



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 08:47 PM EDT

PDB ID : 8G60 / pdb_00008g60
EMDB ID : EMD-29759
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (CR 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 : 2.54 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:

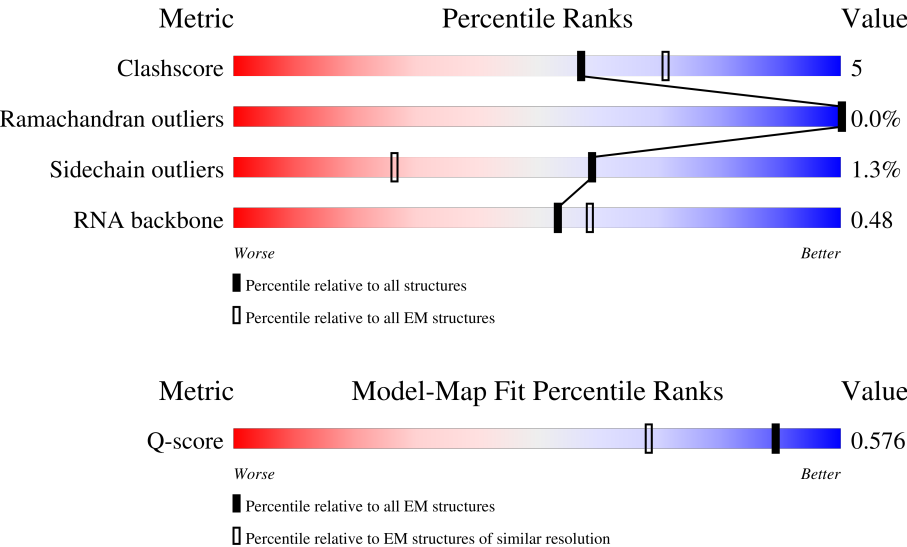
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.54 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.



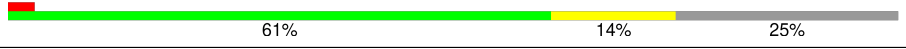
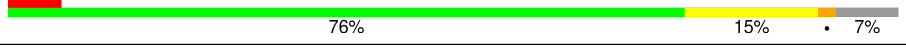
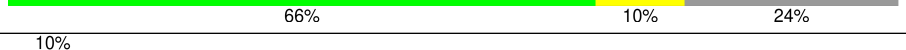
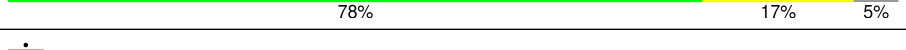
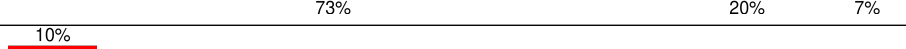
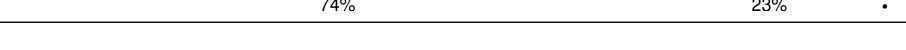
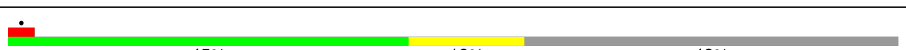
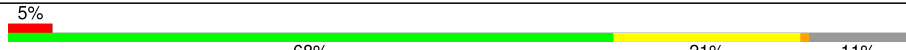
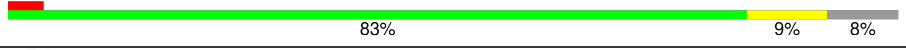
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7403 (2.04 - 3.04)

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	

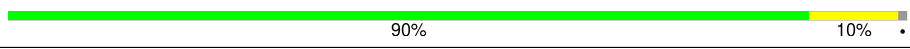
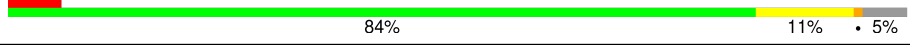
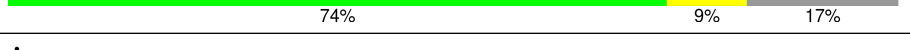
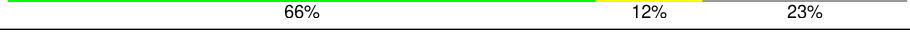
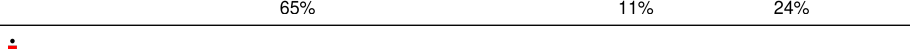
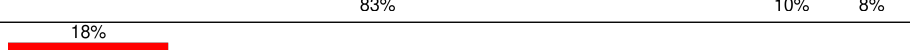
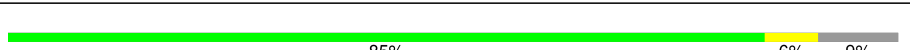
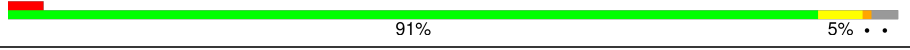
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	Lz	217	
39	LA	257	
40	LB	403	
41	LC	427	
42	LJ	178	
43	LH	192	
44	LE	288	
45	LG	266	
46	Lq	317	
47	LK	165	
48	LO	203	
49	LL	270	
50	LV	140	
51	LM	215	
52	La	148	
53	LN	204	

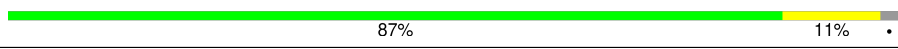
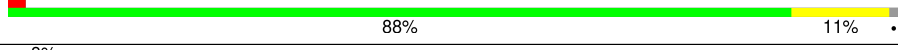
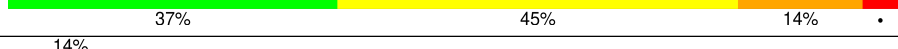
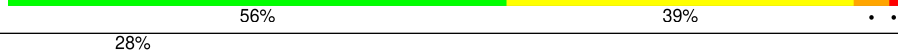
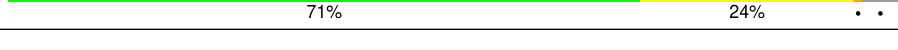
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Mol	Chain	Length	Quality of chain
54	LI	214	
55	LD	297	
56	LQ	188	
57	LR	196	
58	LS	176	
59	LT	160	
60	LP	184	
61	LU	128	
62	LX	156	
63	LY	145	
64	LW	157	
65	LZ	136	
66	Lr	137	
67	Lh	123	
68	Lb	159	
69	LF	248	
70	Lc	115	
71	Ld	125	
72	Le	135	
73	Lf	110	
74	Lg	117	
75	Li	105	
76	Lj	97	
77	Lk	70	
78	Ll	51	

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Mol	Chain	Length	Quality of chain
79	Lm	128	
80	Ln	25	
81	Lo	106	
82	Lp	92	
83	mR	60	
84	At	76	
85	Pt	77	
86	EF	462	

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 223755 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	1654	Total	C	N	O	P	0	0
			35359	15812	6338	11555	1654		

- 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
			3320	1482	585	1097	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3637	Total	C	N	O	P	1	0
			78069	34805	14275	25351	3638		

- 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
			2562	1141	456	845	120		

- Molecule 5 is a protein called eS1.

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 uS2.

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 uS3.

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 uS4.

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 eS4.

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 uS5.

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 eS6.

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 uS7.

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 eS7.

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 uS8.

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 eS8.

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 uS9.

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 uS10.

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 eS10.

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 uS11.

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	142	Total	C	N	O	S	0	0
			1105	696	220	186	3		

- Molecule 21 is a protein called eS12.

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

- Molecule 22 is a protein called uS13.

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 uS14.

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 uS15.

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 uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	145	Total	C	N	O	S	0	0
			1189	757	225	201	6		

- Molecule 26 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1083	680	201	198	4		

- Molecule 27 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	128	Total	C	N	O	S	0	0
			1050	666	198	179	7		

- Molecule 28 is a protein called eS19.

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

- Molecule 29 is a protein called eS21.

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 eS24.

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 eS25.

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 eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 33 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 34 is a protein called eS28.

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

- Molecule 35 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	51	Total	C	N	O	S	0	0
			406	248	92	65	1		

- Molecule 36 is a protein called eS31.

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 RACK1.

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 uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- 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 uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LB	402	Total	C	N	O	S	0	0
			3240	2061	608	557	14		

- Molecule 41 is a protein called uL4.

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

- Molecule 42 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	169	Total	C	N	O	S	0	0
			1358	859	253	240	6		

- Molecule 43 is a protein called uL6.

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 eL6.

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 eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LG	239	Total	C	N	O	S	0	0
			1910	1217	368	321	4		

- Molecule 46 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lq	196	Total	C	N	O	S	0	0
			1506	958	263	276	9		

- Molecule 47 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LK	147	Total	C	N	O	S	0	0
			1121	700	211	207	3		

- Molecule 48 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LO	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 49 is a protein called eL13.

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

- Molecule 50 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LV	133	Total	C	N	O	S	0	0
			989	623	186	175	5		

- Molecule 51 is a protein called eL14.

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

- Molecule 52 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 53 is a protein called eL15.

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

- Molecule 54 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LI	208	Total	C	N	O	S	0	0
			1680	1065	323	278	14		

- Molecule 55 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LD	293	Total	C	N	O	S	0	0
			2387	1511	435	427	14		

- Molecule 56 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ	187	Total	C	N	O	S	0	0
			1511	944	314	248	5		

- Molecule 57 is a protein called eL19.

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

- Molecule 58 is a protein called eL20.

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

- Molecule 59 is a protein called eL21.

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

- Molecule 60 is a protein called uL22.

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

- Molecule 61 is a protein called eL22.

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

- Molecule 62 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 63 is a protein called uL24.

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

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LW	117	Total	C	N	O	S	0	0
			944	592	191	157	4		

- Molecule 65 is a protein called eL27.

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

- Molecule 66 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lr	125	Total	C	N	O	S	0	0
			1005	624	207	169	5		

- Molecule 67 is a protein called uL29.

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

- Molecule 68 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lb	109	Total	C	N	O	S	0	0
			885	552	192	137	4		

- Molecule 69 is a protein called uL30.

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

- Molecule 70 is a protein called eL30.

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

- Molecule 71 is a protein called eL31.

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

- Molecule 72 is a protein called eL32.

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

- Molecule 73 is a protein called eL33.

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

- Molecule 74 is a protein called eL34.

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

- Molecule 75 is a protein called eL36.

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

- Molecule 76 is a protein called eL37.

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

- Molecule 77 is a protein called eL38.

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

- Molecule 78 is a protein called eL39.

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

- Molecule 79 is a protein called eL40.

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

- Molecule 80 is a protein called eL41.

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

- Molecule 81 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lo	104	Total	C	N	O	S	0	0
			852	534	174	138	6		

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	mR	9	Total	C	N	O	P	0	0
			188	84	29	66	9		

- Molecule 84 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	At	76	Total	C	N	O	P	S	0	0
			1630	730	290	532	76	2		

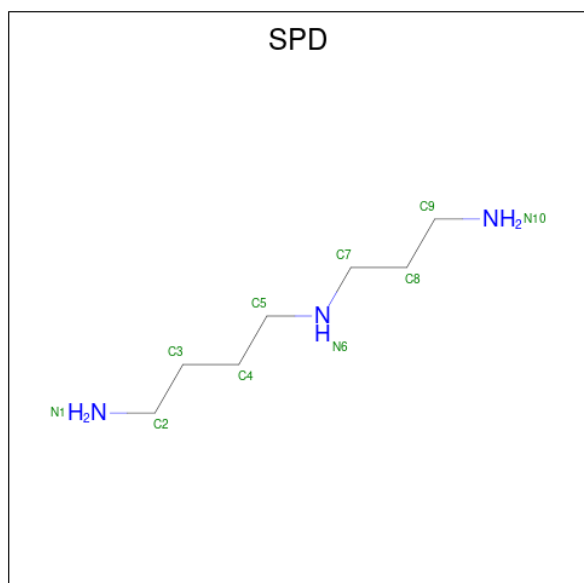
- Molecule 85 is a RNA chain called P-site tRNA.

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

- Molecule 86 is a protein called eEF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	EF	443	Total	C	N	O	S	1	0
			3401	2165	584	635	17		

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



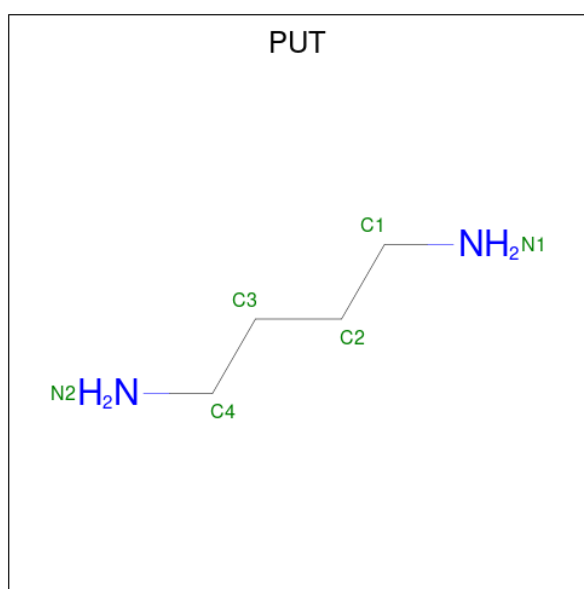
Mol	Chain	Residues	Atoms			AltConf
87	S2	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 88 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



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

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

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

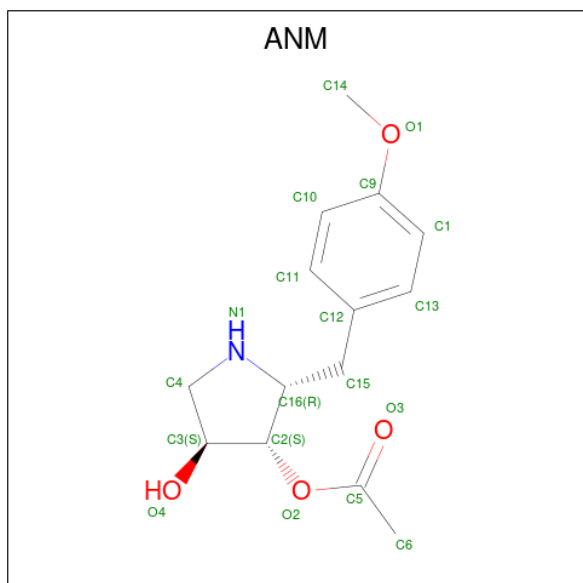
Mol	Chain	Residues	Atoms		AltConf
89	S2	112	Total	Mg	0
			112	112	
89	L8	7	Total	Mg	0
			7	7	
89	L5	307	Total	Mg	0
			307	307	
89	L7	7	Total	Mg	0
			7	7	
89	SG	1	Total	Mg	0
			1	1	
89	SO	1	Total	Mg	0
			1	1	
89	SS	2	Total	Mg	0
			2	2	
89	SN	1	Total	Mg	0
			1	1	
89	SP	1	Total	Mg	0
			1	1	
89	Sa	1	Total	Mg	0
			1	1	
89	LA	1	Total	Mg	0
			1	1	
89	LB	3	Total	Mg	0
			3	3	
89	LC	1	Total	Mg	0
			1	1	
89	LL	1	Total	Mg	0
			1	1	
89	LV	1	Total	Mg	0
			1	1	
89	LN	1	Total	Mg	0
			1	1	

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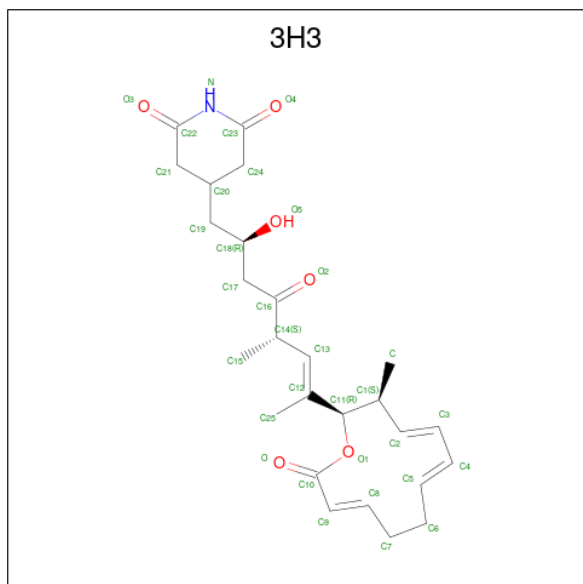
Mol	Chain	Residues	Atoms		AltConf
89	LI	1	Total	Mg	0
			1	1	
89	LR	1	Total	Mg	0
			1	1	
89	LS	1	Total	Mg	0
			1	1	
89	LP	2	Total	Mg	0
			2	2	
89	Le	1	Total	Mg	0
			1	1	
89	Lf	1	Total	Mg	0
			1	1	
89	Lg	2	Total	Mg	0
			2	2	
89	Lj	1	Total	Mg	0
			1	1	
89	Pt	2	Total	Mg	0
			2	2	
89	EF	1	Total	Mg	0
			1	1	

- Molecule 90 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



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

- Molecule 91 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).



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

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
92	L5	10	Total	K	0
			10	10	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

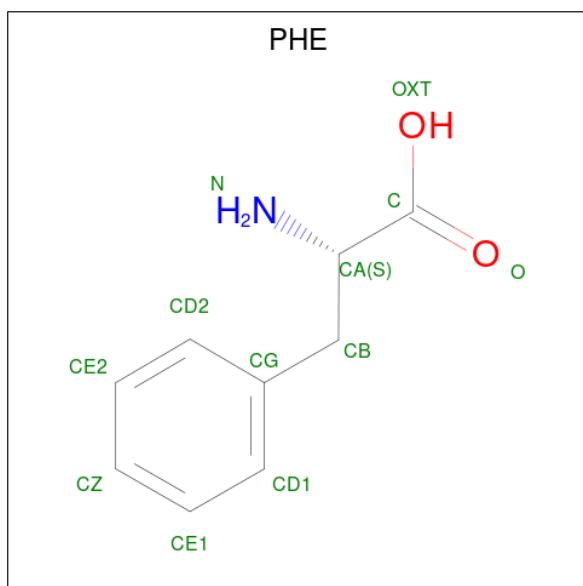
Mol	Chain	Residues	Atoms		AltConf
93	Sd	1	Total	Zn	0
			1	1	
93	Sa	1	Total	Zn	0
			1	1	
93	Lg	1	Total	Zn	0
			1	1	
93	Lj	1	Total	Zn	0
			1	1	
93	Lm	1	Total	Zn	0
			1	1	
93	Lo	1	Total	Zn	0
			1	1	

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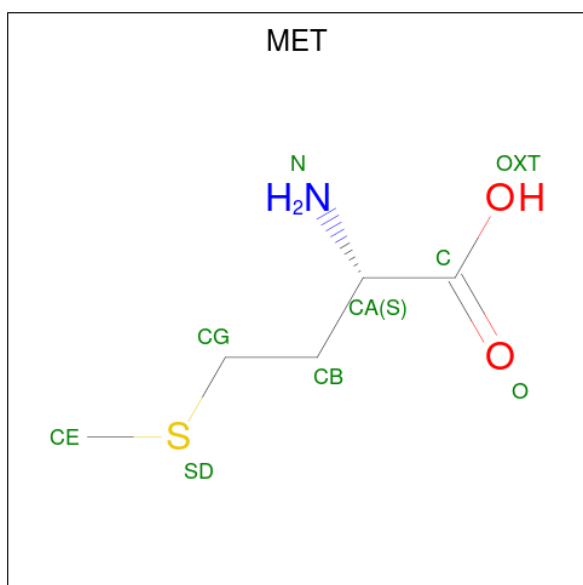
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
93	Lp	1	1	1	0

- Molecule 94 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



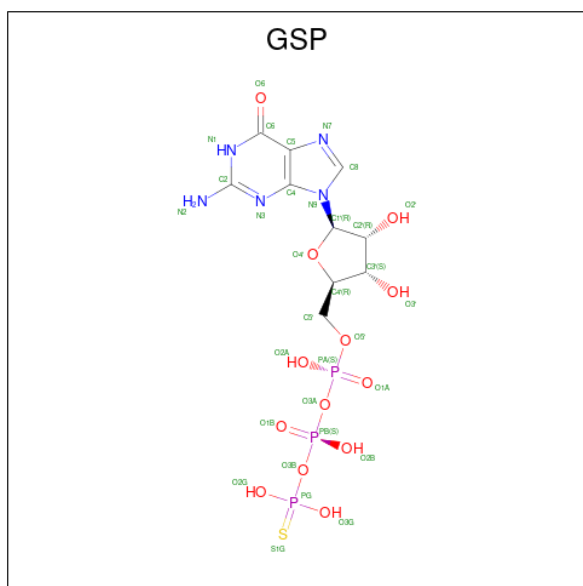
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
94	At	1	11	9	1	1	0

- Molecule 95 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



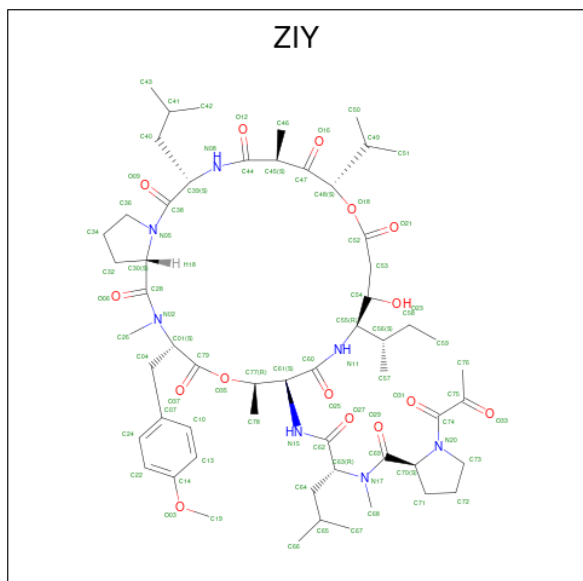
Mol	Chain	Residues	Atoms					AltConf
95	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 96 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms					AltConf	
96	EF	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

- Molecule 97 is plitidepsin (CCD ID: ZIY) (formula: $C_{57}H_{87}N_7O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
97	EF	1	Total	C	N	O	0
			79	57	7	15	

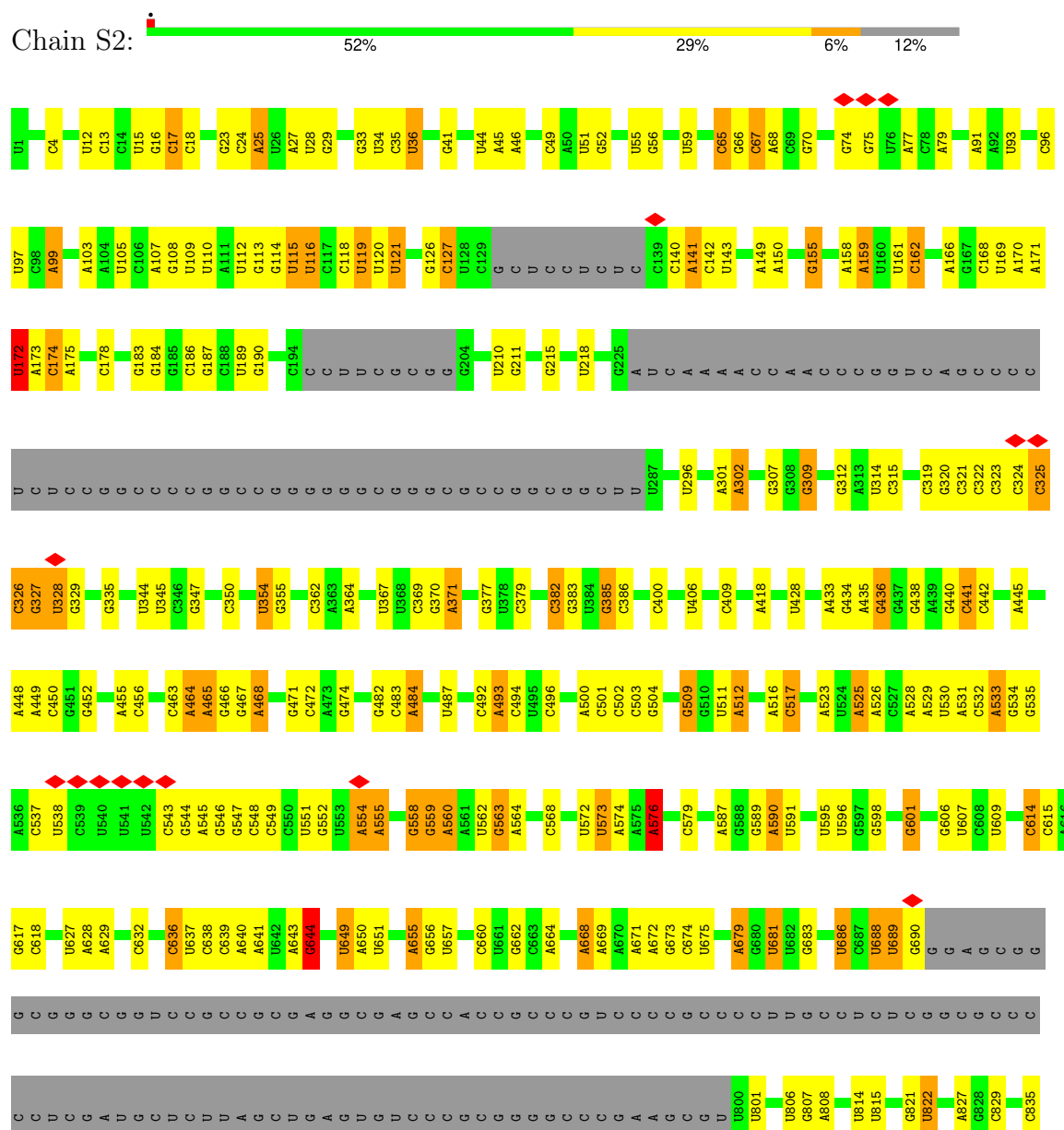
- Molecule 98 is water.

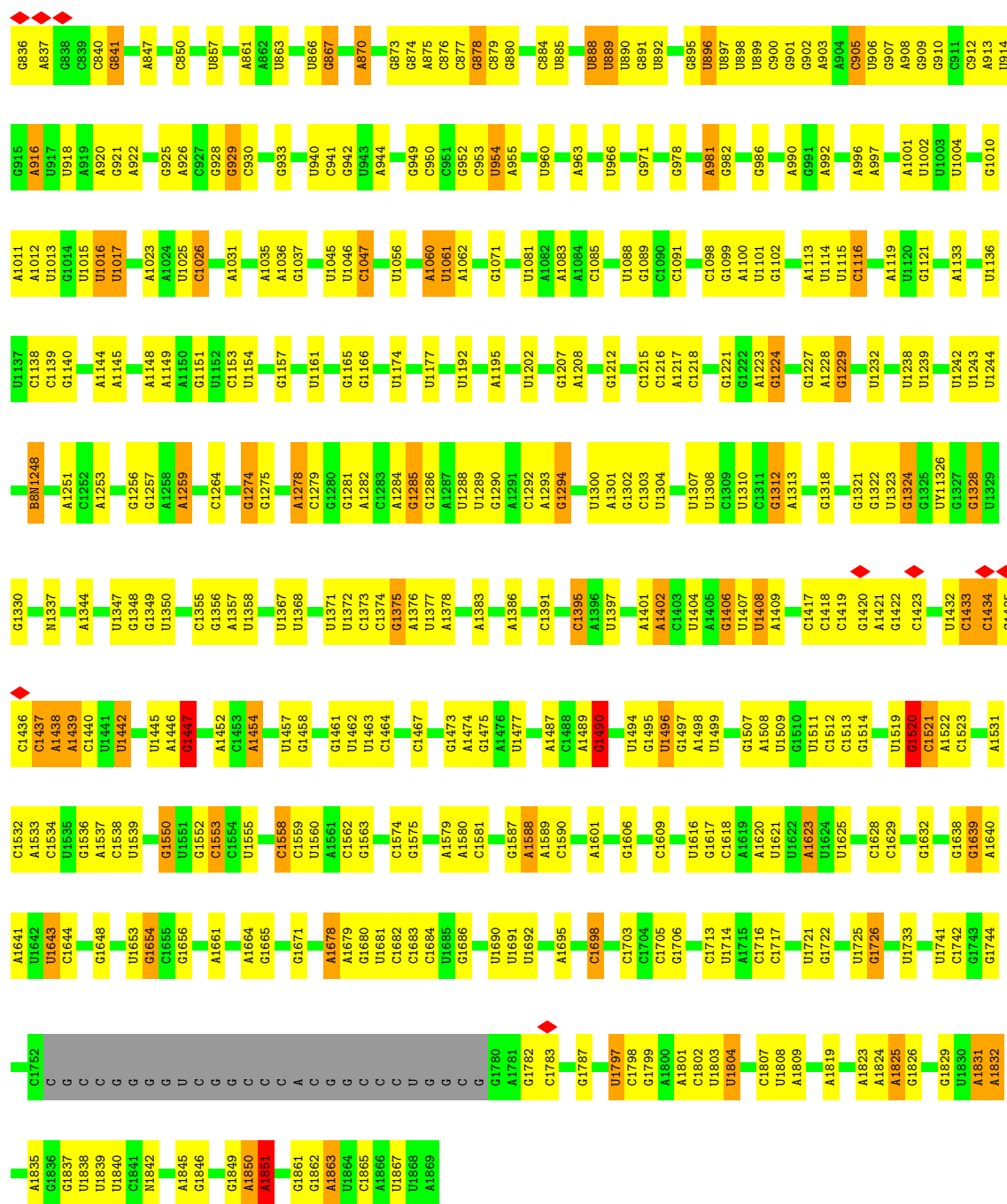
Mol	Chain	Residues	Atoms				AltConf
98	S2	9	Total	O			0
			9	9			
98	L8	3	Total	O			0
			3	3			
98	L5	228	Total	O			0
			228	228			
98	L7	1	Total	O			0
			1	1			
98	SQ	1	Total	O			0
			1	1			
98	SO	1	Total	O			0
			1	1			
98	LA	7	Total	O			0
			7	7			
98	LB	1	Total	O			0
			1	1			
98	LC	1	Total	O			0
			1	1			
98	LH	1	Total	O			0
			1	1			
98	LL	1	Total	O			0
			1	1			
98	LQ	1	Total	O			0
			1	1			
98	LS	1	Total	O			0
			1	1			
98	Lb	2	Total	O			0
			2	2			
98	LF	1	Total	O			0
			1	1			
98	Le	2	Total	O			0
			2	2			
98	Lo	2	Total	O			0
			2	2			

3 Residue-property plots

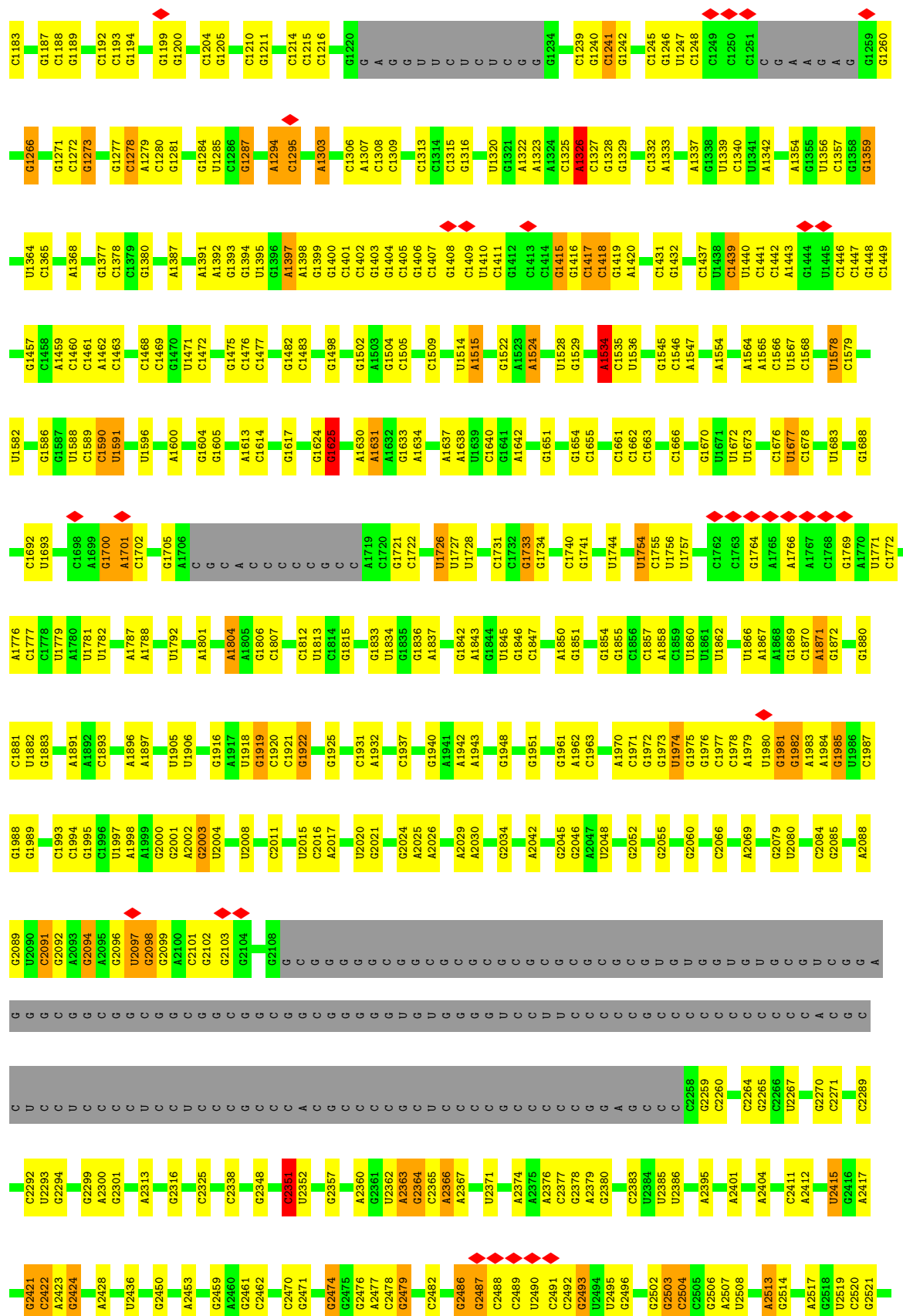
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA

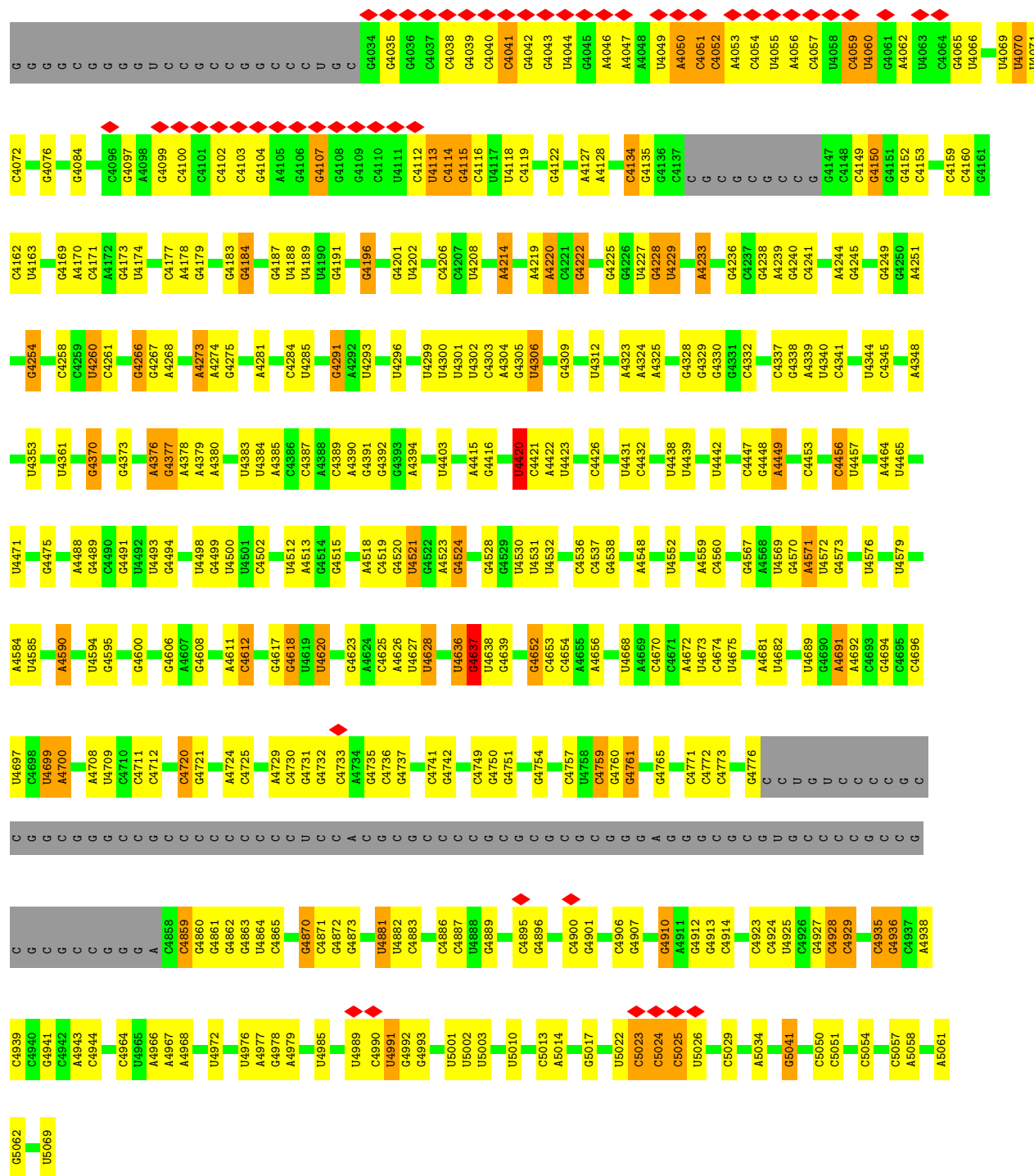




Chain L5: 45% 23% 28%







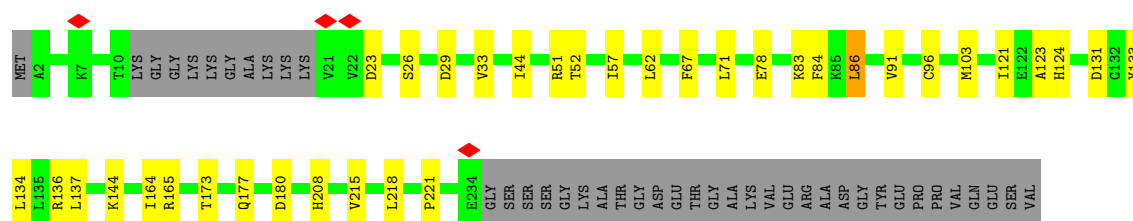
• Molecule 4: 5S rRNA

Chain L7:



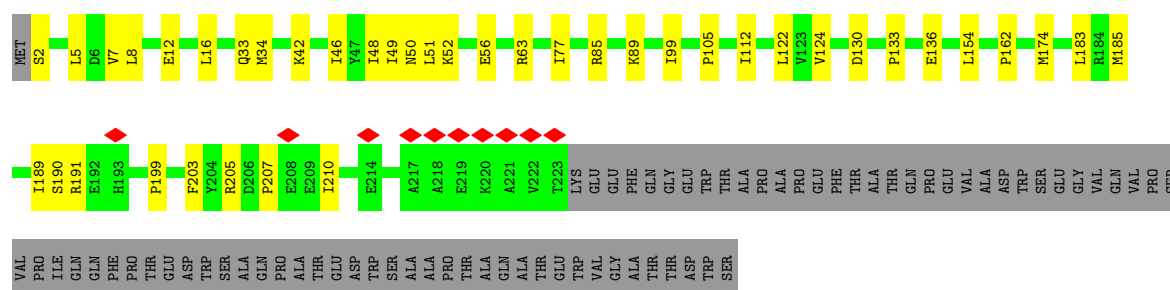
• Molecule 5: eS1

Chain SB: 



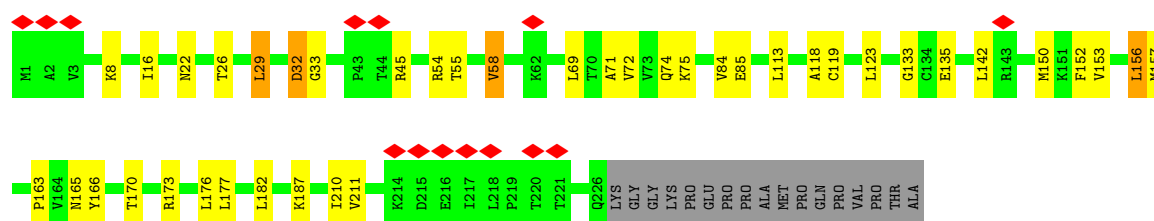
• Molecule 6: uS2

Chain SA: 



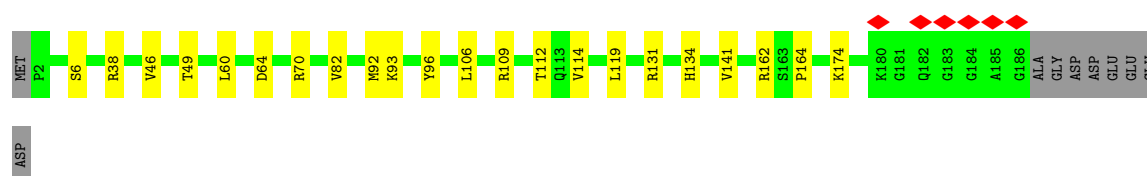
• Molecule 7: uS3

Chain SD: 



• Molecule 8: uS4

Chain SJ: 



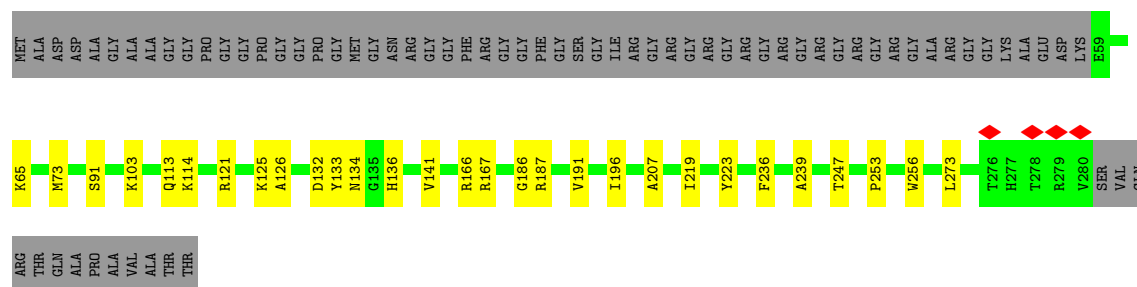
• Molecule 9: eS4

Chain SE: 

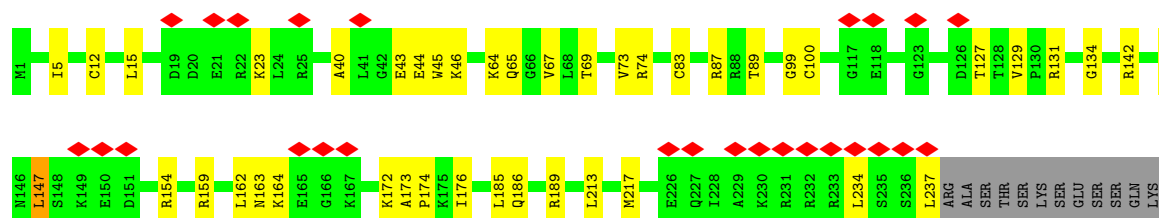
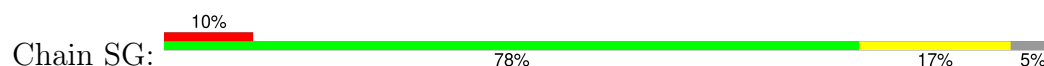




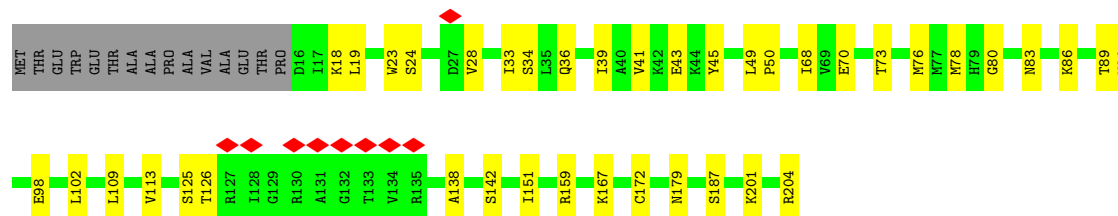
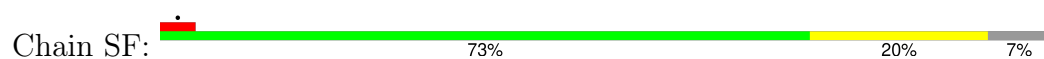
- Molecule 10: uS5



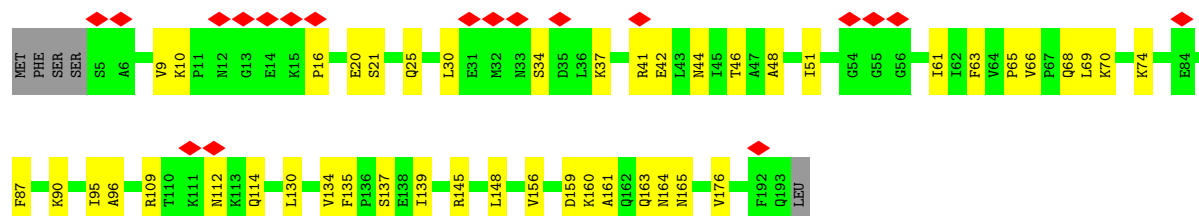
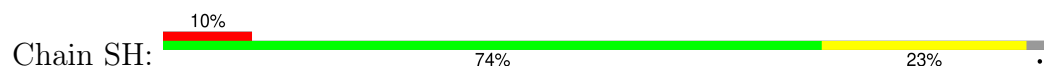
- Molecule 11: eS6



- Molecule 12: uS7

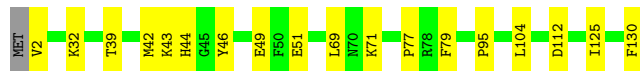


- Molecule 13: eS7



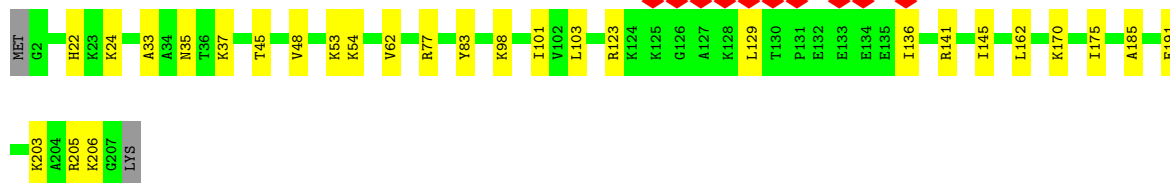
- Molecule 14: uS8

Chain SW:  85% 14%



- Molecule 15: eS8

Chain SI:  5% 86% 13%



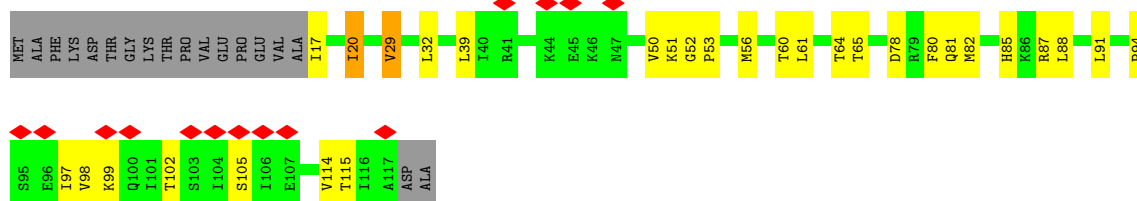
- Molecule 16: uS9

Chain SQ:  83% 14%

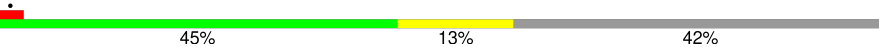


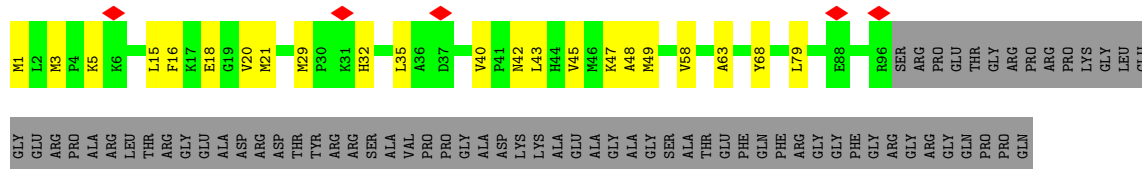
- Molecule 17: uS10

Chain SU:  12% 60% 24% 15%



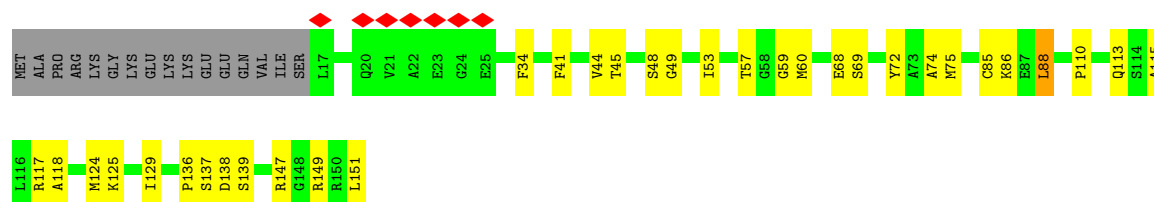
- Molecule 18: eS10

Chain SK:  45% 13% 42%

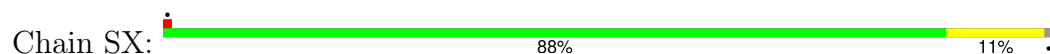


- Molecule 19: uS11

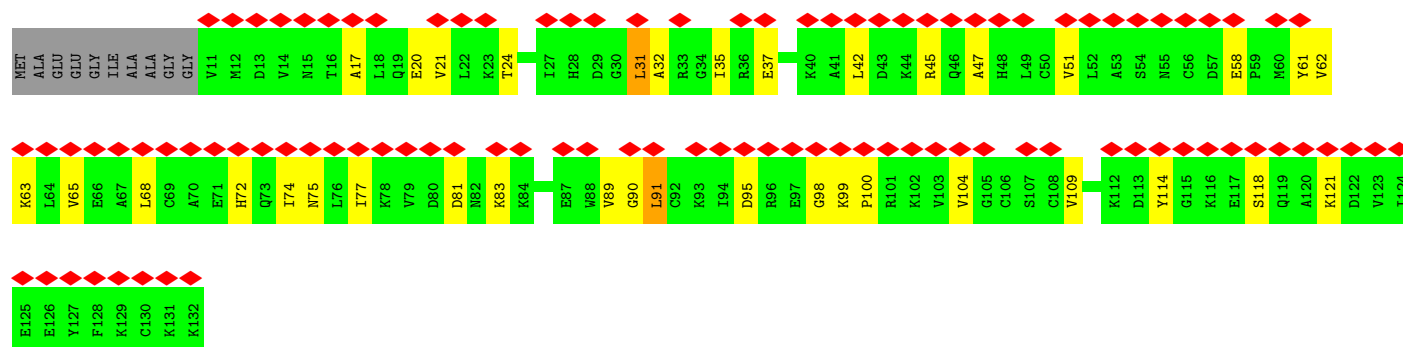
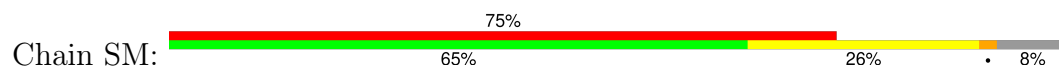
Chain SO:  5% 68% 21% 11%



