



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 09:01 AM EDT

PDB ID : 8G5Y / pdb_00008g5y
EMDB ID : EMD-29757
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (IC state)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-02-14
Resolution : 2.29 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

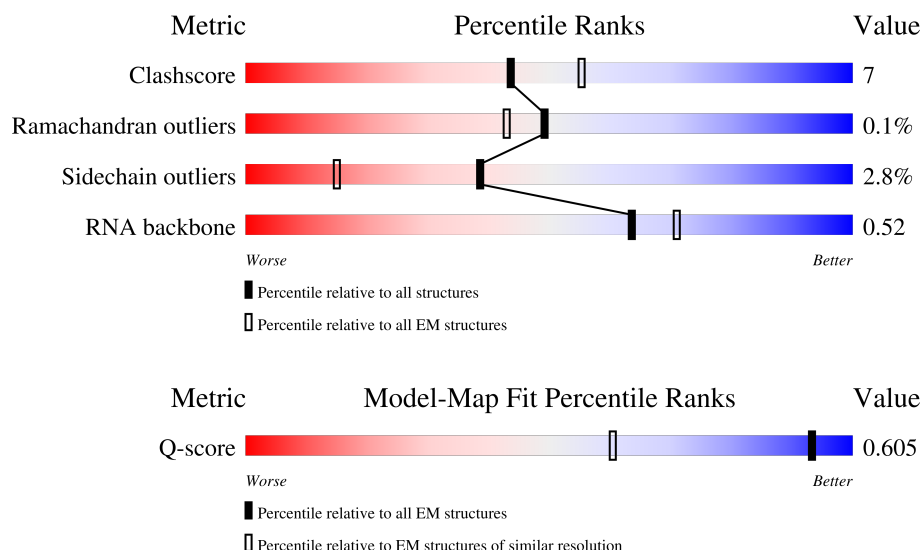
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.29 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.



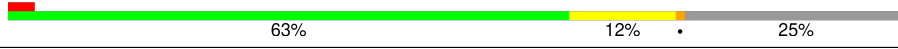
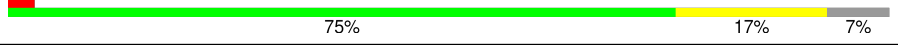
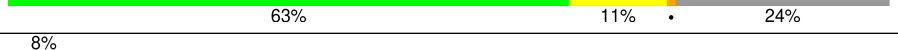
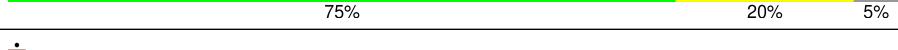
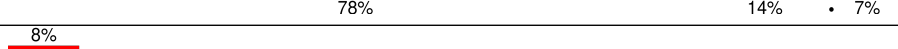
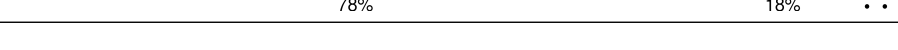
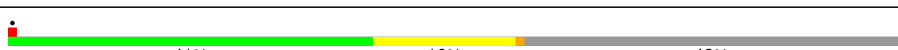
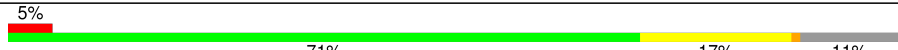
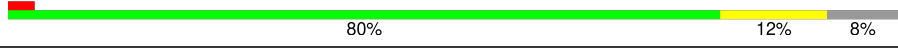
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3699 (1.79 - 2.79)

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	

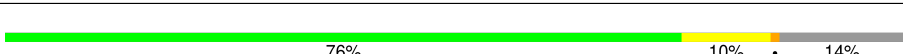
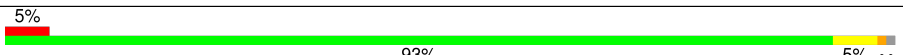
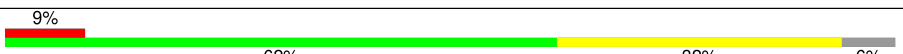
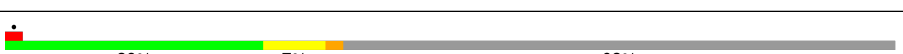
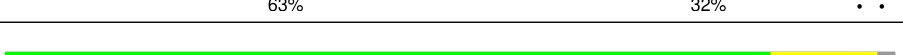
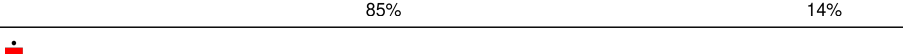
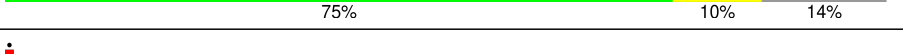
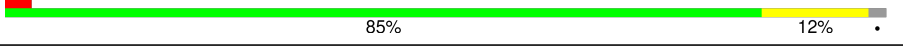
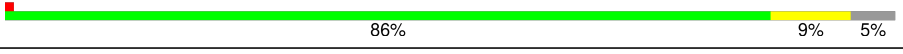
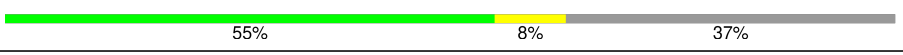
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	SB	264	
6	SA	295	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SG	249	
12	SF	204	
13	SH	194	
14	SW	130	
15	SI	208	
16	SQ	146	
17	SU	119	
18	SK	165	
19	SO	151	
20	SX	143	
21	SM	132	
22	SS	152	
23	Sd	56	
24	SN	151	
25	SL	158	
26	SR	135	
27	SP	145	
28	ST	145	

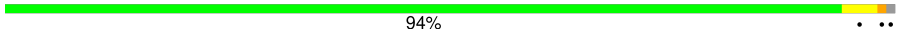
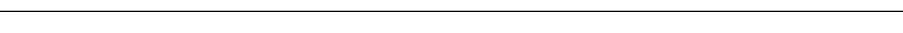
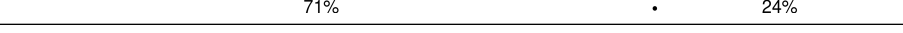
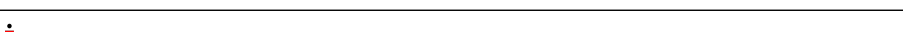
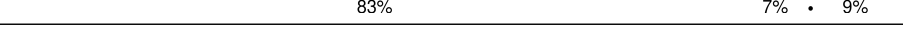
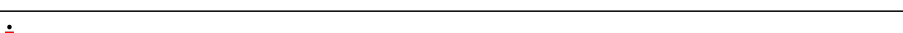
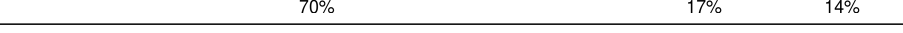
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	Lz	217	
39	LA	257	
40	LB	403	
41	LC	427	
42	LJ	178	
43	LH	192	
44	LE	288	
45	LG	266	
46	LO	203	
47	LL	211	
48	LV	140	
49	LM	215	
50	La	148	
51	LN	204	
52	LI	214	
53	LD	297	

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Mol	Chain	Length	Quality of chain
54	LQ	188	
55	LR	196	
56	LS	176	
57	LT	160	
58	LP	184	
59	LU	128	
60	LX	156	
61	LY	145	
62	LW	157	
63	LZ	136	
64	Lr	137	
65	Lh	123	
66	Lb	159	
67	LF	248	
68	Lc	115	
69	Ld	125	
70	Le	135	
71	Lf	110	
72	Lg	117	
73	Li	105	
74	Lj	97	
75	Lk	70	
76	Ll	51	
77	Lm	128	
78	Ln	25	

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Mol	Chain	Length	Quality of chain
79	Lo	106	
80	Lp	92	
81	mR	60	
82	Pt	77	
83	5A	154	

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
85	PUT	L5	5518	-	-	X	-

2 Entry composition [i](#)

There are 92 unique types of molecules in this entry. The entry contains 219823 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	1680	Total	C	N	O	P	0	0
			35800	16005	6403	11713	1679		

- 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	3721	Total	C	N	O	P	2	0
			79154	35258	14402	25772	3722		

- 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 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 L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	211	Total	C	N	O	S	0	0
			1695	1086	304	297	8		

- Molecule 39 is a protein called uL2.

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

- Molecule 40 is a protein called 60S ribosomal protein L3.

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

- Molecule 41 is a protein called 60S ribosomal protein L4.

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

- Molecule 42 is a protein called 60S ribosomal protein L11.

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

- Molecule 43 is a protein called 60S ribosomal protein L9.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

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

- Molecule 45 is a protein called 60S ribosomal protein L7a.

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

- Molecule 46 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LO	199	Total	C	N	O	S	0	0
			1633	1053	319	256	5		

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LL	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 48 is a protein called 60S ribosomal protein L23.

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

- Molecule 49 is a protein called 60S ribosomal protein L14.

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

- Molecule 50 is a protein called 60S ribosomal protein L27a.

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

- Molecule 51 is a protein called 60S ribosomal protein L15.

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

- Molecule 52 is a protein called 60S ribosomal protein L10.

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

- Molecule 53 is a protein called 60S ribosomal protein L5.

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

- Molecule 54 is a protein called 60S ribosomal protein L18.

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

- Molecule 55 is a protein called 60S ribosomal protein L19.

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

- Molecule 56 is a protein called 60S ribosomal protein L18a.

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

- Molecule 57 is a protein called 60S ribosomal protein L21.

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

- Molecule 58 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LP	153	Total	C	N	O	S	1	0
			1248	780	242	217	9		

- Molecule 59 is a protein called 60S ribosomal protein L22.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L26.

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

- Molecule 62 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LW	118	Total	C	N	O	S	1	0
			955	599	192	159	5		

- Molecule 63 is a protein called 60S ribosomal protein L27.

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

- Molecule 64 is a protein called 60S ribosomal protein L28.

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

- Molecule 65 is a protein called 60S ribosomal protein L35.

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

- Molecule 66 is a protein called 60S ribosomal protein L29.

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

- Molecule 67 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	LF	225	Total	C	N	O	S	0	0
			1869	1202	358	300	9		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 77 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Lm	52	Total	C	N	O	S	0	0
			431	269	90	66	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lo	105	Total	C	N	O	S	2	0
			878	553	180	139	6		

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

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

- Molecule 81 is a RNA chain called mRNA.

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

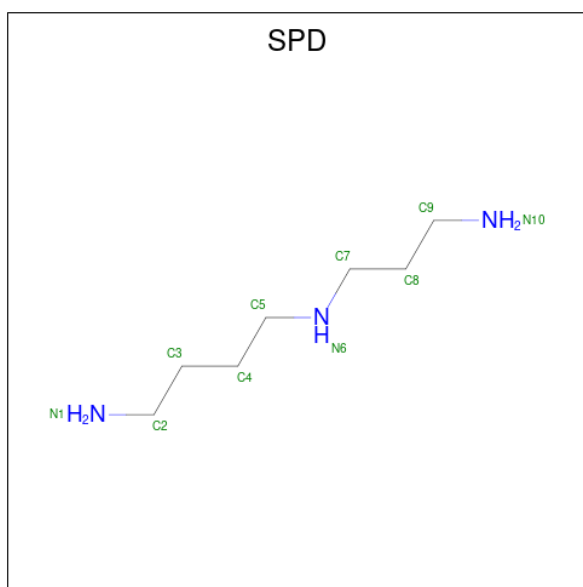
- Molecule 82 is a RNA chain called P-site tRNA.

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

- Molecule 83 is a protein called eIF5A1.

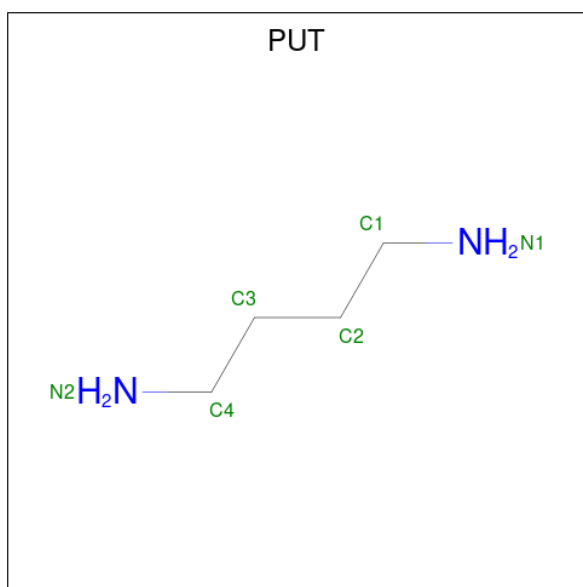
Mol	Chain	Residues	Atoms					AltConf	Trace
83	5A	138	Total	C	N	O	S	1	0
			1073	676	184	204	9		

- Molecule 84 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

- Molecule 85 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

- Molecule 86 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
86	S2	17	Total	K	0
			17	17	

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Mol	Chain	Residues	Atoms	AltConf
86	L8	1	Total K 1 1	0
86	L5	52	Total K 52 52	0
86	L7	1	Total K 1 1	0
86	SL	1	Total K 1 1	0
86	Sa	1	Total K 1 1	0
86	LA	1	Total K 1 1	0
86	LH	1	Total K 1 1	0
86	Lf	1	Total K 1 1	0
86	Lg	1	Total K 1 1	0

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
87	S2	124	Total Mg 124 124	0
87	L8	10	Total Mg 10 10	0
87	L5	344	Total Mg 344 344	0
87	L7	5	Total Mg 5 5	0
87	SJ	1	Total Mg 1 1	0
87	SE	1	Total Mg 1 1	0
87	SC	1	Total Mg 1 1	0
87	SX	1	Total Mg 1 1	0
87	Sd	1	Total Mg 1 1	0
87	SN	1	Total Mg 1 1	0

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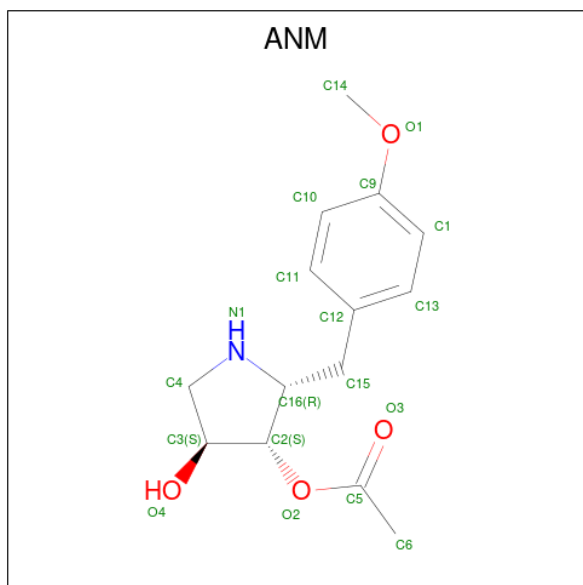
Mol	Chain	Residues	Atoms		AltConf
87	ST	1	Total 1	Mg 1	0
87	Sb	1	Total 1	Mg 1	0
87	LA	2	Total 2	Mg 2	0
87	LB	2	Total 2	Mg 2	0
87	LC	2	Total 2	Mg 2	0
87	LO	1	Total 1	Mg 1	0
87	LL	2	Total 2	Mg 2	0
87	LV	1	Total 1	Mg 1	0
87	LN	1	Total 1	Mg 1	0
87	LI	1	Total 1	Mg 1	0
87	LD	1	Total 1	Mg 1	0
87	LQ	1	Total 1	Mg 1	0
87	LR	2	Total 2	Mg 2	0
87	LS	2	Total 2	Mg 2	0
87	LP	3	Total 3	Mg 3	0
87	Lr	1	Total 1	Mg 1	0
87	Lc	1	Total 1	Mg 1	0
87	Le	1	Total 1	Mg 1	0
87	Lg	1	Total 1	Mg 1	0
87	Lj	1	Total 1	Mg 1	0
87	Lo	1	Total 1	Mg 1	0

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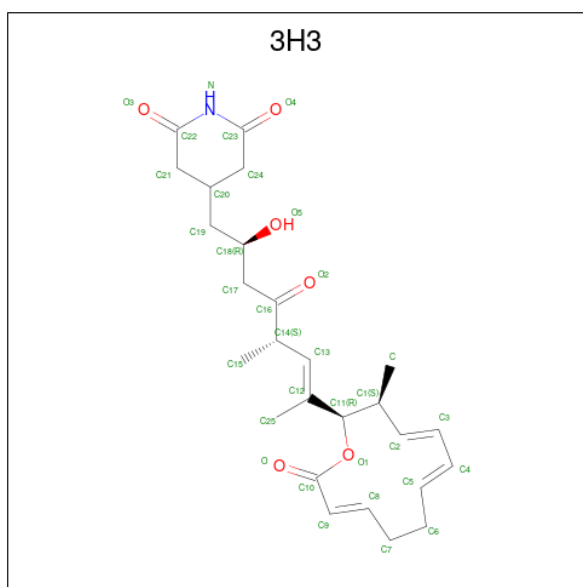
Mol	Chain	Residues	Atoms		AltConf
87	Lp	1	Total	Mg	0
			1	1	
87	Pt	4	Total	Mg	0
			4	4	
87	5A	1	Total	Mg	0
			1	1	

- Molecule 88 is ANISOMYCIN (CCD ID: ANM) (formula: C₁₄H₁₉NO₄).



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

- Molecule 89 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: C₂₆H₃₅NO₆) (labeled as "Ligand of Interest" by depositor).

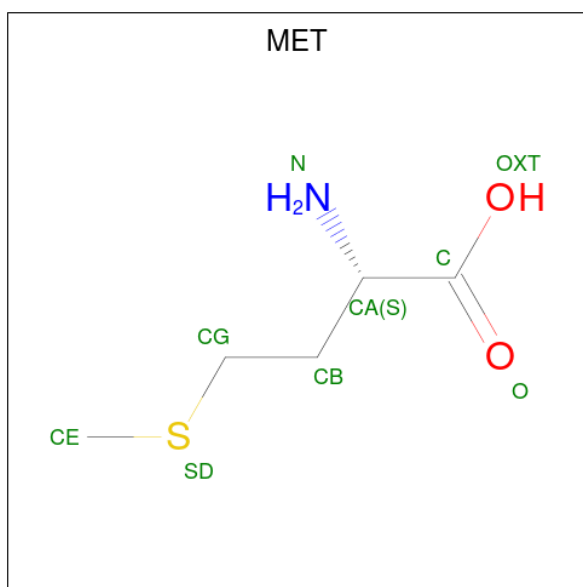


Mol	Chain	Residues	Atoms				AltConf
89	L5	1	Total	C	N	O	0
			33	26	1	6	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 91 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



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

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	S2	123	Total	O	0
			123	123	
92	L8	11	Total	O	0
			11	11	
92	L5	996	Total	O	0
			996	996	
92	L7	8	Total	O	0
			8	8	
92	SA	1	Total	O	0
			1	1	
92	SF	1	Total	O	0
			1	1	
92	SQ	1	Total	O	0
			1	1	
92	SS	1	Total	O	0
			1	1	
92	SN	1	Total	O	0
			1	1	
92	Sa	3	Total	O	0
			3	3	
92	LA	18	Total	O	0
			18	18	

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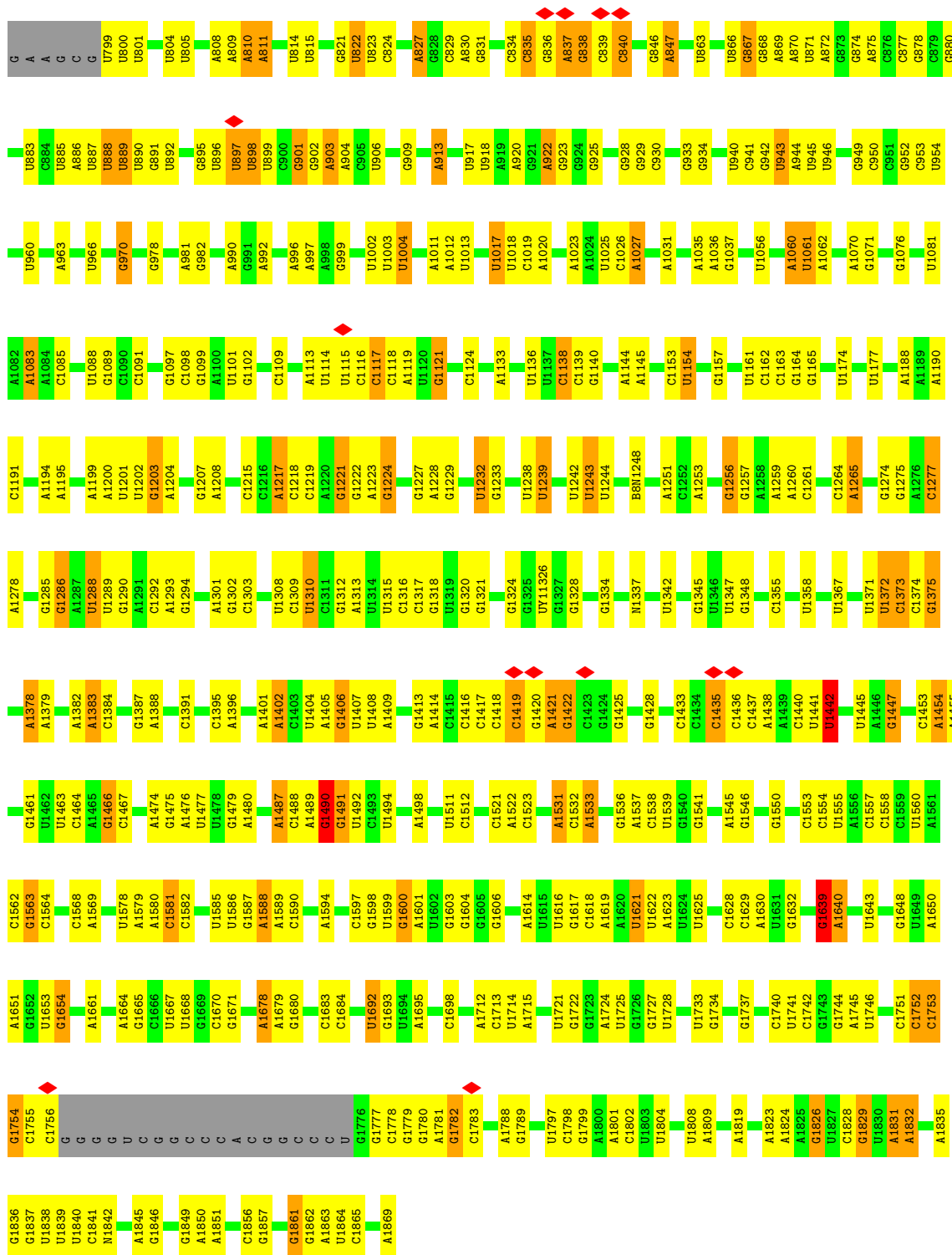
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Mol	Chain	Residues	Atoms		AltConf
92	LB	8	Total 8	O 8	0
92	LC	21	Total 21	O 21	0
92	LO	3	Total 3	O 3	0
92	LL	3	Total 3	O 3	0
92	LV	2	Total 2	O 2	0
92	La	10	Total 10	O 10	0
92	LN	4	Total 4	O 4	0
92	LI	2	Total 2	O 2	0
92	LD	1	Total 1	O 1	0
92	LQ	6	Total 6	O 6	0
92	LR	1	Total 1	O 1	0
92	LT	1	Total 1	O 1	0
92	LP	2	Total 2	O 2	0
92	LX	2	Total 2	O 2	0
92	LZ	1	Total 1	O 1	0
92	Lr	1	Total 1	O 1	0
92	Lb	2	Total 2	O 2	0
92	LF	4	Total 4	O 4	0
92	Lc	1	Total 1	O 1	0
92	Ld	1	Total 1	O 1	0
92	Le	14	Total 14	O 14	0

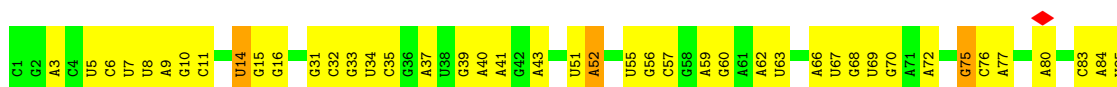
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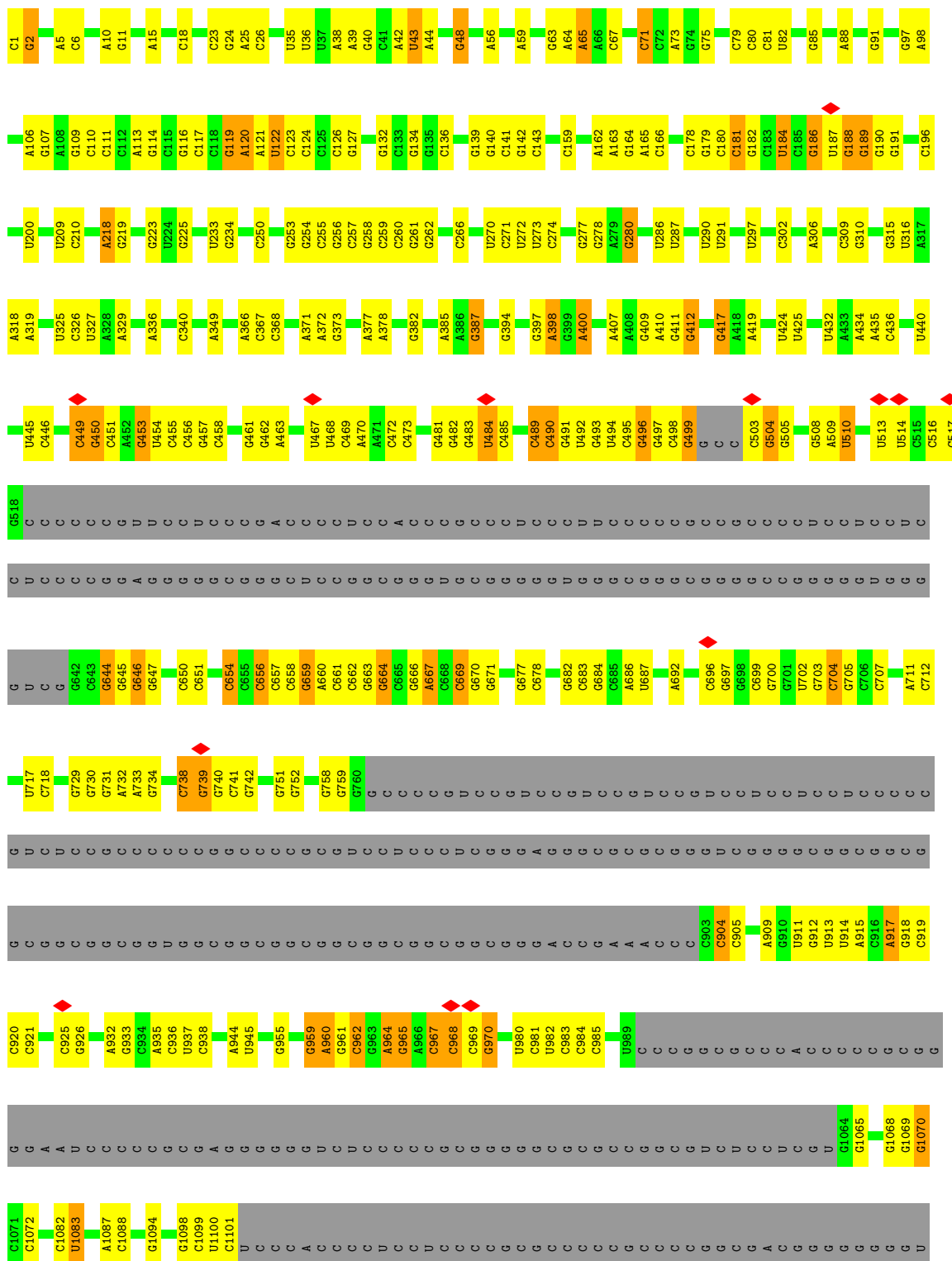
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Mol	Chain	Residues	Atoms		AltConf
92	Lf	3	Total 3	O 3	0
92	Lg	4	Total 4	O 4	0
92	Lj	6	Total 6	O 6	0
92	Ln	1	Total 1	O 1	0
92	Lo	1	Total 1	O 1	0
92	Lp	2	Total 2	O 2	0
92	Pt	1	Total 1	O 1	0
92	5A	1	Total 1	O 1	0



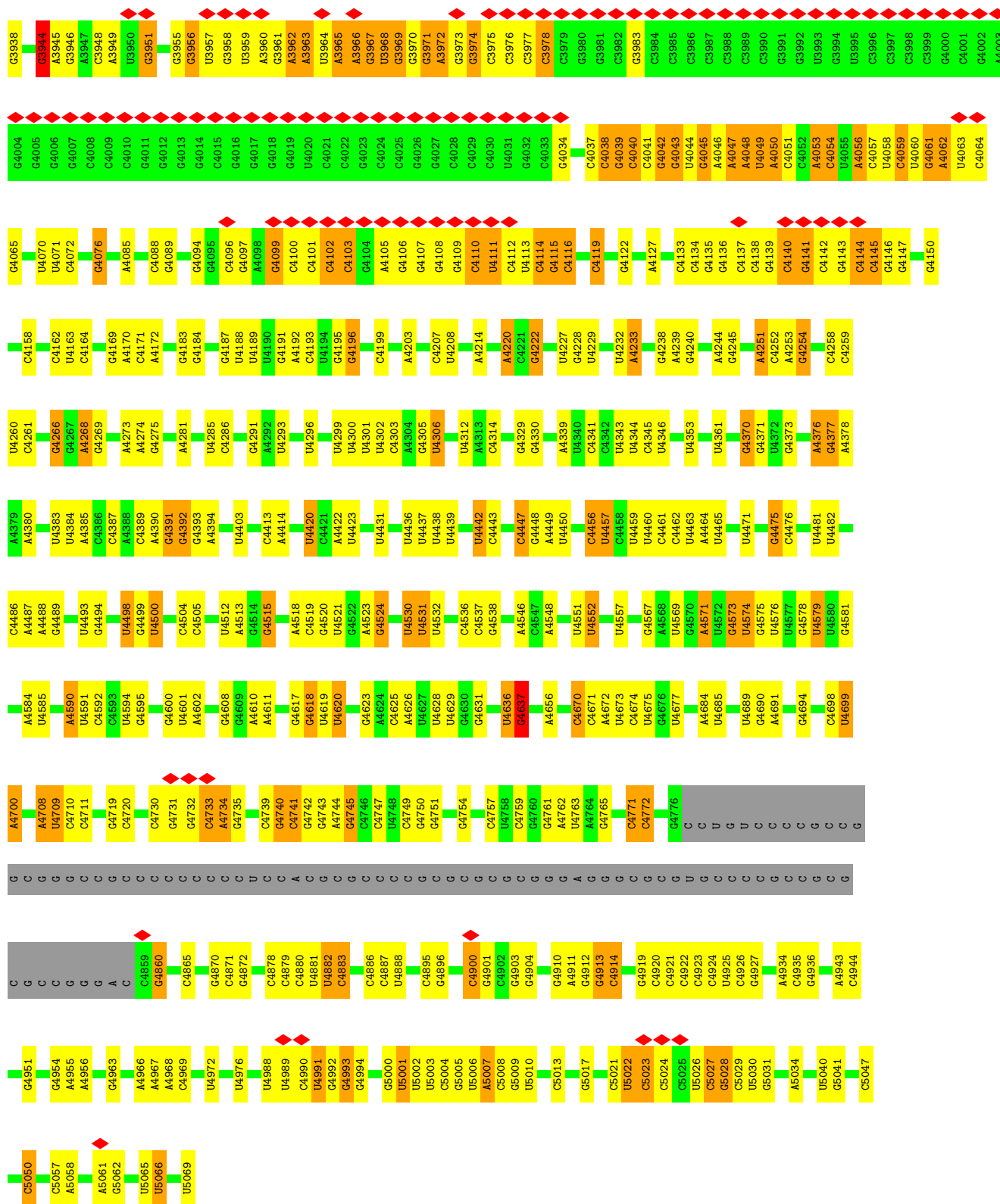
• Molecule 2: 5.8S rRNA









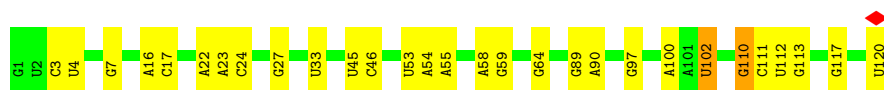


• Molecule 4: 5S rRNA

Chain L7:

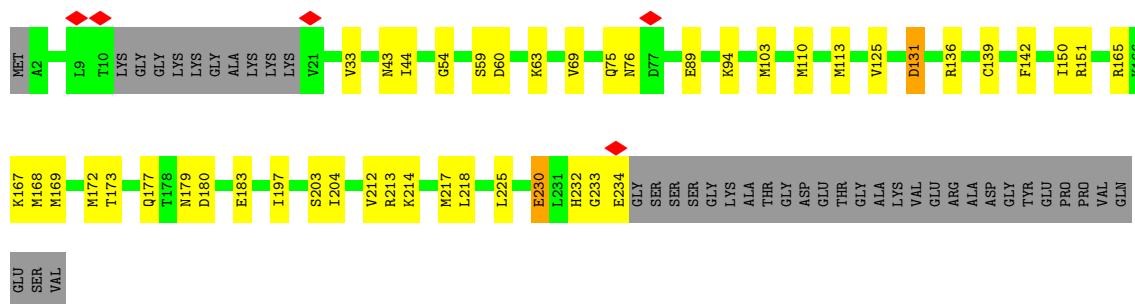
76%

22%



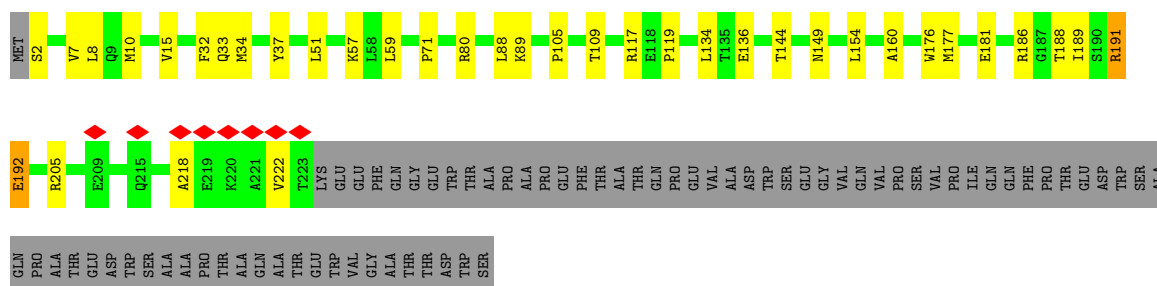
- Molecule 5: 40S ribosomal protein S3a

Chain SB: 67% 16% 16%



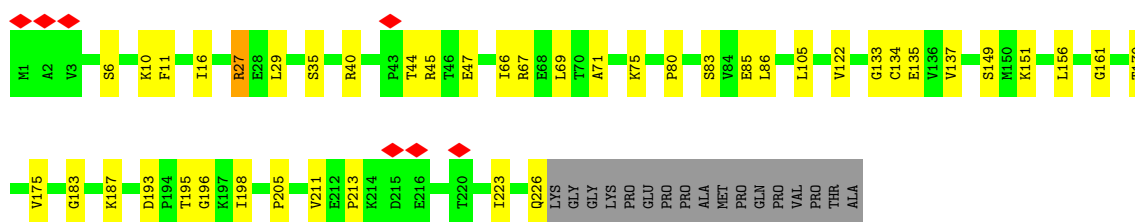
- Molecule 6: 40S ribosomal protein SA

Chain SA: 63% 12% 25%



- Molecule 7: 40S ribosomal protein S3

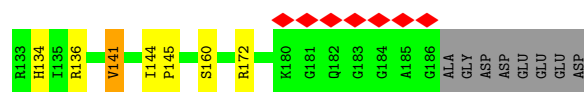
Chain SD: 75% 17% 7%



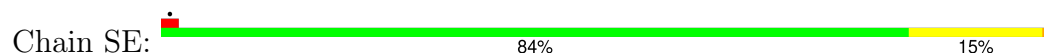
- Molecule 8: 40S ribosomal protein S9

Chain SJ: 74% 20% 5%

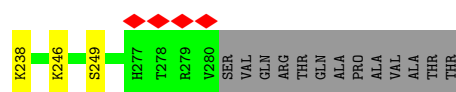
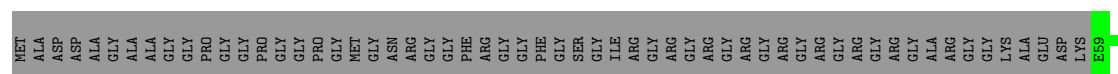




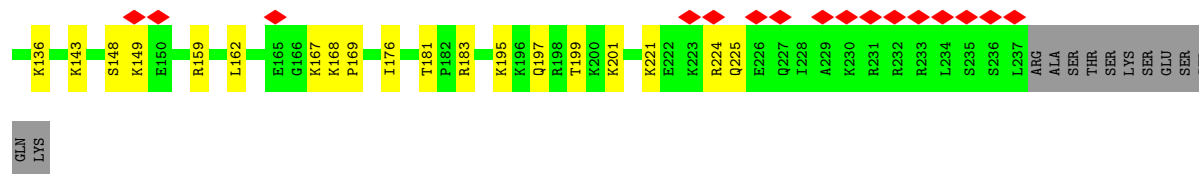
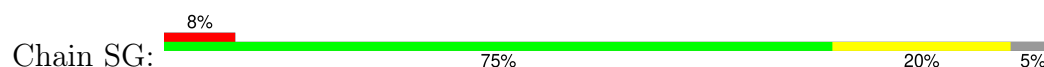
- Molecule 9: 40S ribosomal protein S4, X isoform



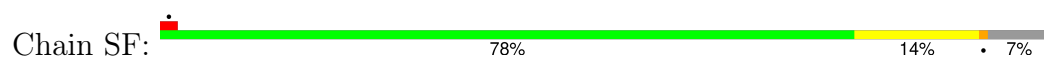
- Molecule 10: 40S ribosomal protein S2



- Molecule 11: 40S ribosomal protein S6

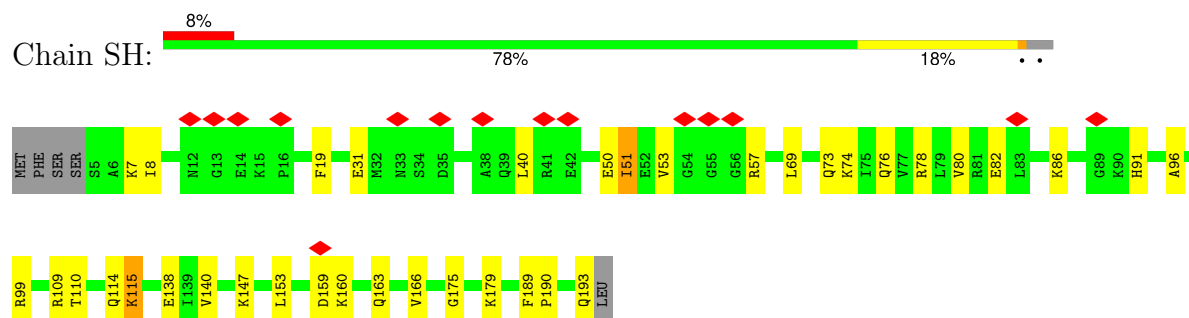


- Molecule 12: 40S ribosomal protein S5

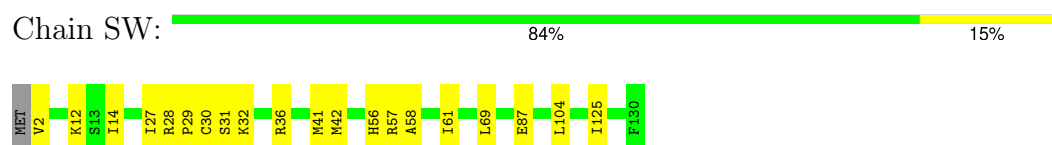




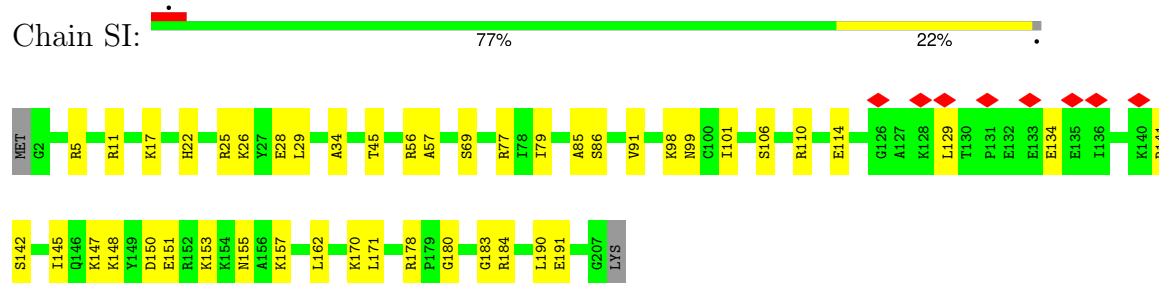
- Molecule 13: 40S ribosomal protein S7



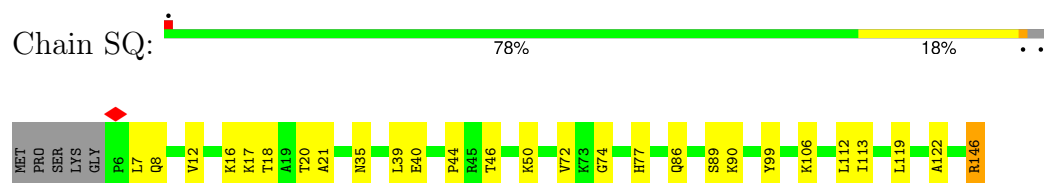
- Molecule 14: 40S ribosomal protein S15a



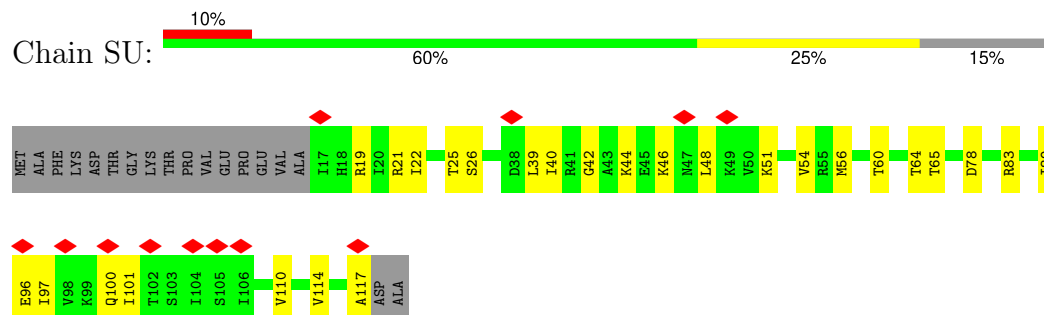
- Molecule 15: 40S ribosomal protein S8



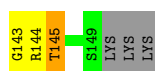
- Molecule 16: 40S ribosomal protein S16



- Molecule 17: 40S ribosomal protein S20



- | NET |
|------|
| S2 |
| L13 |
| R14 |
| V15 |
| L16 |
| N17 |
| I20 |
| D21 |
| G22 |
| K34 |
| G35 |
| V36 |
| G37 |
| D51 |
| L52 |
| T53 |
| K54 |
| R55 |
| A56 |
| V64 |
| V67 |
| I68 |
| M71 |
| Q72 |
| R75 |
| D92 |
| G93 |
| K94 |
| L99 |
| L103 |
| D104 |
| N105 |
| E109 |
| D110 |
| R113 |
| K116 |
| I117 |
| R124 |
| L129 |
| T136 |
| R142 |



- Molecule 23: 40S ribosomal protein S29

Chain Sd: 79% 18% ..



- Molecule 24: 40S ribosomal protein S13

Chain SN: 79% 20% ..



- Molecule 25: 40S ribosomal protein S11

Chain SL: 80% 12% 8%



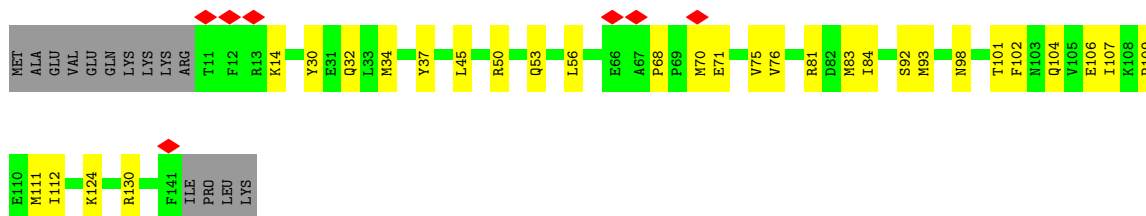
- Molecule 26: 40S ribosomal protein S17

Chain SR: 68% 27% ..



- Molecule 27: 40S ribosomal protein S15

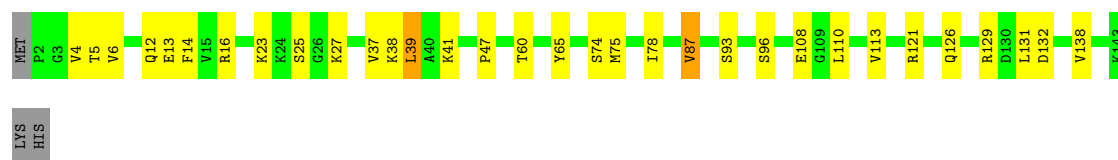
Chain SP: 5% 70% 21% 10%



- Molecule 28: 40S ribosomal protein S19

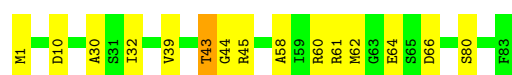


Chain ST:  76% 21% ..



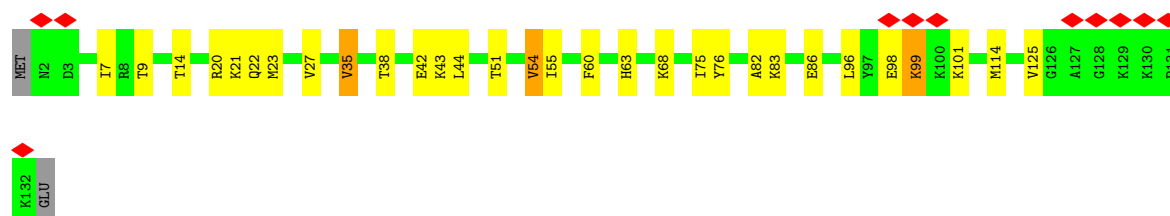
- Molecule 29: 40S ribosomal protein S21

Chain SV:  82% 17% .



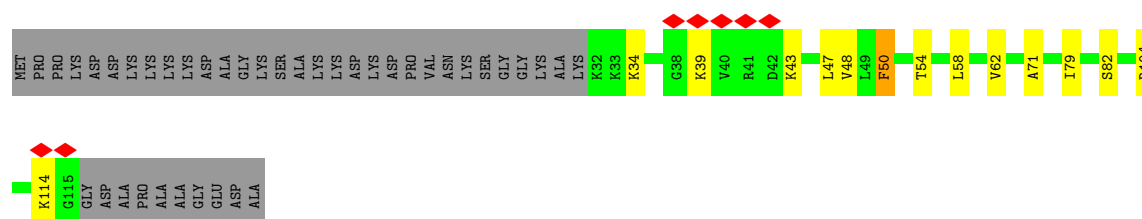
- Molecule 30: 40S ribosomal protein S24

Chain SY:  8% 76% 20% ..



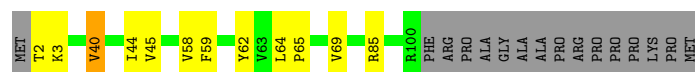
- Molecule 31: 40S ribosomal protein S25

Chain SZ:  6% 56% 10% 33%

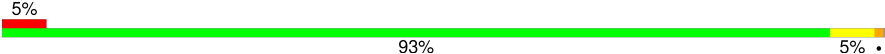


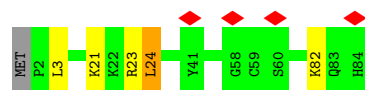
- Molecule 32: 40S ribosomal protein S26

Chain Sa:  76% 10% 14%



- Molecule 33: 40S ribosomal protein S27

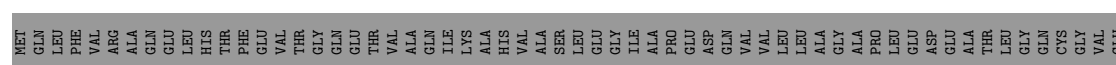
Chain Sb:  5% 93% 5% ..



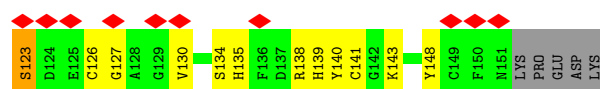
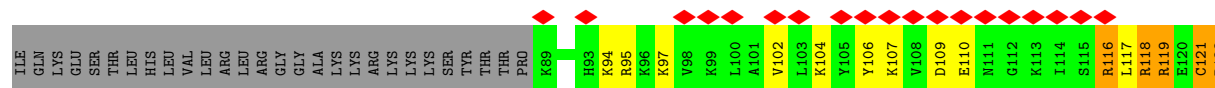
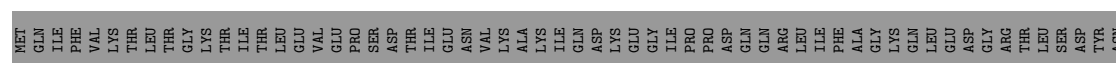
- Molecule 34: 40S ribosomal protein S28



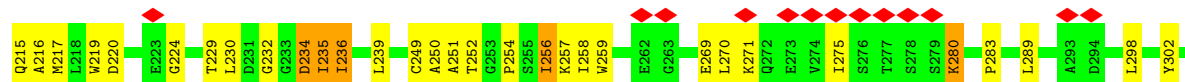
- Molecule 35: FAU ubiquitin-like and ribosomal protein S30

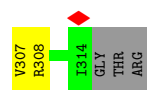


- Molecule 36: Ubiquitin-40S ribosomal protein S27a

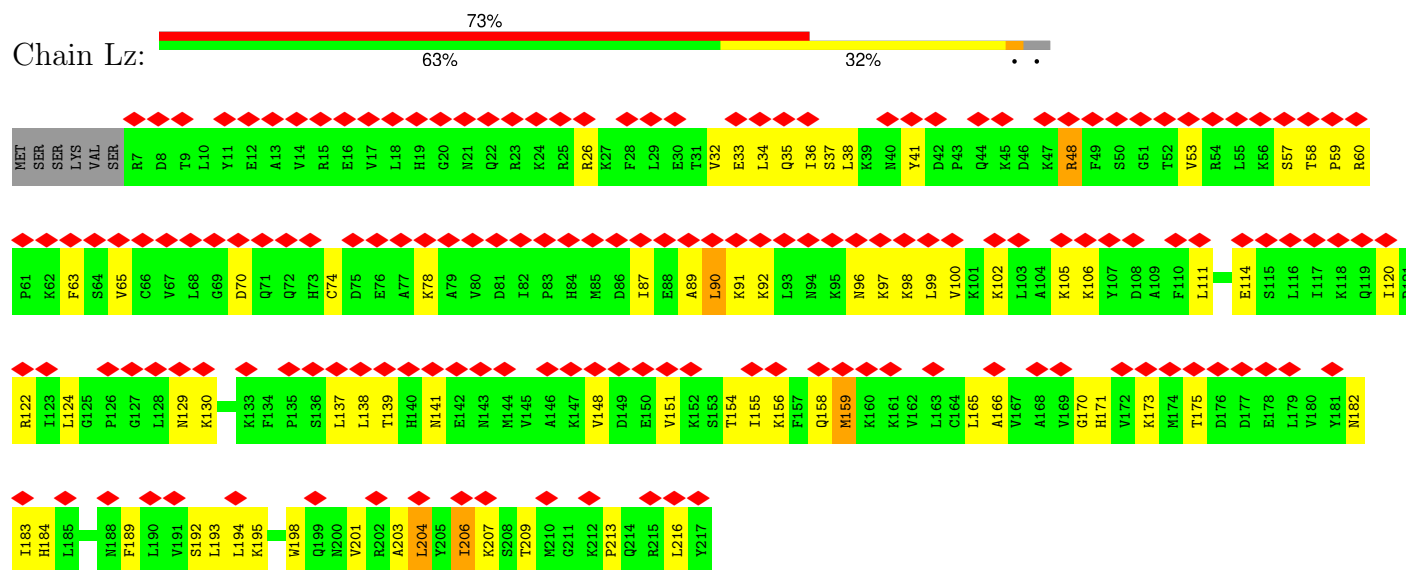


- Molecule 37: Receptor of activated protein C kinase 1

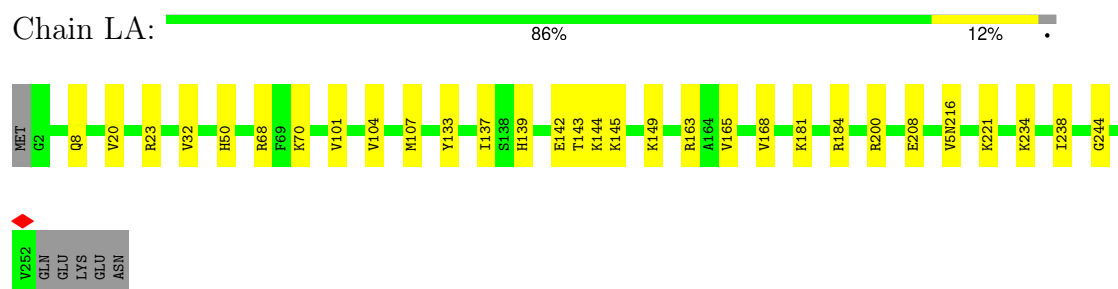




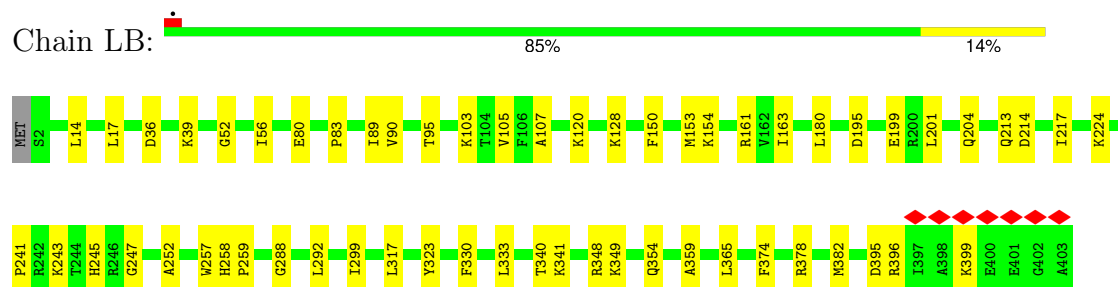
• Molecule 38: 60S ribosomal protein L10a



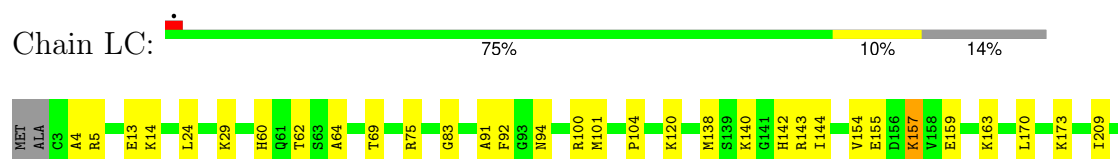
• Molecule 39: uL2

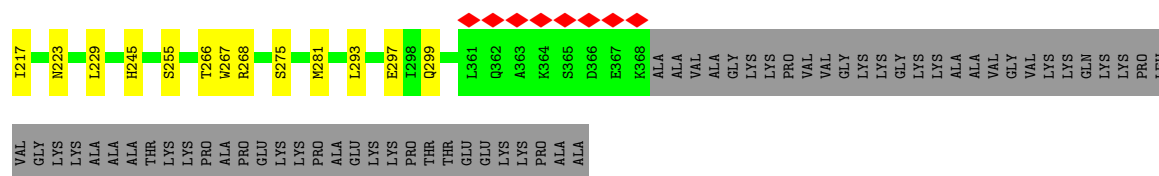


• Molecule 40: 60S ribosomal protein L3

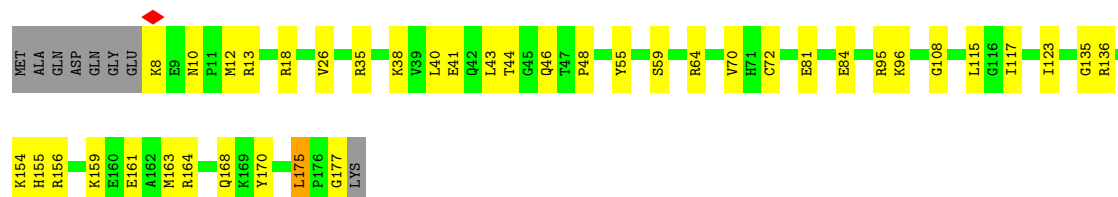
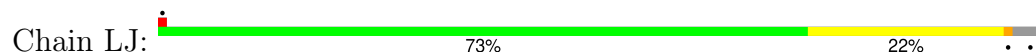


• Molecule 41: 60S ribosomal protein L4

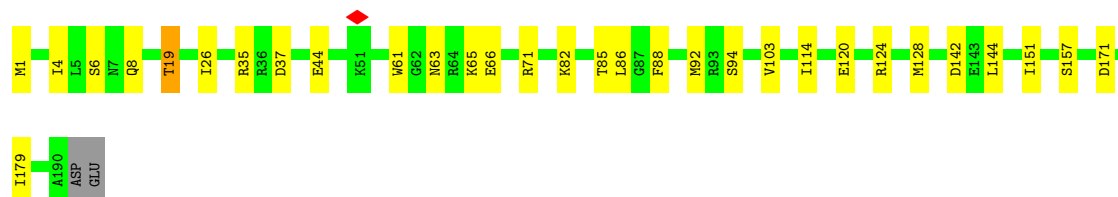
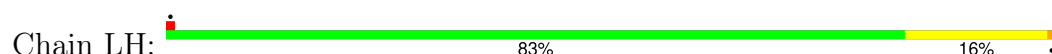




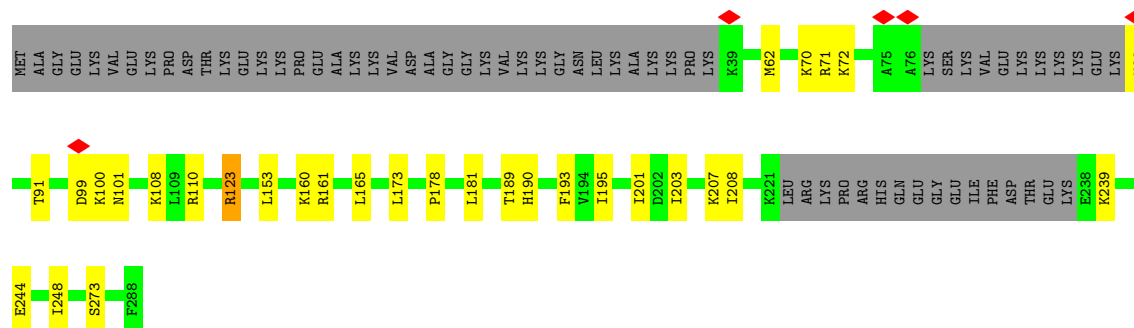
• Molecule 42: 60S ribosomal protein L11



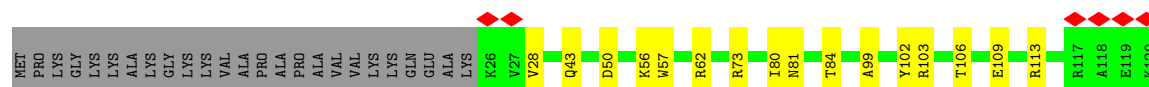
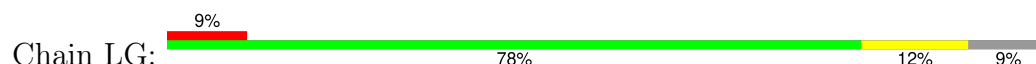
• Molecule 43: 60S ribosomal protein L9



• Molecule 44: 60S ribosomal protein L6

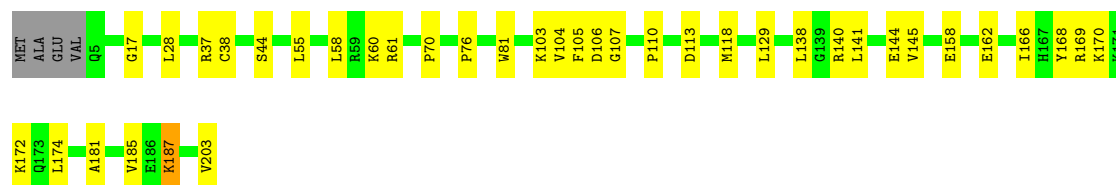
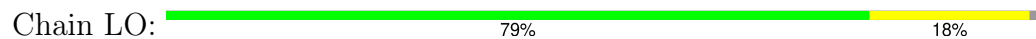


• Molecule 45: 60S ribosomal protein L7a

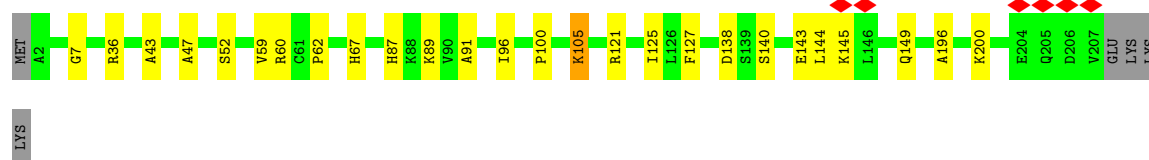
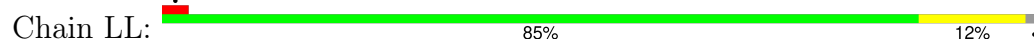




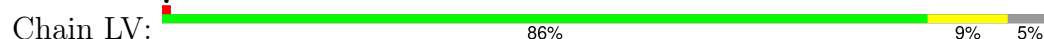
- Molecule 46: 60S ribosomal protein L13a



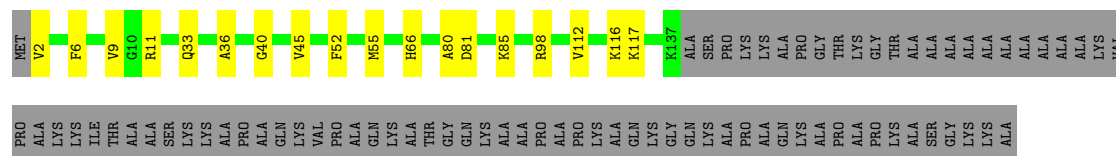
- Molecule 47: 60S ribosomal protein L13



- Molecule 48: 60S ribosomal protein L23



- Molecule 49: 60S ribosomal protein L14



- Molecule 50: 60S ribosomal protein L27a



- Molecule 51: 60S ribosomal protein L15

Chain LN:  88% 11%



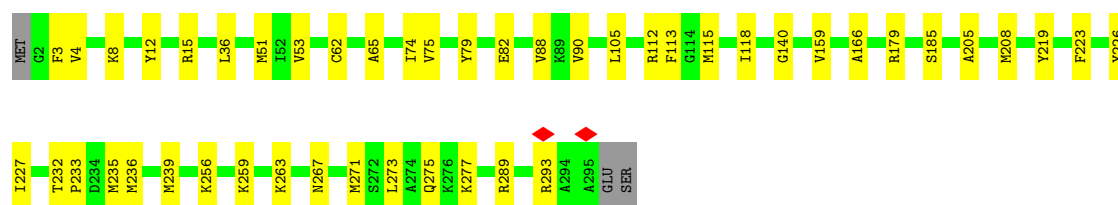
- Molecule 52: 60S ribosomal protein L10

Chain LI:  77% 17% 5%

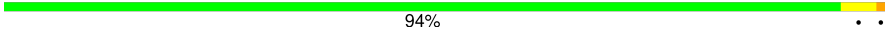


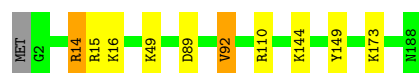
- Molecule 53: 60S ribosomal protein L5

Chain LD:  83% 16%



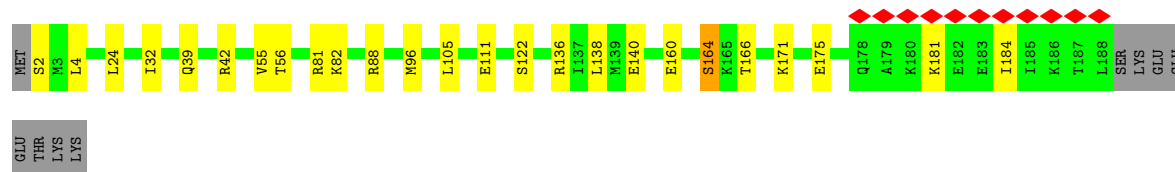
- Molecule 54: 60S ribosomal protein L18

Chain LQ:  94%



- Molecule 55: 60S ribosomal protein L19

Chain LR:  6% 83% 12% 5%



- Molecule 56: 60S ribosomal protein L18a

Chain LS:  90% 10%



- Molecule 57: 60S ribosomal protein L21

Chain LT:  87% 12%



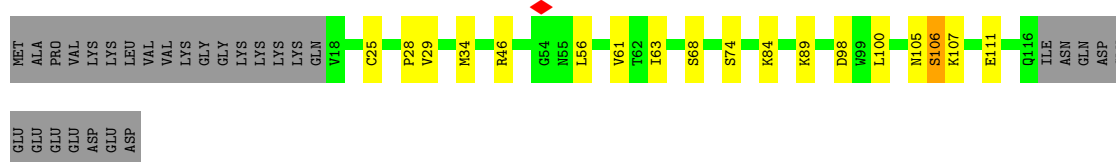
- Molecule 58: 60S ribosomal protein L17

Chain LP:  72% 11% 17%



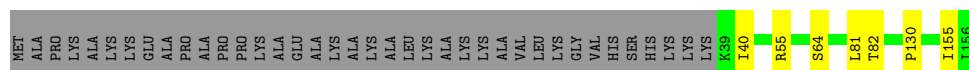
- Molecule 59: 60S ribosomal protein L22

Chain LU:  63% 13% 23%



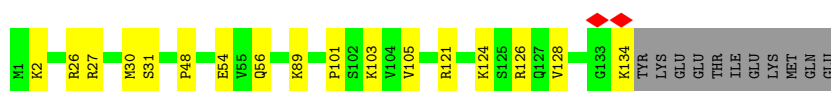
- Molecule 60: 60S ribosomal protein L23a

Chain LX:  71% 24%



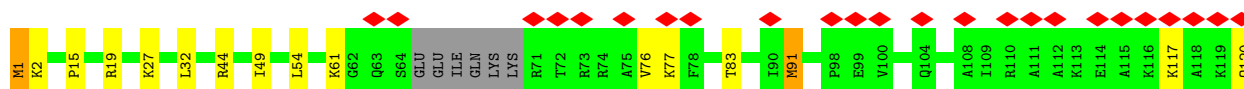
- Molecule 61: 60S ribosomal protein L26

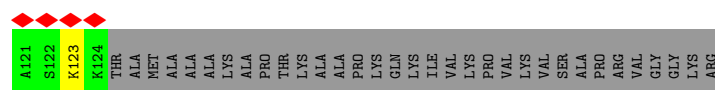
Chain LY:  81% 12% 8%



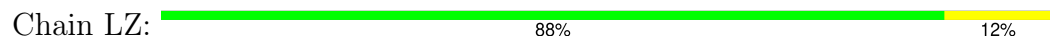
- Molecule 62: 60S ribosomal protein L24

Chain LW:  18% 64% 10% 25%

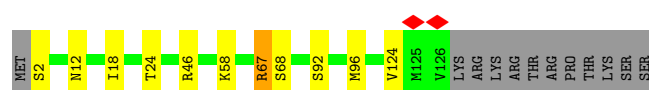
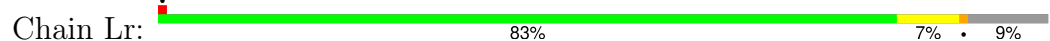




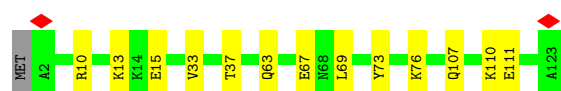
- Molecule 63: 60S ribosomal protein L27



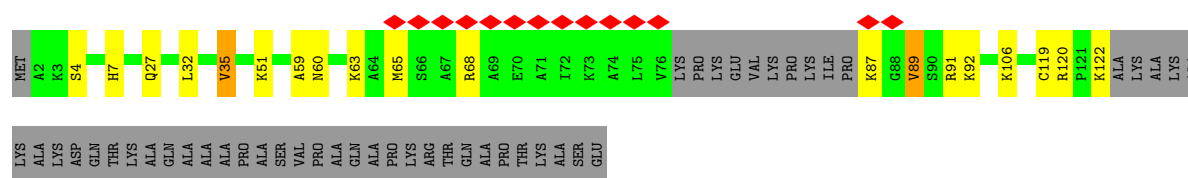
- Molecule 64: 60S ribosomal protein L28



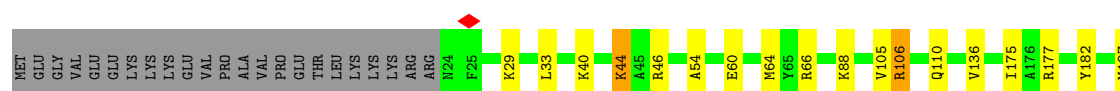
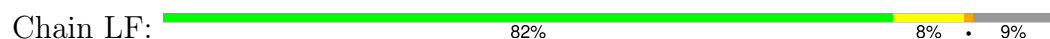
- Molecule 65: 60S ribosomal protein L35



- Molecule 66: 60S ribosomal protein L29



- Molecule 67: 60S ribosomal protein L7

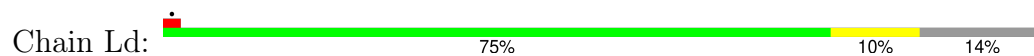


- Molecule 68: 60S ribosomal protein L30

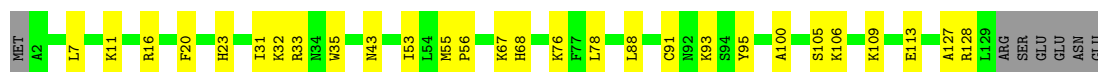




- Molecule 69: 60S ribosomal protein L31



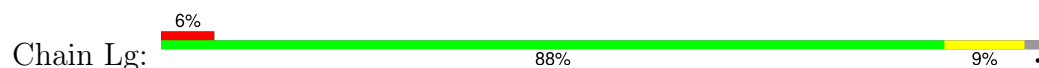
- Molecule 70: 60S ribosomal protein L32



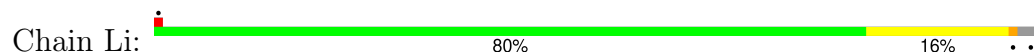
- Molecule 71: 60S ribosomal protein L35a



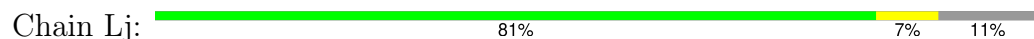
- Molecule 72: 60S ribosomal protein L34



- Molecule 73: 60S ribosomal protein L36



- Molecule 74: 60S ribosomal protein L37



- Molecule 75: 60S ribosomal protein L38

Chain Lk:  74% 23% ..



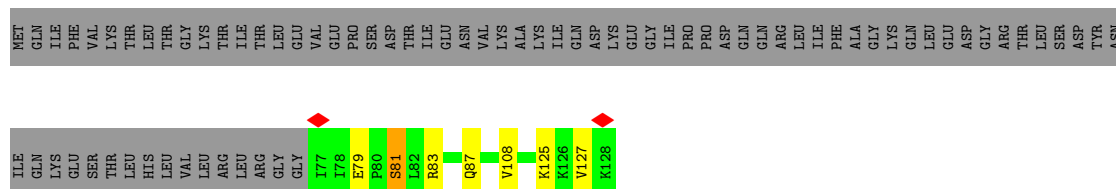
- Molecule 76: 60S ribosomal protein L39

Chain Ll:  90% 8% .



