



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 10:05 PM EDT

PDB ID : 8GLP / pdb_00008glp
EMDB ID : EMD-40205
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria
(Consensus LSU focused refined structure)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Watson, Z.L.;
Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-03-22
Resolution : 1.67 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

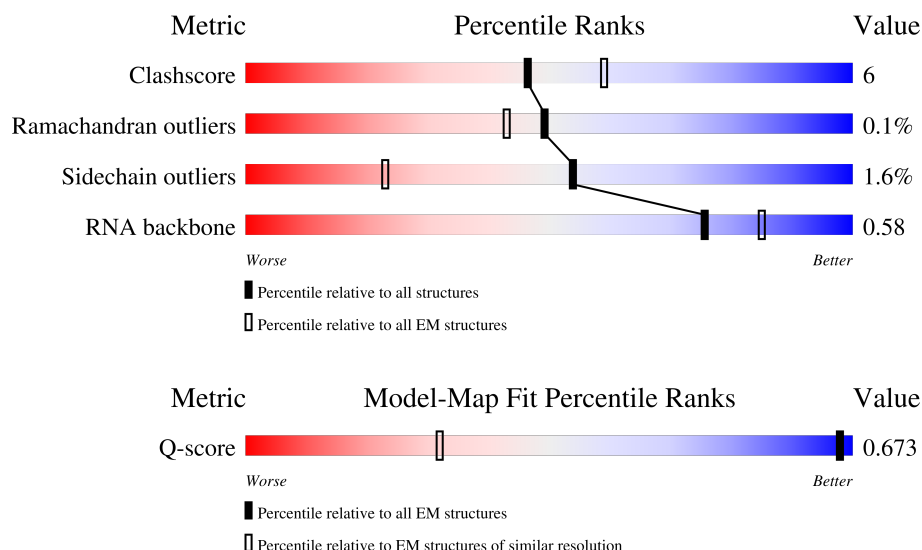
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.67 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.



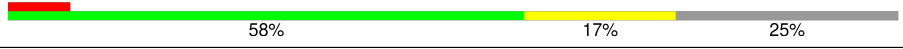
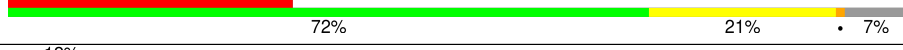
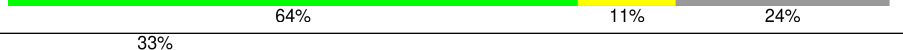
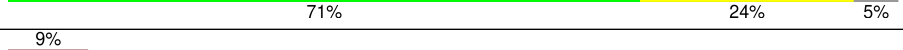
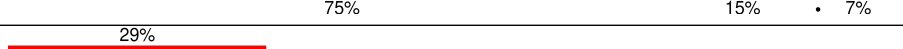
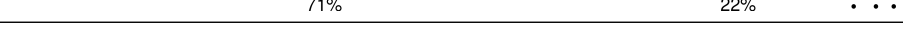
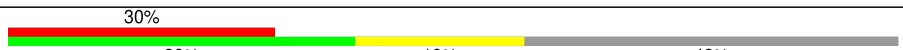
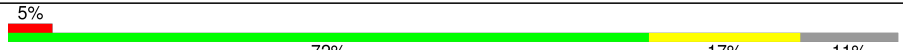
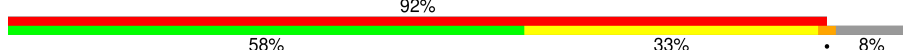
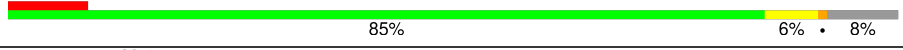
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	465 (1.19 - 2.17)

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	S2	1869	
2	L8	156	
3	L5	5069	

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	SB	264	
6	SA	295	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SG	249	
12	SF	204	
13	SH	194	
14	SW	130	
15	SI	208	
16	SQ	146	
17	SU	119	
18	SK	165	
19	SO	151	
20	SX	143	
21	SM	132	
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23	Sd	56	
24	SN	151	
25	SL	158	
26	SR	135	
27	SP	145	
28	ST	145	

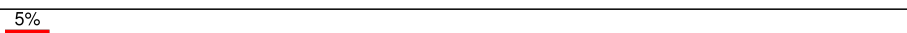
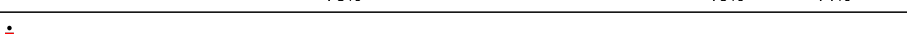
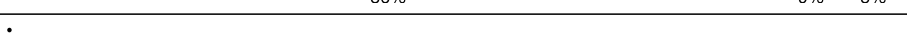
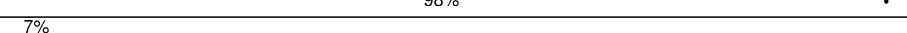
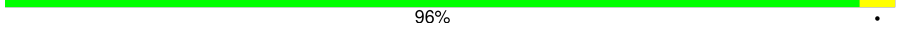
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	LA	257	
39	LB	403	
40	LC	427	
41	LJ	178	
42	LH	192	
43	LE	288	
44	LG	266	
45	LO	203	
46	LL	211	
47	LV	140	
48	LM	215	
49	La	148	
50	LN	204	
51	LI	214	
52	LD	297	
53	LQ	188	

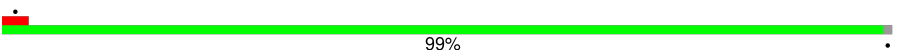
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Mol	Chain	Length	Quality of chain
54	LR	196	
55	LS	176	
56	LT	160	
57	LP	184	
58	LU	128	
59	LX	156	
60	LY	145	
61	LW	157	
62	LZ	136	
63	Lr	137	
64	Lh	123	
65	Lb	159	
66	LF	248	
67	Lc	115	
68	Ld	125	
69	Le	135	
70	Lf	110	
71	Lg	117	
72	Li	105	
73	Lj	97	
74	Lk	70	
75	Ll	51	
76	Lm	128	
77	Ln	25	
78	Lo	106	

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Mol	Chain	Length	Quality of chain
79	Lp	92	
80	mR	60	
81	Pt	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SAC	SA	2	-	X	-	-
82	SPD	L5	5112	-	-	X	-
82	SPD	L5	5114	-	-	X	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 220877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1672	Total	C	N	O	P	0	0
			35736	15981	6403	11681	1671		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3546	Total	C	N	O	P	1	0
			76116	33935	13923	24712	3546		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

- Molecule 6 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SA	222	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

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

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

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 11 is a protein called 40S ribosomal protein S6.

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

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SF	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

- Molecule 13 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S8.

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

- Molecule 16 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SQ	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 18 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 19 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SO	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 20 is a protein called 40S ribosomal protein S23 (uS12).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SX	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SM	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 22 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 23 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	146	Total	C	N	O	S	0	0
			1200	766	226	202	6		

- Molecule 26 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	131	Total	C	N	O	S	0	0
			1078	684	204	183	7		

- Molecule 28 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	ST	142	Total	C	N	O	S	1	0
			1121	707	212	199	3		

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SV	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 30 is a protein called 40S ribosomal protein S24.

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

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	84	Total	C	N	O	S	0	0
			674	433	126	114	1		

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	99	Total	C	N	O	S	1	0
			800	497	168	130	5		

- Molecule 33 is a protein called 40S ribosomal protein S27.

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

- Molecule 34 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sc	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 35 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	50	Total	C	N	O	S	0	0
			394	241	88	64	1		

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a protein called 60S ribosomal protein L8 (uL2).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LA	251	Total	C	N	O	S	1	0
			1930	1209	396	319	6		

- Molecule 39 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 40 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 41 is a protein called 60S ribosomal protein L11.

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

- Molecule 42 is a protein called 60S ribosomal protein L9.

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

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LE	223	Total	C	N	O	S	0	0
			1786	1150	339	293	4		

- Molecule 44 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LG	241	Total	C	N	O	S	0	0
			1926	1228	371	323	4		

- Molecule 45 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LO	202	Total	C	N	O	S	0	0
			1654	1066	322	261	5		

- Molecule 46 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LL	206	Total	C	N	O	S	1	0
			1672	1046	348	274	4		

- Molecule 47 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LV	133	Total	C	N	O	S	0	0
			988	623	186	174	5		

- Molecule 48 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 49 is a protein called 60S ribosomal protein L27a.

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

- Molecule 50 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 51 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LI	203	Total	C	N	O	S	0	0
			1645	1045	317	270	13		

- Molecule 52 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 53 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 54 is a protein called 60S ribosomal protein L19.

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

- Molecule 55 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 56 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LT	159	Total	C	N	O	S	2	0
			1311	833	256	216	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LP	153	Total	C	N	O	S	1	0
			1249	781	243	216	9		

- Molecule 58 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 59 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LX	118	Total	C	N	O	S	0	0
			966	618	181	166	1		

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

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

- Molecule 61 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LW	118	Total	C	N	O	S	0	0
			950	595	192	159	4		

- Molecule 62 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lr	125	Total	C	N	O	S	1	0
			1011	629	208	169	5		

- Molecule 64 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Lb	111	Total	C	N	O	S	0	0
			898	560	195	139	4		

- Molecule 66 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LF	225	Total	C	N	O	S	2	0
			1885	1212	364	300	9		

- Molecule 67 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Le	128	Total	C	N	O	S	1	0
			1061	672	219	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lf	110	Total	C	N	O	S	0	0
			883	560	175	144	4		

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

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

- Molecule 72 is a protein called 60S ribosomal protein L36.

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

- Molecule 73 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lk	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 76 is a protein called 60S ribosomal protein L40 (eL40).

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lm	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

- Molecule 77 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 78 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 79 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lp	91	Total	C	N	O	S	1	0
			715	450	139	119	7		

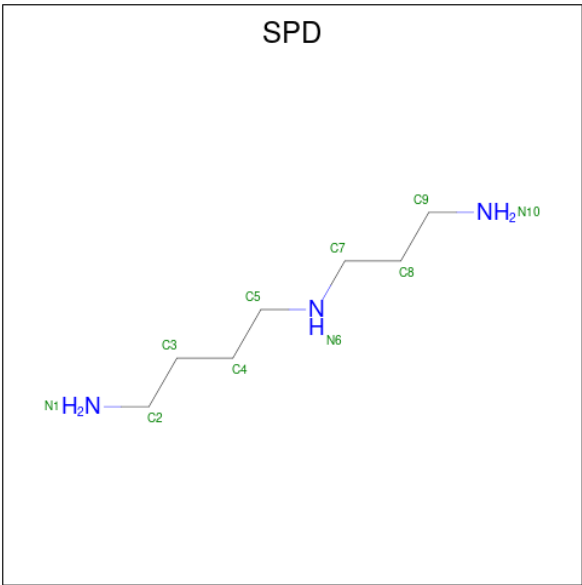
- Molecule 80 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	mR	8	Total	C	N	O	P	0	0
			172	77	32	55	8		

- Molecule 81 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 82 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



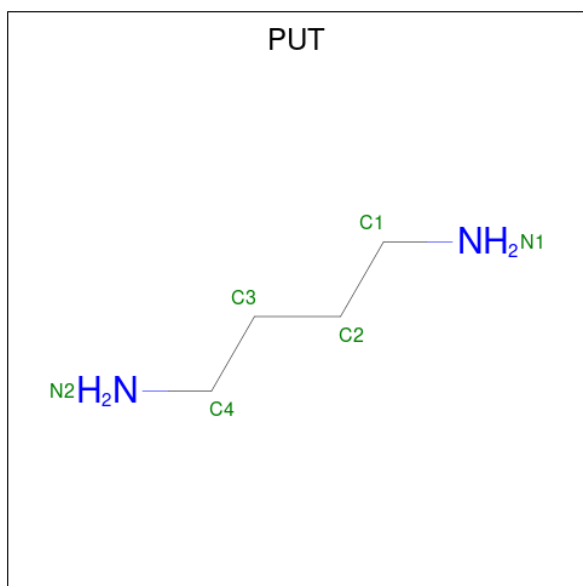
Mol	Chain	Residues	Atoms			AltConf
82	S2	1	Total	C	N	0
			10	7	3	
82	S2	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 83 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
83	S2	1	Total	C	N	0
			6	4	2	
83	L5	1	Total	C	N	0
			6	4	2	
83	L5	1	Total	C	N	0
			6	4	2	
83	L5	1	Total	C	N	0
			6	4	2	
83	L5	1	Total	C	N	0
			6	4	2	
83	L5	1	Total	C	N	0
			6	4	2	
83	L5	1	Total	C	N	0
			6	4	2	
83	L5	1	Total	C	N	0
			6	4	2	

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
84	S2	12	Total 12	K 12	0
84	L8	4	Total 4	K 4	0
84	L5	117	Total 117	K 117	0
84	L7	4	Total 4	K 4	0
84	SO	1	Total 1	K 1	0
84	SL	1	Total 1	K 1	0
84	Sa	1	Total 1	K 1	0
84	LA	3	Total 3	K 3	0
84	LH	1	Total 1	K 1	0
84	LL	1	Total 1	K 1	0
84	LN	1	Total 1	K 1	0
84	LI	1	Total 1	K 1	0
84	LQ	1	Total 1	K 1	0
84	Lb	1	Total 1	K 1	0
84	Le	1	Total 1	K 1	0
84	Lf	1	Total 1	K 1	0
84	Ll	1	Total 1	K 1	0

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	S2	137	Total 137	Mg 137	0
85	L8	16	Total 16	Mg 16	0
85	L5	463	Total 463	Mg 463	0

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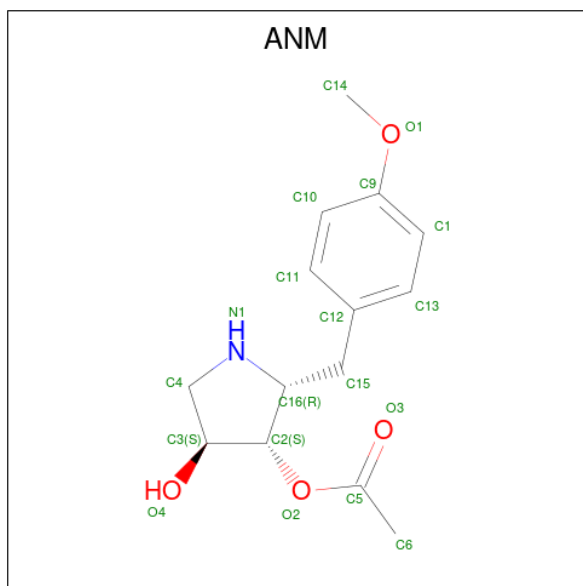
Mol	Chain	Residues	Atoms		AltConf
85	L7	15	Total 15	Mg 15	0
85	SG	1	Total 1	Mg 1	0
85	SX	1	Total 1	Mg 1	0
85	SS	2	Total 2	Mg 2	0
85	Sd	1	Total 1	Mg 1	0
85	SN	1	Total 1	Mg 1	0
85	ST	1	Total 1	Mg 1	0
85	LB	1	Total 1	Mg 1	0
85	LC	1	Total 1	Mg 1	0
85	LH	1	Total 1	Mg 1	0
85	LG	1	Total 1	Mg 1	0
85	LO	2	Total 2	Mg 2	0
85	LL	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	La	1	Total 1	Mg 1	0
85	LN	3	Total 3	Mg 3	0
85	LD	1	Total 1	Mg 1	0
85	LQ	2	Total 2	Mg 2	0
85	LR	1	Total 1	Mg 1	0
85	LS	1	Total 1	Mg 1	0
85	LP	2	Total 2	Mg 2	0

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Mol	Chain	Residues	Atoms		AltConf
85	Lr	3	Total	Mg	0
			3	3	
85	LF	1	Total	Mg	0
			1	1	
85	Lc	1	Total	Mg	0
			1	1	
85	Lf	1	Total	Mg	0
			1	1	
85	Lg	1	Total	Mg	0
			1	1	
85	Lj	2	Total	Mg	0
			2	2	
85	Lo	1	Total	Mg	0
			1	1	
85	Lp	2	Total	Mg	0
			2	2	
85	Pt	2	Total	Mg	0
			2	2	

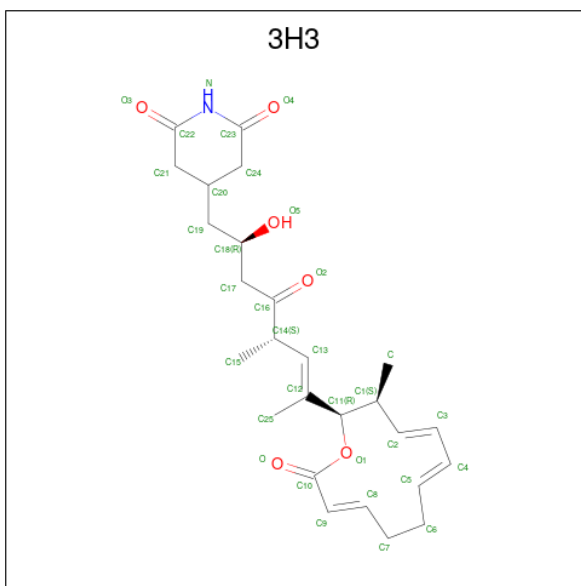
- Molecule 86 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				AltConf
86	L5	1	Total	C	N	O	0
			19	14	1	4	

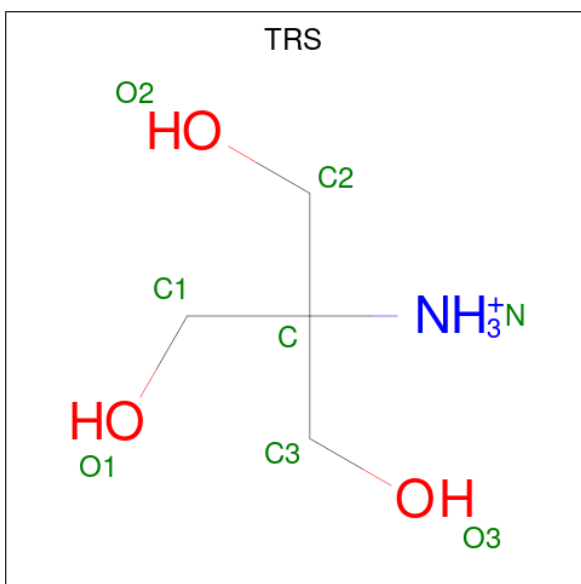
- Molecule 87 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxo-oxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (CCD ID: 3H3)

(formula: $C_{26}H_{35}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
87	L5	1	Total	C	N	O	0
			33	26	1	6	

- Molecule 88 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
88	L5	1	Total	C	N	O	0
			8	4	1	3	

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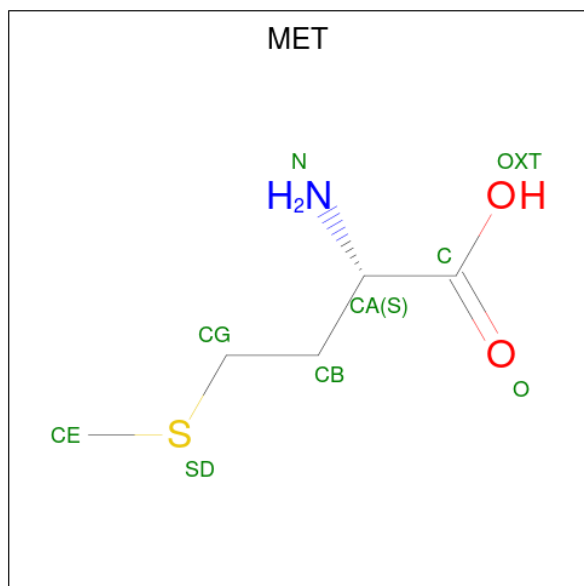
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Mol	Chain	Residues	Atoms				AltConf
88	L5	1	Total	C	N	O	0
			8	4	1	3	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	Sd	1	Total	Zn	0
			1	1	
89	Sa	1	Total	Zn	0
			1	1	
89	Sf	1	Total	Zn	0
			1	1	
89	Lg	1	Total	Zn	0
			1	1	
89	Lj	1	Total	Zn	0
			1	1	
89	Lm	1	Total	Zn	0
			1	1	
89	Lo	1	Total	Zn	0
			1	1	
89	Lp	1	Total	Zn	0
			1	1	

- Molecule 90 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
90	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
91	S2	266	Total	O	0
			266	266	
91	L8	189	Total	O	0
			189	189	
91	L5	5661	Total	O	0
			5661	5661	
91	L7	133	Total	O	0
			133	133	
91	SA	1	Total	O	0
			1	1	
91	SE	1	Total	O	0
			1	1	
91	SF	1	Total	O	0
			1	1	
91	SO	3	Total	O	0
			3	3	
91	SN	3	Total	O	0
			3	3	
91	SL	2	Total	O	0
			2	2	
91	Sa	4	Total	O	0
			4	4	
91	Sb	1	Total	O	0
			1	1	
91	LA	93	Total	O	0
			93	93	
91	LB	113	Total	O	0
			113	113	
91	LC	137	Total	O	0
			137	137	
91	LJ	4	Total	O	0
			4	4	
91	LH	14	Total	O	0
			14	14	
91	LE	28	Total	O	0
			28	28	
91	LG	28	Total	O	0
			28	28	

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Mol	Chain	Residues	Atoms		AltConf
91	LO	69	Total 69	O 69	0
91	LL	62	Total 62	O 62	0
91	LV	25	Total 25	O 25	0
91	LM	10	Total 10	O 10	0
91	La	71	Total 71	O 71	0
91	LN	112	Total 112	O 112	0
91	LI	33	Total 33	O 33	0
91	LD	37	Total 37	O 37	0
91	LQ	81	Total 81	O 81	0
91	LR	34	Total 34	O 34	0
91	LS	51	Total 51	O 51	0
91	LT	58	Total 58	O 58	0
91	LP	44	Total 44	O 44	0
91	LU	1	Total 1	O 1	0
91	LX	15	Total 15	O 15	0
91	LY	23	Total 23	O 23	0
91	LW	8	Total 8	O 8	0
91	LZ	7	Total 7	O 7	0
91	Lr	53	Total 53	O 53	0
91	Lh	10	Total 10	O 10	0
91	Lb	21	Total 21	O 21	0

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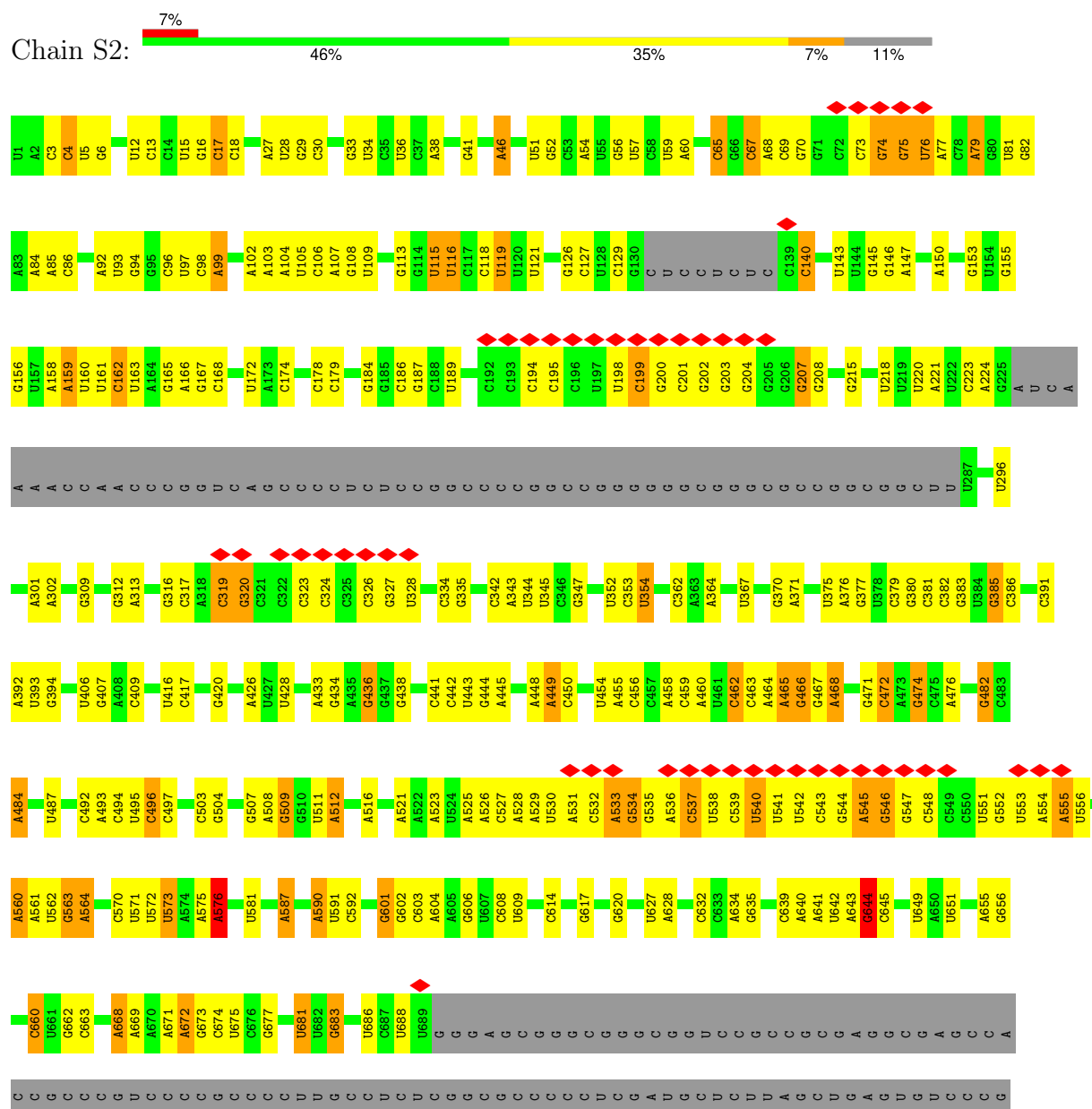
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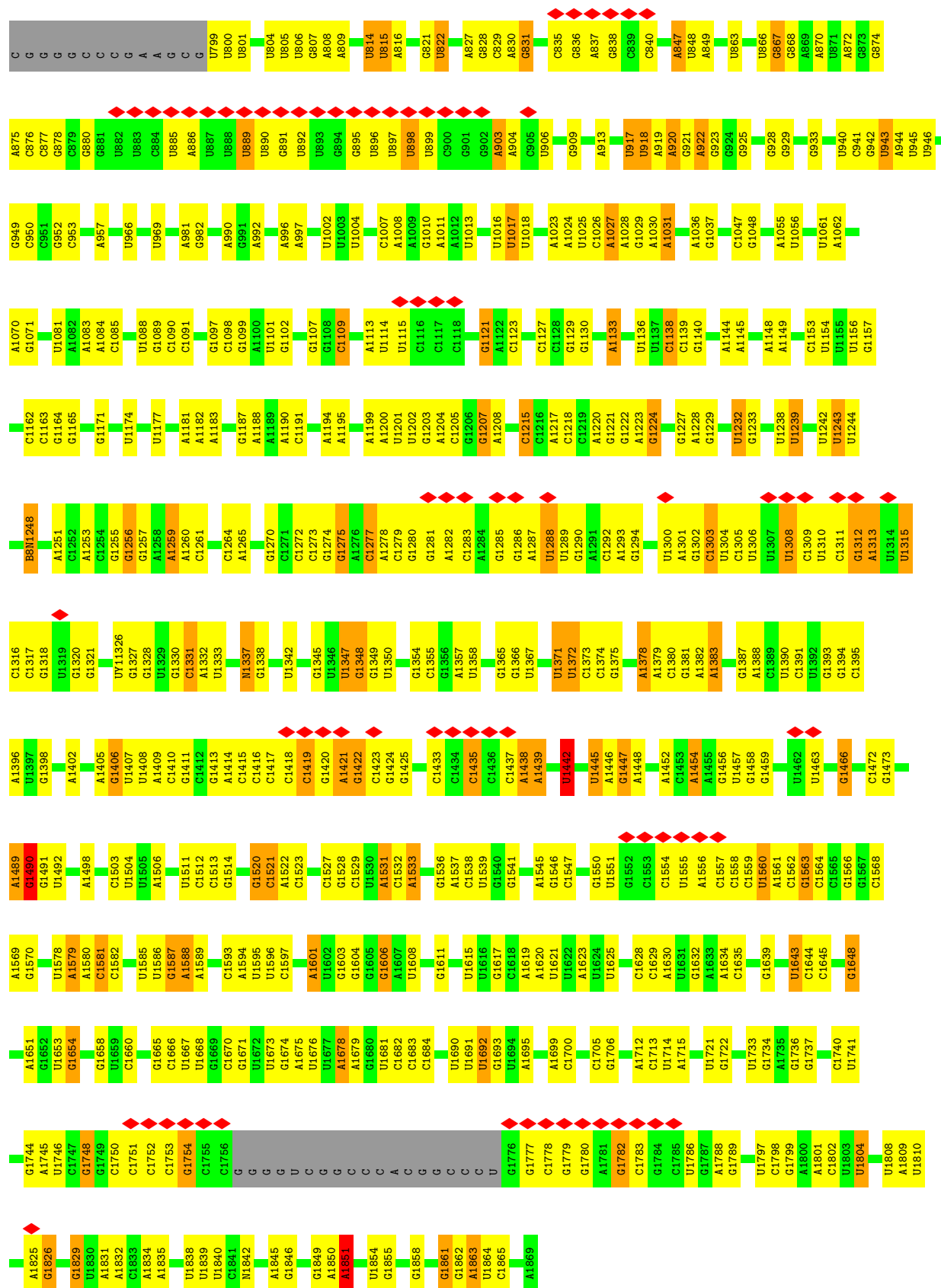
Mol	Chain	Residues	Atoms		AltConf
91	LF	77	Total 77	O 77	0
91	Lc	5	Total 5	O 5	0
91	Ld	20	Total 20	O 20	0
91	Le	71	Total 71	O 71	0
91	Lf	45	Total 45	O 45	0
91	Lg	39	Total 39	O 39	0
91	Li	15	Total 15	O 15	0
91	Lj	36	Total 36	O 36	0
91	Lk	2	Total 2	O 2	0
91	Ll	14	Total 14	O 14	0
91	Lm	8	Total 8	O 8	0
91	Ln	4	Total 4	O 4	0
91	Lo	37	Total 37	O 37	0
91	Lp	24	Total 24	O 24	0
91	Pt	1	Total 1	O 1	0

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.

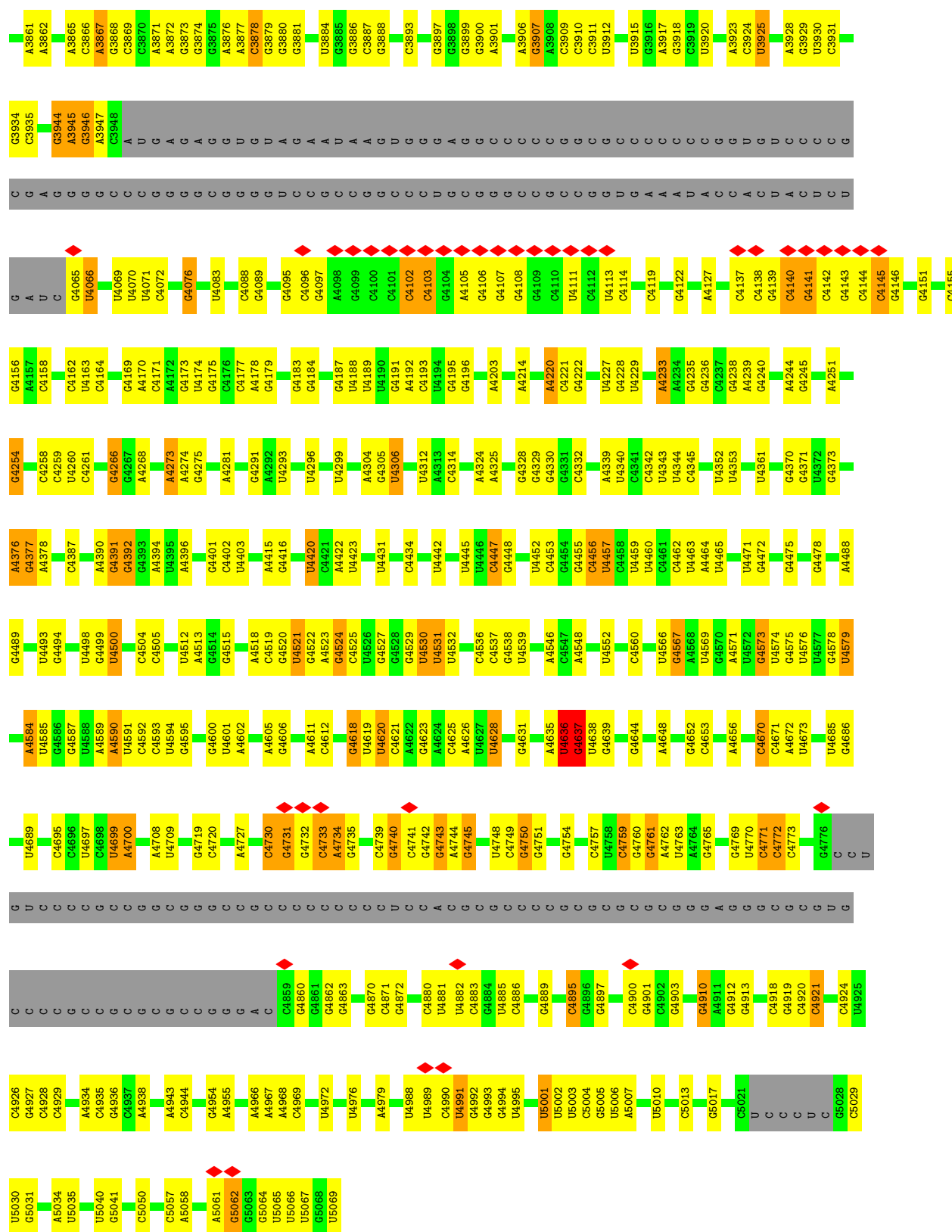
• Molecule 1: 18S rRNA



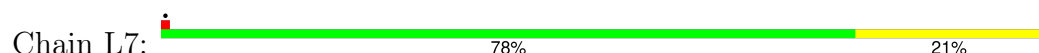


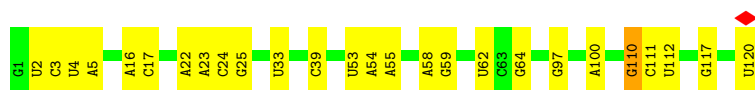






- Molecule 4: 5S rRNA





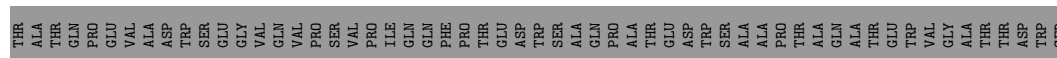
- Molecule 5: 40S ribosomal protein S3a

Chain SB: 70% 14% 16%



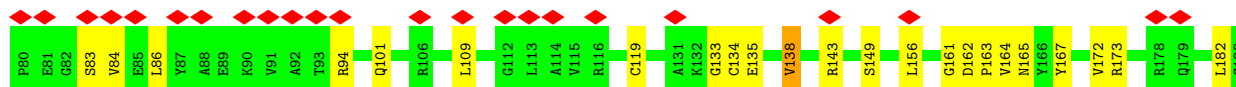
- Molecule 6: 40S ribosomal protein SA

Chain SA: 7% 58% 17% 25%



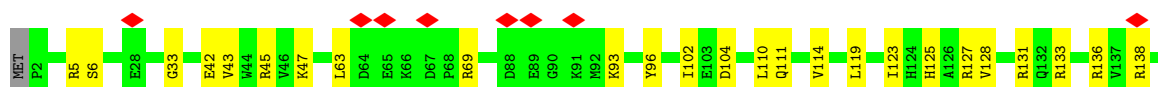
- Molecule 7: 40S ribosomal protein S3

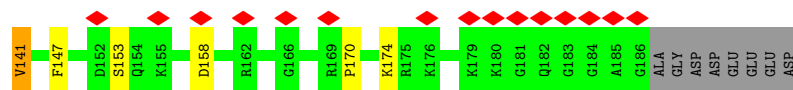
Chain SD: 32% 72% 21% 7%



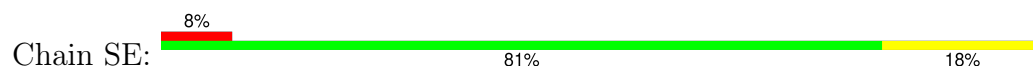
- Molecule 8: 40S ribosomal protein S9

Chain SJ: 12% 79% 15% 5%

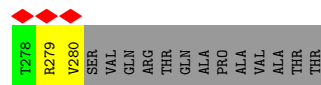
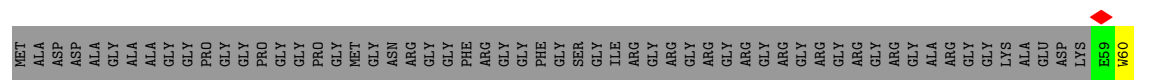




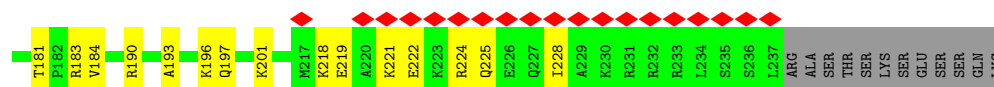
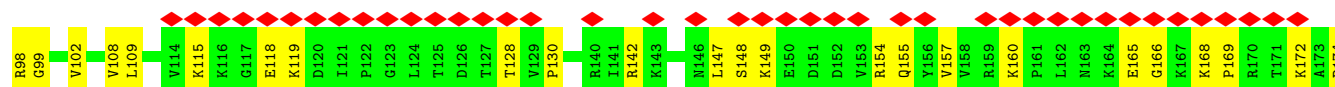
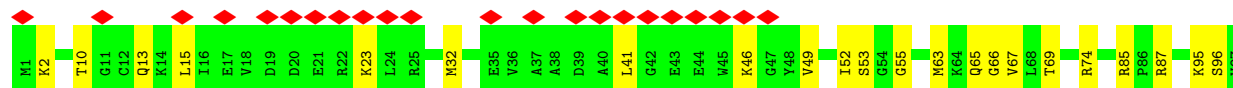
- Molecule 9: 40S ribosomal protein S4, X isoform



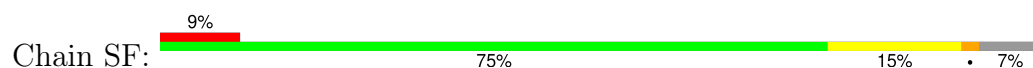
- Molecule 10: 40S ribosomal protein S2

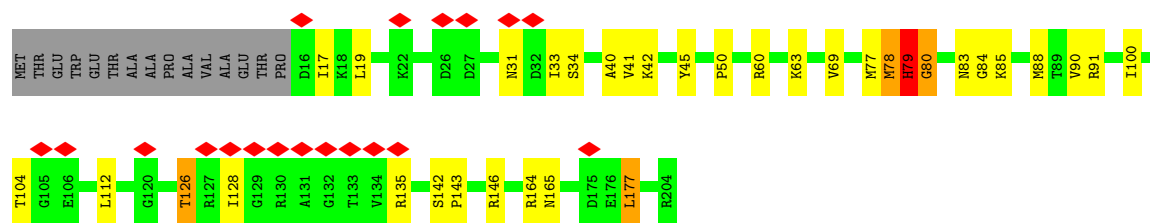


- Molecule 11: 40S ribosomal protein S6

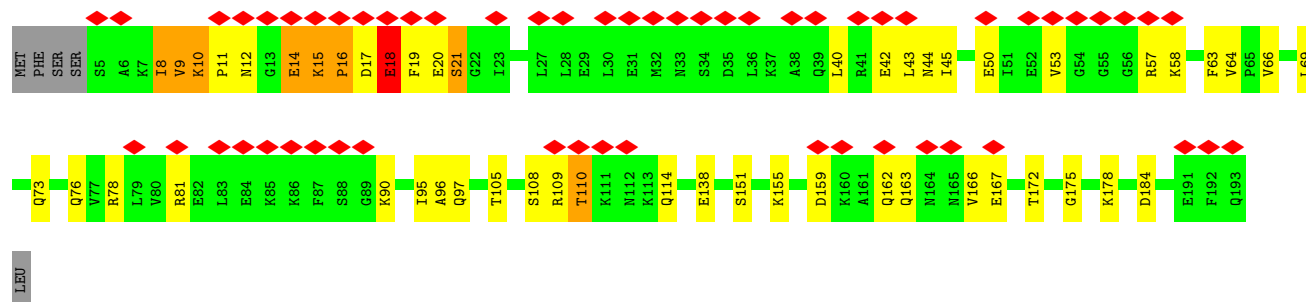


- Molecule 12: 40S ribosomal protein S5

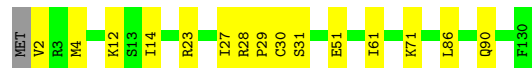
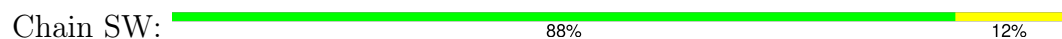




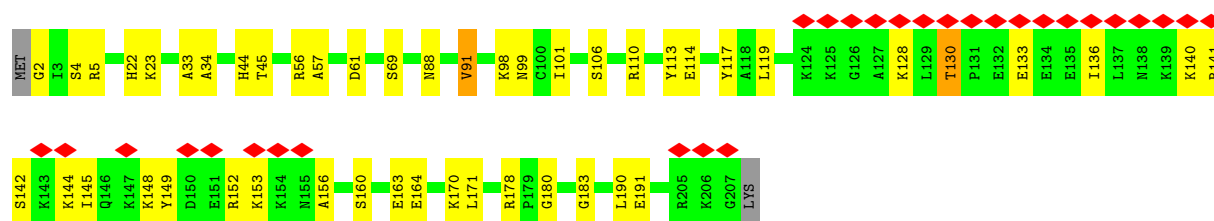
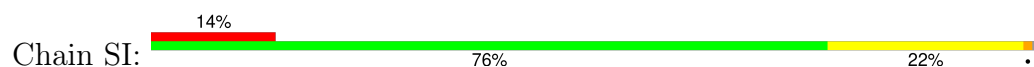
• Molecule 13: 40S ribosomal protein S7



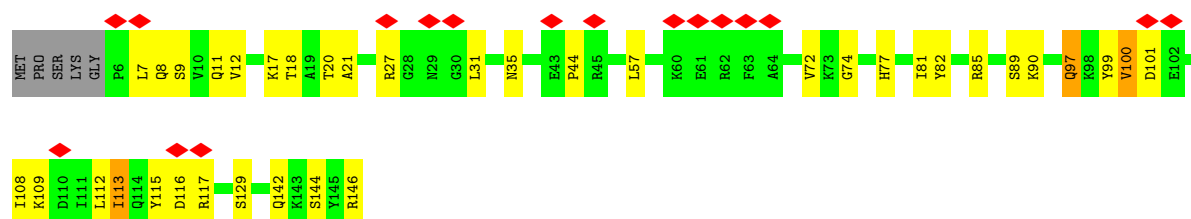
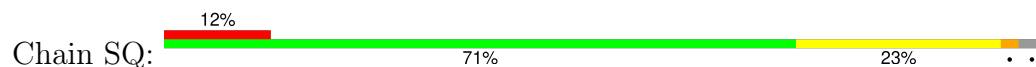
• Molecule 14: 40S ribosomal protein S15a



• Molecule 15: 40S ribosomal protein S8

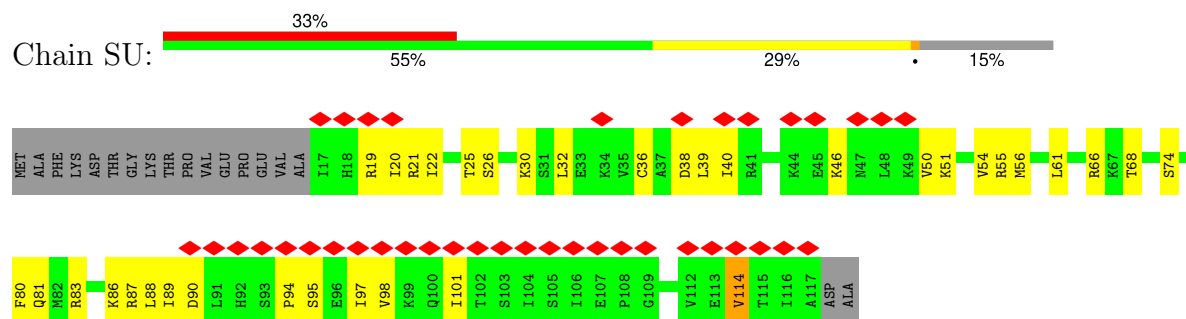


• Molecule 16: 40S ribosomal protein S16



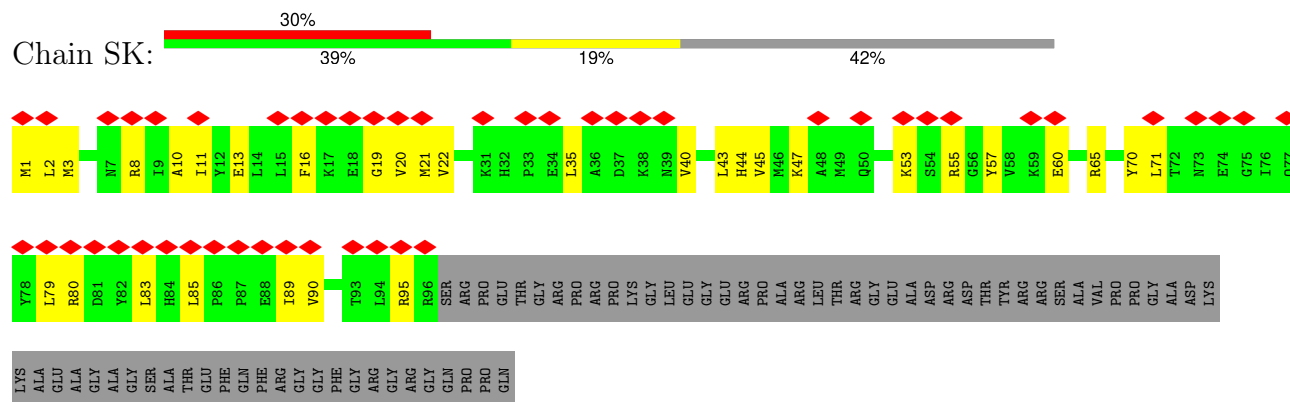
- Molecule 17: 40S ribosomal protein S20

Chain SU:



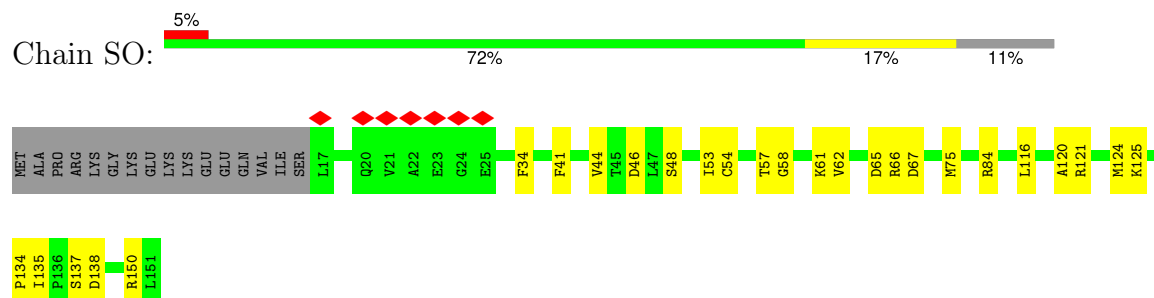
- Molecule 18: 40S ribosomal protein S10

Chain SK:



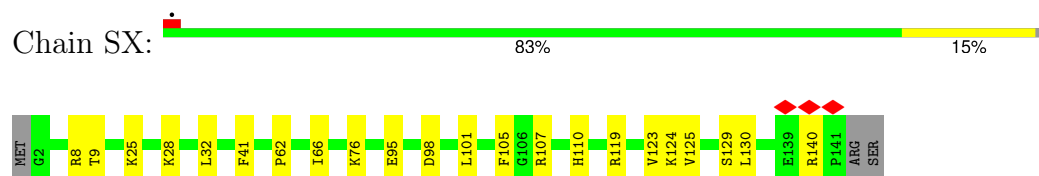
- Molecule 19: 40S ribosomal protein S14

Chain SO:



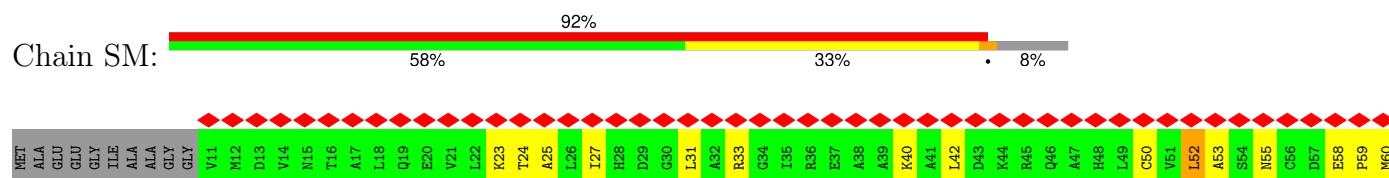
- Molecule 20: 40S ribosomal protein S23 (uS12)

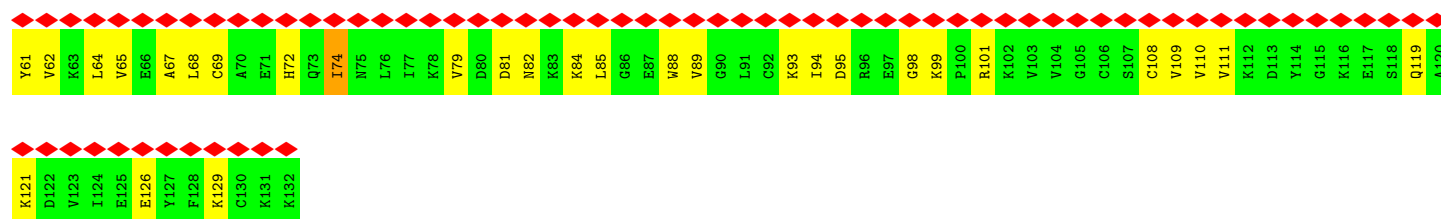
Chain SX:



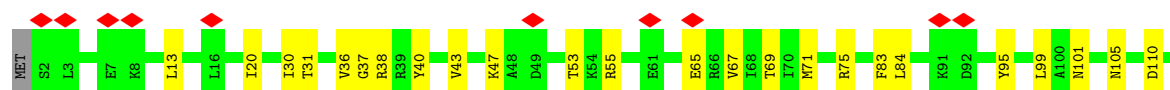
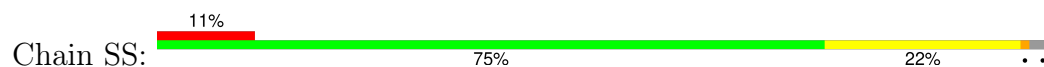
- Molecule 21: 40S ribosomal protein S12

Chain SM:

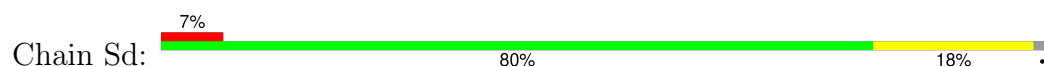




- Molecule 22: 40S ribosomal protein S18



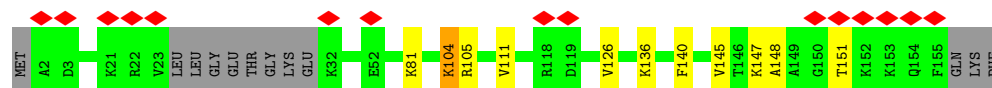
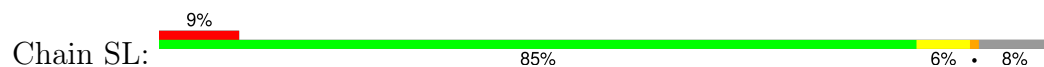
- Molecule 23: 40S ribosomal protein S29



- Molecule 24: 40S ribosomal protein S13



- Molecule 25: 40S ribosomal protein S11

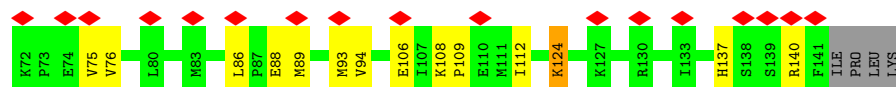
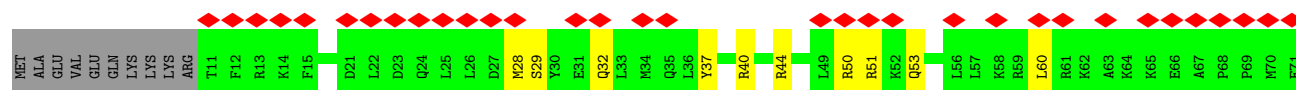
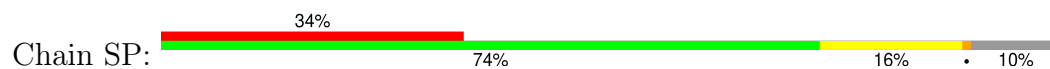


- Molecule 26: 40S ribosomal protein S17

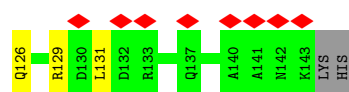
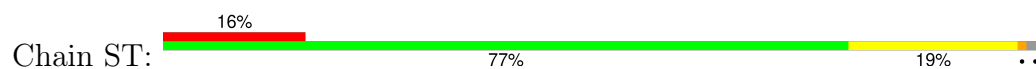




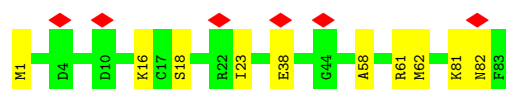
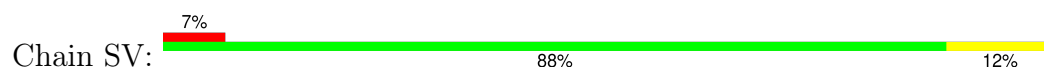
- Molecule 27: 40S ribosomal protein S15



- Molecule 28: 40S ribosomal protein S19



- Molecule 29: 40S ribosomal protein S21



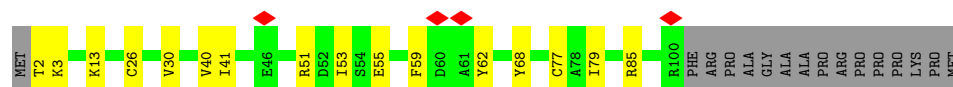
- Molecule 30: 40S ribosomal protein S24



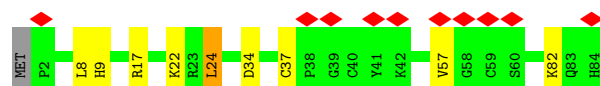
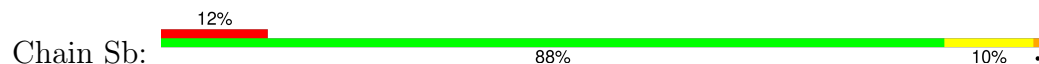
- Molecule 31: 40S ribosomal protein S25



- Molecule 32: 40S ribosomal protein S26



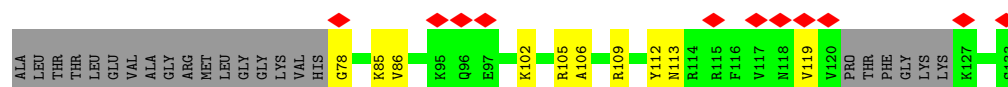
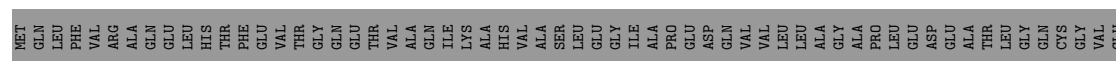
- Molecule 33: 40S ribosomal protein S27



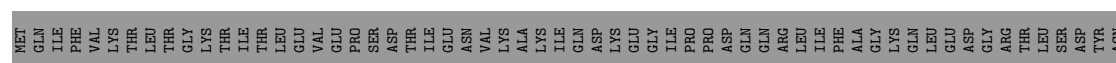
- Molecule 34: 40S ribosomal protein S28



- Molecule 35: FAU ubiquitin-like and ribosomal protein S30

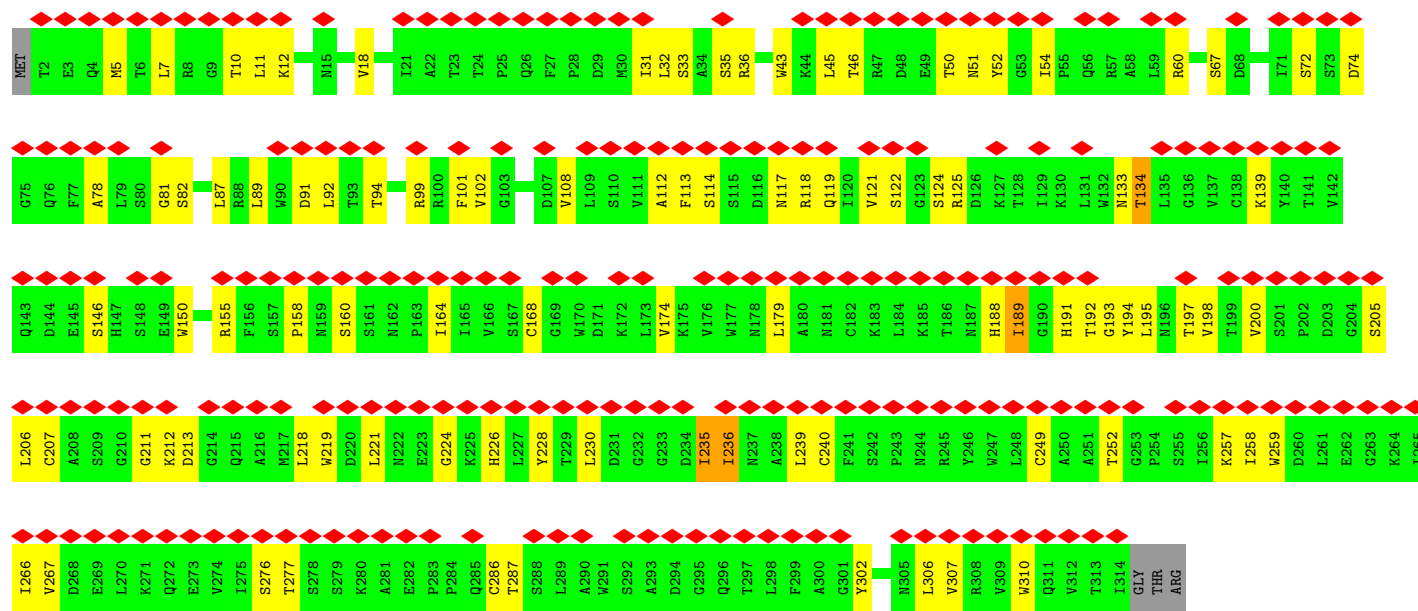
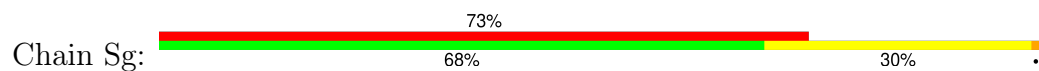


- Molecule 36: Ubiquitin-40S ribosomal protein S27a





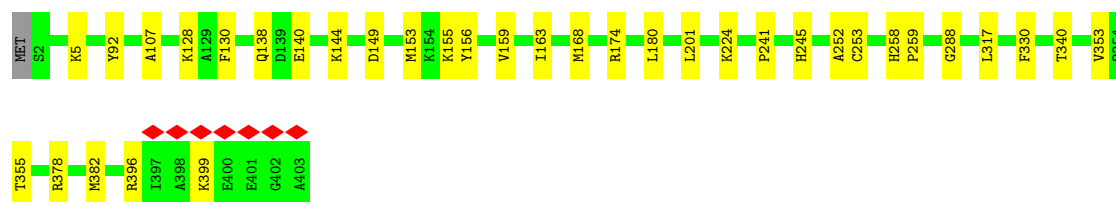
- Molecule 37: Receptor of activated protein C kinase 1



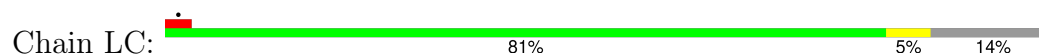
- Molecule 38: 60S ribosomal protein L8 (uL2)

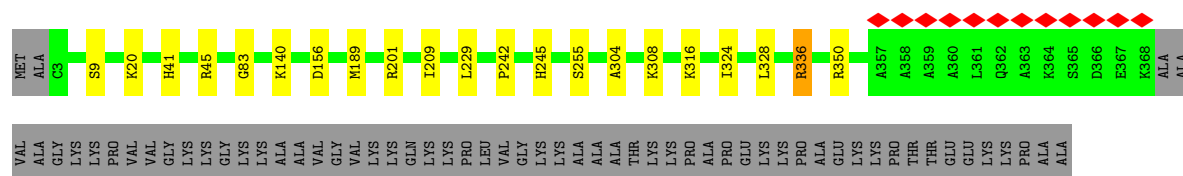


- Molecule 39: 60S ribosomal protein L3



- Molecule 40: 60S ribosomal protein L4

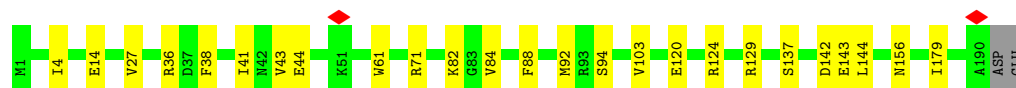
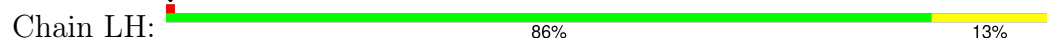




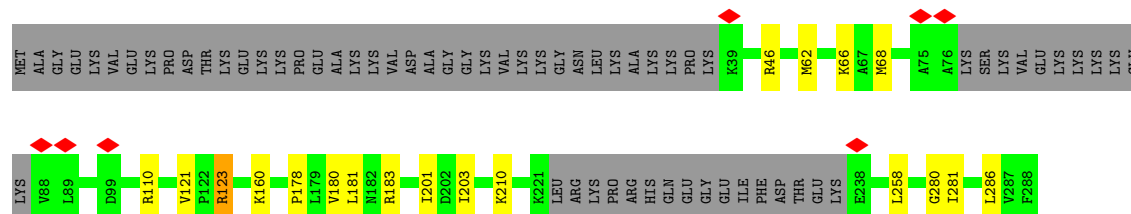
- Molecule 41: 60S ribosomal protein L11



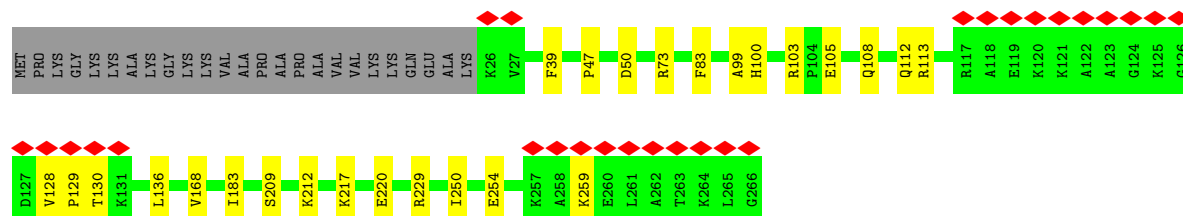
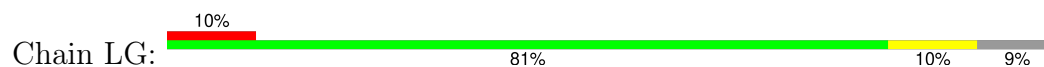
- Molecule 42: 60S ribosomal protein L9



- Molecule 43: 60S ribosomal protein L6



- Molecule 44: 60S ribosomal protein L7a



- Molecule 45: 60S ribosomal protein L13a



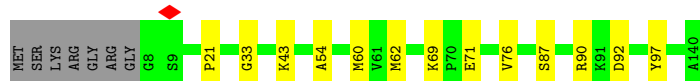
- Molecule 46: 60S ribosomal protein L13

Chain LL:  89% 9%



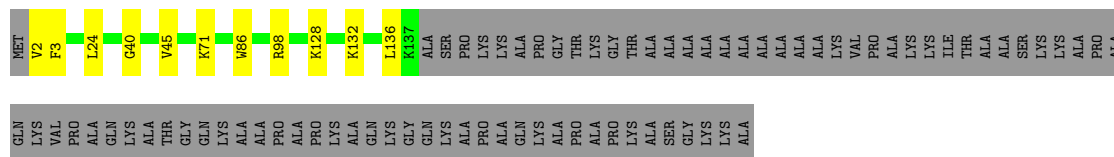
- Molecule 47: 60S ribosomal protein L23

Chain LV:  86% 9% 5%

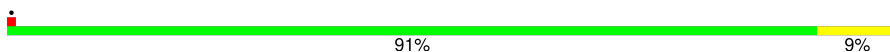


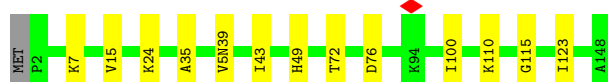
- Molecule 48: 60S ribosomal protein L14

Chain LM:  58% 5% 37%



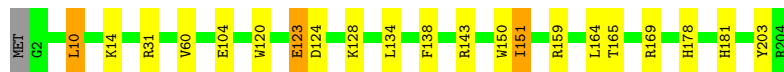
- Molecule 49: 60S ribosomal protein L27a

Chain La:  91% 9%



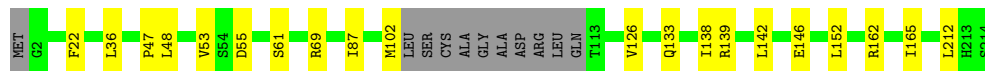
- Molecule 50: 60S ribosomal protein L15

Chain LN:  89% 9%



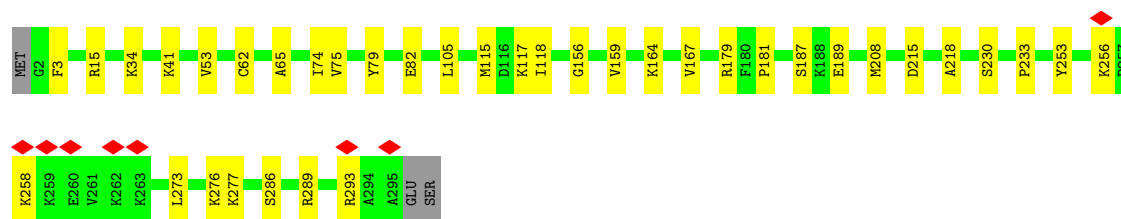
- Molecule 51: 60S ribosomal protein L10

Chain LI:  86% 9% 5%



- Molecule 52: 60S ribosomal protein L5

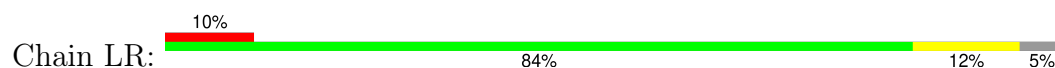
Chain LD:  87% 12%



- Molecule 53: 60S ribosomal protein L18



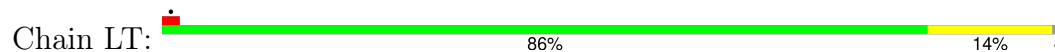
- Molecule 54: 60S ribosomal protein L19



- Molecule 55: 60S ribosomal protein L18a



- Molecule 56: 60S ribosomal protein L21

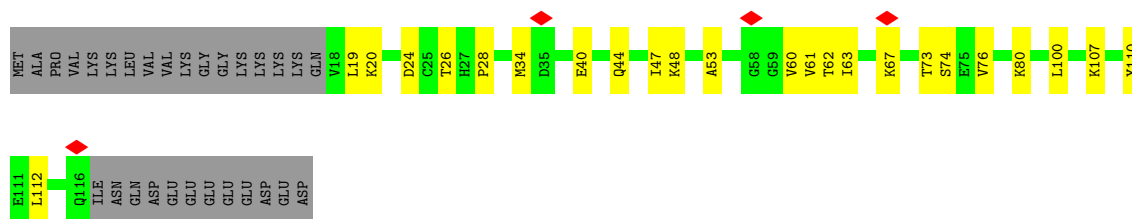


- Molecule 57: 60S ribosomal protein L17

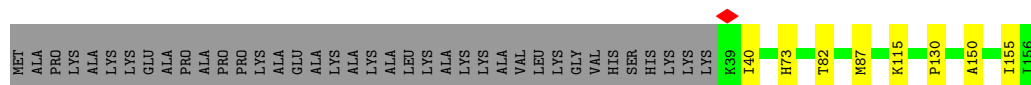


- Molecule 58: 60S ribosomal protein L22

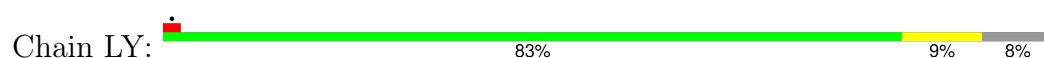




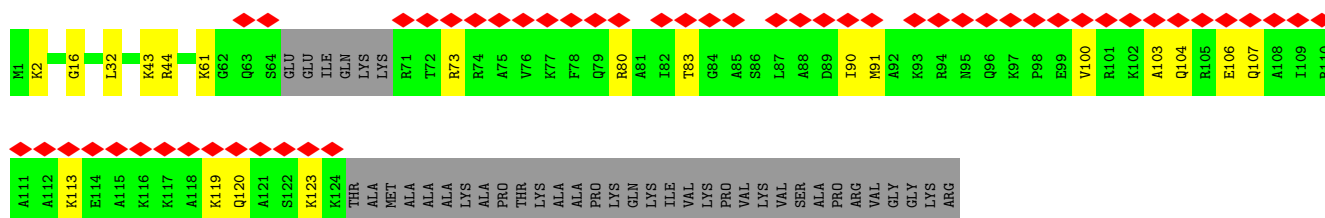
- Molecule 59: 60S ribosomal protein L23a



- Molecule 60: 60S ribosomal protein L26



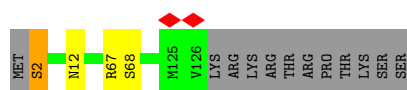
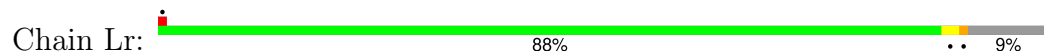
- Molecule 61: 60S ribosomal protein L24



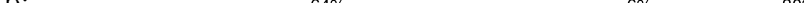
- Molecule 62: 60S ribosomal protein L27

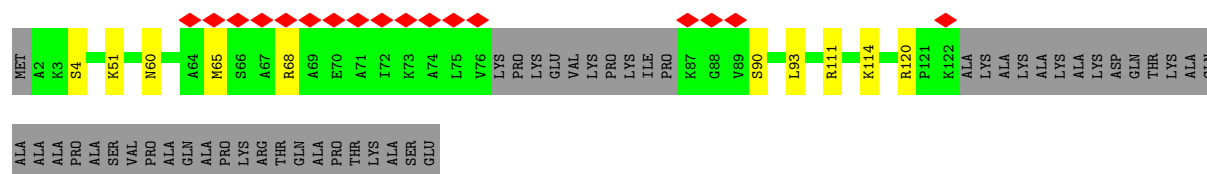


- Molecule 63: 60S ribosomal protein L28

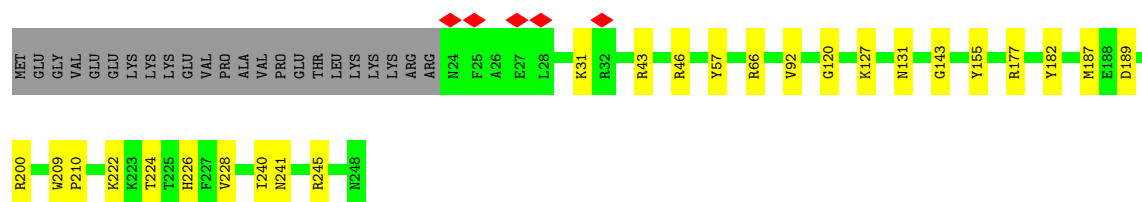


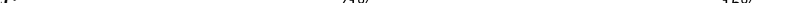
- Molecule 64: 60S ribosomal protein L35

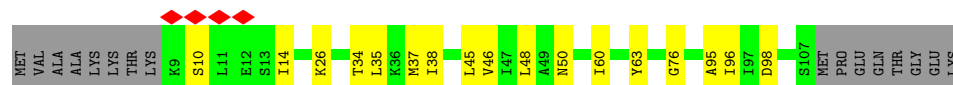
- Chain Lb: 

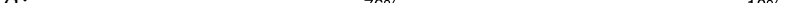


- Chain LF:

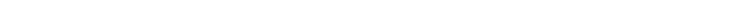


- Chain Lc: 



- Chain Ld: 

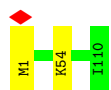


- Chain Le:  86% 9% 5%



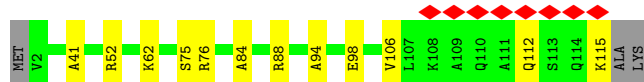
- 
- WORLDWIDE
PDB
PROTEIN DATA BANK

Chain Lf:  98% .



