



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 11:59 PM EDT

PDB ID : 9P8B / pdb_00009p8b
EMDB ID : EMD-71371
Title : In situ human eEF1A-A/T-P-E state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-22
Resolution : 2.48 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

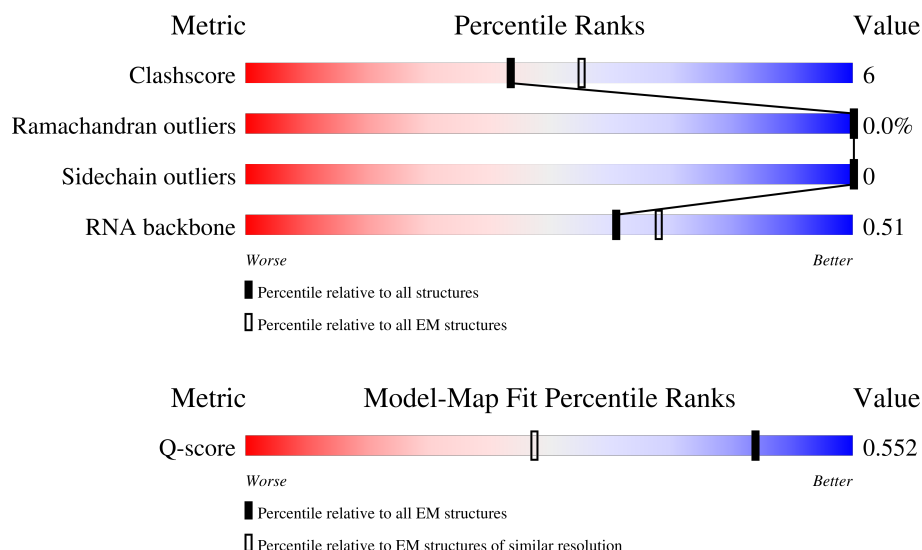
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.48 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	6178 (1.98 - 2.98)

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	CI	31	
2	Pt	74	
3	Et	75	

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Mol	Chain	Length	Quality of chain
4	CF	441	
5	AT	76	
6	L5	3655	
7	L7	120	
8	L8	156	
9	LA	248	
10	LB	402	
11	LC	368	
12	LD	293	
13	LE	250	
14	LF	225	
15	LG	241	
16	LH	190	
17	LI	213	
18	LJ	176	
19	LL	210	
20	LM	139	
21	LN	203	
22	LO	201	
23	LP	153	
24	LQ	187	
25	LR	187	
26	LS	175	
27	LT	159	
28	LU	101	

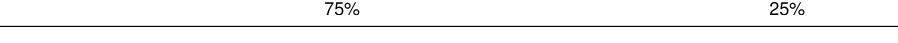
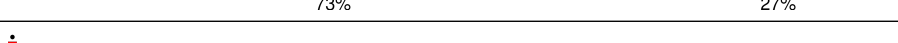
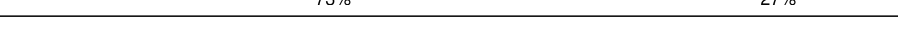
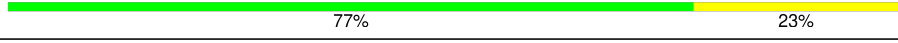
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Mol	Chain	Length	Quality of chain
29	LV	131	
30	LW	124	
31	LX	120	
32	LY	134	
33	LZ	135	
34	La	147	
35	Lb	121	
36	Lc	98	
37	Ld	107	
38	Le	128	
39	Lf	109	
40	Lg	114	
41	Lh	122	
42	Li	102	
43	Lj	86	
44	Lk	69	
45	Ll	50	
46	Lm	52	
47	Ln	24	
48	Lo	105	
49	Lp	91	
50	Lr	125	
51	Ls	196	
52	Lt	157	
53	SD	227	

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Mol	Chain	Length	Quality of chain
54	SF	189	
55	SK	98	
56	SM	122	
57	SP	121	
58	SQ	144	
59	SR	135	
60	SS	145	
61	ST	143	
62	SU	104	
63	SZ	75	
64	Sc	64	
65	Sd	55	
66	Sf	67	
67	Sg	313	
68	SA	221	
69	SB	214	
70	SC	222	
71	SE	262	
72	SG	237	
73	SH	189	
74	SI	206	
75	SJ	185	
76	SL	153	
77	SN	150	
78	SO	140	

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Mol	Chain	Length	Quality of chain
79	SV	83	 73%27%
80	SW	129	 81%19%
81	SX	141	 79%21%
82	SY	131	 78%22%
83	Sa	102	 83%17%
84	Sb	83	 76%24%
85	Se	58	 81%19%
86	S2	1740	 56%36%8%

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 224971 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transcription factor BTF3.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Pt	3	C	U	conflict	GB X64278
Pt	?	-	U	deletion	GB X64278
Pt	?	-	G	deletion	GB X64278
Pt	19	G	U	conflict	GB X64278
Pt	50	U	-	insertion	GB X64278
Pt	74	C	-	insertion	GB X64278

- Molecule 3 is a RNA chain called E site tRNA.

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

- Molecule 4 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	CF	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

- Molecule 5 is a RNA chain called A/T site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AT	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	3655	Total	C	N	O	P	1	0
			78445	34968	14346	25476	3655		

- Molecule 7 is a RNA chain called 5S rRNA.

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

- Molecule 8 is a RNA chain called 5.8S rRNA.

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

- Molecule 9 is a protein called 60S ribosomal protein L8.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 11 is a protein called 60S ribosomal protein L4.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 13 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 14 is a protein called 60S ribosomal protein L7.

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

- Molecule 15 is a protein called 60S ribosomal protein L7a.

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

- Molecule 16 is a protein called 60S ribosomal protein L9.

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

- Molecule 17 is a protein called Ribosomal protein uL16-like.

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

- Molecule 18 is a protein called 60S ribosomal protein L11.

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

- Molecule 19 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 20 is a protein called 60S ribosomal protein L14.

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

- Molecule 21 is a protein called 60S ribosomal protein L15.

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

- Molecule 22 is a protein called 60S ribosomal protein L13a.

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

- Molecule 23 is a protein called 60S ribosomal protein L17.

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

- Molecule 24 is a protein called 60S ribosomal protein L18.

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

- Molecule 25 is a protein called 60S ribosomal protein L19.

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

- Molecule 26 is a protein called 60S ribosomal protein L18a.

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

- Molecule 27 is a protein called 60S ribosomal protein L21.

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

- Molecule 28 is a protein called Heparin-binding protein HBp15.

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

- Molecule 29 is a protein called 60S ribosomal protein L23.

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

- Molecule 30 is a protein called Ribosomal protein L24.

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

- Molecule 31 is a protein called 60S ribosomal protein L23a.

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

- Molecule 32 is a protein called 60S ribosomal protein L26.

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

- Molecule 33 is a protein called 60S ribosomal protein L27.

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

- Molecule 34 is a protein called 60S ribosomal protein L27a.

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

- Molecule 35 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 36 is a protein called 60S ribosomal protein L30.

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

- Molecule 37 is a protein called 60S ribosomal protein L31.

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

- Molecule 38 is a protein called 60S ribosomal protein L32.

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

- Molecule 39 is a protein called 60S ribosomal protein L35a.

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

- Molecule 40 is a protein called 60S ribosomal protein L34.

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

- Molecule 41 is a protein called 60S ribosomal protein L35.

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

- Molecule 42 is a protein called 60S ribosomal protein L36.

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

- Molecule 43 is a protein called 60S ribosomal protein L37.

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

- Molecule 44 is a protein called 60S ribosomal protein L38.

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

- Molecule 45 is a protein called 60S ribosomal protein L39.

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

- Molecule 46 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 47 is a protein called 60S ribosomal protein L41.

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

- Molecule 48 is a protein called 60S ribosomal protein L36a.

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

- Molecule 49 is a protein called 60S ribosomal protein L37a.

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

- Molecule 50 is a protein called 60S ribosomal protein L28.

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

- Molecule 51 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S10.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 57 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 58 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 60 is a protein called 40S ribosomal protein S18.

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

- Molecule 61 is a protein called 40S ribosomal protein S19.

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

- Molecule 62 is a protein called 40S ribosomal protein S20.

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

- Molecule 63 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 64 is a protein called 40S ribosomal protein S28.

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

- Molecule 65 is a protein called 40S ribosomal protein S29.

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

- Molecule 66 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 67 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 68 is a protein called 40S ribosomal protein SA.

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

- Molecule 69 is a protein called 40S ribosomal protein S3a.

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

- Molecule 70 is a protein called 40S ribosomal protein S2.

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

- Molecule 71 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 72 is a protein called 40S ribosomal protein S6.

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

- Molecule 73 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 74 is a protein called 40S ribosomal protein S8.

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

- Molecule 75 is a protein called 40S ribosomal protein S9.

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

- Molecule 76 is a protein called 40S ribosomal protein S11.

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

- Molecule 77 is a protein called 40S ribosomal protein S13.

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

- Molecule 78 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 80 is a protein called 40S ribosomal protein S15a.

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

- Molecule 81 is a protein called 40S ribosomal protein S23.

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

- Molecule 82 is a protein called 40S ribosomal protein S24.

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

- Molecule 83 is a protein called 40S ribosomal protein S26.

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

- Molecule 84 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 85 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 86 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	S2	1740	Total	C	N	O	P	0	0
			36953	16508	6600	12106	1739		

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

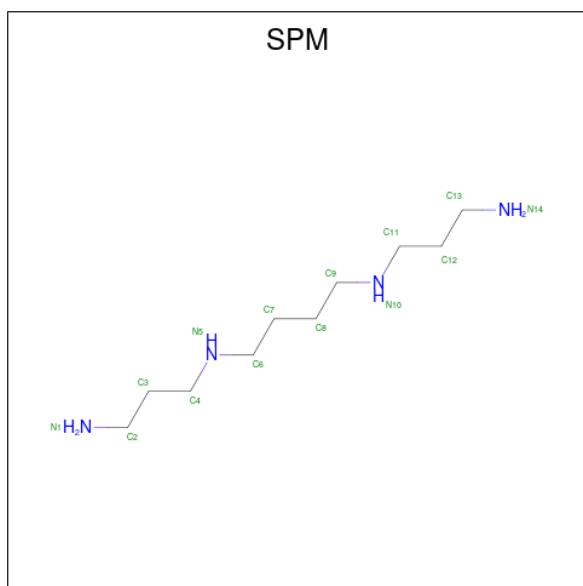
Mol	Chain	Residues	Atoms		AltConf
87	L5	177	Total	Mg	0
			177	177	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LB	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	Lj	1	Total	Mg	0
			1	1	
87	SS	1	Total	Mg	0
			1	1	
87	SG	1	Total	Mg	0
			1	1	
87	S2	26	Total	Mg	0
			26	26	

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



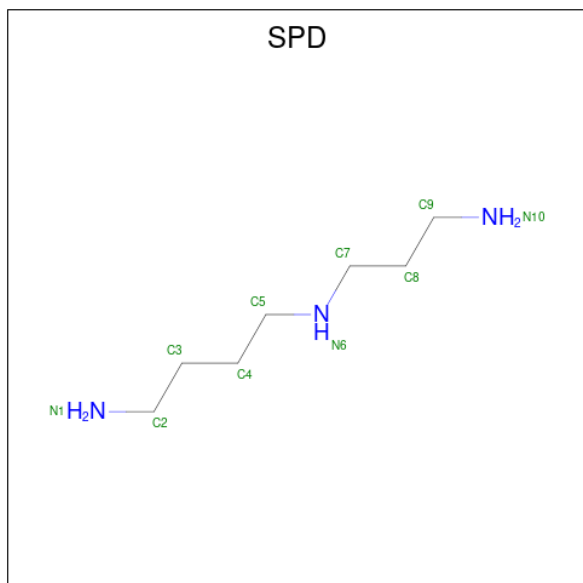
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

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

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



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

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

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

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

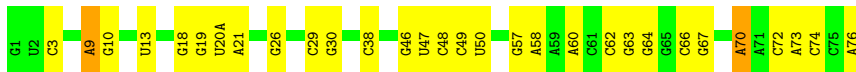
- Molecule 1: Transcription factor BTF3

Chain CI:  77% 23%

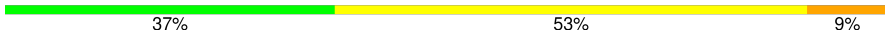


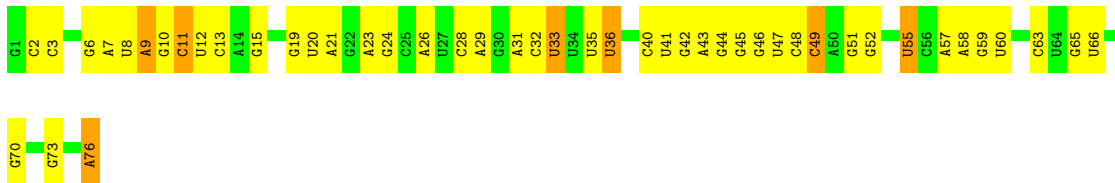
- Molecule 2: P site tRNA

Chain Pt:  59% 38% .



- Molecule 3: E site tRNA

Chain Et:  37% 53% 9%



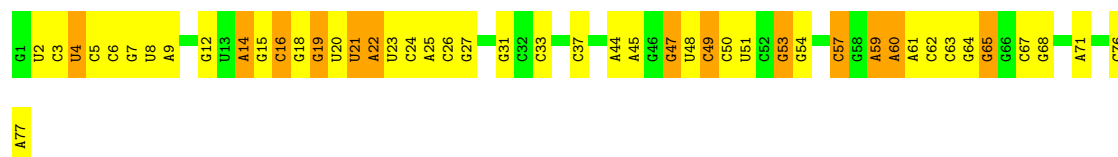
- Molecule 4: Elongation factor 1-alpha 1

Chain CF:  73% 27%

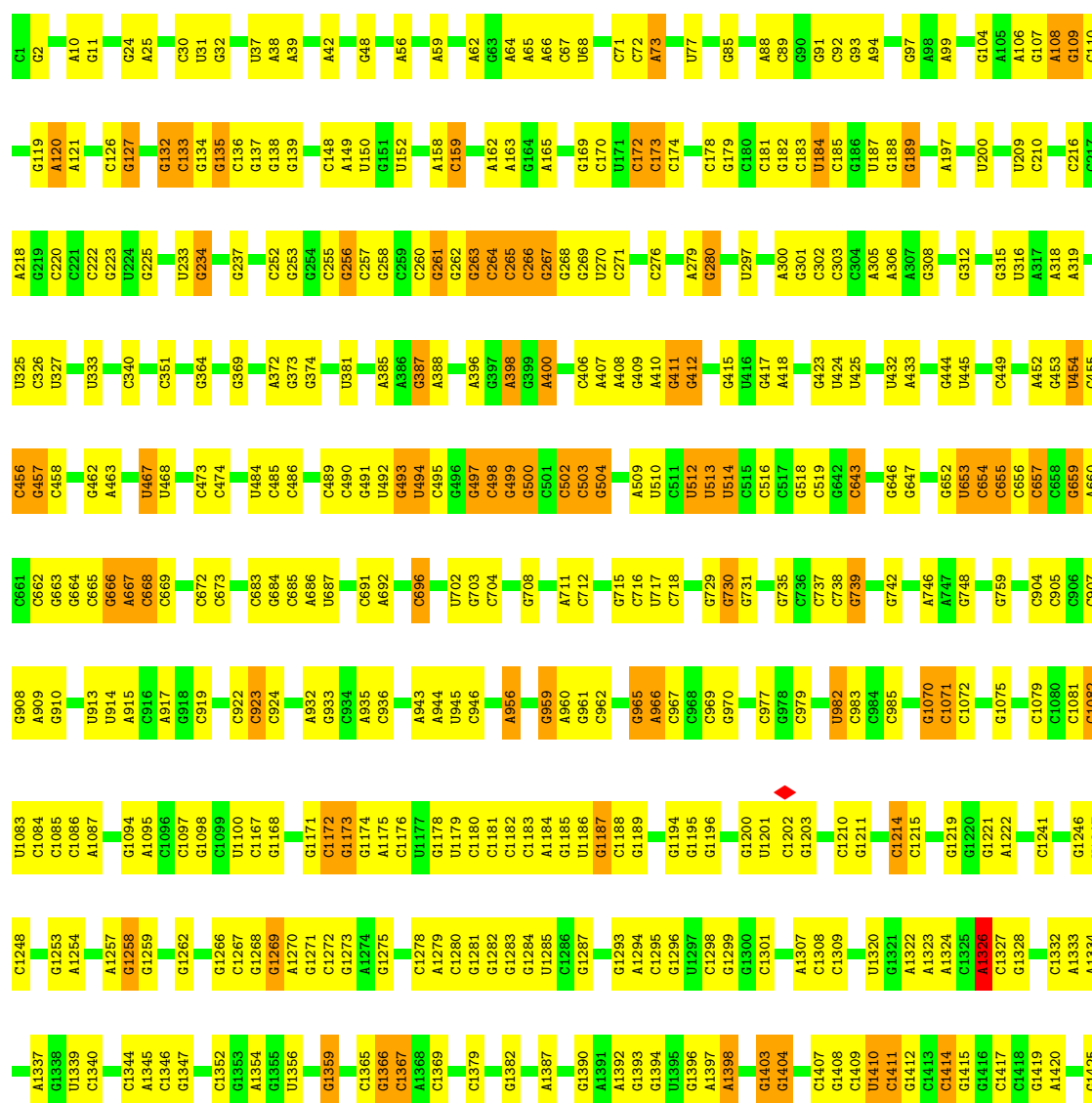




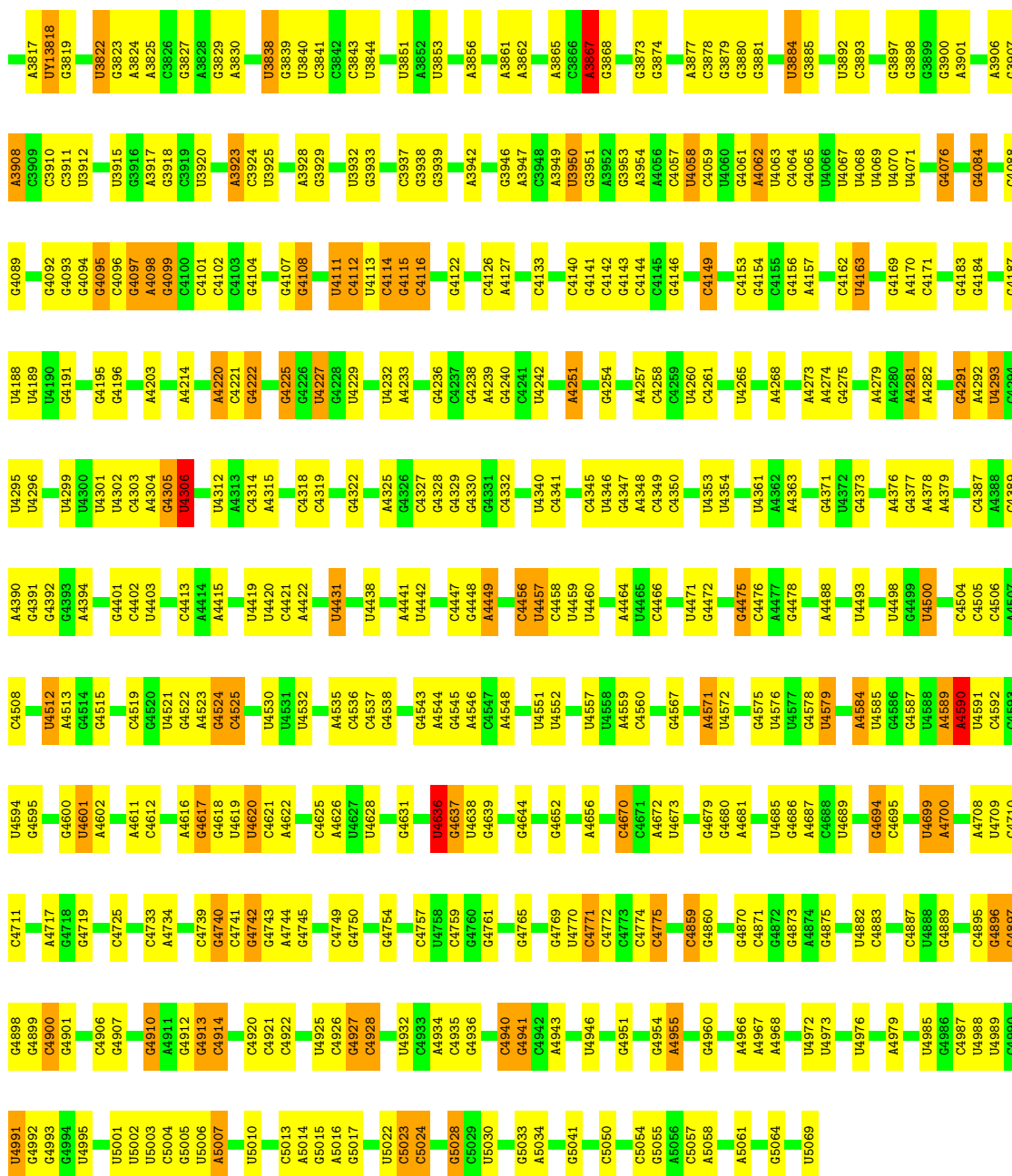
• Molecule 5: A/T site tRNA



• Molecule 6: 28S rRNA

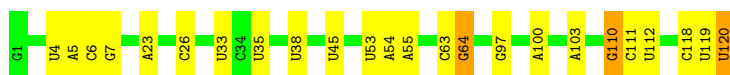


G3698	G3609	A2844	A2743	G2640	C2458	G2326	G2085	A1991	U1882	G1781	G1685	C1566	C1437
A3610	A3610	A2845	A2744	A2641	C2459	U2329	G2092	U1992	A1891	U1782	C1694	G1577	U1438
A3611	A3611	G2847	A2745	C2653	A2460	G2459	A2093	C1993	A1892	U1695	U1578	C1439	
G3615	G3615	G2848	A2746	U2656	G2461	A2332	A2094	C1994	G1896	A1787	U1582		C1442
G3616	U3616	G2849	C2749	G2657	C2462	G2333	A2095	G1995	A1897	C1788	U1588		A1443
G3617	G3617	C2855	G2750	G2658	G2463	G2334	G2096	C1996	C1897	C1789	C1589		G1444
G3618	G3618	C2856	C2751	G2659	C2464	G2335	U2097	U1997	G1898	U1792	U1590		A1445
G3619	G3619	C2857	G2752	G2660	C2465	G2336	G2098	A1998	C1899	A1793	U1591		C1447
A3624	A3624	C2861	A2756	G2662	G2466	A2347	C2101	A1999	G1912	A1794	U1596		C1461
G3625	G3625	A2864	G2757	G2663	U2467	G2348	G2102	G2000	C1913	C1703			A1462
G3626	G3626	U2865	G2759	G2664	U2468	A2349	G2103	A2001	G1914	A1802			G1466
		C2866	G2760	G2665	C2470	U2350	G2104	A2002	A1917	G1803			C1467
A3630	A3630	C2867	G2762	G2666	G2471	C2351	G2105	G2003	U1918	A1804			C1468
		C2867	U2763	G2669		G2352	C2106	U2004	G1919	A1805			
A3635	A3635	A2870	U2764	C2670	G2474	A2360	C2107	G2007	C1920	C1717			G1466
G3636	G3636	A2871	G2765	C2671	G2475	G2361	G2108	U2008	G1921	A1806			C1467
U3637	U3637	A2872	U2766	C2672	A2476	U2362	C2109	A2009	C1922	A1807			C1468
G3638	G3638	G2876	U2767		C2478	A2363	G2111	A2010	G1925	G1721			C1480
U3639	U3639	G2877	C2768	G2675	G2479	G2364	G2112	A2012	G1930	U1726			C1481
U3640	U3640	A2878	U2769	G2676	G2480	A2365	C2249	A2013	U1931	U1727			C1482
U3641	U3641	A2879	C2770	G2677	G2483	A2368	C2250	A2017	G1932	G1624			C1483
					U2484	A2382	G2251	C2018	C1933	G1625			U1494
A3730	A3730	C2892	G2773	C2683	G2485	C2383	G2252	C2019	A1934	G1495			G1496
A3733	A3733	U2893		C2684	G2486			G2020	G1935	G1497			G1499
A3736	A3736	A2894	A2783	U2687	G2487	A2395	C2286	G2021	C1936	A1631			G1499
A3737	A3737	C2899	U2787	G2688	C2488	A2396	G2287	U2020	G1937	A1632			C1499
		U2900	U2788		U2490	A2397	G2288	G2024	G1940	G1734			A1500
A3748	A3748	G2901	U2789	G2689	U2491	U2398	G2289	A2025	A1941	G1735			C1501
		C2902	U2790	A2695	C2492	G2399	C2284	A2026	A1942	A1633			C1502
G3753	G3654	G2903		A2696	U2493	G2400	G2285		A1943	U1638			G1503
		U2904	A2806		U2494	A2401	G2286	A2029	G1948	C1640			G1504
A3760	A3659	C2905	C2702		G2495	A2404	A2276	A2030	G1951	A1742			C1509
U3770	G3660	G2906	G2706	U2707	G2496		G2277			A1743			
	G3661	G2907	U2708	U2708	G2497	G2407	G2278	G2046	G1961	G1750			G1516
A3774	A3662	C2908	C2709	C2709	C2498	U2408	G2279	A2047	A1962	G1751			G1517
A3775	A3663	G2909	G2710	G2710	G2502	U2409	G2284	U2048	A1646	G1752			
G3776	G3664	C3584	G2711	G2711	G2503	C2410	C2289	G2049	G1969	U1647			G1522
G3777	G3665	G3585	G2712	G2712	C2504	A2411	C2289			C1755			A1523
	C3670	A2815			C2505	A2412	C2289	G2055	G1972	U1756			A1524
C3782		G2816			G2506	U2413	C2285	G2056	G1973	U1757			A1534
A3786	C3673	G2822	C2716		A2507	G2414	U2298	G2060	G1974	G1758			A1535
U3786	G3674	G2823	C2717		A2513	U2415	G2299	G2061	G1975	G1759			U1536
	G3684	U2826	C2719		G2516	A2417	G2301	A2069	G1976	G1761			U1537
G3792	C3685	G2827	G2721		A2517	G2421	C2302		G1977	C1762			U1538
		U2828	G2724		G2518	C2422	C2303	C2072	U1978	G1763			G1539
U3796	U3688	A2832	A2725		U2519	A2423	G2306	C2073	U1980	G1764			
A3799	G3689	G2726	G2726		C2520	G2424	G2306	G2076	G1981	A1867			A1547
	C3690	A2835	U2730		G2521	U2425	G2306	G2079	G1982	A1868			C1678
C3808	A2835	U2836	C2731		A2529	G2448	A2313	U2080	A1983	A1869			A1548
	A3604	U2837	C2731		A2537	A2449	G2318		A1984	A1871			A1568
G3811	C3605	U2838	C2739		U2538	G2450	G2318		G1985	C1870			G1569
C3812	U3696	G2839	G2742		U2538		G2321	C2083	U1986	G1768			
U3814	U3697	U2839			C2539			C1987	A1770	G1769			
								U1773					A1563



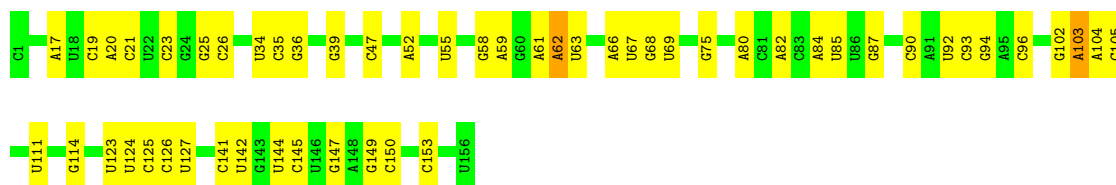
• Molecule 7: 5S rRNA

Chain L7: 80% 18%



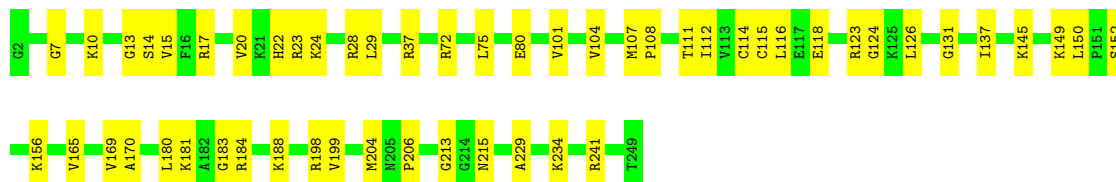
• Molecule 8: 5.8S rRNA

Chain L8: 66% 33%



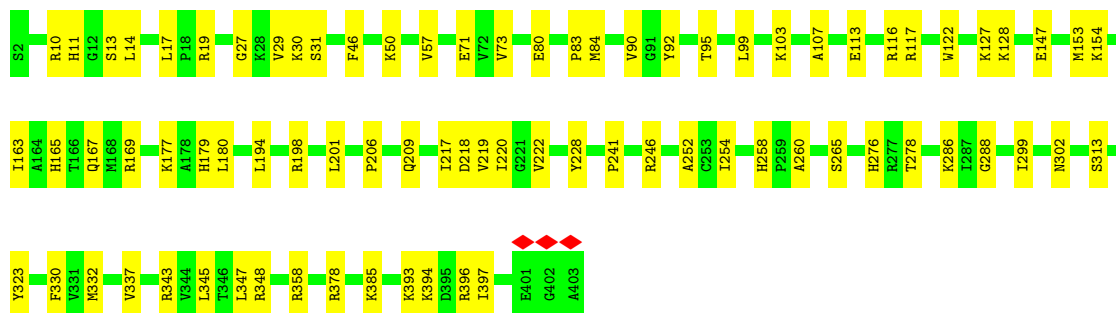
• Molecule 9: 60S ribosomal protein L8

Chain LA: 79% 21%



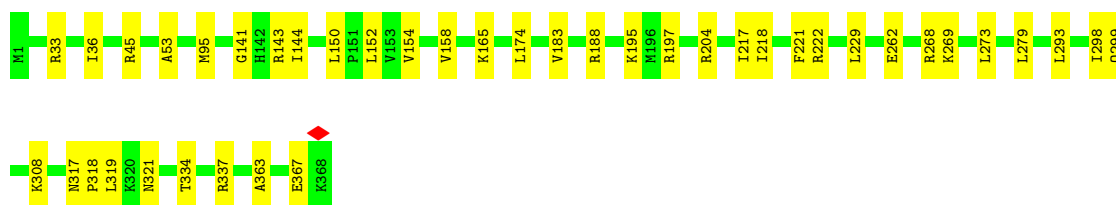
• Molecule 10: Large ribosomal subunit protein uL3

Chain LB: 80% 20%



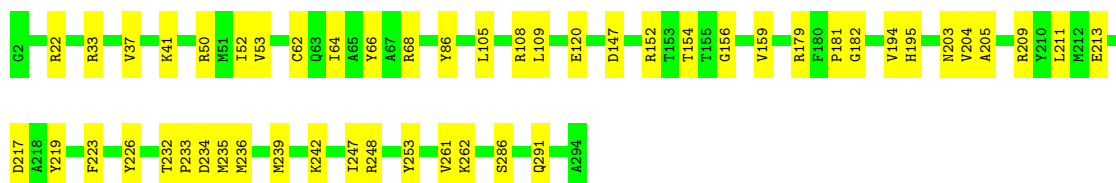
• Molecule 11: 60S ribosomal protein L4

Chain LC: 89% 11%



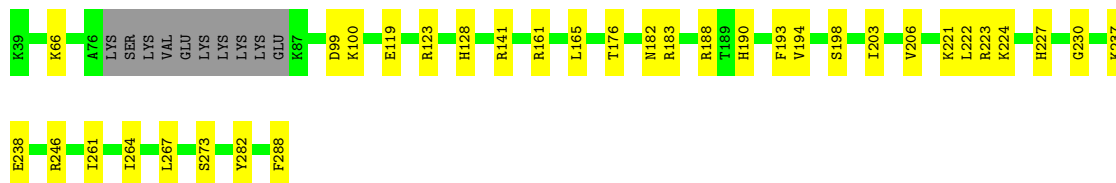
• Molecule 12: Large ribosomal subunit protein uL18

Chain LD: 83% 17%



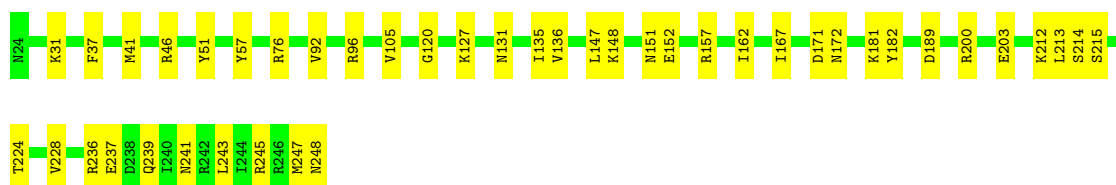
- Molecule 13: Large ribosomal subunit protein eL6

Chain LE:  82% 14%



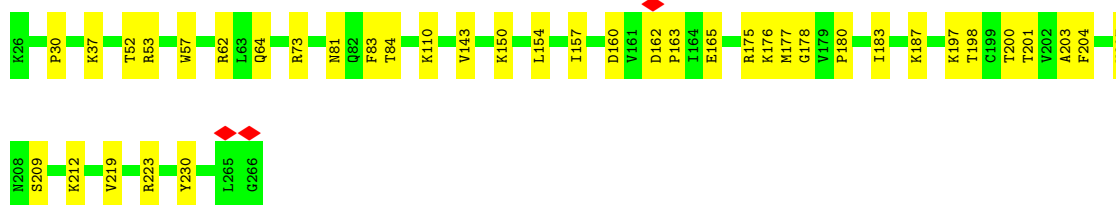
- Molecule 14: 60S ribosomal protein L7

Chain LF:  81% 19%



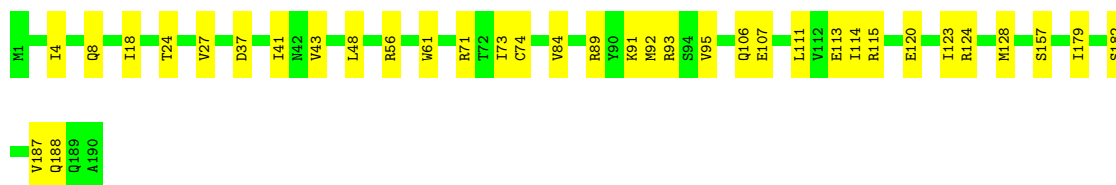
- Molecule 15: 60S ribosomal protein L7a

Chain LG:  84% 16%



- Molecule 16: 60S ribosomal protein L9

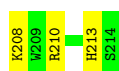
Chain LH:  82% 18%



- Molecule 17: Ribosomal protein uL16-like

Chain LI:  83% 17%





- Molecule 18: 60S ribosomal protein L11

Chain LJ: 78% 19%



- Molecule 19: Large ribosomal subunit protein eL13

Chain LL: 86% 14%



- Molecule 20: 60S ribosomal protein L14

Chain LM: 81% 19%



- Molecule 21: 60S ribosomal protein L15

Chain LN: 86% 14%



- Molecule 22: 60S ribosomal protein L13a

Chain LO: 80% 20%

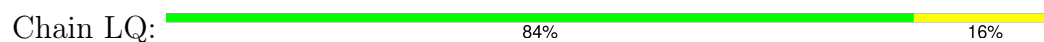


- Molecule 23: 60S ribosomal protein L17

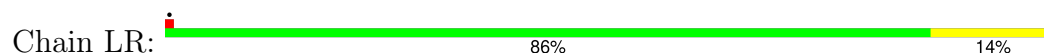
Chain LP: 82% 18%



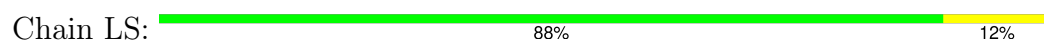
- Molecule 24: 60S ribosomal protein L18



- Molecule 25: 60S ribosomal protein L19



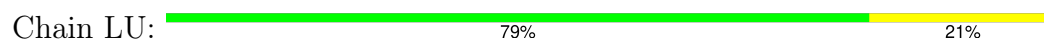
- Molecule 26: 60S ribosomal protein L18a



- Molecule 27: 60S ribosomal protein L21



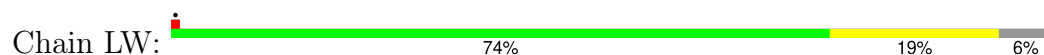
- Molecule 28: Heparin-binding protein HBp15

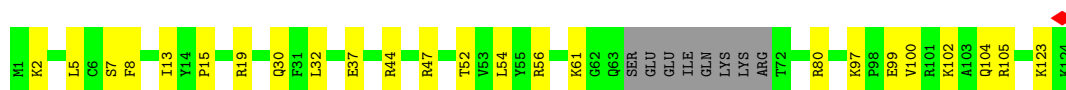


- Molecule 29: 60S ribosomal protein L23



- Molecule 30: Ribosomal protein L24





- Molecule 31: 60S ribosomal protein L23a

Chain LX: 88% 12%



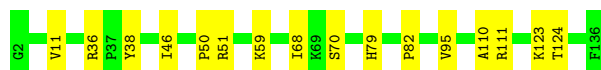
- Molecule 32: 60S ribosomal protein L26

Chain LY: 83% 17%



- Molecule 33: 60S ribosomal protein L27

Chain LZ: 88% 12%



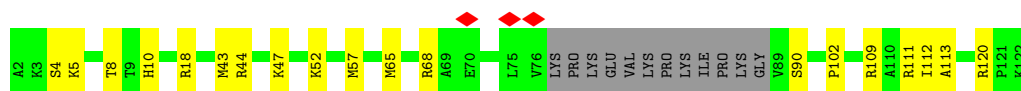
- Molecule 34: 60S ribosomal protein L27a

Chain La: 93% 7%



- Molecule 35: Large ribosomal subunit protein eL29

Chain Lb: 74% 16% 10%



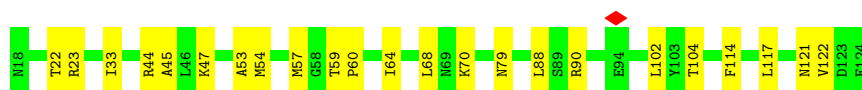
- Molecule 36: 60S ribosomal protein L30

Chain Lc: 80% 20%

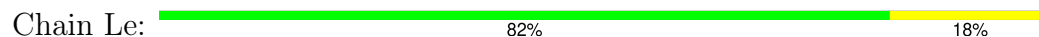


- Molecule 37: 60S ribosomal protein L31

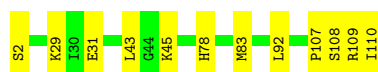
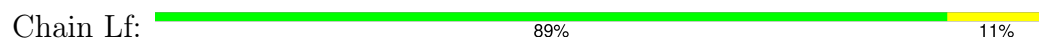
Chain Ld: 79% 21%



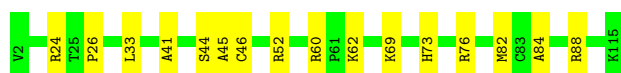
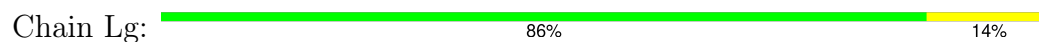
- Molecule 38: 60S ribosomal protein L32



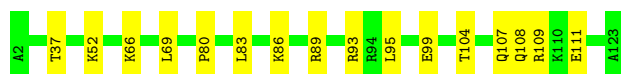
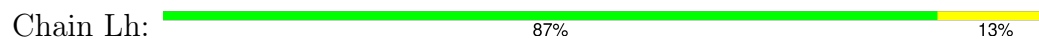
- Molecule 39: 60S ribosomal protein L35a



- Molecule 40: 60S ribosomal protein L34



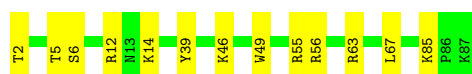
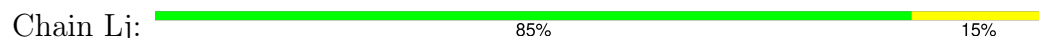
- Molecule 41: 60S ribosomal protein L35



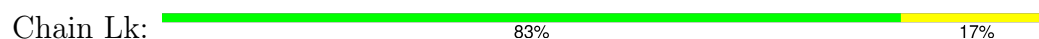
- Molecule 42: 60S ribosomal protein L36



- Molecule 43: 60S ribosomal protein L37



- Molecule 44: 60S ribosomal protein L38





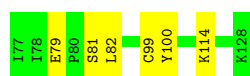
- Molecule 45: 60S ribosomal protein L39

Chain Ll: 86% 14%



- Molecule 46: Large ribosomal subunit protein eL40

Chain Lm: 88% 12%



- Molecule 47: 60S ribosomal protein L41

Chain Ln: 79% 21%



- Molecule 48: 60S ribosomal protein L36a

Chain Lo: 86% 14%



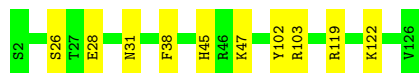
- Molecule 49: 60S ribosomal protein L37a

Chain Lp: 93% 7%



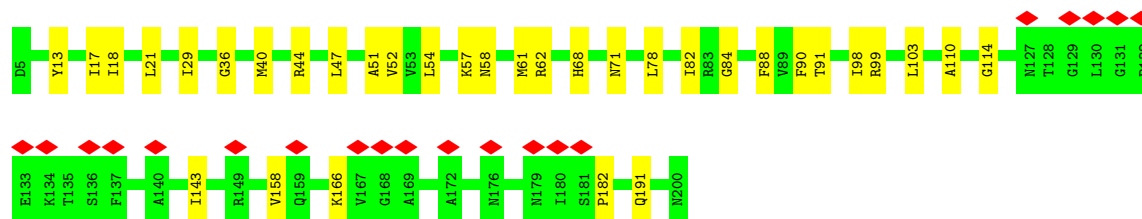
- Molecule 50: 60S ribosomal protein L28

Chain Lr: 92% 8%

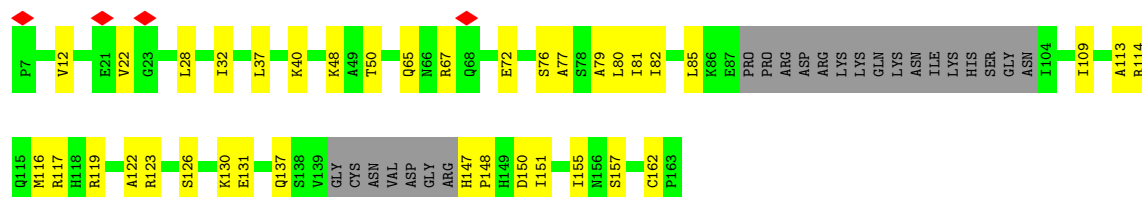


- Molecule 51: 60S acidic ribosomal protein P0

Chain Ls: 10% 83% 17%



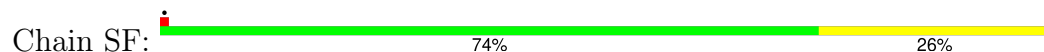
- Molecule 52: Large ribosomal subunit protein uL11



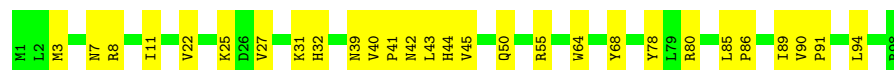
- Molecule 53: Small ribosomal subunit protein uS3



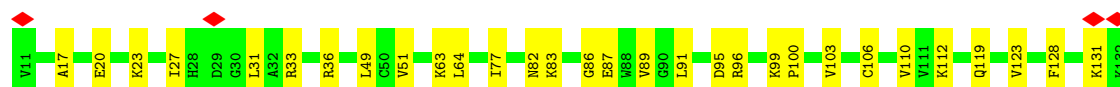
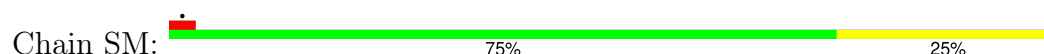
- Molecule 54: 40S ribosomal protein S5



- Molecule 55: 40S ribosomal protein S10



- Molecule 56: Small ribosomal subunit protein eS12



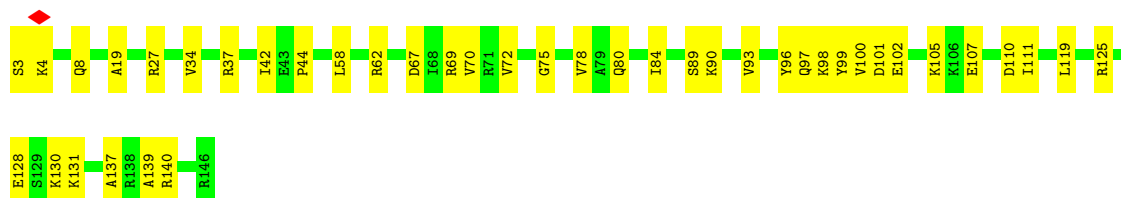
- Molecule 57: Small ribosomal subunit protein uS19

Chain SP:  79% 21%



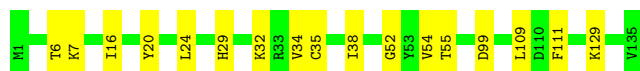
- Molecule 58: Small ribosomal subunit protein uS9

Chain SQ:  72% 28%



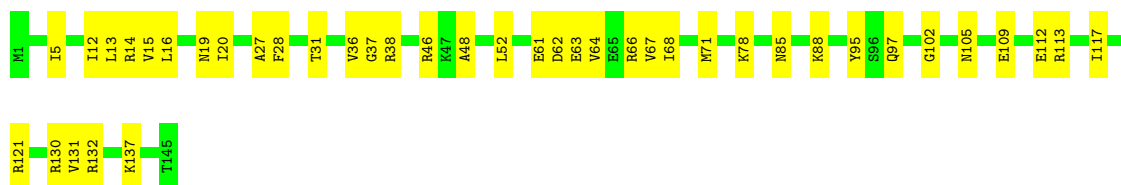
- Molecule 59: Small ribosomal subunit protein eS17

Chain SR:  87% 13%



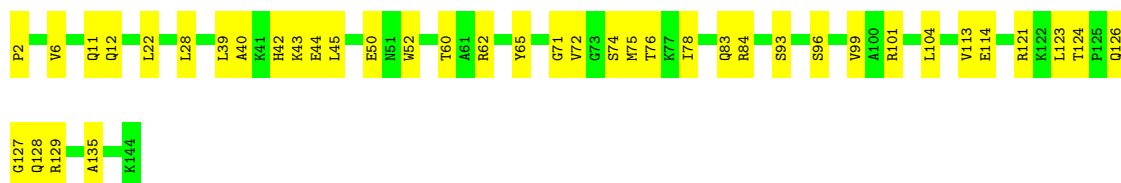
- Molecule 60: 40S ribosomal protein S18

Chain SS:  72% 28%



- Molecule 61: 40S ribosomal protein S19

Chain ST:  72% 28%



- Molecule 62: 40S ribosomal protein S20

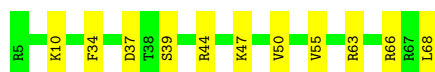
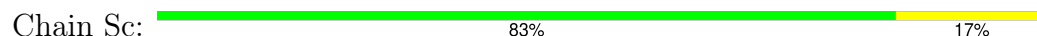
Chain SU:  73% 27%



- Molecule 63: Small ribosomal subunit protein eS25



- Molecule 64: 40S ribosomal protein S28



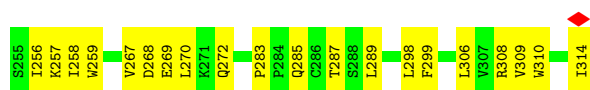
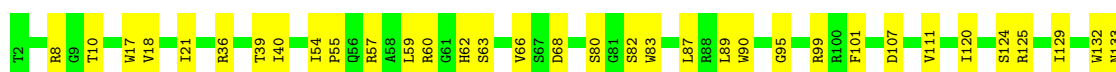
- Molecule 65: 40S ribosomal protein S29



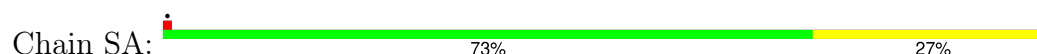
- Molecule 66: Ubiquitin-40S ribosomal protein S27a

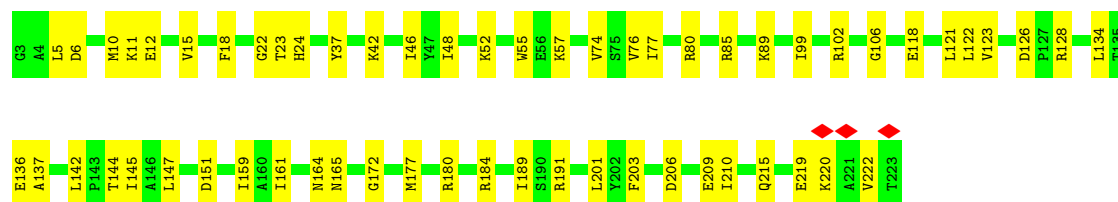


- Molecule 67: Receptor of activated protein C kinase 1



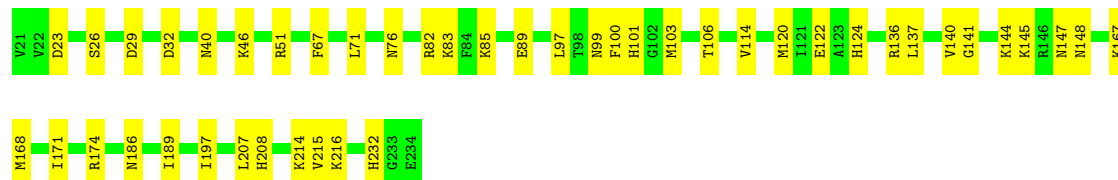
- Molecule 68: 40S ribosomal protein SA





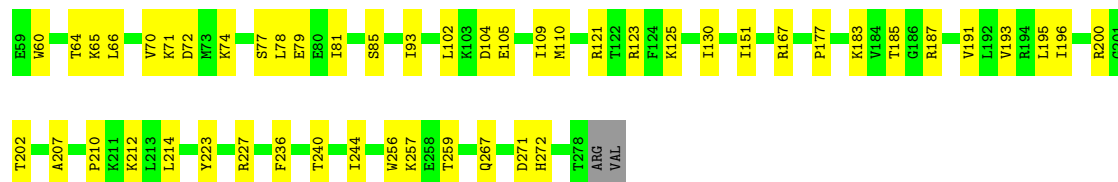
- Molecule 69: 40S ribosomal protein S3a

Chain SB: 79% 21%



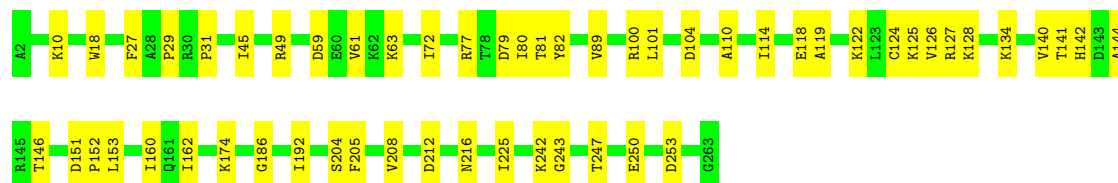
- Molecule 70: 40S ribosomal protein S2

Chain SC: 77% 23%



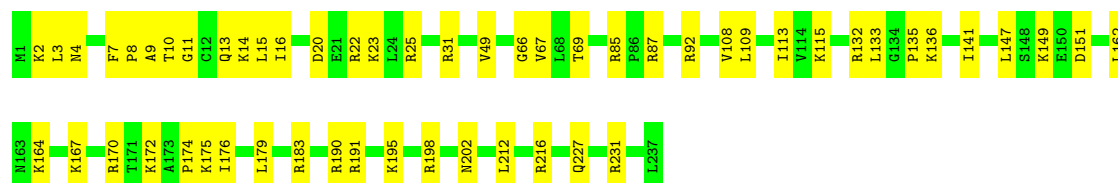
- Molecule 71: Small ribosomal subunit protein eS4, X isoform

Chain SE: 79% 21%



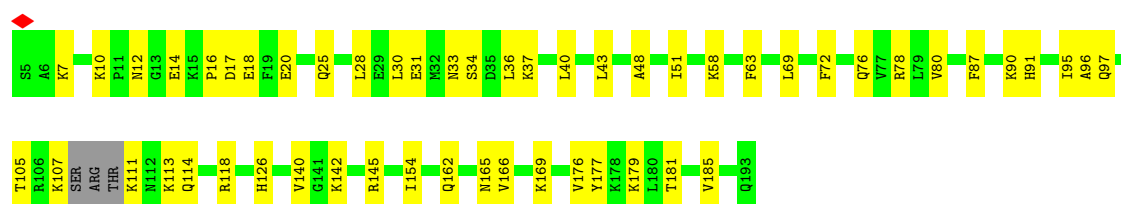
- Molecule 72: 40S ribosomal protein S6

Chain SG: 77% 23%



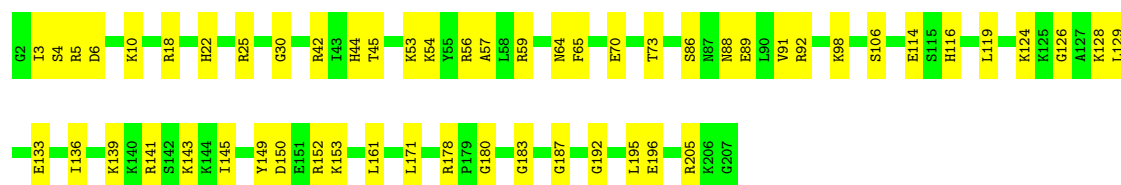
- Molecule 73: Small ribosomal subunit protein eS7

Chain SH:  70% 28%



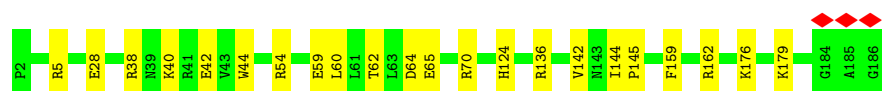
- Molecule 74: 40S ribosomal protein S8

Chain SI:  73% 27%



- Molecule 75: 40S ribosomal protein S9

Chain SJ:  88% 12%



- Molecule 76: 40S ribosomal protein S11

Chain SL:  86% 14%



- Molecule 77: 40S ribosomal protein S13

Chain SN:  87% 13%



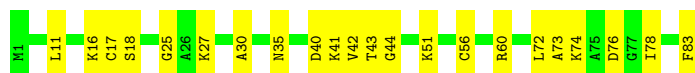
- Molecule 78: Small ribosomal subunit protein uS11

Chain SO:  81% 17%



- Molecule 79: Small ribosomal subunit protein eS21

Chain SV:  73% 27%



- Molecule 80: 40S ribosomal protein S15a

Chain SW:  81% 19%



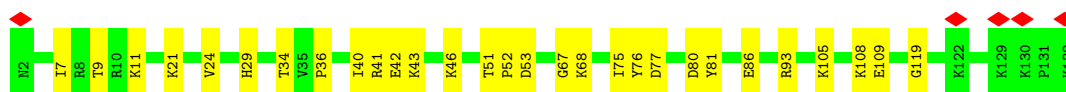
- Molecule 81: 40S ribosomal protein S23

Chain SX:  79% 21%



- Molecule 82: 40S ribosomal protein S24

Chain SY:  78% 22%



- Molecule 83: 40S ribosomal protein S26

Chain Sa:  83% 17%



- Molecule 84: Small ribosomal subunit protein eS27

Chain Sb:  76% 24%



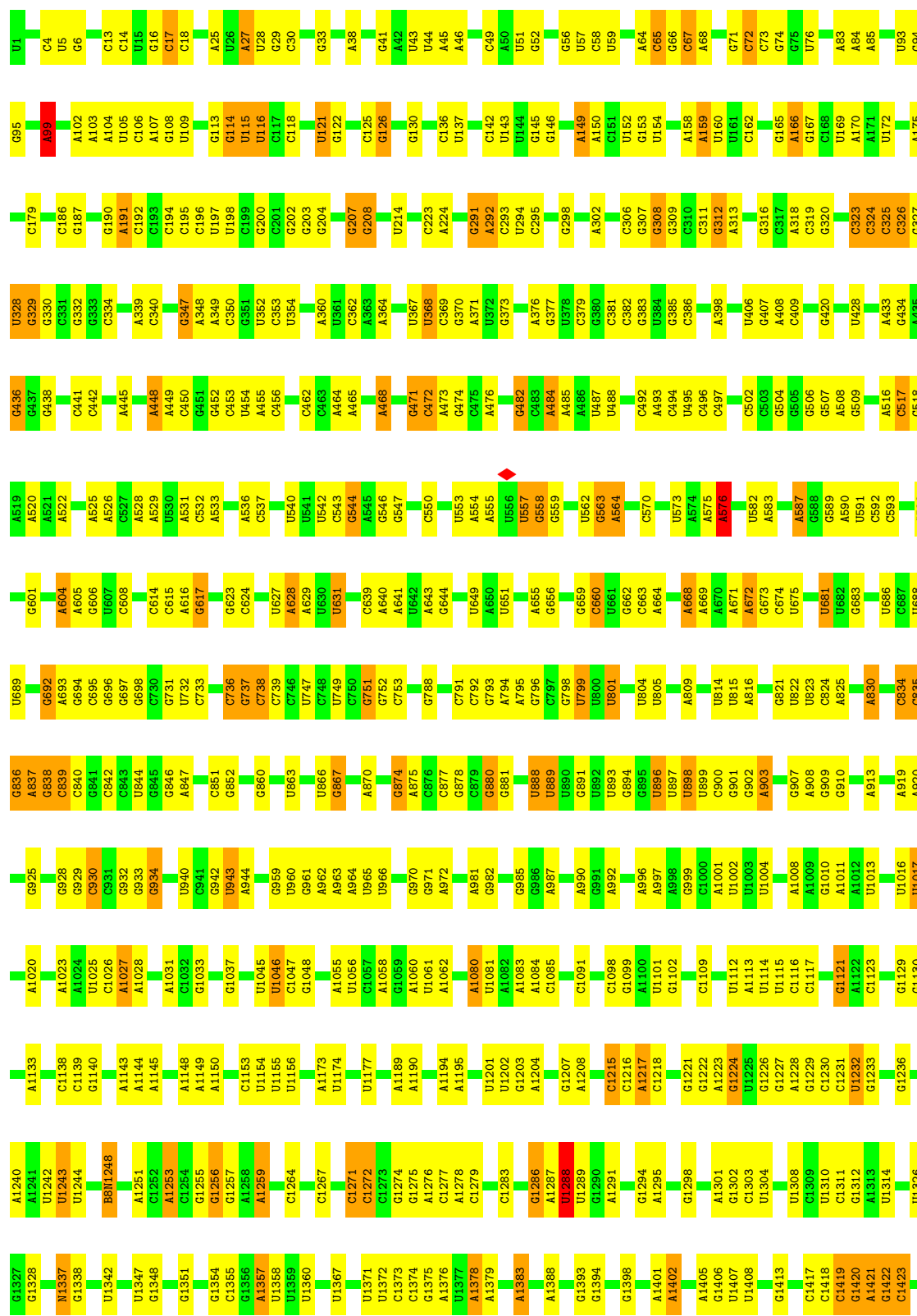
- Molecule 85: Small ribosomal subunit protein eS30

Chain Se:  81% 19%



- Molecule 86: 18S rRNA

Chain S2:



	C1433	G1540	U1621	U1694	A1801
	C1434	G1541	U1622	A1695	C1802
	C1435	G1542	A1623	C1698	U1810
	C1436	U1543		A1699	
	C1437	U1544	C1628	C1705	G1814
	A1438	A1545	A1629	G1706	
	A1439	G1546	A1630		A1825
			U1631		G1826
	U1442		G1632		
	A1446	U1550	A1634		G1829
	G1447	G1551			U1830
	U1448	G1552	A1637		A1831
	G1449	C1553	G1638		A1832
			A1639		
	A1452	A1556			A1835
	C1453	C1557	U1643		U1838
	A1454	C1558	C1644		U1839
		U1560	C1645		U1840
	U1463	A1561			A1845
		G1562	G1648		G1846
	U1477	G1563	U1649		
	U1478		A1650		G1849
	G1479	G1566	A1651		A1850
	A1480	G1567	G1652		A1851
	G1481	C1568	U1653		
	C1482	A1569	G1654		G1740
			G1655		
	A1487	C1574	G1656		G1744
	C1488	G1575	G1657		A1745
	A1489		G1658		
	G1490	U1578	U1659		G1748
	G1491	A1579	C1660		
	U1492	A1580	A1661		C1752
	C1493	C1581	U1662		C1753
	U1494	C1582	A1663		G1754
	G1495		A1664		C1755
	U1496		G1665		G1756
	G1497	U1587	C1666		G1757
	A1498	A1588	U1667		G1758
	U1499	A1589	G1668		G1759
	G1500		U1669		G1760
		C1593	C1670		U1761
	C1512	A1594	G1671		
	C1513	U1595	U1672		C1772
	G1514	U1596	U1673		C1773
		G1597			C1774
	C1518	G1598			U1775
	U1519	U1599	U1676		G1776
	G1520	G1600			G1777
	C1521	A1601	A1679		C1778
		U1602	G1680		G1779
	G1528	G1603	U1681		G1780
		G1604	C1682		A1781
	A1531	G1605	C1683		G1782
	C1532	G1606	C1684		C1783
	A1533		U1685		G1784
		G1610	G1686		G1785
					U1786
	G1536	A1619	U1692		
	A1537	A1620	G1693		U1797
					C1798

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281431	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.368	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0156	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	CI	0.16	0/247	0.30	0/323
2	Pt	0.17	0/1761	0.25	0/2741
3	Et	0.15	0/1778	0.31	0/2767
4	CF	0.14	0/3442	0.38	0/4656
5	AT	0.11	0/1805	0.23	0/2809
6	L5	0.29	0/85098	0.30	0/132762
7	L7	0.27	0/2861	0.25	0/4459
8	L8	0.28	0/3631	0.28	0/5657
9	LA	0.29	0/1936	0.42	0/2596
10	LB	0.26	0/3306	0.40	0/4424
11	LC	0.27	0/2981	0.37	0/4002
12	LD	0.22	0/2428	0.33	0/3252
13	LE	0.22	0/1973	0.40	0/2645
14	LF	0.26	0/1905	0.33	0/2539
15	LG	0.23	0/1960	0.38	0/2637
16	LH	0.23	0/1537	0.36	0/2066
17	LI	0.24	0/1751	0.35	0/2340
18	LJ	0.20	0/1385	0.40	0/1852
19	LL	0.23	0/1732	0.31	0/2315
20	LM	0.26	0/1161	0.40	0/1554
21	LN	0.28	0/1746	0.34	0/2338
22	LO	0.27	0/1682	0.37	0/2250
23	LP	0.28	0/1268	0.41	0/1701
24	LQ	0.28	0/1537	0.37	0/2052
25	LR	0.24	0/1582	0.37	0/2091
26	LS	0.27	0/1493	0.36	0/2003
27	LT	0.24	0/1326	0.33	0/1770
28	LU	0.25	0/839	0.52	0/1126
29	LV	0.25	0/993	0.37	0/1332
30	LW	0.22	0/959	0.37	0/1270
31	LX	0.23	0/1002	0.36	0/1345

