866	PSU	C6-N1-C2	-2.33	120.53	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	4353	PSU	C6-C5-C4	2.33	119.75	118.17
35	S2	1232	PSU	C6-N1-C2	-2.33	120.53	122.69
35	S2	159	A2M	O4'-C1'-C2'	2.33	110.59	106.59
39	L5	1792	PSU	C6-N1-C2	-2.32	120.54	122.69
39	L5	3853	PSU	C6-N1-C2	-2.32	120.54	122.69
35	S2	668	A2M	C6-C5-C4	-2.32	114.01	117.18
39	L5	2815	A2M	C1'-N9-C8	2.32	132.24	127.09
39	L5	3785	A2M	C5-C6-N1	2.32	123.39	117.51
39	L5	1744	PSU	C6-N1-C2	-2.31	120.55	122.69
35	S2	1081	PSU	O2-C2-N1	-2.31	120.41	122.79
39	L5	1524	A2M	C1'-N9-C8	2.30	132.21	127.09
35	S2	1383	A2M	C4'-O4'-C1'	-2.30	104.38	109.47
35	S2	814	PSU	C6-N1-C2	-2.30	120.56	122.69
35	S2	1081	PSU	C6-N1-C2	-2.30	120.56	122.69
39	L5	3822	PSU	O4'-C1'-C2'	2.30	108.33	105.15
39	L5	3785	A2M	O4'-C1'-N9	2.29	112.50	108.09
39	L5	4457	PSU	C6-N1-C2	-2.29	120.56	122.69
35	S2	1056	PSU	C6-C5-C4	2.29	119.72	118.17
39	L5	1871	A2M	O4'-C1'-C2'	2.28	110.51	106.59
39	L5	1781	PSU	C6-N1-C2	-2.28	120.58	122.69
39	L5	4493	PSU	C6-N1-C2	-2.27	120.58	122.69
39	L5	1323	A2M	C4-N9-C1'	-2.26	121.34	126.63
39	L5	3867	A2M	C6-C5-C4	-2.26	114.09	117.18
35	S2	866	PSU	O4'-C1'-C2'	2.26	108.27	105.15
35	S2	1288	OMU	C1'-N1-C2	2.25	121.64	117.59
39	L5	1326	A2M	C6-C5-C4	-2.25	114.10	117.18
35	S2	93	PSU	C6-N1-C2	-2.25	120.60	122.69
39	L5	1534	A2M	C1'-N9-C8	2.25	132.09	127.09
39	L5	1323	A2M	C1'-N9-C8	2.24	132.08	127.09
39	L5	4530	UR3	C6-N1-C2	-2.23	119.97	121.80
35	S2	166	A2M	O4'-C1'-C2'	2.23	110.44	106.59
39	L5	1534	A2M	C4-N9-C1'	-2.23	121.41	126.63
39	L5	400	A2M	C6-C5-C4	-2.23	114.13	117.18
35	S2	468	A2M	C6-C5-C4	-2.23	114.13	117.18
39	L5	4403	PSU	O4'-C1'-C2'	2.23	108.23	105.15
39	L5	2401	A2M	C6-C5-C4	-2.23	114.14	117.18
35	S2	166	A2M	C6-C5-C4	-2.23	114.14	117.18
39	L5	4523	A2M	C6-C5-C4	-2.23	114.14	117.18
39	L5	4532	PSU	C6-N1-C2	-2.23	120.63	122.69
35	S2	121	OMU	O2-C2-N1	-2.22	119.91	122.80
39	L5	3867	A2M	O4'-C1'-C2'	2.22	110.41	106.59
39	L5	3825	A2M	C6-C5-C4	-2.21	114.16	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	1677	PSU	O4'-C1'-C2'	2.20	108.19	105.15
39	L5	3830	A2M	C6-C5-C4	-2.19	114.19	117.18
39	L5	4403	PSU	C6-N1-C2	-2.19	120.66	122.69
39	L5	4571	A2M	C6-C5-C4	-2.19	114.19	117.18
39	L5	3785	A2M	C1'-N9-C8	2.19	131.95	127.09
39	L5	4442	PSU	O4'-C1'-C2'	2.19	108.18	105.15
35	S2	1031	A2M	C6-C5-C4	-2.19	114.19	117.18
39	L5	2401	A2M	C2-N1-C6	-2.18	115.14	118.73
39	L5	3867	A2M	C3'-C2'-C1'	-2.18	98.63	102.81
35	S2	1244	PSU	C6-C5-C4	2.18	119.64	118.17
39	L5	1534	A2M	C2-N1-C6	-2.18	115.15	118.73
35	S2	468	A2M	O4'-C1'-C2'	2.18	110.34	106.59
39	L5	1322	1MA	N1-C6-N6	2.18	125.18	119.71
39	L5	1522	OMG	C2'-C1'-N9	-2.17	110.11	114.24
35	S2	576	A2M	C6-C5-C4	-2.17	114.22	117.18
35	S2	428	OMU	O2-C2-N1	-2.17	119.98	122.80
39	L5	2815	A2M	O4'-C1'-C2'	2.16	110.31	106.59
41	L8	69	PSU	O4'-C1'-C2'	2.15	108.13	105.15
39	L5	3785	A2M	O4'-C4'-C3'	2.15	109.42	105.15
39	L5	2401	A2M	C5-C6-N1	2.15	122.97	117.51
39	L5	400	A2M	C5-C6-N1	2.15	122.97	117.51
39	L5	2787	A2M	C6-C5-C4	-2.15	114.25	117.18
35	S2	484	A2M	C3'-C2'-C1'	-2.14	98.70	102.81
39	L5	398	A2M	C6-C5-C4	-2.14	114.25	117.18
39	L5	3637	PSU	C6-C5-C4	2.14	119.62	118.17
41	L8	69	PSU	C6-C5-C4	2.14	119.62	118.17
35	S2	99	A2M	C2-N1-C6	-2.14	115.22	118.73
39	L5	4361	PSU	C6-N1-C2	-2.13	120.71	122.69
39	L5	2632	PSU	C6-C5-C4	2.13	119.61	118.17
39	L5	4523	A2M	C5-C6-N1	2.13	122.92	117.51
39	L5	4636	PSU	O4'-C1'-C2'	2.13	108.10	105.15
39	L5	400	A2M	O4'-C1'-C2'	2.13	110.25	106.59
39	L5	4571	A2M	O4'-C1'-C2'	2.13	110.25	106.59
39	L5	1524	A2M	C6-C5-C4	-2.12	114.28	117.18
35	S2	159	A2M	O3'-C3'-C4'	-2.12	104.98	111.08
39	L5	4620	OMU	O2-C2-N1	-2.12	120.03	122.80
39	L5	1326	A2M	C5-C6-N1	2.12	122.90	117.51
35	S2	1248	B8N	O4-C4-C5	-2.12	118.91	122.58
35	S2	686	PSU	C6-C5-C4	2.12	119.60	118.17
39	L5	4523	A2M	C2-N1-C6	-2.12	115.25	118.73
35	S2	484	A2M	O4'-C1'-C2'	2.12	110.23	106.59
35	S2	1031	A2M	C5-C6-N1	2.11	122.88	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	400	A2M	C2-N1-C6	-2.11	115.26	118.73
39	L5	2815	A2M	C2-N1-C6	-2.11	115.26	118.73
39	L5	3825	A2M	C2-N1-C6	-2.11	115.26	118.73
35	S2	1337	4AC	C5-C4-N4	-2.11	119.38	122.94
39	L5	2363	A2M	C5-C6-N1	2.11	122.87	117.51
35	S2	27	A2M	C6-C5-C4	-2.11	114.30	117.18
35	S2	1383	A2M	C6-C5-C4	-2.10	114.30	117.18
35	S2	27	A2M	C5-C6-N1	2.10	122.85	117.51
35	S2	27	A2M	O4'-C1'-C2'	2.10	110.20	106.59
39	L5	3782	5MC	C1'-N1-C6	-2.10	117.70	121.15
39	L5	398	A2M	C5-C6-N1	2.10	122.83	117.51
39	L5	1534	A2M	O3'-C3'-C4'	-2.09	105.07	111.08
39	L5	4973	PSU	C6-C5-C4	2.09	119.59	118.17
39	L5	4457	PSU	O4'-C1'-C2'	2.09	108.05	105.15
39	L5	3830	A2M	C5-C6-N1	2.09	122.82	117.51
39	L5	3785	A2M	C6-C5-C4	-2.09	114.33	117.18
39	L5	1326	A2M	C2'-C1'-N9	2.09	117.19	113.75
39	L5	3867	A2M	O3'-C3'-C2'	2.09	117.03	111.19
35	S2	27	A2M	C2-N1-C6	-2.08	115.31	118.73
39	L5	3718	A2M	C6-C5-C4	-2.08	114.33	117.18
35	S2	172	OMU	O2-C2-N1	-2.08	120.09	122.80
35	S2	1031	A2M	C2-N1-C6	-2.08	115.31	118.73
39	L5	2815	A2M	C5-C6-N1	2.08	122.80	117.51
35	S2	484	A2M	C2-N1-C6	-2.08	115.32	118.73
35	S2	484	A2M	C2'-C1'-N9	2.08	117.17	113.75
39	L5	4571	A2M	C5-C6-N1	2.07	122.78	117.51
39	L5	3637	PSU	O2-C2-N1	-2.07	120.65	122.79
39	L5	2787	A2M	C5-C6-N1	2.07	122.76	117.51
39	L5	3808	OMC	C1'-N1-C6	-2.07	116.36	120.78
39	L5	3825	A2M	C5-C6-N1	2.07	122.76	117.51
39	L5	1871	A2M	C4'-O4'-C1'	-2.07	104.90	109.47
35	S2	1248	B8N	C31-N3-C4	2.07	120.11	117.18
35	S2	668	A2M	C5-C6-N1	2.07	122.76	117.51
39	L5	1323	A2M	C5-C6-N1	2.06	122.75	117.51
39	L5	2363	A2M	C2-N1-C6	-2.06	115.34	118.73
39	L5	3825	A2M	O4'-C1'-C2'	2.06	110.14	106.59
39	L5	1323	A2M	C2-N1-C6	-2.06	115.35	118.73
39	L5	4636	PSU	C6-N1-C2	-2.06	120.78	122.69
39	L5	1534	A2M	C5-C6-N1	2.06	122.73	117.51
35	S2	109	PSU	O4'-C1'-C2'	2.05	107.99	105.15
35	S2	159	A2M	C5-C6-N1	2.05	122.71	117.51
35	S2	166	A2M	C5-C6-N1	2.05	122.71	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L5	4523	A2M	C4'-O4'-C1'	-2.05	104.94	109.47
39	L5	2815	A2M	C6-C5-C4	-2.05	114.38	117.18
39	L5	1323	A2M	C6-C5-C4	-2.05	114.38	117.18
39	L5	4571	A2M	C2-N1-C6	-2.04	115.37	118.73
35	S2	99	A2M	C5-C6-N1	2.04	122.70	117.51
35	S2	1383	A2M	C5-C6-N1	2.04	122.69	117.51
39	L5	2401	A2M	O4'-C1'-C2'	2.04	110.10	106.59
39	L5	3867	A2M	C2-N1-C6	-2.04	115.38	118.73
35	S2	159	A2M	C6-C5-C4	-2.04	114.40	117.18
35	S2	484	A2M	C5-C6-N1	2.03	122.67	117.51
35	S2	468	A2M	C5-C6-N1	2.03	122.67	117.51
39	L5	398	A2M	C2-N1-C6	-2.03	115.40	118.73
39	L5	2422	OMC	C1'-N1-C2	2.03	122.92	118.44
39	L5	1326	A2M	C2-N1-C6	-2.03	115.40	118.73
39	L5	2787	A2M	C2-N1-C6	-2.02	115.41	118.73
35	S2	406	PSU	C6-C5-C4	2.02	119.54	118.17
39	L5	3718	A2M	C2-N1-C6	-2.02	115.42	118.73
39	L5	2787	A2M	O4'-C4'-C3'	2.02	109.15	105.15
39	L5	4353	PSU	O4'-C1'-C2'	2.01	107.94	105.15
35	S2	1442	OMU	O2-C2-N1	-2.01	120.17	122.80
35	S2	668	A2M	C2-N1-C6	-2.01	115.42	118.73
35	S2	99	A2M	C6-C5-C4	-2.01	114.43	117.18
39	L5	3718	A2M	C5-C6-N1	2.01	122.62	117.51
39	L5	2363	A2M	C6-C5-C4	-2.01	114.43	117.18
39	L5	4500	PSU	O4'-C1'-C2'	2.00	107.92	105.15
35	S2	1383	A2M	C2-N1-C6	-2.00	115.44	118.73
39	L5	4521	PSU	C6-C5-C4	2.00	119.52	118.17