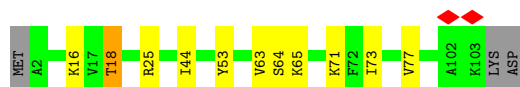
- Molecule 71: 60S ribosomal protein L34

Chain Lg:  7% 87% 10% .



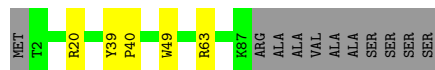
- Molecule 72: 60S ribosomal protein L36

Chain Li:  87% 10% .



- Molecule 73: 60S ribosomal protein L37

Chain Lj:  84% 5% 11%



- Molecule 74: 60S ribosomal protein L38

Chain Lk:  86% 13% .



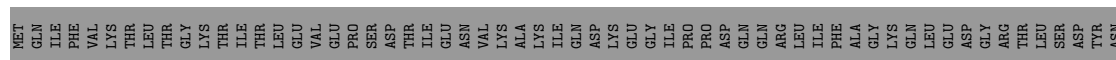
- Molecule 75: 60S ribosomal protein L39

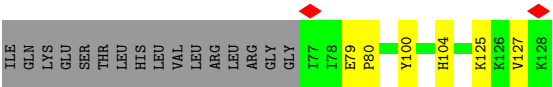
Chain Ll:  78% 20% .



- Molecule 76: 60S ribosomal protein L40 (eL40)

Chain Lm:  36% 5% 59%

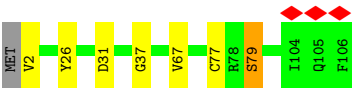




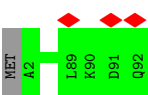
• Molecule 77: 60S ribosomal protein L41



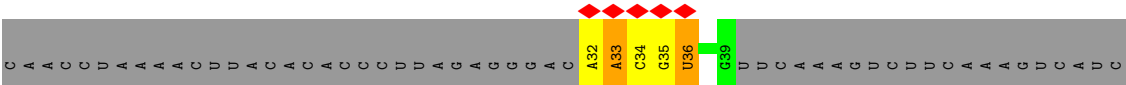
• Molecule 78: 60S ribosomal protein L36a



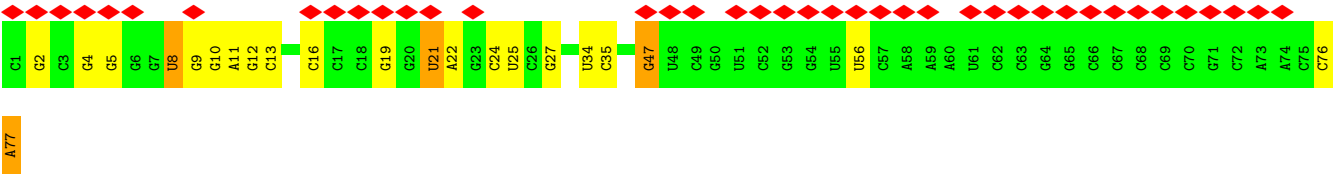
• Molecule 79: 60S ribosomal protein L37a



• Molecule 80: mRNA



• Molecule 81: P-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	845750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	528.64, 528.64, 528.64	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82600003, 0.82600003, 0.82600003	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, 6MZ, HIC, G7M, A2M, 1MA, OMG, PSU, SPD, HY3, MLZ, PUT, SAC, MG, UR3, TRS, B8N, OMU, ANM, UY1, V5N, H2U, 4SU, MA6, K, 3H3, 5MC, M3L, ZN, AME, OMC

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	S2	0.21	0/37935	0.28	0/59125
2	L8	0.28	0/3609	0.31	0/5623
3	L5	0.29	0/82080	0.34	0/128048
4	L7	0.27	0/2858	0.29	0/4455
5	SB	0.15	0/1832	0.29	0/2449
6	SA	0.15	0/1778	0.29	0/2416
7	SD	0.12	0/1784	0.28	0/2403
8	SJ	0.13	0/1550	0.28	0/2069
9	SE	0.13	0/2118	0.30	0/2849
10	SC	0.22	0/1762	0.41	1/2381 (0.0%)
11	SG	0.13	0/1946	0.27	0/2590
12	SF	0.29	0/1515	0.52	1/2037 (0.0%)
13	SH	0.26	0/1540	0.44	0/2064
14	SW	0.17	0/1051	0.36	0/1406
15	SI	0.19	0/1715	0.36	0/2287
16	SQ	0.13	0/1141	0.32	0/1528
17	SU	0.24	0/813	0.47	0/1092
18	SK	0.13	0/834	0.33	0/1125
19	SO	0.16	0/1022	0.33	0/1372
20	SX	0.14	0/1096	0.27	0/1461
21	SM	0.17	0/960	0.53	0/1286
22	SS	0.15	0/1232	0.32	0/1651
23	Sd	0.12	0/469	0.27	0/623
24	SN	0.15	0/1242	0.26	0/1671
25	SL	0.19	0/1221	0.30	0/1632
26	SR	0.16	0/1097	0.43	1/1474 (0.1%)
27	SP	0.19	0/1100	0.36	0/1470
28	ST	0.14	0/1148	0.36	0/1540
29	SV	0.14	0/635	0.27	0/850
30	SY	0.11	0/1083	0.27	0/1438
31	SZ	0.11	0/682	0.29	0/911

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.18	0/816	0.32	0/1093
33	Sb	0.15	0/665	0.32	0/891
34	Sc	0.14	0/514	0.31	0/688
35	Se	0.10	0/396	0.27	0/519
36	Sf	0.12	0/525	0.36	0/695
37	Sg	0.12	0/2493	0.34	0/3394
38	LA	0.23	0/1958	0.39	0/2623
39	LB	0.23	0/3294	0.34	0/4406
40	LC	0.23	0/2968	0.34	0/3985
41	LJ	0.18	0/1385	0.32	0/1852
42	LH	0.23	0/1537	0.34	0/2066
43	LE	0.19	0/1820	0.32	0/2442
44	LG	0.20	0/1959	0.34	0/2637
45	LO	0.25	0/1686	0.35	0/2257
46	LL	0.20	0/1706	0.33	0/2284
47	LV	0.21	0/1002	0.34	0/1345
48	LM	0.21	0/1142	0.31	0/1527
49	La	0.23	0/1178	0.34	0/1573
50	LN	0.28	0/1745	0.40	1/2338 (0.0%)
51	LI	0.20	0/1683	0.31	0/2247
52	LD	0.19	0/2437	0.31	0/3263
53	LQ	0.24	0/1536	0.37	0/2052
54	LR	0.20	0/1582	0.36	0/2091
55	LS	0.24	0/1500	0.33	0/2013
56	LT	0.25	0/1345	0.39	0/1795
57	LP	0.31	0/1279	0.47	2/1716 (0.1%)
58	LU	0.21	0/822	0.39	0/1103
59	LX	0.21	0/983	0.33	0/1323
60	LY	0.21	0/1132	0.32	0/1504
61	LW	0.19	0/964	0.34	0/1278
62	LZ	0.20	0/1141	0.29	0/1521
63	Lr	0.23	0/1020	0.32	0/1367
64	Lh	0.20	0/1022	0.27	0/1351
65	Lb	0.19	0/900	0.36	0/1187
66	LF	0.24	0/1926	0.34	0/2567
67	Lc	0.20	0/780	0.35	0/1046
68	Ld	0.21	0/903	0.34	0/1216
69	Le	0.23	0/1082	0.32	0/1443
70	Lf	0.24	0/902	0.32	0/1208
71	Lg	0.21	0/916	0.31	0/1220
72	Li	0.18	0/843	0.28	0/1115
73	Lj	0.24	0/731	0.36	0/967
74	Lk	0.19	0/574	0.32	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Ll	0.23	0/453	0.32	0/599
76	Lm	0.20	0/433	0.31	0/575
77	Ln	0.21	0/240	0.26	0/305
78	Lo	0.22	0/877	0.29	0/1156
79	Lp	0.22	0/728	0.34	0/967
80	mR	0.09	0/192	0.18	0/297
81	Pt	0.27	0/1721	0.30	0/2679
All	All	0.24	0/222284	0.33	6/325873 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SR	81	ARG	CB-CG-CD	7.09	127.61	111.30
50	LN	123	GLU	CB-CA-C	-5.92	99.20	109.86
57	LP	93[A]	HIS	CA-C-O	5.68	126.57	120.55
57	LP	93[B]	HIS	CA-C-O	5.68	126.57	120.55
10	SC	275	LYS	N-CA-C	-5.16	105.57	111.14
12	SF	79	HIS	CB-CA-C	5.02	120.42	110.42

There are no chirality outliers.

There are no planarity outliers.