- Molecule 77: eL40

Chain Lm:  35% 5% 59%



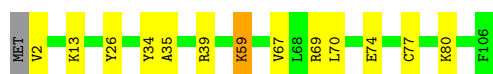
- Molecule 78: 60S ribosomal protein L41

Chain Ln:  84% 16%

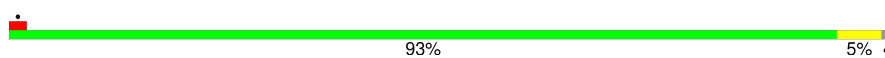


- Molecule 79: 60S ribosomal protein L36a

Chain Lo:  87% 11% ..



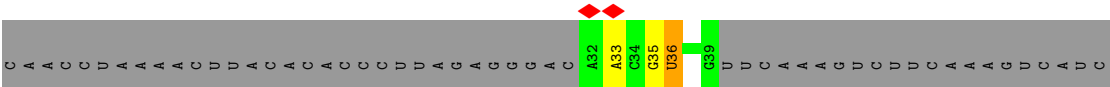
- Molecule 80: 60S ribosomal protein L37a

Chain Lp:  93% 5% .

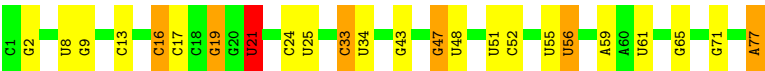


- Molecule 81: mRNA

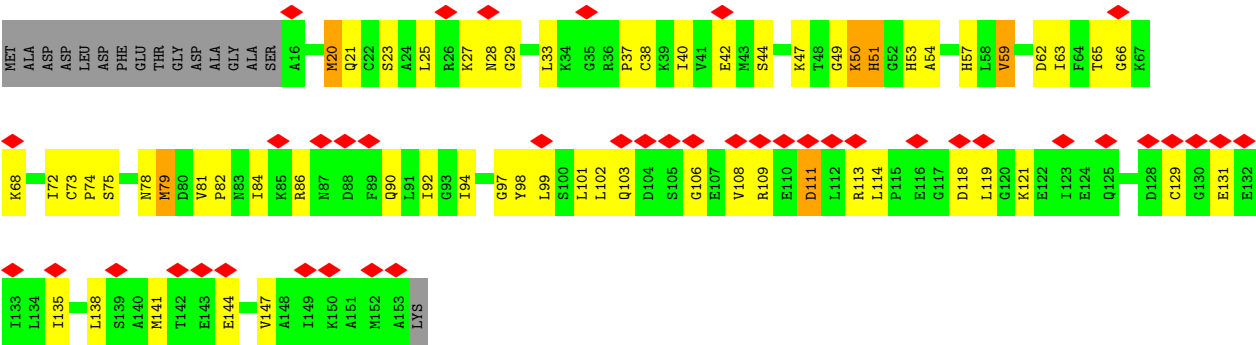
Chain mR:  8% 87%



• Molecule 82: P-site tRNA



• Molecule 83: eIF5A1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55836	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	0.053	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	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: AME, ANM, SAC, HIC, MLZ, ZN, PSU, A2M, H2U, 1MA, 5MC, 4AC, HY3, MA6, 3H3, 6MZ, UR3, MG, PUT, K, 4SU, B8N, G7M, OMU, OMG, UY1, SPD, V5N, 5CT, OMC, M3L

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	0.38	1/38000 (0.0%)	0.37	0/59217
2	L8	0.44	0/3609	0.42	0/5623
3	L5	0.44	3/85432 (0.0%)	0.44	2/133204 (0.0%)
4	L7	0.43	0/2858	0.37	0/4455
5	SB	0.27	0/1832	0.39	0/2449
6	SA	0.31	0/1778	0.39	0/2416
7	SD	0.27	0/1784	0.37	0/2403
8	SJ	0.25	0/1550	0.30	0/2069
9	SE	0.28	0/2118	0.37	0/2849
10	SC	0.29	0/1762	0.35	0/2381
11	SG	0.23	0/1946	0.41	0/2590
12	SF	0.28	0/1515	0.40	0/2037
13	SH	0.23	0/1540	0.42	0/2064
14	SW	0.34	0/1051	0.50	0/1406
15	SI	0.30	0/1715	0.40	0/2287
16	SQ	0.28	0/1141	0.38	0/1528
17	SU	0.28	0/813	0.38	0/1092
18	SK	0.27	0/834	0.47	0/1125
19	SO	0.29	0/1022	0.43	1/1372 (0.1%)
20	SX	0.31	0/1096	0.36	0/1461
21	SM	0.18	0/960	0.49	0/1286
22	SS	0.25	0/1232	0.37	0/1651
23	Sd	0.29	0/469	0.41	0/623
24	SN	0.30	0/1242	0.35	0/1671
25	SL	0.32	0/1221	0.38	0/1632
26	SR	0.40	0/1097	0.57	1/1474 (0.1%)
27	SP	0.25	0/1100	0.39	0/1470
28	ST	0.26	0/1148	0.39	0/1540
29	SV	0.33	0/635	0.40	0/850
30	SY	0.24	0/1083	0.38	0/1438
31	SZ	0.22	0/682	0.33	0/911

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.31	0/816	0.37	0/1093
33	Sb	0.28	0/665	0.39	0/891
34	Sc	0.26	0/514	0.42	0/688
35	Se	0.22	0/396	0.29	0/519
36	Sf	0.44	0/525	0.69	0/695
37	Sg	0.26	0/2493	0.47	0/3394
38	Lz	0.20	0/1723	0.45	0/2313
39	LA	0.38	0/1958	0.48	0/2623
40	LB	0.33	0/3294	0.40	0/4406
41	LC	0.38	0/2968	0.46	0/3985
42	LJ	0.27	0/1385	0.37	0/1852
43	LH	0.29	0/1537	0.32	0/2066
44	LE	0.28	0/1820	0.35	0/2442
45	LG	0.29	0/1959	0.37	0/2637
46	LO	0.35	0/1665	0.41	0/2228
47	LL	0.34	0/1695	0.46	0/2270
48	LV	0.32	0/1002	0.41	0/1345
49	LM	0.30	0/1142	0.32	0/1527
50	La	0.41	0/1178	0.50	0/1573
51	LN	0.43	0/1745	0.51	0/2338
52	LI	0.30	0/1683	0.36	0/2247
53	LD	0.29	0/2437	0.35	0/3263
54	LQ	0.37	0/1536	0.49	0/2052
55	LR	0.29	0/1582	0.34	0/2091
56	LS	0.36	0/1500	0.39	0/2013
57	LT	0.35	0/1345	0.38	0/1795
58	LP	0.35	0/1277	0.41	0/1713
59	LU	0.22	0/822	0.31	0/1103
60	LX	0.33	0/983	0.35	0/1323
61	LY	0.31	0/1132	0.34	0/1504
62	LW	0.28	0/972	0.38	0/1288
63	LZ	0.30	0/1141	0.31	0/1521
64	Lr	0.34	0/1020	0.36	0/1367
65	Lh	0.28	0/1022	0.34	0/1351
66	Lb	0.33	0/900	0.44	0/1187
67	LF	0.36	0/1904	0.43	0/2539
68	Lc	0.29	0/780	0.34	0/1046
69	Ld	0.33	0/903	0.42	0/1216
70	Le	0.41	0/1071	0.48	0/1429
71	Lf	0.36	0/902	0.42	0/1208
72	Lg	0.33	0/916	0.38	0/1220
73	Li	0.29	0/843	0.42	0/1115
74	Lj	0.41	0/731	0.50	0/967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lk	0.26	0/574	0.29	0/761
76	Ll	0.35	0/453	0.40	0/599
77	Lm	0.42	0/425	0.50	1/564 (0.2%)
78	Ln	0.39	0/240	0.45	0/305
79	Lo	0.34	0/888	0.43	0/1170
80	Lp	0.32	0/728	0.41	0/967
81	mR	0.22	0/192	0.33	0/297
82	Pt	0.39	1/1721 (0.1%)	0.37	0/2679
83	5A	0.27	0/1060	0.56	0/1425
All	All	0.38	5/228428 (0.0%)	0.41	5/334784 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
19	SO	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1383	A2M	O3'-P	5.34	1.61	1.56
3	L5	3760	A2M	O3'-P	5.17	1.61	1.56
3	L5	1871	A2M	O3'-P	5.12	1.61	1.56
82	Pt	47	G7M	O3'-P	5.06	1.61	1.56
3	L5	2415	OMU	O3'-P	5.02	1.61	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1670	G	C2'-C3'-O3'	-6.25	104.32	113.70
19	SO	139	SER	N-CA-C	5.84	115.80	108.45
26	SR	81	ARG	CB-CA-C	-5.55	101.36	110.08
3	L5	1624	G	C2'-C3'-O3'	-5.12	101.82	109.50
77	Lm	108	VAL	N-CA-C	-5.05	107.81	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	SO	138	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	35800	0	18101	445	0
2	L8	3316	0	1687	45	0
3	L5	79154	0	39952	877	0
4	L7	2558	0	1296	16	0
5	SB	1806	0	1888	24	0
6	SA	1750	0	1755	25	0
7	SD	1756	0	1852	27	0
8	SJ	1525	0	1640	29	0
9	SE	2076	0	2177	23	0
10	SC	1725	0	1813	21	0
11	SG	1923	0	2089	40	0
12	SF	1494	0	1549	22	0
13	SH	1517	0	1605	27	0
14	SW	1034	0	1080	13	0
15	SI	1686	0	1772	30	0
16	SQ	1123	0	1193	17	0
17	SU	803	0	873	17	0
18	SK	810	0	836	20	0
19	SO	1009	0	1034	17	0
20	SX	1088	0	1149	12	0
21	SM	950	0	987	29	0
22	SS	1214	0	1275	23	0
23	Sd	458	0	448	10	0
24	SN	1214	0	1300	19	0
25	SL	1200	0	1271	11	0
26	SR	1082	0	1137	29	0
27	SP	1078	0	1121	18	0
28	ST	1121	0	1151	20	0
29	SV	639	0	638	9	0
30	SY	1065	0	1142	17	0
31	SZ	674	0	748	10	0
32	Sa	800	0	854	9	0
33	Sb	651	0	672	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Sc	512	0	541	13	0
35	Se	394	0	434	10	0
36	Sf	515	0	521	23	0
37	Sg	2436	0	2393	65	0
38	Lz	1695	0	1799	51	0
39	LA	1930	0	2028	17	0
40	LB	3239	0	3377	37	0
41	LC	2914	0	3087	32	0
42	LJ	1362	0	1399	25	0
43	LH	1518	0	1600	20	0
44	LE	1786	0	1945	18	0
45	LG	1926	0	2074	19	0
46	LO	1633	0	1779	25	0
47	LL	1664	0	1773	22	0
48	LV	988	0	1047	6	0
49	LM	1120	0	1187	11	0
50	La	1162	0	1206	8	0
51	LN	1700	0	1749	20	0
52	LI	1645	0	1694	26	0
53	LD	2391	0	2426	29	0
54	LQ	1512	0	1628	9	0
55	LR	1566	0	1728	12	0
56	LS	1460	0	1502	11	0
57	LT	1311	0	1392	20	0
58	LP	1248	0	1277	13	0
59	LU	808	0	831	11	0
60	LX	966	0	1040	6	0
61	LY	1115	0	1205	13	0
62	LW	955	0	1010	14	0
63	LZ	1115	0	1195	9	0
64	Lr	1011	0	1085	6	0
65	Lh	1014	0	1148	8	0
66	Lb	898	0	983	16	0
67	LF	1869	0	1996	14	0
68	Lc	770	0	809	10	0
69	Ld	888	0	930	7	0
70	Le	1053	0	1147	22	0
71	Lf	883	0	924	6	0
72	Lg	906	0	998	6	0
73	Li	832	0	917	12	0
74	Lj	712	0	744	6	0
75	Lk	568	0	637	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	Ll	443	0	483	3	0
77	Lm	431	0	471	3	0
78	Ln	239	0	289	4	0
79	Lo	878	0	949	10	0
80	Lp	715	0	769	2	0
81	mR	172	0	87	1	0
82	Pt	1645	0	843	12	0
83	5A	1073	0	1098	53	0
84	L5	120	0	228	11	0
84	S2	10	0	19	1	0
85	L5	54	0	108	7	0
85	S2	12	0	24	2	0
86	L5	52	0	0	0	0
86	L7	1	0	0	0	0
86	L8	1	0	0	0	0
86	LA	1	0	0	0	0
86	LH	1	0	0	0	0
86	Lf	1	0	0	0	0
86	Lg	1	0	0	0	0
86	S2	17	0	0	0	0
86	SL	1	0	0	0	0
86	Sa	1	0	0	0	0
87	5A	1	0	0	0	0
87	L5	344	0	0	0	0
87	L7	5	0	0	0	0
87	L8	10	0	0	0	0
87	LA	2	0	0	0	0
87	LB	2	0	0	0	0
87	LC	2	0	0	0	0
87	LD	1	0	0	0	0
87	LI	1	0	0	0	0
87	LL	2	0	0	0	0
87	LN	1	0	0	0	0
87	LO	1	0	0	0	0
87	LP	3	0	0	0	0
87	LQ	1	0	0	0	0
87	LR	2	0	0	0	0
87	LS	2	0	0	0	0
87	LV	1	0	0	0	0
87	Lc	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	Lj	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Lr	1	0	0	0	0
87	Pt	4	0	0	0	0
87	S2	124	0	0	0	0
87	SC	1	0	0	0	0
87	SE	1	0	0	0	0
87	SJ	1	0	0	0	0
87	SN	1	0	0	0	0
87	ST	1	0	0	0	0
87	SX	1	0	0	0	0
87	Sb	1	0	0	0	0
87	Sd	1	0	0	0	0
88	L5	19	0	18	0	0
89	L5	33	0	35	3	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
90	Sd	1	0	0	0	0
90	Sf	1	0	0	0	0
91	Pt	8	0	8	1	0
92	5A	1	0	0	0	0
92	L5	996	0	0	3	0
92	L7	8	0	0	0	0
92	L8	11	0	0	0	0
92	LA	18	0	0	0	0
92	LB	8	0	0	0	0
92	LC	21	0	0	0	0
92	LD	1	0	0	0	0
92	LF	4	0	0	0	0
92	LI	2	0	0	0	0
92	LL	3	0	0	0	0
92	LN	4	0	0	0	0
92	LO	3	0	0	0	0
92	LP	2	0	0	0	0
92	LQ	6	0	0	0	0
92	LR	1	0	0	0	0
92	LT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	LV	2	0	0	0	0
92	LX	2	0	0	0	0
92	LZ	1	0	0	0	0
92	La	10	0	0	0	0
92	Lb	2	0	0	0	0
92	Lc	1	0	0	0	0
92	Ld	1	0	0	0	0
92	Le	14	0	0	0	0
92	Lf	3	0	0	0	0
92	Lg	4	0	0	0	0
92	Lj	6	0	0	0	0
92	Ln	1	0	0	0	0
92	Lo	1	0	0	0	0
92	Lp	2	0	0	0	0
92	Lr	1	0	0	0	0
92	Pt	1	0	0	0	0
92	S2	123	0	0	1	0
92	SA	1	0	0	0	0
92	SF	1	0	0	0	0
92	SN	1	0	0	0	0
92	SQ	1	0	0	0	0
92	SS	1	0	0	0	0
92	Sa	3	0	0	0	0
All	All	219823	0	162699	2463	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 7.