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	L8	75	OMG	C1'-C2'-O2'-CM2
35	S2	27	A2M	C1'-C2'-O2'-CM'
35	S2	159	A2M	C1'-C2'-O2'-CM'
35	S2	462	OMC	C1'-C2'-O2'-CM2
35	S2	601	OMG	C1'-C2'-O2'-CM2
35	S2	644	OMG	O4'-C4'-C5'-O5'
35	S2	799	OMU	C3'-C4'-C5'-O5'
35	S2	799	OMU	O4'-C4'-C5'-O5'
35	S2	801	PSU	C3'-C4'-C5'-O5'
35	S2	867	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
35	S2	1031	A2M	C1'-C2'-O2'-CM'
35	S2	1272	OMC	O4'-C4'-C5'-O5'
35	S2	1288	OMU	O4'-C4'-C5'-O5'
35	S2	1337	4AC	N3-C4-N4-C7
35	S2	1383	A2M	C1'-C2'-O2'-CM'
35	S2	1442	OMU	O4'-C4'-C5'-O5'
39	L5	400	A2M	C1'-C2'-O2'-CM'
39	L5	1326	A2M	O4'-C4'-C5'-O5'
39	L5	1326	A2M	C1'-C2'-O2'-CM'
39	L5	1340	OMC	C1'-C2'-O2'-CM2
39	L5	1625	OMG	O4'-C4'-C5'-O5'
39	L5	1677	PSU	C2'-C1'-C5-C4
39	L5	2351	OMC	C1'-C2'-O2'-CM2
39	L5	2364	OMG	C1'-C2'-O2'-CM2
39	L5	2787	A2M	C1'-C2'-O2'-CM'
39	L5	2824	OMC	C1'-C2'-O2'-CM2
39	L5	3701	OMC	C2'-C1'-N1-C2
39	L5	3701	OMC	O4'-C4'-C5'-O5'
39	L5	3792	OMG	O4'-C4'-C5'-O5'
39	L5	3808	OMC	C1'-C2'-O2'-CM2
39	L5	3867	A2M	C1'-C2'-O2'-CM'
39	L5	4196	OMG	C1'-C2'-O2'-CM2
39	L5	4590	A2M	O4'-C4'-C5'-O5'
39	L5	4637	OMG	O4'-C4'-C5'-O5'
35	S2	99	A2M	O4'-C4'-C5'-O5'
35	S2	644	OMG	C3'-C4'-C5'-O5'
35	S2	683	OMG	C3'-C4'-C5'-O5'
35	S2	1272	OMC	C3'-C4'-C5'-O5'
39	L5	1323	A2M	O4'-C4'-C5'-O5'
39	L5	1326	A2M	C3'-C4'-C5'-O5'
39	L5	1536	PSU	C3'-C4'-C5'-O5'
39	L5	1536	PSU	O4'-C4'-C5'-O5'
39	L5	1625	OMG	C3'-C4'-C5'-O5'
39	L5	2364	OMG	O4'-C4'-C5'-O5'
39	L5	2815	A2M	O4'-C4'-C5'-O5'
39	L5	4500	PSU	C3'-C4'-C5'-O5'
39	L5	4500	PSU	O4'-C4'-C5'-O5'
39	L5	4590	A2M	C3'-C4'-C5'-O5'
39	L5	3701	OMC	C2'-C1'-N1-C6
35	S2	576	A2M	O4'-C4'-C5'-O5'
35	S2	801	PSU	O4'-C4'-C5'-O5'
35	S2	867	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
35	S2	1442	OMU	C3'-C4'-C5'-O5'
39	L5	3701	OMC	C3'-C4'-C5'-O5'
39	L5	4228	OMG	O4'-C4'-C5'-O5'
39	L5	4228	OMG	C3'-C4'-C5'-O5'
35	S2	627	OMU	O4'-C4'-C5'-O5'
35	S2	1288	OMU	C3'-C4'-C5'-O5'
35	S2	428	OMU	C2'-C1'-N1-C6
35	S2	627	OMU	C2'-C1'-N1-C6
39	L5	4447	5MC	C2'-C1'-N1-C6
35	S2	576	A2M	C3'-C4'-C5'-O5'
35	S2	1045	PSU	C3'-C4'-C5'-O5'
39	L5	2787	A2M	C3'-C4'-C5'-O5'
39	L5	3792	OMG	C3'-C4'-C5'-O5'
39	L5	3899	OMG	C3'-C4'-C5'-O5'
39	L5	4637	OMG	C3'-C4'-C5'-O5'
35	S2	683	OMG	O4'-C4'-C5'-O5'
35	S2	1045	PSU	O4'-C4'-C5'-O5'
39	L5	1323	A2M	C3'-C4'-C5'-O5'
39	L5	2364	OMG	C3'-C4'-C5'-O5'
39	L5	2815	A2M	C3'-C4'-C5'-O5'
39	L5	3867	A2M	C3'-C4'-C5'-O5'
35	S2	99	A2M	C3'-C4'-C5'-O5'
35	S2	668	A2M	O4'-C4'-C5'-O5'
35	S2	1248	B8N	N34-C33-C34-O36
39	L5	2787	A2M	C2'-C1'-N9-C8
39	L5	3899	OMG	O4'-C4'-C5'-O5'
35	S2	668	A2M	C3'-C4'-C5'-O5'
39	L5	4590	A2M	C4'-C5'-O5'-P
39	L5	3925	OMU	C1'-C2'-O2'-CM2
39	L5	1524	A2M	C3'-C4'-C5'-O5'
39	L5	4296	PSU	C3'-C4'-C5'-O5'
39	L5	4296	PSU	O4'-C4'-C5'-O5'
35	S2	1383	A2M	O4'-C4'-C5'-O5'
35	S2	428	OMU	C2'-C1'-N1-C2
35	S2	627	OMU	O4'-C1'-N1-C6
39	L5	3851	PSU	C3'-C4'-C5'-O5'
35	S2	428	OMU	O4'-C1'-N1-C6
39	L5	4447	5MC	O4'-C1'-N1-C6
35	S2	1703	OMC	O4'-C4'-C5'-O5'
39	L5	1524	A2M	O4'-C4'-C5'-O5'
35	S2	428	OMU	O4'-C1'-N1-C2
39	L5	3818	UY1	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
35	S2	627	OMU	C2'-C1'-N1-C2
39	L5	4447	5MC	C2'-C1'-N1-C2
35	S2	627	OMU	O4'-C1'-N1-C2
39	L5	4447	5MC	O4'-C1'-N1-C2
39	L5	3785	A2M	C3'-C2'-O2'-CM'
39	L5	4494	OMG	C3'-C2'-O2'-CM2
35	S2	576	A2M	C4'-C5'-O5'-P
35	S2	644	OMG	C4'-C5'-O5'-P
39	L5	1534	A2M	C4'-C5'-O5'-P
39	L5	4500	PSU	C4'-C5'-O5'-P
39	L5	3818	UY1	O4'-C1'-C5-C4
39	L5	2787	A2M	C2'-C1'-N9-C4
35	S2	627	OMU	C3'-C4'-C5'-O5'
35	S2	1383	A2M	C3'-C4'-C5'-O5'
39	L5	2422	OMC	C3'-C4'-C5'-O5'
39	L5	4220	6MZ	C3'-C4'-C5'-O5'
39	L5	4618	OMG	C3'-C4'-C5'-O5'
35	S2	1490	OMG	C4'-C5'-O5'-P
39	L5	3887	OMC	C4'-C5'-O5'-P
39	L5	3844	PSU	C4'-C5'-O5'-P
39	L5	2787	A2M	O4'-C4'-C5'-O5'
39	L5	4220	6MZ	O4'-C4'-C5'-O5'
39	L5	2401	A2M	C1'-C2'-O2'-CM'
35	S2	1639	G7M	C3'-C4'-C5'-O5'
39	L5	3818	UY1	O4'-C1'-C5-C6
39	L5	4636	PSU	O4'-C1'-C5-C6
39	L5	1524	A2M	C3'-C2'-O2'-CM'
39	L5	1322	1MA	C2'-C1'-N9-C8
39	L5	1781	PSU	C3'-C4'-C5'-O5'
39	L5	3785	A2M	O4'-C4'-C5'-O5'
39	L5	1322	1MA	C2'-C1'-N9-C4
39	L5	3701	OMC	O4'-C1'-N1-C6
39	L5	4636	PSU	C2'-C1'-C5-C6
35	S2	668	A2M	O4'-C1'-N9-C8
39	L5	3899	OMG	C3'-C2'-O2'-CM2
35	S2	1832	6MZ	N1-C6-N6-C9
39	L5	2422	OMC	O4'-C4'-C5'-O5'
39	L5	3782	5MC	O4'-C4'-C5'-O5'
35	S2	1851	MA6	C4'-C5'-O5'-P
35	S2	1832	6MZ	C5-C6-N6-C9
35	S2	1081	PSU	C4'-C5'-O5'-P
39	L5	1326	A2M	C4'-C5'-O5'-P

There are no ring outliers.

61 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	S2	681	PSU	1	0
35	S2	116	OMU	3	0
39	L5	3920	PSU	1	0
35	S2	867	OMG	1	0
39	L5	1534	A2M	1	0
39	L5	4536	OMC	1	0
39	L5	4456	OMC	1	0
35	S2	27	A2M	2	0
35	S2	428	OMU	2	0
39	L5	1781	PSU	1	0
35	S2	601	OMG	1	0
39	L5	3822	PSU	2	0
39	L5	3867	A2M	3	0
39	L5	1683	PSU	1	0
35	S2	93	PSU	1	0
39	L5	2351	OMC	2	0
39	L5	4523	A2M	1	0
39	L5	4196	OMG	1	0
35	S2	1232	PSU	2	0
35	S2	1850	MA6	2	0
35	S2	576	A2M	2	0
39	L5	4623	OMG	1	0
39	L5	3830	A2M	1	0
39	L5	3782	5MC	1	0
39	L5	4353	PSU	1	0
35	S2	1288	OMU	1	0
35	S2	462	OMC	2	0
35	S2	1328	OMG	1	0
35	S2	509	OMG	1	0
39	L5	3701	OMC	1	0
39	L5	4571	A2M	1	0
39	L5	1871	A2M	1	0
39	L5	400	A2M	1	0
35	S2	166	A2M	1	0
39	L5	2824	OMC	1	0
35	S2	99	A2M	2	0
39	L5	3718	A2M	2	0
39	L5	2422	OMC	1	0
35	S2	484	A2M	1	0
39	L5	4457	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	L5	3808	OMC	1	0
41	L8	75	OMG	2	0
39	L5	3818	UY1	1	0
39	L5	4431	PSU	1	0
35	S2	644	OMG	1	0
35	S2	1383	A2M	1	0
39	L5	4521	PSU	1	0
39	L5	4620	OMU	2	0
35	S2	1337	4AC	3	0
35	S2	649	PSU	1	0
35	S2	1639	G7M	1	0
39	L5	4392	OMG	1	0
39	L5	2364	OMG	1	0
39	L5	1340	OMC	2	0
35	S2	121	OMU	1	0
35	S2	1031	A2M	2	0
35	S2	159	A2M	2	0
39	L5	2363	A2M	1	0
35	S2	1842	4AC	1	0
39	L5	2632	PSU	1	0
39	L5	1326	A2M	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 241 ligands modelled in this entry, 224 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.90	0
88	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPD	L5	5287	-	9,9,9	0.33	0	8,8,8	0.81	0
87	SPM	L5	5291	-	13,13,13	0.34	0	12,12,12	0.83	0
87	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	0.94	0
88	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.97	0
87	SPM	L5	5263	-	13,13,13	0.34	0	12,12,12	0.96	0
88	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.83	0
87	SPM	L5	5264	-	13,13,13	0.37	0	12,12,12	1.07	0
88	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.85	0
87	SPM	L5	5288	-	13,13,13	0.35	0	12,12,12	0.98	0
88	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.77	0
87	SPM	L5	5258	-	13,13,13	0.36	0	12,12,12	0.93	0
88	SPD	L8	201	-	9,9,9	0.32	0	8,8,8	0.90	0
88	SPD	L5	5285	-	9,9,9	0.34	0	8,8,8	0.94	0
88	SPD	LN	301	-	9,9,9	0.35	0	8,8,8	0.92	0
87	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L5	5283	-	-	1/7/7/7	-
88	SPD	L5	5286	-	-	2/7/7/7	-
88	SPD	L5	5287	-	-	2/7/7/7	-
87	SPM	L5	5291	-	-	4/11/11/11	-
87	SPM	L5	5267	-	-	4/11/11/11	-
88	SPD	L5	5261	-	-	0/7/7/7	-
87	SPM	L5	5263	-	-	4/11/11/11	-
88	SPD	L5	5290	-	-	4/7/7/7	-
87	SPM	L5	5264	-	-	7/11/11/11	-
88	SPD	L5	5289	-	-	3/7/7/7	-
87	SPM	L5	5288	-	-	4/11/11/11	-
88	SPD	L5	5284	-	-	3/7/7/7	-
87	SPM	L5	5258	-	-	4/11/11/11	-
88	SPD	L8	201	-	-	4/7/7/7	-
88	SPD	L5	5285	-	-	4/7/7/7	-
88	SPD	LN	301	-	-	2/7/7/7	-
87	SPM	L5	5292	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5264	SPM	N5-C6-C7-C8
88	L5	5284	SPD	C3-C4-C5-N6
87	L5	5263	SPM	N10-C11-C12-C13
87	L5	5292	SPM	N10-C11-C12-C13
88	L5	5285	SPD	N6-C7-C8-C9
88	L5	5289	SPD	N6-C7-C8-C9
87	L5	5263	SPM	C7-C6-N5-C4
87	L5	5291	SPM	C8-C9-N10-C11
88	LN	301	SPD	C8-C7-N6-C5
87	L5	5291	SPM	C7-C8-C9-N10
88	L8	201	SPD	C3-C4-C5-N6
88	L5	5285	SPD	C3-C4-C5-N6
87	L5	5267	SPM	C7-C8-C9-N10
87	L5	5264	SPM	C6-C7-C8-C9
87	L5	5288	SPM	C2-C3-C4-N5
88	L8	201	SPD	N6-C7-C8-C9
88	L5	5286	SPD	C3-C4-C5-N6
87	L5	5288	SPM	C12-C11-N10-C9
88	L8	201	SPD	C8-C7-N6-C5
87	L5	5258	SPM	C7-C6-N5-C4
88	L5	5290	SPD	C4-C5-N6-C7
88	L5	5285	SPD	C2-C3-C4-C5
87	L5	5267	SPM	C6-C7-C8-C9
88	L5	5286	SPD	C2-C3-C4-C5
88	L5	5290	SPD	C3-C4-C5-N6
87	L5	5288	SPM	C8-C9-N10-C11
87	L5	5258	SPM	C2-C3-C4-N5
87	L5	5267	SPM	C8-C9-N10-C11
87	L5	5288	SPM	N1-C2-C3-C4
87	L5	5292	SPM	C11-C12-C13-N14
87	L5	5292	SPM	C6-C7-C8-C9
87	L5	5264	SPM	C8-C9-N10-C11
87	L5	5258	SPM	C6-C7-C8-C9
88	L8	201	SPD	C2-C3-C4-C5
87	L5	5263	SPM	C3-C4-N5-C6
88	L5	5285	SPD	C7-C8-C9-N10
88	L5	5287	SPD	C8-C7-N6-C5