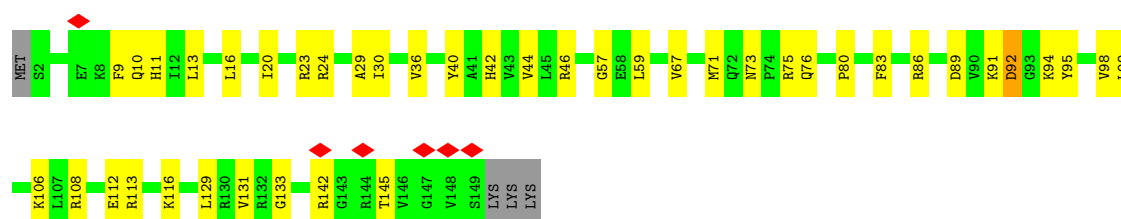
• Molecule 20: uS12



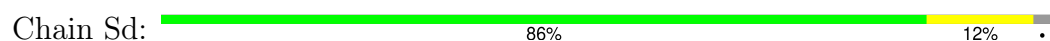
• Molecule 21: eS12



• Molecule 22: uS13



• Molecule 23: uS14



• Molecule 24: uS15





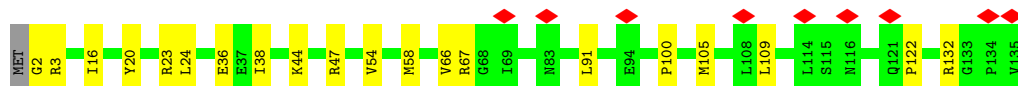
• Molecule 25: uS17

Chain SL: 83% 9% 8%



• Molecule 26: eS17

Chain SR: 7% 84% 15%



• Molecule 27: uS19

Chain SP: 8% 78% 10% 12%



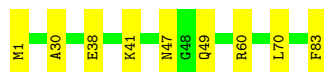
• Molecule 28: eS19

Chain ST: 88% 11%



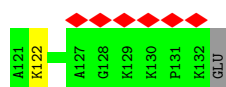
• Molecule 29: eS21

Chain SV: 89% 11%

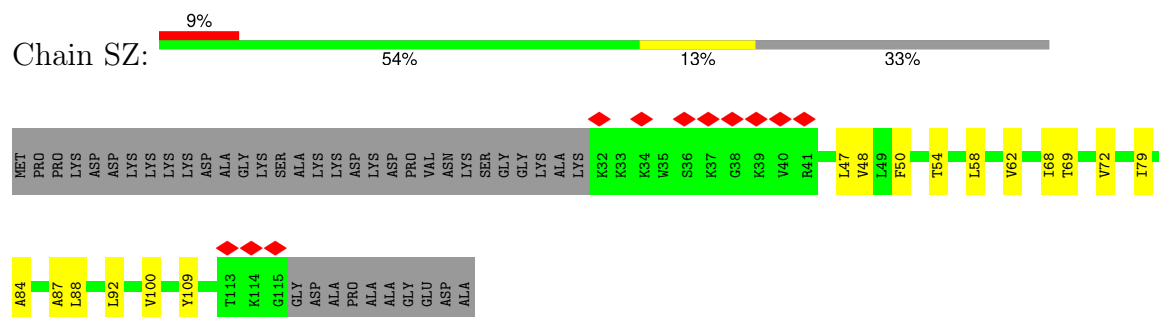


• Molecule 30: eS24

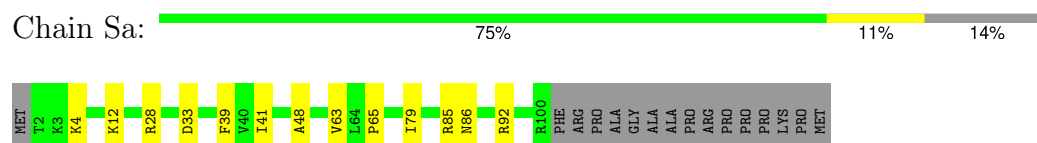
Chain SY: 8% 73% 25%



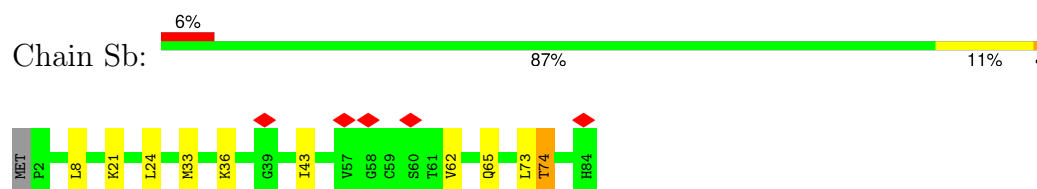
- Molecule 31: eS25



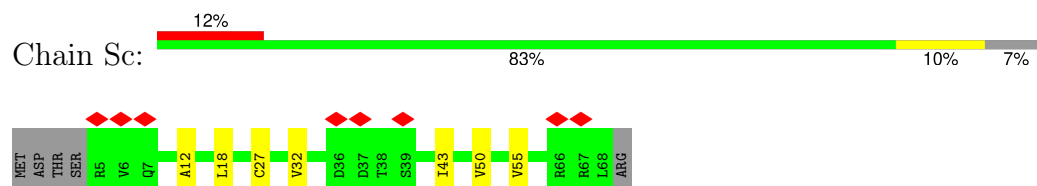
- Molecule 32: eS26



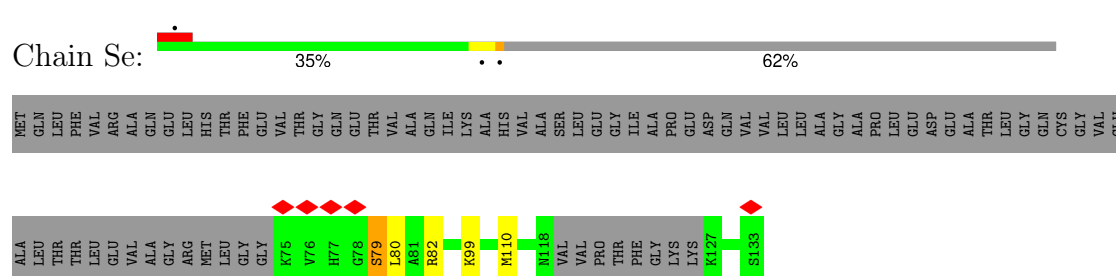
- Molecule 33: eS27



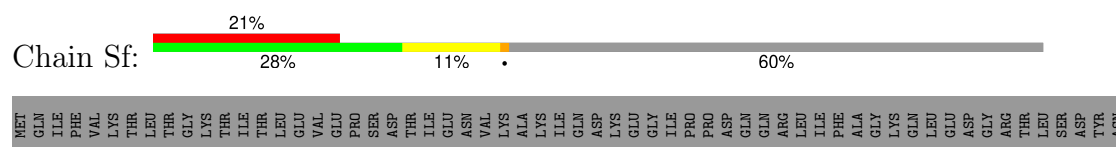
- Molecule 34: eS28

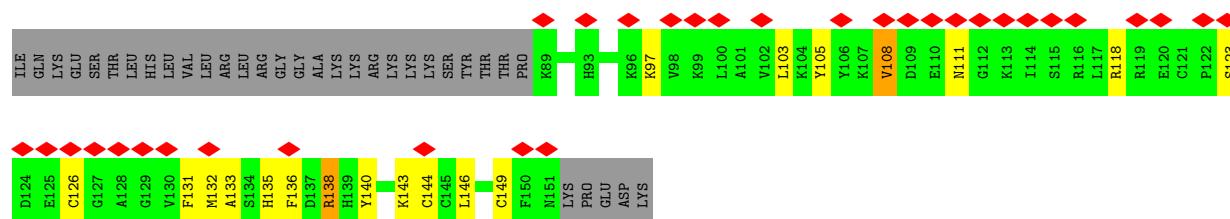


- Molecule 35: eS30

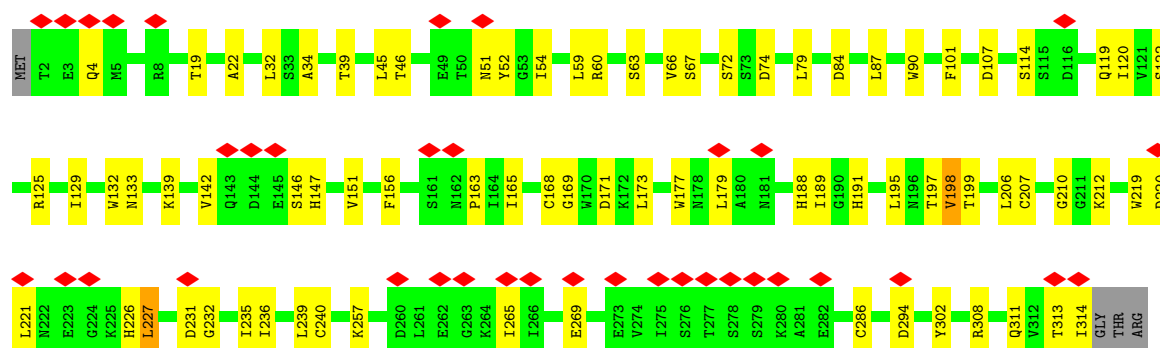
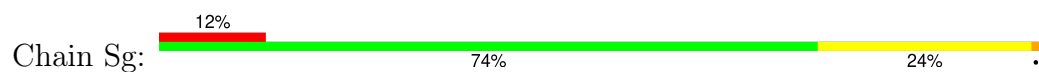


- Molecule 36: eS31

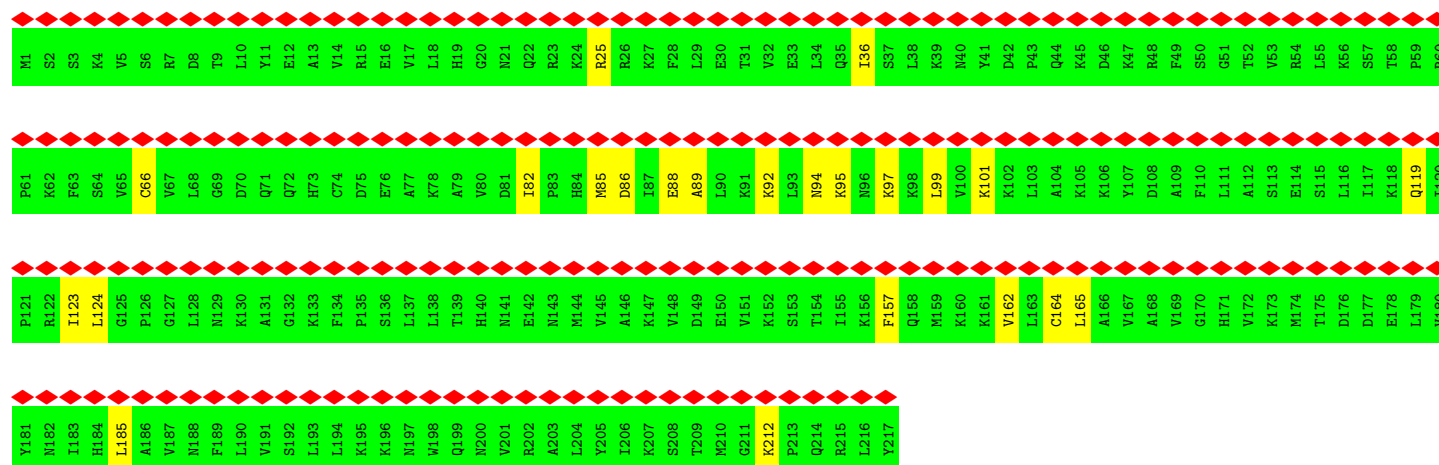
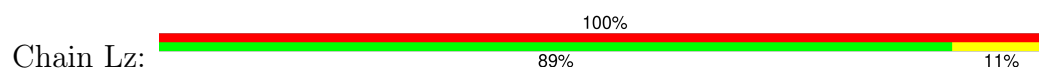




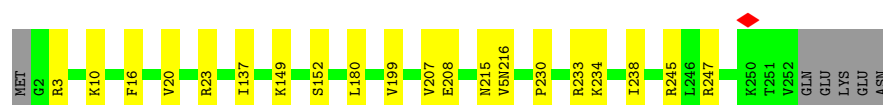
• Molecule 37: RACK1



• Molecule 38: uL1

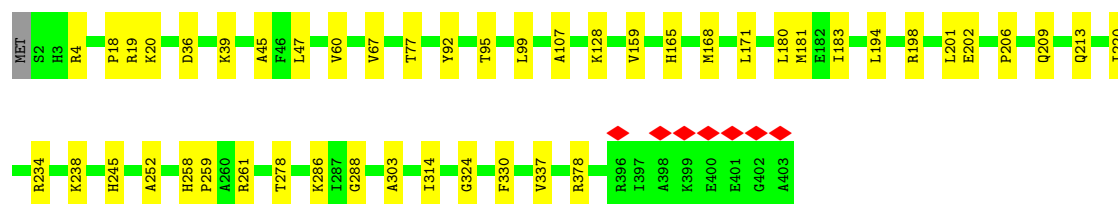


• Molecule 39: uL2



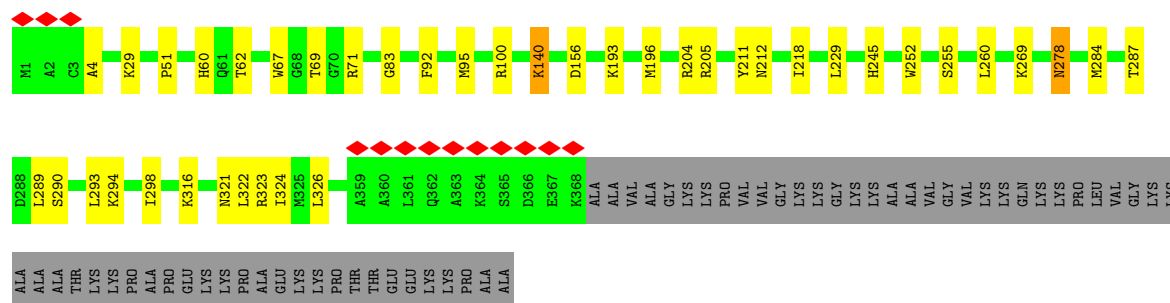
• Molecule 40: uL3

Chain LB:  88% 12%



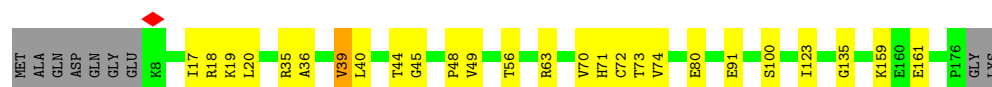
• Molecule 41: uL4

Chain LC:  77% 9% 14%



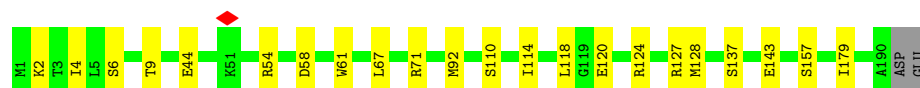
• Molecule 42: uL5

Chain LJ:  80% 14% 5%



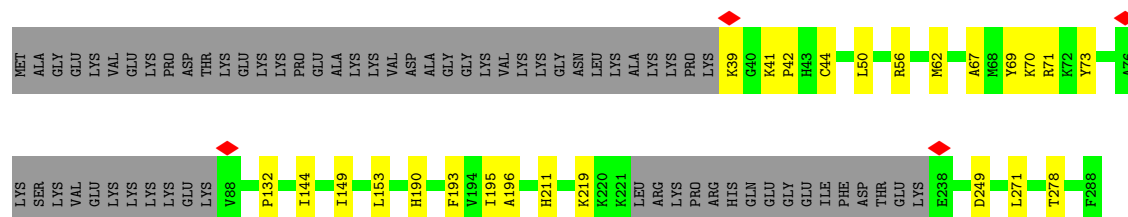
• Molecule 43: uL6

Chain LH:  88% 11%

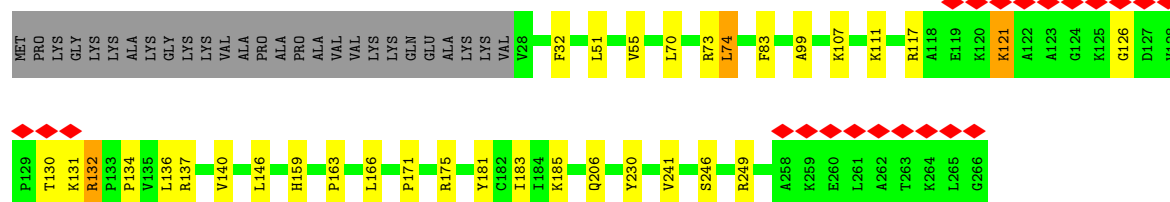
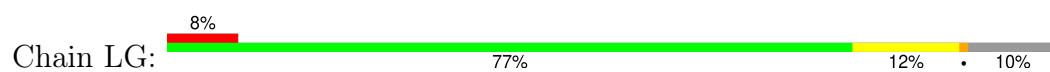


• Molecule 44: eL6

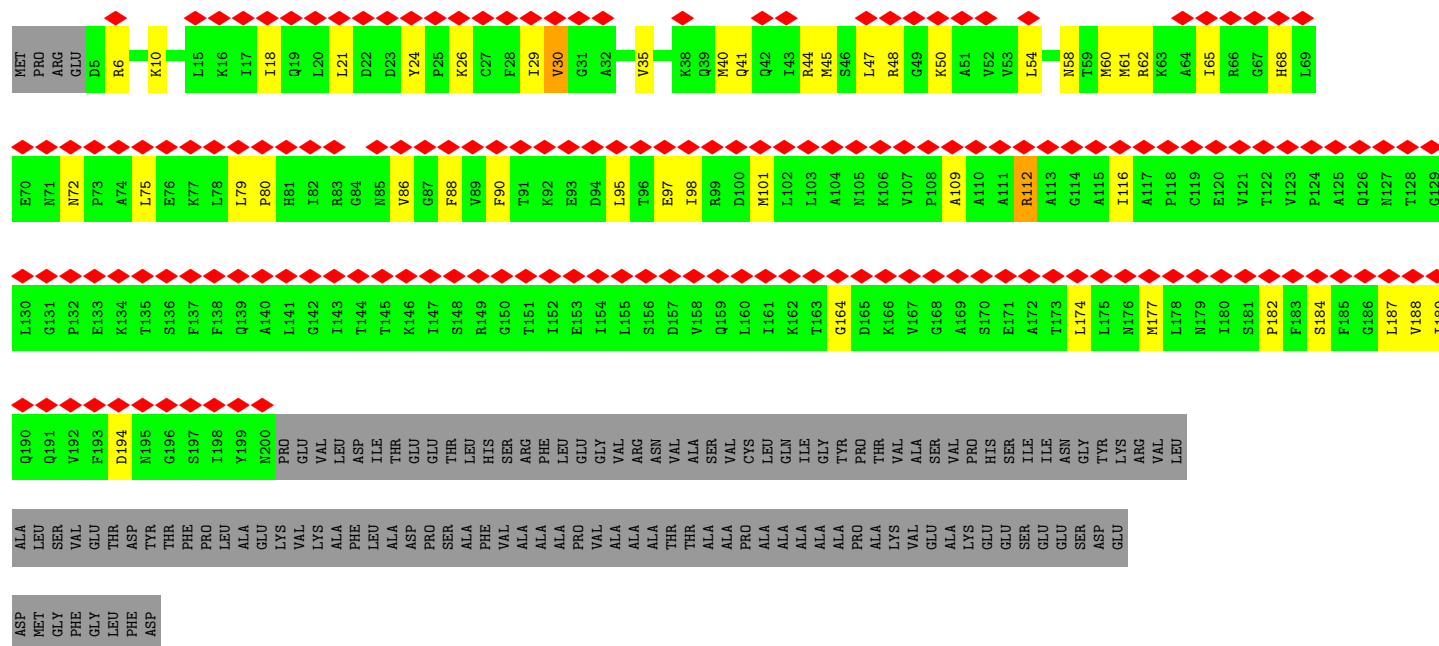
Chain LE:  69% 9% 23%



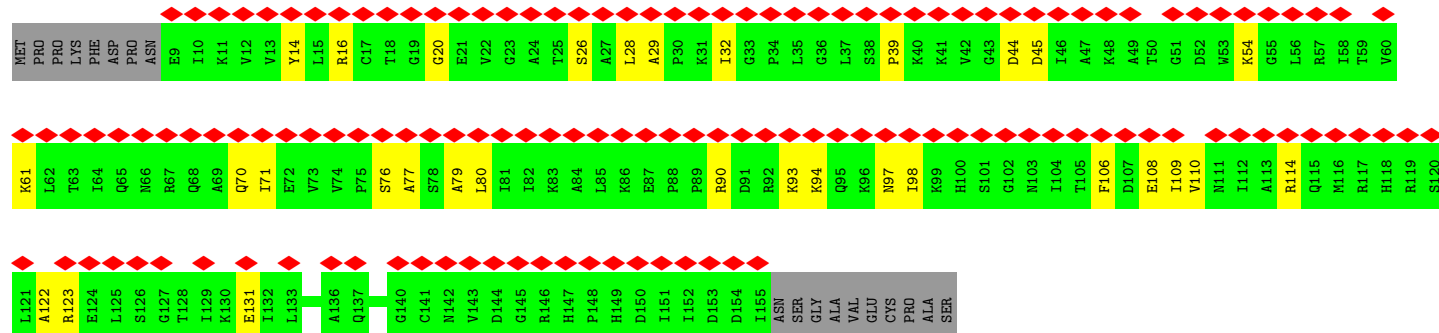
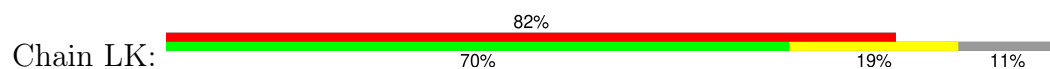
• Molecule 45: eL8



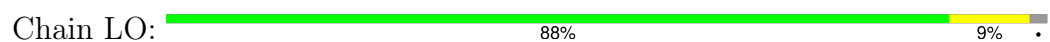
- Molecule 46: uL10

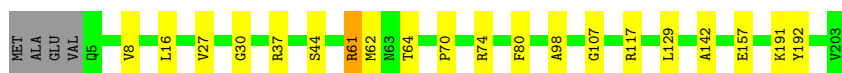


- Molecule 47: uL11



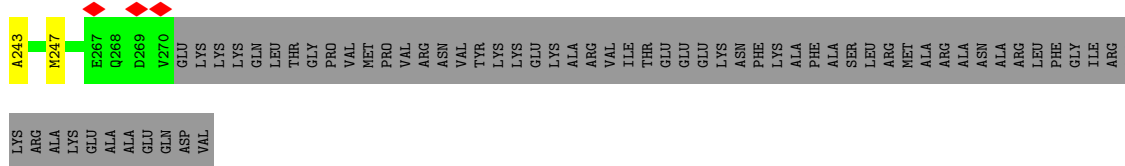
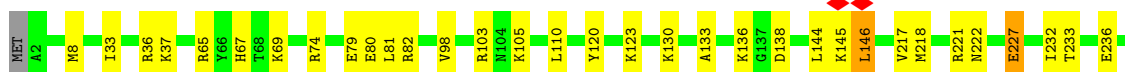
- Molecule 48: uL13





• Molecule 49: eL13

Chain LL:



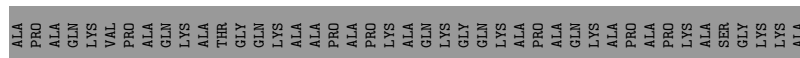
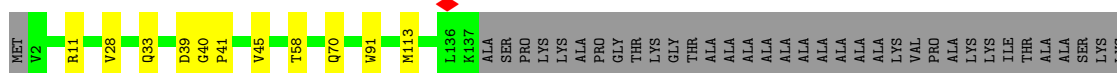
• Molecule 50: uL14

Chain LV:



• Molecule 51: eL14

Chain LM:



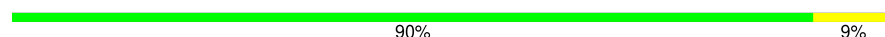
• Molecule 52: uL15

Chain La:



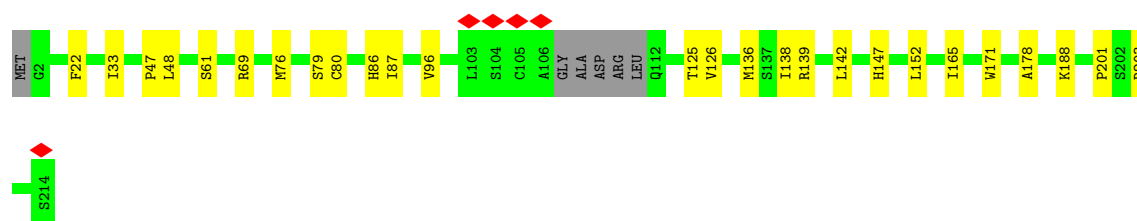
• Molecule 53: eL15

Chain LN:



• Molecule 54: uL16

Chain LI:  85% 12%



- Molecule 55: uL18

Chain LD:  91% 8%



- Molecule 56: eL18

Chain LQ:  90% 10%



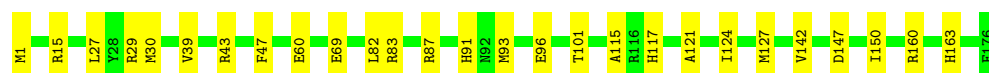
- Molecule 57: eL19

Chain LR:  6% 84% 11% 5%



- Molecule 58: eL20

Chain LS:  85% 15%



- Molecule 59: eL21

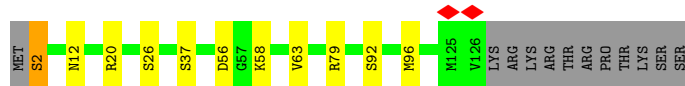
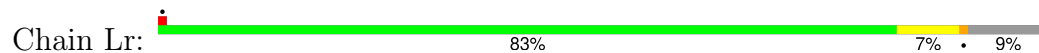
Chain LT:  88% 12%



- Molecule 60: uL22

Chain LP:  74% 9% 17%

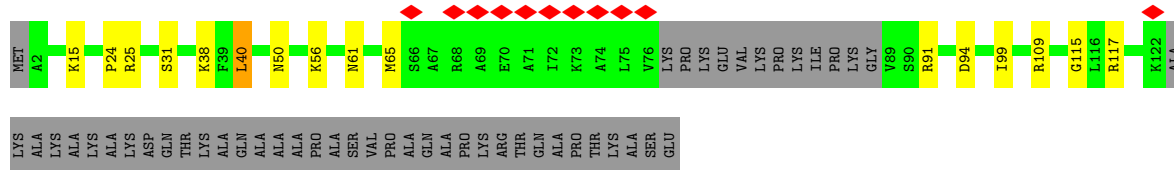
• Molecule 66: eL28



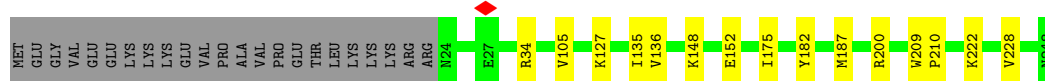
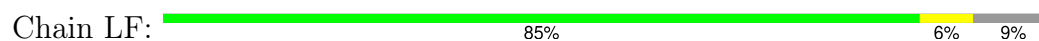
• Molecule 67: uL29



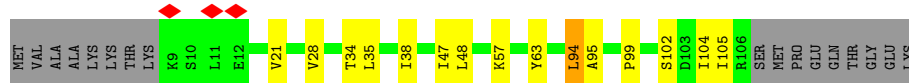
• Molecule 68: eL29



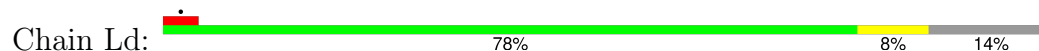
• Molecule 69: uL30



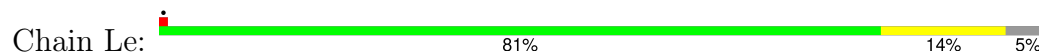
• Molecule 70: eL30

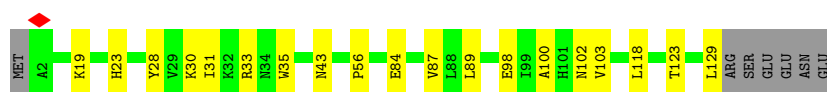


• Molecule 71: eL31



• Molecule 72: eL32





• Molecule 73: eL33

Chain Lf: 90% 9% .



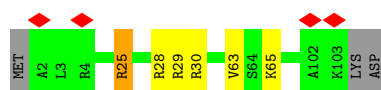
• Molecule 74: eL34

Chain Lg: 6% 87% 10% .



• Molecule 75: eL36

Chain Li: 91% 5% . .



• Molecule 76: eL37

Chain Lj: 79% 9% 11%



• Molecule 77: eL38

Chain Lk: 87% 10% . .



• Molecule 78: eL39

Chain Ll: 80% 16% . .



• Molecule 79: eL40

Chain Lm: 38% 59%

MET GLN ILE PHE VAL THR LEU THR GLY THR LYS THR ILE THR LEU VAL GLU VAL GLU PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLY ILE PRO PRO ASP GLN GLN ARG LEU ILE PHE ALA GLY LYS LEU LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN

ILE GLN LYS GLU SER THR LEU HIS VAL LEU ARG ARG GLY ILE I77 I78 R83 C99 K114 K128

• Molecule 80: eL41

Chain Ln:  84% 16%

M1 R12 R15 K25

• Molecule 81: eL42

Chain Lo:  87% 11%

MET V2 T10 K14 S32 L33 Y34 A35 K38 R39 K61 S79 M82 H90 Q105 PHE

• Molecule 82: eL43

Chain Lp:  88% 11%

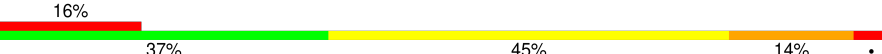
MET A2 G9 Y18 V26 E30 M47 K48 R49 W55 H56 C57 V79 I83 D91 Q92

• Molecule 83: mRNA

Chain mR:  8% 8% 5% 85%

C A A C C U A A A A C U U A C A C A G G G G A C A C34 G35 U40 U41 C42 A A A G U C U U C A A A G U C A U C

• Molecule 84: A-site tRNA

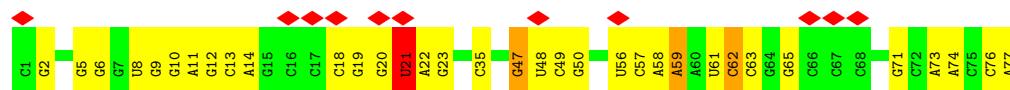
Chain At:  16% 37% 45% 14%

G1 A7 U8 A9 G10 C11 U12 C13 A14 G15 U16 C17 G18 G19 U20 A21 G22 A23 G27 G28 G29 G30 A31 U32 U33 G34 A35 A36 A37 A38 U39 C40 C41 C42 C43 C44 U45 C46 U47 C48 C49 U50 U51 G52 A58 U59 U60 G63 A64 G65 U66 C67 C68 A73 C74

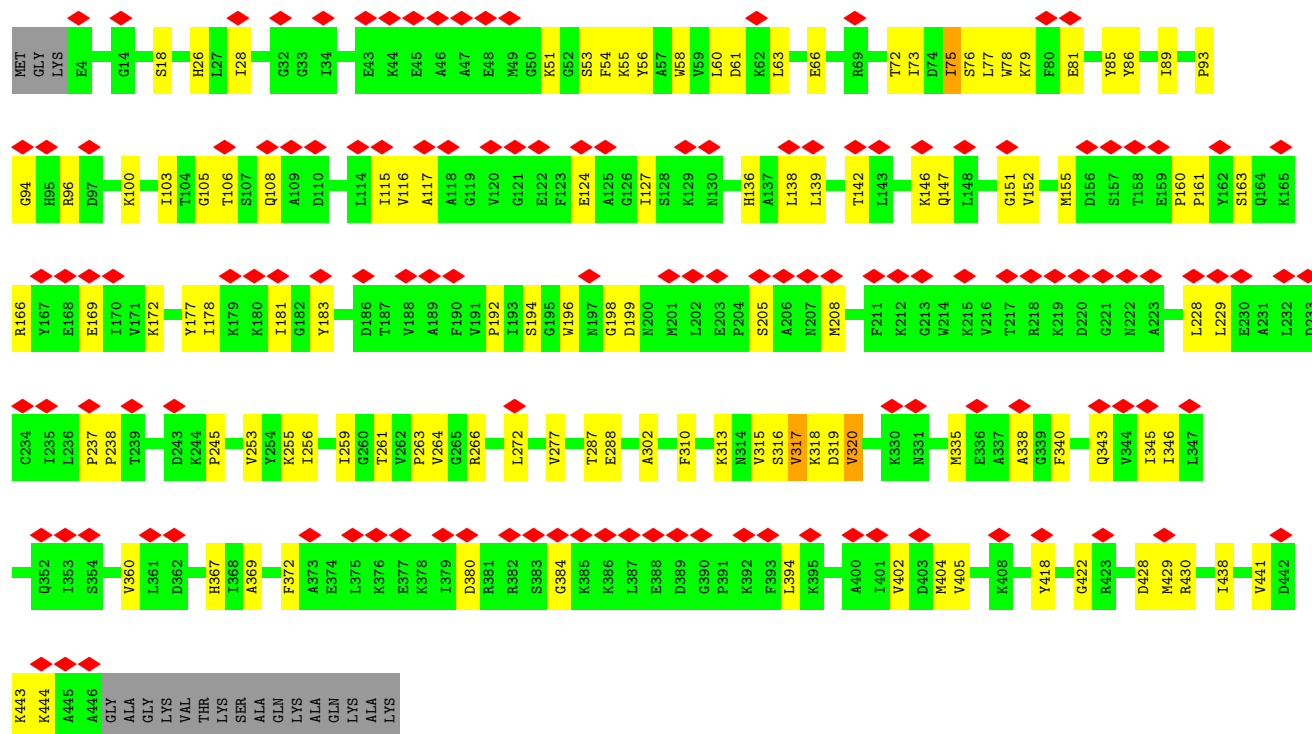
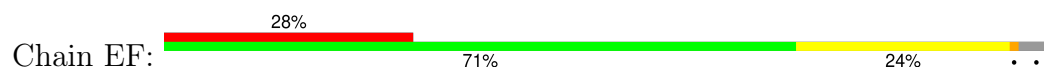
C75 A76

• Molecule 85: P-site tRNA

Chain Pt:  14% 56% 39%



• Molecule 86: eEF1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21942	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	0.045	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: SPD, B8N, UR3, M3L, OMG, MG, 4SU, ANM, 5MC, ZN, OMU, GSP, 3H3, PUT, ZIY, MLY, 4AC, PSU, H2U, MIA, K, HIC, AME, 6MZ, OMC, SAC, A2M, G7M, 1MA, MA6, V5N, HY3, MLZ, UY1

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	0.42	7/37514 (0.0%)	0.53	1/58464 (0.0%)
2	L8	0.44	0/3613	0.51	0/5627
3	L5	0.45	4/84265 (0.0%)	0.54	5/131451 (0.0%)
4	L7	0.43	0/2862	0.45	0/4459
5	SB	0.37	0/1832	0.52	0/2449
6	SA	0.65	0/1778	0.89	0/2416
7	SD	0.63	0/1784	0.92	1/2403 (0.0%)
8	SJ	0.46	0/1550	0.70	0/2069
9	SE	0.50	0/2118	0.72	0/2849
10	SC	0.45	0/1762	0.62	0/2381
11	SG	0.54	0/1946	0.74	0/2590
12	SF	0.41	0/1515	0.56	0/2037
13	SH	0.37	0/1540	0.56	0/2064
14	SW	0.38	0/1051	0.50	0/1406
15	SI	0.58	0/1715	0.78	0/2287
16	SQ	0.49	0/1141	0.74	0/1528
17	SU	0.71	0/813	1.04	0/1092
18	SK	0.43	0/834	0.59	0/1125
19	SO	0.47	0/1022	0.76	3/1372 (0.2%)
20	SX	0.38	0/1113	0.52	0/1483
21	SM	0.45	0/950	0.70	0/1275
22	SS	0.48	0/1232	0.77	0/1651
23	Sd	0.34	0/469	0.47	0/623
24	SN	0.47	1/1242 (0.1%)	0.62	1/1671 (0.1%)
25	SL	0.35	0/1209	0.40	0/1616
26	SR	0.34	0/1098	0.58	0/1474
27	SP	0.56	0/1071	0.86	0/1432
28	ST	0.64	0/1131	0.95	1/1515 (0.1%)
29	SV	0.54	0/635	0.76	0/850
30	SY	0.66	0/1083	1.04	0/1438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	SZ	0.57	0/682	0.77	0/911
32	Sa	0.43	0/805	0.65	0/1079
33	Sb	0.42	0/664	0.60	0/891
34	Sc	0.23	0/508	0.30	0/680
35	Se	0.60	0/409	0.97	1/535 (0.2%)
36	Sf	0.79	0/525	1.12	1/695 (0.1%)
37	Sg	0.61	0/2493	0.89	2/3394 (0.1%)
38	Lz	0.30	0/1769	0.51	0/2371
39	LA	0.51	0/1958	0.66	1/2623 (0.0%)
40	LB	0.43	0/3295	0.56	1/4406 (0.0%)
41	LC	0.54	0/2981	0.77	1/4002 (0.0%)
42	LJ	0.48	0/1381	0.71	1/1847 (0.1%)
43	LH	0.38	0/1537	0.52	0/2066
44	LE	0.44	0/1820	0.62	0/2442
45	LG	0.45	0/1943	0.63	0/2616
46	Lq	0.47	0/1529	0.75	0/2063
47	LK	0.45	0/1135	0.64	0/1529
48	LO	0.43	0/1666	0.57	0/2228
49	LL	0.55	0/1695	0.73	0/2270
50	LV	0.38	0/1003	0.52	0/1345
51	LM	0.37	0/1142	0.48	0/1527
52	La	0.56	0/1179	0.77	0/1573
53	LN	0.57	0/1746	0.77	0/2338
54	LI	0.46	0/1718	0.65	0/2293
55	LD	0.51	0/2433	0.74	0/3258
56	LQ	0.39	0/1535	0.52	0/2050
57	LR	0.49	0/1582	0.72	0/2091
58	LS	0.45	0/1500	0.58	0/2013
59	LT	0.48	0/1326	0.64	0/1770
60	LP	0.46	0/1268	0.65	0/1701
61	LU	0.45	0/822	0.75	0/1103
62	LX	0.34	0/984	0.39	0/1323
63	LY	0.56	0/1132	0.86	1/1504 (0.1%)
64	LW	0.48	0/958	0.69	1/1270 (0.1%)
65	LZ	0.57	0/1130	0.80	0/1507
66	Lr	0.50	0/1011	0.67	0/1356
67	Lh	0.42	0/1023	0.56	0/1351
68	Lb	0.53	0/887	0.78	0/1171
69	LF	0.38	0/1905	0.45	0/2539
70	Lc	0.61	0/774	0.87	0/1038
71	Ld	0.37	0/903	0.45	0/1216
72	Le	0.54	0/1071	0.70	0/1429
73	Lf	0.48	0/895	0.57	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Lg	0.39	0/916	0.52	0/1220
75	Li	0.33	0/843	0.46	0/1115
76	Lj	0.50	0/720	0.67	0/952
77	Lk	0.34	0/574	0.41	0/761
78	Ll	0.69	0/453	1.01	1/599 (0.2%)
79	Lm	0.41	0/425	0.58	0/564
80	Ln	0.42	0/240	0.59	0/305
81	Lo	0.39	0/854	0.54	0/1125
82	Lp	0.48	0/718	0.66	0/953
83	mR	0.27	0/208	0.41	0/321
84	At	0.43	0/1650	0.58	0/2566
85	Pt	0.39	1/1721 (0.1%)	0.49	0/2679
86	EF	0.43	1/3424 (0.0%)	0.66	2/4639 (0.0%)
All	All	0.46	14/233356 (0.0%)	0.60	25/341508 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1678	A2M	O3'-P	6.93	1.63	1.56
1	S2	166	A2M	O3'-P	6.79	1.63	1.56
3	L5	3760	A2M	O3'-P	6.41	1.62	1.56
1	S2	1442	OMU	O3'-P	6.24	1.62	1.56
1	S2	1031	A2M	O3'-P	5.89	1.62	1.56
85	Pt	8	4SU	O3'-P	5.75	1.62	1.56
1	S2	590	A2M	O3'-P	5.69	1.61	1.56
3	L5	4571	A2M	O3'-P	5.35	1.61	1.56
3	L5	1871	A2M	O3'-P	5.35	1.61	1.56
24	SN	136	PRO	C-O	-5.30	1.20	1.25
1	S2	428	OMU	O3'-P	5.22	1.61	1.56
3	L5	3925	OMU	O3'-P	5.18	1.61	1.56
1	S2	1804	OMU	O3'-P	5.03	1.61	1.56
86	EF	177[A]	TYR	C-O	5.02	1.30	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	SO	139	SER	N-CA-C	8.65	119.68	108.34
1	S2	1520	G	C2'-C3'-O3'	-8.26	101.31	113.70
19	SO	138	ASP	CB-CA-C	7.78	125.70	110.30
63	LY	110	LYS	N-CA-C	-6.69	99.99	109.96
3	L5	1590	C	C2'-C3'-O3'	-6.69	103.67	113.70
3	L5	2786	C	C2'-C3'-O3'	-6.45	104.03	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	EF	177[A]	TYR	CA-C-O	6.29	127.09	120.42
36	Sf	136	PHE	CB-CA-C	-6.20	101.14	110.88
19	SO	137	SER	N-CA-C	-6.13	104.29	110.97
86	EF	177[A]	TYR	N-CA-C	6.04	117.94	111.36
28	ST	125	PRO	N-CA-C	-5.91	105.67	113.65
37	Sg	171	ASP	N-CA-C	-5.89	105.95	113.01
7	SD	33	GLY	CA-C-O	-5.60	117.76	122.29
42	LJ	45	GLY	N-CA-C	-5.52	106.58	115.08
35	Se	79	SER	N-CA-C	5.51	115.51	108.24
64	LW	98	PRO	N-CA-C	5.48	119.07	110.80
39	LA	215	ASN	CB-CA-C	5.43	120.41	110.10
3	L5	4233	A	C2'-C3'-O3'	-5.28	101.58	109.50
40	LB	4	ARG	CB-CA-C	5.28	118.48	109.72
78	Ll	31	THR	CB-CA-C	5.26	118.42	109.84
37	Sg	52	TYR	N-CA-C	-5.22	105.71	111.71
41	LC	140	LYS	N-CA-C	-5.16	106.57	112.92
3	L5	1524	A2M	OP1-P-O3'	5.09	116.40	105.20
24	SN	133	ARG	CB-CA-C	5.09	119.53	111.23
3	L5	5041	G	C2'-C3'-O3'	-5.08	106.09	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	35359	0	17896	289	0
2	L8	3320	0	1686	24	0
3	L5	78069	0	39524	572	0
4	L7	2562	0	1295	12	0
5	SB	1806	0	1888	23	0
6	SA	1750	0	1755	24	0
7	SD	1756	0	1852	28	0
8	SJ	1525	0	1640	16	0
9	SE	2076	0	2177	25	0
10	SC	1725	0	1813	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	SG	1923	0	2088	34	0
12	SF	1494	0	1549	27	0
13	SH	1517	0	1605	27	0
14	SW	1034	0	1080	13	0
15	SI	1686	0	1772	17	0
16	SQ	1123	0	1193	10	0
17	SU	803	0	873	19	0
18	SK	810	0	836	15	0
19	SO	1009	0	1034	21	0
20	SX	1105	0	1167	12	0
21	SM	940	0	965	25	0
22	SS	1214	0	1275	29	0
23	Sd	458	0	448	9	0
24	SN	1214	0	1301	9	0
25	SL	1189	0	1262	8	0
26	SR	1083	0	1137	18	0
27	SP	1050	0	1094	10	0
28	ST	1112	0	1146	10	0
29	SV	639	0	638	6	0
30	SY	1065	0	1142	19	0
31	SZ	674	0	748	10	0
32	Sa	792	0	841	8	0
33	Sb	650	0	672	7	0
34	Sc	506	0	536	5	0
35	Se	406	0	445	4	0
36	Sf	515	0	525	10	0
37	Sg	2436	0	2393	42	0
38	Lz	1741	0	1854	16	0
39	LA	1930	0	2028	13	0
40	LB	3240	0	3377	30	0
41	LC	2927	0	3104	31	0
42	LJ	1358	0	1396	12	0
43	LH	1518	0	1601	14	0
44	LE	1786	0	1945	15	0
45	LG	1910	0	2052	19	0
46	Lq	1506	0	1562	27	0
47	LK	1121	0	1184	18	0
48	LO	1634	0	1779	13	0
49	LL	1664	0	1773	22	0
50	LV	989	0	1047	14	0
51	LM	1120	0	1187	7	0
52	La	1163	0	1206	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	LN	1701	0	1749	16	0
54	LI	1680	0	1728	18	0
55	LD	2387	0	2423	14	0
56	LQ	1511	0	1628	12	0
57	LR	1566	0	1729	10	0
58	LS	1460	0	1502	21	0
59	LT	1298	0	1366	17	0
60	LP	1242	0	1269	10	0
61	LU	808	0	831	8	0
62	LX	967	0	1040	13	0
63	LY	1115	0	1205	8	0
64	LW	944	0	994	15	0
65	LZ	1107	0	1182	10	0
66	Lr	1005	0	1072	9	0
67	Lh	1015	0	1148	8	0
68	Lb	885	0	967	12	0
69	LF	1870	0	1996	10	0
70	Lc	764	0	804	7	0
71	Ld	888	0	930	7	0
72	Le	1053	0	1147	12	0
73	Lf	876	0	912	6	0
74	Lg	906	0	998	10	0
75	Li	832	0	917	4	0
76	Lj	705	0	736	7	0
77	Lk	568	0	637	5	0
78	Ll	443	0	483	5	0
79	Lm	431	0	470	2	0
80	Ln	239	0	289	4	0
81	Lo	852	0	920	7	0
82	Lp	708	0	756	6	0
83	mR	188	0	96	5	0
84	At	1630	0	839	32	0
85	Pt	1645	0	843	15	0
86	EF	3401	0	3462	75	0
87	L5	70	0	133	2	0
87	S2	10	0	19	0	0
88	L5	48	0	96	1	0
88	S2	12	0	24	0	0
89	EF	1	0	0	0	0
89	L5	307	0	0	0	0
89	L7	7	0	0	0	0
89	L8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	LA	1	0	0	0	0
89	LB	3	0	0	0	0
89	LC	1	0	0	0	0
89	LI	1	0	0	0	0
89	LL	1	0	0	0	0
89	LN	1	0	0	0	0
89	LP	2	0	0	0	0
89	LR	1	0	0	0	0
89	LS	1	0	0	0	0
89	LV	1	0	0	0	0
89	Le	1	0	0	0	0
89	Lf	1	0	0	0	0
89	Lg	2	0	0	0	0
89	Lj	1	0	0	0	0
89	Pt	2	0	0	0	0
89	S2	112	0	0	0	0
89	SG	1	0	0	0	0
89	SN	1	0	0	0	0
89	SO	1	0	0	0	0
89	SP	1	0	0	0	0
89	SS	2	0	0	0	0
89	Sa	1	0	0	0	0
90	L5	19	0	19	0	0
91	L5	33	0	35	4	0
92	L5	10	0	0	0	0
93	Lg	1	0	0	0	0
93	Lj	1	0	0	0	0
93	Lm	1	0	0	0	0
93	Lo	1	0	0	0	0
93	Lp	1	0	0	0	0
93	Sa	1	0	0	0	0
93	Sd	1	0	0	0	0
94	At	11	0	8	2	0
95	Pt	8	0	8	0	0
96	EF	32	0	12	1	0
97	EF	79	0	0	1	0
98	L5	228	0	0	2	0
98	L7	1	0	0	0	0
98	L8	3	0	0	0	0
98	LA	7	0	0	0	0
98	LB	1	0	0	0	0
98	LC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
98	LF	1	0	0	0	0
98	LH	1	0	0	0	0
98	LL	1	0	0	0	0
98	LQ	1	0	0	0	0
98	LS	1	0	0	0	0
98	Lb	2	0	0	0	0
98	Le	2	0	0	0	0
98	Lo	2	0	0	0	0
98	S2	9	0	0	0	0
98	SO	1	0	0	0	0
98	SQ	1	0	0	0	0
All	All	223755	0	167808	1884	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 5.