All (2463) 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)
37:Sg:212:LYS:HA	37:Sg:235:ILE:HD12	1.34	1.03
1:S2:394:G:H5''	25:SL:81:LYS:HB3	1.39	1.02
3:L5:1194:G:H3'	3:L5:1195:G:H21	1.35	0.91
12:SF:165:ASN:HD21	12:SF:167:LYS:HG2	1.36	0.91
26:SR:79:GLU:HA	26:SR:83:ASN:HD21	1.35	0.90
3:L5:3692:A:H62	3:L5:3823:G:H21	1.19	0.88
12:SF:41:VAL:HG23	12:SF:42:LYS:HG3	1.55	0.88
3:L5:2089:G:H1	3:L5:2096:G:H1	1.22	0.88
42:LJ:96:LYS:HE2	42:LJ:163:MET:HE1	1.57	0.87
3:L5:5021:C:H2'	3:L5:5022:U:H4'	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:LT:4:THR:HG22	57:LT:6:GLY:H	1.37	0.85
3:L5:1698:C:H2'	3:L5:1699:A:N7	1.93	0.84
36:Sf:123:SER:HB3	36:Sf:126:CYS:HB3	1.61	0.83
48:LV:33:GLY:HA3	48:LV:69:LYS:HD2	1.61	0.82
6:SA:89:LYS:NZ	26:SR:82:ASP:HA	1.94	0.82
59:LU:28:PRO:HB2	59:LU:34:MET:HG2	1.61	0.81
1:S2:925:G:H1	1:S2:1017:U:H3	1.26	0.81
11:SG:22:ARG:HD2	11:SG:25:ARG:HH21	1.45	0.81
1:S2:928:G:H1	1:S2:1013:U:H3	1.29	0.80
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.17	0.80
11:SG:32:MET:HE2	11:SG:54:GLY:HA3	1.62	0.79
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.13	0.79
1:S2:195:C:H2'	1:S2:196:C:H6	1.49	0.78
13:SH:110:THR:O	13:SH:110:THR:HG22	1.83	0.78
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.66	0.77
40:LB:317:LEU:HD11	40:LB:382:MET:HG2	1.67	0.77
1:S2:195:C:H2'	1:S2:196:C:C6	2.20	0.77
3:L5:1194:G:H2'	3:L5:1195:G:H5'	1.68	0.76
4:L7:117:G:H5'	53:LD:256:LYS:HD2	1.66	0.76
78:Ln:20:MET:HE3	78:Ln:20:MET:HA	1.67	0.76
43:LH:44:GLU:HG3	49:LM:2:VAL:HG12	1.67	0.76
1:S2:1751:C:H2'	1:S2:1752:C:H5'	1.68	0.76
37:Sg:87:LEU:HB2	37:Sg:101:PHE:HB2	1.68	0.76
1:S2:1581:C:H5'	1:S2:1582:C:H5	1.50	0.76
56:LS:30:MET:HE1	56:LS:47:PHE:HB2	1.67	0.76
38:Lz:139:THR:HG23	38:Lz:141:ASN:H	1.50	0.75
3:L5:4691:A:H5'	43:LH:71:ARG:HH11	1.52	0.75
3:L5:2492:C:H2'	3:L5:2493:G:H8	1.52	0.75
13:SH:73:GLN:HA	13:SH:76:GLN:HB2	1.69	0.75
1:S2:970:G:H5''	3:L5:3711:A:H1'	1.67	0.74
3:L5:4113:U:H2'	3:L5:4114:C:C6	2.23	0.74
46:LO:168:TYR:CE2	46:LO:172:LYS:HD2	2.23	0.74
68:Lc:34:THR:HG23	68:Lc:95:ALA:HB2	1.70	0.74
1:S2:164:A:H3'	1:S2:165:G:H21	1.52	0.73
10:SC:176:LYS:HD3	10:SC:177:PRO:HD2	1.70	0.73
3:L5:4741:C:H5'	3:L5:4900:C:N3	2.03	0.73
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.71	0.73
3:L5:2517:A:H5'	72:Lg:62:LYS:HD3	1.71	0.72
36:Sf:106:TYR:HE1	36:Sf:116:ARG:HD2	1.53	0.72
12:SF:165:ASN:ND2	12:SF:167:LYS:HG2	2.04	0.72
38:Lz:195:LYS:H	38:Lz:195:LYS:HD2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LV:13:LYS:HE2	48:LV:128:LEU:HD11	1.71	0.72
53:LD:289:ARG:HD2	53:LD:293:ARG:HH21	1.54	0.72
1:S2:1523:C:H4'	22:SS:145:THR:HA	1.71	0.72
61:LY:121:ARG:HB3	61:LY:121:ARG:HH11	1.55	0.72
3:L5:1974:U:C2	3:L5:1976:G:H5'	2.24	0.72
43:LH:94:SER:HB2	43:LH:142:ASP:HB3	1.72	0.72
51:LN:158:HIS:HB3	51:LN:161:MET:HG3	1.72	0.71
1:S2:70:G:H21	1:S2:79:A:H2	1.38	0.71
64:Lr:46:ARG:HH22	64:Lr:67:ARG:HD2	1.54	0.71
11:SG:181:THR:HG22	11:SG:183:ARG:H	1.53	0.71
52:LI:48:LEU:HB2	52:LI:142:LEU:HD12	1.71	0.71
1:S2:1289:U:H4'	18:SK:2:LEU:HD21	1.71	0.71
3:L5:196:C:H4'	61:LY:126:ARG:HG3	1.72	0.71
30:SY:27:VAL:HG11	30:SY:35:VAL:HG11	1.72	0.71
73:Li:79:THR:HG22	73:Li:82:ARG:H	1.54	0.71
3:L5:2490:U:H1'	3:L5:2491:C:C5	2.26	0.70
36:Sf:95:ARG:HH21	36:Sf:97:LYS:HG2	1.55	0.70
6:SA:10:MET:HE2	6:SA:15:VAL:HG22	1.72	0.70
39:LA:181:LYS:HG3	39:LA:184:ARG:HG3	1.73	0.70
3:L5:704:C:H42	3:L5:707:C:H41	1.40	0.70
15:SI:142:SER:HB3	15:SI:145:ILE:HG22	1.72	0.70
52:LI:47:PRO:HG2	52:LI:142:LEU:HD13	1.74	0.70
83:5A:25:LEU:HD11	83:5A:79:MET:HG3	1.73	0.70
37:Sg:302:TYR:HE2	37:Sg:308:ARG:HB2	1.57	0.70
3:L5:48:G:H8	85:L5:5518:PUT:H32	1.57	0.69
22:SS:15:VAL:HG12	22:SS:16:LEU:HD12	1.73	0.69
50:La:6:ARG:HH11	50:La:6:ARG:HG3	1.56	0.69
3:L5:4457:PSU:H1'	40:LB:252:ALA:HB3	1.74	0.69
3:L5:3962:A:H61	3:L5:3965:A:H1'	1.56	0.69
3:L5:4924:C:H2'	3:L5:4925:U:C6	2.28	0.69
19:SO:53:ILE:HG23	19:SO:88:LEU:HD23	1.75	0.69
21:SM:25:ALA:HB1	21:SM:31:LEU:HD21	1.73	0.69
1:S2:377:G:H5''	15:SI:98:LYS:HB3	1.76	0.68
26:SR:79:GLU:HA	26:SR:83:ASN:ND2	2.08	0.68
3:L5:291:U:H5'	85:L5:5518:PUT:H42	1.75	0.68
3:L5:411:G:H4'	3:L5:412:G:H5''	1.75	0.68
22:SS:13:LEU:HB2	22:SS:20:ILE:HB	1.75	0.68
53:LD:112:ARG:HH21	53:LD:113:PHE:HE1	1.40	0.68
35:Se:119:VAL:HG12	35:Se:120:VAL:HG12	1.76	0.68
12:SF:165:ASN:HD21	12:SF:167:LYS:CG	2.07	0.68
1:S2:1228:A:H2'	1:S2:1229:G:H8	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1545:A:H2'	1:S2:1546:G:C8	2.29	0.68
36:Sf:119:ARG:HH12	36:Sf:148:TYR:HD2	1.42	0.68
9:SE:211:LYS:HD2	9:SE:215:GLY:HA2	1.75	0.68
3:L5:964:A:H2'	3:L5:965:G:H4'	1.74	0.67
1:S2:196:C:H2'	1:S2:197:U:C6	2.29	0.67
1:S2:1546:G:H5'	16:SQ:18:THR:HG21	1.75	0.67
1:S2:1536:G:H2'	1:S2:1537:A:C8	2.29	0.67
83:5A:101:LEU:HD11	83:5A:135:ILE:HB	1.76	0.67
39:LA:137:ILE:HD11	39:LA:149:LYS:HB2	1.76	0.67
1:S2:433:A:H5''	15:SI:22:HIS:HB3	1.76	0.67
9:SE:139:LEU:HB2	9:SE:150:PRO:HG3	1.74	0.67
12:SF:78:MET:O	12:SF:79:HIS:HB2	1.94	0.67
18:SK:65:ARG:HD3	23:Sd:25:SER:HB3	1.77	0.67
42:LJ:55:TYR:HA	42:LJ:64:ARG:HG3	1.75	0.67
13:SH:190:PRO:HG2	13:SH:193:GLN:HE22	1.58	0.67
1:S2:455:A:H2'	1:S2:456:C:C6	2.30	0.67
3:L5:184:U:H2'	3:L5:186:G:C8	2.30	0.67
3:L5:2809:G:N7	84:L5:5511:SPD:H92	2.08	0.67
3:L5:2488:C:H2'	3:L5:2489:C:C6	2.30	0.66
37:Sg:83:TRP:HA	37:Sg:107:ASP:HB3	1.76	0.66
1:S2:640:A:H2'	1:S2:641:A:C8	2.30	0.66
1:S2:1751:C:C2'	1:S2:1752:C:H5'	2.24	0.66
3:L5:1194:G:H3'	3:L5:1195:G:N2	2.09	0.66
3:L5:658:C:H2'	3:L5:659:G:C8	2.31	0.66
57:LT:111:GLU:HB3	57:LT:115:LYS:NZ	2.11	0.66
1:S2:551:U:H2'	1:S2:552:G:C8	2.29	0.66
17:SU:51:LYS:HB2	17:SU:90:ASP:HB2	1.78	0.66
37:Sg:252:THR:HG21	37:Sg:257:LYS:HD2	1.77	0.66
3:L5:1590:C:H4'	3:L5:2857:A:H5'	1.77	0.66
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.30	0.66
58:LP:125:MET:HE2	58:LP:143:PRO:HG3	1.78	0.66
8:SJ:47:LYS:HG3	8:SJ:102:ILE:HD12	1.77	0.66
24:SN:120:SER:O	24:SN:124:ARG:HG3	1.95	0.66
9:SE:19:MET:SD	9:SE:108:ARG:HD2	2.36	0.65
26:SR:66:VAL:HG23	26:SR:67:ARG:H	1.61	0.65
43:LH:92:MET:HE2	43:LH:179:ILE:HG22	1.76	0.65
3:L5:2021:G:H2'	3:L5:2022:C:H5'	1.78	0.65
13:SH:160:LYS:HA	13:SH:163:GLN:HB2	1.78	0.65
19:SO:56:VAL:HG13	19:SO:60:MET:HE2	1.79	0.65
6:SA:59:LEU:HD22	6:SA:181:GLU:HG2	1.77	0.65
3:L5:48:G:H5'	85:L5:5518:PUT:N2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.32	0.65
3:L5:4966:A:H5''	40:LB:128:LYS:HG3	1.78	0.65
15:SI:106:SER:HB3	15:SI:171:LEU:HG	1.78	0.65
1:S2:202:G:H3'	1:S2:203:G:H5''	1.77	0.65
48:LV:62:MET:HE3	48:LV:76:VAL:HG12	1.78	0.65
1:S2:553:U:H2'	1:S2:555:A:H8	1.62	0.65
15:SI:98:LYS:HG3	15:SI:178:ARG:HG3	1.79	0.65
1:S2:981:A:H2'	1:S2:982:G:C8	2.32	0.64
3:L5:493:G:H22	3:L5:661:C:H1'	1.62	0.64
3:L5:1801:A:H4'	57:LT:102:ARG:HD3	1.80	0.64
3:L5:1992:U:H4'	3:L5:2002:A:H2	1.61	0.64
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.32	0.64
3:L5:3722:G:H2'	3:L5:3723:A2M:H8	1.77	0.64
1:S2:1780:G:H2'	1:S2:1781:A:O4'	1.98	0.64
37:Sg:217:MET:HG2	37:Sg:229:THR:OG1	1.98	0.64
23:Sd:27:ARG:HG2	23:Sd:27:ARG:HH11	1.62	0.64
38:Lz:120:ILE:HG23	38:Lz:124:LEU:HD12	1.78	0.64
63:LZ:92:ASP:HB3	63:LZ:95:VAL:HG12	1.79	0.64
5:SB:230:GLU:HA	5:SB:234:GLU:HA	1.78	0.64
24:SN:42:LYS:HE3	24:SN:80:LEU:HD21	1.80	0.64
3:L5:2461:G:H5'	51:LN:104:GLU:OE1	1.97	0.63
37:Sg:269:GLU:HG2	37:Sg:271:LYS:HE3	1.78	0.63
38:Lz:70:ASP:HA	38:Lz:87:ILE:HD11	1.78	0.63
15:SI:101:ILE:HD12	15:SI:190:LEU:HD11	1.80	0.63
1:S2:944:A:H5''	19:SO:134:PRO:HB3	1.79	0.63
3:L5:1703:C:H2'	3:L5:1704:C:C6	2.33	0.63
8:SJ:136:ARG:HG2	8:SJ:160:SER:HA	1.80	0.63
65:Lh:13:LYS:HE3	65:Lh:15:GLU:HB2	1.80	0.63
3:L5:4883:C:H1'	71:Lf:1:MET:HG2	1.80	0.63
1:S2:107:A:H2'	1:S2:108:G:C8	2.33	0.63
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.33	0.63
8:SJ:93:LYS:HE2	8:SJ:96:TYR:HE2	1.63	0.63
3:L5:1411:C:H2'	3:L5:1412:G:C8	2.33	0.63
6:SA:89:LYS:HZ2	26:SR:82:ASP:HA	1.63	0.63
14:SW:28:ARG:HB3	14:SW:29:PRO:HD3	1.81	0.63
38:Lz:114:GLU:HG2	38:Lz:137:LEU:HD21	1.79	0.63
57:LT:39:ILE:HG13	57:LT:102:ARG:HG3	1.79	0.63
13:SH:138:GLU:H	13:SH:159:ASP:HB2	1.63	0.62
73:Li:80:HIS:NE2	73:Li:84:LYS:HD2	2.14	0.62
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.34	0.62
50:La:134:GLU:OE1	50:La:138:LYS:HE3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:373:G:OP2	74:Lj:36:LYS:HE2	1.99	0.62
3:L5:2022:C:H2'	3:L5:2023:C:C2	2.33	0.62
62:LW:117:LYS:HA	62:LW:120:GLN:HB3	1.80	0.62
1:S2:532:C:H2'	1:S2:533:A:C8	2.35	0.62
3:L5:71:C:H1'	47:LL:62:PRO:O	1.99	0.62
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.34	0.62
3:L5:1771:U:H2'	3:L5:1772:C:H6	1.64	0.62
20:SX:124:LYS:HA	20:SX:129:SER:HA	1.82	0.62
57:LT:4:THR:HG22	57:LT:6:GLY:N	2.13	0.62
3:L5:280:G:H5''	51:LN:14:LYS:HE2	1.82	0.62
3:L5:1296:G:H2'	3:L5:1297:U:C6	2.34	0.62
3:L5:4119:C:H5	72:Lg:100:GLN:HG2	1.65	0.62
59:LU:56:LEU:HD11	59:LU:63:ILE:HD12	1.82	0.62
3:L5:965:G:H1'	3:L5:2093:A:H61	1.64	0.62
3:L5:2486:G:H2'	3:L5:2487:G:C8	2.35	0.62
9:SE:45:ILE:HA	9:SE:61:VAL:HG11	1.82	0.62
1:S2:1751:C:H42	1:S2:1782:G:N2	1.98	0.62
3:L5:184:U:H1'	3:L5:188:G:H1'	1.81	0.62
3:L5:496:G:H2'	3:L5:497:G:C8	2.34	0.62
3:L5:1417:C:H2'	3:L5:1418:C:O4'	1.99	0.62
1:S2:615:C:O2	35:Se:85:LYS:HE2	2.00	0.61
1:S2:880:G:H1	1:S2:906:U:H3	1.48	0.61
15:SI:141:ARG:H	15:SI:141:ARG:HD2	1.65	0.61
38:Lz:38:LEU:HD13	38:Lz:41:TYR:HE2	1.65	0.61
41:LC:281:MET:HE2	54:LQ:110:ARG:CZ	2.30	0.61
1:S2:1217:A:H2'	1:S2:1218:C:C6	2.35	0.61
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.35	0.61
62:LW:120:GLN:HA	62:LW:123:LYS:HE2	1.81	0.61
1:S2:809:A:H2'	1:S2:810:A:C8	2.35	0.61
1:S2:1091:C:HO2'	14:SW:2:VAL:N	1.98	0.61
3:L5:1242:G:H5'	66:Lb:122:LYS:HD2	1.82	0.61
3:L5:4110:C:H2'	3:L5:4111:U:C6	2.35	0.61
21:SM:81:ASP:HB3	21:SM:84:LYS:HB3	1.83	0.61
1:S2:1536:G:H2'	1:S2:1537:A:H8	1.63	0.61
37:Sg:249:CYS:HB3	37:Sg:258:ILE:HD13	1.82	0.61
3:L5:2492:C:H2'	3:L5:2493:G:C8	2.33	0.61
3:L5:424:U:H2'	3:L5:425:U:C6	2.36	0.61
3:L5:1960:A:H5''	3:L5:1961:G:C8	2.35	0.61
3:L5:4114:C:H2'	3:L5:4115:G:N3	2.15	0.61
3:L5:1756:U:H2'	3:L5:1757:U:C6	2.35	0.61
32:Sa:59:PHE:HB2	32:Sa:62:TYR:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1490:OMG:C8	1:S2:1490:OMG:H5'	2.35	0.61
63:LZ:87:VAL:HG22	63:LZ:89:ILE:HG12	1.82	0.61
3:L5:1771:U:H2'	3:L5:1772:C:C6	2.35	0.60
3:L5:1420:A:H5''	3:L5:1420:A:H8	1.66	0.60
3:L5:2696:A:H5'	75:Lk:70:LYS:HG2	1.83	0.60
1:S2:153:G:H21	11:SG:13:GLN:NE2	1.99	0.60
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.65	0.60
41:LC:138:MET:HG2	41:LC:144:ILE:HD11	1.82	0.60
41:LC:209:ILE:HB	41:LC:229:LEU:HD13	1.82	0.60
57:LT:51:GLY:HA3	57:LT:92:ARG:HG3	1.83	0.60
10:SC:196:ILE:HB	10:SC:223:TYR:HB2	1.83	0.60
40:LB:36:ASP:HB3	40:LB:39:LYS:HG3	1.83	0.60
57:LT:111:GLU:HB3	57:LT:115:LYS:HZ2	1.65	0.60
3:L5:260:C:H2'	3:L5:261:G:H8	1.66	0.60
3:L5:2862:G:OP2	84:L5:5508:SPD:H52	2.02	0.60
8:SJ:60:LEU:HD22	8:SJ:70:ARG:HA	1.83	0.60
37:Sg:156:PHE:HE1	37:Sg:179:LEU:HD11	1.65	0.60
83:5A:20:MET:HE3	83:5A:81:VAL:HG21	1.84	0.60
1:S2:1490:OMG:H5'	1:S2:1490:OMG:H8	1.65	0.60
19:SO:34:PHE:HB3	19:SO:41:PHE:HB2	1.82	0.60
53:LD:62:CYS:HB3	53:LD:105:LEU:HD22	1.84	0.60
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.37	0.60
15:SI:150:ASP:HA	15:SI:153:LYS:HG2	1.83	0.60
54:LQ:16:LYS:HA	54:LQ:16:LYS:HE3	1.84	0.60
83:5A:42:GLU:HG3	83:5A:59:VAL:HG12	1.84	0.60
3:L5:1759:G:H1	3:L5:1773:U:H3	1.49	0.60
73:Li:2:ALA:N	73:Li:5:TYR:HH	2.00	0.60
1:S2:1395:C:O2'	1:S2:1396:A:H5'	2.02	0.60
3:L5:711:A:H2'	3:L5:712:C:C6	2.37	0.60
3:L5:1481:C:O2'	3:L5:1482:G:H5'	2.01	0.60
11:SG:130:PRO:HG2	62:LW:83:THR:HG22	1.83	0.60
42:LJ:84:GLU:HG2	42:LJ:170:TYR:HE1	1.66	0.60
1:S2:1421:A:H1'	1:S2:1422:G:H2'	1.82	0.59
7:SD:27:ARG:HB3	18:SK:61:GLN:OE1	2.01	0.59
64:Lr:92:SER:O	64:Lr:96:MET:HG3	2.02	0.59
1:S2:942:G:H2'	1:S2:943:U:C6	2.37	0.59
25:SL:91:ASP:HB3	25:SL:104:LYS:HE2	1.83	0.59
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.37	0.59
3:L5:4113:U:H2'	3:L5:4114:C:H6	1.67	0.59
1:S2:534:G:H2'	1:S2:535:G:H8	1.66	0.59
3:L5:162:A:H2'	3:L5:163:A:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:120:ILE:HB	37:Sg:132:TRP:HB2	1.84	0.59
1:S2:799:U:H6	13:SH:109:ARG:HG2	1.67	0.59
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.37	0.59
6:SA:89:LYS:HZ1	26:SR:82:ASP:HA	1.64	0.59
15:SI:57:ALA:HB2	15:SI:183:GLY:HA2	1.84	0.59
41:LC:140:LYS:HE3	41:LC:245:HIS:HB2	1.83	0.59
61:LY:30:MET:HB3	61:LY:101:PRO:HG3	1.85	0.59
1:S2:810:A:H5''	1:S2:811:A:H5'	1.84	0.59
3:L5:3648:A:H1'	3:L5:3785:A2M:N6	2.18	0.59
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.03	0.59
3:L5:4629:U:O3'	62:LW:19:ARG:HD2	2.03	0.59
36:Sf:121:CYS:HB3	36:Sf:126:CYS:SG	2.42	0.59
3:L5:2478:C:H2'	3:L5:2479:G:H5'	1.84	0.59
10:SC:187:ARG:HD3	10:SC:192:LEU:HD12	1.85	0.59
27:SP:37:TYR:HE1	27:SP:112:ILE:HG22	1.67	0.59
29:SV:43:THR:HB	29:SV:45:ARG:HG3	1.85	0.59
51:LN:138:PHE:HA	51:LN:143:ARG:HD2	1.85	0.59
1:S2:996:A:H2'	1:S2:997:A:C8	2.37	0.59
1:S2:1826:G:HO2'	3:L5:3759:A:HO2'	1.45	0.59
70:Le:109:LYS:O	70:Le:113:GLU:HG3	2.03	0.59
1:S2:16:G:H2'	1:S2:17:C:C6	2.38	0.59
3:L5:492:U:H2'	3:L5:493:G:C8	2.38	0.59
49:LM:36:ALA:HB3	49:LM:55:MET:HE1	1.85	0.59
3:L5:4208:U:OP2	57:LT:4:THR:HG21	2.03	0.58
61:LY:121:ARG:HB3	61:LY:121:ARG:NH1	2.18	0.58
3:L5:2838:G:H5'	40:LB:247:GLY:HA3	1.84	0.58
58:LP:125:MET:HE3	58:LP:141:SER:OG	2.03	0.58
1:S2:877:C:H2'	1:S2:878:G:C8	2.39	0.58
3:L5:664:G:H21	3:L5:667:A:N6	2.01	0.58
6:SA:117:ARG:HG3	6:SA:119:PRO:HD3	1.85	0.58
21:SM:55:ASN:HD21	21:SM:81:ASP:HA	1.68	0.58
37:Sg:11:LEU:HB2	37:Sg:307:VAL:HB	1.85	0.58
54:LQ:89:ASP:HB3	54:LQ:92:VAL:HG12	1.84	0.58
40:LB:378:ARG:HG2	62:LW:32:LEU:HD21	1.86	0.58
44:LE:91:THR:HG22	44:LE:108:LYS:HA	1.84	0.58
3:L5:738:C:N4	3:L5:741:C:H4'	2.18	0.58
3:L5:2018:C:H2'	3:L5:2019:C:C6	2.39	0.58
1:S2:846:G:C6	9:SE:19:MET:HE3	2.39	0.58
3:L5:962:C:H42	3:L5:1701:A:H1'	1.68	0.58
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.04	0.58
37:Sg:133:ASN:HD21	37:Sg:139:LYS:HD3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Lc:37:MET:HA	68:Lc:37:MET:HE2	1.85	0.58
1:S2:1229:G:H21	28:ST:87:VAL:HG22	1.69	0.58
3:L5:3922:G:N7	83:5A:72:ILE:HG12	2.18	0.58
3:L5:4115:G:H4'	3:L5:4116:C:H5'	1.85	0.58
28:ST:5:THR:HG22	28:ST:132:ASP:OD2	2.03	0.58
1:S2:562:U:H2'	1:S2:563:G:C8	2.38	0.58
3:L5:188:G:H4'	3:L5:189:G:H5'	1.86	0.58
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.39	0.58
3:L5:4384:U:H3'	83:5A:50[B]:5CT:H12	1.86	0.58
5:SB:173:THR:O	5:SB:177:GLN:HG2	2.03	0.58
30:SY:55:ILE:HD13	30:SY:75:ILE:HG12	1.86	0.58
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.18	0.58
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.39	0.57
21:SM:12:MET:O	21:SM:12:MET:HE3	2.04	0.57
36:Sf:122:PRO:O	36:Sf:123:SER:HB2	2.03	0.57
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.39	0.57
1:S2:587:A:H5'	1:S2:592:C:H41	1.68	0.57
1:S2:1801:A:H2'	1:S2:1802:C:C6	2.39	0.57
3:L5:664:G:H21	3:L5:667:A:H61	1.52	0.57
9:SE:165:GLU:HG3	9:SE:166:THR:HG23	1.86	0.57
37:Sg:230:LEU:HD21	37:Sg:259:TRP:CD2	2.38	0.57
58:LP:54:GLN:HA	58:LP:83:TRP:CD1	2.39	0.57
1:S2:1639:G7M:H2'	1:S2:1640:A:C8	2.39	0.57
52:LI:201:PRO:HB2	52:LI:203:ARG:HG2	1.85	0.57
61:LY:56:GLN:HG2	61:LY:105:VAL:HG12	1.86	0.57
3:L5:1765:A:H8	3:L5:1767:A:N7	2.02	0.57
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.40	0.57
7:SD:193:ASP:OD2	7:SD:198:ILE:HG12	2.04	0.57
29:SV:58:ALA:O	29:SV:62:MET:HG3	2.04	0.57
41:LC:5:ARG:HD2	41:LC:24:LEU:O	2.04	0.57
3:L5:1756:U:H2'	3:L5:1757:U:H6	1.69	0.57
10:SC:204:ILE:HG22	10:SC:206:SER:HB3	1.85	0.57
47:LL:144:LEU:HD12	47:LL:145:LYS:HG2	1.86	0.57
3:L5:2557:G:H1	3:L5:2570:U:H3	1.52	0.57
40:LB:163:ILE:HG22	40:LB:180:LEU:HD22	1.85	0.57
56:LS:30:MET:HE3	56:LS:32:ILE:HD11	1.87	0.57
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.20	0.57
3:L5:2485:U:H3	3:L5:2493:G:H1	1.50	0.57
24:SN:133:ARG:NH1	25:SL:150:GLY:HA3	2.20	0.57
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.70	0.57
42:LJ:18:ARG:HG3	42:LJ:135:GLY:HA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:145:G:H2'	1:S2:146:G:C8	2.40	0.56
1:S2:923:G:N7	84:S2:1901:SPD:H51	2.19	0.56
1:S2:1421:A:H4'	1:S2:1422:G:H5'	1.85	0.56
3:L5:496:G:H2'	3:L5:497:G:H8	1.69	0.56
3:L5:1082:C:H2'	3:L5:1083:U:O4'	2.05	0.56
47:LL:100:PRO:O	73:Li:25:ARG:NH1	2.34	0.56
1:S2:190:G:H1'	1:S2:209:A:H61	1.70	0.56
1:S2:1754:G:H2'	1:S2:1755:C:C6	2.39	0.56
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.39	0.56
3:L5:2412:A:H2'	3:L5:2413:U:C6	2.39	0.56
3:L5:2862:G:N7	84:L5:5508:SPD:N10	2.53	0.56
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.86	0.56
6:SA:51:LEU:HB2	26:SR:105:MET:HE1	1.88	0.56
1:S2:209:A:H2'	1:S2:210:U:H5'	1.87	0.56
3:L5:2363:A2M:H2'	3:L5:2364:OMG:O4'	2.05	0.56
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.40	0.56
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.40	0.56
5:SB:179:ASN:HD22	5:SB:183:GLU:HB3	1.69	0.56
6:SA:191:ARG:HG3	6:SA:191:ARG:O	2.05	0.56
15:SI:148:LYS:HA	15:SI:151:GLU:HG2	1.87	0.56
17:SU:60:THR:HG23	17:SU:83:ARG:HD3	1.88	0.56
26:SR:70:SER:HB2	26:SR:73:LEU:HD12	1.87	0.56
37:Sg:45:LEU:HD23	37:Sg:52:TYR:CE2	2.40	0.56
45:LG:102:TYR:OH	45:LG:211:ASP:OD2	2.21	0.56
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.06	0.56
8:SJ:30:LYS:O	8:SJ:34:GLU:HG3	2.05	0.56
30:SY:83:LYS:HD3	30:SY:96:LEU:HD22	1.87	0.56
35:Se:102:LYS:HD3	35:Se:106:ALA:HB1	1.87	0.56
1:S2:874:G:H2'	1:S2:875:A:H8	1.69	0.56
3:L5:1755:C:N3	53:LD:3:PHE:HB3	2.21	0.56
3:L5:4140:C:H2'	3:L5:4141:G:N3	2.20	0.56
4:L7:23:A:H2'	4:L7:24:C:C6	2.40	0.56
53:LD:205:ALA:HB2	53:LD:236:MET:HE2	1.86	0.56
53:LD:208:MET:HB2	53:LD:233:PRO:HG3	1.87	0.56
1:S2:1217:A:H2'	1:S2:1218:C:H6	1.69	0.56
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.40	0.56
3:L5:4903:G:H2'	3:L5:4904:G:O4'	2.06	0.56
11:SG:22:ARG:HH11	11:SG:25:ARG:HH21	1.52	0.56
12:SF:19:LEU:HD21	12:SF:69:VAL:HG11	1.88	0.56
3:L5:1:C:H5''	3:L5:2:G:C8	2.40	0.56
3:L5:48:G:H5'	85:L5:5518:PUT:HN22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1970:A:O3'	3:L5:2000:G:H8	1.89	0.56
3:L5:2494:U:H2'	3:L5:2495:U:O4'	2.04	0.56
34:Sc:13:ARG:HB2	34:Sc:35:MET:HE3	1.86	0.56
68:Lc:57:LYS:O	68:Lc:61:GLU:HG3	2.05	0.56
73:Li:63:VAL:HG23	73:Li:65:LYS:HG3	1.87	0.56
1:S2:17:C:H2'	1:S2:18:C:C6	2.41	0.56
1:S2:837:A:N1	1:S2:838:G:N2	2.47	0.56
1:S2:1408:U:H2'	1:S2:1409:A:C8	2.40	0.56
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.41	0.56
3:L5:3956:G:H2'	3:L5:3966:A:H1'	1.87	0.56
12:SF:49:LEU:HD12	16:SQ:50:LYS:HG2	1.87	0.56
46:LO:37:ARG:HA	46:LO:107:GLY:H	1.71	0.56
3:L5:4199:C:H4'	83:5A:47:LYS:HD2	1.87	0.56
63:LZ:50:PRO:HD3	63:LZ:68:ILE:HG12	1.88	0.56
1:S2:808:A:C2'	1:S2:809:A:H5'	2.36	0.56
3:L5:3983:G:H5''	3:L5:4034:G:H22	1.71	0.56
18:SK:35:LEU:HD12	18:SK:35:LEU:O	2.06	0.56
27:SP:56:LEU:HD23	27:SP:83:MET:HG2	1.87	0.56
52:LI:87:ILE:HG12	52:LI:138:ILE:HG12	1.88	0.56
52:LI:152:LEU:HB3	52:LI:165:ILE:HD12	1.88	0.56
1:S2:118:C:H1'	1:S2:445:A:C5	2.41	0.55
3:L5:1766:A:H3'	22:SS:116:LYS:HA	1.87	0.55
8:SJ:114:VAL:HG13	8:SJ:119:LEU:HB2	1.88	0.55
40:LB:80:GLU:OE1	40:LB:323:TYR:OH	2.24	0.55
38:Lz:156:LYS:HE3	38:Lz:158:GLN:HB3	1.88	0.55
45:LG:234:ARG:HH21	73:Li:46:GLU:HG3	1.71	0.55
3:L5:1236:C:H2'	3:L5:1237:C:C6	2.42	0.55
3:L5:1404:G:H2'	3:L5:1405:C:C6	2.41	0.55
16:SQ:146:ARG:HD2	82:Pt:33:OMC:OP2	2.06	0.55
20:SX:68:LYS:HB3	20:SX:91:LEU:HD22	1.88	0.55
1:S2:455:A:H2'	1:S2:456:C:H6	1.71	0.55
1:S2:1017:U:H5'	24:SN:55:ARG:HD3	1.88	0.55
3:L5:126:C:H2'	3:L5:127:G:H8	1.72	0.55
16:SQ:89:SER:HB3	16:SQ:112:LEU:HD13	1.89	0.55
1:S2:201:C:H5''	1:S2:202:G:N2	2.22	0.55
3:L5:1401:C:H2'	3:L5:1402:C:H6	1.71	0.55
22:SS:124:ARG:NH2	22:SS:129:LEU:HB3	2.21	0.55
1:S2:67:C:C5	11:SG:162:LEU:HB3	2.41	0.55
1:S2:1037:G:H4'	1:S2:1845:A:H4'	1.87	0.55
9:SE:31:PRO:HG2	9:SE:38:LEU:HG	1.89	0.55
37:Sg:24:THR:HG22	37:Sg:27:PHE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:118:ARG:NH1	37:Sg:118:ARG:HB2	2.20	0.55
42:LJ:95:ARG:HH21	42:LJ:177:GLY:H	1.53	0.55
58:LP:39:MET:HG2	58:LP:43:LYS:HD3	1.88	0.55
68:Lc:20:LEU:HB3	68:Lc:102:SER:HB3	1.88	0.55
1:S2:199:C:H3'	1:S2:200:G:H5''	1.88	0.55
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.42	0.55
63:LZ:103:ASP:HB3	63:LZ:106:LEU:HD12	1.88	0.55
3:L5:162:A:H2'	3:L5:163:A:H8	1.71	0.55
7:SD:211:VAL:O	26:SR:20:TYR:OH	2.25	0.55
1:S2:170:A:H2'	1:S2:171:A:C8	2.42	0.55
40:LB:292:LEU:HD12	40:LB:299:ILE:HB	1.88	0.55
1:S2:140:C:H42	1:S2:313:A:H61	1.55	0.55
1:S2:1754:G:H2'	1:S2:1755:C:H6	1.72	0.55
3:L5:508:G:O2'	3:L5:510:U:OP2	2.25	0.55
15:SI:11:ARG:NH2	15:SI:17:LYS:HE3	2.22	0.55
52:LI:43:VAL:HG21	52:LI:197:VAL:HG13	1.89	0.55
3:L5:1292:C:H3'	3:L5:1293:G:H21	1.72	0.54
36:Sf:135:HIS:HB2	36:Sf:138:ARG:O	2.07	0.54
6:SA:34:MET:HE2	6:SA:149:ASN:O	2.07	0.54
46:LO:61:ARG:HA	46:LO:70:PRO:HD2	1.89	0.54
1:S2:1667:U:H2'	1:S2:1668:U:C6	2.43	0.54
3:L5:1195:G:H2'	3:L5:1196:G:C8	2.42	0.54
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.42	0.54
3:L5:2481:G:H2'	3:L5:2482:C:C6	2.42	0.54
27:SP:30:TYR:O	27:SP:34:MET:HG3	2.06	0.54
37:Sg:108:VAL:HA	37:Sg:124:SER:HA	1.89	0.54
39:LA:101:VAL:HG22	39:LA:165:VAL:HG22	1.89	0.54
1:S2:200:G:H3'	1:S2:201:C:H6	1.73	0.54
3:L5:3938:G:OP2	51:LN:24:ARG:HD3	2.07	0.54
11:SG:78:SER:HB3	11:SG:92:ARG:HG2	1.89	0.54
26:SR:66:VAL:HG23	26:SR:67:ARG:N	2.22	0.54
38:Lz:57:SER:HB3	38:Lz:182:ASN:HD21	1.73	0.54
75:Lk:36:VAL:HG13	75:Lk:43:TYR:HB2	1.88	0.54
1:S2:1025:U:H2'	1:S2:1026:C:O4'	2.07	0.54
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.42	0.54
3:L5:4266:G:N3	3:L5:4266:G:H2'	2.22	0.54
21:SM:73:GLN:CD	21:SM:73:GLN:H	2.15	0.54
31:SZ:50:PHE:HB2	31:SZ:54:THR:HB	1.89	0.54
1:S2:827:A:H5'	8:SJ:8:VAL:HG12	1.90	0.54
3:L5:1406:G:H2'	3:L5:1407:C:C6	2.43	0.54
3:L5:4061:G:H2'	3:L5:4062:A:H5''	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4140:C:H5''	3:L5:4141:G:C5	2.42	0.54
3:L5:4739:C:H2'	3:L5:4740:G:H5'	1.88	0.54
83:5A:20:MET:HG3	83:5A:21:GLN:N	2.22	0.54
83:5A:97:GLY:HA2	83:5A:114:LEU:HD11	1.89	0.54
1:S2:561:A:O2'	8:SJ:134:HIS:NE2	2.37	0.54
1:S2:1678:A2M:O2'	1:S2:1679:A:H5'	2.08	0.54
3:L5:1969:G:H2'	3:L5:1999:A:H2	1.71	0.54
3:L5:3707:U:H2'	3:L5:3708:C:H6	1.71	0.54
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.42	0.54
43:LH:19:THR:HG23	43:LH:26:ILE:HB	1.90	0.54
83:5A:98:TYR:HE1	83:5A:113:ARG:HD2	1.71	0.54
1:S2:902:G:H2'	1:S2:903:A:H8	1.73	0.54
1:S2:1407:U:H2'	1:S2:1408:U:C6	2.43	0.54
1:S2:1564:C:P	28:ST:121:ARG:HH22	2.31	0.54
3:L5:704:C:H42	3:L5:707:C:N4	2.05	0.54
3:L5:5027:C:H6	15:SI:77:ARG:HH12	1.56	0.54
56:LS:76:LYS:HB3	56:LS:131:GLU:HG3	1.90	0.54
1:S2:385:G:H3'	25:SL:136:LYS:HB2	1.89	0.54
1:S2:1408:U:H2'	1:S2:1409:A:H8	1.71	0.54
3:L5:48:G:C8	85:L5:5518:PUT:H32	2.41	0.54
3:L5:491:G:H2'	3:L5:492:U:C6	2.43	0.54
3:L5:2292:C:H2'	3:L5:2293:U:C6	2.43	0.54
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.43	0.54
3:L5:3971:G:HO2'	38:Lz:209:THR:HG1	1.51	0.54
1:S2:200:G:H3'	1:S2:201:C:C6	2.44	0.53
1:S2:551:U:H4'	35:Se:113:ASN:HB3	1.89	0.53
3:L5:23:C:H2'	3:L5:24:G:O4'	2.08	0.53
3:L5:4114:C:H3'	3:L5:4115:G:H21	1.71	0.53
1:S2:199:C:H3'	1:S2:200:G:H8	1.72	0.53
1:S2:316:G:OP2	11:SG:183:ARG:HD3	2.09	0.53
1:S2:1317:C:H2'	1:S2:1318:G:H8	1.73	0.53
3:L5:258:G:H2'	3:L5:259:C:C5	2.43	0.53
3:L5:733:A:H2'	3:L5:734:G:O4'	2.09	0.53
3:L5:1811:G:H4'	66:Lb:60:ASN:HD22	1.73	0.53
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.08	0.53
36:Sf:126:CYS:SG	36:Sf:143:LYS:HE2	2.47	0.53
69:Ld:64:ILE:HG23	69:Ld:68:LEU:HD23	1.88	0.53
83:5A:65:THR:HG22	83:5A:66:GLY:H	1.72	0.53
83:5A:138:LEU:HD22	83:5A:147:VAL:HG11	1.90	0.53
1:S2:115:U:H2'	1:S2:116:OMU:C6	2.38	0.53
1:S2:1797:U:H2'	1:S2:1798:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1939:A:H5'	3:L5:1940:G:H5'	1.90	0.53
3:L5:2486:G:H2'	3:L5:2487:G:H8	1.72	0.53
18:SK:79:LEU:O	18:SK:83:LEU:HD12	2.08	0.53
37:Sg:236:ILE:HG22	37:Sg:250:ALA:HB1	1.90	0.53
67:LF:182:TYR:HB3	67:LF:200:ARG:HG3	1.90	0.53
1:S2:525:A:H2'	1:S2:526:A:H8	1.73	0.53
3:L5:2004:U:N3	3:L5:2016:C:H1'	2.23	0.53
3:L5:2023:C:H2'	3:L5:2024:G:O4'	2.08	0.53
41:LC:140:LYS:HB3	41:LC:142:HIS:HD2	1.73	0.53
58:LP:45:THR:O	58:LP:49:LYS:HE3	2.09	0.53
1:S2:808:A:H2'	1:S2:809:A:H5'	1.90	0.53
1:S2:1264:C:H4'	1:S2:1265:A:O5'	2.08	0.53
2:L8:5:U:H2'	2:L8:6:C:C6	2.43	0.53
3:L5:699:C:H2'	3:L5:700:G:H8	1.73	0.53
3:L5:2478:C:C2'	3:L5:2479:G:H5'	2.38	0.53
3:L5:4546:A:OP1	83:5A:50[A]:5CT:H14	2.09	0.53
21:SM:31:LEU:HD22	21:SM:111:VAL:HA	1.91	0.53
28:ST:108:GLU:HG3	28:ST:113:VAL:HG12	1.91	0.53
59:LU:46:ARG:NH2	59:LU:89:LYS:HE3	2.24	0.53
1:S2:1124:C:H5''	5:SB:150:ILE:HG12	1.90	0.53
3:L5:372:A:OP1	74:Lj:36:LYS:HE3	2.09	0.53
3:L5:2083:C:P	54:LQ:14:ARG:HH22	2.31	0.53
3:L5:2591:A:H2'	3:L5:2592:U:H6	1.73	0.53
7:SD:105:LEU:HB2	7:SD:122:VAL:HG21	1.90	0.53
77:Lm:79:GLU:OE1	77:Lm:81:SER:HB3	2.09	0.53
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.44	0.53
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.73	0.53
25:SL:111:VAL:HG12	25:SL:140:PHE:HB2	1.91	0.53
42:LJ:10:ASN:HB3	42:LJ:13:ARG:HG3	1.91	0.53
68:Lc:35:LEU:O	68:Lc:39:ARG:HG2	2.08	0.53
1:S2:1752:C:O2'	1:S2:1782:G:H5'	2.09	0.53
3:L5:286:U:H2'	3:L5:287:U:C6	2.43	0.53
3:L5:462:G:H2'	3:L5:463:A:C8	2.43	0.53
3:L5:2002:A:N3	3:L5:2002:A:H2'	2.23	0.53
3:L5:2488:C:H2'	3:L5:2489:C:O4'	2.08	0.53
3:L5:3746:A:H5''	39:LA:244:GLY:HA3	1.91	0.53
37:Sg:29:ASP:CG	37:Sg:47:ARG:HH12	2.16	0.53
1:S2:377:G:H5'	15:SI:99:ASN:HB2	1.90	0.53
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.44	0.53
9:SE:124:CYS:HB3	9:SE:141:THR:HB	1.91	0.53
38:Lz:34:LEU:HD21	38:Lz:183:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:LD:79:TYR:O	53:LD:82:GLU:HG2	2.09	0.53
1:S2:15:U:H2'	1:S2:16:G:O4'	2.09	0.53
1:S2:1101:U:H2'	1:S2:1102:G:C8	2.44	0.53
1:S2:1144:A:H2'	1:S2:1145:A:C8	2.44	0.53
3:L5:1693:U:OP2	54:LQ:49:LYS:HE3	2.08	0.53
3:L5:2491:C:H2'	3:L5:2492:C:C6	2.44	0.53
3:L5:3705:G:H2'	3:L5:3706:C:C6	2.44	0.53
1:S2:1425:G:H21	28:ST:5:THR:HG21	1.74	0.52
1:S2:1597:C:H4'	1:S2:1603:G:O6	2.09	0.52
2:L8:92:U:H2'	2:L8:93:C:O4'	2.10	0.52
3:L5:116:G:H2'	3:L5:117:C:C6	2.43	0.52
9:SE:100:ARG:HH12	9:SE:122:LYS:HA	1.74	0.52
1:S2:59:U:H5''	1:S2:503:C:N4	2.24	0.52
1:S2:1600:G:H5'	31:SZ:43:LYS:HG3	1.90	0.52
3:L5:2020:U:H2'	3:L5:2021:G:C8	2.44	0.52
3:L5:3960:A:H2	3:L5:4045:G:H4'	1.74	0.52
3:L5:4475:G:N7	77:Lm:125:LYS:HE3	2.24	0.52
19:SO:93:LEU:HG	19:SO:124:MET:HE2	1.91	0.52
53:LD:223:PHE:HB3	53:LD:226:TYR:HB2	1.91	0.52
58:LP:23:ARG:HG3	58:LP:125:MET:HE1	1.90	0.52
3:L5:669:C:H5'	64:Lr:68:SER:HB2	1.91	0.52
10:SC:114:LYS:HG2	10:SC:121:ARG:HG3	1.90	0.52
10:SC:184:VAL:HG23	10:SC:195:LEU:HB2	1.91	0.52
18:SK:13:GLU:O	18:SK:17:LYS:N	2.31	0.52
21:SM:84:LYS:HG3	21:SM:85:LEU:N	2.25	0.52
40:LB:14:LEU:HD22	40:LB:17:LEU:HD11	1.92	0.52
1:S2:186:C:H2'	1:S2:187:G:H8	1.75	0.52
1:S2:1076:G:OP2	24:SN:107:LYS:HE2	2.10	0.52
2:L8:70:G:H5''	61:LY:27:ARG:CZ	2.40	0.52
3:L5:469:C:H2'	3:L5:470:A:H8	1.75	0.52
3:L5:1294:A:H1'	3:L5:1295:C:H5	1.75	0.52
44:LE:165:LEU:HB3	44:LE:208:ILE:HD11	1.89	0.52
1:S2:1453:C:C5	1:S2:1455:A:H1'	2.44	0.52
1:S2:1780:G:C2	1:S2:1781:A:H1'	2.45	0.52
3:L5:1942:A:H61	3:L5:2039:G:H2'	1.75	0.52
3:L5:2488:C:H2'	3:L5:2489:C:H6	1.72	0.52
3:L5:3930:U:H2'	3:L5:3931:C:C6	2.44	0.52
3:L5:4260:U:H2'	3:L5:4261:C:H6	1.74	0.52
70:Le:35:TRP:CH2	70:Le:55:MET:HG2	2.44	0.52
2:L8:5:U:H2'	2:L8:6:C:H6	1.75	0.52
3:L5:962:C:N4	3:L5:1701:A:H1'	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1412:G:H2'	3:L5:1413:C:O4'	2.10	0.52
3:L5:4232:U:H4'	3:L5:4233:A:O4'	2.10	0.52
5:SB:131:ASP:OD2	5:SB:180:ASP:HB2	2.10	0.52
6:SA:57:LYS:HE3	6:SA:160:ALA:O	2.10	0.52
77:Lm:83:ARG:O	77:Lm:87:GLN:HG3	2.10	0.52
1:S2:1114:U:H3	1:S2:1119:A:H62	1.56	0.52
1:S2:1466:G:H5'	26:SR:4:VAL:HG22	1.91	0.52
1:S2:1861:G:H5''	32:Sa:3:LYS:HA	1.90	0.52
3:L5:661:C:H2'	3:L5:662:C:C6	2.45	0.52
3:L5:960:A:H2'	3:L5:970:G:N7	2.23	0.52
27:SP:93:MET:HE1	27:SP:106:GLU:HA	1.90	0.52
47:LL:200:LYS:HD3	47:LL:200:LYS:N	2.25	0.52
67:LF:60:GLU:O	67:LF:64:MET:HG3	2.10	0.52
69:Ld:33:ILE:HG22	69:Ld:44:ARG:HG3	1.90	0.52
1:S2:199:C:H5''	1:S2:200:G:C8	2.45	0.52
1:S2:1203:G:H2'	1:S2:1204:A:C8	2.44	0.52
3:L5:225:G:OP2	41:LC:223:ASN:HB2	2.10	0.52
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.45	0.52
3:L5:4100:C:H2'	3:L5:4101:C:O4'	2.09	0.52
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.45	0.52
38:Lz:59:PRO:HA	38:Lz:170:GLY:HA2	1.91	0.52
3:L5:1501:C:O2	3:L5:1501:C:H2'	2.10	0.52
3:L5:1698:C:H2'	3:L5:1699:A:C5	2.44	0.52
3:L5:2374:A:H5'	69:Ld:64:ILE:O	2.10	0.52
7:SD:75:LYS:HE2	18:SK:18:GLU:HG2	1.92	0.52
30:SY:98:GLU:C	30:SY:99:LYS:HD3	2.35	0.52
53:LD:235:MET:HE2	53:LD:235:MET:O	2.09	0.52
1:S2:1154:U:O4	10:SC:227:ARG:HD2	2.10	0.52
1:S2:1823:A:H2'	1:S2:1824:A:O4'	2.10	0.52
3:L5:1739:G:H5''	4:L7:102:U:H1'	1.92	0.52
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	1.90	0.52
18:SK:1:MET:HE1	18:SK:44:HIS:CD2	2.45	0.52
56:LS:52:LYS:HB2	56:LS:54:MET:HG2	1.92	0.52
57:LT:92:ARG:HB3	57:LT:94:GLU:OE2	2.09	0.52
38:Lz:37:SER:HB3	38:Lz:203:ALA:HB3	1.92	0.51
1:S2:196:C:O2'	1:S2:197:U:H5'	2.10	0.51
1:S2:928:G:H2'	1:S2:929:G:C8	2.45	0.51
1:S2:1778:C:H2'	1:S2:1779:G:C8	2.44	0.51
3:L5:1647:U:OP1	84:L5:5509:SPD:N6	2.43	0.51
3:L5:2756:G:N7	63:LZ:51:ARG:NH2	2.57	0.51
3:L5:3723:A2M:H2'	3:L5:3724:A2M:H8	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:SW:32:LYS:HE3	14:SW:36:ARG:NH2	2.25	0.51
22:SS:92:ASP:OD2	22:SS:94:LYS:HG2	2.10	0.51
34:Sc:17:VAL:HG22	34:Sc:30:VAL:HG12	1.91	0.51
36:Sf:95:ARG:NH2	36:Sf:97:LYS:HG2	2.24	0.51
56:LS:76:LYS:NZ	56:LS:100:LEU:O	2.43	0.51
67:LF:40:LYS:O	67:LF:44:LYS:HG3	2.10	0.51
1:S2:945:U:H2'	1:S2:946:U:C6	2.46	0.51
1:S2:1754:G:C6	1:S2:1755:C:N4	2.78	0.51
3:L5:453:G:H2'	3:L5:453:G:N3	2.24	0.51
3:L5:3733:A:H2'	3:L5:3734:PSU:O4'	2.10	0.51
3:L5:4099:G:H22	3:L5:4110:C:H42	1.56	0.51
6:SA:33:GLN:HB3	6:SA:154:LEU:HD12	1.91	0.51
26:SR:34:VAL:O	26:SR:38:ILE:HG13	2.10	0.51
26:SR:77:GLU:HG3	26:SR:78:ARG:N	2.24	0.51
79:Lo:26:TYR:HB3	79:Lo:67:VAL:HB	1.93	0.51
3:L5:111:C:OP1	65:Lh:110:LYS:NZ	2.31	0.51
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.76	0.51
3:L5:1698:C:H42	3:L5:1704:C:N4	2.08	0.51
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.10	0.51
16:SQ:12:VAL:HG11	16:SQ:90:LYS:HB3	1.93	0.51
28:ST:74:SER:O	28:ST:78:ILE:HD12	2.10	0.51
1:S2:1139:C:H2'	1:S2:1140:G:O4'	2.11	0.51
1:S2:1568:C:H2'	1:S2:1569:A:C8	2.45	0.51
3:L5:911:U:H2'	3:L5:912:G:O4'	2.11	0.51
3:L5:1273:G:H2'	3:L5:1274:A:O4'	2.11	0.51
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.11	0.51
3:L5:2493:G:H2'	3:L5:2494:U:C6	2.46	0.51
3:L5:4498:OMU:O5'	3:L5:4498:OMU:H6	2.11	0.51
3:L5:4546:A:O3'	83:5A:50[B]:5CT:H4	2.11	0.51
4:L7:111:C:H2'	4:L7:112:U:O4'	2.11	0.51
36:Sf:119:ARG:CZ	36:Sf:139:HIS:HE1	2.23	0.51
38:Lz:204:LEU:HD12	38:Lz:216:LEU:HD22	1.92	0.51
40:LB:288:GLY:HA3	40:LB:330:PHE:CZ	2.46	0.51
1:S2:367:U:H4'	1:S2:371:A:C8	2.46	0.51
1:S2:463:C:O2'	1:S2:466:G:O6	2.27	0.51
1:S2:1779:G:H2'	1:S2:1780:G:C8	2.45	0.51
3:L5:259:C:H2'	3:L5:260:C:H6	1.75	0.51
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.46	0.51
4:L7:110:G:H2'	4:L7:111:C:C6	2.46	0.51
8:SJ:109:ARG:HB2	8:SJ:112:THR:HG22	1.93	0.51
20:SX:68:LYS:HE2	35:Se:83:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:SS:105:ASN:O	22:SS:109:GLU:HG3	2.10	0.51
27:SP:109:PRO:O	27:SP:112:ILE:HG12	2.10	0.51
83:5A:82:PRO:HG2	83:5A:84:ILE:HD11	1.92	0.51
1:S2:913:A:P	13:SH:99:ARG:HH12	2.33	0.51
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.46	0.51
3:L5:1969:G:H3'	3:L5:1970:A:H8	1.76	0.51
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.76	0.51
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.45	0.51
10:SC:165:VAL:HG21	10:SC:217:ALA:HB1	1.93	0.51
17:SU:26:SER:HB2	17:SU:110:VAL:HA	1.93	0.51
53:LD:208:MET:HE3	53:LD:233:PRO:HA	1.92	0.51
1:S2:1227:G:C2	1:S2:1228:A:C8	2.98	0.51
30:SY:14:THR:HG22	30:SY:21:LYS:HG2	1.92	0.51
34:Sc:67:ARG:HD2	34:Sc:68:LEU:HG	1.92	0.51
36:Sf:106:TYR:CE1	36:Sf:116:ARG:HD2	2.42	0.51
46:LO:103:LYS:HB3	46:LO:105:PHE:CE2	2.46	0.51
51:LN:201:HIS:O	51:LN:204:ARG:HD3	2.11	0.51
1:S2:1161:U:OP2	20:SX:4:CYS:HB3	2.11	0.51
3:L5:657:C:H2'	3:L5:658:C:C6	2.46	0.51
3:L5:664:G:N2	3:L5:667:A:H61	2.08	0.51
3:L5:2591:A:H2'	3:L5:2592:U:C6	2.45	0.51
3:L5:2838:G:H5'	40:LB:247:GLY:CA	2.40	0.51
3:L5:3944:OMG:O3'	5:SB:54:GLY:HA2	2.11	0.51
38:Lz:38:LEU:HD13	38:Lz:41:TYR:CE2	2.45	0.51
38:Lz:48:ARG:HD2	38:Lz:159:MET:HE3	1.92	0.51
38:Lz:96:ASN:HB3	38:Lz:99:LEU:HG	1.92	0.51
41:LC:60:HIS:HA	41:LC:92:PHE:CE1	2.46	0.51
45:LG:129:PRO:O	45:LG:130:THR:HG22	2.11	0.51
75:Lk:67:LYS:HE2	75:Lk:69:LEU:HD23	1.93	0.51
1:S2:178:C:H2'	1:S2:179:C:C6	2.46	0.51
1:S2:1113:A:H2'	1:S2:1114:U:C6	2.46	0.51
1:S2:1387:G:H2'	1:S2:1388:A:O4'	2.10	0.51
3:L5:3668:C:H5'	39:LA:8:GLN:O	2.11	0.51
3:L5:4187:G:OP1	84:L5:5504:SPD:H52	2.11	0.51
11:SG:67:VAL:HG12	11:SG:69:THR:HG22	1.92	0.51
13:SH:57:ARG:HH12	13:SH:91:HIS:CE1	2.29	0.51
30:SY:54:VAL:HG22	30:SY:76:TYR:HB2	1.92	0.51
1:S2:531:A:H2'	1:S2:532:C:C6	2.46	0.50
1:S2:677:G:N1	1:S2:1027:A:OP2	2.33	0.50
3:L5:2019:C:H2'	3:L5:2020:U:C6	2.46	0.50
41:LC:4:ALA:O	41:LC:29:LYS:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:LD:208:MET:HB3	53:LD:219:TYR:HE1	1.74	0.50
1:S2:804:U:H2'	1:S2:805:U:C6	2.47	0.50
1:S2:1550:G:O2'	1:S2:1558:C:O2	2.27	0.50
3:L5:456:C:H2'	3:L5:457:G:C8	2.46	0.50
3:L5:1420:A:H5''	3:L5:1420:A:C8	2.44	0.50
3:L5:1577:G:H5'	3:L5:1578:U:H5''	1.93	0.50
3:L5:1855:G:H2'	3:L5:1856:C:O4'	2.12	0.50
13:SH:110:THR:O	13:SH:110:THR:CG2	2.55	0.50
44:LE:207:LYS:N	44:LE:207:LYS:HD2	2.25	0.50
47:LL:127:PHE:HA	47:LL:143:GLU:OE1	2.10	0.50
70:Le:35:TRP:CZ2	70:Le:56:PRO:HD2	2.46	0.50
1:S2:12:U:H2'	1:S2:13:C:C6	2.45	0.50
1:S2:74:G:H2'	1:S2:75:G:O4'	2.12	0.50
1:S2:1808:U:H2'	1:S2:1809:A:C8	2.47	0.50
3:L5:181:C:H2'	3:L5:182:G:H8	1.75	0.50
3:L5:1567:U:H2'	3:L5:1568:C:H6	1.76	0.50
3:L5:3978:C:H2'	3:L5:4034:G:H21	1.77	0.50
24:SN:102:LEU:HD11	24:SN:112:LYS:HA	1.93	0.50
60:LX:64:SER:HB2	65:Lh:69:LEU:HD13	1.92	0.50
1:S2:1383:A2M:H2'	1:S2:1384:C:C6	2.47	0.50
1:S2:1454:A:H5''	26:SR:3:ARG:HD2	1.94	0.50
1:S2:1598:G:OP2	31:SZ:82:SER:OG	2.21	0.50
2:L8:32:C:H2'	2:L8:33:G:O4'	2.11	0.50
3:L5:2022:C:H2'	3:L5:2023:C:N1	2.26	0.50
3:L5:3602:C:H2'	3:L5:3603:G:C8	2.47	0.50
3:L5:3727:A:H2'	3:L5:3728:A:C8	2.47	0.50
3:L5:4043:G:H2'	3:L5:4044:U:C6	2.47	0.50
3:L5:4488:A:H4'	3:L5:4489:G:C8	2.47	0.50
13:SH:190:PRO:HG2	13:SH:193:GLN:NE2	2.26	0.50
37:Sg:155:ARG:O	37:Sg:165:ILE:HD12	2.11	0.50
3:L5:325:U:H2'	3:L5:326:C:C6	2.47	0.50
3:L5:1409:C:H2'	3:L5:1410:U:H4'	1.94	0.50
3:L5:1788:A:H2'	52:LI:22:PHE:CZ	2.45	0.50
3:L5:3956:G:C6	3:L5:3966:A:C6	3.00	0.50
11:SG:22:ARG:HD2	11:SG:25:ARG:NH2	2.22	0.50
16:SQ:44:PRO:HD3	16:SQ:77:HIS:HB3	1.93	0.50
42:LJ:84:GLU:HG2	42:LJ:170:TYR:CE1	2.47	0.50
43:LH:26:ILE:HG13	43:LH:35:ARG:HG3	1.93	0.50
65:Lh:107:GLN:O	65:Lh:111:GLU:HG3	2.11	0.50
70:Le:67:LYS:HG2	70:Le:68:HIS:CD2	2.46	0.50
1:S2:538:U:H2'	1:S2:539:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.77	0.50
1:S2:1683:C:H2'	1:S2:1684:C:H6	1.77	0.50
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.11	0.50
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.47	0.50
11:SG:118:GLU:HG2	11:SG:119:LYS:HD3	1.92	0.50
15:SI:11:ARG:HH22	15:SI:17:LYS:HE3	1.76	0.50
15:SI:26:LYS:HG3	15:SI:29:LEU:HD23	1.94	0.50
27:SP:130:ARG:HG3	27:SP:130:ARG:HH11	1.77	0.50
34:Sc:12:ALA:HB1	34:Sc:32:VAL:HB	1.92	0.50
44:LE:244:GLU:O	44:LE:248:ILE:HG12	2.12	0.50
1:S2:1428:G:N2	1:S2:1585:U:H5'	2.26	0.50
3:L5:258:G:H2'	3:L5:259:C:C6	2.46	0.50
3:L5:1969:G:H3'	3:L5:1970:A:C8	2.47	0.50
3:L5:2489:C:HO2'	3:L5:2490:U:H6	1.59	0.50
6:SA:134:LEU:HD22	6:SA:144:THR:HG21	1.91	0.50
1:S2:67:C:H5	11:SG:162:LEU:HB3	1.77	0.50
1:S2:1487:A:O2'	1:S2:1488:C:H5'	2.12	0.50
1:S2:1606:G:N2	1:S2:1632:G:H1'	2.27	0.50
3:L5:1769:G:H2'	3:L5:1770:A:H8	1.75	0.50
3:L5:3976:C:H42	3:L5:4038:C:H41	1.59	0.50
29:SV:62:MET:HE2	29:SV:64:GLU:HG3	1.94	0.50
37:Sg:191:HIS:CG	37:Sg:195:LEU:HD21	2.46	0.50
47:LL:105:LYS:HD3	47:LL:105:LYS:N	2.26	0.50
1:S2:1286:G:N1	21:SM:37:GLU:OE1	2.45	0.50
1:S2:1653:U:H2'	1:S2:1654:G:C8	2.47	0.50
3:L5:683:C:H2'	3:L5:684:G:O4'	2.11	0.50
3:L5:1401:C:H2'	3:L5:1402:C:C6	2.47	0.50
3:L5:1761:G:H1	3:L5:1771:U:H3	1.58	0.50
3:L5:2416:G:N2	3:L5:2427:G:N7	2.54	0.50
3:L5:2727:C:H2'	3:L5:2728:U:C6	2.47	0.50
3:L5:4437:U:C2	3:L5:4515:G:H5'	2.46	0.50
31:SZ:58:LEU:HD12	31:SZ:62:VAL:HG21	1.92	0.50
32:Sa:45:VAL:HB	32:Sa:64:LEU:HD13	1.93	0.50
1:S2:1288:OMU:O2'	1:S2:1289:U:H5'	2.12	0.49
2:L8:43:A:H4'	74:Lj:22:CYS:O	2.12	0.49
3:L5:254:G:H2'	3:L5:255:C:C6	2.46	0.49
3:L5:449:C:OP1	3:L5:450:G:H4'	2.11	0.49
3:L5:1069:G:H2'	3:L5:1070:G:O4'	2.12	0.49
3:L5:2758:G:O2'	3:L5:2765:A:N3	2.40	0.49
8:SJ:111:GLN:NE2	8:SJ:127:ARG:HB2	2.27	0.49
53:LD:51:MET:CE	53:LD:166:ALA:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:25:A:H2'	3:L5:26:C:C6	2.48	0.49
4:L7:89:G:H2'	4:L7:90:A:C8	2.47	0.49
7:SD:133:GLY:HA3	7:SD:156:LEU:O	2.12	0.49
27:SP:75:VAL:HG22	27:SP:93:MET:HB3	1.94	0.49
59:LU:46:ARG:HH21	59:LU:89:LYS:HE3	1.77	0.49
83:5A:44:SER:OG	83:5A:57:HIS:HB3	2.12	0.49
1:S2:190:G:H1'	1:S2:209:A:N6	2.26	0.49
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.12	0.49
3:L5:1961:G:N2	3:L5:2024:G:O2'	2.44	0.49
3:L5:3948:C:H2'	3:L5:3949:A:C8	2.47	0.49
20:SX:100:VAL:HG12	20:SX:125:VAL:HG23	1.93	0.49
1:S2:51:U:H2'	1:S2:52:G:C8	2.46	0.49
1:S2:420:G:O2'	1:S2:660:C:N3	2.46	0.49
1:S2:898:U:H2'	1:S2:899:U:C6	2.48	0.49
1:S2:1712:A:H2'	1:S2:1713:C:C6	2.47	0.49
1:S2:1752:C:H2'	1:S2:1753:C:C6	2.47	0.49
3:L5:1705:G:H2'	3:L5:1706:A:C8	2.48	0.49
11:SG:56:ASN:HB2	11:SG:108:VAL:HG12	1.94	0.49
3:L5:440:U:H4'	71:Lf:91:ASN:O	2.13	0.49
3:L5:2434:G:O2'	3:L5:2527:A:N1	2.45	0.49
3:L5:3710:G:H21	3:L5:3711:A:H61	1.60	0.49
3:L5:4530:UR3:H2'	3:L5:4531:PSU:H2'	1.94	0.49
26:SR:11:LYS:O	26:SR:15:VAL:HG23	2.13	0.49
53:LD:115:MET:HA	53:LD:118:ILE:HD12	1.93	0.49
1:S2:178:C:H2'	1:S2:179:C:H6	1.77	0.49
1:S2:1221:G:H2'	1:S2:1222:G:C8	2.47	0.49
1:S2:1277:C:H2'	1:S2:1278:A:H8	1.77	0.49
3:L5:1564:A:H2'	3:L5:1565:A:C8	2.47	0.49
3:L5:2414:G:H2'	3:L5:2415:OMU:H6	1.93	0.49
5:SB:110:MET:HE2	5:SB:213:ARG:HD2	1.94	0.49
8:SJ:28:GLU:HG2	8:SJ:43:VAL:HG11	1.95	0.49
19:SO:125:LYS:HB3	32:Sa:58:VAL:HG13	1.93	0.49
38:Lz:65:VAL:HG11	38:Lz:148:VAL:HG23	1.95	0.49
45:LG:81:ASN:O	45:LG:84:THR:OG1	2.29	0.49
58:LP:41:ILE:HD12	58:LP:150:LEU:HD21	1.95	0.49
1:S2:543:C:H3'	1:S2:544:G:C8	2.47	0.49
1:S2:824:C:O2	8:SJ:144:ILE:HG21	2.13	0.49
3:L5:4145:C:H2'	3:L5:4146:G:C8	2.48	0.49
5:SB:136:ARG:HB2	5:SB:218:LEU:HD11	1.95	0.49
6:SA:71:PRO:HB3	6:SA:186:ARG:HH22	1.78	0.49
12:SF:167:LYS:HA	31:SZ:71:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:254:PRO:HB3	37:Sg:283:PRO:HB2	1.95	0.49
51:LN:159:ARG:HB3	51:LN:164:LEU:HB2	1.95	0.49
59:LU:28:PRO:HB3	59:LU:100:LEU:HD11	1.93	0.49
76:Ll:23:ILE:HD11	76:Ll:28:ARG:CZ	2.43	0.49
83:5A:49:GLY:O	83:5A:50[A]:5CT:H2O	2.12	0.49
1:S2:1755:C:H2'	1:S2:1756:C:C6	2.48	0.49
2:L8:141:C:H2'	2:L8:142:U:C6	2.48	0.49
3:L5:126:C:H2'	3:L5:127:G:C8	2.47	0.49
3:L5:650:C:H2'	3:L5:651:C:C6	2.48	0.49
3:L5:2485:U:H2'	3:L5:2486:G:C8	2.48	0.49
3:L5:2664:G:H4'	3:L5:2677:G:H4'	1.94	0.49
5:SB:103:MET:HE1	5:SB:212:VAL:O	2.13	0.49
7:SD:170:THR:HG23	7:SD:187:LYS:HG2	1.95	0.49
12:SF:136:ARG:HB2	12:SF:203:ASN:ND2	2.27	0.49
13:SH:76:GLN:O	13:SH:80:VAL:HG23	2.13	0.49
37:Sg:125:ARG:HG2	37:Sg:150:TRP:CG	2.48	0.49
41:LC:91:ALA:O	41:LC:92:PHE:HB2	2.13	0.49
41:LC:293:LEU:O	41:LC:299:GLN:NE2	2.45	0.49
47:LL:200:LYS:HD3	47:LL:200:LYS:H	1.76	0.49
65:Lh:73:TYR:HA	65:Lh:76:LYS:HG3	1.94	0.49
1:S2:319:C:H2'	1:S2:320:G:C8	2.48	0.49
1:S2:452:G:H2'	1:S2:453:C:C6	2.48	0.49
1:S2:1098:C:H2'	1:S2:1099:G:C8	2.48	0.49
2:L8:110:U:O2'	2:L8:111:U:H4'	2.13	0.49
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.48	0.49
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.13	0.49
3:L5:2000:G:H3'	3:L5:2000:G:N3	2.28	0.49
3:L5:2065:G:H2'	3:L5:2066:C:O4'	2.13	0.49
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.48	0.49
3:L5:3966:A:H2'	3:L5:3967:G:H5'	1.94	0.49
3:L5:4143:G:H2'	3:L5:4144:C:C6	2.48	0.49
6:SA:37:TYR:OH	6:SA:57:LYS:HE2	2.13	0.49
8:SJ:30:LYS:HE2	35:Se:116:PHE:CE1	2.46	0.49
17:SU:19:ARG:HG3	17:SU:117:ALA:HA	1.95	0.49
19:SO:57:THR:OG1	19:SO:60:MET:HG3	2.13	0.49
36:Sf:143:LYS:HD3	36:Sf:143:LYS:N	2.28	0.49
46:LO:55:LEU:HD23	46:LO:58:LEU:HD12	1.95	0.49
55:LR:81:ARG:HG2	55:LR:88:ARG:CZ	2.43	0.49
1:S2:17:C:O2'	1:S2:1194:A:N1	2.41	0.49
1:S2:1745:A:H1'	11:SG:66:GLY:HA2	1.95	0.49
3:L5:106:A:H2'	3:L5:107:G:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1850:A:H2'	3:L5:1851:G:C8	2.48	0.49
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.95	0.49
3:L5:3641:U:C6	3:L5:3645:U:C4	3.01	0.49
3:L5:3690:U:OP2	39:LA:200:ARG:HD2	2.12	0.49
3:L5:3717:A:N1	3:L5:3933:G:H1'	2.28	0.49
3:L5:4750:G:H2'	3:L5:4751:G:C8	2.48	0.49
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.13	0.49
8:SJ:45:ARG:O	8:SJ:49:THR:HG23	2.12	0.49
13:SH:53:VAL:HG12	13:SH:175:GLY:HA3	1.95	0.49
18:SK:53:LYS:HG3	18:SK:60:GLU:HB2	1.95	0.49
44:LE:173:LEU:HB2	44:LE:189:THR:HG22	1.94	0.49
55:LR:181:LYS:HA	55:LR:184:ILE:HD12	1.95	0.49
57:LT:103:ASP:O	57:LT:107:LYS:HG2	2.13	0.49
1:S2:1088:U:H4'	1:S2:1089:G:OP2	2.13	0.48
3:L5:1210:C:H41	67:LF:66:ARG:CZ	2.26	0.48
3:L5:2326:G:H5''	70:Le:127:ALA:HB2	1.94	0.48
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.78	0.48
3:L5:4968:A:H2'	3:L5:4969:C:C6	2.48	0.48
6:SA:218:ALA:O	6:SA:222:VAL:HG12	2.12	0.48
45:LG:209:SER:HA	45:LG:212:LYS:HG3	1.95	0.48
47:LL:60:ARG:HD2	47:LL:67:HIS:O	2.12	0.48
65:Lh:63:GLN:O	65:Lh:67:GLU:HG2	2.13	0.48
83:5A:23:SER:HB2	83:5A:75:SER:HB3	1.95	0.48
1:S2:155:G:H4'	11:SG:15:LEU:HD22	1.94	0.48
1:S2:835:C:N4	1:S2:838:G:O6	2.46	0.48
2:L8:15:G:H1'	3:L5:419:A:N6	2.28	0.48
3:L5:65:A:N6	3:L5:75:G:H1'	2.28	0.48
3:L5:223:G:H4'	3:L5:225:G:N7	2.28	0.48
3:L5:469:C:H2'	3:L5:470:A:C8	2.48	0.48
3:L5:670:G:H2'	3:L5:671:G:H8	1.78	0.48
3:L5:1591:U:OP2	40:LB:243:LYS:HE3	2.14	0.48
3:L5:1699:A:H3'	3:L5:1699:A:H8	1.77	0.48
3:L5:4057:C:H2'	3:L5:4058:U:C6	2.48	0.48
8:SJ:29:LEU:HD12	35:Se:116:PHE:HE2	1.79	0.48
9:SE:151:ASP:HB3	9:SE:154:ILE:HG13	1.95	0.48
11:SG:168:LYS:HG2	11:SG:169:PRO:HD2	1.94	0.48
15:SI:34:ALA:HB2	15:SI:56:ARG:HD2	1.94	0.48
31:SZ:47:LEU:HD12	31:SZ:79:ILE:HG22	1.94	0.48
40:LB:258:HIS:HA	40:LB:259:PRO:C	2.37	0.48
52:LI:38:ARG:HG2	52:LI:41:ALA:HB2	1.95	0.48
70:Le:35:TRP:HH2	70:Le:55:MET:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Lk:26:LYS:HB2	75:Lk:69:LEU:HD12	1.95	0.48
1:S2:1406:G:H2'	1:S2:1407:U:C6	2.48	0.48
3:L5:79:C:H2'	3:L5:80:C:H6	1.78	0.48
3:L5:1248:C:H2'	3:L5:1249:C:H6	1.78	0.48
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.78	0.48
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.49	0.48
14:SW:104:LEU:HD23	14:SW:125:ILE:HA	1.95	0.48
29:SV:62:MET:HE1	33:Sb:3:LEU:HD21	1.94	0.48
37:Sg:302:TYR:CE2	37:Sg:308:ARG:HD2	2.48	0.48
1:S2:166:A2M:O2'	1:S2:167:G:H5'	2.13	0.48
1:S2:449:A:H4'	9:SE:3:ARG:HD3	1.95	0.48
1:S2:1416:C:P	28:ST:129:ARG:HH11	2.36	0.48
1:S2:1594:A:N7	31:SZ:104:ARG:HD3	2.28	0.48
1:S2:1597:C:H4'	1:S2:1603:G:C6	2.48	0.48
1:S2:1714:U:H2'	1:S2:1715:A:C8	2.49	0.48
1:S2:1746:U:P	11:SG:31:ARG:HH12	2.35	0.48
1:S2:1752:C:H2'	1:S2:1753:C:H6	1.78	0.48
3:L5:1452:A:H2'	3:L5:1453:G:O4'	2.13	0.48
3:L5:1699:A:H3'	3:L5:1699:A:C8	2.49	0.48
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.95	0.48
3:L5:2849:A:O2'	3:L5:2855:G:N7	2.46	0.48
3:L5:3749:C:H4'	39:LA:221:LYS:O	2.14	0.48
3:L5:4207:C:OP2	57:LT:4:THR:HG23	2.12	0.48
15:SI:69:SER:HB2	25:SL:21:LYS:HB2	1.94	0.48
21:SM:20:GLU:HG2	21:SM:21:VAL:N	2.27	0.48
53:LD:53:VAL:HG11	53:LD:159:VAL:HA	1.95	0.48
1:S2:38:A:OP1	8:SJ:5:ARG:HG3	2.13	0.48
1:S2:352:U:H2'	1:S2:353:C:C6	2.48	0.48
1:S2:388:U:H2'	1:S2:389:A:C8	2.49	0.48
3:L5:481:G:O2'	3:L5:482:G:H5'	2.14	0.48
3:L5:2862:G:N3	3:L5:3624:A:H2'	2.28	0.48
3:L5:3955:G:H2'	3:L5:3956:G:C8	2.48	0.48
3:L5:4220:6MZ:H2'	3:L5:4222:G:H5''	1.96	0.48
21:SM:127:TYR:HA	21:SM:130:CYS:HB2	1.95	0.48
68:Lc:38:ILE:HG21	68:Lc:63:TYR:HB3	1.95	0.48
1:S2:224:A:H2'	1:S2:225:G:O4'	2.13	0.48
2:L8:40:A:H2'	2:L8:41:A:C8	2.47	0.48
2:L8:67:U:H2'	2:L8:68:G:H8	1.79	0.48
2:L8:106:G:H4'	2:L8:137:A:H5'	1.96	0.48
3:L5:699:C:H2'	3:L5:700:G:C8	2.48	0.48
3:L5:3962:A:H2	3:L5:3963:A:H3'	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4057:C:H2'	3:L5:4058:U:H6	1.78	0.48
3:L5:4109:G:H2'	3:L5:4110:C:H6	1.77	0.48
3:L5:4734:A:H2'	3:L5:4735:G:C8	2.48	0.48
6:SA:8:LEU:HD11	29:SV:39:VAL:HG21	1.95	0.48
21:SM:79:VAL:HG11	21:SM:85:LEU:HB2	1.95	0.48
43:LH:85:THR:HG22	43:LH:86:LEU:HG	1.95	0.48
47:LL:87:HIS:CE1	47:LL:89:LYS:HG3	2.48	0.48
1:S2:1035:A:H2'	1:S2:1036:A:O4'	2.14	0.48
1:S2:1545:A:H5''	16:SQ:74:GLY:HA2	1.95	0.48
3:L5:394:G:N2	3:L5:397:G:OP2	2.41	0.48
3:L5:1567:U:H2'	3:L5:1568:C:C6	2.49	0.48
3:L5:3951:G:H22	3:L5:4062:A:H1'	1.79	0.48
3:L5:3962:A:N6	3:L5:3965:A:H1'	2.27	0.48
1:S2:543:C:H3'	1:S2:544:G:H8	1.78	0.48
1:S2:563:G:O2'	1:S2:564:A:H8	1.96	0.48
1:S2:1121:G:O2'	5:SB:204:ILE:O	2.31	0.48
3:L5:25:A:H2'	3:L5:26:C:H6	1.78	0.48
3:L5:368:C:O4'	41:LC:83:GLY:HA3	2.14	0.48
3:L5:702:U:H2'	3:L5:703:G:O4'	2.14	0.48
3:L5:1767:A:H3'	3:L5:1767:A:N3	2.28	0.48
3:L5:3602:C:H2'	3:L5:3603:G:H8	1.78	0.48
3:L5:4923:C:H2'	3:L5:4924:C:H6	1.78	0.48
22:SS:67:VAL:O	22:SS:71:MET:HG3	2.13	0.48
37:Sg:195:LEU:HA	37:Sg:211:GLY:HA3	1.94	0.48
1:S2:940:U:H2'	1:S2:941:C:C6	2.49	0.48
3:L5:660:A:N7	3:L5:661:C:N4	2.61	0.48
3:L5:2406:G:N7	76:LI:2:SER:N	2.62	0.48
3:L5:3911:C:H4'	3:L5:4196:OMG:HM22	1.96	0.48
3:L5:4042:G:H2'	3:L5:4043:G:C8	2.48	0.48
3:L5:4370:OMG:HM23	3:L5:4370:OMG:H1'	1.61	0.48
3:L5:4691:A:H5'	43:LH:71:ARG:NH1	2.24	0.48
13:SH:51:ILE:HG21	13:SH:179:LYS:HG2	1.96	0.48
43:LH:4:ILE:HG12	43:LH:61:TRP:CH2	2.49	0.48
43:LH:103:VAL:HG11	43:LH:144:LEU:HD21	1.95	0.48
52:LI:62:SER:HB3	52:LI:93:PRO:HG3	1.96	0.48
1:S2:1292:C:N3	36:Sf:138:ARG:NH2	2.59	0.48
2:L8:16:G:N2	3:L5:417:G:H1'	2.29	0.48
3:L5:163:A:H2'	3:L5:164:G:H8	1.78	0.48
3:L5:489:C:H2'	3:L5:490:C:C6	2.49	0.48
3:L5:1698:C:C6	67:LF:177:ARG:HD3	2.49	0.48
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.48	0.48
3:L5:4207:C:H3'	57:LT:4:THR:HG21	1.96	0.48
8:SJ:136:ARG:HA	8:SJ:141:VAL:HA	1.96	0.48
22:SS:55:ARG:NE	31:SZ:48:VAL:HG21	2.28	0.48
56:LS:81:TRP:HZ3	56:LS:130:GLU:HG2	1.79	0.48
79:Lo:35:ALA:O	79:Lo:39:ARG:HG3	2.13	0.48
1:S2:294:U:OP1	25:SL:36:TYR:OH	2.31	0.47
1:S2:1097:G:H4'	6:SA:32:PHE:CD1	2.49	0.47
1:S2:1383:A2M:H2'	1:S2:1384:C:H6	1.79	0.47
3:L5:5:A:H2'	3:L5:6:C:O4'	2.14	0.47
37:Sg:20:GLN:HG2	37:Sg:69:VAL:H	1.79	0.47
42:LJ:12:MET:HE2	42:LJ:12:MET:HA	1.97	0.47
50:La:6:ARG:HG3	50:La:6:ARG:NH1	2.25	0.47
51:LN:24:ARG:CZ	51:LN:24:ARG:HA	2.44	0.47
1:S2:1406:G:H2'	1:S2:1407:U:H6	1.79	0.47
2:L8:84:A:C5	2:L8:88:A:H4'	2.49	0.47
2:L8:127:U:H3'	2:L8:128:C:H6	1.78	0.47
3:L5:435:A:OP1	84:L5:5512:SPD:H31	2.14	0.47
3:L5:2093:A:C4	3:L5:2094:G:C6	3.02	0.47
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.79	0.47
24:SN:25:TRP:CD2	33:Sb:82:LYS:HE2	2.49	0.47
24:SN:54:LEU:HB3	24:SN:60:VAL:HB	1.96	0.47
37:Sg:207:CYS:SG	37:Sg:219:TRP:HB2	2.54	0.47
38:Lz:92:LYS:C	38:Lz:92:LYS:HD2	2.39	0.47
38:Lz:130:LYS:HA	38:Lz:130:LYS:HD3	1.72	0.47
1:S2:115:U:H2'	1:S2:116:OMU:H6	1.96	0.47
1:S2:163:U:OP1	11:SG:85:ARG:N	2.45	0.47
1:S2:555:A:H2'	1:S2:556:U:C6	2.49	0.47
1:S2:1201:U:H2'	1:S2:1202:U:C6	2.49	0.47
3:L5:119:G:H3'	3:L5:120:A:H5''	1.96	0.47
3:L5:445:U:H2'	3:L5:446:C:C6	2.49	0.47
3:L5:1969:G:H2'	3:L5:1999:A:C2	2.48	0.47
3:L5:3712:A:H2'	3:L5:3713:U:C6	2.49	0.47
3:L5:3878:C:N4	3:L5:4518:A:C4	2.81	0.47
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.79	0.47
3:L5:4880:C:H2'	3:L5:4881:U:O4'	2.14	0.47
19:SO:98:ARG:HB3	19:SO:132:VAL:HG23	1.96	0.47
22:SS:75:ARG:HE	22:SS:75:ARG:HB3	1.47	0.47
37:Sg:87:LEU:HD21	37:Sg:122:SER:HB3	1.95	0.47
2:L8:76:C:H2'	2:L8:77:A:O4'	2.14	0.47
3:L5:738:C:H5''	3:L5:739:G:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1952:G:H4'	56:LS:93:MET:HB3	1.96	0.47
3:L5:4376:A:H5''	3:L5:4377:G:O5'	2.15	0.47
4:L7:3:C:H2'	4:L7:4:U:C6	2.49	0.47
29:SV:30:ALA:O	29:SV:60:ARG:HD3	2.13	0.47
41:LC:69:THR:HG22	41:LC:75:ARG:HD3	1.95	0.47
49:LM:36:ALA:HB2	49:LM:52:PHE:CE1	2.50	0.47
1:S2:70:G:OP2	11:SG:167:LYS:NZ	2.37	0.47
1:S2:449:A:H5''	92:S2:2102:HOH:O	2.13	0.47
1:S2:1218:C:H2'	1:S2:1219:C:H6	1.79	0.47
2:L8:85:U:H5'	2:L8:87:G:O4'	2.14	0.47
2:L8:88:A:H2'	2:L8:89:U:O4'	2.15	0.47
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.50	0.47
3:L5:3701:OMC:N4	3:L5:3745:U:H2'	2.29	0.47
3:L5:4573:G:H2'	3:L5:4574:U:O4'	2.14	0.47
3:L5:4618:OMG:H5''	48:LV:15:ARG:HB2	1.96	0.47
40:LB:56:ILE:HD13	40:LB:365:LEU:HD22	1.96	0.47
60:LX:82:THR:HG22	60:LX:155:ILE:HG23	1.97	0.47
67:LF:209:TRP:CD1	67:LF:210:PRO:HD2	2.49	0.47
70:Le:23:HIS:HA	70:Le:53:ILE:HD12	1.97	0.47
1:S2:1670:C:H2'	1:S2:1671:G:C8	2.50	0.47
3:L5:498:C:H42	3:L5:656:C:H42	1.63	0.47
3:L5:1701:A:H3'	3:L5:1701:A:OP1	2.14	0.47
3:L5:1763:C:H2'	3:L5:1764:G:C8	2.50	0.47
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.49	0.47
3:L5:3703:G:H5'	83:5A:68:LYS:HE3	1.97	0.47
37:Sg:20:GLN:HE21	37:Sg:21:ILE:H	1.62	0.47
1:S2:677:G:OP1	24:SN:124:ARG:HD2	2.14	0.47
3:L5:260:C:H2'	3:L5:261:G:C8	2.46	0.47
3:L5:1989:G:H2'	3:L5:1990:A:C8	2.50	0.47
3:L5:3604:A:H2'	3:L5:3605:C:C6	2.49	0.47
3:L5:4740:G:O2'	3:L5:4742:G:H5'	2.15	0.47
3:L5:4919:G:H2'	3:L5:4920:C:C6	2.50	0.47
11:SG:2:LYS:HB3	11:SG:15:LEU:HD11	1.95	0.47
13:SH:19:PHE:CE2	13:SH:50:GLU:HB2	2.50	0.47
13:SH:69:LEU:HD13	13:SH:96:ALA:HB2	1.97	0.47
13:SH:115:LYS:HE2	13:SH:115:LYS:HB2	1.62	0.47
14:SW:56:HIS:C	14:SW:57:ARG:HG3	2.40	0.47
21:SM:121:LYS:H	21:SM:121:LYS:HD3	1.80	0.47
27:SP:14:LYS:HD2	27:SP:14:LYS:HA	1.65	0.47
30:SY:114:MET:HA	30:SY:125:VAL:HG21	1.96	0.47
37:Sg:191:HIS:CD2	37:Sg:195:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lz:97:LYS:HE2	38:Lz:97:LYS:HB2	1.73	0.47
82:Pt:55:U:H2'	82:Pt:56:PSU:O4'	2.14	0.47
2:L8:5:U:O2'	2:L8:6:C:H5'	2.15	0.47
2:L8:108:A:C2	2:L8:112:G:C6	3.03	0.47
3:L5:290:U:H4'	85:L5:5518:PUT:H31	1.96	0.47
3:L5:493:G:N2	3:L5:661:C:O2'	2.47	0.47
3:L5:1881:OMC:C2	3:L5:1881:OMC:HM23	2.50	0.47
3:L5:4571:A2M:HM'3	3:L5:4571:A2M:H1'	1.80	0.47
3:L5:4887:C:H2'	3:L5:4888:U:O4'	2.14	0.47
17:SU:94:PRO:HG2	17:SU:97:ILE:HG12	1.97	0.47
58:LP:45:THR:HG22	58:LP:49:LYS:CE	2.45	0.47
1:S2:186:C:H2'	1:S2:187:G:C8	2.49	0.47
1:S2:1373:C:OP1	26:SR:7:LYS:N	2.47	0.47
1:S2:1778:C:H5''	62:LW:77:LYS:HE2	1.95	0.47
1:S2:1828:C:H2'	1:S2:1829:G:O4'	2.15	0.47
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.50	0.47
7:SD:66:ILE:HD11	7:SD:86:LEU:HB3	1.97	0.47
11:SG:148:SER:OG	11:SG:149:LYS:N	2.47	0.47
16:SQ:112:LEU:HD22	16:SQ:119:LEU:HD13	1.97	0.47
24:SN:103:GLU:HA	24:SN:106:ARG:NH1	2.29	0.47
34:Sc:15:THR:HG22	34:Sc:16:LYS:H	1.80	0.47
37:Sg:14:HIS:CE1	37:Sg:35:SER:HB3	2.50	0.47
38:Lz:26:ARG:HA	38:Lz:26:ARG:NE	2.29	0.47
52:LI:184:MET:HE3	52:LI:189:ARG:HH21	1.79	0.47
66:Lb:63:LYS:HA	66:Lb:63:LYS:HD3	1.80	0.47
71:Lf:78:HIS:HB2	71:Lf:85:ARG:HG3	1.96	0.47
80:Lp:38:THR:HA	80:Lp:45:THR:HA	1.95	0.47
1:S2:223:C:H2'	1:S2:224:A:C8	2.50	0.47
1:S2:595:U:H2'	1:S2:596:U:C6	2.50	0.47
1:S2:888:U:O2'	1:S2:889:U:H5'	2.14	0.47
2:L8:56:G:H2'	2:L8:57:C:O4'	2.15	0.47
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.49	0.47
3:L5:4268:A:H2'	3:L5:4269:G:O4'	2.15	0.47
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.50	0.47
9:SE:107:GLY:HA2	9:SE:189:LEU:HG	1.96	0.47
12:SF:126:THR:HG21	34:Sc:27:CYS:SG	2.55	0.47
15:SI:25:ARG:HB2	15:SI:28:GLU:HG2	1.97	0.47
40:LB:195:ASP:O	40:LB:199:GLU:HG2	2.14	0.47
41:LC:154:VAL:HG21	41:LC:170:LEU:HD11	1.97	0.47
45:LG:103:ARG:HG2	45:LG:193:LEU:O	2.14	0.47
45:LG:136:LEU:HD22	45:LG:202:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LG:255:LYS:HZ2	45:LG:255:LYS:C	2.22	0.47
52:LI:47:PRO:HB3	52:LI:171:TRP:CZ2	2.50	0.47
54:LQ:144:LYS:HD3	54:LQ:149:TYR:CD1	2.50	0.47
70:Le:16:ARG:HD3	70:Le:20:PHE:CE2	2.51	0.47
1:S2:1070:A:H2'	1:S2:1071:G:O4'	2.15	0.46
3:L5:1535:C:N3	3:L5:1637:A:H5'	2.30	0.46
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.14	0.46
3:L5:1884:C:H4'	3:L5:2070:U:C4	2.51	0.46
3:L5:2701:U:H2'	3:L5:2702:C:C6	2.50	0.46
3:L5:2814:C:H5'	3:L5:2815:A2M:OP2	2.15	0.46
3:L5:3615:G:C5	62:LW:49:ILE:HD12	2.50	0.46
3:L5:4138:C:H2'	3:L5:4139:G:C8	2.50	0.46
3:L5:4341:C:C2	89:L5:5523:3H3:H14	2.50	0.46
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.50	0.46
11:SG:52:ILE:HG23	11:SG:109:LEU:HD11	1.97	0.46
22:SS:51:ASP:O	22:SS:54:LYS:HG2	2.15	0.46
22:SS:64:VAL:O	22:SS:68:ILE:HG13	2.15	0.46
22:SS:142:ARG:HH11	22:SS:144:ARG:HH22	1.62	0.46
31:SZ:34:LYS:HE3	31:SZ:34:LYS:HB3	1.72	0.46
1:S2:159:A2M:O5'	1:S2:159:A2M:H8	2.15	0.46
1:S2:1124:C:OP1	5:SB:151:ARG:HG3	2.16	0.46
1:S2:1779:G:C6	1:S2:1780:G:C6	3.03	0.46
3:L5:1952:G:H5'	56:LS:95:ARG:NH1	2.30	0.46
14:SW:14:ILE:HG13	14:SW:27:ILE:HD11	1.98	0.46
21:SM:60:MET:HA	21:SM:63:LYS:NZ	2.29	0.46
21:SM:126:GLU:CD	21:SM:129:LYS:HE2	2.40	0.46
31:SZ:114:LYS:HE3	31:SZ:114:LYS:HB3	1.74	0.46
42:LJ:48:PRO:HB2	42:LJ:70:VAL:HG22	1.98	0.46
52:LI:61:SER:HA	52:LI:126:VAL:HG12	1.97	0.46
1:S2:949:G:H2'	1:S2:950:C:C6	2.50	0.46
1:S2:1692:PSU:H2'	1:S2:1693:G:C8	2.50	0.46
1:S2:1831:A:H2'	1:S2:1832:6MZ:H8	1.97	0.46
3:L5:982:U:H2'	3:L5:983:C:C6	2.50	0.46
3:L5:1194:G:H2'	3:L5:1195:G:C5'	2.43	0.46
3:L5:2798:A:H5''	92:L5:6379:HOH:O	2.15	0.46
3:L5:2862:G:H4'	3:L5:3625:G:N7	2.29	0.46
9:SE:174:LYS:HB3	9:SE:174:LYS:HE3	1.59	0.46
17:SU:54:VAL:HG12	17:SU:56:MET:HE3	1.98	0.46
20:SX:95:GLU:O	20:SX:98:ASP:HB2	2.15	0.46
36:Sf:143:LYS:HD3	36:Sf:143:LYS:H	1.81	0.46
60:LX:55:ARG:HD3	60:LX:55:ARG:HA	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:5A:37:PRO:O	83:5A:63:ILE:HG12	2.16	0.46
1:S2:51:U:H2'	1:S2:52:G:H8	1.81	0.46
3:L5:377:A:H2'	3:L5:378:A:O4'	2.15	0.46
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.51	0.46
3:L5:1774:C:H2'	3:L5:1775:A:O4'	2.15	0.46
3:L5:1855:G:OP1	66:Lb:4:SER:HB2	2.14	0.46
3:L5:1967:A:H2'	3:L5:1968:G:C8	2.51	0.46
3:L5:2474:G:N2	3:L5:2503:G:H5''	2.30	0.46
3:L5:2489:C:H1'	3:L5:2490:U:C5	2.50	0.46
3:L5:3974:G:H4'	3:L5:4050:A:C8	2.50	0.46
3:L5:4385:A:C4	83:5A:50[A]:5CT:H13	2.51	0.46
3:L5:5013:C:H41	3:L5:5029:C:P	2.39	0.46
12:SF:22:LYS:HE3	12:SF:22:LYS:HB3	1.67	0.46
19:SO:75:MET:HB3	19:SO:75:MET:HE2	1.80	0.46
27:SP:68:PRO:HD2	27:SP:71:GLU:HG2	1.97	0.46
37:Sg:125:ARG:HG2	37:Sg:150:TRP:CD2	2.51	0.46
38:Lz:159:MET:HB3	38:Lz:165:LEU:HD21	1.97	0.46
41:LC:155:GLU:HG3	41:LC:157:LYS:HG2	1.96	0.46
46:LO:76:PRO:HB2	46:LO:106:ASP:OD1	2.15	0.46
70:Le:23:HIS:HD2	70:Le:43:ASN:HD21	1.63	0.46
1:S2:29:G:H2'	1:S2:30:C:C6	2.51	0.46
1:S2:1232:PSU:H2'	1:S2:1233:G:C8	2.50	0.46
1:S2:1630:A:H5''	22:SS:37:GLY:H	1.80	0.46
3:L5:79:C:H2'	3:L5:80:C:C6	2.51	0.46
3:L5:658:C:H2'	3:L5:659:G:H8	1.80	0.46
3:L5:1203:G:H2'	3:L5:1204:C:C6	2.50	0.46
3:L5:1702:C:H3'	3:L5:1703:C:H6	1.79	0.46
3:L5:1959:U:C5'	3:L5:1961:G:H1'	2.46	0.46
3:L5:2045:G:O2'	3:L5:2046:G:H5''	2.16	0.46
3:L5:2487:G:N3	3:L5:2488:C:H1'	2.31	0.46
3:L5:3812:C:OP1	3:L5:3813:A:O2'	2.32	0.46
3:L5:4134:C:H2'	3:L5:4135:G:O4'	2.15	0.46
8:SJ:65:GLU:O	8:SJ:66:LYS:HG2	2.15	0.46
13:SH:31:GLU:HG3	13:SH:40:LEU:HB3	1.97	0.46
24:SN:16:LEU:HD11	24:SN:62:GLN:HG3	1.96	0.46
27:SP:75:VAL:HG21	27:SP:104:GLN:NE2	2.31	0.46
41:LC:266:THR:O	41:LC:267:TRP:HB2	2.15	0.46
53:LD:88:VAL:HA	53:LD:239:MET:HE2	1.97	0.46
1:S2:438:G:N3	1:S2:438:G:H5''	2.31	0.46
1:S2:443:U:H2'	1:S2:444:G:O4'	2.16	0.46
1:S2:1407:U:H2'	1:S2:1408:U:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L8:127:U:H3'	2:L8:128:C:C6	2.50	0.46
3:L5:494:U:H2'	3:L5:495:C:C6	2.51	0.46
3:L5:1359:G:H4'	51:LN:203:TYR:HB2	1.97	0.46
3:L5:4254:G:H2'	3:L5:4254:G:N3	2.31	0.46
3:L5:5006:U:H4'	3:L5:5007:A:H5'	1.97	0.46
12:SF:33:ILE:HD11	34:Sc:11:LEU:HD23	1.98	0.46
22:SS:113:ARG:O	22:SS:117:ILE:HG12	2.16	0.46
37:Sg:213:ASP:OD2	37:Sg:215:GLN:HB2	2.16	0.46
44:LE:178:PRO:HD2	44:LE:181:LEU:HD12	1.98	0.46
51:LN:60:VAL:HG22	51:LN:134:LEU:HB2	1.96	0.46
51:LN:178:HIS:HA	51:LN:181:HIS:NE2	2.31	0.46
75:Lk:8:ILE:HD13	75:Lk:45:LEU:HD21	1.97	0.46
1:S2:35:C:H5''	1:S2:579:C:H5''	1.97	0.46
1:S2:170:A:H4'	11:SG:136:LYS:HD3	1.98	0.46
1:S2:1229:G:H21	28:ST:87:VAL:CG2	2.28	0.46
3:L5:1440:U:H3	3:L5:2105:A:H2	1.63	0.46
3:L5:1699:A:H2'	3:L5:1700:G:C8	2.51	0.46
3:L5:1764:G:H3'	3:L5:1765:A:N3	2.31	0.46
3:L5:1942:A:N6	3:L5:2039:G:H2'	2.31	0.46
3:L5:2021:G:C2'	3:L5:2022:C:H5'	2.44	0.46
3:L5:2484:A:H2'	3:L5:2485:U:C6	2.51	0.46
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.81	0.46
3:L5:4192:A:H2'	3:L5:4193:C:C6	2.51	0.46
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.96	0.46
21:SM:18:LEU:HA	21:SM:21:VAL:HG12	1.98	0.46
37:Sg:256:ILE:HD11	37:Sg:289:LEU:HD11	1.98	0.46
44:LE:190:HIS:HB3	44:LE:193:PHE:HD2	1.81	0.46
71:Lf:63:LYS:HD3	71:Lf:63:LYS:HA	1.62	0.46
82:Pt:19:G:O6	82:Pt:56:PSU:H1'	2.15	0.46
1:S2:159:A2M:HM'3	1:S2:159:A2M:H1'	1.70	0.46
1:S2:462:OMC:HM23	1:S2:462:OMC:H1'	1.74	0.46
2:L8:8:U:H2'	2:L8:9:A:C8	2.51	0.46
2:L8:67:U:H2'	2:L8:68:G:C8	2.51	0.46
2:L8:140:C:H2'	2:L8:141:C:C6	2.51	0.46
3:L5:40:G:N2	3:L5:4380:A:H62	2.14	0.46
3:L5:498:C:H42	3:L5:656:C:N4	2.14	0.46
3:L5:1564:A:OP1	24:SN:140:LYS:HE3	2.15	0.46
3:L5:3976:C:N4	3:L5:4038:C:H41	2.13	0.46
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.81	0.46
6:SA:88:LEU:HD12	26:SR:81:ARG:HH12	1.79	0.46
10:SC:167:ARG:HG2	10:SC:219:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SF:40:ALA:HB1	12:SF:45:TYR:CG	2.51	0.46
18:SK:80:ARG:HH22	18:SK:90:VAL:HG23	1.80	0.46
20:SX:107:ARG:HB3	20:SX:110:HIS:HB3	1.97	0.46
37:Sg:197:THR:HG23	37:Sg:239:LEU:HD12	1.97	0.46
66:Lb:89:VAL:HG22	66:Lb:91:ARG:HD2	1.97	0.46
67:LF:44:LYS:HB3	67:LF:44:LYS:HE2	1.56	0.46
83:5A:86:ARG:NH1	83:5A:86:ARG:HB2	2.31	0.46
83:5A:103:GLN:NE2	83:5A:109:ARG:HB2	2.30	0.46
1:S2:77:A:H1'	11:SG:176:ILE:HD12	1.97	0.46
1:S2:355:G:OP1	25:SL:92:TYR:OH	2.30	0.46
1:S2:376:A:H2'	1:S2:377:G:O4'	2.14	0.46
1:S2:1190:A:H2'	1:S2:1191:C:O4'	2.16	0.46
3:L5:165:A:H2'	3:L5:166:C:C6	2.51	0.46
3:L5:1524:A2M:HM'2	3:L5:1525:A:O5'	2.15	0.46
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.16	0.46
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.81	0.46
3:L5:2607:C:H5''	55:LR:96:MET:HE1	1.98	0.46
3:L5:3951:G:H22	3:L5:4061:G:H22	1.64	0.46
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.50	0.46
3:L5:4071:U:H2'	3:L5:4072:C:C6	2.51	0.46
3:L5:4109:G:H2'	3:L5:4110:C:C6	2.51	0.46
15:SI:56:ARG:NH1	15:SI:180:GLY:O	2.48	0.46
40:LB:154:LYS:HB2	40:LB:154:LYS:HE2	1.68	0.46
40:LB:213:GLN:HG3	40:LB:214:ASP:CG	2.41	0.46
45:LG:99:ALA:HB1	45:LG:136:LEU:HD11	1.96	0.46
47:LL:121:ARG:HG3	47:LL:121:ARG:NH1	2.31	0.46
62:LW:61:LYS:HA	62:LW:61:LYS:HD3	1.69	0.46
82:Pt:16:C:H5''	82:Pt:17:C:OP2	2.16	0.46
1:S2:528:A:H2'	1:S2:529:A:H8	1.81	0.46
1:S2:547:G:H2'	1:S2:548:C:C6	2.51	0.46
1:S2:834:C:N4	1:S2:835:C:H41	2.13	0.46
3:L5:424:U:H2'	3:L5:425:U:H6	1.81	0.46
3:L5:1100:U:H1'	3:L5:1196:G:N2	2.31	0.46
3:L5:2347:A:C4	70:Le:31:ILE:HD11	2.51	0.46
3:L5:4481:U:H2'	3:L5:4482:U:C6	2.51	0.46
3:L5:5027:C:H4'	3:L5:5028:G:H5'	1.97	0.46
9:SE:102:ILE:HG21	9:SE:239:PRO:HD3	1.98	0.46
10:SC:194:ARG:HD3	10:SC:196:ILE:HD11	1.97	0.46
13:SH:140:VAL:HG12	24:SN:19:ARG:HD3	1.97	0.46
22:SS:143:GLY:C	22:SS:144:ARG:HE	2.24	0.46
47:LL:121:ARG:HG3	47:LL:121:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LV:21:PRO:HA	48:LV:54:ALA:HA	1.97	0.46
61:LY:2:LYS:HE3	61:LY:2:LYS:HB3	1.70	0.46
73:Li:73:ILE:O	73:Li:77:VAL:HG22	2.16	0.46
1:S2:534:G:H2'	1:S2:535:G:C8	2.47	0.45
3:L5:445:U:H2'	3:L5:446:C:O4'	2.16	0.45
3:L5:984:C:H2'	3:L5:985:C:H6	1.80	0.45
3:L5:2046:G:C4	46:LO:60:LYS:HD2	2.50	0.45
3:L5:2415:OMU:HM23	3:L5:2415:OMU:H1'	1.72	0.45
3:L5:2693:G:H2'	3:L5:2694:G:N2	2.31	0.45
3:L5:3971:G:O2'	38:Lz:209:THR:OG1	2.26	0.45
3:L5:4384:U:OP1	83:5A:50[B]:5CT:H9	2.16	0.45
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.77	0.45
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.14	0.45
16:SQ:8:GLN:HG3	16:SQ:99:TYR:CG	2.51	0.45
37:Sg:32:LEU:HD21	37:Sg:42:MET:HG2	1.98	0.45
38:Lz:98:LYS:O	38:Lz:102:LYS:HG2	2.16	0.45
54:LQ:15:ARG:C	54:LQ:16:LYS:HD2	2.41	0.45
1:S2:195:C:C2	1:S2:205:G:C2	3.04	0.45
1:S2:874:G:H21	13:SH:114:GLN:HE21	1.63	0.45
1:S2:1538:C:H2'	1:S2:1539:U:C6	2.50	0.45
3:L5:1637:A:OP1	3:L5:1639:U:H5	1.99	0.45
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.52	0.45
6:SA:191:ARG:NH2	29:SV:44:GLY:O	2.50	0.45
11:SG:224:ARG:NH1	11:SG:225:GLN:HG3	2.31	0.45
12:SF:75:SER:HB3	12:SF:155:CYS:SG	2.56	0.45
15:SI:34:ALA:HB2	15:SI:56:ARG:CD	2.46	0.45
30:SY:63:HIS:CD2	30:SY:68:LYS:HG2	2.51	0.45
30:SY:82:ALA:O	30:SY:86:GLU:HB3	2.16	0.45