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Mol	Chain	Res	Type	Atoms
88	L5	5289	SPD	C7-C8-C9-N10
87	L5	5291	SPM	C6-C7-C8-C9
87	L5	5264	SPM	C12-C11-N10-C9
88	L5	5283	SPD	C2-C3-C4-C5
87	L5	5264	SPM	C7-C8-C9-N10
87	L5	5263	SPM	N5-C6-C7-C8
88	L5	5284	SPD	N6-C7-C8-C9
87	L5	5264	SPM	C2-C3-C4-N5
87	L5	5292	SPM	C8-C9-N10-C11
88	L5	5290	SPD	C8-C7-N6-C5
87	L5	5264	SPM	C7-C6-N5-C4
88	L5	5287	SPD	N6-C7-C8-C9
88	L5	5289	SPD	C2-C3-C4-C5
87	L5	5258	SPM	C3-C4-N5-C6
88	LN	301	SPD	C4-C5-N6-C7
88	L5	5284	SPD	C2-C3-C4-C5
88	L5	5290	SPD	N1-C2-C3-C4
87	L5	5267	SPM	C11-C12-C13-N14
87	L5	5291	SPM	C7-C6-N5-C4

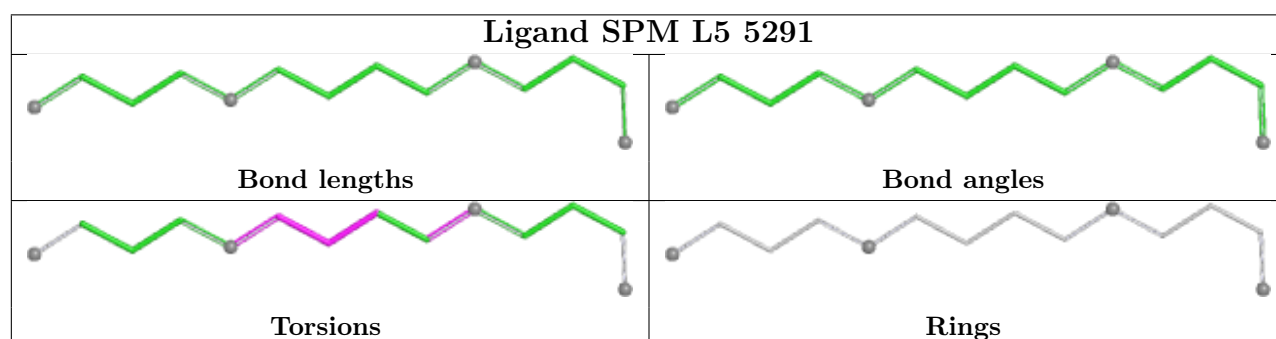
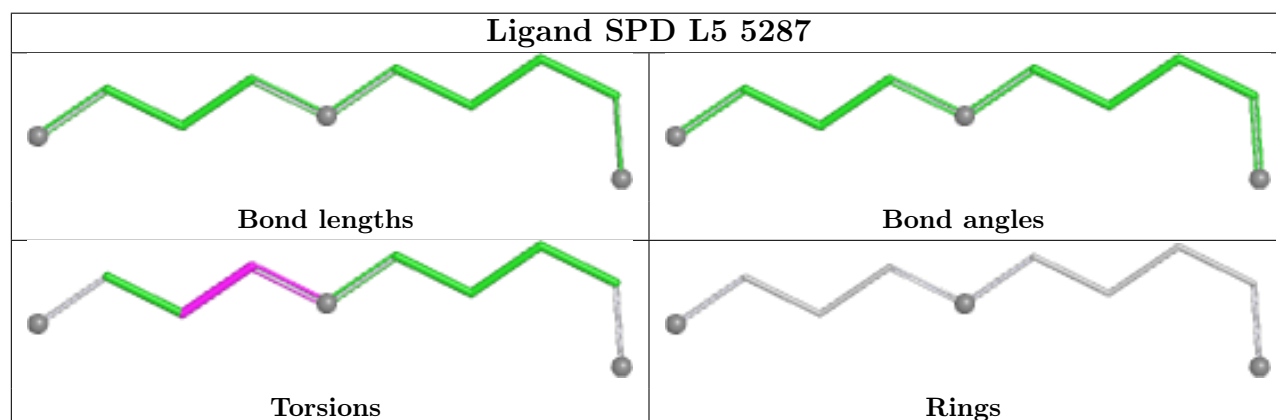
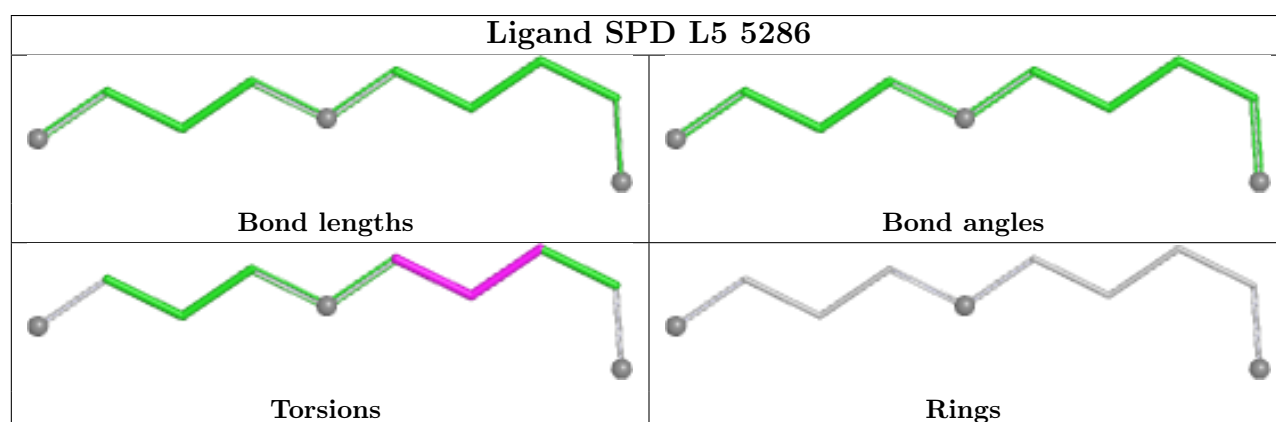
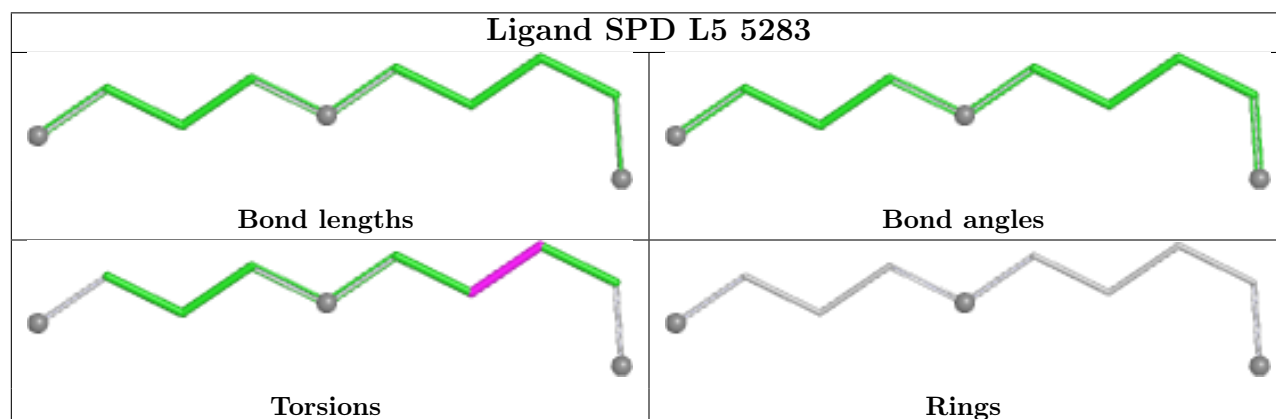
There are no ring outliers.