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LY	0.24	0/1132	0.36	0/1504
33	LZ	0.23	0/1130	0.37	0/1507
34	La	0.26	0/1191	0.32	0/1591
35	Lb	0.21	0/889	0.38	0/1175
36	Lc	0.25	0/774	0.38	0/1038
37	Ld	0.25	0/903	0.38	0/1216
38	Le	0.27	0/1071	0.33	0/1429
39	Lf	0.28	0/895	0.37	0/1198
40	Lg	0.25	0/916	0.33	0/1220
41	Lh	0.22	0/1023	0.33	0/1351
42	Li	0.21	0/843	0.30	0/1115
43	Lj	0.28	0/720	0.40	0/952
44	Lk	0.21	0/575	0.42	0/761
45	Ll	0.26	0/454	0.30	0/599
46	Lm	0.23	0/435	0.35	0/575
47	Ln	0.26	0/231	0.35	0/294
48	Lo	0.26	0/876	0.35	0/1156
49	Lp	0.25	0/718	0.34	0/953
50	Lr	0.25	0/1017	0.33	0/1364
51	Ls	0.13	0/1519	0.34	0/2052
52	Lt	0.16	0/1009	0.48	0/1363
53	SD	0.15	0/1793	0.30	0/2414
54	SF	0.18	0/1516	0.37	0/2037
55	SK	0.18	0/851	0.46	0/1147
56	SM	0.14	0/950	0.39	0/1275
57	SP	0.17	0/1003	0.39	0/1342
58	SQ	0.18	0/1160	0.40	0/1553
59	SR	0.19	0/1105	0.47	0/1484
60	SS	0.18	0/1216	0.38	0/1628
61	ST	0.17	0/1131	0.38	0/1515
62	SU	0.19	0/831	0.49	0/1115
63	SZ	0.19	0/604	0.46	0/810
64	Sc	0.19	0/508	0.39	0/680
65	Sd	0.18	0/470	0.32	0/623
66	Sf	0.15	0/560	0.46	0/745
67	Sg	0.15	0/2493	0.39	0/3394
68	SA	0.19	0/1778	0.37	0/2416
69	SB	0.19	0/1765	0.38	0/2362
70	SC	0.21	0/1744	0.36	0/2357
71	SE	0.18	0/2118	0.36	0/2849
72	SG	0.16	0/1946	0.36	0/2590
73	SH	0.18	0/1519	0.42	0/2033
74	SI	0.21	0/1715	0.37	0/2287

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SJ	0.17	0/1550	0.32	0/2069
76	SL	0.21	0/1268	0.31	0/1696
77	SN	0.19	0/1232	0.27	0/1656
78	SO	0.23	0/1037	0.41	0/1391
79	SV	0.20	0/643	0.38	0/860
80	SW	0.23	0/1051	0.35	0/1406
81	SX	0.20	0/1116	0.37	0/1490
82	SY	0.18	0/1083	0.42	0/1438
83	Sa	0.22	0/836	0.35	0/1121
84	Sb	0.20	0/665	0.37	0/891
85	Se	0.16	0/465	0.38	0/612
86	S2	0.24	0/39756	0.28	0/61939
All	All	0.25	0/236904	0.33	0/347312