All (1884) 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)
84:At:44:G:H1'	84:At:45:U:H2'	1.42	1.01
3:L5:209:U:H5''	63:LY:59:ARG:HD2	1.49	0.93
21:SM:91:LEU:HD21	21:SM:104:VAL:H	1.38	0.88
21:SM:32:ALA:HB1	21:SM:37:GLU:HB3	1.61	0.82
3:L5:4041:C:H1'	38:Lz:101:LYS:HG3	1.60	0.82
36:Sf:138:ARG:HB2	36:Sf:149:CYS:HA	1.61	0.82
1:S2:928:G:H1	1:S2:1013:U:H3	1.30	0.80
61:LU:48:LYS:HG2	61:LU:53:ALA:HB2	1.62	0.80
3:L5:4152:G:H2'	3:L5:4153:C:H6	1.47	0.80
1:S2:925:G:H1	1:S2:1017:U:H3	1.29	0.79
64:LW:97:LYS:HA	64:LW:101:ARG:HE	1.47	0.78
37:Sg:87:LEU:HB2	37:Sg:101:PHE:HB2	1.66	0.78
11:SG:69:THR:HG21	11:SG:73:VAL:HG13	1.65	0.77
11:SG:67:VAL:HB	11:SG:99:GLY:HA2	1.65	0.76
3:L5:691:C:H2'	3:L5:692:A:C8	2.22	0.74
37:Sg:199:THR:HG21	37:Sg:240:CYS:HA	1.68	0.74
60:LP:17:SER:HB2	60:LP:98:ALA:HB2	1.71	0.73
1:S2:888:U:H1'	1:S2:889:U:H2'	1.70	0.72
86:EF:178:ILE:HB	86:EF:183:TYR:HB2	1.70	0.72
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.73	0.71
47:LK:76:SER:HB3	47:LK:79:ALA:HB2	1.71	0.71
16:SQ:19:ALA:HB2	16:SQ:75:GLY:HA3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:mR:41:U:H3	84:At:34:G:H1	1.38	0.70
78:Ll:23:ILE:HD11	78:Ll:28:ARG:HE	1.56	0.69
42:LJ:36:ALA:HA	42:LJ:39:VAL:HG13	1.74	0.69
86:EF:335:MET:HE2	86:EF:443:LYS:HB3	1.75	0.69
49:LL:80:GLU:HG3	49:LL:110:LEU:HD12	1.75	0.68
3:L5:2351:OMC:HM23	41:LC:95:MET:HG3	1.74	0.68
65:LZ:50:PRO:HD3	65:LZ:68:ILE:HG12	1.76	0.68
1:S2:640:A:H2'	1:S2:641:A:C8	2.28	0.68
3:L5:4966:A:H5''	40:LB:128:LYS:HG3	1.75	0.68
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.29	0.68
39:LA:137:ILE:HD11	39:LA:149:LYS:HB2	1.76	0.68
1:S2:806:U:H3	1:S2:857:U:H3	1.41	0.68
7:SD:16:ILE:HG21	23:Sd:22:ARG:HH11	1.59	0.68
3:L5:1970:A:H4'	3:L5:2000:G:H8	1.59	0.67
3:L5:1754:U:HO2'	3:L5:1755:C:H6	1.40	0.67
52:La:72:THR:HG22	52:La:110:LYS:HB3	1.77	0.67
3:L5:4152:G:H2'	3:L5:4153:C:C6	2.29	0.67
27:SP:49:LEU:HD22	27:SP:53:GLN:HG2	1.77	0.67
37:Sg:147:HIS:CE1	37:Sg:169:GLY:H	2.13	0.67
85:Pt:19:G:H21	85:Pt:59:A:H5'	1.59	0.67
1:S2:1114:U:H3	1:S2:1119:A:H62	1.41	0.67
1:S2:874:G:H21	13:SH:114:GLN:HE22	1.41	0.67
40:LB:206:PRO:HG2	40:LB:209:GLN:HG3	1.76	0.67
85:Pt:48:U:H4'	85:Pt:49:C:H5'	1.76	0.67
38:Lz:36:ILE:H	38:Lz:165:LEU:HD12	1.59	0.66
86:EF:108:GLN:HB2	86:EF:266:ARG:HD3	1.77	0.66
3:L5:2101:C:H2'	3:L5:2102:G:C8	2.31	0.66
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.78	0.66
37:Sg:120:ILE:HB	37:Sg:132:TRP:HB2	1.78	0.66
1:S2:1144:A:H2'	1:S2:1145:A:C8	2.32	0.65
62:LX:82:THR:HG21	67:Lh:37:THR:HG22	1.77	0.65
1:S2:1274:G:H4'	18:SK:47:LYS:HE2	1.77	0.65
11:SG:67:VAL:HG12	11:SG:69:THR:HG22	1.78	0.65
84:At:9:A:H62	84:At:23:A:H62	1.42	0.65
1:S2:1101:U:H2'	1:S2:1102:G:C8	2.32	0.65
3:L5:181:C:H2'	3:L5:182:G:H8	1.62	0.65
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.32	0.65
11:SG:131:ARG:HD2	64:LW:82:ILE:HG12	1.79	0.65
62:LX:82:THR:HG22	62:LX:155:ILE:HG23	1.79	0.65
85:Pt:20:G:H3'	85:Pt:21:H2U:H62	1.78	0.65
9:SE:104:ASP:HB3	9:SE:110:ALA:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Lo:33:LEU:HA	81:Lo:38:LYS:HG2	1.80	0.64
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.32	0.64
84:At:32:PSU:H1'	84:At:38:A:N6	2.11	0.64
37:Sg:34:ALA:HB1	37:Sg:66:VAL:HG23	1.79	0.64
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.33	0.64
22:SS:13:LEU:HB2	22:SS:20:ILE:HB	1.80	0.64
37:Sg:219:TRP:CD1	37:Sg:226:HIS:HA	2.33	0.64
39:LA:245[B]:ARG:HH11	39:LA:245[B]:ARG:HG3	1.62	0.64
6:SA:203:PHE:HZ	26:SR:91:LEU:HD11	1.63	0.64
42:LJ:19:LYS:HB2	42:LJ:73:THR:HG23	1.80	0.63
70:Lc:34:THR:HG23	70:Lc:95:ALA:HB2	1.81	0.63
65:LZ:33:THR:HG23	65:LZ:36:ARG:H	1.62	0.63
18:SK:16:PHE:HB2	18:SK:79:LEU:HD23	1.79	0.63
40:LB:92:TYR:HB3	40:LB:99:LEU:HD22	1.81	0.63
12:SF:49:LEU:HD12	16:SQ:50:LYS:HG2	1.80	0.63
45:LG:134:PRO:HB3	45:LG:206:GLN:HG3	1.80	0.63
79:Lm:78:ILE:HG21	79:Lm:83:ARG:HH21	1.64	0.63
1:S2:1606:G:H3'	28:ST:86:GLY:HA3	1.80	0.63
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.28	0.63
3:L5:4859:C:H3'	3:L5:4860:G:H8	1.64	0.63
37:Sg:286:CYS:HA	37:Sg:302:TYR:HD1	1.64	0.63
20:SX:107:ARG:HD3	20:SX:112:VAL:HG12	1.81	0.63
40:LB:261:ARG:HB2	48:LO:64:THR:HG21	1.80	0.62
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.34	0.62
1:S2:530:U:H3	1:S2:555:A:H61	1.45	0.62
7:SD:150:MET:HE2	7:SD:152:PHE:HZ	1.64	0.62
1:S2:502:C:H5'	9:SE:66:MET:HE3	1.81	0.62
50:LV:43:LYS:HG3	50:LV:60:MET:HG2	1.82	0.62
3:L5:2016:C:H2'	3:L5:2017:A:H8	1.63	0.62
86:EF:116:VAL:HB	86:EF:152:VAL:HG12	1.82	0.62
12:SF:34:SER:HA	34:Sc:55:VAL:HB	1.82	0.61
18:SK:3:MET:HE1	18:SK:48:ALA:HB2	1.82	0.61
86:EF:63:LEU:HB3	86:EF:66:GLU:HG3	1.81	0.61
1:S2:1091:C:HO2'	14:SW:2:VAL:N	1.98	0.61
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	1.82	0.61
50:LV:13:LYS:HB2	50:LV:128:LEU:HD11	1.82	0.61
76:Lj:31:LYS:HB3	76:Lj:33:THR:HG22	1.81	0.61
85:Pt:9:G:H5''	85:Pt:47:G7M:H1'	1.81	0.61
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.35	0.61
86:EF:75:ILE:HG21	86:EF:105:GLY:HA3	1.82	0.61
86:EF:103:ILE:HD11	86:EF:139:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:4:GLN:HE22	37:Sg:314:ILE:HD12	1.65	0.61
7:SD:54:ARG:O	7:SD:58:VAL:HG13	2.01	0.61
53:LN:45:PRO:O	53:LN:49:ARG:HG3	2.00	0.61
3:L5:2091:C:H1'	3:L5:2094:G:H1'	1.83	0.61
11:SG:43:GLU:HA	11:SG:46:LYS:HD3	1.83	0.61
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.83	0.60
45:LG:99:ALA:HB1	45:LG:136:LEU:HD11	1.81	0.60
60:LP:54:GLN:HA	60:LP:83:TRP:CD1	2.36	0.60
1:S2:1536:G:H2'	1:S2:1537:A:C8	2.35	0.60
5:SB:52:THR:HG23	5:SB:57:ILE:HA	1.83	0.60
13:SH:87:PHE:HB3	13:SH:90:LYS:HD2	1.82	0.60
75:Li:63:VAL:HG23	75:Li:65:LYS:HG3	1.84	0.60
3:L5:4993:G:H22	3:L5:5058:A:H2	1.50	0.60
25:SL:18:GLN:HG2	25:SL:33:LEU:HD11	1.84	0.60
8:SJ:60:LEU:HD22	8:SJ:70:ARG:HA	1.84	0.60
40:LB:213:GLN:HE22	40:LB:286:LYS:HA	1.66	0.60
7:SD:8:LYS:HG2	17:SU:61:LEU:HD11	1.83	0.60
86:EF:272:LEU:HB3	86:EF:302:ALA:HB3	1.84	0.60
1:S2:367:U:H4'	1:S2:371:A:C8	2.37	0.60
22:SS:73:ASN:HB3	22:SS:76:GLN:HE22	1.65	0.60
65:LZ:100:VAL:HG21	65:LZ:110:ALA:HB2	1.84	0.60
54:LI:201:PRO:HB2	54:LI:203:ARG:HG2	1.82	0.59
22:SS:23:ARG:HG2	31:SZ:48:VAL:HG11	1.84	0.59
39:LA:245[B]:ARG:NH1	39:LA:247:ARG:HH12	1.99	0.59
1:S2:433:A:H5''	15:SI:22:HIS:HB3	1.83	0.59
9:SE:151:ASP:HB3	9:SE:154:ILE:HG13	1.83	0.59
83:mR:40:U:H2'	83:mR:41:U:C6	2.38	0.59
49:LL:103:ARG:HD3	75:Li:25:ARG:HD2	1.84	0.59
41:LC:284:MET:HE2	41:LC:287:THR:HA	1.83	0.59
48:LO:61:ARG:HA	48:LO:70:PRO:HD2	1.84	0.59
9:SE:133:THR:HG22	9:SE:134:LYS:HG2	1.85	0.59
42:LJ:20:LEU:HB3	42:LJ:74:VAL:HG23	1.84	0.59
86:EF:160:PRO:HG2	86:EF:163:SER:HA	1.85	0.59
38:Lz:157:PHE:HZ	38:Lz:165:LEU:HD13	1.68	0.59
46:Lq:72:ASN:HB3	46:Lq:75:LEU:HD23	1.84	0.59
49:LL:144:LEU:HD12	49:LL:145:LYS:HG2	1.85	0.59
3:L5:1971:C:H2'	3:L5:1972:G:H8	1.68	0.58
86:EF:79:M3L:HG2	86:EF:86:TYR:HE1	1.68	0.58
3:L5:1405:C:H2'	3:L5:1406:G:C8	2.38	0.58
9:SE:213:ALA:HB3	9:SE:244:ILE:HD11	1.84	0.58
12:SF:76:MET:HB2	12:SF:89:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:377:G:H5'	15:SI:98:LYS:HB3	1.85	0.58
8:SJ:6:SER:HB3	9:SE:23:LEU:HD21	1.86	0.58
54:LI:87:ILE:HG12	54:LI:138:ILE:HG12	1.85	0.58
41:LC:193:LYS:HD2	41:LC:196:MET:HE2	1.86	0.58
1:S2:309:G:OP2	15:SI:53:LYS:NZ	2.31	0.58
1:S2:1278:A:H2'	1:S2:1279:C:C6	2.39	0.58
17:SU:50:VAL:HG12	17:SU:52:GLY:H	1.68	0.58
65:LZ:17:ARG:HD3	74:Lg:75:SER:HB3	1.86	0.58
12:SF:28:VAL:HG11	12:SF:113:VAL:HG21	1.86	0.58
12:SF:28:VAL:HG21	12:SF:109:LEU:HB3	1.86	0.58
27:SP:13:ARG:O	27:SP:14:LYS:HG3	2.04	0.58
1:S2:1797:U:H2'	1:S2:1798:C:C6	2.39	0.58
3:L5:1726:U:H5'	69:LF:135:ILE:HD11	1.86	0.58
3:L5:2543:A:H2	3:L5:2773:G:H22	1.50	0.58
6:SA:42:LYS:HD2	6:SA:48:ILE:HD11	1.85	0.58
25:SL:126:VAL:HG12	25:SL:145:VAL:HG22	1.84	0.58
38:Lz:85:MET:HB2	38:Lz:89:ALA:HB2	1.86	0.58
41:LC:212:ASN:HD22	41:LC:255:SER:HB3	1.68	0.58
64:LW:97:LYS:HA	64:LW:101:ARG:NE	2.16	0.58
40:LB:107:ALA:HB2	40:LB:201:LEU:HD22	1.86	0.57
68:Lb:91:ARG:HB3	68:Lb:94:ASP:HB2	1.86	0.57
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.38	0.57
36:Sf:123:SER:HB3	36:Sf:126:CYS:HB2	1.87	0.57
5:SB:123:ALA:HB2	5:SB:165:ARG:HG3	1.86	0.57
37:Sg:142:VAL:HG12	37:Sg:146:SER:HB3	1.86	0.57
9:SE:19:MET:SD	9:SE:108:ARG:HD2	2.45	0.57
46:Lq:174:LEU:HA	46:Lq:177:MET:HE2	1.87	0.57
49:LL:123:LYS:HD2	49:LL:218:MET:HE2	1.87	0.57
1:S2:1825:A:O4'	83:mR:40:U:H1'	2.05	0.57
11:SG:64:LYS:HB2	11:SG:83:CYS:SG	2.45	0.57
13:SH:44:ASN:H	13:SH:68:GLN:HE22	1.53	0.57
22:SS:113:ARG:HA	22:SS:116:LYS:HE3	1.86	0.57
25:SL:33:LEU:HD12	25:SL:34:PRO:HD2	1.86	0.57
1:S2:870:A:H62	1:S2:916:A:H5'	1.69	0.57
1:S2:1520:G:N3	1:S2:1520:G:H2'	2.19	0.57
17:SU:61:LEU:HD22	17:SU:82:MET:HE2	1.87	0.57
86:EF:124:GLU:HA	86:EF:127:ILE:HG12	1.86	0.57
1:S2:546:G:H2'	1:S2:547:G:C8	2.39	0.56
24:SN:93:LYS:HA	24:SN:150:VAL:HG21	1.87	0.56
38:Lz:97:LYS:HE3	38:Lz:99:LEU:HB3	1.87	0.56
72:Le:23:HIS:HD2	72:Le:43:ASN:HD21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1406:G:H2'	1:S2:1407:U:C6	2.41	0.56
6:SA:183:LEU:HB3	6:SA:189:ILE:HG12	1.88	0.56
84:At:34:G:H3'	84:At:35:A:H8	1.70	0.56
3:L5:1971:C:C5	3:L5:2000:G:H2'	2.41	0.56
38:Lz:162:VAL:HG12	38:Lz:164:CYS:H	1.68	0.56
49:LL:130:LYS:HB3	49:LL:133:ALA:HB3	1.88	0.56
1:S2:1432:U:H4'	1:S2:1437:C:H2'	1.88	0.56
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.40	0.56
6:SA:5:LEU:HD13	29:SV:41:LYS:HA	1.86	0.56
1:S2:528:A:H2'	1:S2:529:A:C8	2.41	0.56
3:L5:1971:C:H2'	3:L5:1972:G:C8	2.41	0.56
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.40	0.56
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.87	0.56
10:SC:191:VAL:HG11	10:SC:236:PHE:HA	1.87	0.56
31:SZ:47:LEU:HB2	31:SZ:79:ILE:HG22	1.87	0.56
40:LB:18:PRO:HG2	40:LB:20:LYS:HD2	1.87	0.56
86:EF:338:ALA:HB2	86:EF:444:LYS:HD2	1.86	0.56
86:EF:346:ILE:HG13	86:EF:394:LEU:HD21	1.88	0.56
1:S2:981:A:H2'	1:S2:982:G:C8	2.41	0.56
1:S2:1808:U:H2'	1:S2:1809:A:C8	2.41	0.56
21:SM:91:LEU:HD11	21:SM:104:VAL:HB	1.87	0.56
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.40	0.55
7:SD:113:LEU:HD22	7:SD:118:ALA:HB2	1.87	0.55
43:LH:92:MET:HE2	43:LH:179:ILE:HG22	1.88	0.55
86:EF:28:ILE:HD11	86:EF:89:ILE:HD11	1.88	0.55
66:Lr:63:VAL:HG22	66:Lr:79:ARG:HG2	1.88	0.55
22:SS:92:ASP:C	22:SS:94:LYS:H	2.15	0.55
1:S2:70:G:H21	1:S2:79:A:H62	1.52	0.55
27:SP:75:VAL:HG12	27:SP:93:MET:HB3	1.87	0.55
1:S2:1725:U:H2'	1:S2:1726:G:C8	2.42	0.55
3:L5:93:G:H2'	3:L5:94:A:C8	2.41	0.55
3:L5:1437:C:H1'	3:L5:2098:G:H5'	1.88	0.55
30:SY:12:PHE:HZ	30:SY:21:LYS:HE3	1.71	0.55
49:LL:243:ALA:HB1	49:LL:247:MET:HE1	1.89	0.55
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.72	0.55
43:LH:44:GLU:HB3	43:LH:58:ASP:HB2	1.88	0.55
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.89	0.55
18:SK:35:LEU:HD23	18:SK:40:VAL:HG21	1.89	0.55
65:LZ:95:VAL:HG12	65:LZ:110:ALA:HA	1.89	0.55
1:S2:906:U:H2'	1:S2:907:G:C8	2.42	0.55
1:S2:1825:A:H3'	3:L5:3760:A2M:H2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:LI:33:ILE:HB	54:LI:69:ARG:NH1	2.21	0.55
15:SI:62:VAL:HA	15:SI:77:ARG:HA	1.89	0.55
26:SR:66:VAL:HG12	26:SR:67:ARG:H	1.71	0.55
1:S2:1312:G:H4'	18:SK:5:LYS:HZ1	1.72	0.54
3:L5:1994:C:H2'	3:L5:1995:G:H8	1.71	0.54
55:LD:83:LEU:HB3	55:LD:88:VAL:HB	1.90	0.54
40:LB:258:HIS:HA	40:LB:259:PRO:C	2.31	0.54
54:LI:152:LEU:HB3	54:LI:165:ILE:HD12	1.88	0.54
1:S2:1323:U:H2'	1:S2:1324:G:C8	2.42	0.54
1:S2:1639:G7M:H2'	1:S2:1640:A:C8	2.42	0.54
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.22	0.54
3:L5:4772:C:H2'	3:L5:4773:C:C6	2.43	0.54
40:LB:36:ASP:HB3	40:LB:39:LYS:HG3	1.89	0.54
3:L5:184:U:H2'	3:L5:186:G:H1'	1.88	0.54
60:LP:105:LYS:HG3	60:LP:107:LEU:HD13	1.89	0.54
1:S2:907:G:H2'	1:S2:908:A:C8	2.43	0.54
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.71	0.54
5:SB:103:MET:HG3	5:SB:215:VAL:HB	1.88	0.54
86:EF:315:VAL:HG13	86:EF:319:ASP:HB2	1.90	0.54
3:L5:728:U:H2'	3:L5:730:G:H5'	1.89	0.54
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.43	0.54
60:LP:2:VAL:HG23	60:LP:3:ARG:H	1.73	0.54
1:S2:15:U:H2'	1:S2:16:G:O4'	2.08	0.54
1:S2:681:PSU:H4'	20:SX:9:THR:HG22	1.90	0.54
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.71	0.54
3:L5:3601:C:H2'	3:L5:3602:C:C6	2.43	0.54
46:Lq:30:VAL:HG21	46:Lq:187:LEU:HD12	1.90	0.54
3:L5:25:A:H2'	3:L5:26:C:C6	2.43	0.54
26:SR:100:PRO:HG2	26:SR:122:PRO:HG3	1.89	0.54
1:S2:162:C:H5''	11:SG:87:ARG:HH22	1.73	0.54
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.43	0.54
12:SF:33:ILE:HA	12:SF:36:GLN:HG2	1.90	0.54
84:At:33:U:H1'	84:At:36:A:N7	2.23	0.54
3:L5:4611:A:H2'	3:L5:4612:C:C6	2.43	0.53
40:LB:168:MET:HA	40:LB:171:LEU:HD12	1.90	0.53
54:LI:61:SER:HA	54:LI:126:VAL:HG12	1.88	0.53
84:At:27:G:H2'	84:At:28:G:C8	2.43	0.53
1:S2:940:U:H3	1:S2:1002:U:H3	1.57	0.53
1:S2:1037:G:H4'	1:S2:1845:A:H4'	1.90	0.53
3:L5:1377:G:H21	3:L5:1380:G:H5'	1.73	0.53
10:SC:103:LYS:HD2	10:SC:133:TYR:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SI:45:THR:HG23	15:SI:53:LYS:HG3	1.90	0.53
42:LJ:18:ARG:HG3	42:LJ:135:GLY:HA3	1.90	0.53
69:LF:105:VAL:HG13	69:LF:136:VAL:HG12	1.90	0.53
13:SH:145:ARG:HH21	14:SW:49:GLU:HB2	1.72	0.53
60:LP:33:ALA:HB1	60:LP:117:ILE:HG12	1.91	0.53
86:EF:169:GLU:HA	86:EF:172:LYS:HE3	1.91	0.53
3:L5:25:A:H2'	3:L5:26:C:H6	1.72	0.53
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.43	0.53
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.43	0.53
32:Sa:4:LYS:HE3	32:Sa:92:ARG:CZ	2.38	0.53
61:LU:28:PRO:HB2	61:LU:34:MET:HG2	1.91	0.53
3:L5:1985:G:H1'	3:L5:2003:G:H2'	1.91	0.53
61:LU:100:LEU:HD13	61:LU:112:LEU:HD23	1.91	0.53
84:At:38:A:H2'	84:At:39:PSU:C6	2.44	0.53
1:S2:639:C:H2'	1:S2:640:A:C8	2.44	0.53
1:S2:1312:G:H4'	18:SK:5:LYS:NZ	2.23	0.53
3:L5:1655:C:C5	52:La:26:ARG:HD2	2.44	0.53
11:SG:142:ARG:HA	11:SG:147:LEU:HB2	1.89	0.53
37:Sg:87:LEU:HD21	37:Sg:122:SER:HB3	1.90	0.53
49:LL:227:GLU:HG3	52:La:100:ILE:HB	1.90	0.53
3:L5:492:U:H2'	3:L5:493:G:C8	2.44	0.53
1:S2:944:A:H1'	19:SO:136:PRO:HB3	1.91	0.53
42:LJ:17:ILE:HD12	42:LJ:80:GLU:HG2	1.91	0.53
7:SD:133:GLY:HA3	7:SD:156:LEU:O	2.08	0.53
36:Sf:108:VAL:HG13	36:Sf:111:ASN:HA	1.90	0.53
38:Lz:92:LYS:HA	38:Lz:97:LYS:HD2	1.90	0.53
41:LC:60:HIS:NE2	41:LC:100:ARG:HD3	2.23	0.53
17:SU:20:ILE:HG12	17:SU:98:VAL:HG11	1.91	0.52
44:LE:153:LEU:HD11	44:LE:195:ILE:HG13	1.91	0.52
46:Lq:18:ILE:HD12	46:Lq:21:LEU:HD21	1.91	0.52
86:EF:94:GLY:HA2	86:EF:136:HIS:HE1	1.74	0.52
1:S2:1808:U:H2'	1:S2:1809:A:H8	1.74	0.52
3:L5:1439:C:H5'	69:LF:34:ARG:HH22	1.75	0.52
5:SB:144:LYS:HD3	5:SB:208:HIS:HB3	1.91	0.52
9:SE:55:ALA:HB1	9:SE:60:GLU:HB2	1.91	0.52
21:SM:63:LYS:HB3	36:Sf:108:VAL:HG11	1.90	0.52
21:SM:74:ILE:HG13	21:SM:75:ASN:H	1.74	0.52
24:SN:16:LEU:HD12	24:SN:17:PRO:HD2	1.91	0.52
86:EF:85:TYR:CE1	86:EF:237:PRO:HG3	2.45	0.52
3:L5:189:G:H2'	3:L5:190:G:C8	2.44	0.52
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.45	0.52
44:LE:41:LYS:HD2	44:LE:42:PRO:HD2	1.91	0.52
3:L5:3604:A:H2'	3:L5:3605:C:C6	2.45	0.52
7:SD:22:ASN:O	7:SD:26:THR:HG23	2.09	0.52
12:SF:76:MET:HB2	12:SF:89:THR:CG2	2.39	0.52
21:SM:51:VAL:HG23	21:SM:77:ILE:HG13	1.90	0.52
30:SY:25:ILE:HD13	30:SY:44:LEU:HD11	1.91	0.52
40:LB:47:LEU:HG	40:LB:181:MET:SD	2.50	0.52
69:LF:182:TYR:HB3	69:LF:200:ARG:HG3	1.92	0.52
3:L5:1245:C:H2'	3:L5:1246:G:C8	2.44	0.52
3:L5:2421:G:H5'	3:L5:2421:G:N3	2.24	0.52
72:Le:28:TYR:HB3	72:Le:30:LYS:HG2	1.91	0.52
1:S2:551:U:H2'	1:S2:552:G:C8	2.45	0.52
3:L5:495:C:H2'	3:L5:496:G:C8	2.44	0.52
3:L5:1463:C:H5''	68:Lb:31:SER:HB3	1.91	0.52
3:L5:1564:A:H2'	3:L5:1565:A:C8	2.44	0.52
4:L7:3:C:H2'	4:L7:4:U:C6	2.45	0.52
5:SB:173:THR:O	5:SB:177:GLN:HG3	2.10	0.52
8:SJ:106:LEU:O	8:SJ:112:THR:HG21	2.09	0.52
30:SY:40:ILE:O	30:SY:44:LEU:HB2	2.10	0.52
3:L5:106:A:H2'	3:L5:107:G:O4'	2.10	0.52
19:SO:129:ILE:O	32:Sa:65:PRO:HG3	2.10	0.52
21:SM:21:VAL:HG13	21:SM:114:TYR:CE1	2.45	0.52
1:S2:1438:A:H2'	1:S2:1439:A:C8	2.44	0.52
3:L5:208:A:C2	3:L5:233:U:H5''	2.45	0.52
3:L5:1446:C:H2'	3:L5:1447:C:O4'	2.10	0.52
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.10	0.52
13:SH:51:ILE:HD13	13:SH:61:ILE:HD11	1.92	0.52
21:SM:31:LEU:HD13	21:SM:109:VAL:HG13	1.91	0.52
45:LG:73:ARG:HD3	45:LG:241:VAL:O	2.10	0.52
26:SR:44:LYS:HG3	26:SR:47:ARG:HH21	1.75	0.52
46:Lq:26:LYS:NZ	46:Lq:95:LEU:HD21	2.25	0.52
49:LL:217:VAL:HG12	49:LL:218:MET:HG3	1.91	0.52
54:LI:76:MET:HE2	54:LI:138:ILE:HG21	1.91	0.52
1:S2:1101:U:H2'	1:S2:1102:G:H8	1.75	0.51
3:L5:1204:C:H2'	3:L5:1205:G:C8	2.45	0.51
13:SH:70:LYS:O	13:SH:74:LYS:HG2	2.10	0.51
3:L5:1776:A:H2'	3:L5:1777:C:C6	2.45	0.51
3:L5:2045:G:C6	48:LO:62:MET:HA	2.46	0.51
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.10	0.51
3:L5:2492:C:H2'	3:L5:2493:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:At:51:U:H3	84:At:63:G:H1	1.59	0.51
86:EF:360:VAL:HA	86:EF:369:ALA:HA	1.92	0.51
20:SX:60:LYS:HG3	20:SX:116:PRO:HG3	1.93	0.51
30:SY:99:LYS:HB3	30:SY:101:LYS:HD3	1.92	0.51
37:Sg:147:HIS:CE1	37:Sg:169:GLY:N	2.79	0.51
48:LO:16:LEU:HD12	48:LO:80:PHE:HD1	1.75	0.51
49:LL:120:TYR:HA	49:LL:218:MET:HE1	1.92	0.51
86:EF:255:LYS:HB2	86:EF:317:VAL:HG21	1.92	0.51
1:S2:1536:G:H2'	1:S2:1537:A:H8	1.76	0.51
3:L5:3602:C:H2'	3:L5:3603:G:C8	2.45	0.51
3:L5:4220:6MZ:H2'	3:L5:4222:G:H5''	1.93	0.51
3:L5:4376:A:H5''	3:L5:4377:G:O5'	2.11	0.51
8:SJ:46:VAL:HA	8:SJ:49:THR:HG22	1.92	0.51
55:LD:205:ALA:HA	55:LD:208:MET:HE3	1.92	0.51
1:S2:537:C:H2'	1:S2:538:U:C6	2.46	0.51
1:S2:1454:A:H5''	26:SR:3:ARG:HH11	1.75	0.51
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.45	0.51
7:SD:142:LEU:HD13	7:SD:150:MET:SD	2.51	0.51
21:SM:21:VAL:HG13	21:SM:114:TYR:HE1	1.76	0.51
39:LA:20:VAL:HA	39:LA:23:ARG:HG3	1.92	0.51
48:LO:27:VAL:HG23	48:LO:98:ALA:HB1	1.93	0.51
59:LT:39:ILE:HG13	59:LT:102:ARG:HG3	1.91	0.51
73:Lf:50:VAL:HG22	73:Lf:69:VAL:HG22	1.93	0.51
1:S2:314:U:H2'	1:S2:315:C:C6	2.45	0.51
1:S2:379:C:H5'	15:SI:33:ALA:HA	1.92	0.51
1:S2:1461:G:H2'	1:S2:1464:C:H41	1.76	0.51
2:L8:141:C:H2'	2:L8:142:U:C6	2.44	0.51
9:SE:160:ILE:HD12	9:SE:169:ILE:HG12	1.93	0.51
86:EF:263:PRO:HD2	86:EF:310:PHE:O	2.10	0.51
1:S2:1499:U:H4'	7:SD:176:LEU:HD11	1.91	0.51
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.46	0.51
3:L5:1701:A:H2'	3:L5:1702:C:O4'	2.10	0.51
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.45	0.51
3:L5:4694:G:H4'	43:LH:71:ARG:HH12	1.76	0.51
3:L5:4923:C:H2'	3:L5:4924:C:C6	2.45	0.51
18:SK:18:GLU:HG3	18:SK:20:VAL:HG22	1.93	0.51
24:SN:40:LEU:HD13	24:SN:53:ILE:HD11	1.93	0.51
1:S2:158:A:H2'	1:S2:159:A2M:O4'	2.11	0.51
1:S2:1457:U:H2'	1:S2:1458:G:C8	2.46	0.51
3:L5:741:C:H3'	3:L5:742:G:H5''	1.92	0.51
3:L5:2374:A:H5'	71:Ld:64:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SA:199:PRO:HG2	26:SR:91:LEU:HD12	1.93	0.51
11:SG:131:ARG:HH21	64:LW:80:ARG:H	1.59	0.51
41:LC:218:ILE:HA	41:LC:229:LEU:HD22	1.91	0.51
45:LG:70:LEU:O	45:LG:74:LEU:HG	2.11	0.51
85:Pt:5:G:H2'	85:Pt:6:G:H8	1.76	0.51
1:S2:455:A:H2'	1:S2:456:C:C6	2.46	0.51
1:S2:806:U:H2'	1:S2:807:G:C8	2.46	0.51
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.46	0.51
12:SF:167:LYS:HE3	12:SF:172:CYS:SG	2.51	0.51
13:SH:65:PRO:HD2	13:SH:68:GLN:HE21	1.75	0.51
2:L8:152:U:H2'	2:L8:153:C:O4'	2.11	0.51
3:L5:982:U:H2'	3:L5:983:C:C6	2.46	0.51
3:L5:2292:C:H2'	3:L5:2293:U:C6	2.46	0.51
3:L5:2569:G:H2'	3:L5:2570:U:C6	2.46	0.51
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.45	0.51
3:L5:4861:G:H2'	3:L5:4862:G:C8	2.46	0.51
7:SD:75:LYS:HD3	18:SK:20:VAL:HG23	1.91	0.51
19:SO:85:CYS:HB2	19:SO:124:MET:HE3	1.93	0.51
21:SM:45:ARG:HA	21:SM:72:HIS:CE1	2.46	0.51
31:SZ:92:LEU:HD22	31:SZ:109:TYR:HE1	1.76	0.51
45:LG:131:LYS:O	45:LG:132:ARG:C	2.54	0.51
84:At:32:PSU:H1'	84:At:38:A:C6	2.46	0.51
1:S2:382:C:H2'	1:S2:383:G:H8	1.76	0.50
1:S2:545:A:H2'	1:S2:546:G:C8	2.47	0.50
1:S2:1705:C:H2'	1:S2:1706:G:C8	2.46	0.50
3:L5:162:A:H2'	3:L5:163:A:C8	2.46	0.50
3:L5:396:A:H2'	3:L5:397:G:C8	2.46	0.50
3:L5:683:C:H2'	3:L5:684:G:O4'	2.11	0.50
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.11	0.50
4:L7:110:G:H2'	4:L7:111:C:C6	2.47	0.50
37:Sg:168:CYS:HB3	37:Sg:198:VAL:HG13	1.93	0.50
62:LX:89:LYS:HE3	62:LX:137:TYR:CD1	2.46	0.50
85:Pt:57:C:H2'	85:Pt:58:A:C8	2.46	0.50
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.47	0.50
3:L5:2299:G:OP2	41:LC:204:ARG:HD2	2.11	0.50
3:L5:2669:C:H2'	3:L5:2670:C:O4'	2.11	0.50
19:SO:34:PHE:HB3	19:SO:41:PHE:HB2	1.93	0.50
45:LG:107:LYS:HE3	45:LG:111:LYS:HE3	1.93	0.50
46:Lq:6:ARG:O	46:Lq:10:LYS:HG2	2.11	0.50
1:S2:688:U:H4'	1:S2:689:U:O5'	2.11	0.50
2:L8:86:U:H3'	2:L8:87:G:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.46	0.50
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.73	0.50
13:SH:160:LYS:HA	13:SH:163:GLN:HB2	1.93	0.50
44:LE:149:ILE:HD12	44:LE:271:LEU:HD21	1.93	0.50
86:EF:245:PRO:HG2	86:EF:418:TYR:OH	2.11	0.50
1:S2:1035:A:H2'	1:S2:1036:A:O4'	2.11	0.50
3:L5:962:C:H2'	3:L5:1701:A:N1	2.26	0.50
12:SF:102:LEU:HD11	31:SZ:100:VAL:HG21	1.92	0.50
37:Sg:191:HIS:CE1	37:Sg:195:LEU:HD21	2.46	0.50
1:S2:941:C:H2'	1:S2:942:G:C8	2.47	0.50
3:L5:1509:C:H5''	52:La:2:PRO:HD3	1.92	0.50
3:L5:2000:G:H4'	3:L5:2017:A:N1	2.26	0.50
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.12	0.50
3:L5:4910:G:H22	48:LO:107:GLY:HA3	1.76	0.50
13:SH:139:ILE:HG23	13:SH:156:VAL:HG13	1.93	0.50
20:SX:21:LYS:HE2	20:SX:27:TYR:CE1	2.47	0.50
41:LC:290:SER:O	41:LC:294:LYS:HG2	2.12	0.50
50:LV:129:TRP:HB3	50:LV:132:ILE:HD12	1.93	0.50
1:S2:560:A:H5'	8:SJ:174:LYS:HD3	1.92	0.50
1:S2:1606:G:N2	1:S2:1632:G:H1'	2.26	0.50
3:L5:1554:A:H5'	82:Lp:9:GLY:C	2.36	0.50
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.47	0.50
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.46	0.50
36:Sf:105:TYR:HB3	36:Sf:131:PHE:CE2	2.47	0.50
46:Lq:24:TYR:HD2	46:Lq:90:PHE:HB3	1.75	0.50
63:LY:31:SER:HA	63:LY:48:PRO:HA	1.94	0.50
1:S2:899:U:H2'	1:S2:900:C:O4'	2.12	0.50
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.12	0.50
1:S2:1606:G:H5''	28:ST:86:GLY:C	2.36	0.50
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.12	0.50
3:L5:1590:C:H4'	3:L5:2857:A:H5'	1.94	0.50
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.47	0.50
3:L5:4169:G:H4'	3:L5:4171:C:C2	2.47	0.50
19:SO:147:ARG:HA	32:Sa:28:ARG:HD2	1.93	0.50
46:Lq:58:ASN:HB3	46:Lq:62:ARG:HH21	1.77	0.50
56:LQ:178:ARG:HA	56:LQ:184:ARG:O	2.12	0.50
84:At:33:U:H2'	84:At:35:A:OP2	2.12	0.50
1:S2:77:A:C8	11:SG:154:ARG:HG2	2.47	0.50
4:L7:111:C:H2'	4:L7:112:U:O4'	2.12	0.50
12:SF:73:THR:HG23	12:SF:89:THR:HG22	1.94	0.50
19:SO:151:LEU:HD23	19:SO:151:LEU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LG:175:ARG:HD2	45:LG:230:TYR:CD2	2.47	0.50
1:S2:464:A:H3'	1:S2:465:A:H8	1.77	0.50
3:L5:4520:G:H2'	3:L5:4521:PSU:O4'	2.12	0.50
11:SG:159:ARG:HD3	11:SG:173:ALA:HB2	1.94	0.50
50:LV:35:LYS:HD3	50:LV:68:GLY:HA2	1.94	0.50
1:S2:548:C:H2'	1:S2:549:C:C6	2.47	0.49
1:S2:1139:C:H2'	1:S2:1140:G:O4'	2.12	0.49
3:L5:2565:A:H3'	3:L5:2566:G:H8	1.77	0.49
15:SI:48:VAL:HG11	15:SI:54:LYS:HD2	1.94	0.49
15:SI:141:ARG:HB3	15:SI:145:ILE:HG13	1.93	0.49
58:LS:1:MET:HG3	58:LS:39:VAL:HG11	1.93	0.49
72:Le:35:TRP:CZ2	72:Le:56:PRO:HD2	2.47	0.49
84:At:29:G:H2'	84:At:30:G:H8	1.77	0.49
1:S2:115:U:H2'	1:S2:116:OMU:C6	2.43	0.49
1:S2:1025:U:H2'	1:S2:1026:C:O4'	2.12	0.49
3:L5:1981:G:H3'	3:L5:1982:G:H8	1.76	0.49
12:SF:39:ILE:HG22	12:SF:41:VAL:HG23	1.94	0.49
12:SF:73:THR:O	12:SF:89:THR:HG21	2.12	0.49
30:SY:56:PHE:HB2	30:SY:74:MET:HB2	1.93	0.49
58:LS:60:GLU:HB3	59:LT:136:ARG:HH22	1.77	0.49
86:EF:155:MET:HE1	86:EF:192:PRO:HB2	1.94	0.49
86:EF:194:SER:HB3	86:EF:199:ASP:HB2	1.95	0.49
1:S2:954:U:H2'	1:S2:955:A:C8	2.47	0.49
3:L5:260:C:H2'	3:L5:261:G:C8	2.47	0.49
3:L5:456:C:H2'	3:L5:457:G:C8	2.47	0.49
3:L5:2459:G:H2'	3:L5:2461:G:OP2	2.12	0.49
3:L5:4928:C:H2'	3:L5:4929:C:C6	2.47	0.49
41:LC:316:LYS:HB2	41:LC:324:ILE:HG13	1.93	0.49
1:S2:636:C:H2'	1:S2:637:U:O4'	2.11	0.49
1:S2:926:A:H61	1:S2:1015:U:H3	1.59	0.49
1:S2:1060:A:H4'	1:S2:1061:U:H5''	1.94	0.49
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.28	0.49
22:SS:73:ASN:HB3	22:SS:76:GLN:NE2	2.26	0.49
28:ST:21:PHE:HE2	28:ST:133:ARG:HH22	1.59	0.49
31:SZ:69:THR:H	31:SZ:72:VAL:HG12	1.77	0.49
37:Sg:22:ALA:HB3	37:Sg:32:LEU:HB2	1.94	0.49
44:LE:67:ALA:HA	44:LE:69:TYR:CE2	2.47	0.49
1:S2:4:C:H4'	10:SC:207:ALA:HB2	1.94	0.49
2:L8:8:U:H2'	2:L8:9:A:C8	2.47	0.49
3:L5:4966:A:H2'	3:L5:4967:A:O4'	2.12	0.49
3:L5:2267:U:OP1	66:Lr:37:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SA:85:ARG:HD3	6:SA:203:PHE:O	2.12	0.49
86:EF:58:TRP:HA	86:EF:61:ASP:HB2	1.93	0.49
1:S2:573:PSU:O4	1:S2:576:A2M:H8	2.12	0.49
3:L5:286:U:H2'	3:L5:287:U:C6	2.47	0.49
3:L5:1391:A:OP1	87:L5:5106:SPD:H52	2.13	0.49
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.48	0.49
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.48	0.49
6:SA:105:PRO:HA	6:SA:136:GLU:OE2	2.12	0.49
9:SE:100:ARG:HB2	9:SE:114:ILE:HD13	1.93	0.49
40:LB:220:ILE:HG12	40:LB:278:THR:HG23	1.95	0.49
1:S2:909:G:H2'	1:S2:910:G:H8	1.78	0.49
1:S2:1511:U:H2'	1:S2:1512:C:C6	2.48	0.49
1:S2:1681:U:H2'	1:S2:1682:C:C6	2.48	0.49
3:L5:304:C:H2'	3:L5:305:A:O4'	2.13	0.49
3:L5:2491:C:H2'	3:L5:2492:C:C6	2.48	0.49
3:L5:4449:A:H5''	98:L5:5567:HOH:O	2.12	0.49
24:SN:84:LEU:HD22	24:SN:88:LEU:HD23	1.95	0.49
1:S2:1408:U:H2'	1:S2:1409:A:C8	2.48	0.49
5:SB:33:VAL:HG12	5:SB:44:ILE:HD12	1.94	0.49
11:SG:213:LEU:HD11	11:SG:217:MET:HE3	1.95	0.49
17:SU:65:THR:HG21	23:Sd:40:ARG:HB2	1.94	0.49
37:Sg:133:ASN:HB2	37:Sg:139:LYS:HD3	1.94	0.49
64:LW:97:LYS:HG2	64:LW:101:ARG:HH21	1.78	0.49
1:S2:532:C:H2'	1:S2:533:A:C8	2.47	0.49
3:L5:170:C:H2'	3:L5:171:U:C6	2.48	0.49
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.48	0.49
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.13	0.49
3:L5:1972:G:H2'	3:L5:1973:G:C8	2.48	0.49
3:L5:1975:G:H2'	47:LK:16:ARG:HE	1.77	0.49
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.48	0.49
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.48	0.49
3:L5:4370:OMG:HM21	91:L5:5117:3H3:O	2.13	0.49
7:SD:32:ASP:O	7:SD:54:ARG:HB2	2.13	0.49
9:SE:100:ARG:HH21	9:SE:118:GLU:HG2	1.78	0.49
40:LB:378:ARG:HG2	64:LW:32:LEU:HD21	1.95	0.49
86:EF:199:ASP:HB3	86:EF:205:SER:HB2	1.95	0.49
1:S2:1259:A:H1'	1:S2:1264:C:H42	1.77	0.48
3:L5:325:U:H2'	3:L5:326:C:C6	2.48	0.48
3:L5:4611:A:H2	43:LH:120:GLU:HG2	1.78	0.48
6:SA:42:LYS:HD3	6:SA:46:ILE:HB	1.93	0.48
28:ST:42:HIS:HB3	28:ST:93:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:188:HIS:HB3	37:Sg:219:TRP:CZ3	2.48	0.48
45:LG:246:SER:HA	45:LG:249:ARG:HG2	1.93	0.48
86:EF:340:PHE:HB3	86:EF:441:VAL:HG13	1.95	0.48
1:S2:530:U:H2'	1:S2:531:A:C8	2.47	0.48
1:S2:1293:A:H2'	1:S2:1294:G:C8	2.48	0.48
3:L5:1460:C:H5''	56:LQ:144:LYS:HG3	1.95	0.48
4:L7:3:C:H2'	4:L7:4:U:H6	1.78	0.48
20:SX:107:ARG:HB3	20:SX:110:HIS:HB3	1.95	0.48
46:Lq:40:MET:HG3	46:Lq:44:ARG:HE	1.77	0.48
55:LD:211:LEU:HB3	55:LD:219:TYR:HB2	1.96	0.48
1:S2:1839:U:H2'	1:S2:1840:U:C6	2.48	0.48
3:L5:40:G:N2	3:L5:4380:A:H62	2.11	0.48
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.47	0.48
3:L5:4341:C:C2	91:L5:5117:3H3:H14	2.48	0.48
18:SK:29:MET:HG3	18:SK:42:ASN:OD1	2.13	0.48
32:Sa:85:ARG:HG3	32:Sa:86:ASN:O	2.13	0.48
47:LK:28:LEU:HA	47:LK:32:ILE:HD13	1.95	0.48
1:S2:808:A:H5''	9:SE:187:ALA:HB3	1.96	0.48
1:S2:909:G:H2'	1:S2:910:G:C8	2.48	0.48
1:S2:1417:C:H2'	1:S2:1418:C:C6	2.49	0.48
1:S2:1623:A:O5'	22:SS:133:GLY:HA3	2.14	0.48
2:L8:89:U:H2'	2:L8:90:C:C6	2.49	0.48
3:L5:1727:U:H2'	3:L5:1728:U:C6	2.49	0.48
3:L5:2748:C:H5''	74:Lg:65:MET:CE	2.43	0.48
3:L5:3774:A:H2'	3:L5:3775:A:C8	2.48	0.48
55:LD:55:VAL:HG22	55:LD:60:ILE:HG12	1.94	0.48
71:Ld:75:LYS:HE3	71:Ld:79:ASN:O	2.13	0.48
77:Lk:23:VAL:HG11	77:Lk:60:LEU:HD21	1.93	0.48
3:L5:1392:A:H2'	3:L5:1393:G:C8	2.48	0.48
3:L5:1788:A:H2'	54:LI:22:PHE:CZ	2.48	0.48
3:L5:2423:A:H2'	3:L5:2424:OMG:C8	2.49	0.48
1:S2:511:U:H2'	1:S2:512:A2M:H8	1.95	0.48
1:S2:867:OMG:HM23	1:S2:867:OMG:H1'	1.60	0.48
1:S2:1098:C:H2'	1:S2:1099:G:C8	2.49	0.48
1:S2:1725:U:H2'	1:S2:1726:G:H8	1.79	0.48
3:L5:758:G:H2'	3:L5:759:G:H8	1.78	0.48
3:L5:1094:G:H2'	3:L5:1095:A:C8	2.48	0.48
3:L5:2563:C:H3'	3:L5:2564:G:H8	1.79	0.48
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.49	0.48
3:L5:4302:U:H4'	59:LT:5:LYS:HD2	1.95	0.48
25:SL:75:GLY:HA3	25:SL:88:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Lq:112:ARG:NH1	46:Lq:182:PRO:HG2	2.28	0.48
86:EF:72:THR:O	86:EF:93:PRO:HB3	2.13	0.48
2:L8:70:G:H5''	63:LY:27:ARG:CZ	2.44	0.48
3:L5:218:A:H2'	3:L5:218:A:N3	2.28	0.48
3:L5:1081:C:H2'	3:L5:1082:C:C6	2.49	0.48
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.48	0.48
46:Lq:10:LYS:HD2	46:Lq:60:MET:SD	2.54	0.48
48:LO:8:VAL:HG12	48:LO:117:ARG:HG3	1.96	0.48
54:LI:171:TRP:HB2	54:LI:178:ALA:HA	1.94	0.48
56:LQ:43:PHE:CD2	56:LQ:133:GLY:HA3	2.48	0.48
86:EF:380:ASP:HB3	86:EF:384:GLY:H	1.78	0.48
2:L8:83:C:H4'	2:L8:84:A:C5	2.49	0.48
3:L5:1397:A:C8	52:La:114:LYS:HD2	2.49	0.48
3:L5:1402:C:H2'	3:L5:1403:G:C8	2.49	0.48
3:L5:1417:C:H2'	3:L5:1418:C:O4'	2.12	0.48
3:L5:2474:G:N2	3:L5:2502:G:H2'	2.28	0.48
3:L5:3762:PSU:H2'	3:L5:3763:A:C8	2.48	0.48
3:L5:3906:A:H5''	41:LC:69:THR:OG1	2.14	0.48
11:SG:69:THR:O	11:SG:99:GLY:HA3	2.13	0.48
12:SF:68:ILE:HD11	12:SF:151:ILE:HD11	1.96	0.48
13:SH:130:LEU:HD21	13:SH:156:VAL:HG21	1.96	0.48
21:SM:35:ILE:HG12	21:SM:61:TYR:CE1	2.48	0.48
37:Sg:168:CYS:O	37:Sg:168:CYS:SG	2.71	0.48
1:S2:35:C:H2'	1:S2:36:PSU:H6	1.79	0.48
3:L5:258:G:H2'	3:L5:259:C:C6	2.49	0.48
3:L5:1771:U:H2'	3:L5:1772:C:C6	2.49	0.48
3:L5:4862:G:H2'	3:L5:4863:G:C8	2.48	0.48
16:SQ:49:TYR:O	16:SQ:53:GLU:HG3	2.14	0.48
19:SO:74:ALA:HB1	19:SO:115:ALA:HB2	1.96	0.48
44:LE:50:LEU:HD22	44:LE:56:ARG:HA	1.96	0.48
55:LD:88:VAL:HA	55:LD:239:MET:HE2	1.95	0.48
84:At:29:G:H2'	84:At:30:G:C8	2.49	0.48
1:S2:1217:A:H2'	1:S2:1218:C:C6	2.49	0.48
1:S2:1322:G:H2'	1:S2:1323:U:O4'	2.13	0.48
3:L5:1524:A2M:H62	3:L5:1651:G:H22	1.61	0.48
3:L5:2694:G:H5''	3:L5:2696:A:N7	2.29	0.48
20:SX:68:LYS:HB3	20:SX:91:LEU:HD22	1.96	0.48
46:Lq:47:LEU:HD13	46:Lq:50:LYS:HE2	1.94	0.48
50:LV:129:TRP:CB	50:LV:132:ILE:HD12	2.44	0.48
3:L5:1590:C:H3'	3:L5:1591:U:H4'	1.96	0.47
3:L5:1801:A:H4'	59:LT:102:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2476:G:H2'	3:L5:2477:A:C8	2.50	0.47
3:L5:2732:G:H2'	3:L5:2733:C:C6	2.49	0.47
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.78	0.47
3:L5:4881:U:C4	51:LM:113:MET:HG3	2.49	0.47
15:SI:162:LEU:HD11	15:SI:191:GLU:HG2	1.96	0.47
58:LS:83:ARG:HA	58:LS:91:HIS:O	2.14	0.47
61:LU:22:THR:O	61:LU:109:SER:HA	2.14	0.47
2:L8:141:C:H5''	53:LN:60:VAL:HG11	1.96	0.47
3:L5:2588:C:H5''	3:L5:2589:C:H5''	1.95	0.47
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.49	0.47
3:L5:3603:G:H2'	3:L5:3604:A:C8	2.49	0.47
74:Lg:69:LYS:HG2	74:Lg:73:HIS:CD2	2.49	0.47
1:S2:1026:C:H4'	1:S2:1161:U:H4'	1.97	0.47
3:L5:268:G:H2'	3:L5:269:G:H8	1.79	0.47
3:L5:1193:C:H2'	3:L5:1194:G:H8	1.80	0.47
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.49	0.47
3:L5:4389:C:H2'	3:L5:4390:A:H8	1.78	0.47
4:L7:58:A:H2'	4:L7:59:G:C8	2.50	0.47
17:SU:60:THR:HG23	17:SU:81:GLN:HG3	1.96	0.47
21:SM:62:VAL:O	21:SM:65:VAL:HG12	2.15	0.47
43:LH:9:THR:HG21	43:LH:54:ARG:HD2	1.96	0.47
86:EF:60:LEU:HD21	86:EF:78:TRP:HB2	1.96	0.47
2:L8:16:G:N2	3:L5:417:G:H1'	2.28	0.47
23:Sd:30:LEU:HA	23:Sd:39:CYS:HA	1.95	0.47
32:Sa:39:PHE:CD2	32:Sa:41:ILE:HD11	2.49	0.47
43:LH:4:ILE:HG12	43:LH:61:TRP:CH2	2.49	0.47
49:LL:81:LEU:HD11	49:LL:98:VAL:HG22	1.96	0.47
50:LV:62:MET:HE3	50:LV:76:VAL:HG12	1.96	0.47
59:LT:133:ALA:HB3	69:LF:127:LYS:HB2	1.96	0.47
71:Ld:40:LYS:C	71:Ld:43:PRO:HD2	2.40	0.47
86:EF:318:M3L:HM12	86:EF:318:M3L:HD3	1.73	0.47
1:S2:12:U:H2'	1:S2:13:C:C6	2.49	0.47
1:S2:107:A:H2'	1:S2:108:G:C8	2.50	0.47
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.50	0.47
3:L5:1303:A:C2	72:Le:33:ARG:HD3	2.49	0.47
3:L5:2478:C:H2'	3:L5:2479:G:C8	2.49	0.47
5:SB:134:LEU:HG	5:SB:218:LEU:HD12	1.95	0.47
13:SH:21:SER:O	13:SH:25:GLN:HG2	2.15	0.47
17:SU:56:MET:HE3	17:SU:88:LEU:HD12	1.97	0.47
34:Sc:12:ALA:HB1	34:Sc:32:VAL:HB	1.96	0.47
43:LH:114:ILE:HB	43:LH:124:ARG:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:51:U:H2'	1:S2:52:G:C8	2.50	0.47
3:L5:1325:C:C4	3:L5:3879:G:H5''	2.50	0.47
3:L5:1756:U:H2'	3:L5:1757:U:H6	1.80	0.47
3:L5:2871:A:H2'	3:L5:2872:C:O4'	2.15	0.47
3:L5:4886:C:H2'	3:L5:4887:C:H6	1.80	0.47
6:SA:51:LEU:H	26:SR:105:MET:CE	2.28	0.47
16:SQ:51:LEU:HG	16:SQ:81:ILE:HG23	1.96	0.47
45:LG:163:PRO:HG3	53:LN:43:THR:O	2.15	0.47
49:LL:8:MET:HE3	49:LL:8:MET:HB2	1.84	0.47
56:LQ:72:LEU:HB2	56:LQ:75:ARG:HD2	1.96	0.47
1:S2:17:C:H2'	1:S2:18:C:C6	2.50	0.47
1:S2:1558:C:H2'	1:S2:1559:C:C6	2.50	0.47
2:L8:56:G:H2'	2:L8:57:C:O4'	2.14	0.47
3:L5:18:C:H4'	53:LN:138:PHE:CD1	2.50	0.47
3:L5:139:G:H2'	3:L5:140:G:C8	2.49	0.47
3:L5:1247:U:H2'	3:L5:1248:C:C6	2.50	0.47
3:L5:3707:U:H2'	3:L5:3708:C:H6	1.80	0.47
3:L5:3848:U:OP1	88:L5:5116:PUT:H22	2.15	0.47
3:L5:4114:C:H2'	3:L5:4115:G:N3	2.29	0.47
3:L5:4696:C:H2'	3:L5:4697:U:O4'	2.15	0.47
6:SA:50:ASN:HA	26:SR:105:MET:HE3	1.96	0.47
8:SJ:114:VAL:HG13	8:SJ:119:LEU:HB2	1.95	0.47
19:SO:86:LYS:HG3	19:SO:124:MET:HE2	1.97	0.47
19:SO:149:ARG:NH1	19:SO:151:LEU:HD13	2.29	0.47
22:SS:92:ASP:C	22:SS:94:LYS:N	2.73	0.47
40:LB:303:ALA:HB2	40:LB:314:ILE:HA	1.97	0.47
46:Lq:29:ILE:HG23	46:Lq:88:PHE:HE1	1.80	0.47
46:Lq:116:ILE:HB	46:Lq:164:GLY:HA2	1.96	0.47
47:LK:90:ARG:HB2	47:LK:94:LYS:HD3	1.95	0.47
50:LV:36:ASN:OD1	50:LV:67:LYS:HG2	2.15	0.47
52:La:95:THR:HG23	52:La:97:ALA:H	1.78	0.47
59:LT:72:VAL:HG21	59:LT:96:ILE:HD13	1.97	0.47
71:Ld:64:ILE:HG23	71:Ld:68:LEU:HD23	1.96	0.47
1:S2:1344:A:N6	1:S2:1386:A:H5'	2.30	0.47
3:L5:288:G:H2'	3:L5:289:C:C6	2.49	0.47
3:L5:929:A:H3'	3:L5:930:G:H8	1.80	0.47
3:L5:2893:U:H5''	15:SI:205:ARG:HH12	1.79	0.47
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.50	0.47
9:SE:123:LEU:HD11	9:SE:236:ILE:HG23	1.96	0.47
19:SO:59:GLY:HA2	19:SO:68:GLU:HG2	1.95	0.47
55:LD:60:ILE:HB	55:LD:80:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Ld:61:ASP:CG	71:Ld:63:ARG:HH21	2.23	0.47
1:S2:385:G:H3'	25:SL:136:LYS:HB2	1.96	0.47
3:L5:270:U:H2'	3:L5:271:C:C6	2.50	0.47
3:L5:1756:U:H2'	3:L5:1757:U:C6	2.50	0.47
3:L5:2379:A:H2'	3:L5:2380:G:O4'	2.15	0.47
3:L5:4060:U:O2	3:L5:4062:A:N6	2.48	0.47
40:LB:107:ALA:HB1	40:LB:202:GLU:HG3	1.97	0.47
58:LS:39:VAL:HG22	69:LF:228:VAL:HA	1.97	0.47
62:LX:77:ILE:HD13	62:LX:100:VAL:HG12	1.96	0.47
86:EF:85:TYR:HE1	86:EF:237:PRO:HG3	1.79	0.47
1:S2:155:G:H4'	11:SG:15:LEU:HD22	1.96	0.47
1:S2:301:A:H2'	1:S2:302:A:O4'	2.15	0.47
1:S2:877:C:H42	1:S2:909:G:H1	1.63	0.47
1:S2:1850:MA6:H92	1:S2:1851:MA6:H93	1.97	0.47
3:L5:176:G:H2'	3:L5:177:G:C8	2.50	0.47
3:L5:1475:G:H2'	3:L5:1476:C:C6	2.49	0.47
3:L5:2627:C:H2'	3:L5:2628:U:C6	2.50	0.47
3:L5:4300:U:H2'	3:L5:4301:U:C6	2.50	0.47
3:L5:4524:G:N3	40:LB:252:ALA:HB1	2.30	0.47
6:SA:207:PRO:HA	6:SA:210:ILE:HB	1.97	0.47
12:SF:86:LYS:O	12:SF:90:VAL:HG23	2.15	0.47
13:SH:30:LEU:O	13:SH:34:SER:OG	2.28	0.47
19:SO:44:VAL:HG12	19:SO:53:ILE:HB	1.97	0.47
38:Lz:101:LYS:HE3	38:Lz:101:LYS:HB3	1.71	0.47
39:LA:234:LYS:HG2	39:LA:238:ILE:HG12	1.96	0.47
41:LC:322:LEU:O	41:LC:326:LEU:HG	2.15	0.47
46:Lq:188:VAL:HG22	46:Lq:189:ILE:H	1.80	0.47
58:LS:15:ARG:HB3	58:LS:27:LEU:HD23	1.97	0.47
84:At:11:C:H2'	84:At:12:U:C6	2.49	0.47
3:L5:89:C:OP1	3:L5:294:G:H1'	2.14	0.46
3:L5:1981:G:H3'	3:L5:1982:G:C8	2.50	0.46
31:SZ:50:PHE:HE2	31:SZ:87:ALA:HB2	1.80	0.46
40:LB:92:TYR:HB2	40:LB:159:VAL:HB	1.96	0.46
45:LG:137:ARG:HG3	45:LG:146:LEU:HD11	1.97	0.46
46:Lq:79:LEU:HB3	46:Lq:80:PRO:HD3	1.97	0.46
51:LM:40:GLY:HA3	51:LM:45:VAL:HB	1.96	0.46
54:LI:188:LYS:HD3	54:LI:188:LYS:HA	1.75	0.46
84:At:28:G:H2'	84:At:29:G:C8	2.50	0.46
86:EF:18:SER:HA	86:EF:117:ALA:HB2	1.95	0.46
1:S2:1439:A:H2'	1:S2:1440:C:O4'	2.15	0.46
3:L5:73:A:H5''	49:LL:105:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:516:C:H2'	3:L5:517:C:C6	2.50	0.46
3:L5:667:A:H2'	3:L5:668:C:C6	2.50	0.46
3:L5:717:U:H2'	3:L5:718:C:C6	2.50	0.46
3:L5:2503:G:H3'	3:L5:2504:C:H4'	1.97	0.46
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.50	0.46
7:SD:16:ILE:HD13	23:Sd:50:ILE:HG12	1.96	0.46
40:LB:288:GLY:HA3	40:LB:330:PHE:CE2	2.50	0.46
47:LK:44:ASP:OD1	47:LK:45:ASP:N	2.48	0.46
76:Lj:25:LYS:O	76:Lj:25:LYS:HD3	2.16	0.46
1:S2:328:U:H5'	64:LW:109:ILE:HD11	1.97	0.46
1:S2:543:C:H3'	1:S2:544:G:H8	1.79	0.46
1:S2:674:C:H2'	1:S2:675:U:C6	2.50	0.46
1:S2:1115:U:H2'	1:S2:1116:C:H5''	1.97	0.46
3:L5:120:A:H2'	3:L5:149:A:H61	1.80	0.46
3:L5:2436:U:C4	62:LX:130:PRO:HG3	2.51	0.46
3:L5:3657:U:OP1	39:LA:245[B]:ARG:HD3	2.16	0.46
3:L5:4864:U:H2'	3:L5:4865:C:O4'	2.15	0.46
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.50	0.46
5:SB:71:LEU:HG	5:SB:78:GLU:HG2	1.97	0.46
19:SO:75:MET:HG3	19:SO:118:ALA:HB2	1.96	0.46
22:SS:89:ASP:HB3	22:SS:92:ASP:O	2.15	0.46
42:LJ:44:THR:HG21	42:LJ:72:CYS:SG	2.54	0.46
47:LK:110:VAL:O	47:LK:114:ARG:HG3	2.15	0.46
70:Lc:48:LEU:HD13	70:Lc:57:LYS:HG2	1.97	0.46
86:EF:205:SER:HB3	86:EF:208:MET:HB3	1.96	0.46
1:S2:639:C:H2'	1:S2:640:A:H8	1.81	0.46
2:L8:96:C:H5''	67:Lh:66:LYS:HD2	1.96	0.46
3:L5:1415:G:H2'	3:L5:1416:G:C8	2.51	0.46
3:L5:2008:U:H1'	3:L5:2011:C:H5	1.79	0.46
5:SB:67:PHE:CE2	19:SO:48:SER:HB3	2.50	0.46
9:SE:211:LYS:NZ	9:SE:215:GLY:O	2.48	0.46
30:SY:21:LYS:HB2	30:SY:75:ILE:HB	1.98	0.46
36:Sf:133:ALA:HB1	36:Sf:135:HIS:HD2	1.80	0.46
43:LH:128:MET:SD	43:LH:157:SER:HB3	2.55	0.46
44:LE:190:HIS:HB3	44:LE:193:PHE:HD2	1.80	0.46
46:Lq:109:ALA:H	46:Lq:184:SER:HB2	1.81	0.46
49:LL:233:THR:OG1	49:LL:236:GLU:HG3	2.15	0.46
62:LX:81:LEU:HD22	62:LX:83:THR:HG23	1.97	0.46
1:S2:149:A:H3'	1:S2:150:A:H8	1.81	0.46
1:S2:344:U:H2'	1:S2:345:U:C6	2.50	0.46
1:S2:434:G:H2'	1:S2:435:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:8:U:H2'	3:L5:9:C:O4'	2.16	0.46
3:L5:946:C:H2'	3:L5:947:C:C6	2.51	0.46
3:L5:4524:G:OP2	3:L5:4524:G:H4'	2.14	0.46
7:SD:72:VAL:HG22	18:SK:68:TYR:HD2	1.81	0.46
15:SI:175:ILE:HD12	15:SI:185:ALA:HB1	1.98	0.46
33:Sb:65:GLN:HE22	33:Sb:74:THR:HG23	1.79	0.46
37:Sg:212:LYS:HA	37:Sg:235:ILE:HG13	1.97	0.46
45:LG:171:PRO:HB3	45:LG:181:TYR:CE2	2.51	0.46
57:LR:74:ARG:O	57:LR:76:MET:HG2	2.16	0.46
60:LP:2:VAL:HG23	60:LP:3:ARG:N	2.31	0.46
1:S2:118:C:H1'	1:S2:445:A:C5	2.51	0.46
1:S2:878:G:H22	1:S2:908:A:H2	1.61	0.46
1:S2:1628:C:H2'	1:S2:1629:C:C6	2.51	0.46
3:L5:981:C:H4'	44:LE:39:LYS:HD3	1.97	0.46
3:L5:1988:G:H2'	3:L5:1989:G:C8	2.51	0.46
3:L5:2102:G:H2'	3:L5:2103:G:C8	2.51	0.46
3:L5:2869:U:O2'	3:L5:2881:A:N7	2.44	0.46
3:L5:4691:A:H2'	3:L5:4692:A:O4'	2.16	0.46
19:SO:57:THR:H	19:SO:60:MET:HE3	1.80	0.46
37:Sg:79:LEU:HD22	37:Sg:120:ILE:HD12	1.98	0.46
37:Sg:156:PHE:HE1	37:Sg:179:LEU:HD11	1.81	0.46
46:Lq:62:ARG:O	46:Lq:65:ILE:HG12	2.15	0.46
83:mR:40:U:H2'	83:mR:41:U:H6	1.79	0.46
85:Pt:5:G:H2'	85:Pt:6:G:C8	2.50	0.46
86:EF:256:ILE:HB	86:EF:259:ILE:HB	1.98	0.46
1:S2:321:C:H2'	1:S2:322:C:C6	2.51	0.46
1:S2:595:U:H2'	1:S2:596:U:C6	2.51	0.46
1:S2:900:C:H2'	1:S2:901:G:C8	2.51	0.46
1:S2:1496:U:H4'	23:Sd:24:CYS:HB2	1.97	0.46
1:S2:1713:C:H2'	1:S2:1714:U:C6	2.51	0.46
2:L8:127:U:H2'	2:L8:128:C:O4'	2.15	0.46
3:L5:462:G:H2'	3:L5:463:A:C8	2.50	0.46
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.81	0.46
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.31	0.46
3:L5:4653:C:H2'	3:L5:4654:C:C6	2.50	0.46
13:SH:69:LEU:HD22	13:SH:96:ALA:HB2	1.96	0.46
42:LJ:56:THR:HG23	42:LJ:63:ARG:HA	1.97	0.46
46:Lq:18:ILE:HD11	46:Lq:68:HIS:CG	2.51	0.46
47:LK:93:LYS:HD2	47:LK:94:LYS:O	2.16	0.46
62:LX:82:THR:HA	62:LX:87:MET:HE3	1.98	0.46
77:Lk:23:VAL:HG23	77:Lk:64:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:928:G:H2'	1:S2:929:G:C8	2.51	0.46
1:S2:1825:A:H3'	3:L5:3760:A2M:C2	2.46	0.46
3:L5:352:G:C6	41:LC:196:MET:HE3	2.51	0.46
3:L5:1306:C:H2'	3:L5:1307:A:C8	2.50	0.46
3:L5:1850:A:H2'	3:L5:1851:G:C8	2.51	0.46
3:L5:1872:G:O2'	3:L5:4219:A:N3	2.47	0.46
3:L5:2066:C:O2'	73:Lf:79:GLY:HA2	2.16	0.46
3:L5:2542:G:H2'	3:L5:2543:A:C8	2.51	0.46
3:L5:4301:U:OP1	59:LT:78:LYS:NZ	2.48	0.46
6:SA:33:GLN:HB3	6:SA:154:LEU:HD12	1.98	0.46
16:SQ:97:GLN:NE2	16:SQ:105:LYS:HE2	2.31	0.46
41:LC:289:LEU:O	41:LC:293:LEU:HG	2.16	0.46
45:LG:32:PHE:CE2	65:LZ:55:ALA:HA	2.51	0.46
46:Lq:26:LYS:HE2	46:Lq:194:ASP:HB2	1.98	0.46
84:At:73:A:H2'	84:At:74:C:C6	2.50	0.46
1:S2:168:C:H4'	11:SG:131:ARG:HB3	1.98	0.46
2:L8:88:A:H2'	2:L8:89:U:O4'	2.16	0.46
3:L5:65:A:N6	3:L5:75:G:H1'	2.31	0.46
3:L5:366:A:H2'	3:L5:367:C:O4'	2.16	0.46
3:L5:1247:U:H2'	3:L5:1248:C:H6	1.80	0.46
3:L5:3937:C:H1'	53:LN:125:SER:HB3	1.98	0.46
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.15	0.46
4:L7:23:A:H2'	4:L7:24:C:C6	2.50	0.46
6:SA:52:LYS:O	6:SA:56:GLU:HG2	2.16	0.46
9:SE:160:ILE:HB	9:SE:169:ILE:HG23	1.98	0.46
22:SS:10:GLN:O	22:SS:11:HIS:HB2	2.16	0.46
26:SR:54:VAL:O	26:SR:58:MET:HG2	2.16	0.46
30:SY:46:LYS:HE2	30:SY:46:LYS:HB2	1.60	0.46
37:Sg:302:TYR:CE2	37:Sg:308:ARG:HB2	2.51	0.46
39:LA:3:ARG:HG2	39:LA:207:VAL:HG22	1.98	0.46
45:LG:121:LYS:HB3	45:LG:126:GLY:HA2	1.98	0.46
49:LL:65:ARG:HA	52:La:69:PHE:CD2	2.51	0.46
61:LU:27:HIS:HB2	61:LU:28:PRO:HD3	1.96	0.46
70:Lc:35:LEU:HD12	70:Lc:35:LEU:HA	1.78	0.46
1:S2:1823:A:H2'	1:S2:1824:A:O4'	2.16	0.46
3:L5:6:C:H2'	3:L5:7:C:C6	2.51	0.46
3:L5:1400:G:H2'	3:L5:1401:C:C6	2.50	0.46
3:L5:4173:G:H2'	3:L5:4174:U:C6	2.51	0.46
3:L5:4681:A:H2'	3:L5:4682:U:O4'	2.16	0.46
7:SD:170:THR:HG23	7:SD:187:LYS:HG2	1.98	0.46
22:SS:42:HIS:O	22:SS:46:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:SS:80:PRO:HG2	22:SS:83:PHE:HB2	1.97	0.46
45:LG:140:VAL:HG21	45:LG:166:LEU:O	2.16	0.46
56:LQ:6:ARG:HG2	56:LQ:8:ASN:OD1	2.16	0.46
1:S2:35:C:H2'	1:S2:36:PSU:C6	2.51	0.45
2:L8:113:C:H2'	2:L8:114:G:O4'	2.16	0.45
3:L5:455:C:H2'	3:L5:456:C:C6	2.52	0.45
3:L5:2491:C:O2'	3:L5:2492:C:O4'	2.33	0.45
3:L5:3865:A:H2'	3:L5:3866:C:C6	2.51	0.45
5:SB:121:ILE:HG21	5:SB:164:ILE:HG22	1.98	0.45
11:SG:134:GLY:HA2	64:LW:82:ILE:HD13	1.99	0.45
21:SM:45:ARG:HA	21:SM:72:HIS:HE1	1.80	0.45
37:Sg:168:CYS:HB3	37:Sg:198:VAL:CG1	2.46	0.45
40:LB:288:GLY:HA3	40:LB:330:PHE:CZ	2.51	0.45
41:LC:67:TRP:HB3	41:LC:71:ARG:HG3	1.98	0.45
41:LC:193:LYS:CD	41:LC:196:MET:HE2	2.46	0.45
55:LD:7:VAL:HG13	55:LD:8:LYS:HG3	1.98	0.45
58:LS:147:ASP:HB3	58:LS:150:ILE:HB	1.99	0.45
70:Lc:102:SER:OG	70:Lc:105:ILE:HB	2.16	0.45
1:S2:91:A:H61	11:SG:89:THR:HG22	1.80	0.45
1:S2:879:C:H2'	1:S2:880:G:C8	2.51	0.45
1:S2:1293:A:H2'	1:S2:1294:G:H8	1.81	0.45
1:S2:1513:C:H2'	1:S2:1514:G:C8	2.51	0.45
3:L5:946:C:H2'	3:L5:947:C:H6	1.82	0.45
3:L5:1700:G:N3	3:L5:2097:U:H1'	2.31	0.45
3:L5:1776:A:H2'	3:L5:1777:C:H6	1.81	0.45
3:L5:1974:U:O2'	3:L5:1975:G:H3'	2.17	0.45
3:L5:2707:U:H5'	3:L5:2707:U:H6	1.82	0.45
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.80	0.45
3:L5:4491:G:H5''	3:L5:4620:OMU:HM21	1.98	0.45
14:SW:51:GLU:CD	33:Sb:8:LEU:HD21	2.40	0.45
14:SW:104:LEU:HD23	14:SW:125:ILE:HA	1.98	0.45
21:SM:42:LEU:HD13	21:SM:68:LEU:HB3	1.97	0.45
27:SP:13:ARG:O	27:SP:14:LYS:CG	2.64	0.45
41:LC:4:ALA:O	41:LC:29:LYS:HE3	2.16	0.45
44:LE:70:LYS:HG3	44:LE:71:ARG:HG3	1.98	0.45
1:S2:525:A:H2'	1:S2:526:A:C8	2.52	0.45
1:S2:996:A:H2'	1:S2:997:A:C8	2.50	0.45
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.51	0.45
30:SY:110:ARG:HG2	30:SY:114:MET:HE2	1.98	0.45
37:Sg:59:LEU:HD23	37:Sg:90:TRP:CE3	2.52	0.45
47:LK:29:ALA:HA	47:LK:39:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LV:25:VAL:HG22	50:LV:38:TYR:HD1	1.81	0.45
1:S2:174:OMC:HM23	1:S2:174:OMC:H1'	1.78	0.45
1:S2:949:G:H2'	1:S2:950:C:C6	2.52	0.45
1:S2:1248:B8N:N34	85:Pt:35:C:OP1	2.49	0.45
1:S2:1310:U:OP1	36:Sf:131:PHE:HB2	2.17	0.45
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.51	0.45
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.51	0.45
3:L5:4071:U:H2'	3:L5:4072:C:C6	2.51	0.45
3:L5:4254:G:H2'	3:L5:4254:G:N3	2.31	0.45
3:L5:4291:G:OP2	81:Lo:10:THR:HG22	2.17	0.45
3:L5:4518:A:O5'	3:L5:4520:G:H4'	2.17	0.45
3:L5:4736:C:H2'	3:L5:4737:G:H8	1.82	0.45
6:SA:7:VAL:HG13	6:SA:8:LEU:HG	1.97	0.45
14:SW:42:MET:HE2	14:SW:42:MET:HB3	1.84	0.45
17:SU:17:ILE:HG13	17:SU:17:ILE:O	2.15	0.45
25:SL:66:VAL:HG11	25:SL:141:ASN:HD22	1.81	0.45
53:LN:182:HIS:H	53:LN:182:HIS:CD2	2.33	0.45
76:Lj:72:ARG:HA	76:Lj:75:ARG:NH1	2.32	0.45
86:EF:60:LEU:HD23	86:EF:60:LEU:HA	1.87	0.45
1:S2:1409:A:H61	1:S2:1432:U:H3	1.63	0.45
3:L5:218:A:H3'	3:L5:219:G:H21	1.82	0.45
3:L5:327:U:O4	75:Li:28:ARG:HA	2.16	0.45
3:L5:488:G:H2'	3:L5:489:C:O4'	2.16	0.45
3:L5:758:G:H2'	3:L5:759:G:C8	2.52	0.45
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.51	0.45
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.52	0.45
5:SB:71:LEU:HD22	5:SB:84:PHE:HE1	1.82	0.45
13:SH:63:PHE:HA	13:SH:95:ILE:O	2.16	0.45
21:SM:95:ASP:HB3	21:SM:98:GLY:H	1.82	0.45
27:SP:25:LEU:HD12	27:SP:28:MET:SD	2.56	0.45
33:Sb:33:MET:HE3	33:Sb:73:LEU:HD21	1.99	0.45
49:LL:69:LYS:HG3	49:LL:222:ASN:HD21	1.82	0.45
54:LI:79:SER:HB2	54:LI:147:HIS:CD2	2.51	0.45
72:Le:28:TYR:HB2	72:Le:31:ILE:HG12	1.98	0.45
86:EF:287:THR:HG21	86:EF:315:VAL:HG23	1.97	0.45
1:S2:162:C:H5''	11:SG:87:ARG:NH2	2.32	0.45
1:S2:960:U:H1'	1:S2:963:A:N7	2.31	0.45
3:L5:126:C:H2'	3:L5:127:G:C8	2.51	0.45
3:L5:222:C:H2'	3:L5:223:G:O4'	2.17	0.45
3:L5:1625:OMG:H3'	53:LN:81:TYR:OH	2.17	0.45
3:L5:4303:C:O2'	3:L5:4304:A:H2'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:141:VAL:HG12	30:SY:65:GLY:HA3	1.98	0.45
27:SP:34:MET:HB3	27:SP:42:ARG:HG3	1.99	0.45
38:Lz:119:GLN:HE22	38:Lz:123:ILE:HD12	1.82	0.45
55:LD:237:GLU:HG2	55:LD:241:LYS:NZ	2.31	0.45
84:At:67:C:H2'	84:At:68:C:C6	2.51	0.45
1:S2:168:C:H5''	11:SG:131:ARG:HD3	1.97	0.45
1:S2:1228:A:H2'	1:S2:1229:G:H8	1.76	0.45
1:S2:1683:C:H2'	1:S2:1684:C:C6	2.52	0.45
3:L5:280:G:H5''	53:LN:14:LYS:HE2	1.98	0.45
3:L5:423:G:H5'	60:LP:26:PHE:HZ	1.82	0.45
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.52	0.45
3:L5:2521:G:H4'	74:Lg:26:PRO:HD2	1.98	0.45
3:L5:4415:A:H2'	3:L5:4416:G:O4'	2.16	0.45
3:L5:4572:U:O2	3:L5:4720:C:H5'	2.16	0.45