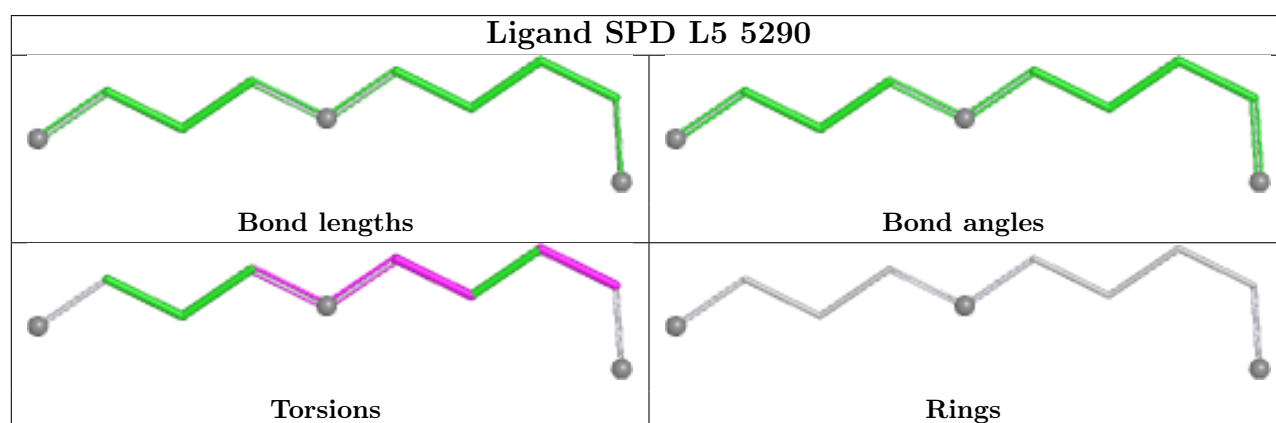
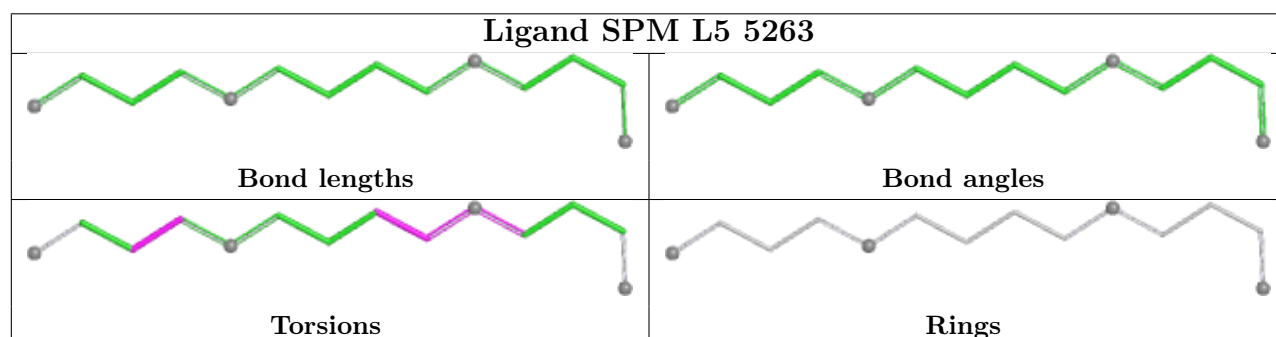
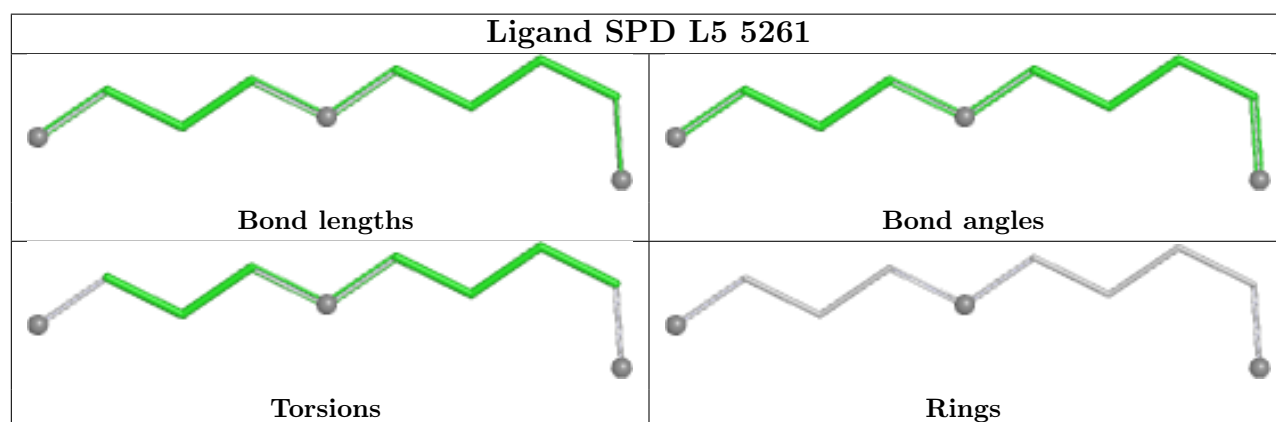
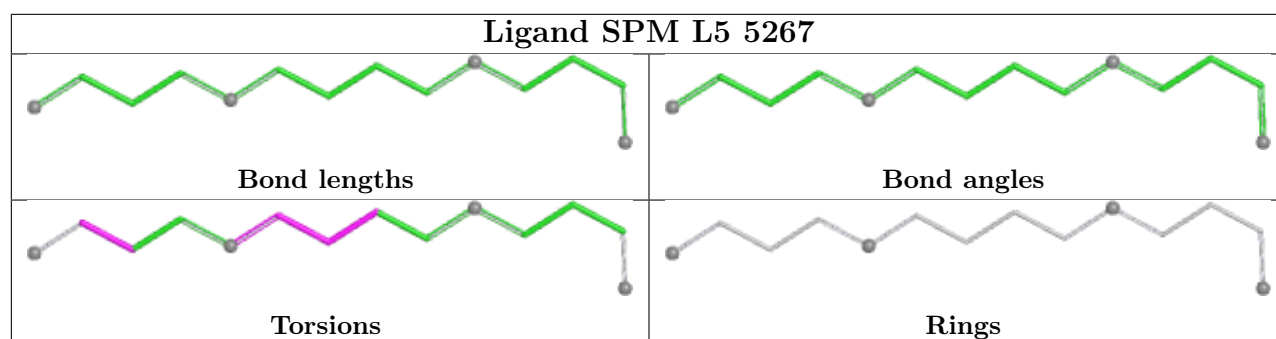
7 monomers are involved in 8 short contacts:

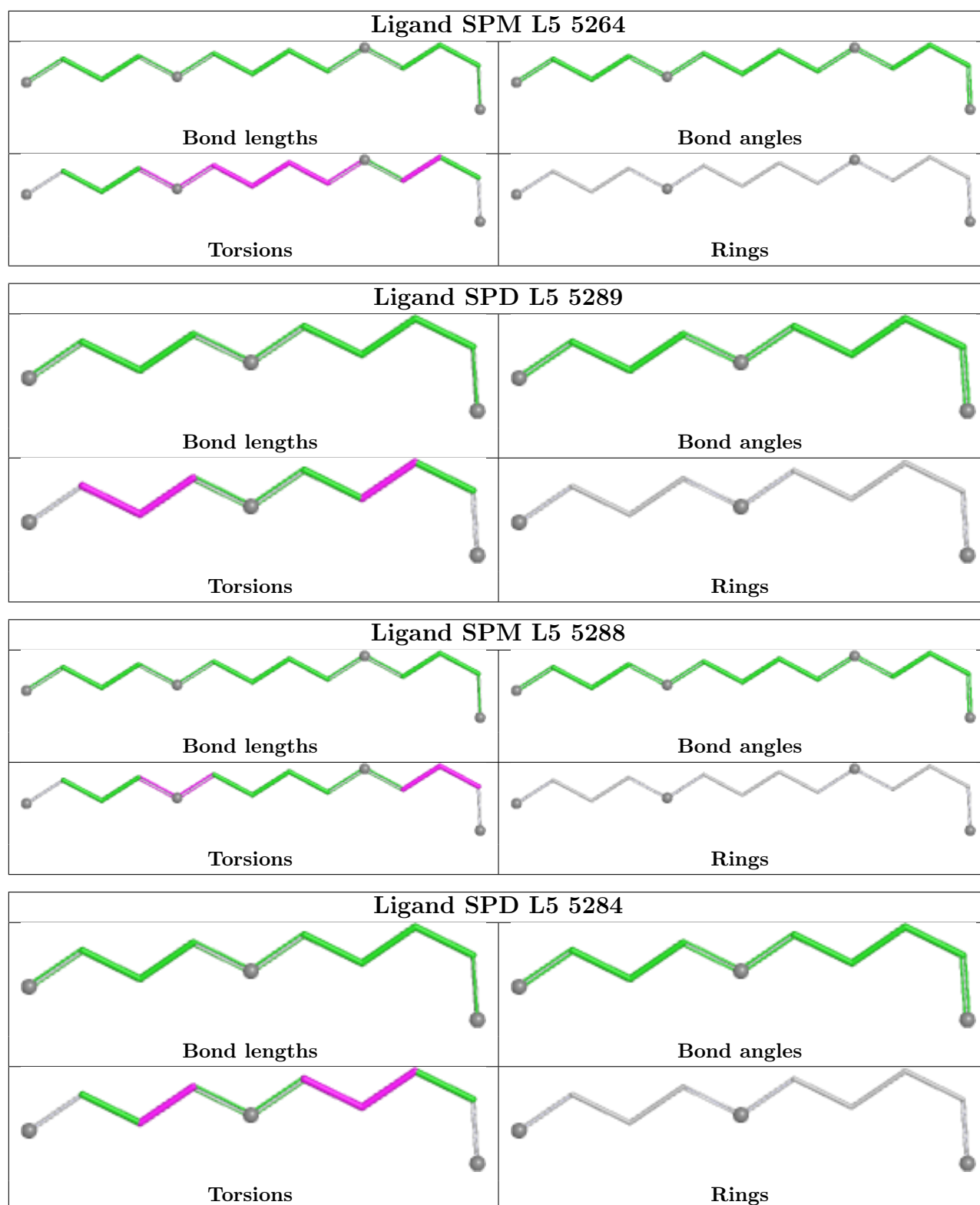
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5286	SPD	1	0
87	L5	5291	SPM	2	0
88	L5	5261	SPD	1	0
87	L5	5263	SPM	1	0
87	L5	5264	SPM	1	0
88	L5	5284	SPD	1	0
87	L5	5292	SPM	1	0

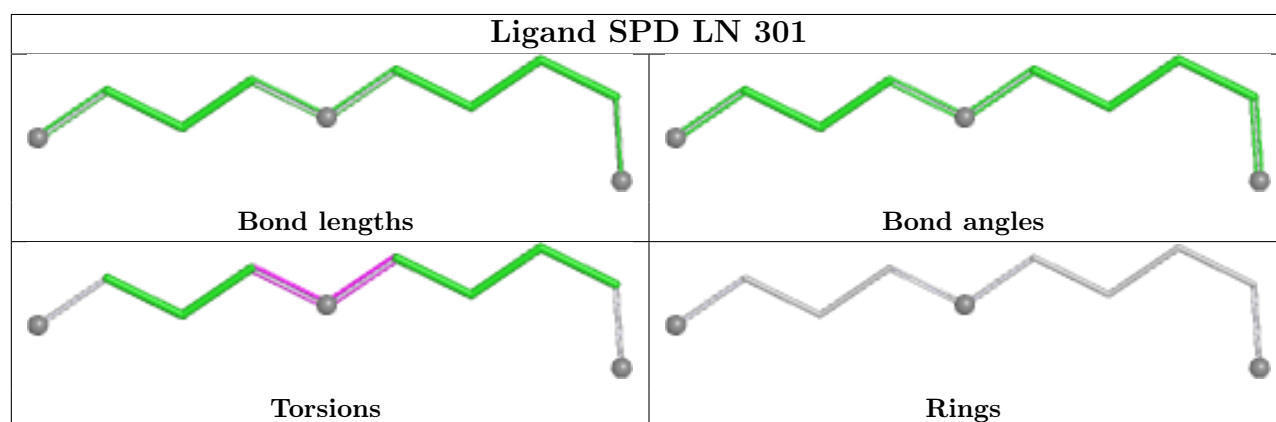
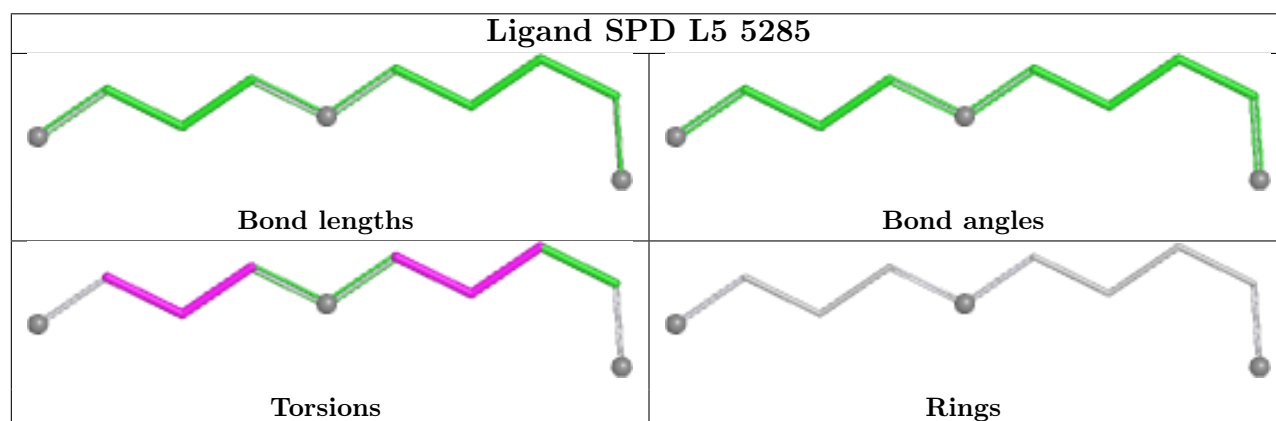
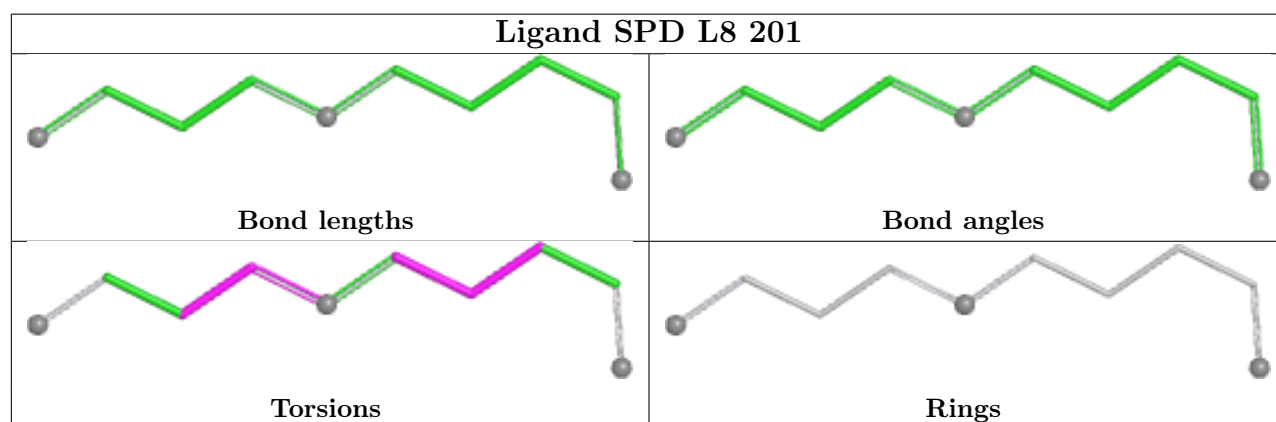
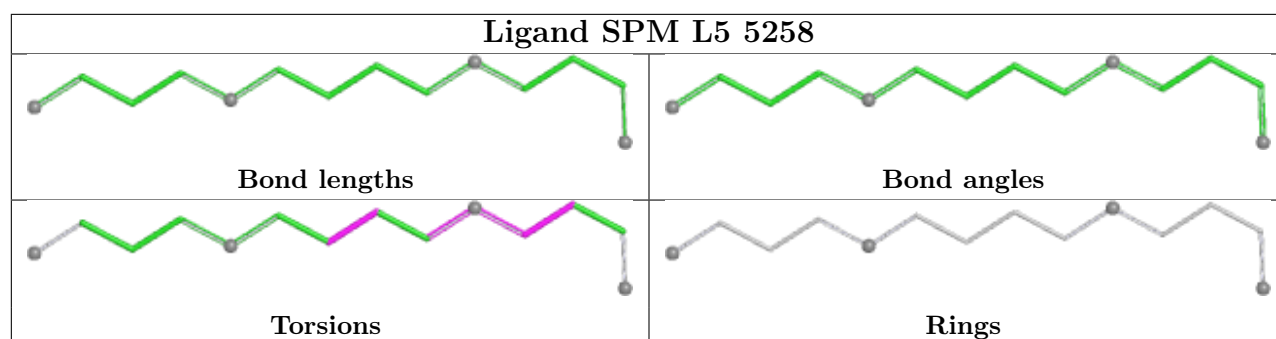
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