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
58	SQ	0	1
78	SO	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
78	SO	137	SER	Peptide
58	SQ	107	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	12	0
2	Pt	1576	0	803	13	0
3	Et	1593	0	810	29	0
4	CF	3383	0	3431	73	0
5	AT	1616	0	824	31	0
6	L5	78445	0	39719	746	0
7	L7	2561	0	1295	15	0
8	L8	3315	0	1685	26	0
9	LA	1898	0	1993	40	0
10	LB	3238	0	3376	58	0
11	LC	2927	0	3104	32	0
12	LD	2382	0	2410	34	0
13	LE	1935	0	2096	27	0
14	LF	1870	0	1996	33	0
15	LG	1927	0	2074	28	0
16	LH	1518	0	1601	22	0
17	LI	1711	0	1749	25	0
18	LJ	1362	0	1399	22	0
19	LL	1701	0	1818	25	0
20	LM	1138	0	1204	20	0
21	LN	1701	0	1749	23	0
22	LO	1650	0	1794	32	0
23	LP	1242	0	1269	19	0
24	LQ	1513	0	1628	20	0
25	LR	1566	0	1729	21	0
26	LS	1453	0	1490	15	0
27	LT	1298	0	1366	18	0
28	LU	825	0	850	15	0
29	LV	979	0	1039	10	0
30	LW	945	0	1003	23	0
31	LX	985	0	1066	9	0
32	LY	1115	0	1205	16	0
33	LZ	1107	0	1182	12	0
34	La	1162	0	1213	10	0
35	Lb	876	0	948	19	0
36	Lc	764	0	804	12	0
37	Ld	888	0	930	14	0
38	Le	1053	0	1147	16	0
39	Lf	876	0	912	10	0
40	Lg	906	0	998	14	0
41	Lh	1015	0	1148	14	0
42	Li	832	0	917	7	0
43	Lj	705	0	737	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Lk	569	0	637	8	0
45	Ll	444	0	483	7	0
46	Lm	429	0	465	5	0
47	Ln	230	0	276	4	0
48	Lo	862	0	929	11	0
49	Lp	708	0	756	5	0
50	Lr	1002	0	1068	6	0
51	Ls	1496	0	1540	22	0
52	Lt	998	0	1032	27	0
53	SD	1765	0	1865	18	0
54	SF	1495	0	1549	40	0
55	SK	827	0	854	21	0
56	SM	940	0	965	18	0
57	SP	985	0	1031	15	0
58	SQ	1142	0	1213	28	0
59	SR	1090	0	1149	14	0
60	SS	1198	0	1261	28	0
61	ST	1112	0	1146	29	0
62	SU	821	0	883	21	0
63	SZ	598	0	656	17	0
64	Sc	506	0	536	11	0
65	Sd	459	0	452	16	0
66	Sf	548	0	551	17	0
67	Sg	2436	0	2393	57	0
68	SA	1741	0	1746	42	0
69	SB	1738	0	1809	31	0
70	SC	1707	0	1791	35	0
71	SE	2076	0	2177	37	0
72	SG	1923	0	2089	49	0
73	SH	1497	0	1590	39	0
74	SI	1686	0	1772	40	0
75	SJ	1525	0	1640	15	0
76	SL	1247	0	1323	14	0
77	SN	1208	0	1294	14	0
78	SO	1024	0	1050	17	0
79	SV	636	0	637	16	0
80	SW	1034	0	1080	19	0
81	SX	1098	0	1167	25	0
82	SY	1065	0	1142	21	0
83	Sa	821	0	870	13	0
84	Sb	651	0	672	15	0
85	Se	459	0	503	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	S2	36953	0	18679	427	0
87	L5	177	0	0	0	0
87	L7	3	0	0	0	0
87	L8	5	0	0	0	0
87	LA	1	0	0	0	0
87	LB	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lj	1	0	0	0	0
87	S2	26	0	0	0	0
87	SG	1	0	0	0	0
87	SS	1	0	0	0	0
88	L5	98	0	182	4	0
89	L5	80	0	152	4	0
89	L8	10	0	19	0	0
89	LN	10	0	19	1	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	224971	0	167887	2490	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 (2490) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:79:ARG:NH1	6:L5:2708:U:O2'	1.68	1.26
6:L5:1996:C:H42	6:L5:2000:G:N2	1.55	1.02
5:AT:51:U:H3	5:AT:65:G:H1	1.02	1.01
3:Et:26:A:H61	3:Et:44:G:H1	1.02	1.00
2:Pt:50:U:H3	2:Pt:64:G:H1	1.10	0.94
6:L5:1996:C:N4	6:L5:2000:G:H22	1.66	0.93
3:Et:26:A:N6	3:Et:44:G:H1	1.65	0.93
86:S2:1748:G:H1	86:S2:1786:U:H3	1.00	0.93
6:L5:3946:G:H1	6:L5:4067:U:H3	1.13	0.92
6:L5:1996:C:H42	6:L5:2000:G:H22	0.96	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:74:LYS:HA	28:LU:116:GLN:O	1.70	0.90
6:L5:2007:G:H21	6:L5:2012:A:H62	1.20	0.87
69:SB:103:MET:HG3	69:SB:215:VAL:HG12	1.56	0.87
66:Sf:126:CYS:SG	66:Sf:144:CYS:N	2.49	0.84
19:LL:64:VAL:HA	19:LL:67:HIS:HD2	1.39	0.84
6:L5:1100:U:H3	6:L5:1194:G:H1	1.27	0.83
86:S2:925:G:H1	86:S2:1017:U:H3	1.30	0.80
70:SC:210:PRO:HB3	70:SC:240:THR:HG21	1.63	0.79
86:S2:1776:G:N2	86:S2:1777:G:N7	2.31	0.79
30:LW:100:VAL:HG12	30:LW:104:GLN:HE22	1.47	0.79
6:L5:1095:A:H2	6:L5:1200:G:H1	1.24	0.77
69:SB:122:GLU:HG2	69:SB:140:VAL:HG12	1.67	0.77
6:L5:4910:G:H4'	10:LB:95:THR:HG22	1.67	0.76
6:L5:5024:C:H41	6:L5:5028:G:H21	1.31	0.75
58:SQ:72:VAL:HG11	58:SQ:80:GLN:HG3	1.68	0.75
70:SC:193:VAL:HG11	70:SC:240:THR:HG22	1.69	0.75
6:L5:3701:OMC:H5	6:L5:3748:A:H62	1.35	0.74
54:SF:134:VAL:HG12	54:SF:135:ARG:HG2	1.68	0.74
23:LP:109:VAL:HA	23:LP:112:LEU:HD13	1.70	0.73
6:L5:2611:A:H5'	6:L5:2688:G:H4'	1.71	0.73
86:S2:94:G:HO2'	86:S2:508:A:HO2'	1.36	0.72
6:L5:1702:C:H4'	11:LC:308:LYS:HD2	1.72	0.72
37:Ld:90:ARG:HD3	37:Ld:102:LEU:HD13	1.72	0.72
4:CF:343:GLN:HE21	4:CF:437:VAL:HG22	1.54	0.72
73:SH:154:ILE:HB	73:SH:185:VAL:HG22	1.71	0.72
67:Sg:247:TRP:HB3	67:Sg:258:ILE:HD11	1.70	0.72
6:L5:497:G:H1	6:L5:657:C:H42	1.38	0.71
6:L5:1982:G:H5'	52:Lt:28:LEU:HD13	1.71	0.71
72:SG:2:LYS:HB2	72:SG:108:VAL:HG12	1.71	0.71
20:LM:15:VAL:HG22	20:LM:50:MET:HE1	1.72	0.71
4:CF:194:SER:HB3	4:CF:199:ASP:HB2	1.72	0.71
6:L5:3594:C:O2	6:L5:3597:G:N2	2.24	0.71
61:ST:12:GLN:NE2	86:S2:1593:C:O2	2.23	0.71
6:L5:4546:A:N7	9:LA:215:ASN:ND2	2.39	0.70
73:SH:105:THR:HG23	73:SH:107:LYS:H	1.56	0.70
6:L5:664:G:N2	6:L5:666:G:O6	2.25	0.70
3:Et:9:A:H2'	3:Et:11:C:H41	1.56	0.70
6:L5:387:G:HO2'	6:L5:412:G:H1	1.39	0.70
9:LA:104:VAL:HA	9:LA:107:MET:HE3	1.73	0.70
71:SE:208:VAL:HG11	71:SE:225:ILE:HG13	1.73	0.70
4:CF:378:LYS:HE2	4:CF:391:PRO:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Et:32:C:OP1	54:SF:135:ARG:NH2	2.25	0.70
80:SW:2:VAL:N	86:S2:1091:C:HO2'	1.90	0.70
6:L5:2484:A:H62	6:L5:2494:U:H3	1.41	0.69
6:L5:2092:G:O2'	6:L5:2262:G:N2	2.26	0.69
6:L5:2351:OMC:HM22	11:LC:95:MET:HG3	1.74	0.69
6:L5:3954:A:H1'	6:L5:4058:U:H5'	1.75	0.69
86:S2:1658:G:OP2	86:S2:1660:C:N4	2.25	0.69
6:L5:184:U:O2	6:L5:253:G:N2	2.23	0.69
6:L5:2702:C:OP1	28:LU:101:ARG:NH2	2.24	0.69
6:L5:4946:U:HO2'	39:Lf:2:SER:N	1.90	0.69
52:Lt:65:GLN:HG3	52:Lt:67:ARG:H	1.57	0.69
56:SM:51:VAL:HG12	56:SM:77:ILE:HB	1.74	0.69
6:L5:3937:C:H1'	21:LN:125:SER:HB3	1.74	0.69
6:L5:4242:U:H3	6:L5:4281:A:H2	1.38	0.68
66:Sf:99:LYS:NZ	86:S2:1287:A:OP1	2.25	0.68
30:LW:80:ARG:NH2	72:SG:8:PRO:O	2.26	0.68
6:L5:748:G:O6	26:LS:98:ARG:NH2	2.26	0.68
53:SD:106:ARG:HG3	53:SD:175:VAL:HG22	1.75	0.68
4:CF:7:HIS:HA	4:CF:86:TYR:O	1.94	0.68
6:L5:1995:G:O2'	52:Lt:122:ALA:O	2.11	0.68
17:LI:205:PRO:HD2	17:LI:208:LYS:HE2	1.76	0.68
5:AT:61:A:OP1	5:AT:63:C:N4	2.26	0.68
6:L5:2007:G:N2	6:L5:2012:A:H62	1.91	0.68
72:SG:183:ARG:NH2	86:S2:316:G:OP2	2.26	0.68
84:Sb:14:GLU:HA	84:Sb:17:ARG:HG2	1.76	0.68
9:LA:107:MET:HB3	9:LA:111:THR:HG21	1.73	0.68
70:SC:187:ARG:NH2	86:S2:1143:A:OP2	2.27	0.67
88:L5:5290:SPM:H112	22:LO:91:LYS:HD3	1.75	0.67
61:ST:124:THR:HG23	61:ST:127:GLY:H	1.60	0.67
6:L5:1669:A:OP1	35:Lb:18:ARG:NH2	2.28	0.67
21:LN:157:LYS:O	21:LN:162:ARG:NH1	2.27	0.67
22:LO:34:VAL:HG22	22:LO:103:LYS:HB2	1.77	0.67
6:L5:665:C:H4'	6:L5:666:G:H5'	1.75	0.67
86:S2:940:U:H3	86:S2:1002:U:H3	1.40	0.67
30:LW:56:ARG:HE	30:LW:61:LYS:HB2	1.59	0.67
3:Et:26:A:N1	3:Et:44:G:N2	2.42	0.67
54:SF:124:ASP:OD1	54:SF:125:SER:N	2.25	0.67
80:SW:71:LYS:NZ	86:S2:1156:U:OP1	2.28	0.67
67:Sg:87:LEU:HB2	67:Sg:101:PHE:HB2	1.77	0.67
6:L5:2458:C:H5''	21:LN:67:ARG:HD2	1.77	0.67
9:LA:29:LEU:O	9:LA:123:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:1414:C:H2'	6:L5:1415:G:H8	1.60	0.66
10:LB:90:VAL:HG23	10:LB:163:ILE:HD11	1.77	0.66
78:SO:104:ARG:NH2	86:S2:959:G:OP1	2.27	0.66
6:L5:2554:U:O2	6:L5:2764:A:N7	2.28	0.66
25:LR:172:ARG:NH1	86:S2:909:G:OP1	2.28	0.66
80:SW:107:SER:HB2	86:S2:860:G:H21	1.59	0.66
5:AT:15:G:N2	5:AT:49:C:C2	2.63	0.66
16:LH:106:GLN:HB2	16:LH:111:LEU:HB3	1.78	0.66
86:S2:747:U:N3	86:S2:796:G:N1	2.44	0.66
55:SK:50:GLN:HE22	86:S2:1276:A:H1'	1.60	0.66
72:SG:132:ARG:NH2	86:S2:152:U:O4'	2.28	0.66
10:LB:222:VAL:O	10:LB:343:ARG:NH1	2.29	0.66
85:Se:41:ARG:NH2	86:S2:639:C:OP1	2.29	0.66
84:Sb:34:ASP:O	84:Sb:79:PHE:HA	1.95	0.66
1:CI:79:ARG:NH1	6:L5:2708:U:HO2'	1.93	0.66
29:LV:35:LYS:HB2	29:LV:67:LYS:HG3	1.76	0.66
60:SS:85:ASN:OD1	60:SS:97:GLN:NE2	2.28	0.66
6:L5:2520:C:O2	6:L5:2640:G:N2	2.28	0.66
44:Lk:8:ILE:HD11	44:Lk:56:LEU:HD13	1.77	0.66
86:S2:533:A:H61	86:S2:550:C:H42	1.44	0.65
8:L8:75:OMG:OP2	32:LY:74:TYR:OH	2.15	0.65
34:La:84:GLU:OE1	34:La:87:ARG:NH2	2.30	0.65
52:Lt:151:ILE:O	52:Lt:155:ILE:HB	1.97	0.65
6:L5:1095:A:N1	6:L5:1200:G:O6	2.29	0.65
72:SG:7:PHE:HD2	72:SG:10:THR:HG22	1.62	0.65
6:L5:4525:C:OP1	10:LB:246:ARG:NH2	2.28	0.65
6:L5:4910:G:N2	22:LO:106:ASP:O	2.30	0.65
51:Ls:58:ASN:ND2	51:Ls:84:GLY:O	2.24	0.65
54:SF:168:THR:OG1	54:SF:171:GLU:OE1	2.15	0.65
72:SG:135:PRO:HG2	72:SG:141:ILE:HG22	1.78	0.65
4:CF:72:THR:HB	4:CF:93:PRO:HA	1.79	0.65
86:S2:1536:G:H2'	86:S2:1537:A:H8	1.62	0.65
4:CF:353:ILE:HB	4:CF:394:LEU:HB2	1.78	0.64
26:LS:76:LYS:NZ	26:LS:100:LEU:O	2.31	0.64
10:LB:10:ARG:NH1	10:LB:11:HIS:O	2.30	0.64
52:Lt:130:LYS:NZ	52:Lt:157:SER:O	2.30	0.64
86:S2:751:G:H1'	86:S2:793:G:H21	1.61	0.64
1:CI:78:HIS:NE2	6:L5:2706:G:N7	2.44	0.64
86:S2:628:A:N6	86:S2:1500:G:O2'	2.30	0.64
6:L5:68:U:OP1	21:LN:178:HIS:ND1	2.31	0.64
44:Lk:54:GLU:OE2	44:Lk:58:GLN:NE2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4281:A:H2'	6:L5:4282:A:H2'	1.79	0.64
23:LP:39:MET:HG2	23:LP:43:LYS:HD3	1.79	0.64
73:SH:114:GLN:HE22	86:S2:874:G:H21	1.45	0.64
27:LT:43:LYS:O	27:LT:58:HIS:ND1	2.31	0.64
68:SA:89:LYS:HD2	68:SA:201:LEU:HG	1.79	0.64
6:L5:2601:A:N6	6:L5:2744:A:OP2	2.28	0.64
86:S2:928:G:H2'	86:S2:929:G:C8	2.32	0.64
6:L5:1994:C:H2'	6:L5:1995:G:C8	2.33	0.64
6:L5:3641:U:OP2	6:L5:3646:A:N6	2.31	0.64
50:Lr:26:SER:OG	50:Lr:28:GLU:OE1	2.15	0.64
53:SD:142:LEU:HD13	53:SD:150:MET:HE2	1.80	0.64
74:SI:98:LYS:HB3	86:S2:377:G:H5'	1.80	0.64
4:CF:201:MET:HG3	4:CF:228:LEU:HD12	1.78	0.63
6:L5:1704:C:O3'	14:LF:46:ARG:NH1	2.31	0.63
28:LU:65:ARG:HG2	28:LU:67:LYS:H	1.63	0.63
62:SU:51:LYS:HB3	62:SU:90:ASP:HB2	1.80	0.63
4:CF:430:ARG:HH12	5:AT:65:G:H4'	1.63	0.63
58:SQ:19:ALA:HB2	58:SQ:75:GLY:HA3	1.81	0.63
75:SJ:162:ARG:NH1	86:S2:582:U:OP1	2.30	0.63
72:SG:22:ARG:HG3	72:SG:25:ARG:HH12	1.64	0.63
86:S2:1829:G:H1'	86:S2:1850:MA6:H2	1.79	0.63
6:L5:1982:G:N2	6:L5:2009:A:O2'	2.32	0.63
6:L5:2495:U:H2'	6:L5:2496:G:H8	1.64	0.63
52:Lt:117:ARG:HE	52:Lt:119:ARG:H	1.45	0.63
71:SE:45:ILE:HG13	71:SE:61:VAL:HG11	1.79	0.63
71:SE:153:LEU:O	71:SE:174:LYS:NZ	2.31	0.63
16:LH:106:GLN:NE2	16:LH:113:GLU:OE2	2.31	0.63
6:L5:3946:G:N2	6:L5:4067:U:O2	2.32	0.63
6:L5:170:C:H42	6:L5:266:C:H42	1.47	0.63
6:L5:4431:PSU:OP2	17:LI:3:ARG:NH2	2.28	0.62
35:Lb:109:ARG:HA	35:Lb:112:ILE:HG12	1.81	0.62
71:SE:79:ASP:HB3	71:SE:82:TYR:HB2	1.81	0.62
6:L5:4092:G:N7	6:L5:4114:C:N4	2.45	0.62
9:LA:137:ILE:HD11	9:LA:149:LYS:HB2	1.82	0.62
67:Sg:252:THR:HG21	67:Sg:257:LYS:HD2	1.81	0.62
6:L5:1100:U:O3'	6:L5:1167:C:N4	2.32	0.62
18:LJ:146:ARG:HG2	18:LJ:147:ARG:HG3	1.81	0.62
6:L5:327:U:O2'	42:Li:30:ARG:NH1	2.32	0.62
6:L5:4987:C:OP2	10:LB:116:ARG:NH2	2.32	0.62
44:Lk:26:LYS:HB2	44:Lk:69:LEU:HD12	1.81	0.62
53:SD:40:ARG:NH2	62:SU:106:ILE:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SU:80:PHE:HB3	65:Sd:52:PHE:HB3	1.81	0.62
86:S2:587:A:H5'	86:S2:592:C:H41	1.64	0.62
5:AT:16:C:O2'	5:AT:19:G:OP1	2.17	0.62
6:L5:67:C:OP2	6:L5:312:G:N2	2.30	0.62
37:Ld:64:ILE:HG23	37:Ld:68:LEU:HD23	1.82	0.62
55:SK:85:LEU:HD21	55:SK:89:ILE:HB	1.80	0.62
71:SE:144:ALA:HB3	86:S2:121:OMU:HM23	1.80	0.62
6:L5:1499:C:OP1	24:LQ:150:ARG:NH2	2.33	0.62
15:LG:209:SER:HA	15:LG:212:LYS:HG3	1.82	0.62
81:SX:105:PHE:HD1	81:SX:121:LYS:HB3	1.65	0.62
86:S2:106:C:H2'	86:S2:107:A:H8	1.65	0.62
86:S2:1417:C:O2	86:S2:1422:G:O6	2.18	0.62
6:L5:2758:G:O2'	6:L5:2765:A:N3	2.30	0.62
6:L5:4992:G:H2'	6:L5:4993:G:C8	2.36	0.61
54:SF:127:ARG:HG2	54:SF:136:ARG:HE	1.64	0.61
68:SA:118:GLU:HG3	70:SC:65:LYS:HE2	1.82	0.61
18:LJ:141:ILE:HA	18:LJ:144:LYS:HD2	1.82	0.61
22:LO:180:GLN:NE2	22:LO:184:ASN:OD1	2.34	0.61
54:SF:34:SER:HA	64:Sc:55:VAL:HG23	1.81	0.61
58:SQ:58:LEU:HB3	58:SQ:62:ARG:HD2	1.82	0.61
74:SI:70:GLU:OE2	76:SL:21:LYS:NZ	2.32	0.61
86:S2:1536:G:H2'	86:S2:1537:A:C8	2.35	0.61
6:L5:3811:G:O2'	6:L5:3814:U:OP2	2.18	0.61
66:Sf:108:VAL:HG12	66:Sf:114:ILE:HA	1.81	0.61
17:LI:87:MET:HG2	17:LI:138:ILE:HG12	1.81	0.61
54:SF:84:GLY:O	86:S2:1673:U:O2'	2.16	0.61
63:SZ:99:LEU:HD21	63:SZ:102:LYS:HB2	1.82	0.61
4:CF:344:VAL:O	4:CF:399:ALA:HA	2.01	0.61
6:L5:2899:C:OP1	25:LR:108:ARG:NH2	2.31	0.61
51:Ls:17:ILE:HD12	51:Ls:54:LEU:HD21	1.82	0.61
86:S2:1422:G:H4'	86:S2:1423:C:H3'	1.82	0.61
6:L5:3796:U:HO2'	86:S2:1720:U:HO2'	1.47	0.61
66:Sf:144:CYS:HB2	66:Sf:146:LEU:HD23	1.82	0.61
76:SL:85:THR:HG21	86:S2:373:G:H4'	1.83	0.61
6:L5:2695:A:OP1	44:Lk:35:LYS:NZ	2.27	0.61
62:SU:70:CYS:SG	86:S2:1491:G:O2'	2.57	0.61
67:Sg:213:ASP:OD2	67:Sg:215:GLN:NE2	2.34	0.61
30:LW:80:ARG:HH22	86:S2:167:G:H4'	1.66	0.61
71:SE:29:PRO:HA	86:S2:496:C:H5'	1.83	0.61
6:L5:1802:A:N3	27:LT:130:ARG:NH2	2.48	0.61
6:L5:3688:U:OP2	9:LA:198:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SD:99:ILE:HG23	53:SD:173:ARG:HH21	1.63	0.61
59:SR:109:LEU:HD13	68:SA:52:LYS:HB2	1.83	0.61
6:L5:2557:G:H1	6:L5:2570:U:H3	1.48	0.60
6:L5:4088:C:OP1	9:LA:37:ARG:NH1	2.34	0.60
53:SD:8:LYS:HG2	62:SU:61:LEU:HD11	1.82	0.60
60:SS:27:ALA:HB2	60:SS:52:LEU:HD12	1.82	0.60
62:SU:26:SER:HB3	62:SU:110:VAL:HA	1.83	0.60
70:SC:200:ARG:O	75:SJ:54:ARG:NH2	2.30	0.60
6:L5:4472:G:O2'	46:Lm:100:TYR:O	2.20	0.60
9:LA:114:CYS:HB3	9:LA:165:VAL:HB	1.84	0.60
21:LN:155:VAL:O	21:LN:162:ARG:NH2	2.33	0.60
86:S2:1228:A:H2'	86:S2:1229:G:C8	2.36	0.60
76:SL:35:ARG:NH2	76:SL:55:TYR:O	2.35	0.60
76:SL:133:PRO:HG2	86:S2:383:G:H21	1.66	0.60
4:CF:93:PRO:HD2	4:CF:102:MET:HB3	1.84	0.60
6:L5:500:G:N2	6:L5:504:G:O2'	2.28	0.60
6:L5:2658:G:N2	6:L5:2676:A:OP2	2.33	0.60
10:LB:107:ALA:HB2	10:LB:201:LEU:HD22	1.82	0.60
56:SM:91:LEU:HD12	56:SM:106:CYS:HB2	1.82	0.60
57:SP:48:GLY:O	57:SP:50:ARG:NH1	2.35	0.60
65:Sd:54:LYS:NZ	86:S2:1482:C:OP1	2.35	0.60
71:SE:49:ARG:NH2	86:S2:496:C:OP1	2.32	0.60
73:SH:177:TYR:O	73:SH:181:THR:HB	2.02	0.60
6:L5:4618:OMG:H5'	29:LV:15:ARG:HB2	1.83	0.60
75:SJ:40:LYS:NZ	86:S2:641:A:OP1	2.32	0.60
54:SF:185:SER:H	54:SF:190:ILE:HD11	1.67	0.60
55:SK:25:LYS:NZ	86:S2:1497:G:N7	2.44	0.60
61:ST:22:LEU:HG	61:ST:28:LEU:HD21	1.82	0.60
82:SY:11:LYS:HB2	82:SY:24:VAL:HG12	1.84	0.60
82:SY:21:LYS:HE2	82:SY:75:ILE:HD11	1.83	0.60
86:S2:1550:G:H3'	86:S2:1579:A:H61	1.66	0.60
4:CF:163:SEP:O2P	4:CF:165:LYS:NZ	2.34	0.60
6:L5:4153:C:H5''	31:LX:38:LYS:HD2	1.83	0.60
25:LR:39:GLN:OE1	25:LR:42:ARG:NH1	2.34	0.60
6:L5:1175:A:H2	6:L5:1185:G:H22	1.49	0.60
6:L5:1366:G:H5''	19:LL:36:ARG:HH12	1.67	0.60
6:L5:2362:U:H2'	6:L5:2363:A2M:H8	1.83	0.60
74:SI:88:ASN:OD1	74:SI:205:ARG:NH2	2.34	0.60
81:SX:107:ARG:HG3	81:SX:110:HIS:HB3	1.83	0.60
86:S2:1277:C:H2'	86:S2:1278:A:H8	1.66	0.60
47:Ln:1:MET:HG3	86:S2:1706:G:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SS:130:ARG:NH2	86:S2:1230:C:OP1	2.35	0.60
63:SZ:58:LEU:HD12	63:SZ:62:VAL:HG21	1.84	0.60
70:SC:183:LYS:HA	70:SC:195:LEU:O	2.02	0.60
12:LD:223:PHE:HB3	12:LD:226:TYR:HB2	1.84	0.60
57:SP:130:ARG:HD3	57:SP:131:PRO:HD2	1.84	0.60
6:L5:500:G:OP1	6:L5:504:G:N2	2.35	0.59
6:L5:1503:A:H62	24:LQ:87:THR:HG21	1.66	0.59
72:SG:66:GLY:HA2	86:S2:1745:A:H1'	1.84	0.59
4:CF:246:LEU:O	4:CF:247:ARG:NH1	2.36	0.59
86:S2:838:G:H1	86:S2:840:C:HO2'	1.48	0.59
4:CF:178:ILE:HB	4:CF:183:TYR:HB2	1.84	0.59
53:SD:172:VAL:HG22	53:SD:185:LYS:HG2	1.85	0.59
86:S2:554:A:HO2'	86:S2:555:A:H8	1.48	0.59
86:S2:874:G:H2'	86:S2:875:A:H8	1.67	0.59
6:L5:4594:U:H2'	6:L5:4595:G:H8	1.67	0.59
68:SA:77:ILE:HG13	68:SA:99:ILE:HB	1.84	0.59
6:L5:659:G:H2'	6:L5:660:A:H8	1.67	0.59
6:L5:4107:G:N2	6:L5:4108:G:O6	2.33	0.59
4:CF:373:ALA:H	4:CF:404:MET:HA	1.68	0.59
6:L5:4097:G:O6	6:L5:4098:A:N6	2.36	0.59
20:LM:100:ARG:HA	20:LM:103:LYS:HG2	1.85	0.59
58:SQ:78:VAL:HG12	86:S2:1673:U:H5''	1.85	0.59
67:Sg:206:LEU:HD12	67:Sg:218:LEU:HD12	1.84	0.59
74:SI:150:ASP:HA	74:SI:153:LYS:HG2	1.84	0.59
82:SY:34:THR:O	86:S2:570:C:O2'	2.20	0.59
6:L5:1703:C:O2'	6:L5:1704:C:O4'	2.21	0.59
6:L5:3868:G:H22	6:L5:3900:G:H1'	1.66	0.59
6:L5:513:U:N3	6:L5:516:C:OP2	2.33	0.58
46:Lm:99:CYS:HB2	46:Lm:114:LYS:HE3	1.85	0.58
6:L5:1339:U:H2'	6:L5:1340:OMC:C6	2.38	0.58
6:L5:1996:C:O3'	51:Ls:44:ARG:NH1	2.35	0.58
6:L5:3717:A:H2'	6:L5:3718:A2M:H8	1.84	0.58
48:Lo:2:VAL:N	48:Lo:90:HIS:O	2.36	0.58
53:SD:32:ASP:OD1	53:SD:57:ASN:ND2	2.35	0.58
69:SB:99:ASN:OD1	69:SB:100:PHE:N	2.37	0.58
79:SV:51:LYS:NZ	79:SV:76:ASP:OD1	2.23	0.58
86:S2:640:A:H2'	86:S2:641:A:C8	2.39	0.58
12:LD:64:ILE:HD13	12:LD:109:LEU:HD22	1.85	0.58
63:SZ:80:ARG:O	86:S2:1598:G:O2'	2.18	0.58
6:L5:1739:G:N3	6:L5:1742:A:N6	2.51	0.58
6:L5:2017:A:O2'	6:L5:2018:C:H6	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:2460:A:OP2	89:LN:301:SPD:N10	2.36	0.58
12:LD:62:CYS:HB3	12:LD:105:LEU:HD22	1.84	0.58
30:LW:80:ARG:NH1	86:S2:167:G:O2'	2.36	0.58
44:Lk:27:LYS:O	44:Lk:70:LYS:NZ	2.35	0.58
76:SL:33:LEU:HD12	76:SL:34:PRO:HD2	1.85	0.58
6:L5:919:C:OP1	20:LM:69:HIS:ND1	2.22	0.58
6:L5:3736:A:H2'	6:L5:3737:A:C8	2.38	0.58
6:L5:4887:C:H42	6:L5:4932:U:H3	1.50	0.58
28:LU:44:GLN:HB2	28:LU:56:LEU:HD21	1.84	0.58
58:SQ:125:ARG:HB2	86:S2:1648:G:H5''	1.86	0.58
67:Sg:68:ASP:HB3	67:Sg:111:VAL:HG22	1.84	0.58
6:L5:2007:G:H21	6:L5:2012:A:N6	1.97	0.58
17:LI:85:PHE:HE2	17:LI:87:MET:HE2	1.67	0.58
32:LY:67:ILE:O	32:LY:84:ARG:NH2	2.36	0.58
56:SM:63:LYS:HD3	56:SM:64:LEU:HD22	1.85	0.58
70:SC:267:GLN:OE1	79:SV:35:ASN:ND2	2.36	0.58
73:SH:7:LYS:HD3	73:SH:10:LYS:HB3	1.84	0.58
6:L5:24:G:N7	43:Lj:46:LYS:NZ	2.50	0.58
6:L5:184:U:O2'	6:L5:189:G:O4'	2.22	0.58
6:L5:1396:G:N7	34:La:110:LYS:NZ	2.49	0.58
6:L5:2020:U:H2'	6:L5:2021:G:H8	1.68	0.58
46:Lm:79:GLU:OE2	46:Lm:81:SER:OG	2.19	0.58
55:SK:31:LYS:HZ3	55:SK:40:VAL:H	1.52	0.58
66:Sf:92:LYS:NZ	86:S2:1271:C:OP1	2.33	0.58
72:SG:176:ILE:HG12	72:SG:179:LEU:HD11	1.86	0.58
56:SM:36:ARG:NH1	86:S2:1310:U:OP1	2.36	0.58
58:SQ:100:VAL:HG22	58:SQ:101:ASP:H	1.68	0.58
78:SO:15:ILE:HG23	78:SO:16:SER:H	1.68	0.58
86:S2:165:G:OP2	86:S2:165:G:N2	2.29	0.58
6:L5:2093:A:N3	6:L5:2094:G:N1	2.51	0.58
6:L5:2468:U:O2'	6:L5:2506:G:N2	2.37	0.58
10:LB:165:HIS:HB3	10:LB:180:LEU:HD23	1.86	0.58
43:Lj:14:LYS:NZ	45:Li:51:LEU:OXT	2.37	0.58
6:L5:4076:G:OP1	15:LG:73:ARG:NE	2.36	0.58
12:LD:120:GLU:O	12:LD:248:ARG:NH1	2.36	0.58
73:SH:165:ASN:O	73:SH:169:LYS:NZ	2.31	0.58
74:SI:22:HIS:HB3	86:S2:433:A:H5''	1.84	0.58
6:L5:935:A:O2'	20:LM:44:GLN:O	2.22	0.57
13:LE:161:ARG:NH1	13:LE:273:SER:OG	2.37	0.57
55:SK:8:ARG:NH2	86:S2:1314:U:O2'	2.37	0.57
72:SG:133:LEU:HD12	86:S2:65:C:C4	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:1961:G:N2	6:L5:2024:G:O2'	2.37	0.57
8:L8:52:A:H5'	45:Ll:21:ARG:HD3	1.86	0.57
11:LC:298:ILE:HD13	24:LQ:131:PRO:HB3	1.85	0.57
6:L5:1094:G:O6	6:L5:1201:U:O2	2.22	0.57
6:L5:2017:A:O2'	6:L5:2018:C:O5'	2.19	0.57
10:LB:10:ARG:NH2	10:LB:265:SER:O	2.36	0.57
6:L5:4098:A:H2'	6:L5:4099:G:H4'	1.86	0.57
72:SG:11:GLY:HA2	86:S2:166:A2M:HM'1	1.86	0.57
6:L5:1992:U:H4'	6:L5:1993:C:H5''	1.86	0.57
6:L5:4873:G:N7	22:LO:179:LYS:NZ	2.49	0.57
67:Sg:107:ASP:HB2	67:Sg:125:ARG:HG3	1.87	0.57
73:SH:63:PHE:HA	73:SH:95:ILE:O	2.05	0.57
3:Et:33:U:OP1	54:SF:135:ARG:NH1	2.38	0.57
61:ST:126:GLN:HB2	61:ST:129:ARG:HH21	1.69	0.57
74:SI:106:SER:HB3	74:SI:171:LEU:HG	1.87	0.57
6:L5:2295:C:O2'	11:LC:45:ARG:NH2	2.38	0.57
10:LB:80:GLU:OE1	10:LB:323:TYR:OH	2.23	0.57
12:LD:41:LYS:NZ	27:LT:32:ARG:O	2.35	0.57
50:Lr:28:GLU:OE2	50:Lr:31:ASN:ND2	2.32	0.57
71:SE:100:ARG:HB2	71:SE:114:ILE:HD13	1.86	0.57
72:SG:92:ARG:O	86:S2:453:C:O2'	2.21	0.57
6:L5:62:A:N3	6:L5:77:U:O2'	2.33	0.57
6:L5:2516:G:O2'	40:Lg:62:LYS:NZ	2.38	0.57
8:L8:62:A:OP1	41:Lh:52:LYS:NZ	2.34	0.57
28:LU:28:PRO:HB2	28:LU:34:MET:HG3	1.87	0.57
67:Sg:63:SER:HB2	86:S2:1398:G:H1'	1.86	0.57
67:Sg:254:PRO:O	67:Sg:272:GLN:NE2	2.38	0.57
81:SX:68:LYS:HB3	81:SX:91:LEU:HD13	1.85	0.57
6:L5:4725:C:OP1	10:LB:103:LYS:NZ	2.37	0.57
21:LN:164:LEU:O	21:LN:169:ARG:NH2	2.37	0.57
51:Ls:68:HIS:O	51:Ls:71:ASN:ND2	2.38	0.57
58:SQ:67:ASP:OD2	58:SQ:69:ARG:NH1	2.38	0.57
58:SQ:80:GLN:O	58:SQ:84:ILE:HG13	2.05	0.57
86:S2:695:C:N4	86:S2:736:C:O2'	2.38	0.57
5:AT:51:U:O4	5:AT:65:G:O6	2.22	0.57
62:SU:85:HIS:ND1	86:S2:1447:G:OP1	2.37	0.57
86:S2:508:A:H3'	86:S2:509:OMG:H8	1.69	0.57
6:L5:966:A:OP2	6:L5:2092:G:N2	2.38	0.56
15:LG:180:PRO:HG3	15:LG:219:VAL:HG13	1.86	0.56
20:LM:71:LYS:O	20:LM:75:GLN:HG3	2.05	0.56
60:SS:5:ILE:N	63:SZ:50:PHE:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SH:12:ASN:ND2	73:SH:14:GLU:OE2	2.38	0.56
6:L5:267:G:OP1	41:Lh:109:ARG:NH2	2.37	0.56
6:L5:1281:G:N1	13:LE:128:HIS:HB2	2.20	0.56
6:L5:5002:U:OP2	10:LB:385:LYS:NZ	2.39	0.56
52:Lt:77:ALA:HB3	52:Lt:80:LEU:HB2	1.87	0.56
78:SO:135:ILE:O	86:S2:943:U:O2'	2.22	0.56
6:L5:1914:C:H4'	22:LO:89:PRO:HD3	1.86	0.56
6:L5:1942:A:H2'	6:L5:1943:A:C8	2.39	0.56
6:L5:2613:C:OP1	40:Lg:24:ARG:NH2	2.38	0.56
7:L7:6:C:O2'	12:LD:50:ARG:NH2	2.38	0.56
10:LB:17:LEU:O	10:LB:19:ARG:N	2.37	0.56
13:LE:165:LEU:HD11	13:LE:176:THR:HG22	1.87	0.56
25:LR:176:ARG:NH2	86:S2:910:G:OP1	2.38	0.56
55:SK:31:LYS:NZ	55:SK:40:VAL:H	2.04	0.56
66:Sf:97:LYS:NZ	86:S2:1289:U:OP2	2.36	0.56
78:SO:134:PRO:HB3	86:S2:944:A:H5''	1.87	0.56
86:S2:1228:A:H2'	86:S2:1229:G:H8	1.70	0.56
2:Pt:50:U:O2	2:Pt:64:G:N2	2.28	0.56
6:L5:1993:C:H2'	6:L5:1994:C:C6	2.41	0.56
6:L5:4094:G:N2	6:L5:4115:G:OP2	2.39	0.56
20:LM:36:ALA:HB3	20:LM:55:MET:HE1	1.87	0.56
72:SG:198:ARG:NH1	86:S2:126:G:OP2	2.37	0.56
78:SO:34:PHE:HB3	78:SO:41:PHE:HB2	1.88	0.56
86:S2:1354:G:N2	86:S2:1357:A:OP2	2.34	0.56
6:L5:966:A:H5''	6:L5:2092:G:H22	1.69	0.56
10:LB:83:PRO:O	10:LB:167:GLN:NE2	2.39	0.56
23:LP:17:SER:HB2	23:LP:98:ALA:HB2	1.88	0.56
54:SF:36:GLN:NE2	54:SF:37:ASP:OD1	2.39	0.56
57:SP:31:GLU:HA	57:SP:34:MET:HE2	1.86	0.56
77:SN:55:ARG:HD3	86:S2:1017:U:H5'	1.88	0.56
86:S2:1226:G:N1	86:S2:1639:G7M:OP2	2.30	0.56
4:CF:94:GLY:HA2	4:CF:136:HIS:HE1	1.70	0.56
6:L5:1079:C:O2	6:L5:1221:G:N2	2.29	0.56
45:Ll:28:ARG:HA	45:Ll:33:ASN:HD22	1.71	0.56
73:SH:111:LYS:HE3	86:S2:796:G:H21	1.71	0.56
82:SY:80:ASP:OD1	82:SY:81:TYR:N	2.39	0.56
4:CF:8:ILE:HB	4:CF:87:VAL:HG12	1.88	0.56
6:L5:2478:C:N3	6:L5:2591:A:O2'	2.39	0.56
6:L5:4220:6MZ:H2'	6:L5:4222:G:H5''	1.88	0.56
6:L5:4340:U:O2	89:L5:5260:SPD:N10	2.39	0.56
23:LP:116:HIS:HB3	23:LP:149:ILE:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Lo:33:LEU:HA	48:Lo:38:LYS:HG2	1.88	0.56
65:Sd:19:ARG:NH2	86:S2:1661:A:OP1	2.38	0.56
86:S2:543:C:H3'	86:S2:544:G:H8	1.71	0.56
6:L5:1969:G:H4'	51:Ls:36:GLY:HA2	1.88	0.56
6:L5:2832:A:OP1	37:Ld:47:LYS:NZ	2.29	0.56
6:L5:3611:A:H2	6:L5:5016:A:H8	1.52	0.56
6:L5:4279:A:H5'	6:L5:4281:A:H1'	1.87	0.56
3:Et:28:C:H2'	3:Et:29:A:H8	1.71	0.56
4:CF:273:LYS:HE2	4:CF:301:GLU:HG2	1.87	0.56
32:LY:4:ASN:HB3	32:LY:7:VAL:HG22	1.86	0.56
6:L5:2407:G:O6	45:Ll:2:SER:N	2.39	0.56
15:LG:165:GLU:OE2	21:LN:26:ARG:NH1	2.36	0.56
22:LO:9:LEU:HD23	22:LO:118:MET:HB2	1.88	0.56
56:SM:96:ARG:NH2	56:SM:100:PRO:O	2.39	0.56
2:Pt:18:G:O2'	2:Pt:57:G:N2	2.30	0.55
6:L5:184:U:H3	6:L5:253:G:H1	1.54	0.55
40:Lg:45:ALA:HB3	40:Lg:82:MET:HE2	1.88	0.55
68:SA:22:GLY:O	68:SA:24:HIS:ND1	2.38	0.55
4:CF:360:VAL:HA	4:CF:369:ALA:HA	1.88	0.55
6:L5:2083:C:OP2	24:LQ:14:ARG:NH2	2.33	0.55
6:L5:4163:U:OP2	15:LG:53:ARG:NH2	2.40	0.55
9:LA:118:GLU:OE2	9:LA:156:LYS:NZ	2.39	0.55
10:LB:219:VAL:HG11	10:LB:337:VAL:HG13	1.88	0.55
70:SC:259:THR:HG23	79:SV:16:LYS:HZ3	1.70	0.55
72:SG:136:LYS:NZ	72:SG:175:LYS:O	2.34	0.55
73:SH:34:SER:OG	73:SH:78:ARG:NH2	2.38	0.55
6:L5:158:A:N1	6:L5:276:C:O2'	2.37	0.55
6:L5:4098:A:N1	6:L5:4112:C:N4	2.53	0.55
17:LI:152:LEU:HB3	17:LI:165:ILE:HD12	1.88	0.55
36:Lc:38:ILE:HD11	36:Lc:46:VAL:HG21	1.89	0.55
52:Lt:50:THR:OG1	52:Lt:72:GLU:OE1	2.23	0.55
62:SU:48:LEU:HG	62:SU:93:SER:HB3	1.88	0.55
6:L5:5023:C:OP2	74:SI:124:LYS:NZ	2.40	0.55
76:SL:103:GLU:HG3	81:SX:11:ARG:HB2	1.87	0.55
86:S2:795:A:H2'	86:S2:796:G:C8	2.42	0.55
6:L5:1759:G:H1	6:L5:1773:U:H3	1.54	0.55
6:L5:4537:C:H2'	6:L5:4538:G:H8	1.70	0.55
26:LS:173:ASN:ND2	26:LS:175:PHE:O	2.40	0.55
71:SE:146:THR:HG21	86:S2:122:G:H21	1.70	0.55
73:SH:31:GLU:HA	73:SH:37:LYS:HG3	1.89	0.55
1:Cl:50:MET:HG3	28:LU:114:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:109:G:OP2	19:LL:74:ARG:NH2	2.35	0.55
9:LA:229:ALA:HB3	9:LA:234:LYS:HB3	1.87	0.55
12:LD:204:VAL:HB	12:LD:236:MET:HE1	1.88	0.55
12:LD:232:THR:OG1	12:LD:234:ASP:OD1	2.20	0.55
14:LF:243:LEU:O	14:LF:247:MET:HB2	2.06	0.55
17:LI:38:ARG:NH1	17:LI:45:GLU:OE1	2.37	0.55
30:LW:100:VAL:O	30:LW:104:GLN:NE2	2.40	0.55
54:SF:39:ILE:HG23	54:SF:68:ILE:HD13	1.88	0.55
64:Sc:37:ASP:OD1	64:Sc:39:SER:OG	2.25	0.55
68:SA:126:ASP:OD1	68:SA:165:ASN:ND2	2.39	0.55
6:L5:1332:C:H2'	6:L5:1333:A:H8	1.72	0.55
58:SQ:4:LYS:HE3	86:S2:1423:C:H41	1.72	0.55
70:SC:109:ILE:HD11	70:SC:151:ILE:HD11	1.88	0.55
2:Pt:20(A):U:O4'	18:LJ:58:ARG:NH2	2.40	0.55
6:L5:702:U:H2'	6:L5:703:G:O4'	2.07	0.55
6:L5:1726:U:H5'	14:LF:135:ILE:HD11	1.89	0.55
6:L5:2318:G:N2	6:L5:2321:G:OP2	2.34	0.55
11:LC:262:GLU:HB3	11:LC:273:LEU:HD13	1.89	0.55
15:LG:57:TRP:O	15:LG:62:ARG:NH1	2.40	0.55
54:SF:40:ALA:HB3	54:SF:67:PRO:HA	1.88	0.55
61:ST:2:PRO:HD2	86:S2:1419:C:H42	1.71	0.55
67:Sg:89:LEU:HB3	67:Sg:99:ARG:HB3	1.88	0.55
71:SE:151:ASP:HA	72:SG:212:LEU:HD21	1.89	0.55
6:L5:121:A:OP1	15:LG:110:LYS:NZ	2.32	0.55
6:L5:261:G:H2'	6:L5:262:G:C8	2.42	0.55
6:L5:4413:C:O2	17:LI:158:LYS:NZ	2.40	0.55
30:LW:105:ARG:NH2	72:SG:149:LYS:O	2.40	0.55
37:Ld:22:THR:HG23	37:Ld:122:VAL:HG13	1.88	0.55
51:Ls:110:ALA:HA	51:Ls:182:PRO:HG2	1.89	0.55
70:SC:102:LEU:HD22	70:SC:130:ILE:HD12	1.87	0.55
72:SG:7:PHE:HD1	72:SG:113:ILE:HB	1.72	0.55
74:SI:91:VAL:HG11	74:SI:205:ARG:HH12	1.72	0.55
86:S2:888:U:H4'	86:S2:889:U:H5'	1.89	0.55
6:L5:1100:U:O4	6:L5:1194:G:O6	2.25	0.55
33:LZ:46:ILE:HA	33:LZ:70:SER:HA	1.88	0.55
61:ST:74:SER:O	61:ST:78:ILE:HD12	2.07	0.55
69:SB:144:LYS:HD3	69:SB:208:HIS:HB3	1.88	0.55
54:SF:171:GLU:OE2	63:SZ:106:GLN:NE2	2.37	0.54
60:SS:36:VAL:HG21	60:SS:71:MET:HE3	1.89	0.54
66:Sf:110:GLU:HG2	66:Sf:113:LYS:HD3	1.89	0.54
78:SO:145:GLY:O	83:Sa:22:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SV:42:VAL:HG23	79:SV:43:THR:HG23	1.88	0.54
86:S2:942:G:H2'	86:S2:943:U:C6	2.42	0.54
86:S2:1255:G:OP1	86:S2:1256:G:O2'	2.23	0.54
6:L5:502:C:H3'	6:L5:503:C:H3'	1.89	0.54
6:L5:2486:G:O6	6:L5:2493:G:O6	2.26	0.54
19:LL:64:VAL:HA	19:LL:67:HIS:CD2	2.31	0.54
26:LS:161:ARG:HD2	26:LS:164:LYS:HB2	1.88	0.54
28:LU:23:LEU:HD23	28:LU:110:TYR:HB2	1.89	0.54
40:Lg:44:SER:OG	40:Lg:46:CYS:SG	2.65	0.54
67:Sg:258:ILE:HG23	67:Sg:267:VAL:HG23	1.89	0.54
6:L5:1328:G:O2'	6:L5:2349:A:OP1	2.25	0.54
9:LA:101:VAL:HG22	9:LA:165:VAL:HG22	1.88	0.54
60:SS:88:LYS:H	60:SS:95:TYR:HD1	1.55	0.54
4:CF:348:ASN:HD21	4:CF:431:GLN:HG3	1.72	0.54
6:L5:2495:U:H2'	6:L5:2496:G:C8	2.42	0.54
44:Lk:24:LYS:HD3	44:Lk:69:LEU:HD21	1.89	0.54
74:SI:143:LYS:NZ	86:S2:202:G:OP1	2.41	0.54
86:S2:981:A:H2'	86:S2:982:G:C8	2.42	0.54
86:S2:1513:C:H2'	86:S2:1514:G:H8	1.72	0.54
6:L5:305:A:OP2	21:LN:15:GLN:NE2	2.36	0.54
6:L5:729:G:H5''	14:LF:76:ARG:HD2	1.90	0.54
6:L5:2845:A:H61	6:L5:3843:C:H42	1.54	0.54
6:L5:4363:A:H5''	48:Lo:36:GLN:HG2	1.89	0.54
19:LL:91:ALA:HB1	19:LL:96:ILE:HB	1.90	0.54
54:SF:30:ILE:HG23	54:SF:117:ILE:HD11	1.89	0.54
59:SR:16:ILE:HD11	59:SR:54:VAL:HG21	1.89	0.54
65:Sd:17:GLY:O	65:Sd:27:ARG:NH1	2.41	0.54
86:S2:1606:G:N2	86:S2:1632:G:H1'	2.22	0.54
4:CF:347:LEU:O	4:CF:396:SER:OG	2.26	0.54
6:L5:223:G:OP2	11:LC:165:LYS:NZ	2.40	0.54
6:L5:1333:A:H2'	6:L5:1334:A:C8	2.43	0.54
6:L5:4620:OMU:OP2	6:L5:4670:C:N4	2.33	0.54
6:L5:4774:C:O2'	6:L5:4775:C:O2	2.25	0.54
22:LO:54:TYR:OH	22:LO:73:PHE:O	2.25	0.54
61:ST:62:ARG:NH2	86:S2:1543:U:OP2	2.36	0.54
67:Sg:8:ARG:HB3	67:Sg:309:VAL:HG13	1.89	0.54
73:SH:10:LYS:NZ	73:SH:16:PRO:O	2.41	0.54
6:L5:4617:G:OP2	10:LB:358:ARG:NH2	2.40	0.54
6:L5:4941:G:OP2	13:LE:188:ARG:NH2	2.32	0.54
12:LD:156:GLY:HA2	12:LD:181:PRO:HG3	1.89	0.54
22:LO:186:GLU:OE1	22:LO:186:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:ST:65:TYR:HE1	61:ST:128:GLN:HG3	1.72	0.54
67:Sg:249:CYS:HB3	67:Sg:258:ILE:HD13	1.90	0.54
6:L5:4967:A:H2'	6:L5:4968:A:C8	2.42	0.54
12:LD:291:GLN:NE2	17:LI:213:HIS:O	2.32	0.54
34:La:87:ARG:HG3	34:La:120:GLN:HE22	1.73	0.54
58:SQ:3:SER:OG	58:SQ:4:LYS:N	2.40	0.54
61:ST:121:ARG:HH21	86:S2:1563:G:H5''	1.71	0.54
1:CI:79:ARG:HH22	6:L5:2708:U:H1'	1.72	0.54
6:L5:1591:U:OP2	6:L5:2856:C:O2'	2.20	0.54
6:L5:1933:G:H2'	6:L5:1934:A:C8	2.43	0.54
6:L5:2745:A:H2'	6:L5:2746:A:C8	2.43	0.54
6:L5:3717:A:H2'	6:L5:3718:A2M:C8	2.38	0.54
9:LA:108:PRO:HB2	49:Lp:86:LEU:HD23	1.90	0.54
52:Lt:82:ILE:HG12	52:Lt:137:GLN:HG2	1.90	0.54
52:Lt:114:ARG:NH2	52:Lt:126:SER:OG	2.41	0.54
55:SK:27:VAL:HB	55:SK:43:LEU:HD12	1.90	0.54
60:SS:109:GLU:HA	60:SS:112:GLU:HG2	1.90	0.54
70:SC:72:ASP:OD2	70:SC:272:HIS:NE2	2.40	0.54
1:CI:50:MET:HG3	28:LU:114:TYR:CE2	2.42	0.54
6:L5:88:A:N7	24:LQ:173:LYS:NZ	2.56	0.54
6:L5:364:G:O6	43:Lj:55:ARG:NH2	2.41	0.54
20:LM:119:ARG:HG3	22:LO:189:ILE:HG23	1.89	0.54
24:LQ:99:LYS:HZ2	24:LQ:121:LEU:HD11	1.73	0.54
39:Lf:43:LEU:O	39:Lf:109:ARG:NH2	2.41	0.54
67:Sg:18:VAL:O	67:Sg:287:THR:OG1	2.26	0.54
67:Sg:129:ILE:HB	67:Sg:142:VAL:HB	1.89	0.54
86:S2:557:U:H2'	86:S2:558:G:C8	2.43	0.54
86:S2:889:U:OP2	86:S2:896:U:N3	2.41	0.54
86:S2:1203:G:H2'	86:S2:1204:A:C8	2.42	0.54
6:L5:4220:6MZ:O5'	6:L5:4220:6MZ:H8	2.09	0.53
8:L8:58:G:N7	43:Lj:63:ARG:NH2	2.44	0.53
14:LF:96:ARG:HH12	14:LF:224:THR:HG22	1.72	0.53
18:LJ:84:GLU:OE2	18:LJ:92:TYR:OH	2.25	0.53
58:SQ:130:LYS:NZ	58:SQ:131:LYS:O	2.41	0.53
68:SA:37:TYR:OH	68:SA:57:LYS:NZ	2.38	0.53
86:S2:118:C:H1'	86:S2:445:A:C5	2.43	0.53
6:L5:1214:C:N3	35:Lb:90:SER:OG	2.41	0.53
6:L5:1734:G:N2	6:L5:1735:U:O4	2.34	0.53
6:L5:1837:A:OP2	27:LT:130:ARG:NH1	2.38	0.53
6:L5:4537:C:H2'	6:L5:4538:G:C8	2.42	0.53
36:Lc:99:PRO:HG3	36:Lc:104:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SU:68:THR:O	65:Sd:40:ARG:NH1	2.40	0.53
68:SA:18:PHE:HD1	68:SA:23:THR:HG21	1.71	0.53
74:SI:10:LYS:O	74:SI:18:ARG:NH1	2.41	0.53
6:L5:4694:G:H4'	16:LH:71:ARG:HH12	1.73	0.53
55:SK:55:ARG:NH1	55:SK:78:TYR:OH	2.41	0.53
70:SC:77:SER:OG	70:SC:79:GLU:OE1	2.26	0.53
78:SO:33:ILE:HB	78:SO:97:LEU:HD23	1.91	0.53
76:SL:128:VAL:HG12	76:SL:142:VAL:HA	1.90	0.53
80:SW:111:MET:HE1	80:SW:119:LYS:HD2	1.89	0.53
84:Sb:20:LYS:NZ	86:S2:1016:U:OP2	2.41	0.53
86:S2:851:C:H5''	86:S2:852:G:H5'	1.89	0.53
3:Et:32:C:H5'	54:SF:134:VAL:HG13	1.90	0.53
53:SD:138:VAL:HG13	53:SD:182:LEU:HD21	1.91	0.53
76:SL:133:PRO:O	86:S2:383:G:O2'	2.25	0.53
81:SX:70:VAL:HG11	81:SX:94:ILE:HG21	1.89	0.53
86:S2:1013:U:OP1	86:S2:1129:G:O2'	2.26	0.53
4:CF:380:ASP:HB2	4:CF:387:LEU:HD21	1.91	0.53
6:L5:1994:C:H2'	6:L5:1995:G:H8	1.73	0.53
6:L5:3911:C:H2'	6:L5:3912:U:H6	1.73	0.53
6:L5:4260:U:H2'	6:L5:4261:C:C6	2.44	0.53
11:LC:218:ILE:HA	11:LC:229:LEU:HD22	1.89	0.53
32:LY:2:LYS:HD2	32:LY:7:VAL:HG23	1.89	0.53
77:SN:70:LYS:NZ	86:S2:1020:A:N7	2.55	0.53
84:Sb:62:VAL:HG23	84:Sb:74:THR:HG21	1.91	0.53
86:S2:1581:C:H5'	86:S2:1582:C:H5	1.74	0.53
4:CF:111:CYS:SG	4:CF:112:ALA:N	2.81	0.53
6:L5:691:C:H2'	6:L5:692:A:C8	2.43	0.53
6:L5:735:G:H5''	20:LM:70:GLN:HG3	1.91	0.53
13:LE:223:ARG:HH22	13:LE:238:GLU:HG3	1.74	0.53
22:LO:168:TYR:CE2	22:LO:172:LYS:HD2	2.44	0.53
63:SZ:106:GLN:HG3	63:SZ:108:ILE:HD11	1.89	0.53
70:SC:257:LYS:O	79:SV:16:LYS:NZ	2.40	0.53
77:SN:66:VAL:HG13	77:SN:67:THR:HG23	1.90	0.53
86:S2:902:G:O2'	86:S2:903:A:O4'	2.27	0.53
4:CF:214:TRP:HZ2	4:CF:231:ALA:HB2	1.74	0.53
6:L5:71:C:H1'	19:LL:62:PRO:O	2.09	0.53
23:LP:118:GLN:OE1	23:LP:120:ASN:ND2	2.41	0.53
32:LY:76:LYS:HE2	45:Ll:31:THR:HB	1.89	0.53
51:Ls:29:ILE:HG22	51:Ls:88:PHE:HD1	1.72	0.53
54:SF:78:MET:HE3	86:S2:1222:G:H5''	1.90	0.53
84:Sb:11:SER:N	84:Sb:14:GLU:OE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Pt:38:C:O2'	86:S2:1058:A:OP1	2.27	0.53
29:LV:92:ASP:O	30:LW:2:LYS:NZ	2.42	0.53
50:Lr:38:PHE:O	50:Lr:45:HIS:NE2	2.31	0.53
86:S2:455:A:H2'	86:S2:456:C:H6	1.74	0.53
5:AT:14:A:H3'	5:AT:15:G:H8	1.74	0.53
6:L5:267:G:H2'	6:L5:268:G:H8	1.74	0.53
6:L5:1756:U:O2'	6:L5:1758:G:OP2	2.24	0.53
30:LW:123:LYS:HD2	86:S2:320:G:H5''	1.90	0.53
55:SK:3:MET:HE1	55:SK:11:ILE:HD12	1.90	0.53
68:SA:85:ARG:NH1	68:SA:203:PHE:O	2.40	0.53
4:CF:13:ILE:HD12	4:CF:136:HIS:HB3	1.91	0.52
5:AT:57:C:H5	6:L5:2009:A:H1'	1.74	0.52
6:L5:1241:C:O2'	35:Lb:120:ARG:O	2.27	0.52
6:L5:1258:G:H2'	6:L5:1259:G:C8	2.44	0.52
6:L5:1548:G:O2'	6:L5:2812:A:N3	2.38	0.52
6:L5:2084:C:O2	24:LQ:16:LYS:NZ	2.42	0.52
11:LC:293:LEU:O	11:LC:299:GLN:NE2	2.39	0.52
35:Lb:102:PRO:O	35:Lb:109:ARG:NH2	2.41	0.52
58:SQ:131:LYS:HB2	58:SQ:140:ARG:HH22	1.74	0.52
60:SS:48:ALA:O	60:SS:66:ARG:NH2	2.42	0.52
64:Sc:66:ARG:HH12	64:Sc:68:LEU:HD23	1.74	0.52
85:Se:58:ASN:ND2	86:S2:608:C:O4'	2.42	0.52
86:S2:553:U:O4	86:S2:554:A:N6	2.40	0.52
86:S2:1773:C:H2'	86:S2:1774:C:H5''	1.91	0.52
4:CF:215:LYS:HZ3	4:CF:222:ASN:HB3	1.73	0.52
5:AT:67:C:H2'	5:AT:68:G:C8	2.44	0.52
39:Lf:78:HIS:HB3	39:Lf:83:MET:HB3	1.91	0.52
43:Lj:2:THR:HB	43:Lj:6:SER:HB2	1.90	0.52
83:Sa:41:ILE:HD12	83:Sa:68:TYR:HD2	1.74	0.52
6:L5:2624:G:OP2	28:LU:97:ARG:NH2	2.42	0.52
6:L5:5016:A:C2	6:L5:5033:G:N2	2.74	0.52
24:LQ:15:ARG:NH1	24:LQ:52:PHE:O	2.41	0.52
76:SL:3:ASP:OD1	76:SL:4:ILE:N	2.42	0.52
6:L5:93:G:H2'	6:L5:94:A:C8	2.45	0.52
6:L5:2568:C:H2'	6:L5:2569:G:H8	1.73	0.52
6:L5:4612:C:C2	16:LH:120:GLU:HB2	2.44	0.52
6:L5:4717:A:OP2	10:LB:30:LYS:NZ	2.32	0.52
22:LO:54:TYR:CD1	22:LO:145:VAL:HG21	2.44	0.52
56:SM:82:ASN:OD1	56:SM:83:LYS:N	2.42	0.52
57:SP:79:HIS:HD2	86:S2:1298:G:C4	2.28	0.52
70:SC:60:TRP:O	70:SC:71:LYS:NZ	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SG:13:GLN:NE2	86:S2:153:G:N3	2.57	0.52
6:L5:2696:A:OP1	44:Lk:26:LYS:NZ	2.42	0.52
51:Ls:99:ARG:HG3	51:Ls:103:LEU:HD13	1.92	0.52
70:SC:207:ALA:HB2	86:S2:4:C:H4'	1.92	0.52
73:SH:51:ILE:HG21	73:SH:179:LYS:HG2	1.91	0.52
86:S2:1777:G:H2'	86:S2:1778:C:H6	1.73	0.52
14:LF:41:MET:HE2	35:Lb:113:ALA:HB2	1.90	0.52
22:LO:197:LYS:NZ	22:LO:203:VAL:O	2.42	0.52
54:SF:60:ARG:HD2	86:S2:1679:A:H2'	1.92	0.52
58:SQ:42:ILE:HG23	58:SQ:44:PRO:HD2	1.91	0.52
60:SS:15:VAL:HG12	60:SS:16:LEU:HG	1.91	0.52
71:SE:125:LYS:O	71:SE:142:HIS:N	2.42	0.52
4:CF:281:ALA:HB2	4:CF:334:PRO:HB2	1.92	0.52
6:L5:1270:A:H8	6:L5:2106:G:H21	1.57	0.52
6:L5:2745:A:H2'	6:L5:2746:A:H8	1.75	0.52
6:L5:2756:G:O6	33:LZ:51:ARG:NH2	2.30	0.52
41:Lh:80:PRO:HD2	41:Lh:83:LEU:HD12	1.91	0.52
58:SQ:89:SER:OG	58:SQ:119:LEU:O	2.25	0.52
62:SU:40:ILE:O	62:SU:44:LYS:HG2	2.09	0.52
68:SA:10:MET:HE3	68:SA:55:TRP:HB2	1.90	0.52
77:SN:64:ARG:NH2	86:S2:919:A:OP2	2.41	0.52
52:Lt:119:ARG:NH1	52:Lt:123:ARG:HH12	2.08	0.52
53:SD:161:GLY:HA3	86:S2:1388:A:H61	1.75	0.52
65:Sd:2:GLY:N	86:S2:1271:C:O2	2.42	0.52
86:S2:367:U:H4'	86:S2:371:A:C8	2.45	0.52
86:S2:1010:G:H2'	86:S2:1011:A:C8	2.45	0.52
86:S2:1405:A:H2'	86:S2:1406:G:O4'	2.10	0.52
6:L5:2517:A:H5'	40:Lg:62:LYS:HD3	1.91	0.52
6:L5:4601:U:H2'	6:L5:4602:A:H8	1.75	0.52
13:LE:264:ILE:HD11	13:LE:267:LEU:HD22	1.92	0.52
52:Lt:85:LEU:HD13	52:Lt:109:ILE:HD12	1.90	0.52
61:ST:11:GLN:HB2	86:S2:1542:C:H4'	1.92	0.52
76:SL:61:PRO:HG3	76:SL:141:ASN:HB3	1.92	0.52
6:L5:4478:G:O2'	6:L5:4602:A:N1	2.42	0.52
8:L8:39:G:OP1	41:Lh:86:LYS:NZ	2.43	0.52
69:SB:32:ASP:OD1	69:SB:46:LYS:NZ	2.38	0.52
72:SG:20:ASP:HB3	72:SG:23:LYS:HB2	1.91	0.52
4:CF:215:LYS:NZ	4:CF:216:VAL:O	2.43	0.51
6:L5:1961:G:O2'	6:L5:2025:A:N6	2.44	0.51
6:L5:3823:G:OP2	6:L5:3823:G:N2	2.35	0.51
37:Ld:23:ARG:HG2	37:Ld:121:ASN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SQ:140:ARG:HB2	86:S2:1644:C:H4'	1.92	0.51
82:SY:119:GLY:HA2	86:S2:85:A:H5'	1.91	0.51
4:CF:76:SER:N	4:CF:91:ASP:OD1	2.40	0.51
6:L5:268:G:H2'	6:L5:269:G:H8	1.75	0.51
6:L5:1070:G:O2'	6:L5:1071:C:O5'	2.26	0.51
6:L5:1509:C:H5''	34:La:2:PRO:HD3	1.92	0.51
11:LC:363:ALA:O	11:LC:367:GLU:HB3	2.10	0.51
55:SK:85:LEU:HD12	55:SK:86:PRO:HD2	1.91	0.51
66:Sf:102:VAL:HG22	66:Sf:104:LYS:HG2	1.92	0.51
80:SW:6:VAL:HG12	80:SW:34:ILE:HD11	1.93	0.51
80:SW:6:VAL:HG13	80:SW:29:PRO:HB2	1.91	0.51
68:SA:76:VAL:HG12	68:SA:123:VAL:HB	1.91	0.51
69:SB:167:LYS:O	69:SB:171:ILE:HG12	2.10	0.51
72:SG:3:LEU:HD23	72:SG:109:LEU:HB3	1.91	0.51
72:SG:191:ARG:HH12	86:S2:312:G:H2'	1.75	0.51
73:SH:162:GLN:HE22	73:SH:166:VAL:HB	1.75	0.51
80:SW:111:MET:HE3	80:SW:116:ALA:HA	1.93	0.51
86:S2:672:A:N6	86:S2:1027:A:OP1	2.41	0.51
86:S2:1130:G:OP2	86:S2:1130:G:N2	2.34	0.51
86:S2:1748:G:O6	86:S2:1786:U:O4	2.28	0.51
86:S2:1801:A:H2'	86:S2:1802:C:C6	2.46	0.51
3:Et:23:A:H2'	3:Et:24:G:C8	2.45	0.51
6:L5:1718:C:O2'	14:LF:181:LYS:NZ	2.43	0.51
6:L5:3898:G:H5'	10:LB:254:ILE:HG13	1.92	0.51
10:LB:50:LYS:HB2	10:LB:345:LEU:HD11	1.92	0.51
21:LN:146:PRO:HB2	41:Lh:104:THR:HG23	1.93	0.51
57:SP:37:TYR:O	60:SS:88:LYS:NZ	2.43	0.51
81:SX:124:LYS:NZ	86:S2:29:G:OP1	2.40	0.51
86:S2:1610:G:O6	86:S2:1630:A:N6	2.43	0.51
6:L5:1268:G:N7	35:Lb:111:ARG:NH2	2.53	0.51
6:L5:1411:C:H2'	6:L5:1412:G:C8	2.45	0.51
6:L5:4274:A:H2'	6:L5:4275:G:C8	2.45	0.51
6:L5:4967:A:H2'	6:L5:4968:A:H8	1.75	0.51
63:SZ:41:ARG:HH12	63:SZ:44:LEU:HG	1.75	0.51
66:Sf:103:LEU:HB2	66:Sf:105:TYR:CE2	2.45	0.51
69:SB:26:SER:O	69:SB:51:ARG:NH2	2.43	0.51
81:SX:48:LYS:HB3	81:SX:75:ILE:HD12	1.91	0.51
6:L5:1683:PSU:OP1	34:La:44:ASN:ND2	2.42	0.51
13:LE:141:ARG:NH2	39:Lf:110:ILE:O	2.44	0.51
15:LG:157:ILE:HA	15:LG:201:THR:HG22	1.93	0.51
21:LN:46:ASP:OD1	21:LN:47:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SS:28:PHE:O	60:SS:31:THR:OG1	2.25	0.51
70:SC:121:ARG:NH1	70:SC:123:ARG:HE	2.09	0.51
86:S2:525:A:H2'	86:S2:526:A:H8	1.75	0.51
6:L5:308:G:OP2	6:L5:308:G:N2	2.35	0.51
6:L5:1867:A:H2'	6:L5:1868:A:C8	2.46	0.51
10:LB:288:GLY:HA3	10:LB:330:PHE:CE1	2.46	0.51
14:LF:171:ASP:OD1	14:LF:172:ASN:N	2.43	0.51
18:LJ:104:ASN:HD22	18:LJ:133:VAL:HG13	1.75	0.51
51:Ls:29:ILE:HG22	51:Ls:88:PHE:CD1	2.46	0.51
56:SM:23:LYS:O	56:SM:27:ILE:HG12	2.10	0.51
62:SU:96:GLU:OE1	62:SU:99:LYS:N	2.36	0.51
67:Sg:239:LEU:HD11	67:Sg:248:LEU:HD21	1.93	0.51
71:SE:204:SER:OG	71:SE:205:PHE:N	2.39	0.51
71:SE:247:THR:N	71:SE:250:GLU:OE2	2.39	0.51
74:SI:3:ILE:O	74:SI:30:GLY:N	2.42	0.51
86:S2:145:G:H2'	86:S2:146:G:C8	2.45	0.51
5:AT:53:G:H2'	5:AT:54:G:H8	1.75	0.51
10:LB:57:VAL:HG22	10:LB:73:VAL:HG22	1.93	0.51
74:SI:45:THR:HG23	74:SI:53:LYS:HG3	1.93	0.51
84:Sb:67:THR:OG1	84:Sb:70:LYS:O	2.21	0.51
51:Ls:13:TYR:O	51:Ls:17:ILE:HG12	2.11	0.51
71:SE:31:PRO:HA	71:SE:81:THR:HB	1.93	0.51
71:SE:126:VAL:HA	71:SE:141:THR:HA	1.93	0.51
86:S2:57:U:OP1	86:S2:504:G:O2'	2.29	0.51
86:S2:964:A:H2'	86:S2:965:U:H6	1.76	0.51
86:S2:1421:A:H5''	86:S2:1422:G:H2'	1.92	0.51
86:S2:1588:A:H2'	86:S2:1589:A:C8	2.46	0.51
4:CF:266:ARG:HD3	4:CF:305:GLY:HA2	1.93	0.51
16:LH:92:MET:HE2	16:LH:179:ILE:HG22	1.93	0.51
37:Ld:59:THR:OG1	37:Ld:104:THR:OG1	2.25	0.51
42:Li:55:ARG:O	42:Li:59:GLU:HG2	2.11	0.51
60:SS:14:ARG:HH11	60:SS:19:ASN:HB3	1.76	0.51
65:Sd:12:ARG:NH1	86:S2:1513:C:OP1	2.31	0.51
70:SC:191:VAL:HG11	70:SC:236:PHE:HA	1.93	0.51
73:SH:10:LYS:HE3	73:SH:17:ASP:HB3	1.93	0.51
4:CF:108:GLN:HE22	4:CF:251:GLN:HG3	1.76	0.50
6:L5:351:C:OP2	11:LC:197:ARG:NH1	2.34	0.50
6:L5:2102:G:H1'	6:L5:2103:G:C8	2.46	0.50
6:L5:4636:PSU:N1	37:Ld:79:ASN:OD1	2.43	0.50
6:L5:4896:G:H2'	6:L5:4897:G:C8	2.47	0.50
16:LH:107:GLU:N	16:LH:107:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LO:126:VAL:HG13	22:LO:127:VAL:HG13	1.92	0.50
82:SY:108:LYS:NZ	86:S2:506:G:OP1	2.38	0.50
4:CF:42:PHE:HE1	4:CF:67:ARG:HH21	1.59	0.50
6:L5:387:G:O2'	6:L5:412:G:N1	2.36	0.50
6:L5:717:U:H2'	6:L5:718:C:C6	2.46	0.50
6:L5:1438:U:H4'	14:LF:31:LYS:HE3	1.93	0.50
6:L5:4927:G:H5''	6:L5:4928:C:H5	1.76	0.50
22:LO:10:ASP:OD2	22:LO:37:ARG:NH2	2.44	0.50
57:SP:56:LEU:HD22	57:SP:80:LEU:HD11	1.92	0.50
61:ST:44:GLU:HG3	61:ST:45:LEU:HD12	1.93	0.50
69:SB:40:ASN:HD21	69:SB:76:ASN:HB2	1.77	0.50
75:SJ:136:ARG:NH1	75:SJ:159:PHE:O	2.40	0.50
86:S2:28:U:H2'	86:S2:29:G:H8	1.76	0.50
86:S2:107:A:H2'	86:S2:108:G:C8	2.46	0.50
4:CF:58:TRP:HA	4:CF:61:ASP:HB2	1.92	0.50
6:L5:2577:C:OP1	33:LZ:111:ARG:NH2	2.44	0.50
8:L8:21:C:OP1	11:LC:195:LYS:NZ	2.42	0.50
19:LL:7:GLY:O	34:La:49:HIS:NE2	2.40	0.50
67:Sg:40:ILE:HB	67:Sg:59:LEU:HB2	1.93	0.50
83:Sa:41:ILE:HD12	83:Sa:68:TYR:CD2	2.45	0.50
86:S2:1033:G:N1	86:S2:1080:A:O2'	2.39	0.50
86:S2:1845:A:H2'	86:S2:1846:G:C8	2.46	0.50
1:CI:78:HIS:NE2	6:L5:2706:G:C8	2.75	0.50
6:L5:2018:C:H2'	6:L5:2019:C:C6	2.46	0.50
6:L5:4589:A:N1	6:L5:4621:C:O2'	2.41	0.50
17:LI:207:ASP:OD1	17:LI:210:ARG:NH1	2.44	0.50
30:LW:7:SER:OG	30:LW:8:PHE:N	2.45	0.50
54:SF:22:LYS:HG3	54:SF:23:TRP:CD2	2.46	0.50
68:SA:128:ARG:NH2	68:SA:151:ASP:O	2.44	0.50
5:AT:44:A:H2'	5:AT:45:A:C8	2.46	0.50
6:L5:418:A:C2	8:L8:17:A:H1'	2.47	0.50
6:L5:1802:A:H5''	6:L5:1803:G:H5'	1.93	0.50
6:L5:3732:A:H2'	6:L5:3733:A:H8	1.76	0.50
11:LC:144:ILE:HG13	11:LC:144:ILE:O	2.11	0.50
28:LU:36:ALA:HB1	28:LU:70:ILE:HD11	1.93	0.50
68:SA:137:ALA:HB1	68:SA:142:LEU:HB3	1.94	0.50
73:SH:140:VAL:HG12	77:SN:19:ARG:HD3	1.94	0.50
75:SJ:38:ARG:N	75:SJ:42:GLU:OE2	2.30	0.50
86:S2:436:OMG:OP2	86:S2:471:G:O2'	2.23	0.50
5:AT:24:C:H2'	5:AT:25:A:C8	2.47	0.50
6:L5:1697:G:H22	6:L5:2084:C:P	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:3707:U:H2'	6:L5:3708:C:C6	2.46	0.50
6:L5:5064:G:N2	23:LP:75:GLN:HE22	2.10	0.50
10:LB:378:ARG:HE	30:LW:32:LEU:HD21	1.75	0.50
25:LR:92:LYS:HG2	25:LR:96:MET:HE3	1.94	0.50
67:Sg:57:ARG:HE	67:Sg:95:GLY:HA3	1.76	0.50
70:SC:78:LEU:HD12	70:SC:81:ILE:HD12	1.93	0.50
70:SC:196:ILE:HB	70:SC:223:TYR:HB2	1.92	0.50
86:S2:455:A:H2'	86:S2:456:C:C6	2.46	0.50
2:Pt:3:C:H42	2:Pt:70:A:H61	1.58	0.50
6:L5:654:C:H2'	6:L5:655:C:C6	2.47	0.50
6:L5:2300:A:N7	11:LC:143:ARG:NH1	2.60	0.50
6:L5:3910:C:H2'	6:L5:3911:C:C6	2.47	0.50
23:LP:107:LEU:HD13	23:LP:152:GLU:HG3	1.93	0.50
67:Sg:176:VAL:HG23	67:Sg:185:LYS:HB2	1.94	0.50
74:SI:133:GLU:HA	74:SI:136:ILE:HG12	1.92	0.50
86:S2:159:A2M:O5'	86:S2:159:A2M:H8	2.12	0.50
6:L5:137:G:H2'	6:L5:138:G:H8	1.77	0.50
6:L5:1617:G:H1'	6:L5:2513:A:N6	2.26	0.50
18:LJ:38:LYS:HD2	18:LJ:123:ILE:HD11	1.94	0.50
62:SU:79:ARG:NH2	86:S2:1669:G:OP1	2.42	0.50
72:SG:135:PRO:HA	86:S2:169:U:H5''	1.93	0.50
72:SG:190:ARG:NH2	86:S2:334:C:OP2	2.40	0.50
86:S2:482:G:N1	86:S2:485:A:OP2	2.39	0.50
3:Et:9:A:O2'	3:Et:45:G:N3	2.44	0.50
6:L5:1655:C:OP2	34:La:26:ARG:NH1	2.45	0.50
6:L5:3697:U:H5''	6:L5:3698:G:H5'	1.93	0.50
6:L5:4239:A:H2'	6:L5:4240:G:C8	2.47	0.50
6:L5:4591:U:H2'	6:L5:4592:C:C6	2.47	0.50
8:L8:141:C:H2'	8:L8:142:U:C6	2.47	0.50
10:LB:147:GLU:OE2	10:LB:198:ARG:NH2	2.32	0.50
12:LD:182:GLY:HA2	12:LD:194:VAL:HG23	1.93	0.50
16:LH:48:LEU:HD21	16:LH:56:ARG:HB2	1.93	0.50
49:Lp:75:SER:O	49:Lp:79:VAL:HG23	2.12	0.50
55:SK:22:VAL:HG22	55:SK:68:TYR:HD1	1.76	0.50
55:SK:64:TRP:HB3	65:Sd:23:VAL:HA	1.94	0.50
67:Sg:195:LEU:HA	67:Sg:211:GLY:HA3	1.93	0.50
70:SC:85:SER:OG	79:SV:25:GLY:O	2.29	0.50
73:SH:20:GLU:HG2	73:SH:48:ALA:HB3	1.93	0.50
74:SI:141:ARG:HD3	74:SI:145:ILE:HG21	1.93	0.50
78:SO:45:THR:HA	78:SO:52:THR:HA	1.94	0.50
82:SY:51:THR:OG1	82:SY:53:ASP:OD1	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:SY:119:GLY:O	86:S2:84:A:O2'	2.27	0.50
86:S2:149:A:H3'	86:S2:150:A:H8	1.76	0.50
4:CF:15:HIS:NE2	4:CF:133:THR:OG1	2.30	0.49
6:L5:1628:C:OP1	9:LA:14:SER:OG	2.29	0.49
6:L5:2809:G:O2'	6:L5:4644:G:OP1	2.28	0.49
9:LA:181:LYS:HB2	9:LA:184:ARG:HG3	1.94	0.49
10:LB:218:ASP:OD2	10:LB:348:ARG:NH2	2.32	0.49
19:LL:111:GLN:O	19:LL:115:GLN:HG2	2.12	0.49
61:ST:60:THR:HG22	61:ST:75:MET:HE2	1.94	0.49
69:SB:97:LEU:HB3	69:SB:232:HIS:NE2	2.27	0.49
86:S2:960:U:O2'	86:S2:962:A:N7	2.37	0.49
6:L5:1662:C:H2'	6:L5:1663:C:C6	2.47	0.49
6:L5:3641:U:H5	6:L5:3646:A:N7	2.09	0.49
14:LF:157:ARG:HE	14:LF:248:ASN:HB2	1.77	0.49
54:SF:60:ARG:NH2	86:S2:1679:A:OP1	2.43	0.49
54:SF:141:VAL:HG12	64:Sc:47:LYS:HG2	1.92	0.49
68:SA:184:ARG:HE	68:SA:191:ARG:HA	1.77	0.49
72:SG:170:ARG:HG3	86:S2:72:C:N3	2.27	0.49
86:S2:1562:C:H2'	86:S2:1563:G:H8	1.76	0.49
6:L5:433:A:C2	6:L5:3867:A2M:H4'	2.46	0.49
10:LB:394:LYS:HA	10:LB:397:ILE:HG12	1.94	0.49
12:LD:217:ASP:N	12:LD:217:ASP:OD1	2.41	0.49
13:LE:190:HIS:HB3	13:LE:193:PHE:HD2	1.77	0.49
16:LH:18:ILE:HG12	16:LH:27:VAL:HG22	1.94	0.49
30:LW:2:LYS:HE3	30:LW:15:PRO:HB3	1.94	0.49
51:Ls:143:ILE:HD12	51:Ls:158:VAL:HG11	1.95	0.49
56:SM:49:LEU:HD21	56:SM:123:VAL:HG11	1.94	0.49
81:SX:28:LYS:HE2	81:SX:32:LEU:HD22	1.93	0.49
82:SY:105:LYS:NZ	86:S2:507:G:O6	2.36	0.49
86:S2:1337:4AC:O5'	86:S2:1337:4AC:H6	2.12	0.49
6:L5:173:C:OP1	19:LL:129:ARG:NH1	2.46	0.49
6:L5:325:U:H2'	6:L5:326:C:C6	2.47	0.49
6:L5:512:U:H3	6:L5:647:G:H1	1.60	0.49
6:L5:1283:G:N1	6:L5:2076:G:OP1	2.33	0.49
6:L5:3659:G:OP1	9:LA:241:ARG:NH1	2.45	0.49
10:LB:258:HIS:HA	10:LB:260:ALA:N	2.26	0.49
12:LD:66:TYR:HE2	12:LD:68:ARG:HE	1.60	0.49
26:LS:27:LEU:HB3	27:LT:148:PRO:HB3	1.94	0.49
52:Lt:76:SER:OG	52:Lt:116:MET:SD	2.69	0.49
65:Sd:46:TYR:O	65:Sd:50:ILE:HD12	2.12	0.49
77:SN:14:SER:HB3	86:S2:1016:U:H5''	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:SW:3:ARG:HH22	80:SW:28:ARG:HH21	1.60	0.49
80:SW:44:HIS:NE2	80:SW:112:ASP:OD2	2.42	0.49
83:Sa:8:ASN:ND2	86:S2:1861:G:OP1	2.42	0.49
86:S2:928:G:H1	86:S2:1013:U:H3	1.59	0.49
6:L5:10:A:H2'	6:L5:11:G:C8	2.48	0.49
6:L5:1480:C:O2'	6:L5:1482:G:OP2	2.31	0.49
6:L5:1516:G:O2'	19:LL:18:TRP:NE1	2.45	0.49
6:L5:3880:G:H2'	6:L5:3881:G:C8	2.47	0.49
6:L5:4188:U:H2'	6:L5:4189:U:C6	2.48	0.49
54:SF:81:ARG:O	54:SF:85:LYS:NZ	2.34	0.49
60:SS:46:ARG:NH1	61:ST:50:GLU:OE2	2.45	0.49
86:S2:1288:OMU:HN3	86:S2:1311:C:H42	1.60	0.49
86:S2:1720:U:H5''	86:S2:1721:U:H5''	1.94	0.49
4:CF:11:VAL:HG12	4:CF:90:ILE:HB	1.93	0.49
4:CF:364:HIS:CD2	4:CF:365:THR:H	2.30	0.49
6:L5:2279:A:O2'	38:Le:48:ARG:NH2	2.46	0.49
6:L5:2491:C:H2'	6:L5:2492:C:C6	2.47	0.49
6:L5:2739:C:O2	9:LA:188:LYS:NZ	2.43	0.49
6:L5:3615:G:H1'	30:LW:44:ARG:HD3	1.95	0.49
6:L5:3720:G:H22	6:L5:3733:A:H2	1.58	0.49
79:SV:73:ALA:HB1	79:SV:78:ILE:HB	1.95	0.49
86:S2:49:C:H2'	86:S2:472:C:H41	1.76	0.49
6:L5:2101:C:H2'	6:L5:2102:G:C8	2.47	0.49
6:L5:2539:C:H2'	6:L5:2540:C:C6	2.48	0.49
6:L5:2568:C:H2'	6:L5:2569:G:C8	2.48	0.49
6:L5:4459:U:H2'	6:L5:4460:U:C6	2.47	0.49
10:LB:299:ILE:HB	10:LB:313:SER:HB3	1.94	0.49
33:LZ:50:PRO:HD3	33:LZ:68:ILE:HG12	1.95	0.49
60:SS:132:ARG:NH1	86:S2:1623:A:N1	2.60	0.49
71:SE:104:ASP:HB3	71:SE:110:ALA:HB2	1.93	0.49
73:SH:87:PHE:HB3	73:SH:90:LYS:HD2	1.95	0.49
74:SI:116:HIS:O	74:SI:152:ARG:NH2	2.38	0.49
75:SJ:60:LEU:HD22	75:SJ:70:ARG:HA	1.95	0.49
86:S2:1098:C:H2'	86:S2:1099:G:C8	2.47	0.49
86:S2:1407:U:H2'	86:S2:1408:U:C6	2.47	0.49
1:CI:78:HIS:CD2	6:L5:2706:G:N7	2.81	0.49
6:L5:1646:A:O2'	43:Lj:49:TRP:O	2.25	0.49
6:L5:1985:G:N2	6:L5:2003:G:O2'	2.46	0.49
6:L5:4699:U:H1'	6:L5:4700:A:H5''	1.94	0.49
22:LO:119:VAL:N	26:LS:168:THR:O	2.44	0.49
29:LV:87:SER:OG	30:LW:19:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SR:32:LYS:NZ	86:S2:1452:A:OP2	2.45	0.49
68:SA:106:GLY:N	68:SA:136:GLU:OE2	2.34	0.49
86:S2:207:G:H3'	86:S2:208:G:H8	1.78	0.49
86:S2:1277:C:H2'	86:S2:1278:A:C8	2.47	0.49
86:S2:1528:G:O2'	86:S2:1666:C:OP1	2.30	0.49
6:L5:148:C:OP2	15:LG:197:LYS:NZ	2.42	0.49
6:L5:280:G:H5''	21:LN:14:LYS:HE2	1.93	0.49
6:L5:308:G:O6	21:LN:12:ARG:NH1	2.46	0.49
6:L5:2764:A:H2'	6:L5:2765:A:H8	1.78	0.49
6:L5:2835:A:O2'	10:LB:228:TYR:O	2.27	0.49
6:L5:4966:A:H5''	10:LB:128:LYS:HG3	1.93	0.49
10:LB:217:ILE:HD12	10:LB:347:LEU:HB3	1.95	0.49
81:SX:128:VAL:HG23	81:SX:138:LYS:HD2	1.95	0.49
82:SY:7:ILE:HG12	82:SY:43:LYS:HD3	1.94	0.49
82:SY:41:ARG:NH2	82:SY:52:PRO:O	2.45	0.49
6:L5:1097:C:H2'	6:L5:1098:G:C8	2.48	0.49
6:L5:1332:C:H2'	6:L5:1333:A:C8	2.47	0.49
6:L5:1500:A:H5''	6:L5:1501:C:H5''	1.95	0.49
6:L5:1743:A:N1	6:L5:1789:C:O2'	2.44	0.49
6:L5:1998:A:O2'	6:L5:1999:A:O4'	2.29	0.49
6:L5:2744:A:H2'	6:L5:2745:A:C8	2.47	0.49
6:L5:4225:G:OP1	17:LI:24:ARG:NH2	2.39	0.49
6:L5:4457:PSU:H1'	10:LB:252:ALA:HB3	1.95	0.49
6:L5:4935:C:H2'	6:L5:4936:G:C8	2.47	0.49
18:LJ:22:LEU:HD22	18:LJ:128:LEU:HD12	1.94	0.49
19:LL:56:ARG:NH1	19:LL:74:ARG:O	2.40	0.49
30:LW:56:ARG:HE	30:LW:61:LYS:CB	2.26	0.49
47:Ln:12:ARG:HG2	47:Ln:15:ARG:HH21	1.78	0.49
54:SF:49:LEU:HD12	54:SF:50:PRO:HD2	1.94	0.49
54:SF:161:ALA:O	54:SF:165:ASN:ND2	2.40	0.49
55:SK:41:PRO:HG2	55:SK:44:HIS:CG	2.48	0.49
72:SG:172:LYS:NZ	86:S2:67:C:OP2	2.34	0.49
77:SN:29:THR:OG1	77:SN:31:ASP:OD1	2.27	0.49
6:L5:158:A:H5''	6:L5:159:C:H2'	1.96	0.48
6:L5:2716:C:O3'	28:LU:107:LYS:NZ	2.46	0.48
6:L5:3664:G:H2'	6:L5:3665:G:H8	1.78	0.48
26:LS:99:ASP:OD1	26:LS:100:LEU:N	2.43	0.48
38:Le:108:ARG:HD2	38:Le:128:ARG:HB2	1.93	0.48
58:SQ:96:TYR:HA	58:SQ:100:VAL:HG12	1.95	0.48
69:SB:171:ILE:HG22	69:SB:174:ARG:HE	1.78	0.48
85:Se:11:LYS:O	85:Se:15:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:S2:84:A:N3	86:S2:150:A:O2'	2.46	0.48
5:AT:67:C:H2'	5:AT:68:G:H8	1.78	0.48
6:L5:1326:A2M:H2'	6:L5:1327:C:C6	2.48	0.48
6:L5:1503:A:H4'	6:L5:1504:G:H5'	1.95	0.48
11:LC:154:VAL:HG11	11:LC:174:LEU:HD11	1.95	0.48
13:LE:119:GLU:HG3	38:Le:7:LEU:HD22	1.94	0.48
35:Lb:5:LYS:HE2	35:Lb:8:THR:HB	1.94	0.48
73:SH:69:LEU:HD13	73:SH:96:ALA:HB2	1.96	0.48
79:SV:30:ALA:O	79:SV:60:ARG:HD3	2.13	0.48
84:Sb:49:HIS:ND1	84:Sb:69:GLY:O	2.46	0.48
86:S2:1533:A:H62	86:S2:1602:U:H3	1.61	0.48
86:S2:1568:C:H2'	86:S2:1569:A:C8	2.48	0.48
86:S2:1595:U:H2'	86:S2:1596:U:C6	2.48	0.48
6:L5:121:A:H62	6:L5:152:U:H3	1.62	0.48
6:L5:369:G:N2	6:L5:372:A:OP2	2.42	0.48
6:L5:497:G:N2	6:L5:498:C:H41	2.11	0.48
6:L5:1344:C:H1'	19:LL:10:LEU:HD11	1.95	0.48
6:L5:1866:U:OP1	17:LI:4:ARG:NH1	2.36	0.48
6:L5:2903:G:H1'	6:L5:2904:U:H5	1.78	0.48
6:L5:3619:G:H22	6:L5:3624:A:H1'	1.77	0.48
6:L5:4940:C:O2'	13:LE:246:ARG:NH2	2.45	0.48
9:LA:180:LEU:HD22	49:Lp:18:TYR:HB3	1.96	0.48
38:Le:91:CYS:HB3	38:Le:95:TYR:HD2	1.77	0.48
64:Sc:39:SER:HB2	83:Sa:51:ARG:HH12	1.77	0.48
66:Sf:95:ARG:HH12	86:S2:1291:A:H62	1.60	0.48
67:Sg:207:CYS:HB3	67:Sg:221:LEU:HD21	1.95	0.48
68:SA:134:LEU:HD21	68:SA:144:THR:HG21	1.96	0.48
74:SI:54:LYS:NZ	86:S2:381:C:OP2	2.45	0.48
3:Et:55:U:H2'	3:Et:57:A:N7	2.28	0.48
5:AT:3:C:H42	5:AT:71:A:H61	1.60	0.48
6:L5:467:U:C4	6:L5:468:U:H1'	2.48	0.48
6:L5:1320:U:O2'	6:L5:1891:A:N1	2.45	0.48
6:L5:1461:C:H2'	6:L5:1462:A:C8	2.48	0.48
6:L5:4584:A:H2'	6:L5:4585:U:O4'	2.13	0.48
16:LH:41:ILE:HG22	16:LH:43:VAL:HG13	1.95	0.48
16:LH:61:TRP:CZ3	20:LM:33:GLN:HG3	2.49	0.48
17:LI:54:SER:HB3	17:LI:135:ILE:HD11	1.95	0.48
23:LP:54:GLN:HA	23:LP:83:TRP:CD1	2.47	0.48
31:LX:122:ALA:N	31:LX:139:ARG:O	2.43	0.48
67:Sg:82:SER:OG	67:Sg:83:TRP:N	2.45	0.48
69:SB:85:LYS:HB2	69:SB:101:HIS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SI:89:GLU:OE1	74:SI:92:ARG:NH2	2.46	0.48
86:S2:5:U:H2'	86:S2:6:G:H8	1.78	0.48
86:S2:106:C:H2'	86:S2:107:A:C8	2.46	0.48
86:S2:1144:A:H2'	86:S2:1145:A:C8	2.48	0.48
86:S2:1652:G:H1	86:S2:1672:U:H3	1.60	0.48
6:L5:1095:A:N1	6:L5:1200:G:C6	2.81	0.48
6:L5:1324:A:O2'	6:L5:1326:A2M:OP1	2.24	0.48
6:L5:2049:G:HO2'	6:L5:3884:PSU:HO2'	1.54	0.48
6:L5:2588:C:OP1	6:L5:2768:C:O2'	2.27	0.48
6:L5:4769:G:H5''	22:LO:176:ARG:HD3	1.96	0.48
11:LC:268:ARG:NH1	11:LC:269:LYS:HE2	2.29	0.48
15:LG:150:LYS:NZ	15:LG:177:MET:O	2.46	0.48
82:SY:29:HIS:O	82:SY:67:GLY:HA2	2.14	0.48
86:S2:1115:U:O2'	86:S2:1117:C:OP2	2.30	0.48
6:L5:1326:A2M:HM'3	6:L5:1326:A2M:H1'	1.63	0.48
6:L5:4347:G:H2'	6:L5:4348:A:C8	2.48	0.48
74:SI:25:ARG:HA	86:S2:448:A:H5''	1.95	0.48
86:S2:1438:A:H2'	86:S2:1439:A:C8	2.49	0.48
3:Et:35:U:H2'	3:Et:36:U:H6	1.78	0.48
6:L5:172:C:H4'	6:L5:173:C:H5'	1.96	0.48
6:L5:423:G:H21	23:LP:118:GLN:NE2	2.10	0.48
6:L5:500:G:H1'	6:L5:504:G:H3'	1.95	0.48
6:L5:4345:C:H2'	6:L5:4346:U:C6	2.48	0.48
10:LB:153:MET:HB3	10:LB:194:LEU:HD11	1.95	0.48
18:LJ:63:ARG:HH11	48:Lo:106:PHE:HB2	1.79	0.48
54:SF:142:SER:HB3	64:Sc:50:VAL:HG22	1.94	0.48
55:SK:32:HIS:CD2	55:SK:45:VAL:HG11	2.48	0.48
56:SM:128:PHE:HA	56:SM:131:LYS:HG2	1.96	0.48
58:SQ:110:ASP:OD1	58:SQ:111:ILE:HD12	2.13	0.48
63:SZ:42:ASP:OD1	63:SZ:42:ASP:N	2.44	0.48
66:Sf:139:HIS:O	66:Sf:147:THR:HA	2.13	0.48
67:Sg:166:VAL:HG12	67:Sg:176:VAL:HG12	1.95	0.48
72:SG:202:ASN:ND2	86:S2:125:C:OP1	2.39	0.48
73:SH:51:ILE:HD11	73:SH:176:VAL:HG12	1.96	0.48
74:SI:57:ALA:HB2	74:SI:183:GLY:HA2	1.95	0.48
86:S2:17:C:O2'	86:S2:1194:A:N1	2.38	0.48
86:S2:1337:4AC:H2'	86:S2:1338:G:H8	1.78	0.48
86:S2:1435:C:O2'	86:S2:1436:C:O4'	2.30	0.48
5:AT:3:C:H2'	5:AT:4:U:H6	1.77	0.48
6:L5:1367:C:O2'	6:L5:1369:C:OP2	2.26	0.48
6:L5:2583:C:OP2	40:Lg:76:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4113:U:H4'	6:L5:4115:G:C6	2.48	0.48
6:L5:4897:G:OP1	20:LM:128:LYS:NZ	2.45	0.48
11:LC:141:GLY:O	11:LC:204:ARG:NH1	2.35	0.48
16:LH:114:ILE:HB	16:LH:124:ARG:HB2	1.95	0.48
19:LL:142:GLU:HA	19:LL:146:LEU:HD12	1.95	0.48
25:LR:127:VAL:HG12	25:LR:132:PHE:HD2	1.78	0.48
28:LU:63:ILE:HD13	28:LU:72:VAL:HG22	1.96	0.48
60:SS:64:VAL:O	60:SS:68:ILE:HG12	2.13	0.48
86:S2:329:G:H2'	86:S2:330:G:C8	2.49	0.48
86:S2:907:G:H2'	86:S2:908:A:C8	2.48	0.48
6:L5:2411:C:H2'	6:L5:2412:A:C8	2.49	0.48
6:L5:4305:G:N7	27:LT:87:LYS:NZ	2.53	0.48
6:L5:4769:G:OP1	22:LO:176:ARG:NH1	2.43	0.48
8:L8:19:C:H2'	8:L8:20:A:C8	2.48	0.48
12:LD:234:ASP:OD1	12:LD:235:MET:N	2.47	0.48
14:LF:127:LYS:HB2	27:LT:133:ALA:HB3	1.96	0.48
14:LF:237:GLU:HG2	26:LS:38:VAL:HG22	1.96	0.48
62:SU:56:MET:HB2	62:SU:86:LYS:HG3	1.95	0.48
69:SB:168:MET:HB2	69:SB:197:ILE:HD13	1.96	0.48
73:SH:30:LEU:O	73:SH:33:ASN:ND2	2.47	0.48
4:CF:323:GLY:HA2	4:CF:365:THR:HB	1.96	0.48
6:L5:138:G:H2'	6:L5:139:G:H8	1.79	0.48
6:L5:737:C:C5	6:L5:739:G:H5''	2.49	0.48
6:L5:1095:A:C2	6:L5:1200:G:N1	2.65	0.48
6:L5:2018:C:H2'	6:L5:2019:C:H6	1.79	0.48
6:L5:2846:G:OP1	29:LV:85:ARG:NH2	2.47	0.48
6:L5:3732:A:H2'	6:L5:3733:A:C8	2.49	0.48
7:L7:23:A:N3	7:L7:118:C:O2'	2.36	0.48
12:LD:86:TYR:HE1	12:LD:247:ILE:HG13	1.78	0.48
23:LP:114:ILE:HA	23:LP:150:LEU:HD23	1.96	0.48
59:SR:29:HIS:CD2	67:Sg:36:ARG:HH21	2.32	0.48
61:ST:40:ALA:HB3	61:ST:43:LYS:HG2	1.96	0.48
63:SZ:85:ARG:NH2	86:S2:1597:C:OP2	2.39	0.48
71:SE:192:ILE:HG12	71:SE:243:GLY:HA3	1.96	0.48
77:SN:15:ALA:HB2	84:Sb:20:LYS:HD3	1.95	0.48
81:SX:105:PHE:CD1	81:SX:121:LYS:HB3	2.45	0.48
6:L5:374:G:OP2	43:Lj:56:ARG:NH1	2.38	0.47
6:L5:490:C:H2'	6:L5:491:G:C8	2.48	0.47
6:L5:1942:A:H2'	6:L5:1943:A:H8	1.78	0.47
10:LB:27:GLY:HA2	10:LB:276:HIS:CD2	2.49	0.47
28:LU:39:PHE:HD1	28:LU:90:TYR:CD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SF:26:ASP:N	54:SF:26:ASP:OD1	2.46	0.47
54:SF:83:ASN:OD1	86:S2:1651:A:O2'	2.28	0.47
69:SB:171:ILE:HD11	69:SB:197:ILE:HA	1.95	0.47
84:Sb:11:SER:OG	84:Sb:14:GLU:OE1	2.30	0.47
6:L5:178:C:N4	6:L5:179:G:O6	2.47	0.47
6:L5:1176:C:H42	6:L5:1184:A:H61	1.61	0.47
6:L5:4622:A:H4'	10:LB:13:SER:HB2	1.95	0.47
10:LB:14:LEU:HD22	10:LB:17:LEU:HD11	1.94	0.47
19:LL:110:LEU:O	19:LL:114:VAL:HG13	2.15	0.47
29:LV:43:LYS:HE2	29:LV:62:MET:HE3	1.95	0.47
67:Sg:212:LYS:HA	67:Sg:235:ILE:HG13	1.95	0.47
82:SY:105:LYS:O	82:SY:109:GLU:HG2	2.14	0.47
83:Sa:13:LYS:HD3	83:Sa:13:LYS:HA	1.71	0.47
86:S2:325:C:N3	86:S2:326:C:O2'	2.45	0.47
86:S2:1383:A2M:HM'3	86:S2:1383:A2M:H1'	1.64	0.47
6:L5:256:G:H2'	6:L5:257:C:C6	2.49	0.47
6:L5:519:C:H1'	6:L5:643:C:C2	2.49	0.47
6:L5:667:A:H5''	6:L5:668:C:H5''	1.96	0.47
6:L5:2029:A:H2'	6:L5:2030:A:C8	2.48	0.47
6:L5:4095:G:H2'	6:L5:4096:C:C6	2.50	0.47
6:L5:4149:C:OP1	33:LZ:59:LYS:N	2.47	0.47
8:L8:150:C:N4	15:LG:52:THR:O	2.47	0.47
14:LF:213:LEU:HB3	14:LF:247:MET:HG3	1.97	0.47
14:LF:241:ASN:O	14:LF:245:ARG:HG2	2.14	0.47
16:LH:89:ARG:HD3	16:LH:91:LYS:HE3	1.96	0.47
17:LI:36:LEU:HD11	17:LI:69:ARG:HD2	1.97	0.47
25:LR:157:ASP:OD1	25:LR:158:GLN:N	2.47	0.47
41:Lh:89:ARG:O	41:Lh:93:ARG:HG2	2.15	0.47
54:SF:19:LEU:HD11	54:SF:50:PRO:HD3	1.95	0.47
55:SK:42:ASN:HA	55:SK:45:VAL:HG12	1.96	0.47
67:Sg:133:ASN:HB3	67:Sg:139:LYS:HD2	1.97	0.47
72:SG:162:LEU:HG	72:SG:167:LYS:HE3	1.95	0.47
86:S2:1550:G:O2'	86:S2:1558:C:O2	2.25	0.47
6:L5:1461:C:H2'	6:L5:1462:A:H8	1.78	0.47
6:L5:1727:U:OP1	14:LF:131:ASN:ND2	2.46	0.47
6:L5:2811:G:N1	6:L5:2814:C:OP2	2.42	0.47
6:L5:4301:U:OP2	6:L5:4303:C:N4	2.47	0.47
51:Ls:114:GLY:HA2	51:Ls:166:LYS:HD2	1.96	0.47
56:SM:110:VAL:O	56:SM:112:LYS:NZ	2.45	0.47
67:Sg:124:SER:OG	67:Sg:125:ARG:N	2.46	0.47
86:S2:223:C:H2'	86:S2:224:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:S2:329:G:H2'	86:S2:330:G:H8	1.79	0.47
6:L5:97:G:OP1	19:LL:16:LYS:NZ	2.37	0.47
6:L5:170:C:H42	6:L5:266:C:N4	2.12	0.47
6:L5:2284:G:OP1	34:La:7:LYS:NZ	2.43	0.47
6:L5:2411:C:H2'	6:L5:2412:A:H8	1.78	0.47
6:L5:2580:U:OP1	33:LZ:36:ARG:NH1	2.41	0.47
6:L5:2640:G:H2'	6:L5:2641:A:C8	2.50	0.47
6:L5:3917:A:H2'	6:L5:3918:G:H8	1.79	0.47
8:L8:75:OMG:HM23	8:L8:75:OMG:H1'	1.70	0.47
21:LN:140:LYS:HD3	21:LN:140:LYS:HA	1.66	0.47
58:SQ:102:GLU:HA	58:SQ:105:LYS:HB3	1.97	0.47
67:Sg:39:THR:HG22	67:Sg:60:ARG:HG2	1.96	0.47
71:SE:247:THR:OG1	71:SE:250:GLU:OE1	2.33	0.47
72:SG:191:ARG:HH22	86:S2:312:G:H2'	1.80	0.47
86:S2:17:C:H2'	86:S2:18:C:C6	2.49	0.47
86:S2:604:A:N3	86:S2:639:C:O2'	2.42	0.47
86:S2:996:A:H2'	86:S2:997:A:C8	2.49	0.47
6:L5:169:G:O6	6:L5:170:C:N4	2.48	0.47
6:L5:1194:G:H2'	6:L5:1195:G:C8	2.50	0.47
6:L5:3661:G:N7	9:LA:152:SER:OG	2.44	0.47
10:LB:29:VAL:HG12	10:LB:31:SER:H	1.80	0.47
27:LT:102:ARG:O	27:LT:106:LEU:HG	2.14	0.47
61:ST:83:GLN:OE1	61:ST:93:SER:OG	2.30	0.47
86:S2:747:U:C2	86:S2:796:G:N1	2.83	0.47
86:S2:1491:G:H2'	86:S2:1492:U:C6	2.49	0.47
6:L5:99:A:H5''	21:LN:184:ILE:HD12	1.96	0.47
6:L5:257:C:H2'	6:L5:258:G:C8	2.50	0.47
6:L5:1396:G:HO2'	6:L5:1468:C:HO2'	1.56	0.47
6:L5:1846:G:H2'	6:L5:1847:C:C6	2.49	0.47
6:L5:1855:G:OP1	35:Lb:4:SER:HB2	2.14	0.47
6:L5:1899:G:O2'	38:Le:57:ASN:OD1	2.31	0.47
6:L5:2910:G:N2	6:L5:3585:G:O2'	2.47	0.47
6:L5:4251:A:H5''	18:LJ:108:GLY:HA3	1.96	0.47
14:LF:57:TYR:OH	14:LF:189:ASP:OD1	2.30	0.47
16:LH:115:ARG:HD3	16:LH:123:ILE:HD12	1.96	0.47
24:LQ:154:LYS:NZ	24:LQ:159:PRO:O	2.46	0.47
50:Lr:119:ARG:HA	50:Lr:122:LYS:HE3	1.95	0.47
53:SD:32:ASP:OD2	53:SD:65:ARG:NH1	2.48	0.47
53:SD:77:PHE:HB2	53:SD:79:PHE:CE1	2.49	0.47
55:SK:32:HIS:HD2	55:SK:45:VAL:HG11	1.80	0.47
61:ST:84:ARG:NH1	86:S2:1605:G:OP1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sf:105:TYR:HE1	66:Sf:131:PHE:HD2	1.62	0.47
70:SC:110:MET:HG2	70:SC:125:LYS:HB3	1.97	0.47
70:SC:227:ARG:NH2	86:S2:663:C:O2'	2.47	0.47
71:SE:127:ARG:HG3	71:SE:142:HIS:HA	1.96	0.47
79:SV:74:LYS:HZ1	79:SV:83:PHE:HB3	1.80	0.47
86:S2:16:G:H2'	86:S2:17:C:C6	2.50	0.47
86:S2:349:A:H2'	86:S2:350:C:C6	2.49	0.47
86:S2:520:A:O2'	86:S2:825:A:N3	2.40	0.47
4:CF:107:SER:HB3	4:CF:143:LEU:HD13	1.96	0.47
4:CF:287:THR:HG21	4:CF:312:VAL:HB	1.96	0.47
6:L5:1194:G:H2'	6:L5:1195:G:H8	1.80	0.47
6:L5:1877:G:O6	35:Lb:10:HIS:NE2	2.46	0.47
6:L5:1932:A:OP1	22:LO:49:ARG:NH2	2.27	0.47
13:LE:223:ARG:HB3	13:LE:224:LYS:HB2	1.96	0.47
14:LF:182:TYR:HB3	14:LF:200:ARG:HG3	1.96	0.47
16:LH:4:ILE:HG12	16:LH:61:TRP:CH2	2.50	0.47
20:LM:130:LEU:HB3	22:LO:177:LEU:HD11	1.96	0.47
24:LQ:50:ARG:HH21	24:LQ:140:SER:HB2	1.80	0.47
67:Sg:120:ILE:HB	67:Sg:132:TRP:HB2	1.97	0.47
69:SB:23:ASP:N	69:SB:23:ASP:OD1	2.48	0.47
74:SI:4:SER:OG	74:SI:6:ASP:OD2	2.26	0.47
86:S2:66:G:H2'	86:S2:67:C:H4'	1.97	0.47
86:S2:159:A2M:HM'3	86:S2:159:A2M:H1'	1.58	0.47
3:Et:51:G:H2'	3:Et:52:G:C8	2.50	0.47
4:CF:15:HIS:HE1	4:CF:132:GLN:H	1.62	0.47
6:L5:715:G:OP1	11:LC:321:ASN:ND2	2.44	0.47
6:L5:2382:A:N1	6:L5:2829:U:O2'	2.45	0.47
6:L5:3923:A:H2'	6:L5:3924:C:C6	2.50	0.47
6:L5:4441:A:H5''	17:LI:114:GLY:HA2	1.97	0.47
15:LG:154:LEU:HB3	15:LG:204:PHE:HB2	1.97	0.47
51:Ls:91:THR:HG21	51:Ls:98:ILE:HG13	1.97	0.47
75:SJ:64:ASP:OD1	75:SJ:65:GLU:N	2.48	0.47
83:Sa:87:ARG:NH1	83:Sa:94:ASP:OD1	2.48	0.47
85:Se:41:ARG:HG3	85:Se:42:PHE:HD1	1.80	0.47
85:Se:41:ARG:HG3	85:Se:42:PHE:CD1	2.50	0.47
86:S2:1144:A:H5'	86:S2:1355:C:H41	1.80	0.47
86:S2:1736:G:H2'	86:S2:1737:G:C8	2.49	0.47
4:CF:214:TRP:CZ2	4:CF:231:ALA:HB2	2.50	0.47
6:L5:1298:C:H2'	6:L5:1299:G:C8	2.50	0.47
6:L5:2021:G:OP1	51:Ls:58:ASN:N	2.44	0.47
6:L5:3799:A:N3	6:L5:4506:C:O2'	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:3841:OMC:HM23	6:L5:3841:OMC:H1'	1.76	0.47
6:L5:4742:G:H2'	6:L5:4743:G:H8	1.80	0.47
15:LG:162:ASP:HB3	15:LG:163:PRO:HD3	1.96	0.47
18:LJ:56:THR:OG1	18:LJ:64:ARG:N	2.44	0.47
54:SF:187:SER:OG	54:SF:190:ILE:HG12	2.15	0.47
68:SA:206:ASP:HB3	68:SA:209:GLU:OE1	2.15	0.47
86:S2:793:G:H2'	86:S2:794:A:H8	1.80	0.47
5:AT:22:A:H2'	5:AT:23:U:C6	2.51	0.46
5:AT:24:C:N3	5:AT:25:A:N6	2.62	0.46
6:L5:106:A:H2'	6:L5:107:G:O4'	2.15	0.46
6:L5:444:G:H2'	6:L5:445:U:C6	2.50	0.46
6:L5:1188:C:H2'	6:L5:1189:G:H8	1.80	0.46
6:L5:1333:A:H2'	6:L5:1334:A:H8	1.78	0.46
6:L5:1601:A:OP1	43:Lj:5:THR:OG1	2.22	0.46
6:L5:1995:G:H2'	6:L5:1996:C:C6	2.50	0.46
6:L5:2299:G:O6	11:LC:188:ARG:NH2	2.48	0.46
6:L5:3908:A:N7	6:L5:4449:A:N6	2.63	0.46
6:L5:4954:G:H2'	6:L5:4955:A:C8	2.49	0.46
9:LA:206:PRO:HG3	9:LA:213:GLY:HA3	1.96	0.46
12:LD:205:ALA:HB1	12:LD:233:PRO:HB3	1.97	0.46
21:LN:75:VAL:HG21	21:LN:80:THR:HG22	1.97	0.46
53:SD:115:VAL:HG21	53:SD:138:VAL:HG11	1.97	0.46
58:SQ:8:GLN:HG3	58:SQ:27:ARG:HE	1.80	0.46
67:Sg:289:LEU:HD11	67:Sg:298:LEU:HD21	1.97	0.46
82:SY:77:ASP:OD1	82:SY:77:ASP:N	2.47	0.46
86:S2:51:U:H2'	86:S2:52:G:C8	2.50	0.46
86:S2:454:U:H2'	86:S2:455:A:H8	1.80	0.46
86:S2:656:G:N2	86:S2:663:C:H5''	2.30	0.46
86:S2:656:G:H5'	86:S2:662:G:N2	2.30	0.46
86:S2:1692:U:H2'	86:S2:1693:G:C8	2.50	0.46
6:L5:497:G:H21	6:L5:498:C:H41	1.63	0.46
6:L5:2298:U:OP1	11:LC:204:ARG:NE	2.47	0.46
6:L5:3950:U:H3	6:L5:4063:U:H3	1.62	0.46
6:L5:4504:C:H2'	6:L5:4505:C:C6	2.50	0.46
24:LQ:3:VAL:HG13	24:LQ:5:ILE:HG12	1.97	0.46
36:Lc:47:ILE:HD12	36:Lc:94:LEU:HD11	1.96	0.46
53:SD:223:ILE:HD11	67:Sg:189:ILE:HD12	1.97	0.46
55:SK:7:ASN:HB2	55:SK:40:VAL:HG22	1.98	0.46
68:SA:102:ARG:NH1	86:S2:1378:A:OP2	2.46	0.46
70:SC:70:VAL:HG21	70:SC:93:ILE:HG23	1.97	0.46
72:SG:85:ARG:O	72:SG:87:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:S2:528:A:H2'	86:S2:529:A:C8	2.50	0.46
86:S2:1286:G:N2	86:S2:1312:G:O2'	2.49	0.46
86:S2:1337:4AC:H2'	86:S2:1338:G:C8	2.50	0.46
3:Et:12:U:H2'	3:Et:13:C:C6	2.51	0.46
6:L5:907:C:H2'	6:L5:908:G:H8	1.81	0.46
6:L5:908:G:H2'	6:L5:909:A:H8	1.79	0.46
6:L5:1308:C:OP1	22:LO:93:LYS:NZ	2.46	0.46
6:L5:1408:G:O2'	6:L5:1411:C:N4	2.48	0.46
6:L5:1696:C:H5'	6:L5:1719:A:H1'	1.97	0.46
6:L5:2725:A:N6	25:LR:88:ARG:O	2.48	0.46
6:L5:4115:G:O2'	6:L5:4116:C:O5'	2.32	0.46
15:LG:83:PHE:HA	15:LG:183:ILE:HD13	1.97	0.46
22:LO:166:ILE:HG12	22:LO:169:ARG:HH21	1.80	0.46
23:LP:122:ALA:HB3	23:LP:143:PRO:HG2	1.97	0.46
38:Le:76:LYS:HD2	38:Le:98:GLU:CD	2.41	0.46
58:SQ:139:ALA:HB2	86:S2:1650:A:H5''	1.96	0.46
61:ST:42:HIS:NE2	61:ST:43:LYS:HE3	2.30	0.46
61:ST:114:GLU:OE1	61:ST:114:GLU:N	2.47	0.46
81:SX:90:CYS:HA	81:SX:93:PHE:HD2	1.79	0.46
86:S2:51:U:H2'	86:S2:52:G:H8	1.81	0.46
86:S2:468:A2M:HM'3	86:S2:468:A2M:H1'	1.68	0.46
86:S2:693:A:H2'	86:S2:694:G:C8	2.51	0.46
86:S2:962:A:N1	86:S2:1055:A:O2'	2.47	0.46
86:S2:1755:C:H2'	86:S2:1756:C:C6	2.51	0.46