3:L5:4759:C:H2'	3:L5:4760:G:C8	2.52	0.45
17:SU:32:LEU:HD21	17:SU:87:ARG:HG2	1.98	0.45
22:SS:98:VAL:HG11	22:SS:106:LYS:HG3	1.99	0.45
24:SN:31:ASP:OD1	24:SN:32:ASP:N	2.49	0.45
37:Sg:173:LEU:HD22	37:Sg:189:ILE:HG12	1.97	0.45
37:Sg:212:LYS:HD2	37:Sg:235:ILE:HD12	1.99	0.45
37:Sg:220:ASP:HB2	37:Sg:227:LEU:HD13	1.99	0.45
47:LK:106:PHE:HA	47:LK:109:ILE:HG12	1.97	0.45
50:LV:112:MET:HE1	50:LV:117:ILE:HG12	1.99	0.45
70:Lc:47:ILE:HB	70:Lc:94:LEU:HG	1.98	0.45
1:S2:99:A2M:H62	1:S2:433:A:H1'	1.81	0.45
1:S2:1281:G:H2'	1:S2:1282:A:C8	2.52	0.45
3:L5:3640:U:H2'	3:L5:3646:A:N6	2.32	0.45
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.52	0.45
3:L5:4266:G:N3	3:L5:4266:G:H2'	2.31	0.45
13:SH:51:ILE:HD11	13:SH:176:VAL:HG22	1.99	0.45
43:LH:2:LYS:HE2	51:LM:33:GLN:HE22	1.81	0.45
45:LG:51:LEU:O	45:LG:55:VAL:HG23	2.16	0.45
60:LP:4:TYR:OH	60:LP:18:ARG:HB2	2.17	0.45
1:S2:35:C:H5''	1:S2:579:C:H5''	1.98	0.45
1:S2:1401:A:H4'	17:SU:53:PRO:HD2	1.98	0.45
3:L5:106:A:H1'	3:L5:336:A:N3	2.31	0.45
3:L5:2415:OMU:H1'	3:L5:2415:OMU:HM23	1.70	0.45
3:L5:4301:U:H4'	59:LT:54:HIS:CD2	2.52	0.45
13:SH:37:LYS:O	13:SH:41:ARG:HG2	2.17	0.45
17:SU:50:VAL:HG22	17:SU:91:LEU:HD21	1.99	0.45
41:LC:278:ASN:HD22	41:LC:278:ASN:HA	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Lq:6:ARG:HG3	46:Lq:10:LYS:HE2	1.99	0.45
55:LD:64:ILE:HG13	55:LD:109:LEU:HD22	1.99	0.45
94:At:77:PHE:HA	86:EF:264:VAL:HG21	1.99	0.45
86:EF:85:TYR:O	86:EF:86:TYR:C	2.60	0.45
1:S2:528:A:H2'	1:S2:529:A:H8	1.81	0.45
1:S2:877:C:H2'	1:S2:878:G:C8	2.51	0.45
1:S2:905:C:H2'	1:S2:906:U:C6	2.52	0.45
1:S2:1202:U:H4'	10:SC:114:LYS:HE3	1.98	0.45
3:L5:162:A:H2'	3:L5:163:A:H8	1.81	0.45
3:L5:1079:C:H2'	3:L5:1080:C:C6	2.52	0.45
3:L5:4050:A:H5'	3:L5:4051:C:C5	2.52	0.45
6:SA:56:GLU:HG3	29:SV:83:PHE:HD1	1.81	0.45
7:SD:45:ARG:HH21	7:SD:85:GLU:HB2	1.82	0.45
11:SG:162:LEU:HD11	11:SG:172:LYS:HE2	1.98	0.45
40:LB:165:HIS:HB3	40:LB:180:LEU:HD13	1.99	0.45
45:LG:117:ARG:HD2	45:LG:130:THR:HG21	1.99	0.45
47:LK:76:SER:OG	47:LK:77:ALA:N	2.50	0.45
54:LI:47:PRO:HG2	54:LI:142:LEU:CD2	2.47	0.45
76:Lj:39:TYR:CD1	76:Lj:40:PRO:HA	2.51	0.45
84:At:46:G7M:H8	84:At:46:G7M:H2'	1.72	0.45
1:S2:493:A:H1'	1:S2:574:A:H5'	1.99	0.44
1:S2:1088:U:H4'	1:S2:1089:G:OP2	2.17	0.44
1:S2:1473:G:N2	1:S2:1475:G:H3'	2.32	0.44
3:L5:1273:G:C6	44:LE:73:TYR:HB2	2.52	0.44
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.52	0.44
3:L5:4618:OMG:HM23	3:L5:4618:OMG:H1'	1.65	0.44
8:SJ:134:HIS:CE1	8:SJ:164:PRO:HD2	2.52	0.44
9:SE:124:CYS:HB3	9:SE:141:THR:HB	1.99	0.44
10:SC:65:LYS:HE3	10:SC:273:LEU:HD13	1.99	0.44
11:SG:65:GLN:HA	11:SG:100:CYS:HB3	1.99	0.44
50:LV:87:SER:HB3	64:LW:19:ARG:HH21	1.83	0.44
53:LN:71:ARG:O	53:LN:92:LEU:HB2	2.18	0.44
56:LQ:34:PHE:CE1	56:LQ:38:ARG:HG3	2.52	0.44
84:At:16:H2U:H61	84:At:17:C:C4	2.52	0.44
86:EF:160:PRO:O	86:EF:161:PRO:C	2.59	0.44
1:S2:24:C:O2'	1:S2:25:A:H5'	2.17	0.44
1:S2:649:PSU:H2'	1:S2:650:A:C8	2.51	0.44
1:S2:1113:A:H2'	1:S2:1114:U:C6	2.52	0.44
2:L8:19:C:H2'	2:L8:20:A:C8	2.52	0.44
3:L5:299:C:O3'	53:LN:171:SER:HA	2.17	0.44
3:L5:674:G:H2'	3:L5:675:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.52	0.44
3:L5:3946:G:H2'	3:L5:3947:A:C8	2.51	0.44
3:L5:4184:G:H5'	39:LA:233:ARG:HB2	1.99	0.44
8:SJ:93:LYS:HB2	8:SJ:96:TYR:CD2	2.53	0.44
8:SJ:131:ARG:HD2	8:SJ:131:ARG:HA	1.83	0.44
11:SG:234:LEU:HD12	11:SG:237:LEU:HD11	1.98	0.44
30:SY:99:LYS:HA	30:SY:99:LYS:HD2	1.78	0.44
58:LS:121:ALA:HA	58:LS:124:ILE:HD12	1.99	0.44
82:Lp:26:VAL:HG22	82:Lp:30:GLU:HG2	1.98	0.44
84:At:30:G:H3'	84:At:31:A:H8	1.82	0.44
86:EF:166:ARG:O	86:EF:169:GLU:HG3	2.17	0.44
86:EF:402:VAL:HG13	86:EF:404:MET:HE3	2.00	0.44
1:S2:558:G:H2'	1:S2:559:G:C8	2.52	0.44
1:S2:895:G:C6	1:S2:896:U:H1'	2.53	0.44
1:S2:1432:U:H2'	1:S2:1438:A:C8	2.53	0.44
1:S2:1523:C:H4'	22:SS:145:THR:HA	1.98	0.44
3:L5:79:C:H2'	3:L5:80:C:H6	1.82	0.44
3:L5:163:A:H2'	3:L5:164:G:H8	1.81	0.44
3:L5:259:C:H2'	3:L5:260:C:C6	2.53	0.44
3:L5:978:G:OP1	44:LE:62:MET:HE2	2.17	0.44
3:L5:2363:A2M:H2'	3:L5:2364:OMG:O4'	2.18	0.44
3:L5:3911:C:H4'	3:L5:4196:OMG:HM22	1.99	0.44
3:L5:4711:C:H2'	3:L5:4712:C:C6	2.53	0.44
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.52	0.44
11:SG:145:PHE:HB2	11:SG:147:LEU:HD13	1.99	0.44
20:SX:107:ARG:CD	20:SX:112:VAL:HG12	2.46	0.44
28:ST:134:ILE:O	28:ST:138:VAL:HG23	2.17	0.44
57:LR:112:SER:OG	57:LR:114:LYS:HE2	2.16	0.44
74:Lg:94:ALA:O	74:Lg:98:GLU:HG2	2.17	0.44
1:S2:484:A2M:HM'3	1:S2:484:A2M:H1'	1.71	0.44
1:S2:544:G:H2'	1:S2:545:A:C8	2.53	0.44
1:S2:879:C:H2'	1:S2:880:G:H8	1.83	0.44
3:L5:1600:A:H5'	60:LP:133:HIS:HA	1.99	0.44
3:L5:2663:G:H4'	57:LR:117:ARG:HH21	1.82	0.44
3:L5:2872:C:H5''	80:Ln:25:LYS:HD2	2.00	0.44
30:SY:2:ASN:HA	30:SY:32:LYS:HE3	1.99	0.44
58:LS:1:MET:HG3	58:LS:39:VAL:CG1	2.48	0.44
74:Lg:45:ALA:HB3	74:Lg:82:MET:HE2	1.98	0.44
81:Lo:35:ALA:O	81:Lo:39:ARG:HG3	2.17	0.44
1:S2:649:PSU:H2'	1:S2:650:A:H8	1.82	0.44
1:S2:906:U:H2'	1:S2:907:G:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L8:83:C:H4'	2:L8:84:A:C4	2.52	0.44
2:L8:139:G:H2'	2:L8:140:C:O4'	2.17	0.44
3:L5:340:C:H4'	3:L5:341:G:OP2	2.17	0.44
3:L5:424:U:H2'	3:L5:425:U:C6	2.53	0.44
3:L5:1246:G:H2'	3:L5:1247:U:C6	2.53	0.44
3:L5:3723:A2M:HM'3	3:L5:3723:A2M:H1'	1.64	0.44
5:SB:131:ASP:OD2	5:SB:180:ASP:HB2	2.17	0.44
13:SH:9:VAL:HG13	13:SH:9:VAL:O	2.17	0.44
13:SH:148:LEU:HD22	14:SW:49:GLU:HG2	2.00	0.44
21:SM:17:ALA:O	21:SM:21:VAL:HG23	2.17	0.44
28:ST:42:HIS:CD2	28:ST:43:LYS:HE2	2.52	0.44
33:Sb:62:VAL:HG23	33:Sb:74:THR:HG21	2.00	0.44
73:Lf:14:TYR:CD2	73:Lf:23:GLU:HA	2.52	0.44
73:Lf:40:GLU:OE1	73:Lf:109:ARG:NH1	2.49	0.44
80:Ln:12:ARG:HG2	80:Ln:15:ARG:NH2	2.32	0.44
86:EF:346:ILE:HG13	86:EF:394:LEU:CD2	2.48	0.44
3:L5:1441:C:H2'	3:L5:1442:C:C6	2.52	0.44
3:L5:2583:C:OP1	74:Lg:54:ARG:HB2	2.17	0.44
3:L5:4159:C:H2'	3:L5:4160:C:C6	2.52	0.44
3:L5:4273:A:H2'	3:L5:4274:A:C8	2.52	0.44
3:L5:4324:A:H2'	3:L5:4325:A:C8	2.53	0.44
5:SB:83:LYS:HE3	5:SB:83:LYS:HB2	1.82	0.44
12:SF:80:GLY:HA2	12:SF:83:ASN:OD1	2.18	0.44
17:SU:29:VAL:HG23	17:SU:85:HIS:CE1	2.53	0.44
24:SN:88:LEU:HD22	24:SN:135:LEU:HD11	2.00	0.44
26:SR:20:TYR:HD2	26:SR:23:ARG:HD3	1.83	0.44
28:ST:45:LEU:HD23	28:ST:45:LEU:HA	1.84	0.44
1:S2:210:U:H2'	1:S2:211:G:H8	1.81	0.44
1:S2:1804:OMU:HM23	1:S2:1804:OMU:H1'	1.79	0.44
3:L5:1294:A:H1'	3:L5:1295:C:H5	1.82	0.44
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.18	0.44
7:SD:71:ALA:O	7:SD:74:GLN:HG3	2.17	0.44
9:SE:20:LEU:HD21	9:SE:46:ILE:HD12	2.00	0.44
15:SI:103:LEU:HD22	15:SI:170:LYS:HB3	2.00	0.44
25:SL:111:VAL:HG12	25:SL:140:PHE:HB2	2.00	0.44
29:SV:47:ASN:OD1	29:SV:49:GLN:HB2	2.17	0.44
43:LH:6:SER:OG	43:LH:67:LEU:HD22	2.18	0.44
48:LO:44:SER:HB3	48:LO:129:LEU:HD21	1.99	0.44
86:EF:405:VAL:HG13	86:EF:405:VAL:O	2.18	0.44
86:EF:428:ASP:OD1	86:EF:429:MET:N	2.51	0.44
1:S2:618:C:H41	20:SX:67:ARG:NH2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:840:C:H2'	1:S2:841:G:H4'	2.00	0.44
1:S2:952:G:H2'	1:S2:953:C:C6	2.53	0.44
3:L5:2060:G:N2	58:LS:115:ALA:HB2	2.32	0.44
3:L5:2504:C:N4	3:L5:2507:A:H5''	2.32	0.44
3:L5:2550:G:O2'	3:L5:2587:A:N1	2.49	0.44
3:L5:4178:A:H2'	3:L5:4179:G:C8	2.52	0.44
3:L5:4711:C:H2'	3:L5:4712:C:H6	1.82	0.44
3:L5:4870:G:H5''	51:LM:91:TRP:CD2	2.53	0.44
5:SB:180:ASP:OD1	5:SB:180:ASP:N	2.50	0.44
17:SU:80:PHE:HB3	23:Sd:52:PHE:HB3	2.00	0.44
22:SS:24:ARG:HB2	22:SS:29:ALA:HB2	1.99	0.44
58:LS:69:GLU:HG2	58:LS:101:THR:HG22	1.98	0.44
68:Lb:61:ASN:O	68:Lb:65:MET:HG2	2.17	0.44
77:Lk:16:ARG:HE	77:Lk:61:PRO:HG3	1.83	0.44
82:Lp:49:ARG:HG3	82:Lp:55:TRP:CE2	2.53	0.44
1:S2:512:A2M:H4'	1:S2:576:A2M:H2	2.00	0.44
1:S2:1223:A:H2'	1:S2:1224:G:O4'	2.17	0.44
1:S2:1376:A:H2'	1:S2:1377:U:O4'	2.17	0.44
1:S2:1538:C:H2'	1:S2:1539:U:C6	2.53	0.44
1:S2:1706:G:H5'	80:Ln:1:MET:HB2	2.00	0.44
1:S2:1802:C:H2'	1:S2:1803:U:C6	2.53	0.44
2:L8:45:C:H4'	78:Ll:11:ARG:HE	1.83	0.44
3:L5:498:C:H2'	3:L5:499:G:C8	2.53	0.44
3:L5:1077:C:H2'	3:L5:1078:A:C8	2.53	0.44
3:L5:2097:U:H3'	3:L5:2098:G:H4'	2.00	0.44
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.53	0.44
3:L5:4652:G:H2'	3:L5:4653:C:C6	2.52	0.44
7:SD:74:GLN:HB3	7:SD:84:VAL:HG11	2.00	0.44
30:SY:111:LYS:HB3	30:SY:111:LYS:HE3	1.74	0.44
31:SZ:84:ALA:O	31:SZ:88:LEU:HG	2.18	0.44
40:LB:19:ARG:HB2	40:LB:234:ARG:NH2	2.32	0.44
47:LK:70:GLN:NE2	47:LK:71:ILE:O	2.51	0.44
52:La:36:GLY:HA3	52:La:40:HIS:CE1	2.53	0.44
59:LT:18:PRO:HB2	59:LT:21:LYS:HG3	1.99	0.44
61:LU:105:ASN:HB2	61:LU:111:GLU:HB2	1.99	0.44
62:LX:64:SER:HB2	67:Lh:69:LEU:HD13	2.00	0.44
62:LX:87:MET:HE1	62:LX:155:ILE:HG21	2.00	0.44
1:S2:1259:A:H1'	1:S2:1264:C:N4	2.33	0.43
1:S2:1589:A:H2'	1:S2:1590:C:C6	2.53	0.43
3:L5:164:G:H2'	3:L5:165:A:C8	2.53	0.43
3:L5:1087:A:H2'	3:L5:1088:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1395:U:O2	3:L5:1469:C:H4'	2.18	0.43
3:L5:2293:U:H2'	3:L5:2294:G:C8	2.53	0.43
3:L5:2377:C:H2'	3:L5:2378:G:O4'	2.18	0.43
3:L5:4112:C:H2'	3:L5:4113:U:C6	2.53	0.43
3:L5:4208:U:P	59:LT:6:GLY:HA3	2.57	0.43
3:L5:4309:G:H5'	3:L5:4338:G:H5''	2.00	0.43
10:SC:167:ARG:HG2	10:SC:219:ILE:HD13	1.98	0.43
11:SG:5:ILE:HG21	11:SG:45:TRP:HH2	1.83	0.43
21:SM:20:GLU:OE2	21:SM:24:THR:HB	2.17	0.43
22:SS:30:ILE:HG22	22:SS:36:VAL:HG11	1.99	0.43
27:SP:84:ILE:HD13	27:SP:84:ILE:HA	1.81	0.43
37:Sg:39:THR:HG22	37:Sg:60:ARG:HG2	2.00	0.43
37:Sg:165:ILE:HG23	37:Sg:177:TRP:HB2	2.00	0.43
40:LB:60:VAL:HB	40:LB:67:VAL:O	2.18	0.43
43:LH:118:LEU:HD23	43:LH:118:LEU:HA	1.82	0.43
46:Lq:26:LYS:HZ3	46:Lq:95:LEU:HD21	1.83	0.43
86:EF:138:LEU:O	86:EF:142:THR:HG23	2.17	0.43
1:S2:1046:U:H2'	1:S2:1047:C:C6	2.53	0.43
1:S2:1284:A:OP1	1:S2:1285:G:H2'	2.18	0.43
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.53	0.43
3:L5:1359:G:H4'	53:LN:203:TYR:HB2	1.99	0.43
3:L5:1397:A:OP1	52:La:132:ARG:HB2	2.18	0.43
3:L5:2015:U:H2'	3:L5:2016:C:C6	2.53	0.43
3:L5:3642:A:C4	76:Lj:3:LYS:HB3	2.53	0.43
3:L5:3701:OMC:N4	3:L5:3745:U:H2'	2.33	0.43
3:L5:3822:U:H3'	3:L5:3823:G:N2	2.33	0.43
3:L5:4187:G:P	87:L5:5103:SPD:HN6	2.41	0.43
3:L5:4201:G:O2'	3:L5:4202:U:H5'	2.18	0.43
3:L5:4571:A2M:HM'3	3:L5:4571:A2M:H1'	1.83	0.43
3:L5:4611:A:C2	43:LH:120:GLU:HG2	2.53	0.43
13:SH:10:LYS:NZ	13:SH:16:PRO:HD2	2.33	0.43
17:SU:94:PRO:HD2	17:SU:97:ILE:HD13	2.01	0.43
29:SV:30:ALA:O	29:SV:60:ARG:HD3	2.18	0.43
37:Sg:207:CYS:HB2	37:Sg:221:LEU:HD21	2.00	0.43
45:LG:55:VAL:HG21	62:LX:41:ARG:HD2	2.00	0.43
48:LO:37:ARG:HD3	48:LO:157:GLU:OE2	2.18	0.43
65:LZ:119:GLU:O	65:LZ:123:LYS:HG2	2.18	0.43
73:Lf:24:HIS:HA	73:Lf:91:ASN:OD1	2.18	0.43
1:S2:1012:A:H2'	1:S2:1013:U:O4'	2.18	0.43
1:S2:1447:OMG:HM23	1:S2:1447:OMG:H1'	1.62	0.43
1:S2:1801:A:H2'	1:S2:1802:C:C6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1863:A:H1'	32:Sa:79:ILE:HD13	2.01	0.43
3:L5:335:A:H2'	3:L5:336:A:C8	2.53	0.43
3:L5:1082:C:H2'	3:L5:1083:U:O4'	2.19	0.43
3:L5:1329:G:H3'	98:L5:5530:HOH:O	2.18	0.43
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.53	0.43
3:L5:1567:U:H2'	3:L5:1568:C:C6	2.53	0.43
3:L5:4228:OMG:H5''	3:L5:4229:U:O4'	2.19	0.43
7:SD:69:LEU:HA	7:SD:72:VAL:HG12	2.01	0.43
8:SJ:162:ARG:NH1	30:SY:31:GLY:HA2	2.33	0.43
10:SC:166:ARG:HB3	10:SC:247:THR:HB	1.99	0.43
22:SS:75:ARG:HD2	22:SS:95:TYR:O	2.18	0.43
24:SN:38:TYR:CZ	24:SN:78:LYS:HG3	2.52	0.43
66:Lr:92:SER:O	66:Lr:96:MET:HG3	2.17	0.43
72:Le:89:LEU:HD13	72:Le:118:LEU:HD22	1.99	0.43
86:EF:146:LYS:NZ	86:EF:147:GLN:HE21	2.16	0.43
1:S2:28:U:H2'	1:S2:29:G:H8	1.83	0.43
1:S2:1010:G:H2'	1:S2:1011:A:C8	2.53	0.43
2:L8:92:U:H2'	2:L8:93:C:O4'	2.18	0.43
3:L5:1188:C:H2'	3:L5:1189:G:H8	1.83	0.43
3:L5:1378:C:C2	49:LL:221:ARG:HD2	2.53	0.43
3:L5:1845:U:OP1	68:Lb:25:ARG:NE	2.52	0.43
13:SH:10:LYS:HD2	13:SH:46:THR:O	2.18	0.43
13:SH:20:GLU:H	13:SH:20:GLU:CD	2.25	0.43
38:Lz:66:CYS:HB2	38:Lz:82:ILE:HG21	2.01	0.43
77:Lk:60:LEU:HD12	77:Lk:60:LEU:HA	1.79	0.43
1:S2:1522:A:OP2	22:SS:142:ARG:NH1	2.51	0.43
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.83	0.43
3:L5:2034:G:OP1	58:LS:87:ARG:HG3	2.18	0.43
3:L5:2461:G:H2'	3:L5:2462:C:C6	2.53	0.43
3:L5:3724:A2M:HM'3	3:L5:3724:A2M:H1'	1.75	0.43
3:L5:5051:C:O3'	40:LB:324:GLY:HA2	2.18	0.43
7:SD:163:PRO:C	7:SD:165:ASN:N	2.76	0.43
13:SH:20:GLU:HG3	13:SH:48:ALA:HB3	2.00	0.43
13:SH:42:GLU:N	13:SH:42:GLU:OE1	2.52	0.43
14:SW:39:THR:O	14:SW:43:LYS:HG2	2.18	0.43
29:SV:70:LEU:HD21	29:SV:83:PHE:CE2	2.54	0.43
33:Sb:36:LYS:HG2	33:Sb:43:ILE:HG13	1.99	0.43
41:LC:60:HIS:HA	41:LC:92:PHE:HE1	1.84	0.43
53:LN:178:HIS:HA	53:LN:181:HIS:NE2	2.33	0.43
54:LI:47:PRO:HG2	54:LI:142:LEU:HD22	2.00	0.43
80:Ln:12:ARG:HG2	80:Ln:15:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:At:41:C:H2'	84:At:42:C:C6	2.54	0.43
1:S2:440:G:OP1	15:SI:24:LYS:NZ	2.50	0.43
3:L5:1364:U:OP2	49:LL:36:ARG:NH2	2.51	0.43
3:L5:3601:C:H2'	3:L5:3602:C:H6	1.83	0.43
3:L5:4736:C:H2'	3:L5:4737:G:C8	2.53	0.43
7:SD:135:GLU:HG3	7:SD:153:VAL:HG22	2.00	0.43
10:SC:253:PRO:HA	10:SC:256:TRP:CE2	2.53	0.43
11:SG:74:ARG:HE	11:SG:74:ARG:HB3	1.65	0.43
12:SF:23:TRP:HZ2	12:SF:98:GLU:HG2	1.84	0.43
18:SK:21:MET:HG2	18:SK:49:MET:SD	2.59	0.43
19:SO:69:SER:O	19:SO:110:PRO:HG2	2.18	0.43
37:Sg:257:LYS:HG2	37:Sg:269:GLU:HG2	2.01	0.43
51:LM:28:VAL:HG21	51:LM:39:ASP:HB2	2.01	0.43
86:EF:178:ILE:HA	86:EF:181:ILE:HG12	2.01	0.43
86:EF:345:ILE:HG21	97:EF:502:ZIY:O37	2.18	0.43
1:S2:1100:A:H5''	26:SR:132:ARG:NE	2.34	0.43
1:S2:1248:B8N:C4	85:Pt:35:C:H5'	2.49	0.43
1:S2:1395:C:H1'	1:S2:1474:A:C4	2.54	0.43
1:S2:1490:OMG:H1'	1:S2:1490:OMG:HM23	1.68	0.43
3:L5:169:G:H2'	3:L5:170:C:C6	2.54	0.43
3:L5:385:A:N3	3:L5:387:G:H5''	2.34	0.43
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.18	0.43
3:L5:1977:C:H2'	3:L5:1978:C:O4'	2.19	0.43
3:L5:2338:C:H4'	66:Lr:12:ASN:O	2.19	0.43
7:SD:211:VAL:HG12	26:SR:38:ILE:O	2.19	0.43
12:SF:125:SER:HA	12:SF:138:ALA:HA	2.01	0.43
12:SF:126:THR:HG21	34:Sc:27:CYS:SG	2.58	0.43
17:SU:39:LEU:HD11	17:SU:105:SER:HB3	2.01	0.43
37:Sg:107:ASP:HB2	37:Sg:125:ARG:CD	2.49	0.43
37:Sg:294:ASP:OD1	37:Sg:294:ASP:N	2.51	0.43
58:LS:43:ARG:HA	58:LS:43:ARG:HD2	1.75	0.43
86:EF:96:ARG:NH1	86:EF:430:ARG:O	2.51	0.43
1:S2:159:A2M:O5'	1:S2:159:A2M:H8	2.18	0.43
1:S2:502:C:H4'	9:SE:62:LYS:HE3	2.01	0.43
1:S2:921:G:H5'	33:Sb:21:LYS:HD2	2.00	0.43
1:S2:1562:C:H2'	1:S2:1563:G:C8	2.53	0.43
3:L5:1100:U:H2'	3:L5:1101:C:C6	2.54	0.43
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.53	0.43
3:L5:1670:G:N2	3:L5:1854:G:H2'	2.34	0.43
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.54	0.43
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4886:C:H2'	3:L5:4887:C:C6	2.53	0.43
7:SD:150:MET:HE2	7:SD:152:PHE:CZ	2.50	0.43
8:SJ:64:ASP:O	8:SJ:70:ARG:HD3	2.19	0.43
18:SK:32:HIS:CD2	18:SK:45:VAL:HG21	2.54	0.43
41:LC:60:HIS:HA	41:LC:92:PHE:CE1	2.54	0.43
46:Lq:112:ARG:HH12	46:Lq:182:PRO:HG2	1.84	0.43
50:LV:35:LYS:HB2	50:LV:67:LYS:HG3	2.00	0.43
3:L5:35:U:O2'	3:L5:1651:G:H1'	2.19	0.43
3:L5:52:G:H4'	3:L5:1529:G:H4'	2.00	0.43
3:L5:1419:G:C6	52:La:116:LYS:HD2	2.53	0.43
3:L5:1545:G:H2'	3:L5:1546:C:C6	2.54	0.43
3:L5:1630:A:H2	3:L5:3638:G:N3	2.16	0.43
3:L5:2554:U:OP1	3:L5:2554:U:H4'	2.18	0.43
3:L5:4134:C:H2'	3:L5:4135:G:C8	2.54	0.43
5:SB:44:ILE:HD11	5:SB:86:LEU:HD23	2.00	0.43
5:SB:136:ARG:HB2	5:SB:218:LEU:HD11	2.00	0.43
8:SJ:134:HIS:HE1	8:SJ:164:PRO:HD2	1.84	0.43
11:SG:186:GLN:HA	11:SG:189:ARG:HE	1.84	0.43
14:SW:71:LYS:HB3	14:SW:130:PHE:CE1	2.54	0.43
15:SI:203:LYS:O	15:SI:206:LYS:HG2	2.18	0.43
18:SK:1:MET:HE1	18:SK:43:LEU:HG	2.01	0.43
22:SS:36:VAL:HG22	22:SS:40:TYR:CD2	2.54	0.43
26:SR:36:GLU:HG3	26:SR:47:ARG:HD2	2.01	0.43
72:Le:19:LYS:HE2	72:Le:19:LYS:HB3	1.88	0.43
72:Le:23:HIS:CD2	72:Le:43:ASN:HD21	2.35	0.43
86:EF:53:SER:HA	86:EF:196:TRP:CZ2	2.54	0.43
1:S2:533:A:H61	1:S2:551:U:H3	1.67	0.43
1:S2:1741:U:H2'	1:S2:1742:C:O4'	2.19	0.43
3:L5:208:A:H2	3:L5:233:U:H5''	1.82	0.43
3:L5:1666:C:O2'	3:L5:1688:G:H5''	2.19	0.43
3:L5:1893:C:H1'	3:L5:1937:C:O2	2.19	0.43
3:L5:2517:A:H5'	74:Lg:62:LYS:HD3	2.01	0.43
3:L5:4910:G:H4'	40:LB:95:THR:HG22	2.01	0.43
4:L7:7:G:OP1	55:LD:33:ARG:NH1	2.52	0.43
9:SE:103:TYR:HB2	9:SE:182:MET:HE2	1.99	0.43
28:ST:99:VAL:O	28:ST:103:VAL:HG23	2.18	0.43
43:LH:137:SER:HB3	43:LH:143:GLU:HB3	2.01	0.43
45:LG:83:PHE:HA	45:LG:183:ILE:HD13	1.99	0.43
58:LS:30:MET:HE1	58:LS:47:PHE:CG	2.54	0.43
76:Lj:39:TYR:CG	76:Lj:40:PRO:HA	2.53	0.43
86:EF:60:LEU:HD22	86:EF:76:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1678:A2M:H1'	1:S2:1678:A2M:HM'3	1.67	0.42
3:L5:137:G:C2	3:L5:138:G:N7	2.87	0.42
3:L5:1077:C:H2'	3:L5:1078:A:H8	1.85	0.42
3:L5:1882:U:H1'	3:L5:1883:G:C8	2.54	0.42
3:L5:2270:G:H2'	3:L5:2271:C:O4'	2.19	0.42
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.55	0.42
22:SS:108:ARG:O	22:SS:112:GLU:HG2	2.18	0.42
54:LI:96:VAL:HG22	54:LI:125:THR:HG22	2.00	0.42
61:LU:80:LYS:HE2	61:LU:110:TYR:CE2	2.54	0.42
62:LX:119:ILE:HD12	62:LX:140:LEU:HD22	2.01	0.42
66:Lr:20:ARG:HH12	72:Le:84:GLU:CD	2.26	0.42
1:S2:463:C:H2'	1:S2:465:A:N7	2.34	0.42
1:S2:551:U:H2'	1:S2:552:G:H8	1.82	0.42
1:S2:1402:A:H5'	17:SU:51:LYS:O	2.18	0.42
1:S2:1562:C:H2'	1:S2:1563:G:H8	1.85	0.42
6:SA:12:GLU:O	6:SA:16:LEU:HG	2.19	0.42
12:SF:204:ARG:HD2	19:SO:72:TYR:CZ	2.53	0.42
13:SH:134:VAL:O	13:SH:135:PHE:C	2.61	0.42
17:SU:99:LYS:HA	17:SU:99:LYS:HD3	1.85	0.42
21:SM:31:LEU:HD11	21:SM:89:VAL:HG13	2.02	0.42
54:LI:86:HIS:HB3	54:LI:139:ARG:HG2	2.01	0.42
81:Lo:14:LYS:HE3	81:Lo:79:SER:HB2	2.01	0.42
1:S2:1467:C:OP1	26:SR:2:GLY:N	2.52	0.42
3:L5:92:C:C2	52:La:55:LYS:HE3	2.55	0.42
3:L5:123:C:H2'	3:L5:124:C:C6	2.54	0.42
3:L5:138:G:H2'	3:L5:139:G:C8	2.55	0.42
3:L5:270:U:H2'	3:L5:271:C:H6	1.84	0.42
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.54	0.42
3:L5:1721:G:H2'	3:L5:1722:C:O4'	2.18	0.42
3:L5:2267:U:C6	3:L5:2270:G:H4'	2.54	0.42
3:L5:3906:A:H2'	41:LC:69:THR:HG21	2.00	0.42
3:L5:4184:G:C8	39:LA:230:PRO:HG2	2.55	0.42
3:L5:4638:U:H2'	3:L5:4639:G:N3	2.33	0.42
3:L5:4906:C:H2'	3:L5:4907:G:H8	1.84	0.42
3:L5:4923:C:H2'	3:L5:4924:C:H6	1.84	0.42
4:L7:8:G:OP2	55:LD:30:TYR:OH	2.33	0.42
21:SM:58:GLU:O	21:SM:62:VAL:HG23	2.19	0.42
37:Sg:311:GLN:HE22	37:Sg:313:THR:HB	1.84	0.42
38:Lz:124:LEU:HD23	38:Lz:124:LEU:H	1.84	0.42
40:LB:201:LEU:O	40:LB:202:GLU:HB2	2.19	0.42
46:Lq:45:MET:HA	46:Lq:48:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:LI:48:LEU:O	54:LI:139:ARG:HA	2.20	0.42
55:LD:41:LYS:HB2	59:LT:68:THR:O	2.20	0.42
57:LR:136:ARG:O	57:LR:140:GLU:HG2	2.19	0.42
61:LU:63:ILE:HG23	61:LU:70:ILE:HG23	2.01	0.42
1:S2:67:C:H2'	11:SG:164:LYS:HE3	2.00	0.42
1:S2:436:OMG:HM23	1:S2:436:OMG:H1'	1.83	0.42
1:S2:644:OMG:HM23	1:S2:644:OMG:H1'	1.71	0.42
1:S2:1553:C:N4	23:Sd:22:ARG:HG2	2.35	0.42
3:L5:1068:G:H8	44:LE:44:CYS:HG	1.64	0.42
3:L5:1812:C:H2'	3:L5:1813:U:C6	2.54	0.42
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.54	0.42
3:L5:2803:U:H2'	3:L5:2804:OMC:H6	1.84	0.42
3:L5:2832:A:OP1	71:Ld:47:LYS:NZ	2.47	0.42
3:L5:2861:OMC:H2'	3:L5:2862:G:O4'	2.18	0.42
3:L5:3760:A2M:H1'	3:L5:3760:A2M:HM'3	1.79	0.42
3:L5:4488:A:H4'	3:L5:4489:G:C8	2.54	0.42
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.54	0.42
6:SA:77:ILE:HG12	6:SA:99:ILE:HB	2.02	0.42
10:SC:125:LYS:HE2	10:SC:141:VAL:HG11	2.01	0.42
36:Sf:132:MET:HE2	36:Sf:132:MET:HA	2.02	0.42
37:Sg:210:GLY:HA3	37:Sg:236:ILE:HG21	2.01	0.42
47:LK:97:ASN:OD1	47:LK:98:ILE:N	2.52	0.42
64:LW:109:ILE:HD11	64:LW:113:LYS:NZ	2.34	0.42
67:Lh:4:ILE:HG13	67:Lh:53:SER:HB3	2.02	0.42
78:Ll:12:PHE:CE1	78:Ll:51:LEU:HD13	2.54	0.42
86:EF:55:MLY:HB2	86:EF:55:MLY:HE3	1.75	0.42
86:EF:103:ILE:HD13	86:EF:103:ILE:HA	1.94	0.42
1:S2:1328:OMG:H1'	1:S2:1328:OMG:HM23	1.72	0.42
1:S2:1716:C:H2'	1:S2:1717:C:C6	2.54	0.42
3:L5:37:U:H2'	3:L5:38:A:O4'	2.19	0.42
3:L5:113:A:H2'	3:L5:114:G:O4'	2.17	0.42
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.55	0.42
3:L5:1086:C:H2'	3:L5:1087:A:C8	2.55	0.42
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.55	0.42
3:L5:1192:C:H2'	3:L5:1193:C:H6	1.83	0.42
3:L5:1459:A:OP1	56:LQ:65:ARG:NH1	2.53	0.42
3:L5:1692:C:H2'	3:L5:1693:U:C6	2.54	0.42
3:L5:2492:C:H2'	3:L5:2493:G:C8	2.53	0.42
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.84	0.42
4:L7:16:A:H2'	4:L7:17:C:C6	2.54	0.42
6:SA:49:ILE:HG23	6:SA:162:PRO:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SC:132:ASP:OD1	10:SC:136:HIS:HB2	2.19	0.42
12:SF:201:LYS:HA	12:SF:204:ARG:HG3	2.01	0.42
19:SO:45:THR:OG1	19:SO:49:GLY:HA2	2.19	0.42
31:SZ:68:ILE:HB	31:SZ:109:TYR:HB2	2.01	0.42
37:Sg:63:SER:HB2	37:Sg:84:ASP:HB3	2.00	0.42
37:Sg:231:ASP:OD1	37:Sg:232:GLY:N	2.52	0.42
41:LC:205:ARG:HD3	41:LC:205:ARG:HA	1.87	0.42
66:Lr:2:SAC:H2A1	66:Lr:2:SAC:HA	1.85	0.42
85:Pt:19:G:N2	85:Pt:59:A:H5'	2.30	0.42
86:EF:26:HIS:CE1	86:EF:198:GLY:HA3	2.54	0.42
1:S2:127:C:H6	1:S2:127:C:H5'	1.85	0.42
1:S2:367:U:H6	1:S2:367:U:O5'	2.03	0.42
1:S2:829:C:OP1	9:SE:21:ASP:HB2	2.19	0.42
1:S2:902:G:H2'	1:S2:903:A:C8	2.55	0.42
1:S2:1289:U:H2'	1:S2:1290:G:C8	2.55	0.42
3:L5:986:C:H2'	3:L5:987:C:C6	2.54	0.42
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.54	0.42
9:SE:11:ARG:HA	9:SE:28:ALA:HB2	2.01	0.42
11:SG:44:GLU:H	11:SG:44:GLU:CD	2.28	0.42
19:SO:125:LYS:HD3	19:SO:125:LYS:HA	1.81	0.42
20:SX:67:ARG:HG3	20:SX:115:ILE:HG12	2.02	0.42
22:SS:36:VAL:HG22	22:SS:40:TYR:HD2	1.84	0.42
26:SR:66:VAL:HG12	26:SR:67:ARG:N	2.32	0.42
41:LC:140:LYS:HE3	41:LC:245:HIS:HB2	2.02	0.42
41:LC:298:ILE:HD13	56:LQ:131:PRO:HB3	2.01	0.42
57:LR:41:ILE:O	57:LR:45:ILE:HG13	2.20	0.42
57:LR:44:LEU:HD22	57:LR:49:LEU:HD22	2.01	0.42
65:LZ:128:LYS:O	65:LZ:132:GLN:HG3	2.20	0.42
66:Lr:56:ASP:O	66:Lr:58:LYS:N	2.49	0.42
69:LF:209:TRP:CD1	69:LF:210:PRO:HD2	2.55	0.42
84:At:44:G:C2	84:At:45:U:C2	3.08	0.42
86:EF:115:ILE:HA	86:EF:151:GLY:O	2.19	0.42
1:S2:77:A:H1'	11:SG:176:ILE:CD1	2.50	0.42
1:S2:494:C:N4	1:S2:509:OMG:HN22	2.18	0.42
1:S2:1553:C:H41	23:Sd:22:ARG:HG2	1.84	0.42
1:S2:1618:C:H4'	27:SP:50:ARG:HH12	1.84	0.42
3:L5:207:G:H2'	3:L5:208:A:C8	2.54	0.42
3:L5:362:A:N6	78:Ll:37:TYR:O	2.49	0.42
3:L5:1368:A:C8	63:LY:3:PHE:HE1	2.38	0.42
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.54	0.42
3:L5:4978:G:H2'	3:L5:4979:A:H5''	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L7:85:G:OP1	69:LF:222:LYS:HE2	2.19	0.42
7:SD:177:LEU:HD12	7:SD:182:LEU:HD13	2.00	0.42
15:SI:83:TYR:HB3	15:SI:101:ILE:HB	2.01	0.42
31:SZ:58:LEU:HD12	31:SZ:62:VAL:HG21	2.01	0.42
35:Se:110:MET:HE2	35:Se:110:MET:HB3	1.89	0.42
39:LA:10:LYS:HA	39:LA:16:PHE:CD2	2.54	0.42
45:LG:159:HIS:ND1	45:LG:185:LYS:HA	2.34	0.42
55:LD:68:ARG:HD3	55:LD:68:ARG:HA	1.84	0.42
55:LD:179:ARG:HA	55:LD:179:ARG:HD3	1.88	0.42
74:Lg:2:VAL:HG13	74:Lg:2:VAL:O	2.19	0.42
1:S2:884:C:H2'	1:S2:885:U:C6	2.55	0.42
3:L5:1099:C:H2'	3:L5:1100:U:C6	2.54	0.42
3:L5:1320:U:O2'	3:L5:1891:A:N1	2.51	0.42
3:L5:3755:G:O2'	85:Pt:12:G:H5''	2.19	0.42
3:L5:4337:C:N3	81:Lo:61:LYS:HE3	2.35	0.42
4:L7:24:C:H2'	4:L7:25:G:O4'	2.20	0.42
7:SD:29:LEU:HD23	7:SD:29:LEU:HA	1.83	0.42
12:SF:179:ASN:HB3	12:SF:187:SER:HB2	2.01	0.42
20:SX:53:GLU:HA	20:SX:96:GLU:OE1	2.20	0.42
32:Sa:12:LYS:HB2	32:Sa:33:ASP:OD2	2.20	0.42
35:Se:79:SER:H	35:Se:82:ARG:HH12	1.68	0.42
42:LJ:35:ARG:HD2	42:LJ:123:ILE:O	2.19	0.42
48:LO:44:SER:HB3	48:LO:129:LEU:HD11	2.01	0.42
49:LL:146:LEU:HD23	67:Lh:122:LYS:HD3	2.01	0.42
58:LS:93:MET:HE1	58:LS:117:HIS:CE1	2.54	0.42
66:Lr:56:ASP:OD1	66:Lr:56:ASP:N	2.50	0.42
68:Lb:99:ILE:O	68:Lb:109:ARG:NH1	2.52	0.42
72:Le:84:GLU:O	72:Le:87:VAL:HG22	2.19	0.42
1:S2:141:A:H4'	1:S2:142:C:H3'	2.02	0.42
1:S2:189:U:H2'	1:S2:190:G:O4'	2.20	0.42
1:S2:686:PSU:OP1	14:SW:32:LYS:HG3	2.20	0.42
3:L5:67:C:O3'	53:LN:177:GLY:HA3	2.20	0.42
3:L5:1880:G:OP2	3:L5:1881:OMC:HM22	2.20	0.42
3:L5:2385:U:H2'	3:L5:2386:U:C6	2.54	0.42
3:L5:3868:G:N2	3:L5:3900:G:H1'	2.35	0.42
3:L5:3946:G:H2'	3:L5:3947:A:H8	1.85	0.42
3:L5:4056:A:H2'	3:L5:4059:C:H42	1.85	0.42
3:L5:4438:U:H2'	3:L5:4439:U:O4'	2.20	0.42
16:SQ:134:GLY:HA3	16:SQ:139:ALA:O	2.19	0.42
21:SM:35:ILE:HG23	21:SM:61:TYR:HE1	1.84	0.42
21:SM:90:GLY:O	21:SM:91:LEU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LB:194:LEU:O	40:LB:198:ARG:HG3	2.19	0.42
47:LK:20:GLY:H	47:LK:54:LYS:HA	1.85	0.42
47:LK:109:ILE:HG13	47:LK:110:VAL:N	2.34	0.42
48:LO:191:LYS:HE3	48:LO:192:TYR:CZ	2.55	0.42
72:Le:100:ALA:HB3	72:Le:103:VAL:HG23	2.01	0.42
86:EF:422:GLY:O	86:EF:438:ILE:HD12	2.19	0.42
1:S2:554:A:H1'	35:Se:99:LYS:HE3	2.01	0.42
1:S2:1349:G:H21	6:SA:112:ILE:HD11	1.85	0.42
1:S2:1433:C:H3'	1:S2:1434:C:C5	2.55	0.42
1:S2:1616:U:H2'	1:S2:1617:G:O4'	2.20	0.42
2:L8:148:A:H2'	2:L8:149:G:C8	2.55	0.42
3:L5:181:C:H2'	3:L5:182:G:C8	2.49	0.42
3:L5:1281:G:H5'	41:LC:323:ARG:HB2	2.02	0.42
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.20	0.42
3:L5:1578:U:H2'	3:L5:1579:C:C6	2.55	0.42
3:L5:2424:OMG:H1'	3:L5:2424:OMG:HM23	1.80	0.42
3:L5:2748:C:H5''	74:Lg:65:MET:HE3	2.01	0.42
3:L5:4220:6MZ:OP2	59:LT:2:THR:N	2.53	0.42
3:L5:5023:C:H6	3:L5:5023:C:H2'	1.70	0.42
10:SC:196:ILE:HB	10:SC:223:TYR:HB2	2.02	0.42
12:SF:18:LYS:HE2	12:SF:24:SER:HB3	2.00	0.42
30:SY:55:ILE:HD12	30:SY:75:ILE:HD12	2.02	0.42
53:LN:60:VAL:HG22	53:LN:134:LEU:HB2	2.01	0.42
63:LY:24:HIS:CE1	63:LY:25:ILE:HG12	2.55	0.42
70:Lc:38:ILE:HG21	70:Lc:63:TYR:HB3	2.02	0.42
85:Pt:62:C:H2'	85:Pt:63:C:C6	2.55	0.42
1:S2:509:OMG:H1'	1:S2:509:OMG:HM23	1.83	0.41
1:S2:1148:A:H4'	1:S2:1149:A:O4'	2.20	0.41
1:S2:1698:C:H42	83:mR:42:C:H5'	1.85	0.41
3:L5:32:G:H21	3:L5:50:C:H5	1.68	0.41
3:L5:257:C:H2'	3:L5:258:G:O4'	2.20	0.41
3:L5:267:G:H2'	3:L5:268:G:H8	1.84	0.41
3:L5:1204:C:H2'	3:L5:1205:G:H8	1.85	0.41
3:L5:1806:G:H2'	3:L5:1807:C:C6	2.55	0.41
7:SD:210:ILE:HD13	26:SR:16:ILE:HG13	2.02	0.41
12:SF:50:PRO:O	12:SF:70:GLU:HG3	2.20	0.41
14:SW:77:PRO:HD2	14:SW:79:PHE:CZ	2.55	0.41
20:SX:68:LYS:HE3	35:Se:80:LEU:HA	2.01	0.41
21:SM:118:SER:HA	21:SM:121:LYS:HE3	2.02	0.41
22:SS:92:ASP:O	22:SS:94:LYS:N	2.53	0.41
30:SY:36:PRO:HB2	30:SY:39:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LB:77:THR:HG21	40:LB:337:VAL:HG22	2.01	0.41
46:Lq:45:MET:HE2	47:LK:122:ALA:HA	2.02	0.41
67:Lh:82:ASP:OD1	67:Lh:82:ASP:N	2.49	0.41
71:Ld:93:ASN:C	71:Ld:93:ASN:HD22	2.27	0.41
86:EF:26:HIS:HB2	86:EF:56:TYR:CD2	2.55	0.41
86:EF:55:MLY:HE2	86:EF:56:TYR:CZ	2.55	0.41
86:EF:372:PHE:CD1	86:EF:404:MET:HE1	2.55	0.41
1:S2:1100:A:H5''	26:SR:132:ARG:CZ	2.50	0.41
1:S2:1349:G:H2'	1:S2:1350:U:C6	2.55	0.41
1:S2:1807:C:H2'	1:S2:1808:U:O4'	2.20	0.41
2:L8:27:U:H2'	2:L8:28:C:C6	2.55	0.41
3:L5:169:G:H2'	3:L5:170:C:H6	1.85	0.41
3:L5:911:U:H2'	3:L5:912:G:O4'	2.20	0.41
3:L5:1192:C:H2'	3:L5:1193:C:C6	2.55	0.41
3:L5:2404:A:H1'	76:Lj:12:ARG:HD2	2.02	0.41
5:SB:62:LEU:HD21	5:SB:96:CYS:SG	2.60	0.41
5:SB:133:TYR:CE1	5:SB:221:PRO:HD2	2.55	0.41
10:SC:113:GLN:HA	10:SC:121:ARG:O	2.20	0.41
21:SM:47:ALA:O	21:SM:74:ILE:HG12	2.19	0.41
22:SS:91:LYS:HA	27:SP:16:THR:O	2.20	0.41
31:SZ:58:LEU:O	31:SZ:62:VAL:HB	2.20	0.41
38:Lz:119:GLN:NE2	38:Lz:123:ILE:HD12	2.35	0.41
41:LC:211:TYR:HE2	41:LC:229:LEU:HB3	1.84	0.41
42:LJ:48:PRO:HB2	42:LJ:70:VAL:HG22	2.00	0.41
43:LH:110:SER:O	43:LH:127:ARG:HD3	2.20	0.41
49:LL:79:GLU:HG2	49:LL:82:ARG:NH2	2.35	0.41
62:LX:153:ILE:HB	62:LX:155:ILE:HD12	2.02	0.41
63:LY:76:LYS:HE3	78:Ll:31:THR:HG23	2.02	0.41
69:LF:175:ILE:HD11	69:LF:187:MET:SD	2.60	0.41
82:Lp:47:MET:HE2	82:Lp:57:CYS:HB2	2.02	0.41
86:EF:288:GLU:HB2	86:EF:313:LYS:HE2	2.01	0.41
1:S2:186:C:H2'	1:S2:187:G:C8	2.54	0.41
1:S2:601:OMG:HM23	1:S2:601:OMG:H1'	1.82	0.41
1:S2:1401:A:H2'	1:S2:1402:A:C8	2.55	0.41
3:L5:1534:A2M:HM'3	3:L5:1637:A:C4	2.55	0.41
3:L5:2325:C:H4'	72:Le:98:GLU:HG2	2.02	0.41
3:L5:2565:A:H3'	3:L5:2566:G:C8	2.55	0.41
3:L5:4456:OMC:HM23	3:L5:4456:OMC:H1'	1.81	0.41
3:L5:4724:A:H2'	3:L5:4725:C:O4'	2.20	0.41
8:SJ:106:LEU:HD23	8:SJ:109:ARG:HD2	2.02	0.41
9:SE:77:ARG:HD2	9:SE:82:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SU:102:THR:HG21	17:SU:114:VAL:HG11	2.01	0.41
34:Sc:18:LEU:HD11	34:Sc:43:ILE:HD12	2.02	0.41
40:LB:238:LYS:HE2	40:LB:238:LYS:HB2	1.75	0.41
41:LC:156:ASP:OD2	41:LC:255:SER:OG	2.25	0.41
81:Lo:32:SER:O	81:Lo:33:LEU:HB3	2.20	0.41
86:EF:277:VAL:HG22	86:EF:288:GLU:HG2	2.02	0.41
1:S2:120:U:H2'	1:S2:121:OMU:C6	2.51	0.41
1:S2:168:C:H2'	1:S2:169:U:C6	2.56	0.41
1:S2:326:C:H1'	1:S2:327:G:C6	2.55	0.41
1:S2:441:C:H2'	1:S2:442:C:C6	2.55	0.41
1:S2:656:G:H5'	1:S2:662:G:N2	2.34	0.41
1:S2:875:A:H2'	1:S2:876:C:C6	2.55	0.41
3:L5:135:G:H1	67:Lh:75:GLY:HA2	1.86	0.41
3:L5:288:G:H2'	3:L5:289:C:H6	1.85	0.41
3:L5:308:G:O6	53:LN:12:ARG:NH1	2.51	0.41
3:L5:368:C:O4'	41:LC:83:GLY:HA3	2.20	0.41
3:L5:1905:U:H2'	3:L5:1906:U:O4'	2.20	0.41
3:L5:2701:U:H2'	3:L5:2702:C:C6	2.55	0.41
3:L5:2862:G:N3	3:L5:3624:A:H2'	2.36	0.41
3:L5:3619:G:H4'	57:LR:79:GLY:O	2.20	0.41
3:L5:4628:PSU:H4'	64:LW:16:GLY:O	2.20	0.41
3:L5:4760:G:H2'	3:L5:4761:G:O4'	2.21	0.41
14:SW:95:PRO:HD3	14:SW:130:PHE:CD2	2.56	0.41
19:SO:113:GLN:H	19:SO:113:GLN:CD	2.28	0.41
22:SS:71:MET:HB3	22:SS:99:LEU:HD21	2.02	0.41
41:LC:293:LEU:HD22	56:LQ:34:PHE:CD2	2.55	0.41
44:LE:211:HIS:NE2	44:LE:249:ASP:OD2	2.54	0.41
68:Lb:117:ARG:HA	68:Lb:117:ARG:HD3	1.76	0.41
82:Lp:79:VAL:O	82:Lp:83:ILE:HG12	2.20	0.41
86:EF:318:M3L:HB3	86:EF:318:M3L:HE2	1.75	0.41
1:S2:115:U:H2'	1:S2:116:OMU:H6	2.02	0.41
1:S2:679:A:H5''	1:S2:679:A:H8	1.85	0.41
1:S2:1016:U:H5''	24:SN:14:SER:HB3	2.01	0.41
1:S2:1144:A:H5'	1:S2:1355:C:C5	2.54	0.41
3:L5:260:C:H2'	3:L5:261:G:H8	1.86	0.41
3:L5:1342:A:OP1	53:LN:204:ARG:HD2	2.21	0.41
3:L5:1448:G:H2'	3:L5:1449:C:C6	2.56	0.41
3:L5:1974:U:H2'	3:L5:1976:G:OP2	2.20	0.41
7:SD:119:CYS:O	7:SD:123:LEU:HB2	2.20	0.41
9:SE:136:ILE:HD13	9:SE:148:ARG:HH21	1.85	0.41
10:SC:134:ASN:O	10:SC:167:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SG:129:VAL:O	64:LW:80:ARG:NH2	2.54	0.41
13:SH:66:VAL:HG22	13:SH:96:ALA:HB1	2.01	0.41
13:SH:159:ASP:C	13:SH:161:ALA:H	2.29	0.41
15:SI:123:ARG:NH1	15:SI:129:LEU:HG	2.35	0.41
18:SK:15:LEU:HD22	18:SK:49:MET:HE3	2.02	0.41
18:SK:63:ALA:HB3	18:SK:68:TYR:HE1	1.85	0.41
22:SS:44:VAL:HG11	22:SS:71:MET:HG3	2.01	0.41
57:LR:176:ARG:O	57:LR:180:LYS:HG3	2.21	0.41
59:LT:92:ARG:HB3	59:LT:94:GLU:OE1	2.20	0.41
84:At:16:H2U:H61	84:At:17:C:C5	2.56	0.41
84:At:76:A:N6	86:EF:259:ILE:HD12	2.34	0.41
86:EF:54:PHE:CE1	96:EF:501:GSP:H5'2	2.56	0.41
1:S2:67:C:N4	11:SG:163:ASN:O	2.53	0.41
1:S2:468:A2M:HM'3	1:S2:468:A2M:H1'	1.89	0.41
3:L5:4383:U:H2'	3:L5:4384:U:C6	2.55	0.41
5:SB:62:LEU:HD23	5:SB:91:VAL:HG21	2.01	0.41
6:SA:63:ARG:HG3	6:SA:185:MET:HE1	2.02	0.41
6:SA:205:ARG:CZ	6:SA:210:ILE:HD13	2.50	0.41
12:SF:19:LEU:N	12:SF:23:TRP:O	2.50	0.41
16:SQ:113:ILE:HD11	16:SQ:120:LEU:HD12	2.02	0.41
19:SO:88:LEU:HD12	19:SO:88:LEU:HA	1.84	0.41
30:SY:102:THR:HG23	30:SY:107:ARG:HG2	2.03	0.41
42:LJ:100:SER:O	42:LJ:159:LYS:HB2	2.20	0.41
59:LT:39:ILE:CG1	59:LT:102:ARG:HG3	2.51	0.41
84:At:22:G:H2'	84:At:23:A:C8	2.55	0.41
84:At:66:U:H2'	84:At:67:C:C6	2.56	0.41
86:EF:51:LYS:HD2	86:EF:54:PHE:CD2	2.54	0.41
1:S2:96:C:H2'	1:S2:97:U:C6	2.56	0.41
1:S2:325:C:H6	1:S2:325:C:H2'	1.70	0.41
2:L8:28:C:H4'	41:LC:51:PRO:HG2	2.03	0.41
3:L5:189:G:H2'	3:L5:190:G:H8	1.86	0.41
3:L5:1631:A:N7	39:LA:199:VAL:HG21	2.35	0.41
3:L5:1672:U:H2'	3:L5:1673:U:C6	2.55	0.41
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.87	0.41
3:L5:2376:A:H2'	3:L5:2377:C:C6	2.56	0.41
3:L5:4674:C:H2'	3:L5:4675:U:C6	2.56	0.41
5:SB:29:ASP:OD2	5:SB:51:ARG:HG2	2.21	0.41
6:SA:34:MET:HE3	6:SA:34:MET:HB3	1.85	0.41
8:SJ:82:VAL:HG21	8:SJ:92:MET:SD	2.61	0.41
16:SQ:72:VAL:HG11	16:SQ:84:ILE:HD11	2.03	0.41
21:SM:81:ASP:O	21:SM:83:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Sb:24:LEU:HD12	33:Sb:24:LEU:HA	1.85	0.41
37:Sg:151:VAL:HA	37:Sg:169:GLY:HA2	2.03	0.41
37:Sg:163:PRO:C	37:Sg:179:LEU:HD23	2.45	0.41
40:LB:45:ALA:HB3	40:LB:183:ILE:HG23	2.03	0.41
47:LK:26:SER:HB3	47:LK:28:LEU:HD22	2.03	0.41
58:LS:30:MET:HE1	58:LS:47:PHE:CB	2.50	0.41
84:At:30:G:C5	84:At:31:A:C5	3.09	0.41
1:S2:1653:U:H2'	1:S2:1654:G:C8	2.55	0.41
3:L5:691:C:H2'	3:L5:692:A:H8	1.79	0.41
3:L5:905:C:H2'	3:L5:906:C:C6	2.56	0.41
3:L5:1193:C:H2'	3:L5:1194:G:C8	2.56	0.41
3:L5:2555:G:H2'	3:L5:2556:G:H5''	2.02	0.41
3:L5:2758:G:H1'	3:L5:2766:A:H1'	2.03	0.41
3:L5:3883:U:H2'	3:L5:3884:PSU:C6	2.55	0.41
3:L5:4284:C:H2'	3:L5:4285:U:C6	2.56	0.41
3:L5:4341:C:N3	91:L5:5117:3H3:H14	2.36	0.41
5:SB:86:LEU:HD12	5:SB:86:LEU:HA	1.83	0.41
10:SC:186:GLY:HA3	10:SC:239:ALA:O	2.21	0.41
12:SF:43:GLU:C	12:SF:45:TYR:H	2.29	0.41
41:LC:321:ASN:HD22	41:LC:324:ILE:H	1.69	0.41
49:LL:33:ILE:O	49:LL:37:LYS:HG2	2.21	0.41
63:LY:13:LYS:O	63:LY:17:ARG:HD3	2.20	0.41
64:LW:50:ASN:HA	64:LW:55:TYR:CD1	2.55	0.41
64:LW:120:GLN:HA	64:LW:123:LYS:HG2	2.01	0.41
68:Lb:40:LEU:HD12	68:Lb:40:LEU:HA	1.72	0.41
84:At:27:G:H2'	84:At:28:G:H8	1.84	0.41
86:EF:26:HIS:HE1	86:EF:198:GLY:HA3	1.85	0.41
86:EF:100:LYS:HG3	86:EF:367:HIS:CD2	2.56	0.41
1:S2:28:U:H2'	1:S2:29:G:C8	2.55	0.41
1:S2:70:G:N2	1:S2:79:A:H62	2.17	0.41
1:S2:543:C:H3'	1:S2:544:G:C8	2.56	0.41
1:S2:562:U:H2'	1:S2:563:G:C8	2.56	0.41
1:S2:614:C:H5''	1:S2:615:C:C6	2.56	0.41
1:S2:1356:G:H2'	1:S2:1357:A:C8	2.56	0.41
1:S2:1690:U:H2'	1:S2:1691:U:C6	2.56	0.41
2:L8:124:U:H4'	2:L8:125:C:H5'	2.02	0.41
3:L5:164:G:H2'	3:L5:165:A:H8	1.84	0.41
3:L5:498:C:H5'	3:L5:499:G:OP2	2.21	0.41
3:L5:504:G:H8	3:L5:504:G:OP2	2.04	0.41
3:L5:757:G:H2'	3:L5:758:G:H8	1.86	0.41
3:L5:1083:U:H2'	3:L5:1084:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.56	0.41
3:L5:1916:G:H1'	73:Lf:16:ARG:O	2.21	0.41
3:L5:1922:G:OP1	58:LS:160:ARG:HD3	2.20	0.41
3:L5:2267:U:P	66:Lr:37:SER:HB2	2.61	0.41
3:L5:2759:G:N3	3:L5:2764:A:H2	2.19	0.41
3:L5:3712:A:H2	3:L5:3740:G:H22	1.69	0.41
3:L5:3777:G:N2	3:L5:3815:G:H2'	2.36	0.41
3:L5:3969:G:H21	3:L5:4052:C:H5'	1.86	0.41
3:L5:4524:G:C2	40:LB:252:ALA:HB1	2.56	0.41
5:SB:124:HIS:HA	5:SB:137:LEU:O	2.21	0.41
6:SA:130:ASP:O	6:SA:133:PRO:HD2	2.21	0.41
9:SE:205:PHE:HD2	9:SE:221:ARG:CZ	2.34	0.41
11:SG:12:CYS:SG	11:SG:127:THR:HG23	2.61	0.41
12:SF:78:MET:HB2	12:SF:159:ARG:CZ	2.51	0.41
14:SW:44:HIS:NE2	14:SW:112:ASP:OD2	2.51	0.41
14:SW:46:TYR:HB3	14:SW:69:LEU:HD13	2.02	0.41
27:SP:53:GLN:HG3	27:SP:83:MET:SD	2.60	0.41
29:SV:38:GLU:HB2	29:SV:49:GLN:O	2.20	0.41
30:SY:28:LEU:HD13	30:SY:68:LYS:HB2	2.02	0.41
30:SY:45:ALA:HB1	30:SY:50:THR:O	2.21	0.41
30:SY:77:ASP:HB2	30:SY:81:TYR:HD2	1.85	0.41
37:Sg:165:ILE:CG2	37:Sg:177:TRP:HB2	2.51	0.41
39:LA:180:LEU:HD22	82:Lp:18:TYR:HB3	2.03	0.41
42:LJ:91:GLU:HG2	42:LJ:91:GLU:O	2.21	0.41
46:Lq:47:LEU:HD21	46:Lq:101:MET:HE1	2.02	0.41
48:LO:27:VAL:HA	48:LO:30:GLY:O	2.20	0.41
50:LV:72:LEU:HD21	50:LV:113:LYS:HE2	2.03	0.41
56:LQ:154:LYS:O	56:LQ:163:THR:OG1	2.31	0.41
58:LS:96:GLU:HB3	58:LS:142:VAL:HG21	2.02	0.41
65:LZ:22:LYS:NZ	65:LZ:129:TRP:O	2.50	0.41
67:Lh:52:LYS:HA	67:Lh:52:LYS:HD3	1.85	0.41
84:At:30:G:H3'	84:At:31:A:C8	2.56	0.41
84:At:45:U:H3'	84:At:46:G7M:H5''	2.02	0.41
85:Pt:11:A:H2'	85:Pt:12:G:C8	2.56	0.41
86:EF:66:GLU:CD	86:EF:73:ILE:H	2.29	0.41
86:EF:253:VAL:HG21	86:EF:320:VAL:HG23	2.03	0.41
86:EF:261:THR:HG23	86:EF:317:VAL:HA	2.02	0.41
1:S2:1643:PSU:H2'	1:S2:1644:C:C6	2.56	0.41
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.56	0.41
3:L5:1241:C:H2'	3:L5:1242:G:C8	2.56	0.41
3:L5:1471:U:H2'	3:L5:1472:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.56	0.41
3:L5:1812:C:H5''	68:Lb:56:LYS:HE2	2.03	0.41
3:L5:1883:G:O6	3:L5:1896:A:H2	2.04	0.41
3:L5:2486:G:H4'	3:L5:2487:G:H5'	2.03	0.41
3:L5:2558:C:H2'	3:L5:2559:G:C8	2.56	0.41
3:L5:3706:C:H2'	3:L5:3707:U:O4'	2.21	0.41
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.88	0.41
3:L5:4240:G:H2'	3:L5:4241:C:O4'	2.21	0.41
3:L5:4323:A:H2'	3:L5:4324:A:O4'	2.21	0.41
3:L5:4653:C:H2'	3:L5:4654:C:H6	1.86	0.41
17:SU:64:THR:HA	17:SU:78:ASP:O	2.21	0.41
47:LK:108:GLU:H	47:LK:108:GLU:HG2	1.72	0.41
54:LI:76:MET:O	54:LI:80:CYS:HB2	2.20	0.41
60:LP:131:ARG:HG3	60:LP:137:ASN:ND2	2.36	0.41
1:S2:655:A:C8	1:S2:657:U:H2'	2.55	0.40
1:S2:912:C:C2	1:S2:914:U:H1'	2.57	0.40
2:L8:103:A:N3	3:L5:21:G:H1'	2.35	0.40
3:L5:163:A:H2'	3:L5:164:G:C8	2.56	0.40
3:L5:1471:U:H2'	3:L5:1472:C:H6	1.86	0.40
3:L5:2366:A:H2'	3:L5:2367:A:H5''	2.03	0.40
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.56	0.40
3:L5:3663:A:O2'	3:L5:3664:G:H5'	2.21	0.40
3:L5:3845:A:O3'	3:L5:4668:U:H4'	2.21	0.40
3:L5:4340:U:N3	91:L5:5117:3H3:O3	2.50	0.40
3:L5:4618:OMG:H5''	50:LV:15:ARG:HB2	2.02	0.40
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.56	0.40
5:SB:23:ASP:O	5:SB:26:SER:OG	2.34	0.40
7:SD:16:ILE:HG21	23:Sd:22:ARG:NH1	2.31	0.40
10:SC:73:MET:HE3	10:SC:73:MET:HB3	1.90	0.40
16:SQ:11:GLN:HE21	16:SQ:71:ARG:HH12	1.69	0.40
20:SX:57:VAL:CG1	20:SX:116:PRO:HD2	2.51	0.40
37:Sg:72:SER:OG	37:Sg:74:ASP:OD1	2.29	0.40
38:Lz:86:ASP:HB2	38:Lz:88:GLU:OE1	2.22	0.40
41:LC:252:TRP:CH2	41:LC:260:LEU:HD11	2.56	0.40
51:LM:11:ARG:NH1	51:LM:58:THR:O	2.54	0.40
56:LQ:49:LYS:HE2	56:LQ:49:LYS:HB3	1.77	0.40
70:Lc:21:VAL:HG22	70:Lc:99:PRO:O	2.21	0.40
86:EF:237:PRO:HA	86:EF:238:PRO:HD3	1.97	0.40
1:S2:354:OMU:HM22	1:S2:355:G:O4'	2.21	0.40
1:S2:503:C:H6	1:S2:503:C:H2'	1.72	0.40
1:S2:1609:C:OP1	22:SS:131:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1851:MA6:H5''	1:S2:1851:MA6:H8	2.03	0.40
3:L5:1266:G:O6	68:Lb:91:ARG:HB2	2.21	0.40
3:L5:1440:U:H2'	3:L5:1441:C:C6	2.56	0.40
3:L5:3700:C:H2'	3:L5:3746:A:H61	1.86	0.40
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.56	0.40
3:L5:4384:U:O3'	3:L5:4385:A:H3'	2.22	0.40
7:SD:173:ARG:HD3	7:SD:173:ARG:HA	1.92	0.40
10:SC:126:ALA:O	10:SC:141:VAL:HA	2.21	0.40
11:SG:23:LYS:HG3	11:SG:40:ALA:O	2.21	0.40
12:SF:142:SER:HB3	34:Sc:50:VAL:HG22	2.03	0.40
13:SH:164:ASN:OD1	13:SH:165:ASN:N	2.54	0.40
36:Sf:103:LEU:HD13	36:Sf:105:TYR:CD2	2.56	0.40
38:Lz:25:ARG:HH11	38:Lz:212:LYS:HZ2	1.70	0.40
50:LV:112:MET:HE1	50:LV:117:ILE:CG1	2.51	0.40
52:La:98:ALA:HB2	52:La:121:PRO:HB2	2.03	0.40
58:LS:82:LEU:C	58:LS:127:MET:HE2	2.46	0.40
62:LX:151:ASN:OD1	62:LX:156:ILE:HD13	2.21	0.40
86:EF:103:ILE:HA	86:EF:106:THR:HG22	2.03	0.40
86:EF:429:MET:SD	86:EF:429:MET:O	2.79	0.40
1:S2:118:C:H2'	1:S2:119:PSU:O4'	2.20	0.40
1:S2:523:A:OP2	8:SJ:38:ARG:HD3	2.21	0.40
1:S2:1831:A:N6	1:S2:1832:6MZ:H9	2.36	0.40
3:L5:76:A:OP2	49:LL:74:ARG:NH1	2.54	0.40
3:L5:79:C:H2'	3:L5:80:C:C6	2.56	0.40
3:L5:1287:G:C2	44:LE:132:PRO:HG3	2.57	0.40
3:L5:1919:G:H4'	58:LS:163:HIS:CD2	2.57	0.40
3:L5:1993:C:H2'	3:L5:1994:C:C6	2.56	0.40
3:L5:3615:G:C4	64:LW:49:ILE:HD12	2.56	0.40
3:L5:3661:G:N7	39:LA:152:SER:OG	2.52	0.40
3:L5:4065:G:H2'	3:L5:4066:U:C6	2.57	0.40
3:L5:4420:PSU:H2'	3:L5:4421:C:C6	2.56	0.40
3:L5:4977:A:H2'	3:L5:4978:G:O4'	2.21	0.40
21:SM:99:LYS:HB2	21:SM:100:PRO:HD2	2.04	0.40
22:SS:86:ARG:HE	22:SS:89:ASP:CG	2.29	0.40
26:SR:20:TYR:O	26:SR:24:LEU:HG	2.22	0.40
28:ST:30:VAL:HG22	28:ST:53:PHE:CD2	2.56	0.40
36:Sf:118:ARG:HB2	36:Sf:131:PHE:HD2	1.87	0.40
37:Sg:114:SER:HB3	37:Sg:119:GLN:HB2	2.02	0.40
37:Sg:265:ILE:HD12	37:Sg:265:ILE:HA	1.95	0.40
38:Lz:185:LEU:HD23	38:Lz:185:LEU:HA	1.90	0.40
42:LJ:49:VAL:HG23	42:LJ:71:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:LK:14:TYR:CE2	47:LK:61:LYS:HD3	2.56	0.40
49:LL:232:ILE:HD11	52:La:98:ALA:HB3	2.03	0.40
51:LM:41:PRO:HB3	51:LM:70:GLN:HE21	1.86	0.40
57:LR:89:MET:HE3	57:LR:90:PRO:HD2	2.02	0.40
57:LR:181:LYS:HE3	57:LR:185:ILE:HD11	2.03	0.40
65:LZ:67:LYS:HB3	65:LZ:67:LYS:HE2	1.77	0.40
85:Pt:62:C:H2'	85:Pt:63:C:H6	1.87	0.40
85:Pt:73:A:H2'	85:Pt:74:A:C8	2.57	0.40
1:S2:1521:C:OP1	22:SS:129:LEU:HD13	2.21	0.40
3:L5:178:C:H6	3:L5:178:C:H2'	1.69	0.40
3:L5:434:A:H2'	3:L5:435:A:O4'	2.21	0.40
3:L5:4107:G:H3'	3:L5:4107:G:N3	2.37	0.40
3:L5:4637:OMG:H1'	3:L5:4637:OMG:HM23	1.69	0.40
3:L5:4773:C:H42	3:L5:4861:G:H1	1.70	0.40
3:L5:4861:G:H2'	3:L5:4862:G:H8	1.87	0.40
3:L5:4906:C:H2'	3:L5:4907:G:C8	2.57	0.40
3:L5:4941:G:OP1	44:LE:219:LYS:HG3	2.22	0.40
3:L5:5024:C:H2'	3:L5:5025:C:H4'	2.03	0.40
4:L7:1:G:H2'	4:L7:2:U:O4'	2.21	0.40
6:SA:122:LEU:HD21	6:SA:124:VAL:HG13	2.03	0.40
9:SE:75:LYS:HB3	9:SE:75:LYS:HE2	1.88	0.40
15:SI:35:ASN:HB3	15:SI:37:LYS:NZ	2.36	0.40
24:SN:87:ASP:OD1	24:SN:87:ASP:N	2.55	0.40
25:SL:47:PRO:HB2	25:SL:49:GLU:OE1	2.21	0.40
38:Lz:94:ASN:OD1	38:Lz:95:LYS:N	2.51	0.40
44:LE:144:ILE:HG12	44:LE:196:ALA:HB2	2.04	0.40
46:Lq:97:GLU:HG2	46:Lq:98:ILE:N	2.36	0.40
54:LI:69:ARG:HA	54:LI:136:MET:HE1	2.03	0.40
58:LS:29:ARG:NH1	59:LT:148:PRO:O	2.54	0.40
58:LS:29:ARG:NH2	59:LT:150:LEU:HB2	2.37	0.40
59:LT:84:ILE:HG22	68:Lb:24:PRO:HD3	2.04	0.40
81:Lo:2:VAL:N	81:Lo:90:HIS:O	2.54	0.40
84:At:8:4SU:H6	84:At:8:4SU:O5'	2.21	0.40
1:S2:65:C:C6	11:SG:174:PRO:HB3	2.56	0.40
1:S2:172:OMU:O2	1:S2:314:U:H1'	2.21	0.40
3:L5:49:U:H2'	3:L5:50:C:H6	1.86	0.40
3:L5:268:G:H2'	3:L5:269:G:C8	2.56	0.40
3:L5:327:U:O2'	75:Li:30:ARG:HD3	2.21	0.40
3:L5:1094:G:H2'	3:L5:1095:A:H8	1.86	0.40
3:L5:1241:C:C6	68:Lb:115:GLY:HA2	2.56	0.40
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1528:U:H2'	3:L5:1529:G:C8	2.57	0.40
3:L5:1804:A:O4'	3:L5:1806:G:C8	2.74	0.40
3:L5:4149:C:H2'	3:L5:4150:G:O4'	2.22	0.40
16:SQ:86:GLN:HE22	16:SQ:122:ALA:HA	1.85	0.40
19:SO:117:ARG:HH12	32:Sa:48:ALA:HB1	1.85	0.40
22:SS:9:PHE:CZ	22:SS:57:GLY:HA3	2.57	0.40
28:ST:21:PHE:CD2	28:ST:134:ILE:HD11	2.56	0.40
48:LO:74:ARG:O	48:LO:142:ALA:HB1	2.22	0.40
54:LI:86:HIS:HB3	54:LI:139:ARG:CG	2.52	0.40
56:LQ:17:GLU:HG3	56:LQ:18:PRO:O	2.22	0.40
63:LY:62:TYR:CG	63:LY:85:VAL:HG13	2.57	0.40
68:Lb:15:LYS:HB3	68:Lb:15:LYS:HE2	1.90	0.40
69:LF:148:LYS:O	69:LF:152:GLU:HG3	2.21	0.40
77:Lk:24:LYS:HD3	77:Lk:69:LEU:HD21	2.03	0.40
79:Lm:99:CYS:HB2	79:Lm:114:LYS:HD2	2.02	0.40
84:At:8:4SU:H5''	84:At:49:C:H5'	2.03	0.40
94:At:77:PHE:HA	86:EF:264:VAL:CG2	2.51	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%)	214 (98%)	5 (2%)	0	100	100
6	SA	220/295 (75%)	214 (97%)	6 (3%)	0	100	100
7	SD	224/243 (92%)	219 (98%)	4 (2%)	1 (0%)	30	39
8	SJ	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
9	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
10	SC	220/293 (75%)	216 (98%)	4 (2%)	0	100	100
11	SG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	SF	187/204 (92%)	175 (94%)	12 (6%)	0	100	100
13	SH	187/194 (96%)	178 (95%)	9 (5%)	0	100	100
14	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
15	SI	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
16	SQ	139/146 (95%)	137 (99%)	2 (1%)	0	100	100
17	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
18	SK	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
19	SO	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
20	SX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
21	SM	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
22	SS	146/152 (96%)	139 (95%)	6 (4%)	1 (1%)	18	25
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	141/158 (89%)	133 (94%)	8 (6%)	0	100	100
26	SR	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
27	SP	126/145 (87%)	117 (93%)	9 (7%)	0	100	100
28	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
29	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
30	SY	129/133 (97%)	124 (96%)	5 (4%)	0	100	100
31	SZ	82/125 (66%)	78 (95%)	4 (5%)	0	100	100
32	Sa	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
33	Sb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
35	Se	47/133 (35%)	47 (100%)	0	0	100	100
36	Sf	61/156 (39%)	55 (90%)	5 (8%)	1 (2%)	7	9
37	Sg	311/317 (98%)	290 (93%)	21 (7%)	0	100	100
38	Lz	215/217 (99%)	187 (87%)	28 (13%)	0	100	100
39	LA	249/257 (97%)	239 (96%)	10 (4%)	0	100	100
40	LB	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
41	LC	366/427 (86%)	361 (99%)	5 (1%)	0	100	100
42	LJ	167/178 (94%)	166 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
44	LE	217/288 (75%)	210 (97%)	7 (3%)	0	100	100
45	LG	237/266 (89%)	227 (96%)	9 (4%)	1 (0%)	30	39
46	Lq	194/317 (61%)	181 (93%)	13 (7%)	0	100	100
47	LK	145/165 (88%)	131 (90%)	14 (10%)	0	100	100
48	LO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
49	LL	204/270 (76%)	196 (96%)	8 (4%)	0	100	100
50	LV	131/140 (94%)	129 (98%)	2 (2%)	0	100	100
51	LM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
52	La	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	25
53	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
54	LI	204/214 (95%)	193 (95%)	11 (5%)	0	100	100
55	LD	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
56	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
57	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
58	LS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
59	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
60	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
61	LU	97/128 (76%)	90 (93%)	7 (7%)	0	100	100
62	LX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
63	LY	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
64	LW	113/157 (72%)	111 (98%)	2 (2%)	0	100	100
65	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
66	Lr	123/137 (90%)	117 (95%)	6 (5%)	0	100	100
67	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
68	Lb	104/159 (65%)	99 (95%)	5 (5%)	0	100	100
69	LF	223/248 (90%)	215 (96%)	8 (4%)	0	100	100
70	Lc	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
71	Ld	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
72	Le	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
73	Lf	107/110 (97%)	107 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Li	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
76	Lj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
77	Lk	67/70 (96%)	67 (100%)	0	0	100	100
78	Ll	48/51 (94%)	48 (100%)	0	0	100	100
79	Lm	49/128 (38%)	49 (100%)	0	0	100	100
80	Ln	23/25 (92%)	23 (100%)	0	0	100	100
81	Lo	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
82	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
86	EF	437/462 (95%)	413 (94%)	24 (6%)	0	100	100
All	All	12269/13982 (88%)	11858 (97%)	406 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	La	15	VAL
7	SD	157	MET
22	SS	92	ASP
36	Sf	97	LYS
45	LG	132	ARG