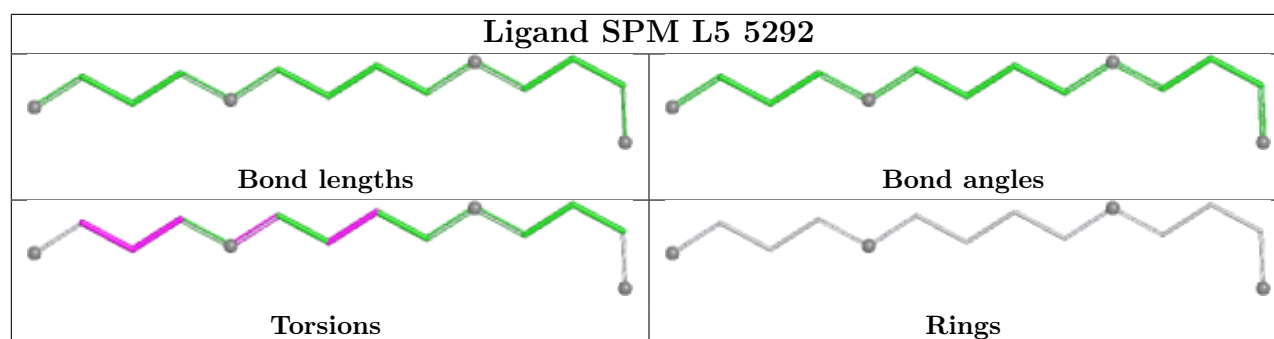
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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
39	L5	10
35	S2	4
66	Lb	1
83	Lt	1
23	SH	1
1	AP	1
2	PE	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	34.81
1	S2	753:C	O3'	785:C	P	28.44
1	L5	2910:G	O3'	3584:C	P	20.91
1	L5	1706:A	O3'	1716:G	P	20.70
1	L5	760:G	O3'	903:C	P	17.16
1	L5	3954:A	O3'	4056:A	P	16.36
1	L5	519:C	O3'	642:G	P	15.44
1	L5	4776:G	O3'	4858:C	P	15.10
1	Lt	87:GLU	C	104:ILE	N	14.14
1	S2	698:G	O3'	730:C	P	14.05
1	L5	2112:G	O3'	2249:C	P	13.37
1	L5	990:C	O3'	1064:G	P	12.99
1	S2	739:C	O3'	746:C	P	12.53
1	L5	1222:A	O3'	1234:G	P	12.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SH	107:LYS	C	111:LYS	N	11.51
1	AP	15:G	O3'	18:G	P	10.75
1	L5	1100:U	O3'	1167:C	P	7.10
1	S2	225:G	O3'	287:U	P	6.72
1	PE	16:C	O3'	18:U	P	5.74

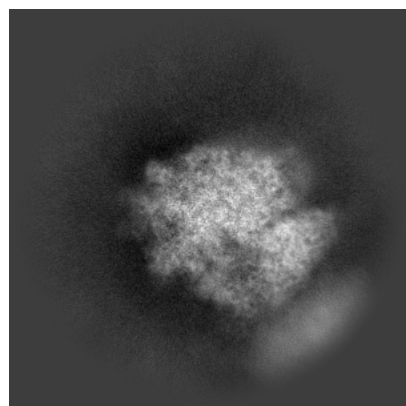
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71377. These allow visual inspection of the internal detail of the map and identification of artifacts.

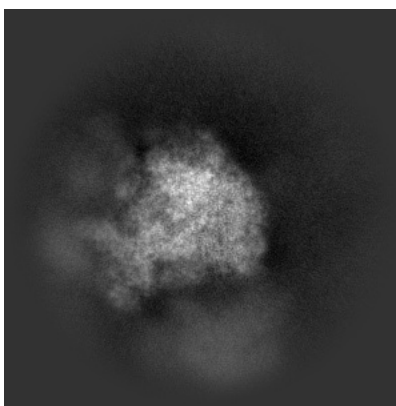
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

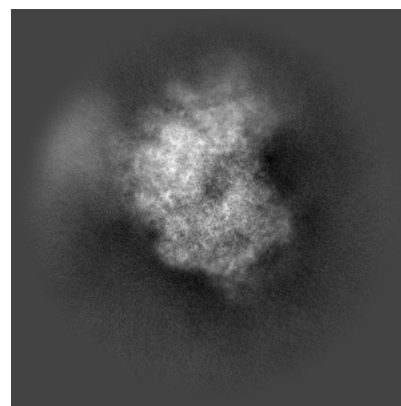
6.1.1 Primary map



X

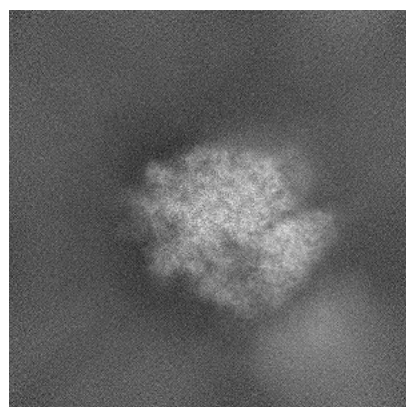


Y

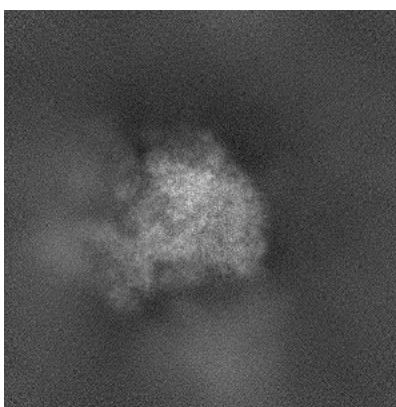


Z

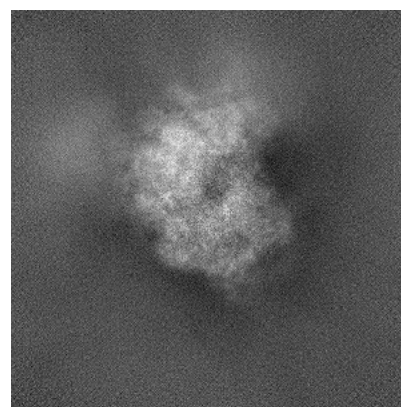
6.1.2 Raw map



X



Y

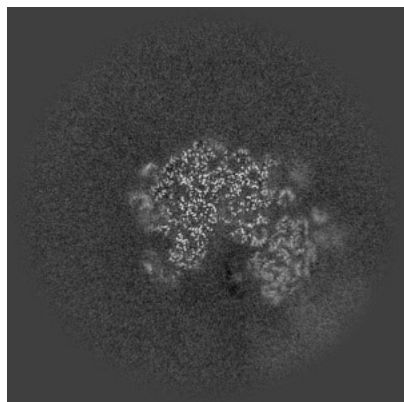


Z

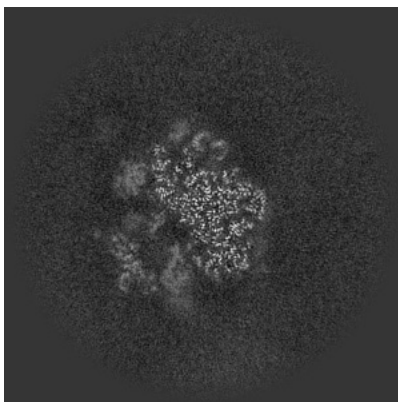
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

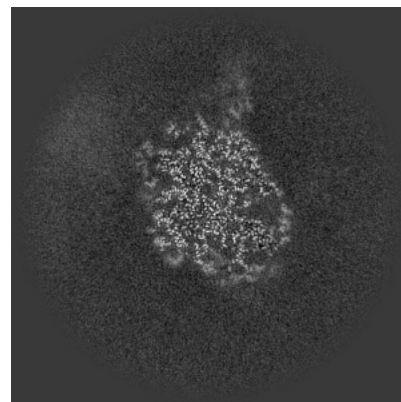
6.2.1 Primary map



X Index: 256

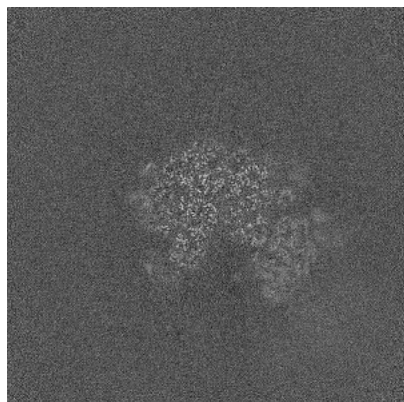


Y Index: 256

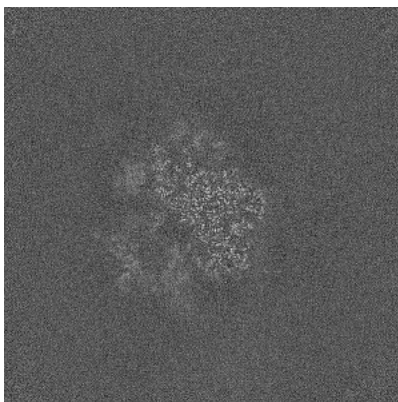


Z Index: 256

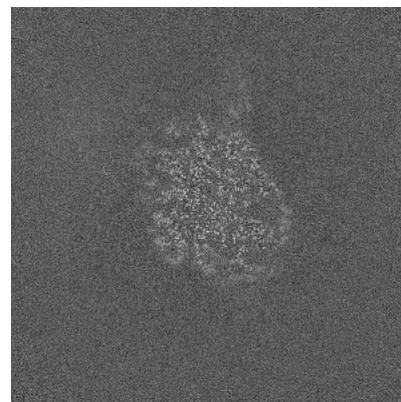
6.2.2 Raw map



X Index: 256



Y Index: 256

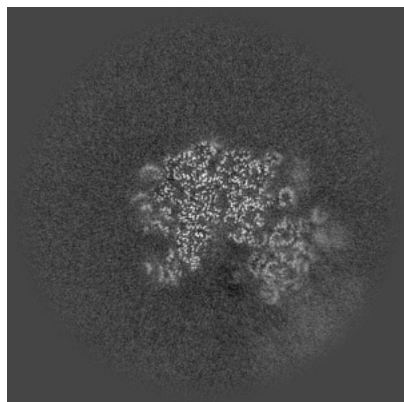


Z Index: 256

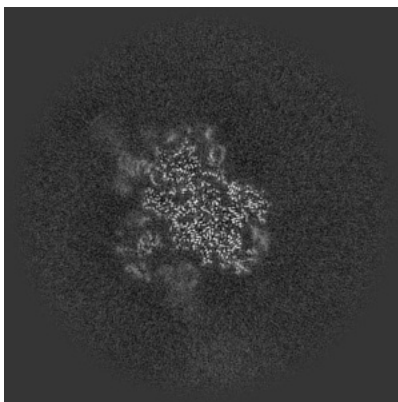
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