4:CF:193:ILE:HG21	4:CF:228:LEU:HD11	1.97	0.46
6:L5:965:G:N2	6:L5:2092:G:H1'	2.30	0.46
18:LJ:83:LEU:HD22	18:LJ:132:VAL:HG11	1.97	0.46
20:LM:96:GLU:O	20:LM:100:ARG:HG2	2.15	0.46
29:LV:42:VAL:HB	29:LV:45:ILE:HG13	1.98	0.46
65:Sd:14:PHE:HB2	86:S2:1661:A:H8	1.81	0.46
69:SB:186:ASN:HA	69:SB:189:ILE:HD12	1.98	0.46
71:SE:100:ARG:NH2	71:SE:118:GLU:OE2	2.48	0.46
73:SH:145:ARG:HE	80:SW:51:GLU:HB2	1.81	0.46
86:S2:598:G:O2'	86:S2:605:A:N1	2.46	0.46
86:S2:1189:A:H2'	86:S2:1190:A:H8	1.81	0.46
86:S2:1656:G:H1	86:S2:1668:U:H3	1.63	0.46
6:L5:2111:G:N2	6:L5:2251:G:O2'	2.48	0.46
6:L5:2112:G:H5''	6:L5:2251:G:H1	1.79	0.46
37:Ld:53:ALA:HA	37:Ld:88:LEU:HD21	1.97	0.46
54:SF:103:LEU:HD11	63:SZ:67:LEU:HD22	1.97	0.46
59:SR:52:GLY:O	59:SR:55:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sf:124:ASP:OD1	66:Sf:124:ASP:N	2.45	0.46
72:SG:2:LYS:HB3	72:SG:15:LEU:HD11	1.97	0.46
75:SJ:145:PRO:HD2	86:S2:522:A:H5''	1.98	0.46
77:SN:5:HIS:HB3	77:SN:117:LEU:HD13	1.98	0.46
86:S2:1643:U:H2'	86:S2:1644:C:C6	2.50	0.46
3:Et:7:A:O2'	3:Et:49:C:O4'	2.30	0.46
3:Et:26:A:N6	3:Et:44:G:N1	2.35	0.46
4:CF:62:LYS:O	4:CF:67:ARG:NH1	2.48	0.46
6:L5:300:A:H2'	6:L5:301:G:H8	1.81	0.46
6:L5:1414:C:H2'	6:L5:1415:G:C8	2.47	0.46
6:L5:1695:U:O2'	6:L5:1719:A:N3	2.39	0.46
6:L5:4476:C:O2'	6:L5:4478:G:OP2	2.26	0.46
6:L5:4543:G:H2'	6:L5:4544:A:C8	2.50	0.46
8:L8:96:C:H5''	41:Lh:66:LYS:HG2	1.98	0.46
13:LE:161:ARG:O	13:LE:182:ASN:ND2	2.49	0.46
14:LF:46:ARG:HH21	35:Lb:102:PRO:HG3	1.81	0.46
36:Lc:48:LEU:HD13	36:Lc:57:LYS:HG3	1.98	0.46
64:Sc:10:LYS:HE2	64:Sc:34:PHE:HD2	1.81	0.46
74:SI:141:ARG:NH2	86:S2:192:C:OP2	2.49	0.46
74:SI:149:TYR:O	74:SI:153:LYS:HG2	2.16	0.46
80:SW:27:ILE:HG13	80:SW:61:ILE:HB	1.97	0.46
84:Sb:68:GLY:O	86:S2:928:G:N2	2.44	0.46
5:AT:18:G:H21	5:AT:59:A:H5'	1.81	0.46
6:L5:455:C:O2'	6:L5:456:C:H5'	2.15	0.46
6:L5:1390:G:N2	6:L5:1393:G:OP2	2.40	0.46
6:L5:3867:A2M:HM'3	6:L5:3867:A2M:H1'	1.65	0.46
10:LB:302:ASN:HB2	10:LB:313:SER:HA	1.98	0.46
54:SF:127:ARG:HG2	54:SF:136:ARG:HB2	1.98	0.46
60:SS:137:LYS:NZ	86:S2:1236:G:O6	2.49	0.46
67:Sg:10:THR:HG22	67:Sg:308:ARG:HG2	1.97	0.46
68:SA:184:ARG:HG2	68:SA:189:ILE:HB	1.97	0.46
69:SB:136:ARG:HB3	69:SB:216:LYS:HG3	1.96	0.46
69:SB:214:LYS:NZ	86:S2:943:U:OP1	2.39	0.46
73:SH:126:HIS:CE1	73:SH:181:THR:HG23	2.51	0.46
81:SX:52:LEU:HD11	81:SX:73:GLN:HB2	1.97	0.46
86:S2:5:U:H2'	86:S2:6:G:C8	2.51	0.46
86:S2:327:G:H5''	86:S2:328:U:C2	2.50	0.46
86:S2:1775:U:H2'	86:S2:1776:G:C2	2.51	0.46
4:CF:127:ILE:HG13	4:CF:134:ARG:HD3	1.97	0.46
6:L5:4088:C:H2'	6:L5:4089:G:C8	2.51	0.46
11:LC:183:VAL:HA	11:LC:204:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LW:7:SER:HB2	30:LW:13:ILE:HD11	1.97	0.46
32:LY:10:ASP:HB3	32:LY:13:LYS:HB2	1.98	0.46
34:La:72:THR:HG22	34:La:110:LYS:HB3	1.98	0.46
70:SC:121:ARG:HH12	70:SC:123:ARG:HE	1.63	0.46
70:SC:271:ASP:OD1	70:SC:272:HIS:N	2.49	0.46
71:SE:134:LYS:N	86:S2:298:G:OP1	2.45	0.46
73:SH:30:LEU:HG	73:SH:33:ASN:HD22	1.81	0.46
74:SI:126:GLY:O	74:SI:128:LYS:NZ	2.48	0.46
86:S2:102:A:H4'	86:S2:104:A:C8	2.51	0.46
86:S2:1189:A:H2'	86:S2:1190:A:C8	2.51	0.46
6:L5:162:A:H2'	6:L5:163:A:C8	2.51	0.46
6:L5:1647:U:OP1	89:L5:5288:SPD:H51	2.16	0.46
6:L5:2474:G:H2'	6:L5:2502:G:N2	2.30	0.46
9:LA:116:LEU:HB3	9:LA:126:LEU:HB2	1.96	0.46
13:LE:261:ILE:HG23	13:LE:267:LEU:HD23	1.97	0.46
52:Lt:28:LEU:HD23	52:Lt:28:LEU:H	1.81	0.46
58:SQ:37:ARG:NH2	86:S2:1543:U:OP1	2.39	0.46
60:SS:37:GLY:N	86:S2:1630:A:H5'	2.31	0.46
72:SG:4:ASN:ND2	86:S2:154:U:O2	2.47	0.46
74:SI:98:LYS:HG3	74:SI:178:ARG:HG2	1.98	0.46
80:SW:62:VAL:HG11	84:Sb:8:LEU:HG	1.97	0.46
82:SY:76:TYR:OH	82:SY:86:GLU:OE1	2.19	0.46
86:S2:420:G:O2'	86:S2:660:C:N3	2.45	0.46
4:CF:255:LYS:HB2	4:CF:317:VAL:HG11	1.98	0.46
6:L5:197:A:N1	6:L5:225:G:O2'	2.47	0.46
6:L5:233:U:HO2'	6:L5:234:G:H8	1.63	0.46
6:L5:417:G:OP1	6:L5:2329:U:O2'	2.28	0.46
6:L5:1398:A:N1	6:L5:1419:G:O2'	2.48	0.46
6:L5:1725:U:H2'	6:L5:1726:U:H6	1.81	0.46
6:L5:2033:A:OP1	17:LI:162:ARG:NH2	2.46	0.46
88:L5:5290:SPM:H31	88:L5:5290:SPM:H62	1.79	0.46
7:L7:120:U:H5''	12:LD:262:LYS:HG2	1.96	0.46
12:LD:181:PRO:HD2	12:LD:195:HIS:CD2	2.51	0.46
14:LF:162:ILE:HD12	14:LF:167:ILE:HB	1.98	0.46
23:LP:52:THR:HG23	23:LP:85:LYS:HG3	1.98	0.46
39:Lf:45:LYS:NZ	39:Lf:108:SER:HA	2.31	0.46
40:Lg:82:MET:HE3	40:Lg:82:MET:HB2	1.88	0.46
50:Lr:47:LYS:O	50:Lr:103:ARG:HD2	2.16	0.46
56:SM:87:GLU:HG3	56:SM:103:VAL:HG11	1.98	0.46
71:SE:59:ASP:O	71:SE:63:LYS:HG3	2.16	0.46
73:SH:33:ASN:ND2	73:SH:36:LEU:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SI:44:HIS:ND1	86:S2:1740:C:OP1	2.38	0.46
86:S2:1420:G:O2'	86:S2:1421:A:N3	2.49	0.46
86:S2:1667:U:H2'	86:S2:1668:U:C6	2.50	0.46
4:CF:178:ILE:HA	4:CF:181:ILE:HG22	1.98	0.45
6:L5:659:G:H2'	6:L5:660:A:C8	2.50	0.45
6:L5:1340:OMC:HM23	6:L5:1340:OMC:H1'	1.75	0.45
6:L5:2580:U:O2'	33:LZ:79:HIS:ND1	2.44	0.45
6:L5:2724:G:O2'	6:L5:2726:G:OP2	2.31	0.45
12:LD:179:ARG:HD3	12:LD:179:ARG:HA	1.72	0.45
15:LG:187:LYS:HB2	15:LG:198:THR:HG23	1.97	0.45
68:SA:74:VAL:HG23	68:SA:121:LEU:HB3	1.97	0.45
76:SL:132:ARG:HD3	86:S2:114:G:H5'	1.97	0.45
81:SX:60:LYS:H	81:SX:114:ASP:HB2	1.81	0.45
4:CF:346:ILE:HD13	4:CF:353:ILE:HD13	1.97	0.45
5:AT:4:U:H2'	5:AT:5:C:H6	1.80	0.45
6:L5:4389:C:H2'	6:L5:4390:A:C8	2.51	0.45
6:L5:4775:C:H41	6:L5:4859:C:N4	2.14	0.45
6:L5:5004:C:H2'	6:L5:5005:G:O4'	2.15	0.45
9:LA:114:CYS:N	9:LA:165:VAL:O	2.49	0.45
16:LH:93:ARG:HG2	16:LH:182:SER:HB3	1.97	0.45
25:LR:175:GLU:O	25:LR:178:GLN:HG3	2.17	0.45
57:SP:22:LEU:HA	57:SP:25:LEU:HB2	1.99	0.45
61:ST:6:VAL:HG12	61:ST:135:ALA:HB2	1.99	0.45
85:Se:31:ARG:NH2	86:S2:525:A:O3'	2.49	0.45
86:S2:115:U:H2'	86:S2:116:OMU:C6	2.46	0.45
86:S2:1010:G:H2'	86:S2:1011:A:H8	1.81	0.45
4:CF:251:GLN:N	4:CF:264:VAL:O	2.48	0.45
6:L5:150:U:OP2	15:LG:200:THR:OG1	2.27	0.45
6:L5:498:C:C2	6:L5:499:G:H1'	2.51	0.45
6:L5:3856:A:H5''	23:LP:83:TRP:O	2.16	0.45
6:L5:4401:G:H2'	6:L5:4402:C:H6	1.80	0.45
18:LJ:15:LEU:HD12	18:LJ:165:TRP:HB2	1.98	0.45
30:LW:19:ARG:NH2	30:LW:37:GLU:OE2	2.50	0.45
33:LZ:123:LYS:O	33:LZ:124:THR:OG1	2.24	0.45
51:Ls:18:ILE:HD12	51:Ls:21:LEU:HD11	1.98	0.45
57:SP:81:ARG:NH1	57:SP:120:SER:OG	2.49	0.45
67:Sg:21:ILE:HG21	67:Sg:299:PHE:HB2	1.98	0.45
73:SH:18:GLU:OE1	73:SH:18:GLU:N	2.49	0.45
74:SI:56:ARG:HA	74:SI:180:GLY:HA2	1.98	0.45
86:S2:932:G:O2'	86:S2:934:G:OP2	2.28	0.45
86:S2:1240:A:N3	86:S2:1267:C:O2'	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CF:166:ARG:O	4:CF:169:GLU:HG2	2.16	0.45
6:L5:318:A:H2'	6:L5:319:A:C8	2.52	0.45
6:L5:1494:U:H2'	6:L5:1495:G:H8	1.81	0.45
6:L5:3595:U:H5''	6:L5:3597:G:OP2	2.16	0.45
10:LB:258:HIS:HA	10:LB:260:ALA:H	1.80	0.45
13:LE:222:LEU:HB2	13:LE:237:LYS:HD2	1.97	0.45
15:LG:73:ARG:HD3	15:LG:73:ARG:HA	1.81	0.45
22:LO:61:ARG:HA	22:LO:70:PRO:HD2	1.98	0.45
61:ST:72:VAL:O	61:ST:76:THR:HG23	2.16	0.45
72:SG:170:ARG:NH1	86:S2:72:C:O2	2.50	0.45
6:L5:252:C:H2'	6:L5:253:G:H8	1.82	0.45
6:L5:1269:G:O2'	6:L5:1270:A:O4'	2.30	0.45
6:L5:1733:G:N3	6:L5:4214:A:H2'	2.31	0.45
6:L5:2072:C:OP1	24:LQ:2:GLY:N	2.50	0.45
6:L5:4508:C:N3	6:L5:4512:U:H5	2.14	0.45
6:L5:4536:OMC:HM22	6:L5:4537:C:O4'	2.17	0.45
8:L8:66:A:H2'	8:L8:67:U:C6	2.51	0.45
8:L8:67:U:H2'	8:L8:68:G:H8	1.81	0.45
12:LD:108:ARG:CZ	12:LD:253:TYR:HB2	2.47	0.45
37:Ld:114:PHE:HA	37:Ld:117:LEU:HD12	1.99	0.45
51:Ls:29:ILE:HD11	51:Ls:191:GLN:HG2	1.97	0.45
58:SQ:98:LYS:O	67:Sg:57:ARG:NH1	2.38	0.45
60:SS:63:GLU:O	60:SS:67:VAL:HG23	2.17	0.45
65:Sd:8:TRP:HZ3	86:S2:1512:C:H5''	1.82	0.45
67:Sg:17:TRP:HB2	67:Sg:36:ARG:HD3	1.98	0.45
70:SC:104:ASP:OD1	70:SC:105:GLU:N	2.49	0.45
72:SG:49:VAL:HB	72:SG:115:LYS:HG2	1.97	0.45
82:SY:68:LYS:HE2	82:SY:68:LYS:HB3	1.78	0.45
84:Sb:42:LYS:HE3	84:Sb:57:VAL:HG22	1.98	0.45
86:S2:1221:G:O2'	86:S2:1676:U:O2	2.33	0.45
3:Et:8:U:H5'	3:Et:49:C:H5''	1.99	0.45
5:AT:4:U:H2'	5:AT:5:C:C6	2.52	0.45
6:L5:303:C:OP2	21:LN:68:ARG:NH2	2.44	0.45
6:L5:327:U:HO2'	42:Li:30:ARG:HH11	1.60	0.45
6:L5:1577:G:O2'	6:L5:1612:G:H4'	2.16	0.45
6:L5:1912:G:N2	22:LO:87:MET:HE2	2.32	0.45
6:L5:2306:G:H1'	6:L5:2332:A:N6	2.32	0.45
6:L5:2611:A:H2'	6:L5:2612:G:C8	2.51	0.45
6:L5:3861:A:H2'	6:L5:3862:A:C8	2.52	0.45
6:L5:3932:U:H2'	6:L5:3933:G:C8	2.52	0.45
6:L5:4345:C:H2'	6:L5:4346:U:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4775:C:H41	6:L5:4859:C:H42	1.65	0.45
9:LA:28:ARG:HD2	9:LA:123:ARG:HG3	1.99	0.45
41:Lh:95:LEU:HD22	41:Lh:99:GLU:HG3	1.97	0.45
58:SQ:97:GLN:HB2	58:SQ:105:LYS:HG3	1.98	0.45
59:SR:99:ASP:OD2	68:SA:42:LYS:NZ	2.31	0.45
68:SA:42:LYS:HD3	68:SA:46:ILE:HB	1.98	0.45
72:SG:7:PHE:CE2	72:SG:9:ALA:HB3	2.51	0.45
85:Se:12:VAL:HG23	86:S2:616:A:H1'	1.97	0.45
86:S2:525:A:H2'	86:S2:526:A:C8	2.51	0.45
86:S2:563:G:O2'	86:S2:564:A:OP1	2.33	0.45
86:S2:929:G:H2'	86:S2:930:C:O4'	2.17	0.45
2:Pt:10:G:N2	2:Pt:26:G:H1'	2.32	0.45
6:L5:162:A:H2'	6:L5:163:A:H8	1.81	0.45
6:L5:381:U:H4'	6:L5:415:G:H5'	1.98	0.45
6:L5:1811:G:H21	35:Lb:57:MET:HE2	1.82	0.45
6:L5:2846:G:O2'	29:LV:19:GLY:O	2.28	0.45
6:L5:3664:G:H2'	6:L5:3665:G:C8	2.52	0.45
6:L5:3726:A:H2'	6:L5:3727:A:C8	2.51	0.45
6:L5:4587:G:OP1	22:LO:61:ARG:NH1	2.46	0.45
10:LB:50:LYS:NZ	10:LB:337:VAL:O	2.47	0.45
12:LD:152:ARG:HG3	12:LD:154:THR:HG23	1.99	0.45
14:LF:37:PHE:HZ	35:Lb:113:ALA:HB1	1.82	0.45
14:LF:182:TYR:CZ	14:LF:203:GLU:HG2	2.52	0.45
42:Li:35:LYS:HE3	42:Li:35:LYS:HB3	1.81	0.45
53:SD:55:THR:HA	53:SD:58:VAL:HG12	1.98	0.45
85:Se:8:ARG:HG2	85:Se:11:LYS:HD3	1.99	0.45
86:S2:29:G:H2'	86:S2:30:C:C6	2.52	0.45
86:S2:629:A:O2'	86:S2:631:U:OP1	2.34	0.45
86:S2:1201:U:H2'	86:S2:1202:U:C6	2.52	0.45
86:S2:1231:C:O2'	86:S2:1253:A:N6	2.50	0.45
86:S2:1232:PSU:H2'	86:S2:1233:G:C8	2.52	0.45
86:S2:1736:G:H2'	86:S2:1737:G:H8	1.82	0.45
4:CF:277:VAL:HA	4:CF:288:GLU:HA	1.99	0.45
6:L5:1613:A:H5''	9:LA:183:GLY:CA	2.47	0.45
6:L5:2521:G:H4'	40:Lg:26:PRO:HD2	1.98	0.45
6:L5:4315:A:OP1	27:LT:69:GLN:NE2	2.47	0.45
6:L5:4524:G:C2	10:LB:252:ALA:HB1	2.52	0.45
20:LM:24:LEU:HB2	20:LM:43:THR:HG21	1.99	0.45
25:LR:19:LYS:HB2	25:LR:19:LYS:HE2	1.82	0.45
57:SP:24:GLN:O	57:SP:28:MET:HB2	2.16	0.45
59:SR:29:HIS:HA	59:SR:32:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SS:62:ASP:OD1	60:SS:62:ASP:N	2.49	0.45
60:SS:121:ARG:HG3	60:SS:131:VAL:HB	1.99	0.45
61:ST:39:LEU:HA	61:ST:39:LEU:HD23	1.74	0.45
63:SZ:91:LEU:HG	63:SZ:96:LEU:HD21	1.99	0.45
68:SA:145:ILE:HG12	68:SA:159:ILE:HB	1.98	0.45
73:SH:142:LYS:HB3	80:SW:54:ASP:HB3	1.98	0.45
84:Sb:42:LYS:HZ1	84:Sb:58:GLY:H	1.65	0.45
2:Pt:29:C:H2'	2:Pt:30:G:H8	1.81	0.45
4:CF:6:THR:O	4:CF:85:TYR:HB2	2.17	0.45
6:L5:2676:A:OP2	6:L5:2676:A:H8	2.00	0.45
6:L5:4093:G:H3'	6:L5:4094:G:H8	1.82	0.45
24:LQ:32:TYR:HD2	24:LQ:51:LEU:HD11	1.80	0.45
36:Lc:65:MET:HE3	36:Lc:65:MET:HB3	1.90	0.45
52:Lt:81:ILE:HD13	52:Lt:113:ALA:HB1	1.99	0.45
72:SG:67:VAL:HG12	72:SG:69:THR:HG22	1.99	0.45
77:SN:83:ASP:OD1	77:SN:84:LEU:N	2.49	0.45
81:SX:105:PHE:CE2	81:SX:112:VAL:HB	2.51	0.45
4:CF:34:ILE:HD11	4:CF:39:ILE:HD12	1.99	0.45
6:L5:424:U:H2'	6:L5:425:U:C6	2.52	0.45
6:L5:3611:A:C2	6:L5:5016:A:H8	2.34	0.45
10:LB:113:GLU:OE2	10:LB:169:ARG:NH1	2.50	0.45
16:LH:8:GLN:HG2	16:LH:74:CYS:SG	2.57	0.45
17:LI:52:MET:HE3	17:LI:163:GLN:HG2	1.99	0.45
41:Lh:107:GLN:O	41:Lh:111:GLU:HG3	2.17	0.45
68:SA:6:ASP:OD1	68:SA:6:ASP:N	2.49	0.45
71:SE:10:LYS:NZ	86:S2:95:G:OP1	2.33	0.45
86:S2:563:G:HO2'	86:S2:564:A:P	2.39	0.45
86:S2:1259:A:N6	86:S2:1519:U:O5'	2.50	0.45
6:L5:965:G:H21	6:L5:2092:G:H1'	1.82	0.44
6:L5:1895:G:OP1	14:LF:96:ARG:NH2	2.47	0.44
6:L5:4742:G:OP1	6:L5:4900:C:N4	2.35	0.44
19:LL:126:LEU:N	19:LL:138:ASP:OD2	2.27	0.44
23:LP:5:SER:OG	23:LP:118:GLN:NE2	2.50	0.44
31:LX:121:VAL:HA	31:LX:140:LEU:HA	1.99	0.44
58:SQ:98:LYS:HE3	58:SQ:99:TYR:CZ	2.53	0.44
67:Sg:62:HIS:NE2	67:Sg:80:SER:OG	2.35	0.44
72:SG:87:ARG:HD3	72:SG:87:ARG:HA	1.70	0.44
86:S2:674:C:H2'	86:S2:675:U:C6	2.52	0.44
86:S2:1139:C:H5	86:S2:1149:A:H62	1.66	0.44
86:S2:1217:A:H2'	86:S2:1218:C:C6	2.50	0.44
86:S2:1681:U:H2'	86:S2:1682:C:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:197:A:N3	6:L5:222:C:O2'	2.49	0.44
6:L5:4302:U:H4'	27:LT:5:LYS:HD3	2.00	0.44
11:LC:150:LEU:O	11:LC:152:LEU:N	2.50	0.44
19:LL:55:ILE:O	19:LL:97:SER:OG	2.32	0.44
37:Ld:54:MET:HE3	37:Ld:60:PRO:HA	1.98	0.44
51:Ls:52:VAL:HG12	51:Ls:90:PHE:HB2	1.99	0.44
67:Sg:191:HIS:ND1	67:Sg:195:LEU:HD21	2.32	0.44
69:SB:29:ASP:OD1	69:SB:29:ASP:N	2.51	0.44
69:SB:145:LYS:HB2	69:SB:145:LYS:HE3	1.73	0.44
78:SO:149:ARG:NH2	86:S2:961:G:OP1	2.50	0.44
81:SX:28:LYS:NZ	86:S2:1189:A:OP1	2.40	0.44
86:S2:99:A2M:H8	86:S2:99:A2M:O5'	2.18	0.44
86:S2:576:A2M:HM'3	86:S2:576:A2M:H1'	1.82	0.44
86:S2:1084:A:OP1	86:S2:1858:G:O2'	2.28	0.44
3:Et:6:G:H2'	3:Et:7:A:C8	2.53	0.44
4:CF:51:LYS:HG2	4:CF:54:PHE:HB2	1.99	0.44
4:CF:273:LYS:HG2	4:CF:276:MET:HE1	2.00	0.44
6:L5:423:G:H5'	23:LP:26:PHE:HZ	1.83	0.44
6:L5:684:G:H5''	13:LE:100:LYS:HE3	1.99	0.44
6:L5:2079:G:H2'	6:L5:2080:U:C6	2.53	0.44
6:L5:4274:A:H2'	6:L5:4275:G:H8	1.82	0.44
6:L5:4291:G:H5'	6:L5:4293:PSU:C6	2.52	0.44
6:L5:4524:G:N3	10:LB:252:ALA:HB1	2.32	0.44
9:LA:131:GLY:H	9:LA:169:VAL:HG13	1.82	0.44
24:LQ:86:ILE:HD11	24:LQ:100:VAL:HG11	1.98	0.44
25:LR:176:ARG:NH1	25:LR:177:LEU:HG	2.33	0.44
37:Ld:57:MET:HG2	37:Ld:88:LEU:HD23	2.00	0.44
55:SK:31:LYS:HZ3	55:SK:39:ASN:N	2.15	0.44
60:SS:38:ARG:HD2	61:ST:45:LEU:HD11	1.99	0.44
61:ST:39:LEU:HD21	61:ST:52:TRP:CZ3	2.53	0.44
62:SU:19:ARG:HB3	62:SU:92:HIS:CD2	2.53	0.44
63:SZ:86:ALA:HA	63:SZ:89:GLN:HE21	1.81	0.44
67:Sg:268:ASP:OD1	67:Sg:269:GLU:N	2.50	0.44
71:SE:101:LEU:HD12	71:SE:101:LEU:HA	1.85	0.44
86:S2:1850:MA6:H8	86:S2:1850:MA6:O5'	2.18	0.44
6:L5:4456:OMC:HM21	10:LB:241:PRO:HD3	1.99	0.44
6:L5:4594:U:H2'	6:L5:4595:G:C8	2.48	0.44
13:LE:183:ARG:HA	13:LE:183:ARG:HD2	1.80	0.44
17:LI:101:LYS:NZ	17:LI:102:MET:O	2.48	0.44
19:LL:140:SER:HA	19:LL:143:GLU:HG2	1.99	0.44
29:LV:107:ASN:ND2	29:LV:111:GLU:OE2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Lm:79:GLU:CD	46:Lm:81:SER:HG	2.21	0.44
57:SP:37:TYR:HB3	57:SP:41:GLN:HB2	1.98	0.44
59:SR:35:CYS:HA	59:SR:38:ILE:HG12	1.99	0.44
68:SA:18:PHE:CD1	68:SA:23:THR:HG21	2.51	0.44
72:SG:136:LYS:HB2	86:S2:65:C:H41	1.83	0.44
86:S2:27:A2M:HM'3	86:S2:27:A2M:H1'	1.63	0.44
86:S2:830:A:OP2	86:S2:846:G:N2	2.50	0.44
5:AT:57:C:C5	6:L5:2009:A:H1'	2.52	0.44
5:AT:60:A:H2'	5:AT:61:A:O4'	2.18	0.44
6:L5:72:C:H5	19:LL:67:HIS:HD1	1.64	0.44
6:L5:138:G:H2'	6:L5:139:G:C8	2.52	0.44
6:L5:662:C:H2'	6:L5:663:G:H8	1.83	0.44
6:L5:979:C:OP2	13:LE:66:LYS:HD3	2.17	0.44
6:L5:1282:G:OP2	13:LE:128:HIS:NE2	2.51	0.44
6:L5:1537:A:H2'	6:L5:1538:U:C6	2.53	0.44
6:L5:1751:A:H2'	6:L5:1752:G:C8	2.53	0.44
6:L5:2347:A:C4	38:Le:31:ILE:HD11	2.53	0.44
6:L5:2570:U:H2'	6:L5:2571:C:C6	2.53	0.44
15:LG:143:VAL:HG22	15:LG:203:ALA:HB2	1.99	0.44
53:SD:27:ARG:NH1	86:S2:1498:A:OP2	2.42	0.44
76:SL:127:THR:HB	76:SL:144:LYS:HB3	1.99	0.44
86:S2:136:C:H5''	86:S2:137:U:H5''	2.00	0.44
86:S2:194:C:H2'	86:S2:195:C:H6	1.83	0.44
86:S2:835:C:H4'	86:S2:836:G:C8	2.53	0.44
86:S2:1215:C:O2'	86:S2:1645:C:OP2	2.34	0.44
86:S2:1628:C:H2'	86:S2:1629:C:C6	2.51	0.44
86:S2:1801:A:H2'	86:S2:1802:C:H6	1.82	0.44
4:CF:274:PRO:HA	4:CF:289:VAL:HG13	2.00	0.44
4:CF:427:ARG:HD2	4:CF:430:ARG:HH21	1.82	0.44
6:L5:1327:C:H2'	6:L5:1328:G:C8	2.53	0.44
6:L5:1818:G:O2'	6:L5:1820:C:OP2	2.27	0.44
6:L5:2864:A:H2'	6:L5:2865:U:C6	2.52	0.44
6:L5:4126:C:OP1	15:LG:37:LYS:NZ	2.51	0.44
11:LC:334:THR:HG22	11:LC:337:ARG:HH21	1.82	0.44
13:LE:198:SER:OG	13:LE:288:PHE:O	2.25	0.44
16:LH:187:VAL:HG12	16:LH:188:GLN:HG3	2.00	0.44
17:LI:48:LEU:O	17:LI:139:ARG:HA	2.17	0.44
53:SD:163:PRO:O	53:SD:167:TYR:HB2	2.18	0.44
86:S2:1037:G:H4'	86:S2:1845:A:H4'	1.98	0.44
86:S2:1653:U:H2'	86:S2:1654:G:C8	2.52	0.44
4:CF:79:LYS:HD2	4:CF:295:HIS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CF:294:MET:HB2	4:CF:299:LEU:HD11	1.99	0.44
4:CF:349:HIS:ND1	4:CF:351:GLY:O	2.51	0.44
6:L5:132:G:H2'	6:L5:133:C:H4'	1.99	0.44
6:L5:268:G:H2'	6:L5:269:G:C8	2.52	0.44
6:L5:1359:G:H4'	21:LN:203:TYR:HB2	2.00	0.44
6:L5:1662:C:H2'	6:L5:1663:C:H6	1.83	0.44
6:L5:2848:G:O2'	6:L5:3838:U:O4	2.25	0.44
6:L5:3813:A:N3	6:L5:4538:G:O2'	2.45	0.44
6:L5:3932:U:H2'	6:L5:3933:G:H8	1.83	0.44
10:LB:165:HIS:HA	10:LB:179:HIS:O	2.17	0.44
13:LE:99:ASP:OD1	13:LE:99:ASP:N	2.50	0.44
40:Lg:69:LYS:HG3	40:Lg:73:HIS:CD2	2.53	0.44
48:Lo:74:GLU:HB3	48:Lo:77:CYS:HB3	2.00	0.44
57:SP:34:MET:HB3	57:SP:42:ARG:HG3	1.98	0.44
62:SU:87:ARG:HH22	86:S2:1447:G:P	2.41	0.44
68:SA:220:LYS:HA	68:SA:220:LYS:HD3	1.84	0.44
72:SG:147:LEU:HD12	72:SG:151:ASP:HB2	2.00	0.44
73:SH:37:LYS:HA	73:SH:40:LEU:HB3	1.99	0.44
78:SO:101:GLY:HA3	78:SO:134:PRO:HD2	1.99	0.44
81:SX:63:ASN:OD1	86:S2:624:C:N4	2.42	0.44
86:S2:494:C:N4	86:S2:509:OMG:HN22	2.16	0.44
86:S2:1221:G:H2'	86:S2:1222:G:C8	2.53	0.44
86:S2:1589:A:N3	86:S2:1653:U:O2'	2.44	0.44
3:Et:43:A:H2'	3:Et:44:G:H8	1.82	0.44
5:AT:3:C:H2'	5:AT:4:U:C6	2.52	0.44
6:L5:1084:C:H2'	6:L5:1085:C:H6	1.83	0.44
6:L5:2326:G:H5''	38:Le:127:ALA:HB1	1.99	0.44
6:L5:3911:C:H2'	6:L5:3912:U:C6	2.51	0.44
7:L7:119:U:C2	12:LD:261:VAL:HG11	2.53	0.44
10:LB:46:PHE:CZ	10:LB:84:MET:HG2	2.52	0.44
12:LD:33:ARG:O	12:LD:37:VAL:HG22	2.18	0.44
15:LG:81:ASN:O	15:LG:84:THR:OG1	2.32	0.44
15:LG:175:ARG:HG2	15:LG:230:TYR:CD2	2.53	0.44
20:LM:115:ALA:HB1	22:LO:192:TYR:HB3	2.00	0.44
21:LN:200:LEU:HD22	21:LN:204:ARG:NH1	2.32	0.44
51:Ls:78:LEU:O	51:Ls:82:ILE:HG12	2.17	0.44
53:SD:215:ASP:OD1	53:SD:216:GLU:N	2.45	0.44
66:Sf:107:LYS:NZ	66:Sf:108:VAL:O	2.51	0.44
74:SI:45:THR:OG1	86:S2:308:G:OP1	2.28	0.44
74:SI:86:SER:OG	86:S2:376:A:N3	2.44	0.44
86:S2:116:OMU:HN3	86:S2:347:G:H1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:S2:659:G:O2'	86:S2:662:G:O2'	2.28	0.44
6:L5:1677:PSU:H4'	6:L5:1680:G:C2	2.53	0.44
6:L5:1741:G:O6	7:L7:103:A:O2'	2.27	0.44
6:L5:3599:A:H2'	6:L5:3600:G:C8	2.52	0.44
14:LF:46:ARG:NH2	35:Lb:102:PRO:HG3	2.33	0.44
30:LW:5:LEU:HD12	30:LW:30:GLN:NE2	2.33	0.44
37:Ld:44:ARG:HA	37:Ld:47:LYS:HE3	1.99	0.44
61:ST:104:LEU:HD22	61:ST:121:ARG:HD2	2.00	0.44
73:SH:18:GLU:C	73:SH:20:GLU:H	2.26	0.44
82:SY:9:THR:HG22	86:S2:837:A:N6	2.32	0.44
86:S2:573:U:O2	86:S2:576:A2M:H8	2.17	0.44
86:S2:1777:G:H2'	86:S2:1778:C:C6	2.53	0.44
6:L5:66:A:O2'	6:L5:326:C:O2	2.36	0.43
6:L5:454:U:H2'	6:L5:455:C:O4'	2.18	0.43
6:L5:2399:G:O2'	6:L5:2822:G:O2'	2.34	0.43
6:L5:2730:U:H2'	6:L5:2731:C:C6	2.53	0.43
6:L5:3873:G:H2'	6:L5:3874:G:C8	2.53	0.43
6:L5:4156:G:H5''	6:L5:4157:A:H2'	2.00	0.43
6:L5:4419:U:OP1	6:L5:4475:G:N2	2.49	0.43
6:L5:4611:A:H2'	6:L5:4612:C:H6	1.83	0.43
6:L5:4743:G:H2'	6:L5:4744:A:C8	2.53	0.43
6:L5:4897:G:H2'	6:L5:4898:G:H8	1.81	0.43
18:LJ:17:ILE:HD12	18:LJ:80:GLU:HG2	2.00	0.43
20:LM:104:MET:HG3	20:LM:108:ASP:HB2	2.00	0.43
20:LM:118:MET:HG2	22:LO:192:TYR:CZ	2.53	0.43
27:LT:28:ALA:O	27:LT:32:ARG:HG2	2.18	0.43
33:LZ:11:VAL:HG12	33:LZ:82:PRO:HA	2.00	0.43
45:Ll:12:PHE:CE2	45:Ll:51:LEU:HD22	2.53	0.43
70:SC:64:THR:HG22	70:SC:66:LEU:H	1.83	0.43
71:SE:72:ILE:HD12	71:SE:77:ARG:HB2	2.00	0.43
83:Sa:12:LYS:HG3	83:Sa:15:ARG:HB2	2.00	0.43
86:S2:495:U:H2'	86:S2:496:C:O4'	2.18	0.43
6:L5:696:C:H42	13:LE:221:LYS:HG3	1.82	0.43
6:L5:711:A:H2'	6:L5:712:C:C6	2.53	0.43
6:L5:3928:A:H2'	6:L5:3929:G:O4'	2.17	0.43
6:L5:4111:U:H2'	6:L5:4112:C:H5	1.83	0.43
8:L8:26:C:O2'	11:LC:53:ALA:O	2.35	0.43
22:LO:88:LEU:HD12	22:LO:99:LEU:HD13	2.01	0.43
56:SM:91:LEU:HD23	56:SM:91:LEU:HA	1.80	0.43
60:SS:102:GLY:HA2	60:SS:105:ASN:HD21	1.83	0.43
64:Sc:10:LYS:HE2	64:Sc:34:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SE:18:TRP:HH2	71:SE:31:PRO:HD3	1.82	0.43
71:SE:80:ILE:HG23	71:SE:81:THR:HG23	2.00	0.43
71:SE:152:PRO:HG2	72:SG:216:ARG:HG3	2.00	0.43
86:S2:186:C:H2'	86:S2:187:G:H8	1.83	0.43
6:L5:473:C:H2'	6:L5:474:C:C6	2.53	0.43
6:L5:1081:C:C2'	6:L5:1082:C:H5'	2.49	0.43
6:L5:4913:G:H4'	6:L5:4914:C:O5'	2.17	0.43
8:L8:102:G:OP2	8:L8:104:A:O2'	2.30	0.43
10:LB:206:PRO:HG2	10:LB:209:GLN:HG3	1.99	0.43
31:LX:127:LEU:HD11	31:LX:135:LYS:HE3	2.01	0.43
59:SR:111:PHE:HE1	68:SA:12:GLU:HG3	1.84	0.43
61:ST:101:ARG:NH2	86:S2:1566:G:N7	2.65	0.43
63:SZ:86:ALA:O	63:SZ:90:GLU:HG2	2.18	0.43
67:Sg:10:THR:HB	67:Sg:306:LEU:HD21	2.00	0.43
68:SA:177:MET:SD	68:SA:180:ARG:NH2	2.92	0.43
70:SC:185:THR:OG1	86:S2:1155:U:OP1	2.27	0.43
72:SG:174:PRO:HB3	86:S2:65:C:C6	2.54	0.43
74:SI:65:PHE:HA	74:SI:187:GLY:O	2.18	0.43
81:SX:54:LYS:NZ	81:SX:94:ILE:O	2.49	0.43
81:SX:107:ARG:HG2	81:SX:112:VAL:HG22	2.00	0.43
86:S2:441:C:H2'	86:S2:442:C:C6	2.53	0.43
86:S2:1047:C:H2'	86:S2:1048:G:O4'	2.18	0.43
4:CF:82:THR:OG1	4:CF:85:TYR:O	2.23	0.43
6:L5:907:C:H2'	6:L5:908:G:C8	2.53	0.43
6:L5:2864:A:H2'	6:L5:2865:U:H6	1.83	0.43
6:L5:2870:A:H2'	6:L5:2871:A:C8	2.53	0.43
6:L5:3684:G:H2'	6:L5:3685:C:C6	2.54	0.43
6:L5:4238:G:H2'	6:L5:4239:A:C8	2.53	0.43
89:L5:5282:SPD:H82	89:L5:5282:SPD:H51	1.78	0.43
13:LE:194:VAL:O	39:Lf:108:SER:OG	2.29	0.43
17:LI:73:ASN:HB2	17:LI:87:MET:HE1	2.00	0.43
59:SR:24:LEU:HD23	59:SR:34:VAL:HG21	2.00	0.43
61:ST:96:SER:HB3	61:ST:99:VAL:HB	1.99	0.43
71:SE:186:GLY:HA3	86:S2:809:A:OP1	2.19	0.43
74:SI:150:ASP:HA	74:SI:153:LYS:CG	2.48	0.43
76:SL:23:VAL:HG23	76:SL:25:LEU:HG	2.00	0.43
79:SV:74:LYS:NZ	79:SV:83:PHE:HB3	2.33	0.43
4:CF:166:ARG:O	4:CF:170:ILE:HG12	2.19	0.43
6:L5:173:C:H2'	6:L5:174:C:C6	2.53	0.43
6:L5:264:C:H2'	6:L5:265:C:C4	2.53	0.43
6:L5:494:U:H2'	6:L5:495:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:1981:G:N1	6:L5:1982:G:O6	2.51	0.43
6:L5:4076:G:H5'	15:LG:73:ARG:HG3	2.00	0.43
9:LA:80:GLU:HB2	9:LA:170:ALA:HA	1.99	0.43
14:LF:236:ARG:HD3	14:LF:239:GLN:HB2	2.01	0.43
16:LH:128:MET:SD	16:LH:157:SER:HB3	2.58	0.43
67:Sg:54:ILE:HD12	67:Sg:55:PRO:HD2	2.00	0.43
74:SI:141:ARG:NE	86:S2:191:A:OP1	2.52	0.43
86:S2:291:G:HO2'	86:S2:292:A:P	2.41	0.43
86:S2:348:A:H2'	86:S2:349:A:C8	2.53	0.43
1:CI:66:GLY:HA3	37:Ld:70:LYS:NZ	2.34	0.43
4:CF:5:LYS:HG3	4:CF:85:TYR:HA	2.00	0.43
6:L5:491:G:H2'	6:L5:492:U:C6	2.54	0.43
6:L5:716:C:OP1	11:LC:317:ASN:HB2	2.19	0.43
6:L5:1466:G:OP2	35:Lb:44:ARG:NH2	2.51	0.43
6:L5:2465:C:H2'	6:L5:2466:G:O4'	2.19	0.43
6:L5:4088:C:H2'	6:L5:4089:G:H8	1.83	0.43
6:L5:4392:OMG:H2'	6:L5:4447:5MC:HM51	2.01	0.43
6:L5:5057:C:H2'	6:L5:5058:A:C8	2.54	0.43
8:L8:58:G:O6	43:Lj:63:ARG:NH1	2.52	0.43
12:LD:203:ASN:OD1	12:LD:203:ASN:N	2.51	0.43
18:LJ:104:ASN:HB2	18:LJ:133:VAL:HA	1.99	0.43
21:LN:90:ASN:O	48:Lo:48:TYR:OH	2.33	0.43
32:LY:22:PRO:HD2	32:LY:25:ILE:HD11	2.00	0.43
69:SB:124:HIS:HA	69:SB:137:LEU:O	2.19	0.43
74:SI:64:ASN:OD1	74:SI:73:THR:HG22	2.18	0.43
74:SI:139:LYS:HE2	74:SI:139:LYS:HB2	1.70	0.43
75:SJ:28:GLU:OE2	75:SJ:44:TRP:NE1	2.41	0.43
86:S2:194:C:H2'	86:S2:195:C:C6	2.53	0.43
86:S2:1278:A:H2'	86:S2:1279:C:C6	2.54	0.43
3:Et:35:U:H2'	3:Et:36:U:C6	2.53	0.43
6:L5:2404:A:H1'	43:Lj:12:ARG:HH21	1.82	0.43
6:L5:2667:C:O4'	25:LR:96:MET:HG2	2.18	0.43
6:L5:3690:U:H2'	6:L5:3691:G:O4'	2.19	0.43
6:L5:4322:G:N2	6:L5:4325:A:OP2	2.43	0.43
7:L7:110:G:H2'	7:L7:111:C:C6	2.54	0.43
9:LA:13:GLY:O	9:LA:17:ARG:HG3	2.18	0.43
9:LA:22:HIS:O	9:LA:24:LYS:NZ	2.49	0.43
10:LB:393:LYS:HG3	10:LB:396:ARG:HH21	1.83	0.43
13:LE:203:ILE:O	13:LE:206:VAL:HG22	2.19	0.43
14:LF:105:VAL:HG13	14:LF:136:VAL:HG12	2.01	0.43
23:LP:76:TRP:CD1	23:LP:76:TRP:H	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LW:52:THR:O	30:LW:56:ARG:HG2	2.18	0.43
54:SF:79:HIS:O	54:SF:81:ARG:N	2.47	0.43
62:SU:38:ASP:OD1	62:SU:39:LEU:N	2.51	0.43
67:Sg:183:LYS:HA	67:Sg:183:LYS:HD2	1.85	0.43
79:SV:17:CYS:HB2	79:SV:56:CYS:HB3	2.01	0.43
82:SY:36:PRO:O	82:SY:40:ILE:HD12	2.18	0.43
86:S2:152:U:H2'	86:S2:153:G:C8	2.54	0.43
86:S2:1243:U:OP2	86:S2:1518:C:O2'	2.25	0.43
3:Et:41:U:O3'	54:SF:198:ARG:NE	2.52	0.43
6:L5:262:G:H2'	6:L5:263:G:C8	2.53	0.43
6:L5:1195:G:H2'	6:L5:1196:G:C8	2.54	0.43
6:L5:3827:G:O2'	6:L5:3829:G:OP2	2.36	0.43
6:L5:4238:G:H2'	6:L5:4239:A:H8	1.84	0.43
7:L7:63:C:H5'	7:L7:64:G:H5''	2.01	0.43
8:L8:36:G:C5	41:Lh:89:ARG:HD3	2.54	0.43
8:L8:144:U:H2'	8:L8:145:C:C6	2.53	0.43
11:LC:279:LEU:HD23	11:LC:279:LEU:HA	1.87	0.43
16:LH:24:THR:HA	16:LH:37:ASP:HA	2.01	0.43
22:LO:124:LEU:HD23	22:LO:124:LEU:HA	1.87	0.43
58:SQ:90:LYS:HA	58:SQ:93:VAL:HG22	2.00	0.43
68:SA:184:ARG:NE	68:SA:191:ARG:HD3	2.33	0.43
69:SB:83:LYS:HD3	69:SB:106:THR:HG22	2.01	0.43
72:SG:14:LYS:HE2	72:SG:16:ILE:HD11	2.01	0.43
75:SJ:5:ARG:HB3	86:S2:38:A:H5''	2.01	0.43
79:SV:18:SER:HB3	79:SV:72:LEU:HD21	2.01	0.43
80:SW:28:ARG:HB3	80:SW:29:PRO:HD3	2.00	0.43
82:SY:9:THR:HG22	86:S2:837:A:H61	1.84	0.43
83:Sa:59:PHE:HB2	83:Sa:62:TYR:HB2	2.01	0.43
86:S2:293:C:O2'	86:S2:294:U:H3'	2.19	0.43
86:S2:517:OMC:H2'	86:S2:518:G:O4'	2.18	0.43
6:L5:922:C:H2'	6:L5:923:C:O4'	2.19	0.43
6:L5:1175:A:H2	6:L5:1185:G:H1	1.66	0.43
6:L5:2421:G:OP2	6:L5:2828:U:H1'	2.19	0.43
6:L5:4887:C:N4	6:L5:4932:U:H3	2.15	0.43
11:LC:318:PRO:O	11:LC:319:LEU:HB2	2.19	0.43
14:LF:147:LEU:O	14:LF:151:ASN:ND2	2.43	0.43
14:LF:214:SER:OG	14:LF:215:SER:N	2.51	0.43
38:Le:35:TRP:CZ2	38:Le:56:PRO:HD2	2.54	0.43
41:Lh:52:LYS:HA	41:Lh:52:LYS:HD3	1.81	0.43
67:Sg:59:LEU:HD23	67:Sg:90:TRP:CD2	2.54	0.43
73:SH:58:LYS:HA	73:SH:58:LYS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:S2:639:C:H2'	86:S2:640:A:C8	2.54	0.43
86:S2:1560:U:O2	86:S2:1575:G:O6	2.37	0.43
86:S2:1683:C:H2'	86:S2:1684:C:H6	1.84	0.43
3:Et:2:C:H2'	3:Et:3:C:C6	2.53	0.43
5:AT:5:C:H2'	5:AT:6:C:H6	1.84	0.43
6:L5:1563:A:N6	86:S2:1028:A:N1	2.66	0.43
6:L5:1683:PSU:H2'	6:L5:1684:A:C8	2.54	0.43
6:L5:1826:G:H4'	35:Lb:43:MET:HE3	2.01	0.43
6:L5:1998:A:N6	51:Ls:40:MET:SD	2.92	0.43
6:L5:2664:G:H4'	6:L5:2677:G:H4'	2.00	0.43
6:L5:2671:C:H2'	6:L5:2672:C:C6	2.54	0.43
7:L7:55:A:H4'	18:LJ:155:HIS:HB2	2.00	0.43
10:LB:154:LYS:HE2	10:LB:154:LYS:HB2	1.70	0.43
18:LJ:77:ALA:O	18:LJ:81:GLU:HG2	2.18	0.43
18:LJ:113:ILE:HD11	60:SS:14:ARG:HD3	2.00	0.43
19:LL:111:GLN:HA	19:LL:114:VAL:HG22	2.01	0.43
32:LY:72:GLN:HE21	32:LY:74:TYR:HD1	1.67	0.43
36:Lc:38:ILE:HG21	36:Lc:63:TYR:HB3	1.99	0.43
55:SK:91:PRO:HB2	55:SK:94:LEU:HD23	2.01	0.43
60:SS:13:LEU:HD22	60:SS:20:ILE:HD11	2.00	0.43
67:Sg:270:LEU:HD13	67:Sg:310:TRP:CE3	2.54	0.43
68:SA:11:LYS:O	68:SA:15:VAL:HG23	2.18	0.43
71:SE:122:LYS:HE2	71:SE:124:CYS:SG	2.58	0.43
86:S2:166:A2M:HM'3	86:S2:166:A2M:H1'	1.68	0.43
86:S2:693:A:H2'	86:S2:694:G:N7	2.33	0.43
86:S2:834:C:H42	86:S2:839:C:H42	1.66	0.43
86:S2:1101:U:H2'	86:S2:1102:G:C8	2.54	0.43
86:S2:1217:A:H2'	86:S2:1218:C:H6	1.83	0.43
3:Et:15:G:N1	3:Et:59:G:N7	2.66	0.42
6:L5:1278:C:H2'	6:L5:1279:A:O4'	2.18	0.42
6:L5:1404:G:N7	6:L5:1408:G:N1	2.67	0.42
6:L5:1613:A:H5''	9:LA:183:GLY:HA2	2.01	0.42
6:L5:1631:A:C2	9:LA:204:MET:HG2	2.53	0.42
6:L5:1847:C:H2'	6:L5:1848:C:C6	2.54	0.42
6:L5:2017:A:HO2'	6:L5:2018:C:C5'	2.31	0.42
6:L5:2809:G:H5''	25:LR:63:CYS:SG	2.59	0.42
6:L5:3654:G:O2'	6:L5:3693:U:OP1	2.28	0.42
6:L5:3782:5MC:OP1	47:Ln:23:ARG:NH2	2.52	0.42
6:L5:4084:G:O6	9:LA:72:ARG:NH2	2.51	0.42
6:L5:4590:A2M:HM'3	6:L5:4590:A2M:H1'	1.79	0.42
6:L5:4859:C:H2'	6:L5:4860:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4927:G:H5''	6:L5:4928:C:C5	2.54	0.42
11:LC:33:ARG:HG2	11:LC:36:ILE:HD12	2.01	0.42
16:LH:95:VAL:HG12	46:Lm:82:LEU:HD13	2.01	0.42
30:LW:47:ARG:HE	30:LW:54:LEU:HD22	1.84	0.42
32:LY:23:SER:HA	32:LY:26:ARG:HB2	2.00	0.42
39:Lf:45:LYS:HA	39:Lf:107:PRO:HD2	2.01	0.42
64:Sc:44:ARG:NH2	64:Sc:63:ARG:HH11	2.17	0.42
70:SC:167:ARG:HB3	70:SC:177:PRO:HB2	2.00	0.42
86:S2:1259:A:H1'	86:S2:1264:C:N4	2.34	0.42
3:Et:51:G:H2'	3:Et:52:G:H8	1.82	0.42
3:Et:76:A:H62	6:L5:4371:G:H5'	1.84	0.42
6:L5:490:C:H2'	6:L5:491:G:H8	1.83	0.42
6:L5:1669:A:H4'	6:L5:1685:G:N2	2.34	0.42
6:L5:3861:A:H2'	6:L5:3862:A:H8	1.84	0.42
6:L5:4327:C:OP1	27:LT:70:HIS:NE2	2.51	0.42
6:L5:5006:U:H4'	6:L5:5007:A:H5'	2.01	0.42
10:LB:92:TYR:HB3	10:LB:99:LEU:HD22	2.00	0.42
11:LC:221:PHE:O	11:LC:222:ARG:HG2	2.20	0.42
27:LT:44:GLY:HA2	27:LT:95:HIS:HB3	2.01	0.42
36:Lc:47:ILE:HB	36:Lc:94:LEU:HG	2.02	0.42
42:Li:76:ARG:HD3	42:Li:76:ARG:HA	1.79	0.42
52:Lt:114:ARG:NH2	52:Lt:162:CYS:SG	2.92	0.42
60:SS:61:GLU:HA	60:SS:64:VAL:HG12	2.01	0.42
61:ST:62:ARG:CZ	86:S2:1542:C:H5''	2.49	0.42
67:Sg:135:LEU:HD23	67:Sg:135:LEU:HA	1.89	0.42
67:Sg:200:VAL:HA	67:Sg:206:LEU:O	2.19	0.42
68:SA:42:LYS:HD2	68:SA:48:ILE:HD11	2.01	0.42
69:SB:147:ASN:OD1	69:SB:148:ASN:N	2.52	0.42
77:SN:29:THR:O	77:SN:33:VAL:HG23	2.19	0.42
86:S2:454:U:H2'	86:S2:455:A:C8	2.54	0.42
86:S2:1139:C:H2'	86:S2:1140:G:O4'	2.18	0.42
86:S2:1705:C:H2'	86:S2:1706:G:C8	2.54	0.42
6:L5:92:C:OP2	6:L5:4341:C:O2'	2.28	0.42
6:L5:457:G:H2'	6:L5:458:C:C6	2.54	0.42
6:L5:1346:C:H2'	6:L5:1347:G:H8	1.84	0.42
6:L5:1979:A:H1'	6:L5:1988:G:N2	2.34	0.42
6:L5:4187:G:OP1	88:L5:5266:SPM:H111	2.19	0.42
6:L5:4742:G:H2'	6:L5:4743:G:C8	2.54	0.42
7:L7:111:C:H2'	7:L7:112:U:O4'	2.19	0.42
10:LB:17:LEU:HD23	10:LB:17:LEU:HA	1.78	0.42
14:LF:92:VAL:O	14:LF:120:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:14:ASN:O	17:LI:128:ARG:NH2	2.24	0.42
22:LO:56:ALA:O	22:LO:60:LYS:HG2	2.18	0.42
35:Lb:43:MET:HE2	35:Lb:47:LYS:NZ	2.34	0.42
36:Lc:18:LEU:O	36:Lc:22:MET:HG2	2.19	0.42
47:Ln:17:ARG:NH1	86:S2:1173:A:OP1	2.53	0.42
58:SQ:110:ASP:OD1	58:SQ:110:ASP:N	2.49	0.42
69:SB:167:LYS:HE2	69:SB:167:LYS:HB2	1.82	0.42
74:SI:161:LEU:HD23	74:SI:195:LEU:HG	2.00	0.42
78:SO:63:LYS:HD3	78:SO:63:LYS:HA	1.87	0.42
78:SO:147:ARG:HH22	86:S2:1854:U:P	2.43	0.42
80:SW:5:ASN:HB3	80:SW:8:ALA:HB3	2.00	0.42
86:S2:1347:U:H2'	86:S2:1348:G:N3	2.34	0.42
86:S2:1540:G:H2'	86:S2:1541:G:H8	1.85	0.42
86:S2:1779:G:H2'	86:S2:1780:G:C8	2.53	0.42
4:CF:250:LEU:HD13	4:CF:263:PRO:HB3	2.00	0.42
5:AT:2:U:H2'	5:AT:3:C:C6	2.55	0.42
6:L5:89:C:OP1	34:La:59:LYS:NZ	2.41	0.42
6:L5:1084:C:H2'	6:L5:1085:C:C6	2.54	0.42
6:L5:1625:OMG:HM23	21:LN:81:TYR:HE2	1.84	0.42
6:L5:2073:C:OP1	14:LF:212:LYS:HE3	2.19	0.42
6:L5:2765:A:H2'	6:L5:2766:A:C8	2.54	0.42
6:L5:2808:G:O3'	25:LR:60:ARG:NH1	2.51	0.42
8:L8:102:G:H5''	43:Lj:39:TYR:HE1	1.83	0.42
10:LB:220:ILE:HG12	10:LB:278:THR:HG23	2.00	0.42
15:LG:176:LYS:HD3	42:Li:43:MET:HE1	2.02	0.42
23:LP:85:LYS:O	23:LP:89:GLU:HG3	2.20	0.42
31:LX:82:THR:HG21	41:Lh:37:THR:HG22	2.01	0.42
48:Lo:78:ARG:O	48:Lo:80:LYS:NZ	2.52	0.42
51:Ls:47:LEU:HD11	51:Ls:51:ALA:HB3	2.02	0.42
69:SB:214:LYS:HE2	69:SB:216:LYS:HE3	2.02	0.42
86:S2:1733:U:H2'	86:S2:1734:G:O4'	2.20	0.42
86:S2:1797:U:H2'	86:S2:1798:C:C6	2.54	0.42
2:Pt:62:C:H2'	2:Pt:63:G:H8	1.84	0.42
6:L5:120:A:H2'	6:L5:149:A:H61	1.85	0.42
6:L5:252:C:H2'	6:L5:253:G:C8	2.54	0.42
6:L5:408:A:O2'	6:L5:411:G:OP2	2.26	0.42
6:L5:1703:C:O2'	6:L5:1704:C:O5'	2.37	0.42
6:L5:2368:A:N6	6:L5:2827:G:O2'	2.51	0.42
6:L5:2424:OMG:H1'	6:L5:2424:OMG:HM23	1.80	0.42
6:L5:2492:C:H2'	6:L5:2493:G:C8	2.54	0.42
6:L5:2558:C:H2'	6:L5:2559:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:2638:G:H22	6:L5:2719:C:P	2.42	0.42
6:L5:3718:A2M:H2'	6:L5:3719:A:O4'	2.19	0.42
6:L5:3937:C:O2'	21:LN:124:ASP:OD1	2.38	0.42
6:L5:4685:U:H2'	6:L5:4686:G:C8	2.54	0.42
9:LA:20:VAL:HA	9:LA:23:ARG:HG3	1.99	0.42
14:LF:228:VAL:HG12	26:LS:38:VAL:HG12	2.02	0.42
20:LM:86:TRP:O	20:LM:89:THR:OG1	2.33	0.42
30:LW:97:LYS:O	30:LW:99:GLU:N	2.51	0.42
68:SA:180:ARG:HH11	68:SA:184:ARG:HH11	1.68	0.42
68:SA:206:ASP:O	68:SA:210:ILE:HD12	2.18	0.42
71:SE:253:ASP:N	71:SE:253:ASP:OD1	2.51	0.42
79:SV:40:ASP:OD1	79:SV:44:GLY:N	2.52	0.42
86:S2:804:U:H2'	86:S2:805:U:C6	2.54	0.42
6:L5:37:U:H2'	6:L5:38:A:O4'	2.19	0.42
6:L5:400:A2M:H1'	6:L5:400:A2M:HM'3	1.63	0.42
6:L5:959:G:C8	13:LE:123:ARG:HG2	2.55	0.42
6:L5:2303:C:H5''	38:Le:104:SER:HB3	2.02	0.42
6:L5:2492:C:H2'	6:L5:2493:G:H8	1.85	0.42
6:L5:2517:A:N3	6:L5:2539:C:O2'	2.50	0.42
6:L5:2607:C:O5'	25:LR:96:MET:HE1	2.20	0.42
6:L5:3725:G:N7	42:Li:67:LYS:NZ	2.50	0.42
8:L8:90:C:H1'	32:LY:24:HIS:HB3	2.01	0.42
27:LT:4:THR:OG1	27:LT:9:ARG:HD3	2.19	0.42
32:LY:74:TYR:HE2	32:LY:77:LYS:HG3	1.85	0.42
48:Lo:4:VAL:HG23	48:Lo:93:LEU:HD23	2.02	0.42
67:Sg:227:LEU:HD23	67:Sg:228:TYR:HB2	2.01	0.42
70:SC:202:THR:HG23	75:SJ:54:ARG:HH22	1.85	0.42
71:SE:128:LYS:HG2	71:SE:140:VAL:HB	2.01	0.42
71:SE:242:LYS:HD3	71:SE:242:LYS:HA	1.75	0.42
72:SG:31:ARG:NH1	86:S2:1745:A:O3'	2.52	0.42
72:SG:164:LYS:HE2	72:SG:164:LYS:HB2	1.90	0.42
72:SG:227:GLN:HB3	72:SG:231:ARG:HH21	1.84	0.42
81:SX:28:LYS:O	81:SX:32:LEU:HB2	2.19	0.42
81:SX:34:THR:HG21	86:S2:1189:A:H4'	2.01	0.42
6:L5:398:A2M:HM'3	6:L5:398:A2M:H1'	1.79	0.42
6:L5:1410:U:H3	35:Lb:52:LYS:NZ	2.17	0.42
6:L5:4535:A:H2'	6:L5:4536:OMC:H6	1.84	0.42
6:L5:4940:C:H5'	6:L5:4941:G:H5''	2.01	0.42
9:LA:7:GLY:HA2	9:LA:10:LYS:HG3	2.02	0.42
12:LD:211:LEU:HB3	12:LD:219:TYR:HB2	2.02	0.42
20:LM:37:LEU:HD12	20:LM:37:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LQ:110:ARG:HG3	24:LQ:120:ILE:HD12	2.01	0.42
26:LS:69:GLU:HG3	26:LS:71:SER:H	1.84	0.42
36:Lc:30:GLY:O	36:Lc:34:THR:OG1	2.26	0.42
37:Ld:33:ILE:HD11	37:Ld:45:ALA:HA	2.00	0.42
43:Lj:67:LEU:HD23	43:Lj:67:LEU:HA	1.87	0.42
45:Ll:28:ARG:HA	45:Ll:33:ASN:ND2	2.33	0.42
63:SZ:48:VAL:HG23	63:SZ:80:ARG:HD2	2.01	0.42
67:Sg:101:PHE:CD2	67:Sg:136:GLY:HA2	2.54	0.42
67:Sg:207:CYS:SG	67:Sg:219:TRP:HB2	2.60	0.42
70:SC:214:LEU:HD22	70:SC:244:ILE:HD11	2.02	0.42
76:SL:48:LYS:HD3	76:SL:52:GLU:OE2	2.20	0.42
81:SX:88:ASP:HA	86:S2:617:G:H4'	2.01	0.42
86:S2:1393:G:H2'	86:S2:1394:G:C8	2.55	0.42
86:S2:1401:A:H2'	86:S2:1402:A:C8	2.54	0.42
5:AT:63:C:H2'	5:AT:64:G:C8	2.54	0.42
6:L5:85:G:O2'	6:L5:97:G:O6	2.31	0.42
6:L5:137:G:H2'	6:L5:138:G:C8	2.53	0.42
6:L5:1281:G:C6	13:LE:128:HIS:HB2	2.55	0.42
6:L5:1444:G:H22	6:L5:2104:G:N2	2.18	0.42
6:L5:1824:G:H5''	27:LT:35:LYS:HE2	2.01	0.42
6:L5:3867:A2M:H2'	6:L5:3868:G:O4'	2.19	0.42
6:L5:4458:C:H2'	6:L5:4459:U:C6	2.55	0.42
6:L5:4859:C:H2'	6:L5:4860:G:C8	2.55	0.42
19:LL:59:VAL:HG21	19:LL:73:GLY:HA3	2.01	0.42
19:LL:194:ILE:HD12	19:LL:194:ILE:HA	1.88	0.42
24:LQ:43:PHE:CD2	24:LQ:133:GLY:HA3	2.55	0.42
27:LT:39:ILE:HG13	27:LT:102:ARG:HE	1.85	0.42
32:LY:47:MET:HE3	32:LY:48:PRO:HD2	2.01	0.42
32:LY:50:ARG:NH1	32:LY:51:LYS:HB3	2.35	0.42
38:Le:98:GLU:HG2	38:Le:123:THR:OG1	2.20	0.42
43:Lj:85:LYS:HB3	43:Lj:85:LYS:HE3	1.71	0.42
54:SF:167:LYS:HA	63:SZ:71:ALA:HB1	2.02	0.42
68:SA:5:LEU:HD11	79:SV:41:LYS:HD2	2.01	0.42
68:SA:215:GLN:O	68:SA:219:GLU:HG2	2.19	0.42
71:SE:212:ASP:OD1	71:SE:216:ASN:N	2.52	0.42
73:SH:63:PHE:HB3	73:SH:97:GLN:HG3	2.01	0.42
85:Se:56:ASN:ND2	86:S2:606:G:O4'	2.48	0.42
86:S2:601:OMG:HM23	86:S2:601:OMG:H1'	1.71	0.42
86:S2:888:U:O2'	86:S2:898:U:N3	2.49	0.42
1:CI:63:ARG:HD2	1:CI:63:ARG:HA	1.85	0.42
2:Pt:9:A:O2'	2:Pt:10:G:N7	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CF:26:HIS:HB3	4:CF:201:MET:HE3	2.01	0.42
6:L5:108:A:N1	6:L5:333:U:O2'	2.50	0.42
6:L5:1178:G:H2'	12:LD:286:SER:HB3	2.01	0.42
6:L5:1392:A:H2'	6:L5:1393:G:C8	2.55	0.42
6:L5:2521:G:H5'	6:L5:2640:G:H1'	2.02	0.42
6:L5:3610:A:H2'	6:L5:3611:A:C8	2.55	0.42
6:L5:4113:U:H4'	6:L5:4115:G:C5	2.55	0.42
6:L5:4195:G:OP1	6:L5:4221:C:O2'	2.36	0.42
10:LB:117:ARG:HA	10:LB:177:LYS:HD2	2.01	0.42
17:LI:51:HIS:CD2	17:LI:168:SER:HB3	2.54	0.42
20:LM:38:VAL:O	20:LM:47:ARG:HA	2.18	0.42
32:LY:50:ARG:HB3	32:LY:53:ASP:OD2	2.20	0.42
52:Lt:147:HIS:HA	52:Lt:148:PRO:HD3	1.83	0.42
56:SM:20:GLU:HG2	56:SM:119:GLN:HB2	2.00	0.42
56:SM:31:LEU:HG	56:SM:33:ARG:HG3	2.01	0.42
57:SP:93:MET:HE1	57:SP:106:GLU:OE1	2.19	0.42
60:SS:78:LYS:HD3	60:SS:78:LYS:HA	1.76	0.42
70:SC:74:LYS:HA	70:SC:74:LYS:HD3	1.89	0.42
73:SH:76:GLN:O	73:SH:80:VAL:HG23	2.20	0.42
78:SO:113:GLN:OE1	83:Sa:46:GLU:N	2.53	0.42
83:Sa:34:LYS:NZ	86:S2:1862:G:N7	2.61	0.42
1:CI:72:ARG:NH2	25:LR:25:ASP:OD2	2.48	0.42
4:CF:164:GLN:O	4:CF:168:GLU:HG2	2.20	0.42
5:AT:15:G:N2	5:AT:49:C:O2	2.52	0.42
6:L5:462:G:H2'	6:L5:463:A:C8	2.54	0.42
6:L5:499:G:H2'	6:L5:499:G:N3	2.35	0.42
6:L5:691:C:H2'	6:L5:692:A:H8	1.85	0.42
6:L5:730:G:OP2	14:LF:76:ARG:NE	2.48	0.42
6:L5:982:U:H2'	6:L5:983:C:C6	2.55	0.42
6:L5:1345:A:H2'	6:L5:1346:C:C6	2.55	0.42
6:L5:1538:U:H2'	6:L5:1539:G:H8	1.85	0.42
6:L5:2335:C:H2'	6:L5:2336:G:H8	1.85	0.42
6:L5:2415:U:H2'	6:L5:2416:G:C8	2.55	0.42
6:L5:2845:A:H61	6:L5:3843:C:N4	2.18	0.42
6:L5:4638:U:H2'	6:L5:4639:G:N3	2.35	0.42
6:L5:4987:C:P	10:LB:116:ARG:HH22	2.42	0.42
8:L8:67:U:H2'	8:L8:68:G:C8	2.55	0.42
8:L8:92:U:H2'	8:L8:93:C:O4'	2.20	0.42
13:LE:227:HIS:HE1	13:LE:230:GLY:HA2	1.83	0.42
18:LJ:35:ARG:O	18:LJ:39:VAL:HG23	2.20	0.42
23:LP:32:THR:HG23	23:LP:58:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LR:105:LEU:HD23	25:LR:138:LEU:HD23	2.01	0.42
36:Lc:82:GLY:HA2	36:Lc:91:VAL:HG12	2.02	0.42
40:Lg:41:ALA:O	40:Lg:52:ARG:HD3	2.20	0.42
54:SF:112:LEU:HD13	54:SF:177:LEU:HD21	2.02	0.42
56:SM:17:ALA:O	56:SM:20:GLU:HG3	2.18	0.42
62:SU:104:ILE:HB	62:SU:106:ILE:HG12	2.01	0.42
64:Sc:44:ARG:HH22	64:Sc:63:ARG:HH11	1.68	0.42
69:SB:71:LEU:HD22	69:SB:82:ARG:HD2	2.02	0.42
78:SO:96:LYS:HD3	78:SO:132:VAL:HG11	2.02	0.42
82:SY:93:ARG:HH21	86:S2:575:A:P	2.42	0.42
86:S2:562:U:H2'	86:S2:563:G:C8	2.55	0.42
86:S2:867:OMG:H1'	86:S2:867:OMG:HM23	1.75	0.42
86:S2:1232:PSU:H2'	86:S2:1233:G:H8	1.85	0.42
86:S2:1759:G:N2	86:S2:1760:G:O6	2.51	0.42
4:CF:348:ASN:ND2	4:CF:431:GLN:HG3	2.35	0.41
6:L5:223:G:H4'	6:L5:225:G:C8	2.54	0.41
6:L5:1870:C:H2'	6:L5:1871:A2M:H8	2.02	0.41
6:L5:2622:G:O6	28:LU:81:ARG:NH2	2.53	0.41
6:L5:2823:G:N7	25:LR:20:LYS:HD3	2.35	0.41
6:L5:3893:C:O2'	6:L5:4979:A:N1	2.50	0.41
6:L5:4524:G:OP1	6:L5:4559:A:N6	2.47	0.41
9:LA:115:CYS:SG	9:LA:124:GLY:HA3	2.60	0.41
25:LR:99:MET:HE2	25:LR:99:MET:HA	2.02	0.41
26:LS:15:ARG:HD2	26:LS:25:PRO:HG2	2.01	0.41
29:LV:111:GLU:H	29:LV:111:GLU:CD	2.28	0.41
35:Lb:65:MET:HG3	35:Lb:68:ARG:HH12	1.85	0.41
52:Lt:79:ALA:HA	52:Lt:82:ILE:HG22	2.01	0.41
61:ST:71:GLY:O	61:ST:75:MET:HG2	2.20	0.41
62:SU:19:ARG:HH11	62:SU:92:HIS:HB3	1.85	0.41
62:SU:32:LEU:CD1	62:SU:85:HIS:HB2	2.50	0.41
86:S2:186:C:H2'	86:S2:187:G:C8	2.55	0.41
86:S2:838:G:N1	86:S2:840:C:O2'	2.50	0.41
86:S2:1597:C:H4'	86:S2:1603:G:O6	2.19	0.41
86:S2:1713:C:H2'	86:S2:1714:U:C6	2.55	0.41
3:Et:43:A:H2'	3:Et:44:G:C8	2.55	0.41
4:CF:229:LEU:HD13	4:CF:232:LEU:HD11	2.02	0.41
4:CF:266:ARG:HA	4:CF:307:ASN:HA	2.02	0.41
6:L5:513:U:H3'	6:L5:514:U:H4'	2.01	0.41
6:L5:1172:C:O2'	6:L5:1173:G:H8	2.03	0.41
6:L5:1382:G:OP1	19:LL:66:TYR:OH	2.34	0.41
6:L5:2264:C:H2'	6:L5:2265:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:3822:PSU:OP1	88:L5:5289:SPM:N5	2.32	0.41
6:L5:4389:C:H2'	6:L5:4390:A:H8	1.85	0.41
7:L7:35:U:O2	7:L7:45:U:O2'	2.35	0.41
10:LB:29:VAL:HA	10:LB:220:ILE:HD13	2.01	0.41
15:LG:178:GLY:O	15:LG:223:ARG:NH2	2.53	0.41
25:LR:35:ALA:HA	25:LR:40:GLN:OE1	2.20	0.41
50:Lr:47:LYS:HB2	50:Lr:102:TYR:CZ	2.55	0.41
53:SD:213:PRO:HB3	59:SR:20:TYR:CE1	2.55	0.41
57:SP:29:SER:HB3	57:SP:32:GLN:NE2	2.34	0.41
73:SH:25:GLN:O	73:SH:28:LEU:HG	2.20	0.41
78:SO:131:ASP:OD1	78:SO:133:THR:OG1	2.33	0.41
86:S2:1348:G:OP2	86:S2:1348:G:N2	2.50	0.41
86:S2:1417:C:O2	86:S2:1422:G:C6	2.74	0.41
6:L5:956:A:H1'	6:L5:2076:G:H5''	2.01	0.41
6:L5:3722:G:H2'	6:L5:3723:A:H8	1.84	0.41
6:L5:4227:OMU:HM23	6:L5:4227:OMU:H1'	1.85	0.41
9:LA:112:ILE:HD11	49:Lp:79:VAL:HG22	2.03	0.41
18:LJ:119:TYR:CG	60:SS:12:ILE:HG12	2.56	0.41
31:LX:64:SER:HB2	41:Lh:69:LEU:HD13	2.01	0.41
54:SF:123:GLU:OE1	64:Sc:63:ARG:NH2	2.53	0.41
62:SU:61:LEU:HB2	62:SU:82:MET:HB3	2.02	0.41
65:Sd:56:ASP:OXT	86:S2:1480:A:O2'	2.32	0.41
67:Sg:283:PRO:O	67:Sg:285:GLN:NE2	2.53	0.41
72:SG:174:PRO:HG3	86:S2:65:C:C2	2.55	0.41
73:SH:118:ARG:HA	73:SH:118:ARG:HD3	1.91	0.41
82:SY:42:GLU:O	82:SY:46:LYS:HG3	2.20	0.41
86:S2:1839:U:H2'	86:S2:1840:U:C6	2.55	0.41
3:Et:28:C:H2'	3:Et:29:A:C8	2.54	0.41
3:Et:32:C:H2'	3:Et:33:U:C2	2.55	0.41
4:CF:34:ILE:HD13	4:CF:59:VAL:HG21	2.03	0.41
6:L5:302:C:H2'	6:L5:303:C:C6	2.55	0.41
6:L5:1869:G:C6	89:L5:5284:SPD:H32	2.55	0.41
6:L5:2409:U:H5	6:L5:2783:A:N1	2.18	0.41
6:L5:3865:A:H61	6:L5:3881:G:H1	1.67	0.41
6:L5:4619:U:H2'	6:L5:4620:OMU:H6	2.01	0.41
11:LC:334:THR:HG21	14:LF:51:TYR:OH	2.20	0.41
24:LQ:69:LYS:HA	24:LQ:69:LYS:HD3	1.90	0.41
60:SS:113:ARG:O	60:SS:117:ILE:HG12	2.19	0.41
65:Sd:13:LYS:HG3	86:S2:1556:A:C8	2.55	0.41
66:Sf:108:VAL:HB	66:Sf:113:LYS:H	1.86	0.41
67:Sg:153:CYS:O	67:Sg:167:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SB:141:GLY:HA3	69:SB:207:LEU:HD23	2.03	0.41
75:SJ:176:LYS:HA	75:SJ:179:LYS:HG2	2.01	0.41
83:Sa:39:PHE:CE2	83:Sa:41:ILE:HD11	2.54	0.41
85:Se:8:ARG:NH1	86:S2:615:C:O3'	2.53	0.41
2:Pt:18:G:H4'	2:Pt:60:A:C2	2.55	0.41
6:L5:2861:OMC:H1'	6:L5:2861:OMC:HM23	1.86	0.41
6:L5:4522:G:O2'	6:L5:4525:C:OP2	2.31	0.41
6:L5:4637:OMG:HM23	6:L5:4637:OMG:H1'	1.78	0.41
10:LB:337:VAL:HG11	10:LB:345:LEU:HD13	2.03	0.41
13:LE:282:TYR:HE1	39:Lf:31:GLU:HG2	1.85	0.41
17:LI:84:GLY:O	17:LI:140:THR:OG1	2.29	0.41
23:LP:95:LEU:HD23	23:LP:95:LEU:HA	1.95	0.41
26:LS:93:MET:HE1	26:LS:117:HIS:CE1	2.55	0.41
36:Lc:50:ASN:ND2	36:Lc:76:GLY:O	2.54	0.41
54:SF:59:LYS:HB3	54:SF:62:ARG:HG3	2.03	0.41
54:SF:60:ARG:HE	86:S2:1679:A:P	2.43	0.41
67:Sg:101:PHE:CE2	67:Sg:136:GLY:HA2	2.55	0.41
67:Sg:125:ARG:HD3	67:Sg:150:TRP:CE2	2.56	0.41
73:SH:43:LEU:HB3	73:SH:72:PHE:CE1	2.56	0.41
86:S2:71:G:H2'	86:S2:72:C:H4'	2.01	0.41
86:S2:1328:OMG:H1'	86:S2:1328:OMG:HM23	1.81	0.41
86:S2:1670:C:H2'	86:S2:1671:G:C8	2.55	0.41
86:S2:1845:A:H2'	86:S2:1846:G:H8	1.84	0.41
5:AT:3:C:N4	5:AT:71:A:H61	2.18	0.41
6:L5:279:A:OP2	21:LN:8:GLN:NE2	2.42	0.41
6:L5:654:C:O3'	11:LC:268:ARG:NH1	2.52	0.41
6:L5:1973:G:O2'	52:Lt:117:ARG:NH2	2.48	0.41
6:L5:2743:A:H2'	6:L5:2744:A:C8	2.56	0.41
6:L5:4318:C:H4'	48:Lo:17:LYS:HA	2.02	0.41
6:L5:4739:C:H2'	6:L5:4740:G:H5'	2.03	0.41
12:LD:52:ILE:HA	12:LD:147:ASP:HB3	2.02	0.41
12:LD:86:TYR:CE1	12:LD:247:ILE:HG13	2.55	0.41
15:LG:30:PRO:HG2	33:LZ:124:THR:HA	2.02	0.41
21:LN:159:ARG:HB3	21:LN:164:LEU:HB2	2.01	0.41
38:Le:19:LYS:HE3	38:Le:19:LYS:HB3	1.90	0.41
38:Le:89:LEU:HD13	38:Le:118:LEU:HD22	2.03	0.41
38:Le:99:ILE:HD13	38:Le:108:ARG:HB2	2.03	0.41
51:Ls:57:LYS:O	51:Ls:61:MET:HG2	2.20	0.41
55:SK:64:TRP:CD2	65:Sd:23:VAL:HG22	2.55	0.41
57:SP:86:LEU:H	57:SP:89:MET:CE	2.33	0.41
70:SC:212:LYS:HE2	70:SC:212:LYS:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SG:191:ARG:NH1	86:S2:312:G:H2'	2.35	0.41
77:SN:7:PRO:HG3	86:S2:996:A:H5''	2.01	0.41
86:S2:352:U:H2'	86:S2:353:C:C6	2.56	0.41
86:S2:382:C:H2'	86:S2:383:G:C8	2.56	0.41
86:S2:1754:G:N7	86:S2:1779:G:N2	2.67	0.41
6:L5:270:U:H2'	6:L5:271:C:C6	2.56	0.41
6:L5:492:U:H2'	6:L5:493:G:O4'	2.20	0.41
6:L5:1174:G:H1	6:L5:1186:U:H3	1.68	0.41
6:L5:1972:G:H2'	6:L5:1973:G:C8	2.56	0.41
6:L5:2060:G:N2	26:LS:115:ALA:HB2	2.36	0.41
6:L5:2422:OMC:HM23	6:L5:2422:OMC:H1'	1.90	0.41
6:L5:2656:U:H5''	33:LZ:38:TYR:HB3	2.02	0.41
6:L5:2844:A:O2'	6:L5:4631:G:H4'	2.21	0.41
6:L5:3689:G:O2'	6:L5:3818:UY1:OP2	2.34	0.41
6:L5:3785:A2M:H2	6:L5:4551:U:O2	2.20	0.41
6:L5:4102:C:H1'	6:L5:4108:G:H1	1.86	0.41
6:L5:4260:U:H2'	6:L5:4261:C:H6	1.83	0.41
8:L8:39:G:H1'	8:L8:103:A:N6	2.36	0.41
8:L8:47:C:H1'	8:L8:61:A:H2'	2.01	0.41
10:LB:286:LYS:HB3	10:LB:332:MET:HB3	2.03	0.41
12:LD:209:ARG:O	12:LD:213:GLU:HG2	2.21	0.41
22:LO:28:LEU:HD23	22:LO:28:LEU:HA	1.95	0.41
26:LS:83:ARG:HG3	26:LS:125:GLN:HB2	2.02	0.41
31:LX:81:LEU:HG	31:LX:83:THR:HG23	2.03	0.41
59:SR:7:LYS:HG3	86:S2:1373:C:OP1	2.20	0.41
59:SR:109:LEU:HG	59:SR:111:PHE:HD2	1.85	0.41
66:Sf:117:LEU:HD12	66:Sf:118:ARG:HD3	2.01	0.41
68:SA:147:LEU:HD13	68:SA:161:ILE:HB	2.03	0.41
71:SE:27:PHE:O	86:S2:495:U:O2'	2.38	0.41
74:SI:114:GLU:HG3	74:SI:119:LEU:O	2.21	0.41
75:SJ:142:VAL:HG12	75:SJ:144:ILE:H	1.85	0.41
80:SW:106:THR:OG1	80:SW:111:MET:HE2	2.21	0.41
86:S2:1374:C:H2'	86:S2:1375:G:O4'	2.21	0.41
5:AT:21:U:C4	5:AT:47:G:H1'	2.55	0.41
5:AT:63:C:H2'	5:AT:64:G:H8	1.85	0.41
6:L5:135:G:N3	6:L5:135:G:H2'	2.36	0.41
6:L5:1308:C:H2'	6:L5:1309:C:C6	2.56	0.41
6:L5:3607:U:H2'	6:L5:3608:A:C8	2.56	0.41
6:L5:4291:G:H4'	6:L5:4292:A:H5''	2.03	0.41
6:L5:4306:OMU:HM23	6:L5:4306:OMU:H1'	1.93	0.41
6:L5:4578:G:H2'	6:L5:4579:PSU:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4770:U:H2'	6:L5:4771:C:C6	2.56	0.41
12:LD:37:VAL:HG12	12:LD:50:ARG:HD3	2.02	0.41
15:LG:160:ASP:OD1	15:LG:160:ASP:N	2.54	0.41
19:LL:18:TRP:CD1	19:LL:18:TRP:H	2.38	0.41
33:LZ:95:VAL:HG12	33:LZ:110:ALA:HA	2.03	0.41
36:Lc:20:LEU:O	36:Lc:24:SER:HB3	2.21	0.41
38:Le:85:LEU:HD21	38:Le:115:ALA:HB2	2.02	0.41
39:Lf:29:LYS:HB2	39:Lf:83:MET:HE1	2.02	0.41
63:SZ:102:LYS:HA	63:SZ:102:LYS:HD3	1.81	0.41
68:SA:80:ARG:HH21	68:SA:126:ASP:HB2	1.86	0.41
69:SB:120:MET:HE1	86:S2:987:A:C6	2.56	0.41
70:SC:64:THR:HG22	70:SC:66:LEU:N	2.35	0.41
72:SG:195:LYS:HD3	86:S2:126:G:H5'	2.03	0.41
73:SH:58:LYS:HB2	73:SH:90:LYS:HG2	2.03	0.41
79:SV:27:LYS:HD3	79:SV:27:LYS:HA	1.86	0.41
81:SX:9:THR:HG22	86:S2:681:PSU:H4'	2.03	0.41
6:L5:260:C:H2'	6:L5:261:G:C8	2.55	0.41
6:L5:262:G:H2'	6:L5:263:G:H8	1.85	0.41
6:L5:1352:C:O2'	6:L5:1356:U:OP1	2.34	0.41
6:L5:1403:G:N2	6:L5:1415:G:C4	2.89	0.41
6:L5:1751:A:H2'	6:L5:1752:G:H8	1.86	0.41
6:L5:2276:A:H2'	6:L5:2277:C:O4'	2.21	0.41
6:L5:2448:G:H2'	6:L5:2449:A:C8	2.56	0.41
6:L5:2461:G:H2'	6:L5:2462:C:C6	2.55	0.41
6:L5:2543:A:H2	6:L5:2773:G:H22	1.68	0.41
6:L5:2876:OMG:HM22	6:L5:2877:G:H5'	2.02	0.41
6:L5:2878:G:OP2	6:L5:2879:A:O2'	2.28	0.41
6:L5:4236:G:H4'	6:L5:4328:G:O2'	2.21	0.41
6:L5:4680:G:H2'	6:L5:4681:A:C8	2.55	0.41
6:L5:4710:C:H2'	6:L5:4711:C:C6	2.56	0.41
6:L5:4749:C:H2'	6:L5:4750:G:O4'	2.21	0.41
6:L5:4920:C:H2'	6:L5:4921:C:H6	1.86	0.41
6:L5:5002:U:H2'	6:L5:5003:U:C6	2.56	0.41
7:L7:7:G:H5''	12:LD:22:ARG:HD3	2.03	0.41
8:L8:149:G:H21	15:LG:64:GLN:HE22	1.69	0.41
10:LB:71:GLU:HB2	30:LW:2:LYS:HD3	2.02	0.41
10:LB:122:TRP:CE2	10:LB:127:LYS:HE3	2.56	0.41
17:LI:207:ASP:HA	17:LI:210:ARG:HG2	2.03	0.41
18:LJ:20:LEU:HD21	18:LJ:130:PHE:CD2	2.56	0.41
20:LM:37:LEU:HD22	26:LS:75:VAL:HG23	2.02	0.41
22:LO:142:ALA:HA	22:LO:145:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LY:74:TYR:CE2	32:LY:77:LYS:HG3	2.56	0.41
38:Le:100:ALA:HB3	38:Le:103:VAL:HG23	2.03	0.41
39:Lf:92:LEU:HD23	39:Lf:92:LEU:HA	1.90	0.41
40:Lg:33:LEU:HD23	40:Lg:33:LEU:HA	1.91	0.41
52:Lt:12:VAL:HG11	52:Lt:65:GLN:N	2.36	0.41
52:Lt:114:ARG:NH1	52:Lt:126:SER:O	2.44	0.41
56:SM:95:ASP:HB3	56:SM:99:LYS:HB3	2.03	0.41
58:SQ:128:GLU:HG2	58:SQ:137:ALA:HB1	2.02	0.41
61:ST:113:VAL:HG22	61:ST:123:LEU:HD23	2.02	0.41
63:SZ:68:ILE:HB	63:SZ:109:TYR:HB2	2.03	0.41
68:SA:122:LEU:HD22	68:SA:137:ALA:HB2	2.01	0.41
68:SA:172:GLY:HA3	68:SA:203:PHE:HD1	1.85	0.41
68:SA:219:GLU:HA	68:SA:222:VAL:HG12	2.03	0.41
71:SE:160:ILE:HD12	71:SE:162:ILE:HD11	2.02	0.41
73:SH:91:HIS:ND1	73:SH:169:LYS:HG2	2.35	0.41
74:SI:42:ARG:HH21	74:SI:59:ARG:NH1	2.19	0.41
74:SI:141:ARG:HA	74:SI:141:ARG:CZ	2.51	0.41
77:SN:37:ILE:HG23	77:SN:50:ILE:HG21	2.03	0.41
79:SV:11:LEU:HD23	79:SV:11:LEU:H	1.85	0.41
80:SW:57:ARG:NH2	84:Sb:26:GLN:HB2	2.36	0.41
80:SW:125:ILE:HA	80:SW:125:ILE:HD12	1.84	0.41
86:S2:43:U:OP2	86:S2:485:A:N6	2.47	0.41
86:S2:484:A2M:H8	86:S2:484:A2M:O5'	2.20	0.41
86:S2:693:A:H2	86:S2:739:C:H4'	1.84	0.41
86:S2:747:U:O2	86:S2:796:G:C2	2.74	0.41
86:S2:1223:A:H2'	86:S2:1224:G:O4'	2.21	0.41
86:S2:1446:A:O2'	86:S2:1447:G:H5''	2.20	0.41
5:AT:6:C:H2'	5:AT:7:G:C8	2.56	0.41
6:L5:126:C:H2'	6:L5:127:G:H8	1.85	0.41
6:L5:267:G:H2'	6:L5:268:G:C8	2.54	0.41
6:L5:1247:U:H2'	6:L5:1248:C:C6	2.56	0.41
6:L5:2412:A:H2'	6:L5:2413:U:C6	2.56	0.41
6:L5:2749:C:H2'	6:L5:2750:G:C8	2.56	0.41
7:L7:4:U:H2'	7:L7:5:A:C8	2.56	0.41
7:L7:26:C:O2'	18:LJ:147:ARG:NH1	2.52	0.41
24:LQ:59:PRO:HG3	24:LQ:143:ARG:HA	2.02	0.41
28:LU:80:LYS:HG2	28:LU:110:TYR:CE2	2.54	0.41
41:Lh:104:THR:O	41:Lh:108:GLN:HG2	2.21	0.41
52:Lt:131:GLU:OE2	52:Lt:155:ILE:HG21	2.21	0.41
54:SF:182:LYS:HE3	54:SF:182:LYS:HB2	1.89	0.41
55:SK:80:ARG:HH22	55:SK:90:VAL:HG12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SM:86:GLY:HA2	56:SM:89:VAL:HG12	2.02	0.41
57:SP:47:ARG:NE	86:S2:1619:A:OP1	2.40	0.41
59:SR:6:THR:HA	86:S2:1373:C:H5'	2.03	0.41
65:Sd:3:HIS:CE1	65:Sd:5:GLN:HB2	2.56	0.41
65:Sd:41:GLN:OE1	65:Sd:41:GLN:N	2.54	0.41
66:Sf:125:GLU:HG2	66:Sf:126:CYS:N	2.36	0.41
68:SA:164:ASN:OD1	68:SA:165:ASN:N	2.54	0.41
69:SB:136:ARG:O	69:SB:215:VAL:HA	2.21	0.41
72:SG:133:LEU:HB2	86:S2:65:C:C2	2.56	0.41
72:SG:136:LYS:O	72:SG:176:ILE:HG13	2.20	0.41
75:SJ:59:GLU:O	75:SJ:62:THR:OG1	2.32	0.41
83:Sa:36:ILE:HD11	83:Sa:75:VAL:HG12	2.02	0.41
86:S2:433:A:H2'	86:S2:434:G:C8	2.57	0.41
86:S2:462:OMC:HM23	86:S2:462:OMC:H1'	1.85	0.41
86:S2:692:G:N7	86:S2:693:A:N6	2.68	0.41
86:S2:815:U:C2	86:S2:816:A:C8	3.09	0.41
86:S2:1025:U:H2'	86:S2:1026:C:O4'	2.21	0.41
86:S2:1540:G:H2'	86:S2:1541:G:C8	2.56	0.41
6:L5:73:A:H5''	19:LL:105:LYS:HD3	2.02	0.40
6:L5:652:G:H2'	6:L5:653:U:C6	2.56	0.40
6:L5:1086:C:H2'	6:L5:1087:A:H8	1.85	0.40
6:L5:1631:A:C8	9:LA:199:VAL:HG21	2.56	0.40
6:L5:1962:A:H2	6:L5:2024:G:H21	1.67	0.40
6:L5:2497:C:H2'	6:L5:2498:C:H6	1.86	0.40
6:L5:4070:U:H2'	6:L5:4071:U:C6	2.56	0.40
9:LA:145:LYS:HA	9:LA:145:LYS:HD3	1.86	0.40
11:LC:158:VAL:HG12	11:LC:217:ILE:HD12	2.02	0.40
12:LD:239:MET:HA	12:LD:242:LYS:NZ	2.35	0.40
14:LF:148:LYS:O	14:LF:152:GLU:HG2	2.21	0.40
15:LG:207:VAL:O	15:LG:212:LYS:NZ	2.55	0.40
17:LI:51:HIS:ND1	17:LI:137:SER:OG	2.49	0.40
25:LR:82:LYS:HA	25:LR:82:LYS:HD2	1.89	0.40
27:LT:50:LYS:HB3	27:LT:50:LYS:HE2	1.80	0.40
32:LY:126:ARG:HG2	32:LY:130:LYS:HE2	2.03	0.40
40:Lg:60:ARG:HD2	40:Lg:60:ARG:HA	1.84	0.40
52:Lt:22:VAL:HA	52:Lt:48:LYS:HG2	2.02	0.40
52:Lt:28:LEU:O	52:Lt:32:ILE:HD12	2.20	0.40
62:SU:52:GLY:HA3	86:S2:1401:A:H4'	2.03	0.40
70:SC:256:TRP:CE2	80:SW:68:ARG:HD3	2.56	0.40
73:SH:17:ASP:OD1	73:SH:17:ASP:N	2.51	0.40
74:SI:192:GLY:O	74:SI:196:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:S2:368:U:H3'	86:S2:369:C:H2'	2.03	0.40
86:S2:496:C:H2'	86:S2:497:C:H6	1.86	0.40
86:S2:880:G:H3'	86:S2:881:G:H8	1.85	0.40
2:Pt:3:C:H42	2:Pt:70:A:N6	2.19	0.40
6:L5:302:C:H2'	6:L5:303:C:H6	1.87	0.40
6:L5:423:G:H2'	6:L5:424:U:C6	2.57	0.40
6:L5:1974:U:H4'	6:L5:1975:G:H3'	2.03	0.40
6:L5:2683:C:H2'	6:L5:2684:C:C6	2.57	0.40
6:L5:4196:OMG:HM23	6:L5:4196:OMG:H1'	1.70	0.40
6:L5:4232:U:H5'	48:Lo:3:ASN:HB3	2.03	0.40
6:L5:4616:A:H2'	6:L5:4617:G:O4'	2.21	0.40
6:L5:4906:C:H2'	6:L5:4907:G:H8	1.86	0.40
6:L5:5015:G:H2'	6:L5:5016:A:C2	2.57	0.40
16:LH:27:VAL:HG12	16:LH:84:VAL:HG21	2.03	0.40
16:LH:43:VAL:HG21	16:LH:73:ILE:HD13	2.03	0.40
31:LX:80:PRO:HA	31:LX:98:PHE:HA	2.01	0.40
52:Lt:114:ARG:O	52:Lt:117:ARG:HG2	2.22	0.40
52:Lt:150:ASP:OD1	52:Lt:151:ILE:N	2.53	0.40
67:Sg:191:HIS:CD2	67:Sg:195:LEU:HD11	2.56	0.40
69:SB:114:VAL:O	86:S2:1869:A:N6	2.53	0.40
74:SI:5:ARG:NE	86:S2:379:C:O2	2.54	0.40
86:S2:64:A:N6	86:S2:83:A:OP2	2.54	0.40
86:S2:835:C:H4'	86:S2:836:G:H8	1.86	0.40
86:S2:1112:U:O2	86:S2:1121:G:O6	2.40	0.40
86:S2:1719:A:N6	86:S2:1814:G:O2'	2.54	0.40
2:Pt:72:C:H3'	2:Pt:73:A:H8	1.86	0.40
4:CF:41:LYS:HA	4:CF:44:LYS:HE2	2.03	0.40
4:CF:146:LYS:NZ	4:CF:423:ARG:HH22	2.20	0.40
4:CF:198:GLY:HA2	4:CF:201:MET:HE1	2.03	0.40
6:L5:31:U:H2'	6:L5:32:G:O4'	2.21	0.40
6:L5:1186:U:H2'	6:L5:1187:G:N3	2.36	0.40
6:L5:1558:A:H2'	6:L5:1559:G:C8	2.56	0.40
6:L5:1794:A:H5''	6:L5:4214:A:H61	1.86	0.40
6:L5:2632:PSU:H2'	6:L5:2633:U:C6	2.56	0.40
6:L5:3951:G:H1'	6:L5:4062:A:H61	1.86	0.40
6:L5:4169:G:H4'	6:L5:4171:C:C2	2.56	0.40
6:L5:4232:U:H5''	48:Lo:3:ASN:O	2.21	0.40
9:LA:75:LEU:HD12	9:LA:75:LEU:HA	1.91	0.40
9:LA:150:LEU:HD11	9:LA:156:LYS:HD2	2.03	0.40
30:LW:102:LYS:HA	30:LW:105:ARG:HG2	2.03	0.40
40:Lg:84:ALA:O	40:Lg:88:ARG:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lk:25:ILE:HD13	44:Lk:57:LYS:HZ3	1.84	0.40
49:Lp:23:ARG:HA	49:Lp:26:VAL:HG12	2.04	0.40
51:Ls:58:ASN:O	51:Ls:62:ARG:NE	2.42	0.40
52:Lt:37:LEU:HA	52:Lt:40:LYS:HE3	2.03	0.40
54:SF:100:ILE:HD11	54:SF:108:PRO:HB3	2.02	0.40
56:SM:112:LYS:HE2	56:SM:112:LYS:HB2	1.83	0.40
58:SQ:34:VAL:HG22	58:SQ:70:VAL:HB	2.03	0.40
67:Sg:230:LEU:HD11	67:Sg:259:TRP:CG	2.56	0.40
67:Sg:251:ALA:HA	67:Sg:256:ILE:HD13	2.04	0.40
69:SB:67:PHE:CE2	78:SO:48:SER:HB3	2.56	0.40
78:SO:140:THR:HB	86:S2:1046:PSU:H1'	2.03	0.40
81:SX:22:TRP:HE3	81:SX:28:LYS:HD2	1.85	0.40
85:Se:36:MET:SD	85:Se:40:ARG:NE	2.87	0.40
86:S2:323:C:H5'	86:S2:324:C:OP1	2.21	0.40
86:S2:737:G:H2'	86:S2:738:C:H4'	2.03	0.40
86:S2:1406:G:H2'	86:S2:1407:U:C6	2.57	0.40
4:CF:134:ARG:HA	4:CF:177:TYR:CE2	2.57	0.40
4:CF:404:MET:N	4:CF:404:MET:SD	2.95	0.40
6:L5:223:G:N7	11:LC:165:LYS:HE3	2.37	0.40
6:L5:1307:A:H2'	6:L5:1308:C:C6	2.57	0.40
6:L5:1494:U:H2'	6:L5:1495:G:C8	2.57	0.40
6:L5:1806:G:H2'	6:L5:1807:C:H6	1.86	0.40
6:L5:3652:A:H2'	6:L5:3653:A:C5	2.56	0.40
6:L5:4153:C:H2'	6:L5:4154:G:H8	1.87	0.40
6:L5:4571:A2M:H2'	6:L5:4572:U:H6	1.86	0.40
7:L7:4:U:H2'	7:L7:5:A:H8	1.86	0.40
7:L7:7:G:OP1	12:LD:33:ARG:NH1	2.52	0.40
9:LA:131:GLY:N	9:LA:169:VAL:HG13	2.36	0.40
12:LD:53:VAL:HG11	12:LD:159:VAL:HA	2.03	0.40
24:LQ:32:TYR:HD1	24:LQ:32:TYR:HA	1.72	0.40
40:Lg:41:ALA:O	40:Lg:52:ARG:NH1	2.49	0.40
71:SE:89:VAL:HG11	71:SE:119:ALA:HB1	2.02	0.40
74:SI:129:LEU:HD12	74:SI:129:LEU:HA	1.91	0.40
81:SX:68:LYS:HG2	81:SX:91:LEU:HD22	2.04	0.40
86:S2:874:G:H2'	86:S2:875:A:C8	2.52	0.40
3:Et:2:C:H2'	3:Et:3:C:H6	1.87	0.40
6:L5:683:C:H2'	6:L5:684:G:O4'	2.21	0.40
6:L5:1081:C:O2'	6:L5:1082:C:H5'	2.21	0.40
6:L5:1419:G:H5''	24:LQ:71:LYS:NZ	2.37	0.40
6:L5:1588:U:H2'	6:L5:1589:C:C6	2.57	0.40
6:L5:1645:C:H2'	6:L5:1646:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4069:U:H2'	6:L5:4070:U:C6	2.57	0.40
6:L5:4305:G:C6	27:LT:80:VAL:HG21	2.56	0.40
6:L5:4415:A:OP1	17:LI:154:ARG:NH2	2.54	0.40
6:L5:4625:C:O2'	6:L5:4626:A:H5'	2.22	0.40
6:L5:4991:U:H2'	6:L5:4992:G:C8	2.56	0.40
9:LA:14:SER:OG	9:LA:15:VAL:N	2.54	0.40
18:LJ:40:LEU:HD23	18:LJ:40:LEU:HA	1.92	0.40
31:LX:88:LYS:HE3	31:LX:88:LYS:HB2	1.95	0.40
54:SF:97:PHE:HA	54:SF:100:ILE:HG12	2.03	0.40
67:Sg:66:VAL:HA	67:Sg:82:SER:HB2	2.03	0.40
67:Sg:314:ILE:HD12	67:Sg:314:ILE:HA	1.92	0.40
68:SA:57:LYS:HA	68:SA:57:LYS:HD2	1.79	0.40
69:SB:89:GLU:OE2	69:SB:99:ASN:HB3	2.21	0.40
73:SH:113:LYS:HA	73:SH:113:LYS:HD2	1.64	0.40
75:SJ:124:HIS:HD2	85:Se:31:ARG:HE	1.69	0.40
77:SN:94:LYS:HE2	77:SN:94:LYS:HB2	1.93	0.40
81:SX:52:LEU:N	81:SX:71:ARG:O	2.53	0.40
84:Sb:33:MET:HE3	84:Sb:48:SER:HA	2.04	0.40
86:S2:1351:G:O2'	86:S2:1378:A:N1	2.55	0.40
86:S2:1360:U:O2'	86:S2:1379:A:OP2	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
4	CF	438/441 (99%)	422 (96%)	16 (4%)	0	100	100
9	LA	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
10	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	LC	366/368 (100%)	351 (96%)	15 (4%)	0	100	100
12	LD	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
13	LE	236/250 (94%)	224 (95%)	12 (5%)	0	100	100
14	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
15	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
16	LH	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
17	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
18	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
19	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
20	LM	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
21	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
22	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
23	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
24	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
25	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
26	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
27	LT	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
28	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
29	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
30	LW	112/124 (90%)	107 (96%)	5 (4%)	0	100	100
31	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
32	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
33	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
34	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
35	Lb	105/121 (87%)	99 (94%)	6 (6%)	0	100	100
36	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
37	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
38	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
39	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
40	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
41	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
43	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
44	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
45	Ll	48/50 (96%)	48 (100%)	0	0	100	100
46	Lm	50/52 (96%)	50 (100%)	0	0	100	100
47	Ln	22/24 (92%)	22 (100%)	0	0	100	100
48	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
49	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
50	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
51	Ls	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
52	Lt	128/157 (82%)	111 (87%)	17 (13%)	0	100	100
53	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
54	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
55	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
56	SM	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
57	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
58	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
59	SR	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	28
60	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
61	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
62	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
63	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
64	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
65	Sd	53/55 (96%)	53 (100%)	0	0	100	100
66	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
67	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
68	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
69	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
70	SC	218/222 (98%)	203 (93%)	15 (7%)	0	100	100
71	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
72	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	SH	182/189 (96%)	169 (93%)	13 (7%)	0	100	100
74	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
75	SJ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
76	SL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
77	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
78	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
79	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
80	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
81	SX	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
82	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
83	Sa	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
84	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
85	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
All	All	12110/12348 (98%)	11587 (96%)	522 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	SR	129	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	25/25 (100%)	25 (100%)	0	100	100
4	CF	365/366 (100%)	365 (100%)	0	100	100
9	LA	190/190 (100%)	190 (100%)	0	100	100
10	LB	348/348 (100%)	348 (100%)	0	100	100
11	LC	306/306 (100%)	306 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	LD	246/247 (100%)	246 (100%)	0	100	100
13	LE	212/222 (96%)	212 (100%)	0	100	100
14	LF	194/194 (100%)	194 (100%)	0	100	100
15	LG	203/205 (99%)	203 (100%)	0	100	100
16	LH	169/169 (100%)	169 (100%)	0	100	100
17	LI	180/180 (100%)	180 (100%)	0	100	100
18	LJ	143/148 (97%)	143 (100%)	0	100	100
19	LL	176/176 (100%)	176 (100%)	0	100	100
20	LM	118/118 (100%)	118 (100%)	0	100	100
21	LN	171/171 (100%)	171 (100%)	0	100	100
22	LO	173/173 (100%)	173 (100%)	0	100	100
23	LP	134/134 (100%)	134 (100%)	0	100	100
24	LQ	164/164 (100%)	164 (100%)	0	100	100
25	LR	166/166 (100%)	166 (100%)	0	100	100
26	LS	156/156 (100%)	156 (100%)	0	100	100
27	LT	139/139 (100%)	139 (100%)	0	100	100
28	LU	91/91 (100%)	91 (100%)	0	100	100
29	LV	101/101 (100%)	101 (100%)	0	100	100
30	LW	95/103 (92%)	95 (100%)	0	100	100
31	LX	108/108 (100%)	108 (100%)	0	100	100
32	LY	124/124 (100%)	124 (100%)	0	100	100
33	LZ	117/117 (100%)	117 (100%)	0	100	100
34	La	120/120 (100%)	120 (100%)	0	100	100
35	Lb	88/101 (87%)	88 (100%)	0	100	100
36	Lc	83/83 (100%)	83 (100%)	0	100	100
37	Ld	98/98 (100%)	98 (100%)	0	100	100
38	Le	114/114 (100%)	114 (100%)	0	100	100
39	Lf	88/88 (100%)	88 (100%)	0	100	100
40	Lg	98/98 (100%)	98 (100%)	0	100	100
41	Lh	109/109 (100%)	109 (100%)	0	100	100
42	Li	86/86 (100%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Lj	73/73 (100%)	73 (100%)	0	100	100
44	Lk	64/64 (100%)	64 (100%)	0	100	100
45	Ll	47/47 (100%)	47 (100%)	0	100	100
46	Lm	48/48 (100%)	48 (100%)	0	100	100
47	Ln	23/23 (100%)	23 (100%)	0	100	100
48	Lo	93/93 (100%)	93 (100%)	0	100	100
49	Lp	74/74 (100%)	74 (100%)	0	100	100
50	Lr	109/109 (100%)	109 (100%)	0	100	100
51	Ls	162/164 (99%)	162 (100%)	0	100	100
52	Lt	107/130 (82%)	107 (100%)	0	100	100
53	SD	190/190 (100%)	190 (100%)	0	100	100
54	SF	159/159 (100%)	159 (100%)	0	100	100
55	SK	89/89 (100%)	89 (100%)	0	100	100
56	SM	102/104 (98%)	102 (100%)	0	100	100
57	SP	107/107 (100%)	107 (100%)	0	100	100
58	SQ	119/119 (100%)	119 (100%)	0	100	100
59	SR	122/122 (100%)	122 (100%)	0	100	100
60	SS	126/126 (100%)	126 (100%)	0	100	100
61	ST	113/113 (100%)	113 (100%)	0	100	100
62	SU	94/94 (100%)	94 (100%)	0	100	100
63	SZ	66/66 (100%)	66 (100%)	0	100	100
64	Sc	57/57 (100%)	57 (100%)	0	100	100
65	Sd	48/48 (100%)	48 (100%)	0	100	100
66	Sf	60/60 (100%)	60 (100%)	0	100	100
67	Sg	272/272 (100%)	272 (100%)	0	100	100
68	SA	183/183 (100%)	183 (100%)	0	100	100
69	SB	195/195 (100%)	195 (100%)	0	100	100
70	SC	186/188 (99%)	186 (100%)	0	100	100
71	SE	224/224 (100%)	224 (100%)	0	100	100
72	SG	207/207 (100%)	207 (100%)	0	100	100
73	SH	166/169 (98%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	SI	178/178 (100%)	178 (100%)	0	100	100
75	SJ	161/161 (100%)	161 (100%)	0	100	100
76	SL	137/137 (100%)	137 (100%)	0	100	100
77	SN	130/130 (100%)	130 (100%)	0	100	100
78	SO	107/110 (97%)	107 (100%)	0	100	100
79	SV	67/67 (100%)	67 (100%)	0	100	100
80	SW	112/112 (100%)	112 (100%)	0	100	100
81	SX	113/113 (100%)	113 (100%)	0	100	100
82	SY	113/113 (100%)	113 (100%)	0	100	100
83	Sa	89/89 (100%)	89 (100%)	0	100	100
84	Sb	75/75 (100%)	75 (100%)	0	100	100
85	Se	47/47 (100%)	47 (100%)	0	100	100
All	All	10512/10587 (99%)	10512 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
4	CF	136	HIS
4	CF	324	ASN
4	CF	331	ASN
4	CF	343	GLN
9	LA	97	ASN
10	LB	68	ASN
10	LB	145	GLN
10	LB	184	GLN
10	LB	203	GLN
10	LB	301	ASN
11	LC	329	ASN
11	LC	347	HIS
14	LF	239	GLN
15	LG	64	GLN
15	LG	112	GLN
16	LH	98	HIS
16	LH	138	GLN
17	LI	59	GLN
18	LJ	112	HIS