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%)	201 (100%)	1 (0%)	81	88
6	SA	183/242 (76%)	179 (98%)	4 (2%)	45	64
7	SD	189/202 (94%)	183 (97%)	6 (3%)	34	51
8	SJ	161/168 (96%)	161 (100%)	0	100	100
9	SE	224/225 (100%)	221 (99%)	3 (1%)	61	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	SC	188/225 (84%)	186 (99%)	2 (1%)	65	79
11	SG	207/218 (95%)	205 (99%)	2 (1%)	68	80
12	SF	159/170 (94%)	159 (100%)	0	100	100
13	SH	168/174 (97%)	165 (98%)	3 (2%)	51	70
14	SW	112/113 (99%)	112 (100%)	0	100	100
15	SI	178/180 (99%)	177 (99%)	1 (1%)	78	87
16	SQ	117/121 (97%)	116 (99%)	1 (1%)	70	82
17	SU	93/107 (87%)	90 (97%)	3 (3%)	34	51
18	SK	87/136 (64%)	86 (99%)	1 (1%)	65	79
19	SO	105/119 (88%)	104 (99%)	1 (1%)	68	80
20	SX	113/114 (99%)	113 (100%)	0	100	100
21	SM	102/108 (94%)	100 (98%)	2 (2%)	48	67
22	SS	128/132 (97%)	125 (98%)	3 (2%)	44	62
23	Sd	48/49 (98%)	48 (100%)	0	100	100
24	SN	131/131 (100%)	131 (100%)	0	100	100
25	SL	131/142 (92%)	131 (100%)	0	100	100
26	SR	121/122 (99%)	120 (99%)	1 (1%)	73	84
27	SP	114/130 (88%)	113 (99%)	1 (1%)	70	82
28	ST	113/115 (98%)	111 (98%)	2 (2%)	51	70
29	SV	66/66 (100%)	66 (100%)	0	100	100
30	SY	113/115 (98%)	107 (95%)	6 (5%)	20	31
31	SZ	74/103 (72%)	73 (99%)	1 (1%)	59	75
32	Sa	86/98 (88%)	85 (99%)	1 (1%)	63	78
33	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	76
34	Sc	57/62 (92%)	57 (100%)	0	100	100
35	Se	41/104 (39%)	41 (100%)	0	100	100
36	Sf	56/140 (40%)	50 (89%)	6 (11%)	6	7
37	Sg	272/275 (99%)	260 (96%)	12 (4%)	25	38
38	Lz	195/196 (100%)	195 (100%)	0	100	100
39	LA	193/198 (98%)	192 (100%)	1 (0%)	81	88
40	LB	347/348 (100%)	347 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	LC	306/348 (88%)	303 (99%)	3 (1%)	68	80
42	LJ	143/149 (96%)	140 (98%)	3 (2%)	47	66
43	LH	169/171 (99%)	169 (100%)	0	100	100
44	LE	196/252 (78%)	195 (100%)	1 (0%)	81	88
45	LG	201/223 (90%)	199 (99%)	2 (1%)	68	80
46	Lq	164/258 (64%)	157 (96%)	7 (4%)	26	39
47	LK	122/137 (89%)	119 (98%)	3 (2%)	42	60
48	LO	171/174 (98%)	170 (99%)	1 (1%)	78	87
49	LL	172/224 (77%)	167 (97%)	5 (3%)	37	55
50	LV	102/107 (95%)	101 (99%)	1 (1%)	68	80
51	LM	116/161 (72%)	116 (100%)	0	100	100
52	La	119/120 (99%)	118 (99%)	1 (1%)	73	84
53	LN	171/172 (99%)	169 (99%)	2 (1%)	63	78
54	LI	177/181 (98%)	177 (100%)	0	100	100
55	LD	247/250 (99%)	245 (99%)	2 (1%)	73	84
56	LQ	164/165 (99%)	164 (100%)	0	100	100
57	LR	166/175 (95%)	161 (97%)	5 (3%)	36	53
58	LS	157/157 (100%)	157 (100%)	0	100	100
59	LT	139/140 (99%)	139 (100%)	0	100	100
60	LP	134/163 (82%)	134 (100%)	0	100	100
61	LU	89/115 (77%)	89 (100%)	0	100	100
62	LX	106/133 (80%)	106 (100%)	0	100	100
63	LY	124/135 (92%)	123 (99%)	1 (1%)	73	84
64	LW	94/126 (75%)	91 (97%)	3 (3%)	34	51
65	LZ	117/118 (99%)	112 (96%)	5 (4%)	26	39
66	Lr	108/120 (90%)	107 (99%)	1 (1%)	70	82
67	Lh	109/110 (99%)	109 (100%)	0	100	100
68	Lb	89/125 (71%)	86 (97%)	3 (3%)	32	48
69	LF	194/215 (90%)	194 (100%)	0	100	100
70	Lc	83/97 (86%)	80 (96%)	3 (4%)	31	46
71	Ld	98/110 (89%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	Le	114/121 (94%)	111 (97%)	3 (3%)	40	59
73	Lf	88/89 (99%)	88 (100%)	0	100	100
74	Lg	98/100 (98%)	98 (100%)	0	100	100
75	Li	86/89 (97%)	84 (98%)	2 (2%)	44	62
76	Lj	73/80 (91%)	73 (100%)	0	100	100
77	Lk	64/65 (98%)	62 (97%)	2 (3%)	35	53
78	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	39
79	Lm	47/115 (41%)	47 (100%)	0	100	100
80	Ln	24/24 (100%)	24 (100%)	0	100	100
81	Lo	91/93 (98%)	90 (99%)	1 (1%)	65	79
82	Lp	74/75 (99%)	74 (100%)	0	100	100
86	EF	363/375 (97%)	354 (98%)	9 (2%)	42	60
All	All	10665/11860 (90%)	10529 (99%)	136 (1%)	59	76