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	S2	35736	0	18087	538	0
2	L8	3316	0	1687	39	0
3	L5	76116	0	38517	709	0
4	L7	2558	0	1295	17	0
5	SB	1806	0	1888	25	0
6	SA	1750	0	1755	35	0
7	SD	1756	0	1852	34	0
8	SJ	1525	0	1640	25	0
9	SE	2076	0	2177	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	SC	1725	0	1813	22	0
11	SG	1923	0	2089	52	0
12	SF	1494	0	1549	25	0
13	SH	1517	0	1605	38	0
14	SW	1034	0	1080	11	0
15	SI	1686	0	1772	33	0
16	SQ	1123	0	1193	24	0
17	SU	803	0	873	27	0
18	SK	810	0	836	25	0
19	SO	1009	0	1034	18	0
20	SX	1088	0	1149	13	0
21	SM	950	0	987	35	0
22	SS	1214	0	1275	21	0
23	Sd	458	0	448	8	0
24	SN	1214	0	1300	8	0
25	SL	1200	0	1271	8	0
26	SR	1082	0	1137	34	0
27	SP	1078	0	1121	19	0
28	ST	1121	0	1151	27	0
29	SV	639	0	638	7	0
30	SY	1065	0	1142	30	0
31	SZ	674	0	748	10	0
32	Sa	800	0	854	10	0
33	Sb	651	0	672	8	0
34	Sc	512	0	541	11	0
35	Se	394	0	434	9	0
36	Sf	515	0	521	21	0
37	Sg	2436	0	2393	68	0
38	LA	1930	0	2028	14	0
39	LB	3239	0	3377	25	0
40	LC	2914	0	3087	18	0
41	LJ	1362	0	1399	15	0
42	LH	1518	0	1600	15	0
43	LE	1786	0	1945	16	0
44	LG	1926	0	2074	16	0
45	LO	1654	0	1799	13	0
46	LL	1672	0	1786	16	0
47	LV	988	0	1047	7	0
48	LM	1120	0	1187	9	0
49	La	1162	0	1206	8	0
50	LN	1700	0	1749	20	0
51	LI	1645	0	1693	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	LD	2391	0	2426	23	0
53	LQ	1512	0	1628	3	0
54	LR	1566	0	1728	16	0
55	LS	1460	0	1502	10	0
56	LT	1311	0	1392	16	0
57	LP	1249	0	1276	11	0
58	LU	808	0	831	13	0
59	LX	966	0	1040	6	0
60	LY	1115	0	1205	11	0
61	LW	950	0	999	17	0
62	LZ	1115	0	1195	9	0
63	Lr	1011	0	1085	5	0
64	Lh	1014	0	1148	7	0
65	Lb	898	0	983	10	0
66	LF	1885	0	2022	19	0
67	Lc	770	0	809	10	0
68	Ld	888	0	930	7	0
69	Le	1061	0	1160	10	0
70	Lf	883	0	923	2	0
71	Lg	906	0	998	8	0
72	Li	832	0	917	9	0
73	Lj	712	0	744	3	0
74	Lk	568	0	637	6	0
75	Ll	443	0	482	8	0
76	Lm	436	0	477	4	0
77	Ln	239	0	289	1	0
78	Lo	870	0	936	5	0
79	Lp	715	0	769	0	0
80	mR	172	0	87	4	0
81	Pt	1645	0	843	11	0
82	L5	130	0	246	27	0
82	S2	20	0	38	2	0
83	L5	48	0	96	3	0
83	S2	6	0	12	0	0
84	L5	117	0	0	0	0
84	L7	4	0	0	0	0
84	L8	4	0	0	0	0
84	LA	3	0	0	0	0
84	LH	1	0	0	0	0
84	LI	1	0	0	0	0
84	LL	1	0	0	0	0
84	LN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	LQ	1	0	0	0	0
84	Lb	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lf	1	0	0	0	0
84	Ll	1	0	0	0	0
84	S2	12	0	0	0	0
84	SL	1	0	0	0	0
84	SO	1	0	0	0	0
84	Sa	1	0	0	0	0
85	L5	463	0	0	0	0
85	L7	15	0	0	0	0
85	L8	16	0	0	0	0
85	LB	1	0	0	0	0
85	LC	1	0	0	0	0
85	LD	1	0	0	0	0
85	LF	1	0	0	0	0
85	LG	1	0	0	0	0
85	LH	1	0	0	0	0
85	LL	1	0	0	0	0
85	LN	3	0	0	0	0
85	LO	2	0	0	0	0
85	LP	2	0	0	0	0
85	LQ	2	0	0	0	0
85	LR	1	0	0	0	0
85	LS	1	0	0	0	0
85	LV	1	0	0	0	0
85	La	1	0	0	0	0
85	Lc	1	0	0	0	0
85	Lf	1	0	0	0	0
85	Lg	1	0	0	0	0
85	Lj	2	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	2	0	0	0	0
85	Lr	3	0	0	0	0
85	Pt	2	0	0	0	0
85	S2	137	0	0	0	0
85	SG	1	0	0	0	0
85	SN	1	0	0	0	0
85	SS	2	0	0	0	0
85	ST	1	0	0	0	0
85	SX	1	0	0	0	0
85	Sd	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L5	19	0	19	1	0
87	L5	33	0	35	2	0
88	L5	16	0	24	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	1	0	0	0	0
89	Sf	1	0	0	0	0
90	Pt	8	0	8	2	0
91	L5	5661	0	0	7	0
91	L7	133	0	0	0	0
91	L8	189	0	0	0	0
91	LA	93	0	0	0	0
91	LB	113	0	0	0	0
91	LC	137	0	0	1	0
91	LD	37	0	0	0	0
91	LE	28	0	0	0	0
91	LF	77	0	0	0	0
91	LG	28	0	0	0	0
91	LH	14	0	0	0	0
91	LI	33	0	0	0	0
91	LJ	4	0	0	0	0
91	LL	62	0	0	1	0
91	LM	10	0	0	0	0
91	LN	112	0	0	0	0
91	LO	69	0	0	0	0
91	LP	44	0	0	1	0
91	LQ	81	0	0	0	0
91	LR	34	0	0	0	0
91	LS	51	0	0	1	0
91	LT	58	0	0	1	0
91	LU	1	0	0	0	0
91	LV	25	0	0	0	0
91	LW	8	0	0	0	0
91	LX	15	0	0	0	0
91	LY	23	0	0	0	0
91	LZ	7	0	0	0	0
91	La	71	0	0	0	0
91	Lb	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	Lc	5	0	0	0	0
91	Ld	20	0	0	0	0
91	Le	71	0	0	2	0
91	Lf	45	0	0	0	0
91	Lg	39	0	0	0	0
91	Lh	10	0	0	0	0
91	Li	15	0	0	0	0
91	Lj	36	0	0	0	0
91	Lk	2	0	0	0	0
91	Ll	14	0	0	0	0
91	Lm	8	0	0	0	0
91	Ln	4	0	0	0	0
91	Lo	37	0	0	0	0
91	Lp	24	0	0	0	0
91	Lr	53	0	0	0	0
91	Pt	1	0	0	1	0
91	S2	266	0	0	1	0
91	SA	1	0	0	0	0
91	SE	1	0	0	1	0
91	SF	1	0	0	0	0
91	SL	2	0	0	0	0
91	SN	3	0	0	0	0
91	SO	3	0	0	0	0
91	Sa	4	0	0	0	0
91	Sb	1	0	0	0	0
All	All	220877	0	158440	2229	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 (2229) 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)
50:LN:123:GLU:HG2	50:LN:128:LYS:HG2	1.38	1.06
1:S2:394:G:H5"	25:SL:81:LYS:HB3	1.45	0.96
1:S2:928:G:H1	1:S2:1013:U:H3	1.16	0.91
27:SP:28:MET:HE3	27:SP:29:SER:H	1.36	0.89
1:S2:925:G:H1	1:S2:1017:U:H3	1.20	0.88
3:L5:1759:G:H1	3:L5:1773:U:H3	1.24	0.85
3:L5:3907:G:H22	90:Pt:78:MET:HG2	1.39	0.83
12:Sf:77:MET:HE3	12:Sf:84:GLY:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2096:G:H21	40:LC:304:ALA:HB1	1.45	0.80
1:S2:543:C:H3'	1:S2:544:G:H8	1.46	0.80
12:SF:41:VAL:HG23	12:SF:42:LYS:HG3	1.65	0.79
21:SM:52:LEU:HD11	21:SM:65:VAL:HG11	1.65	0.78
3:L5:208:A:C2	3:L5:233:U:H5''	2.18	0.78
13:SH:14:GLU:HG2	13:SH:16:PRO:HD3	1.64	0.78
13:SH:8:ILE:HD13	13:SH:45:ILE:HG13	1.65	0.78
28:ST:110:LEU:HD22	28:ST:112:MET:HG2	1.65	0.78
21:SM:60:MET:H	21:SM:60:MET:HE2	1.47	0.78
12:SF:50:PRO:HG2	12:SF:90:VAL:HG22	1.64	0.78
3:L5:3869:OMC:C2	82:L5:5114:SPD:H32	2.18	0.77
56:LT:121:GLU:HG3	56:LT:122:LYS:NZ	2.00	0.76
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.21	0.76
1:S2:1421:A:H1'	1:S2:1422:G:H2'	1.67	0.76
13:SH:109:ARG:NH1	13:SH:110:THR:OG1	2.19	0.76
27:SP:28:MET:HE2	27:SP:32:GLN:HB2	1.68	0.75
47:LV:33:GLY:HA3	47:LV:69:LYS:HD2	1.68	0.75
1:S2:543:C:H3'	1:S2:544:G:C8	2.20	0.75
1:S2:544:G:H3'	1:S2:545:A:H8	1.51	0.74
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.70	0.73
3:L5:4095:G:H1	3:L5:4113:U:H3	1.34	0.73
3:L5:3888:G:H4'	82:L5:5114:SPD:H22	1.71	0.73
3:L5:5064:G:H21	57:LP:75:GLN:HE22	1.34	0.73
20:SX:8:ARG:NH2	25:SL:104:LYS:HG3	2.03	0.73
3:L5:143:C:O4'	44:LG:108:GLN:NE2	2.22	0.72
3:L5:196:C:H4'	60:LY:126:ARG:HG3	1.72	0.72
36:Sf:95:ARG:HH21	36:Sf:97:LYS:HG2	1.54	0.72
21:SM:60:MET:O	21:SM:64:LEU:HD22	1.90	0.72
82:L5:5110:SPD:H91	91:L5:7968:HOH:O	1.88	0.71
1:S2:377:G:H5''	15:SI:98:LYS:HB3	1.72	0.71
81:Pt:77:A:H1'	91:Pt:201:HOH:O	1.90	0.71
3:L5:3722:G:H2'	3:L5:3723:A2M:H8	1.73	0.71
21:SM:81:ASP:HB3	21:SM:84:LYS:HB3	1.70	0.71
39:LB:378:ARG:HG2	61:LW:32:LEU:HD21	1.72	0.71
1:S2:70:G:H21	1:S2:79:A:H2	1.39	0.70
82:L5:5115:SPD:H51	91:L5:5818:HOH:O	1.91	0.70
3:L5:3907:G:N2	90:Pt:78:MET:HG2	2.07	0.70
3:L5:739:G:H5''	3:L5:739:G:H8	1.56	0.70
1:S2:165:G:OP2	1:S2:165:G:N2	2.23	0.70
21:SM:61:TYR:O	21:SM:65:VAL:HG23	1.92	0.70
46:LL:103:ARG:HD3	72:Li:25:ARG:HD2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2416:G:N2	3:L5:2427:G:N7	2.40	0.70
37:Sg:87:LEU:HB2	37:Sg:101:PHE:HB2	1.74	0.70
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.57	0.70
42:LH:94:SER:HB2	42:LH:142:ASP:HB3	1.74	0.69
3:L5:2492:C:H2'	3:L5:2493:G:H8	1.56	0.69
17:SU:40:ILE:HD11	17:SU:89:ILE:HD12	1.74	0.69
30:SY:21:LYS:HB2	30:SY:75:ILE:HB	1.74	0.69
43:LE:210:LYS:H	43:LE:210:LYS:HE2	1.56	0.69
9:SE:45:ILE:HA	9:SE:61:VAL:HG11	1.75	0.69
1:S2:835:C:N4	30:SY:9:THR:O	2.26	0.69
3:L5:1766:A:H5''	22:SS:116:LYS:HG3	1.75	0.69
21:SM:31:LEU:HD22	21:SM:111:VAL:HA	1.74	0.69
6:SA:2:SAC:O	6:SA:63:ARG:NH2	2.26	0.69
27:SP:28:MET:HE3	27:SP:29:SER:N	2.07	0.68
30:SY:9:THR:HB	30:SY:23:MET:HG3	1.74	0.68
3:L5:969:C:H4'	43:LE:123:ARG:HH21	1.58	0.68
3:L5:2099:G:H2'	3:L5:2100:A:O4'	1.92	0.68
22:SS:67:VAL:O	22:SS:71:MET:HG3	1.94	0.68
5:SB:230:GLU:HA	5:SB:234:GLU:HA	1.74	0.68
11:SG:181:THR:HG22	11:SG:183:ARG:H	1.58	0.68
1:S2:1308:U:H2'	1:S2:1309:C:H6	1.58	0.68
21:SM:79:VAL:HB	21:SM:85:LEU:HD23	1.76	0.68
13:SH:17:ASP:O	13:SH:18:GLU:C	2.37	0.68
40:LC:140:LYS:HE3	40:LC:245:HIS:HB2	1.76	0.68
1:S2:672:A:N6	1:S2:1027:A:OP1	2.27	0.67
36:Sf:121:CYS:HB2	36:Sf:132:MET:HE1	1.76	0.67
1:S2:537:C:H2'	1:S2:538:U:C6	2.29	0.67
3:L5:177:G:H2'	3:L5:178:C:H5''	1.76	0.67
21:SM:42:LEU:HD21	21:SM:68:LEU:HB2	1.75	0.67
1:S2:640:A:H2'	1:S2:641:A:C8	2.30	0.67
7:SD:210:ILE:HD13	26:SR:16:ILE:HG13	1.77	0.67
34:Sc:15:THR:HG22	34:Sc:16:LYS:H	1.60	0.67
44:LG:99:ALA:HB1	44:LG:136:LEU:HD11	1.76	0.67
15:SI:141:ARG:H	15:SI:141:ARG:HD2	1.60	0.66
3:L5:738:C:N4	3:L5:741:C:H4'	2.10	0.66
1:S2:1527:C:OP1	16:SQ:142:GLN:NE2	2.28	0.66
3:L5:184:U:H1'	3:L5:188:G:H1'	1.78	0.66
1:S2:1228:A:H2'	1:S2:1229:G:H8	1.61	0.66
37:Sg:118:ARG:HH22	37:Sg:133:ASN:HA	1.60	0.66
18:SK:83:LEU:HB3	18:SK:85:LEU:HD13	1.78	0.66
3:L5:1811:G:H4'	65:Lb:60:ASN:HD22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2089:G:H22	3:L5:2096:G:H1	1.43	0.66
36:Sf:118:ARG:NH1	36:Sf:130:VAL:O	2.28	0.66
1:S2:1546:G:H5'	16:SQ:18:THR:HG21	1.78	0.66
1:S2:1300:U:O2'	27:SP:51:ARG:NH2	2.29	0.66
1:S2:1562:C:H2'	1:S2:1563:G:H8	1.61	0.66
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.78	0.66
3:L5:711:A:H2'	3:L5:712:C:C6	2.31	0.65
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.26	0.65
7:SD:76:ARG:HB2	18:SK:22:VAL:HG11	1.76	0.65
38:LA:137:ILE:HD11	38:LA:149:LYS:HB2	1.79	0.65
3:L5:109:G:OP2	46:LL:74:ARG:NH2	2.26	0.65
21:SM:58:GLU:HG2	21:SM:61:TYR:HB2	1.79	0.65
4:L7:117:G:H5'	52:LD:256:LYS:HD2	1.78	0.65
3:L5:1704:C:O2'	66:LF:46:ARG:NH1	2.30	0.65
47:LV:43:LYS:HG3	47:LV:60:MET:HG2	1.78	0.65
6:SA:52:LYS:HB2	26:SR:109:LEU:HD23	1.79	0.65
1:S2:1417:C:H2'	1:S2:1418:C:C2	2.32	0.65
3:L5:280:G:H5''	50:LN:14:LYS:HE2	1.79	0.65
4:L7:17:C:OP1	41:LJ:156:ARG:NH2	2.30	0.65
28:ST:74:SER:O	28:ST:78:ILE:HD12	1.97	0.65
1:S2:1091:C:HO2'	14:SW:2:VAL:N	1.95	0.64
1:S2:1536:G:H2'	1:S2:1537:A:C8	2.33	0.64
3:L5:739:G:H5''	3:L5:739:G:C8	2.32	0.64
13:SH:163:GLN:O	13:SH:167:GLU:HB3	1.96	0.64
15:SI:142:SER:HB3	15:SI:145:ILE:HG22	1.78	0.64
6:SA:117:ARG:HG3	6:SA:119:PRO:HD3	1.78	0.64
1:S2:1545:A:H2'	1:S2:1546:G:C8	2.32	0.64
3:L5:2486:G:H2'	3:L5:2487:G:H8	1.63	0.64
21:SM:94:ILE:HG23	21:SM:98:GLY:HA2	1.77	0.64
3:L5:1241:C:N3	65:Lb:120:ARG:NH2	2.42	0.64
30:SY:10:ARG:HG3	30:SY:24:VAL:HG13	1.79	0.64
3:L5:3823:G:OP2	3:L5:3823:G:N2	2.25	0.64
3:L5:1703:C:O2'	66:LF:43:ARG:NH2	2.29	0.64
3:L5:4750:G:H2'	3:L5:4751:G:C8	2.32	0.64
1:S2:677:G:N1	1:S2:1027:A:OP2	2.26	0.64
45:LO:168:TYR:CE2	45:LO:172:LYS:HD2	2.33	0.64
3:L5:658:C:H2'	3:L5:659:G:C8	2.33	0.64
1:S2:981:A:H2'	1:S2:982:G:C8	2.33	0.64
3:L5:1940:G:H22	3:L5:4434:C:H5''	1.63	0.64
11:SG:193:ALA:O	11:SG:197:GLN:HG3	1.98	0.64
13:SH:17:ASP:HA	13:SH:20:GLU:CD	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SH:53:VAL:HG11	13:SH:172:THR:HA	1.80	0.64
3:L5:1448:G:H2'	3:L5:1449:C:C6	2.34	0.63
21:SM:55:ASN:HB2	21:SM:82:ASN:HB2	1.78	0.63
26:SR:66:VAL:HG23	26:SR:67:ARG:H	1.63	0.63
1:S2:1541:G:N3	28:ST:12:GLN:NE2	2.47	0.63
3:L5:3887:OMC:CM2	82:L5:5114:SPD:H31	2.28	0.63
30:SY:101:LYS:H	30:SY:101:LYS:HD3	1.63	0.63
37:Sg:212:LYS:HA	37:Sg:235:ILE:HD12	1.80	0.63
42:LH:14:GLU:H	42:LH:14:GLU:CD	2.07	0.63
56:LT:111:GLU:HB3	56:LT:115:LYS:NZ	2.13	0.63
3:L5:2557:G:H1	3:L5:2570:U:H3	1.45	0.63
1:S2:145:G:H2'	1:S2:146:G:C8	2.33	0.63
1:S2:1536:G:H2'	1:S2:1537:A:H8	1.63	0.63
3:L5:1390:G:O3'	82:L5:5109:SPD:H91	1.97	0.63
3:L5:2486:G:H2'	3:L5:2487:G:C8	2.32	0.63
44:LG:209:SER:HA	44:LG:212:LYS:HG3	1.81	0.63
1:S2:1523:C:H4'	22:SS:145:THR:HA	1.81	0.63
3:L5:137:G:OP1	64:Lh:96:ASN:ND2	2.32	0.63
1:S2:462:OMC:H2'	1:S2:463:C:C6	2.34	0.63
1:S2:532:C:H2'	1:S2:533:A:C8	2.34	0.63
3:L5:664:G:H21	3:L5:667:A:N6	1.96	0.63
3:L5:2492:C:H2'	3:L5:2493:G:C8	2.33	0.63
37:Sg:33:SER:OG	37:Sg:43:TRP:NE1	2.23	0.63
3:L5:4734:A:H2'	3:L5:4735:G:C8	2.34	0.63
15:SI:110:ARG:O	15:SI:114:GLU:HG2	1.98	0.62
10:SC:187:ARG:HD3	10:SC:192:LEU:HD12	1.82	0.62
3:L5:4910:G:N2	45:LO:106:ASP:O	2.33	0.62
6:SA:205:ARG:NH1	6:SA:213:GLU:OE1	2.31	0.62
1:S2:455:A:H2'	1:S2:456:C:H6	1.64	0.62
1:S2:463:C:H2'	1:S2:465:A:N7	2.14	0.62
3:L5:2485:U:H2'	3:L5:2486:G:C8	2.35	0.62
22:SS:13:LEU:HB2	22:SS:20:ILE:HB	1.82	0.62
1:S2:928:G:H2'	1:S2:929:G:C8	2.35	0.61
3:L5:4352:U:OP1	46:LL:190[B]:ARG:NH2	2.28	0.61
3:L5:184:U:H2'	3:L5:186:G:C8	2.34	0.61
10:SC:276:THR:HA	10:SC:279:ARG:HE	1.65	0.61
44:LG:250:ILE:O	44:LG:254:GLU:HG2	2.00	0.61
3:L5:1763:C:H2'	3:L5:1764:G:C8	2.35	0.61
32:Sa:59:PHE:HB2	32:Sa:62:TYR:HB2	1.81	0.61
26:SR:37:GLU:OE1	37:Sg:150:TRP:NE1	2.30	0.61
42:LH:92:MET:HE2	42:LH:179:ILE:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1753:C:HO2'	1:S2:1754:G:H8	1.45	0.61
9:SE:11:ARG:HA	9:SE:28:ALA:HB2	1.82	0.61
13:SH:10:LYS:HE3	13:SH:11:PRO:HD2	1.81	0.61
17:SU:56:MET:HG3	17:SU:86:LYS:HE2	1.81	0.61
1:S2:534:G:H2'	1:S2:535:G:H8	1.64	0.61
1:S2:1217:A:H2'	1:S2:1218:C:H6	1.64	0.61
57:LP:94:MET:HG2	57:LP:148:MET:HE3	1.82	0.61
1:S2:535:G:H2'	1:S2:536:A:C8	2.36	0.61
3:L5:669:C:H5'	63:Lr:68:SER:HB2	1.81	0.61
3:L5:4918:C:H2'	3:L5:4919:G:H8	1.66	0.61
18:SK:35:LEU:HD11	18:SK:40:VAL:HG22	1.81	0.61
1:S2:909:G:OP1	54:LR:176:ARG:NH1	2.31	0.61
1:S2:944:A:H5''	19:SO:134:PRO:HB3	1.82	0.61
1:S2:1101:U:H2'	1:S2:1102:G:C8	2.36	0.61
7:SD:143:ARG:HB3	7:SD:143:ARG:HH11	1.65	0.61
1:S2:455:A:H2'	1:S2:456:C:C6	2.36	0.60
3:L5:1765:A:O2'	3:L5:1766:A:OP1	2.19	0.60
12:SF:128:ILE:HB	12:SF:135:ARG:HG2	1.83	0.60
56:LT:88:ARG:NH1	91:LT:201:HOH:O	2.28	0.60
1:S2:874:G:H2'	1:S2:875:A:H8	1.67	0.60
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.36	0.60
56:LT:158:PHE:CE1	56:LT:159:MET:HE3	2.36	0.60
18:SK:20:VAL:HG12	18:SK:70:TYR:HA	1.83	0.60
41:LJ:18:ARG:HG3	41:LJ:135:GLY:HA3	1.82	0.60
1:S2:65:C:H4'	11:SG:172:LYS:HD2	1.82	0.60
82:L5:5112:SPD:H81	91:L5:7544:HOH:O	1.99	0.60
15:SI:160:SER:HA	15:SI:163:GLU:HB2	1.84	0.60
39:LB:317:LEU:HD21	39:LB:382:MET:HG2	1.81	0.60
50:LN:138:PHE:HA	50:LN:143:ARG:HD2	1.83	0.60
1:S2:367:U:H4'	1:S2:371:A:C8	2.35	0.60
16:SQ:8:GLN:OE1	16:SQ:27:ARG:NH2	2.35	0.60
56:LT:51:GLY:HA3	56:LT:92:ARG:HG3	1.83	0.60
1:S2:12:U:H2'	1:S2:13:C:C6	2.37	0.60
14:SW:28:ARG:HB3	14:SW:29:PRO:HD3	1.84	0.60
1:S2:1382:A:H2'	1:S2:1383:A2M:H8	1.84	0.60
3:L5:1188:C:H2'	3:L5:1189:G:H8	1.67	0.60
3:L5:2096:G:N2	40:LC:304:ALA:HB1	2.16	0.60
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.37	0.60
1:S2:1562:C:H2'	1:S2:1563:G:C8	2.37	0.60
3:L5:2297:G:H5''	82:L5:5112:SPD:HN12	1.66	0.60
1:S2:1101:U:H2'	1:S2:1102:G:H8	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.67	0.59
1:S2:84:A:N3	1:S2:150:A:O2'	2.35	0.59
1:S2:543:C:N3	1:S2:544:G:H1'	2.16	0.59
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.38	0.59
42:LH:44:GLU:HG3	48:LM:2:VAL:HG12	1.84	0.59
3:L5:4457:PSU:H1'	39:LB:252:ALA:HB3	1.85	0.59
18:SK:65:ARG:HD3	23:Sd:25:SER:HB3	1.84	0.59
54:LR:136:ARG:O	54:LR:140:GLU:HG3	2.01	0.59
55:LS:1:MET:N	91:LS:301:HOH:O	2.36	0.59
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.37	0.59
3:L5:1940:G:N2	3:L5:4434:C:OP1	2.35	0.59
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.37	0.59
20:SX:98:ASP:OD2	20:SX:140:ARG:NH1	2.35	0.59
1:S2:540:U:H1'	1:S2:544:G:N2	2.17	0.59
1:S2:1568:C:H2'	1:S2:1569:A:C8	2.37	0.59
34:Sc:10:LYS:NZ	34:Sc:36:ASP:OD2	2.27	0.59
56:LT:111:GLU:HB3	56:LT:115:LYS:HZ1	1.65	0.59
3:L5:260:C:H2'	3:L5:261:G:H8	1.68	0.59
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.37	0.59
1:S2:918:PSU:O2'	1:S2:919:A:O4'	2.20	0.59
1:S2:1801:A:H2'	1:S2:1802:C:C6	2.37	0.59
3:L5:233:U:O2'	3:L5:234:G:H2'	2.03	0.59
27:SP:93:MET:HE1	27:SP:106:GLU:HG2	1.82	0.59
1:S2:1008:A:N7	91:S2:2104:HOH:O	2.32	0.59
21:SM:69:CYS:HA	21:SM:74:ILE:HD11	1.84	0.59
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.83	0.59
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.68	0.59
13:SH:63:PHE:HB3	13:SH:97:GLN:HG2	1.85	0.59
1:S2:1259:A:H1'	1:S2:1264:C:H42	1.68	0.58
37:Sg:18:VAL:O	37:Sg:287:THR:OG1	2.20	0.58
1:S2:541:U:H3'	1:S2:542:U:H6	1.68	0.58
1:S2:923:G:N7	82:S2:1901:SPD:H51	2.18	0.58
3:L5:1702:C:H4'	40:LC:308:LYS:HD2	1.85	0.58
75:Ll:25:GLN:OE1	75:Ll:28:ARG:NH2	2.36	0.58
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.39	0.58
16:SQ:97:GLN:OE1	37:Sg:60:ARG:NH1	2.36	0.58
3:L5:12:A:N3	91:L5:5840:HOH:O	2.31	0.58
3:L5:131:C:N4	3:L5:132:G:O6	2.36	0.58
37:Sg:118:ARG:NH2	37:Sg:119:GLN:OE1	2.32	0.58
1:S2:1248:B8N:N34	81:Pt:35:C:OP1	2.36	0.58
3:L5:325:U:H2'	3:L5:326:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1326:A2M:OP2	3:L5:4445:U:O2'	2.21	0.58
22:SS:110:ASP:OD1	22:SS:113:ARG:NH2	2.35	0.58
1:S2:1308:U:H2'	1:S2:1309:C:C6	2.37	0.58
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.39	0.58
3:L5:3869:OMC:N1	82:L5:5114:SPD:H32	2.17	0.58
12:SF:34:SER:HA	34:Sc:55:VAL:HB	1.85	0.58
3:L5:666:G:H5'	63:Lr:67:ARG:NH2	2.19	0.58
1:S2:94:G:OP1	9:SE:6:LYS:NZ	2.37	0.58
3:L5:4966:A:H5''	39:LB:128:LYS:HG3	1.86	0.58
11:SG:221:LYS:HG2	11:SG:224:ARG:HH21	1.67	0.58
1:S2:889:U:H4'	1:S2:890:U:H5'	1.86	0.58
7:SD:162:ASP:OD1	7:SD:165:ASN:ND2	2.32	0.58
9:SE:162:ILE:HG22	9:SE:169:ILE:HA	1.84	0.58
1:S2:377:G:H5'	15:SI:99:ASN:HB2	1.85	0.57
1:S2:537:C:H2'	1:S2:538:U:H6	1.67	0.57
1:S2:1330:G:H4'	1:S2:1331:C:H3'	1.85	0.57
3:L5:2756:G:N7	62:LZ:51:ARG:NH2	2.51	0.57
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.39	0.57
11:SG:98:ARG:NH1	11:SG:99:GLY:O	2.37	0.57
13:SH:69:LEU:HD13	13:SH:96:ALA:HB2	1.85	0.57
37:Sg:31:ILE:HG12	37:Sg:45:LEU:HD11	1.86	0.57
1:S2:107:A:H2'	1:S2:108:G:C8	2.38	0.57
1:S2:541:U:H3'	1:S2:542:U:C6	2.39	0.57
1:S2:1024:A:OP2	24:SN:124:ARG:NH2	2.33	0.57
3:L5:704:C:O2'	3:L5:705:G:OP1	2.21	0.57
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.39	0.57
3:L5:3886:G:O6	82:L5:5114:SPD:H82	2.05	0.57
3:L5:4478:G:O2'	3:L5:4602:A:N1	2.38	0.57
13:SH:14:GLU:O	13:SH:15:LYS:C	2.47	0.57
37:Sg:205:SER:HA	37:Sg:221:LEU:H	1.68	0.57
60:LY:66:GLN:H	60:LY:66:GLN:CD	2.12	0.57
1:S2:1579:A:H4'	1:S2:1581:C:H5	1.69	0.57
1:S2:1416:C:H2'	1:S2:1417:C:C6	2.40	0.57
3:L5:171:U:H4'	3:L5:172:C:H5'	1.85	0.57
3:L5:3878:C:OP2	83:L5:5121:PUT:H12	2.04	0.57
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.40	0.57
11:SG:52:ILE:HD13	11:SG:102:VAL:HG21	1.86	0.57
50:LN:159:ARG:HB3	50:LN:164:LEU:HB2	1.86	0.57
55:LS:71:SER:O	55:LS:76:LYS:NZ	2.37	0.57
64:Lh:15:GLU:CD	64:Lh:15:GLU:H	2.13	0.57
1:S2:15:U:H2'	1:S2:16:G:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:51:U:H2'	1:S2:52:G:C8	2.40	0.57
3:L5:2566:G:H2'	3:L5:2567:G:H8	1.69	0.57
1:S2:140:C:H42	1:S2:313:A:H61	1.52	0.57
12:SF:78:MET:O	12:SF:79:HIS:HB2	2.04	0.57
16:SQ:44:PRO:HD3	16:SQ:77:HIS:HB3	1.85	0.57
50:LN:120:TRP:HE1	50:LN:123:GLU:HG3	1.68	0.57
58:LU:100:LEU:HD13	58:LU:112:LEU:HD23	1.86	0.57
1:S2:528:A:H2'	1:S2:529:A:C8	2.39	0.57
1:S2:534:G:H2'	1:S2:535:G:C8	2.39	0.57
3:L5:4993:G:H22	3:L5:5058:A:H2	1.51	0.57
17:SU:56:MET:HE2	17:SU:56:MET:HA	1.87	0.57
3:L5:4546:A:N7	38:LA:215:ASN:ND2	2.51	0.57
27:SP:93:MET:HE2	27:SP:93:MET:HA	1.87	0.57
62:LZ:30:ASP:O	62:LZ:39:SER:OG	2.20	0.56
1:S2:1520:G:N3	1:S2:1520:G:H2'	2.20	0.56
3:L5:1210:C:H41	66:LF:66[A]:ARG:CZ	2.18	0.56
3:L5:1253:G:H22	3:L5:1256:G:H5'	1.69	0.56
3:L5:1479:G:O2'	3:L5:1480:C:H5'	2.05	0.56
30:SY:27:VAL:HG11	30:SY:35:VAL:HG11	1.87	0.56
37:Sg:179:LEU:H	37:Sg:179:LEU:HD12	1.70	0.56
1:S2:1416:C:OP1	28:ST:129:ARG:NH1	2.38	0.56
1:S2:1750:C:H41	61:LW:73:ARG:HH21	1.52	0.56
3:L5:664:G:N2	3:L5:667:A:H61	2.02	0.56
3:L5:3888:G:C4'	82:L5:5114:SPD:H52	2.35	0.56
17:SU:21:ARG:HD2	17:SU:88:LEU:HD22	1.87	0.56
1:S2:1630:A:H5''	22:SS:37:GLY:H	1.69	0.56
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.21	0.56
1:S2:808:A:H3'	1:S2:809:A:H8	1.70	0.56
3:L5:969:C:N4	43:LE:121:VAL:O	2.38	0.56
8:SJ:136:ARG:HA	8:SJ:141:VAL:HA	1.88	0.56
11:SG:85:ARG:O	11:SG:87:ARG:NH1	2.38	0.56
17:SU:56:MET:HB2	17:SU:86:LYS:HB3	1.88	0.56
26:SR:104:GLU:O	26:SR:108:LEU:HD22	2.05	0.56
37:Sg:67:SER:H	37:Sg:82:SER:HA	1.70	0.56
68:Ld:95:ASP:O	68:Ld:98:SER:OG	2.22	0.56
1:S2:1564:C:P	28:ST:121:ARG:HH22	2.29	0.56
3:L5:4143:G:O2'	3:L5:4144:C:O4'	2.21	0.56
15:SI:128:LYS:HE2	15:SI:130:THR:HG22	1.88	0.56
16:SQ:113:ILE:HG13	16:SQ:117:ARG:HG2	1.86	0.56
1:S2:433:A:H5''	15:SI:22:HIS:HB3	1.87	0.56
3:L5:2494:U:H2'	3:L5:2495:U:O4'	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.06	0.56
14:SW:86:LEU:O	14:SW:90:GLN:HG3	2.06	0.56
30:SY:5:VAL:O	30:SY:43:LYS:NZ	2.39	0.56
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.40	0.56
1:S2:1712:A:H2'	1:S2:1713:C:C6	2.41	0.56
3:L5:1437:C:N3	3:L5:2098:G:H2'	2.21	0.56
37:Sg:230:LEU:HD21	37:Sg:259:TRP:CD2	2.41	0.56
67:Lc:37:MET:HA	67:Lc:37:MET:HE2	1.87	0.56
1:S2:877:C:H2'	1:S2:878:G:C8	2.41	0.56
1:S2:898:U:H2'	1:S2:899:U:O4'	2.06	0.56
1:S2:1579:A:H4'	1:S2:1581:C:C5	2.41	0.56
3:L5:2583:C:OP2	71:Lg:76:ARG:NH1	2.36	0.56
3:L5:4187:G:OP1	82:L5:5115:SPD:H52	2.06	0.56
18:SK:80:ARG:HH22	18:SK:90:VAL:HG12	1.69	0.56
1:S2:969:U:OP2	5:SB:8:ARG:NH1	2.39	0.55
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.87	0.55
10:SC:276:THR:HA	10:SC:279:ARG:HH21	1.72	0.55
67:Lc:34:THR:HG23	67:Lc:95:ALA:HB2	1.87	0.55
3:L5:462:G:H2'	3:L5:463:A:C8	2.41	0.55
3:L5:1961:G:N2	3:L5:2024:G:O2'	2.33	0.55
3:L5:4924:C:O2	3:L5:4926:C:N4	2.35	0.55
43:LE:178:PRO:HD2	43:LE:181:LEU:HD12	1.87	0.55
1:S2:420:G:O2'	1:S2:660:C:N3	2.39	0.55
1:S2:528:A:H2'	1:S2:529:A:H8	1.71	0.55
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.42	0.55
12:SF:19:LEU:HD21	12:SF:69:VAL:HG11	1.89	0.55
26:SR:27:ASP:OD1	26:SR:30:THR:HG23	2.06	0.55
1:S2:1551:U:OP1	7:SD:9:ARG:NH1	2.40	0.55
3:L5:964:A:H2'	3:L5:965:G:H4'	1.88	0.55
3:L5:1755:C:N3	52:LD:3:PHE:HB3	2.21	0.55
6:SA:50:ASN:HB3	6:SA:53:ARG:HG3	1.88	0.55
10:SC:68:ARG:HD2	10:SC:276:THR:HG21	1.87	0.55
13:SH:73:GLN:HA	13:SH:76:GLN:HB2	1.86	0.55
2:L8:141:C:H2'	2:L8:142:U:C6	2.42	0.55
3:L5:968:C:H5'	43:LE:110:ARG:HH22	1.71	0.55
3:L5:3887:OMC:HM22	82:L5:5114:SPD:H31	1.89	0.55
13:SH:18:GLU:HG2	13:SH:19:PHE:H	1.71	0.55
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.42	0.55
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.42	0.55
10:SC:131:GLY:HA3	10:SC:216:MET:HB3	1.87	0.55
3:L5:2488:C:H2'	3:L5:2489:C:O4'	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2758:G:O2'	3:L5:2765:A:N3	2.36	0.55
3:L5:4065:G:H2'	3:L5:4066:U:C6	2.41	0.55
36:Sf:140:TYR:HB3	36:Sf:147:THR:HG23	1.88	0.55
61:LW:120:GLN:HA	61:LW:123:LYS:HE2	1.89	0.55
1:S2:535:G:H2'	1:S2:536:A:H8	1.71	0.55
3:L5:1697:G:H21	3:L5:2084:C:P	2.29	0.55
15:SI:56:ARG:HA	15:SI:180:GLY:HA2	1.88	0.55
19:SO:46:ASP:OD2	19:SO:48:SER:OG	2.24	0.55
42:LH:129:ARG:NE	42:LH:156:ASN:OD1	2.37	0.55
1:S2:1746:U:H4'	11:SG:65:GLN:HE21	1.71	0.55
3:L5:93:G:H2'	3:L5:94:A:C8	2.42	0.55
3:L5:162:A:H2'	3:L5:163:A:C8	2.42	0.55
3:L5:968:C:OP1	43:LE:110:ARG:NH1	2.35	0.55
3:L5:1359:G:H4'	50:LN:203:TYR:HB2	1.88	0.55
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.42	0.55
3:L5:4739:C:H2'	3:L5:4740:G:H5'	1.89	0.55
19:SO:34:PHE:HB3	19:SO:41:PHE:HB2	1.89	0.55
44:LG:105:GLU:OE2	44:LG:113:ARG:NH1	2.40	0.55
59:LX:87:MET:HE1	59:LX:155:ILE:HG22	1.88	0.55
1:S2:639:C:H2'	1:S2:640:A:H8	1.72	0.55
1:S2:1563:G:H2'	1:S2:1564:C:H6	1.72	0.55
6:SA:52:LYS:NZ	29:SV:82:ASN:OD1	2.40	0.55
12:SF:77:MET:HE3	12:SF:84:GLY:C	2.33	0.55
22:SS:38:ARG:HB3	28:ST:45:LEU:HD21	1.88	0.55
66:LF:182:TYR:HB3	66:LF:200:ARG:HG3	1.89	0.55
1:S2:543:C:C2	1:S2:544:G:H1'	2.41	0.54
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.07	0.54
3:L5:1730:U:H1'	56:LT:101:SER:HB3	1.90	0.54
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.42	0.54
6:SA:54:THR:OG1	6:SA:162:PRO:O	2.22	0.54
1:S2:581:U:OP1	8:SJ:133:ARG:NH2	2.34	0.54
1:S2:1217:A:H2'	1:S2:1218:C:C6	2.41	0.54
1:S2:1406:G:H2'	1:S2:1407:U:C6	2.43	0.54
3:L5:1448:G:H1'	3:L5:2098:G:H5'	1.89	0.54
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.07	0.54
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.73	0.54
7:SD:172:VAL:O	7:SD:173:ARG:NH1	2.34	0.54
34:Sc:12:ALA:HB1	34:Sc:32:VAL:HB	1.88	0.54
41:LJ:40:LEU:HD12	41:LJ:70:VAL:HG22	1.90	0.54
41:LJ:43:LEU:HD13	41:LJ:117:ILE:HD11	1.90	0.54
1:S2:1203:G:H2'	1:S2:1204:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:493:G:H22	3:L5:661:C:H1'	1.72	0.54
3:L5:1178:G:HO2'	52:LD:286:SER:HG	1.52	0.54
3:L5:1768:C:H2'	3:L5:1769:G:C8	2.42	0.54
3:L5:3887:OMC:HM21	82:L5:5114:SPD:H31	1.90	0.54
3:L5:4452:U:O4'	86:L5:5101:ANM:H10	2.07	0.54
13:SH:10:LYS:H	13:SH:15:LYS:HD3	1.71	0.54
37:Sg:108:VAL:HA	37:Sg:124:SER:HA	1.88	0.54
1:S2:156:G:H5''	11:SG:2:LYS:HE3	1.89	0.54
1:S2:382:C:H2'	1:S2:383:G:H8	1.73	0.54
1:S2:1283:C:O2'	1:S2:1313:A:N1	2.35	0.54
1:S2:1445:PSU:O2	1:S2:1446:A:N6	2.40	0.54
14:SW:23:ARG:HH11	14:SW:23:ARG:HG3	1.72	0.54
31:SZ:98:LYS:NZ	31:SZ:113:THR:OG1	2.40	0.54
35:Se:102:LYS:HD3	35:Se:106:ALA:HB1	1.89	0.54
36:Sf:119:ARG:HD2	36:Sf:139:HIS:CD2	2.42	0.54
1:S2:391:C:H2'	1:S2:392:A:H8	1.72	0.54
1:S2:551:U:H4'	35:Se:113:ASN:HB3	1.88	0.54
3:L5:1445:U:H2'	3:L5:1446:C:C5	2.42	0.54
6:SA:69:GLU:OE1	6:SA:120:ARG:NH2	2.40	0.54
9:SE:124:CYS:HB3	9:SE:141:THR:HB	1.89	0.54
9:SE:141:THR:OG1	9:SE:143:ASP:OD1	2.24	0.54
21:SM:50:CYS:HB2	21:SM:110:VAL:HG22	1.89	0.54
1:S2:996:A:H2'	1:S2:997:A:C8	2.42	0.54
3:L5:1766:A:N3	3:L5:1767:A:N6	2.55	0.54
50:LN:60:VAL:HG22	50:LN:134:LEU:HB2	1.88	0.54
51:LI:87:ILE:HG12	51:LI:138:ILE:HG12	1.90	0.54
1:S2:545:A:H2'	1:S2:546:G:N7	2.23	0.54
1:S2:828:G:OP1	8:SJ:6:SER:OG	2.25	0.54
14:SW:14:ILE:HG13	14:SW:27:ILE:HD11	1.89	0.54
1:S2:393:U:H4'	1:S2:394:G:H5'	1.89	0.54
1:S2:1452:A:H5''	26:SR:48:ASN:HD22	1.73	0.54
1:S2:1511:U:H2'	1:S2:1512:C:C6	2.42	0.54
1:S2:1651:A:H1'	12:SF:83:ASN:HD22	1.71	0.54
12:SF:143:PRO:HA	12:SF:146:ARG:HG2	1.90	0.54
20:SX:41:PHE:O	20:SX:76:LYS:NZ	2.36	0.54
29:SV:58:ALA:O	29:SV:62:MET:HG3	2.08	0.54
1:S2:495:U:H2'	1:S2:496:C:O4'	2.07	0.54
1:S2:562:U:H2'	1:S2:563:G:C8	2.42	0.54
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.08	0.54
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.43	0.54
17:SU:54:VAL:HB	17:SU:88:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SR:30:THR:O	26:SR:34:VAL:HG23	2.07	0.54
37:Sg:133:ASN:HD21	37:Sg:139:LYS:HD3	1.73	0.54
1:S2:531:A:H2'	1:S2:532:C:H6	1.72	0.54
1:S2:542:U:H2'	1:S2:543:C:C6	2.43	0.54
1:S2:1144:A:H2'	1:S2:1145:A:C8	2.44	0.54
1:S2:1201:U:H2'	1:S2:1202:U:C6	2.43	0.54
18:SK:53:LYS:NZ	18:SK:60:GLU:OE1	2.31	0.54
21:SM:60:MET:H	21:SM:60:MET:CE	2.17	0.54
41:LJ:41:GLU:HG3	41:LJ:48:PRO:HD3	1.90	0.54
52:LD:62:CYS:HB3	52:LD:105:LEU:HD22	1.90	0.54
3:L5:491:G:H2'	3:L5:492:U:C6	2.43	0.53
3:L5:4472:G:O2'	76:Lm:100:TYR:O	2.24	0.53
3:L5:4918:C:H2'	3:L5:4919:G:C8	2.43	0.53
27:SP:37:TYR:HE1	27:SP:112:ILE:HG22	1.73	0.53
37:Sg:252:THR:HG21	37:Sg:257:LYS:HD2	1.90	0.53
67:Lc:48:LEU:HD21	67:Lc:60:ILE:HG21	1.90	0.53
2:L8:85:U:O4	60:LY:50:ARG:NH2	2.40	0.53
3:L5:1959:U:H4'	3:L5:1961:G:H1'	1.88	0.53
3:L5:3887:OMC:O2	82:L5:5114:SPD:H81	2.07	0.53
3:L5:4371:G:H5'	87:L5:5102:3H3:H31	1.89	0.53
6:SA:85:ARG:HB2	26:SR:81:ARG:NH1	2.23	0.53
7:SD:42:THR:HG22	7:SD:43:PRO:HD2	1.90	0.53
13:SH:53:VAL:HG12	13:SH:175:GLY:HA3	1.91	0.53
17:SU:95:SER:HA	17:SU:98:VAL:HG12	1.90	0.53
27:SP:60:LEU:HD13	27:SP:89:MET:HG2	1.89	0.53
1:S2:1706:G:H5'	77:Ln:1:MET:HB2	1.90	0.53
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	1.90	0.53
3:L5:4145:C:H2'	3:L5:4146:G:H8	1.73	0.53
3:L5:5061:A:H5''	3:L5:5062:G:H8	1.73	0.53
21:SM:33:ARG:HD3	21:SM:89:VAL:HG11	1.91	0.53
45:LO:61:ARG:HA	45:LO:70:PRO:HD2	1.89	0.53
46:LL:144:LEU:HD12	46:LL:145:LYS:HG2	1.89	0.53
1:S2:942:G:H2'	1:S2:943:U:C6	2.44	0.53
1:S2:1797:U:H2'	1:S2:1798:C:C6	2.44	0.53
17:SU:81:GLN:OE1	17:SU:83:ARG:NH1	2.40	0.53
42:LH:137:SER:HB3	42:LH:143:GLU:HB3	1.90	0.53
1:S2:1826:G:HO2'	3:L5:3759:A:HO2'	1.57	0.53
3:L5:188:G:H4'	3:L5:189:G:H5'	1.91	0.53
3:L5:666:G:H5'	63:Lr:67:ARG:HH21	1.73	0.53
1:S2:51:U:H2'	1:S2:52:G:H8	1.74	0.53
1:S2:1705:C:H2'	1:S2:1706:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:186:G:OP2	46:LL:44:ARG:NH2	2.39	0.53
3:L5:260:C:H2'	3:L5:261:G:C8	2.44	0.53
3:L5:653:U:H2'	3:L5:654:C:H6	1.74	0.53
18:SK:1:MET:HE1	18:SK:43:LEU:HG	1.91	0.53
41:LJ:55:TYR:HA	41:LJ:64:ARG:HG3	1.91	0.53
51:LI:152:LEU:HB3	51:LI:165:ILE:HD12	1.91	0.53
1:S2:847:A:O2'	9:SE:106:LYS:NZ	2.41	0.53
1:S2:1129:G:OP1	33:Sb:22:LYS:NZ	2.41	0.53
2:L8:148:A:H2'	2:L8:149:G:C8	2.44	0.53
3:L5:4524:G:C2	39:LB:252:ALA:HB1	2.44	0.53
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.43	0.53
28:ST:112:MET:HE2	28:ST:112:MET:HA	1.91	0.53
67:Lc:45:LEU:HD23	67:Lc:96:ILE:HD12	1.91	0.53
3:L5:4744:A:H2'	3:L5:4745:G:O4'	2.08	0.53
31:SZ:79:ILE:HB	31:SZ:83:LEU:HD23	1.91	0.53
37:Sg:12:LYS:HG3	37:Sg:306:LEU:HD22	1.91	0.53
37:Sg:174:VAL:HB	37:Sg:188:HIS:HB2	1.91	0.53
44:LG:108:GLN:O	44:LG:112:GLN:HG2	2.08	0.53
1:S2:379:C:O2	15:SI:5:ARG:NE	2.42	0.53
1:S2:1255:G:OP1	1:S2:1256:G:O2'	2.26	0.53
1:S2:1315:U:H2'	1:S2:1316:C:H6	1.73	0.53
3:L5:1445:U:H2'	3:L5:1446:C:C6	2.43	0.53
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.44	0.53
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.44	0.53
18:SK:90:VAL:O	18:SK:95:ARG:NH1	2.39	0.53
36:Sf:123:SER:HB3	36:Sf:126:CYS:HB3	1.91	0.53
69:Le:89:LEU:HD13	69:Le:118:LEU:HD22	1.91	0.53
1:S2:1017:U:H5'	24:SN:55:ARG:HD3	1.91	0.52
3:L5:116:G:H2'	3:L5:117:C:C6	2.44	0.52
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.73	0.52
44:LG:217:LYS:O	44:LG:220:GLU:HG3	2.08	0.52
1:S2:571:U:O2'	30:SY:60:PHE:O	2.27	0.52
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.44	0.52
37:Sg:118:ARG:O	37:Sg:134:THR:OG1	2.28	0.52
38:LA:234:LYS:HG2	38:LA:238:ILE:HG12	1.92	0.52
1:S2:75:G:O2'	11:SG:155:GLN:OE1	2.27	0.52
9:SE:54:TYR:O	30:SY:15:ASN:ND2	2.42	0.52
12:SF:100:ILE:O	12:SF:104:THR:OG1	2.28	0.52
14:SW:30:CYS:HB2	14:SW:61:ILE:HG13	1.90	0.52
21:SM:126:GLU:OE2	21:SM:129:LYS:HE2	2.10	0.52
27:SP:137:HIS:HA	27:SP:140:ARG:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:ST:111:LYS:NZ	28:ST:126:GLN:HG2	2.23	0.52
1:S2:546:G:H2'	1:S2:547:G:O4'	2.08	0.52
1:S2:553:U:H2'	1:S2:555:A:H8	1.74	0.52
1:S2:1736:G:H2'	1:S2:1737:G:C8	2.45	0.52
3:L5:1743:A:O4'	52:LD:15:ARG:HD2	2.10	0.52
7:SD:163:PRO:O	7:SD:167:TYR:HB2	2.09	0.52
1:S2:74:G:H2'	1:S2:75:G:O4'	2.10	0.52
1:S2:531:A:H2'	1:S2:532:C:C6	2.45	0.52
1:S2:1037:G:H4'	1:S2:1845:A:H4'	1.91	0.52
6:SA:30:LEU:HD21	6:SA:35:GLU:HG2	1.90	0.52
6:SA:85:ARG:HB2	26:SR:81:ARG:HH12	1.75	0.52
8:SJ:136:ARG:HE	8:SJ:158:ASP:HB3	1.75	0.52
13:SH:10:LYS:HB3	13:SH:11:PRO:HD2	1.92	0.52
13:SH:40:LEU:HD23	13:SH:43:LEU:HB2	1.92	0.52
17:SU:20:ILE:HG21	17:SU:98:VAL:HG21	1.91	0.52
46:LL:91:ALA:HB1	46:LL:96:ILE:HB	1.90	0.52
1:S2:536:A:H2'	1:S2:537:C:O4'	2.10	0.52
1:S2:1667:U:H2'	1:S2:1668:U:C6	2.45	0.52
21:SM:119:GLN:HA	21:SM:121:LYS:HZ2	1.74	0.52
37:Sg:11:LEU:HB2	37:Sg:307:VAL:HB	1.90	0.52
69:Le:89:LEU:HD12	91:Le:315:HOH:O	2.09	0.52
1:S2:943:U:O2'	19:SO:135:ILE:O	2.27	0.52
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.10	0.52
1:S2:1753:C:O2'	1:S2:1754:G:H8	1.92	0.52
26:SR:34:VAL:HG12	26:SR:38:ILE:HD13	1.92	0.52
39:LB:140:GLU:O	39:LB:144:LYS:HG3	2.10	0.52
1:S2:553:U:H2'	1:S2:555:A:C8	2.45	0.52
1:S2:1199:A:OP1	32:Sa:2:THR:N	2.42	0.52
3:L5:982:U:H2'	3:L5:983:C:C6	2.45	0.52
3:L5:1294:A:H1'	3:L5:1295:C:H5	1.74	0.52
3:L5:2849:A:O2'	3:L5:2855:G:N7	2.43	0.52
3:L5:2898:G:OP2	54:LR:135:LYS:NZ	2.36	0.52
3:L5:3878:C:N3	91:L5:5862:HOH:O	2.34	0.52
3:L5:3944:OMG:H2'	3:L5:3945:A:H5'	1.91	0.52
7:SD:94:ARG:O	7:SD:101:GLN:NE2	2.43	0.52
18:SK:90:VAL:HG23	18:SK:95:ARG:HH11	1.74	0.52
37:Sg:193:GLY:H	37:Sg:213:ASP:HB3	1.74	0.52
57:LP:54:GLN:HA	57:LP:83:TRP:CD1	2.44	0.52
58:LU:28:PRO:HB3	58:LU:100:LEU:HD11	1.92	0.52
74:Lk:47:ILE:HG22	74:Lk:49:ASP:H	1.74	0.52
1:S2:545:A:H2	1:S2:546:G:O6	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:940:U:H3	1:S2:1002:U:H3	1.56	0.52
3:L5:181:C:H2'	3:L5:182:G:H8	1.73	0.52
38:LA:39:GLY:HA2	38:LA:93:LYS:HG3	1.92	0.52
62:LZ:50:PRO:HD3	62:LZ:68:ILE:HG12	1.91	0.52
1:S2:539:C:H2'	1:S2:540:U:O4'	2.10	0.51
13:SH:8:ILE:HD13	13:SH:45:ILE:CG1	2.39	0.51
16:SQ:21:ALA:HB2	16:SQ:72:VAL:HG23	1.92	0.51
69:Le:35:TRP:CZ2	69:Le:56:PRO:HD2	2.45	0.51
1:S2:186:C:H2'	1:S2:187:G:H8	1.75	0.51
1:S2:1156:U:OP1	14:SW:71:LYS:NZ	2.41	0.51
2:L8:86:U:H3'	2:L8:87:G:H5'	1.93	0.51
2:L8:144:U:H2'	2:L8:145:C:C6	2.46	0.51
11:SG:130:PRO:HG2	61:LW:83:THR:HG22	1.93	0.51
17:SU:51:LYS:HB3	17:SU:90:ASP:HB2	1.91	0.51
39:LB:155:LYS:HD3	39:LB:156:TYR:CZ	2.45	0.51
1:S2:464:A:H3'	1:S2:465:A:H8	1.74	0.51
3:L5:258:G:H2'	3:L5:259:C:C6	2.45	0.51
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.74	0.51
3:L5:4145:C:H2'	3:L5:4146:G:C8	2.45	0.51
13:SH:57:ARG:H	13:SH:57:ARG:HD3	1.73	0.51
18:SK:1:MET:HE3	18:SK:44:HIS:CD2	2.46	0.51
22:SS:65:GLU:O	22:SS:69:THR:HG22	2.10	0.51
1:S2:223:C:H2'	1:S2:224:A:C8	2.46	0.51
1:S2:496:C:H2'	1:S2:497:C:H6	1.76	0.51
1:S2:656:G:H5'	1:S2:662:G:N2	2.26	0.51
1:S2:1393:G:H2'	1:S2:1394:G:C8	2.45	0.51
3:L5:2023:C:H2'	3:L5:2024:G:O4'	2.10	0.51
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.75	0.51
3:L5:4573:G:H2'	3:L5:4574:U:O4'	2.10	0.51
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.45	0.51
4:L7:55:A:H4'	41:LJ:155:HIS:HB2	1.92	0.51
1:S2:1239:PSU:H5'	27:SP:124:LYS:HE3	1.93	0.51
3:L5:717:U:H2'	3:L5:718:C:C6	2.46	0.51
6:SA:71:PRO:HB3	6:SA:186:ARG:HH22	1.75	0.51
21:SM:59:PRO:HA	21:SM:62:VAL:HG22	1.93	0.51
1:S2:1407:U:H2'	1:S2:1408:U:C6	2.46	0.51
3:L5:1414:C:H2'	3:L5:1415:G:C8	2.46	0.51
3:L5:1699:A:O2'	3:L5:1700:G:O4'	2.17	0.51
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.44	0.51
15:SI:140:LYS:H	15:SI:140:LYS:HE2	1.75	0.51
81:Pt:10:G:N2	81:Pt:27:G:H1'	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:207:G:H3'	1:S2:208:G:H8	1.75	0.51
1:S2:1521:C:H2'	22:SS:136:THR:OG1	2.09	0.51
3:L5:469:C:H2'	3:L5:470:A:H8	1.75	0.51
3:L5:3869:OMC:C4	82:L5:5114:SPD:H71	2.45	0.51
5:SB:77:ASP:N	5:SB:77:ASP:OD1	2.43	0.51
7:SD:211:VAL:O	26:SR:20:TYR:OH	2.29	0.51
9:SE:100:ARG:HB2	9:SE:114:ILE:HD13	1.92	0.51
24:SN:25:TRP:CD2	33:Sb:82:LYS:HE3	2.46	0.51
37:Sg:195:LEU:HA	37:Sg:211:GLY:HA3	1.92	0.51
3:L5:3888:G:O4'	82:L5:5114:SPD:H52	2.11	0.51
3:L5:4102:C:N4	3:L5:4103:C:O2	2.44	0.51
17:SU:26:SER:HB3	17:SU:32:LEU:HD13	1.92	0.51
1:S2:538:U:H2'	1:S2:539:C:O4'	2.11	0.51
3:L5:739:G:H4'	3:L5:740:G:OP2	2.11	0.51
37:Sg:7:LEU:HB2	37:Sg:310:TRP:NE1	2.25	0.51
1:S2:1171:G:O2'	1:S2:1187:G:O6	2.22	0.51
1:S2:1338:G:H4'	17:SU:74:SER:H	1.75	0.51
3:L5:23:C:H2'	3:L5:24:G:O4'	2.11	0.51
3:L5:1855:G:OP1	65:Lb:4:SER:HB2	2.11	0.51
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.10	0.51
15:SI:113:TYR:OH	15:SI:156:ALA:O	2.22	0.51
42:LH:44:GLU:OE2	48:LM:2:VAL:N	2.44	0.51
1:S2:1270:G:O2'	1:S2:1301:A:N7	2.44	0.50
1:S2:1279:C:H2'	1:S2:1280:G:H8	1.76	0.50
3:L5:493:G:N2	3:L5:661:C:O2'	2.44	0.50
3:L5:516:C:H2'	3:L5:517:C:C6	2.46	0.50
7:SD:143:ARG:HB3	7:SD:143:ARG:NH1	2.26	0.50
12:SF:88:MET:O	12:SF:91:ARG:HG3	2.11	0.50
15:SI:61:ASP:N	15:SI:61:ASP:OD1	2.44	0.50
68:Ld:19:GLU:OE1	68:Ld:92:ARG:NH1	2.42	0.50
1:S2:115:U:H2'	1:S2:116:OMU:C6	2.42	0.50
1:S2:552:G:H2'	1:S2:553:U:C6	2.46	0.50
1:S2:674:C:H2'	1:S2:675:U:C6	2.46	0.50
1:S2:1740:C:H2'	1:S2:1741:U:C6	2.46	0.50
3:L5:4648:A:OP1	54:LR:62:ARG:NH2	2.44	0.50
6:SA:208:GLU:O	6:SA:211:GLU:HG3	2.11	0.50
15:SI:106:SER:HB3	15:SI:171:LEU:HG	1.92	0.50
37:Sg:35:SER:OG	37:Sg:36:ARG:N	2.44	0.50
43:LE:201:ILE:HG13	43:LE:203:ILE:HG23	1.93	0.50
1:S2:317:C:OP2	11:SG:183:ARG:NH1	2.45	0.50
3:L5:179:G:O6	3:L5:258:G:N2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1881:OMC:C2	3:L5:1881:OMC:HM23	2.46	0.50
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.25	0.50
3:L5:4635:A:O2'	3:L5:4637:OMG:OP1	2.25	0.50
3:L5:4743:G:H2'	3:L5:4744:A:H8	1.77	0.50
3:L5:4750:G:H2'	3:L5:4751:G:H8	1.73	0.50
36:Sf:121:CYS:HB2	36:Sf:132:MET:CE	2.41	0.50
74:Lk:29:LYS:NZ	74:Lk:29:LYS:HB3	2.26	0.50
1:S2:538:U:H2'	1:S2:539:C:C6	2.46	0.50
1:S2:573:PSU:N3	1:S2:576:A2M:OP2	2.29	0.50
1:S2:639:C:H2'	1:S2:640:A:C8	2.46	0.50
1:S2:1692:PSU:H2'	1:S2:1693:G:C8	2.47	0.50
3:L5:1836:G:OP1	56:LT:129:LYS:NZ	2.45	0.50
3:L5:2297:G:N7	82:L5:5112:SPD:N6	2.57	0.50
3:L5:3946:G:H2'	3:L5:3947:A:C8	2.46	0.50
11:SG:32:MET:HE3	11:SG:63:MET:HG2	1.94	0.50
12:SF:79:HIS:O	12:SF:80:GLY:C	2.54	0.50
30:SY:99:LYS:HB2	30:SY:101:LYS:HD2	1.93	0.50
1:S2:65:C:H1'	11:SG:160:LYS:HD3	1.92	0.50
1:S2:494:C:N4	1:S2:509:OMG:HN22	2.09	0.50
1:S2:1088:U:H4'	1:S2:1089:G:OP2	2.11	0.50
1:S2:1227:G:C2	1:S2:1228:A:C8	2.99	0.50
1:S2:1407:U:O2'	16:SQ:11:GLN:NE2	2.30	0.50
1:S2:1578:U:H5''	1:S2:1579:A:O4'	2.11	0.50
3:L5:2412:A:H2'	3:L5:2413:U:C6	2.46	0.50
3:L5:2696:A:H5'	74:Lk:70:LYS:HG2	1.93	0.50
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.76	0.50
4:L7:62:U:OP2	52:LD:276:LYS:NZ	2.37	0.50
28:ST:78:ILE:HD12	28:ST:78:ILE:H	1.76	0.50
59:LX:82:THR:HG21	64:Lh:37:THR:HG22	1.93	0.50
1:S2:1595:U:H2'	1:S2:1596:U:C6	2.46	0.50
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.11	0.50
3:L5:2497:C:H2'	3:L5:2498:C:H6	1.76	0.50
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.46	0.50
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.47	0.50
3:L5:4340:U:N3	87:L5:5102:3H3:O3	2.43	0.50
3:L5:4343:U:O2'	78:Lo:31:ASP:OD1	2.27	0.50
5:SB:124:HIS:HA	5:SB:137:LEU:O	2.12	0.50
7:SD:133:GLY:HA3	7:SD:156:LEU:O	2.11	0.50
19:SO:54:CYS:HB2	19:SO:84:ARG:HG2	1.94	0.50
37:Sg:112:ALA:HB3	37:Sg:121:VAL:HG12	1.94	0.50
48:LM:40:GLY:HA3	48:LM:45:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1113:A:H2'	1:S2:1114:U:C6	2.47	0.50
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.11	0.50
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.47	0.50
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.46	0.50
5:SB:5:LYS:NZ	19:SO:65:ASP:OD2	2.44	0.50
10:SC:276:THR:HG23	10:SC:279:ARG:HH21	1.77	0.50
15:SI:101:ILE:HD12	15:SI:190:LEU:HD11	1.94	0.50
23:Sd:38:MET:HE1	23:Sd:50:ILE:HD11	1.93	0.50
30:SY:20:ARG:NE	30:SY:22:GLN:OE1	2.40	0.50
61:LW:90:ILE:HG22	61:LW:91:MET:HE2	1.93	0.50
1:S2:1130:G:OP2	1:S2:1130:G:N2	2.36	0.50
1:S2:1407:U:H2'	1:S2:1408:U:H6	1.77	0.50
3:L5:946:C:H5'	40:LC:336:ARG:HD3	1.93	0.50
3:L5:1564:A:H2'	3:L5:1565:A:C8	2.47	0.50
3:L5:2493:G:H2'	3:L5:2494:U:C6	2.46	0.50
3:L5:3888:G:H4'	82:L5:5114:SPD:H52	1.93	0.50
3:L5:4456:OMC:HM21	39:LB:241:PRO:HD3	1.91	0.50
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.47	0.50
3:L5:1548:G:O2'	3:L5:2812:A:N3	2.43	0.50
17:SU:94:PRO:HG2	17:SU:97:ILE:HG22	1.94	0.50
21:SM:24:THR:HA	21:SM:27:ILE:HG12	1.93	0.50
28:ST:72:VAL:HG12	28:ST:104:LEU:HD12	1.94	0.50
37:Sg:32:LEU:HD11	37:Sg:92:LEU:HD21	1.93	0.50
1:S2:1779:G:H2'	1:S2:1780:G:C8	2.47	0.49
3:L5:653:U:H2'	3:L5:654:C:C6	2.46	0.49
3:L5:966:A:OP1	3:L5:967:C:N4	2.45	0.49
3:L5:2100:A:H2'	3:L5:2101:C:C6	2.47	0.49
3:L5:4107:G:H2'	3:L5:4108:G:H8	1.76	0.49
3:L5:4897:G:OP1	48:LM:128:LYS:NZ	2.45	0.49
6:SA:85:ARG:NH1	6:SA:203:PHE:O	2.40	0.49
6:SA:137:ALA:HB1	6:SA:142:LEU:HB3	1.94	0.49
10:SC:105:GLU:HB2	10:SC:216:MET:HE1	1.94	0.49
11:SG:2:LYS:HB2	11:SG:108:VAL:HG23	1.93	0.49
1:S2:1406:G:H2'	1:S2:1407:U:H6	1.76	0.49
3:L5:106:A:H2'	3:L5:107:G:O4'	2.12	0.49
3:L5:2814:C:H5'	3:L5:2815:A2M:OP2	2.12	0.49
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.48	0.49
5:SB:165:ARG:O	5:SB:169:MET:HG3	2.12	0.49
9:SE:18:TRP:HH2	9:SE:31:PRO:HD3	1.77	0.49
37:Sg:78:ALA:HB2	37:Sg:92:LEU:HD11	1.95	0.49
54:LR:177:LEU:HB3	54:LR:181:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:334:C:OP2	11:SG:190:ARG:NH2	2.38	0.49
1:S2:1127:C:H4'	33:Sb:17:ARG:HH11	1.78	0.49
1:S2:1207:G:H22	80:mR:36:U:H3'	1.76	0.49
3:L5:2591:A:H2'	3:L5:2592:U:C6	2.47	0.49
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.47	0.49
5:SB:122:GLU:HG2	5:SB:140:VAL:HG23	1.94	0.49
10:SC:66:LEU:HD11	10:SC:81:ILE:HG12	1.95	0.49
1:S2:16:G:H2'	1:S2:17:C:C6	2.47	0.49
1:S2:220:U:H2'	1:S2:221:A:H8	1.77	0.49
1:S2:545:A:H2'	1:S2:545:A:N3	2.28	0.49
1:S2:1513:C:H2'	1:S2:1514:G:H8	1.77	0.49
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.47	0.49
6:SA:145:ILE:HG12	6:SA:159:ILE:HB	1.92	0.49
7:SD:76:ARG:HA	18:SK:22:VAL:HG21	1.94	0.49
13:SH:17:ASP:HB3	13:SH:21:SER:N	2.28	0.49
17:SU:40:ILE:HD12	17:SU:50:VAL:HG21	1.94	0.49
17:SU:55:ARG:HH11	17:SU:87:ARG:HH21	1.60	0.49
18:SK:21:MET:N	18:SK:21:MET:HE3	2.27	0.49
21:SM:99:LYS:HE2	21:SM:101:ARG:HG3	1.94	0.49
37:Sg:197:THR:HG23	37:Sg:239:LEU:HD12	1.95	0.49
1:S2:903:A:H2'	1:S2:904:A:C8	2.47	0.49
1:S2:1748:G:H1	1:S2:1786:U:H3	1.61	0.49
3:L5:411:G:H4'	3:L5:412:G:H5''	1.95	0.49
3:L5:1266:G:N7	65:Lb:90:SER:OG	2.39	0.49
3:L5:2326:G:H5''	69:Le:127:ALA:HB2	1.95	0.49
3:L5:5064:G:N2	57:LP:75:GLN:HE22	2.07	0.49
4:L7:111:C:H2'	4:L7:112:U:O4'	2.13	0.49
5:SB:40:ASN:ND2	5:SB:76:ASN:OD1	2.44	0.49
11:SG:225:GLN:O	11:SG:228:ILE:HG13	2.12	0.49
21:SM:67:ALA:HB2	36:Sf:108:VAL:HG21	1.95	0.49
36:Sf:130:VAL:HG11	36:Sf:143:LYS:HE2	1.94	0.49
1:S2:1679:A:OP1	12:SF:60:ARG:NH2	2.42	0.49
3:L5:2022:C:H3'	3:L5:2023:C:C5	2.47	0.49
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.47	0.49
9:SE:97:GLU:C	9:SE:98:ASN:HD22	2.20	0.49
15:SI:133:GLU:OE1	15:SI:133:GLU:N	2.46	0.49
3:L5:451:C:OP2	3:L5:1294:A:N6	2.45	0.49
3:L5:469:C:H2'	3:L5:470:A:C8	2.48	0.49
3:L5:691:C:H2'	3:L5:692:A:C8	2.48	0.49
3:L5:4589:A:N1	3:L5:4621:C:O2'	2.45	0.49
17:SU:38:ASP:OD1	17:SU:39:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:LI:102:MET:HE2	51:LI:102:MET:HA	1.94	0.49
1:S2:1398:G:H22	1:S2:1448:A:H2	1.61	0.49
3:L5:946:C:C5'	40:LC:336:ARG:HD3	2.43	0.49
3:L5:1245:C:H2'	3:L5:1246:G:H8	1.76	0.49
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.48	0.49
4:L7:110:G:H2'	4:L7:111:C:C6	2.48	0.49
16:SQ:89:SER:HB3	16:SQ:112:LEU:HD13	1.93	0.49
37:Sg:5:MET:HE3	37:Sg:310:TRP:HB3	1.93	0.49
50:LN:120:TRP:HE1	50:LN:123:GLU:CG	2.26	0.49
55:LS:52:LYS:HB2	55:LS:54:MET:HG2	1.95	0.49
65:Lb:65:MET:HA	65:Lb:65:MET:HE2	1.95	0.49
3:L5:162:A:H2'	3:L5:163:A:H8	1.76	0.49
3:L5:1446:C:O2	3:L5:1446:C:H2'	2.12	0.49
3:L5:2520:C:O2	3:L5:2640:G:N2	2.46	0.49
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.48	0.49
16:SQ:115:TYR:CD2	16:SQ:116:ASP:HB2	2.48	0.49
30:SY:14:THR:HG22	30:SY:21:LYS:HG2	1.94	0.49
40:LC:156:ASP:OD2	40:LC:255:SER:OG	2.21	0.49
47:LV:71:GLU:H	47:LV:71:GLU:CD	2.21	0.49
47:LV:87:SER:HA	47:LV:97:TYR:HB3	1.95	0.49
52:LD:79:TYR:O	52:LD:82:GLU:HG2	2.12	0.49
1:S2:804:U:H2'	1:S2:805:U:C6	2.48	0.49
1:S2:1570:G:N7	28:ST:97:LYS:NZ	2.52	0.49
1:S2:1628:C:H2'	1:S2:1629:C:C6	2.48	0.49
3:L5:1087:A:H2'	3:L5:1088:C:C6	2.48	0.49
3:L5:1417:C:H2'	3:L5:1418:C:O4'	2.13	0.49
3:L5:1756:U:H2'	3:L5:1757:U:C6	2.48	0.49
3:L5:1769:G:H2'	3:L5:1770:A:H8	1.78	0.49
3:L5:3723:A2M:H2'	3:L5:3724:A2M:H8	1.95	0.49
3:L5:4140:C:H2'	3:L5:4141:G:C2	2.48	0.49
3:L5:4266:G:N3	3:L5:4266:G:H2'	2.27	0.49
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.76	0.49
11:SG:148:SER:OG	11:SG:149:LYS:N	2.46	0.49
13:SH:17:ASP:HA	13:SH:20:GLU:HB2	1.93	0.49
20:SX:66:ILE:HD12	35:Se:78:GLY:HA3	1.95	0.49
22:SS:101:ASN:O	22:SS:105:ASN:ND2	2.45	0.49
54:LR:39:GLN:NE2	54:LR:42:ARG:HH21	2.11	0.49
56:LT:102:ARG:O	56:LT:106:LEU:HG	2.13	0.49
57:LP:40:HIS:NE2	57:LP:110:ASP:O	2.43	0.49
61:LW:119:LYS:O	61:LW:123:LYS:HG2	2.12	0.49
1:S2:220:U:H2'	1:S2:221:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1030:A:H2'	1:S2:1031:A2M:H8	1.93	0.48
1:S2:1279:C:H2'	1:S2:1280:G:C8	2.47	0.48
1:S2:1304:U:C2	1:S2:1305:C:C5	3.01	0.48
3:L5:683:C:H2'	3:L5:684:G:O4'	2.12	0.48
3:L5:704:C:O2	3:L5:706:C:N4	2.46	0.48
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.48	0.48
3:L5:4169:G:H4'	3:L5:4171:C:C2	2.48	0.48
5:SB:168:MET:O	5:SB:172:MET:HG3	2.13	0.48
11:SG:193:ALA:HA	11:SG:196:LYS:HD3	1.94	0.48
26:SR:65:PRO:HB3	26:SR:73:LEU:HD13	1.94	0.48
1:S2:496:C:H2'	1:S2:497:C:C6	2.48	0.48
1:S2:1310:U:H2'	1:S2:1311:C:C6	2.48	0.48
1:S2:1396:A:O2'	1:S2:1398:G:N7	2.45	0.48
3:L5:666:G:O2'	3:L5:667:A:H5''	2.13	0.48
3:L5:1927:U:OP1	3:L5:1949:U:O2'	2.23	0.48
3:L5:2022:C:OP2	3:L5:2023:C:N4	2.34	0.48
3:L5:4342:C:O3'	78:Lo:37:GLY:HA3	2.13	0.48
3:L5:5061:A:H5''	3:L5:5062:G:C8	2.48	0.48
10:SC:253:PRO:HA	10:SC:256:TRP:CD1	2.48	0.48
37:Sg:7:LEU:HB2	37:Sg:310:TRP:HE1	1.78	0.48
39:LB:396:ARG:O	39:LB:399:LYS:HG3	2.12	0.48
56:LT:157:GLU:HG2	56:LT:160:ALA:HB3	1.94	0.48
72:Li:64:SER:O	72:Li:64:SER:OG	2.31	0.48
1:S2:5:U:H2'	1:S2:6:G:H8	1.77	0.48
1:S2:521:A:OP1	8:SJ:45:ARG:NH1	2.39	0.48
1:S2:1456:G:OP1	26:SR:59:LYS:HE3	2.14	0.48
1:S2:1466:G:H5'	26:SR:4:VAL:HG22	1.95	0.48
3:L5:1253:G:N2	3:L5:1256:G:H5'	2.28	0.48
9:SE:151:ASP:HB3	9:SE:154:ILE:HG13	1.94	0.48
22:SS:75:ARG:HE	22:SS:75:ARG:HB3	1.49	0.48
27:SP:109:PRO:O	27:SP:112:ILE:HG12	2.12	0.48
30:SY:25:ILE:HD11	30:SY:73:GLY:HA3	1.95	0.48
55:LS:81:TRP:HZ3	55:LS:130:GLU:HG2	1.78	0.48
1:S2:1123:C:OP1	5:SB:151:ARG:NH2	2.47	0.48
3:L5:2095:A:H1'	3:L5:2096:G:N7	2.29	0.48
3:L5:5040:U:H5''	39:LB:396:ARG:HH22	1.78	0.48
8:SJ:127:ARG:HD3	35:Se:105:ARG:HD3	1.94	0.48
14:SW:30:CYS:SG	14:SW:31:SER:N	2.85	0.48
52:LD:41:LYS:HB2	56:LT:68:THR:O	2.14	0.48
58:LU:28:PRO:HB2	58:LU:34:MET:HG2	1.94	0.48
1:S2:468:A2M:OP1	11:SG:96:SER:OG	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:540:U:H3'	1:S2:542:U:OP2	2.13	0.48
1:S2:644:OMG:HM23	1:S2:644:OMG:H1'	1.69	0.48
3:L5:1754:U:O2'	3:L5:1755:C:O5'	2.26	0.48
17:SU:22:ILE:HD12	17:SU:114:VAL:HG12	1.95	0.48
22:SS:84:LEU:HD12	22:SS:95:TYR:HB3	1.95	0.48
37:Sg:10:THR:HG21	37:Sg:306:LEU:HD13	1.95	0.48
1:S2:526:A:OP1	35:Se:109:ARG:NH1	2.47	0.48
1:S2:683:OMG:H4'	14:SW:4:MET:HB3	1.96	0.48
1:S2:874:G:H21	13:SH:114:GLN:NE2	2.11	0.48
3:L5:445:U:H2'	3:L5:446:C:O4'	2.13	0.48
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.48	0.48
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.13	0.48
41:LJ:95:ARG:HE	41:LJ:177:GLY:HA2	1.78	0.48
45:LO:190:ASP:OD1	45:LO:191:LYS:N	2.46	0.48
51:LI:55:ASP:OD2	51:LI:162:ARG:NE	2.46	0.48
1:S2:96:C:H2'	1:S2:97:U:C6	2.48	0.48
1:S2:560:A:H5'	8:SJ:174:LYS:HB2	1.96	0.48
1:S2:1845:A:H2'	1:S2:1846:G:H8	1.78	0.48
3:L5:664:G:N2	3:L5:667:A:N6	2.60	0.48
7:SD:134:CYS:SG	7:SD:135:GLU:N	2.86	0.48
21:SM:93:LYS:H	21:SM:93:LYS:HD3	1.78	0.48
28:ST:111:LYS:HD2	28:ST:111:LYS:O	2.14	0.48
51:LI:61:SER:HA	51:LI:126:VAL:HG12	1.95	0.48
52:LD:117:LYS:N	52:LD:117:LYS:HD2	2.29	0.48
1:S2:541:U:H2'	1:S2:542:U:O4'	2.13	0.48
3:L5:1399:G:H2'	3:L5:1400:G:C8	2.49	0.48
3:L5:4770:U:H2'	3:L5:4771:C:C5	2.49	0.48
21:SM:25:ALA:HB1	21:SM:31:LEU:HD21	1.96	0.48
60:LY:64:GLY:HA3	60:LY:66:GLN:HE22	1.79	0.48
81:Pt:4:G:H2'	81:Pt:5:G:H8	1.78	0.48
1:S2:1597:C:H4'	1:S2:1603:G:O6	2.14	0.48
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.60	0.48
8:SJ:110:LEU:HB2	8:SJ:147:PHE:HB3	1.95	0.48
9:SE:165:GLU:HG3	9:SE:166:THR:HG23	1.96	0.48
11:SG:52:ILE:HG23	11:SG:109:LEU:HD11	1.96	0.48
40:LC:41:HIS:CE1	40:LC:45:ARG:HD3	2.48	0.48
1:S2:106:C:H2'	1:S2:107:A:H8	1.79	0.48
1:S2:463:C:O3'	1:S2:464:A:H8	1.96	0.48
1:S2:527:C:H2'	1:S2:528:A:H8	1.79	0.48
1:S2:1839:U:H2'	1:S2:1840:U:C6	2.49	0.48
2:L8:85:U:H5'	2:L8:87:G:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:63:G:OP1	50:LN:169:ARG:NH2	2.46	0.48
3:L5:2297:G:H5''	82:L5:5112:SPD:N1	2.29	0.48
3:L5:3654:G:O2'	3:L5:3693:U:OP1	2.27	0.48
9:SE:72:ILE:HD12	9:SE:77:ARG:HB2	1.96	0.48
11:SG:224:ARG:HH22	11:SG:225:GLN:HG3	1.79	0.48
12:SF:40:ALA:HB1	12:SF:45:TYR:CG	2.49	0.48
15:SI:34:ALA:HB2	15:SI:56:ARG:HD2	1.96	0.48
19:SO:125:LYS:HA	19:SO:125:LYS:HD2	1.70	0.48
52:LD:258:LYS:HE3	52:LD:258:LYS:HB3	1.72	0.48
1:S2:17:C:H2'	1:S2:18:C:C6	2.49	0.47
1:S2:1098:C:H2'	1:S2:1099:G:C8	2.49	0.47
1:S2:1554:C:OP2	1:S2:1555:U:O2'	2.25	0.47
1:S2:1681:U:H2'	1:S2:1682:C:C6	2.49	0.47
3:L5:980:U:H2'	3:L5:981:C:C6	2.49	0.47
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.14	0.47
3:L5:2089:G:H1	3:L5:2096:G:N2	2.12	0.47
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.49	0.47
6:SA:205:ARG:NH2	26:SR:80:ARG:O	2.47	0.47
8:SJ:114:VAL:HG13	8:SJ:119:LEU:HB2	1.95	0.47
38:LA:101:VAL:HG22	38:LA:165:VAL:HG22	1.96	0.47
52:LD:115:MET:HA	52:LD:118:ILE:HD12	1.96	0.47
52:LD:289:ARG:HD2	52:LD:293:ARG:HH21	1.79	0.47
54:LR:171:LYS:O	54:LR:175:GLU:HG2	2.14	0.47
1:S2:159:A2M:O5'	1:S2:159:A2M:H8	2.14	0.47
1:S2:165:G:H4'	11:SG:53:SER:HB2	1.95	0.47
1:S2:525:A:H2'	1:S2:526:A:H8	1.78	0.47
1:S2:1199:A:H2'	1:S2:1200:A:C8	2.49	0.47
1:S2:1513:C:OP1	23:Sd:10:HIS:HB3	2.14	0.47
1:S2:1670:C:H2'	1:S2:1671:G:C8	2.49	0.47
1:S2:1801:A:H2'	1:S2:1802:C:H6	1.75	0.47
2:L8:85:U:H5''	2:L8:86:U:H3'	1.96	0.47
3:L5:3856:A:H5''	57:LP:83:TRP:O	2.14	0.47
3:L5:4635:A:H3'	3:L5:4636:PSU:H4'	1.96	0.47
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.49	0.47
10:SC:174:ILE:O	10:SC:200:ARG:NH1	2.48	0.47
10:SC:191:VAL:HG11	10:SC:236:PHE:HA	1.96	0.47
17:SU:66:ARG:HH11	17:SU:66:ARG:HG3	1.79	0.47
17:SU:80:PHE:HB3	23:Sd:52:PHE:HB3	1.95	0.47
44:LG:83:PHE:HA	44:LG:183:ILE:HD13	1.94	0.47
45:LO:173:GLN:HG2	45:LO:176:ARG:HH21	1.79	0.47
50:LN:120:TRP:NE1	50:LN:123:GLU:HG3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1164:G:O2'	1:S2:1165:G:H5'	2.15	0.47
1:S2:1736:G:H2'	1:S2:1737:G:H8	1.78	0.47
3:L5:1268:G:N7	65:Lb:111:ARG:NH2	2.51	0.47
3:L5:1300:G:H2'	3:L5:1301:C:C6	2.49	0.47
3:L5:1727:U:OP1	66:LF:131:ASN:ND2	2.47	0.47
3:L5:4538:G:H2'	3:L5:4539:U:C6	2.50	0.47
13:SH:42:GLU:HG2	13:SH:43:LEU:HD23	1.96	0.47
24:SN:31:ASP:O	24:SN:35:GLU:HG2	2.14	0.47
31:SZ:58:LEU:HD12	31:SZ:62:VAL:HG21	1.96	0.47
37:Sg:91:ASP:OD2	37:Sg:94:THR:OG1	2.28	0.47
42:LH:36:ARG:HG2	42:LH:38:PHE:CZ	2.49	0.47
75:Ll:25:GLN:CD	75:Ll:28:ARG:HH21	2.22	0.47
1:S2:319:C:H2'	1:S2:320:G:C8	2.50	0.47
3:L5:738:C:H3'	3:L5:739:G:H5''	1.95	0.47
3:L5:985:C:H2'	3:L5:986:C:H6	1.78	0.47
3:L5:1438:U:O3'	66:LF:31:LYS:NZ	2.46	0.47
3:L5:2436:U:C4	59:LX:130:PRO:HG3	2.50	0.47
9:SE:64:ILE:HG23	9:SE:69:PHE:HE1	1.78	0.47
18:SK:55:ARG:HE	18:SK:57:TYR:HE2	1.63	0.47
57:LP:84:PRO:HB2	57:LP:87:SER:HB2	1.95	0.47
58:LU:60:VAL:HG23	58:LU:61:VAL:HG23	1.97	0.47
67:Lc:38:ILE:HG21	67:Lc:63:TYR:HB3	1.96	0.47
1:S2:57:U:OP1	1:S2:504:G:O2'	2.29	0.47
1:S2:73:C:H42	11:SG:168:LYS:HD2	1.79	0.47
1:S2:511:U:H2'	1:S2:512:A2M:H8	1.97	0.47
1:S2:543:C:C4	1:S2:544:G:H1'	2.50	0.47
1:S2:1139:C:H2'	1:S2:1140:G:O4'	2.15	0.47
1:S2:1628:C:OP1	28:ST:38:LYS:NZ	2.47	0.47
3:L5:4524:G:N3	39:LB:252:ALA:HB1	2.30	0.47
3:L5:4652:G:H2'	3:L5:4653:C:C6	2.50	0.47
6:SA:77:ILE:HG21	6:SA:133:PRO:HG3	1.96	0.47
11:SG:49:VAL:HB	11:SG:115:LYS:HB3	1.95	0.47
17:SU:22:ILE:HB	17:SU:89:ILE:HB	1.96	0.47
22:SS:47:LYS:HD3	22:SS:47:LYS:HA	1.72	0.47
28:ST:35:ASP:OD1	28:ST:35:ASP:N	2.48	0.47
40:LC:350:ARG:HG2	40:LC:350:ARG:HH11	1.79	0.47
1:S2:555:A:H2'	1:S2:556:U:C6	2.50	0.47
2:L8:89:U:H2'	2:L8:90:C:C6	2.50	0.47
3:L5:1296:G:H2'	3:L5:1297:U:C6	2.49	0.47
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.50	0.47
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2539:C:H2'	3:L5:2540:C:H6	1.80	0.47
3:L5:4522:G:O2'	3:L5:4525:C:OP2	2.32	0.47
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.14	0.47
6:SA:63:ARG:NH1	29:SV:38:GLU:HA	2.30	0.47
28:ST:42:HIS:NE2	28:ST:43:LYS:HE2	2.29	0.47
50:LN:123:GLU:OE1	50:LN:128:LYS:HE2	2.14	0.47
52:LD:65:ALA:HB2	52:LD:74:ILE:HD13	1.97	0.47
57:LP:17:SER:HB2	57:LP:98:ALA:HB2	1.96	0.47
1:S2:38:A:OP1	8:SJ:5:ARG:HG3	2.14	0.47
1:S2:194:C:H2'	1:S2:195:C:H6	1.80	0.47
1:S2:443:U:H2'	1:S2:444:G:O4'	2.15	0.47
1:S2:641:A:O2'	1:S2:645:C:OP1	2.33	0.47
1:S2:876:C:H2'	1:S2:877:C:C6	2.50	0.47
1:S2:903:A:H2'	1:S2:904:A:H8	1.80	0.47
1:S2:1405:A:H2'	1:S2:1406:G:O4'	2.15	0.47
3:L5:223:G:H4'	3:L5:225:G:N7	2.30	0.47
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.46	0.47
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.14	0.47
3:L5:1754:U:H1'	3:L5:1755:C:H5	1.80	0.47
3:L5:3604:A:H2'	3:L5:3605:C:C6	2.50	0.47
6:SA:134:LEU:HD22	6:SA:144:THR:HG21	1.97	0.47
11:SG:2:LYS:HB3	11:SG:15:LEU:HD11	1.97	0.47
11:SG:32:MET:SD	11:SG:65:GLN:HB2	2.55	0.47
11:SG:181:THR:HG22	11:SG:183:ARG:N	2.29	0.47
13:SH:78:ARG:HE	13:SH:81:ARG:HH22	1.63	0.47
13:SH:105:THR:N	13:SH:108:SER:OG	2.43	0.47
13:SH:155:LYS:NZ	14:SW:51:GLU:OE1	2.46	0.47
19:SO:121:ARG:NH1	34:Sc:40:ARG:HH12	2.12	0.47
23:Sd:39:CYS:SG	23:Sd:42:CYS:HB2	2.55	0.47
36:Sf:94:LYS:HD2	36:Sf:94:LYS:HA	1.57	0.47
39:LB:138:GLN:OE1	39:LB:138:GLN:HA	2.13	0.47
40:LC:316:LYS:HB2	40:LC:324:ILE:HG13	1.96	0.47
46:LL:190[B]:ARG:HG2	46:LL:191:LEU:HG	1.97	0.47
49:La:100:ILE:HD13	49:La:123:ILE:HB	1.97	0.47
1:S2:344:U:H2'	1:S2:345:U:C6	2.50	0.47
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.50	0.47
3:L5:1448:G:H2'	3:L5:1449:C:H6	1.79	0.47
3:L5:2491:C:H2'	3:L5:2492:C:C6	2.50	0.47
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.49	0.47
3:L5:4730:C:H3'	3:L5:4731:G:H21	1.79	0.47
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:SQ:82:TYR:O	16:SQ:85:ARG:HG2	2.15	0.47
26:SR:28:PHE:O	26:SR:32:LYS:HG2	2.15	0.47
37:Sg:158:PRO:HD3	37:Sg:200:VAL:HG21	1.96	0.47
51:LI:146:GLU:CD	51:LI:146:GLU:H	2.23	0.47
58:LU:74:SER:OG	58:LU:76:VAL:O	2.30	0.47
1:S2:484:A2M:H8	1:S2:484:A2M:O5'	2.14	0.47
1:S2:544:G:N3	1:S2:545:A:H1'	2.29	0.47
1:S2:547:G:H2'	1:S2:548:C:C6	2.50	0.47
1:S2:848:U:H2'	1:S2:849:A:H8	1.80	0.47
1:S2:1025:U:OP1	1:S2:1090:C:O2'	2.33	0.47
1:S2:1232:PSU:H2'	1:S2:1233:G:C8	2.50	0.47
1:S2:1611:G:OP2	22:SS:121:ARG:NH2	2.47	0.47
3:L5:1689:G:OP2	83:L5:5117:PUT:N1	2.48	0.47
3:L5:4076:G:OP1	44:LG:73:ARG:NE	2.41	0.47
3:L5:4455:G:H5''	39:LB:5:LYS:HE2	1.96	0.47
18:SK:80:ARG:NH1	18:SK:89:ILE:O	2.36	0.47
32:Sa:51:ARG:O	32:Sa:55:GLU:HG2	2.14	0.47
37:Sg:67:SER:N	37:Sg:81:GLY:O	2.48	0.47
64:Lh:82:ASP:OD1	64:Lh:82:ASP:N	2.48	0.47
1:S2:29:G:H2'	1:S2:30:C:C6	2.49	0.47
1:S2:301:A:H2'	1:S2:302:A:O4'	2.15	0.47
1:S2:1395:C:O2'	1:S2:1396:A:H5'	2.15	0.47
1:S2:1408:U:H2'	1:S2:1409:A:H8	1.80	0.47
1:S2:1745:A:H1'	11:SG:66:GLY:HA2	1.96	0.47
3:L5:186:G:H2'	3:L5:187:U:H4'	1.96	0.47
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.79	0.47
3:L5:2693:G:H2'	3:L5:2694:G:N2	2.30	0.47
3:L5:5034:A:H2'	3:L5:5035:U:O4'	2.15	0.47
37:Sg:12:LYS:HE2	37:Sg:12:LYS:HB2	1.62	0.47
1:S2:539:C:H1'	1:S2:546:G:O6	2.15	0.46
1:S2:1315:U:H4'	18:SK:2:LEU:HD22	1.97	0.46
1:S2:1533:A:H2	1:S2:1536:G:N3	2.13	0.46
1:S2:1560:U:H2'	1:S2:1561:A:H8	1.81	0.46
2:L8:70:G:H5''	60:LY:27:ARG:CZ	2.45	0.46
3:L5:674:G:H2'	3:L5:675:C:C6	2.50	0.46
3:L5:3923:A:H2'	3:L5:3924:C:H6	1.79	0.46
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.49	0.46
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.96	0.46
13:SH:10:LYS:HB2	13:SH:15:LYS:HE3	1.97	0.46
13:SH:14:GLU:N	13:SH:15:LYS:HZ2	2.14	0.46
26:SR:107:LYS:HB3	26:SR:107:LYS:NZ	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:206:LEU:HD22	37:Sg:218:LEU:HD12	1.96	0.46
51:LI:36:LEU:HD13	51:LI:69:ARG:HH11	1.79	0.46
72:Li:63:VAL:HG12	72:Li:65:LYS:HG3	1.96	0.46
1:S2:60:A:N3	1:S2:316:G:O2'	2.44	0.46
1:S2:178:C:H2'	1:S2:179:C:H6	1.80	0.46
1:S2:1292:C:N3	36:Sf:138:ARG:NH2	2.58	0.46
1:S2:1365:G:H2'	1:S2:1366:G:H8	1.80	0.46
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.51	0.46
1:S2:1678:A2M:HM'3	1:S2:1678:A2M:H1'	1.53	0.46
2:L8:106:G:H4'	2:L8:137:A:H5'	1.97	0.46
3:L5:492:U:H2'	3:L5:493:G:C8	2.50	0.46
3:L5:1256:G:H5''	3:L5:1257:A:C8	2.50	0.46
3:L5:1786:A:H2'	3:L5:1789:C:C5	2.50	0.46
3:L5:2516:G:O2'	71:Lg:62:LYS:NZ	2.48	0.46
3:L5:4415:A:H2'	3:L5:4416:G:O4'	2.15	0.46
3:L5:4734:A:H2'	3:L5:4735:G:H8	1.79	0.46
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.50	0.46
11:SG:10:THR:HB	11:SG:128:THR:HA	1.97	0.46
28:ST:73:GLY:O	28:ST:76:THR:OG1	2.33	0.46
40:LC:209:ILE:HB	40:LC:229:LEU:HD13	1.96	0.46
1:S2:1658:G:OP2	1:S2:1660:C:N4	2.46	0.46
1:S2:1808:U:H2'	1:S2:1809:A:C8	2.50	0.46
1:S2:1809:A:H2'	1:S2:1810:U:C6	2.51	0.46
2:L8:67:U:H2'	2:L8:68:G:H8	1.80	0.46
3:L5:286:U:H2'	3:L5:287:U:C6	2.49	0.46
3:L5:3648:A:H1'	3:L5:3785:A2M:N6	2.30	0.46
3:L5:4739:C:C2'	3:L5:4740:G:H5'	2.45	0.46
3:L5:4954:G:H2'	3:L5:4955:A:H8	1.80	0.46
6:SA:158:ASP:N	6:SA:158:ASP:OD1	2.48	0.46
7:SD:22:ASN:O	7:SD:26:THR:OG1	2.29	0.46
55:LS:113:MET:HE3	55:LS:113:MET:HB3	1.78	0.46