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Mol	Chain	Res	Type
19	LL	19	GLN
19	LL	149	GLN
20	LM	34	ASN
21	LN	117	ASN
22	LO	50	ASN
22	LO	199	HIS
23	LP	97	ASN
23	LP	118	GLN
23	LP	137	ASN
26	LS	23	HIS
26	LS	37	HIS
26	LS	108	GLN
27	LT	144	ASN
28	LU	94	ASN
29	LV	77	HIS
30	LW	79	GLN
30	LW	104	GLN
32	LY	61	HIS
34	La	34	ASN
34	La	67	GLN
34	La	120	GLN
35	Lb	60	ASN
38	Le	52	GLN
42	Li	15	HIS
43	Lj	66	HIS
45	Ll	33	ASN
46	Lm	117	HIS
49	Lp	33	GLN
50	Lr	4	HIS
50	Lr	21	ASN
51	Ls	71	ASN
52	Lt	65	GLN
52	Lt	149	HIS
54	SF	29	GLN
55	SK	28	HIS
55	SK	32	HIS
56	SM	19	GLN
58	SQ	48	GLN
62	SU	81	GLN
62	SU	92	HIS
63	SZ	89	GLN
65	Sd	5	GLN

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Mol	Chain	Res	Type
66	Sf	93	HIS
67	Sg	285	GLN
68	SA	9	GLN
68	SA	84	GLN
68	SA	132	GLN
69	SB	76	ASN
69	SB	95	ASN
69	SB	158	HIS
70	SC	267	GLN
72	SG	227	GLN
73	SH	76	GLN
73	SH	114	GLN
73	SH	162	GLN
74	SI	35	ASN
74	SI	52	ASN
76	SL	19	ASN
76	SL	65	ASN
77	SN	105	ASN
79	SV	35	ASN
81	SX	16	HIS
83	Sa	72	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	14 (19%)	0
3	Et	73/75 (97%)	24 (32%)	0
5	AT	74/76 (97%)	27 (36%)	0
6	L5	3643/3655 (99%)	711 (19%)	15 (0%)
7	L7	119/120 (99%)	9 (7%)	0
8	L8	155/156 (99%)	24 (15%)	0
86	S2	1714/1740 (98%)	360 (21%)	4 (0%)
All	All	5850/5896 (99%)	1169 (19%)	19 (0%)

All (1169) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	13	U
2	Pt	19	G
2	Pt	21	A

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Mol	Chain	Res	Type
2	Pt	46	G
2	Pt	47	U
2	Pt	48	C
2	Pt	49	C
2	Pt	58	A
2	Pt	66	C
2	Pt	67	G
2	Pt	70	A
2	Pt	74	C
2	Pt	76	A
3	Et	9	A
3	Et	10	G
3	Et	11	C
3	Et	19	G
3	Et	20	U
3	Et	21	A
3	Et	31	A
3	Et	33	U
3	Et	36	U
3	Et	40	C
3	Et	42	G
3	Et	46	G
3	Et	47	U
3	Et	48	C
3	Et	49	C
3	Et	55	U
3	Et	58	A
3	Et	60	U
3	Et	63	C
3	Et	65	G
3	Et	66	U
3	Et	70	G
3	Et	73	G
3	Et	76	A
5	AT	4	U
5	AT	8	U
5	AT	9	A
5	AT	12	G
5	AT	14	A
5	AT	16	C
5	AT	19	G
5	AT	20	U

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Mol	Chain	Res	Type
5	AT	21	U
5	AT	22	A
5	AT	26	C
5	AT	27	G
5	AT	31	G
5	AT	33	C
5	AT	37	C
5	AT	47	G
5	AT	48	U
5	AT	49	C
5	AT	50	C
5	AT	53	G
5	AT	57	C
5	AT	59	A
5	AT	60	A
5	AT	62	C
5	AT	65	G
5	AT	76	C
5	AT	77	A
6	L5	2	G
6	L5	25	A
6	L5	30	C
6	L5	39	A
6	L5	42	A
6	L5	48	G
6	L5	56	A
6	L5	59	A
6	L5	64	A
6	L5	65	A
6	L5	73	A
6	L5	91	G
6	L5	104	G
6	L5	108	A
6	L5	109	G
6	L5	110	C
6	L5	119	G
6	L5	120	A
6	L5	127	G
6	L5	132	G
6	L5	133	C
6	L5	134	G
6	L5	135	G

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Mol	Chain	Res	Type
6	L5	136	C
6	L5	159	C
6	L5	165	A
6	L5	172	C
6	L5	173	C
6	L5	181	C
6	L5	182	G
6	L5	183	C
6	L5	184	U
6	L5	185	C
6	L5	187	U
6	L5	188	G
6	L5	189	G
6	L5	200	U
6	L5	209	U
6	L5	210	C
6	L5	216	C
6	L5	218	A
6	L5	220	C
6	L5	234	G
6	L5	237	G
6	L5	255	C
6	L5	256	G
6	L5	261	G
6	L5	263	G
6	L5	264	C
6	L5	265	C
6	L5	266	C
6	L5	267	G
6	L5	280	G
6	L5	297	U
6	L5	306	A
6	L5	315	G
6	L5	316	U
6	L5	340	C
6	L5	373	G
6	L5	385	A
6	L5	387	G
6	L5	388	A
6	L5	396	A
6	L5	407	A
6	L5	409	G

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Mol	Chain	Res	Type
6	L5	410	A
6	L5	411	G
6	L5	412	G
6	L5	432	U
6	L5	449	C
6	L5	452	A
6	L5	453	G
6	L5	454	U
6	L5	456	C
6	L5	457	G
6	L5	467	U
6	L5	484	U
6	L5	485	C
6	L5	486	C
6	L5	489	C
6	L5	494	U
6	L5	497	G
6	L5	498	C
6	L5	499	G
6	L5	500	G
6	L5	502	C
6	L5	503	C
6	L5	504	G
6	L5	509	A
6	L5	510	U
6	L5	512	U
6	L5	513	U
6	L5	514	U
6	L5	518	G
6	L5	643	C
6	L5	646	G
6	L5	653	U
6	L5	654	C
6	L5	655	C
6	L5	656	C
6	L5	657	C
6	L5	659	G
6	L5	666	G
6	L5	667	A
6	L5	668	C
6	L5	669	C
6	L5	672	C

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Mol	Chain	Res	Type
6	L5	673	C
6	L5	685	C
6	L5	686	A
6	L5	687	U
6	L5	696	C
6	L5	704	C
6	L5	708	G
6	L5	730	G
6	L5	731	G
6	L5	738	C
6	L5	739	G
6	L5	742	G
6	L5	746	A
6	L5	759	G
6	L5	904	C
6	L5	905	C
6	L5	910	G
6	L5	913	U
6	L5	914	U
6	L5	915	A
6	L5	917	A
6	L5	923	C
6	L5	924	C
6	L5	932	A
6	L5	933	G
6	L5	936	C
6	L5	943	A
6	L5	944	A
6	L5	945	U
6	L5	946	C
6	L5	956	A
6	L5	959	G
6	L5	960	A
6	L5	961	G
6	L5	962	C
6	L5	965	G
6	L5	966	A
6	L5	967	C
6	L5	969	C
6	L5	970	G
6	L5	977	C
6	L5	982	U

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Mol	Chain	Res	Type
6	L5	985	C
6	L5	1070	G
6	L5	1071	C
6	L5	1072	C
6	L5	1075	G
6	L5	1082	C
6	L5	1083	U
6	L5	1168	G
6	L5	1171	G
6	L5	1172	C
6	L5	1173	G
6	L5	1179	U
6	L5	1180	C
6	L5	1181	C
6	L5	1182	C
6	L5	1183	C
6	L5	1187	G
6	L5	1202	C
6	L5	1203	G
6	L5	1210	C
6	L5	1211	G
6	L5	1214	C
6	L5	1215	C
6	L5	1219	G
6	L5	1222	A
6	L5	1246	G
6	L5	1253	G
6	L5	1254	A
6	L5	1257	A
6	L5	1258	G
6	L5	1262	G
6	L5	1266	G
6	L5	1267	C
6	L5	1269	G
6	L5	1271	G
6	L5	1272	C
6	L5	1273	G
6	L5	1275	G
6	L5	1280	C
6	L5	1284	G
6	L5	1285	U
6	L5	1287	G

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Mol	Chain	Res	Type
6	L5	1293	G
6	L5	1294	A
6	L5	1295	C
6	L5	1296	G
6	L5	1301	C
6	L5	1326	A2M
6	L5	1337	A
6	L5	1354	A
6	L5	1359	G
6	L5	1365	C
6	L5	1366	G
6	L5	1367	C
6	L5	1379	C
6	L5	1387	A
6	L5	1394	G
6	L5	1397	A
6	L5	1398	A
6	L5	1403	G
6	L5	1404	G
6	L5	1407	C
6	L5	1409	C
6	L5	1410	U
6	L5	1411	C
6	L5	1414	C
6	L5	1417	C
6	L5	1420	A
6	L5	1425	G
6	L5	1437	C
6	L5	1439	C
6	L5	1442	C
6	L5	1443	A
6	L5	1444	G
6	L5	1446	C
6	L5	1447	C
6	L5	1482	G
6	L5	1483	C
6	L5	1497	A
6	L5	1498	G
6	L5	1502	G
6	L5	1517	G
6	L5	1524	A2M
6	L5	1534	A2M

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Mol	Chain	Res	Type
6	L5	1537	A
6	L5	1547	A
6	L5	1566	C
6	L5	1578	U
6	L5	1591	U
6	L5	1596	U
6	L5	1621	A
6	L5	1624	G
6	L5	1625	OMG
6	L5	1631	A
6	L5	1633	G
6	L5	1634	A
6	L5	1638	A
6	L5	1640	C
6	L5	1641	G
6	L5	1642	A
6	L5	1654	G
6	L5	1661	C
6	L5	1676	C
6	L5	1677	PSU
6	L5	1678	C
6	L5	1694	C
6	L5	1697	G
6	L5	1699	A
6	L5	1700	G
6	L5	1701	A
6	L5	1702	C
6	L5	1704	C
6	L5	1705	G
6	L5	1717	C
6	L5	1718	C
6	L5	1719	A
6	L5	1721	G
6	L5	1726	U
6	L5	1731	C
6	L5	1734	G
6	L5	1742	A
6	L5	1750	G
6	L5	1755	C
6	L5	1757	U
6	L5	1758	G
6	L5	1760	G

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Mol	Chain	Res	Type
6	L5	1761	G
6	L5	1762	C
6	L5	1763	C
6	L5	1764	G
6	L5	1765	A
6	L5	1766	A
6	L5	1767	A
6	L5	1768	C
6	L5	1770	A
6	L5	1787	A
6	L5	1804	A
6	L5	1806	G
6	L5	1810	G
6	L5	1815	G
6	L5	1821	G
6	L5	1822	U
6	L5	1834	U
6	L5	1836	G
6	L5	1837	A
6	L5	1842	G
6	L5	1855	G
6	L5	1869	G
6	L5	1882	U
6	L5	1897	A
6	L5	1917	A
6	L5	1918	U
6	L5	1919	G
6	L5	1920	C
6	L5	1921	C
6	L5	1922	G
6	L5	1925	G
6	L5	1930	U
6	L5	1931	C
6	L5	1932	A
6	L5	1940	G
6	L5	1948	G
6	L5	1951	G
6	L5	1961	G
6	L5	1962	A
6	L5	1974	U
6	L5	1975	G
6	L5	1978	C

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Mol	Chain	Res	Type
6	L5	1980	U
6	L5	1981	G
6	L5	1982	G
6	L5	1983	A
6	L5	1984	A
6	L5	1985	G
6	L5	1986	U
6	L5	1991	A
6	L5	1993	C
6	L5	1997	U
6	L5	1998	A
6	L5	1999	A
6	L5	2001	G
6	L5	2002	A
6	L5	2003	G
6	L5	2004	U
6	L5	2011	C
6	L5	2017	A
6	L5	2018	C
6	L5	2024	G
6	L5	2026	A
6	L5	2046	G
6	L5	2048	U
6	L5	2055	G
6	L5	2056	G
6	L5	2069	A
6	L5	2084	C
6	L5	2085	G
6	L5	2092	G
6	L5	2093	A
6	L5	2095	A
6	L5	2097	U
6	L5	2098	G
6	L5	2101	C
6	L5	2102	G
6	L5	2107	C
6	L5	2110	C
6	L5	2111	G
6	L5	2112	G
6	L5	2250	C
6	L5	2252	G
6	L5	2256	C

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Mol	Chain	Res	Type
6	L5	2261	G
6	L5	2289	C
6	L5	2300	A
6	L5	2301	G
6	L5	2313	A
6	L5	2333	G
6	L5	2348	G
6	L5	2351	OMC
6	L5	2360	A
6	L5	2364	OMG
6	L5	2383	C
6	L5	2395	A
6	L5	2397	G
6	L5	2417	A
6	L5	2425	U
6	L5	2450	G
6	L5	2453	A
6	L5	2464	C
6	L5	2465	C
6	L5	2469	C
6	L5	2471	G
6	L5	2474	G
6	L5	2475	G
6	L5	2478	C
6	L5	2479	G
6	L5	2483	G
6	L5	2484	A
6	L5	2485	U
6	L5	2487	G
6	L5	2488	C
6	L5	2489	C
6	L5	2490	U
6	L5	2494	U
6	L5	2504	C
6	L5	2505	C
6	L5	2506	G
6	L5	2507	A
6	L5	2513	A
6	L5	2519	U
6	L5	2529	A
6	L5	2537	A
6	L5	2544	G

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Mol	Chain	Res	Type
6	L5	2546	G
6	L5	2547	G
6	L5	2554	U
6	L5	2555	G
6	L5	2556	G
6	L5	2560	C
6	L5	2565	A
6	L5	2567	G
6	L5	2573	A
6	L5	2583	C
6	L5	2587	A
6	L5	2589	C
6	L5	2602	G
6	L5	2618	G
6	L5	2627	C
6	L5	2653	C
6	L5	2662	G
6	L5	2669	C
6	L5	2675	G
6	L5	2676	A
6	L5	2687	U
6	L5	2694	G
6	L5	2695	A
6	L5	2696	A
6	L5	2706	G
6	L5	2707	U
6	L5	2708	U
6	L5	2710	C
6	L5	2711	G
6	L5	2712	G
6	L5	2721	G
6	L5	2724	G
6	L5	2726	G
6	L5	2739	C
6	L5	2742	G
6	L5	2743	A
6	L5	2746	A
6	L5	2761	U
6	L5	2763	U
6	L5	2769	U
6	L5	2770	C
6	L5	2788	U

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Mol	Chain	Res	Type
6	L5	2790	U
6	L5	2806	A
6	L5	2814	C
6	L5	2826	U
6	L5	2827	G
6	L5	2829	U
6	L5	2838	G
6	L5	2855	G
6	L5	2867	C
6	L5	2877	G
6	L5	2892	C
6	L5	2894	A
6	L5	2899	C
6	L5	2900	U
6	L5	2902	G
6	L5	2903	G
6	L5	2904	U
6	L5	2905	C
6	L5	2907	G
6	L5	2908	U
6	L5	3590	G
6	L5	3591	C
6	L5	3592	G
6	L5	3594	C
6	L5	3595	U
6	L5	3596	A
6	L5	3597	G
6	L5	3604	A
6	L5	3605	C
6	L5	3616	U
6	L5	3617	G
6	L5	3626	G
6	L5	3630	A
6	L5	3635	A
6	L5	3644	U
6	L5	3646	A
6	L5	3648	A
6	L5	3662	A
6	L5	3664	G
6	L5	3670	C
6	L5	3673	C
6	L5	3674	G

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Mol	Chain	Res	Type
6	L5	3691	G
6	L5	3701	OMC
6	L5	3710	G
6	L5	3711	A
6	L5	3713	U
6	L5	3726	A
6	L5	3727	A
6	L5	3748	A
6	L5	3753	G
6	L5	3760	A
6	L5	3770	U
6	L5	3774	A
6	L5	3775	A
6	L5	3776	G
6	L5	3777	G
6	L5	3785	A2M
6	L5	3786	U
6	L5	3792	OMG
6	L5	3811	G
6	L5	3812	C
6	L5	3814	U
6	L5	3817	A
6	L5	3819	G
6	L5	3824	A
6	L5	3838	U
6	L5	3839	G
6	L5	3840	U
6	L5	3867	A2M
6	L5	3877	A
6	L5	3878	C
6	L5	3879	G
6	L5	3885	G
6	L5	3892	U
6	L5	3897	G
6	L5	3901	A
6	L5	3906	A
6	L5	3907	G
6	L5	3908	A
6	L5	3915	U
6	L5	3923	A
6	L5	3938	G
6	L5	3939	G

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Mol	Chain	Res	Type
6	L5	3942	A
6	L5	3947	A
6	L5	3949	A
6	L5	3950	U
6	L5	3953	G
6	L5	4057	C
6	L5	4058	U
6	L5	4059	C
6	L5	4061	G
6	L5	4062	A
6	L5	4064	C
6	L5	4065	G
6	L5	4068	U
6	L5	4076	G
6	L5	4084	G
6	L5	4095	G
6	L5	4097	G
6	L5	4098	A
6	L5	4099	G
6	L5	4101	C
6	L5	4104	G
6	L5	4108	G
6	L5	4111	U
6	L5	4112	C
6	L5	4114	C
6	L5	4115	G
6	L5	4116	C
6	L5	4122	G
6	L5	4127	A
6	L5	4133	C
6	L5	4140	C
6	L5	4141	G
6	L5	4142	C
6	L5	4143	G
6	L5	4144	C
6	L5	4146	G
6	L5	4149	C
6	L5	4162	C
6	L5	4163	U
6	L5	4170	A
6	L5	4183	G
6	L5	4184	G

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Mol	Chain	Res	Type
6	L5	4191	G
6	L5	4203	A
6	L5	4222	G
6	L5	4225	G
6	L5	4229	U
6	L5	4233	A
6	L5	4251	A
6	L5	4254	G
6	L5	4257	A
6	L5	4258	C
6	L5	4265	U
6	L5	4268	A
6	L5	4273	A
6	L5	4281	A
6	L5	4291	G
6	L5	4295	U
6	L5	4304	A
6	L5	4305	G
6	L5	4306	OMU
6	L5	4314	C
6	L5	4319	C
6	L5	4329	G
6	L5	4330	G
6	L5	4332	C
6	L5	4349	C
6	L5	4350	C
6	L5	4354	U
6	L5	4373	G
6	L5	4376	A
6	L5	4377	G
6	L5	4378	A
6	L5	4379	A
6	L5	4387	C
6	L5	4391	G
6	L5	4394	A
6	L5	4420	U
6	L5	4421	C
6	L5	4422	A
6	L5	4438	U
6	L5	4448	G
6	L5	4449	A
6	L5	4464	A

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Mol	Chain	Res	Type
6	L5	4466	C
6	L5	4475	G
6	L5	4488	A
6	L5	4500	PSU
6	L5	4512	U
6	L5	4513	A
6	L5	4515	G
6	L5	4519	C
6	L5	4524	G
6	L5	4525	C
6	L5	4545	G
6	L5	4548	A
6	L5	4557	U
6	L5	4560	C
6	L5	4567	G
6	L5	4575	G
6	L5	4584	A
6	L5	4589	A
6	L5	4590	A2M
6	L5	4600	G
6	L5	4601	U
6	L5	4617	G
6	L5	4636	PSU
6	L5	4637	OMG
6	L5	4652	G
6	L5	4656	A
6	L5	4670	C
6	L5	4672	A
6	L5	4679	G
6	L5	4687	A
6	L5	4694	G
6	L5	4695	C
6	L5	4700	A
6	L5	4708	A
6	L5	4709	U
6	L5	4719	G
6	L5	4733	C
6	L5	4734	A
6	L5	4740	G
6	L5	4741	C
6	L5	4742	G
6	L5	4745	G

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Mol	Chain	Res	Type
6	L5	4754	G
6	L5	4757	C
6	L5	4759	C
6	L5	4761	G
6	L5	4765	G
6	L5	4771	C
6	L5	4772	C
6	L5	4775	C
6	L5	4859	C
6	L5	4870	G
6	L5	4871	C
6	L5	4875	G
6	L5	4882	U
6	L5	4883	C
6	L5	4889	G
6	L5	4895	C
6	L5	4896	G
6	L5	4897	G
6	L5	4899	G
6	L5	4900	C
6	L5	4901	G
6	L5	4910	G
6	L5	4912	G
6	L5	4914	C
6	L5	4922	C
6	L5	4925	U
6	L5	4926	C
6	L5	4927	G
6	L5	4928	C
6	L5	4934	A
6	L5	4940	C
6	L5	4941	G
6	L5	4943	A
6	L5	4951	G
6	L5	4955	A
6	L5	4960	G
6	L5	4976	U
6	L5	4985	U
6	L5	4988	U
6	L5	4989	U
6	L5	4991	U
6	L5	4995	U

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Mol	Chain	Res	Type
6	L5	5007	A
6	L5	5013	C
6	L5	5014	A
6	L5	5017	G
6	L5	5022	U
6	L5	5023	C
6	L5	5024	C
6	L5	5028	G
6	L5	5030	U
6	L5	5034	A
6	L5	5041	G
6	L5	5050	C
6	L5	5054	C
6	L5	5055	G
6	L5	5061	A
6	L5	5069	U
7	L7	33	U
7	L7	38	U
7	L7	53	U
7	L7	54	A
7	L7	64	G
7	L7	97	G
7	L7	100	A
7	L7	110	G
7	L7	120	U
8	L8	23	C
8	L8	25	G
8	L8	34	U
8	L8	35	C
8	L8	59	A
8	L8	62	A
8	L8	63	U
8	L8	80	A
8	L8	82	A
8	L8	84	A
8	L8	85	U
8	L8	87	G
8	L8	94	G
8	L8	103	A
8	L8	105	C
8	L8	111	U
8	L8	114	G

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Mol	Chain	Res	Type
8	L8	123	U
8	L8	124	U
8	L8	125	C
8	L8	126	C
8	L8	127	U
8	L8	147	G
8	L8	153	C
86	S2	13	C
86	S2	14	C
86	S2	17	C
86	S2	25	A
86	S2	33	G
86	S2	41	G
86	S2	44	U
86	S2	45	A
86	S2	46	A
86	S2	56	G
86	S2	58	C
86	S2	59	U
86	S2	65	C
86	S2	67	C
86	S2	68	A
86	S2	72	C
86	S2	73	C
86	S2	74	G
86	S2	76	U
86	S2	99	A2M
86	S2	103	A
86	S2	113	G
86	S2	114	G
86	S2	115	U
86	S2	126	G
86	S2	130	G
86	S2	142	C
86	S2	143	U
86	S2	149	A
86	S2	158	A
86	S2	160	U
86	S2	162	C
86	S2	170	A
86	S2	175	A
86	S2	179	C

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Mol	Chain	Res	Type
86	S2	190	G
86	S2	191	A
86	S2	196	C
86	S2	197	U
86	S2	198	U
86	S2	200	G
86	S2	203	G
86	S2	204	G
86	S2	207	G
86	S2	208	G
86	S2	214	U
86	S2	291	G
86	S2	292	A
86	S2	295	C
86	S2	302	A
86	S2	306	C
86	S2	307	G
86	S2	308	G
86	S2	309	G
86	S2	311	C
86	S2	312	G
86	S2	313	A
86	S2	318	A
86	S2	319	C
86	S2	323	C
86	S2	324	C
86	S2	325	C
86	S2	326	C
86	S2	328	U
86	S2	329	G
86	S2	332	G
86	S2	339	A
86	S2	340	C
86	S2	347	G
86	S2	360	A
86	S2	362	C
86	S2	364	A
86	S2	368	U
86	S2	370	G
86	S2	385	G
86	S2	386	C
86	S2	398	A

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Mol	Chain	Res	Type
86	S2	407	G
86	S2	408	A
86	S2	409	C
86	S2	436	OMG
86	S2	438	G
86	S2	448	A
86	S2	449	A
86	S2	450	C
86	S2	452	G
86	S2	464	A
86	S2	465	A
86	S2	471	G
86	S2	472	C
86	S2	473	A
86	S2	474	G
86	S2	476	A
86	S2	482	G
86	S2	487	U
86	S2	488	U
86	S2	492	C
86	S2	493	A
86	S2	502	C
86	S2	516	A
86	S2	517	OMC
86	S2	531	A
86	S2	532	C
86	S2	536	A
86	S2	537	C
86	S2	540	U
86	S2	542	U
86	S2	544	G
86	S2	546	G
86	S2	547	G
86	S2	557	U
86	S2	558	G
86	S2	559	G
86	S2	563	G
86	S2	564	A
86	S2	576	A2M
86	S2	583	A
86	S2	587	A
86	S2	589	G

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Mol	Chain	Res	Type
86	S2	590	A
86	S2	591	U
86	S2	593	C
86	S2	604	A
86	S2	614	C
86	S2	617	G
86	S2	623	G
86	S2	628	A
86	S2	631	U
86	S2	643	A
86	S2	644	OMG
86	S2	655	A
86	S2	660	C
86	S2	664	A
86	S2	668	A2M
86	S2	669	A
86	S2	671	A
86	S2	672	A
86	S2	673	G
86	S2	683	OMG
86	S2	688	U
86	S2	689	U
86	S2	692	G
86	S2	696	G
86	S2	697	G
86	S2	698	G
86	S2	731	G
86	S2	732	U
86	S2	733	C
86	S2	736	C
86	S2	737	G
86	S2	738	C
86	S2	749	U
86	S2	751	G
86	S2	752	G
86	S2	753	C
86	S2	788	G
86	S2	791	C
86	S2	792	C
86	S2	798	G
86	S2	799	OMU
86	S2	801	PSU

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Mol	Chain	Res	Type
86	S2	821	G
86	S2	822	U
86	S2	823	U
86	S2	824	C
86	S2	830	A
86	S2	834	C
86	S2	835	C
86	S2	836	G
86	S2	837	A
86	S2	838	G
86	S2	839	C
86	S2	842	C
86	S2	844	U
86	S2	847	A
86	S2	867	OMG
86	S2	870	A
86	S2	874	G
86	S2	877	C
86	S2	878	G
86	S2	880	G
86	S2	888	U
86	S2	889	U
86	S2	891	G
86	S2	893	U
86	S2	894	G
86	S2	896	U
86	S2	897	U
86	S2	898	U
86	S2	899	U
86	S2	900	C
86	S2	901	G
86	S2	903	A
86	S2	913	A
86	S2	920	A
86	S2	930	C
86	S2	933	G
86	S2	934	G
86	S2	943	U
86	S2	963	A
86	S2	970	G
86	S2	971	G
86	S2	972	A

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Mol	Chain	Res	Type
86	S2	985	G
86	S2	990	A
86	S2	992	A
86	S2	999	G
86	S2	1001	A
86	S2	1008	A
86	S2	1017	U
86	S2	1023	A
86	S2	1027	A
86	S2	1060	A
86	S2	1061	U
86	S2	1062	A
86	S2	1080	A
86	S2	1083	A
86	S2	1085	C
86	S2	1109	C
86	S2	1113	A
86	S2	1114	U
86	S2	1116	C
86	S2	1121	G
86	S2	1123	C
86	S2	1133	A
86	S2	1138	C
86	S2	1148	A
86	S2	1150	A
86	S2	1153	C
86	S2	1154	U
86	S2	1195	A
86	S2	1207	G
86	S2	1208	A
86	S2	1215	C
86	S2	1216	C
86	S2	1217	A
86	S2	1224	G
86	S2	1227	G
86	S2	1242	U
86	S2	1243	U
86	S2	1248	B8N
86	S2	1251	A
86	S2	1253	A
86	S2	1256	G
86	S2	1257	G