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SB	86	LEU
6	SA	89	LYS
6	SA	174	MET
6	SA	190	SER
6	SA	191	ARG
7	SD	29	LEU
7	SD	32	ASP
7	SD	55	THR
7	SD	58	VAL
7	SD	156	LEU
7	SD	166	TYR
9	SE	24	THR
9	SE	115	THR
9	SE	173	ILE
10	SC	91	SER
10	SC	187	ARG
11	SG	147	LEU
11	SG	185	LEU
13	SH	109	ARG
13	SH	112	ASN
13	SH	137	SER

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Mol	Chain	Res	Type
15	SI	136	ILE
16	SQ	8	GLN
17	SU	20	ILE
17	SU	29	VAL
17	SU	115	THR
18	SK	58	VAL
19	SO	88	LEU
21	SM	31	LEU
21	SM	91	LEU
22	SS	16	LEU
22	SS	59	LEU
22	SS	67	VAL
26	SR	109	LEU
27	SP	21	ASP
28	ST	38	LYS
28	ST	131	LEU
30	SY	23	MET
30	SY	38	THR
30	SY	44	LEU
30	SY	117	VAL
30	SY	120	THR
30	SY	122	LYS
31	SZ	54	THR
32	Sa	63	VAL
33	Sb	74	THR
36	Sf	108	VAL
36	Sf	138	ARG
36	Sf	140	TYR
36	Sf	143	LYS
36	Sf	144	CYS
36	Sf	146	LEU
37	Sg	19	THR
37	Sg	45	LEU
37	Sg	46	THR
37	Sg	51	ASN
37	Sg	54	ILE
37	Sg	67	SER
37	Sg	129	ILE
37	Sg	197	THR
37	Sg	198	VAL
37	Sg	206	LEU
37	Sg	227	LEU

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Mol	Chain	Res	Type
37	Sg	239	LEU
39	LA	208	GLU
41	LC	62	THR
41	LC	269	LYS
41	LC	278	ASN
42	LJ	39	VAL
42	LJ	40	LEU
42	LJ	161	GLU
44	LE	278	THR
45	LG	74	LEU
45	LG	121	LYS
46	Lq	30	VAL
46	Lq	35	VAL
46	Lq	41	GLN
46	Lq	54	LEU
46	Lq	61	MET
46	Lq	86	VAL
46	Lq	112	ARG
47	LK	80	LEU
47	LK	123	ARG
47	LK	131	GLU
48	LO	61	ARG
49	LL	67	HIS
49	LL	136	LYS
49	LL	138	ASP
49	LL	146	LEU
49	LL	227	GLU
50	LV	48	ARG
52	La	16	SER
53	LN	182	HIS
53	LN	188	ARG
55	LD	123	VAL
55	LD	200	MET
57	LR	177	LEU
57	LR	181	LYS
57	LR	183	GLU
57	LR	187	THR
57	LR	188	LEU
63	LY	46	SER
64	LW	30	GLN
64	LW	83	THR
64	LW	87	LEU

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Mol	Chain	Res	Type
65	LZ	29	ILE
65	LZ	31	ASP
65	LZ	73	LYS
65	LZ	88	ASP
65	LZ	100	VAL
66	Lr	26	SER
68	Lb	38	LYS
68	Lb	40	LEU
68	Lb	50	ASN
70	Lc	28	VAL
70	Lc	94	LEU
70	Lc	104	ILE
72	Le	102	ASN
72	Le	123	THR
72	Le	129	LEU
75	Li	25	ARG
75	Li	29	ARG
77	Lk	57	LYS
77	Lk	60	LEU
78	Ll	17	GLN
78	Ll	47	THR
81	Lo	82	MET
86	EF	75	ILE
86	EF	77	LEU
86	EF	81	GLU
86	EF	228	LEU
86	EF	229	LEU
86	EF	316	SER
86	EF	317	VAL
86	EF	320	VAL
86	EF	343	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
6	SA	29	ASN
6	SA	84	GLN
6	SA	113	GLN
7	SD	159	HIS
7	SD	226	GLN
9	SE	67	GLN
9	SE	98	ASN

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Mol	Chain	Res	Type
9	SE	201	HIS
9	SE	209	HIS
9	SE	260	GLN
10	SC	136	HIS
11	SG	155	GLN
12	SF	29	GLN
13	SH	68	GLN
13	SH	114	GLN
14	SW	15	ASN
14	SW	24	GLN
15	SI	84	ASN
15	SI	111	GLN
15	SI	146	GLN
16	SQ	8	GLN
16	SQ	97	GLN
17	SU	92	HIS
18	SK	32	HIS
20	SX	16	HIS
20	SX	92	ASN
21	SM	119	GLN
22	SS	135	HIS
23	Sd	37	ASN
24	SN	36	GLN
24	SN	58	HIS
24	SN	62	GLN
25	SL	11	GLN
25	SL	39	ASN
25	SL	94	HIS
26	SR	29	HIS
26	SR	56	HIS
26	SR	118	GLN
28	ST	12	GLN
28	ST	51	ASN
28	ST	83	GLN
28	ST	126	GLN
28	ST	137	GLN
29	SV	29	HIS
30	SY	19	GLN
35	Se	132	ASN
37	Sg	311	GLN
38	Lz	35	GLN
38	Lz	73	HIS

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Mol	Chain	Res	Type
38	Lz	197	ASN
40	LB	109	HIS
40	LB	203	GLN
40	LB	213	GLN
41	LC	43	ASN
41	LC	61	GLN
41	LC	278	ASN
41	LC	310	HIS
41	LC	321	ASN
41	LC	338	ASN
42	LJ	23	ASN
42	LJ	46	GLN
42	LJ	71	HIS
42	LJ	97	ASN
43	LH	140	GLN
43	LH	156	ASN
44	LE	284	HIS
45	LG	208	ASN
46	Lq	12	ASN
46	Lq	71	ASN
46	Lq	81	HIS
47	LK	66	ASN
47	LK	142	ASN
48	LO	50	ASN
49	LL	222	ASN
51	LM	33	GLN
51	LM	125	ASN
51	LM	131	GLN
52	La	14	HIS
53	LN	109	HIS
54	LI	147	HIS
56	LQ	21	GLN
57	LR	141	HIS
58	LS	125	GLN
59	LT	90	ASN
59	LT	112	ASN
60	LP	21	ASN
60	LP	25	HIS
62	LX	57	GLN
62	LX	73	HIS
63	LY	18	HIS
63	LY	127	GLN

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Mol	Chain	Res	Type
64	LW	30	GLN
64	LW	50	ASN
64	LW	95	ASN
64	LW	120	GLN
66	Lr	6	GLN
67	Lh	65	GLN
67	Lh	98	HIS
67	Lh	107	GLN
68	Lb	42	ASN
69	LF	119	ASN
69	LF	192	HIS
70	Lc	50	ASN
70	Lc	72	HIS
71	Ld	93	ASN
71	Ld	116	ASN
71	Ld	121	ASN
72	Le	23	HIS
72	Le	52	GLN
73	Lf	20	ASN
73	Lf	21	GLN
76	Lj	48	ASN
76	Lj	57	ASN
78	Ll	17	GLN
78	Ll	25	GLN
81	Lo	45	GLN
86	EF	9	ASN
86	EF	26	HIS
86	EF	147	GLN
86	EF	164	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1648/1869 (88%)	327 (19%)	28 (1%)
2	L8	155/156 (99%)	25 (16%)	1 (0%)
3	L5	3621/5069 (71%)	642 (17%)	54 (1%)
4	L7	119/120 (99%)	12 (10%)	0
83	mR	8/60 (13%)	2 (25%)	0
84	At	75/76 (98%)	24 (32%)	0
85	Pt	76/77 (98%)	16 (21%)	0
All	All	5702/7427 (76%)	1048 (18%)	83 (1%)

All (1048) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	17	C
1	S2	23	G
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	44	U
1	S2	45	A
1	S2	46	A
1	S2	49	C
1	S2	55	U
1	S2	56	G
1	S2	59	U
1	S2	65	C
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	74	G
1	S2	75	G
1	S2	103	A
1	S2	110	U
1	S2	113	G
1	S2	114	G
1	S2	115	U
1	S2	126	G
1	S2	127	C
1	S2	140	C
1	S2	141	A
1	S2	143	U
1	S2	155	G
1	S2	161	U
1	S2	162	C
1	S2	170	A
1	S2	171	A
1	S2	172	OMU
1	S2	173	A
1	S2	175	A
1	S2	178	C
1	S2	183	G
1	S2	184	G
1	S2	215	G
1	S2	302	A
1	S2	307	G

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Mol	Chain	Res	Type
1	S2	309	G
1	S2	312	G
1	S2	319	C
1	S2	320	G
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	335	G
1	S2	347	G
1	S2	350	C
1	S2	362	C
1	S2	364	A
1	S2	370	G
1	S2	371	A
1	S2	382	C
1	S2	385	G
1	S2	386	C
1	S2	400	C
1	S2	409	C
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	465	A
1	S2	466	G
1	S2	467	G
1	S2	471	G
1	S2	472	C
1	S2	474	G
1	S2	482	G
1	S2	483	C
1	S2	487	U
1	S2	492	C
1	S2	493	A
1	S2	496	C

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Mol	Chain	Res	Type
1	S2	500	A
1	S2	501	C
1	S2	504	G
1	S2	516	A
1	S2	517	OMC
1	S2	525	A
1	S2	533	A
1	S2	534	G
1	S2	535	G
1	S2	554	A
1	S2	555	A
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	563	G
1	S2	564	A
1	S2	568	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	606	G
1	S2	607	U
1	S2	614	C
1	S2	617	G
1	S2	628	A
1	S2	629	A
1	S2	632	C
1	S2	636	C
1	S2	638	C
1	S2	643	A
1	S2	644	OMG
1	S2	655	A
1	S2	660	C
1	S2	664	A
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G

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Mol	Chain	Res	Type
1	S2	679	A
1	S2	688	U
1	S2	689	U
1	S2	690	G
1	S2	821	G
1	S2	822	PSU
1	S2	827	A
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	841	G
1	S2	847	A
1	S2	850	C
1	S2	861	A
1	S2	870	A
1	S2	873	G
1	S2	878	G
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	905	C
1	S2	913	A
1	S2	916	A
1	S2	920	A
1	S2	922	A
1	S2	929	G
1	S2	930	C
1	S2	933	G
1	S2	954	U
1	S2	971	G
1	S2	978	G
1	S2	981	A
1	S2	986	G
1	S2	990	A
1	S2	992	A
1	S2	1001	A
1	S2	1016	U

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Mol	Chain	Res	Type
1	S2	1017	U
1	S2	1023	A
1	S2	1026	C
1	S2	1045	U
1	S2	1047	C
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1071	G
1	S2	1083	A
1	S2	1085	C
1	S2	1116	C
1	S2	1121	G
1	S2	1133	A
1	S2	1138	C
1	S2	1151	G
1	S2	1153	C
1	S2	1154	U
1	S2	1157	G
1	S2	1165	G
1	S2	1166	G
1	S2	1192	U
1	S2	1195	A
1	S2	1207	G
1	S2	1208	A
1	S2	1212	G
1	S2	1215	C
1	S2	1216	C
1	S2	1221	G
1	S2	1224	G
1	S2	1227	G
1	S2	1229	G
1	S2	1242	U
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1274	G
1	S2	1275	G
1	S2	1278	A
1	S2	1285	G

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Mol	Chain	Res	Type
1	S2	1286	G
1	S2	1292	C
1	S2	1294	G
1	S2	1300	U
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1304	U
1	S2	1307	U
1	S2	1308	U
1	S2	1312	G
1	S2	1313	A
1	S2	1318	G
1	S2	1321	G
1	S2	1324	G
1	S2	1330	G
1	S2	1348	G
1	S2	1358	U
1	S2	1368	U
1	S2	1371	U
1	S2	1372	U
1	S2	1373	C
1	S2	1375	G
1	S2	1378	A
1	S2	1395	C
1	S2	1397	U
1	S2	1402	A
1	S2	1404	U
1	S2	1406	G
1	S2	1408	U
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1439	A

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Mol	Chain	Res	Type
1	S2	1442	OMU
1	S2	1447	OMG
1	S2	1452	A
1	S2	1454	A
1	S2	1462	U
1	S2	1463	U
1	S2	1477	U
1	S2	1487	A
1	S2	1489	A
1	S2	1490	OMG
1	S2	1494	U
1	S2	1495	G
1	S2	1496	U
1	S2	1497	G
1	S2	1498	A
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1519	U
1	S2	1520	G
1	S2	1521	C
1	S2	1533	A
1	S2	1550	G
1	S2	1552	G
1	S2	1553	C
1	S2	1558	C
1	S2	1560	U
1	S2	1574	C
1	S2	1575	G
1	S2	1580	A
1	S2	1581	C
1	S2	1587	G
1	S2	1588	A
1	S2	1601	A
1	S2	1620	A
1	S2	1621	U
1	S2	1623	A
1	S2	1638	G
1	S2	1641	A
1	S2	1648	G
1	S2	1654	G
1	S2	1656	G

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Mol	Chain	Res	Type
1	S2	1661	A
1	S2	1664	A
1	S2	1665	G
1	S2	1671	G
1	S2	1679	A
1	S2	1680	G
1	S2	1686	G
1	S2	1695	A
1	S2	1698	C
1	S2	1721	U
1	S2	1722	G
1	S2	1726	G
1	S2	1733	U
1	S2	1744	G
1	S2	1782	G
1	S2	1783	C
1	S2	1787	G
1	S2	1797	U
1	S2	1819	A
1	S2	1825	A
1	S2	1826	G
1	S2	1829	G
1	S2	1831	A
1	S2	1835	A
1	S2	1837	G
1	S2	1838	U
1	S2	1849	G
1	S2	1851	MA6
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1865	C
1	S2	1867	U
2	L8	23	C
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	77	A

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Mol	Chain	Res	Type
2	L8	80	A
2	L8	81	C
2	L8	85	U
2	L8	86	U
2	L8	87	G
2	L8	93	C
2	L8	103	A
2	L8	104	A
2	L8	105	C
2	L8	110	U
2	L8	114	G
2	L8	123	U
2	L8	124	U
2	L8	125	C
2	L8	147	G
2	L8	153	C
3	L5	19	G
3	L5	25	A
3	L5	33	A
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	72	C
3	L5	85	G
3	L5	91	G
3	L5	95	G
3	L5	98	A
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	112	C
3	L5	119	G
3	L5	120	A
3	L5	132	G
3	L5	134	G
3	L5	135	G
3	L5	136	C
3	L5	140	G

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Mol	Chain	Res	Type
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	188	G
3	L5	190	G
3	L5	200	U
3	L5	201	C
3	L5	207	G
3	L5	210	C
3	L5	216	C
3	L5	219	G
3	L5	220	C
3	L5	233	U
3	L5	234	G
3	L5	241	G
3	L5	253	G
3	L5	266	C
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	326	C
3	L5	340	C
3	L5	345	C
3	L5	347	A
3	L5	349	A
3	L5	373	G
3	L5	387	G
3	L5	388	A
3	L5	409	G
3	L5	410	A
3	L5	412	G
3	L5	413	G
3	L5	417	G
3	L5	418	A
3	L5	432	U
3	L5	433	A

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Mol	Chain	Res	Type
3	L5	449	C
3	L5	450	G
3	L5	451	C
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	463	A
3	L5	484	U
3	L5	485	C
3	L5	487	G
3	L5	498	C
3	L5	499	G
3	L5	504	G
3	L5	507	G
3	L5	509	A
3	L5	513	U
3	L5	514	U
3	L5	518	G
3	L5	646	G
3	L5	654	C
3	L5	655	C
3	L5	659	G
3	L5	661	C
3	L5	662	C
3	L5	664	G
3	L5	666	G
3	L5	667	A
3	L5	669	C
3	L5	685	C
3	L5	686	A
3	L5	692	A
3	L5	695	G
3	L5	696	C
3	L5	704	C
3	L5	708	G
3	L5	729	G
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	742	G
3	L5	904	C

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Mol	Chain	Res	Type
3	L5	905	C
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	918	G
3	L5	925	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	934	C
3	L5	935	A
3	L5	936	C
3	L5	941	C
3	L5	942	G
3	L5	944	A
3	L5	945	U
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	968	C
3	L5	969	C
3	L5	970	G
3	L5	971	U
3	L5	972	C
3	L5	977	C
3	L5	981	C
3	L5	982	U
3	L5	1070	G
3	L5	1072	C
3	L5	1073	G
3	L5	1084	C
3	L5	1182	C
3	L5	1183	C
3	L5	1187	G
3	L5	1199	G
3	L5	1200	G

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Mol	Chain	Res	Type
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1216	C
3	L5	1239	C
3	L5	1241	C
3	L5	1260	G
3	L5	1266	G
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1277	G
3	L5	1278	C
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1294	A
3	L5	1295	C
3	L5	1303	A
3	L5	1313	C
3	L5	1315	C
3	L5	1323	A
3	L5	1326	A2M
3	L5	1328	G
3	L5	1337	A
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1399	G
3	L5	1404	G
3	L5	1407	C
3	L5	1408	G
3	L5	1409	C
3	L5	1410	U
3	L5	1411	C
3	L5	1415	G

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Mol	Chain	Res	Type
3	L5	1417	C
3	L5	1418	C
3	L5	1420	A
3	L5	1439	C
3	L5	1443	A
3	L5	1457	G
3	L5	1477	C
3	L5	1482	G
3	L5	1483	C
3	L5	1498	G
3	L5	1502	G
3	L5	1515	A
3	L5	1534	A2M
3	L5	1535	C
3	L5	1547	A
3	L5	1566	C
3	L5	1578	U
3	L5	1586	G
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	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1701	A
3	L5	1705	G
3	L5	1726	U
3	L5	1731	C
3	L5	1733	G
3	L5	1734	G
3	L5	1740	C
3	L5	1741	G

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Mol	Chain	Res	Type
3	L5	1754	U
3	L5	1764	G
3	L5	1766	A
3	L5	1769	G
3	L5	1787	A
3	L5	1804	A
3	L5	1815	G
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A
3	L5	1855	G
3	L5	1869	G
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	1951	G
3	L5	1961	G
3	L5	1962	A
3	L5	1963	C
3	L5	1974	U
3	L5	1979	A
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1983	A
3	L5	1984	A
3	L5	1985	G
3	L5	1987	C
3	L5	1997	U
3	L5	1998	A
3	L5	2001	G
3	L5	2002	A

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Mol	Chain	Res	Type
3	L5	2003	G
3	L5	2004	U
3	L5	2024	G
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	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2089	G
3	L5	2091	C
3	L5	2092	G
3	L5	2094	G
3	L5	2096	G
3	L5	2098	G
3	L5	2099	G
3	L5	2259	G
3	L5	2260	C
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2316	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2357	G
3	L5	2360	A
3	L5	2366	A
3	L5	2371	U
3	L5	2383	C
3	L5	2395	A
3	L5	2417	A
3	L5	2421	G
3	L5	2422	OMC
3	L5	2450	G
3	L5	2453	A
3	L5	2470	C
3	L5	2471	G
3	L5	2474	G

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Mol	Chain	Res	Type
3	L5	2479	G
3	L5	2482	C
3	L5	2486	G
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2493	G
3	L5	2503	G
3	L5	2504	C
3	L5	2506	G
3	L5	2513	A
3	L5	2514	G
3	L5	2519	U
3	L5	2554	U
3	L5	2556	G
3	L5	2564	G
3	L5	2573	A
3	L5	2583	C
3	L5	2586	G
3	L5	2587	A
3	L5	2588	C
3	L5	2601	A
3	L5	2602	G
3	L5	2611	A
3	L5	2618	G
3	L5	2627	C
3	L5	2653	C
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	2703	G
3	L5	2705	G
3	L5	2711	G
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2743	A
3	L5	2754	G

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Mol	Chain	Res	Type
3	L5	2760	G
3	L5	2763	U
3	L5	2764	A
3	L5	2765	A
3	L5	2767	U
3	L5	2769	U
3	L5	2770	C
3	L5	2787	A2M
3	L5	2788	U
3	L5	2790	U
3	L5	2795	A
3	L5	2814	C
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2830	G
3	L5	2855	G
3	L5	2867	C
3	L5	2877	G
3	L5	2901	G
3	L5	2902	G
3	L5	2903	G
3	L5	3597	G
3	L5	3598	C
3	L5	3604	A
3	L5	3615	G
3	L5	3618	C
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3662	A
3	L5	3663	A
3	L5	3673	C
3	L5	3674	G
3	L5	3696	C
3	L5	3712	A
3	L5	3713	U
3	L5	3735	G
3	L5	3736	A
3	L5	3748	A
3	L5	3750	G

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Mol	Chain	Res	Type
3	L5	3753	G
3	L5	3760	A2M
3	L5	3761	C
3	L5	3765	G
3	L5	3766	A
3	L5	3774	A
3	L5	3776	G
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3785	A2M
3	L5	3787	G
3	L5	3788	C
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3822	U
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3860	A
3	L5	3876	A
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3892	U
3	L5	3897	G
3	L5	3901	A
3	L5	3905	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3938	G
3	L5	3951	G
3	L5	3952	A
3	L5	3957	U
3	L5	3959	U
3	L5	3960	A
3	L5	3961	G
3	L5	3962	A

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Mol	Chain	Res	Type
3	L5	3963	A
3	L5	3964	U
3	L5	3966	A
3	L5	3968	U
3	L5	3970	G
3	L5	3971	G
3	L5	3972	A
3	L5	3973	G
3	L5	3977	C
3	L5	4035	G
3	L5	4038	C
3	L5	4039	G
3	L5	4040	C
3	L5	4041	C
3	L5	4042	G
3	L5	4043	G
3	L5	4044	U
3	L5	4046	A
3	L5	4047	A
3	L5	4049	U
3	L5	4050	A
3	L5	4051	C
3	L5	4052	C
3	L5	4053	A
3	L5	4054	C
3	L5	4055	U
3	L5	4057	C
3	L5	4059	C
3	L5	4060	U
3	L5	4070	U
3	L5	4076	G
3	L5	4084	G
3	L5	4097	G
3	L5	4099	G
3	L5	4100	C
3	L5	4102	C
3	L5	4103	C
3	L5	4104	G
3	L5	4107	G
3	L5	4113	U
3	L5	4114	C
3	L5	4115	G

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Mol	Chain	Res	Type
3	L5	4116	C
3	L5	4118	U
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4128	A
3	L5	4134	C
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4177	C
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4206	C
3	L5	4214	A
3	L5	4222	G
3	L5	4225	G
3	L5	4229	U
3	L5	4233	A
3	L5	4249	G
3	L5	4251	A
3	L5	4254	G
3	L5	4258	C
3	L5	4260	U
3	L5	4266	G
3	L5	4267	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	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4348	A
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G

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Mol	Chain	Res	Type
3	L5	4378	A
3	L5	4379	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4420	PSU
3	L5	4422	A
3	L5	4426	C
3	L5	4432	C
3	L5	4448	G
3	L5	4449	A
3	L5	4453	C
3	L5	4464	A
3	L5	4465	U
3	L5	4475	G
3	L5	4502	C
3	L5	4512	U
3	L5	4513	A
3	L5	4515	G
3	L5	4519	C
3	L5	4524	G
3	L5	4528	G
3	L5	4548	A
3	L5	4559	A
3	L5	4560	C
3	L5	4567	G
3	L5	4570	G
3	L5	4573	G
3	L5	4590	A2M
3	L5	4600	G
3	L5	4606	G
3	L5	4608	G
3	L5	4612	C
3	L5	4617	G
3	L5	4627	U
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A
3	L5	4691	A

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Mol	Chain	Res	Type
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4720	C
3	L5	4721	G
3	L5	4729	A
3	L5	4730	C
3	L5	4731	G
3	L5	4732	G
3	L5	4733	C
3	L5	4735	G
3	L5	4741	C
3	L5	4742	G
3	L5	4749	C
3	L5	4750	G
3	L5	4751	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4776	G
3	L5	4859	C
3	L5	4870	G
3	L5	4871	C
3	L5	4873	G
3	L5	4881	U
3	L5	4882	U
3	L5	4883	C
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G
3	L5	4913	G
3	L5	4914	C
3	L5	4925	U
3	L5	4927	G
3	L5	4928	C
3	L5	4929	C

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Mol	Chain	Res	Type
3	L5	4935	C
3	L5	4936	G
3	L5	4938	A
3	L5	4939	C
3	L5	4943	A
3	L5	4944	C
3	L5	4964	C
3	L5	4976	U
3	L5	4985	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5025	C
3	L5	5026	U
3	L5	5029	C
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5054	C
3	L5	5061	A
3	L5	5062	G
3	L5	5069	U
4	L7	10	C
4	L7	25	G
4	L7	33	U
4	L7	42	A
4	L7	49	A
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	110	G
4	L7	120	U
83	mR	35	G
83	mR	42	C

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Mol	Chain	Res	Type
84	At	7	A
84	At	9	A
84	At	14	A
84	At	16	H2U
84	At	19	G
84	At	20	H2U
84	At	21	A
84	At	27	G
84	At	32	PSU
84	At	33	U
84	At	34	G
84	At	35	A
84	At	44	G
84	At	45	U
84	At	46	G7M
84	At	47	U
84	At	48	C
84	At	49	C
84	At	52	G
84	At	58	A
84	At	59	U
84	At	60	U
84	At	65	G
84	At	75	C
85	Pt	2	G
85	Pt	10	G
85	Pt	13	C
85	Pt	14	A
85	Pt	18	C
85	Pt	21	H2U
85	Pt	22	A
85	Pt	23	G
85	Pt	50	G
85	Pt	59	A
85	Pt	61	U
85	Pt	62	C
85	Pt	65	G
85	Pt	71	G
85	Pt	76	C
85	Pt	77	A

All (83) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	74	G
1	S2	112	U
1	S2	323	C
1	S2	325	C
1	S2	326	C
1	S2	369	C
1	S2	370	G
1	S2	385	G
1	S2	448	A
1	S2	500	A
1	S2	587	A
1	S2	628	A
1	S2	688	U
1	S2	896	U
1	S2	1016	U
1	S2	1165	G
1	S2	1215	C
1	S2	1285	G
1	S2	1303	C
1	S2	1420	G
1	S2	1422	G
1	S2	1437	C
1	S2	1446	A
1	S2	1494	U
1	S2	1519	U
1	S2	1534	C
1	S2	1555	U
1	S2	1679	A
2	L8	51	U
3	L5	42	A
3	L5	209	U
3	L5	234	G
3	L5	409	G
3	L5	417	G
3	L5	453	G
3	L5	685	C
3	L5	967	C
3	L5	968	C
3	L5	971	U
3	L5	1215	C
3	L5	1240	G
3	L5	1294	A
3	L5	1407	C

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Mol	Chain	Res	Type
3	L5	1410	U
3	L5	1420	A
3	L5	1482	G
3	L5	1613	A
3	L5	1633	G
3	L5	1678	C
3	L5	1700	G
3	L5	1733	G
3	L5	1833	G
3	L5	1961	G
3	L5	1984	A
3	L5	2002	A
3	L5	2025	A
3	L5	2088	A
3	L5	2091	C
3	L5	2097	U
3	L5	2259	G
3	L5	2428	A
3	L5	2503	G
3	L5	2513	A
3	L5	2587	A
3	L5	2652	G
3	L5	2724	G
3	L5	2761	U
3	L5	2789	A
3	L5	2794	C
3	L5	3765	G
3	L5	3876	A
3	L5	3956	G
3	L5	4043	G
3	L5	4115	G
3	L5	4420	PSU
3	L5	4699	U
3	L5	4729	A
3	L5	4731	G
3	L5	4750	G
3	L5	4872	G
3	L5	4927	G
3	L5	4938	A
3	L5	5061	A