38:Lz:74:CYS:O	38:Lz:78:LYS:HE3	2.16	0.45
53:LD:8:LYS:HG2	53:LD:12:TYR:CE2	2.52	0.45
62:LW:1[A]:MET:HG3	62:LW:15:PRO:HG3	1.98	0.45
1:S2:109:PSU:OP1	1:S2:809:A:O2'	2.34	0.45
1:S2:156:G:H5''	11:SG:2:LYS:HE3	1.98	0.45
1:S2:196:C:H2'	1:S2:197:U:H6	1.79	0.45
1:S2:888:U:H2'	1:S2:889:U:C6	2.51	0.45
1:S2:1589:A:H2'	1:S2:1590:C:C6	2.51	0.45
3:L5:1413:C:H5'	3:L5:1414:C:OP2	2.16	0.45
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.51	0.45
3:L5:2480:G:H2'	3:L5:2481:G:C8	2.51	0.45
3:L5:3923:A:H2'	3:L5:3924:C:H6	1.81	0.45
3:L5:3970:G:H2'	3:L5:3971:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
92:L5:6520:HOH:O	50:La:37:GLY:HA3	2.16	0.45
21:SM:45:ARG:HH12	21:SM:72:HIS:HB2	1.81	0.45
26:SR:67:ARG:HD3	26:SR:67:ARG:HA	1.79	0.45
55:LR:171:LYS:O	55:LR:175:GLU:HG2	2.17	0.45
57:LT:103:ASP:O	57:LT:107:LYS:NZ	2.48	0.45
67:LF:175:ILE:HD11	67:LF:187:MET:SD	2.56	0.45
1:S2:199:C:O2	1:S2:199:C:H2'	2.16	0.45
1:S2:573:PSU:O4	1:S2:576:A2M:H8	2.16	0.45
1:S2:1199:A:OP1	32:Sa:2:THR:N	2.50	0.45
1:S2:1616:U:H2'	1:S2:1617:G:O4'	2.16	0.45
2:L8:52:A:H5'	76:Ll:21:ARG:HD3	1.99	0.45
3:L5:3722:G:P	73:Li:68:ARG:HH21	2.40	0.45
3:L5:4107:G:H2'	3:L5:4108:G:C8	2.51	0.45
3:L5:4343:U:H2'	3:L5:4344:U:C6	2.52	0.45
3:L5:4546:A:H4'	83:5A:49:GLY:O	2.16	0.45
5:SB:94:LYS:HA	5:SB:94:LYS:HD2	1.72	0.45
15:SI:157:LYS:HD2	15:SI:157:LYS:HA	1.69	0.45
19:SO:121:ARG:NH1	34:Sc:40:ARG:HH12	2.14	0.45
22:SS:22:GLY:HA2	22:SS:56:ALA:HB3	1.97	0.45
39:LA:133:TYR:HB3	39:LA:168:VAL:HG23	1.99	0.45
46:LO:44:SER:HB3	46:LO:129:LEU:HD11	1.98	0.45
1:S2:344:U:H2'	1:S2:345:U:C6	2.51	0.45
1:S2:416:U:H2'	1:S2:417:C:O4'	2.16	0.45
1:S2:1378:A:H4'	1:S2:1379:A:O5'	2.16	0.45
3:L5:3966:A:C2	3:L5:3967:G:C8	3.05	0.45
26:SR:94:GLU:H	26:SR:94:GLU:CD	2.24	0.45
44:LE:160:LYS:HE2	71:Lf:1:MET:SD	2.57	0.45
44:LE:201:ILE:HG13	44:LE:203:ILE:HG23	1.99	0.45
70:Le:93:LYS:HA	70:Le:93:LYS:HD2	1.68	0.45
83:5A:33:LEU:HB2	83:5A:38:CYS:SG	2.57	0.45
1:S2:149:A:H2'	1:S2:150:A:O4'	2.17	0.45
1:S2:674:C:H2'	1:S2:675:U:C6	2.51	0.45
3:L5:190:G:H2'	3:L5:191:G:C8	2.51	0.45
3:L5:498:C:H2'	3:L5:499:G:C8	2.51	0.45
3:L5:1764:G:C2	3:L5:1769:G:C2	3.05	0.45
3:L5:2695:A:OP1	75:Lk:35:LYS:NZ	2.49	0.45
3:L5:4171:C:H2'	3:L5:4172:A:O4'	2.17	0.45
3:L5:4371:G:H5'	89:L5:5523:3H3:H31	1.97	0.45
3:L5:4486:C:H2'	3:L5:4487:A:O4'	2.17	0.45
5:SB:33:VAL:HG12	5:SB:44:ILE:HD12	1.99	0.45
37:Sg:31:ILE:HG23	37:Sg:45:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:289:LEU:HD22	37:Sg:298:LEU:HD11	1.98	0.45
41:LC:297:GLU:CD	41:LC:297:GLU:H	2.24	0.45
45:LG:217:LYS:HA	45:LG:217:LYS:HD3	1.81	0.45
56:LS:15:ARG:HB3	56:LS:27:LEU:HD23	1.98	0.45
70:Le:11:LYS:HE3	70:Le:11:LYS:HB3	1.73	0.45
1:S2:829:C:OP1	9:SE:21:ASP:HB2	2.17	0.45
2:L8:86:U:H3'	2:L8:87:G:H5'	1.99	0.45
3:L5:472:C:H2'	3:L5:473:C:H6	1.82	0.45
3:L5:1817:U:O2'	3:L5:1818:G:H5'	2.16	0.45
3:L5:1971:C:H2'	3:L5:1972:G:O4'	2.17	0.45
3:L5:3656:A:H2'	3:L5:3657:U:H6	1.82	0.45
4:L7:16:A:H2'	4:L7:17:C:C6	2.51	0.45
10:SC:73:MET:HE3	10:SC:73:MET:HB3	1.77	0.45
10:SC:137:VAL:O	10:SC:162:ILE:HA	2.16	0.45
21:SM:121:LYS:HE2	21:SM:121:LYS:HB2	1.85	0.45
1:S2:1639:G7M:H8	1:S2:1639:G7M:O5'	2.17	0.45
1:S2:1741:U:H2'	1:S2:1742:C:O4'	2.17	0.45
2:L8:125:C:H2'	2:L8:126:C:H5''	1.99	0.45
3:L5:223:G:H4'	3:L5:225:G:C8	2.51	0.45
3:L5:1292:C:H2'	3:L5:1293:G:O4'	2.17	0.45
3:L5:1400:G:H2'	3:L5:1401:C:H6	1.82	0.45
3:L5:1699:A:C8	3:L5:1699:A:C3'	3.00	0.45
3:L5:2366:A:N3	3:L5:3850:C:O2'	2.48	0.45
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.52	0.45
3:L5:3771:C:H4'	82:Pt:13:C:H4'	1.99	0.45
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.52	0.45
3:L5:3966:A:C6	3:L5:3967:G:N7	2.85	0.45
3:L5:3974:G:OP1	3:L5:4040:C:N4	2.50	0.45
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.52	0.45
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.52	0.45
3:L5:5047:C:O2'	3:L5:5050:C:OP2	2.25	0.45
7:SD:29:LEU:HD21	7:SD:69:LEU:HD11	1.99	0.45
8:SJ:3:VAL:HB	8:SJ:5:ARG:HD3	1.97	0.45
21:SM:55:ASN:ND2	21:SM:81:ASP:HA	2.31	0.45
37:Sg:12:LYS:HB3	37:Sg:12:LYS:HE3	1.86	0.45
59:LU:34:MET:HE3	59:LU:34:MET:HB2	1.81	0.45
61:LY:134:LYS:HA	61:LY:134:LYS:HD2	1.84	0.45
62:LW:54:LEU:HD12	62:LW:54:LEU:HA	1.83	0.45
68:Lc:17:ARG:NH1	68:Lc:103:ASP:OD2	2.50	0.45
82:Pt:17:C:O2'	83:5A:28:ASN:HB3	2.17	0.45
1:S2:1447:OMG:HM23	1:S2:1447:OMG:H1'	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:919:C:H2'	3:L5:920:C:H6	1.82	0.45
3:L5:1702:C:H3'	3:L5:1703:C:C6	2.51	0.45
3:L5:2864:A:H5'	55:LR:82:LYS:O	2.17	0.45
3:L5:3967:G:H2'	3:L5:3968:U:O4'	2.17	0.45
3:L5:4251:A:H5''	42:LJ:108:GLY:HA3	1.98	0.45
3:L5:4456:OMC:HM21	40:LB:241:PRO:HD3	1.99	0.45
3:L5:4684:A:H2'	3:L5:4685:U:O4'	2.16	0.45
27:SP:101:THR:OG1	27:SP:102:PHE:N	2.50	0.45
37:Sg:256:ILE:HG23	37:Sg:270:LEU:HD13	1.98	0.45
40:LB:103:LYS:HD3	40:LB:103:LYS:HA	1.79	0.45
52:LI:183:ASP:O	52:LI:187:GLU:HG2	2.17	0.45
53:LD:65:ALA:HB2	53:LD:74:ILE:HD13	1.99	0.45
63:LZ:100:VAL:HG21	63:LZ:110:ALA:HB2	1.99	0.45
70:Le:105:SER:HB3	70:Le:128:ARG:HB3	1.99	0.45
78:Ln:20:MET:CE	78:Ln:23:ARG:HD3	2.47	0.45
3:L5:457:G:H2'	3:L5:458:C:C6	2.52	0.45
3:L5:4199:C:OP1	83:5A:53:HIS:HA	2.16	0.45
3:L5:4258:C:H2'	3:L5:4259:C:H6	1.82	0.45
5:SB:60:ASP:HA	5:SB:63:LYS:HE2	1.98	0.45
5:SB:113:MET:HE3	5:SB:142:PHE:HE1	1.81	0.45
7:SD:226:GLN:HG2	37:Sg:186:THR:HG23	1.99	0.45
30:SY:20:ARG:HD2	30:SY:22:GLN:OE1	2.17	0.45
37:Sg:26:GLN:NE2	37:Sg:73:SER:O	2.50	0.45
38:Lz:34:LEU:O	38:Lz:166:ALA:HA	2.17	0.45
38:Lz:48:ARG:HB2	83:5A:111:ASP:HB3	1.99	0.45
55:LR:55:VAL:HG12	55:LR:56:THR:O	2.17	0.45
83:5A:27:LYS:C	83:5A:29:GLY:H	2.25	0.45
1:S2:382:C:H2'	1:S2:383:G:H8	1.81	0.44
1:S2:1293:A:H2'	1:S2:1294:G:H8	1.81	0.44
1:S2:1618:C:H4'	27:SP:50:ARG:NH2	2.32	0.44
1:S2:1650:A:H2'	1:S2:1651:A:O4'	2.17	0.44
1:S2:1856:C:H2'	1:S2:1857:G:C8	2.52	0.44
2:L8:148:A:H2'	2:L8:149:G:C8	2.52	0.44
3:L5:904:C:H2'	3:L5:905:C:H6	1.82	0.44
3:L5:3938:G:H8	3:L5:3938:G:OP1	2.00	0.44
3:L5:4114:C:H3'	3:L5:4115:G:N2	2.31	0.44
12:SF:44:LYS:H	12:SF:44:LYS:HG3	1.51	0.44
14:SW:42:MET:HE2	14:SW:42:MET:HB3	1.68	0.44
37:Sg:29:ASP:O	37:Sg:45:LEU:HD12	2.16	0.44
38:Lz:171:HIS:ND1	38:Lz:173:LYS:HB2	2.32	0.44
38:Lz:206:ILE:HB	38:Lz:216:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:LI:36:LEU:HD13	52:LI:69:ARG:HD3	1.98	0.44
61:LY:124:LYS:O	61:LY:128:VAL:HG23	2.16	0.44
70:Le:23:HIS:CD2	70:Le:43:ASN:HD21	2.34	0.44
78:Ln:20:MET:HE1	78:Ln:23:ARG:HD3	1.99	0.44
3:L5:516:C:H2'	3:L5:517:C:C6	2.52	0.44
3:L5:738:C:H42	3:L5:741:C:H4'	1.81	0.44
3:L5:1893:C:H1'	3:L5:1937:C:O2	2.17	0.44
3:L5:3640:U:H2'	3:L5:3646:A:N6	2.32	0.44
3:L5:4053:A:H2'	3:L5:4054:C:C6	2.52	0.44
3:L5:4302:U:H2'	3:L5:4303:C:H5'	2.00	0.44
4:L7:55:A:OP1	42:LJ:154:LYS:HE2	2.18	0.44
13:SH:74:LYS:HD3	13:SH:74:LYS:HA	1.63	0.44
13:SH:109:ARG:HD2	13:SH:110:THR:H	1.83	0.44
38:Lz:122:ARG:NH2	83:5A:131:GLU:HA	2.31	0.44
83:5A:79:MET:HE3	83:5A:79:MET:HB3	1.66	0.44
83:5A:121:LYS:HD3	83:5A:121:LYS:HA	1.72	0.44
1:S2:28:U:H2'	1:S2:29:G:H8	1.82	0.44
3:L5:259:C:H2'	3:L5:260:C:C6	2.52	0.44
3:L5:490:C:H2'	3:L5:491:G:C8	2.53	0.44
3:L5:1275:G:H2'	3:L5:1276:C:O4'	2.17	0.44
3:L5:1443:A:N6	3:L5:2103:G:O6	2.50	0.44
3:L5:1999:A:C4	3:L5:1999:A:OP2	2.71	0.44
3:L5:2508:PSU:H2'	3:L5:2509:C:C6	2.52	0.44
3:L5:3615:G:O2'	62:LW:44:ARG:NH2	2.51	0.44
3:L5:3770:PSU:H2'	3:L5:3771:C:C6	2.52	0.44
4:L7:55:A:H4'	42:LJ:155:HIS:HB2	1.99	0.44
8:SJ:111:GLN:HB2	8:SJ:145:PRO:HB3	1.99	0.44
9:SE:116:PRO:O	9:SE:120:LYS:NZ	2.45	0.44
10:SC:206:SER:OG	10:SC:210:PRO:HG2	2.17	0.44
18:SK:90:VAL:HG22	18:SK:91:PRO:HD2	1.99	0.44
36:Sf:118:ARG:NE	36:Sf:134:SER:OG	2.50	0.44
38:Lz:89:ALA:O	38:Lz:92:LYS:HE3	2.18	0.44
38:Lz:96:ASN:O	38:Lz:100:VAL:HG22	2.17	0.44
55:LR:136:ARG:O	55:LR:140:GLU:HG2	2.18	0.44
1:S2:1138:C:O2'	29:SV:61:ARG:HG2	2.17	0.44
1:S2:1162:C:H2'	1:S2:1163:C:O4'	2.17	0.44
1:S2:1293:A:H2'	1:S2:1294:G:C8	2.53	0.44
3:L5:1806:G:H2'	3:L5:1807:C:C6	2.52	0.44
3:L5:2293:U:H2'	3:L5:2294:G:C8	2.53	0.44
3:L5:2489:C:H6	3:L5:2489:C:O5'	2.00	0.44
3:L5:2490:U:C6	3:L5:2491:C:N3	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4059:C:H2'	3:L5:4060:U:C6	2.52	0.44
3:L5:4436:U:H4'	3:L5:4437:U:O5'	2.17	0.44
84:L5:5509:SPD:H52	84:L5:5509:SPD:H82	1.70	0.44
14:SW:30:CYS:SG	14:SW:31:SER:N	2.91	0.44
17:SU:94:PRO:HB2	17:SU:96:GLU:OE2	2.17	0.44
27:SP:45:LEU:HD23	27:SP:45:LEU:HA	1.85	0.44
37:Sg:106:LYS:HB2	37:Sg:126:ASP:HB3	1.99	0.44
39:LA:142:GLU:C	39:LA:144:LYS:H	2.26	0.44
44:LE:161:ARG:NH1	44:LE:273:SER:OG	2.50	0.44
64:Lr:18:ILE:O	64:Lr:24:THR:HA	2.18	0.44
68:Lc:36:LYS:O	68:Lc:40:GLN:HG3	2.18	0.44
1:S2:953:C:H2'	1:S2:954:U:O4'	2.18	0.44
1:S2:1316:C:C2	1:S2:1317:C:C5	3.05	0.44
1:S2:1435:C:H2'	1:S2:1436:C:C5	2.52	0.44
2:L8:103:A:H3'	2:L8:104:A:H5''	2.00	0.44
3:L5:35:U:H2'	3:L5:36:U:H5'	1.99	0.44
3:L5:2890:C:H2'	3:L5:2891:U:C6	2.52	0.44
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.53	0.44
4:L7:58:A:H2'	4:L7:59:G:C8	2.53	0.44
20:SX:60:LYS:HD2	20:SX:116:PRO:HB3	1.98	0.44
34:Sc:13:ARG:NH2	34:Sc:35:MET:HE1	2.31	0.44
40:LB:348:ARG:HG2	40:LB:349:LYS:O	2.18	0.44
50:La:72:THR:HG22	50:La:110:LYS:HB3	2.00	0.44
82:Pt:24:C:H2'	82:Pt:25:U:C6	2.52	0.44
1:S2:65:C:C2	11:SG:133:LEU:HD22	2.52	0.44
1:S2:164:A:H3'	1:S2:165:G:N2	2.28	0.44
1:S2:218:PSU:O4	15:SI:184:ARG:NH2	2.50	0.44
1:S2:444:G:O6	15:SI:26:LYS:HE3	2.17	0.44
1:S2:532:C:O2'	1:S2:533:A:H5'	2.17	0.44
1:S2:1733:U:H2'	1:S2:1734:G:O4'	2.18	0.44
3:L5:717:U:H2'	3:L5:718:C:C6	2.52	0.44
3:L5:1205:G:H2'	3:L5:1206:C:H6	1.82	0.44
3:L5:1418:C:H2'	3:L5:1419:G:O4'	2.18	0.44
3:L5:1630:A:H2	3:L5:3638:G:N3	2.16	0.44
3:L5:1717:C:H2'	3:L5:1718:C:C2	2.53	0.44
3:L5:1968:G:H3'	3:L5:1969:G:H8	1.81	0.44
3:L5:2666:U:O2'	3:L5:2668:G:N7	2.48	0.44
3:L5:2815:A2M:HM'3	3:L5:2815:A2M:H1'	1.73	0.44
3:L5:3965:A:H61	3:L5:4047:A:H2'	1.83	0.44
3:L5:4139:G:N1	3:L5:4140:C:H1'	2.32	0.44
3:L5:4690:G:O6	3:L5:4698:C:H5''	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SD:11:PHE:CZ	17:SU:25:THR:HG22	2.51	0.44
7:SD:16:ILE:HD11	23:Sd:36:LEU:HD23	1.99	0.44
10:SC:246:LYS:HB3	10:SC:246:LYS:HE2	1.65	0.44
14:SW:41:MET:HE1	14:SW:69:LEU:HD11	1.99	0.44
17:SU:46:LYS:HB2	17:SU:48:LEU:HD13	2.00	0.44
18:SK:4:PRO:O	18:SK:8:ARG:HG3	2.18	0.44
22:SS:36:VAL:HG23	22:SS:99:LEU:HD22	1.99	0.44
28:ST:126:GLN:O	28:ST:129:ARG:HB3	2.17	0.44
37:Sg:7:LEU:HD11	37:Sg:308:ARG:HG2	2.00	0.44
37:Sg:232:GLY:HA2	37:Sg:259:TRP:HH2	1.82	0.44
40:LB:107:ALA:HB2	40:LB:201:LEU:HD22	1.98	0.44
49:LM:40:GLY:HA3	49:LM:45:VAL:HB	2.00	0.44
59:LU:105:ASN:OD1	59:LU:111:GLU:HB2	2.18	0.44
74:Lj:39:TYR:CD1	74:Lj:40:PRO:HA	2.53	0.44
1:S2:656:G:H5'	1:S2:662:G:N2	2.33	0.44
1:S2:1261:C:H6	23:Sd:10:HIS:CE1	2.36	0.44
3:L5:1548:G:O2'	3:L5:2812:A:N3	2.44	0.44
3:L5:1699:A:C5	3:L5:1700:G:C6	3.06	0.44
3:L5:1701:A:C5	3:L5:1702:C:C5	3.05	0.44
3:L5:2097:U:O5'	3:L5:2098:G:H5''	2.17	0.44
3:L5:2390:G:H22	3:L5:2825:A:H2	1.64	0.44
3:L5:2583:C:OP2	72:Lg:76:ARG:NH1	2.49	0.44
3:L5:4438:U:H2'	3:L5:4439:U:O4'	2.18	0.44
3:L5:4456:OMC:HM22	3:L5:4457:PSU:H5''	1.99	0.44
20:SX:101:LEU:HB3	20:SX:123:VAL:O	2.17	0.44
30:SY:9:THR:HB	30:SY:23:MET:HG3	1.99	0.44
37:Sg:11:LEU:HB3	37:Sg:43:TRP:CZ3	2.53	0.44
37:Sg:216:ALA:N	37:Sg:230:LEU:O	2.51	0.44
60:LX:81:LEU:HD12	60:LX:81:LEU:HA	1.84	0.44
1:S2:203:G:N2	1:S2:204:G:H1'	2.32	0.44
1:S2:1383:A2M:HM'3	1:S2:1383:A2M:H1'	1.56	0.44
1:S2:1599:U:H4'	1:S2:1600:G:O5'	2.18	0.44
3:L5:43:U:H2'	3:L5:44:A:H5'	1.99	0.44
3:L5:163:A:H2'	3:L5:164:G:C8	2.53	0.44
3:L5:904:C:H2'	3:L5:905:C:C6	2.52	0.44
3:L5:2021:G:H2'	3:L5:2021:G:N3	2.33	0.44
3:L5:2281:U:O2'	3:L5:2282:A:H5'	2.17	0.44
3:L5:2436:U:C4	60:LX:130:PRO:HG3	2.53	0.44
3:L5:2673:G:N3	3:L5:2673:G:H5'	2.33	0.44
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.53	0.44
3:L5:4169:G:H4'	3:L5:4171:C:C2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4383:U:H5''	83:5A:49:GLY:HA2	2.00	0.44
3:L5:4923:C:H2'	3:L5:4924:C:C6	2.52	0.44
7:SD:134:CYS:SG	7:SD:135:GLU:N	2.90	0.44
27:SP:107:ILE:HA	27:SP:111:MET:HE2	2.00	0.44
28:ST:6:VAL:HB	28:ST:65:TYR:CE2	2.53	0.44
42:LJ:40:LEU:HD12	42:LJ:70:VAL:HG13	1.99	0.44
44:LE:62:MET:HE3	44:LE:62:MET:HB3	1.86	0.44
46:LO:141:LEU:O	46:LO:145:VAL:HG22	2.18	0.44
46:LO:187:LYS:HD3	46:LO:187:LYS:HA	1.60	0.44
47:LL:87:HIS:HE1	47:LL:89:LYS:HG3	1.82	0.44
80:Lp:26:VAL:O	80:Lp:30:GLU:HG2	2.18	0.44
1:S2:429:C:O2'	1:S2:811:A:N1	2.48	0.44
1:S2:476:A:N3	1:S2:488:U:O2'	2.44	0.44
3:L5:1699:A:H2'	3:L5:1700:G:N9	2.32	0.44
3:L5:2815:A2M:H2'	3:L5:2816:G:C8	2.53	0.44
3:L5:4442:PSU:O2'	3:L5:4443:C:H5'	2.17	0.44
3:L5:4886:C:H2'	3:L5:4887:C:C6	2.52	0.44
3:L5:4926:C:O2'	3:L5:4927:G:H5'	2.18	0.44
16:SQ:86:GLN:HE22	16:SQ:122:ALA:HA	1.83	0.44
36:Sf:126:CYS:SG	36:Sf:127:GLY:N	2.91	0.44
38:Lz:111:LEU:HD13	38:Lz:138:LEU:HD22	1.99	0.44
40:LB:90:VAL:HG13	40:LB:161:ARG:HB2	2.00	0.44
57:LT:102:ARG:HD2	57:LT:102:ARG:HA	1.75	0.44
75:Lk:12:LEU:HB3	75:Lk:16:ARG:NH2	2.33	0.44
79:Lo:69:ARG:CZ	79:Lo:80:LYS:HD3	2.48	0.44
1:S2:27:A2M:HM'3	1:S2:27:A2M:H1'	1.70	0.43
1:S2:166:A2M:HM'3	1:S2:166:A2M:H1'	1.80	0.43
1:S2:326:C:H5''	1:S2:327:G:H5'	1.99	0.43
1:S2:494:C:N4	1:S2:509:OMG:HN22	2.16	0.43
1:S2:885:U:H2'	1:S2:886:A:C8	2.53	0.43
1:S2:886:A:H2'	1:S2:887:U:O4'	2.18	0.43
3:L5:503:C:H2'	3:L5:504:G:H5''	2.00	0.43
3:L5:1460:C:H5''	54:LQ:144:LYS:HG3	2.00	0.43
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.99	0.43
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.53	0.43
3:L5:3723:A2M:H1'	3:L5:3723:A2M:HM'3	1.61	0.43
3:L5:3909:C:H1'	91:Pt:78:MET:HA	2.00	0.43
3:L5:3945:A:H2'	3:L5:3946:G:C8	2.53	0.43
3:L5:3968:U:H3'	3:L5:3969:G:H8	1.82	0.43
3:L5:4085:A:C5	45:LG:56:LYS:HD3	2.53	0.43
3:L5:5022:U:H2'	3:L5:5023:C:C2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:L5:5513:SPD:H101	84:L5:5513:SPD:H72	1.24	0.43
5:SB:165:ARG:O	5:SB:169:MET:HG3	2.18	0.43
10:SC:114:LYS:HG2	10:SC:121:ARG:CG	2.48	0.43
14:SW:30:CYS:HB2	14:SW:61:ILE:HG13	2.00	0.43
17:SU:42:GLY:HA3	17:SU:101:ILE:HD11	2.00	0.43
18:SK:29:MET:HB3	18:SK:42:ASN:HB2	2.00	0.43
38:Lz:105:LYS:HD3	38:Lz:105:LYS:HA	1.72	0.43
41:LC:101:MET:SD	41:LC:104:PRO:HA	2.58	0.43
70:Le:35:TRP:CE2	70:Le:56:PRO:HD2	2.53	0.43
1:S2:50:A:OP2	1:S2:472:C:N4	2.44	0.43
1:S2:102:A:H4'	1:S2:104:A:C8	2.53	0.43
1:S2:452:G:H2'	1:S2:453:C:H6	1.82	0.43
1:S2:649:PSU:H1'	20:SX:45:SER:HB3	1.99	0.43
1:S2:1164:G:O2'	1:S2:1165:G:H5'	2.17	0.43
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.53	0.43
2:L8:66:A:H2'	2:L8:67:U:C6	2.53	0.43
3:L5:436:C:OP1	84:L5:5512:SPD:H92	2.18	0.43
3:L5:1399:G:H2'	3:L5:1400:G:H8	1.83	0.43
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.52	0.43
3:L5:4053:A:O2'	3:L5:4054:C:H5'	2.17	0.43
3:L5:4145:C:H2'	3:L5:4146:G:H8	1.81	0.43
35:Se:110:MET:HE2	35:Se:110:MET:HB3	1.90	0.43
38:Lz:91:LYS:HE3	38:Lz:91:LYS:HB3	1.72	0.43
44:LE:72:LYS:HB2	66:Lb:119:CYS:HB2	1.99	0.43
45:LG:57:TRP:O	45:LG:62:ARG:NH1	2.51	0.43
46:LO:118:MET:HE2	56:LS:169:THR:HG23	2.00	0.43
49:LM:9:VAL:HG21	49:LM:66:HIS:HB3	1.99	0.43
62:LW:2:LYS:HE3	62:LW:2:LYS:HB2	1.57	0.43
1:S2:1003:U:H2'	1:S2:1004:PSU:C6	2.53	0.43
1:S2:1541:G:N3	28:ST:12:GLN:NE2	2.65	0.43
1:S2:1745:A:O3'	11:SG:31:ARG:NH1	2.51	0.43
3:L5:1:C:H5''	3:L5:2:G:H8	1.82	0.43
3:L5:67:C:N4	3:L5:326:C:H5'	2.33	0.43
3:L5:456:C:H2'	3:L5:457:G:H8	1.83	0.43
3:L5:937:U:H2'	3:L5:938:C:C6	2.53	0.43
3:L5:1303:A:N7	70:Le:33:ARG:NH2	2.66	0.43
3:L5:1314:C:C2	3:L5:1315:C:C5	3.06	0.43
3:L5:1479:G:H2'	3:L5:1480:C:C6	2.52	0.43
3:L5:1601:A:C8	3:L5:3643:A:C8	3.06	0.43
3:L5:1871:A2M:H1'	3:L5:4195:G:O6	2.19	0.43
3:L5:2019:C:H2'	3:L5:2020:U:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3710:G:O2'	3:L5:3712:A:N6	2.51	0.43
7:SD:205:PRO:HA	26:SR:42:PRO:HG2	2.00	0.43
14:SW:32:LYS:O	14:SW:36:ARG:HG3	2.18	0.43
21:SM:51:VAL:HB	21:SM:109:VAL:HG13	2.00	0.43
30:SY:101:LYS:HE2	30:SY:101:LYS:HB2	1.83	0.43
38:Lz:53:VAL:HG12	38:Lz:155:ILE:HD11	1.99	0.43
38:Lz:207:LYS:HB3	38:Lz:213:PRO:HA	2.00	0.43
66:Lb:65:MET:HA	66:Lb:68:ARG:CZ	2.47	0.43
79:Lo:74:GLU:HB3	79:Lo:77:CYS:HB3	1.99	0.43
1:S2:1011:A:H2'	1:S2:1012:A:O4'	2.18	0.43
1:S2:1391:OMC:H4'	23:Sd:55:LEU:HD13	2.01	0.43
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.73	0.43
3:L5:1374:G:OP1	41:LC:120:LYS:HD2	2.18	0.43
3:L5:1679:A:N1	3:L5:4391:G:O2'	2.47	0.43
3:L5:1833:G:N2	3:L5:1835:G:O4'	2.52	0.43
3:L5:1959:U:H5''	3:L5:1961:G:H1'	2.01	0.43
3:L5:2387:G:H5'	55:LR:24:LEU:O	2.18	0.43
3:L5:3951:G:N2	3:L5:4062:A:H1'	2.33	0.43
3:L5:4878:C:H2'	3:L5:4879:C:H6	1.83	0.43
3:L5:4966:A:H2'	3:L5:4967:A:O4'	2.19	0.43
89:L5:5523:3H3:H2	79:Lo:59:LYS:NZ	2.33	0.43
15:SI:129:LEU:HG	15:SI:134:GLU:OE1	2.18	0.43
21:SM:23:LYS:HA	21:SM:23:LYS:HD3	1.67	0.43
25:SL:37:TYR:CE2	25:SL:51:ILE:HG12	2.53	0.43
26:SR:30:THR:O	26:SR:34:VAL:HG23	2.19	0.43
46:LO:166:ILE:O	46:LO:170:LYS:HG3	2.18	0.43
53:LD:263:LYS:HD2	53:LD:263:LYS:HA	1.85	0.43
83:5A:98:TYR:CE1	83:5A:113:ARG:HD2	2.52	0.43
1:S2:562:U:H4'	8:SJ:132:GLN:HB3	2.00	0.43
1:S2:1395:C:H1'	1:S2:1474:A:C5	2.53	0.43
3:L5:6:C:H5''	45:LG:197:LYS:HG2	1.99	0.43
3:L5:1999:A:H8	3:L5:2000:G:O4'	2.01	0.43
3:L5:2004:U:C2	3:L5:2016:C:H1'	2.54	0.43
3:L5:2478:C:C5	3:L5:2479:G:C8	3.06	0.43
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.85	0.43
3:L5:4524:G:C2	40:LB:252:ALA:HB1	2.54	0.43
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.83	0.43
4:L7:3:C:H2'	4:L7:4:U:H6	1.81	0.43
4:L7:27:G:H21	4:L7:55:A:N6	2.16	0.43
6:SA:188:THR:HG22	6:SA:189:ILE:HG23	1.99	0.43
6:SA:192:GLU:H	6:SA:192:GLU:HG2	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SF:176:GLU:OE2	12:SF:187:SER:OG	2.36	0.43
22:SS:110:ASP:OD1	22:SS:113:ARG:NH2	2.49	0.43
32:Sa:40:VAL:HG13	32:Sa:69:VAL:HB	2.00	0.43
43:LH:65:LYS:HD3	43:LH:65:LYS:HA	1.73	0.43
1:S2:207:G:H3'	1:S2:208:G:H8	1.83	0.43
1:S2:1144:A:H5'	1:S2:1355:C:C5	2.54	0.43
1:S2:1751:C:H42	1:S2:1782:G:H22	1.66	0.43
2:L8:123:U:H5''	2:L8:124:U:H5	1.83	0.43
3:L5:309:C:H5''	3:L5:310:G:O4'	2.19	0.43
3:L5:682:G:H2'	3:L5:683:C:C6	2.54	0.43
3:L5:1589:C:H2'	3:L5:1590:C:C6	2.52	0.43
3:L5:3656:A:H2'	3:L5:3657:U:C6	2.53	0.43
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.81	0.43
3:L5:3917:A:H2'	3:L5:3918:G:C8	2.53	0.43
3:L5:3963:A:H61	3:L5:4048:A:H62	1.66	0.43
3:L5:4102:C:C4	3:L5:4103:C:H1'	2.53	0.43
3:L5:4674:C:H2'	3:L5:4675:U:C6	2.54	0.43
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.53	0.43
5:SB:125:VAL:HG22	5:SB:172:MET:HE3	1.99	0.43
8:SJ:131:ARG:HA	8:SJ:131:ARG:HD2	1.66	0.43
10:SC:191:VAL:HG11	10:SC:236:PHE:HA	2.00	0.43
11:SG:68:LEU:HD23	11:SG:100:CYS:SG	2.59	0.43
15:SI:79:ILE:HG21	15:SI:170:LYS:HE3	2.01	0.43
27:SP:130:ARG:HG3	27:SP:130:ARG:NH1	2.33	0.43
30:SY:38:THR:O	30:SY:42:GLU:HG2	2.18	0.43
37:Sg:236:ILE:CG2	37:Sg:250:ALA:HB1	2.48	0.43
41:LC:94:ASN:HA	41:LC:100:ARG:O	2.19	0.43
52:LI:184:MET:HE3	52:LI:189:ARG:HE	1.83	0.43
1:S2:74:G:H22	11:SG:159:ARG:NH2	2.16	0.43
1:S2:553:U:H2'	1:S2:555:A:C8	2.48	0.43
1:S2:1017:U:H2'	1:S2:1018:U:C6	2.53	0.43
2:L8:31:G:H2'	2:L8:32:C:O4'	2.18	0.43
3:L5:123:C:H2'	3:L5:124:C:C6	2.53	0.43
3:L5:329:A:H4'	51:LN:170:LYS:NZ	2.34	0.43
3:L5:434:A:H2'	3:L5:435:A:O4'	2.18	0.43
3:L5:495:C:H2'	3:L5:496:G:O4'	2.19	0.43
3:L5:1087:A:H2'	3:L5:1088:C:C6	2.54	0.43
3:L5:1399:G:H2'	3:L5:1400:G:C8	2.53	0.43
3:L5:1535:C:H2'	3:L5:1536:PSU:O4'	2.17	0.43
3:L5:1925:G:OP1	49:LM:33:GLN:NE2	2.52	0.43
3:L5:2685:C:H2'	3:L5:2686:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.83	0.43
3:L5:4143:G:H3'	3:L5:4143:G:N3	2.33	0.43
4:L7:17:C:OP1	42:LJ:156:ARG:NH2	2.51	0.43
17:SU:97:ILE:O	17:SU:100:GLN:HG3	2.18	0.43
21:SM:94:ILE:HG23	21:SM:98:GLY:HA2	1.99	0.43
24:SN:87:ASP:OD1	24:SN:87:ASP:N	2.51	0.43
26:SR:36:GLU:HG3	26:SR:47:ARG:HD2	2.00	0.43
28:ST:13:GLU:HG2	28:ST:16:ARG:NH2	2.34	0.43
28:ST:108:GLU:OE2	28:ST:121:ARG:NH1	2.52	0.43
37:Sg:235:ILE:HG13	37:Sg:236:ILE:N	2.31	0.43
38:Lz:193:LEU:HD12	38:Lz:194:LEU:HD12	2.00	0.43
39:LA:68:ARG:HD2	39:LA:70:LYS:HE3	1.99	0.43
42:LJ:35:ARG:HG2	42:LJ:123:ILE:HA	2.01	0.43
43:LH:63:ASN:OD1	43:LH:66:GLU:HG3	2.18	0.43
46:LO:181:ALA:O	46:LO:185:VAL:HG22	2.19	0.43
57:LT:49:GLN:HA	57:LT:52:MET:SD	2.59	0.43
58:LP:117:ILE:HD12	58:LP:148:MET:HE2	2.01	0.43
83:5A:50[A]:5CT:H20	83:5A:50[A]:5CT:H5	1.75	0.43
1:S2:160:U:O2'	1:S2:161:U:H3'	2.18	0.43
1:S2:201:C:C4	1:S2:202:G:C5	3.06	0.43
1:S2:349:A:OP2	85:S2:1902:PUT:H41	2.19	0.43
1:S2:528:A:H2'	1:S2:529:A:C8	2.54	0.43
1:S2:1117:C:H2'	1:S2:1118:C:C6	2.54	0.43
1:S2:1740:C:H2'	1:S2:1741:U:C6	2.53	0.43
3:L5:10:A:H2'	3:L5:11:G:C8	2.54	0.43
3:L5:63:G:OP1	51:LN:169:ARG:NH2	2.52	0.43
3:L5:88:A:N7	54:LQ:173:LYS:NZ	2.66	0.43
3:L5:1248:C:H2'	3:L5:1249:C:C6	2.54	0.43
3:L5:1400:G:H2'	3:L5:1401:C:C6	2.53	0.43
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.18	0.43
3:L5:2108:G:H2'	3:L5:2109:G:O4'	2.19	0.43
3:L5:2384:U:H2'	3:L5:2385:U:C6	2.54	0.43
3:L5:3963:A:N6	3:L5:4048:A:H62	2.17	0.43
3:L5:4520:G:H8	3:L5:4520:G:O5'	2.02	0.43
3:L5:4896:G:N2	3:L5:4926:C:H41	2.17	0.43
21:SM:30:GLY:O	21:SM:31:LEU:HD23	2.19	0.43
36:Sf:104:LYS:O	36:Sf:104:LYS:HG2	2.19	0.43
37:Sg:236:ILE:H	37:Sg:236:ILE:HG12	1.66	0.43
45:LG:106:THR:OG1	45:LG:109:GLU:HG3	2.18	0.43
46:LO:140:ARG:O	46:LO:144:GLU:HG3	2.18	0.43
47:LL:144:LEU:HD12	47:LL:145:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:108:G:H5''	1:S2:810:A:H4'	2.01	0.43
1:S2:495:U:O2'	9:SE:27:PHE:O	2.37	0.43
3:L5:920:C:H2'	3:L5:921:C:H6	1.82	0.43
3:L5:1653:A:H2'	3:L5:1655:C:C4	2.54	0.43
3:L5:1730:U:H1'	57:LT:101:SER:HB3	2.00	0.43
3:L5:3951:G:H1	3:L5:4061:G:H1	1.66	0.43
3:L5:4039:G:H4'	3:L5:4049:U:H2'	2.00	0.43
3:L5:4258:C:H2'	3:L5:4259:C:C6	2.53	0.43
3:L5:4762:A:H2'	3:L5:4763:U:O4'	2.19	0.43
4:L7:22:A:H2'	4:L7:23:A:C8	2.53	0.43
18:SK:1:MET:HE2	18:SK:47:LYS:HB2	2.00	0.43
22:SS:68:ILE:O	22:SS:72:GLN:HG3	2.19	0.43
32:Sa:64:LEU:HD23	32:Sa:64:LEU:HA	1.83	0.43
34:Sc:13:ARG:HG3	34:Sc:14:VAL:N	2.34	0.43
46:LO:76:PRO:HB3	46:LO:138:LEU:HG	2.01	0.43
52:LI:205:PRO:HG2	52:LI:208:LYS:HG3	2.01	0.43
55:LR:4:LEU:HD22	55:LR:32:ILE:HG22	2.01	0.43
55:LR:105:LEU:HD23	55:LR:138:LEU:HD23	2.00	0.43
83:5A:29:GLY:O	83:5A:40:ILE:HG22	2.17	0.43
1:S2:75:G:N2	11:SG:159:ARG:HD2	2.34	0.43
1:S2:441:C:H2'	1:S2:442:C:C6	2.54	0.43
1:S2:1286:G:O6	21:SM:37:GLU:HG3	2.19	0.43
1:S2:1554:C:OP2	1:S2:1555:U:O2'	2.37	0.43
2:L8:102:G:OP2	2:L8:104:A:O2'	2.32	0.43
3:L5:751:G:H2'	3:L5:752:G:O4'	2.19	0.43
3:L5:1297:U:OP1	71:Lf:56:ASN:HB2	2.19	0.43
3:L5:2478:C:C3'	3:L5:2479:G:H5'	2.49	0.43
3:L5:3846:C:H2'	3:L5:3847:C:H6	1.84	0.43
3:L5:3955:G:C2	3:L5:3956:G:C5	3.07	0.43
3:L5:3972:A:P	38:Lz:60:ARG:HH22	2.42	0.43
3:L5:4102:C:N4	3:L5:4103:C:O2	2.52	0.43
13:SH:109:ARG:HH11	13:SH:110:THR:H	1.66	0.43
21:SM:50:CYS:SG	21:SM:51:VAL:N	2.92	0.43
22:SS:142:ARG:CD	22:SS:142:ARG:H	2.32	0.43
34:Sc:46:VAL:HG22	34:Sc:56:LEU:HD21	2.01	0.43
43:LH:82:LYS:HE2	43:LH:88:PHE:CE1	2.54	0.43
52:LI:93:PRO:HB2	52:LI:125:THR:HB	2.00	0.43
67:LF:105:VAL:HG13	67:LF:136:VAL:HG12	2.00	0.43
72:Lg:5:LEU:HD21	72:Lg:30:ILE:HG22	2.00	0.43
1:S2:171:A:C4	1:S2:173:A:C8	3.08	0.42
1:S2:375:U:H2'	1:S2:376:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:512:A2M:H4'	1:S2:576:A2M:H2	2.01	0.42
1:S2:1476:A:H4'	1:S2:1477:U:H5''	2.01	0.42
1:S2:1546:G:C5'	16:SQ:18:THR:HG21	2.47	0.42
3:L5:121:A:H5'	3:L5:122:U:OP2	2.18	0.42
3:L5:644:G:H2'	3:L5:645:G:C8	2.53	0.42
3:L5:656:C:C2	3:L5:657:C:C5	3.07	0.42
3:L5:917:A:H2'	3:L5:918:G:O4'	2.19	0.42
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.54	0.42
3:L5:1600:A:H5'	58:LP:133:HIS:HA	2.00	0.42
3:L5:1992:U:H4'	3:L5:2002:A:C2	2.49	0.42
3:L5:2861:OMC:OP2	84:L5:5508:SPD:N10	2.52	0.42
3:L5:3705:G:H2'	3:L5:3706:C:H6	1.82	0.42
3:L5:3729:PSU:H5'	79:Lo:34:TYR:OH	2.19	0.42
3:L5:4039:G:H1'	3:L5:4040:C:C5	2.54	0.42
5:SB:217:MET:HE2	5:SB:217:MET:HB2	1.67	0.42
15:SI:162:LEU:HD23	15:SI:162:LEU:HA	1.91	0.42
37:Sg:211:GLY:N	37:Sg:236:ILE:HG13	2.33	0.42
49:LM:6:PHE:H	49:LM:11:ARG:NH2	2.17	0.42
52:LI:36:LEU:HD23	52:LI:87:ILE:HB	2.01	0.42
53:LD:208:MET:HB3	53:LD:219:TYR:CE1	2.53	0.42
1:S2:99:A2M:H2'	1:S2:100:U:O4'	2.19	0.42
1:S2:571:U:O2'	30:SY:60:PHE:O	2.34	0.42
1:S2:1101:U:H2'	1:S2:1102:G:H8	1.83	0.42
1:S2:1223:A:H2'	1:S2:1224:G:O4'	2.18	0.42
1:S2:1413:G:H2'	1:S2:1414:A:H8	1.84	0.42
3:L5:1205:G:H2'	3:L5:1206:C:C6	2.53	0.42
3:L5:1414:C:H2'	3:L5:1415:G:C8	2.53	0.42
3:L5:1606:U:O4	84:L5:5506:SPD:H21	2.19	0.42
3:L5:1873:A:H5'	66:Lb:7:HIS:O	2.19	0.42
3:L5:1959:U:C2	3:L5:1961:G:N2	2.87	0.42
3:L5:3846:C:H2'	3:L5:3847:C:C6	2.54	0.42
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.18	0.42
3:L5:4140:C:H2'	3:L5:4141:G:C2	2.54	0.42
3:L5:4462:C:O2'	3:L5:4463:U:H5'	2.19	0.42
19:SO:83:GLN:O	19:SO:87:GLU:HG2	2.19	0.42
19:SO:113:GLN:OE1	32:Sa:45:VAL:HA	2.19	0.42
20:SX:105:PHE:HE2	20:SX:115:ILE:HD12	1.85	0.42
36:Sf:94:LYS:HA	36:Sf:94:LYS:HD2	1.68	0.42
36:Sf:107:LYS:HB2	36:Sf:107:LYS:HE2	1.82	0.42
37:Sg:107:ASP:OD2	37:Sg:125:ARG:HD2	2.18	0.42
38:Lz:151:VAL:HA	38:Lz:154:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:LA:32:VAL:HG22	39:LA:163:ARG:CZ	2.49	0.42
40:LB:89:ILE:HG22	40:LB:153:MET:HE1	2.01	0.42
42:LJ:43:LEU:HD13	42:LJ:117:ILE:HD11	2.00	0.42
53:LD:273:LEU:HG	53:LD:277:LYS:HD2	2.01	0.42
57:LT:91:VAL:CG1	57:LT:95:HIS:HB2	2.49	0.42
66:Lb:106:LYS:HE3	66:Lb:106:LYS:HB2	1.85	0.42
70:Le:78:LEU:HD11	70:Le:100:ALA:HA	2.02	0.42
78:Ln:16:LYS:HA	78:Ln:16:LYS:HD2	1.81	0.42
1:S2:52:G:H2'	1:S2:53:C:C6	2.54	0.42
1:S2:555:A:H2'	1:S2:556:U:H6	1.84	0.42
1:S2:563:G:N7	8:SJ:172:ARG:NH1	2.67	0.42
1:S2:1388:A:C2	7:SD:205:PRO:HG2	2.54	0.42
1:S2:1621:U:O2'	1:S2:1622:U:H2'	2.19	0.42
1:S2:1755:C:H2'	1:S2:1756:C:H6	1.83	0.42
3:L5:18:C:H4'	51:LN:138:PHE:CD1	2.55	0.42
3:L5:1852:U:H5''	50:La:22:ILE:HD12	2.01	0.42
3:L5:3871:A:H2'	3:L5:3872:A:C8	2.54	0.42
3:L5:4383:U:OP1	83:5A:49:GLY:HA3	2.19	0.42
3:L5:4694:G:OP1	3:L5:4694:G:N2	2.49	0.42
5:SB:168:MET:HG2	5:SB:197:ILE:HG21	2.00	0.42
39:LA:104:VAL:O	39:LA:139:HIS:HE1	2.02	0.42
41:LC:62:THR:HG23	41:LC:92:PHE:CZ	2.54	0.42
42:LJ:64:ARG:HE	42:LJ:64:ARG:HB3	1.67	0.42
45:LG:80:ILE:HD11	51:LN:18:VAL:HG23	2.01	0.42
47:LL:91:ALA:HB1	47:LL:96:ILE:HB	2.01	0.42
55:LR:39:GLN:NE2	55:LR:42:ARG:HH21	2.17	0.42
59:LU:29:VAL:HG21	59:LU:68:SER:OG	2.20	0.42
68:Lc:38:ILE:HD11	68:Lc:46:VAL:HG21	2.00	0.42
83:5A:54:ALA:O	83:5A:74:PRO:HA	2.20	0.42
1:S2:201:C:H5''	1:S2:202:G:H21	1.84	0.42
1:S2:1060:A:H4'	1:S2:1061:U:H5''	2.01	0.42
1:S2:1320:G:H2'	1:S2:1321:G:O4'	2.18	0.42
1:S2:1474:A:H2'	1:S2:1475:G:O4'	2.19	0.42
1:S2:1578:U:H5''	1:S2:1579:A:O4'	2.19	0.42
3:L5:280:G:OP2	51:LN:14:LYS:NZ	2.47	0.42
3:L5:1271:G:C6	3:L5:2108:G:N1	2.88	0.42
3:L5:1433:A:H2'	3:L5:1434:G:H5'	2.02	0.42
3:L5:1883:G:O6	3:L5:1896:A:H2	2.02	0.42
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.54	0.42
3:L5:2300:A:N7	41:LC:143:ARG:NH1	2.68	0.42
3:L5:2750:G:H2'	3:L5:2751:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3899:OMG:H5''	40:LB:257:TRP:CD1	2.54	0.42
3:L5:4551:U:H2'	3:L5:4552:PSU:C6	2.54	0.42
3:L5:4708:A:N3	3:L5:4709:U:H5'	2.34	0.42
6:SA:109:THR:HG23	6:SA:136:GLU:HG2	2.01	0.42
7:SD:71:ALA:O	7:SD:75:LYS:HG3	2.19	0.42
13:SH:147:LYS:HE2	13:SH:153:LEU:HB2	2.00	0.42
24:SN:130:LYS:HG3	24:SN:135:LEU:HB2	2.01	0.42
36:Sf:141:CYS:HB2	36:Sf:143:LYS:NZ	2.34	0.42
37:Sg:271:LYS:N	37:Sg:271:LYS:HD2	2.35	0.42
40:LB:52:GLY:HA2	40:LB:341:LYS:HE3	2.02	0.42
46:LO:38:CYS:HB2	46:LO:106:ASP:OD1	2.18	0.42
46:LO:174:LEU:HD23	46:LO:174:LEU:HA	1.83	0.42
57:LT:127:GLN:NE2	57:LT:129:LYS:O	2.52	0.42
61:LY:26:ARG:O	61:LY:30:MET:HG3	2.18	0.42
61:LY:31:SER:HA	61:LY:48:PRO:HA	2.01	0.42
66:Lb:87:LYS:HD2	66:Lb:87:LYS:HA	1.75	0.42
75:Lk:57:LYS:HE2	75:Lk:57:LYS:HB2	1.78	0.42
79:Lo:59:LYS:HE3	79:Lo:59:LYS:HB2	1.82	0.42
83:5A:21:GLN:HA	83:5A:78:ASN:CG	2.43	0.42
2:L8:14:OMU:HM23	2:L8:14:OMU:H1'	1.63	0.42
2:L8:126:C:H42	3:L5:2543:A:H4'	1.85	0.42
3:L5:959:G:O2'	3:L5:2263:A:N6	2.52	0.42
3:L5:1638:A:OP1	3:L5:1638:A:H3'	2.19	0.42
3:L5:1689:G:OP2	85:L5:5515:PUT:N1	2.52	0.42
3:L5:3837:C:H2'	3:L5:3838:U:O4'	2.19	0.42
3:L5:4461:C:O2'	3:L5:4462:C:H5'	2.19	0.42
3:L5:4922:C:C2	3:L5:4923:C:C5	3.07	0.42
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.55	0.42
3:L5:5002:U:H4'	40:LB:374:PHE:O	2.19	0.42
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.19	0.42
3:L5:5030:U:H2'	3:L5:5031:G:H8	1.83	0.42
5:SB:139:CYS:HB2	5:SB:172:MET:SD	2.59	0.42
9:SE:127:ARG:HG3	9:SE:142:HIS:HA	2.01	0.42
20:SX:25:LYS:HE2	20:SX:25:LYS:HB2	1.75	0.42
28:ST:39:LEU:HD22	28:ST:47:PRO:HG3	2.00	0.42
30:SY:7:ILE:CD1	30:SY:43:LYS:HD2	2.50	0.42
30:SY:101:LYS:H	30:SY:101:LYS:HD3	1.84	0.42
32:Sa:44:ILE:HG21	32:Sa:65:PRO:HG2	2.02	0.42
45:LG:158:ALA:HB2	45:LG:190:LEU:HD12	2.00	0.42
47:LL:140:SER:HA	47:LL:143:GLU:HB2	2.00	0.42
49:LM:80:ALA:C	49:LM:81:ASP:OD1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Le:91:CYS:HB2	70:Le:95:TYR:HD2	1.84	0.42
83:5A:50[B]:5CT:H9	83:5A:50[B]:5CT:H3	1.37	0.42
1:S2:929:G:H2'	1:S2:930:C:O4'	2.19	0.42
1:S2:1083:A:N7	1:S2:1841:C:O2'	2.49	0.42
3:L5:318:A:H2'	3:L5:319:A:C8	2.54	0.42
3:L5:968:C:OP1	44:LE:110:ARG:NH2	2.52	0.42
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.54	0.42
3:L5:2052:G:O3'	46:LO:17:GLY:HA3	2.20	0.42
3:L5:4611:A:H2	43:LH:120:GLU:HG3	1.83	0.42
19:SO:47:LEU:HD23	19:SO:47:LEU:HA	1.81	0.42
23:Sd:27:ARG:HG2	23:Sd:27:ARG:NH1	2.32	0.42
23:Sd:38:MET:HE1	23:Sd:50:ILE:HD11	2.02	0.42
27:SP:83:MET:HE3	27:SP:84:ILE:O	2.20	0.42
33:Sb:21:LYS:C	33:Sb:23:ARG:H	2.28	0.42
37:Sg:110:SER:OG	37:Sg:155:ARG:NH2	2.53	0.42
38:Lz:102:LYS:O	38:Lz:106:LYS:HD3	2.20	0.42
48:LV:87:SER:HA	48:LV:97:TYR:HB3	2.02	0.42
66:Lb:27:GLN:OE1	66:Lb:27:GLN:HA	2.19	0.42
1:S2:495:U:H2'	1:S2:496:C:O4'	2.19	0.42
1:S2:1256:G:O6	17:SU:65:THR:HG23	2.20	0.42
1:S2:1754:G:C4	1:S2:1755:C:C5	3.07	0.42
1:S2:1788:A:H2'	1:S2:1789:G:O4'	2.20	0.42
1:S2:1839:U:H2'	1:S2:1840:U:C6	2.54	0.42
3:L5:113:A:H2'	3:L5:114:G:O4'	2.19	0.42
3:L5:959:G:H8	3:L5:959:G:OP2	2.02	0.42
3:L5:3716:C:H3'	3:L5:3735:G:H22	1.85	0.42
3:L5:3956:G:O6	3:L5:4056:A:N1	2.53	0.42
3:L5:4112:C:C2	3:L5:4113:U:C6	3.08	0.42
3:L5:4392:OMG:H2'	3:L5:4447:5MC:HM51	2.02	0.42
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.54	0.42
5:SB:165:ARG:HG2	5:SB:169:MET:HE3	2.01	0.42
13:SH:166:VAL:HG23	13:SH:189:PHE:HZ	1.83	0.42
24:SN:39:LYS:HE2	24:SN:39:LYS:HB2	1.79	0.42
37:Sg:211:GLY:O	37:Sg:236:ILE:HG12	2.19	0.42
37:Sg:249:CYS:HB3	37:Sg:258:ILE:CD1	2.48	0.42
38:Lz:87:ILE:H	38:Lz:87:ILE:HD12	1.84	0.42
40:LB:217:ILE:HD11	40:LB:333:LEU:HD21	2.00	0.42
51:LN:47:LYS:HD2	51:LN:50:ARG:HH11	1.85	0.42
61:LY:89:LYS:HB3	61:LY:89:LYS:HE3	1.80	0.42
64:Lr:46:ARG:NH2	64:Lr:67:ARG:HD2	2.29	0.42
67:LF:54:ALA:HB2	67:LF:188:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Li:16:LYS:HA	73:Li:16:LYS:HD3	1.66	0.42
82:Pt:51:U:H2'	82:Pt:52:C:C6	2.54	0.42
83:5A:94:ILE:HA	83:5A:99:LEU:HA	2.01	0.42
1:S2:89:C:H5''	85:S2:1903:PUT:H41	2.00	0.42
1:S2:566:U:H3'	1:S2:567:C:C6	2.54	0.42
1:S2:658:U:H4'	1:S2:659:G:O5'	2.19	0.42
1:S2:1836:G:H4'	1:S2:1837:G:C4	2.54	0.42
3:L5:190:G:H2'	3:L5:191:G:H8	1.85	0.42
3:L5:677:G:H2'	3:L5:678:C:C6	2.54	0.42
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.55	0.42
3:L5:1741:G:N3	3:L5:1781:PSU:H5''	2.35	0.42
3:L5:1983:A:OP1	3:L5:1983:A:H4'	2.19	0.42
3:L5:4344:U:H2'	3:L5:4345:C:H6	1.85	0.42
3:L5:4882:U:OP1	49:LM:117:LYS:NZ	2.52	0.42
3:L5:5000:G:H4'	40:LB:382:MET:HE1	2.02	0.42
8:SJ:23:SER:O	8:SJ:27:GLN:HG3	2.20	0.42
19:SO:44:VAL:HG12	19:SO:53:ILE:HB	2.00	0.42
22:SS:34:LYS:HB3	22:SS:103:LEU:HD23	2.00	0.42
23:Sd:48:LYS:HB2	23:Sd:48:LYS:HE3	1.59	0.42
26:SR:109:LEU:HD22	26:SR:111:PHE:CE2	2.55	0.42
27:SP:81:ARG:NH1	27:SP:98:ASN:HA	2.35	0.42
28:ST:14:PHE:HA	28:ST:138:VAL:HG21	2.02	0.42
37:Sg:280:LYS:HD2	37:Sg:280:LYS:HA	1.58	0.42
38:Lz:35:GLN:HA	38:Lz:165:LEU:O	2.20	0.42
42:LJ:159:LYS:O	42:LJ:163:MET:HG3	2.20	0.42
43:LH:1:MET:HE3	43:LH:1:MET:HB2	1.83	0.42
46:LO:28:LEU:HD23	46:LO:28:LEU:HA	1.89	0.42
47:LL:7:GLY:O	50:La:49:HIS:NE2	2.51	0.42
47:LL:196:ALA:O	47:LL:200:LYS:HD3	2.20	0.42
52:LI:66:GLU:OE1	52:LI:69:ARG:NH1	2.52	0.42
65:Lh:10:ARG:NH1	65:Lh:63:GLN:OE1	2.51	0.42
74:Lj:36:LYS:HA	74:Lj:36:LYS:HD3	1.85	0.42
83:5A:62:ASP:HB3	83:5A:65:THR:H	1.84	0.42
1:S2:99:A2M:H8	1:S2:99:A2M:O5'	2.20	0.42
1:S2:379:C:O2	15:SI:5:ARG:NE	2.51	0.42
1:S2:1512:C:H5''	23:Sd:8:TRP:CZ3	2.55	0.42
2:L8:144:U:H2'	2:L8:145:C:C6	2.55	0.42
3:L5:106:A:H1'	3:L5:336:A:N3	2.35	0.42
3:L5:218:A:C5	41:LC:173:LYS:HD3	2.55	0.42
3:L5:669:C:OP1	3:L5:669:C:H4'	2.20	0.42
3:L5:1297:U:O2'	3:L5:1298:C:H5'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1811:G:H4'	66:Lb:60:ASN:ND2	2.35	0.42
3:L5:2011:C:H3'	3:L5:2012:A:H8	1.85	0.42
3:L5:3967:G:H2'	3:L5:3968:U:C4'	2.50	0.42
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.55	0.42
3:L5:4345:C:H2'	3:L5:4346:U:C6	2.55	0.42
3:L5:4618:OMG:HM23	3:L5:4618:OMG:H1'	1.89	0.42
3:L5:4744:A:H2'	3:L5:4745:G:O4'	2.19	0.42
92:L5:6026:HOH:O	41:LC:69:THR:HG21	2.18	0.42
37:Sg:48:ASP:OD1	37:Sg:50:THR:OG1	2.34	0.42
39:LA:234:LYS:HG2	39:LA:238:ILE:HG12	2.00	0.42
53:LD:115:MET:HE1	53:LD:140:GLY:O	2.19	0.42
68:Lc:50:ASN:HB2	68:Lc:76:GLY:C	2.45	0.42
69:Ld:93:ASN:C	69:Ld:95:ASP:H	2.26	0.42
73:Li:99:LYS:HE3	73:Li:99:LYS:HB3	1.80	0.42
82:Pt:59:A:O2'	82:Pt:61:U:OP2	2.24	0.42
83:5A:20:MET:HE2	83:5A:20:MET:HB2	1.65	0.42
1:S2:952:G:H2'	1:S2:953:C:C6	2.55	0.42
1:S2:960:U:H1'	1:S2:963:A:N7	2.34	0.42
1:S2:1317:C:H2'	1:S2:1318:G:C8	2.54	0.42
1:S2:1355:C:O3'	10:SC:238:LYS:NZ	2.52	0.42
1:S2:1401:A:HO2'	1:S2:1402:A:H8	1.66	0.42
1:S2:1405:A:H2'	1:S2:1406:G:O4'	2.20	0.42
1:S2:1511:U:H2'	1:S2:1512:C:C6	2.54	0.42
1:S2:1628:C:H2'	1:S2:1629:C:C6	2.55	0.42
2:L8:10:G:H2'	2:L8:11:C:O4'	2.20	0.42
3:L5:302:C:OP1	51:LN:68:ARG:HB3	2.19	0.42
3:L5:650:C:H2'	3:L5:651:C:H6	1.84	0.42
3:L5:1300:G:H2'	3:L5:1301:C:C6	2.55	0.42
3:L5:2100:A:H2'	3:L5:2101:C:C6	2.55	0.42
3:L5:2519:U:C2	3:L5:2520:C:C5	3.08	0.42
3:L5:2638:G:O2'	3:L5:2639:U:H5'	2.20	0.42
3:L5:3970:G:O6	3:L5:4053:A:N6	2.53	0.42
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.20	0.42
3:L5:4872:G:C2	46:LO:203:VAL:HG23	2.54	0.42
10:SC:169:TYR:CD2	10:SC:173:LYS:HA	2.55	0.42
11:SG:2:LYS:HG2	11:SG:17:GLU:HG3	2.02	0.42
11:SG:43:GLU:HA	11:SG:46:LYS:HE2	2.01	0.42
11:SG:201:LYS:HB3	11:SG:201:LYS:HE3	1.79	0.42
12:SF:78:MET:O	12:SF:79:HIS:CB	2.67	0.42
19:SO:61:LYS:HA	19:SO:61:LYS:HD2	1.77	0.42
21:SM:29:ASP:OD1	21:SM:30:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SM:30:GLY:O	21:SM:112:LYS:HG3	2.20	0.42
21:SM:33:ARG:H	21:SM:37:GLU:HB2	1.85	0.42
25:SL:97:ARG:CZ	25:SL:97:ARG:HB3	2.50	0.42
29:SV:32:ILE:HG12	29:SV:60:ARG:HD2	2.02	0.42
40:LB:224:LYS:HG2	40:LB:340:THR:HG22	2.02	0.42
46:LO:81:TRP:HB2	46:LO:104:VAL:HG21	2.02	0.42
49:LM:80:ALA:O	49:LM:85:LYS:HE3	2.20	0.42
55:LR:160:GLU:O	55:LR:164:SER:OG	2.35	0.42
65:Lh:33:VAL:O	65:Lh:37:THR:HG23	2.19	0.42
1:S2:839:C:H3'	1:S2:840:C:C5'	2.50	0.41
1:S2:901:G:H2'	1:S2:902:G:O4'	2.19	0.41
1:S2:1442:OMU:HM23	1:S2:1442:OMU:H1'	1.72	0.41
3:L5:967:C:H3'	3:L5:968:C:C6	2.55	0.41
3:L5:1700:G:C8	3:L5:1700:G:O5'	2.73	0.41
3:L5:1743:A:O4'	53:LD:15:ARG:HD2	2.20	0.41
3:L5:3718:A2M:H1'	3:L5:3718:A2M:HM'3	1.82	0.41
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.87	0.41
3:L5:4285:U:H2'	3:L5:4286:C:C6	2.55	0.41
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.72	0.41
7:SD:193:ASP:OD1	7:SD:196:GLY:N	2.53	0.41
7:SD:213:PRO:HG3	26:SR:19:LYS:HB3	2.01	0.41
8:SJ:129:LEU:HD23	8:SJ:129:LEU:HA	1.88	0.41
9:SE:112:HIS:CE1	9:SE:239:PRO:HA	2.55	0.41
16:SQ:39:LEU:HB3	16:SQ:40:GLU:OE2	2.19	0.41
26:SR:83:ASN:O	26:SR:84:TYR:C	2.63	0.41
43:LH:8:GLN:HE22	43:LH:71:ARG:HG3	1.85	0.41
46:LO:113:ASP:OD1	46:LO:113:ASP:N	2.53	0.41
59:LU:61:VAL:HG22	59:LU:74:SER:HB2	2.02	0.41
67:LF:106:ARG:O	67:LF:110:GLN:HG3	2.20	0.41
75:Lk:47:ILE:HG22	75:Lk:49:ASP:H	1.84	0.41
82:Pt:21:H2U:H2'	82:Pt:21:H2U:H61	1.80	0.41
1:S2:1404:U:P	17:SU:21:ARG:HH22	2.43	0.41
3:L5:1391:A:H2'	3:L5:1392:A:O4'	2.20	0.41
3:L5:2404:A:O2'	74:Lj:12:ARG:HD2	2.20	0.41
3:L5:2513:A:OP1	72:Lg:11:LEU:HD13	2.20	0.41
3:L5:2741:U:H2'	39:LA:50:HIS:CD2	2.55	0.41
3:L5:3712:A:H2'	3:L5:3713:U:N1	2.34	0.41
3:L5:4300:U:H2'	3:L5:4301:U:C6	2.55	0.41
17:SU:22:ILE:HD12	17:SU:89:ILE:HB	2.02	0.41
39:LA:143:THR:HG22	39:LA:145:LYS:HG2	2.01	0.41
40:LB:83:PRO:HB2	40:LB:204:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:LJ:136:ARG:NH2	42:LJ:161:GLU:OE1	2.54	0.41
52:LI:54:SER:HB2	52:LI:135:ILE:HD11	2.01	0.41
70:Le:88:LEU:HA	70:Le:91:CYS:SG	2.60	0.41
83:5A:20:MET:O	83:5A:79:MET:N	2.48	0.41
1:S2:149:A:H2'	1:S2:150:A:C8	2.55	0.41
1:S2:530:U:O4	1:S2:531:A:N6	2.52	0.41
1:S2:535:G:H2'	1:S2:536:A:C8	2.55	0.41
1:S2:641:A:H2'	1:S2:642:U:O4'	2.20	0.41
1:S2:867:OMG:O2'	1:S2:868:G:H5'	2.20	0.41
1:S2:1395:C:H1'	1:S2:1474:A:C4	2.56	0.41
1:S2:1617:G:N2	1:S2:1619:A:H3'	2.35	0.41
2:L8:6:C:H2'	2:L8:7:U:H6	1.86	0.41
3:L5:81:C:H2'	3:L5:82:U:O4'	2.20	0.41
3:L5:326:C:O2'	3:L5:327:U:H5'	2.20	0.41
3:L5:1704:C:O3'	67:LF:46:ARG:NH1	2.54	0.41
3:L5:2590:G:H2'	3:L5:2754:G:N2	2.36	0.41
3:L5:4733:C:H4'	3:L5:4734:A:O5'	2.21	0.41
3:L5:4872:G:O6	49:LM:98:ARG:HG3	2.20	0.41
7:SD:10:LYS:HB3	7:SD:10:LYS:HE3	1.76	0.41
7:SD:40:ARG:HB2	7:SD:47:GLU:HB2	2.02	0.41
8:SJ:20:PHE:HA	8:SJ:25:LEU:HD11	2.01	0.41
12:SF:30:ILE:HG23	12:SF:117:ILE:HD11	2.00	0.41
18:SK:92:ALA:HA	18:SK:95:ARG:HH11	1.85	0.41
19:SO:88:LEU:HD12	19:SO:88:LEU:HA	1.80	0.41
36:Sf:119:ARG:HG2	36:Sf:139:HIS:ND1	2.35	0.41
43:LH:88:PHE:CE2	43:LH:151:ILE:HB	2.56	0.41
45:LG:50:ASP:HB2	60:LX:40:ILE:HD12	2.02	0.41
51:LN:20:ARG:O	51:LN:24:ARG:HG2	2.20	0.41
81:mR:35:G:H2'	81:mR:36:U:H5''	2.01	0.41
83:5A:92:ILE:HD11	83:5A:108:VAL:HG13	2.02	0.41
1:S2:203:G:P	15:SI:147:LYS:HD2	2.61	0.41
1:S2:420:G:H1'	1:S2:661:U:O2	2.20	0.41
1:S2:1019:C:H2'	1:S2:1020:A:O4'	2.21	0.41
1:S2:1334:G:O3'	7:SD:183:GLY:HA3	2.21	0.41
3:L5:123:C:H2'	3:L5:124:C:H6	1.85	0.41
3:L5:273:U:H2'	3:L5:274:C:O4'	2.20	0.41
3:L5:1401:C:OP1	66:Lb:51:LYS:HD2	2.20	0.41
3:L5:1409:C:H2'	3:L5:1410:U:C4'	2.50	0.41
3:L5:1472:C:H2'	3:L5:1473:U:C6	2.55	0.41
3:L5:1586:G:O2'	3:L5:1587:G:H5'	2.20	0.41
3:L5:1979:A:H2	3:L5:1987:C:N4	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2508:PSU:H2'	3:L5:2509:C:H6	1.85	0.41
3:L5:2622:G:OP2	59:LU:84:LYS:NZ	2.53	0.41
3:L5:4860:G:H5''	46:LO:169:ARG:HD3	2.02	0.41
3:L5:5021:C:C2'	3:L5:5022:U:H4'	2.38	0.41
7:SD:137:VAL:HG22	7:SD:151:LYS:HG3	2.02	0.41
10:SC:120:GLN:H	10:SC:120:GLN:HG2	1.58	0.41
24:SN:93:LYS:HA	24:SN:150:VAL:HG21	2.01	0.41
30:SY:101:LYS:HD3	30:SY:101:LYS:N	2.35	0.41
38:Lz:192:SER:OG	38:Lz:193:LEU:N	2.53	0.41
40:LB:105:VAL:HG11	40:LB:150:PHE:CZ	2.56	0.41
45:LG:159:HIS:ND1	45:LG:185:LYS:HA	2.35	0.41
69:Ld:43:PRO:O	69:Ld:47:LYS:HG3	2.21	0.41
83:5A:79:MET:H	83:5A:79:MET:HG2	1.78	0.41
1:S2:618:C:H2'	1:S2:619:A:O4'	2.20	0.41
1:S2:890:U:N3	1:S2:897:U:H5	2.17	0.41
1:S2:940:U:H3	1:S2:1002:U:H3	1.69	0.41
1:S2:1466:G:H2'	1:S2:1467:C:C6	2.55	0.41
1:S2:1724:A:H2'	1:S2:1725:U:C6	2.55	0.41
3:L5:1292:C:H3'	3:L5:1293:G:N2	2.35	0.41
3:L5:1364:U:OP2	47:LL:36:ARG:NH1	2.52	0.41
3:L5:1700:G:N7	3:L5:1704:C:N3	2.69	0.41
3:L5:2045:G:OP2	3:L5:4461:C:H4'	2.21	0.41
3:L5:2393:C:H2'	3:L5:2394:G:H5'	2.02	0.41
3:L5:2607:C:H2'	3:L5:2608:G:H8	1.86	0.41
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.56	0.41
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.56	0.41
3:L5:5040:U:H5''	40:LB:396:ARG:HH22	1.85	0.41
16:SQ:146:ARG:HH11	82:Pt:34:U:P	2.42	0.41
28:ST:41:LYS:HE3	28:ST:93:SER:OG	2.20	0.41
37:Sg:146:SER:HA	37:Sg:177:TRP:HH2	1.86	0.41
37:Sg:206:LEU:HD23	37:Sg:206:LEU:HA	1.88	0.41
38:Lz:90:LEU:HD12	38:Lz:124:LEU:HD21	2.02	0.41
39:LA:107:MET:O	39:LA:139:HIS:NE2	2.43	0.41
41:LC:13:GLU:HG2	41:LC:155:GLU:OE2	2.20	0.41
47:LL:47:ALA:O	47:LL:149:GLN:HB2	2.20	0.41
53:LD:271:MET:HE3	53:LD:275:GLN:HB3	2.02	0.41
73:Li:35:LYS:HE3	73:Li:35:LYS:HB3	1.81	0.41
1:S2:11:A:N1	1:S2:1200:A:H2	2.18	0.41
1:S2:199:C:H3'	1:S2:200:G:C8	2.55	0.41
1:S2:564:A:H2'	1:S2:565:G:O4'	2.20	0.41
1:S2:639:C:H2'	1:S2:640:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1418:C:N3	1:S2:1421:A:H2	2.19	0.41
1:S2:1845:A:H2'	1:S2:1846:G:H8	1.85	0.41
2:L8:37:A:H5''	2:L8:39:G:O4'	2.20	0.41
3:L5:1789:C:H2'	3:L5:1790:U:C6	2.55	0.41
3:L5:2683:C:H2'	3:L5:2684:C:H6	1.86	0.41
3:L5:4113:U:O2'	3:L5:4114:C:H5'	2.20	0.41
3:L5:4476:C:H2'	43:LH:171:ASP:OD2	2.21	0.41
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.56	0.41
17:SU:44:LYS:HE2	17:SU:44:LYS:HB2	1.81	0.41
18:SK:2:LEU:HD12	18:SK:2:LEU:HA	1.90	0.41
38:Lz:151:VAL:O	38:Lz:154:THR:HG22	2.21	0.41
40:LB:354:GLN:HB3	40:LB:359:ALA:HB1	2.03	0.41
53:LD:223:PHE:O	53:LD:227:ILE:HD12	2.21	0.41
56:LS:43:ARG:HD2	56:LS:43:ARG:HA	1.76	0.41
62:LW:91:MET:N	62:LW:91:MET:SD	2.93	0.41
1:S2:1221:G:H2'	1:S2:1222:G:H8	1.86	0.41
1:S2:1416:C:H2'	1:S2:1417:C:C6	2.56	0.41
1:S2:1440:C:O2'	1:S2:1441:U:H5'	2.20	0.41
1:S2:1461:G:H2'	1:S2:1464:C:H41	1.86	0.41
3:L5:329:A:H4'	51:LN:170:LYS:HZ2	1.86	0.41
3:L5:366:A:H2'	3:L5:367:C:O4'	2.21	0.41
3:L5:382:G:H4'	3:L5:407:A:N1	2.36	0.41
3:L5:980:U:H2'	3:L5:981:C:C6	2.55	0.41
3:L5:1321:G:H2'	3:L5:3876:A:N7	2.36	0.41
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.86	0.41
3:L5:1483:C:H4'	3:L5:1484:G:O4'	2.21	0.41
3:L5:1699:A:H2'	3:L5:1700:G:O4'	2.21	0.41
3:L5:2395:A:H1'	3:L5:2806:A:N3	2.35	0.41
3:L5:2787:A2M:CM'	3:L5:2789:A:H3'	2.51	0.41
3:L5:4099:G:N2	3:L5:4110:C:H42	2.18	0.41
3:L5:4107:G:H2'	3:L5:4108:G:H8	1.85	0.41
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.56	0.41
3:L5:4914:C:O5'	3:L5:4914:C:H6	2.04	0.41
9:SE:44:LEU:HD23	9:SE:44:LEU:HA	1.84	0.41
15:SI:110:ARG:O	15:SI:114:GLU:HG2	2.21	0.41
16:SQ:35:ASN:OD1	16:SQ:72:VAL:HG12	2.20	0.41
28:ST:25:SER:C	28:ST:27:LYS:H	2.28	0.41
37:Sg:101:PHE:CD2	37:Sg:136:GLY:HA2	2.56	0.41
38:Lz:60:ARG:HB3	38:Lz:63:PHE:HB2	2.03	0.41
41:LC:13:GLU:CD	41:LC:157:LYS:HD3	2.45	0.41
61:LY:103:LYS:HA	61:LY:103:LYS:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:LF:88:LYS:HB2	67:LF:88:LYS:HE2	1.87	0.41
83:5A:27:LYS:O	83:5A:28:ASN:HB2	2.21	0.41
1:S2:333:G:OP1	11:SG:197:GLN:NE2	2.53	0.41
1:S2:472:C:H4'	1:S2:474:G:OP1	2.20	0.41
1:S2:1454:A:C8	26:SR:3:ARG:HG3	2.56	0.41
3:L5:654:C:H5'	41:LC:268:ARG:NH2	2.36	0.41
3:L5:2396:A:C8	3:L5:2814:C:H2'	2.56	0.41
3:L5:4076:G:OP1	45:LG:73:ARG:NE	2.33	0.41
3:L5:5008:C:H2'	3:L5:5009:G:O4'	2.20	0.41
10:SC:178:HIS:CE1	10:SC:200:ARG:HG2	2.56	0.41
14:SW:12:LYS:HB2	14:SW:12:LYS:HE3	1.92	0.41
16:SQ:16:LYS:O	16:SQ:17:LYS:C	2.63	0.41
26:SR:20:TYR:CD1	26:SR:38:ILE:HD13	2.55	0.41
33:Sb:24:LEU:HD23	33:Sb:24:LEU:HA	1.78	0.41
34:Sc:13:ARG:HH21	34:Sc:35:MET:HE1	1.86	0.41
41:LC:64:ALA:HB3	41:LC:92:PHE:CE2	2.56	0.41
63:LZ:89:ILE:HD11	63:LZ:121:ARG:HG2	2.03	0.41
67:LF:29:LYS:HE3	67:LF:33:LEU:HD11	2.02	0.41
70:Le:106:LYS:HB3	70:Le:106:LYS:HE2	1.79	0.41
72:Lg:45:ALA:HB3	72:Lg:82:MET:HE3	2.02	0.41
79:Lo:70:LEU:O	79:Lo:80:LYS:HA	2.20	0.41
1:S2:19:A:H2'	1:S2:20:G:O4'	2.21	0.41
1:S2:163:U:OP1	11:SG:84:TYR:HA	2.20	0.41
1:S2:202:G:C5	1:S2:203:G:C8	3.09	0.41
1:S2:484:A2M:HM'3	1:S2:484:A2M:H1'	1.85	0.41
1:S2:1144:A:H5'	1:S2:1355:C:H41	1.86	0.41
1:S2:1378:A:C4	6:SA:105:PRO:HB2	2.54	0.41
3:L5:504:G:H2'	3:L5:505:G:H8	1.85	0.41
3:L5:1300:G:H2'	3:L5:1301:C:O4'	2.21	0.41
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.21	0.41
3:L5:1803:G:C5	57:LT:109:VAL:HG22	2.56	0.41
3:L5:2338:C:H4'	64:Lr:12:ASN:O	2.21	0.41
3:L5:2633:U:H2'	3:L5:2634:C:H6	1.85	0.41
3:L5:4059:C:H2'	3:L5:4060:U:H6	1.85	0.41
3:L5:4745:G:H22	3:L5:4955:A:H2	1.64	0.41
3:L5:4886:C:H2'	3:L5:4887:C:H6	1.85	0.41
3:L5:5065:U:H2'	3:L5:5066:U:O4'	2.20	0.41
5:SB:167:LYS:HE2	5:SB:167:LYS:HB2	1.73	0.41
5:SB:233:GLY:O	5:SB:234:GLU:HG2	2.21	0.41
6:SA:176:TRP:CE3	6:SA:177:MET:HG2	2.56	0.41
7:SD:67:ARG:NE	18:SK:93:THR:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SD:226:GLN:NE2	37:Sg:224:GLY:O	2.54	0.41
10:SC:88:ILE:O	10:SC:160:LEU:HD22	2.21	0.41
11:SG:22:ARG:HH11	11:SG:25:ARG:NH2	2.17	0.41
11:SG:95:LYS:HE3	11:SG:95:LYS:HB3	1.82	0.41
24:SN:46:THR:OG1	24:SN:49:GLN:HG3	2.20	0.41
24:SN:130:LYS:HB3	24:SN:130:LYS:HE3	1.96	0.41
26:SR:100:PRO:HG3	26:SR:122:PRO:HG3	2.03	0.41
28:ST:14:PHE:HZ	28:ST:131:LEU:HD13	1.85	0.41
34:Sc:18:LEU:HB2	34:Sc:29:GLN:HB3	2.03	0.41
35:Se:85:LYS:HG3	35:Se:86:VAL:N	2.35	0.41
37:Sg:258:ILE:HD13	37:Sg:258:ILE:HA	1.97	0.41
41:LC:159:GLU:HA	41:LC:217:ILE:HB	2.02	0.41
41:LC:163:LYS:HB3	41:LC:163:LYS:HE3	1.88	0.41
42:LJ:95:ARG:HE	42:LJ:95:ARG:HB3	1.61	0.41
43:LH:114:ILE:HB	43:LH:124:ARG:HB2	2.02	0.41
43:LH:128:MET:SD	43:LH:157:SER:HB3	2.61	0.41
44:LE:99:ASP:OD1	44:LE:100:LYS:N	2.51	0.41
44:LE:153:LEU:HD11	44:LE:195:ILE:HG13	2.03	0.41
46:LO:110:PRO:HA	46:LO:113:ASP:OD1	2.21	0.41
46:LO:158:GLU:O	46:LO:162:GLU:HG3	2.21	0.41
53:LD:179:ARG:HA	53:LD:179:ARG:HD3	1.85	0.41
58:LP:85:LYS:O	58:LP:89:GLU:HG3	2.21	0.41
63:LZ:23:ALA:HA	63:LZ:45:GLY:HA2	2.03	0.41
66:Lb:32:LEU:O	66:Lb:35:VAL:HG13	2.21	0.41
66:Lb:59:ALA:O	66:Lb:63:LYS:HG2	2.21	0.41
69:Ld:23:ARG:HB3	69:Ld:25:TYR:CE1	2.56	0.41
73:Li:32:ARG:HE	73:Li:32:ARG:HB2	1.72	0.41
83:5A:50[B]:5CT:H14	83:5A:51:HIS:HE1	1.85	0.41
83:5A:90:GLN:HB3	83:5A:102:LEU:HB3	2.01	0.41
1:S2:57:U:OP1	1:S2:504:G:O2'	2.33	0.41
1:S2:354:OMU:HM22	1:S2:355:G:O4'	2.21	0.41
1:S2:563:G:N3	1:S2:564:A:C8	2.89	0.41
1:S2:575:A:H2'	1:S2:576:A2M:O4'	2.20	0.41
1:S2:1289:U:H2'	1:S2:1290:G:C8	2.56	0.41
1:S2:1372:U:H2'	1:S2:1373:C:O4'	2.20	0.41
1:S2:1533:A:C2	1:S2:1536:G:N3	2.89	0.41
2:L8:75:OMG:HM23	2:L8:75:OMG:H1'	1.82	0.41
3:L5:38:A:H5''	50:La:35:ALA:HB2	2.03	0.41
3:L5:85:G:O2'	3:L5:97:G:O6	2.36	0.41
3:L5:1364:U:OP2	47:LL:36:ARG:NH2	2.50	0.41
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1755:C:C2	53:LD:3:PHE:HB3	2.55	0.41
3:L5:2000:G:N3	3:L5:2000:G:H5''	2.36	0.41
3:L5:2392:C:H2'	3:L5:2393:C:C6	2.56	0.41
3:L5:3971:G:H1'	38:Lz:33:GLU:OE2	2.21	0.41
3:L5:3973:G:H5'	3:L5:4040:C:H2'	2.02	0.41
3:L5:4208:U:H4'	3:L5:4274:A:C2	2.56	0.41
4:L7:45:U:H2'	4:L7:46:C:O4'	2.20	0.41
5:SB:113:MET:HE3	5:SB:142:PHE:CE1	2.56	0.41
6:SA:176:TRP:HZ3	6:SA:177:MET:HE2	1.86	0.41
12:SF:167:LYS:HG3	12:SF:172:CYS:SG	2.61	0.41
12:SF:192:LYS:HD3	12:SF:192:LYS:HA	1.84	0.41
13:SH:86:LYS:HE3	13:SH:86:LYS:HB3	1.83	0.41
15:SI:85:ALA:O	25:SL:8:ARG:HD2	2.21	0.41
18:SK:49:MET:HA	18:SK:52:LEU:HG	2.03	0.41
26:SR:18:GLU:HG2	26:SR:69:ILE:HG12	2.01	0.41
40:LB:120:LYS:HA	40:LB:120:LYS:HD3	1.83	0.41
52:LI:48:LEU:O	52:LI:139:ARG:HA	2.21	0.41
52:LI:206:LEU:HD12	52:LI:206:LEU:HA	1.93	0.41
58:LP:41:ILE:HD13	58:LP:99:GLU:HG3	2.01	0.41
59:LU:106:SER:OG	59:LU:107:LYS:N	2.53	0.41
70:Le:7:LEU:HB2	70:Le:93:LYS:HB3	2.03	0.41
70:Le:32:LYS:HA	70:Le:32:LYS:HD3	1.85	0.41
75:Lk:61:PRO:HA	75:Lk:62:PRO:HD3	1.98	0.41
79:Lo:13:LYS:HB3	79:Lo:13:LYS:HE3	1.90	0.41
1:S2:512:A2M:HM'3	1:S2:512:A2M:H1'	1.88	0.40
1:S2:570:C:H3'	1:S2:571:U:C6	2.56	0.40
1:S2:668:A2M:HM'3	1:S2:668:A2M:H1'	1.67	0.40
1:S2:847:A:O2'	9:SE:106:LYS:NZ	2.54	0.40
1:S2:1388:A:N6	7:SD:161:GLY:HA3	2.36	0.40
2:L8:6:C:H2'	2:L8:7:U:C6	2.56	0.40
2:L8:60:G:O6	2:L8:96:C:O2'	2.38	0.40
3:L5:385:A:N3	3:L5:387:G:H5''	2.36	0.40
3:L5:1437:C:C4	3:L5:2098:G:C6	3.09	0.40
3:L5:1738:A:O2'	3:L5:1739:G:H5'	2.21	0.40
3:L5:2078:C:H2'	3:L5:2079:G:O4'	2.21	0.40
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.56	0.40
11:SG:195:LYS:O	11:SG:199:THR:HG22	2.21	0.40
36:Sf:109:ASP:O	36:Sf:110:GLU:HG3	2.21	0.40
38:Lz:111:LEU:HD23	38:Lz:111:LEU:HA	1.87	0.40
38:Lz:198:TRP:O	38:Lz:201:VAL:HG22	2.21	0.40
41:LC:14:LYS:HE2	41:LC:14:LYS:HB2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:LC:60:HIS:HA	41:LC:92:PHE:HE1	1.84	0.40
42:LJ:44:THR:HG21	42:LJ:72:CYS:SG	2.60	0.40
47:LL:43:ALA:O	47:LL:47:ALA:HA	2.21	0.40
63:LZ:109:LYS:HE2	63:LZ:109:LYS:HB3	1.55	0.40
83:5A:118:ASP:OD1	83:5A:119:LEU:N	2.54	0.40
1:S2:184:G:H2'	1:S2:185:G:H8	1.86	0.40
1:S2:441:C:H4'	1:S2:1737:G:O2'	2.21	0.40
1:S2:598:G:O2'	1:S2:605:A:N1	2.44	0.40
1:S2:644:OMG:H1'	1:S2:644:OMG:HM23	1.72	0.40
1:S2:1533:A:C8	1:S2:1604:G:H1'	2.56	0.40
2:L8:115:G:H2'	2:L8:116:C:H6	1.87	0.40
3:L5:180:C:H2'	3:L5:181:C:C1'	2.51	0.40
3:L5:1687:U:H2'	3:L5:1688:G:C8	2.57	0.40
3:L5:1806:G:H2'	3:L5:1807:C:H6	1.85	0.40
3:L5:2481:G:N1	3:L5:2498:C:N3	2.69	0.40
3:L5:3777:G:N2	3:L5:3815:G:H2'	2.36	0.40
3:L5:4208:U:H4'	3:L5:4274:A:H2	1.86	0.40
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.86	0.40
7:SD:45:ARG:HH21	7:SD:85:GLU:HG2	1.84	0.40
9:SE:10:LYS:HD3	9:SE:10:LYS:HA	1.88	0.40
14:SW:57:ARG:O	14:SW:58:ALA:C	2.61	0.40
16:SQ:21:ALA:HB2	16:SQ:72:VAL:HG23	2.04	0.40
17:SU:64:THR:HA	17:SU:78:ASP:O	2.22	0.40
22:SS:142:ARG:HB2	22:SS:144:ARG:NH2	2.36	0.40
23:Sd:53:ILE:C	23:Sd:53:ILE:HD12	2.46	0.40
28:ST:60:THR:HG23	28:ST:75:MET:HE3	2.02	0.40
39:LA:20:VAL:HG12	39:LA:23:ARG:HD2	2.02	0.40
42:LJ:175:LEU:HD12	42:LJ:175:LEU:HA	1.86	0.40
47:LL:125:ILE:HA	47:LL:138:ASP:OD2	2.22	0.40
52:LI:91:LEU:HD12	52:LI:135:ILE:HG23	2.02	0.40
83:5A:109:ARG:NH2	83:5A:144:GLU:OE2	2.53	0.40
1:S2:546:G:C6	1:S2:547:G:C6	3.09	0.40
1:S2:573:PSU:O2'	1:S2:575:A:N7	2.49	0.40
1:S2:624:C:H5'	1:S2:625:G:OP2	2.21	0.40
1:S2:1239:PSU:H5'	27:SP:124:LYS:HD2	2.03	0.40
3:L5:659:G:H3'	3:L5:660:A:H8	1.85	0.40
3:L5:732:A:H2'	3:L5:733:A:O4'	2.21	0.40
3:L5:1249:C:H2'	3:L5:1250:C:C6	2.57	0.40
3:L5:1411:C:H2'	3:L5:1412:G:H8	1.85	0.40
3:L5:1701:A:C6	3:L5:1702:C:C4	3.09	0.40
3:L5:3692:A:C2'	3:L5:3693:U:H5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3713:U:H2'	3:L5:3714:G:H8	1.86	0.40
3:L5:3779:A:H2'	3:L5:3780:G:O4'	2.21	0.40
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.86	0.40
8:SJ:63:LEU:HD11	8:SJ:69:ARG:NH1	2.36	0.40
9:SE:212:ASP:OD1	9:SE:244:ILE:HD13	2.21	0.40
16:SQ:106:LYS:HB2	16:SQ:106:LYS:HE2	1.85	0.40
17:SU:39:LEU:HD23	17:SU:39:LEU:HA	1.84	0.40
19:SO:54:CYS:HB2	19:SO:84:ARG:HG2	2.03	0.40
21:SM:63:LYS:HA	21:SM:66:GLU:OE1	2.22	0.40
42:LJ:164:ARG:O	42:LJ:168:GLN:HG3	2.21	0.40
52:LI:101:LYS:HD2	52:LI:101:LYS:HA	1.83	0.40
53:LD:208:MET:HG2	53:LD:223:PHE:CE2	2.57	0.40
58:LP:116:HIS:HB3	58:LP:149:ILE:HB	2.03	0.40
69:Ld:19:GLU:HG2	69:Ld:102:LEU:HD11	2.03	0.40
82:Pt:77:A:OP1	82:Pt:77:A:H4'	2.22	0.40
1:S2:25:A:HO2'	1:S2:26:U:H6	1.67	0.40
1:S2:187:G:C6	1:S2:188:C:C4	3.09	0.40
1:S2:210:U:H2'	1:S2:211:G:C8	2.56	0.40
1:S2:922:A:H2'	1:S2:923:G:O4'	2.21	0.40
1:S2:1310:U:H4'	36:Sf:143:LYS:HD2	2.02	0.40
1:S2:1418:C:H2'	1:S2:1419:C:O4'	2.21	0.40
2:L8:16:G:C2	3:L5:417:G:N3	2.90	0.40
3:L5:400:A2M:HM'3	3:L5:400:A2M:H1'	1.94	0.40
3:L5:483:G:H4'	3:L5:484:U:C5'	2.51	0.40
3:L5:646:G:H3'	3:L5:647:G:H8	1.87	0.40
3:L5:1207:C:H2'	3:L5:1208:G:H8	1.85	0.40
3:L5:1406:G:N1	3:L5:1412:G:C6	2.89	0.40
3:L5:2489:C:O2	3:L5:2490:U:C5	2.75	0.40
3:L5:3876:A:H5''	3:L5:3877:A:C8	2.57	0.40
7:SD:80:PRO:HD2	7:SD:83:SER:OG	2.21	0.40
12:SF:125:SER:HB3	12:SF:136:ARG:HB3	2.04	0.40
13:SH:40:LEU:HD23	13:SH:40:LEU:HA	1.93	0.40
18:SK:92:ALA:HA	18:SK:95:ARG:HD3	2.03	0.40
37:Sg:251:ALA:HA	37:Sg:256:ILE:HD13	2.03	0.40
42:LJ:8:LYS:HD3	42:LJ:8:LYS:HA	1.90	0.40
44:LE:70:LYS:HG3	44:LE:71:ARG:HG3	2.03	0.40
52:LI:115:MET:HE3	52:LI:115:MET:HB3	1.91	0.40
52:LI:166:HIS:CE1	57:LT:159:MET:HB2	2.56	0.40
66:Lb:65:MET:SD	66:Lb:68:ARG:NH1	2.94	0.40
75:Lk:67:LYS:HE2	75:Lk:69:LEU:CD2	2.52	0.40
83:5A:103:GLN:HB2	83:5A:106:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1491:G:H2'	1:S2:1492:U:C6	2.56	0.40
1:S2:1562:C:C2'	1:S2:1563:G:H5'	2.52	0.40
1:S2:1562:C:O2'	1:S2:1563:G:H5'	2.21	0.40
1:S2:1727:G:H2'	1:S2:1728:U:C6	2.57	0.40
1:S2:1801:A:H2'	1:S2:1802:C:H6	1.82	0.40
3:L5:371:A:N3	3:L5:1531:U:O2'	2.49	0.40
3:L5:670:G:H2'	3:L5:671:G:C8	2.55	0.40
3:L5:959:G:O4'	44:LE:123:ARG:HD2	2.21	0.40
3:L5:1818:G:O2'	3:L5:1819:G:H5''	2.21	0.40
3:L5:2415:OMU:H2'	3:L5:2416:G:C8	2.56	0.40
3:L5:2694:G:H5''	3:L5:2696:A:N7	2.36	0.40
3:L5:2804:OMC:HM23	3:L5:2804:OMC:H1'	1.87	0.40
3:L5:3692:A:H62	3:L5:3823:G:N2	2.01	0.40
3:L5:3761:C:H2'	3:L5:3762:PSU:O4'	2.20	0.40
3:L5:3948:C:H2'	3:L5:3949:A:H8	1.86	0.40
3:L5:3956:G:C2	3:L5:3966:A:C2	3.10	0.40
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.22	0.40
3:L5:4413:C:H2'	3:L5:4414:A:O4'	2.22	0.40
3:L5:4670:C:O3'	3:L5:4671:C:H3'	2.22	0.40
3:L5:4992:G:H2'	3:L5:4993:G:N3	2.36	0.40
8:SJ:29:LEU:HD12	35:Se:116:PHE:CE2	2.57	0.40
8:SJ:60:LEU:O	8:SJ:63:LEU:HB2	2.21	0.40
12:SF:156:THR:O	12:SF:160:GLU:HG3	2.22	0.40
13:SH:78:ARG:O	13:SH:82:GLU:HG2	2.21	0.40
18:SK:61:GLN:O	18:SK:68:TYR:N	2.55	0.40
21:SM:48:HIS:C	21:SM:49:LEU:HD12	2.46	0.40
28:ST:110:LEU:HD23	28:ST:110:LEU:HA	1.92	0.40
38:Lz:189:PHE:O	38:Lz:193:LEU:HG	2.21	0.40
40:LB:396:ARG:O	40:LB:399:LYS:HG3	2.21	0.40
42:LJ:41:GLU:HG3	42:LJ:46:GLN:O	2.21	0.40
44:LE:91:THR:HG22	44:LE:108:LYS:HG3	2.03	0.40
53:LD:51:MET:HE1	53:LD:166:ALA:HB2	2.02	0.40
62:LW:27:LYS:HB3	62:LW:27:LYS:HE2	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SB	219/264 (83%)	213 (97%)	6 (3%)	0	100	100
6	SA	220/295 (75%)	215 (98%)	5 (2%)	0	100	100
7	SD	224/243 (92%)	212 (95%)	12 (5%)	0	100	100
8	SJ	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
9	SE	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
10	SC	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
11	SG	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
12	SF	187/204 (92%)	180 (96%)	6 (3%)	1 (0%)	24	31
13	SH	187/194 (96%)	179 (96%)	8 (4%)	0	100	100
14	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
15	SI	204/208 (98%)	197 (97%)	7 (3%)	0	100	100
16	SQ	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
17	SU	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
18	SK	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
19	SO	133/151 (88%)	129 (97%)	3 (2%)	1 (1%)	16	20
20	SX	137/143 (96%)	134 (98%)	3 (2%)	0	100	100
21	SM	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
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%)	147 (99%)	2 (1%)	0	100	100
25	SL	142/158 (90%)	138 (97%)	4 (3%)	0	100	100
26	SR	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
27	SP	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
28	ST	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
29	SV	81/83 (98%)	81 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	SY	129/133 (97%)	126 (98%)	3 (2%)	0	100	100
31	SZ	82/125 (66%)	79 (96%)	3 (4%)	0	100	100
32	Sa	98/115 (85%)	98 (100%)	0	0	100	100
33	Sb	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
34	Sc	63/69 (91%)	59 (94%)	4 (6%)	0	100	100
35	Se	46/133 (35%)	45 (98%)	0	1 (2%)	5	4
36	Sf	61/156 (39%)	49 (80%)	10 (16%)	2 (3%)	3	2
37	Sg	311/317 (98%)	287 (92%)	23 (7%)	1 (0%)	36	46
38	Lz	209/217 (96%)	201 (96%)	8 (4%)	0	100	100
39	LA	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
40	LB	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
41	LC	364/427 (85%)	359 (99%)	5 (1%)	0	100	100
42	LJ	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
43	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
44	LE	217/288 (75%)	212 (98%)	5 (2%)	0	100	100
45	LG	239/266 (90%)	230 (96%)	9 (4%)	0	100	100
46	LO	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
47	LL	204/211 (97%)	195 (96%)	9 (4%)	0	100	100
48	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
49	LM	134/215 (62%)	130 (97%)	4 (3%)	0	100	100
50	La	144/148 (97%)	143 (99%)	1 (1%)	0	100	100
51	LN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
52	LI	199/214 (93%)	197 (99%)	2 (1%)	0	100	100
53	LD	292/297 (98%)	286 (98%)	6 (2%)	0	100	100
54	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
55	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
56	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
57	LT	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
58	LP	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
59	LU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
60	LX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	LY	132/145 (91%)	132 (100%)	0	0	100	100
62	LW	114/157 (73%)	110 (96%)	4 (4%)	0	100	100
63	LZ	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
64	Lr	124/137 (90%)	124 (100%)	0	0	100	100
65	Lh	120/123 (98%)	120 (100%)	0	0	100	100
66	Lb	106/159 (67%)	104 (98%)	2 (2%)	0	100	100
67	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
68	Lc	97/115 (84%)	97 (100%)	0	0	100	100
69	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
70	Le	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
71	Lf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
72	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
73	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
74	Lj	85/97 (88%)	83 (98%)	2 (2%)	0	100	100
75	Lk	67/70 (96%)	67 (100%)	0	0	100	100
76	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
77	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
78	Ln	23/25 (92%)	23 (100%)	0	0	100	100
79	Lo	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
80	Lp	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
83	5A	135/154 (88%)	127 (94%)	7 (5%)	1 (1%)	18	23
All	All	11638/13133 (89%)	11331 (97%)	300 (3%)	7 (0%)	49	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	SF	79	HIS
35	Se	119	VAL
37	Sg	234	ASP
83	5A	141	MET
19	SO	138	ASP
36	Sf	123	SER
36	Sf	122	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%)	190 (94%)	12 (6%)	18	26
6	SA	183/242 (76%)	178 (97%)	5 (3%)	39	58
7	SD	189/202 (94%)	181 (96%)	8 (4%)	26	40
8	SJ	161/168 (96%)	158 (98%)	3 (2%)	50	69
9	SE	224/225 (100%)	216 (96%)	8 (4%)	31	47
10	SC	188/225 (84%)	181 (96%)	7 (4%)	30	45
11	SG	207/218 (95%)	201 (97%)	6 (3%)	37	55
12	SF	159/170 (94%)	156 (98%)	3 (2%)	50	69
13	SH	168/174 (97%)	164 (98%)	4 (2%)	43	62
14	SW	112/113 (99%)	111 (99%)	1 (1%)	70	84
15	SI	178/180 (99%)	173 (97%)	5 (3%)	38	56
16	SQ	117/121 (97%)	112 (96%)	5 (4%)	26	39
17	SU	93/107 (87%)	90 (97%)	3 (3%)	34	51
18	SK	87/136 (64%)	83 (95%)	4 (5%)	24	36
19	SO	105/119 (88%)	101 (96%)	4 (4%)	29	44
20	SX	111/114 (97%)	108 (97%)	3 (3%)	39	58
21	SM	104/108 (96%)	96 (92%)	8 (8%)	12	16
22	SS	128/132 (97%)	124 (97%)	4 (3%)	35	52
23	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	40
24	SN	131/131 (100%)	124 (95%)	7 (5%)	20	30
25	SL	132/142 (93%)	127 (96%)	5 (4%)	29	44
26	SR	121/122 (99%)	106 (88%)	15 (12%)	4	5
27	SP	117/130 (90%)	112 (96%)	5 (4%)	26	39
28	ST	114/115 (99%)	107 (94%)	7 (6%)	17	24
29	SV	66/66 (100%)	62 (94%)	4 (6%)	17	24
30	SY	113/115 (98%)	108 (96%)	5 (4%)	25	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	SZ	74/103 (72%)	72 (97%)	2 (3%)	39	58
32	Sa	87/98 (89%)	84 (97%)	3 (3%)	32	49
33	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	77
34	Sc	58/62 (94%)	54 (93%)	4 (7%)	14	20
35	Se	40/104 (38%)	38 (95%)	2 (5%)	22	33
36	Sf	56/140 (40%)	48 (86%)	8 (14%)	3	3
37	Sg	272/275 (99%)	250 (92%)	22 (8%)	11	14
38	Lz	189/196 (96%)	178 (94%)	11 (6%)	18	26
39	LA	193/198 (98%)	192 (100%)	1 (0%)	81	90
40	LB	347/348 (100%)	345 (99%)	2 (1%)	78	89
41	LC	305/348 (88%)	302 (99%)	3 (1%)	68	82
42	LJ	143/149 (96%)	137 (96%)	6 (4%)	26	40
43	LH	169/171 (99%)	166 (98%)	3 (2%)	51	70
44	LE	196/252 (78%)	192 (98%)	4 (2%)	48	67
45	LG	203/223 (91%)	199 (98%)	4 (2%)	48	67
46	LO	171/174 (98%)	170 (99%)	1 (1%)	78	89
47	LL	172/177 (97%)	169 (98%)	3 (2%)	53	72
48	LV	102/107 (95%)	101 (99%)	1 (1%)	68	82
49	LM	116/161 (72%)	114 (98%)	2 (2%)	53	72
50	La	119/120 (99%)	117 (98%)	2 (2%)	53	72
51	LN	171/172 (99%)	171 (100%)	0	100	100
52	LI	173/181 (96%)	171 (99%)	2 (1%)	63	79
53	LD	247/250 (99%)	239 (97%)	8 (3%)	34	51
54	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	79
55	LR	166/175 (95%)	161 (97%)	5 (3%)	36	53
56	LS	157/157 (100%)	155 (99%)	2 (1%)	61	77
57	LT	141/140 (101%)	141 (100%)	0	100	100
58	LP	135/163 (83%)	133 (98%)	2 (2%)	57	75
59	LU	89/115 (77%)	86 (97%)	3 (3%)	32	49
60	LX	106/133 (80%)	106 (100%)	0	100	100
61	LY	124/135 (92%)	123 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LW	96/126 (76%)	92 (96%)	4 (4%)	26	40
63	LZ	118/118 (100%)	117 (99%)	1 (1%)	73	86
64	Lr	109/120 (91%)	106 (97%)	3 (3%)	38	56
65	Lh	109/110 (99%)	109 (100%)	0	100	100
66	Lb	90/125 (72%)	86 (96%)	4 (4%)	25	38
67	LF	194/215 (90%)	192 (99%)	2 (1%)	68	82
68	Lc	84/97 (87%)	83 (99%)	1 (1%)	63	79
69	Ld	98/110 (89%)	97 (99%)	1 (1%)	68	82
70	Le	114/121 (94%)	113 (99%)	1 (1%)	70	84
71	Lf	89/89 (100%)	89 (100%)	0	100	100
72	Lg	98/100 (98%)	95 (97%)	3 (3%)	35	52
73	Li	86/89 (97%)	84 (98%)	2 (2%)	44	63
74	Lj	74/80 (92%)	72 (97%)	2 (3%)	39	58
75	Lk	64/65 (98%)	62 (97%)	2 (3%)	35	52
76	Ll	47/48 (98%)	47 (100%)	0	100	100
77	Lm	47/115 (41%)	45 (96%)	2 (4%)	26	39
78	Ln	24/24 (100%)	23 (96%)	1 (4%)	26	40
79	Lo	94/93 (101%)	93 (99%)	1 (1%)	65	81
80	Lp	75/75 (100%)	74 (99%)	1 (1%)	61	77
83	5A	114/127 (90%)	107 (94%)	7 (6%)	17	24
All	All	10142/11170 (91%)	9851 (97%)	291 (3%)	38	55