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Mol	Chain	Res	Type
86	S2	1259	A
86	S2	1271	C
86	S2	1272	OMC
86	S2	1274	G
86	S2	1275	G
86	S2	1283	C
86	S2	1286	G
86	S2	1288	OMU
86	S2	1294	G
86	S2	1295	A
86	S2	1301	A
86	S2	1302	G
86	S2	1303	C
86	S2	1304	U
86	S2	1308	U
86	S2	1342	U
86	S2	1357	A
86	S2	1358	U
86	S2	1371	U
86	S2	1372	U
86	S2	1376	A
86	S2	1378	A
86	S2	1402	A
86	S2	1413	G
86	S2	1418	C
86	S2	1419	C
86	S2	1420	G
86	S2	1421	A
86	S2	1422	G
86	S2	1423	C
86	S2	1433	C
86	S2	1435	C
86	S2	1437	C
86	S2	1438	A
86	S2	1439	A
86	S2	1442	OMU
86	S2	1449	G
86	S2	1454	A
86	S2	1463	U
86	S2	1478	U
86	S2	1487	A
86	S2	1489	A

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Mol	Chain	Res	Type
86	S2	1490	OMG
86	S2	1492	U
86	S2	1494	U
86	S2	1495	G
86	S2	1497	G
86	S2	1498	A
86	S2	1521	C
86	S2	1531	A
86	S2	1533	A
86	S2	1544	C
86	S2	1546	G
86	S2	1552	G
86	S2	1553	C
86	S2	1556	A
86	S2	1558	C
86	S2	1574	C
86	S2	1575	G
86	S2	1578	U
86	S2	1580	A
86	S2	1581	C
86	S2	1587	G
86	S2	1588	A
86	S2	1600	G
86	S2	1604	G
86	S2	1606	G
86	S2	1621	U
86	S2	1623	A
86	S2	1631	U
86	S2	1633	A
86	S2	1634	A
86	S2	1637	A
86	S2	1648	G
86	S2	1654	G
86	S2	1663	A
86	S2	1665	G
86	S2	1683	C
86	S2	1686	G
86	S2	1695	A
86	S2	1698	C
86	S2	1699	A
86	S2	1715	A
86	S2	1721	U

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Mol	Chain	Res	Type
86	S2	1722	G
86	S2	1744	G
86	S2	1745	A
86	S2	1752	C
86	S2	1753	C
86	S2	1754	G
86	S2	1755	C
86	S2	1757	G
86	S2	1759	G
86	S2	1761	U
86	S2	1772	C
86	S2	1773	C
86	S2	1774	C
86	S2	1777	G
86	S2	1782	G
86	S2	1783	C
86	S2	1784	G
86	S2	1786	U
86	S2	1798	C
86	S2	1810	U
86	S2	1825	A
86	S2	1826	G
86	S2	1831	A
86	S2	1835	A
86	S2	1838	U
86	S2	1849	G
86	S2	1851	MA6
86	S2	1861	G
86	S2	1862	G
86	S2	1863	A
86	S2	1865	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L5	406	C
6	L5	493	G
6	L5	914	U
6	L5	1082	C
6	L5	1590	C
6	L5	1633	G
6	L5	1703	C

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Mol	Chain	Res	Type
6	L5	1977	C
6	L5	2416	G
6	L5	2675	G
6	L5	2760	G
6	L5	3673	C
6	L5	4600	G
6	L5	4699	U
6	L5	4913	G
86	S2	291	G
86	S2	563	G
86	S2	688	U
86	S2	1477	U

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

179 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	$\# Z > 2$
6	OMG	L5	3899	6	23,26,27	0.63	0	32,38,41	0.54	0
6	OMG	L5	2364	6,87	23,26,27	0.59	0	32,38,41	0.45	0
6	OMC	L5	3869	6	19,22,23	0.62	0	25,31,34	0.71	0
6	OMG	L5	1625	6	23,26,27	0.55	0	32,38,41	0.50	0
6	PSU	L5	2839	6	18,21,22	1.08	2 (11%)	21,30,33	2.01	5 (23%)
6	OMG	L5	1316	6	23,26,27	0.64	0	32,38,41	0.55	0
86	PSU	S2	649	86	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)
6	A2M	L5	400	6	22,25,26	1.24	3 (13%)	30,36,39	1.60	9 (30%)
8	OMG	L8	75	8	23,26,27	0.53	0	32,38,41	0.48	0
6	A2M	L5	1871	6,87	22,25,26	1.26	3 (13%)	30,36,39	1.62	6 (20%)
6	PSU	L5	4431	6	18,21,22	1.04	1 (5%)	21,30,33	1.90	4 (19%)
86	A2M	S2	668	87,86	22,25,26	1.32	2 (9%)	30,36,39	1.63	7 (23%)
6	PSU	L5	5010	6	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
6	PSU	L5	4403	6	18,21,22	1.03	1 (5%)	21,30,33	1.98	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OMG	S2	1328	86	23,26,27	0.48	0	32,38,41	0.44	0
86	B8N	S2	1248	86	25,29,30	3.25	6 (24%)	28,42,45	1.98	7 (25%)
6	OMU	L5	4227	6	19,22,23	3.27	7 (36%)	25,31,34	1.87	5 (20%)
86	OMU	S2	428	86	19,22,23	3.32	7 (36%)	25,31,34	1.87	5 (20%)
6	A2M	L5	1524	6	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)
6	A2M	L5	1323	6	22,25,26	1.20	2 (9%)	30,36,39	1.60	9 (30%)
6	OMC	L5	2861	6	19,22,23	0.63	0	25,31,34	0.77	1 (4%)
4	SEP	CF	163	4	8,9,10	1.61	1 (12%)	7,12,14	1.29	1 (14%)
86	A2M	S2	1383	86	22,25,26	1.18	1 (4%)	30,36,39	1.62	7 (23%)
86	OMG	S2	509	86	23,26,27	0.51	0	32,38,41	0.50	0
6	6MZ	L5	4220	6	26,26,26	2.73	6 (23%)	36,39,39	2.90	16 (44%)
6	A2M	L5	3825	6	22,25,26	1.17	2 (9%)	30,36,39	1.58	8 (26%)
6	A2M	L5	4571	6	22,25,26	1.28	3 (13%)	30,36,39	1.59	9 (30%)
6	A2M	L5	2815	6	22,25,26	1.18	2 (9%)	30,36,39	1.54	8 (26%)
6	PSU	L5	1782	6	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
6	PSU	L5	2632	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
6	5MC	L5	4447	6	19,22,23	0.87	0	26,32,35	0.65	0
6	A2M	L5	3718	6	22,25,26	1.13	1 (4%)	30,36,39	1.55	6 (20%)
86	4AC	S2	1842	86	21,24,25	0.39	0	28,34,37	0.48	0
6	PSU	L5	1862	6	18,21,22	1.04	1 (5%)	21,30,33	2.01	4 (19%)
86	A2M	S2	1031	86	22,25,26	1.16	2 (9%)	30,36,39	1.59	6 (20%)
6	UY1	L5	3818	6	19,22,23	4.82	10 (52%)	21,31,34	2.00	5 (23%)
86	OMU	S2	1326	86	19,22,23	3.32	7 (36%)	25,31,34	1.84	5 (20%)
6	A2M	L5	3867	6	22,25,26	1.27	2 (9%)	30,36,39	1.50	9 (30%)
86	OMG	S2	683	86	23,26,27	0.54	0	32,38,41	0.48	0
6	OMG	L5	3744	6	23,26,27	0.56	0	32,38,41	0.46	0
6	OMU	L5	3925	6	19,22,23	3.21	7 (36%)	25,31,34	1.94	5 (20%)
6	A2M	L5	3785	6,87	22,25,26	1.15	1 (4%)	30,36,39	1.63	10 (33%)
86	OMG	S2	1490	86	23,26,27	0.57	0	32,38,41	0.50	0
86	OMC	S2	1391	86	19,22,23	0.56	0	25,31,34	0.68	0
6	PSU	L5	4689	6	18,21,22	1.07	2 (11%)	21,30,33	2.07	4 (19%)
86	PSU	S2	1046	86	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
6	1MA	L5	1322	6,87	21,25,26	0.63	0	30,37,40	0.80	2 (6%)
6	PSU	L5	1781	6	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
6	OMC	L5	4536	6	19,22,23	0.65	0	25,31,34	0.75	0
86	OMG	S2	436	86	23,26,27	0.51	0	32,38,41	0.54	0
86	PSU	S2	863	86	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PSU	S2	801	86	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
6	PSU	L5	4361	6	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
6	PSU	L5	4312	6	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
6	OMG	L5	4499	6	23,26,27	0.54	0	32,38,41	0.45	0
6	PSU	L5	4521	6,87	18,21,22	1.11	3 (16%)	21,30,33	2.05	6 (28%)
6	A2M	L5	4523	6,87	22,25,26	1.27	3 (13%)	30,36,39	1.58	8 (26%)
6	OMG	L5	2424	6	23,26,27	0.57	0	32,38,41	0.44	0
86	PSU	S2	681	86	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
6	OMC	L5	3701	6	19,22,23	0.71	0	25,31,34	1.74	4 (16%)
6	OMG	L5	4494	6	23,26,27	0.58	0	32,38,41	0.50	0
86	PSU	S2	686	86	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
6	A2M	L5	2363	6,87	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
6	OMC	L5	1340	6	19,22,23	0.67	0	25,31,34	0.80	0
86	OMG	S2	601	86	23,26,27	0.52	0	32,38,41	0.43	0
6	PSU	L5	3844	6	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
86	PSU	S2	1244	86	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L5	4296	6	18,21,22	1.05	1 (5%)	21,30,33	1.95	4 (19%)
86	4AC	S2	1337	86	21,24,25	0.40	0	28,34,37	0.81	2 (7%)
86	OMU	S2	121	86	19,22,23	3.29	7 (36%)	25,31,34	1.82	5 (20%)
86	6MZ	S2	1832	87,86	26,26,26	2.83	5 (19%)	36,39,39	2.03	10 (27%)
6	OMC	L5	2804	6	19,22,23	0.63	0	25,31,34	0.67	0
86	A2M	S2	576	86	22,25,26	1.18	1 (4%)	30,36,39	1.54	6 (20%)
6	OMG	L5	2876	6	23,26,27	0.56	0	32,38,41	0.56	0
6	OMG	L5	4370	6	23,26,27	0.57	0	32,38,41	0.52	0
86	PSU	S2	866	86	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
86	A2M	S2	468	86	22,25,26	1.24	1 (4%)	30,36,39	1.57	7 (23%)
6	PSU	L5	3822	6	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
6	OMU	L5	2837	6	19,22,23	3.24	7 (36%)	25,31,34	1.88	5 (20%)
86	OMC	S2	517	86	19,22,23	0.56	0	25,31,34	0.64	0
6	PSU	L5	1683	6	18,21,22	1.09	2 (11%)	21,30,33	2.11	5 (23%)
6	A2M	L5	3830	6	22,25,26	1.17	1 (4%)	30,36,39	1.57	6 (20%)
6	PSU	L5	1536	6	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
6	PSU	L5	4457	6	18,21,22	1.05	2 (11%)	21,30,33	2.09	6 (28%)
6	PSU	L5	1860	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	4 (19%)
6	PSU	L5	1677	6	18,21,22	1.05	1 (5%)	21,30,33	1.91	3 (14%)
6	PSU	L5	4636	6	18,21,22	1.10	1 (5%)	21,30,33	2.04	6 (28%)
6	OMG	L5	4637	6	23,26,27	0.57	0	32,38,41	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMG	L5	4623	6	23,26,27	0.59	0	32,38,41	0.58	0
86	PSU	S2	406	86	18,21,22	1.06	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L5	4552	6	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)
86	OMG	S2	867	86	23,26,27	0.51	0	32,38,41	0.45	0
86	OMG	S2	644	86	23,26,27	0.49	0	32,38,41	0.49	0
86	PSU	S2	109	86	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
86	PSU	S2	1045	86	18,21,22	1.06	1 (5%)	21,30,33	1.96	4 (19%)
86	PSU	S2	1174	86	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
6	PSU	L5	3884	6	18,21,22	1.08	2 (11%)	21,30,33	1.96	4 (19%)
6	OMC	L5	3887	6	19,22,23	0.60	0	25,31,34	0.67	0
6	OMC	L5	2351	6,87	19,22,23	0.67	0	25,31,34	0.90	1 (4%)
6	OMG	L5	4196	6,2	23,26,27	0.56	0	32,38,41	0.45	0
6	A2M	L5	1326	6	22,25,26	1.21	2 (9%)	30,36,39	1.51	9 (30%)
86	OMU	S2	627	86	19,22,23	3.38	7 (36%)	25,31,34	1.80	5 (20%)
8	PSU	L8	55	8	18,21,22	1.04	1 (5%)	21,30,33	1.98	4 (19%)
6	A2M	L5	1534	6,87	22,25,26	1.22	3 (13%)	30,36,39	1.44	7 (23%)
86	PSU	S2	105	86	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
86	PSU	S2	1177	86	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
6	OMG	L5	4228	6	23,26,27	0.55	0	32,38,41	0.65	0
86	G7M	S2	1639	2,86	23,26,27	2.63	9 (39%)	34,39,42	2.53	11 (32%)
6	OMG	L5	4618	6	23,26,27	0.56	0	32,38,41	0.53	0
6	OMG	L5	4392	6	23,26,27	0.59	0	32,38,41	0.48	0
6	UR3	L5	4530	6	19,22,23	2.63	7 (36%)	26,32,35	1.58	2 (7%)
6	A2M	L5	398	6	22,25,26	1.20	1 (4%)	30,36,39	1.63	7 (23%)
6	OMC	L5	4456	6	19,22,23	0.71	1 (5%)	25,31,34	0.77	1 (4%)
86	A2M	S2	166	86	22,25,26	1.23	1 (4%)	30,36,39	1.59	7 (23%)
86	OMU	S2	172	86	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
6	OMC	L5	3808	6,87	19,22,23	0.69	0	25,31,34	0.81	1 (4%)
6	PSU	L5	4576	6	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
6	PSU	L5	4471	6	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
6	A2M	L5	2787	6	22,25,26	1.15	1 (4%)	30,36,39	1.50	7 (23%)
86	MA6	S2	1850	86	23,26,27	1.28	2 (8%)	33,38,41	3.36	12 (36%)
6	PSU	L5	4532	6	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
86	OMU	S2	799	86	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
6	PSU	L5	3695	6	18,21,22	1.05	2 (11%)	21,30,33	2.00	5 (23%)
6	A2M	L5	4590	6	22,25,26	1.17	1 (4%)	30,36,39	1.53	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	A2M	S2	159	86	22,25,26	1.15	1 (4%)	30,36,39	1.51	7 (23%)
6	PSU	L5	5001	6	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
6	PSU	L5	3639	6	18,21,22	1.08	2 (11%)	21,30,33	2.06	5 (23%)
86	OMU	S2	116	86	19,22,23	3.30	7 (36%)	25,31,34	1.76	5 (20%)
6	OMC	L5	2422	6,87	19,22,23	0.63	0	25,31,34	0.69	0
8	PSU	L8	69	8	18,21,22	1.08	1 (5%)	21,30,33	2.04	6 (28%)
6	OMG	L5	1522	6	23,26,27	0.58	0	32,38,41	0.64	1 (3%)
86	PSU	S2	966	87,86	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
86	PSU	S2	1056	86	18,21,22	1.07	2 (11%)	21,30,33	1.97	5 (23%)
86	OMC	S2	462	86	19,22,23	0.54	0	25,31,34	0.69	0
86	PSU	S2	1232	86	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
86	OMU	S2	1288	86	19,22,23	3.40	7 (36%)	25,31,34	1.75	5 (20%)
6	OMC	L5	2365	6,87	19,22,23	0.63	0	25,31,34	0.59	0
86	PSU	S2	814	86	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
86	MA6	S2	1851	86	23,26,27	1.28	2 (8%)	33,38,41	3.42	12 (36%)
6	PSU	L5	1792	6	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
86	PSU	S2	93	86	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
6	OMC	L5	3841	6	19,22,23	0.63	0	25,31,34	0.72	0
6	OMG	L5	3627	6	23,26,27	0.55	0	32,38,41	0.61	0
6	PSU	L5	4673	6,87	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
6	PSU	L5	3853	6,87	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
6	PSU	L5	4579	6	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
6	OMG	L5	3792	6	23,26,27	0.56	0	32,38,41	0.47	0
6	A2M	L5	2401	6	22,25,26	1.21	1 (4%)	30,36,39	1.64	7 (23%)
86	PSU	S2	651	86	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)
86	OMC	S2	1703	86	19,22,23	0.61	0	25,31,34	0.59	0
6	PSU	L5	4293	6	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
6	PSU	L5	4628	6	18,21,22	1.01	1 (5%)	21,30,33	1.86	5 (23%)
86	OMU	S2	354	86	19,22,23	3.25	7 (36%)	25,31,34	1.88	5 (20%)
6	OMC	L5	2824	6	19,22,23	0.61	0	25,31,34	0.63	0
86	A2M	S2	27	86	22,25,26	1.19	1 (4%)	30,36,39	1.55	7 (23%)
6	PSU	L5	4493	6	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
6	OMU	L5	4498	6	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
6	PSU	L5	4353	6	18,21,22	1.10	2 (11%)	21,30,33	2.05	6 (28%)
6	OMU	L5	4620	6	19,22,23	3.17	7 (36%)	25,31,34	1.71	4 (16%)
86	PSU	S2	1081	86	18,21,22	1.03	1 (5%)	21,30,33	1.96	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PSU	S2	1367	86	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
86	A2M	S2	99	87,86	22,25,26	1.19	1 (4%)	30,36,39	1.57	7 (23%)
86	OMC	S2	1272	86	19,22,23	0.55	0	25,31,34	0.85	1 (4%)
6	PSU	L5	1582	6	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
6	PSU	L5	4299	6	18,21,22	1.05	1 (5%)	21,30,33	1.88	4 (19%)
6	5MC	L5	3782	6,87	19,22,23	0.69	0	26,32,35	0.80	1 (3%)
6	PSU	L5	4442	6	18,21,22	1.09	1 (5%)	21,30,33	2.03	6 (28%)
6	PSU	L5	4500	6	18,21,22	1.14	2 (11%)	21,30,33	2.05	5 (23%)
6	PSU	L5	1744	6,87	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L5	4973	6	18,21,22	1.05	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L5	3637	6	18,21,22	1.08	1 (5%)	21,30,33	2.02	5 (23%)
6	PSU	L5	3920	6,87	18,21,22	1.05	2 (11%)	21,30,33	1.97	5 (23%)
86	OMC	S2	174	86	19,22,23	0.53	0	25,31,34	0.65	0
86	PSU	S2	1004	86	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
6	PSU	L5	4972	6	18,21,22	1.02	1 (5%)	21,30,33	1.92	5 (23%)
86	OMU	S2	1442	86	19,22,23	3.33	7 (36%)	25,31,34	1.78	5 (20%)
86	A2M	S2	484	86	22,25,26	1.17	1 (4%)	30,36,39	1.47	7 (23%)
6	PSU	L5	3851	6	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
6	OMU	L5	4306	6	19,22,23	3.22	7 (36%)	25,31,34	1.88	5 (20%)

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
6	OMG	L5	3899	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	2364	6,87	-	2/9/27/28	0/3/3/3
6	OMC	L5	3869	6	-	1/9/27/28	0/2/2/2
6	OMG	L5	1625	6	-	2/9/27/28	0/3/3/3
6	PSU	L5	2839	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	1316	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	649	86	-	0/7/25/26	0/2/2/2
6	A2M	L5	400	6	-	1/9/27/28	0/3/3/3
8	OMG	L8	75	8	-	1/9/27/28	0/3/3/3
6	A2M	L5	1871	6,87	-	0/9/27/28	0/3/3/3
6	PSU	L5	4431	6	-	0/7/25/26	0/2/2/2
86	A2M	S2	668	87,86	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L5	5010	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4403	6	-	0/7/25/26	0/2/2/2
86	OMG	S2	1328	86	-	0/9/27/28	0/3/3/3
86	B8N	S2	1248	86	-	4/16/34/35	0/2/2/2
6	OMU	L5	4227	6	-	0/9/27/28	0/2/2/2
86	OMU	S2	428	86	-	6/9/27/28	0/2/2/2
6	A2M	L5	1524	6	-	2/9/27/28	0/3/3/3
6	A2M	L5	1323	6	-	2/9/27/28	0/3/3/3
6	OMC	L5	2861	6	-	0/9/27/28	0/2/2/2
4	SEP	CF	163	4	-	6/6/8/10	-
86	A2M	S2	1383	86	-	3/9/27/28	0/3/3/3
86	OMG	S2	509	86	-	0/9/27/28	0/3/3/3
6	6MZ	L5	4220	6	-	2/12/28/28	0/3/3/3
6	A2M	L5	3825	6	-	0/9/27/28	0/3/3/3
6	A2M	L5	4571	6	-	0/9/27/28	0/3/3/3
6	A2M	L5	2815	6	-	2/9/27/28	0/3/3/3
6	PSU	L5	1782	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	2632	6	-	0/7/25/26	0/2/2/2
6	5MC	L5	4447	6	-	4/7/25/26	0/2/2/2
6	A2M	L5	3718	6	-	0/9/27/28	0/3/3/3
86	4AC	S2	1842	86	-	0/11/29/30	0/2/2/2
6	PSU	L5	1862	6	-	0/7/25/26	0/2/2/2
86	A2M	S2	1031	86	-	0/9/27/28	0/3/3/3
6	UY1	L5	3818	6	-	2/9/27/28	0/2/2/2
86	OMU	S2	1326	86	-	0/9/27/28	0/2/2/2
6	A2M	L5	3867	6	-	2/9/27/28	0/3/3/3
86	OMG	S2	683	86	-	2/9/27/28	0/3/3/3
6	OMG	L5	3744	6	-	0/9/27/28	0/3/3/3
6	OMU	L5	3925	6	-	0/9/27/28	0/2/2/2
6	A2M	L5	3785	6,87	-	1/9/27/28	0/3/3/3
86	OMG	S2	1490	86	-	1/9/27/28	0/3/3/3
86	OMC	S2	1391	86	-	0/9/27/28	0/2/2/2
6	PSU	L5	4689	6	-	0/7/25/26	0/2/2/2
86	PSU	S2	1046	86	-	0/7/25/26	0/2/2/2
6	1MA	L5	1322	6,87	-	2/7/25/26	0/3/3/3
6	PSU	L5	1781	6	-	1/7/25/26	0/2/2/2
6	OMC	L5	4536	6	-	0/9/27/28	0/2/2/2
86	OMG	S2	436	86	-	2/9/27/28	0/3/3/3
86	PSU	S2	863	86	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PSU	S2	801	86	-	2/7/25/26	0/2/2/2
6	PSU	L5	4361	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4312	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4499	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4521	6,87	-	0/7/25/26	0/2/2/2
6	A2M	L5	4523	6,87	-	0/9/27/28	0/3/3/3
6	OMG	L5	2424	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	681	86	-	0/7/25/26	0/2/2/2
6	OMC	L5	3701	6	-	6/9/27/28	0/2/2/2
6	OMG	L5	4494	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	686	86	-	0/7/25/26	0/2/2/2
6	A2M	L5	2363	6,87	-	0/9/27/28	0/3/3/3
6	OMC	L5	1340	6	-	1/9/27/28	0/2/2/2
86	OMG	S2	601	86	-	1/9/27/28	0/3/3/3
6	PSU	L5	3844	6	-	1/7/25/26	0/2/2/2
86	PSU	S2	1244	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	4296	6	-	0/7/25/26	0/2/2/2
86	4AC	S2	1337	86	-	1/11/29/30	0/2/2/2
86	OMU	S2	121	86	-	0/9/27/28	0/2/2/2
86	6MZ	S2	1832	87,86	-	3/12/28/28	0/3/3/3
6	OMC	L5	2804	6	-	0/9/27/28	0/2/2/2
86	A2M	S2	576	86	-	3/9/27/28	0/3/3/3
6	OMG	L5	2876	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	4370	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	866	86	-	0/7/25/26	0/2/2/2
86	A2M	S2	468	86	-	0/9/27/28	0/3/3/3
6	PSU	L5	3822	6	-	0/7/25/26	0/2/2/2
6	OMU	L5	2837	6	-	0/9/27/28	0/2/2/2
86	OMC	S2	517	86	-	2/9/27/28	0/2/2/2
6	PSU	L5	1683	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	3830	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	1536	6	-	2/7/25/26	0/2/2/2
6	PSU	L5	4457	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1860	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1677	6	-	3/7/25/26	0/2/2/2
6	PSU	L5	4636	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4637	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	4623	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	406	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	4552	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OMG	S2	867	86	-	3/9/27/28	0/3/3/3
86	OMG	S2	644	86	-	3/9/27/28	0/3/3/3
86	PSU	S2	109	86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1045	86	-	2/7/25/26	0/2/2/2
86	PSU	S2	1174	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	3884	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	3887	6	-	1/9/27/28	0/2/2/2
6	OMC	L5	2351	6,87	-	2/9/27/28	0/2/2/2
6	OMG	L5	4196	6,2	-	1/9/27/28	0/3/3/3
6	A2M	L5	1326	6	-	4/9/27/28	0/3/3/3
86	OMU	S2	627	86	-	1/9/27/28	0/2/2/2
8	PSU	L8	55	8	-	0/7/25/26	0/2/2/2
6	A2M	L5	1534	6,87	-	1/9/27/28	0/3/3/3
86	PSU	S2	105	86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1177	86	-	0/7/25/26	0/2/2/2
6	OMG	L5	4228	6	-	0/9/27/28	0/3/3/3
86	G7M	S2	1639	2,86	-	2/7/25/26	0/3/3/3
6	OMG	L5	4618	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	4392	6	-	0/9/27/28	0/3/3/3
6	UR3	L5	4530	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	398	6	-	1/9/27/28	0/3/3/3
6	OMC	L5	4456	6	-	0/9/27/28	0/2/2/2
86	A2M	S2	166	86	-	1/9/27/28	0/3/3/3
86	OMU	S2	172	86	-	0/9/27/28	0/2/2/2
6	OMC	L5	3808	6,87	-	0/9/27/28	0/2/2/2
6	PSU	L5	4576	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4471	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	2787	6	-	5/9/27/28	0/3/3/3
86	MA6	S2	1850	86	-	0/11/29/30	0/3/3/3
6	PSU	L5	4532	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	799	86	-	2/9/27/28	0/2/2/2
6	PSU	L5	3695	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	4590	6	-	3/9/27/28	0/3/3/3
86	A2M	S2	159	86	-	1/9/27/28	0/3/3/3
6	PSU	L5	5001	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3639	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	116	86	-	0/9/27/28	0/2/2/2
6	OMC	L5	2422	6,87	-	2/9/27/28	0/2/2/2
8	PSU	L8	69	8	-	0/7/25/26	0/2/2/2
6	OMG	L5	1522	6	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PSU	S2	966	87,86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1056	86	-	0/7/25/26	0/2/2/2
86	OMC	S2	462	86	-	0/9/27/28	0/2/2/2
86	PSU	S2	1232	86	-	0/7/25/26	0/2/2/2
86	OMU	S2	1288	86	-	2/9/27/28	0/2/2/2
6	OMC	L5	2365	6,87	-	0/9/27/28	0/2/2/2
86	PSU	S2	814	86	-	0/7/25/26	0/2/2/2
86	MA6	S2	1851	86	-	1/11/29/30	0/3/3/3
6	PSU	L5	1792	6	-	0/7/25/26	0/2/2/2
86	PSU	S2	93	86	-	0/7/25/26	0/2/2/2
6	OMC	L5	3841	6	-	1/9/27/28	0/2/2/2
6	OMG	L5	3627	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4673	6,87	-	0/7/25/26	0/2/2/2
6	PSU	L5	3853	6,87	-	0/7/25/26	0/2/2/2
6	PSU	L5	4579	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	3792	6	-	2/9/27/28	0/3/3/3
6	A2M	L5	2401	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	651	86	-	0/7/25/26	0/2/2/2
86	OMC	S2	1703	86	-	1/9/27/28	0/2/2/2
6	PSU	L5	4293	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4628	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	354	86	-	0/9/27/28	0/2/2/2
6	OMC	L5	2824	6	-	0/9/27/28	0/2/2/2
86	A2M	S2	27	86	-	1/9/27/28	0/3/3/3
6	PSU	L5	4493	6	-	0/7/25/26	0/2/2/2
6	OMU	L5	4498	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	4353	6	-	0/7/25/26	0/2/2/2
6	OMU	L5	4620	6	-	0/9/27/28	0/2/2/2
86	PSU	S2	1081	86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1367	86	-	0/7/25/26	0/2/2/2
86	A2M	S2	99	87,86	-	2/9/27/28	0/3/3/3
86	OMC	S2	1272	86	-	2/9/27/28	0/2/2/2
6	PSU	L5	1582	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4299	6	-	0/7/25/26	0/2/2/2
6	5MC	L5	3782	6,87	-	1/7/25/26	0/2/2/2
6	PSU	L5	4442	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4500	6	-	3/7/25/26	0/2/2/2
6	PSU	L5	1744	6,87	-	0/7/25/26	0/2/2/2
6	PSU	L5	4973	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3637	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3920	6,87	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OMC	S2	174	86	-	0/9/27/28	0/2/2/2
86	PSU	S2	1004	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	4972	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	1442	86	-	2/9/27/28	0/2/2/2
86	A2M	S2	484	86	-	0/9/27/28	0/3/3/3
6	PSU	L5	3851	6	-	1/7/25/26	0/2/2/2
6	OMU	L5	4306	6	-	0/9/27/28	0/2/2/2

All (299) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	1832	6MZ	C6-N6	12.72	1.48	1.34
6	L5	3818	UY1	C6-C5	12.47	1.49	1.35
6	L5	4220	6MZ	C6-N6	11.82	1.47	1.34
6	L5	3818	UY1	C2-N1	11.60	1.51	1.36
86	S2	1288	OMU	C2-N1	8.58	1.51	1.38
86	S2	799	OMU	C2-N1	8.31	1.51	1.38
86	S2	627	OMU	C2-N1	8.18	1.51	1.38
86	S2	1442	OMU	C2-N1	8.10	1.51	1.38
86	S2	172	OMU	C2-N1	8.09	1.51	1.38
86	S2	428	OMU	C2-N1	8.08	1.51	1.38
86	S2	116	OMU	C2-N1	8.08	1.51	1.38
86	S2	1248	B8N	C4-N3	-8.04	1.26	1.40
86	S2	1326	OMU	C2-N1	8.02	1.51	1.38
86	S2	121	OMU	C2-N1	8.00	1.51	1.38
6	L5	4227	OMU	C2-N1	7.97	1.50	1.38
6	L5	2837	OMU	C2-N1	7.86	1.50	1.38
6	L5	4306	OMU	C2-N1	7.85	1.50	1.38
86	S2	354	OMU	C2-N1	7.84	1.50	1.38
6	L5	3925	OMU	C2-N1	7.82	1.50	1.38
86	S2	1248	B8N	C6-N1	7.78	1.55	1.36
6	L5	4498	OMU	C2-N1	7.64	1.50	1.38
6	L5	4620	OMU	C2-N1	7.60	1.50	1.38
6	L5	3818	UY1	C2-N3	7.57	1.49	1.37
86	S2	627	OMU	C2-N3	6.96	1.50	1.38
86	S2	1248	B8N	C4-C5	6.91	1.63	1.47
86	S2	1442	OMU	C2-N3	6.87	1.49	1.38
86	S2	799	OMU	C2-N3	6.86	1.49	1.38
86	S2	116	OMU	C2-N3	6.84	1.49	1.38
86	S2	1288	OMU	C2-N3	6.83	1.49	1.38
86	S2	1326	OMU	C2-N3	6.81	1.49	1.38
86	S2	428	OMU	C2-N3	6.79	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	172	OMU	C2-N3	6.77	1.49	1.38
86	S2	121	OMU	C2-N3	6.72	1.49	1.38
6	L5	4227	OMU	C2-N3	6.68	1.49	1.38
86	S2	354	OMU	C2-N3	6.58	1.49	1.38
6	L5	2837	OMU	C2-N3	6.57	1.49	1.38
6	L5	4306	OMU	C2-N3	6.53	1.49	1.38
6	L5	4498	OMU	C2-N3	6.51	1.49	1.38
6	L5	3925	OMU	C2-N3	6.45	1.49	1.38
6	L5	4620	OMU	C2-N3	6.40	1.49	1.38
86	S2	1639	G7M	C4-N3	6.40	1.48	1.34
6	L5	4530	UR3	C6-C5	6.20	1.49	1.35
6	L5	4530	UR3	C2-N1	5.98	1.46	1.38
86	S2	627	OMU	C6-C5	5.89	1.48	1.35
86	S2	1288	OMU	C6-C5	5.88	1.48	1.35
86	S2	1248	B8N	C2-N1	5.86	1.56	1.39
86	S2	799	OMU	C6-C5	5.83	1.48	1.35
86	S2	172	OMU	C6-C5	5.80	1.48	1.35
86	S2	428	OMU	C6-C5	5.79	1.48	1.35
86	S2	1442	OMU	C6-C5	5.79	1.48	1.35
86	S2	1326	OMU	C6-C5	5.78	1.48	1.35
6	L5	4620	OMU	O4-C4	-5.72	1.13	1.24
86	S2	121	OMU	C6-C5	5.71	1.48	1.35
86	S2	354	OMU	C6-C5	5.71	1.48	1.35
6	L5	3925	OMU	O4-C4	-5.71	1.13	1.24
6	L5	4498	OMU	C6-C5	5.68	1.48	1.35
6	L5	4227	OMU	C6-C5	5.67	1.48	1.35
6	L5	4306	OMU	O4-C4	-5.66	1.13	1.24
86	S2	116	OMU	C6-C5	5.65	1.48	1.35
6	L5	2837	OMU	C6-C5	5.63	1.48	1.35
6	L5	4498	OMU	O4-C4	-5.62	1.13	1.24
6	L5	4227	OMU	O4-C4	-5.59	1.13	1.24
6	L5	2837	OMU	O4-C4	-5.58	1.13	1.24
86	S2	116	OMU	O4-C4	-5.57	1.13	1.24
86	S2	354	OMU	O4-C4	-5.56	1.13	1.24
6	L5	4306	OMU	C6-C5	5.56	1.48	1.35
6	L5	4620	OMU	C6-C5	5.56	1.48	1.35
86	S2	1326	OMU	O4-C4	-5.55	1.13	1.24
6	L5	3925	OMU	C6-C5	5.54	1.47	1.35
6	L5	4530	UR3	C2-N3	5.49	1.49	1.39
86	S2	121	OMU	O4-C4	-5.48	1.13	1.24
86	S2	428	OMU	O4-C4	-5.48	1.13	1.24
86	S2	799	OMU	O4-C4	-5.47	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	627	OMU	O4-C4	-5.46	1.13	1.24
86	S2	1442	OMU	O4-C4	-5.46	1.13	1.24
86	S2	1288	OMU	O4-C4	-5.44	1.13	1.24
86	S2	172	OMU	O4-C4	-5.43	1.13	1.24
86	S2	1639	G7M	C2-N3	5.28	1.46	1.33
6	L5	3818	UY1	C6-N1	5.26	1.44	1.36
86	S2	1248	B8N	C6-C5	5.17	1.42	1.35
86	S2	1639	G7M	C5-N7	-5.05	1.33	1.39
86	S2	1639	G7M	C2-N2	4.83	1.45	1.34
86	S2	627	OMU	C4-N3	4.47	1.46	1.38
6	L5	3818	UY1	C4-N3	4.37	1.47	1.38
86	S2	1442	OMU	C4-N3	4.35	1.46	1.38
86	S2	172	OMU	C4-N3	4.32	1.46	1.38
86	S2	1288	OMU	C4-N3	4.32	1.46	1.38
86	S2	1326	OMU	C4-N3	4.31	1.46	1.38
86	S2	428	OMU	C4-N3	4.28	1.45	1.38
86	S2	116	OMU	C4-N3	4.25	1.45	1.38
86	S2	121	OMU	C4-N3	4.20	1.45	1.38
86	S2	799	OMU	C4-N3	4.20	1.45	1.38
86	S2	354	OMU	C4-N3	4.15	1.45	1.38
6	L5	4498	OMU	C4-N3	4.06	1.45	1.38
6	L5	2837	OMU	C4-N3	4.05	1.45	1.38
6	L5	4227	OMU	C4-N3	4.05	1.45	1.38
6	L5	4306	OMU	C4-N3	4.00	1.45	1.38
6	L5	3925	OMU	C4-N3	3.84	1.45	1.38
6	L5	4620	OMU	C4-N3	3.81	1.45	1.38
6	L5	3818	UY1	O4-C4	-3.76	1.16	1.23
86	S2	1639	G7M	C5-C6	3.72	1.53	1.43
6	L5	2401	A2M	O5'-C5'	-3.70	1.33	1.44
86	S2	801	PSU	C6-C5	3.60	1.39	1.35
6	L5	3825	A2M	O5'-C5'	-3.55	1.33	1.44
6	L5	2787	A2M	O5'-C5'	-3.53	1.33	1.44
4	CF	163	SEP	P-O1P	3.53	1.61	1.50
86	S2	668	A2M	O5'-C5'	-3.53	1.33	1.44
86	S2	1248	B8N	C1'-C5	3.52	1.58	1.50
6	L5	3785	A2M	O5'-C5'	-3.49	1.34	1.44
86	S2	93	PSU	C6-C5	3.48	1.39	1.35
86	S2	99	A2M	O5'-C5'	-3.48	1.34	1.44
6	L5	3830	A2M	O5'-C5'	-3.48	1.34	1.44
6	L5	3844	PSU	C6-C5	3.47	1.39	1.35
6	L5	1326	A2M	O5'-C5'	-3.47	1.34	1.44
6	L5	5010	PSU	C6-C5	3.46	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	4500	PSU	C6-C5	3.46	1.39	1.35
6	L5	1871	A2M	O5'-C5'	-3.46	1.34	1.44
86	S2	1367	PSU	C6-C5	3.46	1.39	1.35
86	S2	1031	A2M	O5'-C5'	-3.46	1.34	1.44
6	L5	400	A2M	O5'-C5'	-3.46	1.34	1.44
86	S2	1232	PSU	C6-C5	3.46	1.39	1.35
6	L5	1323	A2M	O5'-C5'	-3.45	1.34	1.44
86	S2	468	A2M	O5'-C5'	-3.44	1.34	1.44
6	L5	4220	6MZ	C5-C4	-3.44	1.33	1.39
86	S2	1244	PSU	C6-C5	3.44	1.39	1.35
6	L5	1524	A2M	O5'-C5'	-3.43	1.34	1.44
86	S2	866	PSU	C6-C5	3.42	1.39	1.35
6	L5	2363	A2M	O5'-C5'	-3.42	1.34	1.44
86	S2	966	PSU	C6-C5	3.41	1.39	1.35
86	S2	1383	A2M	O5'-C5'	-3.40	1.34	1.44
6	L5	4220	6MZ	C5-N7	-3.40	1.32	1.39
86	S2	1004	PSU	C6-C5	3.40	1.39	1.35
86	S2	27	A2M	O5'-C5'	-3.40	1.34	1.44
6	L5	2815	A2M	O5'-C5'	-3.40	1.34	1.44
86	S2	651	PSU	C6-C5	3.39	1.39	1.35
6	L5	1860	PSU	C6-C5	3.39	1.39	1.35
6	L5	4571	A2M	O5'-C5'	-3.39	1.34	1.44
86	S2	105	PSU	C6-C5	3.38	1.39	1.35
6	L5	2632	PSU	C6-C5	3.38	1.39	1.35
86	S2	576	A2M	O5'-C5'	-3.38	1.34	1.44
6	L5	4552	PSU	C6-C5	3.37	1.39	1.35
6	L5	4312	PSU	C6-C5	3.37	1.39	1.35
86	S2	863	PSU	C6-C5	3.37	1.39	1.35
6	L5	1782	PSU	C6-C5	3.36	1.39	1.35
6	L5	5001	PSU	C6-C5	3.36	1.39	1.35
86	S2	1177	PSU	C6-C5	3.35	1.39	1.35
6	L5	3867	A2M	O5'-C5'	-3.35	1.34	1.44
86	S2	814	PSU	C6-C5	3.32	1.39	1.35
6	L5	398	A2M	O5'-C5'	-3.32	1.34	1.44
86	S2	166	A2M	O5'-C5'	-3.32	1.34	1.44
6	L5	4590	A2M	O5'-C5'	-3.32	1.34	1.44
86	S2	109	PSU	C6-C5	3.31	1.39	1.35
6	L5	3718	A2M	O5'-C5'	-3.31	1.34	1.44
86	S2	484	A2M	O5'-C5'	-3.31	1.34	1.44
6	L5	4523	A2M	O5'-C5'	-3.30	1.34	1.44
6	L5	3818	UY1	O2-C2	-3.30	1.16	1.23
6	L5	4576	PSU	C6-C5	3.30	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1781	PSU	C6-C5	3.29	1.38	1.35
6	L5	4493	PSU	C6-C5	3.28	1.38	1.35
6	L5	3818	UY1	C1'-C5	3.27	1.57	1.50
86	S2	1174	PSU	C6-C5	3.27	1.38	1.35
86	S2	1045	PSU	C6-C5	3.26	1.38	1.35
86	S2	1046	PSU	C6-C5	3.26	1.38	1.35
86	S2	686	PSU	C6-C5	3.26	1.38	1.35
6	L5	1744	PSU	C6-C5	3.25	1.38	1.35
6	L5	4532	PSU	C6-C5	3.25	1.38	1.35
6	L5	4636	PSU	C6-C5	3.24	1.38	1.35
86	S2	649	PSU	C6-C5	3.23	1.38	1.35
6	L5	3853	PSU	C6-C5	3.23	1.38	1.35
86	S2	406	PSU	C6-C5	3.23	1.38	1.35
6	L5	1862	PSU	C6-C5	3.23	1.38	1.35
8	L8	69	PSU	C6-C5	3.21	1.38	1.35
6	L5	4353	PSU	C6-C5	3.21	1.38	1.35
6	L5	3822	PSU	C6-C5	3.20	1.38	1.35
6	L5	4579	PSU	C6-C5	3.20	1.38	1.35
6	L5	4673	PSU	C6-C5	3.20	1.38	1.35
6	L5	4521	PSU	C6-C5	3.19	1.38	1.35
6	L5	1683	PSU	C6-C5	3.19	1.38	1.35
6	L5	4442	PSU	C6-C5	3.19	1.38	1.35
86	S2	1832	6MZ	C5-N7	-3.18	1.33	1.39
6	L5	3637	PSU	C6-C5	3.18	1.38	1.35
6	L5	4296	PSU	C6-C5	3.18	1.38	1.35
6	L5	4293	PSU	C6-C5	3.18	1.38	1.35
86	S2	681	PSU	C6-C5	3.18	1.38	1.35
86	S2	159	A2M	O5'-C5'	-3.16	1.35	1.44
6	L5	4973	PSU	C6-C5	3.15	1.38	1.35
6	L5	4299	PSU	C6-C5	3.15	1.38	1.35
6	L5	4431	PSU	C6-C5	3.14	1.38	1.35
86	S2	1056	PSU	C6-C5	3.14	1.38	1.35
8	L8	55	PSU	C6-C5	3.13	1.38	1.35
6	L5	4361	PSU	C6-C5	3.13	1.38	1.35
6	L5	4471	PSU	C6-C5	3.12	1.38	1.35
6	L5	1582	PSU	C6-C5	3.12	1.38	1.35
6	L5	2839	PSU	C6-C5	3.11	1.38	1.35
6	L5	3884	PSU	C6-C5	3.10	1.38	1.35
86	S2	1832	6MZ	C5-C4	-3.10	1.33	1.39
6	L5	4689	PSU	C6-C5	3.09	1.38	1.35
6	L5	1534	A2M	O5'-C5'	-3.09	1.35	1.44
6	L5	4972	PSU	C6-C5	3.08	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	1851	MA6	C6-N6	3.07	1.45	1.36
86	S2	1850	MA6	C6-N6	3.06	1.45	1.36
6	L5	3695	PSU	C6-C5	3.06	1.38	1.35
86	S2	1081	PSU	C6-C5	3.05	1.38	1.35
86	S2	668	A2M	O4'-C4'	-3.04	1.38	1.45
6	L5	3851	PSU	C6-C5	3.04	1.38	1.35
6	L5	1792	PSU	C6-C5	3.03	1.38	1.35
6	L5	4220	6MZ	C8-N9	-3.00	1.32	1.37
6	L5	4628	PSU	C6-C5	2.99	1.38	1.35
6	L5	3639	PSU	C6-C5	2.93	1.38	1.35
86	S2	1832	6MZ	C8-N9	-2.93	1.32	1.37
6	L5	3920	PSU	C6-C5	2.93	1.38	1.35
6	L5	1536	PSU	C6-C5	2.92	1.38	1.35
6	L5	4403	PSU	C6-C5	2.88	1.38	1.35
86	S2	627	OMU	C5-C4	2.87	1.49	1.43
6	L5	4457	PSU	C6-C5	2.84	1.38	1.35
86	S2	1288	OMU	C5-C4	2.80	1.49	1.43
6	L5	1677	PSU	C6-C5	2.79	1.38	1.35
86	S2	799	OMU	C5-C4	2.79	1.49	1.43
86	S2	1326	OMU	C5-C4	2.78	1.49	1.43
86	S2	172	OMU	C5-C4	2.77	1.49	1.43
6	L5	4530	UR3	O2-C2	-2.76	1.17	1.22
86	S2	1639	G7M	C2-N1	2.75	1.44	1.37
86	S2	428	OMU	C5-C4	2.71	1.49	1.43
86	S2	1442	OMU	C5-C4	2.70	1.49	1.43
6	L5	4498	OMU	C5-C4	2.68	1.49	1.43
86	S2	1288	OMU	C6-N1	2.68	1.44	1.38
86	S2	627	OMU	C6-N1	2.65	1.44	1.38
6	L5	4227	OMU	C5-C4	2.65	1.49	1.43
86	S2	121	OMU	C5-C4	2.64	1.49	1.43
86	S2	354	OMU	C5-C4	2.63	1.49	1.43
6	L5	2837	OMU	C5-C4	2.62	1.49	1.43
86	S2	1639	G7M	O6-C6	-2.62	1.18	1.23
86	S2	1442	OMU	C6-N1	2.62	1.44	1.38
86	S2	799	OMU	C6-N1	2.62	1.44	1.38
6	L5	3925	OMU	C5-C4	2.61	1.49	1.43
6	L5	1524	A2M	O4'-C4'	-2.61	1.39	1.45
6	L5	4571	A2M	O4'-C4'	-2.60	1.39	1.45
86	S2	1851	MA6	C5-C4	-2.59	1.34	1.39
86	S2	116	OMU	C5-C4	2.57	1.49	1.43
86	S2	121	OMU	C6-N1	2.56	1.44	1.38
6	L5	4498	OMU	C6-N1	2.56	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	354	OMU	C6-N1	2.55	1.44	1.38
86	S2	428	OMU	C6-N1	2.54	1.44	1.38
6	L5	2363	A2M	O4'-C4'	-2.53	1.39	1.45
6	L5	1534	A2M	O4'-C4'	-2.53	1.39	1.45
86	S2	1850	MA6	C5-C4	-2.52	1.34	1.39
86	S2	1326	OMU	C6-N1	2.52	1.44	1.38
6	L5	4220	6MZ	C6-N1	-2.48	1.31	1.35
6	L5	4306	OMU	C5-C4	2.47	1.49	1.43
6	L5	4620	OMU	C6-N1	2.47	1.44	1.38
86	S2	172	OMU	C6-N1	2.45	1.43	1.38
6	L5	4530	UR3	C6-N1	2.43	1.43	1.38
6	L5	2837	OMU	C6-N1	2.43	1.43	1.38
86	S2	116	OMU	C6-N1	2.43	1.43	1.38
6	L5	4306	OMU	C6-N1	2.42	1.43	1.38
6	L5	4620	OMU	C5-C4	2.40	1.48	1.43
6	L5	3867	A2M	O4'-C4'	-2.40	1.39	1.45
6	L5	4227	OMU	C6-N1	2.39	1.43	1.38
86	S2	1639	G7M	C6-N1	2.38	1.43	1.38
6	L5	3925	OMU	C6-N1	2.37	1.43	1.38
6	L5	1323	A2M	O4'-C4'	-2.36	1.39	1.45
6	L5	1326	A2M	O4'-C4'	-2.31	1.39	1.45
6	L5	1871	A2M	O4'-C4'	-2.29	1.39	1.45
6	L5	2815	A2M	O4'-C4'	-2.29	1.39	1.45
6	L5	4523	A2M	O3'-C3'	-2.26	1.37	1.43
86	S2	1832	6MZ	C6-N1	-2.25	1.31	1.35
6	L5	3818	UY1	O4'-C1'	-2.22	1.40	1.43
86	S2	1639	G7M	C4-N9	-2.19	1.32	1.38
6	L5	4530	UR3	C5-C4	2.19	1.49	1.43
6	L5	4523	A2M	O4'-C4'	-2.19	1.40	1.45
6	L5	400	A2M	O3'-C3'	-2.17	1.37	1.43
6	L5	4353	PSU	C4-C5	-2.14	1.38	1.44
6	L5	4689	PSU	C4-C5	-2.11	1.38	1.44
6	L5	4521	PSU	C4-C5	-2.11	1.38	1.44
6	L5	3884	PSU	C4-C5	-2.10	1.38	1.44
6	L5	4293	PSU	C4-C5	-2.07	1.38	1.44
6	L5	3639	PSU	C4-C5	-2.07	1.38	1.44
6	L5	3825	A2M	O4'-C4'	-2.06	1.40	1.45
6	L5	2839	PSU	C4-C5	-2.05	1.38	1.44
6	L5	1871	A2M	O3'-C3'	-2.05	1.37	1.43
6	L5	3695	PSU	C4-C5	-2.04	1.38	1.44
6	L5	4500	PSU	C4-C5	-2.04	1.38	1.44
6	L5	400	A2M	O4'-C4'	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	1031	A2M	O4'-C4'	-2.03	1.40	1.45
6	L5	4521	PSU	O4'-C1'	-2.03	1.41	1.43
6	L5	4456	OMC	C4-N3	-2.03	1.30	1.34
86	S2	1177	PSU	C4-C5	-2.03	1.38	1.44
6	L5	1683	PSU	C4-C5	-2.03	1.38	1.44
6	L5	4530	UR3	C3U-N3	2.02	1.50	1.47
6	L5	4552	PSU	C4-C5	-2.02	1.38	1.44
6	L5	4220	6MZ	C4-N9	-2.02	1.33	1.37
86	S2	1056	PSU	C4-C5	-2.02	1.38	1.44
6	L5	3818	UY1	C4-C5	2.01	1.49	1.44
6	L5	4312	PSU	C4-C5	-2.01	1.38	1.44
6	L5	1534	A2M	O3'-C3'	-2.01	1.38	1.43
6	L5	3920	PSU	C4-C5	-2.01	1.38	1.44
6	L5	4571	A2M	O3'-C3'	-2.01	1.38	1.43
86	S2	109	PSU	C4-C5	-2.01	1.38	1.44
6	L5	4457	PSU	C4-C5	-2.00	1.38	1.44