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

244 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PSU	L5	2632	3	18,21,22	1.45	4 (22%)	21,30,33	2.11	3 (14%)
3	OMG	L5	3899	3	23,26,27	1.23	3 (13%)	32,38,41	2.19	7 (21%)
3	PSU	L5	4500	3	18,21,22	1.59	5 (27%)	21,30,33	2.08	5 (23%)
3	OMC	L5	4456	3	19,22,23	0.94	0	25,31,34	1.00	1 (4%)
3	PSU	L5	2508	3	18,21,22	1.43	3 (16%)	21,30,33	1.98	4 (19%)
3	OMG	L5	4637	3	23,26,27	1.29	4 (17%)	32,38,41	2.11	7 (21%)
3	1MA	L5	1322	89,3	21,25,26	1.34	5 (23%)	30,37,40	1.75	6 (20%)
85	G7M	Pt	47	85	23,26,27	1.87	2 (8%)	34,39,42	1.08	1 (2%)
1	PSU	S2	406	1	18,21,22	1.51	4 (22%)	21,30,33	2.14	3 (14%)
1	UY1	S2	1326	89,1	19,22,23	1.36	3 (15%)	21,31,34	2.22	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.55	3 (16%)	21,30,33	1.77	4 (19%)
3	OMG	L5	4623	3	23,26,27	1.28	4 (17%)	32,38,41	2.04	8 (25%)
3	A2M	L5	1326	3	22,25,26	1.48	4 (18%)	30,36,39	2.09	11 (36%)
1	OMU	S2	627	1	19,22,23	1.26	3 (15%)	25,31,34	1.97	5 (20%)
3	OMC	L5	3869	3	19,22,23	0.81	0	25,31,34	1.05	1 (4%)
3	PSU	L5	5001	3	18,21,22	1.42	4 (22%)	21,30,33	2.13	4 (19%)
29	AME	SV	1	29	9,10,11	3.33	2 (22%)	9,11,13	3.74	3 (33%)
3	OMG	L5	3744	3	23,26,27	1.22	4 (17%)	32,38,41	2.07	7 (21%)
1	A2M	S2	590	1	22,25,26	1.47	3 (13%)	30,36,39	2.12	7 (23%)
3	PSU	L5	4299	3	18,21,22	1.55	4 (22%)	21,30,33	2.08	4 (19%)
3	OMU	L5	4498	3	19,22,23	1.31	3 (15%)	25,31,34	1.97	5 (20%)
3	6MZ	L5	4220	3	22,25,26	1.34	5 (22%)	29,36,39	2.19	10 (34%)
1	PSU	S2	1056	1	18,21,22	1.48	3 (16%)	21,30,33	2.18	4 (19%)
1	OMU	S2	1442	89,1	19,22,23	1.34	3 (15%)	25,31,34	1.93	5 (20%)
3	A2M	L5	400	3	22,25,26	1.46	5 (22%)	30,36,39	2.17	10 (33%)
3	PSU	L5	5010	3	18,21,22	1.52	4 (22%)	21,30,33	2.11	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	573	1	18,21,22	1.40	3 (16%)	21,30,33	2.04	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.83	0	25,31,34	1.08	2 (8%)
79	M3L	Lm	98	79	10,11,12	0.38	0	9,14,16	0.09	0
1	PSU	S2	218	1	18,21,22	1.49	4 (22%)	21,30,33	2.15	4 (19%)
3	PSU	L5	3639	3	18,21,22	1.56	5 (27%)	21,30,33	2.00	3 (14%)
1	A2M	S2	468	1	22,25,26	1.48	5 (22%)	30,36,39	2.13	9 (30%)
1	PSU	S2	1232	1	18,21,22	1.54	4 (22%)	21,30,33	2.13	3 (14%)
3	PSU	L5	4532	3	18,21,22	1.57	4 (22%)	21,30,33	2.21	6 (28%)
1	A2M	S2	27	89,1	22,25,26	1.43	4 (18%)	30,36,39	2.09	9 (30%)
1	OMC	S2	1391	1	19,22,23	0.84	0	25,31,34	1.05	2 (8%)
1	PSU	S2	1244	1	18,21,22	1.46	4 (22%)	21,30,33	2.07	3 (14%)
81	MLZ	Lo	53	81	8,9,10	0.63	0	4,9,11	0.89	0
86	M3L	EF	318	86	10,11,12	0.48	0	9,14,16	0.10	0
1	PSU	S2	572	1	18,21,22	1.40	4 (22%)	21,30,33	2.05	4 (19%)
1	OMG	S2	601	1	23,26,27	1.28	3 (13%)	32,38,41	1.90	5 (15%)
1	PSU	S2	681	1	18,21,22	1.55	5 (27%)	21,30,33	2.23	3 (14%)
1	OMU	S2	121	1	19,22,23	1.47	4 (21%)	25,31,34	1.78	5 (20%)
1	OMG	S2	683	1	23,26,27	1.22	4 (17%)	32,38,41	2.09	7 (21%)
3	PSU	L5	3762	3	18,21,22	1.37	2 (11%)	21,30,33	2.15	5 (23%)
3	PSU	L5	4442	3	18,21,22	1.53	5 (27%)	21,30,33	2.27	5 (23%)
3	OMG	L5	4392	3	23,26,27	1.32	4 (17%)	32,38,41	2.02	7 (21%)
3	OMG	L5	4494	3	23,26,27	1.28	4 (17%)	32,38,41	1.98	5 (15%)
3	PSU	L5	4576	3	18,21,22	1.52	3 (16%)	21,30,33	1.87	5 (23%)
1	PSU	S2	34	1	18,21,22	1.43	4 (22%)	21,30,33	2.08	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.81	1 (5%)	25,31,34	0.92	0
1	PSU	S2	1243	1	18,21,22	1.55	4 (22%)	21,30,33	2.30	5 (23%)
86	MLY	EF	55	86	9,10,11	0.48	0	6,11,13	0.89	0
3	PSU	L5	4689	3	18,21,22	1.48	3 (16%)	21,30,33	2.17	5 (23%)
3	A2M	L5	4523	89,3	22,25,26	1.40	4 (18%)	30,36,39	2.22	11 (36%)
1	OMC	S2	517	1	19,22,23	0.83	0	25,31,34	1.03	2 (8%)
1	PSU	S2	1004	1	18,21,22	1.58	4 (22%)	21,30,33	1.97	3 (14%)
3	PSU	L5	1744	3,92	18,21,22	1.45	3 (16%)	21,30,33	2.13	3 (14%)
3	OMC	L5	3808	3	19,22,23	0.77	0	25,31,34	0.86	0
1	PSU	S2	109	1	18,21,22	1.53	4 (22%)	21,30,33	2.17	3 (14%)
2	OMG	L8	75	2	23,26,27	1.22	3 (13%)	32,38,41	2.07	7 (21%)
3	PSU	L5	4531	3	18,21,22	1.46	3 (16%)	21,30,33	2.42	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	2422	89,3	19,22,23	0.82	0	25,31,34	0.98	1 (4%)
3	A2M	L5	2815	89,3	22,25,26	1.60	5 (22%)	30,36,39	1.98	9 (30%)
3	PSU	L5	3764	3	18,21,22	1.50	3 (16%)	21,30,33	2.11	4 (19%)
1	PSU	S2	649	1	18,21,22	1.51	4 (22%)	21,30,33	2.18	4 (19%)
86	M3L	EF	36	86	10,11,12	0.51	0	9,14,16	0.49	0
1	PSU	S2	105	1	18,21,22	1.59	5 (27%)	21,30,33	2.26	5 (23%)
40	HIC	LB	245	40	10,11,12	1.17	1 (10%)	9,14,16	1.33	2 (22%)
1	OMG	S2	436	1	23,26,27	1.24	3 (13%)	32,38,41	1.98	6 (18%)
3	A2M	L5	2363	89,3	22,25,26	1.48	4 (18%)	30,36,39	2.01	9 (30%)
3	OMG	L5	3627	3	23,26,27	1.26	4 (17%)	32,38,41	2.11	8 (25%)
2	PSU	L8	69	2	18,21,22	1.55	6 (33%)	21,30,33	2.27	5 (23%)
3	PSU	L5	1782	3	18,21,22	1.55	4 (22%)	21,30,33	2.07	5 (23%)
3	PSU	L5	4361	3	18,21,22	1.49	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.59	5 (27%)	21,30,33	2.00	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.58	5 (27%)	21,30,33	2.21	3 (14%)
20	HY3	SX	62	20	7,8,9	1.58	1 (14%)	7,10,12	1.29	0
3	A2M	L5	2787	89,3	22,25,26	1.44	5 (22%)	30,36,39	2.26	8 (26%)
3	OMC	L5	2861	3	19,22,23	0.71	0	25,31,34	0.79	1 (4%)
3	A2M	L5	2401	3	22,25,26	1.40	4 (18%)	30,36,39	2.08	11 (36%)
1	OMU	S2	116	1	19,22,23	1.32	3 (15%)	25,31,34	1.84	4 (16%)
1	A2M	S2	1678	1	22,25,26	1.44	4 (18%)	30,36,39	2.10	10 (33%)
1	PSU	S2	686	1	18,21,22	1.49	4 (22%)	21,30,33	2.21	3 (14%)
1	OMU	S2	1288	1	19,22,23	1.24	3 (15%)	25,31,34	1.87	5 (20%)
3	PSU	L5	4423	3	18,21,22	1.40	4 (22%)	21,30,33	2.07	3 (14%)
1	PSU	S2	36	1	18,21,22	1.54	5 (27%)	21,30,33	2.11	3 (14%)
3	PSU	L5	4457	3	18,21,22	1.51	4 (22%)	21,30,33	2.17	5 (23%)
1	OMG	S2	509	89,1	23,26,27	1.22	3 (13%)	32,38,41	2.00	7 (21%)
1	PSU	S2	1625	1	18,21,22	1.40	2 (11%)	21,30,33	2.05	3 (14%)
3	PSU	L5	4420	3	18,21,22	1.55	5 (27%)	21,30,33	2.04	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.48	4 (22%)	21,30,33	1.95	4 (19%)
1	PSU	S2	296	1	18,21,22	1.39	4 (22%)	21,30,33	2.12	4 (19%)
3	OMU	L5	4227	3	19,22,23	1.41	2 (10%)	25,31,34	2.02	5 (20%)
3	PSU	L5	3851	3	18,21,22	1.59	4 (22%)	21,30,33	2.22	6 (28%)
3	A2M	L5	398	3	22,25,26	1.47	4 (18%)	30,36,39	2.07	8 (26%)
3	PSU	L5	4636	3	18,21,22	1.47	3 (16%)	21,30,33	2.17	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	H2U	Pt	21	85	18,21,22	1.01	2 (11%)	19,30,33	0.91	0
3	OMG	L5	1316	3	23,26,27	1.37	4 (17%)	32,38,41	2.02	7 (21%)
3	A2M	L5	3760	1,3	22,25,26	1.48	5 (22%)	30,36,39	2.22	9 (30%)
3	A2M	L5	3785	3	22,25,26	1.41	5 (22%)	30,36,39	2.48	11 (36%)
3	A2M	L5	1534	89,3	22,25,26	1.54	5 (22%)	30,36,39	2.13	10 (33%)
1	PSU	S2	1445	1	18,21,22	1.56	5 (27%)	21,30,33	2.23	4 (19%)
1	G7M	S2	1639	1,85	23,26,27	2.39	5 (21%)	34,39,42	3.11	10 (29%)
39	V5N	LA	216	39	8,11,12	1.36	1 (12%)	8,14,16	1.92	2 (25%)
3	PSU	L5	1677	3	18,21,22	1.56	4 (22%)	21,30,33	2.28	6 (28%)
84	PSU	At	39	84	18,21,22	1.36	2 (11%)	21,30,33	2.12	4 (19%)
3	A2M	L5	4571	3	22,25,26	1.52	5 (22%)	30,36,39	1.94	9 (30%)
1	PSU	S2	1643	89,1	18,21,22	1.55	5 (27%)	21,30,33	2.16	5 (23%)
1	PSU	S2	93	1	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
1	PSU	S2	1081	1	18,21,22	1.58	5 (27%)	21,30,33	2.20	5 (23%)
1	PSU	S2	1692	1	18,21,22	1.44	4 (22%)	21,30,33	2.18	4 (19%)
3	PSU	L5	4493	3	18,21,22	1.60	4 (22%)	21,30,33	2.26	5 (23%)
1	PSU	S2	863	1	18,21,22	1.47	3 (16%)	21,30,33	2.04	3 (14%)
52	V5N	La	39	52	8,11,12	1.52	1 (12%)	8,14,16	1.95	2 (25%)
1	OMG	S2	1490	89,1	23,26,27	1.28	4 (17%)	32,38,41	2.02	7 (21%)
3	UR3	L5	4530	3	19,22,23	0.86	1 (5%)	26,32,35	2.02	5 (19%)
1	PSU	S2	814	1	18,21,22	1.52	4 (22%)	21,30,33	2.16	5 (23%)
1	6MZ	S2	1832	89,1	22,25,26	1.46	5 (22%)	29,36,39	2.14	10 (34%)
3	OMG	L5	1522	3	23,26,27	0.95	2 (8%)	32,38,41	2.15	9 (28%)
3	5MC	L5	4447	3	19,22,23	1.58	3 (15%)	26,32,35	1.57	3 (11%)
3	OMG	L5	4499	3	23,26,27	1.22	3 (13%)	32,38,41	2.02	6 (18%)
1	A2M	S2	576	1	22,25,26	1.51	6 (27%)	30,36,39	2.11	9 (30%)
3	OMC	L5	2365	89,3	19,22,23	0.82	0	25,31,34	0.93	1 (4%)
3	A2M	L5	3825	3	22,25,26	1.37	4 (18%)	30,36,39	2.24	9 (30%)
3	PSU	L5	1683	89,3	18,21,22	1.67	5 (27%)	21,30,33	2.16	3 (14%)
1	A2M	S2	166	1	22,25,26	1.44	4 (18%)	30,36,39	2.21	11 (36%)
3	PSU	L5	4569	3	18,21,22	1.46	5 (27%)	21,30,33	2.24	4 (19%)
3	PSU	L5	3920	89,3	18,21,22	1.57	4 (22%)	21,30,33	2.31	4 (19%)
3	OMG	L5	3944	3	23,26,27	1.25	3 (13%)	32,38,41	2.19	9 (28%)
3	PSU	L5	3715	3	18,21,22	1.42	4 (22%)	21,30,33	2.06	4 (19%)
3	OMG	L5	2364	3	23,26,27	1.14	3 (13%)	32,38,41	2.22	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	1881	89,3	19,22,23	0.78	0	25,31,34	0.90	0
1	PSU	S2	1239	1	18,21,22	1.48	4 (22%)	21,30,33	2.11	4 (19%)
66	SAC	Lr	2	66	7,8,9	3.69	2 (28%)	7,9,11	4.53	4 (57%)
3	OMG	L5	3792	3	23,26,27	1.22	3 (13%)	32,38,41	2.05	5 (15%)
3	UY1	L5	3818	89,3	19,22,23	1.40	4 (21%)	21,31,34	2.12	4 (19%)
85	PSU	Pt	56	85	18,21,22	1.39	3 (16%)	21,30,33	2.08	4 (19%)
3	OMU	L5	4306	3	19,22,23	1.41	3 (15%)	25,31,34	2.10	5 (20%)
1	OMG	S2	1328	1	23,26,27	1.26	4 (17%)	32,38,41	1.97	7 (21%)
1	PSU	S2	651	1	18,21,22	1.44	4 (22%)	21,30,33	2.02	4 (19%)
3	PSU	L5	4579	3	18,21,22	1.52	4 (22%)	21,30,33	2.15	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.48	5 (22%)	30,36,39	2.27	9 (30%)
1	A2M	S2	1383	1	22,25,26	1.41	3 (13%)	30,36,39	2.36	9 (30%)
3	OMC	L5	3701	3,92	19,22,23	0.96	0	25,31,34	1.22	2 (8%)
3	PSU	L5	3768	3	18,21,22	1.53	4 (22%)	21,30,33	1.92	3 (14%)
1	OMU	S2	1804	1	19,22,23	1.34	3 (15%)	25,31,34	1.85	5 (20%)
3	PSU	L5	1536	3	18,21,22	1.68	6 (33%)	21,30,33	2.21	4 (19%)
3	OMG	L5	2876	3	23,26,27	1.26	4 (17%)	32,38,41	2.00	6 (18%)
84	H2U	At	20	84	18,21,22	1.01	2 (11%)	19,30,33	1.17	2 (10%)
3	PSU	L5	2839	3	18,21,22	1.52	6 (33%)	21,30,33	2.18	4 (19%)
1	OMG	S2	1447	1	23,26,27	1.30	4 (17%)	32,38,41	2.11	8 (25%)
3	OMG	L5	1625	89,3	23,26,27	1.27	4 (17%)	32,38,41	1.96	6 (18%)
1	PSU	S2	1174	89,1	18,21,22	1.54	5 (27%)	21,30,33	2.02	4 (19%)
3	OMG	L5	4370	3	23,26,27	1.20	4 (17%)	32,38,41	1.96	5 (15%)
1	OMU	S2	428	1	19,22,23	1.23	2 (10%)	25,31,34	2.06	6 (24%)
1	PSU	S2	815	1	18,21,22	1.48	3 (16%)	21,30,33	2.04	5 (23%)
3	A2M	L5	1871	89,3	22,25,26	1.53	5 (22%)	30,36,39	2.22	11 (36%)
6	SAC	SA	2	6	7,8,9	3.67	2 (28%)	7,9,11	4.12	4 (57%)
3	PSU	L5	3844	3	18,21,22	1.60	5 (27%)	21,30,33	2.14	3 (14%)
3	PSU	L5	1582	3	18,21,22	1.54	5 (27%)	21,30,33	1.96	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.38	3 (16%)	21,30,33	1.86	4 (19%)
3	OMG	L5	4228	3	23,26,27	1.25	4 (17%)	32,38,41	2.07	9 (28%)
1	PSU	S2	609	1	18,21,22	1.41	4 (22%)	21,30,33	2.08	3 (14%)
3	PSU	L5	4628	3	18,21,22	1.43	4 (22%)	21,30,33	1.98	4 (19%)
84	PSU	At	32	84	18,21,22	1.43	3 (16%)	21,30,33	2.06	5 (23%)
1	4AC	S2	1337	1	21,24,25	1.09	1 (4%)	28,34,37	1.25	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3724	3	22,25,26	1.39	4 (18%)	30,36,39	2.13	11 (36%)
1	A2M	S2	668	89,1	22,25,26	1.50	5 (22%)	30,36,39	1.97	8 (26%)
3	PSU	L5	4296	3	18,21,22	1.46	4 (22%)	21,30,33	2.26	4 (19%)
84	4SU	At	8	84	18,21,22	1.99	4 (22%)	25,30,33	2.55	7 (28%)
1	OMU	S2	172	1	19,22,23	1.36	4 (21%)	25,31,34	2.14	9 (36%)
3	PSU	L5	3770	3	18,21,22	1.44	2 (11%)	21,30,33	2.07	3 (14%)
1	B8N	S2	1248	1	25,29,30	0.92	1 (4%)	28,42,45	1.58	7 (25%)
3	OMC	L5	2351	3	19,22,23	0.90	1 (5%)	25,31,34	0.99	1 (4%)
1	PSU	S2	119	1	18,21,22	1.47	4 (22%)	21,30,33	2.15	5 (23%)
3	OMU	L5	4620	3	19,22,23	1.37	3 (15%)	25,31,34	2.00	6 (24%)
1	PSU	S2	1238	1	18,21,22	1.52	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	4312	3	18,21,22	1.55	4 (22%)	21,30,33	2.04	4 (19%)
1	PSU	S2	1347	1	18,21,22	1.44	4 (22%)	21,30,33	2.10	3 (14%)
1	OMC	S2	174	89,1	19,22,23	0.86	0	25,31,34	0.99	1 (4%)
3	OMC	L5	2804	3	19,22,23	0.83	0	25,31,34	1.01	1 (4%)
3	PSU	L5	3729	3	18,21,22	1.49	3 (16%)	21,30,33	2.18	4 (19%)
1	PSU	S2	1136	1	18,21,22	1.50	3 (16%)	21,30,33	2.06	4 (19%)
1	A2M	S2	1031	1	22,25,26	1.47	4 (18%)	30,36,39	2.14	10 (33%)
1	A2M	S2	159	1	22,25,26	1.48	4 (18%)	30,36,39	2.16	8 (26%)
3	A2M	L5	1524	3	22,25,26	1.56	4 (18%)	30,36,39	1.97	8 (26%)
3	PSU	L5	3695	89,3	18,21,22	1.49	3 (16%)	21,30,33	2.22	6 (28%)
3	A2M	L5	3867	3	22,25,26	1.50	5 (22%)	30,36,39	2.04	7 (23%)
3	PSU	L5	4521	89,3	18,21,22	1.60	5 (27%)	21,30,33	2.37	6 (28%)
2	PSU	L8	55	2	18,21,22	1.45	3 (16%)	21,30,33	2.24	4 (19%)
1	PSU	S2	1177	1	18,21,22	1.46	4 (22%)	21,30,33	2.08	3 (14%)
1	MA6	S2	1850	1	23,26,27	1.44	5 (21%)	33,38,41	2.09	10 (30%)
3	PSU	L5	3637	89,3	18,21,22	1.58	3 (16%)	21,30,33	2.25	6 (28%)
3	A2M	L5	3723	3	22,25,26	1.45	5 (22%)	30,36,39	2.04	11 (36%)
84	MIA	At	37	84	28,31,32	2.32	6 (21%)	38,44,47	2.79	14 (36%)
3	PSU	L5	1860	3	18,21,22	1.55	4 (22%)	21,30,33	2.11	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.74	0	25,31,34	0.66	0
3	PSU	L5	4972	3	18,21,22	1.53	4 (22%)	21,30,33	2.06	4 (19%)
3	OMU	L5	2415	3	19,22,23	1.41	3 (15%)	25,31,34	1.94	4 (16%)
2	OMU	L8	14	2,3	19,22,23	1.45	4 (21%)	25,31,34	2.00	6 (24%)
68	MLZ	Lb	5	68	8,9,10	0.94	0	4,9,11	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	M3L	EF	79	86	10,11,12	0.48	0	9,14,16	0.11	0
1	OMG	S2	644	1	23,26,27	1.20	4 (17%)	32,38,41	2.13	7 (21%)
3	PSU	L5	1792	3	18,21,22	1.50	4 (22%)	21,30,33	2.21	4 (19%)
1	A2M	S2	99	89,1	22,25,26	1.46	4 (18%)	30,36,39	2.08	9 (30%)
3	A2M	L5	4590	3	22,25,26	1.50	5 (22%)	30,36,39	2.10	10 (33%)
1	PSU	S2	918	1	18,21,22	1.45	3 (16%)	21,30,33	2.38	5 (23%)
3	PSU	L5	1781	3	18,21,22	1.39	2 (11%)	21,30,33	2.12	4 (19%)
3	OMG	L5	2424	3	23,26,27	1.23	3 (13%)	32,38,41	1.94	5 (15%)
3	PSU	L5	2843	3	18,21,22	1.55	4 (22%)	21,30,33	2.19	4 (19%)
3	OMC	L5	3887	3	19,22,23	0.83	0	25,31,34	0.87	0
3	OMC	L5	1340	3	19,22,23	0.85	0	25,31,34	0.94	0
3	OMG	L5	4196	89,3,85	23,26,27	1.25	4 (17%)	32,38,41	1.92	5 (15%)
1	OMU	S2	354	1	19,22,23	1.47	3 (15%)	25,31,34	2.10	5 (20%)
1	MA6	S2	1851	1	23,26,27	1.46	5 (21%)	33,38,41	2.04	10 (30%)
1	PSU	S2	966	1	18,21,22	1.53	4 (22%)	21,30,33	1.99	5 (23%)
1	OMC	S2	1703	1	19,22,23	0.81	1 (5%)	25,31,34	0.81	1 (4%)
1	A2M	S2	512	1	22,25,26	1.44	5 (22%)	30,36,39	2.22	9 (30%)
1	OMC	S2	462	1	19,22,23	0.89	0	25,31,34	0.87	0
1	PSU	S2	801	1	18,21,22	1.40	3 (16%)	21,30,33	2.11	3 (14%)
1	A2M	S2	484	1	22,25,26	1.49	5 (22%)	30,36,39	2.02	7 (23%)
3	A2M	L5	3718	3	22,25,26	1.52	4 (18%)	30,36,39	1.88	6 (20%)
1	OMG	S2	867	1	23,26,27	1.21	4 (17%)	32,38,41	1.97	7 (21%)
3	OMU	L5	3925	3	19,22,23	1.39	3 (15%)	25,31,34	1.86	5 (20%)
85	OMC	Pt	33	85	19,22,23	0.82	0	25,31,34	0.82	0
3	5MC	L5	3782	89,3	19,22,23	1.64	3 (15%)	26,32,35	1.35	3 (11%)
84	H2U	At	16	84	18,21,22	1.02	2 (11%)	19,30,33	0.92	1 (5%)
1	4AC	S2	1842	1	21,24,25	1.03	2 (9%)	28,34,37	1.23	4 (14%)
3	PSU	L5	1779	3	18,21,22	1.58	5 (27%)	21,30,33	2.12	3 (14%)
1	PSU	S2	822	1	18,21,22	1.50	4 (22%)	21,30,33	2.25	4 (19%)
3	PSU	L5	4673	3	18,21,22	1.36	3 (16%)	21,30,33	1.87	3 (14%)
1	PSU	S2	1367	1	18,21,22	1.56	3 (16%)	21,30,33	2.15	5 (23%)
85	4SU	Pt	8	85	18,21,22	1.96	4 (22%)	25,30,33	2.24	5 (20%)
3	PSU	L5	4403	3	18,21,22	1.58	4 (22%)	21,30,33	2.17	6 (28%)
3	PSU	L5	3734	3	18,21,22	1.41	4 (22%)	21,30,33	2.26	4 (19%)
3	PSU	L5	3853	89,3	18,21,22	1.60	4 (22%)	21,30,33	1.89	5 (23%)
3	OMG	L5	4618	3	23,26,27	1.27	4 (17%)	32,38,41	2.08	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	L5	2837	3	19,22,23	1.31	3 (15%)	25,31,34	2.00	5 (20%)
1	PSU	S2	866	1	18,21,22	1.51	4 (22%)	21,30,33	1.84	3 (14%)
3	PSU	L5	4552	3	18,21,22	1.63	5 (27%)	21,30,33	2.21	3 (14%)
3	PSU	L5	3758	3	18,21,22	1.42	4 (22%)	21,30,33	2.02	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.58	4 (22%)	21,30,33	2.13	4 (19%)
84	G7M	At	46	84	23,26,27	2.39	6 (26%)	34,39,42	2.99	10 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	1MA	L5	1322	89,3	-	1/7/25/26	0/3/3/3
85	G7M	Pt	47	85	-	0/7/25/26	0/3/3/3
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	UY1	S2	1326	89,1	-	1/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
1	OMU	S2	627	1	-	0/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
29	AME	SV	1	29	-	2/9/10/12	-
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	590	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	89,1	-	2/9/27/28	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
79	M3L	Lm	98	79	-	0/9/10/12	-
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	89,1	-	1/9/27/28	0/3/3/3
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
81	MLZ	Lo	53	81	-	2/7/8/10	-
86	M3L	EF	318	86	-	7/9/10/12	-
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1243	1	-	1/7/25/26	0/2/2/2
86	MLY	EF	55	86	-	3/8/9/11	-
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	89,3	-	0/9/27/28	0/3/3/3
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	3,92	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
2	OMG	L8	75	2	-	0/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	2422	89,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2815	89,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3764	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
86	M3L	EF	36	86	-	0/9/10/12	-
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HIC	LB	245	40	-	0/5/6/8	0/1/1/1
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	89,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3627	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	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
3	A2M	L5	2787	89,3	-	5/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1288	1	-	3/9/27/28	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	89,1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3851	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
85	H2U	Pt	21	85	-	3/7/38/39	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3760	1,3	-	3/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1534	89,3	-	2/9/27/28	0/3/3/3
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	G7M	S2	1639	1,85	-	0/7/25/26	0/3/3/3
39	V5N	LA	216	39	-	1/9/10/12	0/1/1/1
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
84	PSU	At	39	84	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1643	89,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
52	V5N	La	39	52	-	1/9/10/12	0/1/1/1
1	OMG	S2	1490	89,1	-	2/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	6MZ	S2	1832	89,1	-	2/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
1	A2M	S2	576	1	-	3/9/27/28	0/3/3/3
3	OMC	L5	2365	89,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1683	89,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	89,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3944	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	1881	89,3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
66	SAC	Lr	2	66	-	2/7/8/10	-
3	OMG	L5	3792	3	-	1/9/27/28	0/3/3/3
3	UY1	L5	3818	89,3	-	2/9/27/28	0/2/2/2
85	PSU	Pt	56	85	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
1	OMG	S2	1328	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
3	OMC	L5	3701	3,92	-	4/9/27/28	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
84	H2U	At	20	84	-	6/7/38/39	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	1/9/27/28	0/3/3/3
3	OMG	L5	1625	89,3	-	3/9/27/28	0/3/3/3
1	PSU	S2	1174	89,1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
1	OMU	S2	428	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	89,3	-	0/9/27/28	0/3/3/3
6	SAC	SA	2	6	-	1/7/8/10	-
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
84	PSU	At	32	84	-	3/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	4/11/29/30	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	668	89,1	-	3/9/27/28	0/3/3/3
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
84	4SU	At	8	84	-	1/7/25/26	0/2/2/2
1	OMU	S2	172	1	-	4/9/27/28	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
3	OMC	L5	2351	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	174	89,1	-	1/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3729	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	1031	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	0/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3695	89,3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3867	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4521	89,3	-	0/7/25/26	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
3	PSU	L5	3637	89,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
84	MIA	At	37	84	-	2/15/33/34	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
2	OMU	L8	14	2,3	-	1/9/27/28	0/2/2/2
68	MLZ	Lb	5	68	-	2/7/8/10	-
86	M3L	EF	79	86	-	3/9/10/12	-
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
1	A2M	S2	99	89,1	-	1/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	918	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4196	89,3,85	-	0/9/27/28	0/3/3/3
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	MA6	S2	1851	1	-	2/11/29/30	0/3/3/3
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
1	OMC	S2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
85	OMC	Pt	33	85	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	89,3	-	0/7/25/26	0/2/2/2
84	H2U	At	16	84	-	3/7/38/39	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	1/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
85	4SU	Pt	8	85	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	89,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
84	G7M	At	46	84	-	2/7/25/26	0/3/3/3