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SB	43	ASN
5	SB	59	SER
5	SB	69	VAL
5	SB	75	GLN
5	SB	76	ASN
5	SB	89	GLU
5	SB	131	ASP
5	SB	203	SER
5	SB	214	LYS
5	SB	225	LEU

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Mol	Chain	Res	Type
5	SB	230	GLU
5	SB	232	HIS
6	SA	7	VAL
6	SA	80	ARG
6	SA	191	ARG
6	SA	192	GLU
6	SA	205	ARG
7	SD	6	SER
7	SD	27	ARG
7	SD	35	SER
7	SD	44	THR
7	SD	149	SER
7	SD	175	VAL
7	SD	195	THR
7	SD	223	ILE
8	SJ	64	ASP
8	SJ	112	THR
8	SJ	141	VAL
9	SE	19	MET
9	SE	49	ARG
9	SE	115	THR
9	SE	148	ARG
9	SE	194	VAL
9	SE	211	LYS
9	SE	230	LYS
9	SE	246	LEU
10	SC	98	LEU
10	SC	101	SER
10	SC	120	GLN
10	SC	137	VAL
10	SC	184	VAL
10	SC	206	SER
10	SC	249	SER
11	SG	78	SER
11	SG	103	ASP
11	SG	127	THR
11	SG	129	VAL
11	SG	143	LYS
11	SG	221	LYS
12	SF	28	VAL
12	SF	91	ARG
12	SF	165	ASN

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Mol	Chain	Res	Type
13	SH	7	LYS
13	SH	8	ILE
13	SH	51	ILE
13	SH	115	LYS
14	SW	87	GLU
15	SI	45	THR
15	SI	86	SER
15	SI	91	VAL
15	SI	155	ASN
15	SI	191	GLU
16	SQ	7	LEU
16	SQ	20	THR
16	SQ	46	THR
16	SQ	113	ILE
16	SQ	146	ARG
17	SU	40	ILE
17	SU	93	SER
17	SU	114	VAL
18	SK	37	ASP
18	SK	89	ILE
18	SK	90	VAL
18	SK	95	ARG
19	SO	17	LEU
19	SO	103	ASN
19	SO	113	GLN
19	SO	137	SER
20	SX	25	LYS
20	SX	32	LEU
20	SX	105	PHE
21	SM	16	THR
21	SM	20	GLU
21	SM	45	ARG
21	SM	65	VAL
21	SM	74	ILE
21	SM	75	ASN
21	SM	84	LYS
21	SM	109	VAL
22	SS	17	ASN
22	SS	53	THR
22	SS	136	THR
22	SS	145	THR
23	Sd	30	LEU

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Mol	Chain	Res	Type
23	Sd	38	MET
24	SN	21	SER
24	SN	30	SER
24	SN	86	GLU
24	SN	123[A]	HIS
24	SN	123[B]	HIS
24	SN	133	ARG
24	SN	142	GLU
25	SL	19	ASN
25	SL	23	VAL
25	SL	39	ASN
25	SL	147	LYS
25	SL	155	PHE
26	SR	8	THR
26	SR	32	LYS
26	SR	40	ILE
26	SR	43	SER
26	SR	76	GLU
26	SR	79	GLU
26	SR	80	ARG
26	SR	81	ARG
26	SR	82	ASP
26	SR	83	ASN
26	SR	88	VAL
26	SR	89	SER
26	SR	109	LEU
26	SR	117	LEU
26	SR	118	GLN
27	SP	32	GLN
27	SP	53	GLN
27	SP	70	MET
27	SP	76	VAL
27	SP	92	SER
28	ST	4	VAL
28	ST	23	LYS
28	ST	37	VAL
28	ST	38	LYS
28	ST	39	LEU
28	ST	87	VAL
28	ST	96	SER
29	SV	10	ASP
29	SV	43	THR

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Mol	Chain	Res	Type
29	SV	66	ASP
29	SV	80	SER
30	SY	35	VAL
30	SY	44	LEU
30	SY	51	THR
30	SY	54	VAL
30	SY	99	LYS
31	SZ	39	LYS
31	SZ	50	PHE
32	Sa	40	VAL
32	Sa	85[A]	ARG
32	Sa	85[B]	ARG
33	Sb	24	LEU
34	Sc	36	ASP
34	Sc	50	VAL
34	Sc	57	THR
34	Sc	61	SER
35	Se	114	ARG
35	Se	120	VAL
36	Sf	102	VAL
36	Sf	116	ARG
36	Sf	117	LEU
36	Sf	118	ARG
36	Sf	119	ARG
36	Sf	121	CYS
36	Sf	130	VAL
36	Sf	140	TYR
37	Sg	33	SER
37	Sg	57	ARG
37	Sg	89	LEU
37	Sg	105	THR
37	Sg	107	ASP
37	Sg	108	VAL
37	Sg	113	PHE
37	Sg	117	ASN
37	Sg	134	THR
37	Sg	140	TYR
37	Sg	141	THR
37	Sg	155	ARG
37	Sg	177	TRP
37	Sg	182	CYS
37	Sg	212	LYS

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Mol	Chain	Res	Type
37	Sg	220	ASP
37	Sg	234	ASP
37	Sg	235	ILE
37	Sg	236	ILE
37	Sg	256	ILE
37	Sg	275	ILE
37	Sg	280	LYS
38	Lz	32	VAL
38	Lz	36	ILE
38	Lz	48	ARG
38	Lz	58	THR
38	Lz	90	LEU
38	Lz	129	ASN
38	Lz	159	MET
38	Lz	175	THR
38	Lz	184	HIS
38	Lz	204	LEU
38	Lz	206	ILE
39	LA	208	GLU
40	LB	95	THR
40	LB	395	ASP
41	LC	157	LYS
41	LC	255	SER
41	LC	275	SER
42	LJ	26	VAL
42	LJ	38	LYS
42	LJ	59	SER
42	LJ	81	GLU
42	LJ	115	LEU
42	LJ	175	LEU
43	LH	6	SER
43	LH	19	THR
43	LH	37	ASP
44	LE	88	VAL
44	LE	101	ASN
44	LE	123	ARG
44	LE	239	LYS
45	LG	28	VAL
45	LG	43	GLN
45	LG	113	ARG
45	LG	250	ILE
46	LO	187	LYS

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Mol	Chain	Res	Type
47	LL	52	SER
47	LL	59	VAL
47	LL	105	LYS
48	LV	118	THR
49	LM	112	VAL
49	LM	116	LYS
50	La	95	THR
50	La	116	LYS
52	LI	53	VAL
52	LI	142	LEU
53	LD	4	VAL
53	LD	36	LEU
53	LD	75	VAL
53	LD	90	VAL
53	LD	185	SER
53	LD	232	THR
53	LD	259	LYS
53	LD	267	ASN
54	LQ	14	ARG
54	LQ	92	VAL
55	LR	2	SER
55	LR	111	GLU
55	LR	122	SER
55	LR	164	SER
55	LR	166	THR
56	LS	6	THR
56	LS	150	ILE
58	LP	75[A]	GLN
58	LP	75[B]	GLN
59	LU	25	CYS
59	LU	98	ASP
59	LU	106	SER
61	LY	54	GLU
62	LW	1[A]	MET
62	LW	1[B]	MET
62	LW	76	VAL
62	LW	91	MET
63	LZ	99	ASP
64	Lr	58	LYS
64	Lr	67	ARG
64	Lr	124	VAL
66	Lb	35	VAL

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Mol	Chain	Res	Type
66	Lb	89	VAL
66	Lb	92	LYS
66	Lb	120	ARG
67	LF	44	LYS
67	LF	106	ARG
68	Lc	94	LEU
69	Ld	118	GLN
70	Le	76	LYS
72	Lg	28	ASN
72	Lg	43	LYS
72	Lg	48	VAL
73	Li	18	THR
73	Li	79	THR
74	Lj	20	ARG
74	Lj	55	ARG
75	Lk	36	VAL
75	Lk	54	GLU
77	Lm	81	SER
77	Lm	127	VAL
78	Ln	25	LYS
79	Lo	59	LYS
80	Lp	63	THR
83	5A	20	MET
83	5A	51	HIS
83	5A	59	VAL
83	5A	73	CYS
83	5A	79	MET
83	5A	111	ASP
83	5A	129	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
5	SB	147	ASN
5	SB	158	HIS
5	SB	179	ASN
5	SB	186	ASN
6	SA	29	ASN
6	SA	169	HIS
7	SD	101	GLN
7	SD	159	HIS
8	SJ	140	GLN

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Mol	Chain	Res	Type
8	SJ	182	GLN
9	SE	36	HIS
10	SC	115	GLN
10	SC	120	GLN
11	SG	13	GLN
11	SG	65	GLN
11	SG	155	GLN
11	SG	163	ASN
12	SF	101	HIS
13	SH	73	GLN
13	SH	91	HIS
13	SH	193	GLN
14	SW	24	GLN
14	SW	64	ASN
15	SI	64	ASN
15	SI	116	HIS
15	SI	167	GLN
16	SQ	77	HIS
17	SU	47	ASN
18	SK	66	HIS
19	SO	20	GLN
20	SX	16	HIS
20	SX	61	GLN
20	SX	92	ASN
21	SM	55	ASN
22	SS	17	ASN
24	SN	58	HIS
24	SN	69	ASN
25	SL	19	ASN
25	SL	39	ASN
25	SL	94	HIS
26	SR	93	GLN
27	SP	54	HIS
30	SY	15	ASN
32	Sa	86	ASN
36	Sf	139	HIS
37	Sg	162	ASN
37	Sg	222	ASN
37	Sg	237	ASN
37	Sg	305	ASN
39	LA	22	HIS
40	LB	145	GLN

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Mol	Chain	Res	Type
40	LB	203	GLN
40	LB	209	GLN
40	LB	354	GLN
41	LC	21	ASN
41	LC	38	ASN
41	LC	187	GLN
41	LC	329	ASN
42	LJ	46	GLN
42	LJ	97	ASN
43	LH	8	GLN
43	LH	98	HIS
43	LH	138	GLN
43	LH	169	ASN
43	LH	189	GLN
45	LG	206	GLN
46	LO	42	ASN
46	LO	167	HIS
49	LM	66	HIS
50	La	89	ASN
51	LN	32	GLN
52	LI	59	GLN
52	LI	73	ASN
53	LD	111	ASN
53	LD	131	ASN
53	LD	250	ASN
53	LD	282	GLN
55	LR	40	GLN
55	LR	143	HIS
56	LS	37	HIS
57	LT	79	GLN
57	LT	90	ASN
57	LT	98	HIS
59	LU	41	GLN
59	LU	44	GLN
62	LW	95	ASN
65	Lh	98	HIS
65	Lh	101	ASN
67	LF	58	HIS
69	Ld	116	ASN
70	Le	23	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1667/1869 (89%)	296 (17%)	2 (0%)
2	L8	155/156 (99%)	26 (16%)	0
3	L5	3651/5069 (72%)	642 (17%)	20 (0%)
4	L7	119/120 (99%)	11 (9%)	0
81	mR	7/60 (11%)	2 (28%)	0
82	Pt	76/77 (98%)	11 (14%)	0
All	All	5675/7351 (77%)	988 (17%)	22 (0%)

All (988) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	45	A
1	S2	46	A
1	S2	55	U
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	80	G
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	155	G
1	S2	162	C
1	S2	163	U
1	S2	168	C
1	S2	184	G
1	S2	197	U
1	S2	198	U

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Mol	Chain	Res	Type
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	205	G
1	S2	207	G
1	S2	209	A
1	S2	215	G
1	S2	216	C
1	S2	225	G
1	S2	302	A
1	S2	309	G
1	S2	312	G
1	S2	319	C
1	S2	320	G
1	S2	323	C
1	S2	324	C
1	S2	327	G
1	S2	328	U
1	S2	351	G
1	S2	362	C
1	S2	364	A
1	S2	370	G
1	S2	377	G
1	S2	381	C
1	S2	385	G
1	S2	386	C
1	S2	407	G
1	S2	409	C
1	S2	413	G
1	S2	418	A
1	S2	438	G
1	S2	441	C
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
1	S2	466	G
1	S2	467	G

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Mol	Chain	Res	Type
1	S2	471	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	523	A
1	S2	525	A
1	S2	533	A
1	S2	534	G
1	S2	544	G
1	S2	553	U
1	S2	554	A
1	S2	555	A
1	S2	560	A
1	S2	563	G
1	S2	564	A
1	S2	566	U
1	S2	570	C
1	S2	576	A2M
1	S2	587	A
1	S2	589	G
1	S2	590	A2M
1	S2	591	U
1	S2	598	G
1	S2	608	C
1	S2	614	C
1	S2	620	G
1	S2	624	C
1	S2	628	A
1	S2	632	C
1	S2	634	A
1	S2	643	A
1	S2	644	OMG
1	S2	655	A
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A

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Mol	Chain	Res	Type
1	S2	673	G
1	S2	688	U
1	S2	689	U
1	S2	800	U
1	S2	810	A
1	S2	811	A
1	S2	821	G
1	S2	822	PSU
1	S2	823	U
1	S2	827	A
1	S2	830	A
1	S2	831	G
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	840	C
1	S2	847	A
1	S2	869	A
1	S2	870	A
1	S2	871	U
1	S2	872	A
1	S2	883	U
1	S2	888	U
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
1	S2	901	G
1	S2	903	A
1	S2	904	A
1	S2	909	G
1	S2	913	A
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	933	G
1	S2	934	G
1	S2	943	U

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Mol	Chain	Res	Type
1	S2	970	G
1	S2	978	G
1	S2	990	A
1	S2	992	A
1	S2	999	G
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1083	A
1	S2	1085	C
1	S2	1109	C
1	S2	1115	U
1	S2	1116	C
1	S2	1117	C
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	1188	A
1	S2	1195	A
1	S2	1203	G
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1217	A
1	S2	1221	G
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	1260	A
1	S2	1265	A
1	S2	1274	G

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Mol	Chain	Res	Type
1	S2	1275	G
1	S2	1277	C
1	S2	1285	G
1	S2	1286	G
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1308	U
1	S2	1309	C
1	S2	1310	U
1	S2	1312	G
1	S2	1313	A
1	S2	1315	U
1	S2	1324	G
1	S2	1342	U
1	S2	1345	G
1	S2	1348	G
1	S2	1358	U
1	S2	1371	U
1	S2	1372	U
1	S2	1373	C
1	S2	1375	G
1	S2	1378	A
1	S2	1382	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	1433	C
1	S2	1435	C
1	S2	1437	C
1	S2	1438	A
1	S2	1442	OMU
1	S2	1454	A
1	S2	1463	U
1	S2	1466	G
1	S2	1479	G
1	S2	1480	A
1	S2	1487	A
1	S2	1489	A

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Mol	Chain	Res	Type
1	S2	1490	OMG
1	S2	1491	G
1	S2	1494	U
1	S2	1498	A
1	S2	1521	C
1	S2	1522	A
1	S2	1531	A
1	S2	1533	A
1	S2	1553	C
1	S2	1557	C
1	S2	1560	U
1	S2	1563	G
1	S2	1580	A
1	S2	1581	C
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A
1	S2	1600	G
1	S2	1601	A
1	S2	1614	A
1	S2	1621	U
1	S2	1623	A
1	S2	1639	G7M
1	S2	1640	A
1	S2	1648	G
1	S2	1654	G
1	S2	1661	A
1	S2	1664	A
1	S2	1665	G
1	S2	1680	G
1	S2	1695	A
1	S2	1698	C
1	S2	1721	U
1	S2	1722	G
1	S2	1744	G
1	S2	1752	C
1	S2	1753	C
1	S2	1754	G
1	S2	1777	G
1	S2	1782	G
1	S2	1783	C
1	S2	1819	A

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Mol	Chain	Res	Type
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	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1869	A
2	L8	3	A
2	L8	34	U
2	L8	35	C
2	L8	51	U
2	L8	52	A
2	L8	59	A
2	L8	62	A
2	L8	63	U
2	L8	72	A
2	L8	80	A
2	L8	83	C
2	L8	86	U
2	L8	87	G
2	L8	103	A
2	L8	104	A
2	L8	105	C
2	L8	109	C
2	L8	110	U
2	L8	111	U
2	L8	112	G
2	L8	114	G
2	L8	123	U
2	L8	124	U
2	L8	126	C
2	L8	127	U
2	L8	147	G
3	L5	2	G
3	L5	15	A
3	L5	39	A
3	L5	42	A

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Mol	Chain	Res	Type
3	L5	43	U
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	71	C
3	L5	73	A
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	122	U
3	L5	132	G
3	L5	134	G
3	L5	136	C
3	L5	139	G
3	L5	140	G
3	L5	141	C
3	L5	142	G
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	250	C
3	L5	253	G
3	L5	256	G

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Mol	Chain	Res	Type
3	L5	257	C
3	L5	262	G
3	L5	266	C
3	L5	270	U
3	L5	271	C
3	L5	272	U
3	L5	277	G
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	432	U
3	L5	449	C
3	L5	450	G
3	L5	451	C
3	L5	453	G
3	L5	454	U
3	L5	455	C
3	L5	461	G
3	L5	467	U
3	L5	468	U
3	L5	484	U
3	L5	485	C
3	L5	489	C
3	L5	490	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	646	G
3	L5	654	C

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Mol	Chain	Res	Type
3	L5	656	C
3	L5	659	G
3	L5	663	G
3	L5	664	G
3	L5	666	G
3	L5	667	A
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	729	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	758	G
3	L5	759	G
3	L5	904	C
3	L5	909	A
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	925	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
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

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Mol	Chain	Res	Type
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	1068	G
3	L5	1070	G
3	L5	1072	C
3	L5	1083	U
3	L5	1094	G
3	L5	1098	G
3	L5	1099	C
3	L5	1101	C
3	L5	1169	G
3	L5	1170	G
3	L5	1175	A
3	L5	1182	C
3	L5	1183	C
3	L5	1185	G
3	L5	1187	G
3	L5	1196	G
3	L5	1199	G
3	L5	1201	U
3	L5	1211	G
3	L5	1215	C
3	L5	1216	C
3	L5	1239	C
3	L5	1241	C
3	L5	1242	G
3	L5	1246	G
3	L5	1252	C
3	L5	1253	G
3	L5	1254	A
3	L5	1257	A
3	L5	1259	G
3	L5	1266	G
3	L5	1270	A
3	L5	1272	C
3	L5	1273	G
3	L5	1276	C
3	L5	1279	A

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Mol	Chain	Res	Type
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1293	G
3	L5	1294	A
3	L5	1297	U
3	L5	1303	A
3	L5	1304	C
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	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1403	G
3	L5	1407	C
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	1437	C
3	L5	1439	C
3	L5	1443	A
3	L5	1444	G
3	L5	1445	U
3	L5	1446	C
3	L5	1448	G
3	L5	1457	G
3	L5	1482	G
3	L5	1483	C
3	L5	1484	G
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G

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Mol	Chain	Res	Type
3	L5	1534	A2M
3	L5	1535	C
3	L5	1547	A
3	L5	1554	A
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1613	A
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	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1691	G
3	L5	1698	C
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1703	C
3	L5	1704	C
3	L5	1734	G
3	L5	1750	G
3	L5	1761	G
3	L5	1765	A
3	L5	1766	A
3	L5	1768	C
3	L5	1769	G
3	L5	1775	A
3	L5	1787	A
3	L5	1789	C
3	L5	1804	A
3	L5	1833	G
3	L5	1834	U
3	L5	1836	G

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Mol	Chain	Res	Type
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A
3	L5	1855	G
3	L5	1869	G
3	L5	1892	A
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	1948	G
3	L5	1961	G
3	L5	1962	A
3	L5	1966	C
3	L5	1968	G
3	L5	1969	G
3	L5	1970	A
3	L5	1971	C
3	L5	1972	G
3	L5	1974	U
3	L5	1976	G
3	L5	1983	A
3	L5	1984	A
3	L5	1985	G
3	L5	1987	C
3	L5	1992	U
3	L5	1993	C
3	L5	1994	C
3	L5	1997	U
3	L5	1998	A
3	L5	1999	A
3	L5	2000	G
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2004	U

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Mol	Chain	Res	Type
3	L5	2011	C
3	L5	2018	C
3	L5	2019	C
3	L5	2021	G
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	2052	G
3	L5	2055	G
3	L5	2062	C
3	L5	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2096	G
3	L5	2097	U
3	L5	2099	G
3	L5	2102	G
3	L5	2103	G
3	L5	2106	G
3	L5	2107	C
3	L5	2108	G
3	L5	2110	C
3	L5	2112	G
3	L5	2259	G
3	L5	2261	G
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2333	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2384	U
3	L5	2395	A

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Mol	Chain	Res	Type
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	2485	U
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
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	2529	A
3	L5	2554	U
3	L5	2567	G
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2601	A
3	L5	2653	C
3	L5	2660	A
3	L5	2662	G
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	2712	G

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Mol	Chain	Res	Type
3	L5	2726	G
3	L5	2735	G
3	L5	2739	C
3	L5	2743	A
3	L5	2761	U
3	L5	2763	U
3	L5	2764	A
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2794	C
3	L5	2795	A
3	L5	2796	G
3	L5	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2838	G
3	L5	2855	G
3	L5	2877	G
3	L5	2899	C
3	L5	3596	A
3	L5	3599	A
3	L5	3606	U
3	L5	3615	G
3	L5	3616	U
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	3713	U
3	L5	3714	G
3	L5	3748	A
3	L5	3753	G
3	L5	3760	A2M
3	L5	3761	C
3	L5	3766	A
3	L5	3776	G
3	L5	3777	G

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Mol	Chain	Res	Type
3	L5	3783	A
3	L5	3784	A
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3822	U
3	L5	3839	G
3	L5	3840	U
3	L5	3876	A
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3897	G
3	L5	3898	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3909	C
3	L5	3915	U
3	L5	3944	OMG
3	L5	3951	G
3	L5	3956	G
3	L5	3957	U
3	L5	3958	G
3	L5	3959	U
3	L5	3961	G
3	L5	3962	A
3	L5	3963	A
3	L5	3965	A
3	L5	3966	A
3	L5	3967	G
3	L5	3968	U
3	L5	3969	G
3	L5	3971	G
3	L5	3972	A
3	L5	3974	G
3	L5	3975	C
3	L5	3977	C
3	L5	3978	C
3	L5	4037	C
3	L5	4038	C

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Mol	Chain	Res	Type
3	L5	4039	G
3	L5	4040	C
3	L5	4041	C
3	L5	4042	G
3	L5	4043	G
3	L5	4045	G
3	L5	4046	A
3	L5	4047	A
3	L5	4048	A
3	L5	4049	U
3	L5	4050	A
3	L5	4051	C
3	L5	4053	A
3	L5	4054	C
3	L5	4056	A
3	L5	4059	C
3	L5	4061	G
3	L5	4062	A
3	L5	4063	U
3	L5	4064	C
3	L5	4065	G
3	L5	4076	G
3	L5	4094	G
3	L5	4096	C
3	L5	4097	G
3	L5	4099	G
3	L5	4102	C
3	L5	4103	C
3	L5	4105	A
3	L5	4106	G
3	L5	4110	C
3	L5	4111	U
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4133	C
3	L5	4136	G
3	L5	4137	C
3	L5	4140	C

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Mol	Chain	Res	Type
3	L5	4141	G
3	L5	4142	C
3	L5	4144	C
3	L5	4145	C
3	L5	4147	G
3	L5	4150	G
3	L5	4158	C
3	L5	4162	C
3	L5	4163	U
3	L5	4164	C
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4214	A
3	L5	4222	G
3	L5	4229	U
3	L5	4233	A
3	L5	4251	A
3	L5	4252	C
3	L5	4253	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	4306	OMU
3	L5	4314	C
3	L5	4329	G
3	L5	4330	G
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	4393	G
3	L5	4394	A

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Mol	Chain	Res	Type
3	L5	4420	PSU
3	L5	4422	A
3	L5	4448	G
3	L5	4449	A
3	L5	4450	U
3	L5	4464	A
3	L5	4465	U
3	L5	4475	G
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
3	L5	4557	U
3	L5	4567	G
3	L5	4573	G
3	L5	4574	U
3	L5	4575	G
3	L5	4581	G
3	L5	4590	A2M
3	L5	4600	G
3	L5	4608	G
3	L5	4610	A
3	L5	4617	G
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A
3	L5	4677	U
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

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Mol	Chain	Res	Type
3	L5	4740	G
3	L5	4741	C
3	L5	4745	G
3	L5	4747	C
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	4860	G
3	L5	4865	C
3	L5	4870	G
3	L5	4871	C
3	L5	4882	U
3	L5	4883	C
3	L5	4895	C
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4911	A
3	L5	4912	G
3	L5	4914	C
3	L5	4943	A
3	L5	4944	C
3	L5	4951	G
3	L5	4956	A
3	L5	4963	G
3	L5	4976	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	4994	G
3	L5	5007	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5026	U
3	L5	5027	C

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Mol	Chain	Res	Type
3	L5	5028	G
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5061	A
3	L5	5062	G
3	L5	5066	U
3	L5	5069	U
4	L7	7	G
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	102	U
4	L7	110	G
4	L7	113	G
4	L7	120	U
81	mR	33	A
81	mR	36	U
82	Pt	2	G
82	Pt	9	G
82	Pt	16	C
82	Pt	19	G
82	Pt	21	H2U
82	Pt	43	G
82	Pt	47	G7M
82	Pt	48	U
82	Pt	65	G
82	Pt	71	G
82	Pt	77	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	1490	OMG
1	S2	1753	C
3	L5	42	A
3	L5	278	G
3	L5	417	G
3	L5	955	G

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Mol	Chain	Res	Type
3	L5	1482	G
3	L5	1613	A
3	L5	1633	G
3	L5	1677	PSU
3	L5	1700	G
3	L5	1733	G
3	L5	2794	C
3	L5	3876	A
3	L5	3958	G
3	L5	3964	U
3	L5	4115	G
3	L5	4449	A
3	L5	4699	U
3	L5	4913	G
3	L5	4993	G
3	L5	5026	U

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

235 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
1	6MZ	S2	1832	86,1,87	22,25,26	1.49	5 (22%)	29,36,39	2.20	9 (31%)
3	OMG	L5	4196	82,87,3	23,26,27	1.22	4 (17%)	32,38,41	1.94	6 (18%)
3	A2M	L5	400	3	22,25,26	1.50	4 (18%)	30,36,39	2.03	6 (20%)
3	A2M	L5	4590	3	22,25,26	1.53	4 (18%)	30,36,39	2.02	10 (33%)
1	PSU	S2	1238	1	18,21,22	1.42	4 (22%)	21,30,33	2.06	4 (19%)
1	A2M	S2	1031	1	22,25,26	1.44	4 (18%)	30,36,39	2.18	10 (33%)
1	OMU	S2	354	1	19,22,23	1.28	3 (15%)	25,31,34	1.77	4 (16%)
3	OMG	L5	4499	3	23,26,27	1.27	4 (17%)	32,38,41	2.03	7 (21%)
3	PSU	L5	4673	87,3	18,21,22	1.45	3 (16%)	21,30,33	2.08	5 (23%)
1	G7M	S2	1639	82,1	23,26,27	2.40	6 (26%)	34,39,42	3.00	10 (29%)

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	1.53	4 (18%)	30,36,39	1.97	7 (23%)
1	OMU	S2	116	1	19,22,23	1.29	3 (15%)	25,31,34	1.77	4 (16%)
3	PSU	L5	3851	87,3	18,21,22	1.48	4 (22%)	21,30,33	2.15	6 (28%)
1	B8N	S2	1248	1	25,29,30	0.86	1 (4%)	28,42,45	1.76	6 (21%)
3	OMU	L5	4306	3	19,22,23	1.23	3 (15%)	25,31,34	1.59	5 (20%)
3	OMU	L5	2415	3	19,22,23	1.32	4 (21%)	25,31,34	1.81	5 (20%)
1	PSU	S2	1244	1	18,21,22	1.43	4 (22%)	21,30,33	2.14	3 (14%)
3	PSU	L5	3639	3	18,21,22	1.72	4 (22%)	21,30,33	2.04	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.56	4 (18%)	30,36,39	2.08	12 (40%)
3	UY1	L5	3818	86,87,3	19,22,23	1.51	4 (21%)	21,31,34	2.00	4 (19%)
3	PSU	L5	4457	3	18,21,22	1.55	4 (22%)	21,30,33	1.94	4 (19%)
1	PSU	S2	1692	1	18,21,22	1.46	4 (22%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3744	3	23,26,27	1.20	4 (17%)	32,38,41	2.03	6 (18%)
3	OMU	L5	4227	3	19,22,23	1.27	2 (10%)	25,31,34	1.84	5 (20%)
1	PSU	S2	863	1	18,21,22	1.42	4 (22%)	21,30,33	2.07	3 (14%)
1	PSU	S2	918	1	18,21,22	1.57	5 (27%)	21,30,33	2.30	5 (23%)
1	PSU	S2	109	86,1	18,21,22	1.66	6 (33%)	21,30,33	2.37	4 (19%)
3	PSU	L5	1860	3	18,21,22	1.40	3 (16%)	21,30,33	2.00	5 (23%)
3	A2M	L5	3867	3	22,25,26	1.57	5 (22%)	30,36,39	2.23	11 (36%)
3	PSU	L5	4552	3	18,21,22	1.51	5 (27%)	21,30,33	2.03	4 (19%)
3	OMG	L5	4618	3	23,26,27	1.18	4 (17%)	32,38,41	2.13	8 (25%)
3	PSU	L5	4361	3	18,21,22	1.42	3 (16%)	21,30,33	2.10	5 (23%)
82	OMC	Pt	33	82	19,22,23	0.79	1 (5%)	25,31,34	0.74	0
3	PSU	L5	3844	3	18,21,22	1.51	5 (27%)	21,30,33	2.09	4 (19%)
3	A2M	L5	2363	87,3	22,25,26	1.55	5 (22%)	30,36,39	2.04	9 (30%)
3	OMG	L5	4637	86,3	23,26,27	1.26	3 (13%)	32,38,41	1.94	6 (18%)
2	PSU	L8	55	2	18,21,22	1.45	3 (16%)	21,30,33	2.08	5 (23%)
40	HIC	LB	245	40	10,11,12	1.44	2 (20%)	9,14,16	1.06	1 (11%)
1	A2M	S2	668	1,87	22,25,26	1.51	5 (22%)	30,36,39	2.10	10 (33%)
3	OMG	L5	1316	3	23,26,27	1.32	4 (17%)	32,38,41	2.20	8 (25%)
3	A2M	L5	3723	3	22,25,26	1.47	4 (18%)	30,36,39	2.04	8 (26%)
3	PSU	L5	3920	87,3	18,21,22	1.45	3 (16%)	21,30,33	2.34	4 (19%)
1	PSU	S2	406	1	18,21,22	1.44	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	3729	3	18,21,22	1.42	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	1779	3	18,21,22	1.43	4 (22%)	21,30,33	2.09	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	4571	3	22,25,26	1.50	4 (18%)	30,36,39	2.09	7 (23%)
1	A2M	S2	484	1	22,25,26	1.49	4 (18%)	30,36,39	2.03	7 (23%)
1	A2M	S2	1383	1	22,25,26	1.49	5 (22%)	30,36,39	2.26	11 (36%)
3	PSU	L5	4531	3	18,21,22	1.41	4 (22%)	21,30,33	2.11	3 (14%)
3	OMC	L5	3887	3	19,22,23	0.82	0	25,31,34	0.82	0
3	PSU	L5	4353	3	18,21,22	1.53	4 (22%)	21,30,33	2.30	3 (14%)
3	PSU	L5	4576	3	18,21,22	1.43	4 (22%)	21,30,33	2.11	3 (14%)
1	OMC	S2	1703	1,87	19,22,23	0.75	0	25,31,34	0.74	0
3	A2M	L5	3785	3	22,25,26	1.47	5 (22%)	30,36,39	2.30	12 (40%)
1	A2M	S2	159	1	22,25,26	1.46	4 (18%)	30,36,39	2.15	9 (30%)
3	PSU	L5	4521	86,87,3	18,21,22	1.49	3 (16%)	21,30,33	2.20	5 (23%)
1	PSU	S2	1136	1	18,21,22	1.45	3 (16%)	21,30,33	2.23	4 (19%)
1	A2M	S2	590	1	22,25,26	1.47	4 (18%)	30,36,39	2.10	7 (23%)
3	PSU	L5	4500	3	18,21,22	1.39	4 (22%)	21,30,33	2.20	4 (19%)
3	PSU	L5	3715	3	18,21,22	1.42	4 (22%)	21,30,33	2.22	4 (19%)
3	PSU	L5	3762	3	18,21,22	1.40	3 (16%)	21,30,33	2.07	4 (19%)
1	PSU	S2	105	1	18,21,22	1.51	4 (22%)	21,30,33	2.19	4 (19%)
1	OMU	S2	1804	1	19,22,23	1.33	4 (21%)	25,31,34	1.92	5 (20%)
3	OMC	L5	3701	86,3	19,22,23	0.82	0	25,31,34	1.00	1 (4%)
3	6MZ	L5	4220	3	22,25,26	1.42	4 (18%)	29,36,39	2.29	11 (37%)
3	PSU	L5	3637	86,87,3	18,21,22	1.40	3 (16%)	21,30,33	2.44	4 (19%)
1	PSU	S2	822	1	18,21,22	1.46	3 (16%)	21,30,33	2.29	5 (23%)
3	A2M	L5	2815	87,3	22,25,26	1.34	4 (18%)	30,36,39	2.23	7 (23%)
1	OMG	S2	644	1	23,26,27	1.23	3 (13%)	32,38,41	1.98	6 (18%)
3	OMG	L5	3899	3	23,26,27	1.26	4 (17%)	32,38,41	2.16	8 (25%)
2	PSU	L8	69	2	18,21,22	1.46	4 (22%)	21,30,33	2.10	5 (23%)
3	PSU	L5	2508	3	18,21,22	1.33	3 (16%)	21,30,33	1.98	4 (19%)
1	A2M	S2	99	1,87	22,25,26	1.49	4 (18%)	30,36,39	2.12	7 (23%)
1	OMG	S2	867	1	23,26,27	1.18	3 (13%)	32,38,41	1.94	6 (18%)
3	PSU	L5	1862	3	18,21,22	1.57	3 (16%)	21,30,33	1.99	5 (23%)
3	OMC	L5	2824	3	19,22,23	0.81	1 (5%)	25,31,34	0.84	0
66	MLZ	Lb	5	66	8,9,10	0.94	0	4,9,11	1.13	0
1	PSU	S2	1643	1,87	18,21,22	1.49	3 (16%)	21,30,33	2.16	5 (23%)
3	PSU	L5	2839	3	18,21,22	1.62	3 (16%)	21,30,33	1.94	4 (19%)
79	MLZ	Lo	53	79	8,9,10	0.74	0	4,9,11	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3734	3	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
29	AME	SV	1	29	9,10,11	3.24	2 (22%)	9,11,13	3.93	3 (33%)
1	A2M	S2	1678	1	22,25,26	1.46	4 (18%)	30,36,39	2.10	9 (30%)
1	PSU	S2	1232	1	18,21,22	1.51	4 (22%)	21,30,33	2.16	4 (19%)
3	OMU	L5	4498	87,3	19,22,23	1.32	3 (15%)	25,31,34	1.88	5 (20%)
3	OMG	L5	4370	3	23,26,27	1.21	4 (17%)	32,38,41	2.03	6 (18%)
3	PSU	L5	5010	3	18,21,22	1.49	4 (22%)	21,30,33	2.15	4 (19%)
3	PSU	L5	3758	3	18,21,22	1.45	4 (22%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3792	3	23,26,27	1.23	4 (17%)	32,38,41	1.92	6 (18%)
1	PSU	S2	34	1	18,21,22	1.45	4 (22%)	21,30,33	2.20	4 (19%)
3	5MC	L5	4447	86,3	19,22,23	1.71	3 (15%)	26,32,35	1.32	3 (11%)
3	PSU	L5	4431	3	18,21,22	1.43	3 (16%)	21,30,33	2.00	4 (19%)
50	V5N	La	39	50	8,11,12	1.50	1 (12%)	8,14,16	1.93	2 (25%)
3	PSU	L5	4312	3	18,21,22	1.41	3 (16%)	21,30,33	2.02	4 (19%)
3	OMC	L5	4456	3	19,22,23	0.82	1 (5%)	25,31,34	0.71	0
3	OMC	L5	3841	3	19,22,23	0.80	1 (5%)	25,31,34	0.94	0
1	PSU	S2	1056	1	18,21,22	1.44	4 (22%)	21,30,33	2.14	6 (28%)
1	PSU	S2	1367	1	18,21,22	1.48	4 (22%)	21,30,33	2.12	3 (14%)
3	OMG	L5	4392	3	23,26,27	1.24	4 (17%)	32,38,41	2.04	7 (21%)
3	OMC	L5	2861	3	19,22,23	0.73	0	25,31,34	0.73	0
3	A2M	L5	1534	87,3	22,25,26	1.55	5 (22%)	30,36,39	2.12	11 (36%)
1	OMC	S2	174	1	19,22,23	0.78	0	25,31,34	0.89	1 (4%)
1	OMG	S2	1490	1,87	23,26,27	1.28	4 (17%)	32,38,41	2.17	7 (21%)
3	OMC	L5	2365	87,3	19,22,23	0.77	0	25,31,34	0.79	0
3	OMG	L5	3944	3	23,26,27	1.20	3 (13%)	32,38,41	1.98	6 (18%)
1	OMU	S2	121	1	19,22,23	1.32	3 (15%)	25,31,34	1.80	4 (16%)
1	PSU	S2	866	1	18,21,22	1.43	4 (22%)	21,30,33	2.10	3 (14%)
3	PSU	L5	1536	3	18,21,22	1.40	3 (16%)	21,30,33	2.27	4 (19%)
1	PSU	S2	1174	1,87	18,21,22	1.46	4 (22%)	21,30,33	2.10	4 (19%)
3	OMU	L5	4620	3	19,22,23	1.25	3 (15%)	25,31,34	1.92	5 (20%)
3	PSU	L5	4293	3	18,21,22	1.48	3 (16%)	21,30,33	2.15	5 (23%)
3	PSU	L5	4296	3	18,21,22	1.45	4 (22%)	21,30,33	2.18	4 (19%)
1	OMG	S2	601	1	23,26,27	1.24	3 (13%)	32,38,41	1.93	5 (15%)
2	OMG	L8	75	2	23,26,27	1.23	4 (17%)	32,38,41	1.94	7 (21%)
1	PSU	S2	1004	1	18,21,22	1.60	5 (27%)	21,30,33	2.19	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	S2	1447	1	23,26,27	1.22	3 (13%)	32,38,41	2.05	6 (18%)
3	PSU	L5	1677	3	18,21,22	1.53	5 (27%)	21,30,33	2.38	4 (19%)
3	OMG	L5	2876	3	23,26,27	1.29	3 (13%)	32,38,41	2.01	6 (18%)
82	H2U	Pt	21	82	18,21,22	0.98	2 (11%)	19,30,33	0.94	1 (5%)
82	G7M	Pt	47	82	23,26,27	1.83	2 (8%)	34,39,42	1.11	1 (2%)
3	PSU	L5	4689	3	18,21,22	1.49	4 (22%)	21,30,33	2.20	5 (23%)
3	PSU	L5	4532	3	18,21,22	1.58	3 (16%)	21,30,33	1.97	5 (23%)
3	1MA	L5	1322	87,3	21,25,26	1.39	4 (19%)	30,37,40	1.73	6 (20%)
3	OMC	L5	2804	3	19,22,23	0.79	0	25,31,34	0.98	2 (8%)
3	OMC	L5	1881	87,3	19,22,23	0.82	0	25,31,34	1.06	1 (4%)
82	4SU	Pt	8	82	18,21,22	2.14	5 (27%)	25,30,33	2.48	6 (24%)
1	OMU	S2	172	1	19,22,23	1.28	4 (21%)	25,31,34	1.87	5 (20%)
1	PSU	S2	572	1	18,21,22	1.44	3 (16%)	21,30,33	2.13	5 (23%)
1	OMG	S2	1328	86,1	23,26,27	1.21	3 (13%)	32,38,41	1.98	5 (15%)
3	OMU	L5	3925	3	19,22,23	1.33	2 (10%)	25,31,34	2.02	5 (20%)
3	PSU	L5	4636	3	18,21,22	1.52	4 (22%)	21,30,33	2.11	5 (23%)
3	A2M	L5	2401	3	22,25,26	1.48	5 (22%)	30,36,39	2.11	10 (33%)
1	OMU	S2	1288	1	19,22,23	1.29	3 (15%)	25,31,34	1.99	6 (24%)
1	PSU	S2	966	1	18,21,22	1.44	4 (22%)	21,30,33	2.07	3 (14%)
3	PSU	L5	2632	3	18,21,22	1.44	4 (22%)	21,30,33	2.05	5 (23%)
1	PSU	S2	814	1	18,21,22	1.45	3 (16%)	21,30,33	2.04	3 (14%)
1	PSU	S2	119	1	18,21,22	1.38	4 (22%)	21,30,33	2.13	4 (19%)
1	OMC	S2	517	1	19,22,23	0.77	0	25,31,34	0.70	0
3	A2M	L5	3724	3	22,25,26	1.44	5 (22%)	30,36,39	2.08	11 (36%)
3	PSU	L5	1792	3	18,21,22	1.41	4 (22%)	21,30,33	2.05	3 (14%)
3	OMG	L5	2364	3	23,26,27	1.41	4 (17%)	32,38,41	2.05	8 (25%)
3	OMG	L5	2424	3	23,26,27	1.24	3 (13%)	32,38,41	1.98	6 (18%)
1	PSU	S2	609	1	18,21,22	1.44	4 (22%)	21,30,33	2.10	3 (14%)
1	A2M	S2	576	1	22,25,26	1.51	5 (22%)	30,36,39	2.02	9 (30%)
3	PSU	L5	1782	3	18,21,22	1.41	3 (16%)	21,30,33	2.13	3 (14%)
1	PSU	S2	801	1	18,21,22	1.39	3 (16%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.51	4 (22%)	21,30,33	2.15	3 (14%)
3	PSU	L5	3764	3	18,21,22	1.45	4 (22%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4423	3	18,21,22	1.47	3 (16%)	21,30,33	2.19	5 (23%)
3	A2M	L5	2787	3	22,25,26	1.52	4 (18%)	30,36,39	2.30	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	36	1	18,21,22	1.44	4 (22%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4569	3	18,21,22	1.46	4 (22%)	21,30,33	2.30	6 (28%)
83	5CT	5A	50[B]	-	13,14,15	1.10	1 (7%)	8,15,17	0.99	0
1	OMU	S2	428	1	19,22,23	1.25	3 (15%)	25,31,34	1.86	5 (20%)
1	OMC	S2	1391	1	19,22,23	0.79	0	25,31,34	0.83	0
3	PSU	L5	4972	3	18,21,22	1.63	5 (27%)	21,30,33	2.33	5 (23%)
3	PSU	L5	1582	3	18,21,22	1.51	4 (22%)	21,30,33	2.11	5 (23%)
3	PSU	L5	4403	3	18,21,22	1.48	4 (22%)	21,30,33	2.15	5 (23%)
1	PSU	S2	649	1	18,21,22	1.40	4 (22%)	21,30,33	2.19	3 (14%)
1	4AC	S2	1337	1	21,24,25	1.05	1 (4%)	28,34,37	1.17	4 (14%)
3	A2M	L5	1871	87,3	22,25,26	1.35	5 (22%)	30,36,39	2.39	11 (36%)
3	OMC	L5	4536	3	19,22,23	0.87	2 (10%)	25,31,34	0.96	2 (8%)
1	PSU	S2	1177	1	18,21,22	1.56	4 (22%)	21,30,33	2.05	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.47	4 (18%)	30,36,39	2.31	11 (36%)
1	OMG	S2	509	1,87	23,26,27	1.19	3 (13%)	32,38,41	2.03	5 (15%)
3	OMG	L5	4494	87,3	23,26,27	1.27	3 (13%)	32,38,41	2.14	7 (21%)
1	PSU	S2	686	1	18,21,22	1.43	4 (22%)	21,30,33	2.12	3 (14%)
1	4AC	S2	1842	1	21,24,25	1.07	1 (4%)	28,34,37	1.31	6 (21%)
1	A2M	S2	27	1,87	22,25,26	1.46	4 (18%)	30,36,39	2.08	11 (36%)
1	PSU	S2	1081	1	18,21,22	1.47	4 (22%)	21,30,33	2.09	5 (23%)
82	PSU	Pt	56	82	18,21,22	1.35	3 (16%)	21,30,33	2.10	4 (19%)
3	OMU	L5	2837	3	19,22,23	1.35	3 (15%)	25,31,34	2.04	6 (24%)
3	OMG	L5	3627	3	23,26,27	1.24	4 (17%)	32,38,41	2.09	7 (21%)
3	OMG	L5	1522	3	23,26,27	1.14	2 (8%)	32,38,41	2.08	11 (34%)
1	PSU	S2	1347	1	18,21,22	1.51	4 (22%)	21,30,33	2.11	4 (19%)
3	A2M	L5	3825	3	22,25,26	1.57	4 (18%)	30,36,39	2.01	9 (30%)
1	OMU	S2	1442	1,87	19,22,23	1.28	3 (15%)	25,31,34	1.80	4 (16%)
1	PSU	S2	296	1	18,21,22	1.43	4 (22%)	21,30,33	2.11	4 (19%)
3	PSU	L5	4493	87,3	18,21,22	1.43	4 (22%)	21,30,33	2.03	3 (14%)
3	OMG	L5	4623	3	23,26,27	1.27	4 (17%)	32,38,41	1.99	6 (18%)
3	PSU	L5	1683	86,3	18,21,22	1.45	4 (22%)	21,30,33	2.22	3 (14%)
3	A2M	L5	3760	1,87,3	22,25,26	1.49	5 (22%)	30,36,39	2.12	9 (30%)
3	UR3	L5	4530	3	19,22,23	0.82	1 (5%)	26,32,35	1.83	3 (11%)
3	PSU	L5	5001	87,3	18,21,22	1.55	4 (22%)	21,30,33	2.23	5 (23%)
3	PSU	L5	3770	3	18,21,22	1.49	5 (27%)	21,30,33	2.14	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5MC	L5	3782	87,3	19,22,23	1.80	3 (15%)	26,32,35	1.19	3 (11%)
3	OMG	L5	1625	86,87,3	23,26,27	1.28	3 (13%)	32,38,41	2.10	8 (25%)
3	OMG	L5	4228	3	23,26,27	1.19	4 (17%)	32,38,41	2.02	9 (28%)
6	SAC	SA	2	6	7,8,9	3.81	2 (28%)	7,9,11	4.43	3 (42%)
1	PSU	S2	651	1	18,21,22	1.46	4 (22%)	21,30,33	2.14	4 (19%)
1	PSU	S2	681	1	18,21,22	1.48	4 (22%)	21,30,33	2.17	4 (19%)
20	HY3	SX	62	20	7,8,9	1.35	1 (14%)	7,10,12	1.57	2 (28%)
64	SAC	Lr	2	64	7,8,9	3.82	2 (28%)	7,9,11	4.07	3 (42%)
3	OMC	L5	3808	87,3	19,22,23	0.80	1 (5%)	25,31,34	0.82	1 (4%)
3	PSU	L5	1744	87,3	18,21,22	1.45	3 (16%)	21,30,33	2.09	3 (14%)
1	A2M	S2	512	1	22,25,26	1.43	4 (18%)	30,36,39	2.17	9 (30%)
1	PSU	S2	1243	1	18,21,22	1.46	4 (22%)	21,30,33	2.14	4 (19%)
1	PSU	S2	1239	1	18,21,22	1.45	4 (22%)	21,30,33	2.15	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.51	5 (22%)	30,36,39	2.27	9 (30%)
3	PSU	L5	3768	3	18,21,22	1.41	4 (22%)	21,30,33	2.15	4 (19%)
1	OMG	S2	683	1	23,26,27	1.19	4 (17%)	32,38,41	2.01	7 (21%)
1	PSU	S2	218	1	18,21,22	1.42	4 (22%)	21,30,33	2.10	4 (19%)
1	PSU	S2	1445	1	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
1	A2M	S2	468	1	22,25,26	1.47	5 (22%)	30,36,39	2.12	10 (33%)
1	A2M	S2	166	1	22,25,26	1.47	4 (18%)	30,36,39	2.25	9 (30%)
1	PSU	S2	815	1	18,21,22	1.41	4 (22%)	21,30,33	2.05	4 (19%)
3	A2M	L5	398	3	22,25,26	1.48	4 (18%)	30,36,39	2.21	10 (33%)
1	OMG	S2	436	1	23,26,27	1.24	3 (13%)	32,38,41	2.13	6 (18%)
3	PSU	L5	3884	87,3	18,21,22	1.44	3 (16%)	21,30,33	2.30	5 (23%)
1	PSU	S2	573	1	18,21,22	1.43	3 (16%)	21,30,33	2.09	4 (19%)
1	OMU	S2	627	1	19,22,23	1.23	3 (15%)	25,31,34	1.85	5 (20%)
3	PSU	L5	4628	3	18,21,22	1.45	6 (33%)	21,30,33	2.19	5 (23%)
2	OMU	L8	14	2,3	19,22,23	1.30	3 (15%)	25,31,34	1.65	5 (20%)
39	V5N	LA	216	39	8,11,12	1.62	1 (12%)	8,14,16	1.68	1 (12%)
3	PSU	L5	3853	87,3	18,21,22	1.43	3 (16%)	21,30,33	2.30	4 (19%)
3	PSU	L5	4299	3	18,21,22	1.53	5 (27%)	21,30,33	2.12	5 (23%)
3	A2M	L5	4523	87,3	22,25,26	1.42	4 (18%)	30,36,39	2.49	11 (36%)
3	PSU	L5	4442	3	18,21,22	1.48	5 (27%)	21,30,33	2.16	6 (28%)
1	MA6	S2	1851	1	23,26,27	1.44	4 (17%)	33,38,41	2.18	11 (33%)
1	PSU	S2	93	1	18,21,22	1.54	3 (16%)	21,30,33	1.96	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4579	3	18,21,22	1.46	4 (22%)	21,30,33	2.04	3 (14%)
3	PSU	L5	4471	3	18,21,22	1.42	3 (16%)	21,30,33	1.97	3 (14%)
3	PSU	L5	3695	3	18,21,22	1.41	4 (22%)	21,30,33	2.17	5 (23%)
1	UY1	S2	1326	1,87	19,22,23	1.49	4 (21%)	21,31,34	2.32	4 (19%)
1	PSU	S2	1625	1	18,21,22	1.45	4 (22%)	21,30,33	2.11	4 (19%)
1	MA6	S2	1850	1	23,26,27	1.39	5 (21%)	33,38,41	2.21	11 (33%)
77	M3L	Lm	98	77	10,11,12	0.57	0	9,14,16	0.50	0
83	5CT	5A	50[A]	87	13,14,15	1.09	1 (7%)	8,15,17	1.32	1 (12%)
3	PSU	L5	2843	3	18,21,22	1.47	3 (16%)	21,30,33	2.25	5 (23%)
3	PSU	L5	4420	3	18,21,22	1.49	5 (27%)	21,30,33	2.02	3 (14%)
1	OMC	S2	462	1	19,22,23	0.78	0	25,31,34	0.81	0
3	OMC	L5	3869	3	19,22,23	0.81	1 (5%)	25,31,34	1.07	1 (4%)
3	OMC	L5	2351	87,3	19,22,23	0.80	0	25,31,34	1.22	2 (8%)
3	OMC	L5	1340	3	19,22,23	0.73	0	25,31,34	0.95	0
3	OMC	L5	2422	87,3	19,22,23	0.80	0	25,31,34	0.81	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
1	6MZ	S2	1832	86,1,87	-	1/9/27/28	0/3/3/3
3	OMG	L5	4196	82,87,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4673	87,3	-	0/7/25/26	0/2/2/2
1	G7M	S2	1639	82,1	-	0/7/25/26	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	3851	87,3	-	1/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
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
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
3	UY1	L5	3818	86,87,3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	86,1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
82	OMC	Pt	33	82	-	0/9/27/28	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4637	86,3	-	1/9/27/28	0/3/3/3
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
40	HIC	LB	245	40	-	0/5/6/8	0/1/1/1
1	A2M	S2	668	1,87	-	5/9/27/28	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	1,87	-	0/9/27/28	0/2/2/2
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4521	86,87,3	-	2/7/25/26	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
3	OMC	L5	3701	86,3	-	4/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3637	86,87,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
3	A2M	L5	2815	87,3	-	4/9/27/28	0/3/3/3
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	99	1,87	-	0/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
66	MLZ	Lb	5	66	-	0/7/8/10	-
1	PSU	S2	1643	1,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
79	MLZ	Lo	53	79	-	3/7/8/10	-
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
29	AME	SV	1	29	-	3/9/10/12	-
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	87,3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	86,3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
50	V5N	La	39	50	-	0/9/10/12	0/1/1/1
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1534	87,3	-	2/9/27/28	0/3/3/3
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	1490	1,87	-	3/9/27/28	0/3/3/3
3	OMC	L5	2365	87,3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1174	1,87	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
2	OMG	L8	75	2	-	0/9/27/28	0/3/3/3
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	3/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
82	H2U	Pt	21	82	-	3/7/38/39	0/2/2/2
82	G7M	Pt	47	82	-	1/7/25/26	0/3/3/3
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
3	OMC	L5	2804	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	1881	87,3	-	0/9/27/28	0/2/2/2
82	4SU	Pt	8	82	-	0/7/25/26	0/2/2/2
1	OMU	S2	172	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1328	86,1	-	1/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	1288	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3764	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	3/9/27/28	0/3/3/3
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
83	5CT	5A	50[B]	-	-	9/13/14/16	-
1	OMU	S2	428	1	-	2/9/27/28	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
1	OMG	S2	509	1,87	-	0/9/27/28	0/3/3/3
3	OMG	L5	4494	87,3	-	0/9/27/28	0/3/3/3
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	A2M	S2	27	1,87	-	1/9/27/28	0/3/3/3
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
82	PSU	Pt	56	82	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
1	OMU	S2	1442	1,87	-	3/9/27/28	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1683	86,3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3760	1,87,3	-	6/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	86,87,3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	1/9/27/28	0/3/3/3
6	SAC	SA	2	6	-	4/7/8/10	-
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
64	SAC	Lr	2	64	-	4/7/8/10	-
3	OMC	L5	3808	87,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	512	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	166	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	3884	87,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	573	1	-	1/7/25/26	0/2/2/2
1	OMU	S2	627	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
2	OMU	L8	14	2,3	-	1/9/27/28	0/2/2/2
39	V5N	LA	216	39	-	1/9/10/12	0/1/1/1
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	87,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	3/11/29/30	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3695	3	-	1/7/25/26	0/2/2/2
1	UY1	S2	1326	1,87	-	1/9/27/28	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
77	M3L	Lm	98	77	-	0/9/10/12	-
83	5CT	5A	50[A]	87	-	9/13/14/16	-
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2351	87,3	-	2/9/27/28	0/2/2/2
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2422	87,3	-	2/9/27/28	0/2/2/2