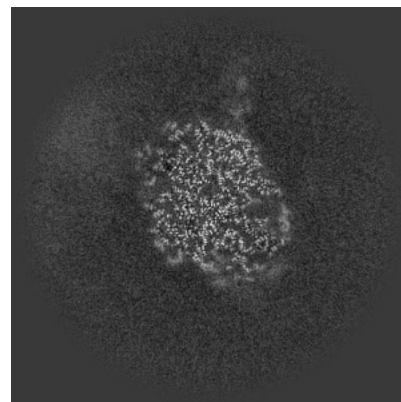
6.3.1 Primary map



X Index: 253

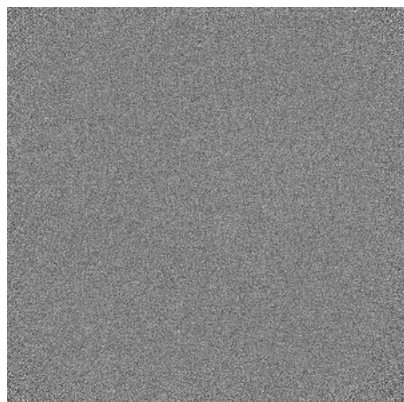


Y Index: 243

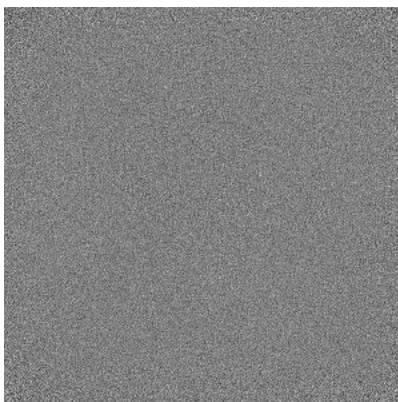


Z Index: 258

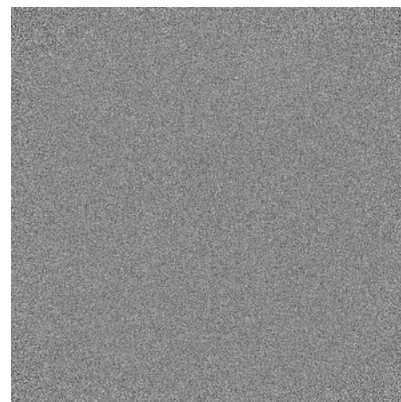
6.3.2 Raw map



X Index: 0



Y Index: 0

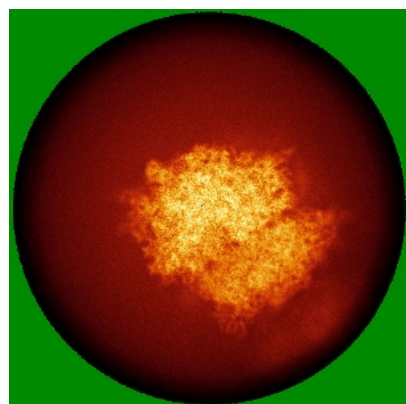


Z Index: 0

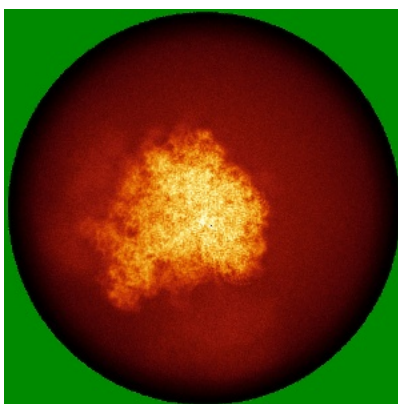
The images above show the largest variance slices of the map in three orthogonal directions.

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

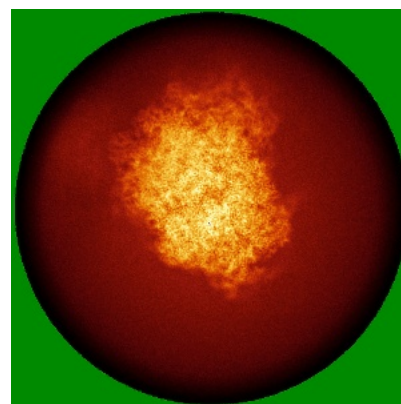
6.4.1 Primary map



X

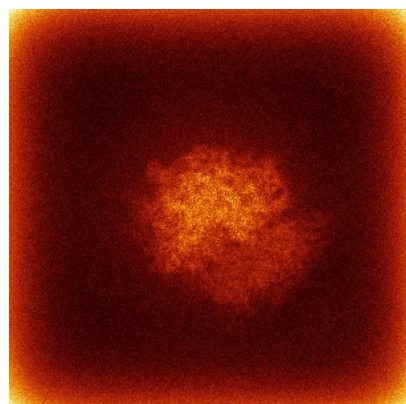


Y

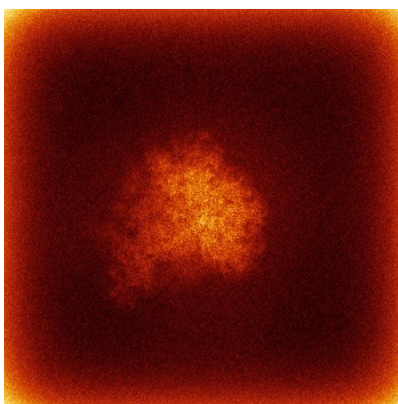


Z

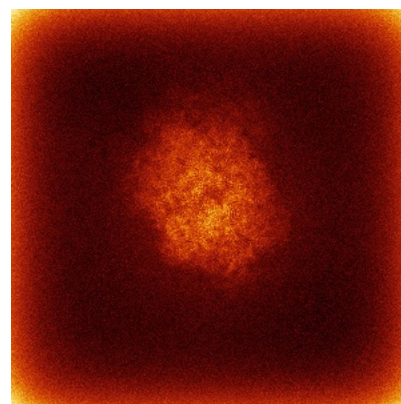
6.4.2 Raw map



X



Y

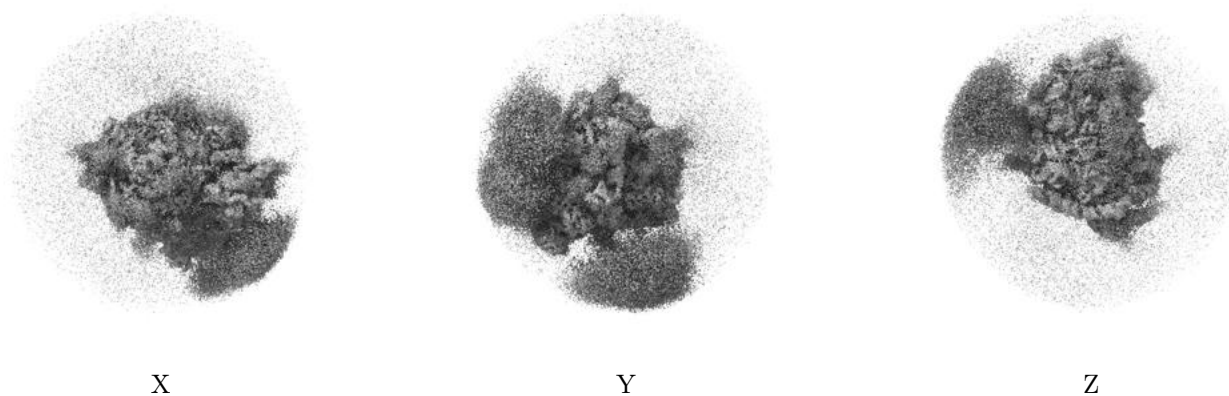


Z

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

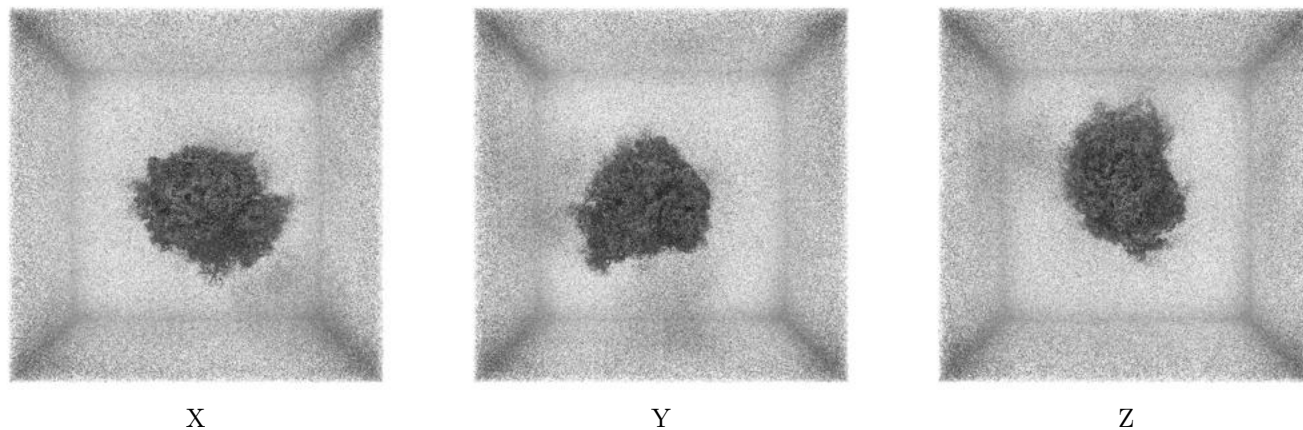
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0126. 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.

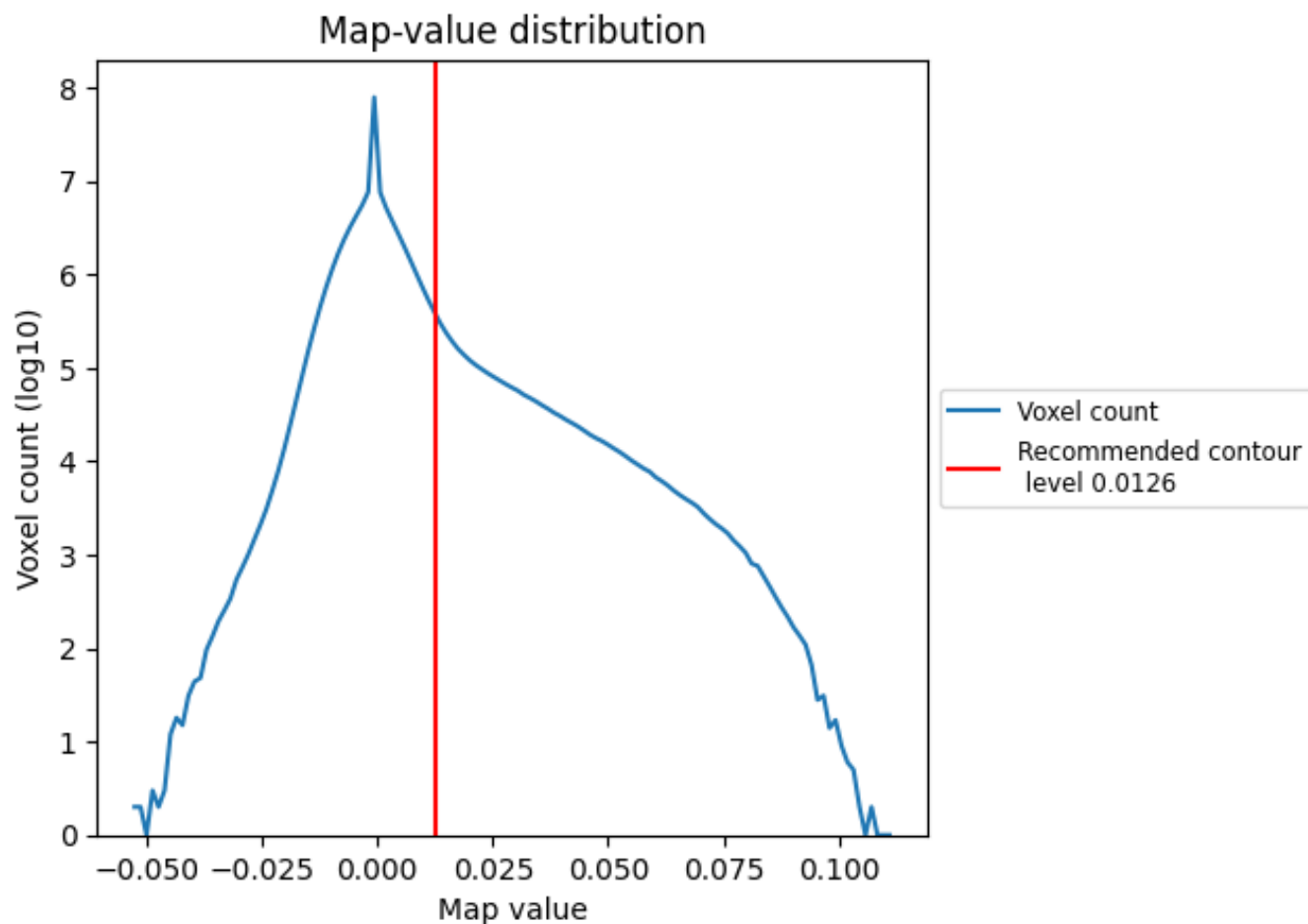
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