1:S2:376:A:H2'	1:S2:377:G:O4'	2.15	0.46
1:S2:507:G:O6	30:SY:105:LYS:NZ	2.48	0.46
1:S2:530:U:H2'	1:S2:531:A:C8	2.51	0.46
1:S2:1308:U:O2	36:Sf:140:TYR:OH	2.34	0.46
1:S2:1347:PSU:H2'	1:S2:1348:G:N3	2.30	0.46
1:S2:1520:G:N3	1:S2:1520:G:C2'	2.78	0.46
1:S2:1589:A:N3	1:S2:1653:U:O2'	2.41	0.46
1:S2:1606:G:N2	1:S2:1632:G:H1'	2.31	0.46
2:L8:87:G:H8	2:L8:87:G:OP2	1.99	0.46
3:L5:209:U:C4	3:L5:233:U:C4	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.51	0.46
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.80	0.46
3:L5:4488:A:H4'	3:L5:4489:G:C8	2.50	0.46
8:SJ:131:ARG:HD2	8:SJ:131:ARG:HA	1.72	0.46
1:S2:178:C:H2'	1:S2:179:C:C6	2.50	0.46
1:S2:352:U:H2'	1:S2:353:C:C6	2.50	0.46
1:S2:462:OMC:HM23	1:S2:462:OMC:H1'	1.60	0.46
1:S2:551:U:H2'	1:S2:552:G:C8	2.51	0.46
1:S2:1277:C:H2'	1:S2:1278:A:H8	1.80	0.46
1:S2:1354:G:N2	1:S2:1357:A:OP2	2.43	0.46
1:S2:1418:C:H2'	1:S2:1419:C:O4'	2.16	0.46
1:S2:1861:G:H5''	32:Sa:3:LYS:HA	1.96	0.46
3:L5:4401:G:H2'	3:L5:4402:C:H6	1.79	0.46
3:L5:4759:C:OP2	45:LO:171:LYS:NZ	2.39	0.46
6:SA:89:LYS:HD2	6:SA:201:LEU:HG	1.97	0.46
11:SG:219:GLU:O	11:SG:222:GLU:HG2	2.16	0.46
19:SO:44:VAL:HG12	19:SO:53:ILE:HB	1.97	0.46
21:SM:31:LEU:O	21:SM:33:ARG:NH2	2.49	0.46
39:LB:92:TYR:HB2	39:LB:159:VAL:HB	1.96	0.46
1:S2:1221:G:O2'	1:S2:1676:U:O2	2.30	0.46
1:S2:1365:G:H2'	1:S2:1366:G:C8	2.51	0.46
1:S2:1562:C:O2'	1:S2:1563:G:H5'	2.15	0.46
3:L5:1704:C:OP2	66:LF:177:ARG:NH2	2.49	0.46
3:L5:2296:G:H3'	82:L5:5112:SPD:H21	1.98	0.46
3:L5:3893:C:O2'	3:L5:4979:A:N1	2.44	0.46
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.50	0.46
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.51	0.46
3:L5:4113:U:H2'	3:L5:4114:C:C6	2.51	0.46
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.50	0.46
5:SB:125:VAL:HG22	5:SB:172:MET:HE3	1.96	0.46
6:SA:34:MET:HE2	6:SA:149:ASN:O	2.16	0.46
8:SJ:111:GLN:NE2	8:SJ:127:ARG:HB2	2.31	0.46
11:SG:67:VAL:HG12	11:SG:69:THR:HG22	1.98	0.46
21:SM:85:LEU:O	21:SM:89:VAL:HG23	2.15	0.46
31:SZ:50:PHE:HB2	31:SZ:54:THR:HB	1.96	0.46
54:LR:105:LEU:HD22	54:LR:135:LYS:HG2	1.98	0.46
65:Lb:65:MET:HE1	65:Lb:68:ARG:HH12	1.81	0.46
81:Pt:24:C:H2'	81:Pt:25:U:C6	2.50	0.46
1:S2:512:A2M:H4'	1:S2:576:A2M:H2	1.96	0.46
1:S2:829:C:OP1	9:SE:21:ASP:HB2	2.16	0.46
1:S2:952:G:H2'	1:S2:953:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1289:U:H2'	1:S2:1290:G:C8	2.51	0.46
3:L5:1774:C:H2'	3:L5:1775:A:O4'	2.15	0.46
3:L5:2099:G:C6	3:L5:2100:A:C5	3.04	0.46
3:L5:2424:OMG:HM23	3:L5:2424:OMG:H1'	1.78	0.46
3:L5:4518:A:O5'	3:L5:4520:G:H4'	2.16	0.46
4:L7:3:C:H2'	4:L7:4:U:C6	2.50	0.46
4:L7:3:C:H2'	4:L7:4:U:H6	1.79	0.46
13:SH:63:PHE:HA	13:SH:95:ILE:O	2.16	0.46
58:LU:48:LYS:HG2	58:LU:53:ALA:HB2	1.97	0.46
67:Lc:26:LYS:HB2	67:Lc:98:ASP:HB3	1.97	0.46
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.15	0.46
3:L5:3724:A2M:HM'3	3:L5:3724:A2M:H1'	1.70	0.46
3:L5:4994:G:H2'	3:L5:4995:U:C6	2.50	0.46
7:SD:46:THR:HG22	7:SD:83:SER:O	2.14	0.46
8:SJ:138:ARG:NH2	8:SJ:153:SER:OG	2.48	0.46
9:SE:107:GLY:HA2	9:SE:189:LEU:HG	1.97	0.46
12:SF:31:ASN:N	12:SF:31:ASN:OD1	2.49	0.46
22:SS:31:THR:HG22	22:SS:31:THR:O	2.14	0.46
50:LN:120:TRP:HE1	50:LN:123:GLU:CD	2.24	0.46
78:Lo:26:TYR:HB3	78:Lo:67:VAL:HB	1.98	0.46
1:S2:1349:G:H2'	1:S2:1350:U:C6	2.51	0.46
82:S2:1902:SPD:HN11	82:S2:1902:SPD:H42	1.49	0.46
3:L5:38:A:H5''	49:La:35:ALA:HB2	1.98	0.46
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.51	0.46
3:L5:1765:A:HO2'	3:L5:1766:A:P	2.38	0.46
3:L5:2093:A:O2'	3:L5:2094:G:O4'	2.31	0.46
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.81	0.46
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.51	0.46
3:L5:4258:C:H2'	3:L5:4259:C:H6	1.80	0.46
13:SH:78:ARG:HB3	13:SH:78:ARG:CZ	2.46	0.46
18:SK:3:MET:HE2	18:SK:3:MET:HB2	1.78	0.46
18:SK:10:ALA:O	18:SK:13:GLU:HG3	2.16	0.46
27:SP:50:ARG:HB2	27:SP:53:GLN:NE2	2.31	0.46
28:ST:110:LEU:O	28:ST:111:LYS:HG3	2.15	0.46
34:Sc:66:ARG:HA	34:Sc:66:ARG:HD2	1.69	0.46
39:LB:163:ILE:HG22	39:LB:180:LEU:HD22	1.97	0.46
39:LB:224:LYS:HG2	39:LB:340:THR:HG22	1.98	0.46
67:Lc:50:ASN:HB2	67:Lc:76:GLY:C	2.41	0.46
68:Ld:23:ARG:HB3	68:Ld:25:TYR:CE1	2.50	0.46
1:S2:1317:C:H2'	1:S2:1318:G:C8	2.51	0.46
3:L5:1:C:H5''	3:L5:2:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:385:A:N3	3:L5:387:G:H5''	2.31	0.46
3:L5:677:G:H2'	3:L5:678:C:C6	2.50	0.46
3:L5:1204:C:H2'	3:L5:1205:G:H8	1.81	0.46
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.50	0.46
3:L5:1672:U:H2'	3:L5:1673:U:C6	2.50	0.46
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.51	0.46
9:SE:174:LYS:HE3	9:SE:174:LYS:HB3	1.64	0.46
21:SM:53:ALA:HB2	21:SM:85:LEU:HD11	1.97	0.46
39:LB:258:HIS:HA	39:LB:259:PRO:C	2.40	0.46
57:LP:135:ARG:NH1	91:LP:304:HOH:O	2.47	0.46
61:LW:43:LYS:HB2	61:LW:43:LYS:HE2	1.70	0.46
1:S2:67:C:OP2	11:SG:172:LYS:NZ	2.32	0.45
1:S2:1025:U:H2'	1:S2:1026:C:O4'	2.15	0.45
2:L8:140:C:H2'	2:L8:141:C:C6	2.52	0.45
3:L5:268:G:H2'	3:L5:269:G:H8	1.81	0.45
3:L5:984:C:H2'	3:L5:985:C:H6	1.81	0.45
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.50	0.45
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.51	0.45
3:L5:2489:C:O2'	3:L5:2490:U:O5'	2.33	0.45
3:L5:3869:OMC:C2	82:L5:5114:SPD:C3	2.95	0.45
8:SJ:111:GLN:HE21	8:SJ:123:ILE:HG13	1.80	0.45
15:SI:98:LYS:HG3	15:SI:178:ARG:HG3	1.96	0.45
37:Sg:72:SER:HB2	37:Sg:117:ASN:ND2	2.31	0.45
37:Sg:87:LEU:HD21	37:Sg:122:SER:HB3	1.98	0.45
65:Lb:51:LYS:HB3	65:Lb:51:LYS:HE3	1.80	0.45
1:S2:199:C:O2	1:S2:199:C:H2'	2.15	0.45
1:S2:544:G:H3'	1:S2:545:A:C8	2.42	0.45
1:S2:1700:C:O2	1:S2:1834:A:N6	2.49	0.45
3:L5:223:G:H4'	3:L5:225:G:C8	2.51	0.45
3:L5:703:G:H2'	3:L5:704:C:H5''	1.98	0.45
3:L5:2900:U:H2'	3:L5:2901:G:C8	2.51	0.45
6:SA:34:MET:HE3	6:SA:34:MET:HB3	1.78	0.45
11:SG:118:GLU:HG2	11:SG:119:LYS:HD3	1.97	0.45
13:SH:138:GLU:H	13:SH:159:ASP:HB2	1.81	0.45
27:SP:93:MET:HE1	27:SP:106:GLU:HA	1.99	0.45
33:Sb:8:LEU:HB3	33:Sb:9:HIS:CE1	2.52	0.45
62:LZ:89:ILE:HD11	62:LZ:121:ARG:HG2	1.96	0.45
67:Lc:38:ILE:HD11	67:Lc:46:VAL:HG21	1.97	0.45
3:L5:208:A:H2	3:L5:233:U:OP1	1.99	0.45
3:L5:394:G:N2	3:L5:397:G:OP2	2.43	0.45
3:L5:1689:G:N7	83:L5:5117:PUT:H42	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.30	0.45
3:L5:1756:U:H2'	3:L5:1757:U:H6	1.81	0.45
3:L5:3727:A:H2'	3:L5:3728:A:C8	2.52	0.45
5:SB:123:ALA:HB2	5:SB:165:ARG:HG3	1.98	0.45
7:SD:7:LYS:HD2	17:SU:25:THR:HG21	1.99	0.45
9:SE:112:HIS:NE2	9:SE:237:SER:O	2.50	0.45
25:SL:148:ALA:O	25:SL:151:THR:OG1	2.33	0.45
78:Lo:77:CYS:SG	78:Lo:79:SER:HB2	2.56	0.45
1:S2:540:U:O2	1:S2:543:C:H5	1.99	0.45
1:S2:1220:A:H2'	1:S2:1221:G:O4'	2.17	0.45
1:S2:1320:G:H2'	1:S2:1321:G:O4'	2.17	0.45
1:S2:1528:G:H2'	1:S2:1529:C:C6	2.51	0.45
1:S2:1617:G:N2	1:S2:1619:A:H3'	2.32	0.45
1:S2:1683:C:H2'	1:S2:1684:C:H6	1.81	0.45
3:L5:1364:U:OP2	46:LL:36:ARG:NH1	2.47	0.45
3:L5:1631:A:C2	38:LA:204:MET:HG2	2.51	0.45
3:L5:3871:A:H2'	3:L5:3872:A:C8	2.51	0.45
6:SA:10:MET:HG3	6:SA:55:TRP:CE3	2.52	0.45
28:ST:99:VAL:O	28:ST:103:VAL:HG23	2.17	0.45
37:Sg:125:ARG:HG2	37:Sg:150:TRP:CG	2.51	0.45
45:LO:181:ALA:O	45:LO:185:VAL:HG22	2.17	0.45
1:S2:536:A:H2'	1:S2:537:C:C6	2.52	0.45
1:S2:681:PSU:H4'	20:SX:9:THR:HG22	1.98	0.45
1:S2:885:U:H2'	1:S2:886:A:C8	2.52	0.45
3:L5:2098:G:H8	3:L5:2098:G:O5'	1.99	0.45
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.16	0.45
3:L5:4392:OMG:H2'	3:L5:4447:5MC:HM51	1.99	0.45
10:SC:167:ARG:HG2	10:SC:219:ILE:HD13	1.98	0.45
18:SK:47:LYS:HD3	18:SK:47:LYS:HA	1.78	0.45
21:SM:58:GLU:HG2	21:SM:61:TYR:CB	2.44	0.45
30:SY:39:GLU:O	30:SY:43:LYS:HG3	2.17	0.45
36:Sf:119:ARG:HD2	36:Sf:139:HIS:NE2	2.31	0.45
40:LC:350:ARG:HG2	40:LC:350:ARG:NH1	2.32	0.45
56:LT:117:LYS:O	56:LT:121:GLU:HG2	2.17	0.45
69:Le:82:VAL:HG13	69:Le:114:ARG:HG2	1.98	0.45
1:S2:575:A:H2'	1:S2:576:A2M:O4'	2.17	0.45
1:S2:587:A:H5'	1:S2:592:C:H41	1.82	0.45
1:S2:1288:OMU:N3	1:S2:1311:C:O2	2.40	0.45
1:S2:1311:C:H2'	1:S2:1312:G:C4	2.52	0.45
2:L8:5:U:H2'	2:L8:6:C:H6	1.81	0.45
3:L5:661:C:H2'	3:L5:662:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:733:A:H2'	3:L5:734:G:O4'	2.16	0.45
3:L5:738:C:H3'	3:L5:739:G:C5'	2.47	0.45
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.98	0.45
3:L5:5013:C:H41	3:L5:5029:C:P	2.39	0.45
4:L7:117:G:OP1	52:LD:253:TYR:OH	2.30	0.45
11:SG:201:LYS:HE3	11:SG:201:LYS:HB3	1.66	0.45
15:SI:170:LYS:HE3	15:SI:170:LYS:HB2	1.70	0.45
31:SZ:48:VAL:HA	31:SZ:83:LEU:HD22	1.98	0.45
58:LU:40:GLU:O	58:LU:44:GLN:HG3	2.16	0.45
72:Li:16:LYS:HA	72:Li:16:LYS:HD3	1.69	0.45
1:S2:436:OMG:OP2	1:S2:471:G:O2'	2.32	0.45
1:S2:831:G:N7	30:SY:11:LYS:NZ	2.65	0.45
1:S2:1438:A:H2'	1:S2:1439:A:C8	2.52	0.45
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.52	0.45
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.52	0.45
7:SD:32:ASP:OD1	7:SD:33:GLY:N	2.49	0.45
18:SK:11:ILE:HG12	18:SK:45:VAL:HG22	1.99	0.45
26:SR:10:LYS:HG2	26:SR:53:TYR:CE2	2.52	0.45
26:SR:50:ILE:O	26:SR:54:VAL:HG23	2.17	0.45
26:SR:109:LEU:HD13	26:SR:111:PHE:HD2	1.81	0.45
61:LW:104:GLN:O	61:LW:107:GLN:HG3	2.17	0.45
76:Lm:79:GLU:HG2	76:Lm:80:PRO:HD2	1.99	0.45
1:S2:54:A:OP1	30:SY:111:LYS:NZ	2.47	0.45
1:S2:601:OMG:HM23	1:S2:601:OMG:H1'	1.68	0.45
1:S2:814:PSU:OP1	9:SE:22:LYS:NZ	2.47	0.45
1:S2:1408:U:H2'	1:S2:1409:A:C8	2.52	0.45
1:S2:1740:C:OP1	15:SI:44:HIS:ND1	2.35	0.45
3:L5:158:A:N1	3:L5:276:C:O2'	2.41	0.45
3:L5:408:A:O2'	3:L5:411:G:OP2	2.28	0.45
3:L5:2083:C:P	53:LQ:14:ARG:HH22	2.39	0.45
3:L5:2091:C:H1'	3:L5:2094:G:H1'	1.99	0.45
3:L5:3641:U:C6	3:L5:3645:U:C4	3.04	0.45
3:L5:3930:U:H2'	3:L5:3931:C:C6	2.51	0.45
4:L7:58:A:H2'	4:L7:59:G:C8	2.52	0.45
10:SC:60:TRP:C	10:SC:61:MET:HE2	2.41	0.45
17:SU:66:ARG:HG3	17:SU:66:ARG:NH1	2.32	0.45
30:SY:12:PHE:HA	30:SY:23:MET:HB3	1.99	0.45
30:SY:54:VAL:HG22	30:SY:76:TYR:HB2	1.97	0.45
31:SZ:98:LYS:HB3	31:SZ:98:LYS:HE2	1.63	0.45
42:LH:4:ILE:HG12	42:LH:61:TRP:CH2	2.52	0.45
49:La:76:ASP:HB3	49:La:115:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:46:A:N1	1:S2:434:G:H1'	2.32	0.45
1:S2:917:U:H2'	1:S2:918:PSU:C6	2.52	0.45
1:S2:1678:A2M:O2'	1:S2:1679:A:H5'	2.16	0.45
3:L5:2041:A:N7	3:L5:4434:C:O2'	2.50	0.45
3:L5:2101:C:H2'	3:L5:2102:G:O4'	2.17	0.45
3:L5:2478:C:O2	3:L5:2591:A:O2'	2.30	0.45
3:L5:2664:G:H4'	3:L5:2677:G:H4'	1.98	0.45
5:SB:131:ASP:OD2	5:SB:180:ASP:HB2	2.17	0.45
7:SD:223:ILE:HD11	37:Sg:189:ILE:HD12	1.98	0.45
68:Ld:51:LYS:HB2	68:Ld:51:LYS:NZ	2.32	0.45
80:mR:35:G:H2'	80:mR:36:U:H5''	1.98	0.45
1:S2:1133:A:H4'	32:Sa:13:LYS:HD2	1.99	0.45
1:S2:1533:A:C8	1:S2:1604:G:H1'	2.52	0.45
3:L5:738:C:H42	3:L5:741:C:H4'	1.81	0.45
3:L5:2461:G:H5'	50:LN:104:GLU:OE2	2.17	0.45
3:L5:3689:G:O2'	3:L5:3818:UY1:OP2	2.31	0.45
8:SJ:93:LYS:HE2	8:SJ:96:TYR:HE2	1.82	0.45
16:SQ:115:TYR:HD2	16:SQ:116:ASP:HB2	1.81	0.45
24:SN:110:ASP:O	24:SN:114:ARG:HG2	2.17	0.45
37:Sg:89:LEU:HD21	37:Sg:99:ARG:HB3	1.99	0.45
37:Sg:114:SER:HB3	37:Sg:119:GLN:HB2	1.99	0.45
43:LE:281:ILE:HG23	43:LE:286:LEU:HD21	1.99	0.45
45:LO:88:LEU:HD12	45:LO:99:LEU:HD13	1.98	0.45
1:S2:77:A:C8	11:SG:154:ARG:HG2	2.53	0.44
1:S2:1317:C:H2'	1:S2:1318:G:H8	1.82	0.44
3:L5:1186:U:H2'	3:L5:1187:G:N3	2.31	0.44
3:L5:1416:G:H2'	3:L5:1417:C:C6	2.52	0.44
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.52	0.44
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.51	0.44
3:L5:4927:G:OP2	3:L5:4927:G:N2	2.41	0.44
8:SJ:63:LEU:HD11	8:SJ:69:ARG:CZ	2.47	0.44
18:SK:1:MET:HE2	18:SK:47:LYS:HB2	1.99	0.44
19:SO:66:ARG:HG3	19:SO:67:ASP:OD1	2.16	0.44
1:S2:602:G:OP2	1:S2:603:C:O2'	2.29	0.44
1:S2:1566:G:N7	28:ST:101:ARG:NH2	2.59	0.44
2:L8:75:OMG:HM23	2:L8:75:OMG:H1'	1.77	0.44
3:L5:182:G:H2'	3:L5:183:C:H6	1.83	0.44
3:L5:456:C:H2'	3:L5:457:G:H8	1.83	0.44
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.82	0.44
3:L5:3934:G:H2'	3:L5:3935:C:C6	2.53	0.44
3:L5:4102:C:C4	3:L5:4103:C:H1'	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4195:G:OP1	3:L5:4221:C:O2'	2.30	0.44
3:L5:4920:C:H2'	3:L5:4921:C:H6	1.82	0.44
6:SA:109:THR:HG23	6:SA:136:GLU:HG2	1.99	0.44
9:SE:36:HIS:CG	9:SE:85:GLY:HA3	2.52	0.44
11:SG:218:LYS:HE3	11:SG:218:LYS:HB3	1.74	0.44
15:SI:133:GLU:O	15:SI:136:ILE:HG13	2.17	0.44
27:SP:44:ARG:HH21	27:SP:53:GLN:HE21	1.65	0.44
29:SV:81:LYS:HD3	29:SV:81:LYS:HA	1.73	0.44
51:LI:47:PRO:HG2	51:LI:142:LEU:HG	1.99	0.44
62:LZ:41:ALA:HB2	62:LZ:77:TYR:HE1	1.82	0.44
1:S2:160:U:O2'	1:S2:161:U:H3'	2.16	0.44
1:S2:1421:A:H4'	1:S2:1422:G:H5'	2.00	0.44
3:L5:25:A:H2'	3:L5:26:C:C6	2.53	0.44
3:L5:259:C:H2'	3:L5:260:C:C6	2.52	0.44
3:L5:3723:A2M:HM'3	3:L5:3723:A2M:H1'	1.72	0.44
3:L5:4530:UR3:H2'	3:L5:4531:PSU:H2'	1.99	0.44
3:L5:4695:C:OP2	42:LH:71:ARG:NH2	2.51	0.44
10:SC:116:THR:OG1	10:SC:119:GLY:O	2.29	0.44
12:SF:126:THR:HG23	34:Sc:47:LYS:HE2	1.99	0.44
20:SX:95:GLU:O	20:SX:98:ASP:HB2	2.18	0.44
23:Sd:48:LYS:HE3	23:Sd:48:LYS:HB2	1.66	0.44
33:Sb:24:LEU:HA	33:Sb:24:LEU:HD23	1.76	0.44
52:LD:208:MET:HB3	52:LD:233:PRO:HG3	1.97	0.44
59:LX:73:HIS:ND1	59:LX:115:LYS:HD3	2.32	0.44
69:Le:35:TRP:CE2	69:Le:56:PRO:HD2	2.52	0.44
80:mR:32:A:O2'	80:mR:33:A:O4'	2.35	0.44
1:S2:65:C:C6	11:SG:174:PRO:HB3	2.53	0.44
1:S2:99:A2M:H8	1:S2:99:A2M:O5'	2.17	0.44
1:S2:1643:PSU:H2'	1:S2:1644:C:C6	2.53	0.44
3:L5:2588:C:OP1	3:L5:2768:C:O2'	2.29	0.44
3:L5:4628:PSU:H4'	61:LW:16:GLY:O	2.18	0.44
3:L5:5030:U:H2'	3:L5:5031:G:H8	1.81	0.44
22:SS:30:ILE:HG13	22:SS:36:VAL:HG11	2.00	0.44
39:LB:149:ASP:O	39:LB:153:MET:HG3	2.18	0.44
50:LN:165:THR:O	50:LN:169:ARG:HB2	2.18	0.44
61:LW:119:LYS:HA	61:LW:119:LYS:HD2	1.79	0.44
1:S2:186:C:H2'	1:S2:187:G:C8	2.50	0.44
1:S2:535:G:C4	1:S2:536:A:C8	3.06	0.44
1:S2:880:G:H1	1:S2:906:U:H3	1.65	0.44
1:S2:1148:A:H4'	1:S2:1149:A:O4'	2.17	0.44
1:S2:1265:A:H4'	1:S2:1327:G:P	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4770:U:H2'	3:L5:4771:C:C6	2.52	0.44
5:SB:138:PHE:O	5:SB:213:ARG:N	2.51	0.44
8:SJ:33:GLY:HA3	35:Se:112:TYR:CD1	2.52	0.44
10:SC:76:LYS:HE2	10:SC:76:LYS:HA	2.00	0.44
11:SG:168:LYS:HG2	11:SG:169:PRO:HD2	1.98	0.44
43:LE:280:GLY:H	45:LO:2:ALA:HB2	1.83	0.44
72:Li:73:ILE:O	72:Li:77:VAL:HG22	2.18	0.44
1:S2:28:U:H2'	1:S2:29:G:H8	1.83	0.44
1:S2:1804:OMU:HM23	1:S2:1804:OMU:H1'	1.75	0.44
2:L8:19:C:H2'	2:L8:20:A:C8	2.52	0.44
3:L5:172:C:H2'	3:L5:173:C:C6	2.52	0.44
3:L5:2374:A:H5'	68:Ld:64:ILE:O	2.18	0.44
3:L5:2519:U:H1'	3:L5:2520:C:C6	2.52	0.44
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.53	0.44
7:SD:226:GLN:NE2	37:Sg:224:GLY:O	2.51	0.44
33:Sb:34:ASP:CG	33:Sb:82:LYS:HZ3	2.26	0.44
44:LG:259:LYS:HD3	44:LG:259:LYS:HA	1.84	0.44
48:LM:24:LEU:HD11	48:LM:86:TRP:CG	2.53	0.44
56:LT:146:LYS:HB2	56:LT:146:LYS:HE2	1.76	0.44
64:Lh:27:GLU:OE2	64:Lh:46:LYS:HE3	2.18	0.44
69:Le:90:MET:HB2	91:Le:329:HOH:O	2.17	0.44
1:S2:433:A:H2'	1:S2:434:G:C8	2.53	0.44
1:S2:1305:C:C2	1:S2:1306:U:C5	3.06	0.44
1:S2:1690:U:H2'	1:S2:1691:U:C6	2.53	0.44
3:L5:140:G:H5'	3:L5:141:C:OP2	2.17	0.44
3:L5:182:G:H2'	3:L5:183:C:C6	2.53	0.44
3:L5:1248:C:H2'	3:L5:1249:C:H6	1.82	0.44
3:L5:1418:C:H2'	3:L5:1419:G:O4'	2.17	0.44
3:L5:1437:C:H1'	3:L5:2097:U:O2'	2.18	0.44
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.53	0.44
3:L5:1830:G:H4'	65:Lb:68:ARG:NH1	2.33	0.44
3:L5:1884:C:H4'	3:L5:2070:U:C4	2.53	0.44
3:L5:4254:G:H2'	3:L5:4254:G:N3	2.33	0.44
3:L5:4529:G:H2'	3:L5:4530:UR3:O4'	2.18	0.44
5:SB:131:ASP:OD1	5:SB:131:ASP:N	2.39	0.44
11:SG:95:LYS:HE3	11:SG:95:LYS:HB3	1.83	0.44
15:SI:130:THR:OG1	15:SI:133:GLU:OE1	2.34	0.44
26:SR:101:ASP:N	26:SR:101:ASP:OD1	2.50	0.44
62:LZ:109:LYS:HE2	62:LZ:109:LYS:HB3	1.56	0.44
74:Lk:52:LYS:HA	74:Lk:55:LYS:HG2	1.99	0.44
1:S2:167:G:O2'	61:LW:80:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:441:C:OP2	15:SI:2:GLY:N	2.51	0.44
1:S2:465:A:H4'	1:S2:466:G:O5'	2.18	0.44
1:S2:525:A:H5''	35:Se:106:ALA:HB2	1.98	0.44
1:S2:538:U:H1'	1:S2:547:G:N2	2.33	0.44
1:S2:571:U:H5''	30:SY:37:LYS:HG3	2.00	0.44
1:S2:1538:C:H2'	1:S2:1539:U:C6	2.53	0.44
3:L5:1785:C:OP1	51:LI:133:GLN:NE2	2.42	0.44
3:L5:1880:G:C8	3:L5:1881:OMC:HM22	2.53	0.44
4:L7:16:A:H2'	4:L7:17:C:C6	2.53	0.44
13:SH:19:PHE:CE2	13:SH:50:GLU:HB2	2.53	0.44
20:SX:28:LYS:HE2	20:SX:32:LEU:HD22	2.00	0.44
50:LN:150:TRP:CH2	50:LN:151:ILE:HD12	2.52	0.44
69:Le:23:HIS:HA	69:Le:53:ILE:HD12	2.00	0.44
71:Lg:94:ALA:O	71:Lg:98:GLU:HG2	2.18	0.44
1:S2:799:U:H4'	13:SH:109:ARG:HE	1.83	0.44
1:S2:1084:A:OP1	1:S2:1858:G:O2'	2.24	0.44
1:S2:1456:G:H2'	1:S2:1457:U:C6	2.52	0.44
1:S2:1532:C:O2'	1:S2:1601:A:N1	2.51	0.44
3:L5:180:C:H2'	3:L5:181:C:C1'	2.48	0.44
3:L5:478:G:H2'	3:L5:479:G:H8	1.82	0.44
3:L5:1437:C:H2'	3:L5:1438:U:O4'	2.18	0.44
3:L5:1510:G:H2'	3:L5:1511:U:C6	2.53	0.44
3:L5:1761:G:H1	3:L5:1771:U:H3	1.66	0.44
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.82	0.44
3:L5:4376:A:H5''	3:L5:4377:G:O5'	2.18	0.44
3:L5:4611:A:H2'	3:L5:4612:C:H6	1.83	0.44
8:SJ:47:LYS:HG3	8:SJ:102:ILE:HD12	2.00	0.44
15:SI:69:SER:OG	15:SI:191:GLU:OE1	2.35	0.44
17:SU:36:CYS:SG	17:SU:87:ARG:HG3	2.58	0.44
37:Sg:194:TYR:CE2	37:Sg:212:LYS:HD2	2.53	0.44
43:LE:66:LYS:HE2	43:LE:68:MET:SD	2.58	0.44
46:LL:121:ARG:HA	46:LL:121:ARG:HD2	1.78	0.44
58:LU:24:ASP:OD1	58:LU:26:THR:HG23	2.17	0.44
61:LW:103:ALA:HA	61:LW:106:GLU:HG2	1.99	0.44
1:S2:1390:U:H2'	1:S2:1391:OMC:C6	2.53	0.43
2:L8:14:OMU:HM23	2:L8:14:OMU:H1'	1.60	0.43
2:L8:66:A:H2'	2:L8:67:U:C6	2.53	0.43
2:L8:127:U:H2'	2:L8:128:C:O4'	2.18	0.43
3:L5:667:A:O5'	3:L5:667:A:C8	2.71	0.43
3:L5:961:G:O2'	3:L5:963:G:N7	2.49	0.43
3:L5:1589:C:H2'	3:L5:1590:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1704:C:O3'	66:LF:46:ARG:NH1	2.51	0.43
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.52	0.43
3:L5:2438:A:O2'	3:L5:2440:U:OP2	2.36	0.43
3:L5:4140:C:H2'	3:L5:4141:G:N3	2.33	0.43
3:L5:4895:C:H1'	48:LM:132:LYS:HE2	2.00	0.43
8:SJ:43:VAL:HG12	8:SJ:47:LYS:HD2	2.00	0.43
16:SQ:12:VAL:HG11	16:SQ:90:LYS:HB3	2.00	0.43
36:Sf:109:ASP:C	36:Sf:110:GLU:HG3	2.43	0.43
38:LA:206:PRO:HG3	38:LA:213:GLY:HA3	2.00	0.43
75:Ll:26:TRP:CD1	75:Ll:26:TRP:H	2.36	0.43
1:S2:102:A:H4'	1:S2:104:A:C8	2.53	0.43
1:S2:867:OMG:HM23	1:S2:867:OMG:H1'	1.64	0.43
3:L5:37:U:H2'	3:L5:38:A:O4'	2.18	0.43
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.83	0.43
3:L5:2382:A:N1	3:L5:2829:U:O2'	2.45	0.43
3:L5:4733:C:H4'	3:L5:4734:A:H5'	1.99	0.43
3:L5:4872:G:O6	48:LM:98:ARG:HG3	2.18	0.43
10:SC:257:LYS:O	29:SV:16:LYS:NZ	2.43	0.43
11:SG:74:ARG:HE	11:SG:74:ARG:HB3	1.71	0.43
37:Sg:191:HIS:CD2	37:Sg:195:LEU:HD21	2.53	0.43
54:LR:105:LEU:HD23	54:LR:138:LEU:HD23	2.00	0.43
75:Ll:23:ILE:HD11	75:Ll:28:ARG:NH1	2.33	0.43
81:Pt:4:G:H2'	81:Pt:5:G:C8	2.53	0.43
1:S2:118:C:H2'	1:S2:119:PSU:O4'	2.18	0.43
1:S2:641:A:H2'	1:S2:642:U:O4'	2.17	0.43
1:S2:1673:U:H2'	1:S2:1674:G:O4'	2.17	0.43
3:L5:424:U:H2'	3:L5:425:U:C6	2.53	0.43
3:L5:969:C:H4'	43:LE:123:ARG:NH2	2.29	0.43
3:L5:2094:G:H3'	3:L5:2095:A:H5''	2.00	0.43
3:L5:3869:OMC:C1'	82:L5:5114:SPD:H32	2.47	0.43
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.17	0.43
10:SC:277:HIS:HA	10:SC:280:VAL:HG23	2.00	0.43
45:LO:177:LEU:HD23	45:LO:177:LEU:HA	1.85	0.43
46:LL:162:LYS:HD2	46:LL:162:LYS:HA	1.63	0.43
48:LM:3:PHE:CZ	55:LS:155:PRO:HB3	2.53	0.43
55:LS:69:GLU:HG2	55:LS:101:THR:HG22	2.00	0.43
59:LX:150:ALA:HB1	59:LX:155:ILE:HB	2.00	0.43
62:LZ:17:ARG:HD3	71:Lg:75:SER:HB3	2.00	0.43
1:S2:542:U:C4	1:S2:543:C:C4	3.07	0.43
1:S2:1410:C:H2'	1:S2:1411:G:H8	1.83	0.43
1:S2:1442:OMU:HM23	1:S2:1442:OMU:H1'	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1454:A:O4'	26:SR:3:ARG:NH1	2.51	0.43
2:L8:67:U:H2'	2:L8:68:G:C8	2.53	0.43
3:L5:5:A:H2'	3:L5:6:C:O4'	2.19	0.43
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.18	0.43
3:L5:1567:U:H2'	3:L5:1568:C:C6	2.53	0.43
3:L5:1695:U:H2'	3:L5:1696:C:C6	2.52	0.43
3:L5:1697:G:N2	3:L5:2084:C:OP1	2.47	0.43
3:L5:3786:U:O2	3:L5:3814:U:H4'	2.18	0.43
5:SB:121:ILE:HG12	5:SB:161:VAL:HG13	2.00	0.43
11:SG:46:LYS:HB2	11:SG:119:LYS:HZ1	1.84	0.43
22:SS:142:ARG:HB2	22:SS:144:ARG:NH2	2.34	0.43
40:LC:20:LYS:HB2	40:LC:20:LYS:HE2	1.80	0.43
44:LG:129:PRO:O	44:LG:130:THR:OG1	2.33	0.43
50:LN:178:HIS:HA	50:LN:181:HIS:NE2	2.34	0.43
54:LR:76:MET:HE3	54:LR:76:MET:HB3	1.85	0.43
54:LR:89:MET:HE3	54:LR:90:PRO:HD2	1.98	0.43
1:S2:4:C:H4'	10:SC:207:ALA:HB2	2.00	0.43
1:S2:1204:A:H2'	1:S2:1205:C:C6	2.53	0.43
1:S2:1679:A:P	12:SF:60:ARG:HE	2.42	0.43
3:L5:173:C:H2'	3:L5:174:C:C6	2.53	0.43
3:L5:1074:G:H2'	3:L5:1075:G:H8	1.83	0.43
3:L5:1397:A:N1	3:L5:1498:G:O2'	2.48	0.43
3:L5:1771:U:H2'	3:L5:1772:C:H6	1.83	0.43
3:L5:2020:U:C2	3:L5:2021:G:C8	3.06	0.43
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.82	0.43
3:L5:2900:U:H2'	3:L5:2901:G:H8	1.84	0.43
8:SJ:33:GLY:HA3	35:Se:112:TYR:CG	2.54	0.43
11:SG:23:LYS:HD3	11:SG:41:LEU:HA	2.01	0.43
16:SQ:100:VAL:HG12	16:SQ:101:ASP:H	1.83	0.43
21:SM:95:ASP:OD1	21:SM:98:GLY:N	2.51	0.43
27:SP:124:LYS:HE2	27:SP:124:LYS:HB2	1.81	0.43
43:LE:160:LYS:HE2	70:Lf:1:MET:SD	2.57	0.43
47:LV:90:ARG:HB2	47:LV:92:ASP:OD1	2.18	0.43
54:LR:39:GLN:HE21	54:LR:42:ARG:HH21	1.67	0.43
61:LW:61:LYS:HA	61:LW:61:LYS:HD3	1.74	0.43
1:S2:949:G:H2'	1:S2:950:C:C6	2.54	0.43
1:S2:957:A:OP1	19:SO:57:THR:OG1	2.34	0.43
1:S2:1190:A:H2'	1:S2:1191:C:O4'	2.19	0.43
1:S2:1563:G:H2'	1:S2:1564:C:C6	2.53	0.43
1:S2:1683:C:N3	34:Sc:24:GLN:HG3	2.32	0.43
2:L8:6:C:H2'	2:L8:7:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:18:C:H4'	50:LN:138:PHE:CD1	2.54	0.43
3:L5:478:G:H2'	3:L5:479:G:C8	2.54	0.43
3:L5:1788:A:H2'	51:LI:22:PHE:CZ	2.53	0.43
3:L5:2484:A:H2'	3:L5:2485:U:C6	2.52	0.43
3:L5:2634:C:H2'	3:L5:2635:U:C6	2.53	0.43
3:L5:3711:A:N6	3:L5:3736:A:OP1	2.52	0.43
7:SD:224:SER:HB3	37:Sg:188:HIS:CD2	2.53	0.43
19:SO:116:LEU:HG	32:Sa:53:ILE:HD11	2.00	0.43
36:Sf:139:HIS:NE2	36:Sf:148:TYR:HB2	2.33	0.43
37:Sg:50:THR:OG1	37:Sg:51:ASN:N	2.51	0.43
42:LH:27:VAL:HG12	42:LH:84:VAL:HG21	2.01	0.43
42:LH:82:LYS:HE2	42:LH:88:PHE:CE1	2.54	0.43
57:LP:116:HIS:HB3	57:LP:149:ILE:HB	1.99	0.43
58:LU:20:LYS:HB2	58:LU:20:LYS:NZ	2.33	0.43
1:S2:29:G:H4'	20:SX:129:SER:HB2	2.01	0.43
1:S2:1017:U:H2'	1:S2:1018:U:H6	1.83	0.43
1:S2:1109:C:C6	26:SR:126:MET:HE3	2.54	0.43
1:S2:1597:C:H4'	1:S2:1603:G:C6	2.54	0.43
2:L8:141:C:H2'	2:L8:142:U:H6	1.82	0.43
3:L5:1302:U:C2	69:Le:17:THR:HB	2.53	0.43
3:L5:1303:A:C2	69:Le:33[B]:ARG:HD2	2.53	0.43
3:L5:1383:G:H2'	3:L5:1384:C:C6	2.54	0.43
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.84	0.43
11:SG:119:LYS:HE2	11:SG:119:LYS:HB2	1.77	0.43
37:Sg:5:MET:CE	37:Sg:310:TRP:HB3	2.48	0.43
68:Ld:29:ILE:O	68:Ld:33:ILE:HG12	2.18	0.43
1:S2:385:G:H3'	25:SL:136:LYS:HB2	2.01	0.43
1:S2:441:C:H2'	1:S2:442:C:C6	2.54	0.43
1:S2:1138:C:O2'	29:SV:61:ARG:HD2	2.19	0.43
1:S2:1278:A:H2'	1:S2:1279:C:C6	2.53	0.43
1:S2:1779:G:C6	1:S2:1780:G:C6	3.06	0.43
3:L5:2292:C:H2'	3:L5:2293:U:C6	2.53	0.43
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.53	0.43
3:L5:5065:U:H2'	3:L5:5066:U:O4'	2.19	0.43
21:SM:72:HIS:O	21:SM:72:HIS:ND1	2.48	0.43
26:SR:67:ARG:HD3	26:SR:67:ARG:HA	1.74	0.43
26:SR:79:GLU:HA	26:SR:83:ASN:ND2	2.34	0.43
27:SP:50:ARG:HB2	27:SP:53:GLN:HE22	1.83	0.43
1:S2:1435:C:H41	17:SU:19:ARG:NH2	2.17	0.43
3:L5:52:G:H4'	3:L5:1529:G:H4'	2.00	0.43
3:L5:451:C:O2'	3:L5:1293:G:H2'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:457:G:H2'	3:L5:458:C:C6	2.54	0.43
3:L5:490:C:H2'	3:L5:491:G:C8	2.53	0.43
3:L5:3668:C:H5'	38:LA:8:GLN:O	2.19	0.43
3:L5:4727:A:H5'	39:LB:130:PHE:H	1.84	0.43
3:L5:4994:G:OP1	39:LB:174:ARG:NH1	2.51	0.43
7:SD:213:PRO:HB3	26:SR:20:TYR:CE1	2.53	0.43
17:SU:98:VAL:HA	17:SU:101:ILE:HG22	2.00	0.43
27:SP:75:VAL:HG22	27:SP:93:MET:HB3	2.01	0.43
30:SY:56:PHE:O	30:SY:74:MET:N	2.46	0.43
38:LA:107:MET:O	38:LA:139:HIS:NE2	2.46	0.43
39:LB:107:ALA:HB2	39:LB:201:LEU:HD22	2.00	0.43
1:S2:380:G:N1	1:S2:383:G:OP2	2.40	0.43
1:S2:454:U:H2'	1:S2:455:A:H8	1.84	0.43
1:S2:1047:C:H2'	1:S2:1048:G:O4'	2.19	0.43
1:S2:1229:G:H21	28:ST:87:VAL:HG22	1.83	0.43
1:S2:1293:A:H2'	1:S2:1294:G:C8	2.54	0.43
1:S2:1345:G:N7	1:S2:1371:U:O2'	2.40	0.43
1:S2:1536:G:C2	1:S2:1537:A:C5	3.07	0.43
3:L5:123:C:H2'	3:L5:124:C:H6	1.84	0.43
3:L5:1764:G:N7	3:L5:1765:A:N6	2.67	0.43
3:L5:1817:U:O2'	3:L5:1818:G:H5'	2.19	0.43
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.82	0.43
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.53	0.43
3:L5:3813:A:N3	3:L5:4538:G:O2'	2.47	0.43
5:SB:219:LYS:HE2	5:SB:219:LYS:HB3	1.80	0.43
49:La:72:THR:HG22	49:La:110:LYS:HB3	2.00	0.43
1:S2:158:A:H2'	1:S2:159:A2M:O4'	2.19	0.42
1:S2:326:C:H2'	61:LW:113:LYS:HZ3	1.83	0.42
1:S2:459:C:H2'	1:S2:460:A:O4'	2.19	0.42
1:S2:815:PSU:C4	1:S2:816:A:C8	3.07	0.42
1:S2:1387:G:H2'	1:S2:1388:A:O4'	2.19	0.42
3:L5:984:C:H2'	3:L5:985:C:C6	2.53	0.42
3:L5:1472:C:H2'	3:L5:1473:U:C6	2.54	0.42
3:L5:2434:G:O2'	3:L5:2527:A:N1	2.46	0.42
3:L5:4139:G:C2	3:L5:4140:C:H1'	2.54	0.42
4:L7:24:C:H2'	4:L7:25:G:O4'	2.19	0.42
5:SB:183:GLU:HA	5:SB:183:GLU:OE2	2.19	0.42
13:SH:9:VAL:HG13	13:SH:44:ASN:ND2	2.33	0.42
21:SM:93:LYS:HG2	21:SM:101:ARG:HH12	1.83	0.42
30:SY:55:ILE:HD12	30:SY:75:ILE:HD13	2.01	0.42
31:SZ:47:LEU:HD12	31:SZ:79:ILE:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:191:HIS:CG	37:Sg:195:LEU:HD21	2.53	0.42
41:LJ:44:THR:HG21	41:LJ:72:CYS:SG	2.59	0.42
43:LE:68:MET:HE3	43:LE:68:MET:HB3	1.82	0.42
51:LI:48:LEU:O	51:LI:139:ARG:HA	2.19	0.42
52:LD:215:ASP:HB3	52:LD:218:ALA:HB3	2.01	0.42
56:LT:28:ALA:HA	56:LT:31:MET:HB2	2.01	0.42
71:Lg:84:ALA:O	71:Lg:88:ARG:HG3	2.20	0.42
1:S2:560:A:O5'	8:SJ:174:LYS:HD3	2.19	0.42
1:S2:1215:C:O2'	1:S2:1645:C:OP2	2.32	0.42
1:S2:1281:G:H2'	1:S2:1282:A:C8	2.54	0.42
1:S2:1303:C:H2'	1:S2:1304:U:H6	1.84	0.42
1:S2:1447:OMG:HM23	1:S2:1447:OMG:H1'	1.83	0.42
1:S2:1733:U:H2'	1:S2:1734:G:O4'	2.20	0.42
3:L5:28:C:H4'	3:L5:61:A:H4'	2.00	0.42
3:L5:456:C:H2'	3:L5:457:G:C8	2.54	0.42
3:L5:1245:C:H2'	3:L5:1246:G:C8	2.53	0.42
3:L5:1558:A:H2'	3:L5:1559:G:C8	2.55	0.42
3:L5:1702:C:H3'	3:L5:1703:C:C6	2.54	0.42
3:L5:4071:U:H2'	3:L5:4072:C:C6	2.54	0.42
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.54	0.42
3:L5:5066:U:H2'	3:L5:5067:U:C6	2.54	0.42
9:SE:3:ARG:NH2	91:SE:301:HOH:O	2.51	0.42
13:SH:66:VAL:HG22	13:SH:96:ALA:HB1	2.01	0.42
15:SI:117:TYR:HB3	15:SI:119:LEU:HD12	2.00	0.42
19:SO:58:GLY:O	19:SO:62:VAL:HG22	2.19	0.42
28:ST:74:SER:O	28:ST:77:LYS:N	2.52	0.42
36:Sf:118:ARG:NH1	36:Sf:120:GLU:HG2	2.33	0.42
37:Sg:82:SER:O	37:Sg:108:VAL:HG22	2.19	0.42
40:LC:328:LEU:HD13	66:LF:187:MET:HE2	2.01	0.42
42:LH:41:ILE:HG22	42:LH:43:VAL:HG13	2.01	0.42
52:LD:34:LYS:HE2	56:LT:30:TYR:CZ	2.54	0.42
58:LU:19:LEU:O	58:LU:73:THR:HA	2.18	0.42
1:S2:99:A2M:HM'3	1:S2:99:A2M:H1'	1.88	0.42
1:S2:1260:A:C2	1:S2:1620:A:C4	3.07	0.42
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.78	0.42
3:L5:1452:A:H2'	3:L5:1453:G:O4'	2.19	0.42
3:L5:1940:G:H1	3:L5:4434:C:H5''	1.84	0.42
3:L5:2634:C:H2'	3:L5:2635:U:H6	1.84	0.42
3:L5:4566:U:H2'	3:L5:4567:G:O4'	2.19	0.42
6:SA:212:LYS:O	6:SA:215:GLN:HG3	2.19	0.42
7:SD:70:THR:HA	7:SD:86:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SE:19:MET:SD	9:SE:108:ARG:HD2	2.60	0.42
15:SI:57:ALA:HB2	15:SI:183:GLY:HA2	2.00	0.42
19:SO:75:MET:HE2	19:SO:75:MET:HB3	1.97	0.42
19:SO:124:MET:HE3	19:SO:124:MET:HB3	1.81	0.42
19:SO:150:ARG:H	19:SO:150:ARG:HG2	1.66	0.42
26:SR:79:GLU:HA	26:SR:83:ASN:HD21	1.84	0.42
30:SY:100:LYS:HE3	30:SY:100:LYS:HB3	1.82	0.42
33:Sb:8:LEU:HD12	33:Sb:8:LEU:HA	1.86	0.42
39:LB:288:GLY:HA3	39:LB:330:PHE:CZ	2.54	0.42
47:LV:21:PRO:HA	47:LV:54:ALA:HA	2.00	0.42
75:Ll:20:ASN:ND2	75:Ll:42:ARG:O	2.47	0.42
75:Ll:48:LYS:HA	75:Ll:48:LYS:HD2	1.88	0.42
1:S2:106:C:H2'	1:S2:107:A:C8	2.55	0.42
1:S2:945:U:H2'	1:S2:946:U:C6	2.54	0.42
1:S2:1520:G:H3'	1:S2:1521:C:C5	2.55	0.42
1:S2:1615:U:O4	27:SP:40:ARG:NH2	2.52	0.42
2:L8:5:U:H2'	2:L8:6:C:C6	2.53	0.42
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.54	0.42
3:L5:2079:G:H2'	3:L5:2080:U:H6	1.85	0.42
3:L5:4083:U:OP1	38:LA:123:ARG:NH1	2.52	0.42
7:SD:138:VAL:CG1	7:SD:182:LEU:HD21	2.49	0.42
10:SC:248:TYR:O	29:SV:23:ILE:HG21	2.20	0.42
20:SX:130:LEU:HD12	20:SX:130:LEU:HA	1.90	0.42
27:SP:108:LYS:HD3	27:SP:108:LYS:HA	1.70	0.42
28:ST:65:TYR:HB2	28:ST:131:LEU:HD12	2.02	0.42
58:LU:80:LYS:HE2	58:LU:110:TYR:CE2	2.53	0.42
60:LY:134:LYS:HA	60:LY:134:LYS:HD2	1.76	0.42
1:S2:354:OMU:HM23	1:S2:354:OMU:H1'	1.82	0.42
1:S2:920:A:O2'	1:S2:922:A:OP1	2.26	0.42
1:S2:1472:C:H2'	1:S2:1473:G:O4'	2.18	0.42
1:S2:1528:G:O2'	1:S2:1666:C:OP1	2.31	0.42
1:S2:1648:G:N7	16:SQ:17:LYS:HE2	2.33	0.42
2:L8:125:C:H2'	2:L8:126:C:H5''	2.02	0.42
3:L5:318:A:H2'	3:L5:319:A:C8	2.54	0.42
3:L5:368:C:O4'	40:LC:83:GLY:HA3	2.20	0.42
3:L5:690:C:H2'	3:L5:691:C:H6	1.84	0.42
3:L5:960:A:H2'	3:L5:970:G:N7	2.35	0.42
3:L5:1567:U:H2'	3:L5:1568:C:H6	1.83	0.42
3:L5:2808:G:O3'	54:LR:60:ARG:NH1	2.53	0.42
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.84	0.42
3:L5:4155:C:H2'	3:L5:4156:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4475:G:N7	76:Lm:125:LYS:HE3	2.34	0.42
3:L5:4885:U:H2'	3:L5:4886:C:H6	1.84	0.42
6:SA:15:VAL:HG12	6:SA:16:LEU:HD23	2.00	0.42
7:SD:119:CYS:SG	7:SD:138:VAL:HG21	2.60	0.42
12:SF:112:LEU:HD13	12:SF:177:LEU:HD21	2.01	0.42
16:SQ:7:LEU:HD12	16:SQ:7:LEU:HA	1.90	0.42
16:SQ:57:LEU:HD11	16:SQ:115:TYR:CD2	2.55	0.42
37:Sg:207:CYS:HB3	37:Sg:221:LEU:HD21	2.01	0.42
44:LG:168:VAL:CG1	50:LN:10:LEU:HD11	2.49	0.42
60:LY:89:LYS:HB3	60:LY:89:LYS:HE3	1.88	0.42
1:S2:634:A:H2'	1:S2:635:G:C8	2.54	0.42
1:S2:940:U:H2'	1:S2:941:C:C6	2.54	0.42
1:S2:1674:G:H4'	12:SF:77:MET:HE1	2.02	0.42
1:S2:1788:A:H2'	1:S2:1789:G:O4'	2.19	0.42
1:S2:1854:U:H2'	1:S2:1855:G:H8	1.84	0.42
3:L5:68:U:OP1	50:LN:178:HIS:ND1	2.35	0.42
3:L5:1743:A:N1	3:L5:1789:C:O2'	2.49	0.42
3:L5:2018:C:H2'	3:L5:2019:C:H6	1.83	0.42
3:L5:4174:U:H2'	3:L5:4175:G:H8	1.84	0.42
6:SA:2:SAC:OG	6:SA:3:GLY:N	2.50	0.42
6:SA:205:ARG:HB3	6:SA:210:ILE:HG13	2.00	0.42
15:SI:22:HIS:ND1	15:SI:23:LYS:O	2.44	0.42
24:SN:38:TYR:CZ	24:SN:78:LYS:HD3	2.55	0.42
30:SY:35:VAL:HG13	30:SY:40:ILE:HD11	2.02	0.42
37:Sg:72:SER:OG	37:Sg:74:ASP:OD1	2.31	0.42
52:LD:164:LYS:HA	52:LD:167:VAL:HG22	2.01	0.42
1:S2:496:C:OP1	9:SE:29:PRO:HG3	2.19	0.42
1:S2:1070:A:H2'	1:S2:1071:G:O4'	2.20	0.42
1:S2:1349:G:H21	6:SA:112:ILE:HD11	1.83	0.42
1:S2:1415:C:N4	1:S2:1416:C:H41	2.17	0.42
1:S2:1490:OMG:HM23	1:S2:1490:OMG:H1'	1.74	0.42
1:S2:1587:G:H2'	28:ST:77:LYS:HG2	2.00	0.42
3:L5:288:G:H2'	3:L5:289:C:C6	2.55	0.42
3:L5:987:C:H2'	3:L5:988:C:H6	1.85	0.42
3:L5:1685:G:H2'	3:L5:1686:C:C6	2.55	0.42
3:L5:1893:C:H1'	3:L5:1937:C:O2	2.19	0.42
3:L5:2045:G:O2'	3:L5:2046:G:H5''	2.19	0.42
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.55	0.42
3:L5:3707:U:H2'	3:L5:3708:C:H6	1.85	0.42
3:L5:4652:G:H2'	3:L5:4653:C:H6	1.84	0.42
3:L5:4862:G:H2'	3:L5:4863:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SD:8:LYS:HB3	17:SU:61:LEU:HD21	2.00	0.42
8:SJ:170:PRO:O	8:SJ:174:LYS:HB3	2.19	0.42
11:SG:142:ARG:HA	11:SG:147:LEU:HB2	2.00	0.42
16:SQ:77:HIS:O	16:SQ:81:ILE:HG12	2.20	0.42
17:SU:46:LYS:HE3	17:SU:97:ILE:HD11	2.01	0.42
25:SL:104:LYS:HZ3	25:SL:105:ARG:C	2.25	0.42
26:SR:66:VAL:HG23	26:SR:67:ARG:N	2.33	0.42
28:ST:23:LYS:HE2	28:ST:23:LYS:HB3	1.85	0.42
37:Sg:102:VAL:HG23	37:Sg:102:VAL:O	2.20	0.42
37:Sg:259:TRP:HE1	37:Sg:266:ILE:HG12	1.84	0.42
37:Sg:286:CYS:HA	37:Sg:302:TYR:HA	2.00	0.42
65:Lb:93:LEU:HD23	65:Lb:93:LEU:HA	1.88	0.42
1:S2:532:C:H2'	1:S2:533:A:H8	1.79	0.42
1:S2:921:G:C6	33:Sb:22:LYS:HA	2.54	0.42
1:S2:1162:C:H2'	1:S2:1163:C:O4'	2.20	0.42
1:S2:1308:U:H1'	36:Sf:135:HIS:NE2	2.34	0.42
1:S2:1315:U:H5'	18:SK:1:MET:O	2.19	0.42
1:S2:1503:C:H2'	1:S2:1504:U:C6	2.55	0.42
2:L8:123:U:H5''	2:L8:124:U:H5	1.85	0.42
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.84	0.42
3:L5:1399:G:H2'	3:L5:1400:G:H8	1.83	0.42
3:L5:1705:G:H2'	3:L5:1706:A:C8	2.55	0.42
3:L5:1846:G:H2'	3:L5:1847:C:H6	1.85	0.42
3:L5:4994:G:H2'	3:L5:4995:U:H6	1.84	0.42
9:SE:127:ARG:HG3	9:SE:142:HIS:HA	2.01	0.42
20:SX:101:LEU:HB3	20:SX:123:VAL:HG13	2.01	0.42
41:LJ:64:ARG:HE	41:LJ:64:ARG:HB3	1.66	0.42
53:LQ:43:PHE:CD2	53:LQ:133:GLY:HA3	2.54	0.42
63:Lr:2:SAC:H2A1	63:Lr:2:SAC:HA	1.79	0.42
1:S2:382:C:H2'	1:S2:383:G:C8	2.51	0.42
1:S2:1207:G:N2	80:mR:36:U:H3'	2.35	0.42
1:S2:1372:U:H2'	1:S2:1373:C:O4'	2.20	0.42
1:S2:1413:G:H2'	1:S2:1414:A:H8	1.85	0.42
1:S2:1422:G:C6	1:S2:1424:G:C6	3.07	0.42
1:S2:1666:C:H2'	1:S2:1667:U:C6	2.55	0.42
1:S2:1808:U:H2'	1:S2:1809:A:H8	1.84	0.42
3:L5:163:A:H2'	3:L5:164:G:C8	2.55	0.42
3:L5:269:G:H2'	3:L5:270:U:C6	2.55	0.42
3:L5:1249:C:H2'	3:L5:1250:C:H6	1.85	0.42
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.54	0.42
3:L5:1695:U:O2'	3:L5:1719:A:N3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2023:C:O5'	3:L5:2023:C:H6	2.02	0.42
3:L5:2747:U:H2'	3:L5:2748:C:C6	2.54	0.42
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.84	0.42
3:L5:4273:A:H2'	3:L5:4274:A:C8	2.55	0.42
3:L5:4324:A:H2'	3:L5:4325:A:C8	2.55	0.42
3:L5:4340:U:O2	82:L5:5103:SPD:N10	2.53	0.42
10:SC:102:LEU:HD23	10:SC:102:LEU:HA	1.84	0.42
11:SG:55:GLY:H	11:SG:63:MET:HE3	1.84	0.42
18:SK:16:PHE:HB2	18:SK:79:LEU:HD23	2.00	0.42
21:SM:23:LYS:HD3	21:SM:23:LYS:HA	1.59	0.42
25:SL:111:VAL:HG12	25:SL:140:PHE:HB2	2.00	0.42
28:ST:110:LEU:O	28:ST:110:LEU:HD23	2.20	0.42
54:LR:179:ALA:HA	54:LR:182:GLU:OE1	2.19	0.42
66:LF:57:TYR:OH	66:LF:189:ASP:OD1	2.30	0.42
71:Lg:112:GLN:HA	71:Lg:115:LYS:HB2	2.01	0.42
1:S2:118:C:H1'	1:S2:445:A:C5	2.54	0.42
1:S2:189:U:OP1	15:SI:152:ARG:NH2	2.50	0.42
1:S2:1653:U:H2'	1:S2:1654:G:C8	2.55	0.42
1:S2:1863:A:H1'	32:Sa:79:ILE:HD13	2.01	0.42
3:L5:382:G:H4'	3:L5:407:A:N1	2.34	0.42
3:L5:1591:U:H5''	3:L5:4527:G:OP1	2.20	0.42
3:L5:1613:A:H5'	38:LA:183:GLY:HA2	2.02	0.42
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.19	0.42
3:L5:1811:G:H2'	3:L5:1812:C:H6	1.85	0.42
3:L5:4233:A:C4	3:L5:4235:G:N7	2.88	0.42
3:L5:4593:C:H2'	3:L5:4594:U:H6	1.85	0.42
7:SD:40:ARG:HA	7:SD:40:ARG:HD2	1.79	0.42
7:SD:68:GLU:O	7:SD:72:VAL:HG22	2.20	0.42
16:SQ:146:ARG:NH1	81:Pt:34:U:OP2	2.39	0.42
25:SL:126:VAL:HG12	25:SL:145:VAL:HG22	2.01	0.42
30:SY:102:THR:OG1	30:SY:103:SER:N	2.53	0.42
41:LJ:95:ARG:HH21	41:LJ:177:GLY:H	1.67	0.42
43:LE:46:ARG:HB2	43:LE:62:MET:HE1	2.01	0.42
50:LN:31:ARG:HD3	50:LN:124:ASP:OD2	2.20	0.42
55:LS:43:ARG:HD2	55:LS:43:ARG:HA	1.71	0.42
1:S2:98:C:OP2	1:S2:426:A:O2'	2.27	0.41
1:S2:1121:G:O2'	5:SB:204:ILE:O	2.33	0.41
1:S2:1221:G:H2'	1:S2:1222:G:C8	2.55	0.41
1:S2:1223:A:H2'	1:S2:1224:G:O4'	2.20	0.41
1:S2:1261:C:O2	23:Sd:10:HIS:NE2	2.53	0.41
1:S2:1558:C:H2'	1:S2:1559:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1634:A:H2'	1:S2:1635:C:O4'	2.20	0.41
3:L5:702:U:H2'	3:L5:703:G:O4'	2.20	0.41
3:L5:2338:C:H4'	63:Lr:12:ASN:O	2.19	0.41
3:L5:2566:G:H2'	3:L5:2567:G:C8	2.52	0.41
3:L5:5030:U:H2'	3:L5:5031:G:C8	2.55	0.41
4:L7:4:U:H2'	4:L7:5:A:H8	1.85	0.41
5:SB:168:MET:HG2	5:SB:197:ILE:HG21	2.01	0.41
5:SB:233:GLY:O	5:SB:234:GLU:HG2	2.20	0.41
19:SO:120:ALA:HB2	32:Sa:53:ILE:HD13	2.01	0.41
20:SX:124:LYS:HA	20:SX:129:SER:HA	2.02	0.41
22:SS:36:VAL:HG23	22:SS:99:LEU:HD22	2.01	0.41
32:Sa:26:CYS:HB3	32:Sa:77:CYS:SG	2.60	0.41
32:Sa:41:ILE:HG12	32:Sa:68:TYR:CD2	2.54	0.41
36:Sf:118:ARG:NH2	36:Sf:128:ALA:O	2.33	0.41
37:Sg:78:ALA:O	37:Sg:89:LEU:HA	2.19	0.41
52:LD:53:VAL:HG11	52:LD:159:VAL:HA	2.02	0.41
52:LD:179:ARG:HA	52:LD:179:ARG:HD3	1.87	0.41
60:LY:64:GLY:HA3	60:LY:66:GLN:NE2	2.35	0.41
66:LF:92:VAL:O	66:LF:120:GLY:HA2	2.20	0.41
66:LF:209:TRP:CD1	66:LF:210:PRO:HD2	2.55	0.41
74:Lk:50:LYS:HA	74:Lk:50:LYS:HD3	1.83	0.41
1:S2:5:U:H2'	1:S2:6:G:C8	2.54	0.41
1:S2:159:A2M:H2	1:S2:468:A2M:O4'	2.20	0.41
1:S2:919:A:H4'	1:S2:920:A:O5'	2.20	0.41
1:S2:1454:A:C8	26:SR:3:ARG:HG3	2.56	0.41
1:S2:1458:G:H2'	1:S2:1459:G:C8	2.55	0.41
1:S2:1712:A:H2'	1:S2:1713:C:H6	1.81	0.41
2:L8:6:C:H2'	2:L8:7:U:H6	1.85	0.41
2:L8:58:G:O6	73:Lj:63:ARG:NH1	2.50	0.41
3:L5:113:A:H2'	3:L5:114:G:O4'	2.19	0.41
3:L5:704:C:HO2'	3:L5:705:G:P	2.40	0.41
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.85	0.41
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.55	0.41
3:L5:4306:OMU:OP2	53:LQ:159:PRO:HD2	2.20	0.41
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.82	0.41
3:L5:4928:C:H2'	3:L5:4929:C:C6	2.55	0.41
12:SF:164:ARG:HE	31:SZ:41:ARG:NH1	2.17	0.41
15:SI:88:ASN:O	15:SI:91:VAL:HG13	2.20	0.41
21:SM:99:LYS:HE3	21:SM:99:LYS:HB2	1.98	0.41
37:Sg:206:LEU:HD23	37:Sg:206:LEU:HA	1.89	0.41
37:Sg:219:TRP:CZ3	37:Sg:226:HIS:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:236:ILE:H	37:Sg:236:ILE:HG12	1.52	0.41
41:LJ:95:ARG:O	41:LJ:98:ASN:HB2	2.19	0.41
57:LP:10:ASN:OD1	57:LP:13:LYS:HD3	2.20	0.41
66:LF:155:TYR:CD1	66:LF:187:MET:HE3	2.55	0.41
66:LF:241:ASN:O	66:LF:245:ARG:HG2	2.19	0.41
1:S2:153:G:H21	11:SG:13:GLN:NE2	2.19	0.41
1:S2:1491:G:H2'	1:S2:1492:U:C6	2.55	0.41
2:L8:112:G:OP1	3:L5:2779:C:O2'	2.30	0.41
3:L5:259:C:H2'	3:L5:260:C:H6	1.85	0.41
3:L5:959:G:H8	3:L5:959:G:OP2	2.04	0.41
3:L5:1415:G:H2'	3:L5:1416:G:C8	2.55	0.41
3:L5:2297:G:H4'	40:LC:242:PRO:HB2	2.02	0.41
3:L5:2415:OMU:HM23	3:L5:2415:OMU:H1'	1.74	0.41
3:L5:3909:C:O2	3:L5:4396:A:N1	2.53	0.41
3:L5:4174:U:H2'	3:L5:4175:G:C8	2.55	0.41
3:L5:4880:C:H2'	3:L5:4881:U:O4'	2.20	0.41
3:L5:5006:U:H4'	3:L5:5007:A:H5'	2.03	0.41
91:L5:7459:HOH:O	60:LY:18:HIS:HE1	2.03	0.41
11:SG:118:GLU:HG2	11:SG:119:LYS:N	2.35	0.41
16:SQ:85:ARG:NH2	16:SQ:116:ASP:OD2	2.39	0.41
25:SL:147:LYS:HB3	25:SL:147:LYS:HE3	1.67	0.41
30:SY:114:MET:HA	30:SY:125:VAL:HG21	2.02	0.41
39:LB:168:MET:HE3	39:LB:168:MET:HB3	1.87	0.41
64:Lh:13:LYS:HB2	64:Lh:16:GLU:HG3	2.02	0.41
1:S2:13:C:H4'	1:S2:1355:C:O2	2.20	0.41
1:S2:458:A:H2'	1:S2:459:C:O4'	2.21	0.41
1:S2:472:C:H4'	1:S2:474:G:OP1	2.20	0.41
1:S2:876:C:H2'	1:S2:877:C:H6	1.85	0.41
1:S2:1229:G:H21	28:ST:87:VAL:CG2	2.34	0.41
1:S2:1337:4AC:H2'	1:S2:1338:G:C8	2.56	0.41
3:L5:163:A:H2'	3:L5:164:G:H8	1.84	0.41
3:L5:3615:G:O2'	61:LW:44:ARG:NH2	2.53	0.41
3:L5:3664:G:H2'	3:L5:3665:G:C8	2.55	0.41
3:L5:3925:OMU:H1'	3:L5:3925:OMU:HM23	1.82	0.41
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.19	0.41
7:SD:7:LYS:HD3	7:SD:7:LYS:HA	1.77	0.41
16:SQ:35:ASN:OD1	16:SQ:72:VAL:HG12	2.21	0.41
21:SM:65:VAL:HA	21:SM:68:LEU:HG	2.01	0.41
40:LC:201:ARG:NH2	91:LC:611:HOH:O	2.53	0.41
46:LL:165:LYS:HE3	46:LL:165:LYS:HB2	1.74	0.41
58:LU:47:ILE:HD12	58:LU:63:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:LY:2:LYS:HE3	60:LY:2:LYS:HB3	1.68	0.41
72:Li:44:ILE:HD13	72:Li:44:ILE:HA	1.90	0.41
1:S2:436:OMG:HM23	1:S2:436:OMG:H1'	1.87	0.41
1:S2:449:A:H4'	9:SE:3:ARG:HD3	2.02	0.41
1:S2:529:A:H2'	1:S2:530:U:C6	2.54	0.41
1:S2:1272:C:H2'	1:S2:1273:C:C6	2.56	0.41
1:S2:1281:G:H2'	1:S2:1282:A:H8	1.86	0.41
1:S2:1778:C:H2'	1:S2:1779:G:C8	2.55	0.41
3:L5:1762:C:H2'	3:L5:1763:C:C6	2.55	0.41
3:L5:2406:G:N7	75:Ll:2:SER:N	2.68	0.41
3:L5:2497:C:H2'	3:L5:2498:C:C6	2.54	0.41
3:L5:3733:A:H2'	3:L5:3734:PSU:O4'	2.20	0.41
3:L5:4220:6MZ:O5'	3:L5:4220:6MZ:H8	2.20	0.41
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.20	0.41
3:L5:4462:C:O2'	3:L5:4463:U:H5'	2.21	0.41
3:L5:4587:G:OP1	45:LO:61:ARG:NH1	2.52	0.41
8:SJ:125:HIS:HA	8:SJ:128:VAL:HG22	2.02	0.41
9:SE:10:LYS:HA	9:SE:10:LYS:HD3	1.86	0.41
11:SG:46:LYS:HB2	11:SG:119:LYS:NZ	2.35	0.41
12:SF:77:MET:HE3	12:SF:84:GLY:CA	2.51	0.41
15:SI:149:TYR:O	15:SI:153:LYS:HD3	2.19	0.41
18:SK:19:GLY:HA2	18:SK:71:LEU:HD12	2.02	0.41
22:SS:40:TYR:O	22:SS:43:VAL:HG12	2.20	0.41
26:SR:5:ARG:O	26:SR:10:LYS:HE2	2.20	0.41
46:LL:34:ARG:HD2	91:LL:440:HOH:O	2.21	0.41
47:LV:62:MET:HE3	47:LV:76:VAL:HG12	2.03	0.41
60:LY:108:ARG:HH11	60:LY:108:ARG:HG3	1.84	0.41
67:Lc:10:SER:O	67:Lc:14:ILE:HG22	2.20	0.41
81:Pt:11:A:H2'	81:Pt:12:G:C8	2.55	0.41
1:S2:59:U:H5''	1:S2:503:C:N4	2.36	0.41
1:S2:416:U:H2'	1:S2:417:C:O4'	2.21	0.41
1:S2:482:G:OP1	20:SX:76:LYS:HA	2.20	0.41
1:S2:1408:U:C2	1:S2:1409:A:C8	3.08	0.41
1:S2:1593:C:H2'	1:S2:1594:A:H8	1.85	0.41
2:L8:8:U:H2'	2:L8:9:A:C8	2.54	0.41
3:L5:181:C:H2'	3:L5:182:G:C8	2.55	0.41
3:L5:699:C:H2'	3:L5:700:G:C8	2.55	0.41
3:L5:1767:A:H3'	3:L5:1767:A:N3	2.35	0.41
3:L5:2018:C:H2'	3:L5:2019:C:C6	2.55	0.41
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.85	0.41
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.85	0.41
3:L5:4637:OMG:H2'	3:L5:4638:U:C6	2.56	0.41
3:L5:4762:A:H2'	3:L5:4763:U:O4'	2.20	0.41
3:L5:4769:G:H5''	45:LO:176:ARG:HD3	2.02	0.41
4:L7:22:A:H2'	4:L7:23:A:C8	2.55	0.41
5:SB:40:ASN:HD22	5:SB:76:ASN:CG	2.28	0.41
6:SA:203:PHE:HZ	26:SR:91:LEU:HD11	1.86	0.41
7:SD:205:PRO:HA	26:SR:42:PRO:HG2	2.01	0.41
13:SH:58:LYS:O	13:SH:90:LYS:HA	2.20	0.41
18:SK:3:MET:HG2	18:SK:8:ARG:HG2	2.02	0.41
30:SY:82:ALA:O	30:SY:86:GLU:HB3	2.20	0.41
35:Se:85:LYS:HG3	35:Se:86:VAL:N	2.35	0.41
36:Sf:144:CYS:SG	36:Sf:146:LEU:HD23	2.60	0.41
39:LB:353:VAL:HG12	39:LB:355:THR:HG23	2.02	0.41
41:LJ:118:LYS:HE3	41:LJ:118:LYS:HB3	1.76	0.41
42:LH:103:VAL:HG11	42:LH:144:LEU:HD21	2.02	0.41
62:LZ:60:LYS:HE2	62:LZ:60:LYS:HB2	1.85	0.41
1:S2:656:G:N2	1:S2:663:C:H5''	2.35	0.41
1:S2:1287:A:H2'	1:S2:1288:OMU:O4'	2.20	0.41
1:S2:1378:A:H4'	1:S2:1379:A:O5'	2.21	0.41
2:L8:56:G:H2'	2:L8:57:C:O4'	2.20	0.41
2:L8:88:A:H2'	2:L8:89:U:O4'	2.21	0.41
3:L5:205:C:N3	3:L5:209:U:H5	2.19	0.41
3:L5:434:A:H2'	3:L5:435:A:O4'	2.21	0.41
3:L5:652:G:H2'	3:L5:653:U:C6	2.55	0.41
3:L5:732:A:H2'	3:L5:733:A:O4'	2.21	0.41
3:L5:921:C:H2'	3:L5:922:C:H6	1.86	0.41
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.55	0.41
3:L5:2097:U:O3'	3:L5:2098:G:H8	2.04	0.41
3:L5:2293:U:H2'	3:L5:2294:G:C8	2.56	0.41
3:L5:2553:A:OP2	3:L5:2574:G:O2'	2.36	0.41
3:L5:2809:G:O2'	3:L5:4644:G:OP1	2.30	0.41
3:L5:2871:A:H2'	3:L5:2872:C:O4'	2.21	0.41
3:L5:4697:U:H4'	76:Lm:104:HIS:CD2	2.56	0.41
3:L5:4748:U:OP1	70:Lf:54:LYS:HE2	2.21	0.41
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.56	0.41
6:SA:87:VAL:HG12	6:SA:175:TRP:CE2	2.55	0.41
30:SY:44:LEU:HD23	30:SY:44:LEU:HA	1.85	0.41
30:SY:109:GLU:HB3	30:SY:113:ARG:HH21	1.86	0.41
34:Sc:14:VAL:HG22	34:Sc:32:VAL:HG12	2.03	0.41
1:S2:1028:A:H2'	1:S2:1029:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1097:G:H4'	6:SA:32:PHE:CD1	2.56	0.41
1:S2:1348:G:C8	1:S2:1349:G:C8	3.09	0.41
1:S2:1513:C:P	23:Sd:12:ARG:HH22	2.43	0.41
1:S2:1713:C:H2'	1:S2:1714:U:C6	2.56	0.41
3:L5:689:U:H2'	3:L5:690:C:H6	1.86	0.41
3:L5:1677:PSU:H4'	3:L5:1680:G:N1	2.36	0.41
3:L5:2284:G:OP1	49:La:7:LYS:NZ	2.46	0.41
3:L5:4638:U:H2'	3:L5:4639:G:N3	2.35	0.41
91:L5:5875:HOH:O	49:La:24:LYS:HE3	2.20	0.41
8:SJ:42:GLU:HG3	8:SJ:45:ARG:NH2	2.35	0.41
9:SE:124:CYS:HA	9:SE:142:HIS:CE1	2.55	0.41
15:SI:144:LYS:HE3	15:SI:145:ILE:HB	2.02	0.41
24:SN:93:LYS:HA	24:SN:150:VAL:HG21	2.02	0.41
34:Sc:44:ARG:HE	34:Sc:44:ARG:HB3	1.78	0.41
38:LA:117:GLU:HG2	38:LA:124:GLY:H	1.86	0.41
44:LG:39:PHE:CD1	44:LG:47:PRO:HD3	2.55	0.41
44:LG:50:ASP:HB2	59:LX:40:ILE:HD12	2.03	0.41
44:LG:128:VAL:O	44:LG:130:THR:HG23	2.21	0.41
46:LL:7:GLY:O	49:La:49:HIS:NE2	2.50	0.41
55:LS:11:LYS:HE3	55:LS:29:ARG:HD3	2.01	0.41
68:Ld:93:ASN:O	68:Ld:94:GLU:HB3	2.20	0.41
71:Lg:41:ALA:O	71:Lg:52:ARG:HD3	2.20	0.41
1:S2:174:OMC:HM23	1:S2:174:OMC:H1'	1.85	0.41
1:S2:561:A:H2'	1:S2:562:U:C6	2.55	0.41
1:S2:806:U:H2'	1:S2:807:G:C8	2.56	0.41
1:S2:1016:U:H5'	24:SN:15:ALA:O	2.20	0.41
1:S2:1410:C:H2'	1:S2:1411:G:C8	2.56	0.41
1:S2:1438:A:H2'	1:S2:1439:A:H8	1.86	0.41
1:S2:1714:U:H2'	1:S2:1715:A:C8	2.56	0.41
2:L8:52:A:H5'	75:Ll:21:ARG:HD3	2.03	0.41
2:L8:80:A:H8	2:L8:84:A:OP1	2.03	0.41
3:L5:123:C:H2'	3:L5:124:C:C6	2.56	0.41
3:L5:644:G:H2'	3:L5:645:G:C8	2.56	0.41
3:L5:737:C:C5	3:L5:740:G:H5'	2.56	0.41
3:L5:740:G:OP2	48:LM:71:LYS:NZ	2.53	0.41
3:L5:1244:G:H2'	3:L5:1245:C:C6	2.55	0.41
3:L5:1577:G:H5'	3:L5:1578:U:H5''	2.03	0.41
3:L5:1773:U:H2'	3:L5:1774:C:H6	1.85	0.41
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.55	0.41
3:L5:2741:U:H2'	38:LA:50:HIS:CD2	2.55	0.41
3:L5:3701:OMC:N4	3:L5:3745:U:H2'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3865:A:H2'	3:L5:3866:C:C6	2.55	0.41
3:L5:4178:A:H2'	3:L5:4179:G:C8	2.56	0.41
3:L5:4352:U:P	46:LL:190[B]:ARG:HH22	2.40	0.41
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.85	0.41
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.20	0.41
82:L5:5114:SPD:H71	82:L5:5114:SPD:H41	1.35	0.41
5:SB:147:ASN:OD1	5:SB:148:ASN:N	2.54	0.41
7:SD:161:GLY:O	7:SD:164:VAL:HG12	2.20	0.41
8:SJ:111:GLN:NE2	8:SJ:123:ILE:HG13	2.35	0.41
10:SC:78:LEU:HD12	10:SC:81:ILE:HD12	2.03	0.41
14:SW:12:LYS:HB2	14:SW:12:LYS:HE3	1.94	0.41
15:SI:145:ILE:O	15:SI:148:LYS:HG2	2.21	0.41
21:SM:85:LEU:HA	21:SM:88:TRP:HB2	2.03	0.41
30:SY:56:PHE:HB2	30:SY:74:MET:HB2	2.03	0.41
36:Sf:104:LYS:HD3	36:Sf:104:LYS:HA	1.83	0.41
36:Sf:126:CYS:SG	36:Sf:127:GLY:N	2.94	0.41
37:Sg:11:LEU:HD21	37:Sg:52:TYR:HD2	1.85	0.41
37:Sg:230:LEU:HD21	37:Sg:259:TRP:CE2	2.56	0.41
37:Sg:240:CYS:SG	37:Sg:249:CYS:HB2	2.60	0.41
37:Sg:258:ILE:O	37:Sg:267:VAL:HG12	2.21	0.41
44:LG:100:HIS:HA	44:LG:103:ARG:HG3	2.03	0.41
54:LR:99:MET:HE2	54:LR:99:MET:HA	2.03	0.41
54:LR:178:GLN:OE1	54:LR:178:GLN:HA	2.20	0.41
61:LW:80:ARG:HE	61:LW:80:ARG:HB3	1.69	0.41
66:LF:222:LYS:HE3	66:LF:224:THR:OG1	2.21	0.41
1:S2:162:C:H2'	1:S2:163:U:O4'	2.21	0.41
1:S2:1651:A:H1'	12:SF:83:ASN:ND2	2.36	0.41
1:S2:1782:G:H1	61:LW:73:ARG:NE	2.19	0.41
2:L8:16:G:N2	3:L5:417:G:H1'	2.36	0.41
2:L8:128:C:H2'	2:L8:129:C:H6	1.85	0.41
3:L5:654:C:C2	3:L5:655:C:C5	3.09	0.41
3:L5:656:C:H2'	3:L5:657:C:H6	1.85	0.41
3:L5:699:C:H2'	3:L5:700:G:H8	1.85	0.41
3:L5:1328:G:O2'	3:L5:2349:A:OP1	2.37	0.41
3:L5:2414:G:H2'	3:L5:2415:OMU:H6	2.03	0.41
3:L5:2693:G:H2'	3:L5:2694:G:C2	2.56	0.41
3:L5:3770:PSU:OP1	81:Pt:25:U:O2'	2.37	0.41
3:L5:3771:C:H4'	81:Pt:13:C:H4'	2.03	0.41
3:L5:4670:C:O3'	3:L5:4671:C:H3'	2.21	0.41
3:L5:4926:C:O2'	3:L5:4927:G:H5'	2.21	0.41
4:L7:58:A:H2'	4:L7:59:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SB:103:MET:HG2	5:SB:104:ASP:N	2.36	0.41
7:SD:218:LEU:HD12	37:Sg:192:THR:HA	2.02	0.41
19:SO:61:LYS:HA	19:SO:61:LYS:HD2	1.84	0.41
21:SM:31:LEU:HB2	21:SM:33:ARG:HH12	1.85	0.41
28:ST:77:LYS:HE3	28:ST:77:LYS:HB2	1.81	0.41
38:LA:173:GLY:O	38:LA:176:ASP:HB2	2.20	0.41
46:LL:108:GLU:OE2	72:Li:18:THR:HG22	2.21	0.41
56:LT:133:ALA:HB3	66:LF:127:LYS:HB2	2.03	0.41
62:LZ:14:LEU:O	71:Lg:88:ARG:HG2	2.21	0.41
66:LF:143:GLY:HA3	66:LF:240:ILE:HB	2.03	0.41
1:S2:540:U:C2'	1:S2:543:C:H41	2.34	0.40
1:S2:867:OMG:O2'	1:S2:868:G:H5'	2.21	0.40
1:S2:1275:G:H5''	1:S2:1506:A:H61	1.86	0.40
2:L8:92:U:H2'	2:L8:93:C:O4'	2.21	0.40
3:L5:134:G:O6	64:Lh:74:LYS:HG3	2.21	0.40
3:L5:1646:A:O2'	73:Lj:49:TRP:O	2.34	0.40
3:L5:4605:A:H2'	3:L5:4606:G:O4'	2.21	0.40
3:L5:4618:OMG:HM23	3:L5:4618:OMG:H1'	1.82	0.40
9:SE:118:GLU:OE2	9:SE:237:SER:N	2.52	0.40
11:SG:165:GLU:HB2	11:SG:166:GLY:H	1.67	0.40
12:SF:142:SER:HB2	34:Sc:50:VAL:HG13	2.03	0.40
20:SX:107:ARG:HB3	20:SX:110:HIS:HB3	2.04	0.40
26:SR:27:ASP:OD1	26:SR:30:THR:N	2.37	0.40
43:LE:183:ARG:HD2	43:LE:183:ARG:HA	1.78	0.40
46:LL:200:LYS:HE3	46:LL:200:LYS:HB3	1.83	0.40
52:LD:156:GLY:HA2	52:LD:181:PRO:HG3	2.03	0.40
74:Lk:8:ILE:HD13	74:Lk:45:LEU:HD21	2.02	0.40
1:S2:85:A:H2'	1:S2:86:C:H6	1.86	0.40
1:S2:1144:A:H5'	1:S2:1355:C:H41	1.86	0.40
1:S2:1489:A:O2'	1:S2:1490:OMG:OP1	2.32	0.40
1:S2:1545:A:H5''	16:SQ:74:GLY:HA2	2.03	0.40
1:S2:1550:G:H3'	1:S2:1579:A:N6	2.30	0.40
1:S2:1678:A2M:OP2	12:SF:63:LYS:NZ	2.48	0.40
1:S2:1829:G:H21	1:S2:1851:MA6:C2	2.35	0.40
3:L5:255:C:N4	3:L5:256:G:N7	2.69	0.40
3:L5:729:G:H5'	3:L5:729:G:N3	2.36	0.40
3:L5:1248:C:H2'	3:L5:1249:C:C6	2.56	0.40
3:L5:1699:A:H2'	3:L5:1700:G:C8	2.55	0.40
3:L5:1858:A:H2'	3:L5:1859:C:H6	1.86	0.40
3:L5:2862:G:H4'	3:L5:3625:G:N7	2.36	0.40
3:L5:4137:C:H2'	3:L5:4138:C:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4304:A:C2	49:La:43:ILE:HG23	2.55	0.40
3:L5:4521:PSU:H1'	39:LB:253:CYS:SG	2.61	0.40
3:L5:4968:A:H2'	3:L5:4969:C:C6	2.57	0.40
4:L7:2:U:H2'	4:L7:3:C:C6	2.56	0.40
5:SB:83:LYS:HE3	5:SB:83:LYS:HB2	1.88	0.40
7:SD:206:ASP:OD1	7:SD:206:ASP:N	2.53	0.40
9:SE:57:THR:O	9:SE:61:VAL:HG23	2.21	0.40
73:Lj:39:TYR:CD1	73:Lj:40:PRO:HA	2.57	0.40
1:S2:69:C:H2'	1:S2:70:G:O4'	2.22	0.40
1:S2:81:U:H2'	1:S2:82:G:O4'	2.21	0.40
1:S2:540:U:H2'	1:S2:543:C:H41	1.86	0.40
1:S2:563:G:O2'	1:S2:564:A:H8	2.04	0.40
1:S2:806:U:H2'	1:S2:807:G:H8	1.87	0.40
1:S2:1007:C:H2'	1:S2:1008:A:C8	2.55	0.40
1:S2:1036:A:H4'	1:S2:1855:G:N2	2.36	0.40
1:S2:1181:A:H2'	1:S2:1182:A:C8	2.57	0.40
1:S2:1648:G:H22	1:S2:1675:A:P	2.45	0.40
1:S2:1746:U:H4'	11:SG:65:GLN:NE2	2.36	0.40
2:L8:47:C:H1'	2:L8:61:A:H2'	2.03	0.40
2:L8:144:U:H2'	2:L8:145:C:H6	1.85	0.40
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.56	0.40
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.82	0.40
3:L5:2065:G:H2'	3:L5:2066:C:O4'	2.21	0.40
3:L5:4188:U:H2'	3:L5:4189:U:H6	1.84	0.40
3:L5:4760:G:H2'	3:L5:4761:G:O4'	2.22	0.40
4:L7:39:C:H4'	41:LJ:47:THR:HG23	2.02	0.40
6:SA:33:GLN:HB3	6:SA:154:LEU:HD12	2.03	0.40
13:SH:162:GLN:O	13:SH:166:VAL:HG22	2.21	0.40
16:SQ:108:ILE:HG13	16:SQ:109:LYS:N	2.36	0.40
41:LJ:153:ALA:HA	41:LJ:156:ARG:HG3	2.03	0.40
42:LH:120:GLU:OE2	42:LH:124:ARG:NH1	2.46	0.40
43:LE:180:VAL:HG21	43:LE:258:LEU:HD11	2.02	0.40
52:LD:273:LEU:HG	52:LD:277:LYS:HD2	2.01	0.40
55:LS:39:VAL:HG22	66:LF:228:VAL:HA	2.03	0.40
66:LF:226:HIS:ND1	66:LF:228:VAL:HG22	2.36	0.40
81:Pt:8:4SU:O2'	81:Pt:22:A:N1	2.47	0.40
1:S2:342:C:C2	1:S2:343:A:C8	3.09	0.40
1:S2:375:U:H2'	1:S2:376:A:C8	2.56	0.40
1:S2:379:C:H5'	15:SI:33:ALA:HA	2.02	0.40
1:S2:1380:C:H2'	1:S2:1381:G:O4'	2.21	0.40
1:S2:1424:G:C5	1:S2:1425:G:N7	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1608:U:OP1	22:SS:134:GLN:NE2	2.46	0.40
2:L8:40:A:H2'	2:L8:41:A:C8	2.57	0.40
3:L5:240:G:H2'	3:L5:241:G:O4'	2.21	0.40
3:L5:518:G:N2	3:L5:643:C:H2'	2.37	0.40
3:L5:667:A:H2'	3:L5:668:C:C6	2.56	0.40
3:L5:751:G:H2'	3:L5:752:G:O4'	2.21	0.40
3:L5:1205:G:H2'	3:L5:1206:C:H6	1.86	0.40
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.88	0.40
3:L5:2500:U:H2'	3:L5:2501:C:C6	2.57	0.40
3:L5:2602:G:H2'	3:L5:2603:C:H6	1.85	0.40
3:L5:2654:C:H2'	3:L5:2655:C:C6	2.55	0.40
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.56	0.40
3:L5:4390:A:H2'	3:L5:4391:G:O4'	2.21	0.40
3:L5:4401:G:H2'	3:L5:4402:C:C6	2.57	0.40
3:L5:4452:U:C4	3:L5:4531:PSU:C2	3.10	0.40
3:L5:4635:A:OP1	3:L5:4636:PSU:O2'	2.36	0.40
9:SE:44:LEU:HD12	9:SE:44:LEU:HA	1.88	0.40
11:SG:181:THR:HB	11:SG:184:VAL:HG23	2.04	0.40
13:SH:178:LYS:NZ	13:SH:184:ASP:OD1	2.34	0.40
16:SQ:8:GLN:HG3	16:SQ:99:TYR:CE1	2.56	0.40
22:SS:55:ARG:NE	31:SZ:48:VAL:HG21	2.36	0.40
31:SZ:69:THR:OG1	31:SZ:72:VAL:HG12	2.21	0.40
37:Sg:168:CYS:HB3	37:Sg:198:VAL:HB	2.04	0.40
45:LO:76:PRO:HB3	45:LO:138:LEU:HG	2.02	0.40
58:LU:19:LEU:HD23	58:LU:19:LEU:HA	1.97	0.40
67:Lc:35:LEU:HD23	67:Lc:35:LEU:HA	1.90	0.40
1:S2:17:C:O2'	1:S2:1194:A:N1	2.46	0.40
1:S2:76:U:H5'	1:S2:77:A:OP2	2.21	0.40
1:S2:116:OMU:HM23	1:S2:116:OMU:H1'	1.71	0.40
1:S2:1010:G:H2'	1:S2:1011:A:C8	2.57	0.40
3:L5:306:A:OP1	72:Li:53:TYR:HE1	2.05	0.40
3:L5:1075:G:H2'	3:L5:1076:C:C6	2.57	0.40
3:L5:1201:U:H2'	3:L5:1202:C:C6	2.57	0.40
3:L5:1472:C:H2'	3:L5:1473:U:H6	1.87	0.40
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.57	0.40
3:L5:2442:G:O2'	3:L5:2512:A:N3	2.54	0.40
3:L5:3725:G:O6	72:Li:71:LYS:HE2	2.21	0.40
3:L5:4173:G:H2'	3:L5:4174:U:C6	2.57	0.40
7:SD:109:LEU:HD12	7:SD:184:ILE:HD11	2.03	0.40
10:SC:183:LYS:HA	10:SC:195:LEU:O	2.21	0.40
37:Sg:67:SER:OG	37:Sg:108:VAL:O	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:218:LEU:HD21	37:Sg:228:TYR:HB2	2.04	0.40
37:Sg:276:SER:OG	37:Sg:277:THR:N	2.53	0.40
52:LD:187:SER:HB2	52:LD:189:GLU:OE2	2.22	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	
5	SB	219/264 (83%)	217 (99%)	2 (1%)	0	100	100
6	SA	220/295 (75%)	214 (97%)	6 (3%)	0	100	100
7	SD	224/243 (92%)	213 (95%)	11 (5%)	0	100	100
8	SJ	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
9	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
10	SC	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
11	SG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
12	SF	187/204 (92%)	179 (96%)	6 (3%)	2 (1%)	11	1
13	SH	187/194 (96%)	176 (94%)	9 (5%)	2 (1%)	11	1
14	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
15	SI	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
16	SQ	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
17	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
18	SK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
19	SO	133/151 (88%)	128 (96%)	4 (3%)	1 (1%)	16	4
20	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
21	SM	120/132 (91%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	SS	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
23	Sd	53/56 (95%)	53 (100%)	0	0	100	100
24	SN	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
25	SL	142/158 (90%)	139 (98%)	3 (2%)	0	100	100
26	SR	132/135 (98%)	121 (92%)	11 (8%)	0	100	100
27	SP	129/145 (89%)	126 (98%)	3 (2%)	0	100	100
28	ST	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
29	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
30	SY	129/133 (97%)	126 (98%)	3 (2%)	0	100	100
31	SZ	82/125 (66%)	78 (95%)	4 (5%)	0	100	100
32	Sa	98/115 (85%)	98 (100%)	0	0	100	100
33	Sb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	Sc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
35	Se	46/133 (35%)	45 (98%)	0	1 (2%)	5	0
36	Sf	61/156 (39%)	53 (87%)	8 (13%)	0	100	100
37	Sg	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
38	LA	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
39	LB	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
40	LC	364/427 (85%)	361 (99%)	3 (1%)	0	100	100
41	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
42	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
43	LE	217/288 (75%)	212 (98%)	5 (2%)	0	100	100
44	LG	239/266 (90%)	230 (96%)	9 (4%)	0	100	100
45	LO	200/203 (98%)	199 (100%)	1 (0%)	0	100	100
46	LL	205/211 (97%)	198 (97%)	7 (3%)	0	100	100
47	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
48	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
49	La	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	5
50	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
51	LI	199/214 (93%)	198 (100%)	1 (0%)	0	100	100
52	LD	292/297 (98%)	288 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	LQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
54	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
55	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
56	LT	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
57	LP	152/184 (83%)	150 (99%)	2 (1%)	0	100	100
58	LU	97/128 (76%)	95 (98%)	1 (1%)	1 (1%)	12	2
59	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
60	LY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
61	LW	114/157 (73%)	109 (96%)	5 (4%)	0	100	100
62	LZ	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
63	Lr	124/137 (90%)	124 (100%)	0	0	100	100
64	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
65	Lb	106/159 (67%)	103 (97%)	3 (3%)	0	100	100
66	LF	225/248 (91%)	219 (97%)	6 (3%)	0	100	100
67	Lc	97/115 (84%)	97 (100%)	0	0	100	100
68	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
69	Le	127/135 (94%)	127 (100%)	0	0	100	100
70	Lf	108/110 (98%)	108 (100%)	0	0	100	100
71	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
72	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
73	Lj	85/97 (88%)	85 (100%)	0	0	100	100
74	Lk	67/70 (96%)	67 (100%)	0	0	100	100
75	Ll	48/51 (94%)	48 (100%)	0	0	100	100
76	Lm	50/128 (39%)	50 (100%)	0	0	100	100
77	Ln	23/25 (92%)	23 (100%)	0	0	100	100
78	Lo	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
79	Lp	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	11301/12762 (89%)	11033 (98%)	260 (2%)	8 (0%)	49	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	Se	119	VAL