All (776) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	Lr	2	SAC	OAC-C1A	9.03	1.43	1.23
6	SA	2	SAC	OAC-C1A	8.95	1.43	1.23
29	SV	1	AME	OT-CT1	8.80	1.42	1.23
82	Pt	47	G7M	C8-N7	7.19	1.45	1.33
1	S2	1639	G7M	C8-N7	7.09	1.45	1.33
3	L5	3782	5MC	C5-C4	6.56	1.49	1.44
3	L5	4447	5MC	C5-C4	6.14	1.48	1.44
1	S2	1639	G7M	C5-N7	-5.84	1.32	1.39
82	Pt	8	4SU	C4-S4	-5.67	1.58	1.68
3	L5	3825	A2M	C5-C4	4.63	1.47	1.39
3	L5	2787	A2M	C5-C4	4.62	1.47	1.39
3	L5	3760	A2M	C5-C4	4.54	1.47	1.39
1	S2	576	A2M	C5-C4	4.49	1.47	1.39
3	L5	1534	A2M	C5-C4	4.48	1.47	1.39
3	L5	4523	A2M	C5-C4	4.48	1.47	1.39
1	S2	1383	A2M	C5-C4	4.47	1.47	1.39
3	L5	4532	PSU	C6-C5	4.46	1.40	1.35
1	S2	159	A2M	C5-C4	4.45	1.47	1.39
1	S2	590	A2M	C5-C4	4.44	1.47	1.39
3	L5	3723	A2M	C5-C4	4.41	1.47	1.39
3	L5	3830	A2M	C5-C4	4.40	1.46	1.39
3	L5	4590	A2M	C5-C4	4.37	1.46	1.39
3	L5	3867	A2M	C5-C4	4.37	1.46	1.39
1	S2	484	A2M	C5-C4	4.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3718	A2M	C5-C4	4.35	1.46	1.39
1	S2	99	A2M	C5-C4	4.32	1.46	1.39
1	S2	1832	6MZ	C5-C4	4.32	1.46	1.39
1	S2	166	A2M	C5-C4	4.31	1.46	1.39
3	L5	398	A2M	C5-C4	4.31	1.46	1.39
3	L5	400	A2M	C5-C4	4.27	1.46	1.39
1	S2	468	A2M	C5-C4	4.26	1.46	1.39
1	S2	27	A2M	C5-C4	4.19	1.46	1.39
3	L5	3724	A2M	C5-C4	4.18	1.46	1.39
64	Lr	2	SAC	C1A-N	4.15	1.47	1.34
3	L5	1326	A2M	C5-C4	4.14	1.46	1.39
3	L5	1524	A2M	C5-C4	4.13	1.46	1.39
82	Pt	8	4SU	C4-N3	-4.13	1.33	1.37
6	SA	2	SAC	C1A-N	4.13	1.47	1.34
1	S2	1678	A2M	C5-C4	4.11	1.46	1.39
3	L5	4571	A2M	C5-C4	4.11	1.46	1.39
1	S2	512	A2M	C5-C4	4.08	1.46	1.39
1	S2	668	A2M	C5-C4	4.08	1.46	1.39
3	L5	2401	A2M	C5-C4	4.07	1.46	1.39
3	L5	3639	PSU	C4-N3	-4.07	1.31	1.38
1	S2	1031	A2M	C5-C4	4.05	1.46	1.39
1	S2	1851	MA6	C5-C4	4.03	1.46	1.39
39	LA	216	V5N	CG-ND1	-4.02	1.33	1.37
3	L5	4220	6MZ	C5-C4	4.01	1.46	1.39
3	L5	2815	A2M	C5-C4	3.90	1.46	1.39
3	L5	3785	A2M	C5-C4	3.88	1.46	1.39
82	Pt	47	G7M	C8-N9	3.84	1.46	1.35
1	S2	1850	MA6	C5-C4	3.78	1.45	1.39
3	L5	1871	A2M	C5-C4	3.77	1.45	1.39
3	L5	2839	PSU	C6-C5	3.76	1.39	1.35
1	S2	1639	G7M	C8-N9	3.74	1.45	1.35
3	L5	1582	PSU	C6-C5	3.70	1.39	1.35
83	5A	50[A]	5CT	O-C	3.66	1.33	1.20
83	5A	50[B]	5CT	O-C	3.66	1.33	1.20
29	SV	1	AME	CT1-N	3.65	1.46	1.34
3	L5	4972	PSU	C4-N3	-3.64	1.32	1.38
1	S2	93	PSU	C6-C5	3.63	1.39	1.35
50	La	39	V5N	CG-ND1	-3.60	1.34	1.37
3	L5	4457	PSU	C6-C5	3.57	1.39	1.35
3	L5	4293	PSU	C6-C5	3.51	1.39	1.35
1	S2	1177	PSU	C4-N3	-3.51	1.32	1.38
3	L5	3884	PSU	C4-N3	-3.50	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4498	OMU	C4-N3	-3.49	1.32	1.38
3	L5	3639	PSU	C6-C5	3.49	1.39	1.35
3	L5	4442	PSU	C4-N3	-3.48	1.32	1.38
3	L5	2843	PSU	C4-N3	-3.46	1.32	1.38
3	L5	1862	PSU	C6-C5	3.44	1.39	1.35
3	L5	4521	PSU	C6-C5	3.42	1.39	1.35
3	L5	3925	OMU	C4-N3	-3.42	1.32	1.38
3	L5	1862	PSU	C4-N3	-3.41	1.32	1.38
3	L5	2363	A2M	C5-C4	3.41	1.45	1.39
1	S2	105	PSU	C4-N3	-3.41	1.32	1.38
3	L5	3818	UY1	C4-N3	-3.40	1.32	1.38
3	L5	5001	PSU	C4-N3	-3.40	1.32	1.38
1	S2	109	PSU	C4-N3	-3.40	1.32	1.38
3	L5	2839	PSU	C4-N3	-3.39	1.32	1.38
3	L5	2364	OMG	C6-N1	-3.38	1.32	1.38
1	S2	1347	PSU	C4-N3	-3.37	1.32	1.38
1	S2	1004	PSU	C4-N3	-3.36	1.32	1.38
3	L5	2837	OMU	C2-N3	-3.35	1.32	1.38
82	Pt	8	4SU	C5-C4	-3.32	1.38	1.42
1	S2	1326	UY1	C4-N3	-3.32	1.32	1.38
3	L5	4423	PSU	C4-N3	-3.31	1.32	1.38
3	L5	4689	PSU	C4-N3	-3.31	1.32	1.38
1	S2	1643	PSU	C4-N3	-3.30	1.32	1.38
1	S2	93	PSU	C4-N3	-3.30	1.32	1.38
1	S2	681	PSU	C4-N3	-3.30	1.32	1.38
3	L5	4361	PSU	C4-N3	-3.30	1.32	1.38
3	L5	2508	PSU	C6-C5	3.30	1.38	1.35
3	L5	1781	PSU	C4-N3	-3.27	1.32	1.38
3	L5	3867	A2M	C5-N7	-3.27	1.33	1.39
3	L5	2837	OMU	C4-N3	-3.27	1.33	1.38
1	S2	866	PSU	C6-C5	3.27	1.38	1.35
3	L5	1683	PSU	C6-C5	3.27	1.38	1.35
2	L8	14	OMU	C4-N3	-3.27	1.33	1.38
3	L5	4552	PSU	C4-N3	-3.27	1.32	1.38
3	L5	4494	OMG	C6-N1	-3.26	1.32	1.38
1	S2	354	OMU	C4-N3	-3.26	1.33	1.38
3	L5	4299	PSU	C4-N3	-3.25	1.32	1.38
1	S2	918	PSU	C4-N3	-3.25	1.32	1.38
3	L5	2839	PSU	C2-N3	-3.24	1.32	1.37
3	L5	3920	PSU	C6-C5	3.24	1.38	1.35
3	L5	2415	OMU	C4-N3	-3.23	1.33	1.38
3	L5	3637	PSU	C6-C5	3.23	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1136	PSU	C4-N3	-3.23	1.32	1.38
1	S2	406	PSU	C4-N3	-3.23	1.32	1.38
3	L5	4673	PSU	C4-N3	-3.23	1.32	1.38
3	L5	4636	PSU	C6-C5	3.22	1.38	1.35
3	L5	3695	PSU	C4-N3	-3.21	1.32	1.38
3	L5	4403	PSU	C4-N3	-3.21	1.32	1.38
20	SX	62	HY3	C3-CA	-3.21	1.51	1.55
1	S2	686	PSU	C4-N3	-3.20	1.32	1.38
3	L5	2876	OMG	C6-N1	-3.20	1.32	1.38
1	S2	1232	PSU	C6-C5	3.19	1.38	1.35
3	L5	1326	A2M	C5-N7	-3.19	1.33	1.39
3	L5	3758	PSU	C4-N3	-3.18	1.32	1.38
3	L5	3853	PSU	C4-N3	-3.18	1.32	1.38
3	L5	4227	OMU	C4-N3	-3.18	1.33	1.38
3	L5	1582	PSU	C4-N3	-3.17	1.32	1.38
3	L5	2363	A2M	C5-N7	-3.17	1.33	1.39
1	S2	1639	G7M	C5-C4	3.17	1.46	1.38
1	S2	1842	4AC	C4-N4	-3.17	1.35	1.39
1	S2	1243	PSU	C4-N3	-3.17	1.32	1.38
1	S2	1232	PSU	C4-N3	-3.16	1.32	1.38
3	L5	4569	PSU	C6-C5	3.16	1.38	1.35
1	S2	121	OMU	C4-N3	-3.16	1.33	1.38
1	S2	1239	PSU	C4-N3	-3.16	1.32	1.38
2	L8	55	PSU	C4-N3	-3.15	1.33	1.38
3	L5	5010	PSU	C4-N3	-3.15	1.33	1.38
1	S2	1177	PSU	C6-C5	3.15	1.38	1.35
3	L5	4431	PSU	C4-N3	-3.14	1.33	1.38
1	S2	966	PSU	C4-N3	-3.14	1.33	1.38
1	S2	1081	PSU	C4-N3	-3.14	1.33	1.38
3	L5	3729	PSU	C4-N3	-3.14	1.33	1.38
3	L5	3825	A2M	C5-N7	-3.13	1.33	1.39
1	S2	1367	PSU	C4-N3	-3.13	1.33	1.38
3	L5	4493	PSU	C4-N3	-3.12	1.33	1.38
3	L5	4293	PSU	C4-N3	-3.12	1.33	1.38
1	S2	863	PSU	C4-N3	-3.12	1.33	1.38
1	S2	822	PSU	C4-N3	-3.12	1.33	1.38
2	L8	69	PSU	C4-N3	-3.11	1.33	1.38
3	L5	3734	PSU	C6-C5	3.11	1.38	1.35
1	S2	1174	PSU	C6-C5	3.11	1.38	1.35
3	L5	1316	OMG	C5-N7	-3.11	1.32	1.39
3	L5	1782	PSU	C4-N3	-3.11	1.33	1.38
1	S2	601	OMG	C6-N1	-3.10	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3715	PSU	C4-N3	-3.10	1.33	1.38
3	L5	4353	PSU	C6-C5	3.10	1.38	1.35
3	L5	1625	OMG	C6-N1	-3.10	1.33	1.38
1	S2	1081	PSU	C6-C5	3.10	1.38	1.35
1	S2	119	PSU	C4-N3	-3.09	1.33	1.38
1	S2	572	PSU	C6-C5	3.09	1.38	1.35
1	S2	1804	OMU	C4-N3	-3.09	1.33	1.38
1	S2	573	PSU	C6-C5	3.09	1.38	1.35
3	L5	3718	A2M	C5-N7	-3.09	1.33	1.39
1	S2	99	A2M	C5-N7	-3.09	1.33	1.39
3	L5	4579	PSU	C4-N3	-3.09	1.33	1.38
3	L5	1779	PSU	C4-N3	-3.08	1.33	1.38
3	L5	4296	PSU	C4-N3	-3.08	1.33	1.38
1	S2	815	PSU	C4-N3	-3.07	1.33	1.38
3	L5	3851	PSU	C6-C5	3.07	1.38	1.35
1	S2	36	PSU	C4-N3	-3.07	1.33	1.38
1	S2	966	PSU	C6-C5	3.06	1.38	1.35
3	L5	3770	PSU	C6-C5	3.06	1.38	1.35
1	S2	651	PSU	C4-N3	-3.06	1.33	1.38
1	S2	609	PSU	C6-C5	3.06	1.38	1.35
3	L5	1683	PSU	C4-N3	-3.06	1.33	1.38
3	L5	4471	PSU	C4-N3	-3.06	1.33	1.38
3	L5	4499	OMG	C6-N1	-3.05	1.33	1.38
1	S2	1625	PSU	C6-C5	3.05	1.38	1.35
1	S2	1238	PSU	C4-N3	-3.05	1.33	1.38
3	L5	3729	PSU	C6-C5	3.05	1.38	1.35
3	L5	4636	PSU	C4-N3	-3.05	1.33	1.38
3	L5	1326	A2M	C4-N9	-3.05	1.31	1.37
1	S2	296	PSU	C4-N3	-3.05	1.33	1.38
3	L5	3768	PSU	C4-N3	-3.04	1.33	1.38
3	L5	1625	OMG	C5-C4	3.04	1.47	1.38
3	L5	2632	PSU	C4-N3	-3.04	1.33	1.38
1	S2	218	PSU	C4-N3	-3.03	1.33	1.38
3	L5	4353	PSU	C4-N3	-3.03	1.33	1.38
1	S2	814	PSU	C4-N3	-3.03	1.33	1.38
3	L5	3920	PSU	C4-N3	-3.03	1.33	1.38
3	L5	1744	PSU	C6-C5	3.03	1.38	1.35
3	L5	3627	OMG	C6-N1	-3.02	1.33	1.38
3	L5	4576	PSU	C4-N3	-3.02	1.33	1.38
3	L5	3844	PSU	C4-N3	-3.02	1.33	1.38
3	L5	1316	OMG	C6-N1	-3.02	1.33	1.38
3	L5	4637	OMG	C6-N1	-3.01	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4306	OMU	C4-N3	-3.01	1.33	1.38
1	S2	801	PSU	C4-N3	-3.01	1.33	1.38
3	L5	5010	PSU	C6-C5	3.01	1.38	1.35
1	S2	1244	PSU	C4-N3	-3.00	1.33	1.38
1	S2	644	OMG	C6-N1	-3.00	1.33	1.38
1	S2	1056	PSU	C4-N3	-3.00	1.33	1.38
1	S2	1692	PSU	C6-C5	2.99	1.38	1.35
3	L5	3762	PSU	C6-C5	2.99	1.38	1.35
1	S2	116	OMU	C4-N3	-2.99	1.33	1.38
1	S2	1174	PSU	C4-N3	-2.99	1.33	1.38
1	S2	1625	PSU	C4-N3	-2.99	1.33	1.38
3	L5	2363	A2M	C4-N9	-2.99	1.31	1.37
1	S2	609	PSU	C4-N3	-2.99	1.33	1.38
1	S2	649	PSU	C4-N3	-2.98	1.33	1.38
1	S2	1031	A2M	C5-N7	-2.98	1.33	1.39
3	L5	4532	PSU	C4-N3	-2.98	1.33	1.38
3	L5	400	A2M	C5-N7	-2.98	1.33	1.39
1	S2	428	OMU	C4-N3	-2.98	1.33	1.38
1	S2	573	PSU	C4-N3	-2.97	1.33	1.38
3	L5	4457	PSU	C4-N3	-2.97	1.33	1.38
3	L5	3770	PSU	C4-N3	-2.97	1.33	1.38
3	L5	4569	PSU	C4-N3	-2.97	1.33	1.38
1	S2	1337	4AC	C4-N4	-2.96	1.35	1.39
1	S2	1442	OMU	C4-N3	-2.96	1.33	1.38
1	S2	1692	PSU	C4-N3	-2.96	1.33	1.38
3	L5	1781	PSU	C6-C5	2.96	1.38	1.35
1	S2	436	OMG	C6-N1	-2.95	1.33	1.38
1	S2	572	PSU	C4-N3	-2.94	1.33	1.38
3	L5	1792	PSU	C4-N3	-2.94	1.33	1.38
2	L8	75	OMG	C6-N1	-2.94	1.33	1.38
3	L5	4579	PSU	C6-C5	2.94	1.38	1.35
3	L5	3899	OMG	C5-C4	2.94	1.46	1.38
3	L5	4521	PSU	C4-N3	-2.94	1.33	1.38
3	L5	1862	PSU	C2-N3	-2.94	1.32	1.37
3	L5	3764	PSU	C4-N3	-2.93	1.33	1.38
3	L5	4620	OMU	C4-N3	-2.93	1.33	1.38
1	S2	34	PSU	C4-N3	-2.93	1.33	1.38
3	L5	4196	OMG	C5-C4	2.93	1.46	1.38
3	L5	4623	OMG	C5-C4	2.93	1.46	1.38
1	S2	814	PSU	C6-C5	2.92	1.38	1.35
1	S2	801	PSU	C6-C5	2.92	1.38	1.35
1	S2	866	PSU	C4-N3	-2.92	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1445	PSU	C4-N3	-2.92	1.33	1.38
3	L5	3792	OMG	C5-C4	2.91	1.46	1.38
1	S2	1643	PSU	C6-C5	2.91	1.38	1.35
3	L5	4571	A2M	C5-N7	-2.91	1.33	1.39
3	L5	2787	A2M	C5-C6	2.90	1.49	1.41
3	L5	2424	OMG	C6-N1	-2.90	1.33	1.38
3	L5	4623	OMG	C6-N1	-2.90	1.33	1.38
1	S2	601	OMG	C5-C4	2.90	1.46	1.38
1	S2	1447	OMG	C5-C4	2.90	1.46	1.38
3	L5	3782	5MC	C6-C5	2.89	1.39	1.34
3	L5	3785	A2M	C5-N7	-2.89	1.33	1.39
1	S2	1328	OMG	C5-C4	2.89	1.46	1.38
3	L5	2424	OMG	C5-C4	2.89	1.46	1.38
3	L5	1744	PSU	C4-N3	-2.89	1.33	1.38
3	L5	1860	PSU	C4-N3	-2.89	1.33	1.38
3	L5	4673	PSU	C6-C5	2.89	1.38	1.35
3	L5	3925	OMU	C2-N3	-2.89	1.32	1.38
1	S2	1447	OMG	C6-N1	-2.89	1.33	1.38
1	S2	1367	PSU	C2-N1	-2.89	1.32	1.36
3	L5	4500	PSU	C6-C5	2.88	1.38	1.35
3	L5	4498	OMU	C2-N3	-2.88	1.32	1.38
1	S2	867	OMG	C5-C4	2.88	1.46	1.38
3	L5	3851	PSU	C4-N3	-2.88	1.33	1.38
3	L5	4227	OMU	C2-N3	-2.88	1.32	1.38
3	L5	4312	PSU	C4-N3	-2.88	1.33	1.38
3	L5	1536	PSU	C6-C5	2.87	1.38	1.35
3	L5	3637	PSU	C4-N3	-2.87	1.33	1.38
3	L5	3762	PSU	C4-N3	-2.87	1.33	1.38
3	L5	3944	OMG	C5-C4	2.87	1.46	1.38
1	S2	686	PSU	C6-C5	2.87	1.38	1.35
3	L5	3734	PSU	C4-N3	-2.87	1.33	1.38
1	S2	1490	OMG	C6-N1	-2.86	1.33	1.38
3	L5	1524	A2M	C5-N7	-2.86	1.33	1.39
3	L5	1534	A2M	C4-N9	-2.86	1.31	1.37
3	L5	2843	PSU	C6-C5	2.86	1.38	1.35
1	S2	1136	PSU	C6-C5	2.86	1.38	1.35
3	L5	5001	PSU	C6-C5	2.86	1.38	1.35
1	S2	172	OMU	C4-N3	-2.86	1.33	1.38
3	L5	2401	A2M	C5-N7	-2.86	1.33	1.39
3	L5	4420	PSU	C6-C5	2.85	1.38	1.35
3	L5	1860	PSU	C6-C5	2.85	1.38	1.35
3	L5	1522	OMG	C5-C4	2.85	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1536	PSU	C4-N3	-2.84	1.33	1.38
3	L5	4590	A2M	C5-N7	-2.84	1.33	1.39
2	L8	55	PSU	C6-C5	2.84	1.38	1.35
3	L5	1534	A2M	C5-N7	-2.84	1.33	1.39
3	L5	4531	PSU	C6-C5	2.84	1.38	1.35
1	S2	1639	G7M	C6-N1	-2.83	1.33	1.38
1	S2	218	PSU	C6-C5	2.83	1.38	1.35
1	S2	1328	OMG	C6-N1	-2.83	1.33	1.38
3	L5	4628	PSU	C4-N3	-2.82	1.33	1.38
1	S2	34	PSU	C6-C5	2.82	1.38	1.35
3	L5	4521	PSU	C2-N3	-2.82	1.32	1.37
3	L5	4299	PSU	C2-N3	-2.82	1.32	1.37
3	L5	4500	PSU	C4-N3	-2.81	1.33	1.38
3	L5	4552	PSU	C6-C5	2.81	1.38	1.35
3	L5	1782	PSU	C6-C5	2.81	1.38	1.35
3	L5	3818	UY1	C2-N3	-2.81	1.32	1.37
3	L5	2876	OMG	C5-C4	2.80	1.46	1.38
3	L5	3825	A2M	C4-N9	-2.80	1.31	1.37
1	S2	1851	MA6	C5-C6	2.80	1.48	1.41
1	S2	918	PSU	C6-C5	2.80	1.38	1.35
3	L5	4220	6MZ	C5-N7	-2.80	1.34	1.39
2	L8	75	OMG	C5-C4	2.80	1.46	1.38
1	S2	651	PSU	C6-C5	2.79	1.38	1.35
1	S2	815	PSU	C6-C5	2.79	1.38	1.35
2	L8	69	PSU	C6-C5	2.79	1.38	1.35
1	S2	1851	MA6	C4-N9	-2.78	1.31	1.37
1	S2	1832	6MZ	C5-N7	-2.78	1.34	1.39
3	L5	1677	PSU	C2-N1	-2.78	1.33	1.36
1	S2	681	PSU	C6-C5	2.78	1.38	1.35
3	L5	1860	PSU	C2-N3	-2.78	1.32	1.37
3	L5	4637	OMG	C5-C4	2.78	1.46	1.38
3	L5	3844	PSU	C6-C5	2.77	1.38	1.35
3	L5	3830	A2M	C5-C6	2.77	1.48	1.41
3	L5	4499	OMG	C5-N7	-2.77	1.33	1.39
1	S2	436	OMG	C5-C4	2.77	1.46	1.38
3	L5	1871	A2M	C5-C6	2.77	1.48	1.41
1	S2	1243	PSU	C6-C5	2.77	1.38	1.35
1	S2	509	OMG	C5-C4	2.77	1.46	1.38
3	L5	4392	OMG	C5-N7	-2.76	1.33	1.39
3	L5	4571	A2M	C5-C6	2.76	1.48	1.41
3	L5	1524	A2M	C4-N9	-2.76	1.31	1.37
1	S2	36	PSU	C6-C5	2.76	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	644	OMG	C5-C4	2.76	1.46	1.38
1	S2	1288	OMU	C4-N3	-2.76	1.33	1.38
3	L5	4228	OMG	C6-N1	-2.76	1.33	1.38
3	L5	1677	PSU	C4-N3	-2.76	1.33	1.38
82	Pt	56	PSU	C6-C5	2.76	1.38	1.35
3	L5	4493	PSU	C6-C5	2.75	1.38	1.35
1	S2	93	PSU	C2-N3	-2.75	1.32	1.37
1	S2	1445	PSU	C6-C5	2.75	1.38	1.35
3	L5	3792	OMG	C5-N7	-2.75	1.33	1.39
1	S2	918	PSU	O4'-C1'	-2.75	1.40	1.43
1	S2	683	OMG	C6-N1	-2.75	1.33	1.38
3	L5	3944	OMG	C6-N1	-2.74	1.33	1.38
3	L5	4689	PSU	C6-C5	2.74	1.38	1.35
3	L5	4471	PSU	C6-C5	2.74	1.38	1.35
3	L5	4196	OMG	C6-N1	-2.74	1.33	1.38
3	L5	3792	OMG	C6-N1	-2.74	1.33	1.38
3	L5	4370	OMG	C5-C4	2.74	1.46	1.38
82	Pt	8	4SU	C2-N3	-2.73	1.33	1.38
3	L5	3744	OMG	C6-N1	-2.73	1.33	1.38
3	L5	4494	OMG	C5-C4	2.73	1.46	1.38
3	L5	3899	OMG	C6-N1	-2.73	1.33	1.38
1	S2	1850	MA6	C5-C6	2.72	1.48	1.41
1	S2	649	PSU	C6-C5	2.72	1.38	1.35
1	S2	1248	B8N	C6-C5	2.72	1.39	1.35
1	S2	1383	A2M	C5-C6	2.72	1.48	1.41
3	L5	4392	OMG	C6-N1	-2.71	1.33	1.38
1	S2	1239	PSU	C6-C5	2.71	1.38	1.35
1	S2	484	A2M	C5-C6	2.71	1.48	1.41
3	L5	4576	PSU	C6-C5	2.71	1.38	1.35
3	L5	4312	PSU	C2-N3	-2.71	1.33	1.37
3	L5	4673	PSU	C2-N3	-2.70	1.33	1.37
3	L5	1534	A2M	C5-C6	2.70	1.48	1.41
82	Pt	56	PSU	C4-N3	-2.70	1.33	1.38
1	S2	1347	PSU	C6-C5	2.70	1.38	1.35
3	L5	2424	OMG	C5-N7	-2.70	1.33	1.39
1	S2	1832	6MZ	C5-C6	2.69	1.48	1.41
3	L5	4499	OMG	C5-C4	2.69	1.46	1.38
3	L5	4420	PSU	C4-N3	-2.69	1.33	1.38
3	L5	3744	OMG	C5-C4	2.68	1.46	1.38
3	L5	4353	PSU	C2-N1	-2.68	1.33	1.36
1	S2	354	OMU	C2-N3	-2.68	1.33	1.38
3	L5	4312	PSU	C6-C5	2.68	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	398	A2M	C5-N7	-2.68	1.34	1.39
3	L5	4972	PSU	C2-N3	-2.68	1.33	1.37
3	L5	1322	1MA	C5-N7	-2.68	1.33	1.39
1	S2	121	OMU	C2-N3	-2.68	1.33	1.38
3	L5	4637	OMG	C5-N7	-2.68	1.33	1.39
1	S2	509	OMG	C6-N1	-2.67	1.33	1.38
3	L5	3768	PSU	C6-C5	2.67	1.38	1.35
3	L5	3639	PSU	C2-N3	-2.67	1.33	1.37
1	S2	1177	PSU	C2-N3	-2.67	1.33	1.37
3	L5	3782	5MC	C6-N1	-2.66	1.33	1.38
3	L5	1625	OMG	C5-N7	-2.66	1.33	1.39
1	S2	668	A2M	C5-C6	2.66	1.48	1.41
3	L5	2415	OMU	C2-N3	-2.66	1.33	1.38
3	L5	3899	OMG	C5-N7	-2.66	1.33	1.39
3	L5	2508	PSU	C4-N3	-2.66	1.33	1.38
3	L5	5001	PSU	C2-N3	-2.65	1.33	1.37
3	L5	2876	OMG	C5-N7	-2.65	1.33	1.39
1	S2	296	PSU	C6-C5	2.65	1.38	1.35
1	S2	576	A2M	C5-C6	2.64	1.48	1.41
3	L5	4431	PSU	C2-N3	-2.64	1.33	1.37
1	S2	668	A2M	C5-N7	-2.64	1.34	1.39
1	S2	1056	PSU	C2-N3	-2.64	1.33	1.37
3	L5	4403	PSU	C2-N1	-2.64	1.33	1.36
1	S2	1347	PSU	C2-N3	-2.63	1.33	1.37
3	L5	3627	OMG	C4-N9	-2.63	1.31	1.38
3	L5	4618	OMG	C5-C4	2.63	1.45	1.38
3	L5	1792	PSU	C6-C5	2.63	1.38	1.35
3	L5	2364	OMG	C5-N7	-2.63	1.33	1.39
3	L5	2364	OMG	C4-N9	-2.63	1.31	1.38
3	L5	4636	PSU	C2-N3	-2.62	1.33	1.37
3	L5	4370	OMG	C6-N1	-2.62	1.33	1.38
3	L5	4293	PSU	C2-N3	-2.62	1.33	1.37
3	L5	4628	PSU	C2-N3	-2.62	1.33	1.37
3	L5	4423	PSU	C6-C5	2.62	1.38	1.35
1	S2	627	OMU	C4-N3	-2.62	1.34	1.38
3	L5	4403	PSU	C2-N3	-2.61	1.33	1.37
3	L5	4420	PSU	O4'-C1'	-2.61	1.40	1.43
3	L5	4431	PSU	C6-C5	2.61	1.38	1.35
1	S2	1238	PSU	C6-C5	2.61	1.38	1.35
1	S2	109	PSU	C2'-C1'	-2.61	1.50	1.53
3	L5	3884	PSU	C2-N3	-2.61	1.33	1.37
3	L5	4618	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	3853	PSU	C2-N3	-2.60	1.33	1.37
3	L5	1779	PSU	C6-C5	2.60	1.38	1.35
3	L5	4296	PSU	C6-C5	2.60	1.38	1.35
1	S2	822	PSU	C6-C5	2.60	1.38	1.35
1	S2	1678	A2M	C5-N7	-2.60	1.34	1.39
1	S2	1244	PSU	C6-C5	2.59	1.38	1.35
3	L5	3723	A2M	C5-N7	-2.59	1.34	1.39
1	S2	668	A2M	C4-N9	-2.59	1.32	1.37
3	L5	4220	6MZ	C4-N9	-2.59	1.32	1.37
3	L5	3760	A2M	C5-N7	-2.59	1.34	1.39
1	S2	681	PSU	C2-N3	-2.59	1.33	1.37
1	S2	590	A2M	C5-N7	-2.59	1.34	1.39
3	L5	398	A2M	C5-C6	2.59	1.48	1.41
1	S2	512	A2M	C5-N7	-2.59	1.34	1.39
3	L5	3853	PSU	C6-C5	2.59	1.38	1.35
1	S2	159	A2M	C5-C6	2.59	1.48	1.41
1	S2	484	A2M	C5-N7	-2.58	1.34	1.39
2	L8	14	OMU	C2-N3	-2.58	1.33	1.38
3	L5	4296	PSU	C2-N3	-2.57	1.33	1.37
1	S2	116	OMU	C2-N3	-2.57	1.33	1.38
82	Pt	21	H2U	C2-N3	-2.57	1.33	1.38
3	L5	4579	PSU	C2-N3	-2.57	1.33	1.37
1	S2	644	OMG	C5-N7	-2.57	1.33	1.39
1	S2	576	A2M	C5-N7	-2.57	1.34	1.39
1	S2	1004	PSU	C2-N3	-2.57	1.33	1.37
3	L5	1522	OMG	C4-N9	-2.56	1.31	1.38
1	S2	428	OMU	C2-N3	-2.56	1.33	1.38
1	S2	109	PSU	C2-N3	-2.56	1.33	1.37
3	L5	3867	A2M	C8-N9	-2.56	1.33	1.37
1	S2	105	PSU	C2-N3	-2.56	1.33	1.37
3	L5	3744	OMG	C5-N7	-2.56	1.33	1.39
3	L5	4494	OMG	C5-N7	-2.56	1.33	1.39
1	S2	166	A2M	C5-C6	2.56	1.48	1.41
3	L5	400	A2M	C5-C6	2.56	1.48	1.41
1	S2	1367	PSU	C2-N3	-2.56	1.33	1.37
1	S2	1490	OMG	C5-C4	2.56	1.45	1.38
1	S2	1442	OMU	C2-N3	-2.56	1.33	1.38
3	L5	3760	A2M	C5-C6	2.55	1.48	1.41
3	L5	1316	OMG	C5-C4	2.55	1.45	1.38
40	LB	245	HIC	CD2-CG	2.55	1.40	1.36
1	S2	1056	PSU	C6-C5	2.55	1.38	1.35
3	L5	4299	PSU	C6-C5	2.55	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	166	A2M	C5-N7	-2.55	1.34	1.39
3	L5	4689	PSU	C2-N3	-2.55	1.33	1.37
1	S2	590	A2M	C5-C6	2.54	1.48	1.41
3	L5	4447	5MC	C6-N1	-2.54	1.33	1.38
3	L5	4392	OMG	C5-C4	2.54	1.45	1.38
3	L5	1322	1MA	C6-N6	2.54	1.34	1.28
3	L5	4623	OMG	C5-N7	-2.54	1.34	1.39
1	S2	683	OMG	C5-C4	2.54	1.45	1.38
1	S2	867	OMG	C6-N1	-2.54	1.34	1.38
3	L5	1536	PSU	C2-N3	-2.53	1.33	1.37
1	S2	1804	OMU	C2-N3	-2.53	1.33	1.38
3	L5	4523	A2M	C5-C6	2.53	1.48	1.41
3	L5	3851	PSU	C2-N3	-2.53	1.33	1.37
3	L5	3627	OMG	C5-C4	2.53	1.45	1.38
1	S2	1174	PSU	C2-N3	-2.53	1.33	1.37
3	L5	3718	A2M	C4-N9	-2.52	1.32	1.37
1	S2	1243	PSU	C2-N3	-2.52	1.33	1.37
3	L5	3867	A2M	C5-C6	2.52	1.48	1.41
1	S2	172	OMU	C2-N3	-2.52	1.33	1.38
1	S2	406	PSU	C2-N3	-2.52	1.33	1.37
3	L5	1322	1MA	C4-N9	-2.52	1.31	1.38
3	L5	4299	PSU	C2-N1	-2.51	1.33	1.36
1	S2	815	PSU	C2-N3	-2.51	1.33	1.37
1	S2	105	PSU	C6-C5	2.51	1.38	1.35
3	L5	3764	PSU	C6-C5	2.51	1.38	1.35
1	S2	1850	MA6	C5-N7	-2.51	1.34	1.39
1	S2	468	A2M	C5-N7	-2.51	1.34	1.39
1	S2	863	PSU	C2-N3	-2.51	1.33	1.37
3	L5	4361	PSU	C6-C5	2.51	1.38	1.35
3	L5	4423	PSU	C2-N3	-2.51	1.33	1.37
3	L5	3785	A2M	C4-N9	-2.51	1.32	1.37
3	L5	1792	PSU	C2-N1	-2.50	1.33	1.36
3	L5	4457	PSU	C2-N3	-2.50	1.33	1.37
1	S2	814	PSU	C2-N3	-2.50	1.33	1.37
1	S2	1804	OMU	C5-C4	-2.49	1.38	1.43
3	L5	4370	OMG	C5-N7	-2.49	1.34	1.39
1	S2	918	PSU	C2-N3	-2.49	1.33	1.37
1	S2	468	A2M	C5-C6	2.48	1.47	1.41
1	S2	1490	OMG	C5-N7	-2.48	1.34	1.39
1	S2	36	PSU	C2-N3	-2.48	1.33	1.37
3	L5	4620	OMU	C2-N3	-2.48	1.33	1.38
3	L5	1677	PSU	O4'-C1'	-2.48	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4590	A2M	C5-C6	2.47	1.47	1.41
3	L5	5010	PSU	C2-N3	-2.47	1.33	1.37
1	S2	1239	PSU	C2-N3	-2.47	1.33	1.37
1	S2	683	OMG	C5-N7	-2.47	1.34	1.39
1	S2	1692	PSU	C2-N3	-2.47	1.33	1.37
3	L5	4228	OMG	C5-C4	2.46	1.45	1.38
3	L5	3724	A2M	C5-C6	2.46	1.47	1.41
3	L5	3758	PSU	C2-N1	-2.46	1.33	1.36
1	S2	1136	PSU	C2-N3	-2.46	1.33	1.37
1	S2	512	A2M	C5-C6	2.46	1.47	1.41
3	L5	2401	A2M	C4-N9	-2.46	1.32	1.37
1	S2	966	PSU	C2-N3	-2.46	1.33	1.37
3	L5	2632	PSU	C6-C5	2.46	1.38	1.35
3	L5	1744	PSU	C2-N3	-2.46	1.33	1.37
1	S2	27	A2M	C5-N7	-2.45	1.34	1.39
3	L5	3830	A2M	C4-N9	-2.45	1.32	1.37
3	L5	4620	OMU	C5-C4	-2.45	1.38	1.43
1	S2	34	PSU	C2-N3	-2.45	1.33	1.37
1	S2	109	PSU	C2-N1	-2.45	1.33	1.36
3	L5	1524	A2M	C5-C6	2.45	1.47	1.41
1	S2	1238	PSU	C2-N3	-2.45	1.33	1.37
1	S2	1326	UY1	C2-N3	-2.45	1.33	1.37
1	S2	1288	OMU	C2-N3	-2.45	1.33	1.38
3	L5	3715	PSU	C2-N3	-2.44	1.33	1.37
1	S2	1643	PSU	C2-N3	-2.44	1.33	1.37
2	L8	55	PSU	C2-N3	-2.44	1.33	1.37
3	L5	2843	PSU	C2-N3	-2.44	1.33	1.37
1	S2	1678	A2M	C5-C6	2.44	1.47	1.41
1	S2	651	PSU	C2-N3	-2.44	1.33	1.37
1	S2	822	PSU	C2-N3	-2.43	1.33	1.37
3	L5	1781	PSU	C2-N3	-2.43	1.33	1.37
1	S2	1081	PSU	C2-N3	-2.43	1.33	1.37
1	S2	99	A2M	C5-C6	2.43	1.47	1.41
3	L5	3844	PSU	C2-N1	-2.43	1.33	1.36
3	L5	2815	A2M	C5-N7	-2.43	1.34	1.39
1	S2	27	A2M	C5-C6	2.43	1.47	1.41
3	L5	4403	PSU	C6-C5	2.42	1.38	1.35
3	L5	3764	PSU	C2-N3	-2.42	1.33	1.37
3	L5	3715	PSU	C6-C5	2.42	1.38	1.35
2	L8	75	OMG	C5-N7	-2.42	1.34	1.39
3	L5	3723	A2M	C5-C6	2.42	1.47	1.41
3	L5	2632	PSU	C2-N3	-2.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3844	PSU	C6-N1	-2.41	1.32	1.36
1	S2	406	PSU	C6-C5	2.41	1.38	1.35
1	S2	1832	6MZ	C4-N9	-2.41	1.32	1.37
3	L5	3695	PSU	C6-C5	2.40	1.38	1.35
3	L5	3724	A2M	C5-N7	-2.40	1.34	1.39
3	L5	4523	A2M	C5-N7	-2.40	1.34	1.39
1	S2	1177	PSU	C2-N1	-2.40	1.33	1.36
3	L5	3718	A2M	C5-C6	2.40	1.47	1.41
1	S2	1347	PSU	C2-N1	-2.39	1.33	1.36
1	S2	159	A2M	C5-N7	-2.39	1.34	1.39
3	L5	3884	PSU	C6-C5	2.39	1.37	1.35
1	S2	1383	A2M	C8-N7	2.39	1.36	1.31
3	L5	1779	PSU	C2-N3	-2.39	1.33	1.37
1	S2	1004	PSU	C2'-C1'	-2.39	1.50	1.53
1	S2	863	PSU	C6-C5	2.39	1.37	1.35
1	S2	218	PSU	C2-N3	-2.38	1.33	1.37
3	L5	4228	OMG	C4-N9	-2.38	1.32	1.38
1	S2	1004	PSU	C2-N1	-2.38	1.33	1.36
3	L5	3830	A2M	C5-N7	-2.38	1.34	1.39
1	S2	1447	OMG	C5-N7	-2.38	1.34	1.39
1	S2	1232	PSU	C2-N3	-2.38	1.33	1.37
1	S2	119	PSU	C6-C5	2.38	1.37	1.35
1	S2	1326	UY1	C6-C5	2.37	1.37	1.35
3	L5	3818	UY1	C6-C5	2.37	1.37	1.35
3	L5	4972	PSU	C6-C5	2.37	1.37	1.35
3	L5	4220	6MZ	C5-C6	2.37	1.47	1.41
3	L5	1871	A2M	C5-N7	-2.37	1.34	1.39
82	Pt	21	H2U	C4-N3	-2.37	1.33	1.37
1	S2	1244	PSU	C2-N3	-2.37	1.33	1.37
3	L5	3818	UY1	C2-N1	-2.37	1.33	1.36
3	L5	1322	1MA	C5-C4	2.37	1.45	1.38
3	L5	3825	A2M	C5-C6	2.37	1.47	1.41
3	L5	3744	OMG	C4-N9	-2.36	1.32	1.38
1	S2	509	OMG	C5-N7	-2.36	1.34	1.39
3	L5	3899	OMG	C4-N9	-2.36	1.32	1.38
3	L5	4532	PSU	C2-N3	-2.35	1.33	1.37
1	S2	296	PSU	C2-N3	-2.35	1.33	1.37
3	L5	2401	A2M	C5-C6	2.35	1.47	1.41
1	S2	1004	PSU	C6-C5	2.35	1.37	1.35
1	S2	1850	MA6	C4-N9	-2.35	1.32	1.37
3	L5	4576	PSU	C2-N1	-2.35	1.33	1.36
3	L5	3758	PSU	C2-N3	-2.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3758	PSU	C6-C5	2.35	1.37	1.35
3	L5	4531	PSU	C4-N3	-2.34	1.34	1.38
3	L5	1582	PSU	C2-N3	-2.34	1.33	1.37
3	L5	3768	PSU	C2-N3	-2.34	1.33	1.37
3	L5	4306	OMU	C2-N3	-2.34	1.33	1.38
3	L5	1779	PSU	C2-N1	-2.33	1.33	1.36
1	S2	436	OMG	C5-N7	-2.32	1.34	1.39
3	L5	3920	PSU	C2-N3	-2.32	1.33	1.37
3	L5	3867	A2M	C4-N9	-2.32	1.32	1.37
1	S2	1442	OMU	C5-C4	-2.32	1.38	1.43
1	S2	576	A2M	C4-N9	-2.32	1.32	1.37
3	L5	4442	PSU	C2-N3	-2.32	1.33	1.37
1	S2	1851	MA6	C5-N7	-2.32	1.34	1.39
1	S2	172	OMU	C5-C4	-2.31	1.38	1.43
3	L5	3627	OMG	C5-N7	-2.31	1.34	1.39
3	L5	4228	OMG	C5-N7	-2.31	1.34	1.39
1	S2	105	PSU	C2-N1	-2.31	1.33	1.36
1	S2	27	A2M	C4-N9	-2.31	1.32	1.37
1	S2	116	OMU	C5-C4	-2.31	1.38	1.43
1	S2	627	OMU	C2-N3	-2.31	1.33	1.38
1	S2	1081	PSU	O4'-C1'	-2.31	1.40	1.43
3	L5	4618	OMG	C5-N7	-2.31	1.34	1.39
1	S2	1639	G7M	C4-N9	-2.30	1.32	1.38
1	S2	572	PSU	C2-N3	-2.30	1.33	1.37
3	L5	4552	PSU	C2-N3	-2.30	1.33	1.37
1	S2	406	PSU	C2-N1	-2.30	1.33	1.36
1	S2	109	PSU	C6-C5	2.30	1.37	1.35
3	L5	3764	PSU	C2-N1	-2.30	1.33	1.36
3	L5	1677	PSU	C6-C5	2.29	1.37	1.35
3	L5	4972	PSU	C2-N1	-2.29	1.33	1.36
3	L5	3844	PSU	C2-N3	-2.29	1.33	1.37
1	S2	867	OMG	C5-N7	-2.29	1.34	1.39
1	S2	1625	PSU	C2-N3	-2.29	1.33	1.37
3	L5	3770	PSU	C2-N3	-2.29	1.33	1.37
1	S2	119	PSU	C2-N3	-2.29	1.33	1.37
3	L5	4569	PSU	O4'-C1'	-2.29	1.40	1.43
1	S2	1850	MA6	C8-N9	-2.28	1.33	1.37
1	S2	1031	A2M	C5-C6	2.28	1.47	1.41
3	L5	4576	PSU	C2-N3	-2.28	1.33	1.37
1	S2	1244	PSU	C2-N1	-2.28	1.33	1.36
1	S2	649	PSU	C2-N1	-2.28	1.33	1.36
1	S2	1490	OMG	C4-N9	-2.28	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	801	PSU	C2-N3	-2.28	1.33	1.37
3	L5	4623	OMG	C4-N9	-2.28	1.32	1.38
1	S2	601	OMG	C5-N7	-2.28	1.34	1.39
3	L5	4493	PSU	C2-N3	-2.28	1.33	1.37
3	L5	2364	OMG	C5-C4	2.28	1.44	1.38
3	L5	2632	PSU	C2-N1	-2.27	1.33	1.36
1	S2	918	PSU	C2-N1	-2.27	1.33	1.36
1	S2	649	PSU	C2-N3	-2.27	1.33	1.37
3	L5	3695	PSU	C2-N1	-2.27	1.33	1.36
3	L5	1782	PSU	C2-N3	-2.27	1.33	1.37
3	L5	1781	PSU	C2-N1	-2.27	1.33	1.36
3	L5	1677	PSU	C6-N1	-2.27	1.32	1.36
3	L5	4353	PSU	C2-N3	-2.27	1.33	1.37
2	L8	75	OMG	C4-N9	-2.27	1.32	1.38
3	L5	4196	OMG	C4-N9	-2.27	1.32	1.38
3	L5	3695	PSU	C2-N3	-2.26	1.33	1.37
3	L5	4628	PSU	C2-N1	-2.26	1.33	1.36
3	L5	4628	PSU	C6-N1	-2.26	1.32	1.36
3	L5	5010	PSU	C2-N1	-2.25	1.33	1.36
3	L5	1582	PSU	O4'-C1'	-2.25	1.40	1.43
3	L5	4523	A2M	C4-N9	-2.25	1.33	1.37
3	L5	3762	PSU	C2-N3	-2.24	1.33	1.37
1	S2	354	OMU	C5-C4	-2.24	1.38	1.43
3	L5	4361	PSU	C2-N3	-2.24	1.33	1.37
3	L5	4471	PSU	C2-N3	-2.24	1.33	1.37
3	L5	4536	OMC	C5-C4	-2.23	1.37	1.42
1	S2	1328	OMG	C5-N7	-2.23	1.34	1.39
3	L5	2787	A2M	C8-N9	-2.23	1.33	1.37
1	S2	686	PSU	C2-N3	-2.23	1.33	1.37
2	L8	14	OMU	C5-C4	-2.23	1.38	1.43
3	L5	4569	PSU	C2-N3	-2.23	1.33	1.37
3	L5	4500	PSU	C2-N1	-2.22	1.33	1.36
3	L5	3768	PSU	C2-N1	-2.22	1.33	1.36
3	L5	5001	PSU	C2-N1	-2.22	1.33	1.36
1	S2	1243	PSU	C2-N1	-2.22	1.33	1.36
1	S2	1832	6MZ	C8-N9	-2.22	1.33	1.37
3	L5	2787	A2M	C5-N7	-2.22	1.35	1.39
1	S2	573	PSU	C2-N3	-2.21	1.33	1.37
3	L5	2815	A2M	C8-N9	-2.21	1.33	1.37
1	S2	1031	A2M	C4-N9	-2.21	1.33	1.37
3	L5	4442	PSU	C2-N1	-2.21	1.33	1.36
1	S2	159	A2M	C8-N7	2.21	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4442	PSU	C6-C5	2.20	1.37	1.35
3	L5	3944	OMG	C5-N7	-2.20	1.34	1.39
1	S2	1367	PSU	C6-C5	2.20	1.37	1.35
3	L5	3785	A2M	C8-N9	-2.20	1.33	1.37
3	L5	3770	PSU	C2-N1	-2.19	1.33	1.36
3	L5	4590	A2M	C4-N9	-2.19	1.33	1.37
3	L5	1683	PSU	C2-N1	-2.19	1.33	1.36
2	L8	69	PSU	C2-N1	-2.19	1.33	1.36
1	S2	1238	PSU	C2-N1	-2.18	1.33	1.36
3	L5	3785	A2M	C5-C6	2.18	1.47	1.41
1	S2	218	PSU	C2-N1	-2.18	1.33	1.36
1	S2	1383	A2M	C5-N7	-2.17	1.35	1.39
3	L5	4972	PSU	C2'-C1'	-2.17	1.50	1.53
3	L5	4420	PSU	C2-N1	-2.17	1.33	1.36
1	S2	609	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4196	OMG	C5-N7	-2.16	1.34	1.39
1	S2	651	PSU	C2-N1	-2.16	1.33	1.36
3	L5	1524	A2M	C8-N9	-2.16	1.33	1.37
1	S2	681	PSU	C2-N1	-2.16	1.33	1.36
3	L5	2363	A2M	C8-N9	-2.16	1.33	1.37
3	L5	4493	PSU	C2-N1	-2.15	1.33	1.36
1	S2	1288	OMU	C5-C4	-2.15	1.39	1.43
3	L5	4618	OMG	C4-N9	-2.15	1.32	1.38
1	S2	1174	PSU	C2-N1	-2.15	1.33	1.36
1	S2	1678	A2M	C4-N9	-2.15	1.33	1.37
3	L5	3841	OMC	C6-C5	2.15	1.40	1.35
3	L5	4447	5MC	C6-C5	2.15	1.38	1.34
3	L5	4552	PSU	C2-N1	-2.15	1.33	1.36
3	L5	1871	A2M	C8-N9	-2.15	1.33	1.37
1	S2	609	PSU	C2-N1	-2.15	1.33	1.36
1	S2	119	PSU	C2-N1	-2.15	1.33	1.36
3	L5	4299	PSU	O4'-C1'	-2.15	1.40	1.43
3	L5	4500	PSU	O4'-C1'	-2.14	1.40	1.43
1	S2	109	PSU	C6-N1	-2.14	1.32	1.36
3	L5	4628	PSU	C6-C5	2.14	1.37	1.35
3	L5	4499	OMG	C4-N9	-2.14	1.32	1.38
82	Pt	56	PSU	C2-N3	-2.14	1.33	1.37
3	L5	4571	A2M	C8-N9	-2.14	1.33	1.37
1	S2	468	A2M	C8-N7	2.14	1.35	1.31
3	L5	4296	PSU	C2-N1	-2.14	1.33	1.36
1	S2	468	A2M	C4-N9	-2.14	1.33	1.37
1	S2	296	PSU	C2-N1	-2.13	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	121	OMU	C5-C4	-2.13	1.39	1.43
1	S2	34	PSU	C2-N1	-2.13	1.33	1.36
1	S2	863	PSU	C2-N1	-2.13	1.33	1.36
3	L5	4579	PSU	C2-N1	-2.13	1.33	1.36
1	S2	172	OMU	C6-N1	-2.13	1.33	1.38
3	L5	4689	PSU	C2-N1	-2.13	1.33	1.36
3	L5	3792	OMG	C4-N9	-2.13	1.32	1.38
3	L5	3729	PSU	C2-N3	-2.13	1.34	1.37
3	L5	4457	PSU	C2-N1	-2.13	1.33	1.36
3	L5	1326	A2M	C5-C6	2.12	1.46	1.41
1	S2	484	A2M	C8-N7	2.12	1.35	1.31
1	S2	1239	PSU	C2-N1	-2.12	1.33	1.36
3	L5	2837	OMU	C5-C4	-2.12	1.39	1.43
1	S2	1445	PSU	C2-N3	-2.12	1.34	1.37
1	S2	1232	PSU	C2-N1	-2.12	1.33	1.36
1	S2	512	A2M	C4-N9	-2.11	1.33	1.37
1	S2	1692	PSU	C2-N1	-2.11	1.33	1.36
1	S2	166	A2M	C8-N7	2.11	1.35	1.31
3	L5	3851	PSU	C2-N1	-2.11	1.33	1.36
1	S2	683	OMG	C4-N9	-2.11	1.32	1.38
3	L5	4420	PSU	C2-N3	-2.11	1.34	1.37
1	S2	576	A2M	C8-N7	2.10	1.35	1.31
3	L5	2401	A2M	C8-N9	-2.10	1.34	1.37
3	L5	2824	OMC	C6-N1	-2.10	1.33	1.38
1	S2	1326	UY1	C2-N1	-2.10	1.33	1.36
3	L5	4498	OMU	C5-C4	-2.09	1.39	1.43
3	L5	4552	PSU	O4'-C1'	-2.09	1.41	1.43
3	L5	4536	OMC	C6-N1	-2.09	1.33	1.38
3	L5	1683	PSU	C2-N3	-2.09	1.34	1.37
3	L5	3724	A2M	C4-N9	-2.08	1.33	1.37
3	L5	4531	PSU	C6-N1	-2.08	1.32	1.36
1	S2	686	PSU	C2-N1	-2.08	1.34	1.36
1	S2	866	PSU	C2-N1	-2.08	1.34	1.36
3	L5	4636	PSU	O4'-C1'	-2.07	1.41	1.43
3	L5	3715	PSU	C2-N1	-2.07	1.34	1.36
3	L5	3760	A2M	C4-N9	-2.07	1.33	1.37
1	S2	428	OMU	C5-C4	-2.07	1.39	1.43
3	L5	4456	OMC	C6-N1	-2.07	1.33	1.38
3	L5	2815	A2M	C5-C6	2.07	1.46	1.41
3	L5	398	A2M	C8-N9	-2.06	1.34	1.37
3	L5	3724	A2M	C8-N7	2.06	1.35	1.31
3	L5	2415	OMU	C5-C4	-2.06	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L8	69	PSU	C2-N3	-2.06	1.34	1.37
3	L5	1316	OMG	C4-N9	-2.05	1.32	1.38
3	L5	1792	PSU	C2-N3	-2.05	1.34	1.37
3	L5	4531	PSU	C2-N1	-2.05	1.34	1.36
3	L5	3808	OMC	C6-N1	-2.05	1.33	1.38
1	S2	966	PSU	C2-N1	-2.05	1.34	1.36
3	L5	3760	A2M	C8-N7	2.05	1.35	1.31
1	S2	99	A2M	C8-N9	-2.05	1.34	1.37
3	L5	3869	OMC	C6-C5	2.05	1.39	1.35
3	L5	2508	PSU	C2-N3	-2.05	1.34	1.37
1	S2	590	A2M	C8-N7	2.05	1.35	1.31
1	S2	668	A2M	C8-N9	-2.05	1.34	1.37
3	L5	4306	OMU	C5-C4	-2.05	1.39	1.43
1	S2	627	OMU	C5-C4	-2.04	1.39	1.43
3	L5	3723	A2M	C4-N9	-2.04	1.33	1.37
3	L5	4392	OMG	C4-N9	-2.04	1.32	1.38
3	L5	4530	UR3	C6-C5	2.04	1.39	1.35
3	L5	400	A2M	C4-N9	-2.04	1.33	1.37
40	LB	245	HIC	CZ-NE2	-2.04	1.41	1.46
3	L5	1871	A2M	C4-N9	-2.03	1.33	1.37
82	Pt	8	4SU	C6-N1	-2.03	1.33	1.38
1	S2	36	PSU	C2-N1	-2.03	1.34	1.36
3	L5	3639	PSU	C2-N1	-2.03	1.34	1.36
3	L5	4442	PSU	O4'-C1'	-2.03	1.41	1.43
3	L5	3770	PSU	O4'-C1'	-2.03	1.41	1.43
1	S2	1804	OMU	C6-N1	-2.03	1.33	1.38
1	S2	866	PSU	C2-N3	-2.02	1.34	1.37
3	L5	1534	A2M	C8-N9	-2.02	1.34	1.37
3	L5	2363	A2M	C5-C6	2.02	1.46	1.41
1	S2	1383	A2M	C4-N9	-2.02	1.33	1.37
3	L5	3637	PSU	C2-N3	-2.01	1.34	1.37
3	L5	4370	OMG	C4-N9	-2.01	1.32	1.38
82	Pt	33	OMC	C6-N1	-2.01	1.33	1.38
3	L5	2415	OMU	C2-N1	2.01	1.41	1.38
1	S2	1625	PSU	C2-N1	-2.01	1.34	1.36
1	S2	815	PSU	C2-N1	-2.01	1.34	1.36
1	S2	1056	PSU	C2-N1	-2.00	1.34	1.36
3	L5	4628	PSU	O4'-C1'	-2.00	1.41	1.43