All (705) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	1851	MA6	N1-C6-N6	-12.27	101.91	116.86
86	S2	1850	MA6	N1-C6-N6	-12.02	102.21	116.86
86	S2	1851	MA6	C5-C6-N6	8.20	138.32	125.33
86	S2	1850	MA6	C5-C6-N6	8.04	138.06	125.33
86	S2	1639	G7M	C1'-N9-C4	7.28	147.99	126.49
86	S2	1639	G7M	C1'-N9-C8	-7.19	102.46	126.74
6	L5	3925	OMU	C4-N3-C2	-6.11	119.03	126.61
6	L5	4220	6MZ	OP3-P-OP1	-5.96	87.63	110.83
6	L5	4227	OMU	C4-N3-C2	-5.85	119.35	126.61
86	S2	1851	MA6	N1-C2-N3	-5.81	119.78	128.58
86	S2	428	OMU	C4-N3-C2	-5.79	119.42	126.61
86	S2	1832	6MZ	N1-C2-N3	-5.78	119.84	128.58
6	L5	4220	6MZ	N1-C2-N3	-5.77	119.85	128.58
6	L5	4498	OMU	C4-N3-C2	-5.76	119.45	126.61
86	S2	1326	OMU	C4-N3-C2	-5.76	119.46	126.61
6	L5	4306	OMU	C4-N3-C2	-5.76	119.46	126.61
86	S2	354	OMU	C4-N3-C2	-5.75	119.47	126.61
86	S2	172	OMU	C4-N3-C2	-5.73	119.50	126.61
6	L5	2837	OMU	C4-N3-C2	-5.69	119.55	126.61
86	S2	627	OMU	C4-N3-C2	-5.60	119.66	126.61
6	L5	4530	UR3	C4-N3-C2	-5.60	120.08	124.58
86	S2	121	OMU	C4-N3-C2	-5.56	119.71	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	799	OMU	C4-N3-C2	-5.53	119.74	126.61
6	L5	4220	6MZ	OP3-P-O5'	-5.52	92.28	106.67
86	S2	1850	MA6	N1-C2-N3	-5.51	120.23	128.58
86	S2	1442	OMU	C4-N3-C2	-5.51	119.77	126.61
6	L5	4220	6MZ	C9-N6-C6	-5.46	117.78	122.85
6	L5	1683	PSU	N1-C2-N3	5.45	120.92	115.17
86	S2	1851	MA6	N9-C8-N7	-5.44	106.22	113.94
6	L5	3701	OMC	C1'-N1-C2	5.39	130.35	118.44
6	L5	4689	PSU	N1-C2-N3	5.38	120.84	115.17
6	L5	4457	PSU	C4-N3-C2	-5.37	118.98	126.37
6	L5	3637	PSU	N1-C2-N3	5.31	120.77	115.17
86	S2	1850	MA6	N9-C8-N7	-5.30	106.42	113.94
6	L5	4220	6MZ	OP3-P-OP2	-5.27	88.03	107.80
86	S2	116	OMU	C4-N3-C2	-5.26	120.08	126.61
6	L5	4636	PSU	C4-N3-C2	-5.26	119.13	126.37
86	S2	1288	OMU	C4-N3-C2	-5.25	120.09	126.61
6	L5	4457	PSU	N1-C2-N3	5.25	120.70	115.17
6	L5	1677	PSU	C4-N3-C2	-5.20	119.21	126.37
86	S2	1248	B8N	C5-C4-N3	5.18	125.56	116.15
6	L5	4353	PSU	N1-C2-N3	5.17	120.62	115.17
6	L5	1683	PSU	C4-N3-C2	-5.16	119.27	126.37
6	L5	3637	PSU	C4-N3-C2	-5.15	119.27	126.37
6	L5	3639	PSU	N1-C2-N3	5.14	120.59	115.17
6	L5	4521	PSU	N1-C2-N3	5.13	120.58	115.17
6	L5	4220	6MZ	OP2-P-OP1	5.13	130.82	110.83
6	L5	4552	PSU	N1-C2-N3	5.13	120.57	115.17
6	L5	4403	PSU	C4-N3-C2	-5.11	119.33	126.37
6	L5	1862	PSU	C4-N3-C2	-5.11	119.33	126.37
6	L5	4500	PSU	N1-C2-N3	5.09	120.54	115.17
8	L8	69	PSU	N1-C2-N3	5.09	120.53	115.17
6	L5	1862	PSU	N1-C2-N3	5.08	120.52	115.17
6	L5	4442	PSU	N1-C2-N3	5.06	120.51	115.17
86	S2	1081	PSU	C4-N3-C2	-5.06	119.40	126.37
6	L5	2839	PSU	N1-C2-N3	5.06	120.51	115.17
6	L5	4521	PSU	C4-N3-C2	-5.06	119.40	126.37
6	L5	3695	PSU	C4-N3-C2	-5.05	119.41	126.37
6	L5	4312	PSU	N1-C2-N3	5.05	120.49	115.17
6	L5	4293	PSU	C4-N3-C2	-5.05	119.42	126.37
6	L5	4293	PSU	N1-C2-N3	5.04	120.49	115.17
6	L5	3695	PSU	N1-C2-N3	5.03	120.48	115.17
6	L5	4579	PSU	N1-C2-N3	5.03	120.47	115.17
86	S2	649	PSU	N1-C2-N3	5.03	120.47	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	1056	PSU	C4-N3-C2	-5.02	119.45	126.37
6	L5	3639	PSU	C4-N3-C2	-5.02	119.45	126.37
8	L8	55	PSU	N1-C2-N3	5.01	120.46	115.17
6	L5	3884	PSU	C4-N3-C2	-5.00	119.48	126.37
86	S2	649	PSU	C4-N3-C2	-5.00	119.48	126.37
6	L5	2632	PSU	N1-C2-N3	4.99	120.43	115.17
6	L5	3920	PSU	N1-C2-N3	4.99	120.43	115.17
86	S2	1045	PSU	C4-N3-C2	-4.99	119.50	126.37
6	L5	3853	PSU	N1-C2-N3	4.98	120.42	115.17
8	L8	55	PSU	C4-N3-C2	-4.98	119.51	126.37
6	L5	4636	PSU	N1-C2-N3	4.98	120.42	115.17
6	L5	4973	PSU	C4-N3-C2	-4.98	119.52	126.37
86	S2	1177	PSU	N1-C2-N3	4.98	120.42	115.17
6	L5	4973	PSU	N1-C2-N3	4.98	120.42	115.17
86	S2	1177	PSU	C4-N3-C2	-4.98	119.52	126.37
6	L5	4471	PSU	N1-C2-N3	4.97	120.42	115.17
6	L5	3818	UY1	C4-N3-C2	-4.97	119.52	126.37
8	L8	69	PSU	C4-N3-C2	-4.97	119.53	126.37
6	L5	1744	PSU	N1-C2-N3	4.97	120.41	115.17
86	S2	406	PSU	C4-N3-C2	-4.97	119.53	126.37
86	S2	651	PSU	N1-C2-N3	4.96	120.40	115.17
6	L5	3851	PSU	N1-C2-N3	4.96	120.40	115.17
6	L5	4442	PSU	C4-N3-C2	-4.96	119.54	126.37
6	L5	4689	PSU	C4-N3-C2	-4.96	119.54	126.37
86	S2	406	PSU	N1-C2-N3	4.96	120.40	115.17
6	L5	1860	PSU	N1-C2-N3	4.96	120.40	115.17
86	S2	1045	PSU	N1-C2-N3	4.96	120.40	115.17
6	L5	3844	PSU	N1-C2-N3	4.96	120.40	115.17
6	L5	4620	OMU	C4-N3-C2	-4.95	120.47	126.61
6	L5	4579	PSU	C4-N3-C2	-4.94	119.57	126.37
86	S2	866	PSU	C4-N3-C2	-4.94	119.57	126.37
6	L5	1860	PSU	C4-N3-C2	-4.93	119.58	126.37
6	L5	4353	PSU	C4-N3-C2	-4.93	119.58	126.37
6	L5	4500	PSU	C4-N3-C2	-4.93	119.58	126.37
6	L5	4552	PSU	C4-N3-C2	-4.93	119.58	126.37
6	L5	3822	PSU	N1-C2-N3	4.93	120.36	115.17
6	L5	4296	PSU	C4-N3-C2	-4.92	119.59	126.37
86	S2	1004	PSU	C4-N3-C2	-4.92	119.59	126.37
86	S2	1081	PSU	N1-C2-N3	4.92	120.36	115.17
6	L5	5010	PSU	N1-C2-N3	4.92	120.35	115.17
86	S2	1004	PSU	N1-C2-N3	4.91	120.35	115.17
6	L5	4673	PSU	N1-C2-N3	4.91	120.35	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	2839	PSU	C4-N3-C2	-4.91	119.60	126.37
6	L5	1792	PSU	C4-N3-C2	-4.91	119.61	126.37
86	S2	866	PSU	N1-C2-N3	4.90	120.34	115.17
6	L5	3884	PSU	N1-C2-N3	4.90	120.34	115.17
86	S2	686	PSU	C4-N3-C2	-4.90	119.62	126.37
86	S2	1174	PSU	C4-N3-C2	-4.90	119.63	126.37
6	L5	3853	PSU	C4-N3-C2	-4.89	119.63	126.37
86	S2	1056	PSU	N1-C2-N3	4.89	120.33	115.17
86	S2	105	PSU	N1-C2-N3	4.89	120.32	115.17
86	S2	1046	PSU	C4-N3-C2	-4.88	119.65	126.37
86	S2	863	PSU	C4-N3-C2	-4.87	119.66	126.37
86	S2	651	PSU	C4-N3-C2	-4.87	119.67	126.37
86	S2	1174	PSU	N1-C2-N3	4.86	120.30	115.17
86	S2	1232	PSU	N1-C2-N3	4.86	120.30	115.17
6	L5	4673	PSU	C4-N3-C2	-4.86	119.67	126.37
86	S2	109	PSU	C4-N3-C2	-4.86	119.68	126.37
6	L5	4296	PSU	N1-C2-N3	4.85	120.29	115.17
6	L5	2632	PSU	C4-N3-C2	-4.85	119.69	126.37
6	L5	1782	PSU	N1-C2-N3	4.85	120.28	115.17
6	L5	4493	PSU	C4-N3-C2	-4.85	119.69	126.37
6	L5	4576	PSU	N1-C2-N3	4.85	120.28	115.17
6	L5	4972	PSU	N1-C2-N3	4.84	120.28	115.17
6	L5	3851	PSU	C4-N3-C2	-4.84	119.70	126.37
6	L5	4403	PSU	N1-C2-N3	4.84	120.27	115.17
6	L5	1744	PSU	C4-N3-C2	-4.84	119.71	126.37
6	L5	5010	PSU	C4-N3-C2	-4.83	119.72	126.37
86	S2	1244	PSU	N1-C2-N3	4.83	120.26	115.17
6	L5	4299	PSU	C4-N3-C2	-4.83	119.72	126.37
86	S2	1046	PSU	N1-C2-N3	4.83	120.26	115.17
86	S2	1244	PSU	C4-N3-C2	-4.82	119.73	126.37
6	L5	1792	PSU	N1-C2-N3	4.82	120.25	115.17
6	L5	5001	PSU	N1-C2-N3	4.82	120.25	115.17
6	L5	4532	PSU	C4-N3-C2	-4.82	119.73	126.37
86	S2	1232	PSU	C4-N3-C2	-4.82	119.73	126.37
6	L5	3920	PSU	C4-N3-C2	-4.82	119.73	126.37
6	L5	4312	PSU	C4-N3-C2	-4.82	119.73	126.37
86	S2	966	PSU	N1-C2-N3	4.82	120.25	115.17
6	L5	4431	PSU	C4-N3-C2	-4.82	119.74	126.37
6	L5	4972	PSU	C4-N3-C2	-4.81	119.74	126.37
86	S2	686	PSU	N1-C2-N3	4.81	120.24	115.17
6	L5	1536	PSU	C4-N3-C2	-4.81	119.75	126.37
86	S2	109	PSU	N1-C2-N3	4.81	120.24	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4576	PSU	C4-N3-C2	-4.80	119.76	126.37
86	S2	1367	PSU	N1-C2-N3	4.80	120.23	115.17
86	S2	863	PSU	N1-C2-N3	4.79	120.22	115.17
6	L5	4628	PSU	N1-C2-N3	4.79	120.22	115.17
86	S2	105	PSU	C4-N3-C2	-4.78	119.78	126.37
6	L5	5001	PSU	C4-N3-C2	-4.78	119.78	126.37
6	L5	4431	PSU	N1-C2-N3	4.78	120.21	115.17
6	L5	3822	PSU	C4-N3-C2	-4.78	119.79	126.37
86	S2	814	PSU	C4-N3-C2	-4.78	119.79	126.37
6	L5	1536	PSU	N1-C2-N3	4.77	120.20	115.17
86	S2	1367	PSU	C4-N3-C2	-4.77	119.81	126.37
6	L5	4299	PSU	N1-C2-N3	4.76	120.19	115.17
86	S2	681	PSU	N1-C2-N3	4.76	120.18	115.17
6	L5	4361	PSU	C4-N3-C2	-4.75	119.83	126.37
6	L5	4532	PSU	N1-C2-N3	4.74	120.16	115.17
6	L5	4493	PSU	N1-C2-N3	4.73	120.16	115.17
6	L5	1677	PSU	N1-C2-N3	4.73	120.15	115.17
6	L5	4471	PSU	C4-N3-C2	-4.72	119.86	126.37
86	S2	1832	6MZ	N9-C8-N7	-4.72	107.24	113.94
6	L5	1582	PSU	N1-C2-N3	4.70	120.12	115.17
6	L5	1782	PSU	C4-N3-C2	-4.69	119.91	126.37
6	L5	1781	PSU	C4-N3-C2	-4.67	119.93	126.37
6	L5	4220	6MZ	N9-C8-N7	-4.67	107.31	113.94
6	L5	1781	PSU	N1-C2-N3	4.67	120.09	115.17
6	L5	3844	PSU	C4-N3-C2	-4.67	119.94	126.37
86	S2	801	PSU	N1-C2-N3	4.67	120.09	115.17
6	L5	4361	PSU	N1-C2-N3	4.66	120.09	115.17
86	S2	93	PSU	N1-C2-N3	4.65	120.07	115.17
86	S2	1248	B8N	C4-N3-C2	-4.64	119.90	125.62
86	S2	681	PSU	C4-N3-C2	-4.64	119.97	126.37
6	L5	4628	PSU	C4-N3-C2	-4.64	119.97	126.37
86	S2	93	PSU	C4-N3-C2	-4.63	119.99	126.37
86	S2	966	PSU	C4-N3-C2	-4.61	120.02	126.37
6	L5	1582	PSU	C4-N3-C2	-4.59	120.04	126.37
86	S2	1832	6MZ	C5-C4-N3	-4.55	120.46	126.72
86	S2	801	PSU	C4-N3-C2	-4.55	120.11	126.37
86	S2	814	PSU	N1-C2-N3	4.52	119.94	115.17
86	S2	1639	G7M	C2-N3-C4	4.48	120.01	112.30
6	L5	4220	6MZ	C5-C4-N3	-4.46	120.58	126.72
6	L5	3818	UY1	N1-C2-N3	4.39	119.80	115.17
86	S2	1850	MA6	C5-C4-N3	-4.38	120.69	126.72
6	L5	1871	A2M	C3'-C2'-C1'	-4.32	94.53	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	1851	MA6	C5-C4-N3	-4.26	120.85	126.72
86	S2	1851	MA6	C4-N9-C8	4.25	110.20	105.74
86	S2	1383	A2M	C3'-C2'-C1'	-4.21	94.74	102.81
6	L5	3701	OMC	C1'-N1-C6	-4.20	111.81	120.78
6	L5	4523	A2M	C3'-C2'-C1'	-4.15	94.86	102.81
6	L5	3925	OMU	N3-C2-N1	4.15	120.30	114.89
6	L5	3830	A2M	C3'-C2'-C1'	-4.13	94.90	102.81
86	S2	1850	MA6	C4-N9-C8	4.13	110.07	105.74
86	S2	354	OMU	N3-C2-N1	4.08	120.21	114.89
6	L5	4306	OMU	N3-C2-N1	4.02	120.12	114.89
6	L5	2837	OMU	N3-C2-N1	4.01	120.11	114.89
6	L5	4498	OMU	N3-C2-N1	3.99	120.09	114.89
86	S2	121	OMU	N3-C2-N1	3.98	120.08	114.89
86	S2	1639	G7M	C5-C6-N1	3.97	120.06	111.84
86	S2	1639	G7M	C5-C4-N3	-3.94	120.70	128.15
86	S2	172	OMU	N3-C2-N1	3.91	119.98	114.89
6	L5	4227	OMU	N3-C2-N1	3.91	119.97	114.89
6	L5	398	A2M	C3'-C2'-C1'	-3.90	95.33	102.81
6	L5	3925	OMU	C5-C4-N3	3.89	120.25	114.80
86	S2	799	OMU	N3-C2-N1	3.87	119.92	114.89
86	S2	428	OMU	N3-C2-N1	3.86	119.92	114.89
86	S2	1326	OMU	N3-C2-N1	3.82	119.86	114.89
6	L5	4498	OMU	C5-C4-N3	3.80	120.12	114.80
6	L5	4227	OMU	C5-C4-N3	3.80	120.12	114.80
86	S2	428	OMU	C5-C4-N3	3.75	120.05	114.80
6	L5	4306	OMU	C5-C4-N3	3.73	120.03	114.80
6	L5	4620	OMU	N3-C2-N1	3.72	119.74	114.89
86	S2	1442	OMU	N3-C2-N1	3.72	119.73	114.89
6	L5	4530	UR3	C5-C4-N3	3.70	119.91	115.04
86	S2	1326	OMU	C5-C4-N3	3.69	119.97	114.80
86	S2	1031	A2M	C3'-C2'-C1'	-3.69	95.74	102.81
86	S2	627	OMU	C5-C4-N3	3.67	119.94	114.80
6	L5	398	A2M	O3'-C3'-C2'	3.65	121.40	111.19
86	S2	1851	MA6	C2-N1-C6	3.64	120.73	111.83
6	L5	2401	A2M	O3'-C3'-C2'	3.64	121.37	111.19
86	S2	116	OMU	N3-C2-N1	3.64	119.63	114.89
86	S2	627	OMU	N3-C2-N1	3.64	119.63	114.89
86	S2	1288	OMU	N3-C2-N1	3.64	119.63	114.89
86	S2	354	OMU	C5-C4-N3	3.63	119.89	114.80
86	S2	1442	OMU	C5-C4-N3	3.63	119.89	114.80
86	S2	799	OMU	C5-C4-N3	3.61	119.86	114.80
86	S2	1248	B8N	C1'-C5-C4	3.61	123.09	117.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	99	A2M	C3'-C2'-C1'	-3.60	95.91	102.81
6	L5	3718	A2M	C3'-C2'-C1'	-3.58	95.95	102.81
86	S2	121	OMU	C5-C4-N3	3.58	119.81	114.80
6	L5	2837	OMU	C5-C4-N3	3.55	119.78	114.80
86	S2	1248	B8N	N3-C2-N1	3.54	121.04	116.72
86	S2	116	OMU	C5-C4-N3	3.52	119.72	114.80
86	S2	172	OMU	C5-C4-N3	3.51	119.72	114.80
86	S2	1850	MA6	C2-N1-C6	3.50	120.39	111.83
86	S2	1850	MA6	C4-C5-C6	3.49	119.52	115.91
6	L5	1323	A2M	C2'-C1'-N9	3.48	119.49	113.75
86	S2	1288	OMU	C5-C4-N3	3.48	119.68	114.80
6	L5	4590	A2M	C3'-C2'-C1'	-3.45	96.21	102.81
6	L5	2787	A2M	O3'-C3'-C2'	3.42	120.77	111.19
6	L5	3825	A2M	C3'-C2'-C1'	-3.41	96.27	102.81
86	S2	468	A2M	C3'-C2'-C1'	-3.41	96.27	102.81
86	S2	1832	6MZ	C2-N3-C4	3.41	120.16	111.83
6	L5	4220	6MZ	O5'-P-OP1	3.39	115.61	106.44
86	S2	576	A2M	O3'-C3'-C2'	3.39	120.68	111.19
6	L5	4620	OMU	C5-C4-N3	3.39	119.54	114.80
6	L5	4220	6MZ	C2-N3-C4	3.35	120.01	111.83
86	S2	1639	G7M	O6-C6-C5	-3.35	120.54	128.01
86	S2	27	A2M	C3'-C2'-C1'	-3.34	96.41	102.81
86	S2	1383	A2M	O3'-C3'-C2'	3.34	120.52	111.19
86	S2	166	A2M	O3'-C3'-C2'	3.31	120.44	111.19
6	L5	2401	A2M	C3'-C2'-C1'	-3.29	96.51	102.81
86	S2	576	A2M	C3'-C2'-C1'	-3.29	96.51	102.81
86	S2	1832	6MZ	C5-N7-C8	3.27	108.60	103.45
6	L5	1683	PSU	O2-C2-N1	-3.25	119.44	122.79
6	L5	1534	A2M	C3'-C2'-C1'	-3.24	96.60	102.81
6	L5	4689	PSU	C6-N1-C2	-3.24	119.69	122.69
8	L8	69	PSU	O2-C2-N1	-3.22	119.47	122.79
6	L5	1323	A2M	O3'-C3'-C2'	3.22	120.20	111.19
86	S2	1174	PSU	O2-C2-N1	-3.21	119.47	122.79
86	S2	1851	MA6	C2-N3-C4	3.21	119.68	111.83
86	S2	1850	MA6	N3-C4-N9	3.21	132.63	127.17
86	S2	166	A2M	C3'-C2'-C1'	-3.20	96.68	102.81
6	L5	1524	A2M	O3'-C3'-C2'	3.20	120.14	111.19
6	L5	4579	PSU	O2-C2-N1	-3.20	119.49	122.79
6	L5	3718	A2M	O3'-C3'-C2'	3.19	120.11	111.19
86	S2	668	A2M	C4-N9-C1'	-3.19	119.18	126.63
86	S2	1851	MA6	C5-N7-C8	3.18	108.45	103.45
6	L5	400	A2M	C3'-C2'-C1'	-3.18	96.71	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	2401	A2M	C4-N9-C1'	-3.18	119.19	126.63
6	L5	3830	A2M	O3'-C3'-C2'	3.18	120.08	111.19
86	S2	1851	MA6	C4-C5-C6	3.18	119.20	115.91
6	L5	1871	A2M	O3'-C3'-C2'	3.16	120.02	111.19
86	S2	99	A2M	O3'-C3'-C2'	3.15	120.01	111.19
86	S2	159	A2M	O3'-C3'-C2'	3.15	120.00	111.19
86	S2	1031	A2M	O3'-C3'-C2'	3.14	119.98	111.19
6	L5	2815	A2M	C2'-C1'-N9	3.14	118.92	113.75
86	S2	1850	MA6	C5-N7-C8	3.14	108.38	103.45
6	L5	400	A2M	O3'-C3'-C2'	3.13	119.96	111.19
6	L5	3825	A2M	O3'-C3'-C2'	3.13	119.95	111.19
6	L5	4689	PSU	O2-C2-N1	-3.12	119.57	122.79
86	S2	428	OMU	O4-C4-C5	-3.12	119.78	125.16
86	S2	1850	MA6	C2-N3-C4	3.12	119.44	111.83
6	L5	4500	PSU	O2-C2-N1	-3.11	119.58	122.79
86	S2	1851	MA6	N3-C4-N9	3.10	132.44	127.17
6	L5	3639	PSU	O2-C2-N1	-3.10	119.59	122.79
6	L5	1536	PSU	O2-C2-N1	-3.10	119.59	122.79
86	S2	116	OMU	O4-C4-C5	-3.08	119.85	125.16
86	S2	1639	G7M	N9-C4-N3	3.08	132.11	125.95
6	L5	4306	OMU	O4-C4-C5	-3.07	119.87	125.16
86	S2	468	A2M	O3'-C3'-C2'	3.07	119.77	111.19
6	L5	4576	PSU	O2-C2-N1	-3.07	119.63	122.79
6	L5	3785	A2M	C4'-O4'-C1'	-3.06	102.70	109.47
6	L5	3844	PSU	O2-C2-N1	-3.04	119.65	122.79
6	L5	3818	UY1	C6-C5-C4	3.03	120.22	118.17
86	S2	1442	OMU	O4-C4-C5	-3.03	119.93	125.16
6	L5	4220	6MZ	C4-N9-C8	3.03	108.92	105.74
6	L5	3851	PSU	O2-C2-N1	-3.03	119.67	122.79
86	S2	1639	G7M	C2-N1-C6	-3.03	119.62	125.11
6	L5	4296	PSU	O2-C2-N1	-3.02	119.68	122.79
6	L5	1860	PSU	O2-C2-N1	-3.01	119.68	122.79
6	L5	2839	PSU	O2-C2-N1	-3.01	119.68	122.79
86	S2	627	OMU	O4-C4-C5	-3.01	119.97	125.16
86	S2	27	A2M	O3'-C3'-C2'	3.01	119.61	111.19
86	S2	668	A2M	C1'-N9-C8	3.01	133.77	127.09
6	L5	4457	PSU	O2-C2-N1	-3.00	119.70	122.79
6	L5	1871	A2M	C4-N9-C1'	-2.99	119.64	126.63
6	L5	1862	PSU	O2-C2-N1	-2.99	119.71	122.79
86	S2	649	PSU	O2-C2-N1	-2.99	119.71	122.79
86	S2	468	A2M	C4-N9-C1'	-2.99	119.64	126.63
6	L5	2363	A2M	C3'-C2'-C1'	-2.99	97.09	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4571	A2M	C3'-C2'-C1'	-2.98	97.10	102.81
86	S2	1337	4AC	N4-C4-N3	2.98	118.70	113.87
6	L5	3853	PSU	O2-C2-N1	-2.97	119.72	122.79
6	L5	3920	PSU	O2-C2-N1	-2.97	119.73	122.79
8	L8	55	PSU	O2-C2-N1	-2.96	119.74	122.79
6	L5	4532	PSU	O2-C2-N1	-2.96	119.74	122.79
86	S2	668	A2M	O3'-C3'-C2'	2.96	119.46	111.19
86	S2	1326	OMU	O4-C4-C5	-2.95	120.07	125.16
6	L5	3925	OMU	O4-C4-C5	-2.95	120.07	125.16
6	L5	4227	OMU	O4-C4-C5	-2.95	120.08	125.16
86	S2	1832	6MZ	C4-N9-C8	2.94	108.82	105.74
6	L5	4552	PSU	O2-C2-N1	-2.93	119.76	122.79
86	S2	109	PSU	O2-C2-N1	-2.93	119.77	122.79
86	S2	1639	G7M	CN7-N7-C5	2.93	130.45	126.80
6	L5	3818	UY1	C6-N1-C2	-2.93	119.97	122.69
6	L5	2837	OMU	O4-C4-C5	-2.93	120.11	125.16
6	L5	1744	PSU	O2-C2-N1	-2.92	119.77	122.79
6	L5	4571	A2M	O3'-C3'-C2'	2.92	119.37	111.19
6	L5	4521	PSU	O2-C2-N1	-2.92	119.78	122.79
6	L5	3785	A2M	O3'-C3'-C2'	2.92	119.35	111.19
86	S2	166	A2M	C4-N9-C1'	-2.91	119.83	126.63
86	S2	1004	PSU	O2-C2-N1	-2.91	119.79	122.79
86	S2	121	OMU	O4-C4-C5	-2.91	120.15	125.16
86	S2	1177	PSU	O2-C2-N1	-2.90	119.80	122.79
6	L5	4220	6MZ	N3-C4-N9	2.89	132.09	127.17
6	L5	4220	6MZ	C5-N7-C8	2.89	107.99	103.45
6	L5	5010	PSU	O2-C2-N1	-2.89	119.81	122.79
6	L5	2401	A2M	C1'-N9-C8	2.88	133.50	127.09
6	L5	3825	A2M	C4-N9-C1'	-2.88	119.89	126.63
6	L5	4590	A2M	O3'-C3'-C2'	2.88	119.25	111.19
6	L5	3701	OMC	O2-C2-N3	-2.88	117.79	122.33
6	L5	4498	OMU	O4-C4-C5	-2.88	120.20	125.16
86	S2	1288	OMU	O4-C4-C5	-2.87	120.21	125.16
86	S2	172	OMU	O4-C4-C5	-2.87	120.21	125.16
86	S2	1244	PSU	O2-C2-N1	-2.87	119.83	122.79
86	S2	799	OMU	O4-C4-C5	-2.87	120.21	125.16
86	S2	1031	A2M	C4-N9-C1'	-2.87	119.93	126.63
6	L5	3695	PSU	O2-C2-N1	-2.86	119.83	122.79
6	L5	3867	A2M	C2'-C1'-N9	2.86	118.47	113.75
6	L5	4442	PSU	O2-C2-N1	-2.86	119.84	122.79
86	S2	1367	PSU	O2-C2-N1	-2.86	119.84	122.79
6	L5	398	A2M	C4-N9-C1'	-2.85	119.96	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	354	OMU	O4-C4-C5	-2.85	120.25	125.16
6	L5	4312	PSU	C6-N1-C2	-2.85	120.05	122.69
6	L5	2363	A2M	O3'-C3'-C2'	2.84	119.14	111.19
86	S2	1832	6MZ	N3-C4-N9	2.84	132.00	127.17
6	L5	4590	A2M	C4-N9-C1'	-2.84	120.00	126.63
86	S2	686	PSU	O2-C2-N1	-2.84	119.86	122.79
6	L5	4523	A2M	O3'-C3'-C2'	2.83	119.11	111.19
6	L5	2632	PSU	O2-C2-N1	-2.83	119.87	122.79
86	S2	1383	A2M	C4-N9-C1'	-2.83	120.01	126.63
6	L5	4312	PSU	O2-C2-N1	-2.83	119.87	122.79
6	L5	4293	PSU	O2-C2-N1	-2.83	119.87	122.79
86	S2	27	A2M	C4-N9-C1'	-2.83	120.02	126.63
86	S2	406	PSU	O2-C2-N1	-2.82	119.88	122.79
6	L5	4673	PSU	O2-C2-N1	-2.82	119.88	122.79
86	S2	99	A2M	C4-N9-C1'	-2.81	120.06	126.63
6	L5	2839	PSU	C6-N1-C2	-2.81	120.09	122.69
86	S2	651	PSU	O2-C2-N1	-2.81	119.89	122.79
86	S2	1232	PSU	O2-C2-N1	-2.81	119.89	122.79
6	L5	3844	PSU	C6-N1-C2	-2.80	120.09	122.69
6	L5	4403	PSU	O2-C2-N1	-2.80	119.90	122.79
86	S2	681	PSU	C6-N1-C2	-2.80	120.10	122.69
86	S2	159	A2M	C4-N9-C1'	-2.79	120.11	126.63
86	S2	668	A2M	O4'-C1'-C2'	2.78	111.38	106.59
6	L5	1871	A2M	C1'-N9-C8	2.78	133.26	127.09
6	L5	4431	PSU	O2-C2-N1	-2.77	119.94	122.79
6	L5	4500	PSU	C6-N1-C2	-2.77	120.12	122.69
86	S2	1045	PSU	O2-C2-N1	-2.76	119.94	122.79
86	S2	1081	PSU	O2-C2-N1	-2.76	119.94	122.79
6	L5	1326	A2M	O3'-C3'-C2'	2.76	118.91	111.19
86	S2	484	A2M	O3'-C3'-C2'	2.76	118.91	111.19
6	L5	1677	PSU	O2-C2-N1	-2.76	119.94	122.79
6	L5	4571	A2M	C4-N9-C1'	-2.75	120.19	126.63
86	S2	1046	PSU	O2-C2-N1	-2.75	119.95	122.79
86	S2	966	PSU	O2-C2-N1	-2.75	119.96	122.79
6	L5	3822	PSU	O2-C2-N1	-2.74	119.96	122.79
6	L5	3884	PSU	O2-C2-N1	-2.74	119.96	122.79
6	L5	4972	PSU	O2-C2-N1	-2.74	119.97	122.79
6	L5	4523	A2M	C4-N9-C1'	-2.73	120.24	126.63
6	L5	4353	PSU	O2-C2-N1	-2.73	119.97	122.79
86	S2	866	PSU	O2-C2-N1	-2.73	119.97	122.79
86	S2	468	A2M	C1'-N9-C8	2.73	133.15	127.09
6	L5	4973	PSU	O2-C2-N1	-2.72	119.98	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	1832	6MZ	C4-C5-C6	2.72	119.04	116.78
6	L5	1792	PSU	O2-C2-N1	-2.71	119.99	122.79
86	S2	484	A2M	C4-N9-C1'	-2.71	120.29	126.63
6	L5	1781	PSU	O2-C2-N1	-2.71	120.00	122.79
6	L5	398	A2M	C1'-N9-C8	2.71	133.10	127.09
6	L5	1582	PSU	O2-C2-N1	-2.71	120.00	122.79
86	S2	1031	A2M	C1'-N9-C8	2.70	133.09	127.09
6	L5	4361	PSU	O2-C2-N1	-2.70	120.00	122.79
6	L5	1326	A2M	C4-N9-C1'	-2.70	120.32	126.63
86	S2	576	A2M	C4-N9-C1'	-2.70	120.32	126.63
86	S2	166	A2M	C1'-N9-C8	2.69	133.07	127.09
86	S2	966	PSU	C6-N1-C2	-2.69	120.19	122.69
86	S2	159	A2M	C1'-N9-C8	2.69	133.07	127.09
6	L5	1524	A2M	C4'-O4'-C1'	-2.69	103.54	109.47
6	L5	3867	A2M	C4-N9-C1'	-2.69	120.35	126.63
6	L5	1683	PSU	C6-N1-C2	-2.68	120.20	122.69
6	L5	1326	A2M	C3'-C2'-C1'	-2.68	97.67	102.81
86	S2	1248	B8N	O4-C4-N3	-2.68	115.64	119.99
86	S2	27	A2M	C1'-N9-C8	2.67	133.03	127.09
86	S2	801	PSU	O2-C2-N1	-2.67	120.03	122.79
6	L5	4636	PSU	O2-C2-N1	-2.67	120.03	122.79
86	S2	863	PSU	O2-C2-N1	-2.67	120.03	122.79
6	L5	3825	A2M	C1'-N9-C8	2.67	133.02	127.09
86	S2	99	A2M	C1'-N9-C8	2.67	133.02	127.09
6	L5	2815	A2M	O3'-C3'-C2'	2.67	118.65	111.19
86	S2	484	A2M	C1'-N9-C8	2.67	133.01	127.09
86	S2	1056	PSU	O2-C2-N1	-2.67	120.04	122.79
6	L5	4620	OMU	O4-C4-C5	-2.66	120.58	125.16
6	L5	4353	PSU	C6-N1-C2	-2.66	120.22	122.69
6	L5	3818	UY1	O2-C2-N1	-2.65	120.05	122.79
6	L5	1524	A2M	O4'-C1'-C2'	2.65	111.15	106.59
6	L5	4590	A2M	C1'-N9-C8	2.65	132.97	127.09
6	L5	1782	PSU	O2-C2-N1	-2.64	120.07	122.79
6	L5	4552	PSU	C6-N1-C2	-2.63	120.25	122.69
6	L5	3718	A2M	C1'-N9-C8	2.63	132.94	127.09
6	L5	1782	PSU	C6-N1-C2	-2.63	120.25	122.69
6	L5	3830	A2M	C4-N9-C1'	-2.63	120.48	126.63
6	L5	4353	PSU	C6-C5-C4	2.63	119.95	118.17
6	L5	3785	A2M	C3'-C2'-C1'	-2.63	97.77	102.81
6	L5	2815	A2M	C3'-C2'-C1'	-2.63	97.77	102.81
6	L5	4628	PSU	O2-C2-N1	-2.63	120.08	122.79
6	L5	3822	PSU	C6-N1-C2	-2.63	120.25	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3785	A2M	C4-N9-C1'	-2.62	120.49	126.63
86	S2	159	A2M	C3'-C2'-C1'	-2.62	97.79	102.81
86	S2	105	PSU	O2-C2-N1	-2.62	120.09	122.79
6	L5	4220	6MZ	OP2-P-O5'	2.62	113.50	106.67
6	L5	3695	PSU	C6-N1-C2	-2.62	120.26	122.69
86	S2	1367	PSU	C6-N1-C2	-2.62	120.26	122.69
6	L5	2351	OMC	C1'-N1-C2	2.61	124.22	118.44
86	S2	1383	A2M	C1'-N9-C8	2.61	132.90	127.09
6	L5	4628	PSU	C6-N1-C2	-2.61	120.27	122.69
86	S2	93	PSU	O2-C2-N1	-2.61	120.09	122.79
86	S2	801	PSU	C6-N1-C2	-2.61	120.27	122.69
6	L5	3867	A2M	C1'-N9-C8	2.61	132.88	127.09
6	L5	4293	PSU	C6-N1-C2	-2.60	120.28	122.69
6	L5	3701	OMC	O2-C2-N1	2.60	124.00	118.90
6	L5	3920	PSU	C6-N1-C2	-2.60	120.28	122.69
6	L5	1323	A2M	C3'-C2'-C1'	-2.60	97.83	102.81
6	L5	3718	A2M	C4-N9-C1'	-2.60	120.55	126.63
6	L5	4471	PSU	C6-N1-C2	-2.60	120.28	122.69
6	L5	4576	PSU	C6-N1-C2	-2.60	120.28	122.69
6	L5	3639	PSU	C6-N1-C2	-2.59	120.28	122.69
8	L8	69	PSU	C6-N1-C2	-2.59	120.29	122.69
6	L5	2787	A2M	O4'-C1'-C2'	2.58	111.02	106.59
6	L5	1326	A2M	C1'-N9-C8	2.57	132.81	127.09
6	L5	4579	PSU	C6-N1-C2	-2.57	120.31	122.69
86	S2	1177	PSU	C6-N1-C2	-2.57	120.31	122.69
6	L5	400	A2M	C4-N9-C1'	-2.57	120.63	126.63
6	L5	2632	PSU	C6-N1-C2	-2.56	120.31	122.69
6	L5	4493	PSU	O2-C2-N1	-2.56	120.14	122.79
86	S2	681	PSU	O2-C2-N1	-2.56	120.14	122.79
6	L5	1744	PSU	C6-N1-C2	-2.56	120.31	122.69
6	L5	4471	PSU	O2-C2-N1	-2.56	120.15	122.79
86	S2	1232	PSU	C6-N1-C2	-2.56	120.32	122.69
86	S2	668	A2M	C2'-C1'-N9	2.56	117.96	113.75
4	CF	163	SEP	OG-CB-CA	2.56	110.63	108.14
6	L5	5001	PSU	O2-C2-N1	-2.56	120.15	122.79
6	L5	4442	PSU	C6-N1-C2	-2.55	120.32	122.69
6	L5	5010	PSU	C6-N1-C2	-2.55	120.32	122.69
6	L5	4220	6MZ	C4-C5-C6	2.55	118.90	116.78
6	L5	4673	PSU	C6-N1-C2	-2.55	120.32	122.69
6	L5	400	A2M	C2'-C1'-N9	2.55	117.95	113.75
86	S2	93	PSU	C6-N1-C2	-2.55	120.33	122.69
6	L5	3830	A2M	C1'-N9-C8	2.54	132.74	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1860	PSU	C6-N1-C2	-2.54	120.34	122.69
86	S2	651	PSU	C6-N1-C2	-2.54	120.34	122.69
86	S2	1046	PSU	C6-N1-C2	-2.53	120.34	122.69
86	S2	576	A2M	C1'-N9-C8	2.53	132.70	127.09
6	L5	2363	A2M	C2'-C1'-N9	2.52	117.90	113.75
8	L8	55	PSU	C6-N1-C2	-2.52	120.35	122.69
86	S2	649	PSU	C6-N1-C2	-2.51	120.36	122.69
6	L5	3853	PSU	C6-N1-C2	-2.51	120.36	122.69
86	S2	105	PSU	C6-N1-C2	-2.51	120.36	122.69
6	L5	4220	6MZ	C5-C6-N1	2.51	120.84	118.15
6	L5	2363	A2M	C4-N9-C1'	-2.50	120.77	126.63
86	S2	1004	PSU	C6-N1-C2	-2.50	120.37	122.69
6	L5	4571	A2M	C1'-N9-C8	2.50	132.64	127.09
6	L5	4521	PSU	C6-N1-C2	-2.50	120.37	122.69
86	S2	1174	PSU	C6-N1-C2	-2.49	120.38	122.69
6	L5	4973	PSU	C6-N1-C2	-2.49	120.38	122.69
6	L5	4299	PSU	O2-C2-N1	-2.49	120.22	122.79
6	L5	4523	A2M	C1'-N9-C8	2.48	132.61	127.09
86	S2	866	PSU	C6-C5-C4	2.48	119.85	118.17
6	L5	4500	PSU	C6-C5-C4	2.48	119.84	118.17
86	S2	354	OMU	O2-C2-N1	-2.47	119.58	122.80
6	L5	400	A2M	C1'-N9-C8	2.47	132.58	127.09
6	L5	1536	PSU	C6-N1-C2	-2.47	120.40	122.69
6	L5	5001	PSU	C6-N1-C2	-2.47	120.40	122.69
86	S2	814	PSU	O2-C2-N1	-2.47	120.25	122.79
6	L5	4442	PSU	C6-C5-C4	2.46	119.83	118.17
6	L5	3808	OMC	C1'-N1-C2	2.46	123.87	118.44
6	L5	2363	A2M	C1'-N9-C8	2.45	132.54	127.09
6	L5	4498	OMU	O2-C2-N1	-2.45	119.61	122.80
86	S2	109	PSU	C6-N1-C2	-2.45	120.42	122.69
6	L5	2787	A2M	C4-N9-C1'	-2.45	120.91	126.63
6	L5	4972	PSU	C6-N1-C2	-2.44	120.42	122.69
86	S2	1832	6MZ	C4-C5-N7	-2.44	107.79	110.58
6	L5	2815	A2M	C4-N9-C1'	-2.44	120.92	126.63
6	L5	1323	A2M	O4'-C1'-C2'	2.44	110.78	106.59
86	S2	1244	PSU	C6-N1-C2	-2.43	120.44	122.69
86	S2	1639	G7M	CN7-N7-C8	-2.43	121.11	124.79
86	S2	1272	OMC	C1'-N1-C2	2.43	123.81	118.44
6	L5	3639	PSU	C6-C5-C4	2.43	119.81	118.17
6	L5	3925	OMU	O2-C2-N1	-2.43	119.64	122.80
6	L5	3884	PSU	C6-N1-C2	-2.42	120.44	122.69
6	L5	3851	PSU	C6-N1-C2	-2.42	120.45	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4521	PSU	C6-C5-C4	2.41	119.80	118.17
6	L5	4431	PSU	C6-N1-C2	-2.40	120.46	122.69
6	L5	2861	OMC	C1'-N1-C2	2.40	123.74	118.44
6	L5	1534	A2M	O3'-C3'-C4'	-2.40	104.19	111.08
86	S2	863	PSU	C6-N1-C2	-2.40	120.47	122.69
86	S2	406	PSU	C6-N1-C2	-2.39	120.48	122.69
6	L5	1582	PSU	C6-N1-C2	-2.38	120.48	122.69
86	S2	1045	PSU	C6-N1-C2	-2.38	120.48	122.69
86	S2	484	A2M	O4'-C1'-C2'	2.38	110.68	106.59
6	L5	3785	A2M	C2-N1-C6	-2.38	114.83	118.73
6	L5	3822	PSU	O4'-C1'-C2'	2.37	108.42	105.15
6	L5	2401	A2M	C6-C5-C4	-2.36	113.95	117.18
6	L5	1871	A2M	C6-C5-C4	-2.36	113.95	117.18
6	L5	1781	PSU	C6-N1-C2	-2.36	120.50	122.69
6	L5	4296	PSU	C6-N1-C2	-2.35	120.51	122.69
86	S2	686	PSU	C6-N1-C2	-2.35	120.51	122.69
86	S2	866	PSU	C6-N1-C2	-2.34	120.52	122.69
6	L5	2837	OMU	O2-C2-N1	-2.34	119.75	122.80
6	L5	4571	A2M	C2'-C1'-N9	2.34	117.60	113.75
6	L5	3637	PSU	C6-N1-C2	-2.34	120.52	122.69
6	L5	2815	A2M	C1'-N9-C8	2.34	132.28	127.09
6	L5	4299	PSU	C6-N1-C2	-2.33	120.53	122.69
6	L5	3785	A2M	C1'-N9-C8	2.33	132.27	127.09
6	L5	1524	A2M	C4-N9-C1'	-2.33	121.19	126.63
6	L5	4636	PSU	C6-C5-C4	2.33	119.74	118.17
86	S2	1639	G7M	N9-C8-N7	-2.32	106.84	112.48
6	L5	2787	A2M	C1'-N9-C8	2.32	132.25	127.09
86	S2	1056	PSU	C6-N1-C2	-2.32	120.54	122.69
6	L5	1323	A2M	C4-N9-C1'	-2.31	121.23	126.63
6	L5	4457	PSU	C6-N1-C2	-2.31	120.55	122.69
86	S2	1248	B8N	O4'-C1'-C2'	2.30	108.34	105.15
86	S2	1850	MA6	C1'-N9-C8	-2.30	121.99	127.09
6	L5	4361	PSU	C6-N1-C2	-2.29	120.56	122.69
6	L5	1683	PSU	C6-C5-C4	2.29	119.72	118.17
6	L5	4532	PSU	C6-N1-C2	-2.29	120.57	122.69
6	L5	2363	A2M	O4'-C1'-C2'	2.28	110.52	106.59
86	S2	668	A2M	C6-C5-C4	-2.28	114.06	117.18
6	L5	4590	A2M	C6-C5-C4	-2.27	114.07	117.18
86	S2	468	A2M	C6-C5-C4	-2.27	114.07	117.18
86	S2	428	OMU	O2-C2-N1	-2.27	119.84	122.80
6	L5	4523	A2M	C6-C5-C4	-2.27	114.08	117.18
86	S2	1288	OMU	C1'-N1-C2	2.27	121.67	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1744	PSU	C6-C5-C4	2.27	119.70	118.17
6	L5	1862	PSU	C6-N1-C2	-2.27	120.59	122.69
86	S2	1851	MA6	C1'-N9-C8	-2.26	122.07	127.09
8	L8	69	PSU	O4'-C1'-C2'	2.26	108.28	105.15
6	L5	1323	A2M	C1'-N9-C8	2.26	132.12	127.09
86	S2	172	OMU	O2-C2-N1	-2.26	119.85	122.80
86	S2	1326	OMU	O2-C2-N1	-2.26	119.85	122.80
6	L5	4571	A2M	O4'-C1'-C2'	2.26	110.48	106.59
6	L5	3785	A2M	C5-C6-N1	2.26	123.25	117.51
86	S2	1337	4AC	C5-C4-N4	-2.26	119.14	122.94
6	L5	2815	A2M	O4'-C1'-C2'	2.25	110.47	106.59
6	L5	3825	A2M	C6-C5-C4	-2.25	114.10	117.18
6	L5	3867	A2M	C6-C5-C4	-2.25	114.10	117.18
6	L5	1326	A2M	C2'-C1'-N9	2.25	117.46	113.75
86	S2	166	A2M	C6-C5-C4	-2.24	114.12	117.18
6	L5	1326	A2M	C6-C5-C4	-2.24	114.12	117.18
6	L5	4493	PSU	C6-N1-C2	-2.24	120.61	122.69
6	L5	1524	A2M	C1'-N9-C8	2.23	132.05	127.09
86	S2	27	A2M	C6-C5-C4	-2.23	114.13	117.18
6	L5	3867	A2M	O3'-C3'-C2'	2.23	117.43	111.19
6	L5	1326	A2M	O4'-C1'-C2'	2.23	110.43	106.59
86	S2	1031	A2M	C6-C5-C4	-2.23	114.13	117.18
6	L5	4571	A2M	C6-C5-C4	-2.22	114.15	117.18
6	L5	1322	1MA	N1-C6-N6	2.22	125.29	119.71
86	S2	406	PSU	C6-C5-C4	2.22	119.67	118.17
6	L5	4457	PSU	C6-C5-C4	2.21	119.66	118.17
86	S2	1056	PSU	C6-C5-C4	2.21	119.66	118.17
6	L5	1522	OMG	C2'-C1'-N9	-2.21	110.05	114.24
6	L5	3637	PSU	C6-C5-C4	2.21	119.66	118.17
6	L5	4227	OMU	O2-C2-N1	-2.20	119.93	122.80
6	L5	4403	PSU	O4'-C1'-C2'	2.20	108.20	105.15
86	S2	1383	A2M	C6-C5-C4	-2.20	114.18	117.18
86	S2	814	PSU	C6-N1-C2	-2.20	120.65	122.69
86	S2	1248	B8N	O4-C4-C5	-2.19	118.80	122.58
6	L5	2632	PSU	C6-C5-C4	2.18	119.65	118.17
6	L5	1792	PSU	C6-N1-C2	-2.18	120.67	122.69
86	S2	159	A2M	O4'-C1'-C2'	2.18	110.34	106.59
6	L5	398	A2M	C6-C5-C4	-2.17	114.21	117.18
6	L5	4636	PSU	O4'-C1'-C2'	2.17	108.15	105.15
86	S2	166	A2M	O4'-C1'-C2'	2.17	110.32	106.59
6	L5	400	A2M	C2-N1-C6	-2.17	115.17	118.73
6	L5	4523	A2M	C4'-O4'-C1'	-2.16	104.71	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	116	OMU	O2-C2-N1	-2.16	119.99	122.80
6	L5	4552	PSU	C6-C5-C4	2.15	119.63	118.17
6	L5	3830	A2M	C6-C5-C4	-2.15	114.24	117.18
6	L5	1534	A2M	O4'-C1'-C2'	2.15	110.29	106.59
8	L8	69	PSU	C6-C5-C4	2.15	119.63	118.17
6	L5	3782	5MC	C1'-N1-C6	-2.15	117.61	121.15
6	L5	4442	PSU	O4'-C1'-C2'	2.15	108.12	105.15
86	S2	649	PSU	C6-C5-C4	2.15	119.62	118.17
86	S2	99	A2M	C6-C5-C4	-2.15	114.25	117.18
6	L5	2839	PSU	C6-C5-C4	2.15	119.62	118.17
86	S2	576	A2M	C6-C5-C4	-2.15	114.25	117.18
86	S2	627	OMU	O2-C2-N1	-2.14	120.01	122.80
6	L5	1322	1MA	CM1-N1-C6	-2.14	116.83	120.15
6	L5	1534	A2M	C2-N1-C6	-2.14	115.22	118.73
6	L5	3785	A2M	C6-C5-C4	-2.13	114.26	117.18
6	L5	1534	A2M	C4-N9-C1'	-2.13	121.64	126.63
6	L5	400	A2M	C6-C5-C4	-2.13	114.28	117.18
6	L5	400	A2M	C5-C6-N1	2.12	122.90	117.51
6	L5	3785	A2M	O4'-C1'-N9	2.12	112.16	108.09
6	L5	3785	A2M	O4'-C4'-C3'	2.12	109.36	105.15
86	S2	1081	PSU	C6-N1-C2	-2.11	120.73	122.69
6	L5	3718	A2M	C6-C5-C4	-2.11	114.29	117.18
6	L5	2363	A2M	C2-N1-C6	-2.11	115.26	118.73
86	S2	1081	PSU	O4'-C1'-C2'	2.11	108.07	105.15
6	L5	1323	A2M	C2-N1-C6	-2.11	115.27	118.73
6	L5	398	A2M	C5-C6-N1	2.11	122.86	117.51
86	S2	99	A2M	C2-N1-C6	-2.11	115.27	118.73
6	L5	2401	A2M	O4'-C1'-C2'	2.11	110.21	106.59
6	L5	2363	A2M	C6-C5-C4	-2.10	114.31	117.18
86	S2	1383	A2M	C4'-O4'-C1'	-2.10	104.83	109.47
6	L5	3637	PSU	O2-C2-N1	-2.10	120.63	122.79
6	L5	2363	A2M	C5-C6-N1	2.09	122.83	117.51
6	L5	4523	A2M	C5-C6-N1	2.09	122.82	117.51
86	S2	468	A2M	O4'-C1'-C2'	2.09	110.18	106.59
6	L5	2787	A2M	C6-C5-C4	-2.09	114.33	117.18
6	L5	1524	A2M	C6-C5-C4	-2.09	114.33	117.18
86	S2	799	OMU	C1'-N1-C2	2.09	121.34	117.59
86	S2	484	A2M	O4'-C4'-C3'	2.09	109.29	105.15
6	L5	4306	OMU	O2-C2-N1	-2.08	120.08	122.80
6	L5	3867	A2M	C2-N1-C6	-2.08	115.31	118.73
6	L5	1323	A2M	C5-C6-N1	2.08	122.80	117.51
6	L5	1534	A2M	C1'-N9-C8	2.08	131.71	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1326	A2M	C5-C6-N1	2.08	122.80	117.51
6	L5	4636	PSU	C6-N1-C2	-2.08	120.76	122.69
6	L5	4403	PSU	C6-N1-C2	-2.08	120.76	122.69
86	S2	484	A2M	C6-C5-C4	-2.08	114.34	117.18
86	S2	159	A2M	C6-C5-C4	-2.08	114.34	117.18
6	L5	2787	A2M	C5-C6-N1	2.08	122.79	117.51
6	L5	3825	A2M	C5-C6-N1	2.08	122.78	117.51
6	L5	3830	A2M	C5-C6-N1	2.07	122.78	117.51
6	L5	4403	PSU	C6-C5-C4	2.07	119.57	118.17
86	S2	99	A2M	C5-C6-N1	2.07	122.78	117.51
86	S2	1832	6MZ	OP2-P-OP1	2.07	118.91	110.83
6	L5	400	A2M	O4'-C1'-C2'	2.07	110.16	106.59
6	L5	398	A2M	C2-N1-C6	-2.07	115.33	118.73
6	L5	1871	A2M	C4'-O4'-C1'	-2.07	104.89	109.47
6	L5	1323	A2M	C6-C5-C4	-2.07	114.35	117.18
86	S2	121	OMU	O2-C2-N1	-2.07	120.11	122.80
6	L5	2401	A2M	C5-C6-N1	2.07	122.76	117.51
86	S2	166	A2M	C5-C6-N1	2.07	122.76	117.51
6	L5	4571	A2M	O3'-C3'-C4'	-2.06	105.15	111.08
6	L5	3867	A2M	C3'-C2'-C1'	-2.06	98.85	102.81
6	L5	4457	PSU	O4'-C1'-C2'	2.06	108.00	105.15
6	L5	2815	A2M	C6-C5-C4	-2.06	114.36	117.18
86	S2	468	A2M	C5-C6-N1	2.06	122.75	117.51
6	L5	3867	A2M	O4'-C1'-C2'	2.06	110.13	106.59
6	L5	4456	OMC	C1'-N1-C2	2.05	122.98	118.44
6	L5	4628	PSU	O4'-C1'-C2'	2.05	107.99	105.15
6	L5	4353	PSU	O4'-C1'-C2'	2.05	107.99	105.15
6	L5	2787	A2M	C2-N1-C6	-2.05	115.36	118.73
6	L5	3825	A2M	C2-N1-C6	-2.05	115.37	118.73
6	L5	3867	A2M	C5-C6-N1	2.05	122.71	117.51
86	S2	1383	A2M	C5-C6-N1	2.04	122.70	117.51
6	L5	1534	A2M	C5-C6-N1	2.04	122.69	117.51
86	S2	1442	OMU	O2-C2-N1	-2.04	120.14	122.80
6	L5	4571	A2M	C5-C6-N1	2.04	122.69	117.51
6	L5	4973	PSU	C6-C5-C4	2.04	119.55	118.17
86	S2	27	A2M	C5-C6-N1	2.04	122.68	117.51
6	L5	3825	A2M	O4'-C1'-C2'	2.03	110.09	106.59
6	L5	4972	PSU	C6-C5-C4	2.03	119.55	118.17
6	L5	2815	A2M	C5-C6-N1	2.03	122.66	117.51
86	S2	159	A2M	C5-C6-N1	2.02	122.65	117.51
6	L5	4523	A2M	C2-N1-C6	-2.02	115.41	118.73
6	L5	4521	PSU	O4'-C1'-C2'	2.02	107.94	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	1031	A2M	C5-C6-N1	2.01	122.63	117.51
86	S2	1244	PSU	C6-C5-C4	2.01	119.53	118.17
86	S2	484	A2M	C5-C6-N1	2.01	122.61	117.51
6	L5	3920	PSU	C6-C5-C4	2.01	119.53	118.17
6	L5	1326	A2M	C2-N1-C6	-2.01	115.43	118.73
86	S2	27	A2M	O4'-C1'-C2'	2.01	110.05	106.59
86	S2	576	A2M	C5-C6-N1	2.01	122.61	117.51
6	L5	3718	A2M	C5-C6-N1	2.01	122.61	117.51
6	L5	4590	A2M	C5-C6-N1	2.01	122.60	117.51
6	L5	3695	PSU	O4'-C1'-C2'	2.00	107.92	105.15
86	S2	668	A2M	O3'-C3'-C4'	-2.00	105.34	111.08

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CF	163	SEP	N-CA-CB-OG
4	CF	163	SEP	C-CA-CB-OG
4	CF	163	SEP	CA-CB-OG-P
4	CF	163	SEP	CB-OG-P-O2P
8	L8	75	OMG	C1'-C2'-O2'-CM2
6	L5	1326	A2M	O4'-C4'-C5'-O5'
6	L5	1326	A2M	C1'-C2'-O2'-CM'
6	L5	1340	OMC	C1'-C2'-O2'-CM2
6	L5	1625	OMG	O4'-C4'-C5'-O5'
6	L5	2351	OMC	C1'-C2'-O2'-CM2
6	L5	2787	A2M	C1'-C2'-O2'-CM'
6	L5	3701	OMC	O4'-C4'-C5'-O5'
6	L5	3792	OMG	O4'-C4'-C5'-O5'
6	L5	4196	OMG	C1'-C2'-O2'-CM2
6	L5	4220	6MZ	C5'-O5'-P-OP1
6	L5	4220	6MZ	C5'-O5'-P-OP3
6	L5	4637	OMG	O4'-C4'-C5'-O5'
86	S2	27	A2M	C1'-C2'-O2'-CM'
86	S2	159	A2M	C1'-C2'-O2'-CM'
86	S2	601	OMG	C1'-C2'-O2'-CM2
86	S2	644	OMG	O4'-C4'-C5'-O5'
86	S2	1248	B8N	O4'-C4'-C5'-O5'
86	S2	1272	OMC	O4'-C4'-C5'-O5'
86	S2	1288	OMU	O4'-C4'-C5'-O5'
86	S2	1337	4AC	N3-C4-N4-C7
86	S2	1383	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
86	S2	1442	OMU	O4'-C4'-C5'-O5'
86	S2	1832	6MZ	C5-C6-N6-C9
86	S2	1832	6MZ	N1-C6-N6-C9
6	L5	3701	OMC	C2'-C1'-N1-C2
6	L5	2364	OMG	O4'-C4'-C5'-O5'
6	L5	3701	OMC	C3'-C4'-C5'-O5'
6	L5	4500	PSU	C3'-C4'-C5'-O5'
6	L5	4500	PSU	O4'-C4'-C5'-O5'
6	L5	4590	A2M	O4'-C4'-C5'-O5'
6	L5	4590	A2M	C3'-C4'-C5'-O5'
86	S2	436	OMG	O4'-C4'-C5'-O5'
86	S2	576	A2M	O4'-C4'-C5'-O5'
86	S2	576	A2M	C3'-C4'-C5'-O5'
86	S2	683	OMG	C3'-C4'-C5'-O5'
86	S2	799	OMU	C3'-C4'-C5'-O5'
86	S2	799	OMU	O4'-C4'-C5'-O5'
86	S2	801	PSU	C3'-C4'-C5'-O5'
86	S2	867	OMG	C3'-C4'-C5'-O5'
86	S2	1272	OMC	C3'-C4'-C5'-O5'
86	S2	1288	OMU	C3'-C4'-C5'-O5'
6	L5	1323	A2M	O4'-C4'-C5'-O5'
6	L5	1536	PSU	C3'-C4'-C5'-O5'
6	L5	1536	PSU	O4'-C4'-C5'-O5'
6	L5	1625	OMG	C3'-C4'-C5'-O5'
6	L5	2815	A2M	O4'-C4'-C5'-O5'
6	L5	3792	OMG	C3'-C4'-C5'-O5'
6	L5	3867	A2M	C3'-C4'-C5'-O5'
86	S2	99	A2M	O4'-C4'-C5'-O5'
86	S2	683	OMG	O4'-C4'-C5'-O5'
86	S2	1442	OMU	C3'-C4'-C5'-O5'
6	L5	3701	OMC	C2'-C1'-N1-C6
6	L5	1326	A2M	C3'-C4'-C5'-O5'
86	S2	644	OMG	C3'-C4'-C5'-O5'
6	L5	4447	5MC	C2'-C1'-N1-C6
6	L5	1677	PSU	C3'-C4'-C5'-O5'
6	L5	2364	OMG	C3'-C4'-C5'-O5'
6	L5	2876	OMG	C3'-C4'-C5'-O5'
6	L5	3899	OMG	C3'-C4'-C5'-O5'
6	L5	4637	OMG	C3'-C4'-C5'-O5'
86	S2	436	OMG	C3'-C4'-C5'-O5'
86	S2	517	OMC	C3'-C4'-C5'-O5'
86	S2	668	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
86	S2	668	A2M	C3'-C4'-C5'-O5'
86	S2	1248	B8N	C3'-C4'-C5'-O5'
86	S2	428	OMU	C2'-C1'-N1-C6
6	L5	1677	PSU	O4'-C4'-C5'-O5'
6	L5	2787	A2M	C3'-C4'-C5'-O5'
6	L5	2815	A2M	C3'-C4'-C5'-O5'
86	S2	801	PSU	O4'-C4'-C5'-O5'
86	S2	867	OMG	O4'-C4'-C5'-O5'
6	L5	1524	A2M	O4'-C4'-C5'-O5'
6	L5	1524	A2M	C3'-C4'-C5'-O5'
6	L5	3867	A2M	O4'-C4'-C5'-O5'
86	S2	517	OMC	O4'-C4'-C5'-O5'
6	L5	2787	A2M	C2'-C1'-N9-C8
6	L5	3899	OMG	O4'-C4'-C5'-O5'
6	L5	4618	OMG	C3'-C4'-C5'-O5'
6	L5	1323	A2M	C3'-C4'-C5'-O5'
6	L5	2876	OMG	O4'-C4'-C5'-O5'
86	S2	99	A2M	C3'-C4'-C5'-O5'
6	L5	4590	A2M	C4'-C5'-O5'-P
6	L5	2422	OMC	O4'-C4'-C5'-O5'
86	S2	1045	PSU	O4'-C4'-C5'-O5'
6	L5	3841	OMC	C1'-C2'-O2'-CM2
86	S2	166	A2M	C1'-C2'-O2'-CM'
86	S2	867	OMG	C1'-C2'-O2'-CM2
6	L5	2422	OMC	C3'-C4'-C5'-O5'
6	L5	3851	PSU	C3'-C4'-C5'-O5'
86	S2	428	OMU	O4'-C4'-C5'-O5'
86	S2	1248	B8N	C31-C32-C33-C34
86	S2	1045	PSU	C3'-C4'-C5'-O5'
86	S2	1248	B8N	N34-C33-C34-O36
86	S2	1639	G7M	C3'-C4'-C5'-O5'
6	L5	4447	5MC	O4'-C1'-N1-C6
86	S2	428	OMU	O4'-C1'-N1-C6
6	L5	4447	5MC	O4'-C1'-N1-C2
4	CF	163	SEP	CB-OG-P-O1P
6	L5	3818	UY1	C4'-C5'-O5'-P
6	L5	4447	5MC	C2'-C1'-N1-C2
86	S2	1383	A2M	O4'-C4'-C5'-O5'
6	L5	3701	OMC	O4'-C1'-N1-C6
6	L5	1534	A2M	C4'-C5'-O5'-P
6	L5	4500	PSU	C4'-C5'-O5'-P
6	L5	3818	UY1	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
6	L5	2787	A2M	C2'-C1'-N9-C4
86	S2	428	OMU	C3'-C4'-C5'-O5'
86	S2	1383	A2M	C3'-C4'-C5'-O5'
86	S2	576	A2M	C4'-C5'-O5'-P
6	L5	1781	PSU	C3'-C4'-C5'-O5'
86	S2	428	OMU	C2'-C1'-N1-C2
6	L5	3887	OMC	C4'-C5'-O5'-P
86	S2	627	OMU	O4'-C4'-C5'-O5'
6	L5	3785	A2M	C3'-C2'-O2'-CM'
86	S2	1490	OMG	C4'-C5'-O5'-P
6	L5	3782	5MC	O4'-C4'-C5'-O5'
6	L5	4618	OMG	O4'-C4'-C5'-O5'
86	S2	1703	OMC	O4'-C4'-C5'-O5'
86	S2	644	OMG	C4'-C5'-O5'-P
86	S2	1851	MA6	C4'-C5'-O5'-P
6	L5	398	A2M	O4'-C4'-C5'-O5'
86	S2	428	OMU	O4'-C1'-N1-C2
6	L5	400	A2M	C1'-C2'-O2'-CM'
6	L5	3844	PSU	C4'-C5'-O5'-P
4	CF	163	SEP	CB-OG-P-O3P
6	L5	1677	PSU	O4'-C1'-C5-C6
6	L5	3869	OMC	C3'-C2'-O2'-CM2
6	L5	3701	OMC	O4'-C1'-N1-C2
6	L5	1322	1MA	C2'-C1'-N9-C8
6	L5	2351	OMC	O4'-C4'-C5'-O5'
86	S2	1832	6MZ	O4'-C4'-C5'-O5'
6	L5	2787	A2M	O4'-C1'-N9-C8
86	S2	1639	G7M	O4'-C4'-C5'-O5'
6	L5	1326	A2M	C4'-C5'-O5'-P
6	L5	1322	1MA	C2'-C1'-N9-C4

There are no ring outliers.

68 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L5	1625	OMG	1	0
6	L5	400	A2M	1	0
8	L8	75	OMG	2	0
6	L5	1871	A2M	1	0
6	L5	4431	PSU	1	0
86	S2	1328	OMG	1	0
6	L5	4227	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L5	2861	OMC	1	0
4	CF	163	SEP	1	0
86	S2	1383	A2M	1	0
86	S2	509	OMG	2	0
6	L5	4220	6MZ	2	0
6	L5	4571	A2M	1	0
6	L5	2632	PSU	1	0
6	L5	4447	5MC	1	0
6	L5	3718	A2M	3	0
6	L5	3818	UY1	1	0
6	L5	3867	A2M	3	0
6	L5	3785	A2M	1	0
86	S2	1046	PSU	1	0
6	L5	4536	OMC	2	0
86	S2	436	OMG	1	0
6	L5	2424	OMG	1	0
86	S2	681	PSU	1	0
6	L5	3701	OMC	1	0
6	L5	2363	A2M	1	0
6	L5	1340	OMC	2	0
86	S2	601	OMG	1	0
86	S2	1337	4AC	3	0
86	S2	121	OMU	1	0
86	S2	576	A2M	2	0
6	L5	2876	OMG	1	0
86	S2	468	A2M	1	0
6	L5	3822	PSU	1	0
86	S2	517	OMC	1	0
6	L5	1683	PSU	2	0
6	L5	4457	PSU	1	0
6	L5	1677	PSU	1	0
6	L5	4636	PSU	1	0
6	L5	4637	OMG	1	0
86	S2	867	OMG	1	0
6	L5	3884	PSU	1	0
6	L5	2351	OMC	1	0
6	L5	4196	OMG	1	0
6	L5	1326	A2M	3	0
86	S2	1639	G7M	1	0
6	L5	4618	OMG	1	0
6	L5	4392	OMG	1	0
6	L5	398	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L5	4456	OMC	1	0
86	S2	166	A2M	2	0
86	S2	1850	MA6	2	0
6	L5	4590	A2M	1	0
86	S2	159	A2M	2	0
86	S2	116	OMU	2	0
6	L5	2422	OMC	1	0
86	S2	462	OMC	1	0
86	S2	1232	PSU	2	0
86	S2	1288	OMU	1	0
6	L5	3841	OMC	1	0
6	L5	4579	PSU	1	0
6	L5	4293	PSU	1	0
86	S2	27	A2M	1	0
6	L5	4620	OMU	2	0
86	S2	99	A2M	1	0
6	L5	3782	5MC	1	0
86	S2	484	A2M	1	0
6	L5	4306	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	SPD	L5	5282	-	9,9,9	0.31	0	8,8,8	0.77	0
89	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.84	0
88	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.87	0
88	SPM	L5	5286	87	13,13,13	0.36	0	12,12,12	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.91	0
88	SPM	L5	5262	-	13,13,13	0.36	0	12,12,12	0.88	0
89	SPD	L5	5260	-	9,9,9	0.31	0	8,8,8	0.95	0
88	SPM	L5	5266	-	13,13,13	0.37	0	12,12,12	1.12	0
89	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.82	0
89	SPD	L5	5281	-	9,9,9	0.33	0	8,8,8	0.84	0
89	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.85	0
88	SPM	L5	5289	-	13,13,13	0.36	0	12,12,12	0.86	0
88	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.00	0
89	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.93	0
89	SPD	L5	5288	-	9,9,9	0.33	0	8,8,8	0.80	0
89	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.85	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
89	SPD	L5	5282	-	-	1/7/7/7	-
89	SPD	L5	5285	-	-	1/7/7/7	-
88	SPM	L5	5290	-	-	3/11/11/11	-
88	SPM	L5	5286	87	-	4/11/11/11	-
89	SPD	L5	5283	-	-	4/7/7/7	-
88	SPM	L5	5262	-	-	2/11/11/11	-
89	SPD	L5	5260	-	-	0/7/7/7	-
88	SPM	L5	5266	-	-	5/11/11/11	-
89	SPD	L5	5284	-	-	0/7/7/7	-
89	SPD	L5	5281	-	-	1/7/7/7	-
89	SPD	LN	301	-	-	1/7/7/7	-
88	SPM	L5	5289	-	-	3/11/11/11	-
88	SPM	L5	5258	-	-	2/11/11/11	-
88	SPM	L5	5263	-	-	4/11/11/11	-
89	SPD	L8	202	-	-	3/7/7/7	-
89	SPD	L5	5288	-	-	3/7/7/7	-
89	SPD	L5	5287	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

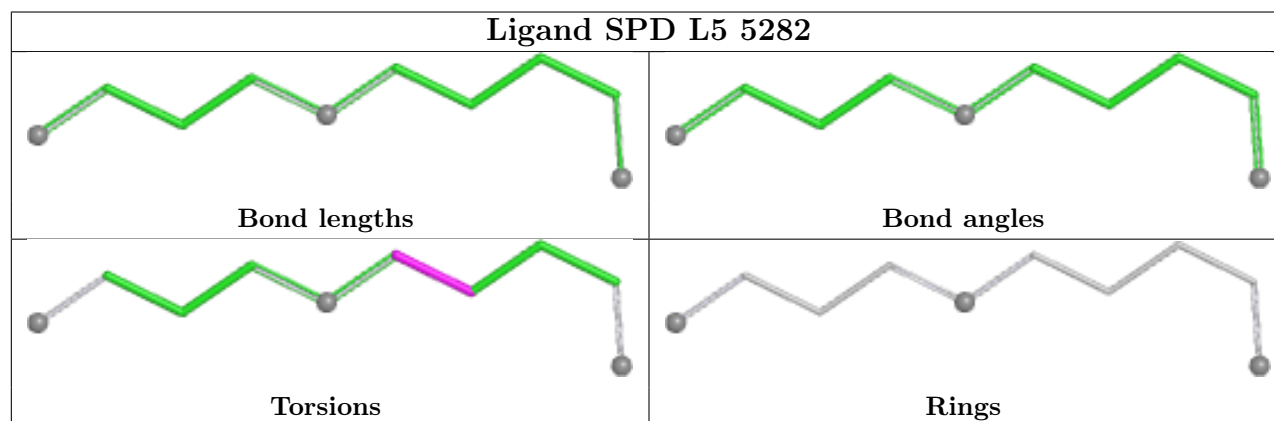
Mol	Chain	Res	Type	Atoms
89	L5	5283	SPD	C3-C4-C5-N6
88	L5	5289	SPM	C7-C8-C9-N10
89	L8	202	SPD	C3-C4-C5-N6
89	L5	5283	SPD	N6-C7-C8-C9
89	L5	5282	SPD	C3-C4-C5-N6
88	L5	5266	SPM	N10-C11-C12-C13
88	L5	5258	SPM	C3-C4-N5-C6
88	L5	5286	SPM	C12-C11-N10-C9
88	L5	5289	SPM	N10-C11-C12-C13
88	L5	5290	SPM	C8-C9-N10-C11
89	L5	5283	SPD	C4-C5-N6-C7
89	L5	5283	SPD	C2-C3-C4-C5
88	L5	5266	SPM	C7-C8-C9-N10
88	L5	5286	SPM	C7-C6-N5-C4
88	L5	5286	SPM	C8-C9-N10-C11
88	L5	5266	SPM	C2-C3-C4-N5
88	L5	5262	SPM	C6-C7-C8-C9
88	L5	5258	SPM	C6-C7-C8-C9
88	L5	5266	SPM	C6-C7-C8-C9
88	L5	5290	SPM	C6-C7-C8-C9
88	L5	5263	SPM	N5-C6-C7-C8
88	L5	5263	SPM	C7-C6-N5-C4
88	L5	5290	SPM	C7-C6-N5-C4
89	L5	5288	SPD	C4-C5-N6-C7
89	L5	5287	SPD	C2-C3-C4-C5
89	L5	5281	SPD	C2-C3-C4-C5
89	LN	301	SPD	C4-C5-N6-C7
88	L5	5263	SPM	N10-C11-C12-C13
88	L5	5286	SPM	N1-C2-C3-C4
89	L5	5288	SPD	C8-C7-N6-C5
88	L5	5266	SPM	N5-C6-C7-C8
89	L5	5288	SPD	N1-C2-C3-C4
88	L5	5263	SPM	C2-C3-C4-N5
89	L8	202	SPD	N6-C7-C8-C9
88	L5	5262	SPM	C3-C4-N5-C6
89	L8	202	SPD	C8-C7-N6-C5
88	L5	5289	SPM	N5-C6-C7-C8
89	L5	5285	SPD	C8-C7-N6-C5

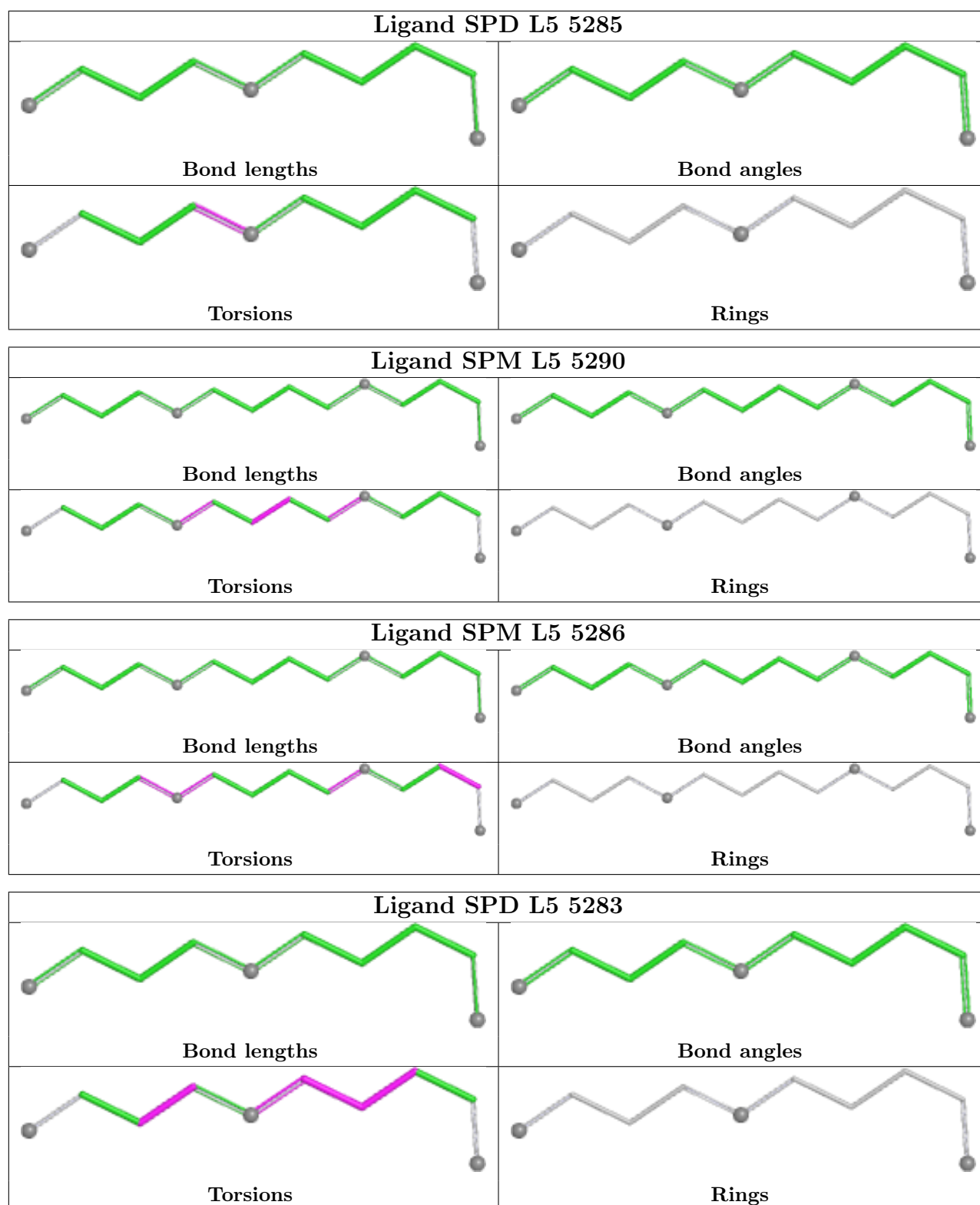
There are no ring outliers.