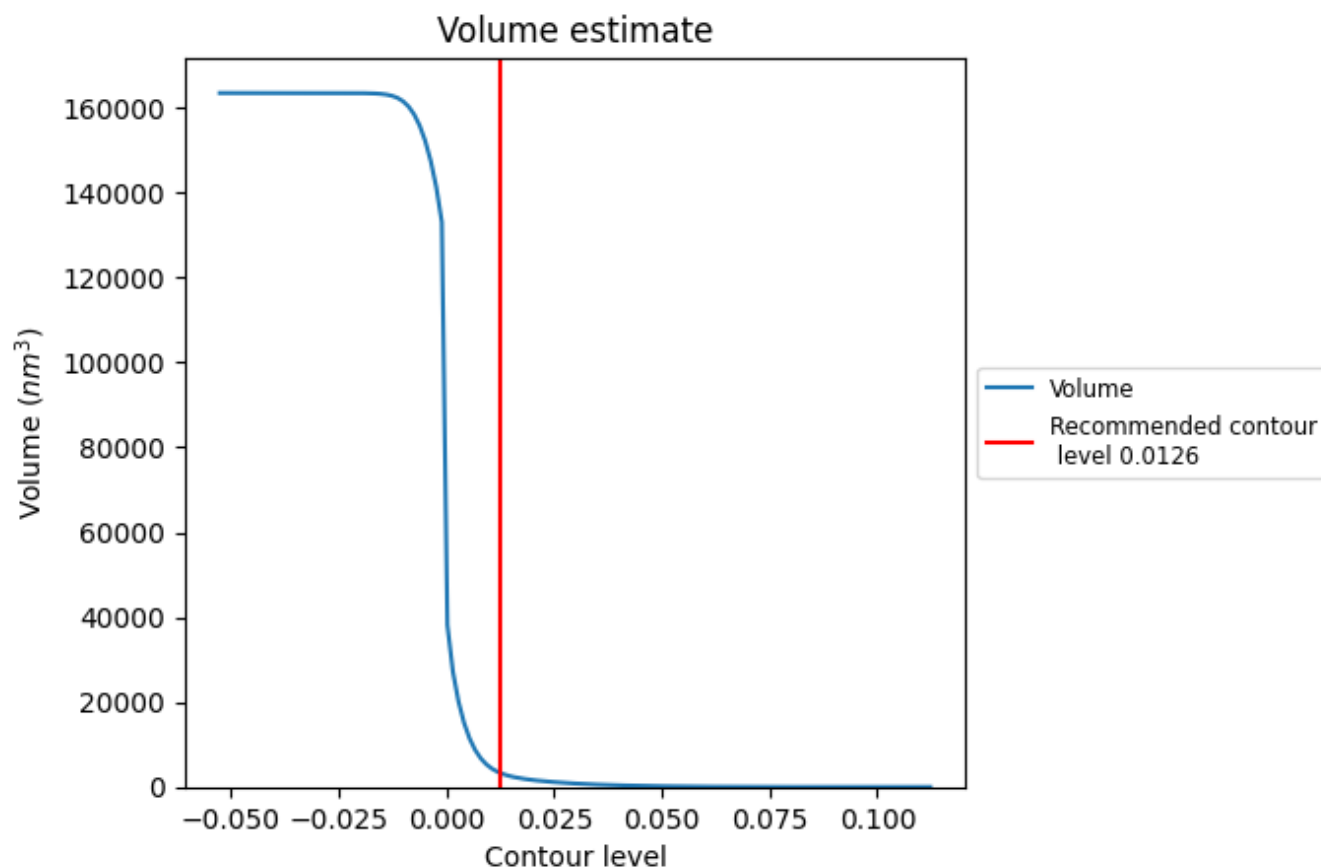
This section contains the results of statistical analysis of the map.

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.

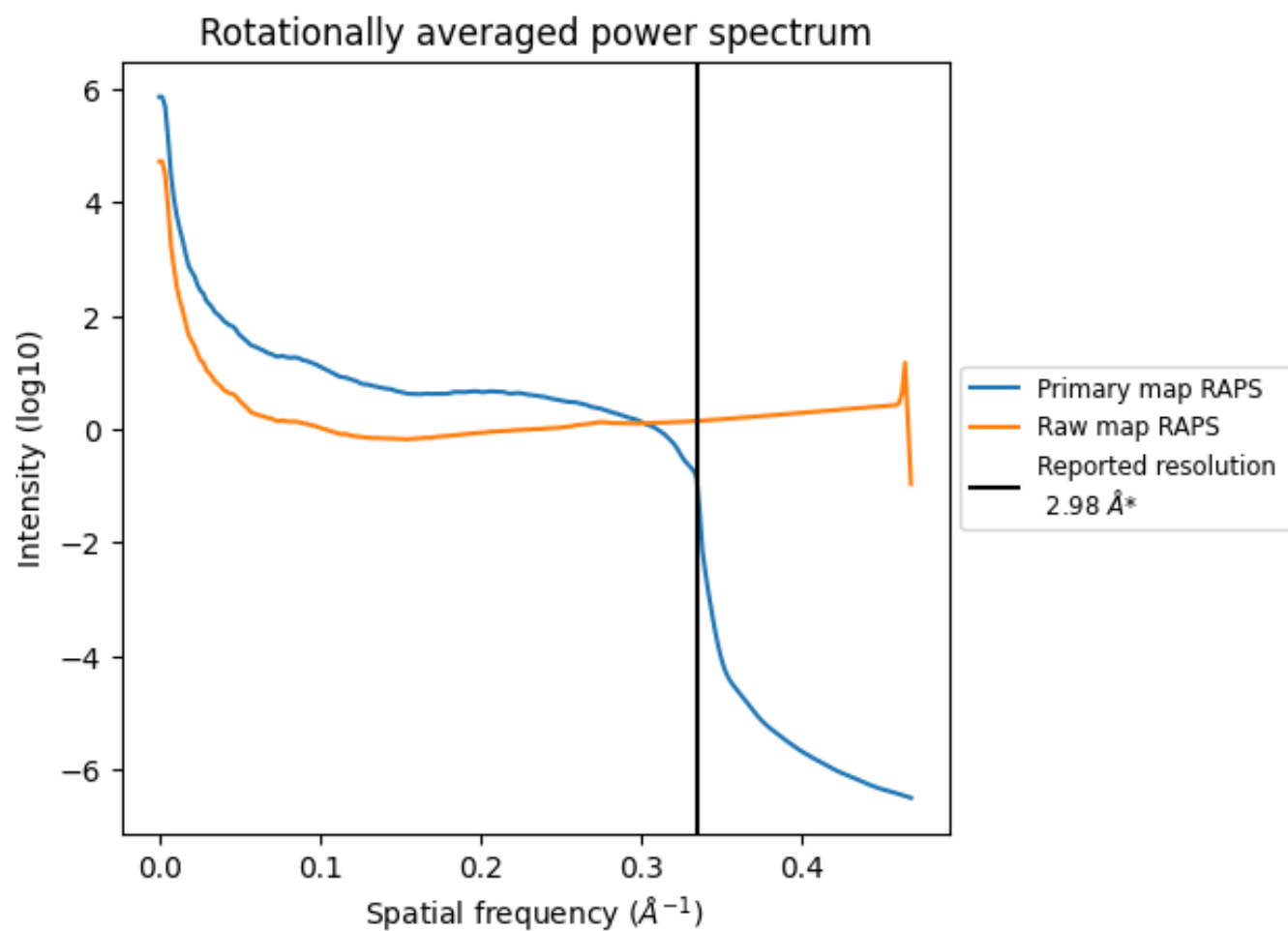
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3255 nm^3 ; this corresponds to an approximate mass of 2941 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

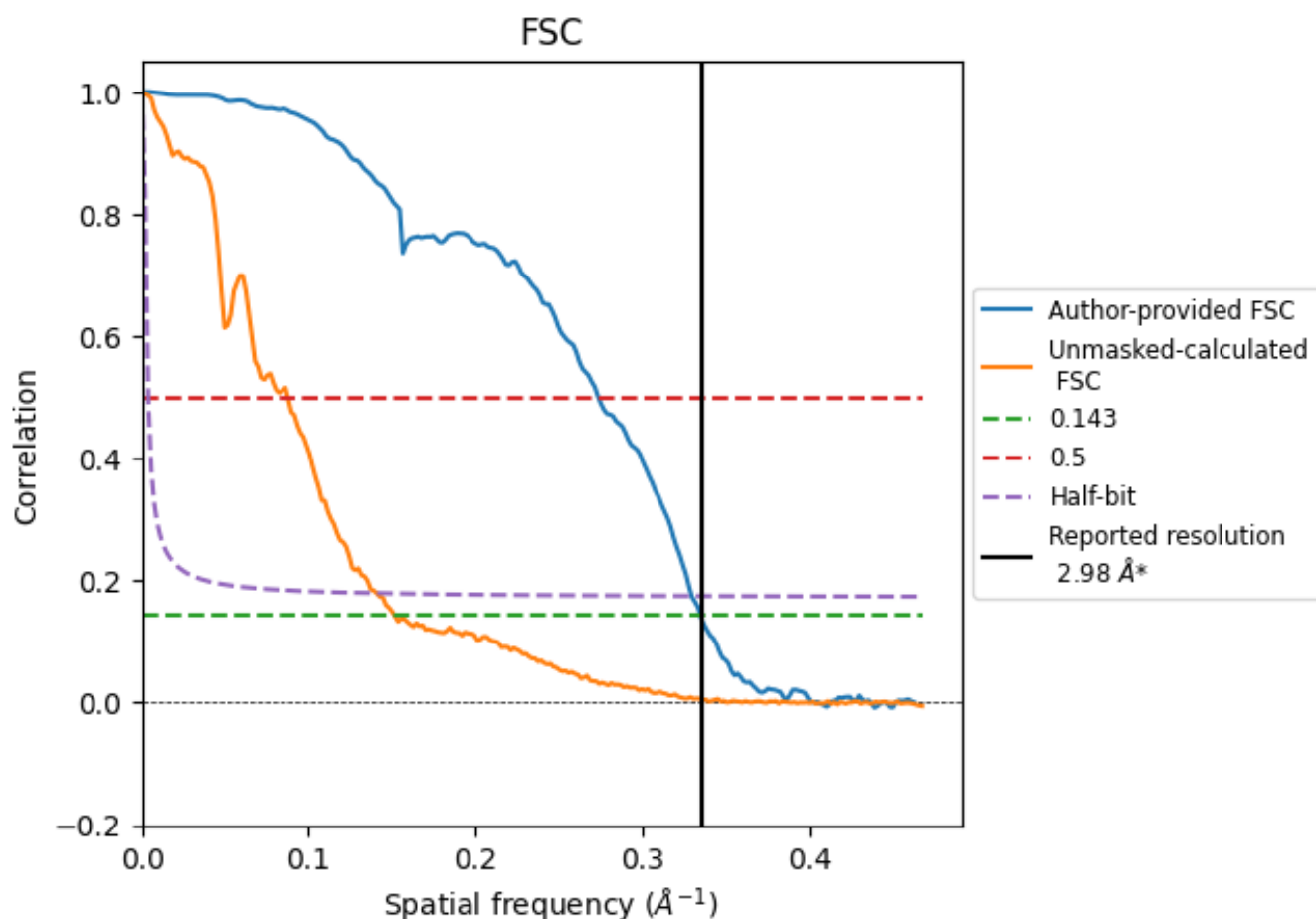


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.336 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