All (1159) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	SA	2	SAC	OAC-C1A-C2A	-8.31	107.26	122.05
1	S2	1639	G7M	CN7-N7-C8	-7.92	112.80	124.79
29	SV	1	AME	OT-CT1-N	-7.88	108.06	121.98
3	L5	3637	PSU	N1-C2-N3	7.64	123.23	115.17
64	Lr	2	SAC	OAC-C1A-N	-7.53	108.67	121.98
1	S2	109	PSU	N1-C2-N3	7.46	123.04	115.17
3	L5	4530	UR3	C4-N3-C2	-7.42	118.61	124.58
82	Pt	8	4SU	C4-N3-C2	-7.40	120.22	127.31
3	L5	4972	PSU	N1-C2-N3	7.34	122.92	115.17
3	L5	4353	PSU	N1-C2-N3	7.13	122.69	115.17
3	L5	2843	PSU	N1-C2-N3	7.12	122.68	115.17
1	S2	918	PSU	N1-C2-N3	7.10	122.66	115.17
3	L5	4442	PSU	N1-C2-N3	7.08	122.64	115.17
1	S2	1639	G7M	N9-C8-N7	-7.08	95.29	112.48
29	SV	1	AME	OT-CT1-CT2	-7.05	109.50	122.05
3	L5	4569	PSU	N1-C2-N3	7.05	122.61	115.17
3	L5	5001	PSU	N1-C2-N3	7.04	122.59	115.17
3	L5	3884	PSU	N1-C2-N3	7.01	122.57	115.17
3	L5	4689	PSU	N1-C2-N3	6.99	122.55	115.17
3	L5	3695	PSU	N1-C2-N3	6.98	122.53	115.17
1	S2	105	PSU	N1-C2-N3	6.95	122.50	115.17
3	L5	3851	PSU	N1-C2-N3	6.95	122.50	115.17
3	L5	4423	PSU	N1-C2-N3	6.94	122.49	115.17
1	S2	1004	PSU	N1-C2-N3	6.92	122.47	115.17
3	L5	1781	PSU	N1-C2-N3	6.92	122.46	115.17
1	S2	34	PSU	N1-C2-N3	6.90	122.45	115.17
3	L5	3920	PSU	N1-C2-N3	6.90	122.44	115.17
3	L5	3853	PSU	N1-C2-N3	6.88	122.43	115.17
1	S2	1136	PSU	N1-C2-N3	6.88	122.42	115.17
3	L5	1536	PSU	N1-C2-N3	6.86	122.40	115.17
3	L5	4293	PSU	N1-C2-N3	6.83	122.37	115.17
3	L5	1683	PSU	N1-C2-N3	6.82	122.36	115.17
1	S2	1326	UY1	N1-C2-N3	6.81	122.35	115.17
3	L5	3639	PSU	N1-C2-N3	6.80	122.34	115.17
1	S2	822	PSU	N1-C2-N3	6.79	122.33	115.17
3	L5	1677	PSU	N1-C2-N3	6.77	122.31	115.17
3	L5	3770	PSU	N1-C2-N3	6.77	122.31	115.17
1	S2	1232	PSU	N1-C2-N3	6.77	122.31	115.17
1	S2	1643	PSU	N1-C2-N3	6.76	122.30	115.17
3	L5	4636	PSU	N1-C2-N3	6.76	122.30	115.17
1	S2	1244	PSU	N1-C2-N3	6.75	122.29	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1243	PSU	N1-C2-N3	6.75	122.28	115.17
1	S2	649	PSU	N1-C2-N3	6.74	122.28	115.17
3	L5	2787	A2M	C5-C4-N3	-6.74	117.43	126.72
1	S2	651	PSU	N1-C2-N3	6.72	122.26	115.17
3	L5	5010	PSU	N1-C2-N3	6.72	122.26	115.17
3	L5	4299	PSU	N1-C2-N3	6.70	122.24	115.17
1	S2	1239	PSU	N1-C2-N3	6.69	122.23	115.17
3	L5	4361	PSU	N1-C2-N3	6.68	122.22	115.17
1	S2	572	PSU	N1-C2-N3	6.68	122.21	115.17
3	L5	3715	PSU	N1-C2-N3	6.67	122.21	115.17
3	L5	1625	OMG	C5-C4-N3	-6.67	117.77	128.39
1	S2	1347	PSU	N1-C2-N3	6.67	122.20	115.17
3	L5	1782	PSU	N1-C2-N3	6.67	122.20	115.17
3	L5	4403	PSU	N1-C2-N3	6.66	122.20	115.17
3	L5	4494	OMG	C5-C4-N3	-6.65	117.81	128.39
82	Pt	8	4SU	C5-C4-N3	6.65	120.93	114.75
3	L5	4500	PSU	N1-C2-N3	6.64	122.17	115.17
1	S2	966	PSU	N1-C2-N3	6.64	122.17	115.17
1	S2	1625	PSU	N1-C2-N3	6.64	122.17	115.17
1	S2	1367	PSU	N1-C2-N3	6.62	122.15	115.17
3	L5	1744	PSU	N1-C2-N3	6.62	122.15	115.17
1	S2	866	PSU	N1-C2-N3	6.61	122.14	115.17
1	S2	119	PSU	N1-C2-N3	6.60	122.13	115.17
1	S2	406	PSU	N1-C2-N3	6.60	122.13	115.17
1	S2	1447	OMG	C5-C4-N3	-6.59	117.90	128.39
1	S2	681	PSU	N1-C2-N3	6.59	122.12	115.17
3	L5	3729	PSU	N1-C2-N3	6.58	122.11	115.17
1	S2	801	PSU	N1-C2-N3	6.57	122.10	115.17
1	S2	1177	PSU	N1-C2-N3	6.57	122.10	115.17
1	S2	573	PSU	N1-C2-N3	6.55	122.08	115.17
1	S2	296	PSU	N1-C2-N3	6.54	122.07	115.17
2	L8	55	PSU	N1-C2-N3	6.54	122.07	115.17
3	L5	3768	PSU	N1-C2-N3	6.53	122.06	115.17
1	S2	686	PSU	N1-C2-N3	6.53	122.06	115.17
3	L5	3762	PSU	N1-C2-N3	6.52	122.05	115.17
3	L5	4532	PSU	N1-C2-N3	6.51	122.03	115.17
1	S2	1056	PSU	N1-C2-N3	6.51	122.03	115.17
3	L5	4493	PSU	N1-C2-N3	6.51	122.03	115.17
1	S2	218	PSU	N1-C2-N3	6.50	122.03	115.17
1	S2	99	A2M	C5-C4-N3	-6.50	117.77	126.72
3	L5	1779	PSU	N1-C2-N3	6.49	122.01	115.17
3	L5	4521	PSU	N1-C2-N3	6.47	122.00	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L8	69	PSU	N1-C2-N3	6.47	121.99	115.17
1	S2	436	OMG	C5-C4-N3	-6.46	118.12	128.39
3	L5	3758	PSU	N1-C2-N3	6.45	121.97	115.17
1	S2	1692	PSU	N1-C2-N3	6.45	121.97	115.17
1	S2	1639	G7M	C8-N7-C5	6.45	115.84	107.78
3	L5	1860	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	1862	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	3818	UY1	N1-C2-N3	6.44	121.96	115.17
3	L5	4628	PSU	N1-C2-N3	6.43	121.95	115.17
3	L5	4296	PSU	N1-C2-N3	6.42	121.94	115.17
1	S2	814	PSU	N1-C2-N3	6.42	121.94	115.17
3	L5	4457	PSU	N1-C2-N3	6.42	121.94	115.17
3	L5	4576	PSU	N1-C2-N3	6.42	121.94	115.17
1	S2	609	PSU	N1-C2-N3	6.40	121.92	115.17
6	SA	2	SAC	OAC-C1A-N	-6.40	110.67	121.98
1	S2	815	PSU	N1-C2-N3	6.39	121.90	115.17
1	S2	36	PSU	N1-C2-N3	6.38	121.90	115.17
82	Pt	56	PSU	N1-C2-N3	6.37	121.89	115.17
3	L5	4579	PSU	N1-C2-N3	6.36	121.88	115.17
3	L5	4673	PSU	N1-C2-N3	6.36	121.88	115.17
3	L5	4531	PSU	N1-C2-N3	6.34	121.86	115.17
1	S2	1238	PSU	N1-C2-N3	6.34	121.86	115.17
64	Lr	2	SAC	OAC-C1A-C2A	-6.34	110.77	122.05
3	L5	3764	PSU	N1-C2-N3	6.34	121.85	115.17
1	S2	1174	PSU	N1-C2-N3	6.33	121.84	115.17
1	S2	863	PSU	N1-C2-N3	6.31	121.83	115.17
3	L5	3734	PSU	N1-C2-N3	6.31	121.82	115.17
3	L5	1792	PSU	N1-C2-N3	6.30	121.81	115.17
3	L5	2424	OMG	C5-C4-N3	-6.30	118.37	128.39
3	L5	2632	PSU	N1-C2-N3	6.28	121.79	115.17
1	S2	1081	PSU	N1-C2-N3	6.27	121.78	115.17
3	L5	1582	PSU	N1-C2-N3	6.26	121.78	115.17
3	L5	4552	PSU	N1-C2-N3	6.26	121.77	115.17
1	S2	1639	G7M	N9-C4-N3	6.25	138.45	125.95
3	L5	4312	PSU	N1-C2-N3	6.24	121.75	115.17
3	L5	4471	PSU	N1-C2-N3	6.23	121.74	115.17
1	S2	1445	PSU	N1-C2-N3	6.22	121.73	115.17
1	S2	93	PSU	N1-C2-N3	6.20	121.71	115.17
1	S2	509	OMG	C5-C4-N3	-6.20	118.52	128.39
3	L5	2839	PSU	N1-C2-N3	6.19	121.70	115.17
1	S2	590	A2M	C5-C4-N3	-6.19	118.20	126.72
1	S2	1328	OMG	C5-C4-N3	-6.16	118.59	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2815	A2M	C5-C4-N3	-6.16	118.24	126.72
1	S2	644	OMG	C5-C4-N3	-6.15	118.60	128.39
3	L5	1316	OMG	C5-C4-N3	-6.12	118.64	128.39
3	L5	1316	OMG	C2-N3-C4	6.11	122.83	112.30
3	L5	4420	PSU	N1-C2-N3	6.11	121.62	115.17
3	L5	4571	A2M	C5-C4-N3	-6.10	118.31	126.72
3	L5	3744	OMG	C5-C4-N3	-6.08	118.71	128.39
3	L5	4499	OMG	C5-C4-N3	-6.08	118.72	128.39
3	L5	4431	PSU	N1-C2-N3	6.05	121.56	115.17
3	L5	398	A2M	C5-C4-N3	-6.05	118.39	126.72
3	L5	400	A2M	C5-C4-N3	-6.04	118.40	126.72
1	S2	159	A2M	C5-C4-N3	-6.04	118.40	126.72
3	L5	4618	OMG	C5-C4-N3	-6.01	118.82	128.39
1	S2	166	A2M	C5-C4-N3	-6.00	118.45	126.72
3	L5	3944	OMG	C5-C4-N3	-5.99	118.86	128.39
1	S2	601	OMG	C5-C4-N3	-5.98	118.88	128.39
3	L5	3792	OMG	C5-C4-N3	-5.96	118.91	128.39
1	S2	867	OMG	C5-C4-N3	-5.95	118.93	128.39
3	L5	3760	A2M	C5-C4-N3	-5.94	118.53	126.72
3	L5	4370	OMG	C5-C4-N3	-5.94	118.94	128.39
3	L5	4392	OMG	C5-C4-N3	-5.93	118.95	128.39
3	L5	4523	A2M	C2'-C1'-N9	-5.90	104.03	113.75
3	L5	3867	A2M	C5-C4-N3	-5.89	118.60	126.72
1	S2	512	A2M	C5-C4-N3	-5.87	118.64	126.72
3	L5	2876	OMG	C5-C4-N3	-5.87	119.05	128.39
3	L5	3899	OMG	C5-C4-N3	-5.86	119.06	128.39
1	S2	484	A2M	C5-C4-N3	-5.86	118.65	126.72
3	L5	2508	PSU	N1-C2-N3	5.85	121.34	115.17
3	L5	3844	PSU	N1-C2-N3	5.85	121.34	115.17
1	S2	1678	A2M	C5-C4-N3	-5.82	118.71	126.72
3	L5	4623	OMG	C5-C4-N3	-5.79	119.17	128.39
1	S2	683	OMG	C5-C4-N3	-5.78	119.19	128.39
1	S2	1490	OMG	C5-C4-N3	-5.77	119.20	128.39
3	L5	4637	OMG	C5-C4-N3	-5.77	119.21	128.39
3	L5	4196	OMG	C5-C4-N3	-5.76	119.22	128.39
3	L5	3718	A2M	C5-C4-N3	-5.76	118.79	126.72
3	L5	4523	A2M	C5-C4-N3	-5.73	118.83	126.72
1	S2	1031	A2M	C5-C4-N3	-5.71	118.85	126.72
3	L5	1871	A2M	C5-C4-N3	-5.71	118.85	126.72
3	L5	3723	A2M	C5-C4-N3	-5.70	118.87	126.72
3	L5	3724	A2M	C5-C4-N3	-5.68	118.90	126.72
3	L5	4494	OMG	C2-N3-C4	5.66	122.05	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3830	A2M	C5-C4-N3	-5.61	118.99	126.72
1	S2	468	A2M	C5-C4-N3	-5.60	119.00	126.72
3	L5	2364	OMG	C5-C4-N3	-5.60	119.48	128.39
3	L5	1522	OMG	C5-C4-N3	-5.55	119.55	128.39
2	L8	75	OMG	C5-C4-N3	-5.53	119.59	128.39
3	L5	3785	A2M	C5-C4-N3	-5.52	119.12	126.72
1	S2	1832	6MZ	C5-C4-N3	-5.50	119.14	126.72
3	L5	3627	OMG	C5-C4-N3	-5.50	119.64	128.39
1	S2	1248	B8N	C4-N3-C2	-5.48	118.88	125.62
1	S2	436	OMG	C2-N3-C4	5.48	121.73	112.30
1	S2	1383	A2M	C5-C4-N3	-5.47	119.18	126.72
1	S2	1850	MA6	C5-C4-N3	-5.46	119.20	126.72
1	S2	576	A2M	C5-C4-N3	-5.45	119.22	126.72
1	S2	27	A2M	C5-C4-N3	-5.43	119.23	126.72
3	L5	2401	A2M	C5-C4-N3	-5.43	119.24	126.72
3	L5	1524	A2M	C5-C4-N3	-5.42	119.25	126.72
3	L5	4618	OMG	C2-N3-C4	5.41	121.62	112.30
3	L5	2815	A2M	N3-C4-N9	5.39	136.34	127.17
3	L5	4392	OMG	C2-N3-C4	5.38	121.57	112.30
3	L5	2363	A2M	C5-C4-N3	-5.38	119.31	126.72
3	L5	4590	A2M	C5-C4-N3	-5.32	119.39	126.72
3	L5	3825	A2M	C5-C4-N3	-5.31	119.41	126.72
3	L5	3925	OMU	N3-C2-N1	5.31	121.80	114.89
3	L5	3744	OMG	C2-N3-C4	5.30	121.42	112.30
3	L5	1524	A2M	N3-C4-N9	5.27	136.12	127.17
3	L5	2424	OMG	C2-N3-C4	5.24	121.33	112.30
1	S2	668	A2M	C5-C4-N3	-5.24	119.51	126.72
3	L5	3830	A2M	C2'-C1'-N9	-5.24	105.14	113.75
3	L5	1534	A2M	C5-C4-N3	-5.22	119.53	126.72
3	L5	4370	OMG	C2-N3-C4	5.21	121.27	112.30
3	L5	3899	OMG	C2-N3-C4	5.21	121.27	112.30
1	S2	1851	MA6	C5-C4-N3	-5.18	119.58	126.72
1	S2	683	OMG	C2-N3-C4	5.18	121.22	112.30
1	S2	428	OMU	C4-N3-C2	-5.17	120.19	126.61
3	L5	4499	OMG	C2-N3-C4	5.16	121.19	112.30
3	L5	4228	OMG	C5-C4-N3	-5.16	120.19	128.39
1	S2	1288	OMU	C4-N3-C2	-5.15	120.21	126.61
1	S2	509	OMG	C2-N3-C4	5.15	121.17	112.30
3	L5	3925	OMU	C4-N3-C2	-5.14	120.23	126.61
3	L5	2876	OMG	N9-C4-N3	5.11	136.17	125.95
1	S2	1328	OMG	C2-N3-C4	5.09	121.07	112.30
1	S2	1447	OMG	C2-N3-C4	5.09	121.06	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3920	PSU	C4-N3-C2	-5.08	119.37	126.37
3	L5	3944	OMG	C2-N3-C4	5.07	121.03	112.30
3	L5	4523	A2M	N3-C4-N9	5.06	135.77	127.17
3	L5	1677	PSU	C4-N3-C2	-5.06	119.41	126.37
3	L5	3637	PSU	C4-N3-C2	-5.05	119.42	126.37
3	L5	4569	PSU	C4-N3-C2	-5.04	119.42	126.37
1	S2	99	A2M	N3-C4-N9	5.03	135.72	127.17
1	S2	1639	G7M	C5-C4-N3	-5.03	118.65	128.15
1	S2	867	OMG	C2-N3-C4	5.02	120.94	112.30
3	L5	3867	A2M	N3-C4-N9	5.01	135.68	127.17
1	S2	1804	OMU	C4-N3-C2	-5.00	120.41	126.61
3	L5	1625	OMG	C2-N3-C4	4.99	120.90	112.30
3	L5	1522	OMG	C2-N3-C4	4.99	120.90	112.30
3	L5	3627	OMG	C2-N3-C4	4.98	120.89	112.30
1	S2	1490	OMG	C2-N3-C4	4.98	120.88	112.30
3	L5	4494	OMG	N9-C4-N3	4.97	135.90	125.95
1	S2	627	OMU	C4-N3-C2	-4.97	120.44	126.61
3	L5	4623	OMG	C2-N3-C4	4.97	120.86	112.30
1	S2	590	A2M	N3-C4-N9	4.97	135.62	127.17
3	L5	4196	OMG	C2-N3-C4	4.96	120.84	112.30
3	L5	2415	OMU	C4-N3-C2	-4.95	120.47	126.61
3	L5	1677	PSU	O2-C2-N1	-4.93	117.70	122.79
3	L5	2364	OMG	C2-N3-C4	4.93	120.79	112.30
1	S2	1447	OMG	N9-C4-N3	4.92	135.80	125.95
3	L5	3884	PSU	C4-N3-C2	-4.92	119.59	126.37
1	S2	601	OMG	C2-N3-C4	4.92	120.77	112.30
3	L5	4498	OMU	C4-N3-C2	-4.91	120.51	126.61
3	L5	4227	OMU	C4-N3-C2	-4.91	120.52	126.61
1	S2	644	OMG	C2-N3-C4	4.91	120.76	112.30
3	L5	4531	PSU	O2-C2-N1	-4.90	117.74	122.79
3	L5	2837	OMU	C4-N3-C2	-4.89	120.54	126.61
3	L5	4972	PSU	C4-N3-C2	-4.88	119.65	126.37
3	L5	2787	A2M	N3-C4-N9	4.86	135.43	127.17
3	L5	3723	A2M	N3-C4-N9	4.86	135.43	127.17
3	L5	4521	PSU	C4-N3-C2	-4.86	119.68	126.37
1	S2	1383	A2M	C2'-C1'-N9	-4.86	105.76	113.75
2	L8	75	OMG	C2-N3-C4	4.83	120.61	112.30
1	S2	172	OMU	C4-N3-C2	-4.81	120.64	126.61
3	L5	4637	OMG	C2-N3-C4	4.81	120.59	112.30
3	L5	1536	PSU	C4-N3-C2	-4.81	119.75	126.37
3	L5	4620	OMU	C4-N3-C2	-4.80	120.66	126.61
3	L5	3792	OMG	C2-N3-C4	4.80	120.56	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3715	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L5	5001	PSU	C4-N3-C2	-4.79	119.77	126.37
1	S2	1442	OMU	C4-N3-C2	-4.79	120.67	126.61
1	S2	109	PSU	C4-N3-C2	-4.79	119.78	126.37
1	S2	1326	UY1	C4-N3-C2	-4.79	119.78	126.37
1	S2	166	A2M	N3-C4-N9	4.78	135.30	127.17
3	L5	2843	PSU	C4-N3-C2	-4.78	119.78	126.37
1	S2	121	OMU	C4-N3-C2	-4.78	120.68	126.61
3	L5	4571	A2M	N3-C4-N9	4.77	135.28	127.17
3	L5	2876	OMG	C2-N3-C4	4.76	120.50	112.30
1	S2	1056	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	1326	A2M	C5-C4-N3	-4.75	120.17	126.72
3	L5	1322	1MA	C5-C4-N3	-4.75	120.28	127.27
3	L5	4628	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	3853	PSU	C4-N3-C2	-4.74	119.84	126.37
3	L5	398	A2M	N3-C4-N9	4.73	135.21	127.17
3	L5	4220	6MZ	C5-C4-N3	-4.73	120.20	126.72
1	S2	512	A2M	N3-C4-N9	4.71	135.18	127.17
1	S2	1678	A2M	N3-C4-N9	4.69	135.15	127.17
3	L5	1871	A2M	C2'-C1'-N9	-4.69	106.03	113.75
1	S2	1639	G7M	C8-N9-C4	4.69	118.71	107.09
1	S2	1136	PSU	C4-N3-C2	-4.69	119.91	126.37
29	SV	1	AME	CT2-CT1-N	-4.69	108.35	116.12
1	S2	644	OMG	N9-C4-N3	4.66	135.27	125.95
3	L5	3792	OMG	N9-C4-N3	4.66	135.27	125.95
3	L5	3760	A2M	N3-C4-N9	4.65	135.08	127.17
1	S2	681	PSU	C4-N3-C2	-4.65	119.96	126.37
3	L5	2787	A2M	C4-C5-N7	-4.65	105.26	110.58
1	S2	116	OMU	C4-N3-C2	-4.64	120.85	126.61
3	L5	400	A2M	N3-C4-N9	4.64	135.06	127.17
3	L5	1316	OMG	N9-C4-N3	4.63	135.21	125.95
1	S2	166	A2M	C2'-C1'-N9	-4.62	106.14	113.75
1	S2	159	A2M	N3-C4-N9	4.62	135.02	127.17
3	L5	4353	PSU	C4-N3-C2	-4.61	120.02	126.37
3	L5	4228	OMG	C2-N3-C4	4.61	120.24	112.30
1	S2	822	PSU	C4-N3-C2	-4.60	120.04	126.37
1	S2	1031	A2M	N3-C4-N9	4.60	134.98	127.17
3	L5	2424	OMG	N9-C4-N3	4.59	135.12	125.95
3	L5	4296	PSU	C4-N3-C2	-4.59	120.06	126.37
3	L5	4498	OMU	C5-C4-N3	4.58	121.22	114.80
3	L5	4353	PSU	O2-C2-N1	-4.58	118.07	122.79
3	L5	1871	A2M	N3-C4-N9	4.58	134.95	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4423	PSU	C4-N3-C2	-4.56	120.08	126.37
3	L5	4361	PSU	C4-N3-C2	-4.56	120.09	126.37
1	S2	436	OMG	N9-C4-N3	4.55	135.06	125.95
3	L5	1322	1MA	C2-N3-C4	4.54	121.44	112.53
1	S2	1328	OMG	N9-C4-N3	4.54	135.03	125.95
82	Pt	47	G7M	N9-C8-N7	-4.54	101.46	112.48
3	L5	4403	PSU	C4-N3-C2	-4.54	120.12	126.37
1	S2	649	PSU	C4-N3-C2	-4.52	120.14	126.37
3	L5	4500	PSU	O2-C2-N1	-4.52	118.13	122.79
1	S2	1692	PSU	C4-N3-C2	-4.51	120.16	126.37
3	L5	4227	OMU	C5-C4-N3	4.51	121.11	114.80
1	S2	1643	PSU	C4-N3-C2	-4.51	120.16	126.37
6	SA	2	SAC	C2A-C1A-N	-4.51	108.64	116.12
3	L5	4689	PSU	C4-N3-C2	-4.50	120.17	126.37
3	L5	1534	A2M	N3-C4-N9	4.49	134.81	127.17
3	L5	4499	OMG	N9-C4-N3	4.49	134.93	125.95
1	S2	105	PSU	C4-N3-C2	-4.49	120.19	126.37
3	L5	3768	PSU	C4-N3-C2	-4.48	120.19	126.37
1	S2	406	PSU	C4-N3-C2	-4.47	120.21	126.37
3	L5	4299	PSU	C4-N3-C2	-4.47	120.21	126.37
3	L5	3944	OMG	N9-C4-N3	4.47	134.90	125.95
1	S2	34	PSU	C4-N3-C2	-4.47	120.21	126.37
1	S2	1832	6MZ	N3-C4-N9	4.46	134.76	127.17
1	S2	1239	PSU	C4-N3-C2	-4.45	120.24	126.37
3	L5	2837	OMU	N3-C2-N1	4.45	120.68	114.89
3	L5	1625	OMG	N9-C4-N3	4.45	134.84	125.95
3	L5	3724	A2M	N3-C4-N9	4.44	134.72	127.17
3	L5	4620	OMU	C5-C4-N3	4.44	121.02	114.80
1	S2	354	OMU	C4-N3-C2	-4.43	121.11	126.61
1	S2	119	PSU	C4-N3-C2	-4.42	120.28	126.37
1	S2	683	OMG	N9-C4-N3	4.42	134.79	125.95
1	S2	1004	PSU	C4-N3-C2	-4.42	120.28	126.37
3	L5	4673	PSU	C4-N3-C2	-4.42	120.28	126.37
1	S2	509	OMG	N9-C4-N3	4.42	134.78	125.95
1	S2	1490	OMG	C2'-C1'-N9	-4.42	105.86	114.24
1	S2	918	PSU	C4-N3-C2	-4.41	120.29	126.37
3	L5	4370	OMG	N9-C4-N3	4.41	134.77	125.95
1	S2	109	PSU	O2-C2-N1	-4.40	118.25	122.79
3	L5	4220	6MZ	N1-C2-N3	-4.40	121.92	128.58
1	S2	1288	OMU	N3-C2-N1	4.40	120.61	114.89
1	S2	867	OMG	N9-C4-N3	4.39	134.74	125.95
1	S2	1174	PSU	C4-N3-C2	-4.39	120.32	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	468	A2M	N3-C4-N9	4.38	134.62	127.17
1	S2	686	PSU	C4-N3-C2	-4.38	120.34	126.37
1	S2	1232	PSU	C4-N3-C2	-4.38	120.34	126.37
1	S2	572	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	512	A2M	C2'-C1'-N9	-4.36	106.58	113.75
3	L5	3758	PSU	C4-N3-C2	-4.35	120.38	126.37
3	L5	3920	PSU	O2-C2-N1	-4.35	118.30	122.79
3	L5	1683	PSU	C4-N3-C2	-4.34	120.39	126.37
2	L8	55	PSU	C4-N3-C2	-4.34	120.39	126.37
3	L5	3785	A2M	N3-C4-N9	4.34	134.55	127.17
1	S2	1442	OMU	N3-C2-N1	4.34	120.54	114.89
1	S2	1081	PSU	C4-N3-C2	-4.34	120.39	126.37
3	L5	1782	PSU	C4-N3-C2	-4.34	120.39	126.37
1	S2	651	PSU	C4-N3-C2	-4.34	120.40	126.37
2	L8	75	OMG	N9-C4-N3	4.33	134.61	125.95
3	L5	2415	OMU	N3-C2-N1	4.33	120.53	114.89
3	L5	3637	PSU	O2-C2-N1	-4.33	118.32	122.79
3	L5	3718	A2M	N3-C4-N9	4.33	134.53	127.17
1	S2	863	PSU	C4-N3-C2	-4.33	120.41	126.37
82	Pt	8	4SU	C5-C4-S4	-4.33	119.36	124.31
1	S2	1851	MA6	C2-N1-C6	4.33	122.39	111.83
3	L5	5010	PSU	C4-N3-C2	-4.32	120.42	126.37
1	S2	484	A2M	N3-C4-N9	4.32	134.51	127.17
3	L5	3825	A2M	N3-C4-N9	4.32	134.51	127.17
1	S2	121	OMU	N3-C2-N1	4.32	120.51	114.89
3	L5	3729	PSU	C4-N3-C2	-4.31	120.43	126.37
1	S2	296	PSU	C4-N3-C2	-4.31	120.43	126.37
3	L5	3762	PSU	C4-N3-C2	-4.31	120.43	126.37
1	S2	116	OMU	C5-C4-N3	4.31	120.83	114.80
1	S2	601	OMG	N9-C4-N3	4.30	134.56	125.95
3	L5	1582	PSU	C4-N3-C2	-4.30	120.44	126.37
1	S2	1238	PSU	C4-N3-C2	-4.30	120.45	126.37
1	S2	1243	PSU	C4-N3-C2	-4.30	120.45	126.37
1	S2	1383	A2M	N3-C4-N9	4.30	134.48	127.17
2	L8	14	OMU	C4-N3-C2	-4.30	121.28	126.61
3	L5	2401	A2M	N3-C4-N9	4.30	134.47	127.17
3	L5	4552	PSU	C4-N3-C2	-4.30	120.45	126.37
1	S2	573	PSU	C4-N3-C2	-4.29	120.46	126.37
1	S2	1804	OMU	N3-C2-N1	4.29	120.48	114.89
82	Pt	56	PSU	C4-N3-C2	-4.29	120.46	126.37
3	L5	4196	OMG	N9-C4-N3	4.29	134.53	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1850	MA6	C2-N1-C6	4.29	122.31	111.83
3	L5	4590	A2M	N3-C4-N9	4.29	134.46	127.17
3	L5	3695	PSU	C4-N3-C2	-4.29	120.47	126.37
1	S2	428	OMU	N3-C2-N1	4.29	120.47	114.89
1	S2	27	A2M	N3-C4-N9	4.27	134.44	127.17
1	S2	218	PSU	C4-N3-C2	-4.27	120.49	126.37
1	S2	1850	MA6	N3-C4-N9	4.26	134.42	127.17
1	S2	815	PSU	C4-N3-C2	-4.26	120.50	126.37
3	L5	1744	PSU	C4-N3-C2	-4.26	120.50	126.37
3	L5	3899	OMG	N9-C4-N3	4.25	134.46	125.95
1	S2	1625	PSU	C4-N3-C2	-4.25	120.52	126.37
3	L5	4498	OMU	N3-C2-N1	4.25	120.42	114.89
1	S2	1244	PSU	C4-N3-C2	-4.25	120.52	126.37
3	L5	4618	OMG	N9-C4-N3	4.24	134.44	125.95
1	S2	1851	MA6	C4-C5-N7	-4.24	105.73	110.58
3	L5	3744	OMG	N9-C4-N3	4.24	134.43	125.95
3	L5	2632	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	4576	PSU	O2-C2-N1	-4.24	118.42	122.79
1	S2	801	PSU	C4-N3-C2	-4.23	120.54	126.37
3	L5	4293	PSU	C4-N3-C2	-4.23	120.54	126.37
1	S2	1850	MA6	C4-C5-N7	-4.23	105.75	110.58
3	L5	4312	PSU	C4-N3-C2	-4.22	120.55	126.37
3	L5	4628	PSU	O2-C2-N1	-4.22	118.44	122.79
3	L5	3770	PSU	C4-N3-C2	-4.22	120.56	126.37
1	S2	1490	OMG	N9-C4-N3	4.22	134.39	125.95
3	L5	4500	PSU	C4-N3-C2	-4.22	120.56	126.37
1	S2	172	OMU	N3-C2-N1	4.21	120.38	114.89
1	S2	428	OMU	C5-C4-N3	4.21	120.70	114.80
1	S2	1347	PSU	C4-N3-C2	-4.21	120.58	126.37
3	L5	2508	PSU	C4-N3-C2	-4.21	120.58	126.37
3	L5	1779	PSU	C4-N3-C2	-4.20	120.58	126.37
3	L5	4220	6MZ	N3-C4-N9	4.20	134.31	127.17
3	L5	2363	A2M	N3-C4-N9	4.20	134.30	127.17
3	L5	3830	A2M	N3-C4-N9	4.20	134.30	127.17
1	S2	354	OMU	N3-C2-N1	4.18	120.34	114.89
1	S2	814	PSU	C4-N3-C2	-4.17	120.62	126.37
1	S2	866	PSU	C4-N3-C2	-4.17	120.62	126.37
3	L5	3853	PSU	O2-C2-N1	-4.17	118.49	122.79
3	L5	4431	PSU	C4-N3-C2	-4.17	120.63	126.37
3	L5	1781	PSU	C4-N3-C2	-4.16	120.64	126.37
3	L5	1683	PSU	O2-C2-N1	-4.16	118.50	122.79
3	L5	3818	UY1	C4-N3-C2	-4.15	120.65	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3764	PSU	C4-N3-C2	-4.14	120.66	126.37
2	L8	69	PSU	C4-N3-C2	-4.14	120.66	126.37
3	L5	4576	PSU	C4-N3-C2	-4.14	120.67	126.37
1	S2	1445	PSU	C4-N3-C2	-4.14	120.67	126.37
3	L5	1524	A2M	C4-N9-C8	4.14	110.08	105.74
3	L5	4227	OMU	N3-C2-N1	4.13	120.27	114.89
3	L5	3627	OMG	N9-C4-N3	4.12	134.20	125.95
1	S2	609	PSU	C4-N3-C2	-4.12	120.69	126.37
3	L5	1522	OMG	N9-C4-N3	4.12	134.19	125.95
1	S2	1031	A2M	C2'-C1'-N9	-4.11	106.98	113.75
1	S2	576	A2M	N3-C4-N9	4.11	134.16	127.17
3	L5	4579	PSU	C4-N3-C2	-4.11	120.71	126.37
3	L5	4636	PSU	C4-N3-C2	-4.10	120.72	126.37
1	S2	1367	PSU	C4-N3-C2	-4.10	120.72	126.37
3	L5	4220	6MZ	C6-C5-N7	4.10	136.90	132.43
3	L5	3760	A2M	C2'-C1'-N9	-4.10	107.01	113.75
3	L5	2837	OMU	C5-C4-N3	4.09	120.53	114.80
3	L5	4623	OMG	N9-C4-N3	4.09	134.12	125.95
3	L5	4442	PSU	C4-N3-C2	-4.09	120.74	126.37
3	L5	2787	A2M	C2-N3-C4	4.08	121.80	111.83
3	L5	1536	PSU	O2-C2-N1	-4.08	118.58	122.79
1	S2	1832	6MZ	C6-C5-N7	4.06	136.85	132.43
2	L8	14	OMU	C5-C4-N3	4.06	120.48	114.80
1	S2	36	PSU	C4-N3-C2	-4.05	120.78	126.37
3	L5	1871	A2M	C2-N3-C4	4.05	121.72	111.83
3	L5	2415	OMU	C5-C4-N3	4.05	120.47	114.80
3	L5	2815	A2M	C2-N3-C4	4.05	121.72	111.83
3	L5	4296	PSU	O2-C2-N1	-4.05	118.61	122.79
82	Pt	8	4SU	N3-C2-N1	4.05	120.16	114.89
1	S2	1804	OMU	C5-C4-N3	4.05	120.47	114.80
3	L5	3844	PSU	C4-N3-C2	-4.04	120.80	126.37
3	L5	4471	PSU	C4-N3-C2	-4.04	120.81	126.37
3	L5	4392	OMG	N9-C4-N3	4.04	134.03	125.95
1	S2	1288	OMU	C5-C4-N3	4.03	120.45	114.80
3	L5	4228	OMG	C6-C5-N7	4.03	137.63	130.29
3	L5	3899	OMG	C6-C5-N7	4.03	137.62	130.29
1	S2	627	OMU	N3-C2-N1	4.02	120.12	114.89
1	S2	121	OMU	C5-C4-N3	4.01	120.42	114.80
1	S2	1367	PSU	O2-C2-N1	-4.01	118.65	122.79
1	S2	1639	G7M	C2-N3-C4	4.00	119.18	112.30
3	L5	1792	PSU	O2-C2-N1	-3.99	118.67	122.79
3	L5	4523	A2M	N3-C2-N1	-3.99	122.54	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	34	PSU	O2-C2-N1	-3.99	118.68	122.79
3	L5	1860	PSU	C4-N3-C2	-3.98	120.89	126.37
3	L5	4420	PSU	C4-N3-C2	-3.98	120.89	126.37
3	L5	2364	OMG	N9-C4-N3	3.97	133.89	125.95
1	S2	966	PSU	C4-N3-C2	-3.97	120.91	126.37
3	L5	3785	A2M	O4'-C1'-N9	3.96	115.69	108.09
3	L5	1792	PSU	C4-N3-C2	-3.96	120.92	126.37
3	L5	1871	A2M	C4-C5-N7	-3.95	106.06	110.58
1	S2	609	PSU	O2-C2-N1	-3.95	118.72	122.79
3	L5	3734	PSU	C4-N3-C2	-3.92	120.97	126.37
3	L5	3844	PSU	O2-C2-N1	-3.92	118.74	122.79
1	S2	627	OMU	C5-C4-N3	3.92	120.29	114.80
1	S2	649	PSU	O2-C2-N1	-3.92	118.75	122.79
3	L5	3627	OMG	C6-C5-N7	3.92	137.43	130.29
1	S2	668	A2M	N3-C4-N9	3.92	133.83	127.17
3	L5	4523	A2M	C2-N3-C4	3.92	121.40	111.83
1	S2	354	OMU	C5-C4-N3	3.92	120.29	114.80
1	S2	1244	PSU	O2-C2-N1	-3.92	118.75	122.79
3	L5	2837	OMU	O2-C2-N1	-3.91	117.70	122.80
1	S2	1177	PSU	C4-N3-C2	-3.90	120.99	126.37
3	L5	3830	A2M	C2-N3-C4	3.90	121.37	111.83
3	L5	3764	PSU	O2-C2-N1	-3.90	118.76	122.79
82	Pt	56	PSU	O2-C2-N1	-3.90	118.76	122.79
3	L5	5010	PSU	O2-C2-N1	-3.90	118.76	122.79
1	S2	1004	PSU	O2-C2-N1	-3.90	118.77	122.79
1	S2	1442	OMU	C5-C4-N3	3.90	120.26	114.80
1	S2	590	A2M	C2-N3-C4	3.90	121.34	111.83
2	L8	69	PSU	O2-C2-N1	-3.89	118.77	122.79
3	L5	2815	A2M	N3-C2-N1	-3.89	122.69	128.58
1	S2	1832	6MZ	C4-C5-N7	-3.89	106.14	110.58
1	S2	93	PSU	C4-N3-C2	-3.88	121.02	126.37
3	L5	2364	OMG	C6-C5-N7	3.88	137.35	130.29
3	L5	3844	PSU	C6-C5-C4	-3.87	115.56	118.17
3	L5	4493	PSU	C4-N3-C2	-3.87	121.04	126.37
3	L5	2401	A2M	C4-C5-N7	-3.87	106.16	110.58
3	L5	1862	PSU	C4-N3-C2	-3.87	121.04	126.37
1	S2	576	A2M	C2'-C1'-N9	-3.87	107.38	113.75
3	L5	1524	A2M	C2-N3-C4	3.87	121.27	111.83
3	L5	3770	PSU	O2-C2-N1	-3.86	118.80	122.79
3	L5	3734	PSU	O2-C2-N1	-3.86	118.81	122.79
3	L5	3715	PSU	O2-C2-N1	-3.86	118.81	122.79
1	S2	119	PSU	O2-C2-N1	-3.86	118.81	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	99	A2M	C2-N3-C4	3.86	121.25	111.83
1	S2	668	A2M	C4-C5-N7	-3.85	106.18	110.58
1	S2	918	PSU	O2-C2-N1	-3.85	118.82	122.79
3	L5	4618	OMG	C6-C5-N7	3.85	137.29	130.29
3	L5	1524	A2M	N3-C2-N1	-3.84	122.77	128.58
1	S2	484	A2M	C2-N3-C4	3.83	121.19	111.83
2	L8	14	OMU	N3-C2-N1	3.83	119.88	114.89
1	S2	166	A2M	C2-N3-C4	3.83	121.18	111.83
1	S2	651	PSU	O2-C2-N1	-3.83	118.84	122.79
1	S2	1445	PSU	O2-C2-N1	-3.83	118.84	122.79
3	L5	3867	A2M	C4-C5-N7	-3.82	106.21	110.58
3	L5	398	A2M	C2'-C1'-N9	-3.82	107.47	113.75
1	S2	159	A2M	C2-N3-C4	3.81	121.13	111.83
3	L5	4571	A2M	C2-N3-C4	3.80	121.10	111.83
1	S2	1248	B8N	N3-C2-N1	3.79	121.35	116.72
3	L5	4220	6MZ	C2-N3-C4	3.79	121.10	111.83
3	L5	398	A2M	C4-C5-N7	-3.79	106.25	110.58
3	L5	3758	PSU	O2-C2-N1	-3.79	118.88	122.79
3	L5	4392	OMG	C6-C5-N7	3.79	137.19	130.29
1	S2	866	PSU	O2-C2-N1	-3.79	118.88	122.79
3	L5	1534	A2M	C4-N9-C8	3.79	109.72	105.74
3	L5	4228	OMG	N9-C4-N3	3.79	133.52	125.95
3	L5	4306	OMU	C4-N3-C2	-3.79	121.91	126.61
3	L5	4306	OMU	N3-C2-N1	3.78	119.81	114.89
1	S2	1326	UY1	O2-C2-N1	-3.78	118.89	122.79
3	L5	4420	PSU	O2-C2-N1	-3.78	118.89	122.79
1	S2	1248	B8N	C31-N3-C4	3.77	122.52	117.18
1	S2	105	PSU	O2-C2-N1	-3.77	118.90	122.79
1	S2	668	A2M	C2-N3-C4	3.77	121.04	111.83
1	S2	172	OMU	C5-C4-N3	3.77	120.08	114.80
1	S2	1678	A2M	C2-N3-C4	3.76	121.03	111.83
1	S2	1136	PSU	O2-C2-N1	-3.76	118.91	122.79
3	L5	4220	6MZ	C9-N6-C6	-3.76	119.36	122.85
3	L5	3825	A2M	C2-N3-C4	3.76	121.00	111.83
1	S2	1232	PSU	O2-C2-N1	-3.75	118.92	122.79
3	L5	3724	A2M	C2-N3-C4	3.75	121.00	111.83
3	L5	3830	A2M	N3-C2-N1	-3.75	122.90	128.58
3	L5	1871	A2M	N3-C2-N1	-3.74	122.91	128.58
1	S2	1625	PSU	O2-C2-N1	-3.74	118.93	122.79
1	S2	296	PSU	O2-C2-N1	-3.73	118.94	122.79
1	S2	822	PSU	O2-C2-N1	-3.72	118.95	122.79
3	L5	1781	PSU	O2-C2-N1	-3.72	118.96	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2632	PSU	O2-C2-N1	-3.71	118.96	122.79
3	L5	2839	PSU	C4-N3-C2	-3.71	121.27	126.37
1	S2	1851	MA6	N3-C4-N9	3.70	133.47	127.17
1	S2	27	A2M	C2-N3-C4	3.70	120.86	111.83
3	L5	1534	A2M	C4-C5-N7	-3.70	106.36	110.58
3	L5	3825	A2M	N3-C2-N1	-3.69	122.99	128.58
1	S2	436	OMG	C6-C5-N7	3.69	137.00	130.29
3	L5	398	A2M	C2-N3-C4	3.69	120.83	111.83
1	S2	1850	MA6	C2-N3-C4	3.69	120.83	111.83
1	S2	512	A2M	C2-N3-C4	3.69	120.83	111.83
1	S2	468	A2M	C2'-C1'-N9	-3.68	107.69	113.75
3	L5	4620	OMU	N3-C2-N1	3.68	119.68	114.89
3	L5	1326	A2M	N3-C2-N1	-3.68	123.01	128.58
1	S2	686	PSU	O2-C2-N1	-3.67	119.00	122.79
3	L5	3830	A2M	C4-C5-N7	-3.67	106.38	110.58
3	L5	4220	6MZ	C4-N9-C8	3.67	109.59	105.74
1	S2	1851	MA6	C2-N3-C4	3.67	120.79	111.83
3	L5	4523	A2M	C4-N9-C8	3.67	109.59	105.74
3	L5	4532	PSU	C4-N3-C2	-3.66	121.32	126.37
1	S2	1639	G7M	CN7-N7-C5	3.66	131.36	126.80
3	L5	3723	A2M	C2-N3-C4	3.66	120.78	111.83
1	S2	468	A2M	C2-N3-C4	3.66	120.76	111.83
3	L5	2363	A2M	C2-N3-C4	3.66	120.76	111.83
1	S2	484	A2M	C4-C5-N7	-3.65	106.41	110.58
3	L5	400	A2M	C2-N3-C4	3.64	120.72	111.83
3	L5	4623	OMG	C6-C5-N7	3.63	136.90	130.29
1	S2	1383	A2M	C4-C5-N7	-3.63	106.43	110.58
1	S2	1639	G7M	C1'-N9-C8	-3.63	114.49	126.74
1	S2	1832	6MZ	N1-C2-N3	-3.62	123.10	128.58
50	La	39	V5N	CD2-CG-ND1	3.62	110.64	105.76
1	S2	1239	PSU	O2-C2-N1	-3.61	119.06	122.79
3	L5	4499	OMG	C6-C5-N7	3.61	136.87	130.29
1	S2	159	A2M	C4-C5-N7	-3.61	106.45	110.58
39	LA	216	V5N	CD2-CG-ND1	3.61	110.63	105.76
3	L5	3768	PSU	O2-C2-N1	-3.61	119.06	122.79
3	L5	3851	PSU	C4-N3-C2	-3.61	121.40	126.37
3	L5	4620	OMU	O4-C4-C5	-3.61	118.94	125.16
3	L5	4493	PSU	O2-C2-N1	-3.60	119.07	122.79
1	S2	1383	A2M	C2-N3-C4	3.60	120.62	111.83
1	S2	1832	6MZ	C2-N3-C4	3.60	120.61	111.83
1	S2	1031	A2M	C2-N3-C4	3.59	120.61	111.83
3	L5	4196	OMG	C6-C5-N7	3.58	136.81	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3785	A2M	C2-N3-C4	3.58	120.58	111.83
1	S2	1243	PSU	O2-C2-N1	-3.58	119.10	122.79
1	S2	668	A2M	N3-C2-N1	-3.58	123.17	128.58
3	L5	4571	A2M	C4-C5-N7	-3.58	106.49	110.58
3	L5	3760	A2M	C2-N3-C4	3.57	120.56	111.83
3	L5	1779	PSU	O2-C2-N1	-3.57	119.10	122.79
3	L5	1782	PSU	O2-C2-N1	-3.57	119.10	122.79
3	L5	1326	A2M	C2-N3-C4	3.57	120.56	111.83
3	L5	3639	PSU	C4-N3-C2	-3.57	121.45	126.37
1	S2	116	OMU	N3-C2-N1	3.57	119.53	114.89
3	L5	3925	OMU	C5-C4-N3	3.56	119.79	114.80
1	S2	863	PSU	O2-C2-N1	-3.56	119.11	122.79
2	L8	75	OMG	C6-C5-N7	3.56	136.76	130.29
3	L5	3867	A2M	C2-N3-C4	3.55	120.50	111.83
3	L5	3785	A2M	C4-C5-N7	-3.55	106.52	110.58
1	S2	27	A2M	C4-C5-N7	-3.54	106.53	110.58
3	L5	4370	OMG	C6-C5-N7	3.53	136.72	130.29
3	L5	3785	A2M	C2'-C1'-N9	-3.53	107.94	113.75
1	S2	576	A2M	C4-C5-N7	-3.53	106.55	110.58
3	L5	2401	A2M	C2-N3-C4	3.53	120.45	111.83
3	L5	1522	OMG	C6-C5-N7	3.52	136.70	130.29
3	L5	1326	A2M	C4-C5-N7	-3.52	106.55	110.58
1	S2	27	A2M	N3-C2-N1	-3.52	123.25	128.58
1	S2	572	PSU	O2-C2-N1	-3.51	119.17	122.79
3	L5	4530	UR3	C5-C4-N3	3.51	119.66	115.04
3	L5	4531	PSU	C4-N3-C2	-3.50	121.55	126.37
3	L5	1316	OMG	C6-C5-N7	3.50	136.66	130.29
1	S2	601	OMG	C6-C5-N7	3.50	136.65	130.29
3	L5	3724	A2M	N3-C2-N1	-3.49	123.30	128.58
3	L5	3729	PSU	O2-C2-N1	-3.49	119.19	122.79
1	S2	1678	A2M	C4-C5-N7	-3.48	106.60	110.58
3	L5	4494	OMG	C6-C5-N7	3.48	136.62	130.29
3	L5	400	A2M	C4-C5-N7	-3.48	106.61	110.58
1	S2	681	PSU	O2-C2-N1	-3.47	119.21	122.79
1	S2	1031	A2M	N3-C2-N1	-3.47	123.32	128.58
1	S2	468	A2M	N3-C2-N1	-3.47	123.33	128.58
1	S2	99	A2M	C4-C5-N7	-3.47	106.62	110.58
3	L5	3724	A2M	C4-C5-N7	-3.46	106.62	110.58
1	S2	1851	MA6	N1-C2-N3	-3.46	123.35	128.58
1	S2	683	OMG	C6-C5-N7	3.45	136.57	130.29
1	S2	1347	PSU	O2-C2-N1	-3.45	119.23	122.79
3	L5	3718	A2M	C2'-C1'-N9	-3.45	108.08	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4636	PSU	O2-C2-N1	-3.45	119.23	122.79
3	L5	2363	A2M	N3-C2-N1	-3.44	123.37	128.58
1	S2	468	A2M	C4-C5-N7	-3.44	106.65	110.58
1	S2	1490	OMG	C6-C5-N7	3.44	136.54	130.29
3	L5	1326	A2M	N3-C4-N9	3.43	133.00	127.17
3	L5	3884	PSU	O2-C2-N1	-3.43	119.25	122.79
1	S2	36	PSU	O2-C2-N1	-3.43	119.25	122.79
1	S2	1850	MA6	N1-C2-N3	-3.43	123.40	128.58
1	S2	573	PSU	O2-C2-N1	-3.43	119.26	122.79
3	L5	1744	PSU	O2-C2-N1	-3.42	119.26	122.79
1	S2	576	A2M	C2-N3-C4	3.42	120.18	111.83
3	L5	4447	5MC	C5-C4-N3	-3.41	118.26	121.75
1	S2	590	A2M	N3-C2-N1	-3.40	123.43	128.58
3	L5	4637	OMG	C6-C5-N7	3.40	136.48	130.29
1	S2	822	PSU	C3'-C2'-C1'	3.40	105.70	101.69
3	L5	3723	A2M	N3-C2-N1	-3.39	123.44	128.58
1	S2	484	A2M	N3-C2-N1	-3.38	123.46	128.58
1	S2	1678	A2M	N3-C2-N1	-3.38	123.46	128.58
3	L5	4972	PSU	O2-C2-N1	-3.38	119.30	122.79
3	L5	4457	PSU	C4-N3-C2	-3.38	121.71	126.37
1	S2	166	A2M	C4-C5-N7	-3.38	106.72	110.58
1	S2	1804	OMU	O4-C4-C5	-3.38	119.34	125.16
1	S2	406	PSU	O2-C2-N1	-3.37	119.31	122.79
3	L5	3744	OMG	C6-C5-N7	3.37	136.42	130.29
3	L5	4423	PSU	O2-C2-N1	-3.37	119.32	122.79
1	S2	166	A2M	N3-C2-N1	-3.36	123.49	128.58
1	S2	1692	PSU	O2-C2-N1	-3.36	119.32	122.79
3	L5	4590	A2M	C2-N3-C4	3.36	120.04	111.83
3	L5	3925	OMU	O2-C2-N1	-3.36	118.42	122.80
1	S2	218	PSU	O2-C2-N1	-3.36	119.32	122.79
1	S2	509	OMG	C6-C5-N7	3.36	136.41	130.29
3	L5	4579	PSU	O2-C2-N1	-3.36	119.33	122.79
3	L5	4689	PSU	O2-C2-N1	-3.36	119.33	122.79
3	L5	3785	A2M	N3-C2-N1	-3.36	123.50	128.58
1	S2	116	OMU	O4-C4-C5	-3.35	119.38	125.16
3	L5	1625	OMG	C6-C5-N7	3.35	136.39	130.29
3	L5	2363	A2M	C4-C5-N7	-3.35	106.75	110.58
1	S2	1328	OMG	C6-C5-N7	3.35	136.38	130.29
1	S2	1174	PSU	O2-C2-N1	-3.35	119.34	122.79
64	Lr	2	SAC	C2A-C1A-N	-3.34	110.58	116.12
1	S2	512	A2M	C4-C5-N7	-3.33	106.77	110.58
3	L5	1534	A2M	C2-N3-C4	3.33	119.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	590	A2M	C4-C5-N7	-3.33	106.78	110.58
3	L5	2876	OMG	C6-C5-N7	3.32	136.34	130.29
1	S2	1031	A2M	C4-C5-N7	-3.32	106.79	110.58
1	S2	966	PSU	O2-C2-N1	-3.31	119.38	122.79
3	L5	3762	PSU	O2-C2-N1	-3.31	119.38	122.79
3	L5	3718	A2M	C2-N3-C4	3.30	119.88	111.83
3	L5	3695	PSU	O2-C2-N1	-3.29	119.39	122.79
3	L5	3944	OMG	C6-C5-N7	3.28	136.26	130.29
3	L5	2401	A2M	N3-C2-N1	-3.27	123.63	128.58
3	L5	4590	A2M	C4-C5-N7	-3.26	106.85	110.58
3	L5	3718	A2M	C4-C5-N7	-3.26	106.86	110.58
3	L5	3760	A2M	C4-C5-N7	-3.26	106.86	110.58
1	S2	159	A2M	N3-C2-N1	-3.25	123.66	128.58
3	L5	4447	5MC	C5-C6-N1	-3.25	119.78	123.31
3	L5	3825	A2M	C4-C5-N7	-3.25	106.87	110.58
1	S2	1238	PSU	O2-C2-N1	-3.24	119.45	122.79
1	S2	867	OMG	C6-C5-N7	3.24	136.18	130.29
3	L5	4306	OMU	C5-C4-N3	3.24	119.33	114.80
1	S2	1643	PSU	O2-C2-N1	-3.23	119.45	122.79
3	L5	3851	PSU	O2-C2-N1	-3.23	119.45	122.79
1	S2	1177	PSU	O2-C2-N1	-3.23	119.46	122.79
1	S2	1383	A2M	N3-C2-N1	-3.23	123.70	128.58
1	S2	801	PSU	O2-C2-N1	-3.22	119.47	122.79
3	L5	4620	OMU	O2-C2-N1	-3.22	118.61	122.80
3	L5	4471	PSU	O2-C2-N1	-3.22	119.47	122.79
1	S2	1850	MA6	C5-N7-C8	3.21	108.49	103.45
3	L5	4403	PSU	O2-C2-N1	-3.20	119.48	122.79
3	L5	4447	5MC	O2-C2-N3	-3.20	117.28	122.33
1	S2	1850	MA6	C4-N9-C8	3.20	109.09	105.74
3	L5	3782	5MC	C5-C6-N1	-3.19	119.84	123.31
3	L5	1582	PSU	C6-C5-C4	-3.18	116.03	118.17
3	L5	4569	PSU	O2-C2-N1	-3.17	119.52	122.79
3	L5	2424	OMG	C6-C5-N7	3.16	136.04	130.29
3	L5	2815	A2M	C4-N9-C8	3.16	109.05	105.74
3	L5	4590	A2M	N3-C2-N1	-3.16	123.80	128.58
3	L5	4523	A2M	C4-C5-N7	-3.15	106.98	110.58
1	S2	1851	MA6	C4-N9-C8	3.15	109.05	105.74
3	L5	3782	5MC	C5-C4-N3	-3.15	118.53	121.75
3	L5	1322	1MA	N9-C4-N3	3.12	134.01	126.90
1	S2	512	A2M	N3-C2-N1	-3.11	123.88	128.58
1	S2	159	A2M	C2'-C1'-N9	-3.11	108.64	113.75
3	L5	3867	A2M	N3-C2-N1	-3.11	123.88	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1677	PSU	C5-C6-N1	-3.11	117.83	122.14
3	L5	4312	PSU	O2-C2-N1	-3.10	119.59	122.79
1	S2	1288	OMU	O4-C4-C5	-3.10	119.81	125.16
3	L5	4571	A2M	N3-C2-N1	-3.09	123.91	128.58
1	S2	1842	4AC	O2-C2-N3	-3.09	117.46	122.33
3	L5	2787	A2M	N3-C2-N1	-3.08	123.92	128.58
1	S2	1383	A2M	C4-N9-C8	3.08	108.97	105.74
1	S2	172	OMU	O4-C4-C5	-3.07	119.86	125.16
1	S2	1326	UY1	C5-C6-N1	-3.07	117.88	122.14
1	S2	814	PSU	O2-C2-N1	-3.07	119.62	122.79
3	L5	4552	PSU	O2-C2-N1	-3.06	119.63	122.79
1	S2	644	OMG	C6-C5-N7	3.06	135.86	130.29
3	L5	4392	OMG	C4-C5-N7	-3.05	105.83	110.67
3	L5	3818	UY1	O2-C2-N1	-3.05	119.64	122.79
1	S2	99	A2M	N3-C2-N1	-3.05	123.97	128.58
3	L5	5001	PSU	O2-C2-N1	-3.05	119.65	122.79
3	L5	1625	OMG	C4-C5-N7	-3.04	105.85	110.67
1	S2	627	OMU	O4-C4-C5	-3.04	119.91	125.16
3	L5	1871	A2M	C5-N7-C8	3.04	108.23	103.45
3	L5	3867	A2M	C5-N7-C8	3.04	108.23	103.45
1	S2	815	PSU	O2-C2-N1	-3.04	119.66	122.79
3	L5	4972	PSU	C5-C6-N1	-3.04	117.92	122.14
3	L5	4299	PSU	O2-C2-N1	-3.04	119.66	122.79
3	L5	2363	A2M	C4-N9-C8	3.03	108.92	105.74
1	S2	1442	OMU	O4-C4-C5	-3.03	119.94	125.16
3	L5	2787	A2M	C5-N7-C8	3.03	108.21	103.45
3	L5	398	A2M	N3-C2-N1	-3.02	124.00	128.58
3	L5	3639	PSU	O2-C2-N1	-3.02	119.67	122.79
3	L5	3867	A2M	C4-N9-C8	3.02	108.91	105.74
2	L8	55	PSU	O2-C2-N1	-3.01	119.68	122.79
1	S2	1851	MA6	C6-C5-N7	3.01	138.24	133.43
1	S2	1056	PSU	O2-C2-N1	-3.01	119.69	122.79
3	L5	2839	PSU	O2-C2-N3	-3.01	116.52	121.86
3	L5	3899	OMG	C4-C5-N7	-3.00	105.92	110.67
3	L5	400	A2M	N3-C2-N1	-2.99	124.06	128.58
3	L5	4293	PSU	O2-C2-N1	-2.99	119.70	122.79
1	S2	1851	MA6	C5-N7-C8	2.99	108.15	103.45
3	L5	4220	6MZ	C4-C5-N7	-2.98	107.18	110.58
3	L5	2351	OMC	C1'-N1-C2	2.97	124.99	118.44
3	L5	2815	A2M	C4-C5-N7	-2.97	107.19	110.58
3	L5	2401	A2M	C5-N7-C8	2.96	108.10	103.45
3	L5	3785	A2M	C4-N9-C8	2.96	108.84	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2401	A2M	C4-N9-C8	2.95	108.84	105.74
3	L5	2508	PSU	O2-C2-N1	-2.95	119.74	122.79
1	S2	1447	OMG	C6-C5-N7	2.95	135.66	130.29
3	L5	4442	PSU	O2-C2-N1	-2.94	119.75	122.79
3	L5	4498	OMU	O4-C4-C5	-2.94	120.09	125.16
3	L5	1871	A2M	C4-N9-C8	2.94	108.83	105.74
1	S2	1288	OMU	C2'-C1'-N1	-2.93	108.69	114.24
3	L5	1534	A2M	C5-N7-C8	2.92	108.04	103.45
3	L5	4227	OMU	O4-C4-C5	-2.92	120.13	125.16
1	S2	1678	A2M	C4-N9-C8	2.90	108.78	105.74
3	L5	3723	A2M	C4-C5-N7	-2.90	107.27	110.58
3	L5	1534	A2M	N3-C2-N1	-2.90	124.20	128.58
3	L5	4457	PSU	O2-C2-N1	-2.88	119.81	122.79
1	S2	576	A2M	N3-C2-N1	-2.88	124.22	128.58
3	L5	3792	OMG	C6-C5-N7	2.88	135.52	130.29
1	S2	428	OMU	O4-C4-C5	-2.87	120.21	125.16
3	L5	4228	OMG	C4-C5-N7	-2.86	106.14	110.67
1	S2	1832	6MZ	C5-N7-C8	2.85	107.94	103.45
3	L5	2843	PSU	C5-C6-N1	-2.85	118.18	122.14
3	L5	1862	PSU	C5-C6-N1	-2.85	118.19	122.14
3	L5	1316	OMG	O6-C6-C5	-2.84	119.03	126.53
1	S2	27	A2M	C2'-C1'-N9	-2.84	109.08	113.75
3	L5	4521	PSU	C6-C5-C4	-2.83	116.26	118.17
1	S2	27	A2M	C4-N9-C8	2.83	108.71	105.74
3	L5	398	A2M	C5-N7-C8	2.82	107.89	103.45
3	L5	4673	PSU	C5-C6-N1	-2.82	118.22	122.14
1	S2	436	OMG	C4-C5-N7	-2.81	106.21	110.67
3	L5	4618	OMG	C4-C5-N7	-2.81	106.21	110.67
3	L5	3723	A2M	C4-N9-C8	2.81	108.69	105.74
1	S2	668	A2M	C4-N9-C8	2.81	108.69	105.74
1	S2	1832	6MZ	C4-N9-C8	2.81	108.69	105.74
3	L5	3830	A2M	C6-C5-N7	2.80	137.49	132.09
3	L5	3715	PSU	C5-C6-N1	-2.80	118.26	122.14
1	S2	1850	MA6	N1-C6-N6	2.79	120.26	116.86
3	L5	4431	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	3760	A2M	N3-C2-N1	-2.78	124.38	128.58
3	L5	3869	OMC	O2-C2-N3	-2.78	117.95	122.33
3	L5	1582	PSU	O2-C2-N1	-2.77	119.93	122.79
3	L5	2364	OMG	C2'-C1'-N9	-2.77	108.99	114.24
3	L5	1326	A2M	O2'-C2'-C1'	2.76	114.23	108.99
1	S2	512	A2M	C4-N9-C8	2.76	108.63	105.74
1	S2	1337	4AC	C6-C5-C4	2.75	120.32	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	121	OMU	O4-C4-C5	-2.75	120.42	125.16
83	5A	50[A]	5CT	C4-C3-C2	-2.75	107.68	113.47
1	S2	354	OMU	O4-C4-C5	-2.74	120.44	125.16
3	L5	4523	A2M	C5-N7-C8	2.73	107.74	103.45
1	S2	668	A2M	C6-C5-N7	2.73	137.35	132.09
3	L5	4361	PSU	O2-C2-N1	-2.72	119.98	122.79
1	S2	509	OMG	C4-C5-N7	-2.71	106.38	110.67
3	L5	2364	OMG	C4-C5-N7	-2.71	106.38	110.67
3	L5	4306	OMU	O2-C2-N1	-2.71	119.28	122.80
3	L5	3627	OMG	C4-C5-N7	-2.70	106.39	110.67
1	S2	1383	A2M	C5-N7-C8	2.70	107.69	103.45
3	L5	2415	OMU	O4-C4-C5	-2.69	120.52	125.16
1	S2	1851	MA6	N9-C8-N7	-2.69	110.12	113.94
3	L5	4306	OMU	O4-C4-C5	-2.69	120.52	125.16
3	L5	4623	OMG	C4-C5-N7	-2.69	106.42	110.67
3	L5	3724	A2M	C4-N9-C8	2.68	108.56	105.74
1	S2	668	A2M	C5-N7-C8	2.68	107.66	103.45
3	L5	4499	OMG	C4-C5-N7	-2.68	106.43	110.67
1	S2	1639	G7M	O6-C6-C5	-2.67	122.06	128.01
20	SX	62	HY3	C4-C3-CA	2.67	105.41	102.51
3	L5	3785	A2M	C5-N7-C8	2.65	107.62	103.45
1	S2	1056	PSU	C5-C6-N1	-2.65	118.46	122.14
1	S2	468	A2M	C4-N9-C8	2.65	108.52	105.74
1	S2	166	A2M	C4-N9-C8	2.64	108.52	105.74
3	L5	1322	1MA	N1-C2-N3	-2.64	122.86	126.00
1	S2	1678	A2M	C5-N7-C8	2.64	107.60	103.45
1	S2	1081	PSU	C6-C5-C4	-2.64	116.39	118.17
3	L5	1871	A2M	C6-C5-N7	2.64	137.17	132.09
3	L5	4571	A2M	C5-N7-C8	2.63	107.58	103.45
3	L5	4220	6MZ	N9-C8-N7	-2.63	110.21	113.94
1	S2	1031	A2M	C4-N9-C8	2.63	108.50	105.74
3	L5	1326	A2M	C6-C5-N7	2.62	137.15	132.09
3	L5	4521	PSU	O2-C2-N3	-2.62	117.20	121.86
3	L5	3920	PSU	C5-C6-N1	-2.62	118.50	122.14
3	L5	4423	PSU	C5-C6-N1	-2.62	118.50	122.14
3	L5	2843	PSU	O2-C2-N3	-2.62	117.21	121.86
1	S2	1031	A2M	C5-N7-C8	2.61	107.55	103.45
1	S2	681	PSU	C5-C6-N1	-2.61	118.52	122.14
3	L5	3825	A2M	C2-N1-C6	2.61	123.01	118.73
3	L5	3782	5MC	O2-C2-N3	-2.61	118.22	122.33
3	L5	1534	A2M	N9-C8-N7	-2.61	110.24	113.94
3	L5	3899	OMG	C2'-C1'-N9	-2.60	109.30	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4220	6MZ	C5-N7-C8	2.60	107.54	103.45
3	L5	3744	OMG	C4-C5-N7	-2.60	106.55	110.67
3	L5	4196	OMG	C4-C5-N7	-2.60	106.55	110.67
3	L5	2843	PSU	O2-C2-N1	-2.60	120.11	122.79
1	S2	1643	PSU	C5-C6-N1	-2.59	118.55	122.14
3	L5	3627	OMG	C2'-C1'-N9	-2.59	109.33	114.24
3	L5	3851	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	4370	OMG	C4-C5-N7	-2.58	106.59	110.67
3	L5	2363	A2M	C5-N7-C8	2.58	107.50	103.45
1	S2	109	PSU	C5-C6-N1	-2.57	118.57	122.14
1	S2	1850	MA6	N9-C8-N7	-2.57	110.28	113.94
1	S2	1328	OMG	C4-C5-N7	-2.57	106.59	110.67
1	S2	159	A2M	C5-N7-C8	2.57	107.49	103.45
1	S2	1447	OMG	C4-C5-N7	-2.57	106.60	110.67
3	L5	4523	A2M	N9-C8-N7	-2.57	110.29	113.94
1	S2	918	PSU	O4'-C1'-C2'	2.56	108.70	105.15
3	L5	4296	PSU	C5-C6-N1	-2.55	118.60	122.14
3	L5	398	A2M	C4-N9-C8	2.55	108.42	105.74
3	L5	5001	PSU	C5-C6-N1	-2.55	118.61	122.14
3	L5	4569	PSU	C5-C6-N1	-2.54	118.62	122.14
3	L5	3724	A2M	C5-N7-C8	2.54	107.44	103.45
3	L5	4623	OMG	C2'-C1'-N9	-2.54	109.43	114.24
3	L5	3718	A2M	N3-C2-N1	-2.54	124.74	128.58
1	S2	27	A2M	C5-N7-C8	2.53	107.43	103.45
1	S2	1337	4AC	O2-C2-N3	-2.53	118.34	122.33
3	L5	2839	PSU	C5-C6-N1	-2.53	118.63	122.14
3	L5	1522	OMG	O6-C6-C5	-2.53	119.86	126.53
3	L5	4523	A2M	C2-N1-C6	2.53	122.88	118.73
3	L5	2787	A2M	C6-C5-N7	2.53	136.96	132.09
1	S2	166	A2M	C5-N7-C8	2.52	107.42	103.45
1	S2	601	OMG	C4-C5-N7	-2.52	106.67	110.67
1	S2	1842	4AC	C6-C5-C4	2.52	120.04	117.00
3	L5	1524	A2M	C4-C5-N7	-2.52	107.71	110.58
3	L5	1316	OMG	C2'-C1'-N9	-2.51	109.47	114.24
3	L5	4532	PSU	O2-C2-N3	-2.51	117.40	121.86
3	L5	400	A2M	C5-N7-C8	2.50	107.39	103.45
3	L5	3851	PSU	C6-C5-C4	-2.50	116.49	118.17
3	L5	1860	PSU	O2-C2-N1	-2.50	120.21	122.79
1	S2	590	A2M	C4-N9-C8	2.50	108.36	105.74
3	L5	3825	A2M	C6-C5-N7	2.49	136.90	132.09
1	S2	512	A2M	C5-N7-C8	2.49	107.36	103.45
3	L5	4590	A2M	C4-N9-C8	2.48	108.35	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1322	1MA	C6-C5-N7	2.48	136.55	132.16
1	S2	590	A2M	C5-N7-C8	2.48	107.35	103.45
3	L5	4637	OMG	C4-C5-N7	-2.48	106.74	110.67
3	L5	3830	A2M	C2-N1-C6	2.48	122.81	118.73
1	S2	1832	6MZ	C2-N1-C6	2.48	123.45	115.24
1	S2	1490	OMG	O6-C6-C5	-2.48	120.00	126.53
3	L5	2401	A2M	C6-C5-N7	2.47	136.86	132.09
1	S2	484	A2M	C5-N7-C8	2.47	107.33	103.45
1	S2	822	PSU	C5-C6-N1	-2.47	118.72	122.14
3	L5	3853	PSU	C6-C5-C4	-2.46	116.51	118.17
1	S2	1490	OMG	C4-C5-N7	-2.46	106.77	110.67
3	L5	4370	OMG	O6-C6-C5	-2.46	120.03	126.53
1	S2	644	OMG	C4-C5-N7	-2.46	106.77	110.67
2	L8	14	OMU	O4-C4-C5	-2.46	120.92	125.16
1	S2	99	A2M	C5-N7-C8	2.46	107.32	103.45
3	L5	4494	OMG	C4-C5-N7	-2.46	106.77	110.67
3	L5	2363	A2M	N9-C8-N7	-2.46	110.45	113.94
1	S2	428	OMU	O2-C2-N1	-2.46	119.60	122.80
1	S2	1136	PSU	C5-C6-N1	-2.45	118.74	122.14
1	S2	668	A2M	C2-N1-C6	2.44	122.74	118.73
1	S2	1851	MA6	C4-N9-C1'	-2.44	120.92	126.63
1	S2	468	A2M	C5-N7-C8	2.43	107.28	103.45
3	L5	3825	A2M	C4-N9-C8	2.43	108.29	105.74
3	L5	1536	PSU	C5-C6-N1	-2.43	118.77	122.14
1	S2	1031	A2M	C2-N1-C6	2.42	122.71	118.73
3	L5	2424	OMG	C4-C5-N7	-2.42	106.83	110.67
1	S2	867	OMG	C4-C5-N7	-2.42	106.83	110.67
3	L5	3744	OMG	O6-C6-C5	-2.42	120.14	126.53
1	S2	27	A2M	C6-C5-N7	2.42	136.75	132.09
3	L5	4552	PSU	C5-C6-N1	-2.41	118.79	122.14
3	L5	4590	A2M	C5-N7-C8	2.41	107.24	103.45
1	S2	406	PSU	C5-C6-N1	-2.41	118.79	122.14
3	L5	4442	PSU	O2-C2-N3	-2.40	117.59	121.86
1	S2	1842	4AC	C1'-N1-C2	2.40	123.75	118.44
3	L5	2876	OMG	C5-C6-N1	2.40	119.36	113.25
3	L5	3944	OMG	C4-C5-N7	-2.40	106.87	110.67
3	L5	4494	OMG	C5-C6-N1	2.40	119.36	113.25
3	L5	1534	A2M	C6-C5-N7	2.39	136.70	132.09
3	L5	4403	PSU	C5-C6-N1	-2.39	118.82	122.14
3	L5	4673	PSU	O2-C2-N1	-2.39	120.32	122.79
3	L5	1862	PSU	O2-C2-N3	-2.39	117.62	121.86
1	S2	34	PSU	C5-C6-N1	-2.39	118.83	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	93	PSU	O2-C2-N3	-2.38	117.63	121.86
1	S2	1383	A2M	N9-C8-N7	-2.37	110.57	113.94
3	L5	2815	A2M	C5-N7-C8	2.37	107.18	103.45
1	S2	683	OMG	C4-C5-N7	-2.37	106.92	110.67
3	L5	3792	OMG	O6-C6-C5	-2.36	120.29	126.53
3	L5	4431	PSU	C6-C5-C4	-2.36	116.58	118.17
3	L5	4220	6MZ	C2-N1-C6	2.36	123.06	115.24
1	S2	1383	A2M	C6-C5-N7	2.36	136.63	132.09
1	S2	484	A2M	C6-C5-N7	2.36	136.63	132.09
1	S2	1850	MA6	C6-C5-N7	2.35	137.19	133.43
3	L5	3899	OMG	O6-C6-C5	-2.35	120.33	126.53
3	L5	4498	OMU	O2-C2-N1	-2.35	119.74	122.80
3	L5	4228	OMG	O6-C6-C5	-2.35	120.34	126.53
3	L5	4590	A2M	C2-N1-C6	2.34	122.58	118.73
3	L5	1625	OMG	O6-C6-C5	-2.34	120.36	126.53
3	L5	3830	A2M	C5-N7-C8	2.34	107.12	103.45
3	L5	2401	A2M	N9-C8-N7	-2.34	110.62	113.94
3	L5	4569	PSU	O4-C4-C5	-2.33	118.21	124.01
50	La	39	V5N	O-C-CA	-2.33	118.77	124.77
1	S2	159	A2M	C4-N9-C8	2.33	108.19	105.74
1	S2	576	A2M	C5-N7-C8	2.33	107.11	103.45
3	L5	4628	PSU	C5-C6-N1	-2.33	118.91	122.14
82	Pt	21	H2U	C5-C6-N1	-2.33	104.47	111.52
3	L5	1524	A2M	N9-C8-N7	-2.33	110.63	113.94
3	L5	1326	A2M	C2-N1-C6	2.33	122.55	118.73
1	S2	1842	4AC	C5-C4-N3	-2.33	118.96	122.60
2	L8	69	PSU	O4'-C1'-C2'	2.32	108.36	105.15
3	L5	1326	A2M	C5-N7-C8	2.32	107.10	103.45
1	S2	576	A2M	C4-N9-C8	2.32	108.17	105.74
3	L5	3639	PSU	C5-C6-N1	-2.32	118.93	122.14
1	S2	1081	PSU	O2-C2-N3	-2.32	117.75	121.86
3	L5	4521	PSU	C5-C6-N1	-2.31	118.93	122.14
3	L5	5001	PSU	O2-C2-N3	-2.31	117.76	121.86
3	L5	4689	PSU	C5-C6-N1	-2.31	118.94	122.14
3	L5	3925	OMU	O4-C4-C5	-2.31	121.18	125.16
3	L5	1524	A2M	O2'-C2'-C1'	-2.31	104.61	108.99
3	L5	3818	UY1	C5-C6-N1	-2.30	118.94	122.14
3	L5	1522	OMG	C5-C6-N1	2.30	119.12	113.25
3	L5	1862	PSU	O2-C2-N1	-2.30	120.42	122.79
3	L5	4972	PSU	O2-C2-N3	-2.30	117.78	121.86
3	L5	1322	1MA	C4-C5-N7	-2.29	107.03	110.67
2	L8	75	OMG	C4-C5-N7	-2.29	107.04	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3785	A2M	N9-C8-N7	-2.29	110.68	113.94
3	L5	1871	A2M	N9-C8-N7	-2.29	110.69	113.94
3	L5	4361	PSU	O2-C2-N3	-2.29	117.80	121.86
3	L5	4673	PSU	O2-C2-N3	-2.29	117.80	121.86
3	L5	4392	OMG	O6-C6-C5	-2.28	120.50	126.53
3	L5	1522	OMG	C8-N9-C4	2.28	110.31	106.03
3	L5	1316	OMG	C5-C6-N1	2.28	119.06	113.25
1	S2	572	PSU	C5-C6-N1	-2.28	118.97	122.14
3	L5	3884	PSU	C5-C6-N1	-2.28	118.98	122.14
1	S2	1174	PSU	C6-C5-C4	-2.27	116.64	118.17
1	S2	1288	OMU	O2-C2-N1	-2.27	119.84	122.80
3	L5	3724	A2M	C6-C5-N7	2.27	136.47	132.09
2	L8	55	PSU	C5-C6-N1	-2.27	118.99	122.14
3	L5	1860	PSU	O2-C2-N3	-2.27	117.83	121.86
3	L5	4618	OMG	O6-C6-C5	-2.27	120.55	126.53
3	L5	1326	A2M	C4-N9-C8	2.27	108.12	105.74
82	Pt	56	PSU	C5-C6-N1	-2.27	119.00	122.14
1	S2	105	PSU	C5-C6-N1	-2.27	119.00	122.14
1	S2	683	OMG	O6-C6-C5	-2.26	120.56	126.53
1	S2	1232	PSU	C5-C6-N1	-2.26	119.00	122.14
1	S2	1804	OMU	O2-C2-N1	-2.26	119.86	122.80
3	L5	4293	PSU	C6-C5-C4	-2.26	116.65	118.17
3	L5	3760	A2M	C5-N7-C8	2.26	107.00	103.45
3	L5	4499	OMG	O6-C6-C5	-2.25	120.59	126.53
1	S2	119	PSU	C5-C6-N1	-2.25	119.02	122.14
1	S2	1081	PSU	O2-C2-N1	-2.25	120.47	122.79
3	L5	4569	PSU	O2-C2-N3	-2.24	117.88	121.86
3	L5	1522	OMG	C2'-C1'-N9	-2.24	109.98	114.24
3	L5	1522	OMG	C4-C5-N7	-2.24	107.12	110.67
1	S2	918	PSU	C5-C6-N1	-2.24	119.03	122.14
3	L5	4228	OMG	C8-N7-C5	2.24	108.25	104.26
3	L5	3830	A2M	C4-N9-C8	2.24	108.09	105.74
3	L5	3724	A2M	C2'-C1'-N9	-2.24	110.07	113.75
3	L5	1326	A2M	O4'-C1'-N9	-2.23	103.80	108.09
3	L5	1524	A2M	C5-N7-C8	2.23	106.95	103.45
3	L5	4392	OMG	C8-N7-C5	2.23	108.23	104.26
3	L5	3944	OMG	O6-C6-C5	-2.23	120.65	126.53
3	L5	3867	A2M	O2'-C2'-C1'	-2.23	104.76	108.99
3	L5	2508	PSU	C5-C6-N1	-2.23	119.05	122.14
3	L5	3899	OMG	C8-N7-C5	2.23	108.23	104.26
3	L5	3825	A2M	C5-N7-C8	2.23	106.95	103.45
3	L5	4442	PSU	O4'-C1'-C2'	2.22	108.22	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1004	PSU	C5-C6-N1	-2.22	119.06	122.14
1	S2	1383	A2M	O4'-C1'-N9	2.22	112.35	108.09
3	L5	4293	PSU	O2-C2-N3	-2.22	117.92	121.86
3	L5	3723	A2M	C5-N7-C8	2.21	106.93	103.45
3	L5	3758	PSU	C5-C6-N1	-2.21	119.07	122.14
3	L5	4628	PSU	O4'-C1'-C2'	2.21	108.21	105.15
1	S2	93	PSU	C5-C6-N1	-2.20	119.08	122.14
1	S2	668	A2M	N9-C8-N7	-2.20	110.81	113.94
1	S2	801	PSU	C5-C6-N1	-2.20	119.08	122.14
3	L5	3792	OMG	C4-C5-N7	-2.20	107.18	110.67
1	S2	1347	PSU	C5-C6-N1	-2.20	119.09	122.14
1	S2	815	PSU	C5-C6-N1	-2.20	119.09	122.14
1	S2	1337	4AC	C5-C4-N3	-2.20	119.16	122.60
1	S2	1248	B8N	O2-C2-N3	-2.19	119.03	121.98
3	L5	3867	A2M	O4'-C1'-N9	2.19	112.29	108.09
3	L5	4637	OMG	O6-C6-C5	-2.18	120.77	126.53
1	S2	159	A2M	C6-C5-N7	2.18	136.30	132.09
1	S2	1239	PSU	C5-C6-N1	-2.18	119.11	122.14
3	L5	3639	PSU	O2-C2-N3	-2.18	117.99	121.86
3	L5	3760	A2M	C4-N9-C8	2.18	108.03	105.74
3	L5	4442	PSU	C5-C6-N1	-2.18	119.12	122.14
3	L5	1881	OMC	O2'-C2'-C1'	2.18	113.12	108.99
1	S2	1447	OMG	O6-C6-C5	-2.18	120.79	126.53
3	L5	2363	A2M	C6-C5-N7	2.17	136.28	132.09
3	L5	4523	A2M	C6-C5-N7	2.17	136.28	132.09
3	L5	4312	PSU	C5-C6-N1	-2.17	119.12	122.14
3	L5	2351	OMC	O2-C2-N3	-2.17	118.91	122.33
1	S2	36	PSU	C5-C6-N1	-2.17	119.12	122.14
2	L8	75	OMG	O6-C6-C5	-2.17	120.81	126.53
3	L5	4299	PSU	C5-C6-N1	-2.17	119.13	122.14
3	L5	1534	A2M	C2-N1-C6	2.17	122.29	118.73
3	L5	4361	PSU	C5-C6-N1	-2.17	119.14	122.14
3	L5	2837	OMU	C2'-C1'-N1	-2.16	110.13	114.24
1	S2	1678	A2M	N9-C8-N7	-2.16	110.87	113.94
3	L5	3785	A2M	C6-C5-N7	2.16	136.25	132.09
3	L5	1625	OMG	C8-N7-C5	2.16	108.11	104.26
3	L5	3762	PSU	C5-C6-N1	-2.16	119.15	122.14
3	L5	4532	PSU	O2-C2-N1	-2.16	120.56	122.79
1	S2	468	A2M	C6-C5-N7	2.15	136.24	132.09
1	S2	867	OMG	O6-C6-C5	-2.15	120.85	126.53
1	S2	1248	B8N	O36-C34-O35	-2.15	119.20	124.08
3	L5	4571	A2M	C4-N9-C8	2.15	108.00	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3851	PSU	O2-C2-N3	-2.15	118.04	121.86
3	L5	1860	PSU	C5-C6-N1	-2.15	119.16	122.14
3	L5	2876	OMG	O6-C6-C5	-2.15	120.87	126.53
1	S2	644	OMG	O6-C6-C5	-2.14	120.87	126.53
3	L5	3723	A2M	C2'-C1'-N9	-2.14	110.22	113.75
3	L5	1316	OMG	C4-C5-N7	-2.14	107.28	110.67
3	L5	3867	A2M	C6-C5-N7	2.14	136.22	132.09
1	S2	1177	PSU	C5-C6-N1	-2.14	119.17	122.14
1	S2	1678	A2M	C6-C5-N7	2.14	136.22	132.09
1	S2	27	A2M	C2-N1-C6	2.14	122.24	118.73
3	L5	2787	A2M	C5'-C4'-C3'	-2.13	107.53	115.21
1	S2	1625	PSU	C5-C6-N1	-2.13	119.18	122.14
3	L5	3695	PSU	O2-C2-N3	-2.13	118.07	121.86
3	L5	2837	OMU	O4-C4-C5	-2.13	121.49	125.16
3	L5	2632	PSU	C5-C6-N1	-2.13	119.19	122.14
3	L5	398	A2M	C6-C5-N7	2.12	136.18	132.09
2	L8	69	PSU	C5-C6-N1	-2.12	119.20	122.14
1	S2	436	OMG	C5-C6-N1	2.12	118.65	113.25
3	L5	3867	A2M	N9-C8-N7	-2.12	110.93	113.94
1	S2	468	A2M	C2-N1-C6	2.12	122.21	118.73
3	L5	4299	PSU	O2-C2-N3	-2.11	118.11	121.86
1	S2	1692	PSU	C5-C6-N1	-2.11	119.21	122.14
3	L5	2804	OMC	C6-C5-C4	2.11	121.00	117.53
3	L5	3627	OMG	O6-C6-C5	-2.11	120.96	126.53
1	S2	627	OMU	O2-C2-N1	-2.11	120.05	122.80
1	S2	576	A2M	C6-C5-N7	2.11	136.16	132.09
3	L5	3764	PSU	C5-C6-N1	-2.11	119.22	122.14
3	L5	1326	A2M	N6-C6-N1	2.10	123.06	118.38
3	L5	4689	PSU	O2-C2-N3	-2.10	118.13	121.86
3	L5	4196	OMG	O6-C6-C5	-2.10	120.99	126.53
1	S2	1056	PSU	O4'-C1'-C2'	2.10	108.05	105.15
3	L5	1522	OMG	N9-C8-N7	-2.10	109.51	113.40
3	L5	5010	PSU	C5-C6-N1	-2.10	119.23	122.14
2	L8	14	OMU	O2-C2-N1	-2.10	120.07	122.80
3	L5	4530	UR3	C3U-N3-C2	2.10	120.98	117.33
3	L5	4227	OMU	O2-C2-N1	-2.10	120.07	122.80
3	L5	3808	OMC	O2-C2-N3	-2.09	119.03	122.33
1	S2	172	OMU	O2-C2-N1	-2.09	120.07	122.80
1	S2	651	PSU	C5-C6-N1	-2.09	119.23	122.14
3	L5	2364	OMG	O6-C6-C5	-2.09	121.01	126.53
3	L5	3785	A2M	C2-N1-C6	2.09	122.17	118.73
3	L5	4228	OMG	N9-C8-N7	-2.09	109.53	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4636	PSU	C5-C6-N1	-2.08	119.25	122.14
3	L5	4590	A2M	O4'-C4'-C3'	-2.08	101.02	105.15
1	S2	99	A2M	C2'-C1'-N9	-2.08	110.32	113.75
1	S2	296	PSU	C5-C6-N1	-2.08	119.25	122.14
1	S2	1337	4AC	O7-C7-N4	2.08	125.17	121.90
3	L5	3768	PSU	C5-C6-N1	-2.08	119.25	122.14
3	L5	3760	A2M	O4'-C1'-N9	2.08	112.08	108.09
1	S2	1842	4AC	N4-C4-N3	2.08	117.24	113.87
3	L5	2804	OMC	O2-C2-N3	-2.08	119.06	122.33
3	L5	3637	PSU	C5-C6-N1	-2.08	119.26	122.14
82	Pt	8	4SU	O2-C2-N1	-2.07	120.10	122.80
1	S2	27	A2M	N9-C8-N7	-2.07	110.99	113.94
3	L5	4590	A2M	C6-C5-N7	2.07	136.09	132.09
3	L5	3884	PSU	O2-C2-N3	-2.07	118.18	121.86
1	S2	1031	A2M	N9-C8-N7	-2.07	111.00	113.94
1	S2	1243	PSU	C5-C6-N1	-2.07	119.27	122.14
1	S2	1248	B8N	O4'-C1'-C2'	2.07	108.02	105.15
3	L5	3718	A2M	C5-N7-C8	2.07	106.70	103.45
3	L5	3724	A2M	N9-C8-N7	-2.07	111.00	113.94
3	L5	4618	OMG	C5-C6-N1	2.07	118.52	113.25
2	L8	75	OMG	C5-C6-N1	2.07	118.52	113.25
3	L5	4423	PSU	O2-C2-N3	-2.07	118.19	121.86
3	L5	3830	A2M	O2'-C2'-C1'	2.07	112.91	108.99
1	S2	218	PSU	C6-C5-C4	-2.07	116.78	118.17
1	S2	93	PSU	O2-C2-N1	-2.06	120.66	122.79
3	L5	2424	OMG	O6-C6-C5	-2.06	121.09	126.53
3	L5	4499	OMG	C5-C6-N1	2.06	118.49	113.25
3	L5	3701	OMC	C5-C6-N1	-2.06	118.49	121.84
3	L5	3729	PSU	C5-C6-N1	-2.06	119.28	122.14
1	S2	683	OMG	C5-C6-N1	2.06	118.49	113.25
3	L5	4500	PSU	O4'-C1'-C2'	2.05	107.99	105.15
3	L5	1871	A2M	C2-N1-C6	2.05	122.10	118.73
3	L5	4457	PSU	O2-C2-N3	-2.05	118.22	121.86
3	L5	1522	OMG	C2-N1-C6	-2.05	121.40	125.11
3	L5	2632	PSU	O4'-C1'-C2'	2.05	107.98	105.15
3	L5	4618	OMG	C8-N7-C5	2.04	107.90	104.26
3	L5	4636	PSU	O4'-C1'-C2'	2.04	107.97	105.15
3	L5	1625	OMG	C2-N1-C6	-2.04	121.41	125.11
40	LB	245	HIC	CB-CG-CD2	-2.04	125.04	129.96
3	L5	2415	OMU	C1'-N1-C2	2.04	121.25	117.59
1	S2	1643	PSU	O2-C2-N3	-2.04	118.24	121.86
3	L5	3734	PSU	O4'-C1'-C2'	2.04	107.97	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	398	A2M	N9-C8-N7	-2.03	111.05	113.94
3	L5	4536	OMC	C6-C5-C4	2.03	120.86	117.53
2	L8	55	PSU	O2-C2-N3	-2.03	118.25	121.86
1	S2	512	A2M	N9-C8-N7	-2.03	111.05	113.94
3	L5	1534	A2M	C2'-C1'-N9	2.03	117.09	113.75
1	S2	573	PSU	C5-C6-N1	-2.03	119.32	122.14
3	L5	1582	PSU	O2-C2-N3	-2.03	118.26	121.86
1	S2	174	OMC	O2-C2-N3	-2.03	119.14	122.33
3	L5	2364	OMG	C5-C6-N1	2.02	118.40	113.25
1	S2	1238	PSU	C5-C6-N1	-2.02	119.33	122.14
1	S2	1056	PSU	O2-C2-N3	-2.02	118.28	121.86
3	L5	4532	PSU	C5-C6-N1	-2.02	119.34	122.14
1	S2	1445	PSU	O4'-C1'-C2'	2.01	107.94	105.15
3	L5	2401	A2M	C2-N1-C6	2.01	122.03	118.73
3	L5	3695	PSU	C5-C6-N1	-2.01	119.35	122.14
3	L5	4228	OMG	C8-N9-C4	2.01	109.79	106.03
82	Pt	8	4SU	C2'-C1'-N1	-2.01	107.66	113.25
20	SX	62	HY3	C3-CA-N	2.01	107.93	103.67
3	L5	3724	A2M	C2-N1-C6	2.01	122.02	118.73
1	S2	1842	4AC	O7-C7-N4	2.00	125.05	121.90
3	L5	1779	PSU	C5-C6-N1	-2.00	119.36	122.14
3	L5	4403	PSU	O2-C2-N3	-2.00	118.31	121.86
1	S2	572	PSU	O4'-C1'-C2'	2.00	107.92	105.15
3	L5	4536	OMC	O2-C2-N3	-2.00	119.17	122.33
1	S2	166	A2M	C6-C5-N7	2.00	135.95	132.09
3	L5	4494	OMG	O6-C6-C5	-2.00	121.25	126.53

There are no chirality outliers.