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Mol	Chain	Res	Type
19	SO	138	ASP
13	SH	18	GLU
12	SF	79	HIS
12	SF	80	GLY
49	La	15	VAL
58	LU	67	LYS
13	SH	16	PRO

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	
5	SB	202/231 (87%)	197 (98%)	5 (2%)	42	16
6	SA	183/242 (76%)	182 (100%)	1 (0%)	81	72
7	SD	189/202 (94%)	181 (96%)	8 (4%)	26	5
8	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	43
9	SE	224/225 (100%)	219 (98%)	5 (2%)	45	19
10	SC	188/225 (84%)	186 (99%)	2 (1%)	65	47
11	SG	207/218 (95%)	206 (100%)	1 (0%)	81	72
12	SF	159/170 (94%)	152 (96%)	7 (4%)	25	4
13	SH	168/174 (97%)	157 (94%)	11 (6%)	15	1
14	SW	112/113 (99%)	112 (100%)	0	100	100
15	SI	178/180 (99%)	173 (97%)	5 (3%)	38	12
16	SQ	117/121 (97%)	109 (93%)	8 (7%)	14	1
17	SU	93/107 (87%)	90 (97%)	3 (3%)	34	9
18	SK	87/136 (64%)	87 (100%)	0	100	100
19	SO	105/119 (88%)	104 (99%)	1 (1%)	68	52
20	SX	111/114 (97%)	107 (96%)	4 (4%)	31	6
21	SM	104/108 (96%)	99 (95%)	5 (5%)	23	4
22	SS	128/132 (97%)	123 (96%)	5 (4%)	28	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	21
24	SN	131/131 (100%)	128 (98%)	3 (2%)	44	18
25	SL	132/142 (93%)	131 (99%)	1 (1%)	73	59
26	SR	121/122 (99%)	115 (95%)	6 (5%)	22	3
27	SP	117/130 (90%)	112 (96%)	5 (4%)	26	5
28	ST	114/115 (99%)	109 (96%)	5 (4%)	25	4
29	SV	66/66 (100%)	65 (98%)	1 (2%)	57	34
30	SY	113/115 (98%)	109 (96%)	4 (4%)	32	7
31	SZ	74/103 (72%)	71 (96%)	3 (4%)	27	5
32	Sa	87/98 (89%)	83 (95%)	4 (5%)	24	4
33	Sb	75/76 (99%)	72 (96%)	3 (4%)	28	5
34	Sc	58/62 (94%)	56 (97%)	2 (3%)	32	8
35	Se	40/104 (38%)	40 (100%)	0	100	100
36	Sf	56/140 (40%)	54 (96%)	2 (4%)	31	6
37	Sg	272/275 (99%)	261 (96%)	11 (4%)	28	5
38	LA	193/198 (98%)	192 (100%)	1 (0%)	81	72
39	LB	347/348 (100%)	347 (100%)	0	100	100
40	LC	305/348 (88%)	303 (99%)	2 (1%)	76	62
41	LJ	143/149 (96%)	143 (100%)	0	100	100
42	LH	169/171 (99%)	169 (100%)	0	100	100
43	LE	196/252 (78%)	195 (100%)	1 (0%)	81	72
44	LG	203/223 (91%)	202 (100%)	1 (0%)	81	72
45	LO	173/174 (99%)	173 (100%)	0	100	100
46	LL	173/177 (98%)	172 (99%)	1 (1%)	78	67
47	LV	102/107 (95%)	102 (100%)	0	100	100
48	LM	116/161 (72%)	115 (99%)	1 (1%)	70	55
49	La	119/120 (99%)	119 (100%)	0	100	100
50	LN	171/172 (99%)	169 (99%)	2 (1%)	63	43
51	LI	173/181 (96%)	171 (99%)	2 (1%)	63	43
52	LD	247/250 (99%)	245 (99%)	2 (1%)	73	59
53	LQ	164/165 (99%)	161 (98%)	3 (2%)	51	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	LR	166/175 (95%)	164 (99%)	2 (1%)	63	43
55	LS	157/157 (100%)	157 (100%)	0	100	100
56	LT	141/140 (101%)	141 (100%)	0	100	100
57	LP	135/163 (83%)	135 (100%)	0	100	100
58	LU	89/115 (77%)	87 (98%)	2 (2%)	45	19
59	LX	106/133 (80%)	106 (100%)	0	100	100
60	LY	124/135 (92%)	121 (98%)	3 (2%)	43	17
61	LW	95/126 (75%)	93 (98%)	2 (2%)	47	21
62	LZ	118/118 (100%)	117 (99%)	1 (1%)	73	59
63	Lr	109/120 (91%)	109 (100%)	0	100	100
64	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	55
65	Lb	90/125 (72%)	89 (99%)	1 (1%)	65	47
66	LF	196/215 (91%)	196 (100%)	0	100	100
67	Lc	84/97 (87%)	84 (100%)	0	100	100
68	Ld	98/110 (89%)	98 (100%)	0	100	100
69	Le	115/121 (95%)	115 (100%)	0	100	100
70	Lf	89/89 (100%)	89 (100%)	0	100	100
71	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	52
72	Li	86/89 (97%)	85 (99%)	1 (1%)	63	43
73	Lj	74/80 (92%)	73 (99%)	1 (1%)	59	36
74	Lk	64/65 (98%)	64 (100%)	0	100	100
75	Ll	47/48 (98%)	46 (98%)	1 (2%)	47	21
76	Lm	48/115 (42%)	47 (98%)	1 (2%)	47	21
77	Ln	24/24 (100%)	24 (100%)	0	100	100
78	Lo	93/93 (100%)	92 (99%)	1 (1%)	65	47
79	Lp	75/75 (100%)	75 (100%)	0	100	100
All	All	9844/10847 (91%)	9686 (98%)	158 (2%)	54	32

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SB	43	ASN
5	SB	53	GLN

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Mol	Chain	Res	Type
5	SB	69	VAL
5	SB	131	ASP
5	SB	232	HIS
6	SA	190	SER
7	SD	35	SER
7	SD	42	THR
7	SD	84	VAL
7	SD	138	VAL
7	SD	149	SER
7	SD	190	LEU
7	SD	195	THR
7	SD	221	THR
8	SJ	104	ASP
8	SJ	141	VAL
9	SE	98	ASN
9	SE	115	THR
9	SE	173	ILE
9	SE	194	VAL
9	SE	236	ILE
10	SC	206	SER
10	SC	275	LYS
11	SG	157	VAL
12	SF	17	ILE
12	SF	33	ILE
12	SF	78	MET
12	SF	85	LYS
12	SF	126	THR
12	SF	165	ASN
12	SF	177	LEU
13	SH	8	ILE
13	SH	9	VAL
13	SH	10	LYS
13	SH	12	ASN
13	SH	14	GLU
13	SH	15	LYS
13	SH	18	GLU
13	SH	21	SER
13	SH	64	VAL
13	SH	110	THR
13	SH	151	SER
15	SI	4	SER
15	SI	45	THR

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Mol	Chain	Res	Type
15	SI	91	VAL
15	SI	130	THR
15	SI	164	GLU
16	SQ	9	SER
16	SQ	20	THR
16	SQ	31	LEU
16	SQ	97	GLN
16	SQ	100	VAL
16	SQ	113	ILE
16	SQ	129	SER
16	SQ	144	SER
17	SU	30	LYS
17	SU	68	THR
17	SU	114	VAL
19	SO	137	SER
20	SX	25	LYS
20	SX	105	PHE
20	SX	119	ARG
20	SX	125	VAL
21	SM	40	LYS
21	SM	52	LEU
21	SM	74	ILE
21	SM	108	CYS
21	SM	109	VAL
22	SS	53	THR
22	SS	83	PHE
22	SS	124	ARG
22	SS	136	THR
22	SS	146	VAL
23	Sd	41	GLN
24	SN	30	SER
24	SN	123[A]	HIS
24	SN	123[B]	HIS
25	SL	104	LYS
26	SR	27	ASP
26	SR	38	ILE
26	SR	89	SER
26	SR	119	VAL
26	SR	124	VAL
26	SR	130	THR
27	SP	76	VAL
27	SP	86	LEU

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Mol	Chain	Res	Type
27	SP	88	GLU
27	SP	94	VAL
27	SP	124	LYS
28	ST	4	VAL
28	ST	25	SER
28	ST	36	THR
28	ST	38	LYS
28	ST	87	VAL
29	SV	18	SER
30	SY	24	VAL
30	SY	35	VAL
30	SY	51	THR
30	SY	125	VAL
31	SZ	50	PHE
31	SZ	58	LEU
31	SZ	82	SER
32	Sa	30	VAL
32	Sa	40	VAL
32	Sa	85[A]	ARG
32	Sa	85[B]	ARG
33	Sb	24	LEU
33	Sb	37	CYS
33	Sb	57	VAL
34	Sc	23	SER
34	Sc	50	VAL
36	Sf	100	LEU
36	Sf	146	LEU
37	Sg	46	THR
37	Sg	54	ILE
37	Sg	113	PHE
37	Sg	134	THR
37	Sg	146	SER
37	Sg	155	ARG
37	Sg	160	SER
37	Sg	164	ILE
37	Sg	189	ILE
37	Sg	235	ILE
37	Sg	236	ILE
38	LA	208	GLU
40	LC	9	SER
40	LC	336	ARG
43	LE	123	ARG

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Mol	Chain	Res	Type
44	LG	229	ARG
46	LL	59	VAL
48	LM	136	LEU
50	LN	10	LEU
50	LN	151	ILE
51	LI	53	VAL
51	LI	212	LEU
52	LD	75	VAL
52	LD	230	SER
53	LQ	14	ARG
53	LQ	92	VAL
53	LQ	172	ARG
54	LR	111	GLU
54	LR	166	THR
58	LU	62	THR
58	LU	107	LYS
60	LY	46	SER
60	LY	113	LYS
60	LY	130	LYS
61	LW	2	LYS
61	LW	100	VAL
62	LZ	100	VAL
64	Lh	97	LYS
65	Lb	114	LYS
71	Lg	106	VAL
72	Li	18	THR
73	Lj	20	ARG
75	Ll	47	THR
76	Lm	127	VAL
78	Lo	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
5	SB	186	ASN
5	SB	208	HIS
7	SD	159	HIS
8	SJ	140	GLN
8	SJ	177	ASN
11	SG	163	ASN
12	SF	79	HIS
12	SF	83	ASN

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Mol	Chain	Res	Type
13	SH	112	ASN
13	SH	168	HIS
15	SI	52	ASN
16	SQ	77	HIS
17	SU	47	ASN
17	SU	100	GLN
18	SK	66	HIS
21	SM	75	ASN
22	SS	11	HIS
23	Sd	26	ASN
24	SN	138	ASN
25	SL	19	ASN
25	SL	121	GLN
25	SL	154	GLN
26	SR	48	ASN
26	SR	56	HIS
28	ST	12	GLN
29	SV	2	GLN
31	SZ	89	GLN
31	SZ	106	GLN
37	Sg	26	GLN
39	LB	203	GLN
39	LB	209	GLN
39	LB	376	HIS
40	LC	38	ASN
40	LC	43	ASN
40	LC	198	ASN
40	LC	212	ASN
40	LC	329	ASN
42	LH	98	HIS
42	LH	102	ASN
42	LH	108	ASN
43	LE	101	ASN
44	LG	141	ASN
45	LO	180	GLN
48	LM	66	HIS
48	LM	131	GLN
49	La	120	GLN
51	LI	59	GLN
51	LI	73	ASN
51	LI	130	HIS
52	LD	45	ASN

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Mol	Chain	Res	Type
52	LD	202	GLN
54	LR	40	GLN
55	LS	23	HIS
56	LT	79	GLN
57	LP	21	ASN
57	LP	75	GLN
57	LP	133	HIS
58	LU	94	ASN
59	LX	93	ASN
59	LX	107	HIS
60	LY	18	HIS
60	LY	56	GLN
60	LY	61	HIS
60	LY	66	GLN
60	LY	72	GLN
60	LY	96	HIS
61	LW	50	ASN
61	LW	95	ASN
67	Lc	19	GLN
67	Lc	72	HIS
68	Ld	116	ASN
69	Le	107	ASN
72	Li	15	HIS
75	Ll	33	ASN
78	Lo	102	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1667/1869 (89%)	255 (15%)	1 (0%)
2	L8	155/156 (99%)	19 (12%)	0
3	L5	3530/5069 (69%)	504 (14%)	15 (0%)
4	L7	119/120 (99%)	8 (6%)	0
80	mR	7/60 (11%)	3 (42%)	0
81	Pt	76/77 (98%)	8 (10%)	0
All	All	5554/7351 (75%)	797 (14%)	16 (0%)

All (797) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C

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Mol	Chain	Res	Type
1	S2	4	C
1	S2	17	C
1	S2	33	G
1	S2	41	G
1	S2	46	A
1	S2	56	G
1	S2	65	C
1	S2	67	C
1	S2	68	A
1	S2	74	G
1	S2	75	G
1	S2	76	U
1	S2	79	A
1	S2	92	A
1	S2	103	A
1	S2	113	G
1	S2	115	U
1	S2	126	G
1	S2	127	C
1	S2	129	C
1	S2	140	C
1	S2	143	U
1	S2	147	A
1	S2	155	G
1	S2	162	C
1	S2	168	C
1	S2	184	G
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	201	C
1	S2	202	G
1	S2	203	G
1	S2	204	G
1	S2	207	G
1	S2	215	G
1	S2	309	G
1	S2	312	G
1	S2	319	C
1	S2	320	G
1	S2	323	C
1	S2	324	C

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Mol	Chain	Res	Type
1	S2	327	G
1	S2	328	U
1	S2	335	G
1	S2	347	G
1	S2	362	C
1	S2	364	A
1	S2	370	G
1	S2	381	C
1	S2	385	G
1	S2	386	C
1	S2	407	G
1	S2	409	C
1	S2	438	G
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	465	A
1	S2	466	G
1	S2	467	G
1	S2	472	C
1	S2	474	G
1	S2	476	A
1	S2	482	G
1	S2	487	U
1	S2	492	C
1	S2	493	A
1	S2	496	C
1	S2	508	A
1	S2	516	A
1	S2	523	A
1	S2	533	A
1	S2	534	G
1	S2	537	C
1	S2	540	U
1	S2	545	A
1	S2	546	G
1	S2	554	A
1	S2	555	A
1	S2	560	A
1	S2	563	G
1	S2	564	A
1	S2	570	C

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Mol	Chain	Res	Type
1	S2	576	A2M
1	S2	587	A
1	S2	590	A2M
1	S2	591	U
1	S2	604	A
1	S2	606	G
1	S2	608	C
1	S2	614	C
1	S2	617	G
1	S2	620	G
1	S2	628	A
1	S2	632	C
1	S2	643	A
1	S2	644	OMG
1	S2	655	A
1	S2	660	C
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	688	U
1	S2	800	U
1	S2	821	G
1	S2	822	PSU
1	S2	827	A
1	S2	830	A
1	S2	831	G
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	840	C
1	S2	847	A
1	S2	870	A
1	S2	872	A
1	S2	889	U
1	S2	891	G
1	S2	892	U
1	S2	895	G
1	S2	896	U
1	S2	897	U
1	S2	898	U

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Mol	Chain	Res	Type
1	S2	903	A
1	S2	913	A
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	933	G
1	S2	943	U
1	S2	990	A
1	S2	992	A
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1055	A
1	S2	1061	U
1	S2	1062	A
1	S2	1083	A
1	S2	1085	C
1	S2	1107	G
1	S2	1109	C
1	S2	1115	U
1	S2	1121	G
1	S2	1133	A
1	S2	1138	C
1	S2	1153	C
1	S2	1154	U
1	S2	1157	G
1	S2	1183	A
1	S2	1188	A
1	S2	1195	A
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1224	G
1	S2	1242	U
1	S2	1243	PSU
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1274	G
1	S2	1275	G

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Mol	Chain	Res	Type
1	S2	1277	C
1	S2	1285	G
1	S2	1286	G
1	S2	1302	G
1	S2	1303	C
1	S2	1308	U
1	S2	1312	G
1	S2	1313	A
1	S2	1315	U
1	S2	1331	C
1	S2	1332	A
1	S2	1333	U
1	S2	1342	U
1	S2	1348	G
1	S2	1358	U
1	S2	1371	U
1	S2	1372	U
1	S2	1378	A
1	S2	1402	A
1	S2	1406	G
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1433	C
1	S2	1435	C
1	S2	1437	C
1	S2	1438	A
1	S2	1439	A
1	S2	1442	OMU
1	S2	1454	A
1	S2	1463	U
1	S2	1466	G
1	S2	1489	A
1	S2	1490	OMG
1	S2	1498	A
1	S2	1521	C
1	S2	1522	A
1	S2	1531	A
1	S2	1533	A
1	S2	1547	C

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Mol	Chain	Res	Type
1	S2	1556	A
1	S2	1557	C
1	S2	1560	U
1	S2	1563	G
1	S2	1579	A
1	S2	1580	A
1	S2	1581	C
1	S2	1582	C
1	S2	1585	U
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A
1	S2	1601	A
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1648	G
1	S2	1654	G
1	S2	1665	G
1	S2	1695	A
1	S2	1699	A
1	S2	1721	U
1	S2	1722	G
1	S2	1744	G
1	S2	1748	G
1	S2	1751	C
1	S2	1752	C
1	S2	1754	G
1	S2	1777	G
1	S2	1782	G
1	S2	1783	C
1	S2	1825	A
1	S2	1826	G
1	S2	1829	G
1	S2	1831	A
1	S2	1835	A
1	S2	1838	U
1	S2	1849	G
1	S2	1851	MA6
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A

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Mol	Chain	Res	Type
1	S2	1864	U
1	S2	1865	C
2	L8	34	U
2	L8	35	C
2	L8	59	A
2	L8	62	A
2	L8	63	U
2	L8	86	U
2	L8	87	G
2	L8	94	G
2	L8	103	A
2	L8	105	C
2	L8	109	C
2	L8	110	U
2	L8	114	G
2	L8	123	U
2	L8	124	U
2	L8	125	C
2	L8	126	C
2	L8	127	U
2	L8	147	G
3	L5	2	G
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	73	A
3	L5	85	G
3	L5	91	G
3	L5	98	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	131	C
3	L5	132	G
3	L5	136	C
3	L5	140	G
3	L5	141	C
3	L5	142	G

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Mol	Chain	Res	Type
3	L5	143	C
3	L5	159	C
3	L5	178	C
3	L5	179	G
3	L5	181	C
3	L5	184	U
3	L5	186	G
3	L5	187	U
3	L5	188	G
3	L5	189	G
3	L5	200	U
3	L5	209	U
3	L5	210	C
3	L5	218	A
3	L5	219	G
3	L5	233	U
3	L5	234	G
3	L5	253	G
3	L5	256	G
3	L5	257	C
3	L5	259	C
3	L5	262	G
3	L5	266	C
3	L5	272	U
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	349	A
3	L5	387	G
3	L5	409	G
3	L5	410	A
3	L5	412	G
3	L5	413	G
3	L5	432	U
3	L5	440	U
3	L5	449	C
3	L5	450	G
3	L5	451	C
3	L5	453	G

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Mol	Chain	Res	Type
3	L5	454	U
3	L5	455	C
3	L5	461	G
3	L5	467	U
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	496	G
3	L5	499	G
3	L5	504	G
3	L5	509	A
3	L5	510	U
3	L5	513	U
3	L5	514	U
3	L5	644	G
3	L5	659	G
3	L5	663	G
3	L5	666	G
3	L5	667	A
3	L5	668	C
3	L5	669	C
3	L5	686	A
3	L5	687	U
3	L5	692	A
3	L5	696	C
3	L5	697	G
3	L5	704	C
3	L5	705	G
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	740	G
3	L5	742	G
3	L5	757	G
3	L5	759	G
3	L5	904	C
3	L5	914	U
3	L5	915	A
3	L5	916	C
3	L5	917	A

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Mol	Chain	Res	Type
3	L5	925	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	936	C
3	L5	943	A
3	L5	944	A
3	L5	945	U
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	964	A
3	L5	965	G
3	L5	967	C
3	L5	968	C
3	L5	969	C
3	L5	970	G
3	L5	1065	G
3	L5	1072	C
3	L5	1073	G
3	L5	1080	C
3	L5	1081	C
3	L5	1094	G
3	L5	1098	G
3	L5	1099	C
3	L5	1101	C
3	L5	1170	G
3	L5	1182	C
3	L5	1183	C
3	L5	1187	G
3	L5	1199	G
3	L5	1200	G
3	L5	1210	C
3	L5	1211	G
3	L5	1215	C
3	L5	1216	C
3	L5	1241	C
3	L5	1253	G
3	L5	1254	A
3	L5	1257	A
3	L5	1258	G

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Mol	Chain	Res	Type
3	L5	1266	G
3	L5	1270	A
3	L5	1272	C
3	L5	1273	G
3	L5	1279	A
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1293	G
3	L5	1302	U
3	L5	1303	A
3	L5	1313	C
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1359	G
3	L5	1366	G
3	L5	1378	C
3	L5	1387	A
3	L5	1397	A
3	L5	1398	A
3	L5	1399	G
3	L5	1410	U
3	L5	1411	C
3	L5	1413	C
3	L5	1414	C
3	L5	1415	G
3	L5	1420	A
3	L5	1435	G
3	L5	1438	U
3	L5	1439	C
3	L5	1443	A
3	L5	1444	G
3	L5	1445	U
3	L5	1446	C
3	L5	1447	C
3	L5	1448	G
3	L5	1498	G
3	L5	1502	G
3	L5	1534	A2M
3	L5	1535	C

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Mol	Chain	Res	Type
3	L5	1547	A
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1614	C
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1638	A
3	L5	1640	C
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1697	G
3	L5	1699	A
3	L5	1701	A
3	L5	1703	C
3	L5	1719	A
3	L5	1721	G
3	L5	1734	G
3	L5	1740	C
3	L5	1750	G
3	L5	1755	C
3	L5	1761	G
3	L5	1764	G
3	L5	1765	A
3	L5	1766	A
3	L5	1768	C
3	L5	1775	A
3	L5	1787	A
3	L5	1789	C
3	L5	1804	A
3	L5	1815	G
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A

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Mol	Chain	Res	Type
3	L5	1855	G
3	L5	1869	G
3	L5	1882	U
3	L5	1897	A
3	L5	1918	U
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1931	C
3	L5	1932	A
3	L5	1940	G
3	L5	1941	A
3	L5	1948	G
3	L5	1961	G
3	L5	1966	C
3	L5	1969	G
3	L5	1970	A
3	L5	2022	C
3	L5	2024	G
3	L5	2025	A
3	L5	2026	A
3	L5	2042	A
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2069	A
3	L5	2084	C
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2096	G
3	L5	2097	U
3	L5	2098	G
3	L5	2099	G
3	L5	2100	A
3	L5	2101	C
3	L5	2102	G
3	L5	2103	G
3	L5	2106	G
3	L5	2107	C

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Mol	Chain	Res	Type
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2314	G
3	L5	2333	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2395	A
3	L5	2397	G
3	L5	2417	A
3	L5	2421	G
3	L5	2470	C
3	L5	2471	G
3	L5	2474	G
3	L5	2475	G
3	L5	2478	C
3	L5	2479	G
3	L5	2483	G
3	L5	2488	C
3	L5	2490	U
3	L5	2503	G
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2513	A
3	L5	2519	U
3	L5	2520	C
3	L5	2554	U
3	L5	2559	G
3	L5	2565	A
3	L5	2567	G
3	L5	2573	A
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2601	A
3	L5	2627	C
3	L5	2653	C
3	L5	2660	A
3	L5	2662	G

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Mol	Chain	Res	Type
3	L5	2669	C
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2708	U
3	L5	2710	C
3	L5	2711	G
3	L5	2735	G
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2761	U
3	L5	2764	A
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2798	A
3	L5	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2855	G
3	L5	2877	G
3	L5	2899	C
3	L5	3597	G
3	L5	3615	G
3	L5	3618	C
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3662	A
3	L5	3673	C
3	L5	3711	A
3	L5	3712	A
3	L5	3714	G
3	L5	3748	A
3	L5	3753	G
3	L5	3754	G
3	L5	3760	A2M
3	L5	3776	G

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Mol	Chain	Res	Type
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3785	A2M
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3915	U
3	L5	3945	A
3	L5	3946	G
3	L5	4066	U
3	L5	4076	G
3	L5	4096	C
3	L5	4097	G
3	L5	4102	C
3	L5	4103	C
3	L5	4105	A
3	L5	4106	G
3	L5	4111	U
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4140	C
3	L5	4141	G
3	L5	4142	C
3	L5	4145	C
3	L5	4151	G
3	L5	4158	C
3	L5	4162	C
3	L5	4163	U
3	L5	4164	C

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Mol	Chain	Res	Type
3	L5	4170	A
3	L5	4177	C
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4222	G
3	L5	4229	U
3	L5	4233	A
3	L5	4251	A
3	L5	4254	G
3	L5	4266	G
3	L5	4268	A
3	L5	4273	A
3	L5	4281	A
3	L5	4291	G
3	L5	4305	G
3	L5	4314	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4420	PSU
3	L5	4422	A
3	L5	4448	G
3	L5	4453	C
3	L5	4464	A
3	L5	4465	U
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4515	G
3	L5	4519	C
3	L5	4524	G
3	L5	4548	A

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Mol	Chain	Res	Type
3	L5	4560	C
3	L5	4567	G
3	L5	4573	G
3	L5	4575	G
3	L5	4584	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4720	C
3	L5	4730	C
3	L5	4731	G
3	L5	4732	G
3	L5	4733	C
3	L5	4734	A
3	L5	4740	G
3	L5	4741	C
3	L5	4742	G
3	L5	4743	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4773	C
3	L5	4860	G
3	L5	4870	G
3	L5	4871	C
3	L5	4882	U
3	L5	4883	C
3	L5	4889	G

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Mol	Chain	Res	Type
3	L5	4895	C
3	L5	4900	C
3	L5	4901	G
3	L5	4903	G
3	L5	4910	G
3	L5	4912	G
3	L5	4913	G
3	L5	4921	C
3	L5	4938	A
3	L5	4943	A
3	L5	4944	C
3	L5	4976	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	5017	G
3	L5	5041	G
3	L5	5050	C
3	L5	5062	G
3	L5	5069	U
4	L7	33	U
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	110	G
4	L7	120	U
80	mR	33	A
80	mR	34	C
80	mR	36	U
81	Pt	2	G
81	Pt	9	G
81	Pt	16	C
81	Pt	19	G
81	Pt	21	H2U
81	Pt	47	G7M
81	Pt	76	C
81	Pt	77	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	1520	G
3	L5	667	A
3	L5	704	C
3	L5	739	G
3	L5	1302	U
3	L5	1590	C
3	L5	1613	A
3	L5	1633	G
3	L5	1754	U
3	L5	1765	A
3	L5	2095	A
3	L5	2097	U
3	L5	2489	C
3	L5	3876	A
3	L5	4699	U
3	L5	4990	C

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

233 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$
3	OMU	L5	2415	3	19,22,23	1.26	3 (15%)	25,31,34	1.81	5 (20%)
1	PSU	S2	1347	1	18,21,22	1.36	3 (16%)	21,30,33	2.04	4 (19%)
3	A2M	L5	1871	85,3	22,25,26	1.47	5 (22%)	30,36,39	2.17	10 (33%)
3	A2M	L5	3825	3	22,25,26	1.46	5 (22%)	30,36,39	2.09	10 (33%)
3	OMG	L5	3899	3	23,26,27	1.20	4 (17%)	32,38,41	2.02	7 (21%)
3	PSU	L5	3920	85,3	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
1	A2M	S2	468	1	22,25,26	1.49	5 (22%)	30,36,39	2.15	10 (33%)
3	PSU	L5	4423	3	18,21,22	1.41	3 (16%)	21,30,33	2.11	4 (19%)
81	4SU	Pt	8	81	18,21,22	1.83	4 (22%)	25,30,33	2.26	5 (20%)
3	OMC	L5	3808	3	19,22,23	0.77	0	25,31,34	0.72	0
3	OMG	L5	4623	3	23,26,27	1.18	4 (17%)	32,38,41	2.01	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	400	3	22,25,26	1.48	5 (22%)	30,36,39	2.01	8 (26%)
3	OMC	L5	2861	3	19,22,23	0.77	0	25,31,34	0.69	0
3	PSU	L5	2508	3	18,21,22	1.37	3 (16%)	21,30,33	2.10	4 (19%)
3	OMU	L5	4620	3	19,22,23	1.28	3 (15%)	25,31,34	1.83	5 (20%)
65	MLZ	Lb	5	84,65	8,9,10	0.83	0	4,9,11	0.68	0
3	A2M	L5	3724	3	22,25,26	1.48	5 (22%)	30,36,39	2.01	8 (26%)
1	OMU	S2	116	1	19,22,23	1.20	3 (15%)	25,31,34	1.79	5 (20%)
1	MA6	S2	1850	1	23,26,27	1.48	4 (17%)	33,38,41	2.09	10 (30%)
1	UY1	S2	1326	85,1	19,22,23	1.33	2 (10%)	21,31,34	2.05	4 (19%)
3	PSU	L5	4312	85,3	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
1	A2M	S2	159	1	22,25,26	1.50	4 (18%)	30,36,39	2.11	9 (30%)
3	A2M	L5	2401	85,3	22,25,26	1.46	4 (18%)	30,36,39	2.11	10 (33%)
3	PSU	L5	4579	3	18,21,22	1.40	4 (22%)	21,30,33	2.06	3 (14%)
3	5MC	L5	4447	84,3	19,22,23	1.51	3 (15%)	26,32,35	1.28	2 (7%)
3	PSU	L5	4299	3	18,21,22	1.40	3 (16%)	21,30,33	2.11	4 (19%)
1	PSU	S2	1367	1	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
1	OMC	S2	517	1	19,22,23	0.78	0	25,31,34	0.79	0
1	PSU	S2	1232	1	18,21,22	1.40	2 (11%)	21,30,33	2.07	3 (14%)
3	A2M	L5	1534	85,3	22,25,26	1.49	4 (18%)	30,36,39	2.06	10 (33%)
3	UR3	L5	4530	3	19,22,23	0.92	0	26,32,35	1.97	3 (11%)
3	PSU	L5	4353	3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
3	PSU	L5	3853	85,84,3	18,21,22	1.40	3 (16%)	21,30,33	2.09	3 (14%)
1	PSU	S2	609	1	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
3	PSU	L5	3729	3	18,21,22	1.39	3 (16%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3792	3	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
3	PSU	L5	4552	3	18,21,22	1.40	4 (22%)	21,30,33	2.06	4 (19%)
3	A2M	L5	2815	85,3	22,25,26	1.47	5 (22%)	30,36,39	2.07	8 (26%)
3	OMG	L5	4392	3	23,26,27	1.21	3 (13%)	32,38,41	2.01	6 (18%)
3	OMU	L5	3925	3	19,22,23	1.29	3 (15%)	25,31,34	1.89	5 (20%)
3	A2M	L5	3785	3	22,25,26	1.46	4 (18%)	30,36,39	2.45	12 (40%)
3	PSU	L5	4532	3	18,21,22	1.50	3 (16%)	21,30,33	2.38	4 (19%)
3	PSU	L5	4403	84,3	18,21,22	1.41	3 (16%)	21,30,33	2.15	5 (23%)
1	PSU	S2	815	1	18,21,22	1.36	3 (16%)	21,30,33	2.05	3 (14%)
3	PSU	L5	4457	3	18,21,22	1.35	3 (16%)	21,30,33	2.17	3 (14%)
3	PSU	L5	4673	85,3	18,21,22	1.41	3 (16%)	21,30,33	2.14	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	1243	1	18,21,22	1.39	3 (16%)	21,30,33	2.06	4 (19%)
1	PSU	S2	966	1	18,21,22	1.38	3 (16%)	21,30,33	2.03	3 (14%)
20	HY3	SX	62	20	7,8,9	1.27	1 (14%)	7,10,12	1.61	2 (28%)
3	UY1	L5	3818	84,3	19,22,23	1.40	4 (21%)	21,31,34	2.23	4 (19%)
3	OMC	L5	2804	3	19,22,23	0.77	0	25,31,34	0.65	0
63	SAC	Lr	2	63	7,8,9	3.86	2 (28%)	7,9,11	4.05	3 (42%)
1	OMU	S2	172	1	19,22,23	1.23	2 (10%)	25,31,34	1.87	5 (20%)
1	A2M	S2	512	1	22,25,26	1.47	4 (18%)	30,36,39	2.18	9 (30%)
3	PSU	L5	2632	3	18,21,22	1.42	4 (22%)	21,30,33	1.99	3 (14%)
3	PSU	L5	4293	3	18,21,22	1.36	3 (16%)	21,30,33	2.06	4 (19%)
76	M3L	Lm	98	76	10,11,12	0.52	0	9,14,16	0.46	0
1	PSU	S2	1056	1	18,21,22	1.36	3 (16%)	21,30,33	2.10	4 (19%)
1	PSU	S2	1625	1	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
3	OMG	L5	1316	3	23,26,27	1.21	4 (17%)	32,38,41	1.90	5 (15%)
3	OMC	L5	4536	3	19,22,23	0.76	0	25,31,34	0.82	0
6	SAC	SA	2	6	7,8,9	3.84	2 (28%)	7,9,11	4.38	3 (42%)
1	OMG	S2	683	1	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
1	OMG	S2	436	1	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
1	PSU	S2	1445	1	18,21,22	1.35	2 (11%)	21,30,33	2.11	5 (23%)
1	4AC	S2	1842	1	21,24,25	0.98	1 (4%)	28,34,37	1.15	3 (10%)
2	OMU	L8	14	84,3,2	19,22,23	1.27	3 (15%)	25,31,34	1.76	5 (20%)
1	PSU	S2	105	1	18,21,22	1.39	3 (16%)	21,30,33	2.08	4 (19%)
1	PSU	S2	572	1	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
1	OMC	S2	462	1	19,22,23	0.86	0	25,31,34	0.99	1 (4%)
3	A2M	L5	4571	3	22,25,26	1.50	5 (22%)	30,36,39	2.00	8 (26%)
1	A2M	S2	1031	1	22,25,26	1.48	5 (22%)	30,36,39	2.08	10 (33%)
3	PSU	L5	4628	3	18,21,22	1.40	4 (22%)	21,30,33	1.99	3 (14%)
1	G7M	S2	1639	81,1	23,26,27	2.37	5 (21%)	34,39,42	3.03	10 (29%)
3	OMG	L5	3944	3	23,26,27	1.18	3 (13%)	32,38,41	2.01	6 (18%)
38	V5N	LA	216	38	8,11,12	1.46	1 (12%)	8,14,16	1.76	2 (25%)
1	PSU	S2	651	1	18,21,22	1.37	3 (16%)	21,30,33	2.07	4 (19%)
2	PSU	L8	55	2	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
1	A2M	S2	99	85,1	22,25,26	1.48	4 (18%)	30,36,39	2.09	8 (26%)
1	OMU	S2	121	1	19,22,23	1.23	3 (15%)	25,31,34	1.82	5 (20%)
1	PSU	S2	863	1	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3744	3	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
3	PSU	L5	4420	3	18,21,22	1.47	4 (22%)	21,30,33	2.01	3 (14%)
2	PSU	L8	69	85,2	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
1	PSU	S2	686	1	18,21,22	1.38	2 (11%)	21,30,33	2.09	4 (19%)
1	4AC	S2	1337	1	21,24,25	1.05	1 (4%)	28,34,37	1.04	2 (7%)
3	A2M	L5	1326	3	22,25,26	1.51	4 (18%)	30,36,39	1.96	7 (23%)
3	PSU	L5	1744	84,3	18,21,22	1.41	3 (16%)	21,30,33	2.03	3 (14%)
1	PSU	S2	119	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	4 (19%)
1	PSU	S2	34	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
3	PSU	L5	3695	84,3	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.40	3 (16%)	21,30,33	2.04	4 (19%)
3	OMG	L5	4637	84,3	23,26,27	1.20	3 (13%)	32,38,41	1.93	6 (18%)
1	PSU	S2	573	1	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
3	OMC	L5	3887	85,3	19,22,23	0.79	0	25,31,34	0.80	0
3	OMG	L5	2424	3	23,26,27	1.21	3 (13%)	32,38,41	1.93	6 (18%)
3	PSU	L5	4569	3	18,21,22	1.42	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	1536	3	18,21,22	1.44	3 (16%)	21,30,33	2.13	3 (14%)
1	A2M	S2	484	1	22,25,26	1.49	4 (18%)	30,36,39	2.11	8 (26%)
1	PSU	S2	918	1	18,21,22	1.44	3 (16%)	21,30,33	2.02	3 (14%)
1	PSU	S2	814	1	18,21,22	1.37	3 (16%)	21,30,33	2.00	3 (14%)
1	PSU	S2	296	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	S2	1244	1	18,21,22	1.37	2 (11%)	21,30,33	2.11	4 (19%)
1	PSU	S2	1238	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	4 (19%)
3	OMC	L5	3869	3	19,22,23	0.78	0	25,31,34	0.77	0
3	OMG	L5	1625	84,3	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
1	PSU	S2	218	1	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)
1	PSU	S2	866	1	18,21,22	1.37	2 (11%)	21,30,33	2.10	4 (19%)
1	OMC	S2	1391	1	19,22,23	0.80	0	25,31,34	0.80	0
1	A2M	S2	590	1	22,25,26	1.51	4 (18%)	30,36,39	2.08	7 (23%)
3	OMC	L5	2422	85,3	19,22,23	0.79	0	25,31,34	0.69	0
3	1MA	L5	1322	85,3	21,25,26	1.32	4 (19%)	30,37,40	1.66	5 (16%)
1	PSU	S2	1174	85,1	18,21,22	1.40	3 (16%)	21,30,33	2.05	4 (19%)
1	OMG	S2	644	1	23,26,27	1.19	3 (13%)	32,38,41	2.00	6 (18%)
1	OMU	S2	1442	85,1	19,22,23	1.23	3 (15%)	25,31,34	1.80	5 (20%)
3	OMG	L5	2364	3	23,26,27	1.20	4 (17%)	32,38,41	1.92	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3718	3	22,25,26	1.50	5 (22%)	30,36,39	1.94	8 (26%)
3	OMU	L5	4227	3	19,22,23	1.26	3 (15%)	25,31,34	1.89	5 (20%)
3	PSU	L5	4531	3	18,21,22	1.33	3 (16%)	21,30,33	2.15	5 (23%)
3	PSU	L5	3768	3	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
1	PSU	S2	1004	1	18,21,22	1.37	2 (11%)	21,30,33	2.06	3 (14%)
3	OMU	L5	2837	3	19,22,23	1.27	3 (15%)	25,31,34	1.89	5 (20%)
3	OMG	L5	4618	84,3	23,26,27	1.18	4 (17%)	32,38,41	2.00	6 (18%)
3	PSU	L5	1860	3	18,21,22	1.43	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.40	3 (16%)	21,30,33	1.92	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.43	3 (16%)	21,30,33	2.14	4 (19%)
3	PSU	L5	5001	85,3	18,21,22	1.44	4 (22%)	21,30,33	2.03	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.43	3 (16%)	21,30,33	2.05	4 (19%)
3	OMU	L5	4498	84,3	19,22,23	1.26	3 (15%)	25,31,34	1.81	5 (20%)
3	A2M	L5	3760	85,3	22,25,26	1.52	4 (18%)	30,36,39	2.07	7 (23%)
3	OMU	L5	4306	3	19,22,23	1.28	3 (15%)	25,31,34	1.76	4 (16%)
1	OMU	S2	428	1	19,22,23	1.21	3 (15%)	25,31,34	1.83	5 (20%)
1	PSU	S2	36	1	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
1	A2M	S2	576	1	22,25,26	1.50	4 (18%)	30,36,39	2.20	10 (33%)
1	PSU	S2	1692	1	18,21,22	1.40	3 (16%)	21,30,33	2.08	4 (19%)
81	OMC	Pt	33	81	19,22,23	0.78	0	25,31,34	0.77	0
81	PSU	Pt	56	81	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.43	3 (16%)	21,30,33	2.15	4 (19%)
1	OMG	S2	601	1	23,26,27	1.19	3 (13%)	32,38,41	1.95	6 (18%)
3	PSU	L5	3715	3	18,21,22	1.37	3 (16%)	21,30,33	2.09	5 (23%)
3	PSU	L5	2843	3	18,21,22	1.38	3 (16%)	21,30,33	2.06	5 (23%)
3	5MC	L5	3782	85,3	19,22,23	1.51	3 (15%)	26,32,35	1.15	2 (7%)
81	G7M	Pt	47	81	23,26,27	1.88	2 (8%)	34,39,42	1.07	1 (2%)
2	OMG	L8	75	2	23,26,27	1.18	3 (13%)	32,38,41	1.97	6 (18%)
3	PSU	L5	3639	3	18,21,22	1.42	3 (16%)	21,30,33	2.05	3 (14%)
1	OMG	S2	1328	1	23,26,27	1.19	3 (13%)	32,38,41	1.96	6 (18%)
3	A2M	L5	1524	3	22,25,26	1.49	4 (18%)	30,36,39	2.03	10 (33%)
1	PSU	S2	1643	85,1	18,21,22	1.40	3 (16%)	21,30,33	2.06	5 (23%)
1	PSU	S2	1239	1	18,21,22	1.37	3 (16%)	21,30,33	2.05	4 (19%)
3	A2M	L5	3723	3	22,25,26	1.49	5 (22%)	30,36,39	2.05	9 (30%)
78	MLZ	Lo	53	78	8,9,10	0.76	0	4,9,11	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	801	1	18,21,22	1.35	3 (16%)	21,30,33	2.05	4 (19%)
3	A2M	L5	398	3	22,25,26	1.49	4 (18%)	30,36,39	2.11	9 (30%)
3	PSU	L5	4972	84,3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
3	PSU	L5	4521	85,84,3	18,21,22	1.43	3 (16%)	21,30,33	2.10	5 (23%)
3	PSU	L5	3851	3	18,21,22	1.43	3 (16%)	21,30,33	2.07	4 (19%)
3	6MZ	L5	4220	3	22,25,26	1.44	4 (18%)	29,36,39	2.12	10 (34%)
3	PSU	L5	4576	3	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)
3	PSU	L5	1862	3	18,21,22	1.38	3 (16%)	21,30,33	2.14	4 (19%)
3	PSU	L5	3758	3	18,21,22	1.38	3 (16%)	21,30,33	2.05	4 (19%)
1	A2M	S2	166	1	22,25,26	1.49	4 (18%)	30,36,39	2.16	10 (33%)
49	V5N	La	39	49	8,11,12	1.51	1 (12%)	8,14,16	1.70	2 (25%)
1	MA6	S2	1851	85,1	23,26,27	1.46	5 (21%)	33,38,41	2.12	10 (30%)
1	PSU	S2	1177	1	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
1	A2M	S2	1383	1	22,25,26	1.46	4 (18%)	30,36,39	2.25	10 (33%)
1	A2M	S2	27	85,1	22,25,26	1.49	4 (18%)	30,36,39	2.08	9 (30%)
3	OMC	L5	4456	3	19,22,23	0.79	0	25,31,34	0.77	1 (4%)
1	A2M	S2	1678	1	22,25,26	1.51	4 (18%)	30,36,39	2.06	8 (26%)
1	OMG	S2	1490	85,1	23,26,27	1.20	3 (13%)	32,38,41	1.94	6 (18%)
3	PSU	L5	1779	3	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.46	3 (16%)	21,30,33	2.07	3 (14%)
3	PSU	L5	1781	3	18,21,22	1.38	3 (16%)	21,30,33	2.04	4 (19%)
3	OMC	L5	2365	85,3	19,22,23	0.76	0	25,31,34	0.77	0
1	B8N	S2	1248	1	25,29,30	0.90	1 (4%)	28,42,45	1.68	6 (21%)
3	PSU	L5	1582	3	18,21,22	1.43	3 (16%)	21,30,33	2.09	4 (19%)
3	OMG	L5	1522	3	23,26,27	1.19	4 (17%)	32,38,41	2.04	8 (25%)
3	OMG	L5	4499	3	23,26,27	1.20	3 (13%)	32,38,41	1.96	6 (18%)
3	A2M	L5	3867	3	22,25,26	1.51	4 (18%)	30,36,39	2.04	10 (33%)
3	PSU	L5	3762	3	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
3	OMG	L5	4370	3	23,26,27	1.22	3 (13%)	32,38,41	1.97	6 (18%)
3	OMC	L5	1340	3	19,22,23	0.76	0	25,31,34	0.73	0
1	PSU	S2	109	1	18,21,22	1.37	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	1677	3	18,21,22	1.44	4 (22%)	21,30,33	2.09	4 (19%)
3	PSU	L5	3770	3	18,21,22	1.54	5 (27%)	21,30,33	2.17	5 (23%)
3	PSU	L5	4493	84,3	18,21,22	1.43	3 (16%)	21,30,33	2.07	4 (19%)
1	PSU	S2	1081	1	18,21,22	1.45	4 (22%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1782	3	18,21,22	1.40	3 (16%)	21,30,33	2.07	4 (19%)
1	OMU	S2	354	1	19,22,23	1.26	3 (15%)	25,31,34	1.86	5 (20%)
1	6MZ	S2	1832	85,84,1	22,25,26	1.50	4 (18%)	29,36,39	2.10	9 (31%)
3	OMC	L5	2824	3	19,22,23	0.78	0	25,31,34	0.78	0
3	PSU	L5	4689	3	18,21,22	1.40	3 (16%)	21,30,33	2.07	3 (14%)
1	PSU	S2	649	1	18,21,22	1.38	3 (16%)	21,30,33	2.09	4 (19%)
1	OMU	S2	1288	1	19,22,23	1.27	4 (21%)	25,31,34	1.76	5 (20%)
3	OMG	L5	2876	3	23,26,27	1.21	3 (13%)	32,38,41	1.99	6 (18%)
81	H2U	Pt	21	81	18,21,22	0.96	2 (11%)	19,30,33	1.00	1 (5%)
3	PSU	L5	4636	85,3	18,21,22	1.43	3 (16%)	21,30,33	2.04	4 (19%)
1	OMC	S2	174	85,1	19,22,23	0.78	0	25,31,34	0.82	0
3	PSU	L5	3764	85,3	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
3	PSU	L5	4442	3	18,21,22	1.39	3 (16%)	21,30,33	2.13	5 (23%)
3	OMC	L5	2351	85,3	19,22,23	0.79	0	25,31,34	0.98	1 (4%)
1	PSU	S2	1136	1	18,21,22	1.37	3 (16%)	21,30,33	2.07	4 (19%)
3	PSU	L5	1792	84,3	18,21,22	1.36	3 (16%)	21,30,33	2.09	4 (19%)
3	OMG	L5	4494	85,3	23,26,27	1.20	3 (13%)	32,38,41	2.01	6 (18%)
1	OMG	S2	509	85,1	23,26,27	1.21	3 (13%)	32,38,41	1.99	6 (18%)
1	OMC	S2	1703	85,1	19,22,23	0.77	0	25,31,34	0.72	0
29	AME	SV	1	29	9,10,11	3.40	2 (22%)	9,11,13	3.64	3 (33%)
1	OMU	S2	1804	1	19,22,23	1.23	3 (15%)	25,31,34	1.85	5 (20%)
3	OMC	L5	3701	84,3	19,22,23	0.79	0	25,31,34	0.88	0
3	OMC	L5	3841	3	19,22,23	0.77	0	25,31,34	0.67	0
3	A2M	L5	4590	3	22,25,26	1.49	5 (22%)	30,36,39	2.11	11 (36%)
1	A2M	S2	668	85,1	22,25,26	1.46	5 (22%)	30,36,39	2.03	10 (33%)
1	PSU	S2	406	1	18,21,22	1.39	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	S2	681	1	18,21,22	1.42	3 (16%)	21,30,33	2.07	4 (19%)
3	OMG	L5	4196	81,3	23,26,27	1.21	3 (13%)	32,38,41	1.95	6 (18%)
3	A2M	L5	3830	3	22,25,26	1.49	5 (22%)	30,36,39	2.13	8 (26%)
3	PSU	L5	4471	85,3	18,21,22	1.41	3 (16%)	21,30,33	2.11	5 (23%)
3	PSU	L5	3637	84,3	18,21,22	1.43	3 (16%)	21,30,33	2.11	5 (23%)
3	PSU	L5	1683	84,3	18,21,22	1.44	4 (22%)	21,30,33	2.16	4 (19%)
1	OMG	S2	867	1	23,26,27	1.17	3 (13%)	32,38,41	1.95	6 (18%)
1	PSU	S2	93	1	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	3734	3	18,21,22	1.36	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4500	85,3	18,21,22	1.38	2 (11%)	21,30,33	2.15	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3627	3	23,26,27	1.19	4 (17%)	32,38,41	2.04	7 (21%)
3	A2M	L5	2363	85,3	22,25,26	1.49	5 (22%)	30,36,39	2.01	9 (30%)
3	PSU	L5	5010	3	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
3	A2M	L5	2787	85,3	22,25,26	1.50	3 (13%)	30,36,39	2.10	8 (26%)
3	A2M	L5	4523	85,3	22,25,26	1.48	5 (22%)	30,36,39	2.15	9 (30%)
39	HIC	LB	245	39	10,11,12	1.39	1 (10%)	9,14,16	1.32	2 (22%)
1	OMU	S2	627	1	19,22,23	1.20	3 (15%)	25,31,34	1.83	5 (20%)
1	PSU	S2	822	1	18,21,22	1.39	3 (16%)	21,30,33	2.11	5 (23%)
3	OMG	L5	4228	3	23,26,27	1.18	4 (17%)	32,38,41	1.98	6 (18%)
3	OMC	L5	1881	85,3	19,22,23	0.78	0	25,31,34	0.94	0
1	OMG	S2	1447	1	23,26,27	1.21	3 (13%)	32,38,41	2.00	6 (18%)

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
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	85,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3920	85,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
81	4SU	Pt	8	81	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
65	MLZ	Lb	5	84,65	-	1/7/8/10	-
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	1/9/27/28	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
1	UY1	S2	1326	85,1	-	2/9/27/28	0/2/2/2
3	PSU	L5	4312	85,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	2401	85,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	84,3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	85,3	-	1/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	85,84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	85,3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3785	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	85,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
3	UY1	L5	3818	84,3	-	2/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
63	SAC	Lr	2	63	-	2/7/8/10	-
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
76	M3L	Lm	98	76	-	0/9/10/12	-
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
6	SAC	SA	2	6	-	5/7/8/10	-
1	OMG	S2	683	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
2	OMU	L8	14	84,3,2	-	1/9/27/28	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
1	G7M	S2	1639	81,1	-	0/7/25/26	0/3/3/3
3	OMG	L5	3944	3	-	1/9/27/28	0/3/3/3
38	V5N	LA	216	38	-	1/9/10/12	0/1/1/1
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	A2M	S2	99	85,1	-	0/9/27/28	0/3/3/3
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4420	3	-	3/7/25/26	0/2/2/2
2	PSU	L8	69	85,2	-	0/7/25/26	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1744	84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	84,3	-	1/9/27/28	0/3/3/3
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	85,3	-	0/9/27/28	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	918	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	1625	84,3	-	1/9/27/28	0/3/3/3
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	590	1	-	4/9/27/28	0/3/3/3
3	OMC	L5	2422	85,3	-	2/9/27/28	0/2/2/2
3	1MA	L5	1322	85,3	-	2/7/25/26	0/3/3/3
1	PSU	S2	1174	85,1	-	0/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
1	OMU	S2	1442	85,1	-	2/9/27/28	0/2/2/2
3	OMG	L5	2364	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4531	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4618	84,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	84,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3760	85,3	-	2/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
81	OMC	Pt	33	81	-	0/9/27/28	0/2/2/2
81	PSU	Pt	56	81	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	85,3	-	0/7/25/26	0/2/2/2
81	G7M	Pt	47	81	-	0/7/25/26	0/3/3/3
2	OMG	L8	75	2	-	0/9/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S2	1328	1	-	1/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	1643	85,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
78	MLZ	Lo	53	78	-	1/7/8/10	-
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4972	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	85,84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
49	V5N	La	39	49	-	0/9/10/12	0/1/1/1
1	MA6	S2	1851	85,1	-	3/11/29/30	0/3/3/3
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	27	85,1	-	1/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	OMG	S2	1490	85,1	-	3/9/27/28	0/3/3/3
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	2365	85,3	-	0/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	1/16/34/35	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	6MZ	S2	1832	85,84,1	-	0/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1288	1	-	2/9/27/28	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
81	H2U	Pt	21	81	-	2/7/38/39	0/2/2/2
3	PSU	L5	4636	85,3	-	2/7/25/26	0/2/2/2
1	OMC	S2	174	85,1	-	0/9/27/28	0/2/2/2
3	PSU	L5	3764	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	85,3	-	2/9/27/28	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	84,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	85,3	-	1/9/27/28	0/3/3/3
1	OMG	S2	509	85,1	-	0/9/27/28	0/3/3/3
1	OMC	S2	1703	85,1	-	0/9/27/28	0/2/2/2
29	AME	SV	1	29	-	1/9/10/12	-
1	OMU	S2	1804	1	-	1/9/27/28	0/2/2/2
3	OMC	L5	3701	84,3	-	4/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	668	85,1	-	4/9/27/28	0/3/3/3
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	81,3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4471	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	84,3	-	0/7/25/26	0/2/2/2
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	85,3	-	1/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	85,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	85,3	-	3/9/27/28	0/3/3/3
3	A2M	L5	4523	85,3	-	0/9/27/28	0/3/3/3
39	HIC	LB	245	39	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	S2	627	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1881	85,3	-	0/9/27/28	0/2/2/2
1	OMG	S2	1447	1	-	2/9/27/28	0/3/3/3