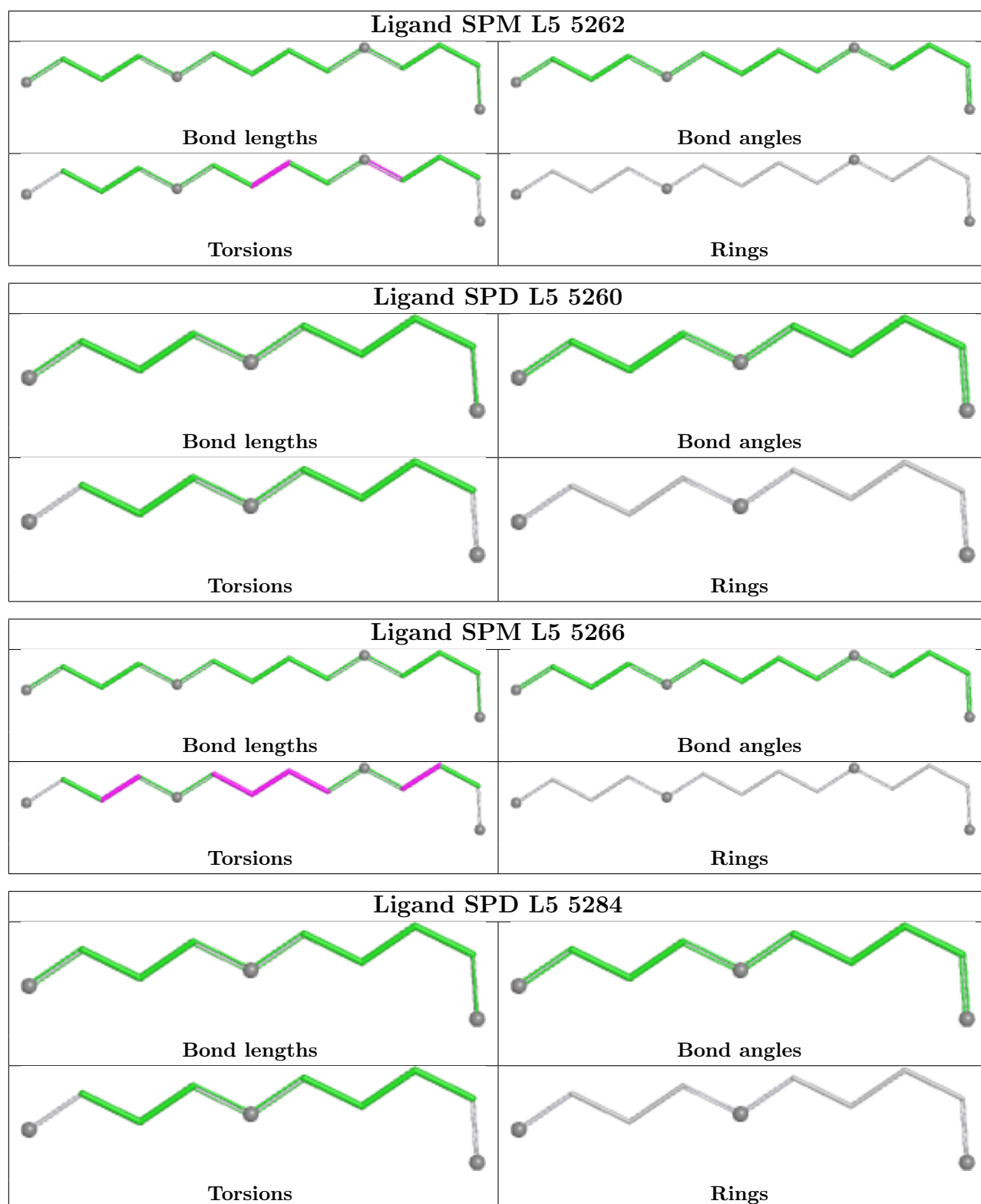
8 monomers are involved in 9 short contacts:

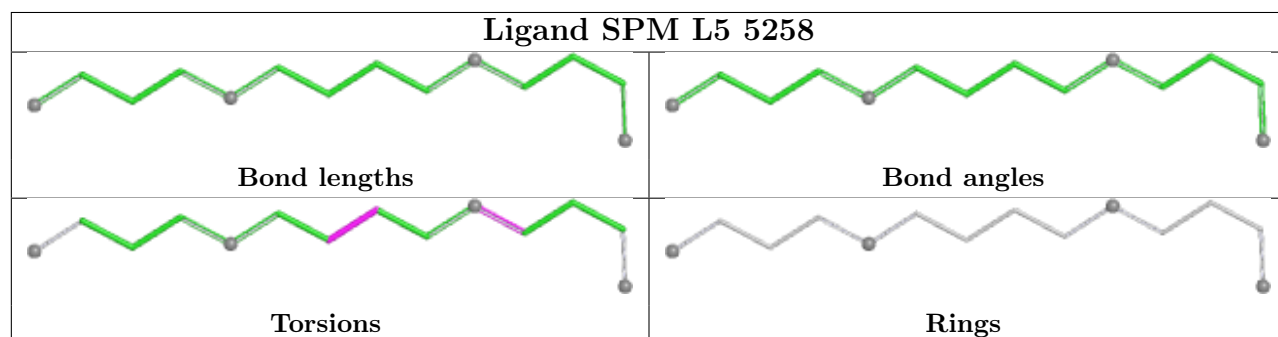
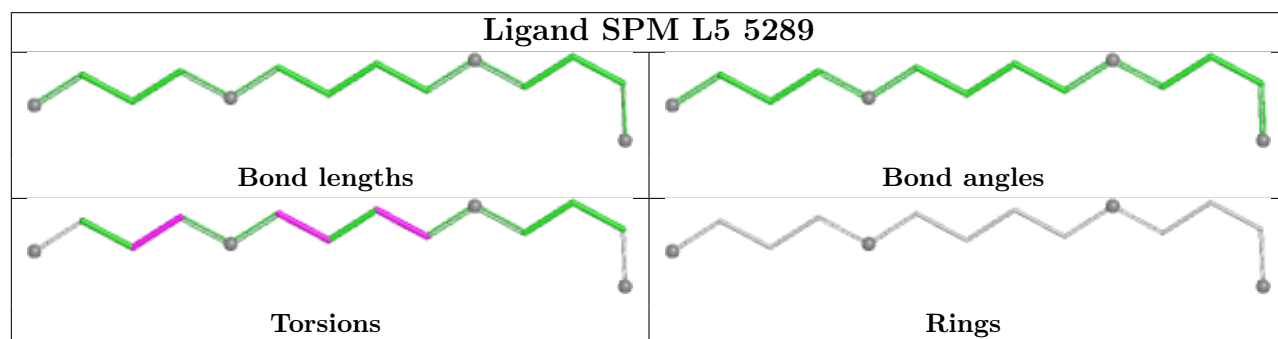
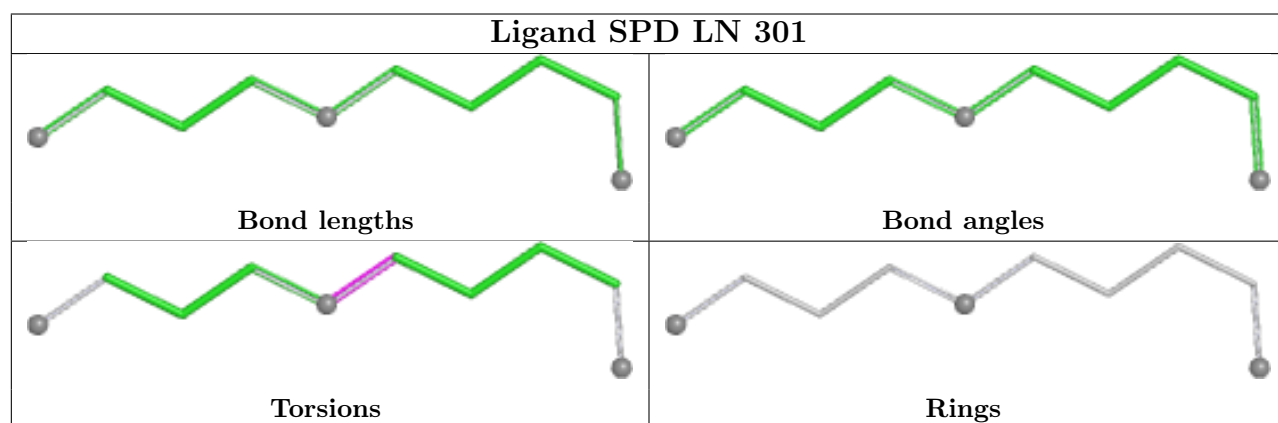
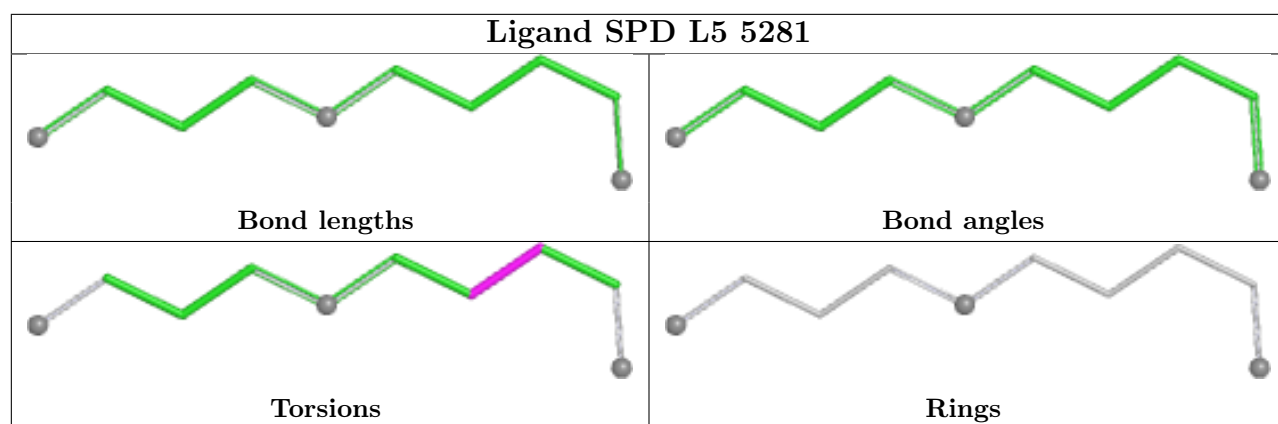
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5282	SPD	1	0
88	L5	5290	SPM	2	0
89	L5	5260	SPD	1	0
88	L5	5266	SPM	1	0
89	L5	5284	SPD	1	0
89	LN	301	SPD	1	0
88	L5	5289	SPM	1	0
89	L5	5288	SPD	1	0

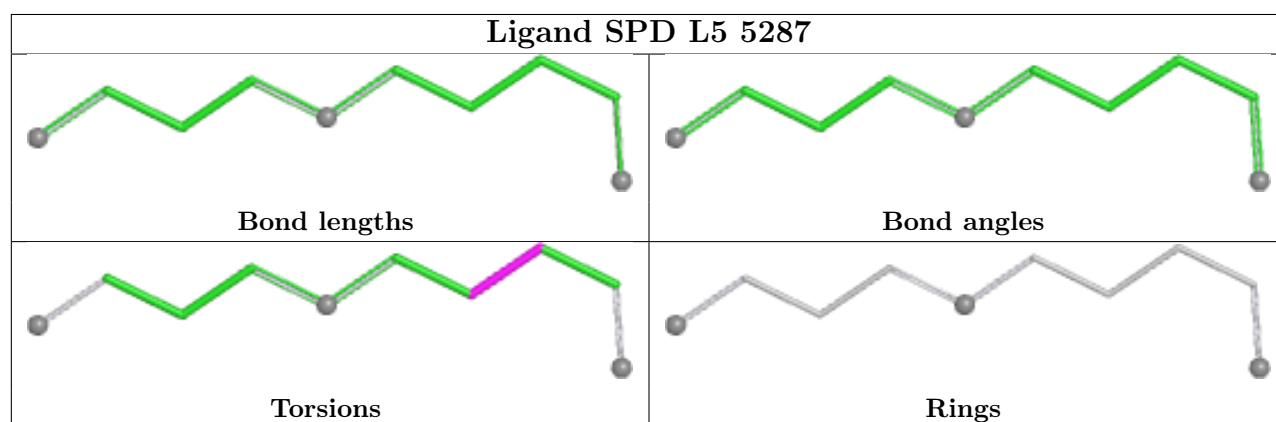
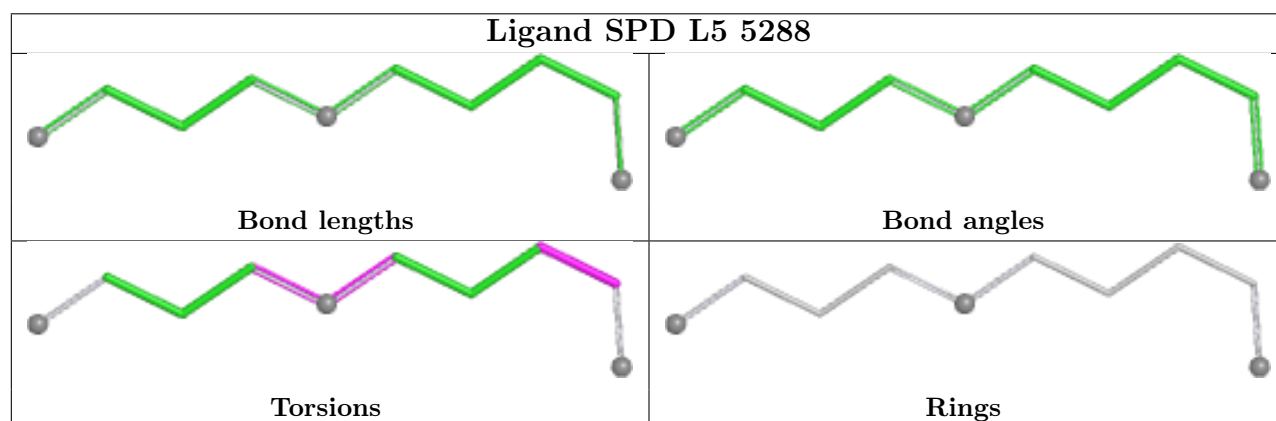
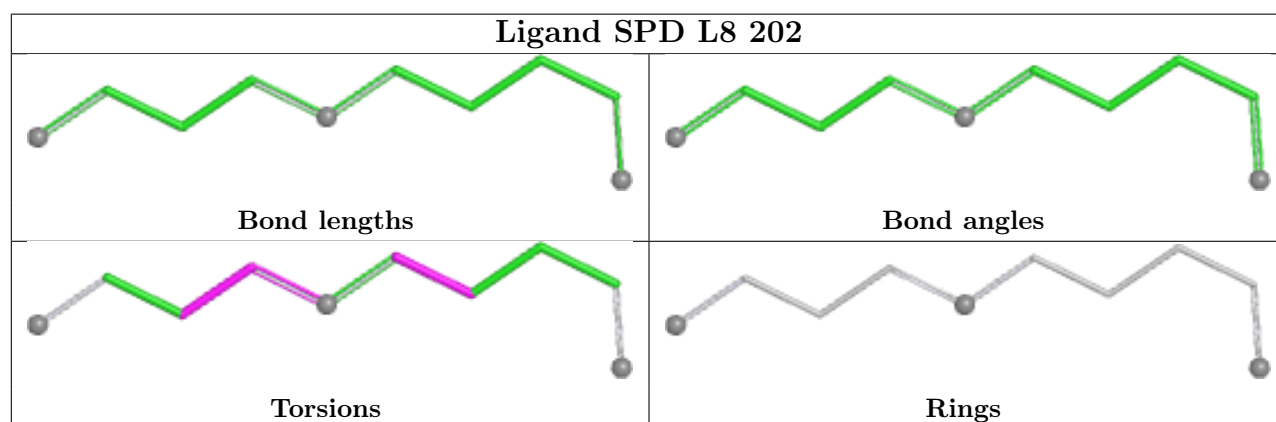
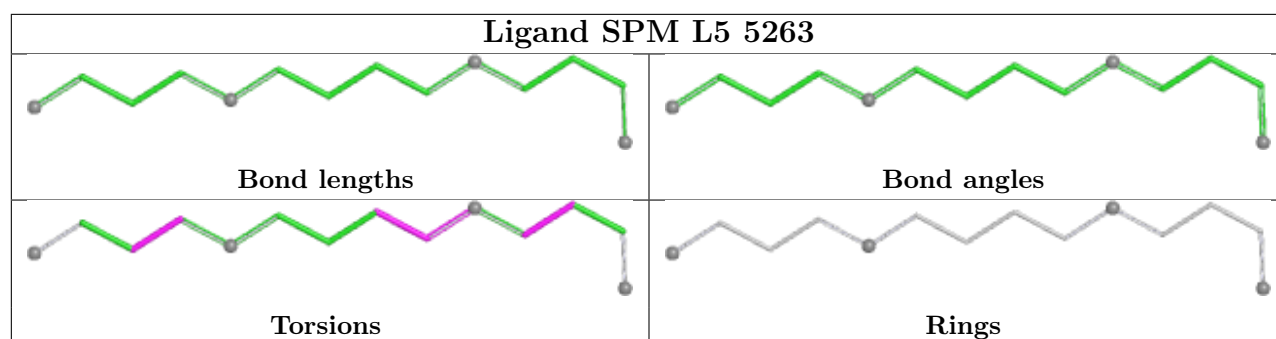
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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
6	L5	10
86	S2	5
2	Pt	1
3	Et	1
5	AT	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	29.36
1	L5	1706:A	O3'	1716:G	P	21.25
1	L5	2910:G	O3'	3584:C	P	21.20
1	L5	760:G	O3'	903:C	P	16.82
1	L5	519:C	O3'	642:G	P	15.80
1	L5	2112:G	O3'	2249:C	P	15.23
1	L5	4776:G	O3'	4858:C	P	15.05
1	S2	698:G	O3'	730:C	P	14.63
1	L5	3954:A	O3'	4056:A	P	13.42
1	S2	739:C	O3'	746:C	P	12.44
1	L5	990:C	O3'	1064:G	P	12.35
1	L5	1222:A	O3'	1234:G	P	10.81
1	Pt	15:G	O3'	18:G	P	10.00
1	S2	225:G	O3'	287:U	P	7.53
1	L5	1100:U	O3'	1167:C	P	7.01
1	Et	16:C	O3'	18:U	P	6.26
1	AT	16:C	O3'	18:G	P	4.46
1	S2	1831:A	O3'	1832:6MZ	P	4.27

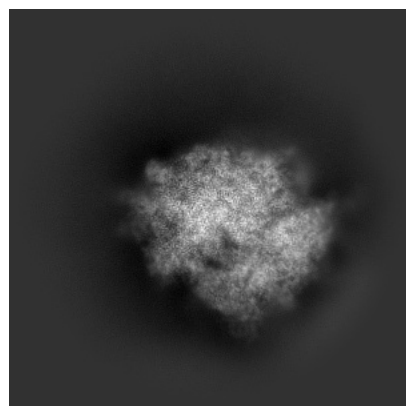
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71371. These allow visual inspection of the internal detail of the map and identification of artifacts.

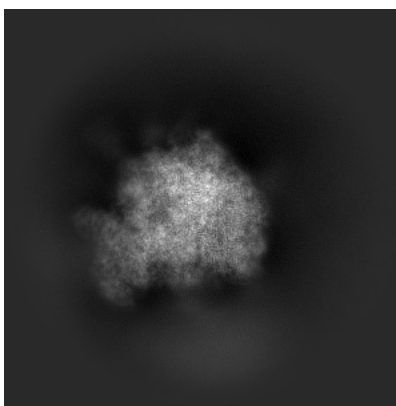
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

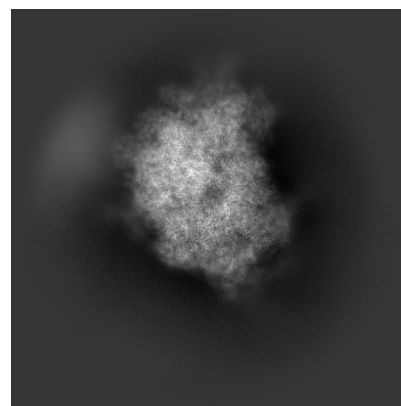
6.1.1 Primary map



X

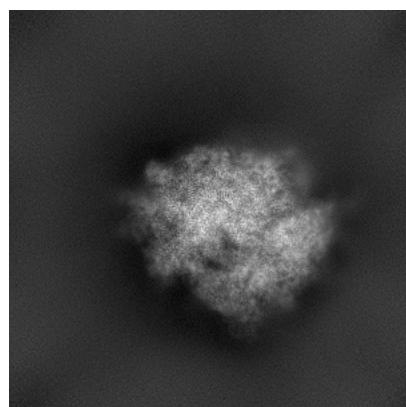


Y

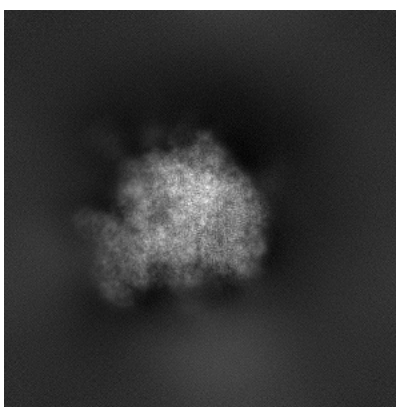


Z

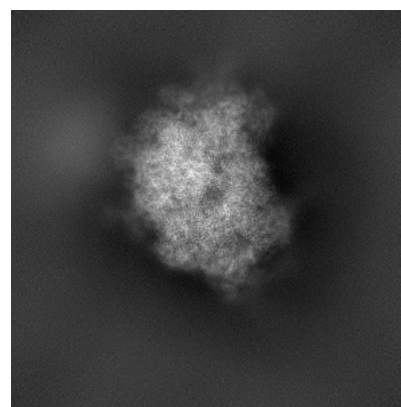
6.1.2 Raw map



X



Y

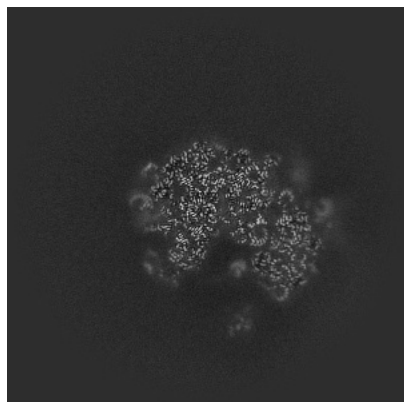


Z

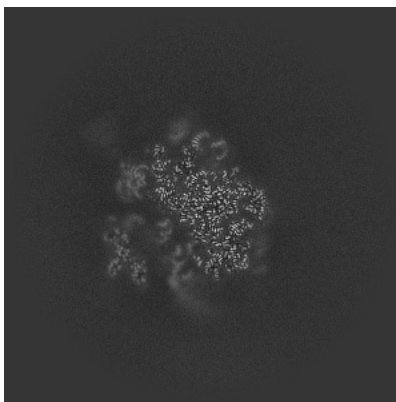
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

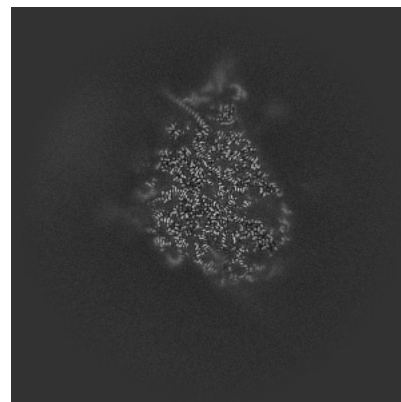
6.2.1 Primary map



X Index: 256

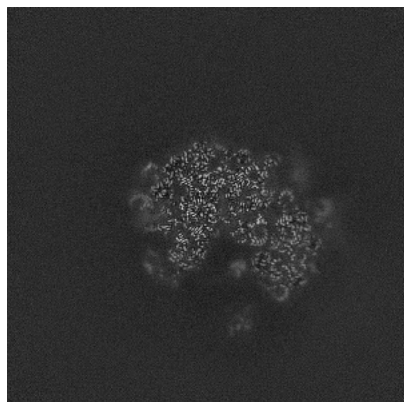


Y Index: 256

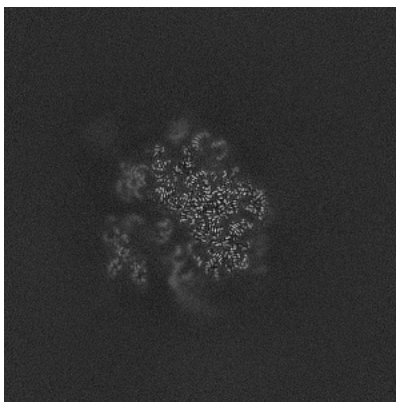


Z Index: 256

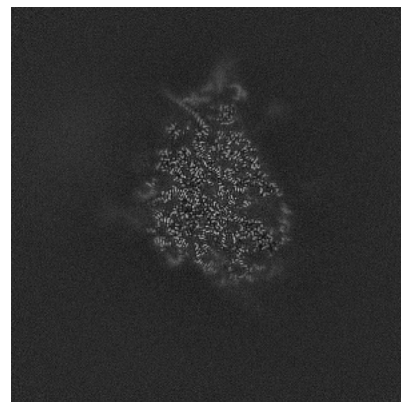
6.2.2 Raw map



X Index: 256



Y Index: 256

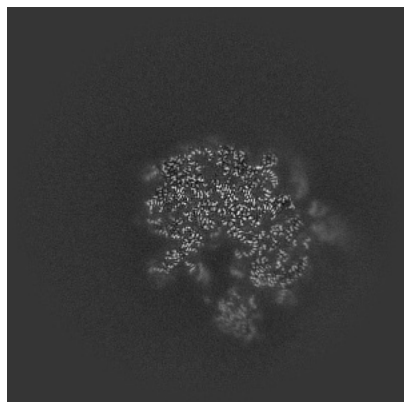


Z Index: 256

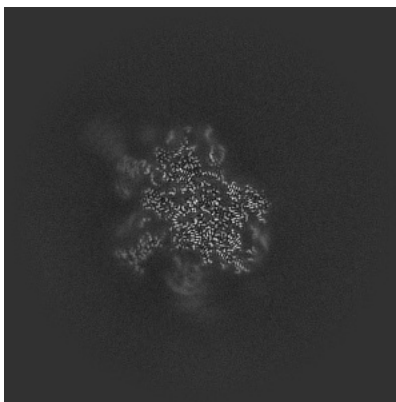
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

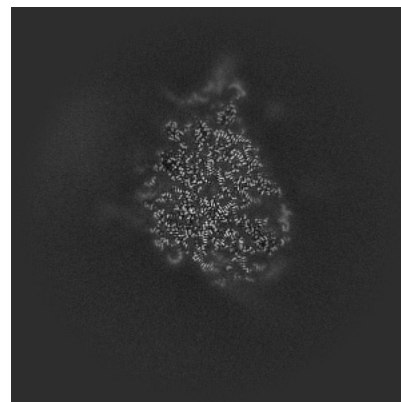
6.3.1 Primary map



X Index: 243

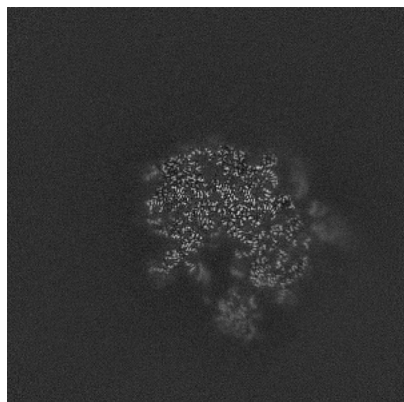


Y Index: 243

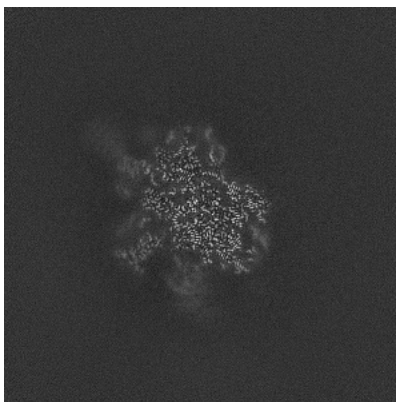


Z Index: 258

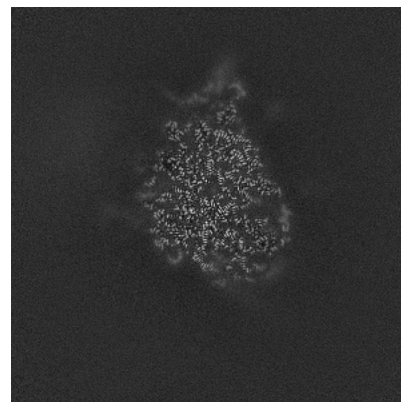
6.3.2 Raw map



X Index: 243



Y Index: 243

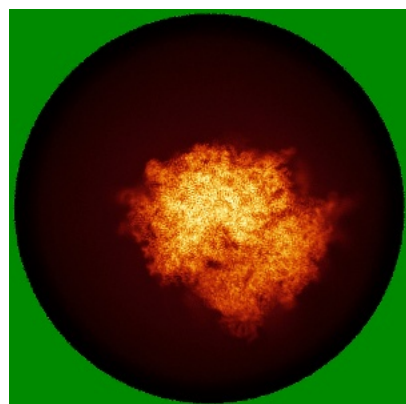


Z Index: 258

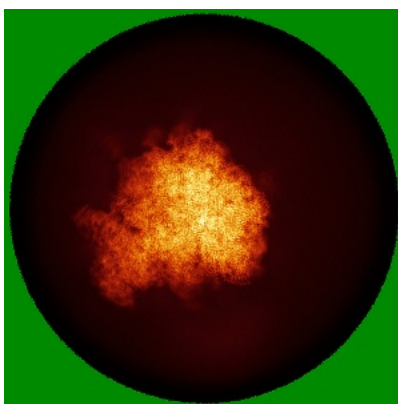
The images above show the largest variance slices of the map in three orthogonal directions.

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

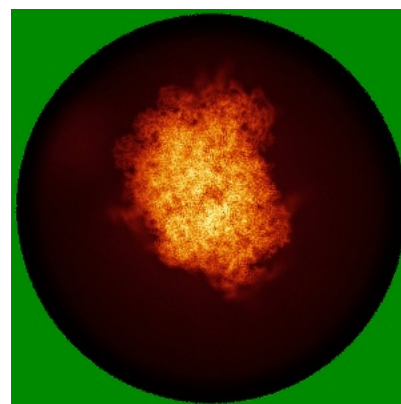
6.4.1 Primary map



X

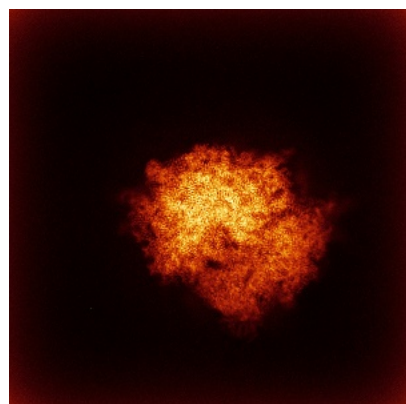


Y

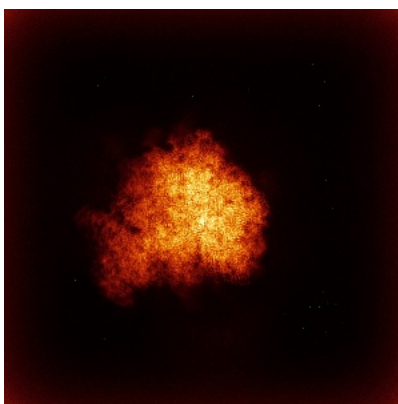


Z

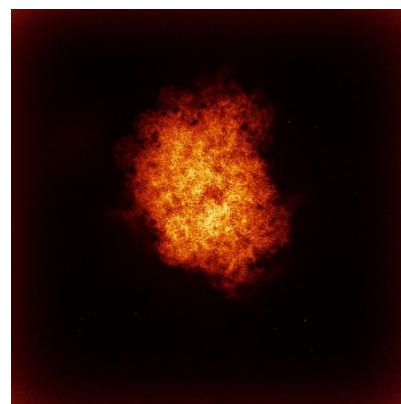
6.4.2 Raw map



X



Y

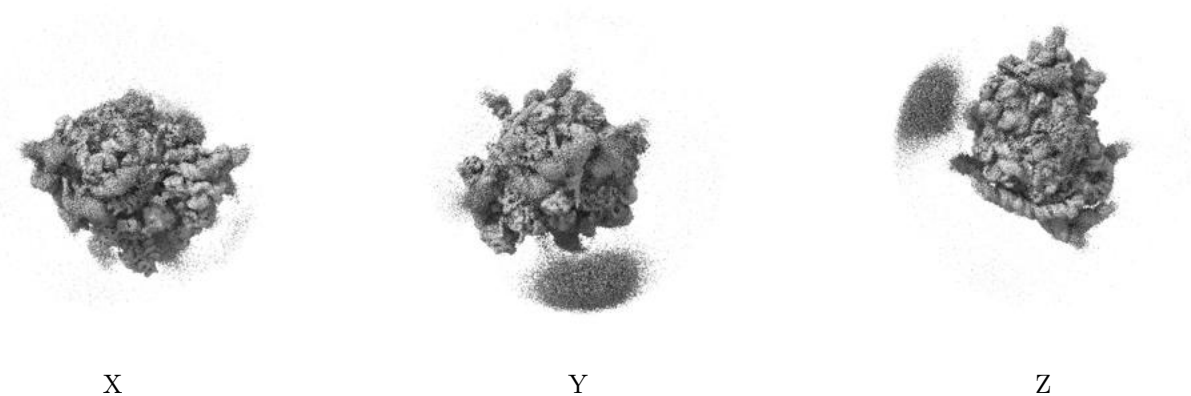


Z

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.

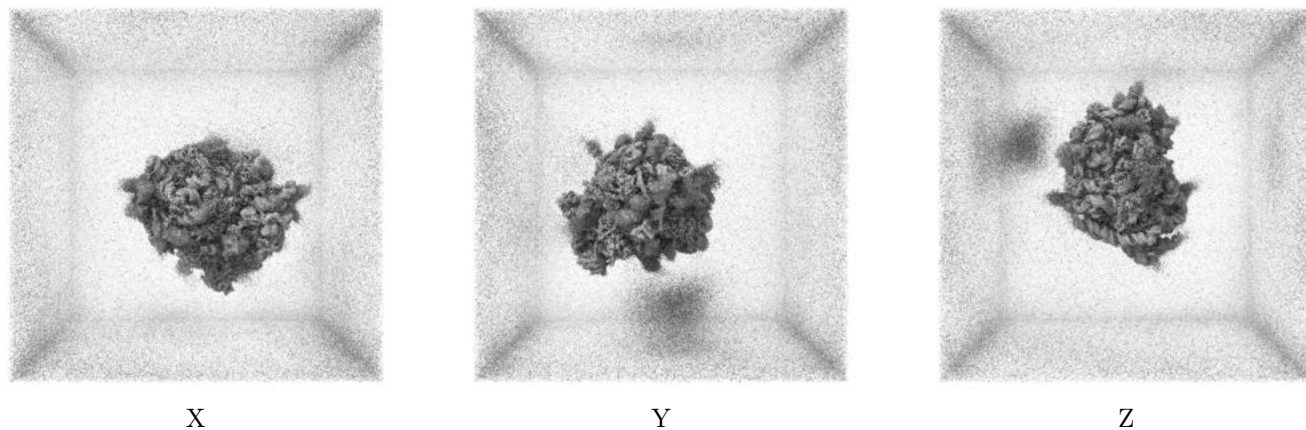
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0156. 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.

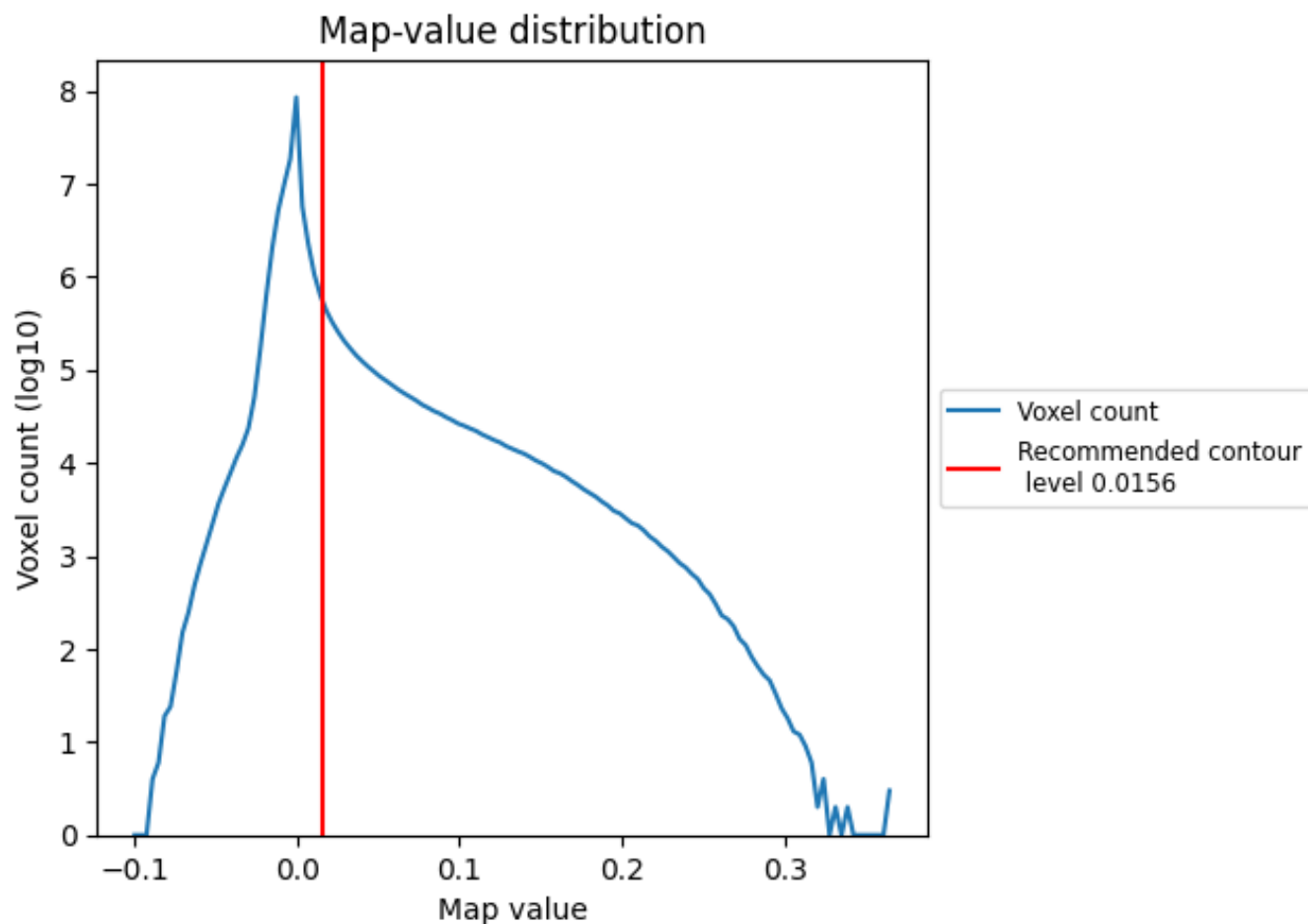
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

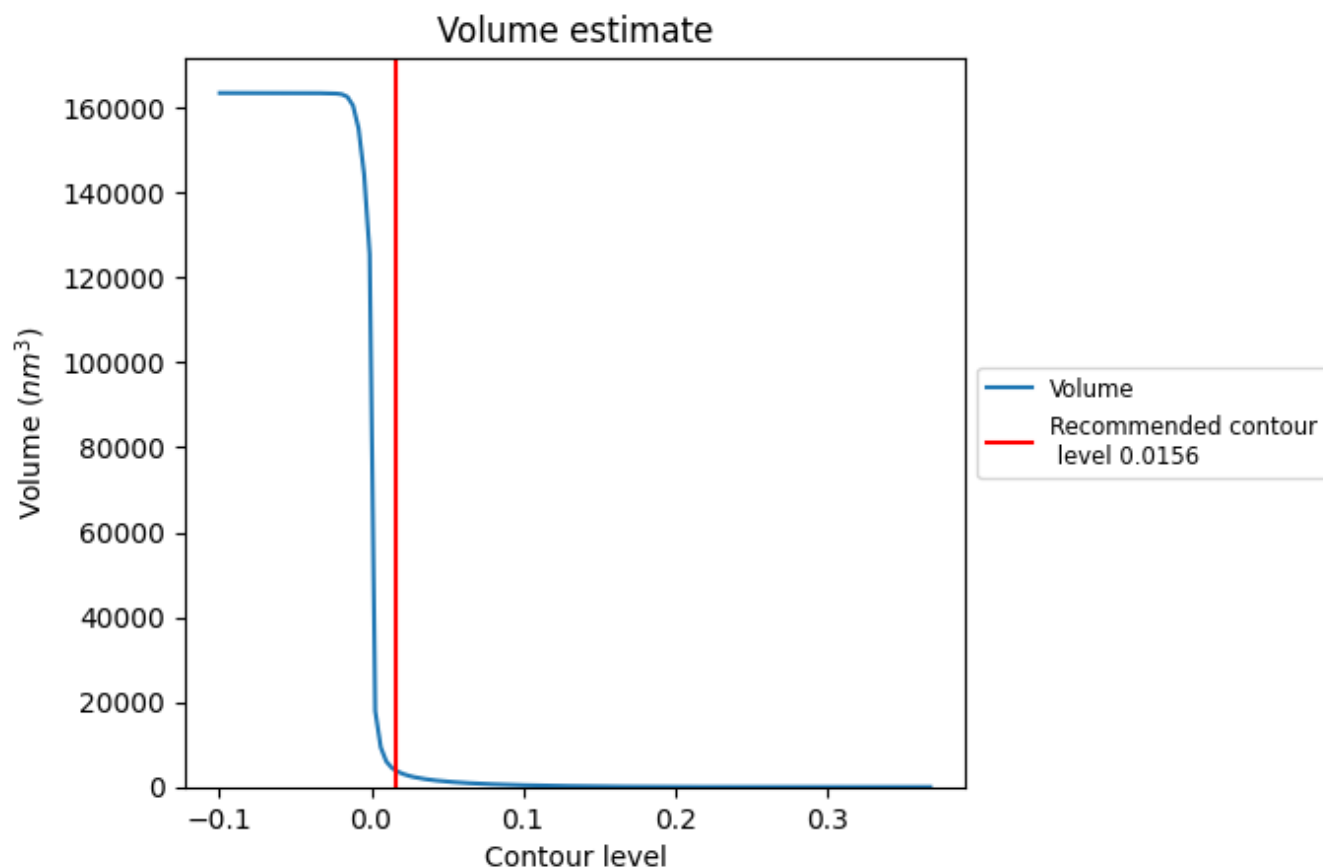
This section contains the results of statistical analysis of the map.

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.

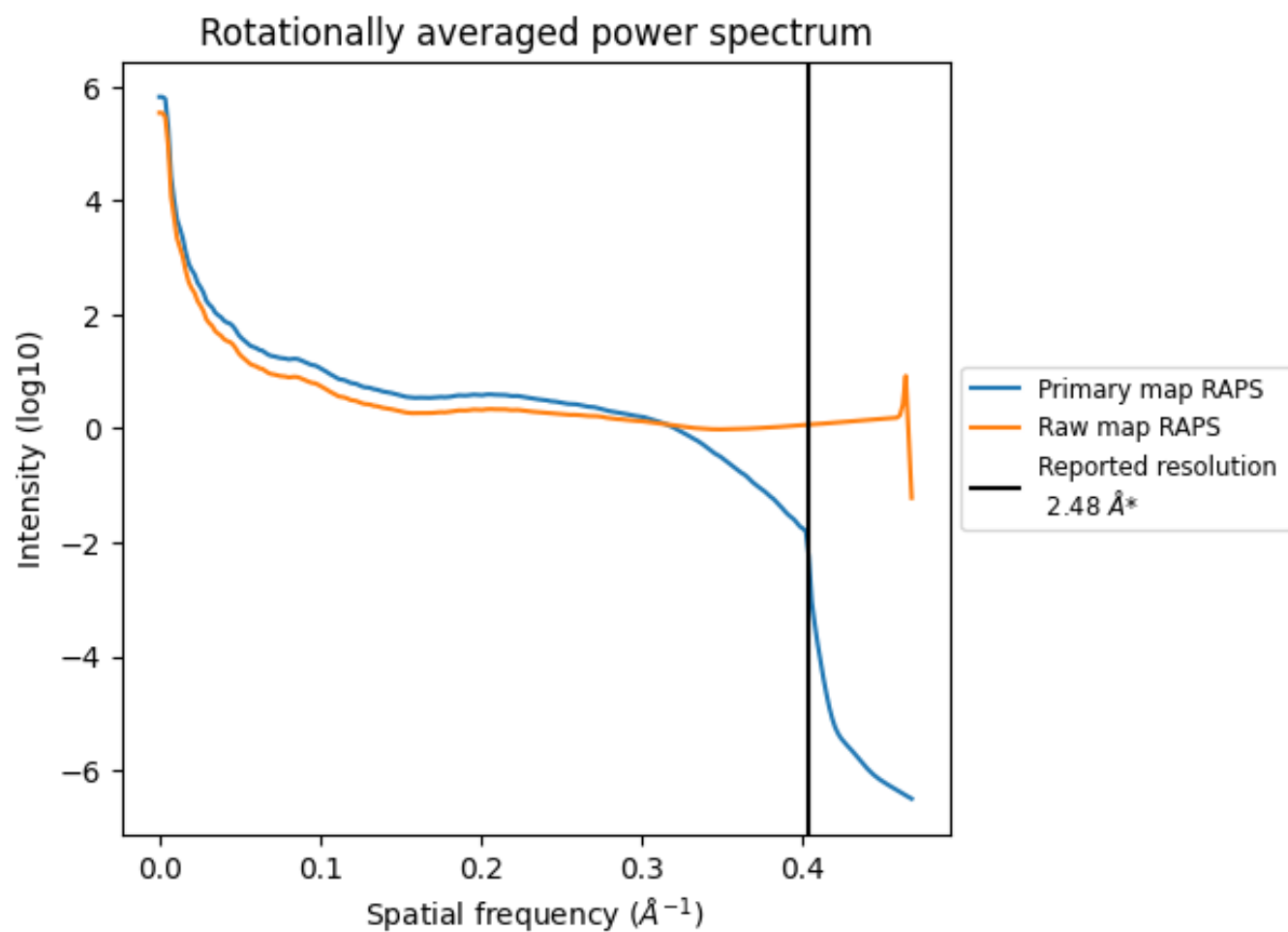
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4043 nm³; this corresponds to an approximate mass of 3652 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 ⓘ

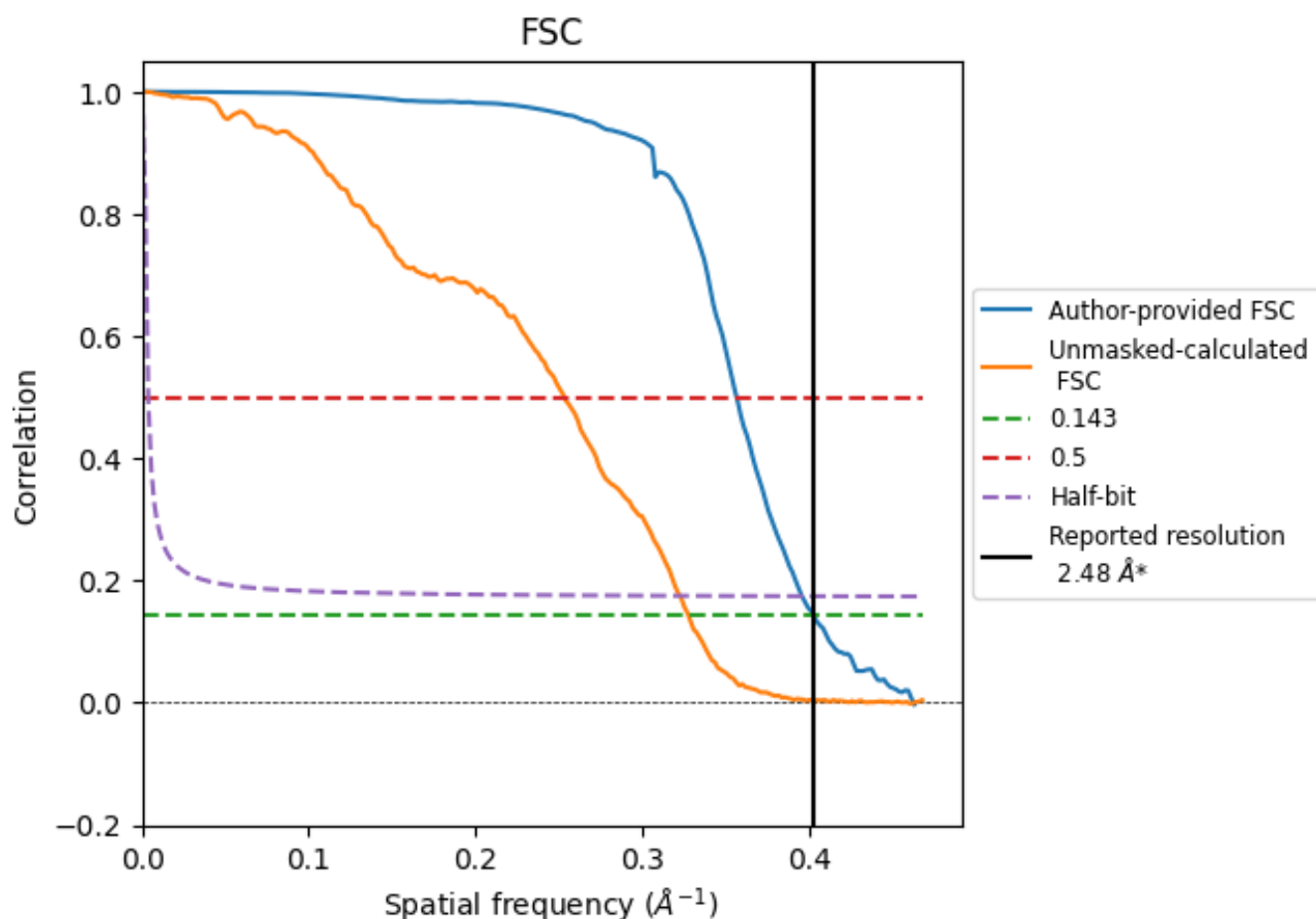


*Reported resolution corresponds to spatial frequency of 0.403 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.403 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

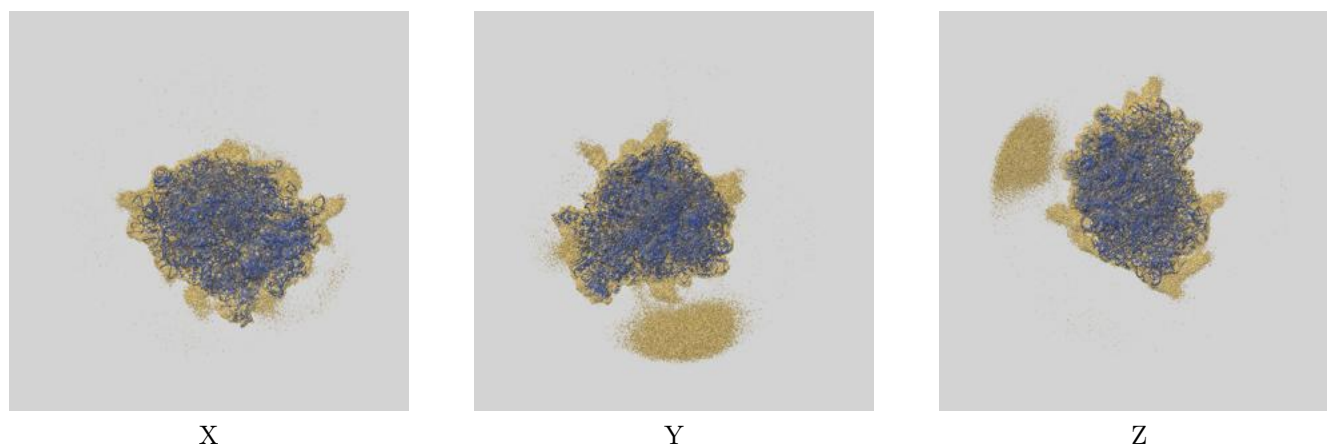
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.80	2.52
Unmasked-calculated*	3.05	3.95	3.10

*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 3.05 differs from the reported value 2.48 by more than 10 %

9 Map-model fit [i](#)

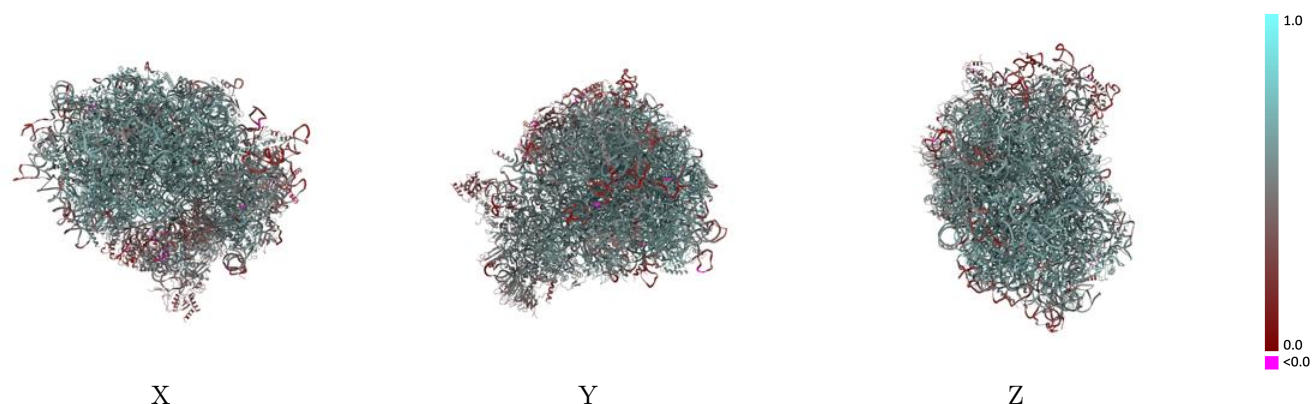
This section contains information regarding the fit between EMDB map EMD-71371 and PDB model 9P8B. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



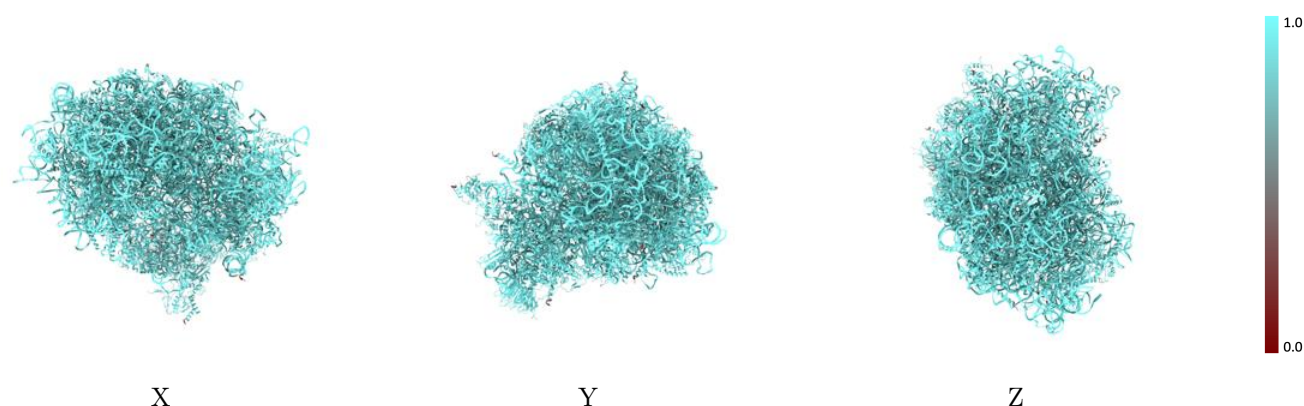
The images above show the 3D surface view of the map at the recommended contour level 0.0156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



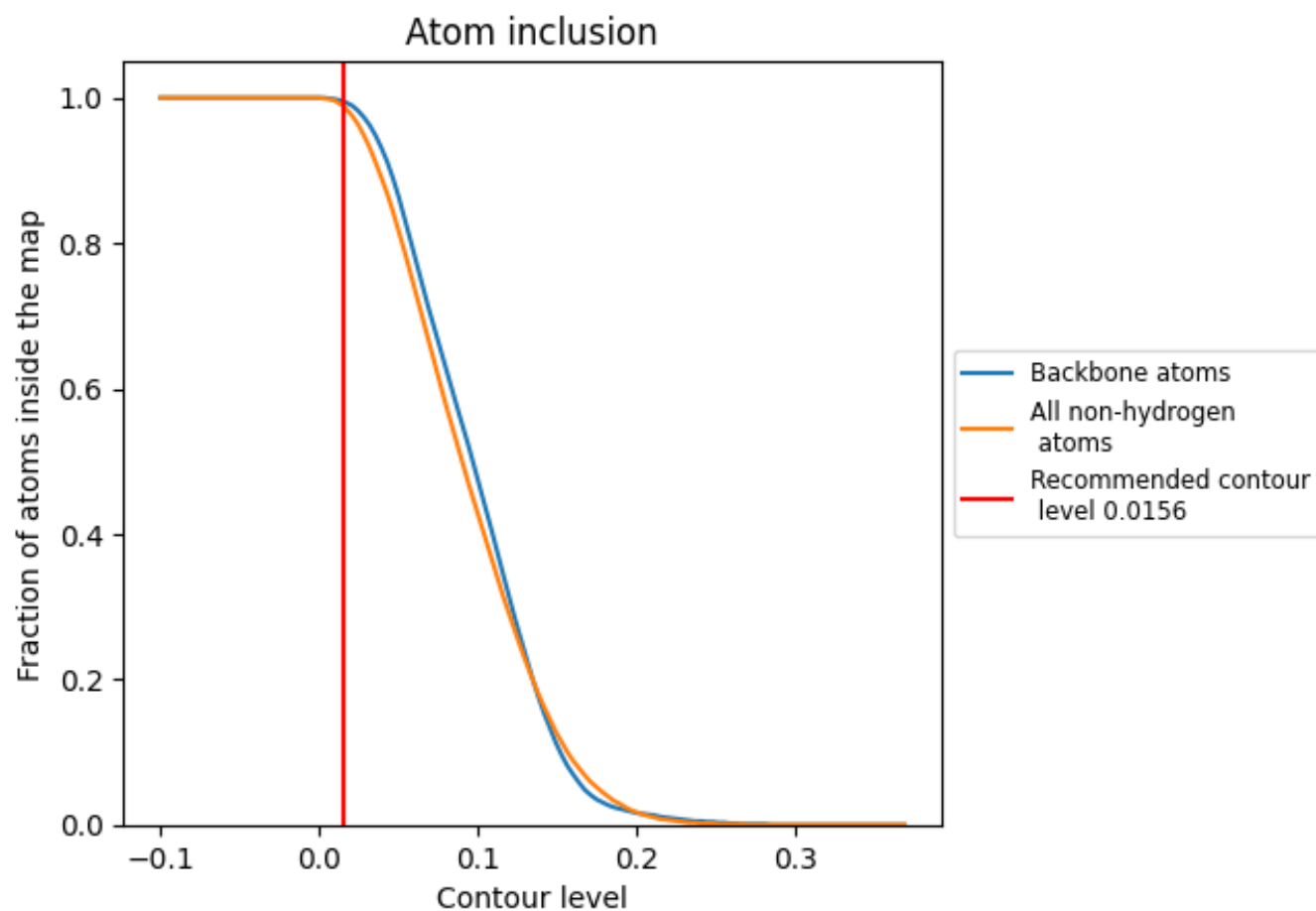
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0156).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.5520
AT	 0.9960	 0.3490
CF	 0.9760	 0.3890
CI	 0.9160	 0.4680
Et	 0.9860	 0.3010
L5	 0.9960	 0.5730
L7	 0.9990	 0.6180
L8	 0.9970	 0.5940
LA	 0.9970	 0.6310
LB	 0.9840	 0.6130
LC	 0.9850	 0.6090
LD	 0.9830	 0.5810
LE	 0.9820	 0.5530
LF	 0.9960	 0.6160
LG	 0.9630	 0.5580
LH	 0.9920	 0.6030
LI	 0.9870	 0.6080
LJ	 0.9770	 0.5650
LL	 0.9710	 0.5890
LM	 0.9920	 0.5940
LN	 0.9990	 0.6420
LO	 0.9910	 0.6160
LP	 0.9920	 0.6220
LQ	 0.9980	 0.6340
LR	 0.9690	 0.5700
LS	 0.9980	 0.6320
LT	 0.9870	 0.5980
LU	 0.9840	 0.5370
LV	 0.9950	 0.6220
LW	 0.9550	 0.4590
LX	 0.9890	 0.5980
LY	 0.9890	 0.6030
LZ	 0.9940	 0.5930
La	 0.9930	 0.6350
Lb	 0.9550	 0.5520



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Chain	Atom inclusion	Q-score
Lc	 0.9830	 0.5850
Ld	 0.9870	 0.5980
Le	 0.9960	 0.6300
Lf	 0.9960	 0.6360
Lg	 0.9870	 0.6090
Lh	 0.9910	 0.5970
Li	 0.9880	 0.5960
Lj	 0.9970	 0.6320
Lk	 0.9770	 0.5460
Ll	 0.9950	 0.6150
Lm	 0.9880	 0.6080
Ln	 1.0000	 0.6140
Lo	 0.9880	 0.6150
Lp	 0.9900	 0.6110
Lr	 0.9920	 0.6180
Ls	 0.8320	 0.2580
Lt	 0.8450	 0.2230
Pt	 0.9920	 0.5420
S2	 0.9980	 0.5360
SA	 0.9710	 0.5280
SB	 0.9850	 0.5660
SC	 0.9920	 0.5620
SD	 0.9830	 0.4910
SE	 0.9950	 0.5420
SF	 0.9740	 0.5060
SG	 0.9750	 0.4590
SH	 0.9650	 0.4700
SI	 0.9790	 0.5480
SJ	 0.9780	 0.5380
SK	 0.9750	 0.4570
SL	 0.9710	 0.5650
SM	 0.8790	 0.2580
SN	 0.9910	 0.5840
SO	 0.9810	 0.5750
SP	 0.9560	 0.4770
SQ	 0.9760	 0.5070
SR	 0.9580	 0.4800
SS	 0.9650	 0.5010
ST	 0.9750	 0.4970
SU	 0.9710	 0.4570
SV	 0.9890	 0.5430
SW	 0.9920	 0.5790

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Chain	Atom inclusion	Q-score
SX	 0.9920	 0.5840
SY	 0.9450	 0.4730
SZ	 0.9360	 0.4820
Sa	 0.9890	 0.5760
Sb	 0.9780	 0.5420
Sc	 0.9590	 0.4800
Sd	 0.9960	 0.5480
Se	 0.9480	 0.4750
Sf	 0.9290	 0.3350
Sg	 0.9690	 0.4420