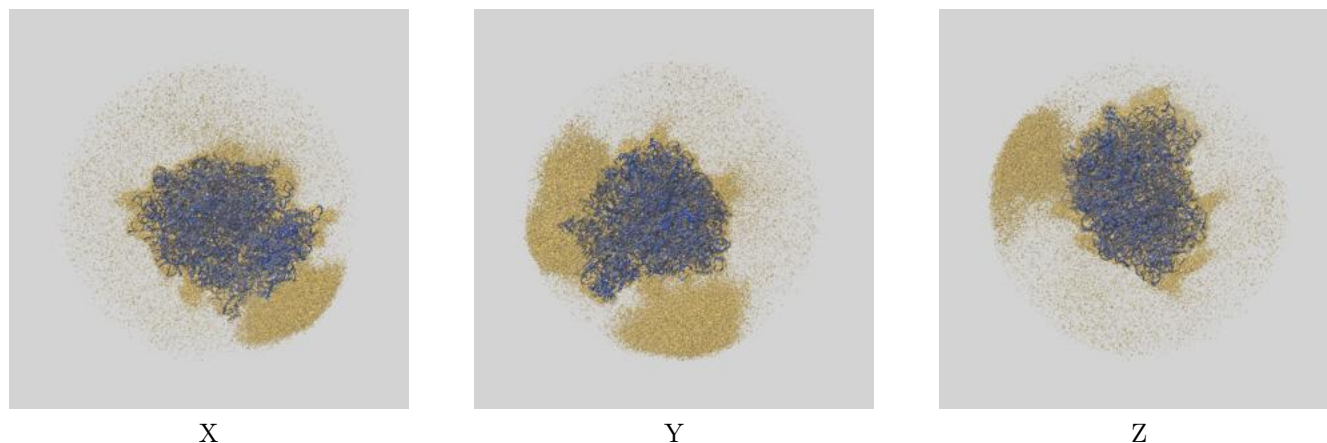
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.65	3.03
Unmasked-calculated*	6.61	11.45	7.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.61 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

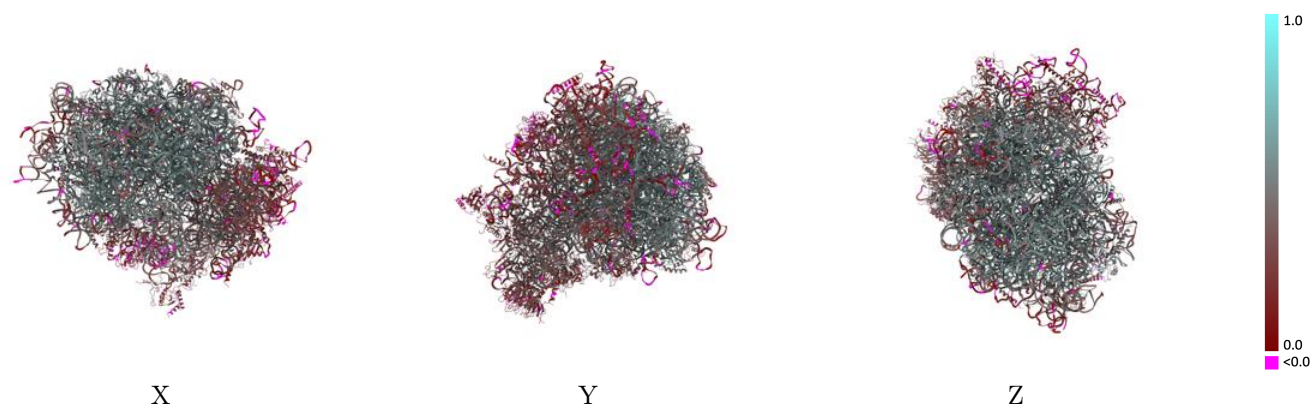
This section contains information regarding the fit between EMDB map EMD-71377 and PDB model 9P8H. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



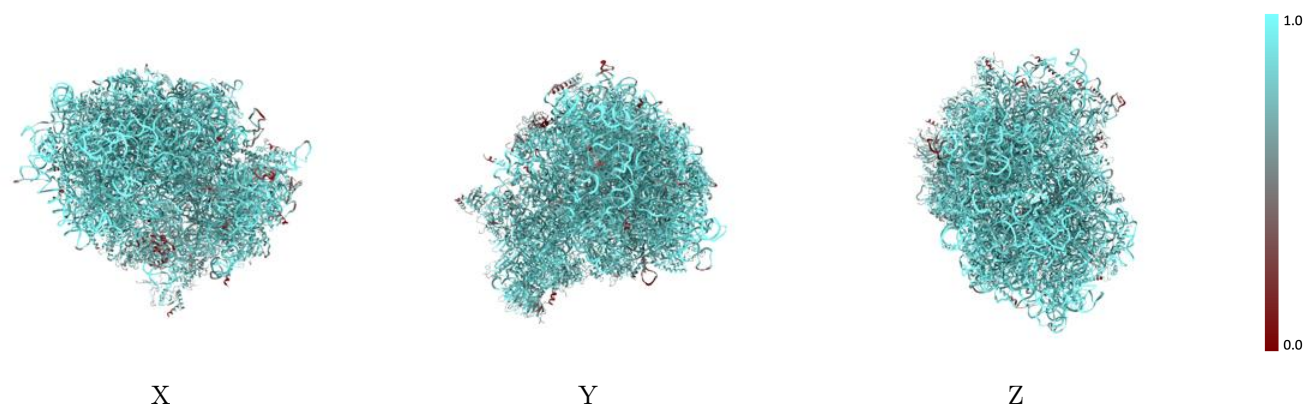
The images above show the 3D surface view of the map at the recommended contour level 0.0126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



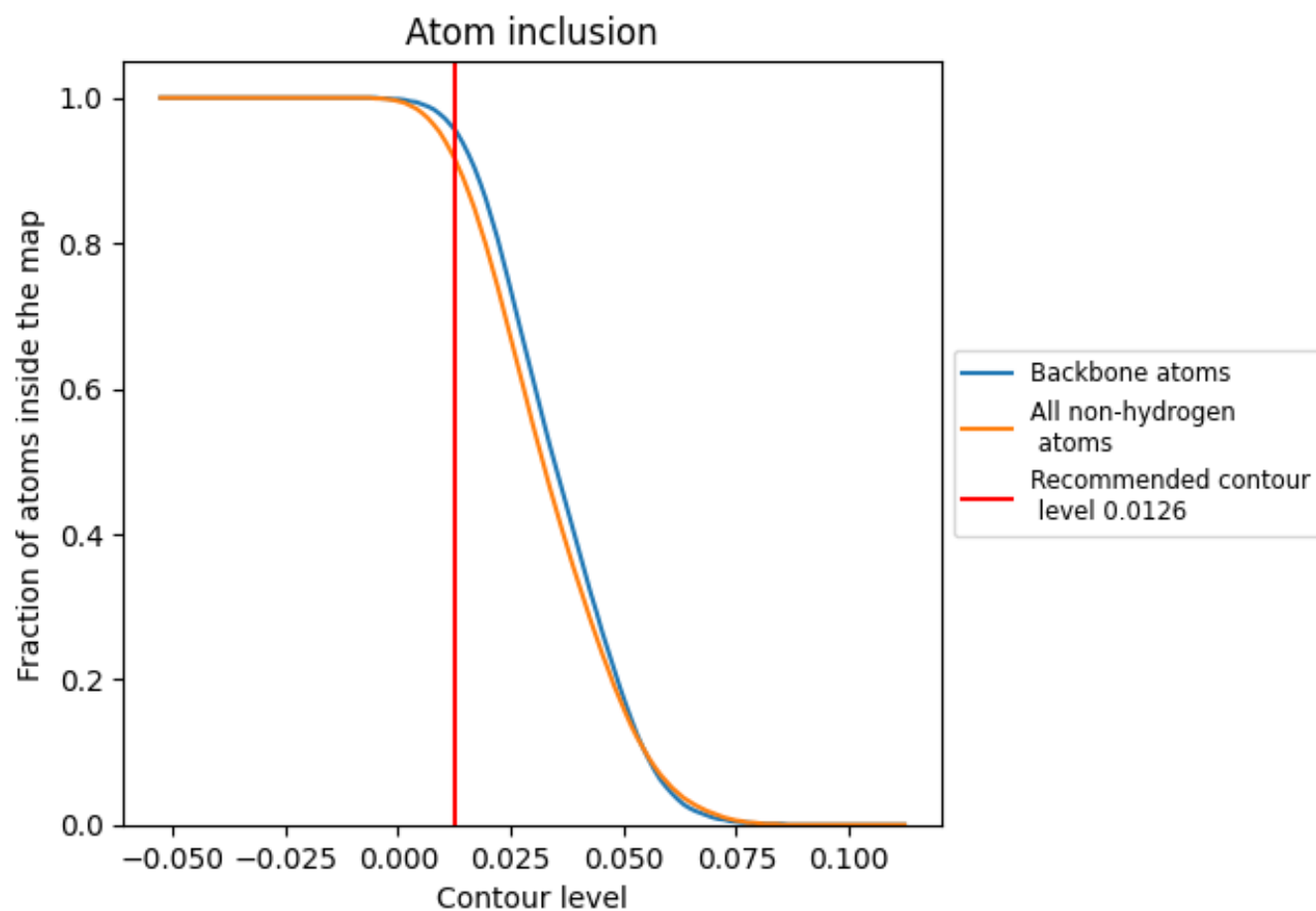
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.4280
AP	 0.7640	 0.2740
CH	 0.6280	 0.2100
CI	 0.7450	 0.3890
L5	 0.9650	 0.4780
L7	 0.9940	 0.5270
L8	 0.9750	 0.5010
LA	 0.9570	 0.5420
LB	 0.9240	 0.5150
LC	 0.9240	 0.5220
LD	 0.9030	 0.4580
LE	 0.8590	 0.4350
LF	 0.9310	 0.5220
LG	 0.8660	 0.4480
LH	 0.8940	 0.4800
LI	 0.8980	 0.4960
LJ	 0.8650	 0.4220
LL	 0.8840	 0.4770
LM	 0.9180	 0.4890
LN	 0.9710	 0.5560
LO	 0.9250	 0.5130
LP	 0.9290	 0.5330
LQ	 0.9490	 0.5460
LR	 0.8820	 0.4480
LS	 0.9420	 0.5410
LT	 0.9010	 0.5060
LU	 0.8750	 0.4200
LV	 0.9210	 0.5210
LW	 0.7530	 0.3210
LX	 0.9030	 0.4950
LY	 0.9190	 0.5040
LZ	 0.9250	 0.4770
La	 0.9470	 0.5420
Lb	 0.8510	 0.4230
Lc	 0.8680	 0.4490



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Chain	Atom inclusion	Q-score
Ld	 0.9040	 0.4960
Le	 0.9460	 0.5440
Lf	 0.9580	 0.5540
Lg	 0.9220	 0.5070
Lh	 0.8920	 0.4840
Li	 0.9080	 0.4720
Lj	 0.9640	 0.5440
Lk	 0.8550	 0.4380
Ll	 0.9270	 0.5200
Lm	 0.9280	 0.5070
Ln	 0.9040	 0.4480
Lo	 0.8850	 0.5060
Lp	 0.9230	 0.5100
Lr	 0.9250	 0.5220
Ls	 0.4990	 0.1240
Lt	 0.4800	 0.0890
PE	 0.9170	 0.3130
S2	 0.9600	 0.3760
SA	 0.8210	 0.3370
SB	 0.8300	 0.3960
SC	 0.8750	 0.3760
SD	 0.8260	 0.3130
SE	 0.8530	 0.2740
SF	 0.8010	 0.3130
SG	 0.7470	 0.2080
SH	 0.7870	 0.2680
SI	 0.8300	 0.3210
SJ	 0.7990	 0.2620
SK	 0.7970	 0.2870
SL	 0.8410	 0.3770
SM	 0.6140	 0.1470
SN	 0.8780	 0.4030
SO	 0.8580	 0.4000
SP	 0.8080	 0.3500
SQ	 0.8360	 0.3080
SR	 0.8000	 0.2860
SS	 0.8110	 0.3490
ST	 0.8300	 0.3240
SU	 0.8060	 0.2770
SV	 0.8330	 0.3340
SW	 0.8910	 0.4240
SX	 0.8210	 0.3750

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Chain	Atom inclusion	Q-score
SY	 0.7140	 0.1870
SZ	 0.7480	 0.2800
Sa	 0.8540	 0.4130
Sb	 0.8260	 0.3540
Sc	 0.7690	 0.2950
Sd	 0.9070	 0.3800
Sf	 0.6620	 0.2080
Sg	 0.7560	 0.2320