All (663) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	Lr	2	SAC	OAC-C1A	9.06	1.43	1.23
6	SA	2	SAC	OAC-C1A	9.05	1.43	1.23
29	SV	1	AME	OT-CT1	9.01	1.43	1.23
81	Pt	47	G7M	C8-N7	7.50	1.45	1.33
1	S2	1639	G7M	C8-N7	7.48	1.45	1.33
3	L5	3782	5MC	C5-C4	5.28	1.48	1.44
3	L5	4447	5MC	C5-C4	5.02	1.47	1.44
81	Pt	8	4SU	C4-S4	-5.02	1.59	1.68
1	S2	1639	G7M	C5-N7	-5.00	1.33	1.39
3	L5	3760	A2M	C5-C4	4.77	1.47	1.39
1	S2	590	A2M	C5-C4	4.75	1.47	1.39
1	S2	159	A2M	C5-C4	4.67	1.47	1.39
1	S2	576	A2M	C5-C4	4.63	1.47	1.39
1	S2	1678	A2M	C5-C4	4.59	1.47	1.39
1	S2	1832	6MZ	C5-C4	4.59	1.47	1.39
1	S2	484	A2M	C5-C4	4.57	1.47	1.39
1	S2	27	A2M	C5-C4	4.54	1.47	1.39
1	S2	166	A2M	C5-C4	4.53	1.47	1.39
1	S2	512	A2M	C5-C4	4.53	1.47	1.39
3	L5	1326	A2M	C5-C4	4.53	1.47	1.39
1	S2	1850	MA6	C5-C4	4.53	1.47	1.39
1	S2	468	A2M	C5-C4	4.51	1.47	1.39
3	L5	400	A2M	C5-C4	4.50	1.47	1.39
3	L5	398	A2M	C5-C4	4.49	1.47	1.39
1	S2	99	A2M	C5-C4	4.48	1.47	1.39
1	S2	1383	A2M	C5-C4	4.47	1.47	1.39
1	S2	1031	A2M	C5-C4	4.46	1.47	1.39
3	L5	4590	A2M	C5-C4	4.44	1.47	1.39
3	L5	2787	A2M	C5-C4	4.44	1.47	1.39
3	L5	3830	A2M	C5-C4	4.43	1.47	1.39
3	L5	3718	A2M	C5-C4	4.42	1.47	1.39
3	L5	1524	A2M	C5-C4	4.41	1.47	1.39
3	L5	3724	A2M	C5-C4	4.40	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4571	A2M	C5-C4	4.39	1.46	1.39
3	L5	3723	A2M	C5-C4	4.39	1.46	1.39
1	S2	1851	MA6	C5-C4	4.37	1.46	1.39
3	L5	4220	6MZ	C5-C4	4.36	1.46	1.39
3	L5	3867	A2M	C5-C4	4.36	1.46	1.39
3	L5	4523	A2M	C5-C4	4.33	1.46	1.39
3	L5	1534	A2M	C5-C4	4.31	1.46	1.39
3	L5	2401	A2M	C5-C4	4.28	1.46	1.39
1	S2	668	A2M	C5-C4	4.26	1.46	1.39
3	L5	2815	A2M	C5-C4	4.26	1.46	1.39
3	L5	2363	A2M	C5-C4	4.26	1.46	1.39
3	L5	1871	A2M	C5-C4	4.26	1.46	1.39
63	Lr	2	SAC	C1A-N	4.24	1.48	1.34
3	L5	3825	A2M	C5-C4	4.23	1.46	1.39
29	SV	1	AME	CT1-N	4.21	1.47	1.34
1	S2	1639	G7M	C8-N9	4.15	1.46	1.35
6	SA	2	SAC	C1A-N	4.14	1.47	1.34
81	Pt	47	G7M	C8-N9	4.05	1.46	1.35
1	S2	1639	G7M	C5-C4	3.69	1.47	1.38
3	L5	4532	PSU	C6-C5	3.62	1.39	1.35
49	La	39	V5N	CG-ND1	-3.57	1.34	1.37
3	L5	3785	A2M	C5-C4	3.50	1.45	1.39
1	S2	1232	PSU	C6-C5	3.40	1.39	1.35
1	S2	609	PSU	C6-C5	3.37	1.39	1.35
1	S2	866	PSU	C6-C5	3.34	1.39	1.35
1	S2	573	PSU	C6-C5	3.33	1.39	1.35
1	S2	572	PSU	C6-C5	3.31	1.39	1.35
38	LA	216	V5N	CG-ND1	-3.31	1.34	1.37
81	Pt	8	4SU	C4-N3	-3.28	1.34	1.37
81	Pt	56	PSU	C6-C5	3.28	1.38	1.35
1	S2	34	PSU	C6-C5	3.27	1.38	1.35
1	S2	1625	PSU	C6-C5	3.27	1.38	1.35
3	L5	3844	PSU	C6-C5	3.26	1.38	1.35
3	L5	4431	PSU	C6-C5	3.26	1.38	1.35
1	S2	1239	PSU	C6-C5	3.25	1.38	1.35
3	L5	3762	PSU	C6-C5	3.25	1.38	1.35
1	S2	863	PSU	C6-C5	3.25	1.38	1.35
1	S2	1643	PSU	C6-C5	3.24	1.38	1.35
3	L5	1683	PSU	C6-C5	3.24	1.38	1.35
1	S2	93	PSU	C6-C5	3.24	1.38	1.35
3	L5	3770	PSU	C4-N3	-3.23	1.32	1.38
3	L5	4972	PSU	C6-C5	3.23	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4673	PSU	C6-C5	3.22	1.38	1.35
1	S2	119	PSU	C6-C5	3.22	1.38	1.35
1	S2	406	PSU	C6-C5	3.22	1.38	1.35
1	S2	649	PSU	C6-C5	3.21	1.38	1.35
1	S2	1243	PSU	C6-C5	3.21	1.38	1.35
3	L5	1860	PSU	C6-C5	3.21	1.38	1.35
1	S2	681	PSU	C6-C5	3.19	1.38	1.35
1	S2	1692	PSU	C6-C5	3.19	1.38	1.35
1	S2	1238	PSU	C6-C5	3.19	1.38	1.35
1	S2	822	PSU	C6-C5	3.19	1.38	1.35
1	S2	686	PSU	C6-C5	3.19	1.38	1.35
3	L5	4493	PSU	C6-C5	3.17	1.38	1.35
3	L5	4500	PSU	C6-C5	3.16	1.38	1.35
3	L5	1536	PSU	C6-C5	3.16	1.38	1.35
1	S2	651	PSU	C6-C5	3.16	1.38	1.35
1	S2	296	PSU	C6-C5	3.15	1.38	1.35
3	L5	2839	PSU	C4-N3	-3.15	1.33	1.38
3	L5	2843	PSU	C4-N3	-3.14	1.33	1.38
3	L5	3639	PSU	C6-C5	3.14	1.38	1.35
1	S2	1244	PSU	C6-C5	3.14	1.38	1.35
1	S2	918	PSU	C6-C5	3.13	1.38	1.35
3	L5	3637	PSU	C4-N3	-3.13	1.33	1.38
1	S2	1136	PSU	C6-C5	3.13	1.38	1.35
3	L5	3851	PSU	C6-C5	3.12	1.38	1.35
1	S2	1004	PSU	C6-C5	3.12	1.38	1.35
3	L5	1744	PSU	C6-C5	3.12	1.38	1.35
1	S2	1367	PSU	C6-C5	3.12	1.38	1.35
3	L5	4569	PSU	C6-C5	3.12	1.38	1.35
3	L5	4299	PSU	C6-C5	3.12	1.38	1.35
3	L5	3925	OMU	C4-N3	-3.12	1.33	1.38
1	S2	36	PSU	C6-C5	3.12	1.38	1.35
3	L5	4420	PSU	C6-C5	3.11	1.38	1.35
1	S2	1447	OMG	C5-C4	3.11	1.47	1.38
1	S2	105	PSU	C6-C5	3.10	1.38	1.35
1	S2	801	PSU	C6-C5	3.10	1.38	1.35
1	S2	1174	PSU	C6-C5	3.10	1.38	1.35
3	L5	4353	PSU	C6-C5	3.10	1.38	1.35
1	S2	1445	PSU	C6-C5	3.10	1.38	1.35
3	L5	5001	PSU	C6-C5	3.10	1.38	1.35
3	L5	5010	PSU	C6-C5	3.08	1.38	1.35
3	L5	2632	PSU	C6-C5	3.08	1.38	1.35
3	L5	4442	PSU	C6-C5	3.08	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3884	PSU	C6-C5	3.08	1.38	1.35
3	L5	3758	PSU	C6-C5	3.08	1.38	1.35
1	S2	1328	OMG	C5-C4	3.08	1.47	1.38
3	L5	3637	PSU	C6-C5	3.07	1.38	1.35
3	L5	1582	PSU	C6-C5	3.07	1.38	1.35
3	L5	1536	PSU	C4-N3	-3.07	1.33	1.38
1	S2	509	OMG	C5-C4	3.07	1.47	1.38
1	S2	966	PSU	C6-C5	3.07	1.38	1.35
1	S2	109	PSU	C6-C5	3.07	1.38	1.35
1	S2	218	PSU	C6-C5	3.06	1.38	1.35
1	S2	1347	PSU	C6-C5	3.06	1.38	1.35
1	S2	1326	UY1	C6-C5	3.06	1.38	1.35
20	SX	62	HY3	C3-CA	-3.05	1.52	1.55
1	S2	1490	OMG	C5-C4	3.05	1.47	1.38
1	S2	601	OMG	C5-C4	3.05	1.47	1.38
3	L5	4306	OMU	C4-N3	-3.05	1.33	1.38
3	L5	4620	OMU	C4-N3	-3.05	1.33	1.38
2	L8	14	OMU	C4-N3	-3.04	1.33	1.38
3	L5	1782	PSU	C6-C5	3.04	1.38	1.35
3	L5	4521	PSU	C4-N3	-3.04	1.33	1.38
1	S2	867	OMG	C5-C4	3.04	1.47	1.38
3	L5	3792	OMG	C5-C4	3.03	1.47	1.38
3	L5	3764	PSU	C6-C5	3.03	1.38	1.35
3	L5	4636	PSU	C6-C5	3.03	1.38	1.35
3	L5	3695	PSU	C4-N3	-3.03	1.33	1.38
3	L5	4431	PSU	C4-N3	-3.03	1.33	1.38
3	L5	2839	PSU	C6-C5	3.03	1.38	1.35
3	L5	4493	PSU	C4-N3	-3.03	1.33	1.38
3	L5	3768	PSU	C6-C5	3.02	1.38	1.35
1	S2	1177	PSU	C6-C5	3.02	1.38	1.35
3	L5	4579	PSU	C6-C5	3.02	1.38	1.35
3	L5	4423	PSU	C6-C5	3.02	1.38	1.35
1	S2	814	PSU	C6-C5	3.02	1.38	1.35
3	L5	4361	PSU	C6-C5	3.01	1.38	1.35
3	L5	3818	UY1	C4-N3	-3.01	1.33	1.38
1	S2	681	PSU	C4-N3	-3.01	1.33	1.38
1	S2	1056	PSU	C6-C5	3.00	1.38	1.35
1	S2	436	OMG	C5-C4	3.00	1.47	1.38
3	L5	2424	OMG	C5-C4	3.00	1.47	1.38
3	L5	4196	OMG	C5-C4	3.00	1.47	1.38
2	L8	69	PSU	C6-C5	3.00	1.38	1.35
3	L5	4296	PSU	C6-C5	3.00	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1625	OMG	C5-C4	3.00	1.47	1.38
3	L5	4296	PSU	C4-N3	-3.00	1.33	1.38
3	L5	3695	PSU	C6-C5	3.00	1.38	1.35
3	L5	2876	OMG	C5-C4	3.00	1.47	1.38
3	L5	3944	OMG	C5-C4	3.00	1.47	1.38
1	S2	644	OMG	C5-C4	3.00	1.47	1.38
2	L8	55	PSU	C6-C5	3.00	1.38	1.35
3	L5	1683	PSU	C4-N3	-2.99	1.33	1.38
3	L5	3729	PSU	C6-C5	2.99	1.38	1.35
3	L5	4353	PSU	C4-N3	-2.99	1.33	1.38
3	L5	4293	PSU	C6-C5	2.99	1.38	1.35
3	L5	4521	PSU	C6-C5	2.99	1.38	1.35
3	L5	1860	PSU	C4-N3	-2.99	1.33	1.38
3	L5	4471	PSU	C4-N3	-2.98	1.33	1.38
3	L5	4689	PSU	C6-C5	2.98	1.38	1.35
3	L5	4569	PSU	C4-N3	-2.97	1.33	1.38
3	L5	4403	PSU	C6-C5	2.97	1.38	1.35
2	L8	55	PSU	C4-N3	-2.97	1.33	1.38
3	L5	1782	PSU	C4-N3	-2.97	1.33	1.38
1	S2	1174	PSU	C4-N3	-2.97	1.33	1.38
3	L5	4471	PSU	C6-C5	2.96	1.38	1.35
3	L5	4552	PSU	C6-C5	2.96	1.38	1.35
3	L5	3853	PSU	C6-C5	2.96	1.38	1.35
3	L5	3884	PSU	C4-N3	-2.96	1.33	1.38
3	L5	3851	PSU	C4-N3	-2.96	1.33	1.38
3	L5	4636	PSU	C4-N3	-2.96	1.33	1.38
3	L5	3920	PSU	C6-C5	2.96	1.38	1.35
3	L5	3734	PSU	C6-C5	2.95	1.38	1.35
3	L5	3785	A2M	C4-N9	-2.95	1.31	1.37
3	L5	5001	PSU	C4-N3	-2.95	1.33	1.38
3	L5	4972	PSU	C4-N3	-2.94	1.33	1.38
3	L5	4576	PSU	C6-C5	2.94	1.38	1.35
3	L5	4499	OMG	C5-C4	2.94	1.46	1.38
3	L5	2837	OMU	C4-N3	-2.94	1.33	1.38
3	L5	4227	OMU	C4-N3	-2.94	1.33	1.38
3	L5	1779	PSU	C4-N3	-2.93	1.33	1.38
3	L5	1744	PSU	C4-N3	-2.93	1.33	1.38
3	L5	4312	PSU	C4-N3	-2.93	1.33	1.38
1	S2	815	PSU	C6-C5	2.93	1.38	1.35
1	S2	1081	PSU	C4-N3	-2.93	1.33	1.38
3	L5	1781	PSU	C6-C5	2.93	1.38	1.35
3	L5	4494	OMG	C5-C4	2.92	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1081	PSU	C6-C5	2.92	1.38	1.35
3	L5	4361	PSU	C4-N3	-2.92	1.33	1.38
3	L5	3818	UY1	C6-C5	2.92	1.38	1.35
3	L5	4370	OMG	C5-C4	2.92	1.46	1.38
3	L5	4299	PSU	C4-N3	-2.92	1.33	1.38
1	S2	683	OMG	C5-C4	2.91	1.46	1.38
3	L5	3853	PSU	C4-N3	-2.91	1.33	1.38
3	L5	3785	A2M	C5-N7	-2.91	1.33	1.39
1	S2	1337	4AC	C4-N4	-2.91	1.35	1.39
3	L5	4447	5MC	C6-C5	2.91	1.39	1.34
3	L5	4531	PSU	C6-C5	2.91	1.38	1.35
3	L5	1862	PSU	C4-N3	-2.91	1.33	1.38
2	L8	75	OMG	C5-C4	2.90	1.46	1.38
1	S2	1136	PSU	C4-N3	-2.90	1.33	1.38
3	L5	3744	OMG	C5-C4	2.90	1.46	1.38
3	L5	1862	PSU	C6-C5	2.90	1.38	1.35
3	L5	4498	OMU	C4-N3	-2.90	1.33	1.38
3	L5	2415	OMU	C4-N3	-2.90	1.33	1.38
3	L5	4552	PSU	C4-N3	-2.90	1.33	1.38
3	L5	4689	PSU	C4-N3	-2.89	1.33	1.38
3	L5	1779	PSU	C6-C5	2.89	1.38	1.35
1	S2	966	PSU	C4-N3	-2.89	1.33	1.38
3	L5	1316	OMG	C5-C4	2.89	1.46	1.38
3	L5	4403	PSU	C4-N3	-2.89	1.33	1.38
3	L5	3715	PSU	C4-N3	-2.89	1.33	1.38
1	S2	354	OMU	C4-N3	-2.88	1.33	1.38
3	L5	4392	OMG	C6-N1	-2.88	1.33	1.38
3	L5	4532	PSU	C4-N3	-2.88	1.33	1.38
1	S2	1177	PSU	C4-N3	-2.88	1.33	1.38
1	S2	105	PSU	C4-N3	-2.88	1.33	1.38
3	L5	2632	PSU	C4-N3	-2.88	1.33	1.38
3	L5	3639	PSU	C4-N3	-2.88	1.33	1.38
3	L5	1582	PSU	C4-N3	-2.88	1.33	1.38
3	L5	4312	PSU	C6-C5	2.87	1.38	1.35
3	L5	2508	PSU	C6-C5	2.87	1.38	1.35
3	L5	2876	OMG	C6-N1	-2.87	1.33	1.38
3	L5	4442	PSU	C4-N3	-2.87	1.33	1.38
3	L5	4370	OMG	C6-N1	-2.87	1.33	1.38
3	L5	1322	1MA	C5-C4	2.86	1.46	1.38
3	L5	4628	PSU	C4-N3	-2.86	1.33	1.38
3	L5	3844	PSU	C4-N3	-2.86	1.33	1.38
3	L5	1677	PSU	C4-N3	-2.86	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1792	PSU	C4-N3	-2.85	1.33	1.38
1	S2	406	PSU	C4-N3	-2.85	1.33	1.38
3	L5	4637	OMG	C5-C4	2.85	1.46	1.38
3	L5	4576	PSU	C4-N3	-2.85	1.33	1.38
3	L5	2843	PSU	C6-C5	2.85	1.38	1.35
3	L5	2508	PSU	C4-N3	-2.85	1.33	1.38
3	L5	4392	OMG	C5-C4	2.84	1.46	1.38
3	L5	5010	PSU	C4-N3	-2.84	1.33	1.38
1	S2	1850	MA6	C5-C6	2.84	1.48	1.41
3	L5	4423	PSU	C4-N3	-2.83	1.33	1.38
1	S2	918	PSU	C4-N3	-2.83	1.33	1.38
1	S2	1851	MA6	C5-C6	2.83	1.48	1.41
2	L8	69	PSU	C4-N3	-2.83	1.33	1.38
3	L5	3764	PSU	C4-N3	-2.82	1.33	1.38
3	L5	4618	OMG	C5-C4	2.82	1.46	1.38
3	L5	3729	PSU	C4-N3	-2.82	1.33	1.38
3	L5	3758	PSU	C4-N3	-2.82	1.33	1.38
3	L5	3768	PSU	C4-N3	-2.82	1.33	1.38
3	L5	2364	OMG	C5-C4	2.82	1.46	1.38
3	L5	4579	PSU	C4-N3	-2.82	1.33	1.38
3	L5	3627	OMG	C5-C4	2.81	1.46	1.38
3	L5	4673	PSU	C4-N3	-2.81	1.33	1.38
3	L5	3770	PSU	C6-C5	2.81	1.38	1.35
3	L5	3715	PSU	C6-C5	2.81	1.38	1.35
3	L5	1781	PSU	C4-N3	-2.81	1.33	1.38
1	S2	801	PSU	C4-N3	-2.81	1.33	1.38
3	L5	4293	PSU	C4-N3	-2.81	1.33	1.38
3	L5	4494	OMG	C6-N1	-2.80	1.33	1.38
1	S2	1326	UY1	C4-N3	-2.80	1.33	1.38
3	L5	3920	PSU	C4-N3	-2.80	1.33	1.38
1	S2	36	PSU	C4-N3	-2.79	1.33	1.38
3	L5	2787	A2M	C5-N7	-2.79	1.34	1.39
1	S2	686	PSU	C4-N3	-2.79	1.33	1.38
1	S2	1238	PSU	C4-N3	-2.79	1.33	1.38
3	L5	4623	OMG	C5-C4	2.79	1.46	1.38
1	S2	1804	OMU	C4-N3	-2.79	1.33	1.38
1	S2	651	PSU	C4-N3	-2.79	1.33	1.38
1	S2	1004	PSU	C4-N3	-2.78	1.33	1.38
1	S2	1692	PSU	C4-N3	-2.78	1.33	1.38
3	L5	4500	PSU	C4-N3	-2.78	1.33	1.38
3	L5	4457	PSU	C4-N3	-2.78	1.33	1.38
1	S2	863	PSU	C4-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1643	PSU	C4-N3	-2.78	1.33	1.38
81	Pt	8	4SU	C5-C4	-2.78	1.39	1.42
3	L5	1792	PSU	C6-C5	2.77	1.38	1.35
1	S2	649	PSU	C4-N3	-2.77	1.33	1.38
3	L5	4457	PSU	C6-C5	2.77	1.38	1.35
3	L5	3734	PSU	C4-N3	-2.77	1.33	1.38
1	S2	1239	PSU	C4-N3	-2.76	1.33	1.38
3	L5	3925	OMU	C2-N3	-2.76	1.33	1.38
3	L5	4228	OMG	C5-C4	2.76	1.46	1.38
3	L5	2424	OMG	C6-N1	-2.76	1.33	1.38
1	S2	93	PSU	C4-N3	-2.76	1.33	1.38
3	L5	1322	1MA	C6-N6	2.76	1.34	1.28
1	S2	34	PSU	C4-N3	-2.76	1.33	1.38
1	S2	1056	PSU	C4-N3	-2.75	1.33	1.38
1	S2	1367	PSU	C4-N3	-2.75	1.33	1.38
1	S2	1625	PSU	C4-N3	-2.74	1.33	1.38
3	L5	1522	OMG	C5-C4	2.74	1.46	1.38
3	L5	4531	PSU	C4-N3	-2.74	1.33	1.38
1	S2	815	PSU	C4-N3	-2.74	1.33	1.38
1	S2	1232	PSU	C4-N3	-2.74	1.33	1.38
1	S2	109	PSU	C4-N3	-2.73	1.33	1.38
3	L5	3899	OMG	C5-C4	2.73	1.46	1.38
3	L5	4637	OMG	C6-N1	-2.73	1.33	1.38
1	S2	172	OMU	C4-N3	-2.73	1.33	1.38
1	S2	1248	B8N	C6-C5	2.73	1.39	1.35
1	S2	218	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1244	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1243	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1347	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1445	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1832	6MZ	C5-C6	2.73	1.48	1.41
1	S2	814	PSU	C4-N3	-2.72	1.33	1.38
1	S2	609	PSU	C4-N3	-2.72	1.33	1.38
3	L5	4628	PSU	C6-C5	2.72	1.38	1.35
3	L5	3792	OMG	C6-N1	-2.72	1.33	1.38
1	S2	121	OMU	C4-N3	-2.72	1.34	1.38
3	L5	1625	OMG	C6-N1	-2.71	1.33	1.38
3	L5	2364	OMG	C6-N1	-2.71	1.33	1.38
1	S2	1442	OMU	C4-N3	-2.71	1.34	1.38
3	L5	4196	OMG	C6-N1	-2.71	1.33	1.38
1	S2	573	PSU	C4-N3	-2.71	1.33	1.38
1	S2	296	PSU	C4-N3	-2.70	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	572	PSU	C4-N3	-2.70	1.33	1.38
1	S2	119	PSU	C4-N3	-2.70	1.33	1.38
1	S2	866	PSU	C4-N3	-2.70	1.33	1.38
3	L5	3867	A2M	C5-N7	-2.70	1.34	1.39
3	L5	1871	A2M	C5-N7	-2.69	1.34	1.39
1	S2	576	A2M	C5-C6	2.68	1.48	1.41
3	L5	3899	OMG	C6-N1	-2.68	1.33	1.38
81	Pt	56	PSU	C4-N3	-2.68	1.33	1.38
3	L5	4420	PSU	C4-N3	-2.68	1.33	1.38
1	S2	159	A2M	C5-C6	2.68	1.48	1.41
1	S2	822	PSU	C4-N3	-2.67	1.33	1.38
1	S2	116	OMU	C4-N3	-2.67	1.34	1.38
3	L5	3762	PSU	C4-N3	-2.67	1.33	1.38
3	L5	4523	A2M	C5-N7	-2.67	1.34	1.39
3	L5	4306	OMU	C2-N3	-2.67	1.33	1.38
3	L5	1677	PSU	C6-C5	2.67	1.38	1.35
3	L5	3760	A2M	C5-C6	2.67	1.48	1.41
1	S2	590	A2M	C5-C6	2.66	1.48	1.41
3	L5	4618	OMG	C6-N1	-2.66	1.33	1.38
3	L5	1522	OMG	C6-N1	-2.66	1.33	1.38
3	L5	3718	A2M	C5-N7	-2.66	1.34	1.39
3	L5	3782	5MC	C6-N1	-2.65	1.33	1.38
3	L5	1534	A2M	C5-N7	-2.65	1.34	1.39
1	S2	509	OMG	C6-N1	-2.65	1.33	1.38
1	S2	1678	A2M	C5-C6	2.65	1.48	1.41
1	S2	484	A2M	C5-C6	2.65	1.48	1.41
3	L5	1326	A2M	C5-N7	-2.65	1.34	1.39
1	S2	166	A2M	C5-C6	2.65	1.48	1.41
1	S2	428	OMU	C4-N3	-2.64	1.34	1.38
3	L5	4220	6MZ	C5-N7	-2.64	1.34	1.39
1	S2	1288	OMU	C4-N3	-2.64	1.34	1.38
3	L5	3825	A2M	C5-N7	-2.64	1.34	1.39
1	S2	468	A2M	C5-C6	2.64	1.48	1.41
3	L5	4499	OMG	C6-N1	-2.64	1.33	1.38
3	L5	3724	A2M	C5-C6	2.64	1.48	1.41
3	L5	3627	OMG	C6-N1	-2.64	1.33	1.38
3	L5	1524	A2M	C5-N7	-2.64	1.34	1.39
1	S2	1447	OMG	C6-N1	-2.64	1.33	1.38
1	S2	1383	A2M	C5-C6	2.63	1.48	1.41
3	L5	3744	OMG	C6-N1	-2.63	1.33	1.38
3	L5	2363	A2M	C5-N7	-2.63	1.34	1.39
1	S2	683	OMG	C6-N1	-2.61	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4571	A2M	C5-C6	2.61	1.48	1.41
1	S2	627	OMU	C4-N3	-2.60	1.34	1.38
3	L5	398	A2M	C5-C6	2.60	1.48	1.41
1	S2	668	A2M	C5-C6	2.60	1.48	1.41
3	L5	4590	A2M	C5-C6	2.60	1.48	1.41
3	L5	2815	A2M	C5-C6	2.59	1.48	1.41
1	S2	644	OMG	C6-N1	-2.59	1.34	1.38
3	L5	3830	A2M	C5-N7	-2.59	1.34	1.39
3	L5	2815	A2M	C5-N7	-2.59	1.34	1.39
39	LB	245	HIC	CD2-CG	2.59	1.40	1.36
3	L5	1534	A2M	C5-C6	2.59	1.48	1.41
3	L5	2401	A2M	C5-N7	-2.59	1.34	1.39
1	S2	512	A2M	C5-C6	2.58	1.48	1.41
1	S2	1328	OMG	C6-N1	-2.58	1.34	1.38
3	L5	1316	OMG	C6-N1	-2.58	1.34	1.38
1	S2	1490	OMG	C6-N1	-2.57	1.34	1.38
3	L5	2837	OMU	C2-N3	-2.57	1.33	1.38
3	L5	3723	A2M	C5-C6	2.57	1.48	1.41
2	L8	14	OMU	C2-N3	-2.57	1.33	1.38
1	S2	436	OMG	C6-N1	-2.57	1.34	1.38
1	S2	27	A2M	C5-C6	2.56	1.48	1.41
3	L5	4498	OMU	C2-N3	-2.56	1.33	1.38
1	S2	1031	A2M	C5-C6	2.56	1.48	1.41
1	S2	99	A2M	C5-C6	2.56	1.48	1.41
3	L5	3944	OMG	C6-N1	-2.55	1.34	1.38
3	L5	3830	A2M	C5-C6	2.55	1.48	1.41
3	L5	400	A2M	C5-C6	2.55	1.48	1.41
3	L5	4620	OMU	C2-N3	-2.55	1.33	1.38
1	S2	601	OMG	C6-N1	-2.54	1.34	1.38
3	L5	1326	A2M	C5-C6	2.54	1.48	1.41
1	S2	99	A2M	C5-N7	-2.54	1.34	1.39
3	L5	4228	OMG	C6-N1	-2.53	1.34	1.38
3	L5	2401	A2M	C5-C6	2.53	1.48	1.41
81	Pt	21	H2U	C2-N3	-2.53	1.33	1.38
3	L5	4623	OMG	C6-N1	-2.52	1.34	1.38
3	L5	3723	A2M	C5-N7	-2.51	1.34	1.39
3	L5	4227	OMU	C2-N3	-2.51	1.33	1.38
3	L5	3770	PSU	C2-N3	-2.51	1.33	1.37
1	S2	1842	4AC	C4-N4	-2.51	1.36	1.39
3	L5	2787	A2M	C5-C6	2.51	1.48	1.41
3	L5	3825	A2M	C5-C6	2.50	1.48	1.41
3	L5	4571	A2M	C5-N7	-2.50	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	398	A2M	C5-N7	-2.50	1.34	1.39
1	S2	1832	6MZ	C5-N7	-2.49	1.34	1.39
3	L5	2415	OMU	C2-N3	-2.49	1.33	1.38
3	L5	400	A2M	C5-N7	-2.48	1.34	1.39
3	L5	3718	A2M	C5-C6	2.47	1.47	1.41
3	L5	3637	PSU	C2-N3	-2.47	1.33	1.37
2	L8	75	OMG	C6-N1	-2.47	1.34	1.38
3	L5	4590	A2M	C5-N7	-2.47	1.34	1.39
3	L5	2363	A2M	C5-C6	2.47	1.47	1.41
3	L5	3782	5MC	C6-C5	2.46	1.38	1.34
1	S2	867	OMG	C6-N1	-2.46	1.34	1.38
3	L5	1524	A2M	C5-C6	2.46	1.47	1.41
1	S2	354	OMU	C2-N3	-2.45	1.33	1.38
1	S2	484	A2M	C5-N7	-2.45	1.34	1.39
1	S2	590	A2M	C5-N7	-2.45	1.34	1.39
3	L5	3867	A2M	C5-C6	2.45	1.47	1.41
3	L5	1677	PSU	O4'-C1'	-2.45	1.40	1.43
3	L5	3724	A2M	C5-N7	-2.45	1.34	1.39
1	S2	1639	G7M	C6-N1	-2.44	1.34	1.38
1	S2	27	A2M	C5-N7	-2.43	1.34	1.39
3	L5	4420	PSU	O4'-C1'	-2.42	1.40	1.43
3	L5	4220	6MZ	C5-C6	2.42	1.47	1.41
3	L5	4523	A2M	C5-C6	2.41	1.47	1.41
3	L5	2424	OMG	C5-N7	-2.41	1.34	1.39
3	L5	2363	A2M	C4-N9	-2.41	1.32	1.37
1	S2	1031	A2M	C5-N7	-2.40	1.34	1.39
1	S2	1678	A2M	C5-N7	-2.39	1.34	1.39
3	L5	1625	OMG	C5-N7	-2.39	1.34	1.39
3	L5	3792	OMG	C5-N7	-2.39	1.34	1.39
3	L5	4531	PSU	C2-N3	-2.38	1.33	1.37
3	L5	4494	OMG	C5-N7	-2.37	1.34	1.39
1	S2	1804	OMU	C2-N3	-2.37	1.33	1.38
3	L5	4392	OMG	C5-N7	-2.37	1.34	1.39
3	L5	2364	OMG	C5-N7	-2.36	1.34	1.39
3	L5	4196	OMG	C5-N7	-2.36	1.34	1.39
1	S2	668	A2M	C5-N7	-2.36	1.34	1.39
1	S2	512	A2M	C5-N7	-2.36	1.34	1.39
3	L5	1871	A2M	C4-N9	-2.35	1.32	1.37
3	L5	4370	OMG	C5-N7	-2.34	1.34	1.39
3	L5	1871	A2M	C5-C6	2.34	1.47	1.41
1	S2	172	OMU	C2-N3	-2.34	1.33	1.38
1	S2	166	A2M	C5-N7	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1383	A2M	C5-N7	-2.34	1.34	1.39
3	L5	1322	1MA	C5-N7	-2.33	1.34	1.39
1	S2	576	A2M	C8-N7	2.33	1.36	1.31
1	S2	159	A2M	C5-N7	-2.33	1.34	1.39
3	L5	1524	A2M	C4-N9	-2.33	1.32	1.37
3	L5	1536	PSU	C2-N3	-2.33	1.33	1.37
3	L5	3899	OMG	C4-N9	-2.33	1.32	1.38
3	L5	4628	PSU	C2-N3	-2.32	1.33	1.37
1	S2	1081	PSU	C2-N3	-2.32	1.33	1.37
1	S2	1851	MA6	C4-N9	-2.32	1.32	1.37
1	S2	1288	OMU	C2-N1	2.32	1.42	1.38
1	S2	576	A2M	C5-N7	-2.31	1.34	1.39
1	S2	468	A2M	C5-N7	-2.31	1.34	1.39
3	L5	4299	PSU	C2-N3	-2.31	1.33	1.37
3	L5	3785	A2M	C8-N9	-2.31	1.33	1.37
1	S2	1850	MA6	C5-N7	-2.31	1.34	1.39
3	L5	2876	OMG	C5-N7	-2.30	1.34	1.39
3	L5	3718	A2M	C4-N9	-2.30	1.32	1.37
1	S2	166	A2M	C8-N7	2.30	1.36	1.31
3	L5	3760	A2M	C5-N7	-2.30	1.34	1.39
3	L5	3627	OMG	C5-N7	-2.30	1.34	1.39
81	Pt	21	H2U	C4-N3	-2.29	1.33	1.37
3	L5	3867	A2M	C4-N9	-2.29	1.32	1.37
3	L5	4637	OMG	C5-N7	-2.29	1.34	1.39
3	L5	4499	OMG	C5-N7	-2.29	1.34	1.39
3	L5	2843	PSU	C2-N3	-2.29	1.33	1.37
3	L5	4498	OMU	C5-C4	-2.29	1.38	1.43
3	L5	1316	OMG	C5-N7	-2.28	1.34	1.39
3	L5	3760	A2M	C8-N7	2.28	1.36	1.31
1	S2	468	A2M	C8-N7	2.28	1.36	1.31
3	L5	2839	PSU	C2-N3	-2.28	1.33	1.37
1	S2	428	OMU	C2-N3	-2.28	1.34	1.38
3	L5	4532	PSU	C2-N3	-2.28	1.33	1.37
3	L5	4220	6MZ	C4-N9	-2.27	1.33	1.37
3	L5	4228	OMG	C4-N9	-2.27	1.32	1.38
3	L5	4447	5MC	C6-N1	-2.27	1.34	1.38
1	S2	509	OMG	C5-N7	-2.26	1.34	1.39
1	S2	1442	OMU	C2-N3	-2.26	1.34	1.38
1	S2	1031	A2M	C4-N9	-2.25	1.33	1.37
1	S2	1851	MA6	C5-N7	-2.25	1.35	1.39
3	L5	4521	PSU	C2-N3	-2.25	1.33	1.37
3	L5	2508	PSU	C2-N3	-2.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	27	A2M	C8-N7	2.24	1.36	1.31
3	L5	4689	PSU	C2-N3	-2.24	1.33	1.37
3	L5	3884	PSU	C2-N3	-2.24	1.33	1.37
3	L5	4312	PSU	C2-N3	-2.24	1.33	1.37
1	S2	668	A2M	C4-N9	-2.24	1.33	1.37
1	S2	121	OMU	C2-N3	-2.23	1.34	1.38
1	S2	159	A2M	C8-N7	2.23	1.36	1.31
3	L5	1522	OMG	C5-N7	-2.22	1.34	1.39
3	L5	4618	OMG	C5-N7	-2.22	1.34	1.39
1	S2	116	OMU	C2-N3	-2.22	1.34	1.38
3	L5	3695	PSU	C2-N3	-2.22	1.33	1.37
3	L5	3899	OMG	C5-N7	-2.22	1.34	1.39
3	L5	1744	PSU	C2-N3	-2.22	1.33	1.37
3	L5	1782	PSU	C2-N3	-2.21	1.33	1.37
1	S2	1678	A2M	C8-N7	2.21	1.35	1.31
3	L5	4523	A2M	C4-N9	-2.21	1.33	1.37
3	L5	4361	PSU	C2-N3	-2.21	1.33	1.37
3	L5	5001	PSU	C2-N3	-2.21	1.33	1.37
1	S2	121	OMU	C5-C4	-2.21	1.38	1.43
1	S2	1447	OMG	C5-N7	-2.21	1.34	1.39
3	L5	1534	A2M	C4-N9	-2.21	1.33	1.37
1	S2	1490	OMG	C5-N7	-2.21	1.34	1.39
1	S2	1850	MA6	C4-N9	-2.21	1.33	1.37
3	L5	4353	PSU	C2-N3	-2.21	1.33	1.37
3	L5	4590	A2M	C8-N7	2.21	1.35	1.31
3	L5	1792	PSU	C2-N3	-2.20	1.33	1.37
3	L5	4431	PSU	C2-N3	-2.20	1.33	1.37
1	S2	512	A2M	C8-N7	2.20	1.35	1.31
1	S2	668	A2M	C8-N7	2.19	1.35	1.31
2	L8	55	PSU	C2-N3	-2.19	1.33	1.37
2	L8	75	OMG	C5-N7	-2.19	1.34	1.39
3	L5	4493	PSU	C2-N3	-2.19	1.33	1.37
3	L5	4579	PSU	C2-N3	-2.19	1.33	1.37
3	L5	4623	OMG	C5-N7	-2.19	1.34	1.39
3	L5	1779	PSU	C2-N3	-2.19	1.33	1.37
3	L5	1316	OMG	C4-N9	-2.19	1.32	1.38
3	L5	4590	A2M	C4-N9	-2.19	1.33	1.37
3	L5	4296	PSU	C2-N3	-2.19	1.33	1.37
3	L5	4471	PSU	C2-N3	-2.19	1.33	1.37
3	L5	3744	OMG	C5-N7	-2.19	1.34	1.39
1	S2	354	OMU	C5-C4	-2.19	1.39	1.43
3	L5	4569	PSU	C2-N3	-2.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	484	A2M	C8-N7	2.18	1.35	1.31
81	Pt	8	4SU	C2-N3	-2.18	1.34	1.38
1	S2	644	OMG	C5-N7	-2.18	1.34	1.39
1	S2	590	A2M	C8-N7	2.18	1.35	1.31
1	S2	1383	A2M	C8-N7	2.18	1.35	1.31
3	L5	1781	PSU	C2-N3	-2.18	1.33	1.37
3	L5	2837	OMU	C5-C4	-2.17	1.39	1.43
3	L5	1860	PSU	C2-N3	-2.17	1.33	1.37
3	L5	4623	OMG	C4-N9	-2.17	1.32	1.38
1	S2	116	OMU	C5-C4	-2.17	1.39	1.43
3	L5	3944	OMG	C5-N7	-2.17	1.34	1.39
3	L5	4571	A2M	C4-N9	-2.17	1.33	1.37
1	S2	601	OMG	C5-N7	-2.17	1.34	1.39
3	L5	4673	PSU	C2-N3	-2.16	1.33	1.37
3	L5	3723	A2M	C8-N7	2.16	1.35	1.31
1	S2	1288	OMU	C2-N3	-2.16	1.34	1.38
1	S2	627	OMU	C2-N3	-2.16	1.34	1.38
3	L5	4228	OMG	C5-N7	-2.16	1.34	1.39
3	L5	3920	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4293	PSU	C2-N3	-2.15	1.33	1.37
1	S2	436	OMG	C5-N7	-2.15	1.34	1.39
3	L5	3825	A2M	C4-N9	-2.15	1.33	1.37
3	L5	2415	OMU	C5-C4	-2.15	1.39	1.43
3	L5	3844	PSU	C2-N3	-2.15	1.33	1.37
3	L5	4620	OMU	C5-C4	-2.15	1.39	1.43
3	L5	1582	PSU	C2-N3	-2.15	1.33	1.37
1	S2	814	PSU	C2-N3	-2.15	1.33	1.37
3	L5	4636	PSU	C2-N3	-2.15	1.33	1.37
1	S2	1288	OMU	C5-C4	-2.14	1.39	1.43
1	S2	681	PSU	C2-N3	-2.14	1.33	1.37
3	L5	3723	A2M	C4-N9	-2.14	1.33	1.37
3	L5	3639	PSU	C2-N3	-2.14	1.34	1.37
3	L5	398	A2M	C8-N7	2.14	1.35	1.31
1	S2	1328	OMG	C5-N7	-2.13	1.34	1.39
3	L5	5010	PSU	C2-N3	-2.13	1.34	1.37
1	S2	1174	PSU	C2-N3	-2.13	1.34	1.37
2	L8	69	PSU	C2-N3	-2.13	1.34	1.37
3	L5	3724	A2M	C8-N7	2.13	1.35	1.31
1	S2	683	OMG	C5-N7	-2.13	1.34	1.39
3	L5	3853	PSU	C2-N3	-2.13	1.34	1.37
1	S2	1851	MA6	C8-N7	2.13	1.35	1.31
3	L5	3818	UY1	O4'-C1'	-2.13	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1347	PSU	C2-N3	-2.13	1.34	1.37
1	S2	1832	6MZ	C4-N9	-2.12	1.33	1.37
3	L5	1862	PSU	C2-N3	-2.12	1.34	1.37
3	L5	2632	PSU	C2-N3	-2.12	1.34	1.37
1	S2	1442	OMU	C5-C4	-2.12	1.39	1.43
3	L5	3729	PSU	C2-N3	-2.12	1.34	1.37
1	S2	1081	PSU	O4'-C1'	-2.11	1.40	1.43
3	L5	4423	PSU	C2-N3	-2.11	1.34	1.37
3	L5	3770	PSU	C2-N1	-2.11	1.33	1.36
3	L5	4227	OMU	C5-C4	-2.11	1.39	1.43
3	L5	4552	PSU	C2-N3	-2.11	1.34	1.37
3	L5	1326	A2M	C4-N9	-2.11	1.33	1.37
3	L5	4628	PSU	C2-N1	-2.10	1.33	1.36
1	S2	105	PSU	C2-N3	-2.10	1.34	1.37
3	L5	1683	PSU	C2-N1	-2.10	1.33	1.36
3	L5	4442	PSU	C2-N3	-2.10	1.34	1.37
3	L5	4972	PSU	C2-N3	-2.10	1.34	1.37
3	L5	3830	A2M	C8-N7	2.10	1.35	1.31
1	S2	428	OMU	C5-C4	-2.10	1.39	1.43
1	S2	966	PSU	C2-N3	-2.09	1.34	1.37
3	L5	4306	OMU	C5-C4	-2.09	1.39	1.43
3	L5	3764	PSU	C2-N3	-2.09	1.34	1.37
3	L5	1322	1MA	C4-N9	-2.09	1.32	1.38
1	S2	109	PSU	C2-N3	-2.09	1.34	1.37
1	S2	468	A2M	C4-N9	-2.09	1.33	1.37
3	L5	1677	PSU	C2-N3	-2.08	1.34	1.37
3	L5	2364	OMG	C4-N9	-2.08	1.32	1.38
1	S2	801	PSU	C2-N3	-2.08	1.34	1.37
3	L5	400	A2M	C4-N9	-2.08	1.33	1.37
1	S2	1177	PSU	C2-N3	-2.08	1.34	1.37
3	L5	3925	OMU	C5-C4	-2.08	1.39	1.43
3	L5	3715	PSU	C2-N3	-2.07	1.34	1.37
3	L5	4457	PSU	C2-N3	-2.07	1.34	1.37
1	S2	1692	PSU	C2-N3	-2.07	1.34	1.37
3	L5	3851	PSU	C2-N3	-2.07	1.34	1.37
1	S2	406	PSU	C2-N3	-2.07	1.34	1.37
1	S2	1804	OMU	C5-C4	-2.07	1.39	1.43
1	S2	1031	A2M	C8-N7	2.07	1.35	1.31
1	S2	99	A2M	C8-N7	2.07	1.35	1.31
3	L5	2632	PSU	C2-N1	-2.06	1.34	1.36
3	L5	3758	PSU	C2-N3	-2.06	1.34	1.37
3	L5	4403	PSU	C2-N3	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4576	PSU	C2-N3	-2.06	1.34	1.37
3	L5	1522	OMG	C4-N9	-2.06	1.32	1.38
3	L5	1683	PSU	C2-N3	-2.05	1.34	1.37
3	L5	3627	OMG	C4-N9	-2.05	1.32	1.38
3	L5	2815	A2M	C4-N9	-2.05	1.33	1.37
3	L5	3818	UY1	C2-N3	-2.05	1.34	1.37
1	S2	867	OMG	C5-N7	-2.05	1.35	1.39
1	S2	822	PSU	O4'-C1'	-2.05	1.41	1.43
3	L5	2401	A2M	C4-N9	-2.05	1.33	1.37
1	S2	1056	PSU	C2-N3	-2.04	1.34	1.37
1	S2	36	PSU	C2-N3	-2.04	1.34	1.37
3	L5	3724	A2M	C4-N9	-2.04	1.33	1.37
1	S2	218	PSU	C2-N3	-2.03	1.34	1.37
1	S2	649	PSU	C2-N3	-2.03	1.34	1.37
3	L5	2363	A2M	C8-N7	2.03	1.35	1.31
1	S2	918	PSU	C2-N3	-2.03	1.34	1.37
3	L5	3770	PSU	C2'-C1'	-2.03	1.51	1.53
3	L5	4571	A2M	C8-N7	2.03	1.35	1.31
2	L8	14	OMU	C5-C4	-2.03	1.39	1.43
3	L5	4523	A2M	C8-N7	2.02	1.35	1.31
1	S2	1243	PSU	C2-N3	-2.02	1.34	1.37
3	L5	400	A2M	C8-N7	2.02	1.35	1.31
3	L5	4420	PSU	C2-N3	-2.02	1.34	1.37
3	L5	2815	A2M	C8-N7	2.02	1.35	1.31
3	L5	3768	PSU	C2-N3	-2.02	1.34	1.37
3	L5	5001	PSU	C2-N1	-2.02	1.34	1.36
3	L5	3718	A2M	C8-N7	2.02	1.35	1.31
1	S2	863	PSU	C2-N3	-2.02	1.34	1.37
1	S2	93	PSU	C2-N3	-2.02	1.34	1.37
1	S2	651	PSU	C2-N3	-2.02	1.34	1.37
1	S2	1136	PSU	C2-N3	-2.02	1.34	1.37
3	L5	4552	PSU	C2-N1	-2.02	1.34	1.36
3	L5	4579	PSU	C2-N1	-2.01	1.34	1.36
3	L5	3830	A2M	C4-N9	-2.01	1.33	1.37
1	S2	627	OMU	C5-C4	-2.01	1.39	1.43
3	L5	3825	A2M	C8-N7	2.01	1.35	1.31
1	S2	1239	PSU	C2-N3	-2.01	1.34	1.37
3	L5	4618	OMG	C4-N9	-2.01	1.33	1.38
1	S2	1643	PSU	C2-N3	-2.00	1.34	1.37
3	L5	1871	A2M	C8-N7	2.00	1.35	1.31
3	L5	3734	PSU	C2-N3	-2.00	1.34	1.37
1	S2	815	PSU	C2-N3	-2.00	1.34	1.37