All (169) 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
6	SA	2	SAC	CB-CA-N-C1A
6	SA	2	SAC	O-C-CA-CB
29	SV	1	AME	OT-CT1-N-CA
64	Lr	2	SAC	C2A-C1A-N-CA
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	159	A2M	C1'-C2'-O2'-CM'
1	S2	166	A2M	C1'-C2'-O2'-CM'
1	S2	462	OMC	C1'-C2'-O2'-CM2
1	S2	484	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
1	S2	644	OMG	O4'-C4'-C5'-O5'
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	668	A2M	C1'-C2'-O2'-CM'
1	S2	867	OMG	C1'-C2'-O2'-CM2
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1288	OMU	C1'-C2'-O2'-CM2
1	S2	1383	A2M	C1'-C2'-O2'-CM'
1	S2	1442	OMU	O4'-C4'-C5'-O5'
1	S2	1447	OMG	C1'-C2'-O2'-CM2
1	S2	1490	OMG	C1'-C2'-O2'-CM2
1	S2	1678	A2M	C1'-C2'-O2'-CM'
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	2415	OMU	C1'-C2'-O2'-CM2
3	L5	2424	OMG	C1'-C2'-O2'-CM2
3	L5	2815	A2M	C1'-C2'-O2'-CM'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	3718	A2M	C1'-C2'-O2'-CM'
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3760	A2M	C1'-C2'-O2'-CM'
3	L5	3925	OMU	C1'-C2'-O2'-CM2
3	L5	4220	6MZ	N1-C6-N6-C9
3	L5	4370	OMG	C1'-C2'-O2'-CM2
3	L5	4420	PSU	O4'-C4'-C5'-O5'
3	L5	4523	A2M	C1'-C2'-O2'-CM'
3	L5	4571	A2M	C1'-C2'-O2'-CM'
3	L5	4590	A2M	C4'-C5'-O5'-P
39	LA	216	V5N	O-C-CA-CB
83	5A	50[A]	5CT	C2-C1-NZ-CE
83	5A	50[A]	5CT	NZ-C1-C2-C3
83	5A	50[A]	5CT	NZ-C1-C2-O1
83	5A	50[A]	5CT	C-CA-CB-CG
83	5A	50[A]	5CT	N-CA-CB-CG
83	5A	50[B]	5CT	CD-CE-NZ-C1
83	5A	50[B]	5CT	NZ-C1-C2-C3
83	5A	50[B]	5CT	NZ-C1-C2-O1
83	5A	50[B]	5CT	C1-C2-C3-C4
83	5A	50[B]	5CT	O1-C2-C3-C4
83	5A	50[B]	5CT	C-CA-CB-CG
83	5A	50[B]	5CT	N-CA-CB-CG
3	L5	3701	OMC	C2'-C1'-N1-C2
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	1442	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	1851	MA6	O4'-C4'-C5'-O5'
3	L5	3944	OMG	O4'-C4'-C5'-O5'
3	L5	3944	OMG	C3'-C4'-C5'-O5'
3	L5	4420	PSU	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
3	L5	4636	PSU	C3'-C4'-C5'-O5'
79	Lo	53	MLZ	CG-CD-CE-NZ
6	SA	2	SAC	C2A-C1A-N-CA
64	Lr	2	SAC	OAC-C1A-N-CA
83	5A	50[A]	5CT	CD-CE-NZ-C1
1	S2	590	A2M	O4'-C4'-C5'-O5'
1	S2	683	OMG	O4'-C4'-C5'-O5'
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C4'-C5'-O5'
82	Pt	21	H2U	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C4
3	L5	1625	OMG	C3'-C2'-O2'-CM2
3	L5	4228	OMG	C3'-C2'-O2'-CM2
1	S2	590	A2M	C3'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
1	S2	576	A2M	O4'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	1447	OMG	C3'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
3	L5	3764	PSU	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
29	SV	1	AME	CA-CB-CG-SD
3	L5	4447	5MC	C2'-C1'-N1-C6
1	S2	1851	MA6	C3'-C4'-C5'-O5'
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
82	Pt	21	H2U	C3'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
3	L5	3764	PSU	O4'-C4'-C5'-O5'
29	SV	1	AME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
64	Lr	2	SAC	C-CA-N-C1A
83	5A	50[B]	5CT	CE-CD-CG-CB
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	4637	OMG	C1'-C2'-O2'-CM2
20	SX	62	HY3	O-C-CA-C3
83	5A	50[A]	5CT	C2-C3-C4-N1
1	S2	822	PSU	C3'-C4'-C5'-O5'
3	L5	3760	A2M	C2'-C1'-N9-C8
1	S2	1248	B8N	C31-C32-C33-N34
83	5A	50[A]	5CT	C1-C2-C3-C4
1	S2	172	OMU	C3'-C2'-O2'-CM2
3	L5	1534	A2M	C3'-C2'-O2'-CM'
83	5A	50[A]	5CT	CG-CD-CE-NZ
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	1781	PSU	C3'-C4'-C5'-O5'
1	S2	668	A2M	C2'-C1'-N9-C8
64	Lr	2	SAC	CB-CA-N-C1A
3	L5	4500	PSU	C4'-C5'-O5'-P
3	L5	3760	A2M	O4'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	1322	1MA	C2'-C1'-N9-C8
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3818	UY1	C4'-C5'-O5'-P
1	S2	573	PSU	O4'-C1'-C5-C4
1	S2	1326	UY1	O4'-C1'-C5-C4
3	L5	3695	PSU	O4'-C1'-C5-C4
3	L5	4521	PSU	O4'-C1'-C5-C4
3	L5	3701	OMC	O4'-C1'-N1-C6
1	S2	1248	B8N	C32-C31-N3-C4
3	L5	3701	OMC	O4'-C1'-N1-C2
1	S2	1447	OMG	O4'-C4'-C5'-O5'
3	L5	3760	A2M	O4'-C1'-N9-C8
1	S2	590	A2M	C4'-C5'-O5'-P
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	1490	OMG	C4'-C5'-O5'-P
1	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	3760	A2M	C3'-C4'-C5'-O5'
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	1322	1MA	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
82	Pt	47	G7M	C4'-C5'-O5'-P
3	L5	3760	A2M	C2'-C1'-N9-C4
1	S2	1328	OMG	C1'-C2'-O2'-CM2
1	S2	1442	OMU	C1'-C2'-O2'-CM2
3	L5	2804	OMC	C1'-C2'-O2'-CM2
3	L5	2815	A2M	C4'-C5'-O5'-P
1	S2	428	OMU	O4'-C1'-N1-C6
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	4521	PSU	O4'-C1'-C5-C6
82	Pt	21	H2U	C4'-C5'-O5'-P
1	S2	428	OMU	C2'-C1'-N1-C6
1	S2	668	A2M	O4'-C1'-N9-C8
3	L5	2787	A2M	O4'-C1'-N9-C8
3	L5	1792	PSU	O4'-C4'-C5'-O5'
1	S2	1081	PSU	C4'-C5'-O5'-P
79	Lo	53	MLZ	CA-CB-CG-CD
1	S2	590	A2M	O4'-C1'-N9-C8
3	L5	4471	PSU	C3'-C4'-C5'-O5'
3	L5	3844	PSU	C4'-C5'-O5'-P
83	5A	50[B]	5CT	CA-CB-CG-CD
3	L5	2401	A2M	C3'-C2'-O2'-CM'
1	S2	1832	6MZ	N1-C6-N6-C9
1	S2	822	PSU	O4'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	2351	OMC	C2'-C1'-N1-C2
1	S2	1248	B8N	N34-C33-C34-O36
3	L5	4220	6MZ	C5-C6-N6-C9
1	S2	1490	OMG	O4'-C4'-C5'-O5'
79	Lo	53	MLZ	N-CA-CB-CG
1	S2	1248	B8N	N34-C33-C34-O35
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C2'-C1'-N1-C6

There are no ring outliers.

88 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1832	6MZ	1	0
3	L5	4196	OMG	2	0
3	L5	400	A2M	1	0
1	S2	354	OMU	1	0
1	S2	1639	G7M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3718	A2M	4	0
1	S2	116	OMU	2	0
3	L5	2415	OMU	3	0
3	L5	4457	PSU	2	0
1	S2	1692	PSU	1	0
1	S2	109	PSU	1	0
3	L5	3867	A2M	2	0
3	L5	4552	PSU	1	0
3	L5	4618	OMG	2	0
82	Pt	33	OMC	1	0
3	L5	2363	A2M	2	0
3	L5	4637	OMG	1	0
1	S2	668	A2M	1	0
3	L5	3723	A2M	3	0
3	L5	3729	PSU	1	0
3	L5	4571	A2M	1	0
1	S2	484	A2M	1	0
1	S2	1383	A2M	3	0
3	L5	4531	PSU	1	0
3	L5	3785	A2M	1	0
1	S2	159	A2M	2	0
3	L5	3762	PSU	1	0
3	L5	3701	OMC	1	0
3	L5	4220	6MZ	1	0
3	L5	2815	A2M	3	0
1	S2	644	OMG	1	0
3	L5	3899	OMG	1	0
3	L5	2508	PSU	2	0
1	S2	99	A2M	2	0
1	S2	867	OMG	1	0
3	L5	3734	PSU	1	0
1	S2	1678	A2M	1	0
1	S2	1232	PSU	1	0
3	L5	4498	OMU	1	0
3	L5	4370	OMG	1	0
3	L5	4447	5MC	1	0
3	L5	4456	OMC	2	0
3	L5	4392	OMG	1	0
3	L5	2861	OMC	1	0
1	S2	1490	OMG	2	0
3	L5	3944	OMG	1	0
3	L5	1536	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4620	OMU	1	0
2	L8	75	OMG	1	0
1	S2	1004	PSU	1	0
1	S2	1447	OMG	1	0
3	L5	2876	OMG	1	0
82	Pt	21	H2U	1	0
3	L5	2804	OMC	1	0
3	L5	1881	OMC	1	0
1	S2	1288	OMU	1	0
3	L5	2632	PSU	1	0
3	L5	3724	A2M	1	0
3	L5	2364	OMG	1	0
1	S2	576	A2M	3	0
3	L5	1781	PSU	1	0
3	L5	2787	A2M	1	0
83	5A	50[B]	5CT	5	0
1	S2	1391	OMC	1	0
1	S2	649	PSU	1	0
3	L5	1871	A2M	2	0
1	S2	509	OMG	1	0
1	S2	27	A2M	1	0
82	Pt	56	PSU	2	0
1	S2	1442	OMU	1	0
3	L5	1683	PSU	1	0
3	L5	4530	UR3	1	0
3	L5	5001	PSU	1	0
3	L5	3770	PSU	1	0
1	S2	512	A2M	2	0
1	S2	1239	PSU	1	0
3	L5	1524	A2M	1	0
1	S2	218	PSU	1	0
1	S2	166	A2M	2	0
3	L5	398	A2M	1	0
1	S2	573	PSU	2	0
2	L8	14	OMU	1	0
3	L5	4442	PSU	1	0
3	L5	4579	PSU	1	0
83	5A	50[A]	5CT	4	0
1	S2	462	OMC	1	0
3	L5	2351	OMC	1	0
3	L5	1340	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 636 ligands modelled in this entry, 609 are monoatomic - leaving 27 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	$\# Z > 2$
91	MET	Pt	78	82	6,7,8	0.65	0	2,7,9	1.36	0
84	SPD	L5	5504	-	9,9,9	0.39	0	8,8,8	1.02	0
85	PUT	L5	5515	-	5,5,5	0.13	0	4,4,4	0.16	0
85	PUT	L5	5518	-	5,5,5	0.18	0	4,4,4	0.22	0
84	SPD	L5	5510	-	9,9,9	0.28	0	8,8,8	0.74	0
84	SPD	L5	5512	-	9,9,9	0.38	0	8,8,8	0.60	0
84	SPD	L5	5505	-	9,9,9	0.42	0	8,8,8	1.10	1 (12%)
85	PUT	L5	5520	-	5,5,5	0.16	0	4,4,4	0.25	0
89	3H3	L5	5523	-	34,34,34	3.30	13 (38%)	36,45,45	3.67	18 (50%)
85	PUT	S2	1903	-	5,5,5	0.07	0	4,4,4	0.15	0
85	PUT	L5	5514	-	5,5,5	0.13	0	4,4,4	0.20	0
84	SPD	L5	5503	-	9,9,9	0.29	0	8,8,8	1.02	1 (12%)
88	ANM	L5	5501	86	20,20,20	1.24	2 (10%)	24,27,27	1.56	6 (25%)
85	PUT	L5	5519	-	5,5,5	0.14	0	4,4,4	0.25	0
84	SPD	L5	5509	-	9,9,9	0.22	0	8,8,8	0.49	0
84	SPD	L5	5506	-	9,9,9	0.16	0	8,8,8	0.22	0
84	SPD	L5	5507	-	9,9,9	0.33	0	8,8,8	0.80	0
84	SPD	L5	5502	-	9,9,9	0.35	0	8,8,8	0.71	0
85	PUT	L5	5517	-	5,5,5	0.11	0	4,4,4	0.13	0
84	SPD	L5	5513	-	9,9,9	0.28	0	8,8,8	0.79	0
85	PUT	L5	5516	-	5,5,5	0.11	0	4,4,4	0.19	0
85	PUT	L5	5522	-	5,5,5	0.07	0	4,4,4	0.14	0
84	SPD	L5	5508	-	9,9,9	0.36	0	8,8,8	0.54	0
84	SPD	L5	5511	-	9,9,9	0.28	0	8,8,8	0.97	1 (12%)
85	PUT	S2	1902	-	5,5,5	0.11	0	4,4,4	0.15	0
84	SPD	S2	1901	-	9,9,9	0.31	0	8,8,8	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	PUT	L5	5521	-	5,5,5	0.07	0	4,4,4	0.21	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
91	MET	Pt	78	82	-	2/5/6/8	-
84	SPD	L5	5504	-	-	4/7/7/7	-
85	PUT	L5	5515	-	-	1/3/3/3	-
85	PUT	L5	5518	-	-	1/3/3/3	-
84	SPD	L5	5510	-	-	4/7/7/7	-
84	SPD	L5	5512	-	-	2/7/7/7	-
84	SPD	L5	5505	-	-	4/7/7/7	-
85	PUT	L5	5520	-	-	1/3/3/3	-
89	3H3	L5	5523	-	-	15/39/51/51	0/1/2/2
85	PUT	S2	1903	-	-	0/3/3/3	-
85	PUT	L5	5514	-	-	0/3/3/3	-
84	SPD	L5	5503	-	-	2/7/7/7	-
88	ANM	L5	5501	86	-	2/10/23/23	0/2/2/2
85	PUT	L5	5519	-	-	1/3/3/3	-
84	SPD	L5	5509	-	-	3/7/7/7	-
84	SPD	L5	5506	-	-	4/7/7/7	-
84	SPD	L5	5507	-	-	4/7/7/7	-
84	SPD	L5	5502	-	-	0/7/7/7	-
85	PUT	L5	5517	-	-	0/3/3/3	-
84	SPD	L5	5513	-	-	2/7/7/7	-
85	PUT	L5	5516	-	-	2/3/3/3	-
85	PUT	L5	5522	-	-	2/3/3/3	-
84	SPD	L5	5508	-	-	2/7/7/7	-
84	SPD	L5	5511	-	-	3/7/7/7	-
85	PUT	S2	1902	-	-	1/3/3/3	-
84	SPD	S2	1901	-	-	4/7/7/7	-
85	PUT	L5	5521	-	-	0/3/3/3	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	L5	5523	3H3	C13-C12	8.94	1.53	1.33
89	L5	5523	3H3	O3-C22	7.66	1.38	1.23
89	L5	5523	3H3	O4-C23	7.27	1.37	1.23
89	L5	5523	3H3	C23-N	6.65	1.48	1.37
89	L5	5523	3H3	C22-N	5.58	1.46	1.37
89	L5	5523	3H3	C3-C2	5.55	1.54	1.33
88	L5	5501	ANM	O2-C5	4.48	1.45	1.35
89	L5	5523	3H3	C19-C20	3.36	1.58	1.53
89	L5	5523	3H3	O1-C11	-3.11	1.39	1.44
89	L5	5523	3H3	C4-C3	2.79	1.53	1.44
89	L5	5523	3H3	O-C10	-2.27	1.17	1.21
89	L5	5523	3H3	O1-C10	2.26	1.39	1.34
88	L5	5501	ANM	O2-C2	-2.23	1.41	1.44
89	L5	5523	3H3	O2-C16	-2.21	1.18	1.21
89	L5	5523	3H3	C24-C20	-2.15	1.49	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	L5	5523	3H3	O3-C22-N	-10.22	104.55	120.30
89	L5	5523	3H3	C22-N-C23	-9.57	114.34	125.87
89	L5	5523	3H3	O4-C23-N	-8.78	106.76	120.30
89	L5	5523	3H3	O3-C22-C21	-6.56	110.10	122.62
89	L5	5523	3H3	C15-C14-C13	-5.99	104.99	110.73
89	L5	5523	3H3	O4-C23-C24	-5.22	112.65	122.62
88	L5	5501	ANM	O2-C5-C6	3.95	118.14	111.09
89	L5	5523	3H3	C25-C12-C13	-3.59	114.34	123.56
89	L5	5523	3H3	C21-C22-N	-3.40	111.80	115.92
89	L5	5523	3H3	C11-C12-C13	-3.17	108.62	119.78
89	L5	5523	3H3	C7-C8-C9	-2.99	119.69	125.92
89	L5	5523	3H3	O1-C10-C9	2.92	117.74	111.39
88	L5	5501	ANM	C15-C16-N1	2.90	114.93	111.21
89	L5	5523	3H3	C4-C3-C2	-2.73	106.06	124.25
89	L5	5523	3H3	C8-C9-C10	-2.70	116.34	122.78
88	L5	5501	ANM	O2-C5-O3	-2.48	118.20	122.99
89	L5	5523	3H3	C1-C2-C3	-2.40	121.15	126.11
88	L5	5501	ANM	C14-O1-C9	2.33	122.48	117.50
89	L5	5523	3H3	C6-C7-C8	-2.26	107.04	112.73
89	L5	5523	3H3	C24-C23-N	-2.22	113.23	115.92
84	L5	5511	SPD	C7-C8-C9	-2.21	106.28	114.17
89	L5	5523	3H3	C25-C12-C11	-2.17	111.67	115.96
84	L5	5505	SPD	C4-C5-N6	-2.16	106.27	112.07
88	L5	5501	ANM	C2-O2-C5	-2.09	114.47	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	L5	5523	3H3	C19-C18-C17	-2.07	108.72	112.96
88	L5	5501	ANM	C15-C12-C11	-2.06	117.07	120.90
84	L5	5503	SPD	C4-C5-N6	-2.01	106.69	112.07

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	S2	1901	SPD	C4-C5-N6-C7
84	L5	5509	SPD	C8-C7-N6-C5
89	L5	5523	3H3	C2-C1-C11-O1
89	L5	5523	3H3	C2-C1-C11-C12
89	L5	5523	3H3	C-C1-C11-O1
89	L5	5523	3H3	C-C1-C11-C12
89	L5	5523	3H3	C1-C11-O1-C10
89	L5	5523	3H3	C12-C11-O1-C10
89	L5	5523	3H3	C9-C10-O1-C11
89	L5	5523	3H3	C12-C13-C14-C16
89	L5	5523	3H3	C25-C12-C13-C14
89	L5	5523	3H3	C1-C11-C12-C25
84	L5	5503	SPD	N6-C7-C8-C9
84	L5	5513	SPD	N6-C7-C8-C9
84	L5	5508	SPD	C3-C4-C5-N6
91	Pt	78	MET	CA-CB-CG-SD
89	L5	5523	3H3	O-C10-O1-C11
84	L5	5504	SPD	C3-C4-C5-N6
84	L5	5511	SPD	C3-C4-C5-N6
89	L5	5523	3H3	C2-C3-C4-C5
84	L5	5504	SPD	N6-C7-C8-C9
84	L5	5506	SPD	N6-C7-C8-C9
84	L5	5506	SPD	C3-C4-C5-N6
84	L5	5511	SPD	N6-C7-C8-C9
89	L5	5523	3H3	O1-C10-C9-C8
84	L5	5507	SPD	C2-C3-C4-C5
85	L5	5518	PUT	N1-C1-C2-C3
84	L5	5511	SPD	C8-C7-N6-C5
85	L5	5522	PUT	C1-C2-C3-C4
84	L5	5510	SPD	N1-C2-C3-C4
91	Pt	78	MET	CB-CG-SD-CE
84	L5	5505	SPD	N6-C7-C8-C9
84	L5	5509	SPD	C4-C5-N6-C7
84	L5	5505	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
84	S2	1901	SPD	N6-C7-C8-C9
84	L5	5503	SPD	C2-C3-C4-C5
85	L5	5515	PUT	C1-C2-C3-C4
84	L5	5510	SPD	N6-C7-C8-C9
84	S2	1901	SPD	C7-C8-C9-N10
84	L5	5509	SPD	C7-C8-C9-N10
84	L5	5513	SPD	C7-C8-C9-N10
89	L5	5523	3H3	O-C10-C9-C8
84	L5	5506	SPD	C2-C3-C4-C5
84	L5	5504	SPD	C4-C5-N6-C7
85	L5	5520	PUT	C1-C2-C3-C4
85	S2	1902	PUT	C1-C2-C3-C4
84	L5	5512	SPD	C2-C3-C4-C5
85	L5	5519	PUT	C1-C2-C3-C4
84	L5	5504	SPD	C7-C8-C9-N10
84	L5	5505	SPD	C7-C8-C9-N10
84	L5	5508	SPD	C2-C3-C4-C5
84	L5	5507	SPD	C4-C5-N6-C7
84	L5	5510	SPD	C4-C5-N6-C7
84	L5	5505	SPD	C2-C3-C4-C5
84	L5	5506	SPD	C4-C5-N6-C7
84	L5	5512	SPD	C4-C5-N6-C7
84	S2	1901	SPD	C8-C7-N6-C5
88	L5	5501	ANM	C11-C12-C15-C16
85	L5	5516	PUT	C1-C2-C3-C4
88	L5	5501	ANM	C13-C12-C15-C16
84	L5	5507	SPD	N1-C2-C3-C4
85	L5	5522	PUT	C2-C3-C4-N2
89	L5	5523	3H3	C12-C13-C14-C15
84	L5	5510	SPD	C7-C8-C9-N10
85	L5	5516	PUT	C2-C3-C4-N2
84	L5	5507	SPD	N6-C7-C8-C9

There are no ring outliers.

14 monomers are involved in 25 short contacts:

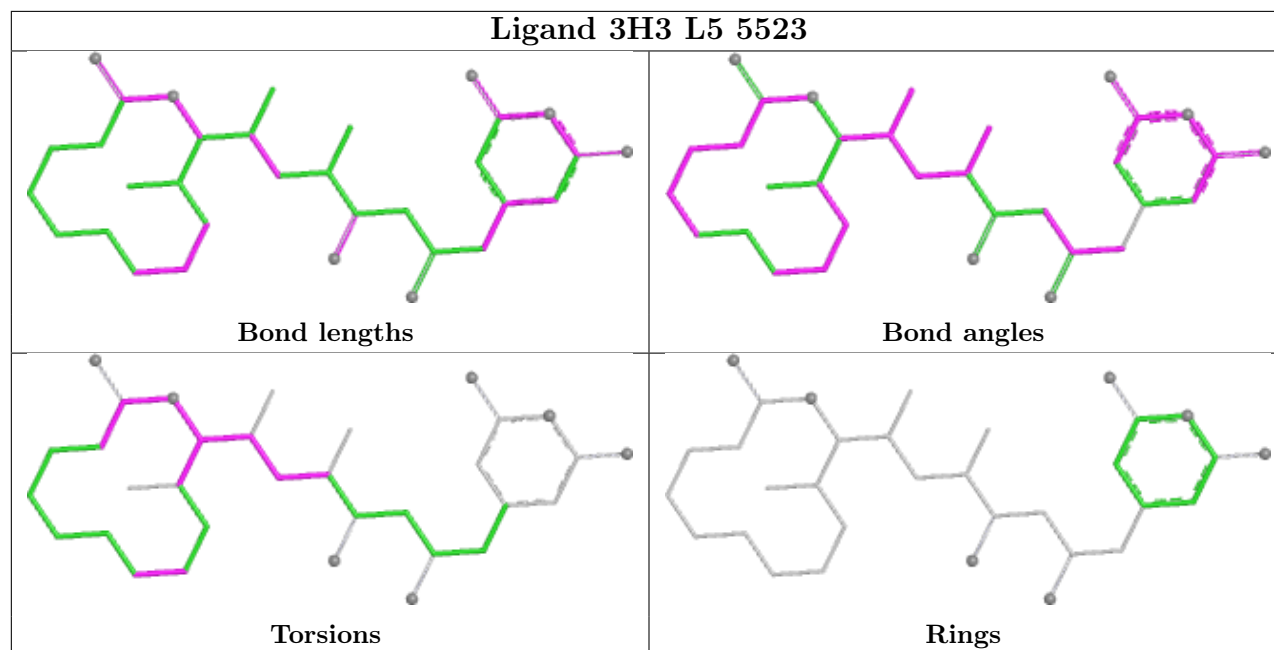
Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	Pt	78	MET	1	0
84	L5	5504	SPD	1	0
85	L5	5515	PUT	1	0
85	L5	5518	PUT	6	0
84	L5	5512	SPD	2	0

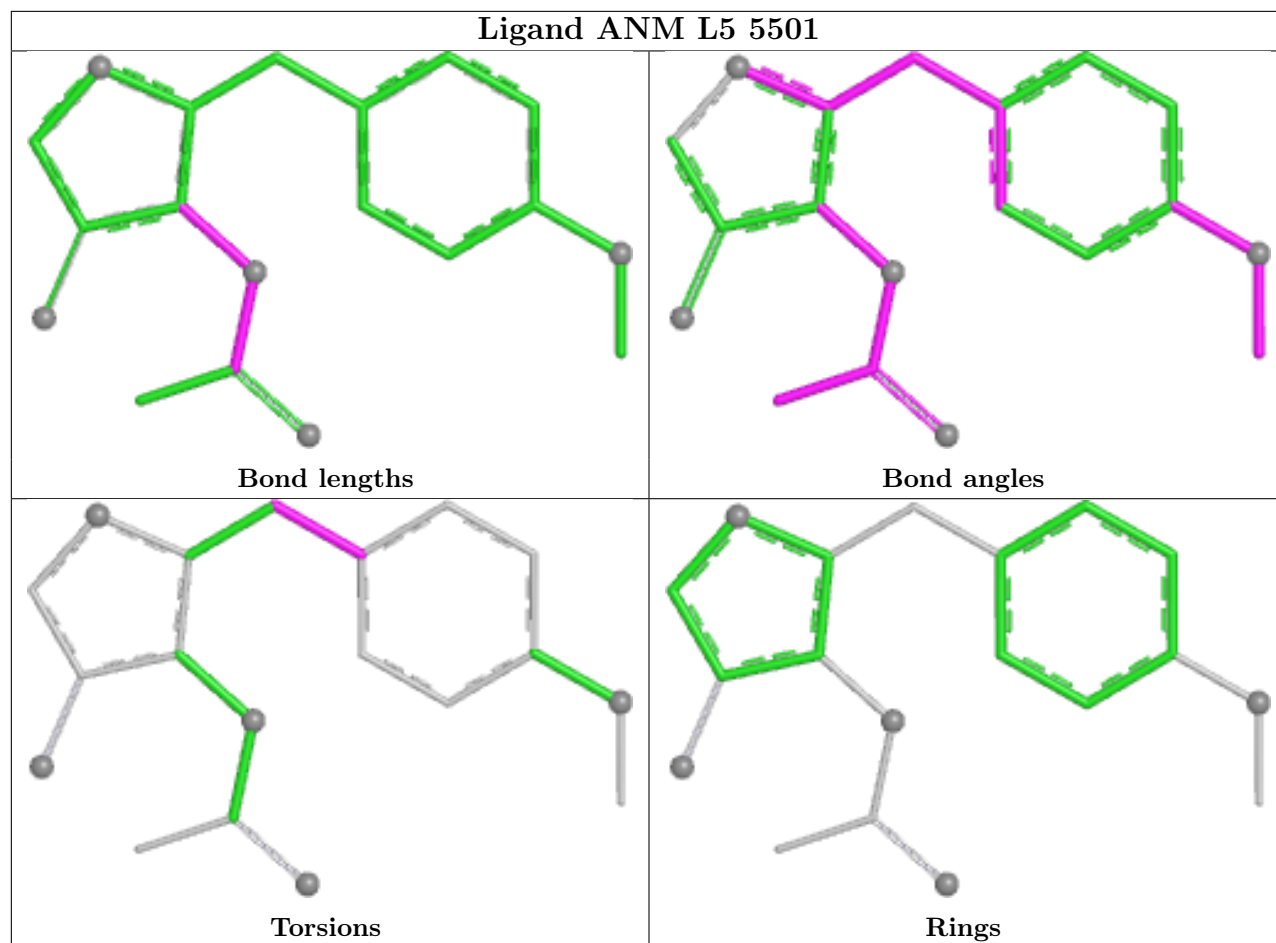
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5523	3H3	3	0
85	S2	1903	PUT	1	0
84	L5	5509	SPD	2	0
84	L5	5506	SPD	1	0
84	L5	5513	SPD	1	0
84	L5	5508	SPD	3	0
84	L5	5511	SPD	1	0
85	S2	1902	PUT	1	0
84	S2	1901	SPD	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

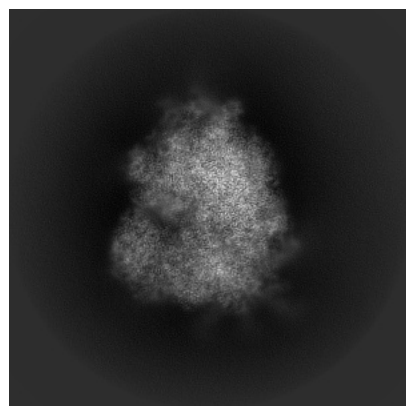
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29757. These allow visual inspection of the internal detail of the map and identification of artifacts.

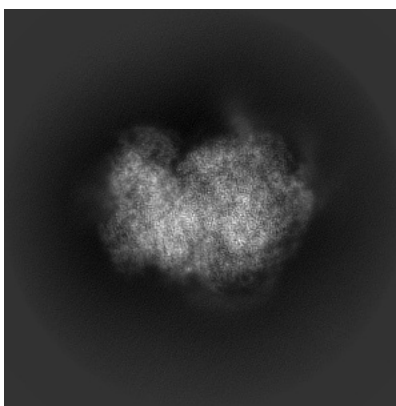
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

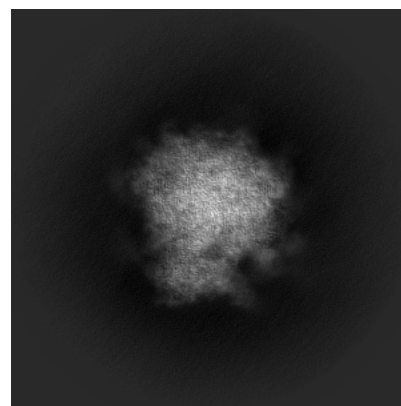
6.1.1 Primary map



X

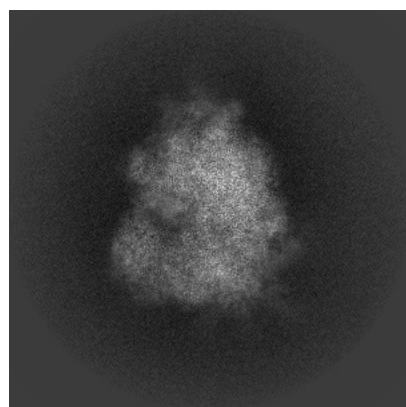


Y

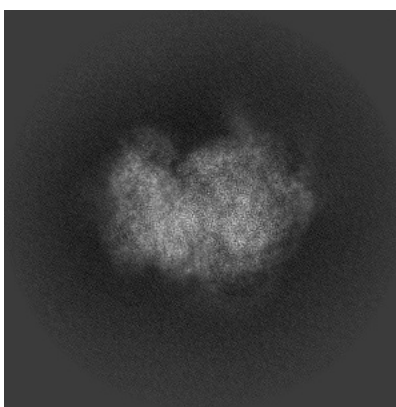


Z

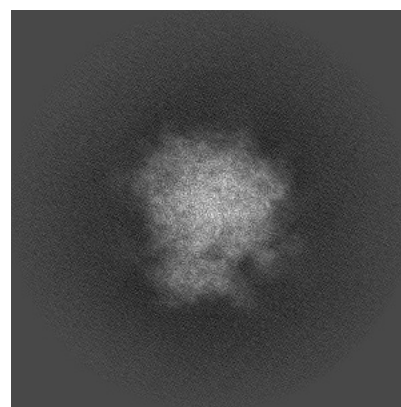
6.1.2 Raw map



X



Y

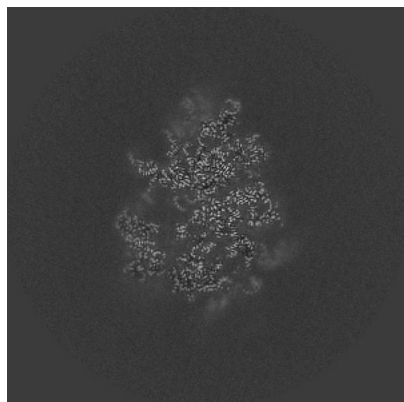


Z

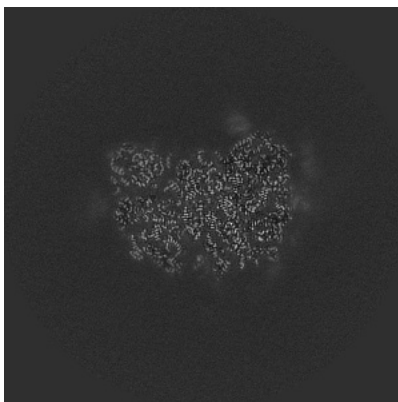
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

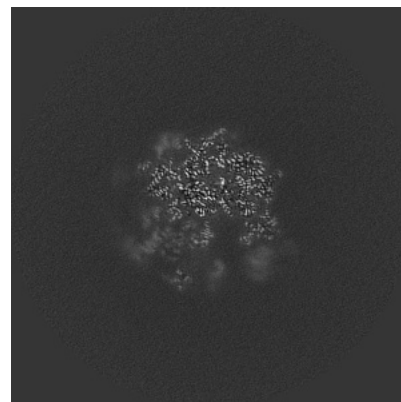
6.2.1 Primary map



X Index: 320

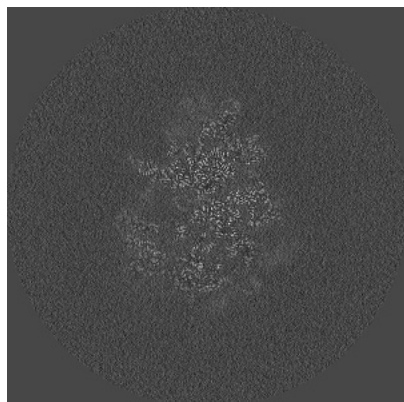


Y Index: 320

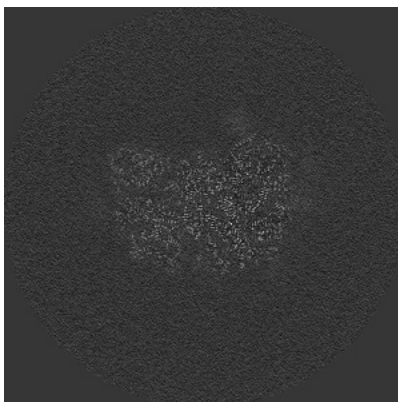


Z Index: 320

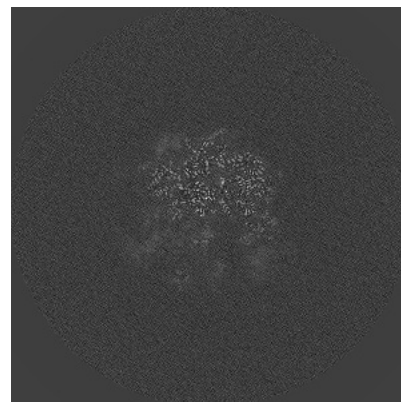
6.2.2 Raw map



X Index: 320



Y Index: 320

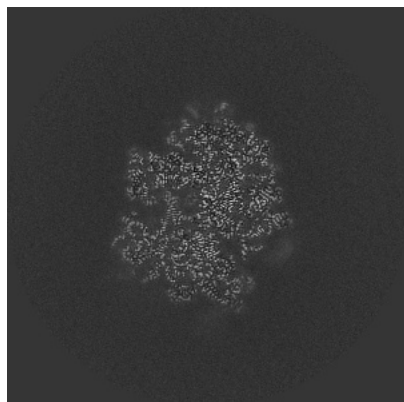


Z Index: 320

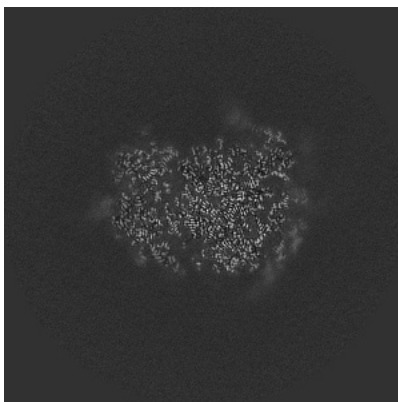
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

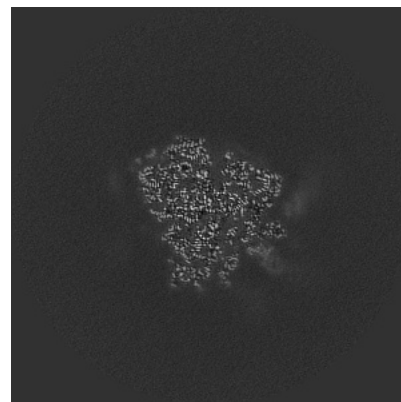
6.3.1 Primary map



X Index: 298

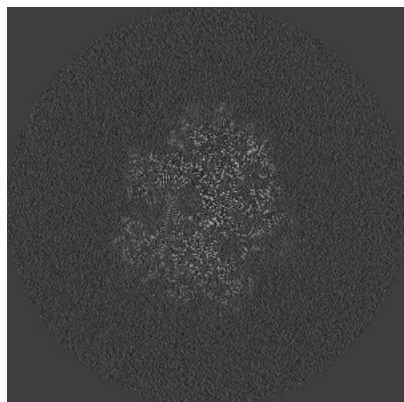


Y Index: 332

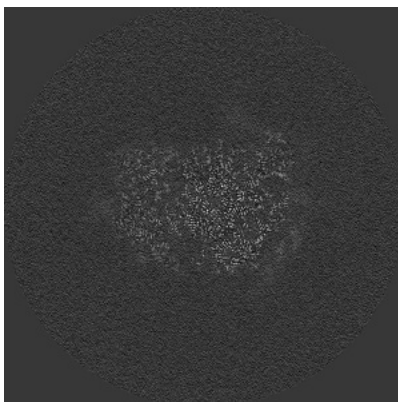


Z Index: 367

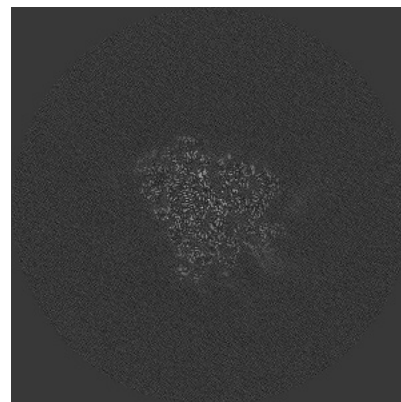
6.3.2 Raw map



X Index: 299



Y Index: 332

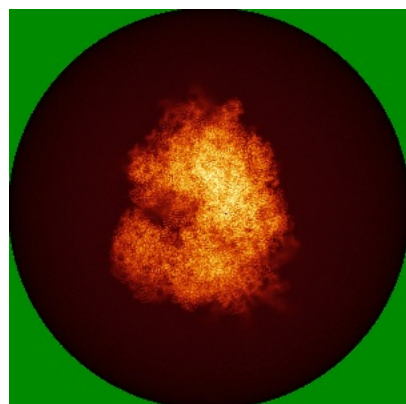


Z Index: 362

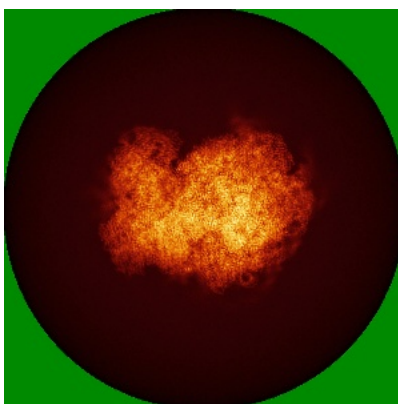
The images above show the largest variance slices of the map in three orthogonal directions.

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

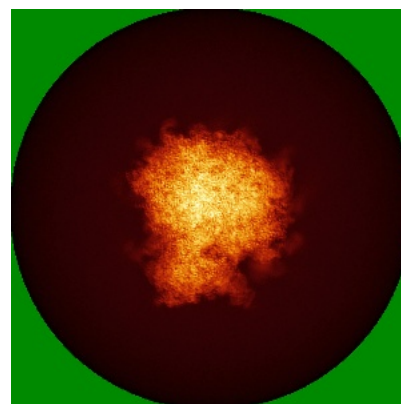
6.4.1 Primary map



X

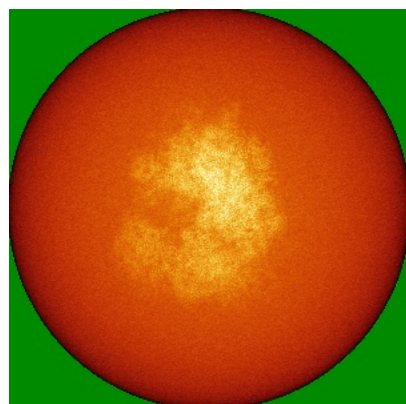


Y

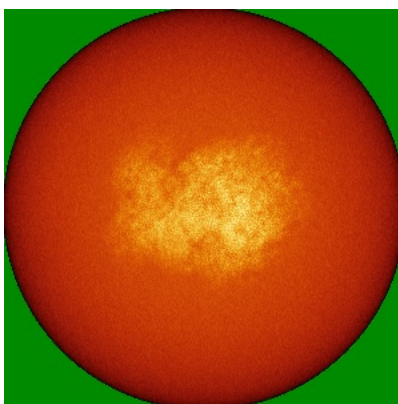


Z

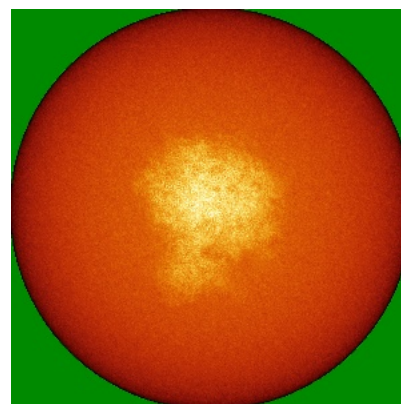
6.4.2 Raw map



X



Y

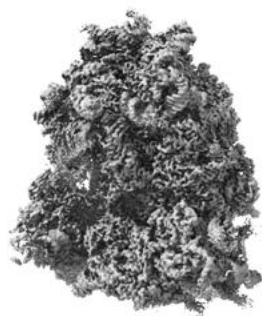


Z

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



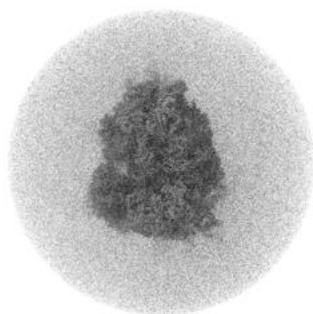
Y



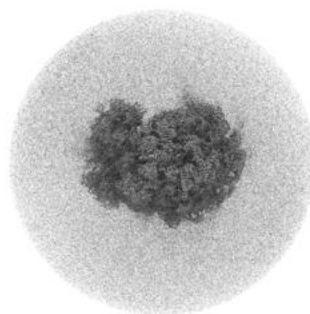
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

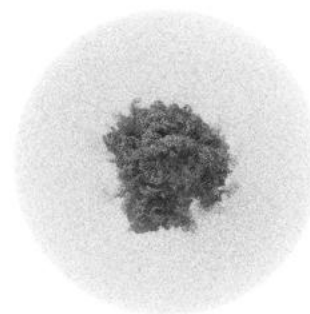
6.5.2 Raw map



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.

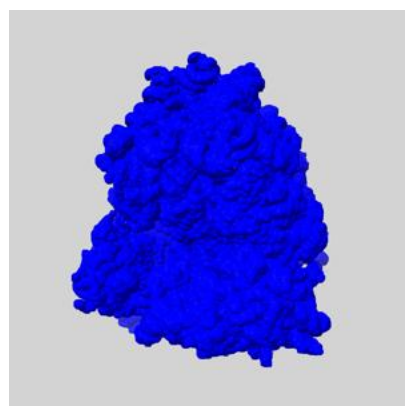
6.6 Mask visualisation [i](#)

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

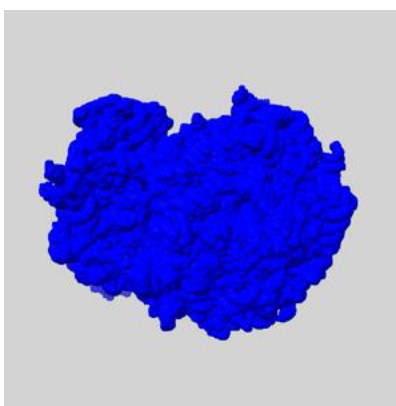
A mask typically either:

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

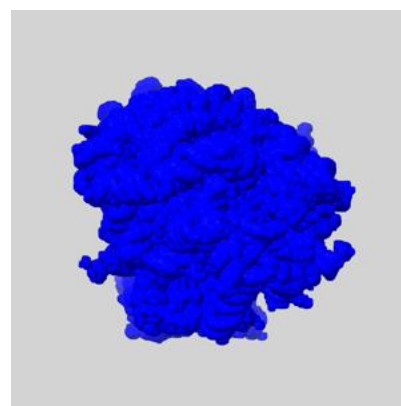
6.6.1 emd_29757_msk_1.map [i](#)



X



Y

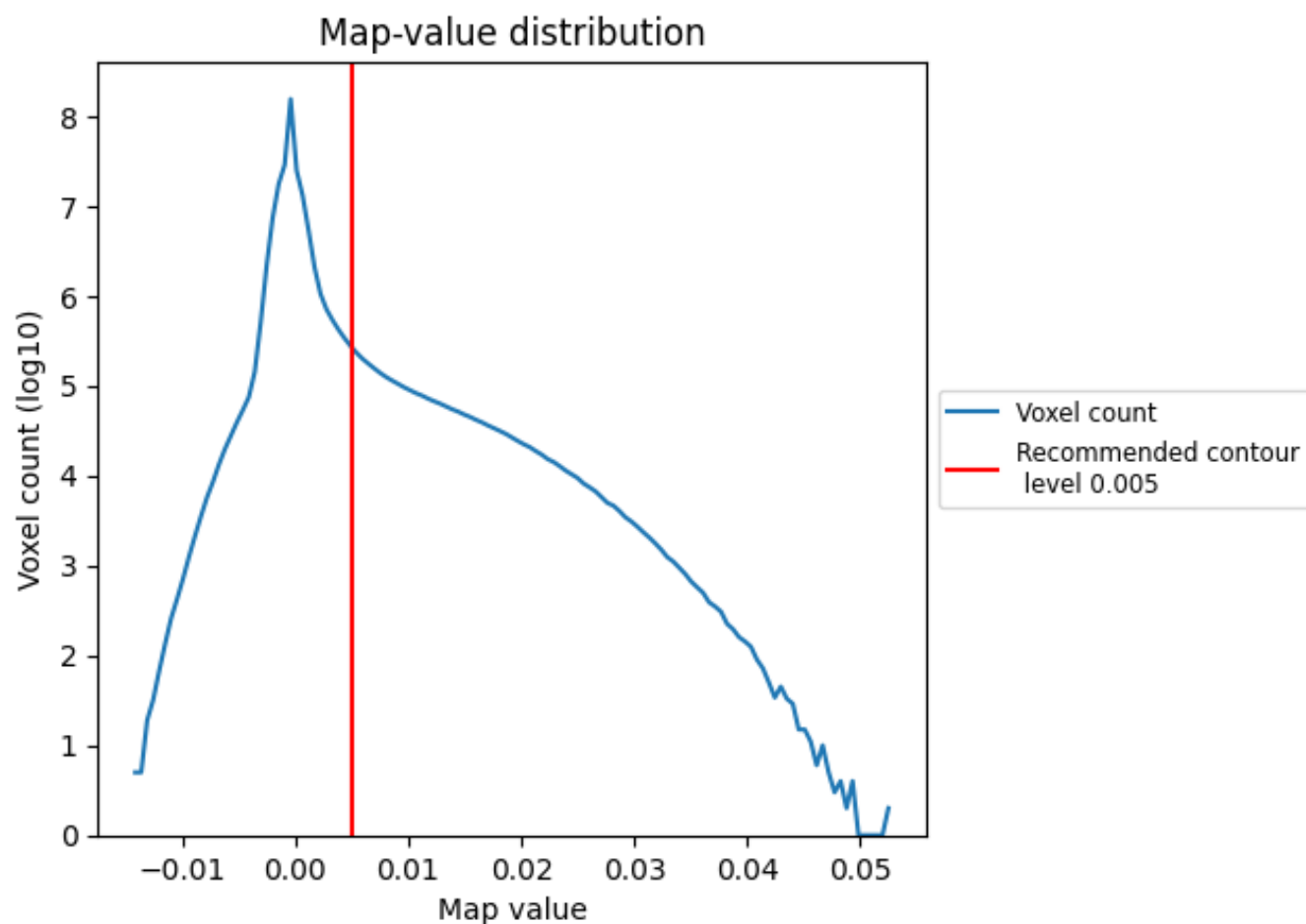


Z

7 Map analysis [i](#)

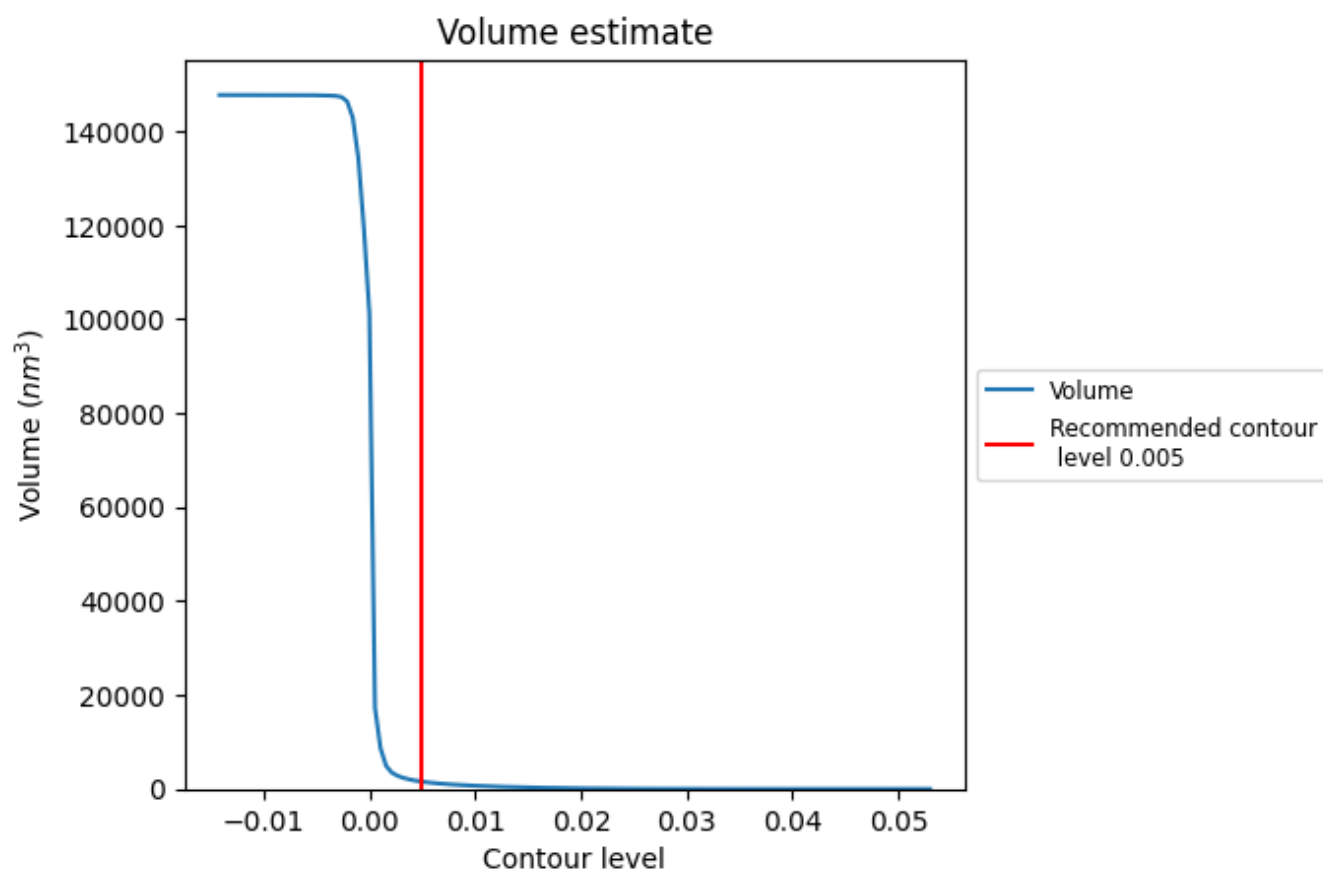
This section contains the results of statistical analysis of the map.

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.

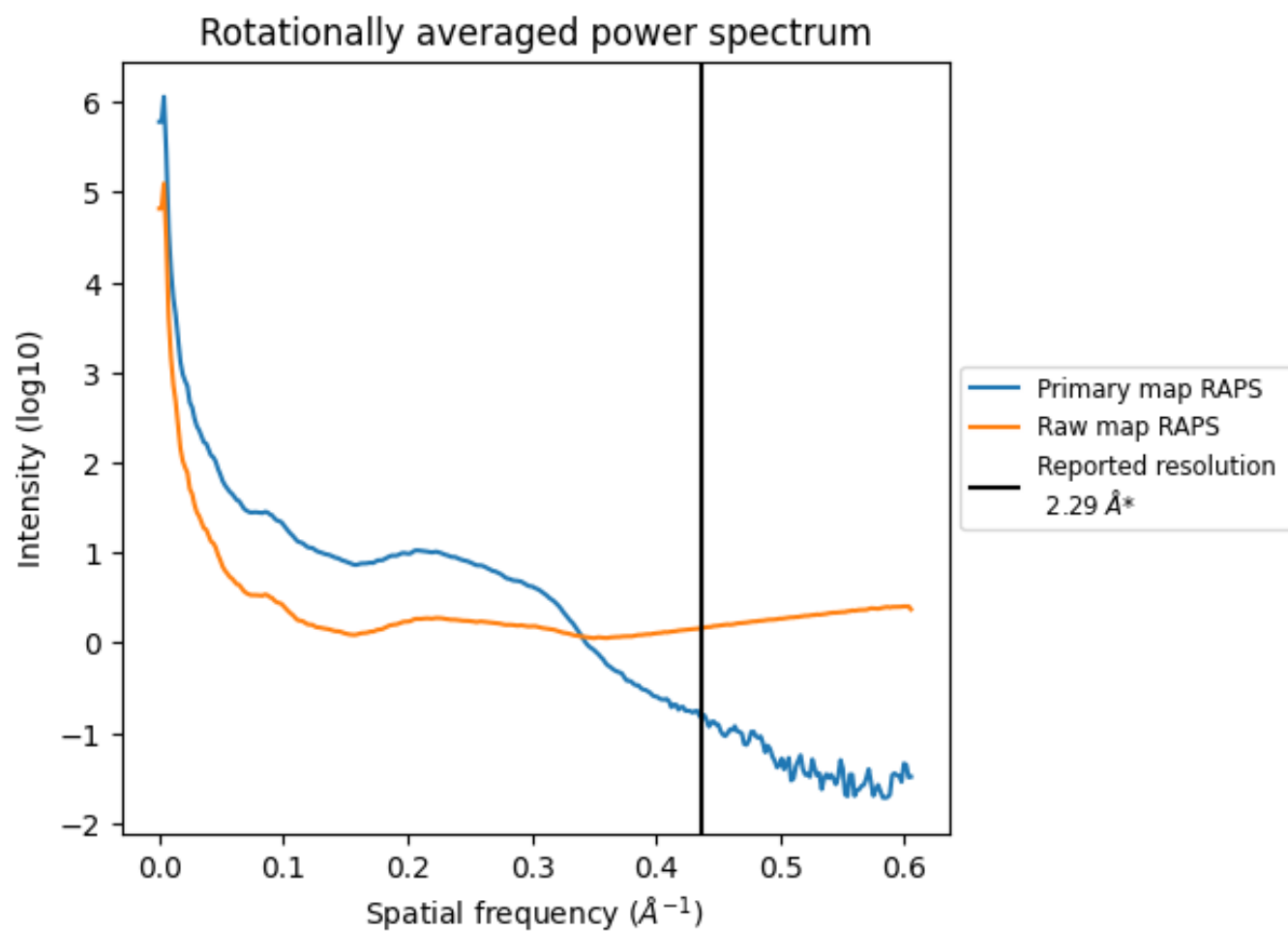
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1549 nm^3 ; this corresponds to an approximate mass of 1399 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 ⓘ

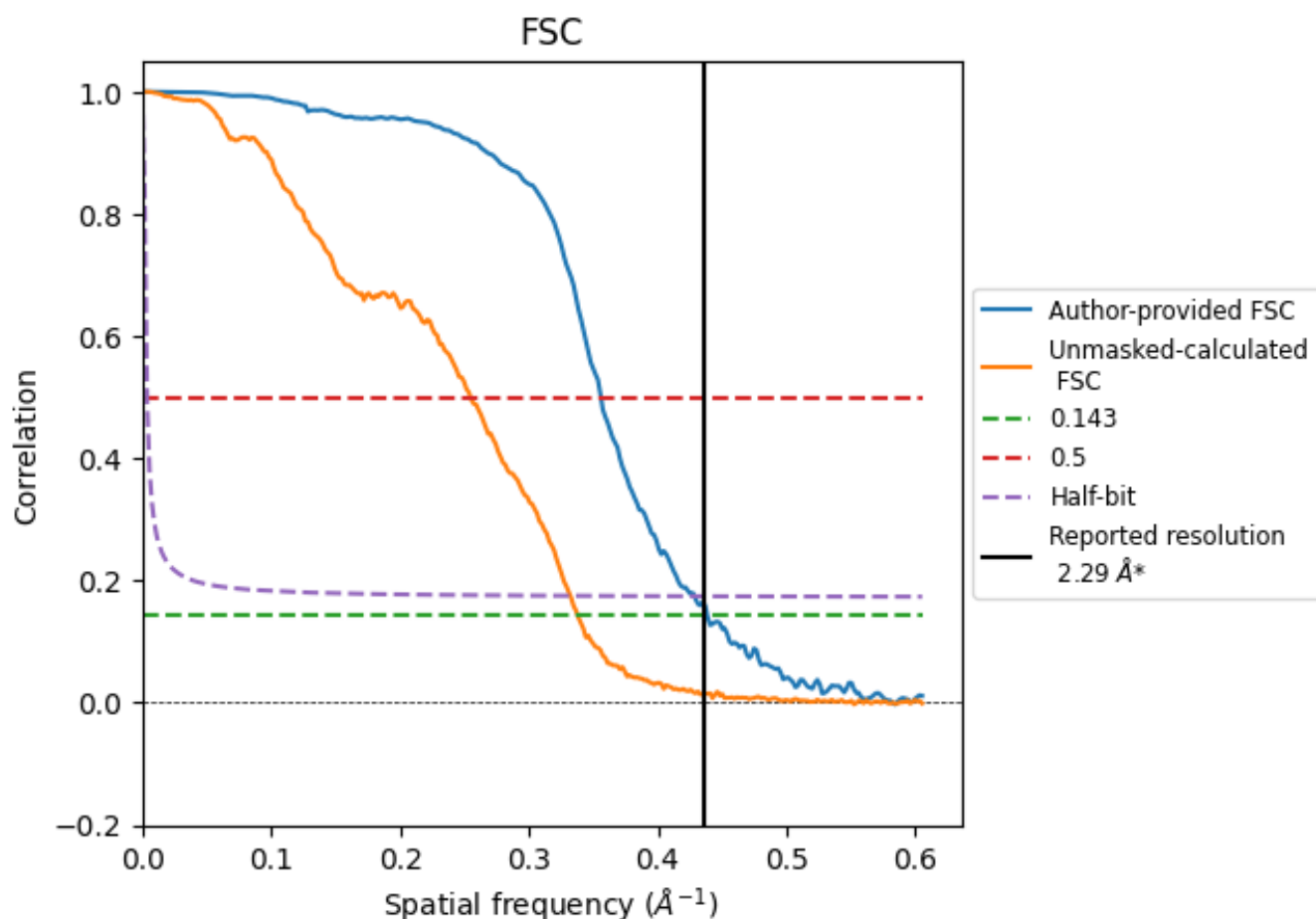


*Reported resolution corresponds to spatial frequency of 0.437 Å⁻¹

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 0.437 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

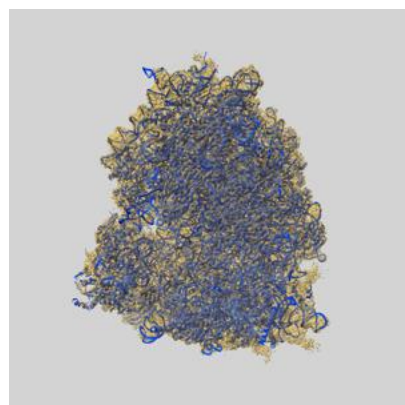
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.28	2.81	2.33
Unmasked-calculated*	2.96	3.92	3.01

*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 2.96 differs from the reported value 2.29 by more than 10 %

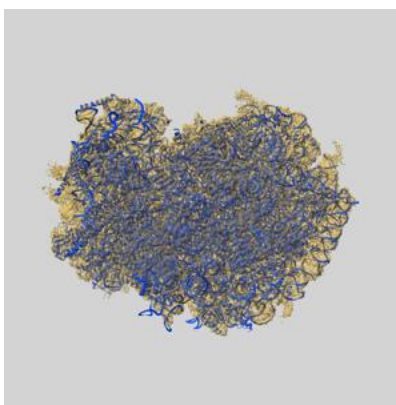
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29757 and PDB model 8G5Y. Per-residue inclusion information can be found in section 3 on page 28.

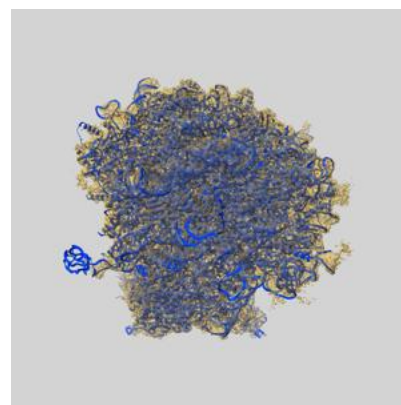
9.1 Map-model overlay [i](#)



X



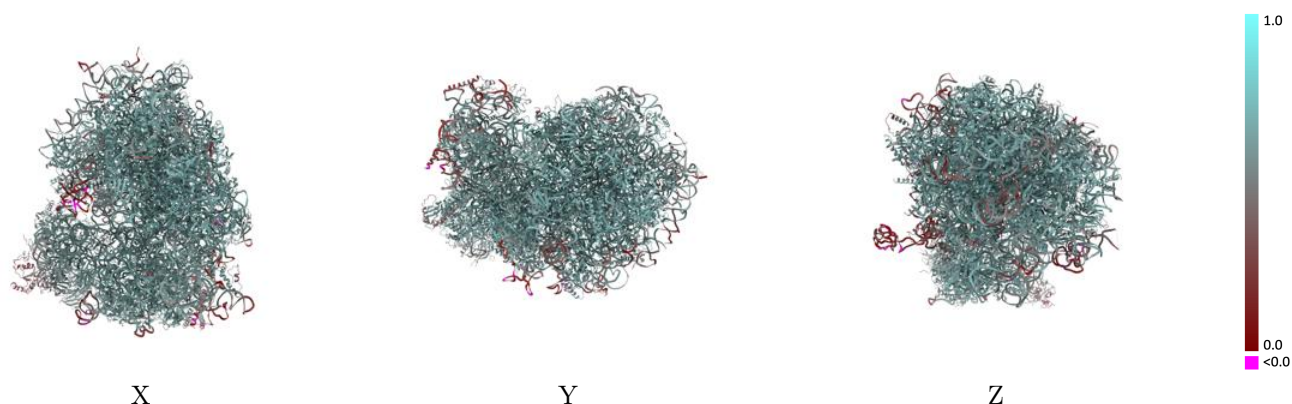
Y



Z

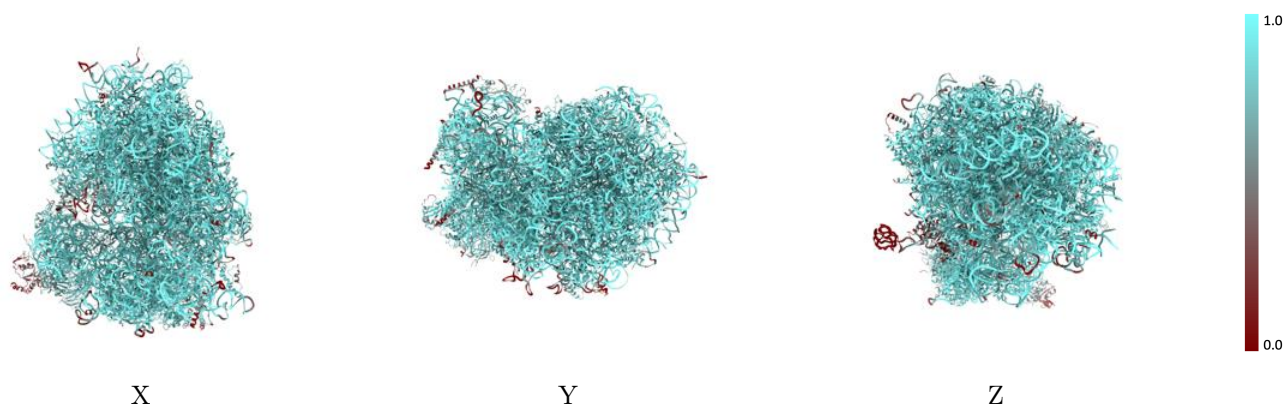
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



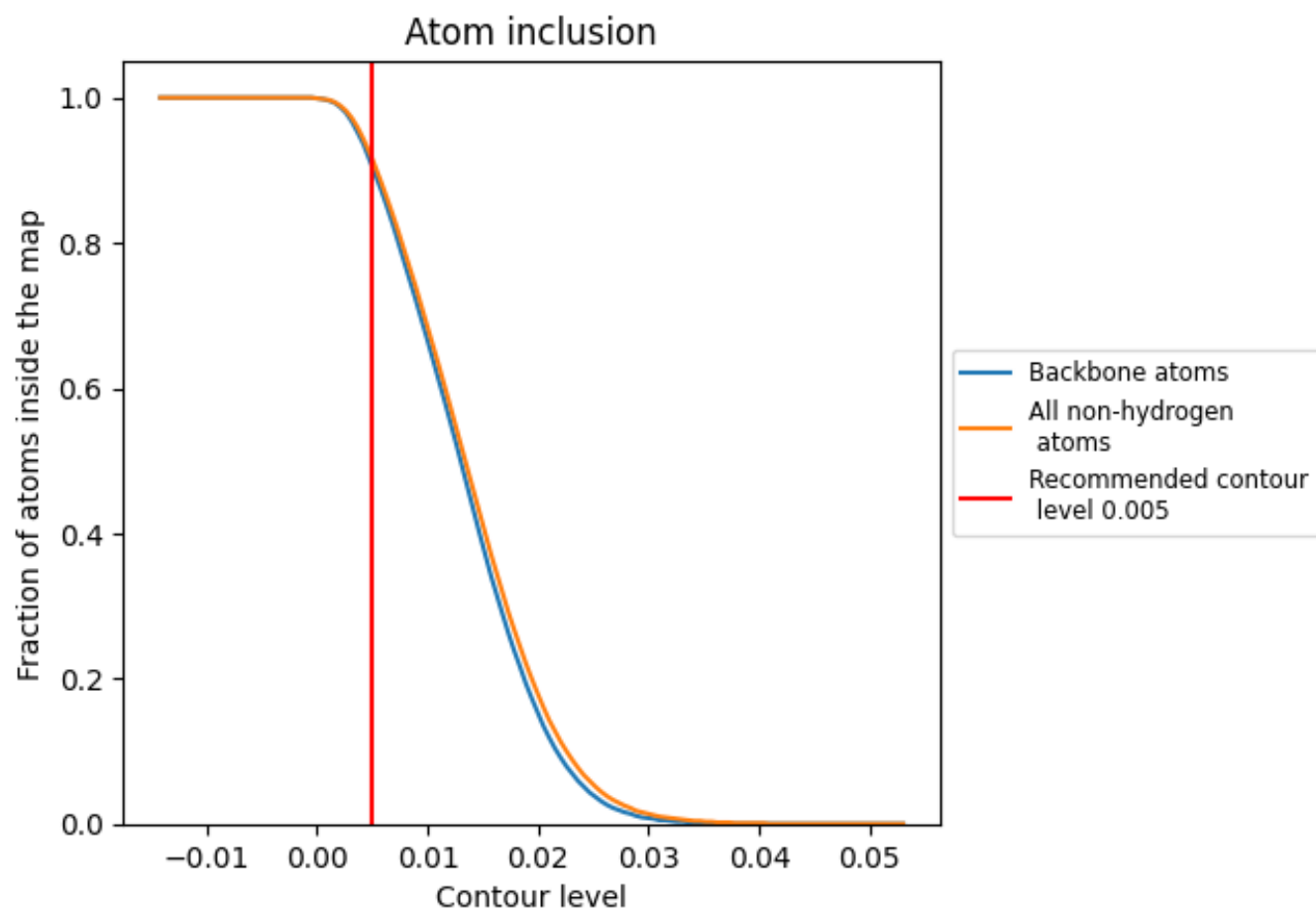
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.6050
5A	 0.5350	 0.4730
L5	 0.9360	 0.5990
L7	 0.9940	 0.6520
L8	 0.9780	 0.6360
LA	 0.9730	 0.6720
LB	 0.9410	 0.6550
LC	 0.9530	 0.6590
LD	 0.9220	 0.6310
LE	 0.9180	 0.6290
LF	 0.9600	 0.6610
LG	 0.8380	 0.5950
LH	 0.9200	 0.6300
LI	 0.9480	 0.6450
LJ	 0.9110	 0.6190
LL	 0.9140	 0.6320
LM	 0.9500	 0.6420
LN	 0.9910	 0.6740
LO	 0.9590	 0.6590
LP	 0.9620	 0.6700
LQ	 0.9780	 0.6750
LR	 0.8830	 0.6220
LS	 0.9750	 0.6590
LT	 0.9380	 0.6500
LU	 0.8470	 0.5820
LV	 0.9540	 0.6580
LW	 0.6950	 0.5080
LX	 0.9400	 0.6470
LY	 0.9260	 0.6400
LZ	 0.9380	 0.6400
La	 0.9810	 0.6760
Lb	 0.8220	 0.5910
Lc	 0.9320	 0.6460
Ld	 0.9240	 0.6330
Le	 0.9800	 0.6750



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Chain	Atom inclusion	Q-score
Lf	 0.9680	 0.6710
Lg	 0.9020	 0.6420
Lh	 0.9280	 0.6430
Li	 0.9010	 0.6210
Lj	 0.9900	 0.6780
Lk	 0.8510	 0.6130
Ll	 0.9620	 0.6510
Lm	 0.9230	 0.6360
Ln	 0.9360	 0.6470
Lo	 0.9480	 0.6490
Lp	 0.9390	 0.6600
Lr	 0.9670	 0.6610
Lz	 0.2670	 0.3690
Pt	 0.9600	 0.5990
S2	 0.9610	 0.5960
SA	 0.9030	 0.6160
SB	 0.8790	 0.6200
SC	 0.9160	 0.6260
SD	 0.8260	 0.5680
SE	 0.9010	 0.6150
SF	 0.8830	 0.6050
SG	 0.7700	 0.5370
SH	 0.7770	 0.5500
SI	 0.8900	 0.6060
SJ	 0.8850	 0.5950
SK	 0.8190	 0.5380
SL	 0.9120	 0.6330
SM	 0.2660	 0.2970
SN	 0.9370	 0.6410
SO	 0.9200	 0.6320
SP	 0.8220	 0.5660
SQ	 0.9090	 0.6100
SR	 0.8150	 0.5660
SS	 0.8920	 0.6040
ST	 0.8930	 0.6030
SU	 0.7750	 0.5470
SV	 0.9090	 0.6230
SW	 0.9680	 0.6480
SX	 0.9460	 0.6390
SY	 0.8040	 0.5550
SZ	 0.7920	 0.5760
Sa	 0.9420	 0.6350

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Chain	Atom inclusion	Q-score
Sb	 0.8420	 0.6070
Sc	 0.8070	 0.5720
Sd	 0.9570	 0.6210
Se	 0.8440	 0.5940
Sf	 0.4420	 0.3830
Sg	 0.7590	 0.5360
mR	 0.6110	 0.5240