All (1085) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1639	G7M	CN7-N7-C8	-8.02	112.64	124.79
6	SA	2	SAC	OAC-C1A-C2A	-7.95	107.89	122.05
3	L5	4530	UR3	C4-N3-C2	-7.75	118.34	124.58
3	L5	4532	PSU	N1-C2-N3	7.59	123.17	115.17
63	Lr	2	SAC	OAC-C1A-N	-7.20	109.27	121.98
29	SV	1	AME	OT-CT1-CT2	-7.13	109.36	122.05
3	L5	3818	UY1	N1-C2-N3	6.96	122.51	115.17
6	SA	2	SAC	OAC-C1A-N	-6.91	109.77	121.98
3	L5	3637	PSU	N1-C2-N3	6.86	122.41	115.17
3	L5	3770	PSU	N1-C2-N3	6.86	122.41	115.17
63	Lr	2	SAC	OAC-C1A-C2A	-6.83	109.89	122.05
3	L5	1683	PSU	N1-C2-N3	6.82	122.37	115.17
81	Pt	8	4SU	C4-N3-C2	-6.80	120.80	127.31
3	L5	2839	PSU	N1-C2-N3	6.80	122.34	115.17
3	L5	4296	PSU	N1-C2-N3	6.78	122.33	115.17
1	S2	1639	G7M	N9-C8-N7	-6.78	96.02	112.48
3	L5	4403	PSU	N1-C2-N3	6.77	122.31	115.17
3	L5	4500	PSU	N1-C2-N3	6.75	122.29	115.17
3	L5	4471	PSU	N1-C2-N3	6.73	122.27	115.17
3	L5	1536	PSU	N1-C2-N3	6.70	122.23	115.17
29	SV	1	AME	OT-CT1-N	-6.69	110.15	121.98
3	L5	4457	PSU	N1-C2-N3	6.68	122.22	115.17
3	L5	4569	PSU	N1-C2-N3	6.66	122.20	115.17
3	L5	1677	PSU	N1-C2-N3	6.66	122.19	115.17
1	S2	1177	PSU	N1-C2-N3	6.63	122.16	115.17
3	L5	4423	PSU	N1-C2-N3	6.63	122.16	115.17
3	L5	4673	PSU	N1-C2-N3	6.62	122.15	115.17
3	L5	1862	PSU	N1-C2-N3	6.62	122.15	115.17
3	L5	4493	PSU	N1-C2-N3	6.61	122.14	115.17
3	L5	1779	PSU	N1-C2-N3	6.59	122.12	115.17
1	S2	1244	PSU	N1-C2-N3	6.59	122.12	115.17
3	L5	3851	PSU	N1-C2-N3	6.59	122.12	115.17
3	L5	4442	PSU	N1-C2-N3	6.57	122.10	115.17
3	L5	4353	PSU	N1-C2-N3	6.57	122.10	115.17
3	L5	4521	PSU	N1-C2-N3	6.57	122.10	115.17
1	S2	649	PSU	N1-C2-N3	6.56	122.09	115.17
1	S2	1056	PSU	N1-C2-N3	6.56	122.09	115.17
3	L5	4576	PSU	N1-C2-N3	6.55	122.08	115.17
3	L5	3729	PSU	N1-C2-N3	6.53	122.06	115.17
1	S2	822	PSU	N1-C2-N3	6.53	122.06	115.17
1	S2	1639	G7M	C8-N7-C5	6.53	115.94	107.78
3	L5	3762	PSU	N1-C2-N3	6.53	122.05	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	686	PSU	N1-C2-N3	6.52	122.05	115.17
1	S2	863	PSU	N1-C2-N3	6.51	122.04	115.17
3	L5	3715	PSU	N1-C2-N3	6.51	122.04	115.17
2	L8	69	PSU	N1-C2-N3	6.51	122.04	115.17
1	S2	406	PSU	N1-C2-N3	6.51	122.03	115.17
1	S2	34	PSU	N1-C2-N3	6.50	122.03	115.17
1	S2	866	PSU	N1-C2-N3	6.50	122.03	115.17
3	L5	4431	PSU	N1-C2-N3	6.50	122.03	115.17
3	L5	1582	PSU	N1-C2-N3	6.50	122.03	115.17
3	L5	4636	PSU	N1-C2-N3	6.50	122.02	115.17
1	S2	1238	PSU	N1-C2-N3	6.50	122.02	115.17
3	L5	3853	PSU	N1-C2-N3	6.50	122.02	115.17
1	S2	1692	PSU	N1-C2-N3	6.49	122.02	115.17
1	S2	918	PSU	N1-C2-N3	6.49	122.02	115.17
3	L5	4299	PSU	N1-C2-N3	6.49	122.02	115.17
1	S2	1136	PSU	N1-C2-N3	6.49	122.02	115.17
3	L5	4689	PSU	N1-C2-N3	6.49	122.02	115.17
1	S2	36	PSU	N1-C2-N3	6.49	122.01	115.17
3	L5	3768	PSU	N1-C2-N3	6.48	122.01	115.17
1	S2	105	PSU	N1-C2-N3	6.48	122.00	115.17
1	S2	1445	PSU	N1-C2-N3	6.47	122.00	115.17
3	L5	2843	PSU	N1-C2-N3	6.47	121.99	115.17
1	S2	1232	PSU	N1-C2-N3	6.47	121.99	115.17
3	L5	2508	PSU	N1-C2-N3	6.46	121.98	115.17
2	L8	55	PSU	N1-C2-N3	6.46	121.98	115.17
1	S2	572	PSU	N1-C2-N3	6.46	121.98	115.17
1	S2	681	PSU	N1-C2-N3	6.45	121.98	115.17
3	L5	1792	PSU	N1-C2-N3	6.45	121.97	115.17
1	S2	1081	PSU	N1-C2-N3	6.45	121.97	115.17
1	S2	1639	G7M	N9-C4-N3	6.45	138.84	125.95
3	L5	4972	PSU	N1-C2-N3	6.44	121.97	115.17
1	S2	815	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	5010	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	1782	PSU	N1-C2-N3	6.44	121.96	115.17
1	S2	119	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	3764	PSU	N1-C2-N3	6.44	121.96	115.17
1	S2	609	PSU	N1-C2-N3	6.43	121.95	115.17
3	L5	3844	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	966	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	1243	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	1367	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	651	PSU	N1-C2-N3	6.41	121.93	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1004	PSU	N1-C2-N3	6.41	121.93	115.17
1	S2	109	PSU	N1-C2-N3	6.40	121.92	115.17
3	L5	3734	PSU	N1-C2-N3	6.40	121.92	115.17
3	L5	3758	PSU	N1-C2-N3	6.38	121.90	115.17
3	L5	1860	PSU	N1-C2-N3	6.38	121.90	115.17
3	L5	4579	PSU	N1-C2-N3	6.38	121.90	115.17
1	S2	296	PSU	N1-C2-N3	6.38	121.89	115.17
3	L5	4312	PSU	N1-C2-N3	6.37	121.89	115.17
3	L5	3920	PSU	N1-C2-N3	6.37	121.89	115.17
3	L5	1744	PSU	N1-C2-N3	6.37	121.89	115.17
1	S2	801	PSU	N1-C2-N3	6.37	121.89	115.17
1	S2	573	PSU	N1-C2-N3	6.37	121.88	115.17
1	S2	1326	UY1	N1-C2-N3	6.35	121.87	115.17
1	S2	1174	PSU	N1-C2-N3	6.35	121.86	115.17
3	L5	3639	PSU	N1-C2-N3	6.35	121.86	115.17
1	S2	1239	PSU	N1-C2-N3	6.34	121.86	115.17
1	S2	1643	PSU	N1-C2-N3	6.34	121.86	115.17
3	L5	4552	PSU	N1-C2-N3	6.34	121.85	115.17
3	L5	2424	OMG	C5-C4-N3	-6.33	118.32	128.39
1	S2	509	OMG	C5-C4-N3	-6.32	118.33	128.39
1	S2	814	PSU	N1-C2-N3	6.32	121.83	115.17
1	S2	218	PSU	N1-C2-N3	6.32	121.83	115.17
81	Pt	56	PSU	N1-C2-N3	6.31	121.83	115.17
3	L5	1781	PSU	N1-C2-N3	6.31	121.83	115.17
1	S2	1447	OMG	C5-C4-N3	-6.31	118.35	128.39
3	L5	5001	PSU	N1-C2-N3	6.31	121.82	115.17
1	S2	590	A2M	C5-C4-N3	-6.30	118.04	126.72
3	L5	4531	PSU	N1-C2-N3	6.30	121.81	115.17
3	L5	4293	PSU	N1-C2-N3	6.28	121.79	115.17
3	L5	4361	PSU	N1-C2-N3	6.28	121.79	115.17
1	S2	644	OMG	C5-C4-N3	-6.27	118.41	128.39
1	S2	93	PSU	N1-C2-N3	6.27	121.79	115.17
3	L5	3695	PSU	N1-C2-N3	6.27	121.79	115.17
1	S2	1625	PSU	N1-C2-N3	6.27	121.78	115.17
3	L5	3792	OMG	C5-C4-N3	-6.26	118.42	128.39
3	L5	4494	OMG	C5-C4-N3	-6.26	118.42	128.39
1	S2	1347	PSU	N1-C2-N3	6.25	121.77	115.17
3	L5	2876	OMG	C5-C4-N3	-6.23	118.48	128.39
3	L5	2632	PSU	N1-C2-N3	6.21	121.72	115.17
3	L5	4392	OMG	C5-C4-N3	-6.18	118.55	128.39
3	L5	2787	A2M	C5-C4-N3	-6.18	118.21	126.72
1	S2	1328	OMG	C5-C4-N3	-6.14	118.61	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	601	OMG	C5-C4-N3	-6.13	118.63	128.39
3	L5	1625	OMG	C5-C4-N3	-6.13	118.64	128.39
3	L5	4628	PSU	N1-C2-N3	6.12	121.63	115.17
3	L5	4420	PSU	N1-C2-N3	6.11	121.61	115.17
3	L5	2815	A2M	C5-C4-N3	-6.11	118.31	126.72
3	L5	3944	OMG	C5-C4-N3	-6.08	118.71	128.39
3	L5	3884	PSU	N1-C2-N3	6.08	121.58	115.17
3	L5	3744	OMG	C5-C4-N3	-6.07	118.73	128.39
1	S2	484	A2M	C5-C4-N3	-6.02	118.43	126.72
3	L5	4196	OMG	C5-C4-N3	-6.01	118.82	128.39
3	L5	2401	A2M	C5-C4-N3	-6.01	118.44	126.72
1	S2	1490	OMG	C5-C4-N3	-6.00	118.83	128.39
1	S2	867	OMG	C5-C4-N3	-5.96	118.90	128.39
1	S2	27	A2M	C5-C4-N3	-5.95	118.52	126.72
1	S2	436	OMG	C5-C4-N3	-5.95	118.92	128.39
1	S2	99	A2M	C5-C4-N3	-5.95	118.53	126.72
3	L5	398	A2M	C5-C4-N3	-5.94	118.54	126.72
1	S2	683	OMG	C5-C4-N3	-5.92	118.96	128.39
3	L5	4499	OMG	C5-C4-N3	-5.92	118.96	128.39
3	L5	4370	OMG	C5-C4-N3	-5.92	118.97	128.39
2	L8	75	OMG	C5-C4-N3	-5.90	119.01	128.39
3	L5	3760	A2M	C5-C4-N3	-5.89	118.61	126.72
3	L5	3830	A2M	C5-C4-N3	-5.87	118.64	126.72
3	L5	4637	OMG	C5-C4-N3	-5.85	119.08	128.39
1	S2	159	A2M	C5-C4-N3	-5.83	118.69	126.72
81	Pt	8	4SU	C5-C4-N3	5.82	120.16	114.75
1	S2	1678	A2M	C5-C4-N3	-5.82	118.71	126.72
3	L5	3825	A2M	C5-C4-N3	-5.81	118.72	126.72
3	L5	2364	OMG	C5-C4-N3	-5.79	119.18	128.39
3	L5	4618	OMG	C5-C4-N3	-5.78	119.20	128.39
3	L5	3723	A2M	C5-C4-N3	-5.78	118.76	126.72
3	L5	3724	A2M	C5-C4-N3	-5.77	118.77	126.72
3	L5	400	A2M	C5-C4-N3	-5.76	118.78	126.72
3	L5	4220	6MZ	C5-C4-N3	-5.75	118.80	126.72
1	S2	512	A2M	C5-C4-N3	-5.75	118.81	126.72
3	L5	3627	OMG	C5-C4-N3	-5.75	119.25	128.39
3	L5	3718	A2M	C5-C4-N3	-5.73	118.83	126.72
3	L5	1522	OMG	C5-C4-N3	-5.71	119.30	128.39
1	S2	1383	A2M	C5-C4-N3	-5.70	118.86	126.72
3	L5	4623	OMG	C5-C4-N3	-5.70	119.32	128.39
1	S2	576	A2M	C5-C4-N3	-5.70	118.87	126.72
1	S2	468	A2M	C5-C4-N3	-5.68	118.89	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1326	A2M	C5-C4-N3	-5.68	118.89	126.72
1	S2	166	A2M	C5-C4-N3	-5.67	118.91	126.72
3	L5	4571	A2M	C5-C4-N3	-5.67	118.91	126.72
3	L5	2363	A2M	C5-C4-N3	-5.65	118.94	126.72
3	L5	3867	A2M	C5-C4-N3	-5.60	119.00	126.72
3	L5	4523	A2M	C5-C4-N3	-5.56	119.06	126.72
3	L5	1524	A2M	C5-C4-N3	-5.56	119.06	126.72
3	L5	1534	A2M	C5-C4-N3	-5.55	119.07	126.72
3	L5	4590	A2M	C5-C4-N3	-5.55	119.08	126.72
1	S2	1832	6MZ	C5-C4-N3	-5.51	119.12	126.72
3	L5	3899	OMG	C5-C4-N3	-5.49	119.65	128.39
1	S2	1639	G7M	C5-C4-N3	-5.48	117.80	128.15
3	L5	1316	OMG	C5-C4-N3	-5.42	119.77	128.39
1	S2	1031	A2M	C5-C4-N3	-5.36	119.33	126.72
1	S2	1248	B8N	C4-N3-C2	-5.35	119.04	125.62
1	S2	668	A2M	C5-C4-N3	-5.35	119.36	126.72
3	L5	1871	A2M	C5-C4-N3	-5.32	119.39	126.72
1	S2	1383	A2M	C2'-C1'-N9	-5.29	105.04	113.75
3	L5	4228	OMG	C5-C4-N3	-5.25	120.03	128.39
1	S2	1850	MA6	C5-C4-N3	-5.24	119.50	126.72
1	S2	1851	MA6	C5-C4-N3	-5.18	119.58	126.72
3	L5	4227	OMU	C4-N3-C2	-5.17	120.20	126.61
3	L5	3944	OMG	C2-N3-C4	5.14	121.15	112.30
3	L5	4392	OMG	C2-N3-C4	5.14	121.15	112.30
2	L8	75	OMG	C2-N3-C4	5.13	121.14	112.30
3	L5	4494	OMG	C2-N3-C4	5.13	121.14	112.30
3	L5	3744	OMG	C2-N3-C4	5.11	121.10	112.30
1	S2	683	OMG	C2-N3-C4	5.09	121.07	112.30
3	L5	3925	OMU	C4-N3-C2	-5.09	120.29	126.61
3	L5	4623	OMG	C2-N3-C4	5.08	121.05	112.30
1	S2	644	OMG	C2-N3-C4	5.08	121.05	112.30
3	L5	4618	OMG	C2-N3-C4	5.07	121.04	112.30
3	L5	4499	OMG	C2-N3-C4	5.07	121.02	112.30
3	L5	3792	OMG	C2-N3-C4	5.06	121.01	112.30
3	L5	1322	1MA	C5-C4-N3	-5.06	119.83	127.27
1	S2	172	OMU	C4-N3-C2	-5.01	120.39	126.61
3	L5	3785	A2M	C5-C4-N3	-5.01	119.82	126.72
3	L5	2876	OMG	C2-N3-C4	5.01	120.92	112.30
1	S2	1328	OMG	C2-N3-C4	5.01	120.92	112.30
1	S2	601	OMG	C2-N3-C4	5.00	120.92	112.30
1	S2	1447	OMG	C2-N3-C4	4.99	120.90	112.30
1	S2	590	A2M	N3-C4-N9	4.99	135.65	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	509	OMG	C2-N3-C4	4.99	120.89	112.30
3	L5	1522	OMG	C2-N3-C4	4.99	120.89	112.30
3	L5	4196	OMG	C2-N3-C4	4.98	120.88	112.30
3	L5	1625	OMG	C2-N3-C4	4.98	120.88	112.30
3	L5	2364	OMG	C2-N3-C4	4.97	120.86	112.30
3	L5	3899	OMG	C2-N3-C4	4.97	120.86	112.30
3	L5	2424	OMG	C2-N3-C4	4.97	120.86	112.30
1	S2	436	OMG	C2-N3-C4	4.96	120.84	112.30
3	L5	3627	OMG	C2-N3-C4	4.95	120.83	112.30
1	S2	428	OMU	C4-N3-C2	-4.95	120.47	126.61
1	S2	1804	OMU	C4-N3-C2	-4.94	120.47	126.61
3	L5	2837	OMU	C4-N3-C2	-4.94	120.47	126.61
1	S2	867	OMG	C2-N3-C4	4.93	120.79	112.30
1	S2	1490	OMG	C2-N3-C4	4.93	120.79	112.30
3	L5	2876	OMG	N9-C4-N3	4.92	135.79	125.95
1	S2	627	OMU	C4-N3-C2	-4.91	120.52	126.61
3	L5	4228	OMG	C2-N3-C4	4.91	120.75	112.30
1	S2	354	OMU	C4-N3-C2	-4.89	120.55	126.61
3	L5	4370	OMG	C2-N3-C4	4.87	120.69	112.30
3	L5	2415	OMU	C4-N3-C2	-4.87	120.57	126.61
3	L5	4637	OMG	C2-N3-C4	4.84	120.64	112.30
3	L5	4498	OMU	C4-N3-C2	-4.81	120.64	126.61
1	S2	1442	OMU	C4-N3-C2	-4.81	120.65	126.61
1	S2	27	A2M	N3-C4-N9	4.80	135.33	127.17
2	L8	14	OMU	C4-N3-C2	-4.80	120.65	126.61
1	S2	576	A2M	C2'-C1'-N9	-4.79	105.87	113.75
3	L5	4220	6MZ	N3-C4-N9	4.78	135.30	127.17
3	L5	2815	A2M	N3-C4-N9	4.78	135.29	127.17
3	L5	2401	A2M	N3-C4-N9	4.76	135.27	127.17
3	L5	3785	A2M	C2'-C1'-N9	-4.75	105.93	113.75
1	S2	121	OMU	C4-N3-C2	-4.74	120.73	126.61
3	L5	3785	A2M	N3-C4-N9	4.74	135.22	127.17
3	L5	3760	A2M	N3-C4-N9	4.73	135.22	127.17
3	L5	3792	OMG	N9-C4-N3	4.73	135.40	125.95
3	L5	4494	OMG	N9-C4-N3	4.72	135.39	125.95
3	L5	1625	OMG	N9-C4-N3	4.71	135.37	125.95
3	L5	4531	PSU	C4-N3-C2	-4.70	119.89	126.37
1	S2	1447	OMG	N9-C4-N3	4.70	135.34	125.95
3	L5	1316	OMG	C2-N3-C4	4.69	120.37	112.30
3	L5	2787	A2M	N3-C4-N9	4.69	135.14	127.17
3	L5	3925	OMU	N3-C2-N1	4.67	120.98	114.89
3	L5	4196	OMG	N9-C4-N3	4.67	135.30	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	99	A2M	N3-C4-N9	4.67	135.11	127.17
3	L5	1871	A2M	C2'-C1'-N9	-4.67	106.07	113.75
1	S2	116	OMU	C4-N3-C2	-4.66	120.83	126.61
1	S2	484	A2M	N3-C4-N9	4.66	135.09	127.17
1	S2	1678	A2M	N3-C4-N9	4.65	135.07	127.17
3	L5	4620	OMU	C4-N3-C2	-4.64	120.85	126.61
1	S2	509	OMG	N9-C4-N3	4.64	135.23	125.95
3	L5	4306	OMU	C4-N3-C2	-4.62	120.88	126.61
3	L5	398	A2M	N3-C4-N9	4.62	135.02	127.17
1	S2	644	OMG	N9-C4-N3	4.62	135.19	125.95
3	L5	3867	A2M	N3-C4-N9	4.61	135.01	127.17
1	S2	512	A2M	N3-C4-N9	4.61	135.01	127.17
3	L5	1326	A2M	N3-C4-N9	4.61	135.01	127.17
3	L5	3830	A2M	N3-C4-N9	4.60	134.99	127.17
3	L5	3825	A2M	N3-C4-N9	4.57	134.94	127.17
3	L5	1322	1MA	C2-N3-C4	4.56	121.48	112.53
3	L5	400	A2M	N3-C4-N9	4.56	134.92	127.17
3	L5	4571	A2M	N3-C4-N9	4.55	134.90	127.17
3	L5	3724	A2M	N3-C4-N9	4.54	134.89	127.17
1	S2	1383	A2M	N3-C4-N9	4.54	134.89	127.17
3	L5	4227	OMU	N3-C2-N1	4.53	120.79	114.89
3	L5	4392	OMG	N9-C4-N3	4.52	135.00	125.95
3	L5	3723	A2M	N3-C4-N9	4.52	134.85	127.17
3	L5	2363	A2M	N3-C4-N9	4.52	134.85	127.17
1	S2	1328	OMG	N9-C4-N3	4.51	134.98	125.95
1	S2	601	OMG	N9-C4-N3	4.51	134.97	125.95
3	L5	3744	OMG	N9-C4-N3	4.50	134.96	125.95
3	L5	3944	OMG	N9-C4-N3	4.50	134.94	125.95
3	L5	2424	OMG	N9-C4-N3	4.49	134.93	125.95
3	L5	3818	UY1	C4-N3-C2	-4.49	120.19	126.37
1	S2	159	A2M	N3-C4-N9	4.49	134.80	127.17
1	S2	1490	OMG	N9-C4-N3	4.48	134.92	125.95
3	L5	2508	PSU	C4-N3-C2	-4.48	120.20	126.37
3	L5	4620	OMU	N3-C2-N1	4.48	120.72	114.89
1	S2	1639	G7M	C2-N3-C4	4.48	120.01	112.30
3	L5	4523	A2M	N3-C4-N9	4.47	134.78	127.17
3	L5	1524	A2M	N3-C4-N9	4.47	134.77	127.17
3	L5	2837	OMU	N3-C2-N1	4.47	120.71	114.89
1	S2	468	A2M	N3-C4-N9	4.47	134.76	127.17
3	L5	1862	PSU	C4-N3-C2	-4.46	120.22	126.37
3	L5	4299	PSU	C4-N3-C2	-4.46	120.23	126.37
3	L5	1522	OMG	N9-C4-N3	4.45	134.86	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1850	MA6	C2-N1-C6	4.44	122.68	111.83
3	L5	4370	OMG	N9-C4-N3	4.44	134.84	125.95
1	S2	576	A2M	N3-C4-N9	4.44	134.72	127.17
1	S2	166	A2M	N3-C4-N9	4.43	134.70	127.17
1	S2	1851	MA6	C2-N1-C6	4.43	122.64	111.83
1	S2	867	OMG	N9-C4-N3	4.42	134.79	125.95
3	L5	4673	PSU	C4-N3-C2	-4.41	120.29	126.37
3	L5	4471	PSU	C4-N3-C2	-4.41	120.30	126.37
3	L5	2839	PSU	C4-N3-C2	-4.41	120.30	126.37
3	L5	1792	PSU	C4-N3-C2	-4.40	120.30	126.37
3	L5	4532	PSU	O2-C2-N1	-4.40	118.25	122.79
1	S2	1804	OMU	N3-C2-N1	4.40	120.61	114.89
2	L8	75	OMG	N9-C4-N3	4.40	134.74	125.95
3	L5	4457	PSU	C4-N3-C2	-4.38	120.34	126.37
3	L5	4637	OMG	N9-C4-N3	4.37	134.69	125.95
1	S2	436	OMG	N9-C4-N3	4.37	134.69	125.95
1	S2	1832	6MZ	N3-C4-N9	4.37	134.59	127.17
3	L5	3920	PSU	C4-N3-C2	-4.36	120.36	126.37
3	L5	4532	PSU	C4-N3-C2	-4.36	120.37	126.37
3	L5	4499	OMG	N9-C4-N3	4.36	134.66	125.95
81	Pt	47	G7M	N9-C8-N7	-4.35	101.92	112.48
2	L8	14	OMU	N3-C2-N1	4.35	120.55	114.89
1	S2	1056	PSU	C4-N3-C2	-4.35	120.38	126.37
1	S2	512	A2M	C2'-C1'-N9	-4.35	106.60	113.75
3	L5	4447	5MC	C5-C6-N1	-4.35	118.59	123.31
6	SA	2	SAC	C2A-C1A-N	-4.34	108.92	116.12
3	L5	3770	PSU	C4-N3-C2	-4.34	120.39	126.37
3	L5	4569	PSU	C4-N3-C2	-4.34	120.39	126.37
1	S2	121	OMU	N3-C2-N1	4.34	120.54	114.89
3	L5	4296	PSU	C4-N3-C2	-4.33	120.40	126.37
3	L5	4442	PSU	C4-N3-C2	-4.33	120.40	126.37
3	L5	1536	PSU	C4-N3-C2	-4.32	120.42	126.37
1	S2	651	PSU	C4-N3-C2	-4.31	120.43	126.37
3	L5	4423	PSU	C4-N3-C2	-4.31	120.43	126.37
1	S2	1445	PSU	C4-N3-C2	-4.31	120.43	126.37
3	L5	1534	A2M	N3-C4-N9	4.31	134.50	127.17
1	S2	866	PSU	C4-N3-C2	-4.31	120.44	126.37
1	S2	681	PSU	C4-N3-C2	-4.31	120.44	126.37
3	L5	3718	A2M	N3-C4-N9	4.31	134.49	127.17
3	L5	1779	PSU	C4-N3-C2	-4.30	120.44	126.37
1	S2	1244	PSU	C4-N3-C2	-4.30	120.44	126.37
3	L5	2415	OMU	N3-C2-N1	4.30	120.49	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	119	PSU	C4-N3-C2	-4.30	120.45	126.37
3	L5	4590	A2M	N3-C4-N9	4.30	134.48	127.17
3	L5	3627	OMG	N9-C4-N3	4.29	134.54	125.95
3	L5	1683	PSU	C4-N3-C2	-4.29	120.46	126.37
3	L5	4618	OMG	N9-C4-N3	4.29	134.53	125.95
3	L5	4500	PSU	C4-N3-C2	-4.29	120.46	126.37
1	S2	572	PSU	C4-N3-C2	-4.29	120.46	126.37
1	S2	406	PSU	C4-N3-C2	-4.29	120.46	126.37
1	S2	172	OMU	N3-C2-N1	4.29	120.47	114.89
3	L5	4293	PSU	C4-N3-C2	-4.29	120.47	126.37
3	L5	3637	PSU	C4-N3-C2	-4.28	120.47	126.37
1	S2	105	PSU	C4-N3-C2	-4.28	120.47	126.37
3	L5	3768	PSU	C4-N3-C2	-4.28	120.47	126.37
3	L5	4523	A2M	C2'-C1'-N9	-4.28	106.70	113.75
1	S2	1326	UY1	C4-N3-C2	-4.28	120.47	126.37
3	L5	2843	PSU	C4-N3-C2	-4.28	120.48	126.37
3	L5	1782	PSU	C4-N3-C2	-4.27	120.49	126.37
1	S2	1177	PSU	C4-N3-C2	-4.27	120.49	126.37
3	L5	1871	A2M	N3-C4-N9	4.27	134.43	127.17
3	L5	4498	OMU	N3-C2-N1	4.27	120.44	114.89
1	S2	1639	G7M	C8-N9-C4	4.26	117.65	107.09
1	S2	1238	PSU	C4-N3-C2	-4.26	120.50	126.37
1	S2	683	OMG	N9-C4-N3	4.26	134.47	125.95
1	S2	1692	PSU	C4-N3-C2	-4.26	120.50	126.37
1	S2	93	PSU	C4-N3-C2	-4.26	120.51	126.37
3	L5	3639	PSU	C4-N3-C2	-4.26	120.51	126.37
3	L5	3729	PSU	C4-N3-C2	-4.26	120.51	126.37
3	L5	1781	PSU	C4-N3-C2	-4.25	120.51	126.37
1	S2	686	PSU	C4-N3-C2	-4.24	120.52	126.37
3	L5	1677	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	3695	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	3785	A2M	C4-N9-C8	4.24	110.19	105.74
1	S2	863	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	3758	PSU	C4-N3-C2	-4.24	120.53	126.37
1	S2	1136	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	5001	PSU	C4-N3-C2	-4.24	120.53	126.37
1	S2	1347	PSU	C4-N3-C2	-4.23	120.54	126.37
1	S2	668	A2M	N3-C4-N9	4.23	134.35	127.17
3	L5	4521	PSU	C4-N3-C2	-4.22	120.55	126.37
1	S2	1174	PSU	C4-N3-C2	-4.22	120.55	126.37
1	S2	296	PSU	C4-N3-C2	-4.22	120.56	126.37
1	S2	1643	PSU	C4-N3-C2	-4.22	120.56	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4972	PSU	C4-N3-C2	-4.22	120.56	126.37
1	S2	354	OMU	N3-C2-N1	4.22	120.38	114.89
1	S2	1239	PSU	C4-N3-C2	-4.21	120.57	126.37
1	S2	649	PSU	C4-N3-C2	-4.21	120.57	126.37
1	S2	36	PSU	C4-N3-C2	-4.21	120.57	126.37
3	L5	1582	PSU	C4-N3-C2	-4.21	120.57	126.37
1	S2	1288	OMU	C4-N3-C2	-4.20	121.40	126.61
2	L8	55	PSU	C4-N3-C2	-4.20	120.58	126.37
3	L5	3764	PSU	C4-N3-C2	-4.20	120.59	126.37
1	S2	801	PSU	C4-N3-C2	-4.20	120.59	126.37
1	S2	1031	A2M	N3-C4-N9	4.20	134.31	127.17
3	L5	4552	PSU	C4-N3-C2	-4.19	120.60	126.37
3	L5	4403	PSU	C4-N3-C2	-4.19	120.60	126.37
3	L5	3715	PSU	C4-N3-C2	-4.19	120.60	126.37
1	S2	166	A2M	C2'-C1'-N9	-4.19	106.86	113.75
3	L5	4457	PSU	O2-C2-N1	-4.18	118.48	122.79
3	L5	5010	PSU	C4-N3-C2	-4.18	120.61	126.37
1	S2	627	OMU	N3-C2-N1	4.17	120.33	114.89
1	S2	34	PSU	C4-N3-C2	-4.17	120.62	126.37
1	S2	1367	PSU	C4-N3-C2	-4.17	120.62	126.37
81	Pt	56	PSU	C4-N3-C2	-4.17	120.62	126.37
2	L8	69	PSU	C4-N3-C2	-4.17	120.63	126.37
3	L5	4579	PSU	C4-N3-C2	-4.17	120.63	126.37
1	S2	1243	PSU	C4-N3-C2	-4.17	120.63	126.37
3	L5	3734	PSU	C4-N3-C2	-4.16	120.64	126.37
1	S2	1442	OMU	N3-C2-N1	4.16	120.31	114.89
3	L5	4312	PSU	C4-N3-C2	-4.16	120.64	126.37
1	S2	815	PSU	C4-N3-C2	-4.16	120.65	126.37
3	L5	4576	PSU	C4-N3-C2	-4.15	120.65	126.37
1	S2	1004	PSU	C4-N3-C2	-4.15	120.65	126.37
1	S2	609	PSU	C4-N3-C2	-4.15	120.65	126.37
3	L5	3853	PSU	C4-N3-C2	-4.15	120.66	126.37
1	S2	109	PSU	C4-N3-C2	-4.15	120.66	126.37
3	L5	4689	PSU	C4-N3-C2	-4.14	120.66	126.37
1	S2	822	PSU	C4-N3-C2	-4.14	120.66	126.37
81	Pt	8	4SU	C5-C4-S4	-4.14	119.58	124.31
3	L5	2364	OMG	N9-C4-N3	4.14	134.23	125.95
3	L5	4353	PSU	C4-N3-C2	-4.14	120.67	126.37
1	S2	116	OMU	N3-C2-N1	4.13	120.27	114.89
3	L5	3762	PSU	C4-N3-C2	-4.13	120.69	126.37
1	S2	354	OMU	C5-C4-N3	4.12	120.57	114.80
1	S2	1232	PSU	C4-N3-C2	-4.12	120.70	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3844	PSU	C4-N3-C2	-4.12	120.70	126.37
1	S2	1081	PSU	C4-N3-C2	-4.11	120.70	126.37
3	L5	4493	PSU	C4-N3-C2	-4.11	120.71	126.37
3	L5	3920	PSU	O2-C2-N1	-4.11	118.55	122.79
1	S2	428	OMU	N3-C2-N1	4.11	120.24	114.89
3	L5	4361	PSU	C4-N3-C2	-4.10	120.73	126.37
1	S2	1850	MA6	N3-C4-N9	4.09	134.13	127.17
1	S2	218	PSU	C4-N3-C2	-4.09	120.73	126.37
3	L5	3851	PSU	C4-N3-C2	-4.09	120.74	126.37
3	L5	4227	OMU	C5-C4-N3	4.09	120.53	114.80
1	S2	1851	MA6	C4-C5-N7	-4.09	105.91	110.58
1	S2	573	PSU	C4-N3-C2	-4.08	120.75	126.37
1	S2	468	A2M	C2'-C1'-N9	-4.08	107.04	113.75
1	S2	918	PSU	C4-N3-C2	-4.07	120.76	126.37
3	L5	1860	PSU	C4-N3-C2	-4.07	120.76	126.37
3	L5	3830	A2M	C2'-C1'-N9	-4.07	107.05	113.75
1	S2	1625	PSU	C4-N3-C2	-4.07	120.77	126.37
3	L5	4306	OMU	N3-C2-N1	4.06	120.18	114.89
3	L5	3785	A2M	O4'-C1'-N9	4.06	115.89	108.09
1	S2	1639	G7M	C1'-N9-C8	-4.04	113.08	126.74
29	SV	1	AME	CT2-CT1-N	-4.04	109.41	116.12
3	L5	3899	OMG	N9-C4-N3	4.04	134.04	125.95
3	L5	1744	PSU	C4-N3-C2	-4.04	120.81	126.37
3	L5	1316	OMG	N9-C4-N3	4.04	134.02	125.95
3	L5	4623	OMG	N9-C4-N3	4.03	134.02	125.95
81	Pt	8	4SU	N3-C2-N1	4.02	120.13	114.89
1	S2	1850	MA6	C4-C5-N7	-4.00	106.01	110.58
1	S2	966	PSU	C4-N3-C2	-4.00	120.86	126.37
3	L5	3925	OMU	C5-C4-N3	3.99	120.40	114.80
1	S2	814	PSU	C4-N3-C2	-3.99	120.88	126.37
3	L5	4306	OMU	C5-C4-N3	3.98	120.38	114.80
3	L5	4636	PSU	C4-N3-C2	-3.97	120.90	126.37
3	L5	2415	OMU	C5-C4-N3	3.97	120.36	114.80
1	S2	428	OMU	C5-C4-N3	3.96	120.35	114.80
2	L8	14	OMU	C5-C4-N3	3.95	120.34	114.80
1	S2	172	OMU	C5-C4-N3	3.95	120.34	114.80
3	L5	4628	PSU	C4-N3-C2	-3.95	120.93	126.37
3	L5	4498	OMU	C5-C4-N3	3.93	120.30	114.80
3	L5	4431	PSU	C4-N3-C2	-3.92	120.98	126.37
1	S2	1804	OMU	C5-C4-N3	3.92	120.28	114.80
3	L5	4576	PSU	O2-C2-N1	-3.91	118.75	122.79
3	L5	4420	PSU	C4-N3-C2	-3.90	120.99	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	822	PSU	O2-C2-N1	-3.90	118.76	122.79
1	S2	1442	OMU	C5-C4-N3	3.90	120.27	114.80
3	L5	2837	OMU	C5-C4-N3	3.90	120.26	114.80
3	L5	2815	A2M	C2-N3-C4	3.90	121.35	111.83
3	L5	2632	PSU	C4-N3-C2	-3.89	121.01	126.37
3	L5	4500	PSU	O2-C2-N1	-3.89	118.78	122.79
1	S2	627	OMU	C5-C4-N3	3.87	120.23	114.80
3	L5	4228	OMG	C6-C5-N7	3.87	137.34	130.29
1	S2	590	A2M	C2-N3-C4	3.87	121.28	111.83
1	S2	116	OMU	C5-C4-N3	3.86	120.21	114.80
1	S2	121	OMU	C5-C4-N3	3.86	120.21	114.80
1	S2	1288	OMU	N3-C2-N1	3.86	119.91	114.89
3	L5	4228	OMG	N9-C4-N3	3.85	133.66	125.95
1	S2	1244	PSU	O2-C2-N1	-3.84	118.83	122.79
3	L5	2787	A2M	C2-N3-C4	3.84	121.21	111.83
1	S2	1851	MA6	N3-C4-N9	3.83	133.69	127.17
3	L5	4530	UR3	C5-C4-N3	3.82	120.08	115.04
3	L5	3853	PSU	O2-C2-N1	-3.82	118.85	122.79
3	L5	3899	OMG	C6-C5-N7	3.81	137.23	130.29
3	L5	1862	PSU	O2-C2-N1	-3.81	118.86	122.79
2	L8	69	PSU	O2-C2-N1	-3.80	118.87	122.79
3	L5	3729	PSU	O2-C2-N1	-3.79	118.88	122.79
3	L5	3818	UY1	O2-C2-N1	-3.79	118.88	122.79
1	S2	1445	PSU	O2-C2-N1	-3.78	118.89	122.79
3	L5	3762	PSU	O2-C2-N1	-3.78	118.89	122.79
3	L5	1582	PSU	O2-C2-N1	-3.78	118.89	122.79
38	LA	216	V5N	CD2-CG-ND1	3.76	110.82	105.76
1	S2	484	A2M	C2-N3-C4	3.75	120.99	111.83
1	S2	512	A2M	C2-N3-C4	3.75	120.99	111.83
3	L5	4590	A2M	C2-N3-C4	3.75	120.98	111.83
1	S2	27	A2M	C2-N3-C4	3.73	120.94	111.83
3	L5	398	A2M	C2-N3-C4	3.73	120.94	111.83
3	L5	2401	A2M	C2-N3-C4	3.73	120.93	111.83
3	L5	4620	OMU	C5-C4-N3	3.72	120.02	114.80
1	S2	1678	A2M	C2-N3-C4	3.72	120.92	111.83
3	L5	3768	PSU	O2-C2-N1	-3.72	118.95	122.79
3	L5	4623	OMG	C6-C5-N7	3.72	137.05	130.29
3	L5	4579	PSU	O2-C2-N1	-3.71	118.96	122.79
3	L5	4403	PSU	O2-C2-N1	-3.71	118.96	122.79
3	L5	3825	A2M	C2-N3-C4	3.71	120.88	111.83
1	S2	1639	G7M	CN7-N7-C5	3.71	131.42	126.80
3	L5	3844	PSU	O2-C2-N1	-3.70	118.97	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3715	PSU	O2-C2-N1	-3.69	118.98	122.79
1	S2	686	PSU	O2-C2-N1	-3.69	118.98	122.79
1	S2	649	PSU	O2-C2-N1	-3.69	118.98	122.79
3	L5	4220	6MZ	C2-N3-C4	3.69	120.85	111.83
1	S2	1832	6MZ	C4-C5-N7	-3.69	106.36	110.58
1	S2	1288	OMU	C5-C4-N3	3.69	119.96	114.80
3	L5	3760	A2M	C2-N3-C4	3.69	120.83	111.83
3	L5	3782	5MC	C5-C6-N1	-3.68	119.31	123.31
3	L5	3724	A2M	C2-N3-C4	3.68	120.82	111.83
1	S2	1383	A2M	C2-N3-C4	3.68	120.82	111.83
1	S2	609	PSU	O2-C2-N1	-3.68	118.99	122.79
1	S2	166	A2M	C2-N3-C4	3.68	120.82	111.83
3	L5	3764	PSU	O2-C2-N1	-3.68	118.99	122.79
1	S2	468	A2M	C2-N3-C4	3.68	120.82	111.83
3	L5	3734	PSU	O2-C2-N1	-3.68	119.00	122.79
81	Pt	56	PSU	O2-C2-N1	-3.68	119.00	122.79
3	L5	3723	A2M	C2-N3-C4	3.67	120.80	111.83
1	S2	1232	PSU	O2-C2-N1	-3.67	119.00	122.79
1	S2	863	PSU	O2-C2-N1	-3.66	119.01	122.79
1	S2	99	A2M	C2-N3-C4	3.66	120.78	111.83
1	S2	159	A2M	C2-N3-C4	3.66	120.77	111.83
3	L5	1683	PSU	O2-C2-N1	-3.66	119.01	122.79
1	S2	1851	MA6	C2-N3-C4	3.66	120.76	111.83
3	L5	3785	A2M	N3-C2-N1	-3.65	123.05	128.58
3	L5	2787	A2M	C4-C5-N7	-3.65	106.41	110.58
1	S2	1243	PSU	O2-C2-N1	-3.65	119.02	122.79
1	S2	576	A2M	C2-N3-C4	3.65	120.75	111.83
3	L5	4571	A2M	C2-N3-C4	3.65	120.75	111.83
1	S2	119	PSU	O2-C2-N1	-3.65	119.03	122.79
3	L5	4420	PSU	O2-C2-N1	-3.65	119.03	122.79
1	S2	918	PSU	O2-C2-N1	-3.65	119.03	122.79
3	L5	2363	A2M	C2-N3-C4	3.65	120.74	111.83
1	S2	36	PSU	O2-C2-N1	-3.64	119.03	122.79
3	L5	4423	PSU	O2-C2-N1	-3.64	119.03	122.79
3	L5	4628	PSU	O2-C2-N1	-3.64	119.03	122.79
3	L5	4552	PSU	O2-C2-N1	-3.64	119.04	122.79
3	L5	4296	PSU	O2-C2-N1	-3.63	119.04	122.79
3	L5	3884	PSU	C4-N3-C2	-3.63	121.37	126.37
3	L5	3867	A2M	C2-N3-C4	3.63	120.69	111.83
1	S2	668	A2M	C2-N3-C4	3.62	120.68	111.83
1	S2	1004	PSU	O2-C2-N1	-3.62	119.06	122.79
3	L5	1779	PSU	O2-C2-N1	-3.62	119.06	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	34	PSU	O2-C2-N1	-3.61	119.06	122.79
1	S2	1692	PSU	O2-C2-N1	-3.61	119.07	122.79
3	L5	4523	A2M	C2-N3-C4	3.61	120.64	111.83
1	S2	109	PSU	O2-C2-N1	-3.59	119.08	122.79
3	L5	4361	PSU	O2-C2-N1	-3.59	119.08	122.79
1	S2	1238	PSU	O2-C2-N1	-3.59	119.09	122.79
3	L5	400	A2M	C2-N3-C4	3.59	120.60	111.83
3	L5	4673	PSU	O2-C2-N1	-3.59	119.09	122.79
3	L5	4590	A2M	N3-C2-N1	-3.59	123.16	128.58
1	S2	1347	PSU	O2-C2-N1	-3.58	119.09	122.79
1	S2	1832	6MZ	C6-C5-N7	3.58	136.33	132.43
3	L5	1871	A2M	C2-N3-C4	3.58	120.58	111.83
3	L5	1534	A2M	C2-N3-C4	3.58	120.57	111.83
3	L5	4521	PSU	O2-C2-N1	-3.57	119.10	122.79
1	S2	866	PSU	O2-C2-N1	-3.57	119.11	122.79
1	S2	576	A2M	C4-C5-N7	-3.57	106.50	110.58
3	L5	4618	OMG	C6-C5-N7	3.57	136.79	130.29
3	L5	3830	A2M	C2-N3-C4	3.57	120.55	111.83
3	L5	5010	PSU	O2-C2-N1	-3.57	119.11	122.79
1	S2	1031	A2M	C2-N3-C4	3.57	120.54	111.83
1	S2	159	A2M	C4-C5-N7	-3.57	106.50	110.58
1	S2	1326	UY1	O2-C2-N1	-3.57	119.11	122.79
3	L5	3627	OMG	C6-C5-N7	3.57	136.78	130.29
1	S2	815	PSU	O2-C2-N1	-3.57	119.11	122.79
1	S2	1851	MA6	N1-C2-N3	-3.56	123.19	128.58
1	S2	296	PSU	O2-C2-N1	-3.56	119.12	122.79
1	S2	1643	PSU	O2-C2-N1	-3.56	119.12	122.79
3	L5	4442	PSU	O2-C2-N1	-3.56	119.12	122.79
3	L5	398	A2M	C4-C5-N7	-3.56	106.52	110.58
3	L5	1534	A2M	C4-C5-N7	-3.55	106.52	110.58
3	L5	3851	PSU	O2-C2-N1	-3.55	119.13	122.79
1	S2	1031	A2M	C4-C5-N7	-3.54	106.53	110.58
1	S2	573	PSU	O2-C2-N1	-3.54	119.13	122.79
3	L5	4293	PSU	O2-C2-N1	-3.54	119.13	122.79
1	S2	1850	MA6	C2-N3-C4	3.54	120.47	111.83
1	S2	1031	A2M	N3-C2-N1	-3.54	123.23	128.58
1	S2	572	PSU	O2-C2-N1	-3.54	119.14	122.79
1	S2	1367	PSU	O2-C2-N1	-3.53	119.15	122.79
3	L5	3825	A2M	C4-C5-N7	-3.53	106.55	110.58
1	S2	166	A2M	C4-C5-N7	-3.52	106.55	110.58
1	S2	651	PSU	O2-C2-N1	-3.52	119.16	122.79
3	L5	4689	PSU	O2-C2-N1	-3.52	119.16	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1832	6MZ	C2-N3-C4	3.52	120.43	111.83
1	S2	1239	PSU	O2-C2-N1	-3.51	119.17	122.79
3	L5	1871	A2M	N3-C2-N1	-3.51	123.27	128.58
3	L5	1524	A2M	C4-C5-N7	-3.51	106.57	110.58
1	S2	1056	PSU	O2-C2-N1	-3.51	119.17	122.79
1	S2	93	PSU	O2-C2-N1	-3.50	119.17	122.79
3	L5	4312	PSU	O2-C2-N1	-3.50	119.17	122.79
3	L5	1792	PSU	O2-C2-N1	-3.50	119.17	122.79
1	S2	668	A2M	N3-C2-N1	-3.50	123.28	128.58
3	L5	2815	A2M	C4-C5-N7	-3.50	106.58	110.58
3	L5	3785	A2M	C2-N3-C4	3.50	120.38	111.83
1	S2	99	A2M	C4-C5-N7	-3.50	106.58	110.58
1	S2	468	A2M	C4-C5-N7	-3.50	106.58	110.58
3	L5	1860	PSU	O2-C2-N1	-3.50	119.18	122.79
3	L5	3830	A2M	C4-C5-N7	-3.49	106.59	110.58
3	L5	400	A2M	C4-C5-N7	-3.49	106.59	110.58
1	S2	683	OMG	C6-C5-N7	3.49	136.63	130.29
3	L5	1677	PSU	O2-C2-N1	-3.48	119.19	122.79
1	S2	218	PSU	O2-C2-N1	-3.48	119.20	122.79
1	S2	1248	B8N	N3-C2-N1	3.48	120.97	116.72
3	L5	1524	A2M	C2-N3-C4	3.48	120.33	111.83
1	S2	1625	PSU	O2-C2-N1	-3.48	119.20	122.79
3	L5	4590	A2M	C4-C5-N7	-3.47	106.61	110.58
3	L5	2401	A2M	C4-C5-N7	-3.47	106.61	110.58
3	L5	4431	PSU	O2-C2-N1	-3.47	119.21	122.79
3	L5	2839	PSU	O2-C2-N1	-3.47	119.21	122.79
3	L5	1781	PSU	O2-C2-N1	-3.47	119.21	122.79
3	L5	3770	PSU	O2-C2-N1	-3.47	119.22	122.79
3	L5	1316	OMG	C6-C5-N7	3.46	136.59	130.29
1	S2	1136	PSU	O2-C2-N1	-3.46	119.22	122.79
1	S2	484	A2M	C4-C5-N7	-3.46	106.62	110.58
1	S2	512	A2M	N3-C2-N1	-3.46	123.34	128.58
1	S2	1177	PSU	O2-C2-N1	-3.46	119.22	122.79
3	L5	1326	A2M	C4-C5-N7	-3.46	106.63	110.58
3	L5	1782	PSU	O2-C2-N1	-3.45	119.23	122.79
1	S2	105	PSU	O2-C2-N1	-3.45	119.23	122.79
3	L5	1326	A2M	C2-N3-C4	3.45	120.25	111.83
1	S2	668	A2M	C4-C5-N7	-3.45	106.64	110.58
3	L5	3723	A2M	C4-C5-N7	-3.44	106.65	110.58
1	S2	966	PSU	O2-C2-N1	-3.44	119.24	122.79
3	L5	3758	PSU	O2-C2-N1	-3.44	119.24	122.79
1	S2	590	A2M	C4-C5-N7	-3.44	106.65	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2632	PSU	O2-C2-N1	-3.44	119.24	122.79
3	L5	3718	A2M	C4-C5-N7	-3.43	106.66	110.58
3	L5	4499	OMG	C6-C5-N7	3.43	136.54	130.29
3	L5	4636	PSU	O2-C2-N1	-3.43	119.25	122.79
3	L5	3724	A2M	C4-C5-N7	-3.43	106.66	110.58
3	L5	3718	A2M	C2-N3-C4	3.43	120.20	111.83
1	S2	1678	A2M	C4-C5-N7	-3.41	106.68	110.58
1	S2	406	PSU	O2-C2-N1	-3.41	119.27	122.79
1	S2	1850	MA6	N1-C2-N3	-3.41	123.42	128.58
3	L5	4220	6MZ	N1-C2-N3	-3.40	123.43	128.58
1	S2	1383	A2M	C4-C5-N7	-3.40	106.69	110.58
3	L5	2364	OMG	C6-C5-N7	3.40	136.48	130.29
3	L5	2363	A2M	C4-C5-N7	-3.40	106.70	110.58
3	L5	1522	OMG	C6-C5-N7	3.40	136.47	130.29
2	L8	75	OMG	C6-C5-N7	3.39	136.46	130.29
3	L5	1536	PSU	O2-C2-N1	-3.39	119.29	122.79
3	L5	4493	PSU	O2-C2-N1	-3.38	119.30	122.79
3	L5	4392	OMG	C6-C5-N7	3.38	136.45	130.29
1	S2	814	PSU	O2-C2-N1	-3.38	119.30	122.79
3	L5	3867	A2M	N3-C2-N1	-3.36	123.49	128.58
3	L5	3639	PSU	O2-C2-N1	-3.36	119.32	122.79
3	L5	4571	A2M	C4-C5-N7	-3.35	106.75	110.58
1	S2	801	PSU	O2-C2-N1	-3.35	119.34	122.79
3	L5	4972	PSU	O2-C2-N1	-3.34	119.34	122.79
1	S2	436	OMG	C6-C5-N7	3.34	136.38	130.29
3	L5	4370	OMG	C6-C5-N7	3.34	136.37	130.29
3	L5	2508	PSU	O2-C2-N1	-3.34	119.34	122.79
3	L5	3867	A2M	C4-C5-N7	-3.34	106.76	110.58
1	S2	1832	6MZ	N1-C2-N3	-3.34	123.53	128.58
1	S2	1337	4AC	N4-C4-N3	3.34	119.28	113.87
3	L5	3760	A2M	C4-C5-N7	-3.34	106.77	110.58
3	L5	3944	OMG	C6-C5-N7	3.33	136.35	130.29
1	S2	1383	A2M	N3-C2-N1	-3.33	123.54	128.58
1	S2	1174	PSU	O2-C2-N1	-3.32	119.36	122.79
1	S2	27	A2M	C4-C5-N7	-3.32	106.79	110.58
3	L5	3744	OMG	C6-C5-N7	3.32	136.33	130.29
3	L5	4523	A2M	N3-C2-N1	-3.31	123.57	128.58
1	S2	512	A2M	C4-C5-N7	-3.31	106.80	110.58
3	L5	398	A2M	N3-C2-N1	-3.29	123.59	128.58
1	S2	166	A2M	N3-C2-N1	-3.29	123.60	128.58
1	S2	1031	A2M	C2'-C1'-N9	-3.28	108.35	113.75
1	S2	867	OMG	C6-C5-N7	3.27	136.25	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4523	A2M	C4-C5-N7	-3.27	106.85	110.58
3	L5	4637	OMG	C6-C5-N7	3.27	136.23	130.29
1	S2	1248	B8N	C31-N3-C4	3.26	121.80	117.18
3	L5	4569	PSU	O2-C2-N1	-3.26	119.42	122.79
1	S2	1678	A2M	N3-C2-N1	-3.26	123.64	128.58
1	S2	1328	OMG	C6-C5-N7	3.26	136.22	130.29
3	L5	2815	A2M	N3-C2-N1	-3.26	123.65	128.58
1	S2	468	A2M	N3-C2-N1	-3.25	123.66	128.58
49	La	39	V5N	CD2-CG-ND1	3.25	110.14	105.76
3	L5	1744	PSU	O2-C2-N1	-3.25	119.44	122.79
1	S2	1081	PSU	O2-C2-N1	-3.25	119.44	122.79
3	L5	4353	PSU	O2-C2-N1	-3.25	119.44	122.79
3	L5	3695	PSU	O2-C2-N1	-3.24	119.44	122.79
3	L5	3825	A2M	N3-C2-N1	-3.24	123.67	128.58
3	L5	4571	A2M	N3-C2-N1	-3.24	123.67	128.58
3	L5	2787	A2M	N3-C2-N1	-3.24	123.67	128.58
1	S2	27	A2M	N3-C2-N1	-3.24	123.68	128.58
3	L5	1534	A2M	N3-C2-N1	-3.23	123.69	128.58
3	L5	1322	1MA	N9-C4-N3	3.23	134.25	126.90
3	L5	4471	PSU	O2-C2-N1	-3.22	119.47	122.79
63	Lr	2	SAC	C2A-C1A-N	-3.21	110.79	116.12
3	L5	3724	A2M	N3-C2-N1	-3.21	123.72	128.58
1	S2	576	A2M	N3-C2-N1	-3.21	123.73	128.58
1	S2	644	OMG	C6-C5-N7	3.21	136.12	130.29
1	S2	484	A2M	N3-C2-N1	-3.20	123.74	128.58
1	S2	601	OMG	C6-C5-N7	3.20	136.11	130.29
1	S2	590	A2M	N3-C2-N1	-3.19	123.75	128.58
2	L8	55	PSU	O2-C2-N1	-3.19	119.50	122.79
1	S2	159	A2M	C2'-C1'-N9	-3.19	108.51	113.75
3	L5	3723	A2M	N3-C2-N1	-3.19	123.76	128.58
3	L5	2363	A2M	N3-C2-N1	-3.18	123.77	128.58
1	S2	462	OMC	C2'-C1'-N1	-3.18	108.21	114.24
3	L5	3760	A2M	N3-C2-N1	-3.18	123.77	128.58
1	S2	1490	OMG	C6-C5-N7	3.17	136.06	130.29
1	S2	116	OMU	O4-C4-C5	-3.17	119.70	125.16
1	S2	681	PSU	O2-C2-N1	-3.17	119.52	122.79
3	L5	4299	PSU	O2-C2-N1	-3.16	119.53	122.79
1	S2	1288	OMU	C1'-N1-C2	3.16	123.26	117.59
1	S2	428	OMU	O4-C4-C5	-3.14	119.75	125.16
3	L5	4196	OMG	C6-C5-N7	3.14	136.00	130.29
1	S2	1442	OMU	O4-C4-C5	-3.13	119.76	125.16
3	L5	2401	A2M	N3-C2-N1	-3.13	123.84	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5001	PSU	O2-C2-N1	-3.13	119.56	122.79
3	L5	4220	6MZ	C4-C5-N7	-3.10	107.03	110.58
1	S2	159	A2M	N3-C2-N1	-3.10	123.89	128.58
1	S2	121	OMU	O4-C4-C5	-3.10	119.81	125.16
3	L5	4494	OMG	C6-C5-N7	3.09	135.92	130.29
1	S2	1447	OMG	C6-C5-N7	3.09	135.91	130.29
1	S2	627	OMU	O4-C4-C5	-3.09	119.83	125.16
1	S2	99	A2M	N3-C2-N1	-3.08	123.92	128.58
3	L5	1871	A2M	C4-C5-N7	-3.07	107.08	110.58
3	L5	400	A2M	N3-C2-N1	-3.07	123.94	128.58
3	L5	1524	A2M	N3-C2-N1	-3.07	123.94	128.58
1	S2	354	OMU	O4-C4-C5	-3.06	119.88	125.16
1	S2	1850	MA6	C4-N9-C8	3.06	108.95	105.74
1	S2	509	OMG	C6-C5-N7	3.05	135.84	130.29
3	L5	3830	A2M	N3-C2-N1	-3.04	123.97	128.58
3	L5	4498	OMU	O4-C4-C5	-3.04	119.91	125.16
3	L5	2876	OMG	C6-C5-N7	3.04	135.82	130.29
3	L5	3867	A2M	C4-N9-C8	3.03	108.92	105.74
3	L5	1625	OMG	C6-C5-N7	3.01	135.77	130.29
1	S2	172	OMU	O4-C4-C5	-3.01	119.98	125.16
1	S2	1842	4AC	C6-C5-C4	3.00	120.61	117.00
3	L5	4227	OMU	O4-C4-C5	-2.99	120.00	125.16
1	S2	99	A2M	C2'-C1'-N9	-2.99	108.83	113.75
1	S2	1804	OMU	O4-C4-C5	-2.99	120.01	125.16
1	S2	668	A2M	C4-N9-C8	2.99	108.87	105.74
1	S2	484	A2M	C2'-C1'-N9	-2.97	108.87	113.75
3	L5	2415	OMU	O4-C4-C5	-2.96	120.05	125.16
3	L5	2363	A2M	C4-N9-C8	2.96	108.84	105.74
3	L5	2424	OMG	C6-C5-N7	2.96	135.67	130.29
1	S2	1288	OMU	O4-C4-C5	-2.95	120.08	125.16
3	L5	4220	6MZ	C6-C5-N7	2.95	135.64	132.43
1	S2	1851	MA6	C4-N9-C8	2.94	108.83	105.74
3	L5	4590	A2M	C2'-C1'-N9	-2.93	108.92	113.75
3	L5	3792	OMG	C6-C5-N7	2.93	135.62	130.29
3	L5	1326	A2M	N3-C2-N1	-2.90	124.19	128.58
3	L5	3718	A2M	C2'-C1'-N9	-2.89	108.99	113.75
3	L5	1524	A2M	C4-N9-C8	2.89	108.77	105.74
3	L5	398	A2M	C2'-C1'-N9	-2.88	109.01	113.75
1	S2	1850	MA6	C5-N7-C8	2.86	107.95	103.45
1	S2	1851	MA6	C5-N7-C8	2.86	107.95	103.45
3	L5	4306	OMU	O4-C4-C5	-2.83	120.28	125.16
1	S2	468	A2M	C4-N9-C8	2.81	108.69	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4220	6MZ	C4-N9-C8	2.80	108.68	105.74
3	L5	2837	OMU	O4-C4-C5	-2.78	120.37	125.16
3	L5	4620	OMU	O4-C4-C5	-2.74	120.44	125.16
3	L5	2843	PSU	O2-C2-N1	-2.73	119.97	122.79
3	L5	2401	A2M	C2'-C1'-N9	-2.73	109.25	113.75
3	L5	4571	A2M	C4-N9-C8	2.73	108.60	105.74
1	S2	1031	A2M	C4-N9-C8	2.73	108.60	105.74
1	S2	27	A2M	C4-N9-C8	2.72	108.59	105.74
3	L5	4623	OMG	C4-C5-N7	-2.72	106.37	110.67
49	La	39	V5N	O-C-CA	-2.71	117.79	124.77
3	L5	3782	5MC	C5-C4-N3	-2.71	118.98	121.75
1	S2	512	A2M	C4-N9-C8	2.71	108.58	105.74
3	L5	3637	PSU	O2-C2-N1	-2.71	120.00	122.79
1	S2	1678	A2M	C4-N9-C8	2.70	108.58	105.74
3	L5	3825	A2M	C4-N9-C8	2.70	108.58	105.74
3	L5	3884	PSU	O2-C2-N1	-2.70	120.00	122.79
1	S2	166	A2M	C4-N9-C8	2.69	108.57	105.74
1	S2	1832	6MZ	C4-N9-C8	2.69	108.57	105.74
3	L5	4523	A2M	C4-N9-C8	2.69	108.57	105.74
1	S2	576	A2M	C4-N9-C8	2.69	108.56	105.74
3	L5	2837	OMU	O2-C2-N1	-2.69	119.30	122.80
1	S2	1383	A2M	C4-N9-C8	2.67	108.54	105.74
3	L5	4392	OMG	C4-C5-N7	-2.67	106.44	110.67
3	L5	2787	A2M	C5-N7-C8	2.66	107.63	103.45
3	L5	3925	OMU	O2-C2-N1	-2.66	119.33	122.80
3	L5	3785	A2M	N9-C8-N7	-2.66	110.17	113.94
3	L5	3718	A2M	N3-C2-N1	-2.65	124.56	128.58
1	S2	1851	MA6	C6-C5-N7	2.64	137.65	133.43
1	S2	1832	6MZ	C5-N7-C8	2.64	107.60	103.45
3	L5	4590	A2M	C4-N9-C8	2.64	108.51	105.74
1	S2	644	OMG	C4-C5-N7	-2.63	106.50	110.67
3	L5	3925	OMU	O4-C4-C5	-2.63	120.62	125.16
1	S2	1842	4AC	C5-C4-N3	-2.63	118.48	122.60
3	L5	3825	A2M	C5-N7-C8	2.63	107.59	103.45
1	S2	1639	G7M	O6-C6-C5	-2.63	122.15	128.01
3	L5	3899	OMG	C4-C5-N7	-2.62	106.52	110.67
3	L5	3723	A2M	C4-N9-C8	2.61	108.48	105.74
3	L5	1326	A2M	C4-N9-C8	2.61	108.47	105.74
1	S2	1328	OMG	C4-C5-N7	-2.61	106.54	110.67
3	L5	4499	OMG	C4-C5-N7	-2.60	106.54	110.67
3	L5	2401	A2M	C4-N9-C8	2.60	108.47	105.74
3	L5	2401	A2M	C5-N7-C8	2.60	107.54	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3760	A2M	C4-N9-C8	2.60	108.47	105.74
3	L5	4220	6MZ	C9-N6-C6	-2.60	120.44	122.85
3	L5	4228	OMG	C4-C5-N7	-2.60	106.55	110.67
20	SX	62	HY3	C4-C3-CA	2.60	105.34	102.51
3	L5	1871	A2M	C4-N9-C8	2.60	108.47	105.74
1	S2	1447	OMG	C4-C5-N7	-2.60	106.56	110.67
3	L5	3724	A2M	C4-N9-C8	2.60	108.46	105.74
3	L5	400	A2M	C4-N9-C8	2.59	108.46	105.74
3	L5	4370	OMG	C4-C5-N7	-2.59	106.56	110.67
1	S2	683	OMG	C4-C5-N7	-2.59	106.56	110.67
3	L5	1534	A2M	C5-N7-C8	2.59	107.52	103.45
3	L5	3627	OMG	C4-C5-N7	-2.59	106.57	110.67
1	S2	166	A2M	C5-N7-C8	2.59	107.51	103.45
3	L5	4498	OMU	O2-C2-N1	-2.58	119.44	122.80
3	L5	4531	PSU	C5-C6-N1	-2.57	118.57	122.14
3	L5	3785	A2M	C4-C5-N7	-2.57	107.64	110.58
3	L5	1534	A2M	C4-N9-C8	2.57	108.44	105.74
1	S2	1842	4AC	N4-C4-N3	2.56	118.03	113.87
3	L5	3744	OMG	C4-C5-N7	-2.56	106.61	110.67
1	S2	601	OMG	C4-C5-N7	-2.56	106.62	110.67
3	L5	3944	OMG	C4-C5-N7	-2.55	106.62	110.67
3	L5	1522	OMG	O6-C6-C5	-2.55	119.79	126.53
1	S2	99	A2M	C5-N7-C8	2.55	107.46	103.45
3	L5	3867	A2M	C5-N7-C8	2.55	107.46	103.45
1	S2	436	OMG	C4-C5-N7	-2.55	106.63	110.67
3	L5	1524	A2M	C5-N7-C8	2.55	107.45	103.45
1	S2	576	A2M	C5-N7-C8	2.54	107.45	103.45
3	L5	398	A2M	C5-N7-C8	2.54	107.45	103.45
3	L5	1326	A2M	C5-N7-C8	2.54	107.45	103.45
1	S2	1383	A2M	C5-N7-C8	2.54	107.44	103.45
1	S2	867	OMG	C4-C5-N7	-2.54	106.64	110.67
1	S2	509	OMG	C4-C5-N7	-2.54	106.65	110.67
3	L5	2815	A2M	C5-N7-C8	2.53	107.43	103.45
1	S2	468	A2M	C5-N7-C8	2.53	107.43	103.45
3	L5	400	A2M	C5-N7-C8	2.53	107.42	103.45
1	S2	1678	A2M	C5-N7-C8	2.53	107.42	103.45
39	LB	245	HIC	NE2-CE1-ND1	-2.52	111.70	112.66
2	L8	14	OMU	O4-C4-C5	-2.52	120.81	125.16
3	L5	3830	A2M	C5-N7-C8	2.52	107.41	103.45
3	L5	3818	UY1	C5-C6-N1	-2.52	118.65	122.14
1	S2	668	A2M	C5-N7-C8	2.52	107.40	103.45
3	L5	1316	OMG	C4-C5-N7	-2.52	106.68	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	159	A2M	C5-N7-C8	2.51	107.40	103.45
3	L5	2815	A2M	C4-N9-C8	2.51	108.37	105.74
1	S2	590	A2M	C5-N7-C8	2.51	107.39	103.45
3	L5	4618	OMG	C4-C5-N7	-2.50	106.70	110.67
1	S2	27	A2M	C5-N7-C8	2.50	107.38	103.45
2	L8	14	OMU	O2-C2-N1	-2.50	119.54	122.80
3	L5	2363	A2M	C5-N7-C8	2.50	107.38	103.45
3	L5	3825	A2M	C2'-C1'-N9	-2.50	109.64	113.75
3	L5	3724	A2M	C5-N7-C8	2.50	107.37	103.45
3	L5	2364	OMG	C4-C5-N7	-2.49	106.72	110.67
3	L5	4590	A2M	C5-N7-C8	2.49	107.36	103.45
3	L5	4620	OMU	O2-C2-N1	-2.49	119.56	122.80
1	S2	484	A2M	C5-N7-C8	2.48	107.36	103.45
1	S2	1031	A2M	C2-N1-C6	2.48	122.81	118.73
3	L5	2424	OMG	C4-C5-N7	-2.48	106.74	110.67
1	S2	116	OMU	O2-C2-N1	-2.47	119.58	122.80
3	L5	3830	A2M	C4-N9-C8	2.47	108.34	105.74
3	L5	4447	5MC	C5-C4-N3	-2.47	119.22	121.75
1	S2	99	A2M	C4-N9-C8	2.47	108.33	105.74
3	L5	4531	PSU	O2-C2-N1	-2.47	120.24	122.79
3	L5	4637	OMG	C4-C5-N7	-2.46	106.77	110.67
2	L8	75	OMG	C4-C5-N7	-2.46	106.77	110.67
1	S2	1031	A2M	C5-N7-C8	2.46	107.31	103.45
3	L5	3723	A2M	C5-N7-C8	2.45	107.31	103.45
1	S2	512	A2M	C5-N7-C8	2.44	107.29	103.45
3	L5	2351	OMC	O2-C2-N3	-2.44	118.48	122.33
3	L5	4571	A2M	C5-N7-C8	2.43	107.27	103.45
3	L5	398	A2M	C4-N9-C8	2.43	108.29	105.74
3	L5	3627	OMG	O6-C6-C5	-2.43	120.12	126.53
3	L5	3760	A2M	C5-N7-C8	2.43	107.26	103.45
1	S2	1490	OMG	C4-C5-N7	-2.42	106.84	110.67
3	L5	2839	PSU	C5-C6-N1	-2.41	118.80	122.14
81	Pt	21	H2U	C5-C6-N1	-2.41	104.24	111.52
3	L5	3637	PSU	O2-C2-N3	-2.40	117.59	121.86
1	S2	172	OMU	O2-C2-N1	-2.40	119.67	122.80
3	L5	4523	A2M	C5-N7-C8	2.40	107.22	103.45
3	L5	2508	PSU	C5-C6-N1	-2.39	118.82	122.14
1	S2	627	OMU	O2-C2-N1	-2.39	119.69	122.80
1	S2	121	OMU	O2-C2-N1	-2.39	119.69	122.80
1	S2	428	OMU	O2-C2-N1	-2.38	119.69	122.80
3	L5	1322	1MA	C6-C5-N7	2.38	136.37	132.16
1	S2	1804	OMU	O2-C2-N1	-2.37	119.71	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4494	OMG	O6-C6-C5	-2.37	120.28	126.53
1	S2	1337	4AC	C6-C5-C4	2.37	119.85	117.00
1	S2	1851	MA6	N9-C8-N7	-2.37	110.58	113.94
3	L5	4532	PSU	C6-N1-C2	-2.37	120.50	122.69
3	L5	4494	OMG	C4-C5-N7	-2.36	106.92	110.67
3	L5	4471	PSU	C5-C6-N1	-2.36	118.86	122.14
3	L5	3792	OMG	C4-C5-N7	-2.36	106.94	110.67
3	L5	2843	PSU	C5-C6-N1	-2.34	118.89	122.14
1	S2	159	A2M	C4-N9-C8	2.34	108.20	105.74
3	L5	1522	OMG	C4-C5-N7	-2.34	106.96	110.67
3	L5	1625	OMG	C4-C5-N7	-2.33	106.97	110.67
1	S2	1445	PSU	C5-C6-N1	-2.33	118.90	122.14
1	S2	1248	B8N	O36-C34-O35	-2.33	118.79	124.08
1	S2	1850	MA6	C6-C5-N7	2.33	137.16	133.43
3	L5	2876	OMG	C4-C5-N7	-2.33	106.98	110.67
3	L5	4227	OMU	O2-C2-N1	-2.33	119.77	122.80
3	L5	4590	A2M	C6-C5-N7	2.33	136.57	132.09
3	L5	4530	UR3	C3U-N3-C4	2.32	121.09	117.87
1	S2	1031	A2M	C6-C5-N7	2.32	136.57	132.09
3	L5	4220	6MZ	C5-N7-C8	2.32	107.09	103.45
1	S2	681	PSU	C5-C6-N1	-2.32	118.92	122.14
39	LB	245	HIC	CB-CG-CD2	-2.31	124.38	129.96
2	L8	69	PSU	O4'-C1'-C2'	2.31	108.35	105.15
1	S2	668	A2M	C6-C5-N7	2.31	136.55	132.09
3	L5	3695	PSU	C5-C6-N1	-2.31	118.94	122.14
1	S2	27	A2M	C2'-C1'-N9	-2.31	109.95	113.75
1	S2	1177	PSU	C5-C6-N1	-2.31	118.94	122.14
3	L5	3792	OMG	O6-C6-C5	-2.31	120.45	126.53
3	L5	4196	OMG	C4-C5-N7	-2.31	107.02	110.67
3	L5	3770	PSU	C5-C6-N1	-2.30	118.94	122.14
3	L5	1522	OMG	C2'-C1'-N9	-2.30	109.87	114.24
3	L5	1322	1MA	C4-C5-N7	-2.30	107.03	110.67
3	L5	3920	PSU	C5-C6-N1	-2.29	118.95	122.14
1	S2	484	A2M	C4-N9-C8	2.29	108.14	105.74
1	S2	1326	UY1	C5-C6-N1	-2.28	118.97	122.14
3	L5	4403	PSU	O4'-C1'-C2'	2.28	108.31	105.15
3	L5	3785	A2M	C5-N7-C8	2.28	107.04	103.45
1	S2	801	PSU	C5-C6-N1	-2.28	118.97	122.14
1	S2	822	PSU	O4'-C1'-C2'	2.28	108.31	105.15
1	S2	572	PSU	C5-C6-N1	-2.27	118.98	122.14
3	L5	4637	OMG	O6-C6-C5	-2.27	120.54	126.53
1	S2	590	A2M	C4-N9-C8	2.27	108.12	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1850	MA6	N9-C8-N7	-2.27	110.72	113.94
3	L5	3637	PSU	C5-C6-N1	-2.27	119.00	122.14
1	S2	1832	6MZ	C2-N1-C6	2.26	122.74	115.24
1	S2	1643	PSU	C5-C6-N1	-2.26	119.00	122.14
3	L5	1862	PSU	C5-C6-N1	-2.26	119.00	122.14
3	L5	4423	PSU	C5-C6-N1	-2.26	119.00	122.14
3	L5	4442	PSU	C5-C6-N1	-2.25	119.01	122.14
3	L5	1792	PSU	C5-C6-N1	-2.25	119.02	122.14
1	S2	1238	PSU	C5-C6-N1	-2.24	119.03	122.14
1	S2	119	PSU	C5-C6-N1	-2.24	119.03	122.14
3	L5	1871	A2M	C5-N7-C8	2.24	106.97	103.45
3	L5	3899	OMG	C2'-C1'-N9	-2.24	109.99	114.24
3	L5	3770	PSU	C3'-C2'-C1'	2.24	104.33	101.69
1	S2	651	PSU	C5-C6-N1	-2.23	119.04	122.14
1	S2	1248	B8N	C1'-C5-C4	2.23	120.99	117.61
1	S2	105	PSU	C5-C6-N1	-2.23	119.05	122.14
3	L5	3723	A2M	C2'-C1'-N9	-2.23	110.09	113.75
3	L5	4196	OMG	O6-C6-C5	-2.22	120.66	126.53
1	S2	668	A2M	N9-C8-N7	-2.22	110.78	113.94
1	S2	1056	PSU	C5-C6-N1	-2.22	119.06	122.14
1	S2	1490	OMG	O6-C6-C5	-2.21	120.69	126.53
3	L5	4569	PSU	C5-C6-N1	-2.21	119.07	122.14
1	S2	354	OMU	O2-C2-N1	-2.21	119.92	122.80
3	L5	1625	OMG	O6-C6-C5	-2.21	120.70	126.53
3	L5	4531	PSU	O2-C2-N3	-2.21	117.94	121.86
2	L8	55	PSU	C5-C6-N1	-2.20	119.08	122.14
3	L5	4521	PSU	C5-C6-N1	-2.20	119.08	122.14
3	L5	3718	A2M	C5-N7-C8	2.20	106.91	103.45
1	S2	1136	PSU	C5-C6-N1	-2.20	119.08	122.14
1	S2	576	A2M	C6-C5-N7	2.20	136.34	132.09
38	LA	216	V5N	O-C-CA	-2.20	119.11	124.77
1	S2	166	A2M	C6-C5-N7	2.20	136.33	132.09
3	L5	4623	OMG	O6-C6-C5	-2.19	120.74	126.53
2	L8	75	OMG	O6-C6-C5	-2.19	120.74	126.53
3	L5	4353	PSU	C5-C6-N1	-2.19	119.10	122.14
3	L5	2876	OMG	O6-C6-C5	-2.19	120.76	126.53
1	S2	1248	B8N	O4'-C1'-C2'	2.19	108.18	105.15
3	L5	2424	OMG	O6-C6-C5	-2.18	120.78	126.53
1	S2	93	PSU	C5-C6-N1	-2.18	119.11	122.14
1	S2	1347	PSU	C5-C6-N1	-2.18	119.12	122.14
1	S2	1244	PSU	C5-C6-N1	-2.18	119.12	122.14
3	L5	4392	OMG	O6-C6-C5	-2.18	120.79	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1779	PSU	C5-C6-N1	-2.17	119.12	122.14
3	L5	2815	A2M	C6-C5-N7	2.17	136.28	132.09
3	L5	4590	A2M	C2-N1-C6	2.17	122.30	118.73
3	L5	1534	A2M	C6-C5-N7	2.17	136.28	132.09
1	S2	1174	PSU	C5-C6-N1	-2.17	119.13	122.14
3	L5	1677	PSU	C5-C6-N1	-2.17	119.14	122.14
3	L5	3715	PSU	C5-C6-N1	-2.16	119.14	122.14
3	L5	3899	OMG	O6-C6-C5	-2.16	120.82	126.53
3	L5	4296	PSU	C5-C6-N1	-2.16	119.14	122.14
3	L5	3758	PSU	C5-C6-N1	-2.16	119.14	122.14
3	L5	2363	A2M	N9-C8-N7	-2.16	110.87	113.94
3	L5	4618	OMG	O6-C6-C5	-2.16	120.83	126.53
1	S2	468	A2M	C6-C5-N7	2.16	136.25	132.09
1	S2	867	OMG	O6-C6-C5	-2.15	120.85	126.53
3	L5	3867	A2M	N9-C8-N7	-2.15	110.88	113.94
3	L5	4228	OMG	O6-C6-C5	-2.15	120.85	126.53
3	L5	2843	PSU	O2-C2-N3	-2.15	118.04	121.86
3	L5	1871	A2M	C6-C5-N7	2.15	136.24	132.09
20	SX	62	HY3	O-C-CA	-2.14	119.19	124.86
3	L5	3825	A2M	C6-C5-N7	2.14	136.21	132.09
1	S2	34	PSU	C5-C6-N1	-2.14	119.17	122.14
1	S2	406	PSU	C5-C6-N1	-2.14	119.17	122.14
3	L5	4442	PSU	O4'-C1'-C2'	2.14	108.11	105.15
3	L5	4299	PSU	C5-C6-N1	-2.13	119.18	122.14
1	S2	1367	PSU	C5-C6-N1	-2.13	119.18	122.14
1	S2	1383	A2M	C6-C5-N7	2.13	136.20	132.09
3	L5	1871	A2M	C2-N1-C6	2.13	122.23	118.73
3	L5	5001	PSU	C5-C6-N1	-2.13	119.19	122.14
1	S2	159	A2M	C6-C5-N7	2.12	136.18	132.09
1	S2	683	OMG	O6-C6-C5	-2.12	120.93	126.53
1	S2	436	OMG	O6-C6-C5	-2.12	120.93	126.53
1	S2	668	A2M	C2-N1-C6	2.12	122.21	118.73
3	L5	3867	A2M	C2-N1-C6	2.12	122.21	118.73
3	L5	4521	PSU	O4'-C1'-C2'	2.12	108.08	105.15
3	L5	3944	OMG	O6-C6-C5	-2.12	120.94	126.53
3	L5	1582	PSU	C5-C6-N1	-2.12	119.20	122.14
1	S2	296	PSU	C5-C6-N1	-2.12	119.20	122.14
3	L5	3724	A2M	C6-C5-N7	2.11	136.17	132.09
3	L5	4972	PSU	C5-C6-N1	-2.11	119.21	122.14
3	L5	1534	A2M	O3'-C3'-C4'	-2.11	105.01	111.08
1	S2	866	PSU	C5-C6-N1	-2.11	119.21	122.14
1	S2	644	OMG	O6-C6-C5	-2.11	120.96	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3744	OMG	O6-C6-C5	-2.11	120.96	126.53
3	L5	3825	A2M	N9-C8-N7	-2.11	110.94	113.94
1	S2	468	A2M	N9-C8-N7	-2.10	110.95	113.94
3	L5	2363	A2M	C6-C5-N7	2.10	136.14	132.09
3	L5	1683	PSU	C5-C6-N1	-2.10	119.23	122.14
3	L5	4523	A2M	C6-C5-N7	2.10	136.14	132.09
1	S2	1243	PSU	C5-C6-N1	-2.10	119.23	122.14
3	L5	4456	OMC	O2-C2-N3	-2.09	119.03	122.33
3	L5	4403	PSU	C5-C6-N1	-2.09	119.23	122.14
1	S2	1447	OMG	O6-C6-C5	-2.09	121.01	126.53
1	S2	166	A2M	N9-C8-N7	-2.09	110.97	113.94
3	L5	3764	PSU	C5-C6-N1	-2.09	119.25	122.14
1	S2	1081	PSU	C5-C6-N1	-2.08	119.25	122.14
3	L5	1781	PSU	C5-C6-N1	-2.08	119.25	122.14
81	Pt	56	PSU	C5-C6-N1	-2.08	119.25	122.14
1	S2	1678	A2M	C6-C5-N7	2.08	136.10	132.09
3	L5	4293	PSU	C5-C6-N1	-2.08	119.26	122.14
3	L5	3734	PSU	C5-C6-N1	-2.07	119.26	122.14
1	S2	601	OMG	O6-C6-C5	-2.07	121.06	126.53
3	L5	5010	PSU	C5-C6-N1	-2.07	119.27	122.14
1	S2	1692	PSU	C5-C6-N1	-2.07	119.27	122.14
3	L5	3785	A2M	C2-N1-C6	2.07	122.13	118.73
1	S2	36	PSU	C5-C6-N1	-2.07	119.27	122.14
3	L5	4493	PSU	C5-C6-N1	-2.07	119.27	122.14
3	L5	3867	A2M	C6-C5-N7	2.07	136.08	132.09
3	L5	398	A2M	C6-C5-N7	2.07	136.07	132.09
1	S2	218	PSU	O4'-C1'-C2'	2.07	108.01	105.15
3	L5	4636	PSU	O4'-C1'-C2'	2.07	108.01	105.15
3	L5	400	A2M	C6-C5-N7	2.07	136.07	132.09
1	S2	686	PSU	C5-C6-N1	-2.06	119.28	122.14
3	L5	2364	OMG	O6-C6-C5	-2.06	121.09	126.53
1	S2	822	PSU	C5-C6-N1	-2.06	119.28	122.14
3	L5	3785	A2M	O4'-C4'-C3'	2.06	109.24	105.15
1	S2	1643	PSU	O4'-C1'-C2'	2.06	108.00	105.15
3	L5	3768	PSU	C5-C6-N1	-2.06	119.28	122.14
3	L5	4499	OMG	O6-C6-C5	-2.06	121.11	126.53
3	L5	3884	PSU	C6-C5-C4	-2.06	116.79	118.17
1	S2	1442	OMU	O2-C2-N1	-2.05	120.13	122.80
1	S2	649	PSU	C5-C6-N1	-2.04	119.31	122.14
1	S2	1239	PSU	C5-C6-N1	-2.04	119.31	122.14
3	L5	3718	A2M	C4-N9-C8	2.04	107.88	105.74
3	L5	1524	A2M	N9-C8-N7	-2.04	111.04	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	512	A2M	C6-C5-N7	2.04	136.02	132.09
1	S2	1328	OMG	O6-C6-C5	-2.04	121.16	126.53
3	L5	1860	PSU	C5-C6-N1	-2.04	119.31	122.14
3	L5	3627	OMG	C2'-C1'-N9	-2.03	110.38	114.24
1	S2	1445	PSU	O4'-C1'-C2'	2.03	107.96	105.15
3	L5	3723	A2M	C6-C5-N7	2.03	136.00	132.09
3	L5	1524	A2M	C6-C5-N7	2.03	136.00	132.09
3	L5	2787	A2M	C6-C5-N7	2.03	136.00	132.09
3	L5	1782	PSU	C5-C6-N1	-2.03	119.33	122.14
3	L5	4471	PSU	O2-C2-N3	-2.03	118.26	121.86
3	L5	4370	OMG	O6-C6-C5	-2.02	121.19	126.53
3	L5	4361	PSU	C5-C6-N1	-2.02	119.33	122.14
3	L5	1522	OMG	C5-C6-N1	2.02	118.41	113.25
3	L5	3715	PSU	O4'-C1'-C2'	2.02	107.95	105.15
3	L5	4571	A2M	C6-C5-N7	2.02	135.99	132.09
1	S2	1383	A2M	N9-C8-N7	-2.02	111.07	113.94
3	L5	2401	A2M	C6-C5-N7	2.02	135.99	132.09
1	S2	509	OMG	O6-C6-C5	-2.02	121.20	126.53
3	L5	4312	PSU	C5-C6-N1	-2.02	119.34	122.14
3	L5	4590	A2M	N9-C8-N7	-2.02	111.07	113.94
3	L5	3851	PSU	C5-C6-N1	-2.01	119.35	122.14
3	L5	2401	A2M	N9-C8-N7	-2.01	111.08	113.94
1	S2	576	A2M	N9-C8-N7	-2.01	111.08	113.94
3	L5	1534	A2M	N9-C8-N7	-2.01	111.08	113.94
1	S2	573	PSU	C5-C6-N1	-2.01	119.35	122.14
3	L5	4220	6MZ	C2-N1-C6	2.01	121.90	115.24
81	Pt	8	4SU	O2-C2-N1	-2.01	120.18	122.80
3	L5	1524	A2M	C2-N1-C6	2.01	122.03	118.73
1	S2	109	PSU	C5-C6-N1	-2.01	119.36	122.14
3	L5	4431	PSU	C5-C6-N1	-2.01	119.36	122.14
3	L5	3729	PSU	C5-C6-N1	-2.01	119.36	122.14
1	S2	27	A2M	N9-C8-N7	-2.00	111.09	113.94
3	L5	2415	OMU	O2-C2-N1	-2.00	120.19	122.80
3	L5	4552	PSU	C5-C6-N1	-2.00	119.36	122.14
3	L5	2787	A2M	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2
6	SA	2	SAC	OAC-C1A-N-CA

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Mol	Chain	Res	Type	Atoms
6	SA	2	SAC	CB-CA-N-C1A
6	SA	2	SAC	O-C-CA-CB
29	SV	1	AME	OT-CT1-N-CA
63	Lr	2	SAC	C2A-C1A-N-CA
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	C1'-C2'-O2'-CM2
1	S2	159	A2M	C1'-C2'-O2'-CM'
1	S2	462	OMC	C1'-C2'-O2'-CM2
1	S2	468	A2M	C1'-C2'-O2'-CM'
1	S2	601	OMG	C1'-C2'-O2'-CM2
1	S2	644	OMG	O4'-C4'-C5'-O5'
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	867	OMG	C1'-C2'-O2'-CM2
1	S2	918	PSU	C2'-C1'-C5-C4
1	S2	1248	B8N	C31-C32-C33-N34
1	S2	1326	UY1	C2'-C1'-C5-C4
1	S2	1328	OMG	C1'-C2'-O2'-CM2
1	S2	1337	4AC	N3-C4-N4-C7
1	S2	1337	4AC	C5-C4-N4-C7
1	S2	1383	A2M	C1'-C2'-O2'-CM'
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1851	MA6	O4'-C4'-C5'-O5'
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	2415	OMU	C1'-C2'-O2'-CM2
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4420	PSU	C2'-C1'-C5-C4
3	L5	4420	PSU	O4'-C4'-C5'-O5'
3	L5	4571	A2M	C1'-C2'-O2'-CM'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	4637	OMG	C1'-C2'-O2'-CM2
20	SX	62	HY3	O-C-CA-C3
38	LA	216	V5N	O-C-CA-CB
3	L5	3701	OMC	C2'-C1'-N1-C6
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	1442	OMU	C3'-C4'-C5'-O5'
1	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	4420	PSU	C3'-C4'-C5'-O5'
3	L5	4636	PSU	C3'-C4'-C5'-O5'
6	SA	2	SAC	C2A-C1A-N-CA

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Mol	Chain	Res	Type	Atoms
63	Lr	2	SAC	OAC-C1A-N-CA
1	S2	576	A2M	O4'-C4'-C5'-O5'
1	S2	1243	PSU	O4'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C4'-C5'-O5'
3	L5	3760	A2M	O4'-C1'-N9-C4
3	L5	2787	A2M	C2'-C1'-N9-C4
1	S2	428	OMU	C2'-C1'-N1-C6
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	1625	OMG	C3'-C2'-O2'-CM2
1	S2	1851	MA6	C3'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
1	S2	590	A2M	O4'-C4'-C5'-O5'
1	S2	590	A2M	C3'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	822	PSU	C3'-C4'-C5'-O5'
1	S2	1447	OMG	C3'-C4'-C5'-O5'
1	S2	1490	OMG	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
1	S2	668	A2M	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	2422	OMC	O4'-C4'-C5'-O5'
81	Pt	21	H2U	O4'-C4'-C5'-O5'
3	L5	3760	A2M	O4'-C1'-N9-C8
78	Lo	53	MLZ	CG-CD-CE-NZ
1	S2	428	OMU	C2'-C1'-N1-C2
1	S2	822	PSU	O4'-C4'-C5'-O5'
3	L5	2422	OMC	C3'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
1	S2	1804	OMU	C1'-C2'-O2'-CM2
3	L5	3718	A2M	C1'-C2'-O2'-CM'
1	S2	668	A2M	C2'-C1'-N9-C8
1	S2	428	OMU	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	2363	A2M	C3'-C2'-O2'-CM'
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	3818	UY1	C4'-C5'-O5'-P
1	S2	1447	OMG	O4'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	3701	OMC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
1	S2	918	PSU	O4'-C1'-C5-C4
1	S2	1326	UY1	O4'-C1'-C5-C4
3	L5	1677	PSU	O4'-C1'-C5-C4
1	S2	428	OMU	O4'-C1'-N1-C2
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	3944	OMG	C3'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	1524	A2M	C3'-C2'-O2'-CM'
6	SA	2	SAC	C-CA-N-C1A
3	L5	1322	1MA	C2'-C1'-N9-C4
1	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	2815	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	1322	1MA	C2'-C1'-N9-C8
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	1288	OMU	C4'-C5'-O5'-P
1	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	3867	A2M	C3'-C4'-C5'-O5'
1	S2	484	A2M	C1'-C2'-O2'-CM'
1	S2	512	A2M	C1'-C2'-O2'-CM'
1	S2	1490	OMG	C1'-C2'-O2'-CM2
3	L5	1677	PSU	O4'-C1'-C5-C6
3	L5	3818	UY1	O4'-C1'-C5-C6
3	L5	4531	PSU	O4'-C1'-C5-C6
1	S2	590	A2M	O4'-C1'-N9-C8
3	L5	4494	OMG	C3'-C2'-O2'-CM2
1	S2	1081	PSU	C4'-C5'-O5'-P
81	Pt	21	H2U	C4'-C5'-O5'-P
3	L5	3729	PSU	O4'-C4'-C5'-O5'
3	L5	2787	A2M	O4'-C1'-N9-C8
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	590	A2M	C2'-C1'-N9-C8
3	L5	3785	A2M	C2'-C1'-N9-C8
1	S2	1288	OMU	C2'-C1'-N1-C2
3	L5	2351	OMC	C2'-C1'-N1-C2
65	Lb	5	MLZ	N-CA-CB-CG
1	S2	668	A2M	O4'-C1'-N9-C8
3	L5	1781	PSU	C3'-C4'-C5'-O5'
3	L5	2351	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

88 monomers are involved in 120 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2415	OMU	2	0
1	S2	1347	PSU	1	0
3	L5	1871	A2M	1	0
1	S2	468	A2M	2	0
81	Pt	8	4SU	1	0
3	L5	4620	OMU	1	0
3	L5	3724	A2M	2	0
1	S2	116	OMU	2	0
1	S2	159	A2M	3	0
3	L5	4579	PSU	1	0
3	L5	4447	5MC	1	0
1	S2	1232	PSU	1	0
3	L5	4530	UR3	2	0
3	L5	2815	A2M	1	0
3	L5	4392	OMG	1	0
3	L5	3925	OMU	1	0
3	L5	3785	A2M	1	0
1	S2	815	PSU	1	0
3	L5	4457	PSU	1	0
3	L5	3818	UY1	1	0
63	Lr	2	SAC	1	0
1	S2	512	A2M	2	0
3	L5	2632	PSU	1	0
3	L5	4536	OMC	1	0
6	SA	2	SAC	2	0
1	S2	683	OMG	1	0
1	S2	436	OMG	2	0
1	S2	1445	PSU	1	0
2	L8	14	OMU	1	0
1	S2	462	OMC	2	0
1	S2	1031	A2M	1	0
3	L5	4628	PSU	1	0
3	L5	3944	OMG	1	0
1	S2	99	A2M	2	0
1	S2	1337	4AC	1	0
3	L5	1326	A2M	1	0
1	S2	119	PSU	1	0
3	L5	4637	OMG	3	0
1	S2	573	PSU	1	0
3	L5	3887	OMC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2424	OMG	1	0
1	S2	484	A2M	1	0
1	S2	918	PSU	2	0
1	S2	814	PSU	1	0
3	L5	3869	OMC	5	0
1	S2	1391	OMC	1	0
1	S2	644	OMG	1	0
1	S2	1442	OMU	1	0
3	L5	2364	OMG	1	0
3	L5	3718	A2M	3	0
3	L5	4531	PSU	2	0
3	L5	4618	OMG	1	0
3	L5	5001	PSU	1	0
3	L5	4306	OMU	1	0
1	S2	576	A2M	3	0
1	S2	1692	PSU	1	0
1	S2	601	OMG	1	0
2	L8	75	OMG	1	0
1	S2	1643	PSU	1	0
1	S2	1239	PSU	1	0
3	L5	3723	A2M	3	0
3	L5	398	A2M	1	0
3	L5	4521	PSU	1	0
3	L5	4220	6MZ	1	0
1	S2	1851	MA6	1	0
1	S2	1383	A2M	1	0
3	L5	4456	OMC	1	0
1	S2	1678	A2M	3	0
1	S2	1490	OMG	2	0
1	S2	1248	B8N	1	0
3	L5	3867	A2M	2	0
3	L5	1340	OMC	2	0
3	L5	1677	PSU	1	0
3	L5	3770	PSU	1	0
1	S2	354	OMU	1	0
1	S2	1288	OMU	2	0
3	L5	2876	OMG	1	0
3	L5	4636	PSU	2	0
1	S2	174	OMC	1	0
3	L5	2351	OMC	1	0
1	S2	509	OMG	1	0
1	S2	1804	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3701	OMC	1	0
1	S2	681	PSU	1	0
1	S2	867	OMG	2	0
3	L5	3734	PSU	1	0
3	L5	1881	OMC	2	0
1	S2	1447	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 860 ligands modelled in this entry, 831 are monoatomic - leaving 29 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	$\# Z > 2$
83	PUT	L5	5121	-	5,5,5	0.14	0	4,4,4	0.23	0
82	SPD	L5	5111	-	9,9,9	0.14	0	8,8,8	0.21	0
82	SPD	L5	5104	-	9,9,9	0.15	0	8,8,8	0.31	0
83	PUT	L5	5119	-	5,5,5	0.08	0	4,4,4	0.13	0
86	ANM	L5	5101	84	20,20,20	1.18	1 (5%)	24,27,27	1.32	2 (8%)
88	TRS	L5	5124	-	7,7,7	0.39	0	9,9,9	0.59	0
82	SPD	L5	5107	-	9,9,9	0.31	0	8,8,8	0.91	0
82	SPD	L5	5105	-	9,9,9	0.18	0	8,8,8	0.26	0
83	PUT	L5	5116	-	5,5,5	0.08	0	4,4,4	0.14	0
87	3H3	L5	5102	-	34,34,34	3.49	12 (35%)	36,45,45	3.81	16 (44%)
82	SPD	L5	5114	-	9,9,9	0.18	0	8,8,8	0.30	0
90	MET	Pt	78	81	6,7,8	0.66	0	2,7,9	1.91	1 (50%)
82	SPD	L5	5113	-	9,9,9	0.15	0	8,8,8	0.21	0
83	PUT	L5	5117	-	5,5,5	0.08	0	4,4,4	0.12	0
82	SPD	L5	5103	-	9,9,9	0.30	0	8,8,8	0.83	0
82	SPD	S2	1902	-	9,9,9	0.32	0	8,8,8	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	PUT	S2	1903	-	5,5,5	0.10	0	4,4,4	0.12	0
82	SPD	S2	1901	-	9,9,9	0.32	0	8,8,8	0.75	0
83	PUT	L5	5118	-	5,5,5	0.08	0	4,4,4	0.15	0
82	SPD	L5	5115	-	9,9,9	0.19	0	8,8,8	0.26	0
83	PUT	L5	5123	-	5,5,5	0.12	0	4,4,4	0.13	0
82	SPD	L5	5112	-	9,9,9	0.18	0	8,8,8	0.27	0
83	PUT	L5	5122	-	5,5,5	0.10	0	4,4,4	0.13	0
82	SPD	L5	5108	-	9,9,9	0.32	0	8,8,8	1.00	0
82	SPD	L5	5106	-	9,9,9	0.21	0	8,8,8	0.24	0
82	SPD	L5	5110	-	9,9,9	0.32	0	8,8,8	0.97	0
88	TRS	L5	5125	-	7,7,7	0.09	0	9,9,9	0.28	0
82	SPD	L5	5109	-	9,9,9	0.15	0	8,8,8	0.24	0
83	PUT	L5	5120	-	5,5,5	0.10	0	4,4,4	0.12	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
83	PUT	L5	5121	-	-	1/3/3/3	-
82	SPD	L5	5111	-	-	3/7/7/7	-
82	SPD	L5	5104	-	-	4/7/7/7	-
83	PUT	L5	5119	-	-	1/3/3/3	-
86	ANM	L5	5101	84	-	0/10/23/23	0/2/2/2
88	TRS	L5	5124	-	-	0/9/9/9	-
82	SPD	L5	5107	-	-	3/7/7/7	-
82	SPD	L5	5105	-	-	5/7/7/7	-
83	PUT	L5	5116	-	-	0/3/3/3	-
87	3H3	L5	5102	-	-	14/39/51/51	0/1/2/2
82	SPD	L5	5114	-	-	5/7/7/7	-
90	MET	Pt	78	81	-	4/5/6/8	-
82	SPD	L5	5113	-	-	6/7/7/7	-
83	PUT	L5	5117	-	-	1/3/3/3	-
82	SPD	L5	5103	-	-	0/7/7/7	-
82	SPD	S2	1902	-	-	5/7/7/7	-
83	PUT	S2	1903	-	-	0/3/3/3	-
82	SPD	S2	1901	-	-	2/7/7/7	-
83	PUT	L5	5118	-	-	0/3/3/3	-
82	SPD	L5	5115	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PUT	L5	5123	-	-	0/3/3/3	-
82	SPD	L5	5112	-	-	5/7/7/7	-
83	PUT	L5	5122	-	-	0/3/3/3	-
82	SPD	L5	5108	-	-	4/7/7/7	-
82	SPD	L5	5106	-	-	2/7/7/7	-
82	SPD	L5	5110	-	-	3/7/7/7	-
88	TRS	L5	5125	-	-	6/9/9/9	-
82	SPD	L5	5109	-	-	4/7/7/7	-
83	PUT	L5	5120	-	-	1/3/3/3	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L5	5102	3H3	C13-C12	9.17	1.53	1.33
87	L5	5102	3H3	O3-C22	8.10	1.39	1.23
87	L5	5102	3H3	O4-C23	7.74	1.38	1.23
87	L5	5102	3H3	C23-N	7.47	1.50	1.37
87	L5	5102	3H3	C22-N	6.59	1.48	1.37
87	L5	5102	3H3	C3-C2	5.67	1.54	1.33
86	L5	5101	ANM	O2-C5	4.49	1.45	1.35
87	L5	5102	3H3	C19-C20	3.44	1.58	1.53
87	L5	5102	3H3	O1-C10	2.92	1.40	1.34
87	L5	5102	3H3	C4-C3	2.90	1.53	1.44
87	L5	5102	3H3	O1-C11	-2.56	1.40	1.44
87	L5	5102	3H3	C24-C20	-2.09	1.50	1.53
87	L5	5102	3H3	O2-C16	-2.06	1.18	1.21

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L5	5102	3H3	C22-N-C23	-12.74	110.52	125.87
87	L5	5102	3H3	O3-C22-N	-7.90	108.12	120.30
87	L5	5102	3H3	O4-C23-N	-7.72	108.39	120.30
87	L5	5102	3H3	O4-C23-C24	-7.07	109.12	122.62
87	L5	5102	3H3	O3-C22-C21	-6.87	109.51	122.62
87	L5	5102	3H3	C8-C9-C10	-5.21	110.34	122.78
87	L5	5102	3H3	C25-C12-C13	-4.65	111.62	123.56
87	L5	5102	3H3	C1-C2-C3	-4.42	116.98	126.11
86	L5	5101	ANM	O2-C5-C6	4.03	118.27	111.09
87	L5	5102	3H3	C24-C23-N	-2.90	112.40	115.92
87	L5	5102	3H3	C21-C22-N	-2.84	112.47	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L5	5102	3H3	C6-C7-C8	-2.82	105.64	112.73
87	L5	5102	3H3	C25-C12-C11	-2.71	110.60	115.96
90	Pt	78	MET	CE-SD-CG	2.70	114.32	100.32
87	L5	5102	3H3	C4-C3-C2	-2.32	108.77	124.25
86	L5	5101	ANM	O2-C5-O3	-2.31	118.52	122.99
87	L5	5102	3H3	C11-C12-C13	-2.28	111.73	119.78
87	L5	5102	3H3	O1-C10-C9	2.13	116.02	111.39
87	L5	5102	3H3	C1-C11-C12	-2.13	109.32	113.19

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	L5	5114	SPD	C4-C5-N6-C7
87	L5	5102	3H3	C2-C1-C11-O1
87	L5	5102	3H3	C2-C1-C11-C12
87	L5	5102	3H3	C-C1-C11-O1
87	L5	5102	3H3	C-C1-C11-C12
87	L5	5102	3H3	C25-C12-C13-C14
87	L5	5102	3H3	C1-C11-C12-C25
87	L5	5102	3H3	O1-C11-C12-C25
88	L5	5125	TRS	C2-C-C1-O1
88	L5	5125	TRS	C3-C-C1-O1
88	L5	5125	TRS	N-C-C1-O1
88	L5	5125	TRS	C1-C-C3-O3
88	L5	5125	TRS	C2-C-C3-O3
88	L5	5125	TRS	N-C-C3-O3
90	Pt	78	MET	N-CA-CB-CG
90	Pt	78	MET	C-CA-CB-CG
82	L5	5114	SPD	C3-C4-C5-N6
82	L5	5104	SPD	N6-C7-C8-C9
82	L5	5105	SPD	N6-C7-C8-C9
87	L5	5102	3H3	O-C10-O1-C11
82	S2	1902	SPD	C3-C4-C5-N6
82	L5	5113	SPD	C3-C4-C5-N6
82	L5	5104	SPD	C3-C4-C5-N6
87	L5	5102	3H3	C2-C3-C4-C5
82	L5	5108	SPD	C3-C4-C5-N6
90	Pt	78	MET	CA-CB-CG-SD
82	L5	5114	SPD	N6-C7-C8-C9
87	L5	5102	3H3	C9-C10-O1-C11
82	S2	1902	SPD	C4-C5-N6-C7

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Mol	Chain	Res	Type	Atoms
82	S2	1902	SPD	N1-C2-C3-C4
82	L5	5109	SPD	C3-C4-C5-N6
87	L5	5102	3H3	C-C1-C2-C3
82	L5	5112	SPD	C3-C4-C5-N6
82	L5	5106	SPD	C8-C7-N6-C5
82	L5	5107	SPD	C7-C8-C9-N10
82	L5	5108	SPD	C7-C8-C9-N10
82	L5	5109	SPD	C8-C7-N6-C5
82	L5	5108	SPD	C2-C3-C4-C5
82	L5	5104	SPD	C4-C5-N6-C7
82	L5	5109	SPD	C2-C3-C4-C5
90	Pt	78	MET	CB-CG-SD-CE
82	L5	5105	SPD	C2-C3-C4-C5
83	L5	5121	PUT	C1-C2-C3-C4
82	L5	5110	SPD	C2-C3-C4-C5
82	L5	5115	SPD	N6-C7-C8-C9
82	S2	1902	SPD	C2-C3-C4-C5
82	L5	5112	SPD	N1-C2-C3-C4
82	S2	1902	SPD	C7-C8-C9-N10
82	L5	5105	SPD	C8-C7-N6-C5
82	L5	5106	SPD	C7-C8-C9-N10
82	L5	5107	SPD	C2-C3-C4-C5
82	L5	5110	SPD	C3-C4-C5-N6
82	L5	5113	SPD	C2-C3-C4-C5
82	L5	5111	SPD	C2-C3-C4-C5
82	L5	5112	SPD	C2-C3-C4-C5
82	L5	5113	SPD	C4-C5-N6-C7
82	L5	5114	SPD	C8-C7-N6-C5
83	L5	5120	PUT	C1-C2-C3-C4
82	L5	5108	SPD	N1-C2-C3-C4
82	L5	5105	SPD	C7-C8-C9-N10
82	L5	5109	SPD	C7-C8-C9-N10
82	L5	5111	SPD	C7-C8-C9-N10
82	L5	5112	SPD	C7-C8-C9-N10
82	L5	5113	SPD	C7-C8-C9-N10
82	L5	5114	SPD	C7-C8-C9-N10
83	L5	5119	PUT	C1-C2-C3-C4
82	L5	5113	SPD	N1-C2-C3-C4
82	L5	5110	SPD	C4-C5-N6-C7
82	L5	5107	SPD	N6-C7-C8-C9
82	L5	5105	SPD	N1-C2-C3-C4
82	S2	1901	SPD	C4-C5-N6-C7

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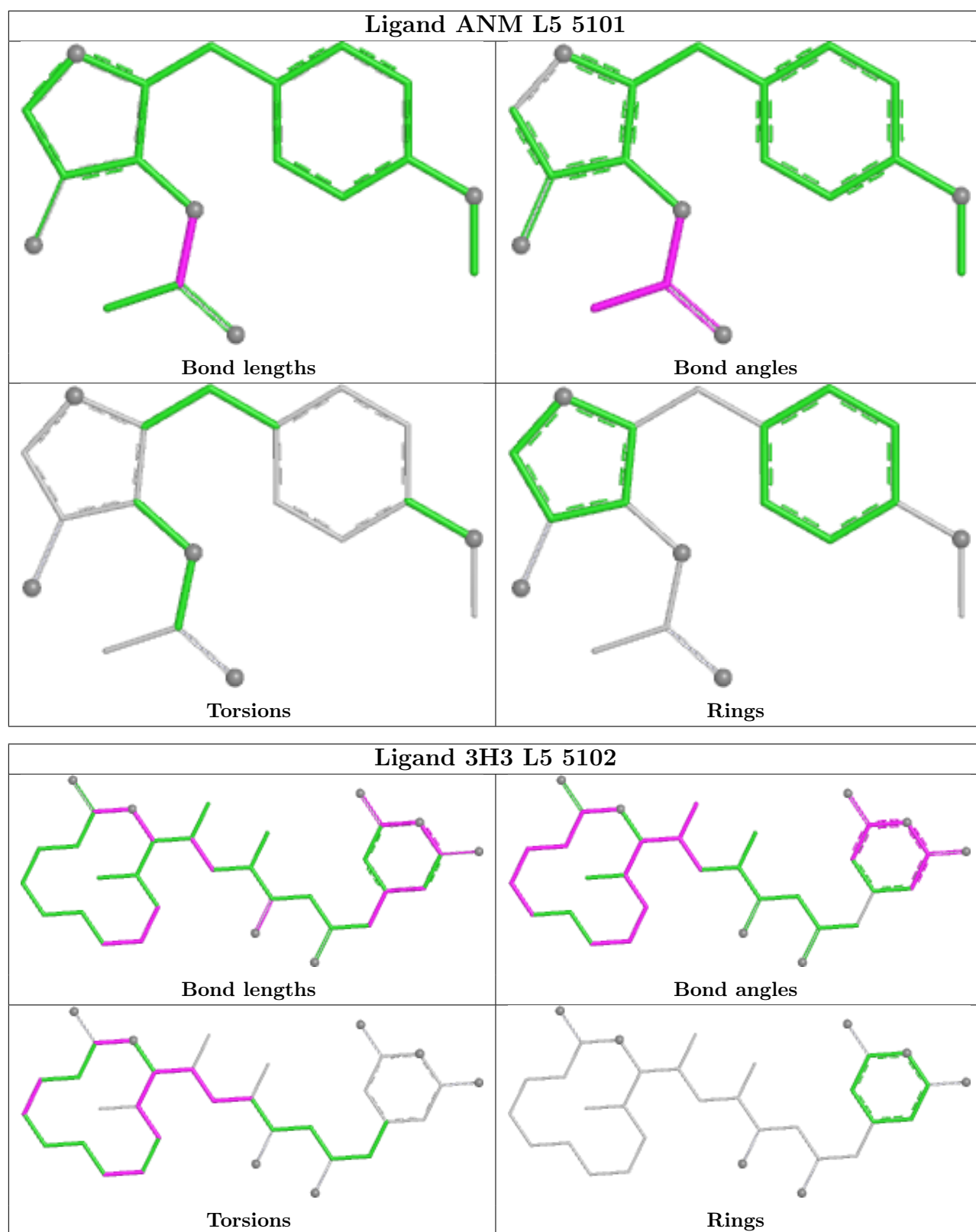
Mol	Chain	Res	Type	Atoms
83	L5	5117	PUT	C1-C2-C3-C4
82	L5	5112	SPD	C4-C5-N6-C7
82	L5	5104	SPD	N1-C2-C3-C4
87	L5	5102	3H3	C6-C7-C8-C9
82	L5	5113	SPD	N6-C7-C8-C9
87	L5	5102	3H3	C12-C13-C14-C15
82	L5	5111	SPD	C8-C7-N6-C5
82	S2	1901	SPD	N6-C7-C8-C9
87	L5	5102	3H3	C11-C1-C2-C3

There are no ring outliers.

13 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	L5	5121	PUT	1	0
86	L5	5101	ANM	1	0
87	L5	5102	3H3	2	0
82	L5	5114	SPD	16	0
90	Pt	78	MET	2	0
83	L5	5117	PUT	2	0
82	L5	5103	SPD	1	0
82	S2	1902	SPD	1	0
82	S2	1901	SPD	1	0
82	L5	5115	SPD	2	0
82	L5	5112	SPD	6	0
82	L5	5110	SPD	1	0
82	L5	5109	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

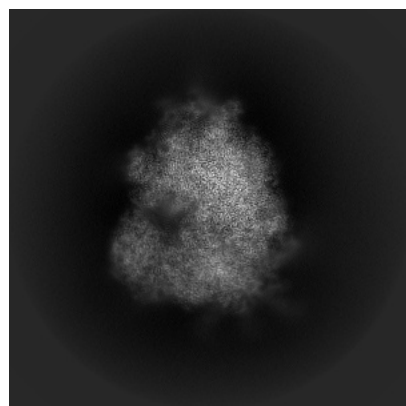
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40205. These allow visual inspection of the internal detail of the map and identification of artifacts.

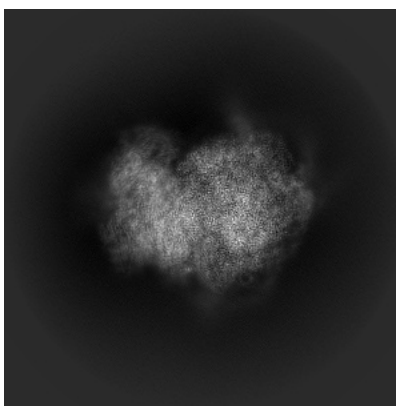
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

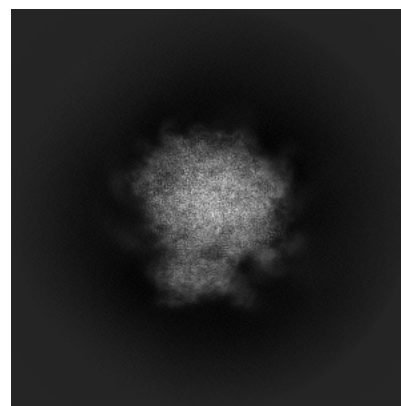
6.1.1 Primary map



X

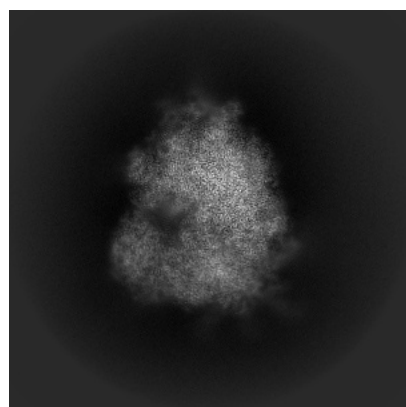


Y

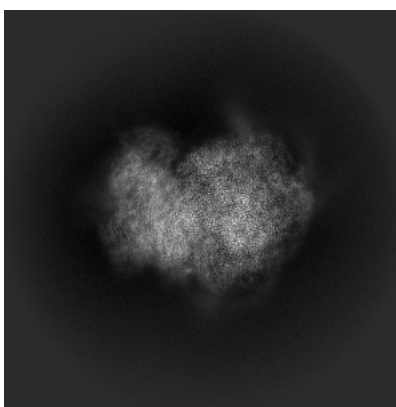


Z

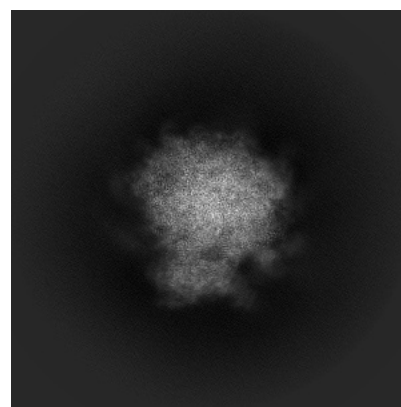
6.1.2 Raw map



X



Y

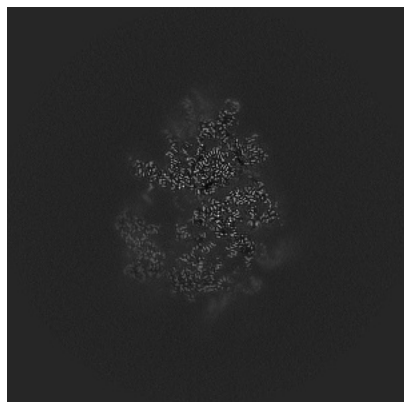


Z

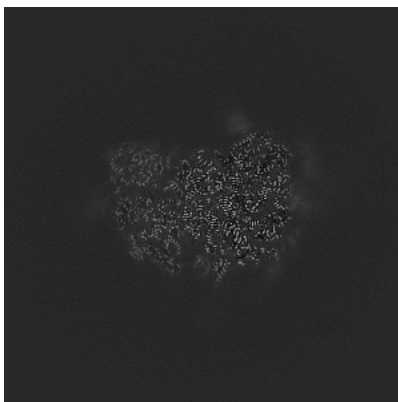
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

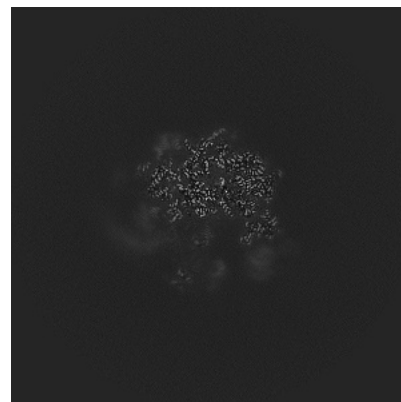
6.2.1 Primary map



X Index: 320

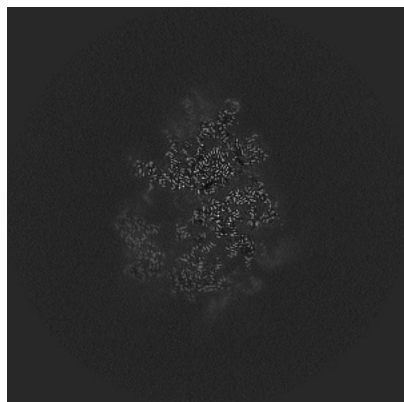


Y Index: 320

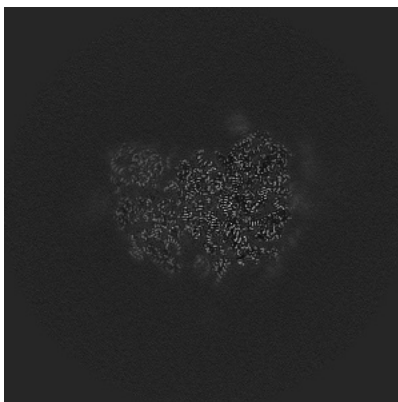


Z Index: 320

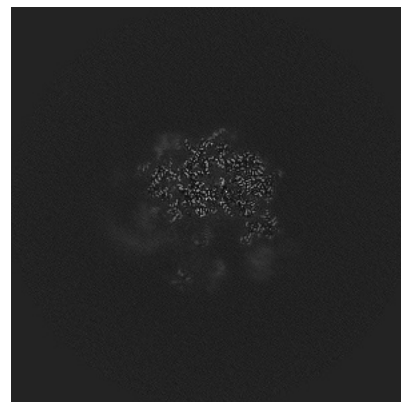
6.2.2 Raw map



X Index: 320



Y Index: 320

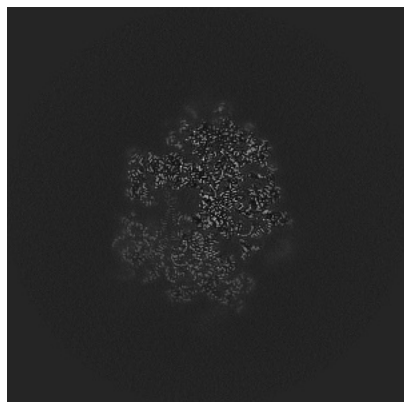


Z Index: 320

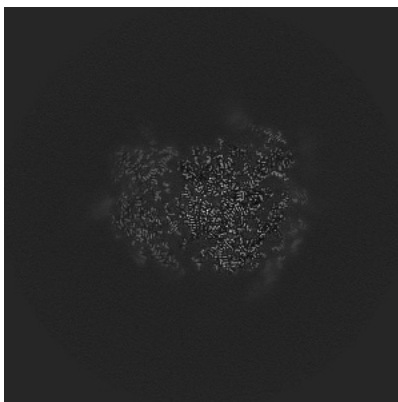
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 299

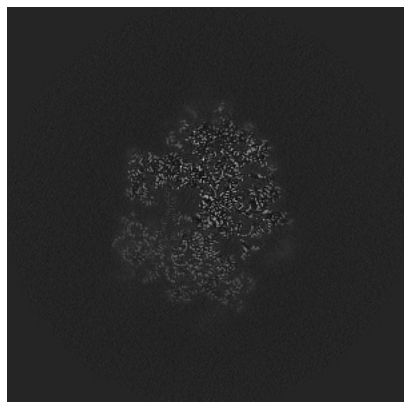


Y Index: 332

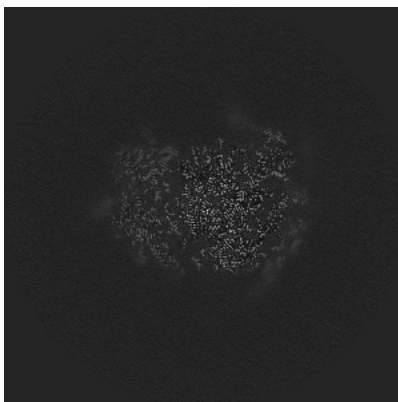


Z Index: 362

6.3.2 Raw map



X Index: 299



Y Index: 332

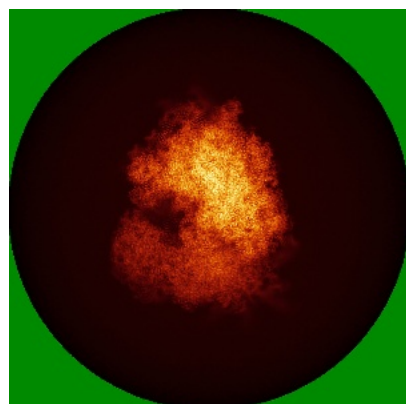


Z Index: 362

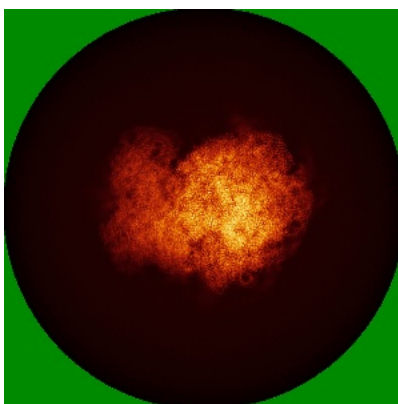
The images above show the largest variance slices of the map in three orthogonal directions.

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

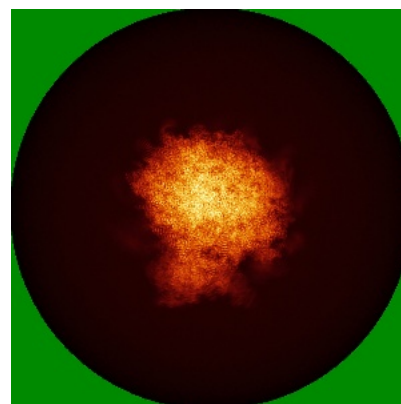
6.4.1 Primary map



X

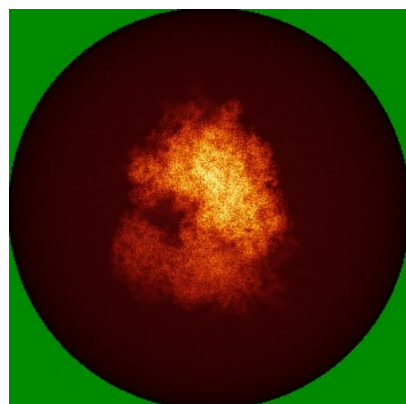


Y

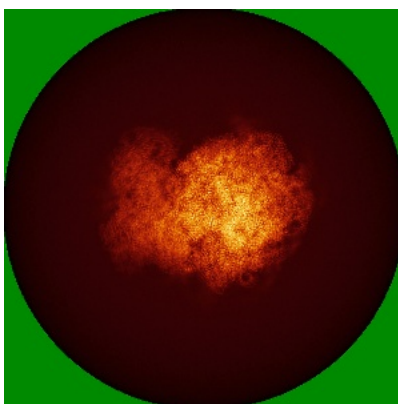


Z

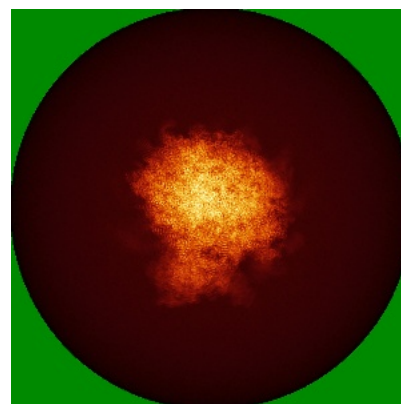
6.4.2 Raw map



X



Y

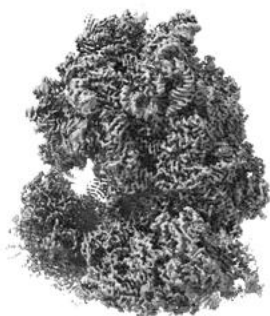


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. 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



X



Y



Z

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.

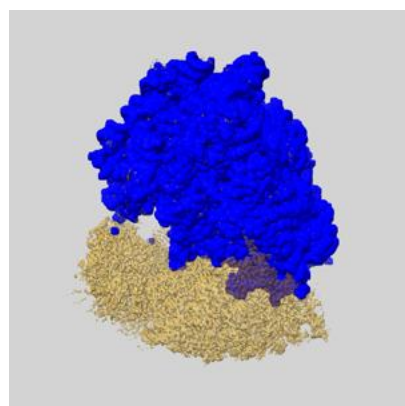
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

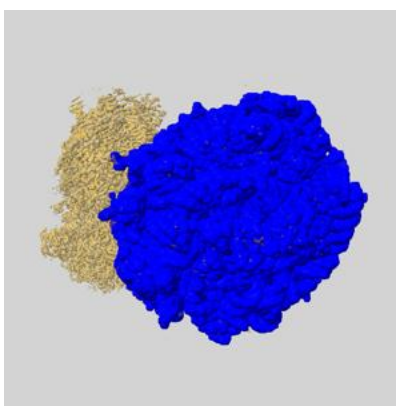
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

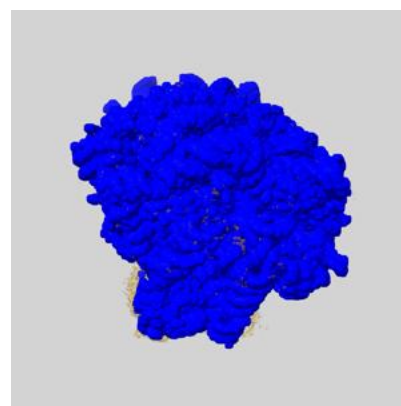
6.6.1 emd_40205_msk_1.map [i](#)



X



Y

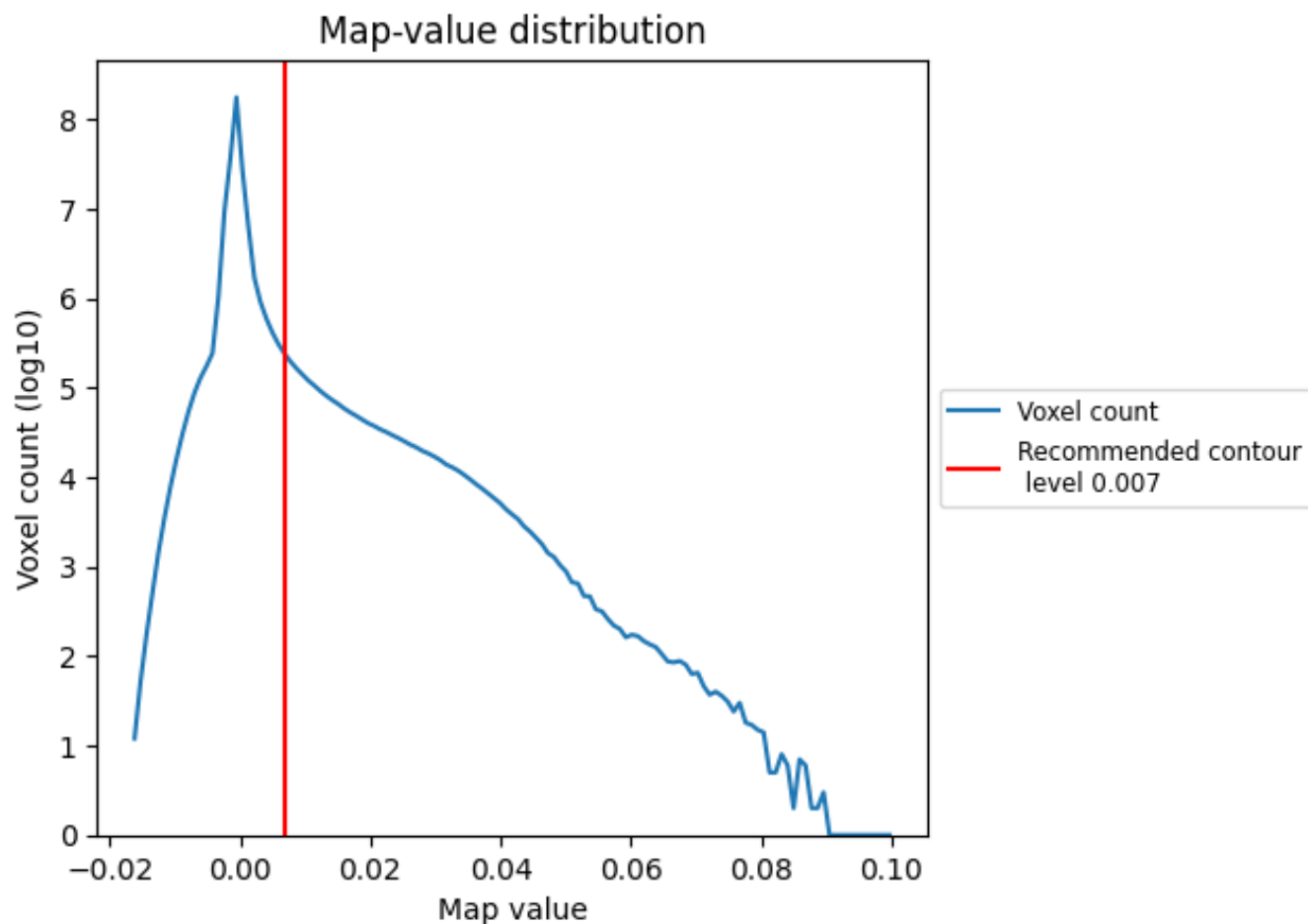


Z

7 Map analysis [i](#)

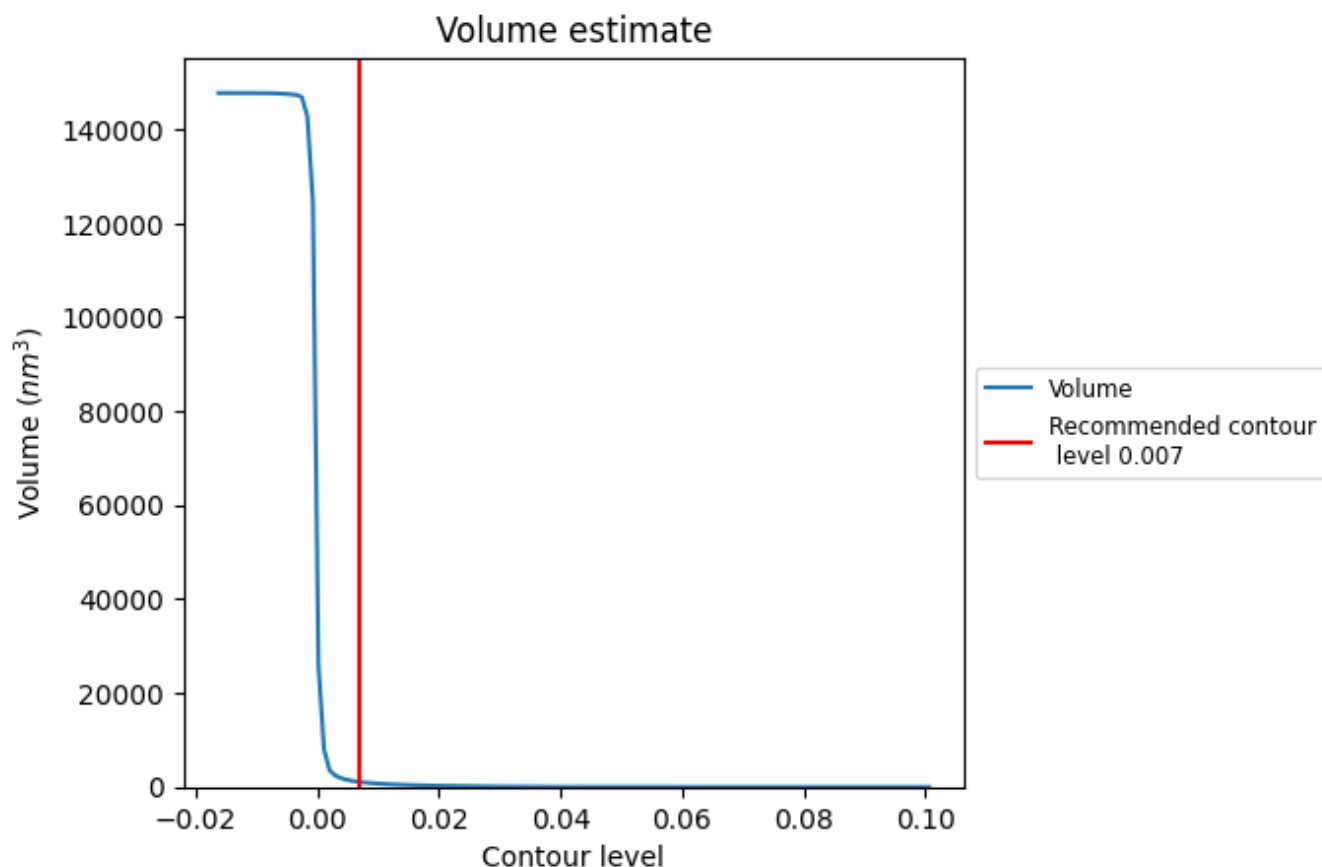
This section contains the results of statistical analysis of the map.

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.

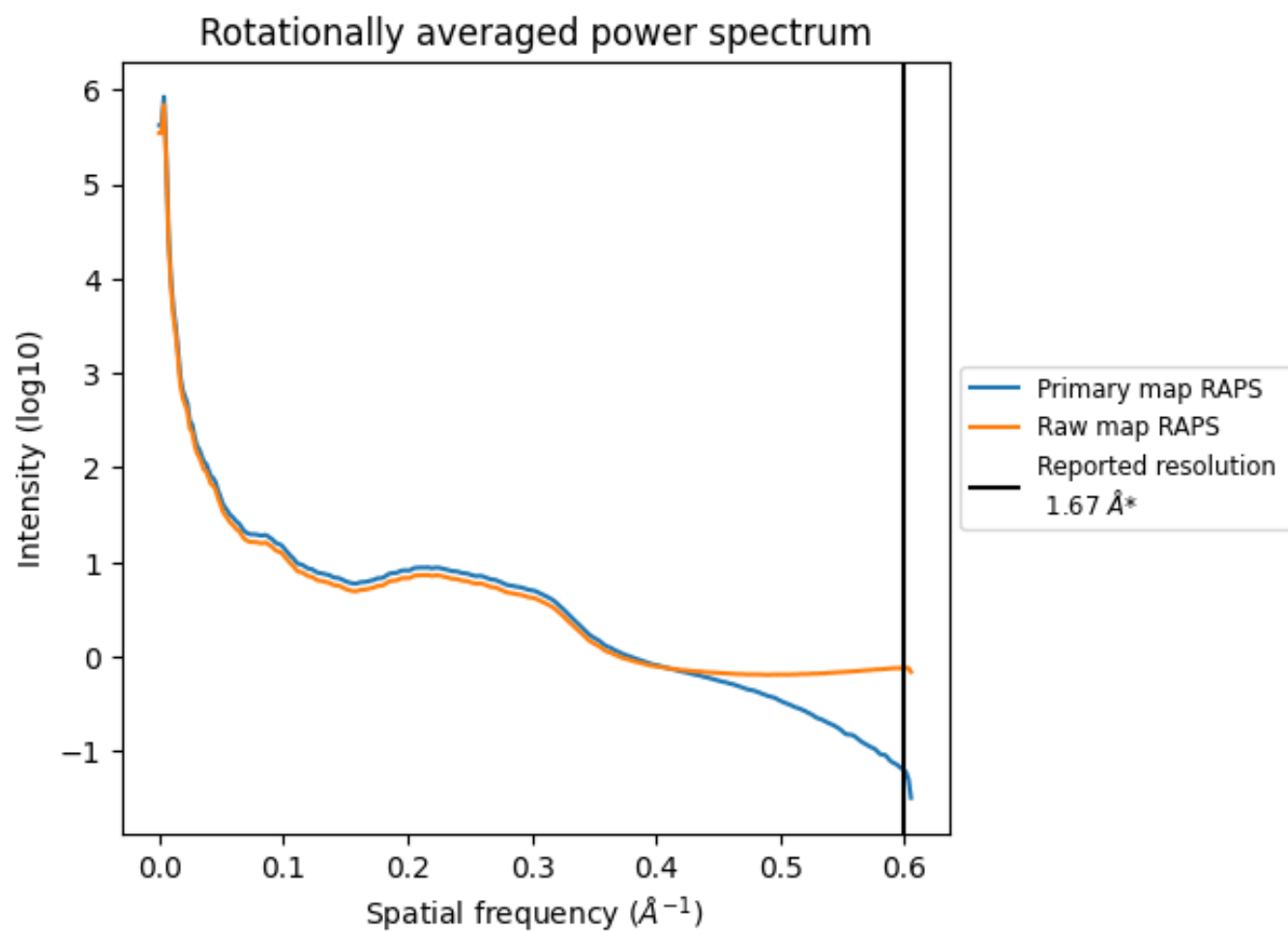
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1063 nm^3 ; this corresponds to an approximate mass of 960 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 ⓘ

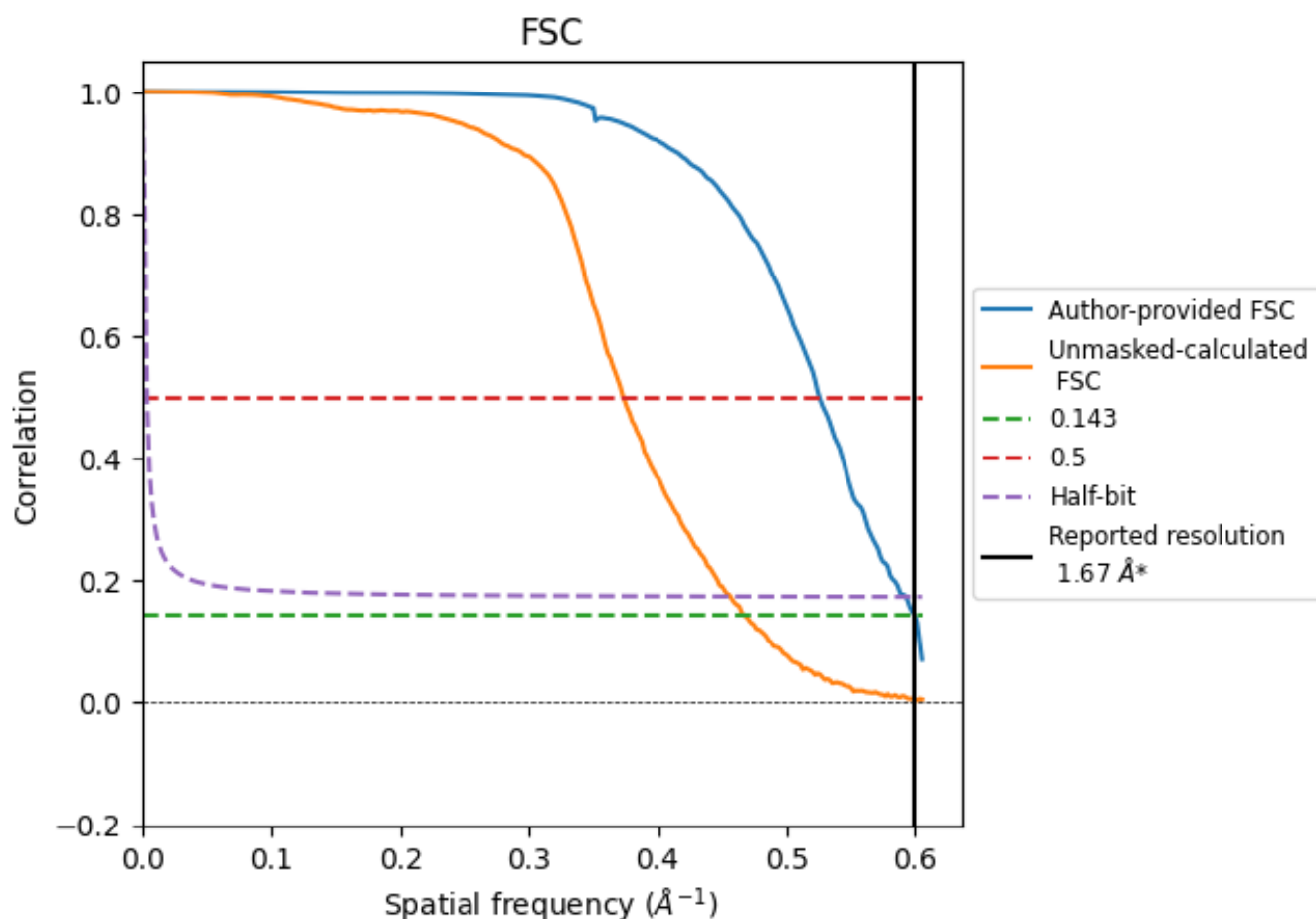


*Reported resolution corresponds to spatial frequency of 0.599 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.599 Å⁻¹

8.2 Resolution estimates [i](#)

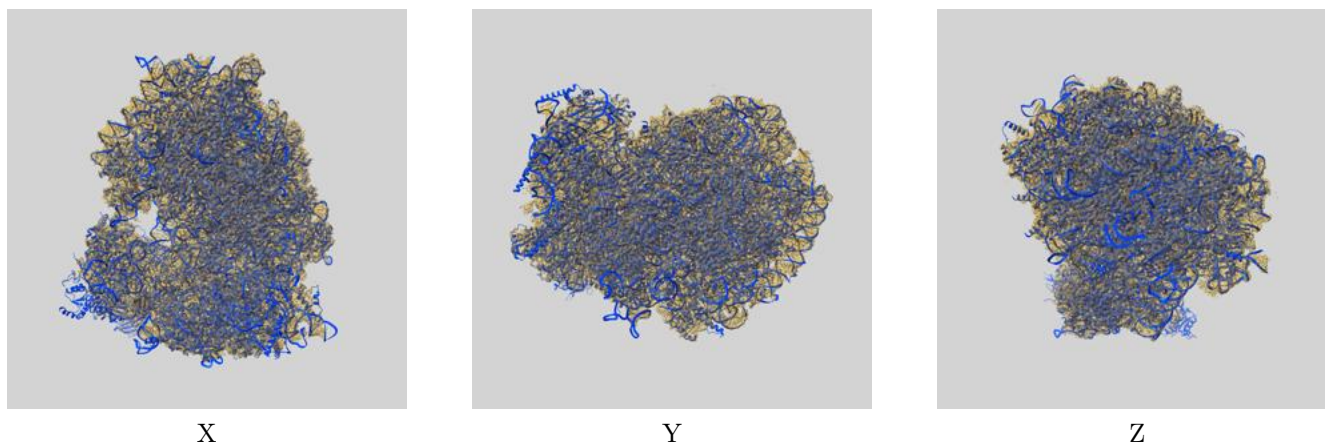
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.67	-	-
Author-provided FSC curve	1.67	1.90	1.69
Unmasked-calculated*	2.14	2.68	2.19

*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 2.14 differs from the reported value 1.67 by more than 10 %

9 Map-model fit [i](#)

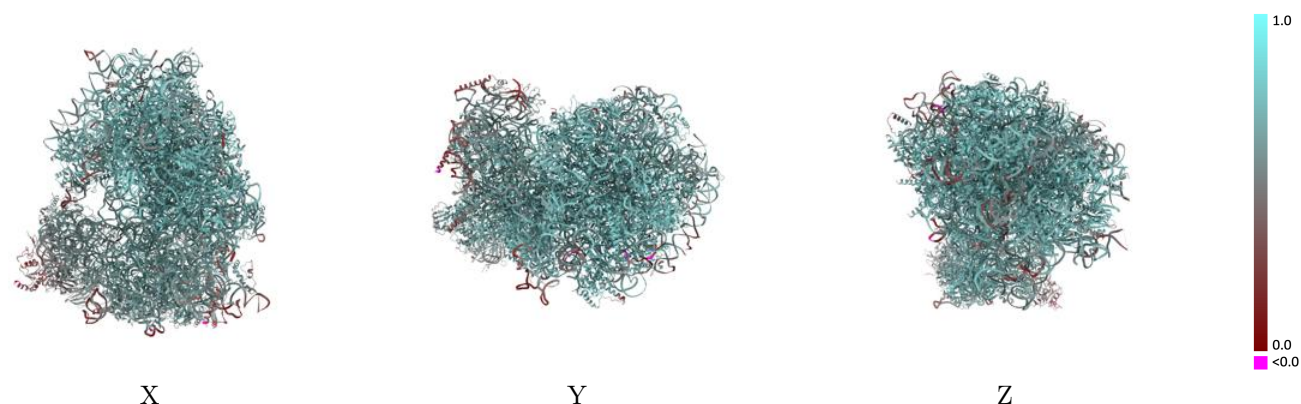
This section contains information regarding the fit between EMDB map EMD-40205 and PDB model 8GLP. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



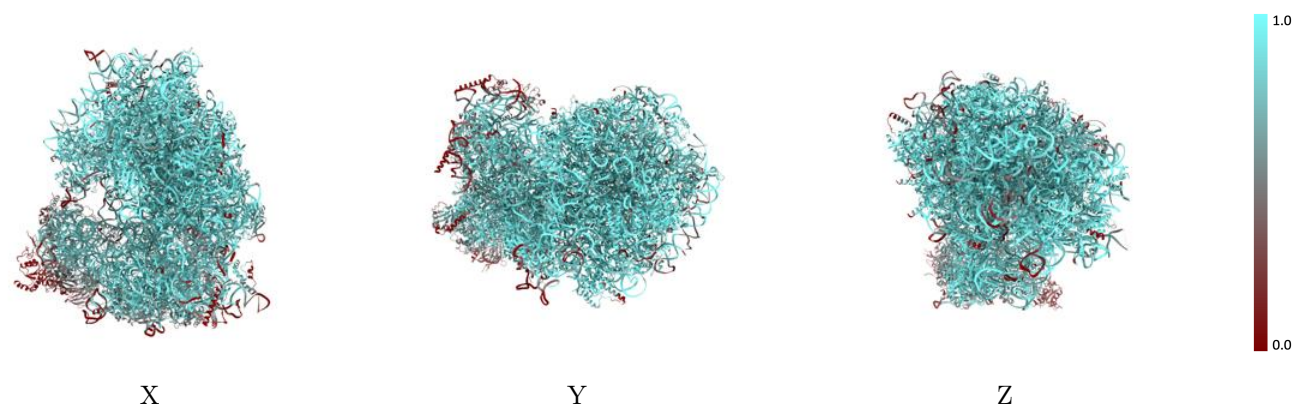
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



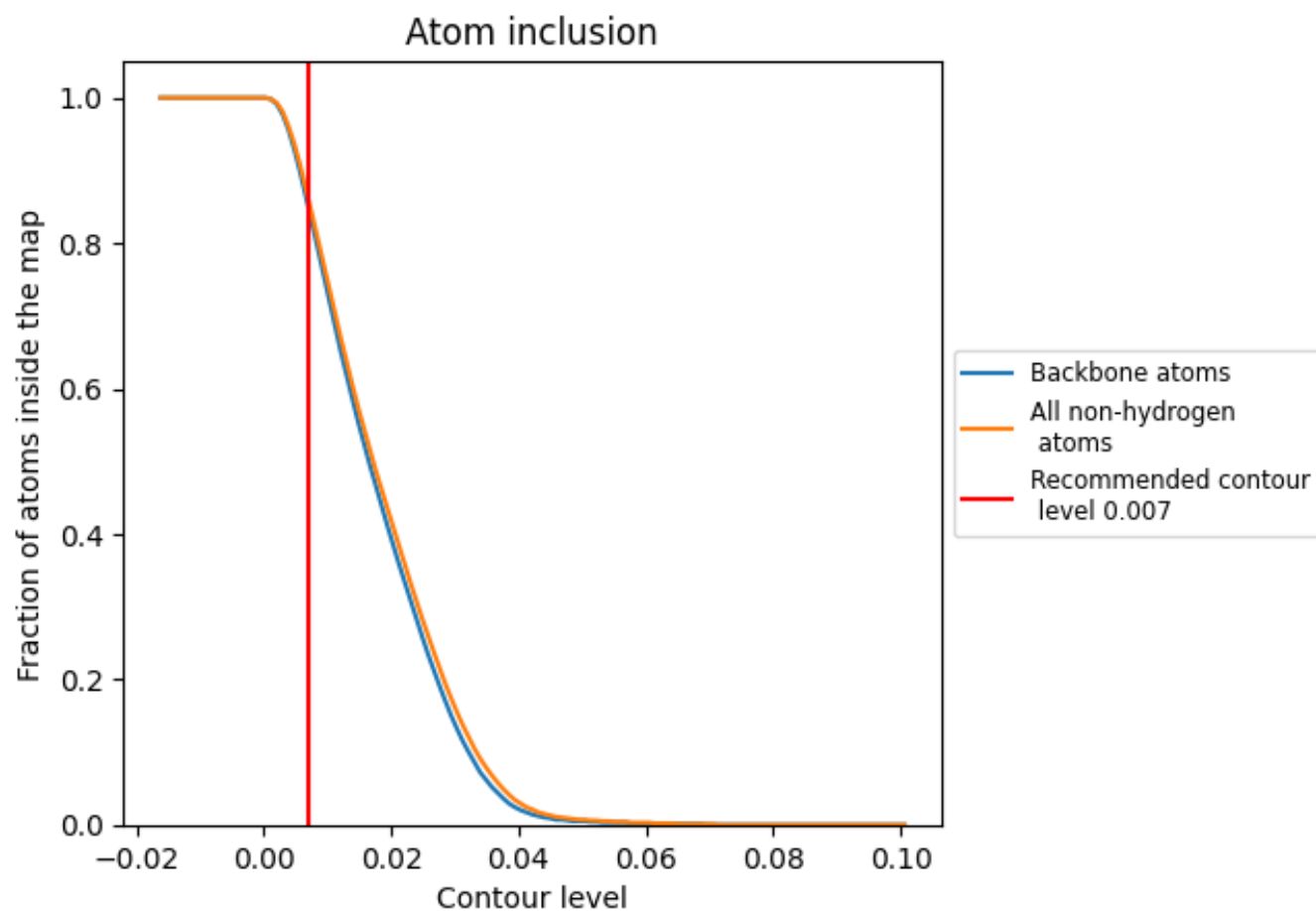
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 86% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.6730
L5	 0.9260	 0.6950
L7	 0.9930	 0.7260
L8	 0.9600	 0.7170
LA	 0.9760	 0.7710
LB	 0.9450	 0.7530
LC	 0.9500	 0.7580
LD	 0.9200	 0.7160
LE	 0.9070	 0.7160
LF	 0.9550	 0.7620
LG	 0.8390	 0.6800
LH	 0.9350	 0.7190
LI	 0.9560	 0.7390
LJ	 0.8800	 0.6850
LL	 0.9100	 0.7240
LM	 0.9490	 0.7300
LN	 0.9980	 0.7780
LO	 0.9540	 0.7570
LP	 0.9600	 0.7640
LQ	 0.9810	 0.7820
LR	 0.8490	 0.6920
LS	 0.9790	 0.7560
LT	 0.9250	 0.7400
LU	 0.8200	 0.6540
LV	 0.9650	 0.7600
LW	 0.5570	 0.5540
LX	 0.9400	 0.7380
LY	 0.9280	 0.7400
LZ	 0.9330	 0.7200
La	 0.9770	 0.7730
Lb	 0.8050	 0.6790
Lc	 0.9110	 0.7260
Ld	 0.9050	 0.7250
Le	 0.9790	 0.7790
Lf	 0.9750	 0.7730



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Chain	Atom inclusion	Q-score
Lg	 0.9050	 0.7370
Lh	 0.9260	 0.7320
Li	 0.9070	 0.7210
Lj	 0.9910	 0.7740
Lk	 0.8270	 0.6840
Ll	 0.9760	 0.7540
Lm	 0.9380	 0.7330
Ln	 0.9500	 0.7320
Lo	 0.9260	 0.7470
Lp	 0.9360	 0.7510
Lr	 0.9660	 0.7620
Pt	 0.4250	 0.6000
S2	 0.8740	 0.6160
SA	 0.7440	 0.6310
SB	 0.7980	 0.6670
SC	 0.8050	 0.6500
SD	 0.5010	 0.5400
SE	 0.7260	 0.6250
SF	 0.6950	 0.6120
SG	 0.5300	 0.5400
SH	 0.5660	 0.5770
SI	 0.7920	 0.6540
SJ	 0.7020	 0.6010
SK	 0.4230	 0.5040
SL	 0.8390	 0.6890
SM	 0.0070	 0.2880
SN	 0.8960	 0.7060
SO	 0.8720	 0.6880
SP	 0.5240	 0.5520
SQ	 0.6820	 0.5980
SR	 0.5890	 0.5660
SS	 0.6750	 0.6080
ST	 0.6510	 0.5890
SU	 0.4910	 0.5240
SV	 0.7630	 0.6480
SW	 0.9200	 0.6950
SX	 0.8780	 0.6760
SY	 0.5720	 0.5590
SZ	 0.5120	 0.5690
Sa	 0.8900	 0.6910
Sb	 0.7210	 0.6440
Sc	 0.5630	 0.5770

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Chain	Atom inclusion	Q-score
Sd	 0.7960	 0.6090
Se	 0.6200	 0.5770
Sf	 0.0620	 0.3100
Sg	 0.2780	 0.4970
mR	 0.2500	 0.4990