All (815) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SV	1	AME	OT-CT1	8.97	1.43	1.23
66	Lr	2	SAC	OAC-C1A	8.84	1.43	1.23
6	SA	2	SAC	OAC-C1A	8.61	1.42	1.23
1	S2	1639	G7M	C8-N7	7.61	1.46	1.33
84	At	46	G7M	C8-N7	7.58	1.46	1.33
85	Pt	47	G7M	C8-N7	7.46	1.45	1.33
84	At	37	MIA	C2-S10	-7.08	1.69	1.75
84	At	37	MIA	C13-C14	6.73	1.52	1.32
3	L5	3782	5MC	C5-C4	5.76	1.48	1.44
84	At	8	4SU	C4-S4	-5.55	1.58	1.68
3	L5	4447	5MC	C5-C4	5.27	1.48	1.44
85	Pt	8	4SU	C4-S4	-5.18	1.59	1.68
84	At	46	G7M	C5-N7	-4.91	1.33	1.39
84	At	37	MIA	C5-C4	4.68	1.47	1.39
1	S2	1639	G7M	C5-N7	-4.66	1.33	1.39
3	L5	3718	A2M	C5-C4	4.51	1.47	1.39
3	L5	3760	A2M	C5-C4	4.51	1.47	1.39
3	L5	4571	A2M	C5-C4	4.43	1.47	1.39
1	S2	1031	A2M	C5-C4	4.42	1.47	1.39
3	L5	4590	A2M	C5-C4	4.42	1.47	1.39
1	S2	576	A2M	C5-C4	4.42	1.47	1.39
1	S2	159	A2M	C5-C4	4.41	1.47	1.39
3	L5	2815	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	2363	A2M	C5-C4	4.36	1.46	1.39
1	S2	590	A2M	C5-C4	4.31	1.46	1.39
3	L5	3867	A2M	C5-C4	4.24	1.46	1.39
1	S2	468	A2M	C5-C4	4.24	1.46	1.39
3	L5	1524	A2M	C5-C4	4.22	1.46	1.39
3	L5	398	A2M	C5-C4	4.20	1.46	1.39
1	S2	1383	A2M	C5-C4	4.20	1.46	1.39
3	L5	1326	A2M	C5-C4	4.20	1.46	1.39
3	L5	3723	A2M	C5-C4	4.18	1.46	1.39
1	S2	484	A2M	C5-C4	4.14	1.46	1.39
3	L5	1534	A2M	C5-C4	4.14	1.46	1.39
1	S2	1850	MA6	C5-C4	4.13	1.46	1.39
6	SA	2	SAC	C1A-N	4.13	1.47	1.34
1	S2	1639	G7M	C8-N9	4.13	1.46	1.35
1	S2	1851	MA6	C5-C4	4.12	1.46	1.39
3	L5	400	A2M	C5-C4	4.10	1.46	1.39
1	S2	512	A2M	C5-C4	4.09	1.46	1.39
3	L5	2401	A2M	C5-C4	4.09	1.46	1.39
1	S2	166	A2M	C5-C4	4.08	1.46	1.39
1	S2	99	A2M	C5-C4	4.07	1.46	1.39
1	S2	27	A2M	C5-C4	4.06	1.46	1.39
3	L5	3724	A2M	C5-C4	4.06	1.46	1.39
3	L5	1871	A2M	C5-C4	4.04	1.46	1.39
85	Pt	47	G7M	C8-N9	4.03	1.46	1.35
1	S2	1678	A2M	C5-C4	4.00	1.46	1.39
84	At	46	G7M	C8-N9	3.98	1.46	1.35
3	L5	4521	PSU	C4-N3	-3.98	1.31	1.38
66	Lr	2	SAC	C1A-N	3.96	1.47	1.34
1	S2	1832	6MZ	C5-C4	3.95	1.46	1.39
29	SV	1	AME	CT1-N	3.93	1.47	1.34
3	L5	3853	PSU	C6-C5	3.93	1.39	1.35
1	S2	1639	G7M	C5-C4	3.90	1.48	1.38
20	SX	62	HY3	C3-CA	-3.89	1.51	1.55
1	S2	668	A2M	C5-C4	3.88	1.46	1.39
3	L5	3825	A2M	C5-C4	3.85	1.45	1.39
3	L5	4523	A2M	C5-C4	3.83	1.45	1.39
3	L5	3830	A2M	C5-C4	3.82	1.45	1.39
3	L5	2843	PSU	C4-N3	-3.76	1.31	1.38
3	L5	2787	A2M	C5-C4	3.70	1.45	1.39
85	Pt	8	4SU	C4-N3	-3.69	1.33	1.37
84	At	8	4SU	C4-N3	-3.67	1.33	1.37
3	L5	3785	A2M	C5-C4	3.66	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4220	6MZ	C5-C4	3.63	1.45	1.39
3	L5	4637	OMG	C6-N1	-3.61	1.32	1.38
1	S2	121	OMU	C4-N3	-3.60	1.32	1.38
52	La	39	V5N	CG-ND1	-3.58	1.34	1.37
3	L5	4299	PSU	C4-N3	-3.58	1.32	1.38
84	At	46	G7M	C5-C4	3.57	1.47	1.38
3	L5	3637	PSU	C4-N3	-3.57	1.32	1.38
1	S2	354	OMU	C4-N3	-3.57	1.32	1.38
3	L5	1683	PSU	C4-N3	-3.57	1.32	1.38
3	L5	4306	OMU	C2-N3	-3.56	1.31	1.38
3	L5	1536	PSU	C4-N3	-3.54	1.32	1.38
1	S2	1232	PSU	C6-C5	3.53	1.39	1.35
3	L5	3770	PSU	C6-C5	3.51	1.39	1.35
3	L5	4552	PSU	C4-N3	-3.50	1.32	1.38
1	S2	1081	PSU	C4-N3	-3.50	1.32	1.38
3	L5	1862	PSU	C4-N3	-3.49	1.32	1.38
1	S2	1367	PSU	C4-N3	-3.48	1.32	1.38
3	L5	4392	OMG	C6-N1	-3.47	1.32	1.38
2	L8	14	OMU	C4-N3	-3.47	1.32	1.38
1	S2	93	PSU	C6-C5	3.46	1.39	1.35
3	L5	4353	PSU	C4-N3	-3.46	1.32	1.38
3	L5	4576	PSU	C4-N3	-3.45	1.32	1.38
1	S2	801	PSU	C6-C5	3.43	1.39	1.35
3	L5	1781	PSU	C6-C5	3.42	1.39	1.35
3	L5	3925	OMU	C4-N3	-3.42	1.32	1.38
1	S2	1136	PSU	C4-N3	-3.42	1.32	1.38
1	S2	966	PSU	C6-C5	3.42	1.39	1.35
3	L5	3764	PSU	C6-C5	3.42	1.39	1.35
3	L5	4312	PSU	C6-C5	3.42	1.39	1.35
3	L5	2415	OMU	C4-N3	-3.40	1.32	1.38
3	L5	3920	PSU	C4-N3	-3.39	1.32	1.38
3	L5	4442	PSU	C4-N3	-3.39	1.32	1.38
3	L5	3695	PSU	C4-N3	-3.38	1.32	1.38
3	L5	1782	PSU	C4-N3	-3.38	1.32	1.38
3	L5	4431	PSU	C4-N3	-3.37	1.32	1.38
1	S2	1367	PSU	C6-C5	3.37	1.39	1.35
1	S2	1625	PSU	C6-C5	3.36	1.39	1.35
3	L5	4972	PSU	C4-N3	-3.35	1.32	1.38
3	L5	2508	PSU	C4-N3	-3.35	1.32	1.38
3	L5	1316	OMG	C5-C4	3.35	1.48	1.38
3	L5	4493	PSU	C4-N3	-3.35	1.32	1.38
1	S2	105	PSU	C4-N3	-3.33	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4471	PSU	C6-C5	3.33	1.39	1.35
3	L5	1524	A2M	C5-N7	-3.33	1.33	1.39
3	L5	2839	PSU	C6-C5	3.32	1.39	1.35
3	L5	4457	PSU	C4-N3	-3.32	1.32	1.38
1	S2	1004	PSU	C4-N3	-3.32	1.32	1.38
3	L5	4361	PSU	C4-N3	-3.32	1.32	1.38
3	L5	4227	OMU	C4-N3	-3.32	1.32	1.38
3	L5	4500	PSU	C4-N3	-3.31	1.32	1.38
1	S2	1174	PSU	C4-N3	-3.31	1.32	1.38
3	L5	1582	PSU	C4-N3	-3.31	1.32	1.38
1	S2	109	PSU	C4-N3	-3.30	1.32	1.38
1	S2	814	PSU	C6-C5	3.30	1.38	1.35
3	L5	3851	PSU	C6-C5	3.29	1.38	1.35
1	S2	1243	PSU	C4-N3	-3.29	1.32	1.38
1	S2	1232	PSU	C4-N3	-3.29	1.32	1.38
1	S2	649	PSU	C4-N3	-3.27	1.32	1.38
84	At	32	PSU	C6-C5	3.27	1.38	1.35
3	L5	1860	PSU	C4-N3	-3.27	1.32	1.38
3	L5	3853	PSU	C4-N3	-3.26	1.32	1.38
1	S2	1238	PSU	C4-N3	-3.26	1.32	1.38
3	L5	1792	PSU	C4-N3	-3.26	1.32	1.38
3	L5	3729	PSU	C4-N3	-3.26	1.32	1.38
3	L5	2837	OMU	C4-N3	-3.25	1.33	1.38
3	L5	3768	PSU	C6-C5	3.24	1.38	1.35
84	At	39	PSU	C6-C5	3.24	1.38	1.35
3	L5	4296	PSU	C4-N3	-3.24	1.32	1.38
3	L5	5010	PSU	C4-N3	-3.24	1.32	1.38
2	L8	55	PSU	C6-C5	3.23	1.38	1.35
1	S2	1445	PSU	C4-N3	-3.23	1.32	1.38
3	L5	2876	OMG	C6-N1	-3.22	1.32	1.38
3	L5	3830	A2M	C5-N7	-3.22	1.33	1.39
1	S2	406	PSU	C4-N3	-3.22	1.32	1.38
1	S2	863	PSU	C6-C5	3.22	1.38	1.35
3	L5	1779	PSU	C4-N3	-3.21	1.32	1.38
3	L5	2787	A2M	C5-N7	-3.21	1.33	1.39
3	L5	4689	PSU	C4-N3	-3.21	1.32	1.38
3	L5	4196	OMG	C6-N1	-3.21	1.32	1.38
1	S2	601	OMG	C6-N1	-3.20	1.32	1.38
3	L5	4306	OMU	C4-N3	-3.20	1.33	1.38
3	L5	4312	PSU	C4-N3	-3.20	1.32	1.38
1	S2	966	PSU	C4-N3	-3.20	1.32	1.38
1	S2	354	OMU	C2-N3	-3.20	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4493	PSU	C6-C5	3.20	1.38	1.35
3	L5	1744	PSU	C6-C5	3.19	1.38	1.35
85	Pt	56	PSU	C6-C5	3.19	1.38	1.35
1	S2	1056	PSU	C4-N3	-3.19	1.32	1.38
3	L5	2815	A2M	C5-N7	-3.19	1.33	1.39
3	L5	4403	PSU	C4-N3	-3.18	1.32	1.38
1	S2	218	PSU	C4-N3	-3.18	1.32	1.38
3	L5	3851	PSU	C4-N3	-3.18	1.32	1.38
3	L5	3637	PSU	C6-C5	3.18	1.38	1.35
1	S2	1347	PSU	C4-N3	-3.18	1.32	1.38
1	S2	686	PSU	C4-N3	-3.18	1.32	1.38
1	S2	681	PSU	C4-N3	-3.17	1.32	1.38
1	S2	1804	OMU	C4-N3	-3.17	1.33	1.38
3	L5	3758	PSU	C4-N3	-3.17	1.32	1.38
3	L5	4420	PSU	O4'-C1'	-3.17	1.39	1.43
3	L5	4620	OMU	C4-N3	-3.17	1.33	1.38
3	L5	4636	PSU	C4-N3	-3.16	1.32	1.38
3	L5	3844	PSU	C6-C5	3.16	1.38	1.35
3	L5	4628	PSU	C4-N3	-3.16	1.32	1.38
3	L5	4494	OMG	C6-N1	-3.16	1.32	1.38
1	S2	1239	PSU	C4-N3	-3.15	1.32	1.38
1	S2	866	PSU	C4-N3	-3.15	1.32	1.38
3	L5	4531	PSU	C6-C5	3.14	1.38	1.35
1	S2	651	PSU	C4-N3	-3.14	1.33	1.38
1	S2	36	PSU	C4-N3	-3.14	1.33	1.38
85	Pt	8	4SU	C5-C4	-3.14	1.38	1.42
1	S2	116	OMU	C4-N3	-3.14	1.33	1.38
1	S2	681	PSU	C6-C5	3.14	1.38	1.35
3	L5	3639	PSU	C4-N3	-3.13	1.33	1.38
1	S2	863	PSU	C4-N3	-3.12	1.33	1.38
1	S2	1643	PSU	C4-N3	-3.11	1.33	1.38
1	S2	1244	PSU	C6-C5	3.11	1.38	1.35
1	S2	866	PSU	C6-C5	3.11	1.38	1.35
3	L5	3818	UY1	C4-N3	-3.11	1.33	1.38
84	At	8	4SU	C5-C4	-3.10	1.38	1.42
3	L5	3764	PSU	C4-N3	-3.10	1.33	1.38
3	L5	4293	PSU	C6-C5	3.10	1.38	1.35
3	L5	3884	PSU	C4-N3	-3.10	1.33	1.38
3	L5	3627	OMG	C6-N1	-3.09	1.33	1.38
3	L5	3844	PSU	C4-N3	-3.09	1.33	1.38
3	L5	4293	PSU	C4-N3	-3.09	1.33	1.38
2	L8	69	PSU	C4-N3	-3.09	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4569	PSU	C4-N3	-3.09	1.33	1.38
3	L5	4972	PSU	C6-C5	3.09	1.38	1.35
1	S2	668	A2M	C5-N7	-3.08	1.33	1.39
1	S2	436	OMG	C6-N1	-3.08	1.33	1.38
1	S2	484	A2M	C5-N7	-3.08	1.33	1.39
3	L5	2632	PSU	C4-N3	-3.08	1.33	1.38
3	L5	3718	A2M	C5-N7	-3.08	1.33	1.39
1	S2	822	PSU	C4-N3	-3.08	1.33	1.38
1	S2	121	OMU	C2-N3	-3.07	1.32	1.38
3	L5	1871	A2M	C5-N7	-3.07	1.33	1.39
3	L5	3715	PSU	C4-N3	-3.07	1.33	1.38
3	L5	4579	PSU	C4-N3	-3.07	1.33	1.38
3	L5	4403	PSU	C6-C5	3.07	1.38	1.35
2	L8	55	PSU	C4-N3	-3.06	1.33	1.38
3	L5	4532	PSU	C4-N3	-3.06	1.33	1.38
1	S2	1177	PSU	C4-N3	-3.06	1.33	1.38
3	L5	4576	PSU	C6-C5	3.06	1.38	1.35
1	S2	119	PSU	C4-N3	-3.05	1.33	1.38
1	S2	1326	UY1	C4-N3	-3.05	1.33	1.38
2	L8	14	OMU	C2-N3	-3.05	1.32	1.38
3	L5	1316	OMG	C6-N1	-3.05	1.33	1.38
3	L5	1779	PSU	C6-C5	3.05	1.38	1.35
1	S2	686	PSU	C6-C5	3.05	1.38	1.35
3	L5	1677	PSU	C4-N3	-3.04	1.33	1.38
3	L5	4471	PSU	C4-N3	-3.04	1.33	1.38
2	L8	75	OMG	C5-C4	3.03	1.47	1.38
1	S2	1239	PSU	C6-C5	3.03	1.38	1.35
1	S2	172	OMU	C4-N3	-3.02	1.33	1.38
3	L5	3825	A2M	C5-N7	-3.02	1.33	1.39
1	S2	573	PSU	C6-C5	3.01	1.38	1.35
3	L5	3851	PSU	C2-N3	-3.01	1.32	1.37
3	L5	4447	5MC	C6-C5	3.01	1.39	1.34
3	L5	1862	PSU	C6-C5	3.01	1.38	1.35
3	L5	2415	OMU	C2-N3	-3.01	1.32	1.38
1	S2	1442	OMU	C4-N3	-3.00	1.33	1.38
3	L5	4403	PSU	C2-N3	-3.00	1.32	1.37
3	L5	4532	PSU	C6-C5	3.00	1.38	1.35
1	S2	815	PSU	C4-N3	-3.00	1.33	1.38
3	L5	1625	OMG	C6-N1	-2.99	1.33	1.38
3	L5	3867	A2M	C5-N7	-2.98	1.33	1.39
1	S2	1692	PSU	C4-N3	-2.98	1.33	1.38
3	L5	3695	PSU	C6-C5	2.98	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1316	OMG	C5-N7	-2.98	1.33	1.39
3	L5	5001	PSU	C4-N3	-2.98	1.33	1.38
1	S2	609	PSU	C6-C5	2.97	1.38	1.35
1	S2	918	PSU	C4-N3	-2.97	1.33	1.38
1	S2	99	A2M	C5-N7	-2.97	1.33	1.39
3	L5	4498	OMU	C4-N3	-2.97	1.33	1.38
3	L5	3920	PSU	C2-N3	-2.97	1.32	1.37
3	L5	2843	PSU	C2-N3	-2.97	1.32	1.37
1	S2	1177	PSU	C6-C5	2.96	1.38	1.35
3	L5	3637	PSU	C2-N3	-2.96	1.32	1.37
3	L5	4392	OMG	C5-C4	2.96	1.46	1.38
3	L5	2839	PSU	C4-N3	-2.96	1.33	1.38
85	Pt	56	PSU	C4-N3	-2.96	1.33	1.38
1	S2	1238	PSU	C6-C5	2.96	1.38	1.35
3	L5	2424	OMG	C5-C4	2.95	1.46	1.38
3	L5	3792	OMG	C5-C4	2.95	1.46	1.38
1	S2	34	PSU	C6-C5	2.95	1.38	1.35
1	S2	509	OMG	C6-N1	-2.94	1.33	1.38
3	L5	4636	PSU	C6-C5	2.94	1.38	1.35
1	S2	1244	PSU	C4-N3	-2.94	1.33	1.38
1	S2	814	PSU	C4-N3	-2.94	1.33	1.38
3	L5	2508	PSU	C6-C5	2.93	1.38	1.35
3	L5	1744	PSU	C4-N3	-2.93	1.33	1.38
1	S2	815	PSU	C6-C5	2.93	1.38	1.35
3	L5	1534	A2M	C5-N7	-2.93	1.33	1.39
3	L5	4299	PSU	C2-N3	-2.92	1.32	1.37
1	S2	918	PSU	C6-C5	2.92	1.38	1.35
3	L5	1782	PSU	C2-N3	-2.92	1.32	1.37
3	L5	4220	6MZ	C5-N7	-2.91	1.33	1.39
3	L5	3899	OMG	C5-C4	2.91	1.46	1.38
1	S2	34	PSU	C4-N3	-2.91	1.33	1.38
3	L5	3899	OMG	C6-N1	-2.91	1.33	1.38
3	L5	3762	PSU	C6-C5	2.90	1.38	1.35
1	S2	867	OMG	C5-C4	2.90	1.46	1.38
1	S2	822	PSU	C6-C5	2.90	1.38	1.35
1	S2	609	PSU	C4-N3	-2.90	1.33	1.38
3	L5	1860	PSU	C6-C5	2.90	1.38	1.35
3	L5	3792	OMG	C6-N1	-2.89	1.33	1.38
3	L5	2876	OMG	C5-C4	2.89	1.46	1.38
1	S2	1056	PSU	C6-C5	2.89	1.38	1.35
3	L5	4499	OMG	C5-C4	2.89	1.46	1.38
1	S2	573	PSU	C4-N3	-2.88	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	LA	216	V5N	CG-ND1	-2.88	1.34	1.37
3	L5	1524	A2M	C4-N9	-2.88	1.31	1.37
3	L5	4623	OMG	C5-C4	2.87	1.46	1.38
1	S2	436	OMG	C5-C4	2.87	1.46	1.38
3	L5	4623	OMG	C6-N1	-2.87	1.33	1.38
3	L5	4227	OMU	C2-N3	-2.87	1.33	1.38
1	S2	601	OMG	C5-C4	2.86	1.46	1.38
3	L5	2363	A2M	C5-N7	-2.86	1.33	1.39
1	S2	1347	PSU	C6-C5	2.86	1.38	1.35
3	L5	2632	PSU	C6-C5	2.85	1.38	1.35
1	S2	1337	4AC	C4-N4	-2.85	1.35	1.39
1	S2	296	PSU	C4-N3	-2.85	1.33	1.38
3	L5	5010	PSU	C6-C5	2.85	1.38	1.35
3	L5	4673	PSU	C4-N3	-2.84	1.33	1.38
3	L5	3925	OMU	C2-N3	-2.84	1.33	1.38
3	L5	1792	PSU	C2-N3	-2.84	1.32	1.37
3	L5	3768	PSU	C4-N3	-2.84	1.33	1.38
84	At	32	PSU	C4-N3	-2.84	1.33	1.38
1	S2	572	PSU	C4-N3	-2.84	1.33	1.38
1	S2	1490	OMG	C6-N1	-2.83	1.33	1.38
1	S2	1326	UY1	C6-C5	2.83	1.38	1.35
1	S2	1248	B8N	C6-C5	2.83	1.39	1.35
3	L5	398	A2M	C5-N7	-2.82	1.33	1.39
3	L5	3639	PSU	C6-C5	2.82	1.38	1.35
3	L5	3734	PSU	C4-N3	-2.82	1.33	1.38
1	S2	296	PSU	C6-C5	2.82	1.38	1.35
3	L5	1683	PSU	C2-N1	-2.82	1.33	1.36
3	L5	4431	PSU	C6-C5	2.82	1.38	1.35
1	S2	1447	OMG	C6-N1	-2.81	1.33	1.38
1	S2	1328	OMG	C5-C4	2.81	1.46	1.38
3	L5	1326	A2M	C5-N7	-2.81	1.34	1.39
3	L5	3785	A2M	C5-N7	-2.81	1.34	1.39
3	L5	4228	OMG	C4-N9	-2.81	1.30	1.38
1	S2	1832	6MZ	C5-N7	-2.81	1.34	1.39
1	S2	1643	PSU	C6-C5	2.80	1.38	1.35
1	S2	1328	OMG	C6-N1	-2.80	1.33	1.38
3	L5	1782	PSU	C6-C5	2.80	1.38	1.35
84	At	37	MIA	C5-C6	2.79	1.48	1.41
3	L5	4618	OMG	C6-N1	-2.79	1.33	1.38
1	S2	1851	MA6	C5-N7	-2.79	1.34	1.39
3	L5	4423	PSU	C4-N3	-2.79	1.33	1.38
1	S2	1136	PSU	C6-C5	2.79	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1683	PSU	C2-N3	-2.78	1.32	1.37
3	L5	4552	PSU	C2-N3	-2.78	1.32	1.37
1	S2	509	OMG	C5-C4	2.78	1.46	1.38
3	L5	3782	5MC	C6-C5	2.77	1.39	1.34
1	S2	683	OMG	C5-C4	2.77	1.46	1.38
3	L5	3744	OMG	C6-N1	-2.77	1.33	1.38
1	S2	1243	PSU	C6-C5	2.77	1.38	1.35
1	S2	1447	OMG	C5-C4	2.77	1.46	1.38
3	L5	1536	PSU	C2-N3	-2.77	1.32	1.37
1	S2	1842	4AC	C4-N4	-2.76	1.35	1.39
3	L5	4521	PSU	C2-N3	-2.76	1.32	1.37
3	L5	4370	OMG	C5-C4	2.76	1.46	1.38
3	L5	4523	A2M	C5-N7	-2.75	1.34	1.39
3	L5	4353	PSU	C6-C5	2.75	1.38	1.35
3	L5	4296	PSU	C6-C5	2.75	1.38	1.35
1	S2	1692	PSU	C6-C5	2.75	1.38	1.35
3	L5	2837	OMU	C2-N3	-2.75	1.33	1.38
3	L5	3729	PSU	C6-C5	2.75	1.38	1.35
3	L5	3639	PSU	C2-N3	-2.75	1.33	1.37
3	L5	4498	OMU	C2-N3	-2.75	1.33	1.38
3	L5	3770	PSU	C4-N3	-2.75	1.33	1.38
3	L5	3944	OMG	C5-C4	2.74	1.46	1.38
1	S2	1490	OMG	C5-C4	2.74	1.46	1.38
3	L5	1322	1MA	C5-C4	2.74	1.46	1.38
3	L5	1536	PSU	C2-N1	-2.74	1.33	1.36
3	L5	4579	PSU	C2-N3	-2.74	1.33	1.37
1	S2	218	PSU	C6-C5	2.74	1.38	1.35
1	S2	105	PSU	C6-C5	2.74	1.38	1.35
1	S2	649	PSU	C6-C5	2.74	1.38	1.35
1	S2	683	OMG	C6-N1	-2.74	1.33	1.38
3	L5	4689	PSU	C6-C5	2.73	1.38	1.35
3	L5	4499	OMG	C6-N1	-2.73	1.33	1.38
1	S2	428	OMU	C4-N3	-2.73	1.33	1.38
3	L5	3734	PSU	C6-C5	2.73	1.38	1.35
3	L5	1322	1MA	C5-N7	-2.72	1.33	1.39
3	L5	1781	PSU	C4-N3	-2.72	1.33	1.38
3	L5	4228	OMG	C5-C4	2.72	1.46	1.38
3	L5	5001	PSU	C6-C5	2.72	1.38	1.35
1	S2	109	PSU	C6-C5	2.72	1.38	1.35
3	L5	1683	PSU	C6-C5	2.72	1.38	1.35
3	L5	3884	PSU	C2-N3	-2.72	1.33	1.37
1	S2	36	PSU	C6-C5	2.71	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	At	46	G7M	C6-N1	-2.71	1.33	1.38
3	L5	4579	PSU	C2-N1	-2.71	1.33	1.36
1	S2	105	PSU	C2-N3	-2.71	1.33	1.37
84	At	16	H2U	C2-N3	-2.70	1.33	1.38
1	S2	572	PSU	C6-C5	2.70	1.38	1.35
1	S2	801	PSU	C4-N3	-2.69	1.33	1.38
1	S2	627	OMU	C4-N3	-2.69	1.34	1.38
3	L5	4312	PSU	C2-N3	-2.69	1.33	1.37
3	L5	2424	OMG	C5-N7	-2.69	1.33	1.39
1	S2	590	A2M	C5-N7	-2.68	1.34	1.39
3	L5	4420	PSU	C4-N3	-2.68	1.33	1.38
1	S2	1851	MA6	C5-C6	2.68	1.48	1.41
3	L5	2424	OMG	C6-N1	-2.68	1.33	1.38
3	L5	4494	OMG	C5-C4	2.67	1.46	1.38
1	S2	1004	PSU	C2-N1	-2.67	1.33	1.36
1	S2	512	A2M	C5-N7	-2.67	1.34	1.39
3	L5	4590	A2M	C5-N7	-2.67	1.34	1.39
1	S2	1136	PSU	C2-N3	-2.67	1.33	1.37
3	L5	1625	OMG	C4-N9	-2.66	1.31	1.38
3	L5	4361	PSU	C6-C5	2.66	1.38	1.35
3	L5	4420	PSU	C6-C5	2.66	1.38	1.35
1	S2	815	PSU	C2-N3	-2.66	1.33	1.37
3	L5	4552	PSU	C2-N1	-2.66	1.33	1.36
1	S2	406	PSU	C6-C5	2.66	1.38	1.35
3	L5	4457	PSU	C6-C5	2.66	1.38	1.35
3	L5	4494	OMG	C5-N7	-2.65	1.33	1.39
3	L5	3884	PSU	C6-C5	2.65	1.38	1.35
3	L5	4569	PSU	C6-C5	2.65	1.38	1.35
3	L5	4353	PSU	C2-N3	-2.65	1.33	1.37
3	L5	4442	PSU	C2-N3	-2.65	1.33	1.37
3	L5	3715	PSU	C6-C5	2.65	1.38	1.35
3	L5	3920	PSU	C6-C5	2.64	1.38	1.35
1	S2	1447	OMG	C5-N7	-2.64	1.33	1.39
3	L5	1860	PSU	C2-N3	-2.64	1.33	1.37
1	S2	1850	MA6	C5-C6	2.64	1.48	1.41
3	L5	3944	OMG	C6-N1	-2.64	1.33	1.38
3	L5	4457	PSU	C2-N3	-2.63	1.33	1.37
1	S2	644	OMG	C5-C4	2.63	1.45	1.38
3	L5	1524	A2M	C8-N9	-2.63	1.33	1.37
3	L5	400	A2M	C5-C6	2.63	1.48	1.41
1	S2	1004	PSU	C2-N3	-2.63	1.33	1.37
3	L5	1582	PSU	C6-C5	2.63	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1056	PSU	C2-N3	-2.63	1.33	1.37
1	S2	116	OMU	C2-N3	-2.63	1.33	1.38
1	S2	1625	PSU	C4-N3	-2.62	1.33	1.38
3	L5	4618	OMG	C5-C4	2.62	1.45	1.38
3	L5	4552	PSU	C6-C5	2.62	1.38	1.35
3	L5	4493	PSU	C2-N3	-2.62	1.33	1.37
3	L5	3844	PSU	C2-N1	-2.62	1.33	1.36
3	L5	1871	A2M	C5-C6	2.62	1.48	1.41
3	L5	4196	OMG	C5-C4	2.62	1.45	1.38
1	S2	1832	6MZ	C4-N9	-2.62	1.32	1.37
1	S2	1804	OMU	C5-C4	-2.61	1.38	1.43
3	L5	3744	OMG	C5-C4	2.61	1.45	1.38
84	At	39	PSU	C4-N3	-2.61	1.34	1.38
1	S2	468	A2M	C5-C6	2.61	1.48	1.41
1	S2	1445	PSU	C6-C5	2.61	1.38	1.35
1	S2	159	A2M	C5-N7	-2.61	1.34	1.39
3	L5	2815	A2M	C5-C6	2.61	1.48	1.41
1	S2	1850	MA6	C4-N9	-2.61	1.32	1.37
3	L5	2364	OMG	C5-C4	2.61	1.45	1.38
1	S2	218	PSU	C2-N3	-2.61	1.33	1.37
1	S2	1238	PSU	C2-N3	-2.60	1.33	1.37
1	S2	576	A2M	C5-N7	-2.60	1.34	1.39
3	L5	3762	PSU	C4-N3	-2.60	1.34	1.38
1	S2	1643	PSU	C2-N1	-2.60	1.33	1.36
1	S2	576	A2M	C5-C6	2.60	1.48	1.41
3	L5	3627	OMG	C5-N7	-2.60	1.33	1.39
1	S2	1288	OMU	C4-N3	-2.59	1.34	1.38
1	S2	166	A2M	C5-N7	-2.59	1.34	1.39
3	L5	2815	A2M	C8-N9	-2.59	1.33	1.37
1	S2	1692	PSU	C2-N3	-2.59	1.33	1.37
3	L5	4576	PSU	C2-N3	-2.58	1.33	1.37
3	L5	4620	OMU	C2-N3	-2.58	1.33	1.38
3	L5	1871	A2M	C4-N9	-2.58	1.32	1.37
1	S2	406	PSU	C2-N1	-2.58	1.33	1.36
1	S2	93	PSU	C4-N3	-2.58	1.34	1.38
3	L5	4471	PSU	C2-N3	-2.58	1.33	1.37
1	S2	1643	PSU	C2-N3	-2.58	1.33	1.37
3	L5	3627	OMG	C5-C4	2.58	1.45	1.38
3	L5	1862	PSU	C2-N3	-2.57	1.33	1.37
1	S2	468	A2M	C5-N7	-2.57	1.34	1.39
1	S2	1081	PSU	C2-N3	-2.57	1.33	1.37
3	L5	4531	PSU	C4-N3	-2.57	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	119	PSU	C6-C5	2.57	1.38	1.35
1	S2	27	A2M	C5-N7	-2.57	1.34	1.39
3	L5	2508	PSU	C2-N3	-2.57	1.33	1.37
3	L5	3758	PSU	C2-N3	-2.57	1.33	1.37
1	S2	644	OMG	C6-N1	-2.57	1.34	1.38
3	L5	1625	OMG	C5-N7	-2.56	1.33	1.39
1	S2	649	PSU	C2-N3	-2.56	1.33	1.37
3	L5	4431	PSU	C2-N3	-2.56	1.33	1.37
1	S2	1174	PSU	C6-C5	2.55	1.38	1.35
3	L5	4637	OMG	C5-N7	-2.55	1.34	1.39
1	S2	866	PSU	C2-N3	-2.55	1.33	1.37
1	S2	1490	OMG	C5-N7	-2.55	1.34	1.39
3	L5	3729	PSU	C2-N3	-2.55	1.33	1.37
3	L5	1862	PSU	C2-N1	-2.55	1.33	1.36
3	L5	3695	PSU	C2-N3	-2.55	1.33	1.37
3	L5	3785	A2M	C4-N9	-2.54	1.32	1.37
3	L5	4623	OMG	C5-N7	-2.54	1.34	1.39
1	S2	651	PSU	C2-N3	-2.54	1.33	1.37
3	L5	3760	A2M	C5-C6	2.54	1.48	1.41
3	L5	4628	PSU	C6-C5	2.54	1.38	1.35
1	S2	1081	PSU	C6-C5	2.54	1.38	1.35
3	L5	4392	OMG	C5-N7	-2.54	1.34	1.39
1	S2	1851	MA6	C4-N9	-2.53	1.32	1.37
1	S2	1004	PSU	C6-C5	2.53	1.38	1.35
3	L5	4370	OMG	C6-N1	-2.53	1.34	1.38
1	S2	966	PSU	C2-N3	-2.53	1.33	1.37
1	S2	1174	PSU	C2-N3	-2.53	1.33	1.37
1	S2	1031	A2M	C5-N7	-2.53	1.34	1.39
1	S2	601	OMG	C5-N7	-2.52	1.34	1.39
3	L5	2363	A2M	C5-C6	2.52	1.48	1.41
3	L5	4689	PSU	C2-N3	-2.52	1.33	1.37
1	S2	1442	OMU	C2-N3	-2.52	1.33	1.38
85	Pt	21	H2U	C2-N3	-2.52	1.33	1.38
84	At	20	H2U	C2-N3	-2.52	1.33	1.38
1	S2	1850	MA6	C5-N7	-2.52	1.34	1.39
3	L5	3723	A2M	C5-N7	-2.51	1.34	1.39
1	S2	1678	A2M	C5-N7	-2.51	1.34	1.39
1	S2	116	OMU	C5-C4	-2.51	1.38	1.43
3	L5	3830	A2M	C4-N9	-2.50	1.32	1.37
1	S2	121	OMU	C5-C4	-2.50	1.38	1.43
1	S2	406	PSU	C2-N3	-2.50	1.33	1.37
3	L5	1779	PSU	C2-N3	-2.50	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4636	PSU	C2-N3	-2.50	1.33	1.37
3	L5	4972	PSU	C2-N3	-2.50	1.33	1.37
3	L5	4532	PSU	C2-N1	-2.50	1.33	1.36
1	S2	1442	OMU	C5-C4	-2.50	1.38	1.43
3	L5	400	A2M	C5-N7	-2.49	1.34	1.39
3	L5	3768	PSU	C2-N3	-2.49	1.33	1.37
3	L5	1536	PSU	C2'-C1'	-2.49	1.50	1.53
3	L5	4423	PSU	C6-C5	2.49	1.38	1.35
3	L5	3853	PSU	C2-N3	-2.49	1.33	1.37
1	S2	1678	A2M	C5-C6	2.49	1.47	1.41
3	L5	1322	1MA	C6-N6	2.49	1.34	1.28
1	S2	1239	PSU	C2-N3	-2.49	1.33	1.37
3	L5	4361	PSU	C2-N3	-2.49	1.33	1.37
3	L5	1792	PSU	C6-C5	2.49	1.38	1.35
1	S2	159	A2M	C5-C6	2.49	1.47	1.41
1	S2	668	A2M	C4-N9	-2.49	1.32	1.37
1	S2	354	OMU	C5-C4	-2.49	1.38	1.43
1	S2	1081	PSU	O4'-C1'	-2.49	1.40	1.43
3	L5	4228	OMG	C6-N1	-2.49	1.34	1.38
85	Pt	8	4SU	C2-N3	-2.49	1.33	1.38
3	L5	1326	A2M	C5-C6	2.48	1.47	1.41
3	L5	1534	A2M	C4-N9	-2.48	1.32	1.37
1	S2	1031	A2M	C5-C6	2.48	1.47	1.41
1	S2	36	PSU	C2-N1	-2.48	1.33	1.36
84	At	16	H2U	C4-N3	-2.47	1.33	1.37
3	L5	4571	A2M	C5-N7	-2.47	1.34	1.39
2	L8	69	PSU	C2'-C1'	-2.47	1.50	1.53
1	S2	27	A2M	C5-C6	2.47	1.47	1.41
3	L5	5010	PSU	C2-N3	-2.47	1.33	1.37
3	L5	4620	OMU	C5-C4	-2.46	1.38	1.43
1	S2	172	OMU	C2-N1	2.46	1.42	1.38
3	L5	2401	A2M	C4-N9	-2.46	1.32	1.37
3	L5	4500	PSU	C2-N3	-2.46	1.33	1.37
3	L5	4571	A2M	C4-N9	-2.46	1.32	1.37
3	L5	4392	OMG	C4-N9	-2.46	1.31	1.38
3	L5	3718	A2M	C4-N9	-2.46	1.32	1.37
3	L5	4361	PSU	C2-N1	-2.46	1.33	1.36
3	L5	2401	A2M	C5-N7	-2.46	1.34	1.39
3	L5	3844	PSU	C2-N3	-2.46	1.33	1.37
3	L5	3851	PSU	C2-N1	-2.45	1.33	1.36
3	L5	3830	A2M	C8-N9	-2.45	1.33	1.37
1	S2	627	OMU	C2-N3	-2.45	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1383	A2M	C5-N7	-2.45	1.34	1.39
3	L5	1582	PSU	C2-N3	-2.44	1.33	1.37
3	L5	4442	PSU	C2-N1	-2.44	1.33	1.36
3	L5	4493	PSU	C2-N1	-2.44	1.33	1.36
3	L5	4571	A2M	C5-C6	2.44	1.47	1.41
3	L5	2632	PSU	C2-N3	-2.44	1.33	1.37
1	S2	590	A2M	C5-C6	2.44	1.47	1.41
3	L5	4299	PSU	C6-C5	2.44	1.38	1.35
3	L5	3760	A2M	C5-N7	-2.44	1.34	1.39
1	S2	119	PSU	C2-N3	-2.44	1.33	1.37
3	L5	4532	PSU	C2-N3	-2.44	1.33	1.37
3	L5	4590	A2M	C5-C6	2.44	1.47	1.41
1	S2	1367	PSU	C2-N3	-2.43	1.33	1.37
3	L5	3944	OMG	C5-N7	-2.43	1.34	1.39
3	L5	3758	PSU	C6-C5	2.43	1.38	1.35
3	L5	4500	PSU	C6-C5	2.43	1.38	1.35
84	At	37	MIA	C8-N7	2.43	1.36	1.31
1	S2	512	A2M	C5-C6	2.42	1.47	1.41
2	L8	69	PSU	C2-N1	-2.42	1.33	1.36
1	S2	1804	OMU	C2-N3	-2.42	1.33	1.38
3	L5	4673	PSU	C6-C5	2.41	1.38	1.35
3	L5	4623	OMG	C4-N9	-2.41	1.31	1.38
1	S2	863	PSU	C2-N3	-2.41	1.33	1.37
1	S2	1639	G7M	C6-N1	-2.41	1.34	1.38
1	S2	867	OMG	C6-N1	-2.41	1.34	1.38
3	L5	4442	PSU	C6-C5	2.41	1.38	1.35
1	S2	1445	PSU	C2-N3	-2.41	1.33	1.37
1	S2	1174	PSU	C2-N1	-2.41	1.33	1.36
1	S2	668	A2M	C8-N9	-2.41	1.33	1.37
1	S2	119	PSU	C2-N1	-2.41	1.33	1.36
3	L5	4431	PSU	C2-N1	-2.41	1.33	1.36
2	L8	55	PSU	C2-N3	-2.41	1.33	1.37
3	L5	4403	PSU	C2-N1	-2.40	1.33	1.36
1	S2	1383	A2M	C5-C6	2.40	1.47	1.41
3	L5	4637	OMG	C5-C4	2.40	1.45	1.38
3	L5	1625	OMG	C5-C4	2.40	1.45	1.38
3	L5	3818	UY1	C2-N3	-2.40	1.33	1.37
3	L5	2815	A2M	C4-N9	-2.39	1.32	1.37
3	L5	3899	OMG	C5-N7	-2.39	1.34	1.39
85	Pt	21	H2U	C4-N3	-2.39	1.33	1.37
1	S2	109	PSU	C2-N1	-2.39	1.33	1.36
3	L5	4498	OMU	C5-C4	-2.39	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L8	69	PSU	C6-C5	2.39	1.37	1.35
3	L5	4296	PSU	C2-N3	-2.39	1.33	1.37
3	L5	4972	PSU	C2-N1	-2.38	1.33	1.36
1	S2	166	A2M	C5-C6	2.38	1.47	1.41
1	S2	1832	6MZ	C5-C6	2.38	1.47	1.41
1	S2	822	PSU	C2-N1	-2.38	1.33	1.36
84	At	20	H2U	C4-N3	-2.38	1.33	1.37
1	S2	109	PSU	C2-N3	-2.38	1.33	1.37
1	S2	681	PSU	C2-N3	-2.38	1.33	1.37
3	L5	2415	OMU	C5-C4	-2.37	1.38	1.43
3	L5	2843	PSU	C6-C5	2.37	1.37	1.35
3	L5	3723	A2M	C4-N9	-2.37	1.32	1.37
1	S2	436	OMG	C5-N7	-2.37	1.34	1.39
3	L5	4353	PSU	C2-N1	-2.37	1.33	1.36
1	S2	668	A2M	C5-C6	2.37	1.47	1.41
1	S2	172	OMU	C2-N3	-2.37	1.33	1.38
1	S2	651	PSU	C6-C5	2.37	1.37	1.35
1	S2	1347	PSU	C2-N3	-2.37	1.33	1.37
1	S2	1243	PSU	C2-N3	-2.36	1.33	1.37
3	L5	4293	PSU	C2-N3	-2.36	1.33	1.37
3	L5	1326	A2M	C4-N9	-2.36	1.32	1.37
1	S2	1328	OMG	C5-N7	-2.35	1.34	1.39
3	L5	4299	PSU	C2-N1	-2.35	1.33	1.36
3	L5	4523	A2M	C5-C6	2.35	1.47	1.41
1	S2	509	OMG	C5-N7	-2.35	1.34	1.39
1	S2	822	PSU	C2-N3	-2.35	1.33	1.37
3	L5	3744	OMG	C5-N7	-2.35	1.34	1.39
3	L5	3723	A2M	C5-C6	2.34	1.47	1.41
3	L5	1792	PSU	C2-N1	-2.34	1.33	1.36
3	L5	4618	OMG	C5-N7	-2.34	1.34	1.39
3	L5	4494	OMG	C4-N9	-2.34	1.32	1.38
3	L5	4579	PSU	C6-C5	2.34	1.37	1.35
2	L8	75	OMG	C6-N1	-2.34	1.34	1.38
1	S2	36	PSU	C2-N3	-2.34	1.33	1.37
3	L5	3844	PSU	C6-N1	-2.34	1.32	1.36
3	L5	3867	A2M	C4-N9	-2.33	1.32	1.37
3	L5	4370	OMG	C5-N7	-2.33	1.34	1.39
3	L5	3724	A2M	C4-N9	-2.33	1.32	1.37
1	S2	1445	PSU	C2'-C1'	-2.33	1.50	1.53
3	L5	1534	A2M	C5-C6	2.33	1.47	1.41
3	L5	5001	PSU	C2-N3	-2.33	1.33	1.37
3	L5	1782	PSU	C2-N1	-2.33	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C2-N1	-2.32	1.33	1.36
1	S2	34	PSU	C2-N3	-2.32	1.33	1.37
3	L5	4628	PSU	C2-N3	-2.32	1.33	1.37
3	L5	3818	UY1	C6-C5	2.32	1.37	1.35
3	L5	4196	OMG	C4-N9	-2.32	1.32	1.38
3	L5	4370	OMG	C4-N9	-2.31	1.32	1.38
3	L5	1779	PSU	C2-N1	-2.31	1.33	1.36
3	L5	4457	PSU	C2-N1	-2.31	1.33	1.36
1	S2	651	PSU	C2-N1	-2.31	1.33	1.36
3	L5	3825	A2M	C4-N9	-2.31	1.32	1.37
1	S2	484	A2M	C5-C6	2.31	1.47	1.41
1	S2	867	OMG	C5-N7	-2.30	1.34	1.39
1	S2	649	PSU	C2-N1	-2.30	1.33	1.36
3	L5	1677	PSU	C2-N3	-2.30	1.33	1.37
3	L5	1522	OMG	C5-C4	2.30	1.45	1.38
3	L5	1677	PSU	C6-C5	2.29	1.37	1.35
3	L5	4569	PSU	C6-N1	-2.29	1.32	1.36
1	S2	1678	A2M	C4-N9	-2.29	1.32	1.37
3	L5	4423	PSU	C2-N1	-2.29	1.33	1.36
3	L5	2364	OMG	C6-N1	-2.29	1.34	1.38
3	L5	1582	PSU	O4'-C1'	-2.29	1.40	1.43
3	L5	4293	PSU	C2-N1	-2.29	1.33	1.36
3	L5	3718	A2M	C5-C6	2.29	1.47	1.41
84	At	8	4SU	C2-N1	2.28	1.42	1.38
3	L5	4499	OMG	C5-N7	-2.28	1.34	1.39
3	L5	3925	OMU	C5-C4	-2.28	1.38	1.43
1	S2	484	A2M	C4-N9	-2.28	1.33	1.37
3	L5	2843	PSU	C2-N1	-2.28	1.33	1.36
1	S2	866	PSU	C2-N1	-2.27	1.33	1.36
3	L5	3724	A2M	C5-N7	-2.27	1.34	1.39
3	L5	2876	OMG	C5-N7	-2.27	1.34	1.39
3	L5	3768	PSU	C2-N1	-2.27	1.33	1.36
1	S2	296	PSU	C2-N3	-2.27	1.33	1.37
1	S2	1445	PSU	C2-N1	-2.27	1.33	1.36
1	S2	686	PSU	C2-N3	-2.27	1.33	1.37
1	S2	1244	PSU	C2-N3	-2.27	1.33	1.37
3	L5	3867	A2M	C8-N9	-2.27	1.33	1.37
3	L5	4521	PSU	C2-N1	-2.26	1.33	1.36
3	L5	3830	A2M	C5-C6	2.26	1.47	1.41
3	L5	4569	PSU	C2-N1	-2.26	1.33	1.36
1	S2	99	A2M	C4-N9	-2.26	1.33	1.37
1	S2	1288	OMU	C2-N3	-2.26	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L8	69	PSU	C6-N1	-2.25	1.32	1.36
1	S2	1031	A2M	C4-N9	-2.25	1.33	1.37
1	S2	814	PSU	C2-N3	-2.25	1.33	1.37
1	S2	1243	PSU	C2-N1	-2.25	1.33	1.36
3	L5	4228	OMG	C5-N7	-2.25	1.34	1.39
3	L5	2632	PSU	C2-N1	-2.24	1.33	1.36
3	L5	4500	PSU	C2-N1	-2.24	1.33	1.36
3	L5	3724	A2M	C5-C6	2.24	1.47	1.41
1	S2	1081	PSU	C2-N1	-2.24	1.33	1.36
1	S2	1851	MA6	C8-N9	-2.24	1.33	1.37
3	L5	4673	PSU	C2-N3	-2.24	1.33	1.37
3	L5	4196	OMG	C5-N7	-2.23	1.34	1.39
3	L5	4628	PSU	C2-N1	-2.23	1.33	1.36
1	S2	1326	UY1	C2-N3	-2.23	1.33	1.37
3	L5	3639	PSU	C2-N1	-2.23	1.33	1.36
3	L5	4618	OMG	C4-N9	-2.23	1.32	1.38
3	L5	2401	A2M	C5-C6	2.23	1.47	1.41
1	S2	1347	PSU	C2-N1	-2.22	1.33	1.36
3	L5	5010	PSU	C2-N1	-2.22	1.33	1.36
1	S2	644	OMG	C4-N9	-2.22	1.32	1.38
1	S2	683	OMG	C5-N7	-2.21	1.34	1.39
1	S2	1232	PSU	C2-N1	-2.21	1.33	1.36
3	L5	2787	A2M	C8-N9	-2.21	1.33	1.37
3	L5	3825	A2M	C5-C6	2.21	1.47	1.41
3	L5	4447	5MC	C6-N1	-2.21	1.34	1.38
3	L5	3920	PSU	C2-N1	-2.21	1.33	1.36
1	S2	576	A2M	C4-N9	-2.21	1.33	1.37
1	S2	1850	MA6	C8-N9	-2.20	1.33	1.37
2	L8	69	PSU	C2-N3	-2.20	1.33	1.37
1	S2	686	PSU	C2-N1	-2.20	1.33	1.36
3	L5	1860	PSU	C2-N1	-2.20	1.33	1.36
1	S2	1239	PSU	C2-N1	-2.20	1.33	1.36
1	S2	218	PSU	C2-N1	-2.19	1.33	1.36
1	S2	644	OMG	C5-N7	-2.19	1.34	1.39
3	L5	1871	A2M	C8-N9	-2.19	1.33	1.37
1	S2	1177	PSU	C2-N3	-2.19	1.33	1.37
1	S2	572	PSU	C2-N3	-2.19	1.33	1.37
1	S2	428	OMU	C2-N3	-2.18	1.34	1.38
3	L5	2364	OMG	C4-N9	-2.18	1.32	1.38
1	S2	1447	OMG	C4-N9	-2.18	1.32	1.38
1	S2	573	PSU	C2-N3	-2.18	1.33	1.37
1	S2	105	PSU	C2'-C1'	-2.18	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3785	A2M	C8-N9	-2.18	1.33	1.37
3	L5	4420	PSU	C2-N3	-2.18	1.33	1.37
1	S2	1490	OMG	C4-N9	-2.18	1.32	1.38
3	L5	2351	OMC	C5-C4	-2.17	1.37	1.42
3	L5	4423	PSU	C2-N3	-2.17	1.33	1.37
1	S2	166	A2M	C4-N9	-2.17	1.33	1.37
3	L5	4306	OMU	C5-C4	-2.17	1.39	1.43
3	L5	3782	5MC	C6-N1	-2.17	1.34	1.38
3	L5	398	A2M	C5-C6	2.16	1.47	1.41
3	L5	4220	6MZ	C4-N9	-2.16	1.33	1.37
1	S2	99	A2M	C5-C6	2.16	1.47	1.41
3	L5	4312	PSU	C2-N1	-2.16	1.33	1.36
3	L5	1534	A2M	C8-N9	-2.16	1.33	1.37
1	S2	576	A2M	C8-N7	2.15	1.35	1.31
3	L5	1683	PSU	C6-N1	-2.15	1.32	1.36
3	L5	3734	PSU	C2-N3	-2.15	1.33	1.37
3	L5	1316	OMG	C4-N9	-2.15	1.32	1.38
3	L5	1322	1MA	C4-N9	-2.14	1.32	1.38
3	L5	3715	PSU	C2-N3	-2.14	1.33	1.37
3	L5	398	A2M	C4-N9	-2.14	1.33	1.37
40	LB	245	HIC	CD2-CG	2.14	1.40	1.36
3	L5	3867	A2M	C5-C6	2.13	1.46	1.41
3	L5	4220	6MZ	C8-N9	-2.13	1.33	1.37
3	L5	400	A2M	C4-N9	-2.13	1.33	1.37
3	L5	4569	PSU	C2-N3	-2.13	1.34	1.37
2	L8	75	OMG	C5-N7	-2.13	1.34	1.39
1	S2	484	A2M	C8-N9	-2.13	1.33	1.37
3	L5	1779	PSU	C2'-C1'	-2.13	1.50	1.53
1	S2	105	PSU	C2-N1	-2.13	1.33	1.36
3	L5	3639	PSU	C2'-C1'	-2.13	1.50	1.53
3	L5	4220	6MZ	C5-C6	2.12	1.47	1.41
1	S2	609	PSU	C2-N1	-2.12	1.33	1.36
85	Pt	56	PSU	C2-N3	-2.12	1.34	1.37
3	L5	2876	OMG	C4-N9	-2.12	1.32	1.38
3	L5	3758	PSU	C2-N1	-2.12	1.33	1.36
3	L5	4523	A2M	C4-N9	-2.12	1.33	1.37
3	L5	1582	PSU	C2-N1	-2.12	1.33	1.36
3	L5	2787	A2M	C4-N9	-2.12	1.33	1.37
1	S2	172	OMU	C5-C4	-2.11	1.39	1.43
3	L5	4590	A2M	C4-N9	-2.11	1.33	1.37
3	L5	2839	PSU	C2-N1	-2.11	1.33	1.36
1	S2	296	PSU	C2-N1	-2.11	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3723	A2M	C8-N7	2.11	1.35	1.31
2	L8	14	OMU	C5-C4	-2.10	1.39	1.43
1	S2	512	A2M	C4-N9	-2.10	1.33	1.37
3	L5	400	A2M	C8-N7	2.10	1.35	1.31
1	S2	1232	PSU	C2-N3	-2.10	1.34	1.37
1	S2	1703	OMC	C6-N1	-2.10	1.33	1.38
3	L5	1536	PSU	C6-C5	2.10	1.37	1.35
1	S2	1692	PSU	C2-N1	-2.10	1.33	1.36
3	L5	3744	OMG	C4-N9	-2.10	1.32	1.38
3	L5	2787	A2M	C5-C6	2.10	1.46	1.41
3	L5	1677	PSU	C2'-C1'	-2.09	1.50	1.53
3	L5	2837	OMU	C5-C4	-2.09	1.39	1.43
3	L5	1536	PSU	C6-N1	-2.09	1.32	1.36
3	L5	3760	A2M	C8-N7	2.09	1.35	1.31
1	S2	867	OMG	C4-N9	-2.09	1.32	1.38
1	S2	1174	PSU	C6-N1	-2.08	1.32	1.36
3	L5	4531	PSU	C2-N1	-2.08	1.33	1.36
3	L5	2839	PSU	C6-N1	-2.08	1.32	1.36
3	L5	3734	PSU	C2-N1	-2.08	1.34	1.36
3	L5	1862	PSU	C6-N1	-2.08	1.32	1.36
1	S2	34	PSU	C2-N1	-2.08	1.34	1.36
1	S2	609	PSU	C2-N3	-2.07	1.34	1.37
3	L5	2839	PSU	O4'-C1'	-2.07	1.41	1.43
3	L5	3841	OMC	C6-N1	-2.07	1.33	1.38
3	L5	3792	OMG	C5-N7	-2.07	1.34	1.39
84	At	46	G7M	C4-N9	-2.07	1.32	1.38
3	L5	3715	PSU	C2-N1	-2.07	1.34	1.36
84	At	32	PSU	C2-N3	-2.07	1.34	1.37
1	S2	681	PSU	C2'-C1'	-2.07	1.50	1.53
1	S2	1177	PSU	C2-N1	-2.07	1.34	1.36
3	L5	3627	OMG	C4-N9	-2.07	1.32	1.38
1	S2	576	A2M	C8-N9	-2.06	1.34	1.37
2	L8	14	OMU	C2-N1	2.06	1.41	1.38
1	S2	918	PSU	C2-N3	-2.06	1.34	1.37
3	L5	1322	1MA	C8-N9	-2.06	1.32	1.37
1	S2	681	PSU	C2-N1	-2.06	1.34	1.36
1	S2	1643	PSU	O4'-C1'	-2.06	1.41	1.43
1	S2	572	PSU	C2-N1	-2.06	1.34	1.36
3	L5	4530	UR3	C5-C4	-2.06	1.38	1.43
3	L5	4521	PSU	O4'-C1'	-2.06	1.41	1.43
84	At	37	MIA	C5-N7	-2.05	1.35	1.39
3	L5	4571	A2M	C8-N7	2.05	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1832	6MZ	C8-N9	-2.05	1.34	1.37
3	L5	4521	PSU	C6-C5	2.05	1.37	1.35
1	S2	468	A2M	C8-N7	2.05	1.35	1.31
3	L5	1522	OMG	C6-N1	-2.05	1.35	1.38
1	S2	627	OMU	C5-C4	-2.04	1.39	1.43
3	L5	4500	PSU	C2'-C1'	-2.04	1.51	1.53
1	S2	1288	OMU	C5-C4	-2.04	1.39	1.43
3	L5	2839	PSU	C2-N3	-2.04	1.34	1.37
3	L5	2363	A2M	C4-N9	-2.04	1.33	1.37
1	S2	1842	4AC	C6-N1	-2.03	1.33	1.38
1	S2	159	A2M	C8-N7	2.03	1.35	1.31
1	S2	468	A2M	C4-N9	-2.03	1.33	1.37
3	L5	4552	PSU	C6-N1	-2.03	1.33	1.36
1	S2	36	PSU	C2'-C1'	-2.03	1.51	1.53
3	L5	3785	A2M	C5-C6	2.03	1.46	1.41
1	S2	512	A2M	C8-N9	-2.03	1.34	1.37
3	L5	4296	PSU	C2-N1	-2.02	1.34	1.36
3	L5	4590	A2M	C8-N7	2.02	1.35	1.31
3	L5	1744	PSU	C2-N3	-2.02	1.34	1.37
3	L5	3764	PSU	C2-N1	-2.02	1.34	1.36
1	S2	27	A2M	C4-N9	-2.02	1.33	1.37
1	S2	1328	OMG	C4-N9	-2.02	1.32	1.38
3	L5	3760	A2M	C4-N9	-2.02	1.33	1.37
3	L5	3853	PSU	C2-N1	-2.02	1.34	1.36
3	L5	5001	PSU	C2-N1	-2.02	1.34	1.36
3	L5	4442	PSU	C6-N1	-2.01	1.33	1.36
3	L5	4431	PSU	C2'-C1'	-2.01	1.51	1.53
3	L5	4637	OMG	C4-N9	-2.01	1.32	1.38
1	S2	801	PSU	C2-N3	-2.01	1.34	1.37
1	S2	1238	PSU	C2-N1	-2.01	1.34	1.36
1	S2	814	PSU	C2'-C1'	-2.01	1.51	1.53
1	S2	966	PSU	C2-N1	-2.00	1.34	1.36
1	S2	121	OMU	C6-N1	-2.00	1.33	1.38
1	S2	683	OMG	C4-N9	-2.00	1.33	1.38
1	S2	1244	PSU	C2-N1	-2.00	1.34	1.36
3	L5	4420	PSU	C2-N1	-2.00	1.34	1.36

All (1204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	At	37	MIA	C12-C13-C14	-9.23	110.44	127.01
1	S2	1639	G7M	CN7-N7-C8	-8.41	112.06	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	At	46	G7M	CN7-N7-C8	-7.88	112.86	124.79
66	Lr	2	SAC	OAC-C1A-N	-7.87	108.06	121.98
3	L5	4521	PSU	N1-C2-N3	7.75	123.35	115.17
6	SA	2	SAC	OAC-C1A-C2A	-7.66	108.41	122.05
84	At	37	MIA	C5-C4-N3	-7.52	119.26	127.18
29	SV	1	AME	OT-CT1-N	-7.41	108.89	121.98
3	L5	4493	PSU	N1-C2-N3	7.40	122.97	115.17
1	S2	1243	PSU	N1-C2-N3	7.38	122.95	115.17
1	S2	105	PSU	N1-C2-N3	7.36	122.93	115.17
3	L5	4530	UR3	C4-N3-C2	-7.32	118.69	124.58
3	L5	4531	PSU	N1-C2-N3	7.29	122.86	115.17
84	At	46	G7M	N9-C8-N7	-7.27	94.82	112.48
1	S2	1367	PSU	N1-C2-N3	7.22	122.78	115.17
3	L5	3920	PSU	N1-C2-N3	7.21	122.77	115.17
3	L5	3851	PSU	N1-C2-N3	7.13	122.69	115.17
1	S2	918	PSU	N1-C2-N3	7.12	122.68	115.17
3	L5	3734	PSU	N1-C2-N3	7.08	122.64	115.17
3	L5	3637	PSU	N1-C2-N3	7.08	122.64	115.17
3	L5	3695	PSU	N1-C2-N3	7.06	122.62	115.17
1	S2	686	PSU	N1-C2-N3	7.04	122.59	115.17
1	S2	1081	PSU	N1-C2-N3	6.98	122.53	115.17
1	S2	1445	PSU	N1-C2-N3	6.97	122.52	115.17
2	L8	55	PSU	N1-C2-N3	6.94	122.49	115.17
3	L5	1683	PSU	N1-C2-N3	6.94	122.49	115.17
1	S2	822	PSU	N1-C2-N3	6.93	122.48	115.17
3	L5	4403	PSU	N1-C2-N3	6.90	122.44	115.17
29	SV	1	AME	OT-CT1-CT2	-6.89	109.78	122.05
3	L5	4552	PSU	N1-C2-N3	6.89	122.44	115.17
3	L5	4353	PSU	N1-C2-N3	6.89	122.44	115.17
3	L5	4296	PSU	N1-C2-N3	6.89	122.44	115.17
1	S2	1232	PSU	N1-C2-N3	6.89	122.43	115.17
3	L5	3844	PSU	N1-C2-N3	6.86	122.41	115.17
1	S2	681	PSU	N1-C2-N3	6.86	122.41	115.17
3	L5	4689	PSU	N1-C2-N3	6.86	122.40	115.17
3	L5	4442	PSU	N1-C2-N3	6.85	122.40	115.17
1	S2	649	PSU	N1-C2-N3	6.84	122.39	115.17
1	S2	1643	PSU	N1-C2-N3	6.84	122.39	115.17
3	L5	4431	PSU	N1-C2-N3	6.83	122.38	115.17
1	S2	109	PSU	N1-C2-N3	6.83	122.37	115.17
3	L5	4569	PSU	N1-C2-N3	6.83	122.37	115.17
1	S2	1639	G7M	N9-C8-N7	-6.81	95.94	112.48
66	Lr	2	SAC	OAC-C1A-C2A	-6.80	109.95	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2839	PSU	N1-C2-N3	6.79	122.33	115.17
1	S2	1056	PSU	N1-C2-N3	6.79	122.33	115.17
3	L5	3729	PSU	N1-C2-N3	6.78	122.32	115.17
3	L5	4636	PSU	N1-C2-N3	6.76	122.30	115.17
3	L5	4312	PSU	N1-C2-N3	6.76	122.30	115.17
1	S2	1692	PSU	N1-C2-N3	6.75	122.29	115.17
3	L5	2632	PSU	N1-C2-N3	6.75	122.29	115.17
1	S2	1326	UY1	N1-C2-N3	6.74	122.28	115.17
3	L5	1860	PSU	N1-C2-N3	6.72	122.26	115.17
1	S2	218	PSU	N1-C2-N3	6.72	122.25	115.17
3	L5	5010	PSU	N1-C2-N3	6.71	122.25	115.17
1	S2	406	PSU	N1-C2-N3	6.70	122.24	115.17
1	S2	1639	G7M	C8-N7-C5	6.70	116.16	107.78
3	L5	1536	PSU	N1-C2-N3	6.70	122.23	115.17
3	L5	2787	A2M	C5-C4-N3	-6.70	117.49	126.72
1	S2	1238	PSU	N1-C2-N3	6.69	122.22	115.17
6	SA	2	SAC	OAC-C1A-N	-6.67	110.19	121.98
3	L5	2843	PSU	N1-C2-N3	6.67	122.20	115.17
1	S2	36	PSU	N1-C2-N3	6.67	122.20	115.17
3	L5	4579	PSU	N1-C2-N3	6.66	122.20	115.17
2	L8	69	PSU	N1-C2-N3	6.66	122.19	115.17
3	L5	1677	PSU	N1-C2-N3	6.65	122.18	115.17
3	L5	1792	PSU	N1-C2-N3	6.65	122.18	115.17
3	L5	1744	PSU	N1-C2-N3	6.63	122.16	115.17
84	At	8	4SU	C4-N3-C2	-6.61	120.98	127.31
3	L5	3764	PSU	N1-C2-N3	6.60	122.13	115.17
3	L5	5001	PSU	N1-C2-N3	6.57	122.10	115.17
1	S2	1177	PSU	N1-C2-N3	6.57	122.10	115.17
3	L5	4500	PSU	N1-C2-N3	6.57	122.10	115.17
84	At	46	G7M	C8-N7-C5	6.57	115.99	107.78
3	L5	4637	OMG	C5-C4-N3	-6.55	117.96	128.39
1	S2	1347	PSU	N1-C2-N3	6.54	122.07	115.17
3	L5	4457	PSU	N1-C2-N3	6.54	122.06	115.17
84	At	39	PSU	N1-C2-N3	6.53	122.06	115.17
1	S2	34	PSU	N1-C2-N3	6.52	122.05	115.17
1	S2	814	PSU	N1-C2-N3	6.52	122.05	115.17
3	L5	1779	PSU	N1-C2-N3	6.52	122.05	115.17
1	S2	1244	PSU	N1-C2-N3	6.51	122.04	115.17
1	S2	863	PSU	N1-C2-N3	6.50	122.03	115.17
3	L5	3899	OMG	C5-C4-N3	-6.50	118.04	128.39
1	S2	1639	G7M	N9-C4-N3	6.50	138.94	125.95
3	L5	4361	PSU	N1-C2-N3	6.49	122.02	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	At	8	4SU	C5-C4-N3	6.49	120.79	114.75
1	S2	801	PSU	N1-C2-N3	6.49	122.01	115.17
3	L5	3762	PSU	N1-C2-N3	6.47	122.00	115.17
3	L5	1781	PSU	N1-C2-N3	6.46	121.98	115.17
3	L5	4299	PSU	N1-C2-N3	6.45	121.97	115.17
3	L5	4972	PSU	N1-C2-N3	6.45	121.97	115.17
1	S2	296	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	3715	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	4423	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	1136	PSU	N1-C2-N3	6.41	121.94	115.17
85	Pt	56	PSU	N1-C2-N3	6.38	121.90	115.17
1	S2	590	A2M	C5-C4-N3	-6.37	117.94	126.72
1	S2	966	PSU	N1-C2-N3	6.37	121.89	115.17
1	S2	119	PSU	N1-C2-N3	6.37	121.89	115.17
1	S2	1625	PSU	N1-C2-N3	6.37	121.88	115.17
1	S2	1174	PSU	N1-C2-N3	6.36	121.88	115.17
1	S2	572	PSU	N1-C2-N3	6.36	121.88	115.17
3	L5	3770	PSU	N1-C2-N3	6.36	121.88	115.17
1	S2	609	PSU	N1-C2-N3	6.35	121.87	115.17
3	L5	4420	PSU	N1-C2-N3	6.35	121.87	115.17
1	S2	573	PSU	N1-C2-N3	6.34	121.86	115.17
1	S2	1239	PSU	N1-C2-N3	6.34	121.85	115.17
3	L5	3639	PSU	N1-C2-N3	6.33	121.85	115.17
3	L5	2424	OMG	C5-C4-N3	-6.31	118.34	128.39
3	L5	3792	OMG	C5-C4-N3	-6.31	118.35	128.39
1	S2	815	PSU	N1-C2-N3	6.29	121.81	115.17
3	L5	3758	PSU	N1-C2-N3	6.27	121.79	115.17
84	At	32	PSU	N1-C2-N3	6.26	121.77	115.17
1	S2	651	PSU	N1-C2-N3	6.25	121.76	115.17
3	L5	1782	PSU	N1-C2-N3	6.22	121.73	115.17
3	L5	3818	UY1	N1-C2-N3	6.21	121.72	115.17
85	Pt	8	4SU	C4-N3-C2	-6.21	121.36	127.31
1	S2	1004	PSU	N1-C2-N3	6.21	121.72	115.17
3	L5	4494	OMG	C5-C4-N3	-6.21	118.51	128.39
3	L5	1862	PSU	N1-C2-N3	6.21	121.72	115.17
3	L5	3768	PSU	N1-C2-N3	6.21	121.71	115.17
3	L5	4532	PSU	N1-C2-N3	6.20	121.71	115.17
1	S2	509	OMG	C5-C4-N3	-6.19	118.54	128.39
1	S2	93	PSU	N1-C2-N3	6.19	121.70	115.17
3	L5	2508	PSU	N1-C2-N3	6.14	121.65	115.17
3	L5	3627	OMG	C5-C4-N3	-6.12	118.65	128.39
3	L5	3853	PSU	N1-C2-N3	6.10	121.61	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	484	A2M	C5-C4-N3	-6.07	118.36	126.72
1	S2	468	A2M	C5-C4-N3	-6.07	118.36	126.72
1	S2	436	OMG	C5-C4-N3	-6.06	118.74	128.39
3	L5	2364	OMG	C5-C4-N3	-6.05	118.77	128.39
1	S2	866	PSU	N1-C2-N3	6.04	121.54	115.17
1	S2	1328	OMG	C5-C4-N3	-6.03	118.80	128.39
1	S2	159	A2M	C5-C4-N3	-6.02	118.43	126.72
3	L5	4628	PSU	N1-C2-N3	6.01	121.51	115.17
84	At	46	G7M	N9-C4-N3	6.01	137.97	125.95
3	L5	4499	OMG	C5-C4-N3	-6.01	118.83	128.39
1	S2	27	A2M	C5-C4-N3	-6.00	118.46	126.72
1	S2	601	OMG	C5-C4-N3	-5.98	118.87	128.39
3	L5	4392	OMG	C5-C4-N3	-5.97	118.89	128.39
1	S2	1490	OMG	C5-C4-N3	-5.95	118.91	128.39
3	L5	4576	PSU	N1-C2-N3	5.94	121.44	115.17
1	S2	512	A2M	C5-C4-N3	-5.92	118.57	126.72
3	L5	4293	PSU	N1-C2-N3	5.90	121.39	115.17
1	S2	1383	A2M	C5-C4-N3	-5.89	118.61	126.72
3	L5	3785	A2M	C5-C4-N3	-5.89	118.61	126.72
3	L5	3830	A2M	C2'-C1'-N9	-5.87	104.09	113.75
3	L5	4673	PSU	N1-C2-N3	5.85	121.34	115.17
2	L8	75	OMG	C5-C4-N3	-5.85	119.08	128.39
3	L5	2876	OMG	C5-C4-N3	-5.84	119.10	128.39
1	S2	1447	OMG	C5-C4-N3	-5.84	119.10	128.39
3	L5	4471	PSU	N1-C2-N3	5.83	121.32	115.17
3	L5	400	A2M	C5-C4-N3	-5.82	118.70	126.72
84	At	37	MIA	N3-C4-N9	5.82	134.37	126.99
1	S2	668	A2M	C5-C4-N3	-5.81	118.71	126.72
1	S2	683	OMG	C5-C4-N3	-5.81	119.15	128.39
1	S2	576	A2M	C5-C4-N3	-5.80	118.73	126.72
3	L5	1582	PSU	N1-C2-N3	5.80	121.29	115.17
3	L5	1316	OMG	C5-C4-N3	-5.79	119.17	128.39
85	Pt	8	4SU	C5-C4-N3	5.78	120.13	114.75
3	L5	4623	OMG	C5-C4-N3	-5.78	119.19	128.39
3	L5	2363	A2M	C5-C4-N3	-5.78	118.76	126.72
3	L5	4618	OMG	C5-C4-N3	-5.78	119.20	128.39
3	L5	398	A2M	C5-C4-N3	-5.76	118.79	126.72
3	L5	4590	A2M	C5-C4-N3	-5.76	118.79	126.72
3	L5	3744	OMG	C5-C4-N3	-5.74	119.25	128.39
3	L5	3760	A2M	C5-C4-N3	-5.73	118.82	126.72
1	S2	1678	A2M	C5-C4-N3	-5.73	118.83	126.72
3	L5	4370	OMG	C5-C4-N3	-5.72	119.28	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3830	A2M	C5-C4-N3	-5.70	118.87	126.72
1	S2	99	A2M	C5-C4-N3	-5.70	118.87	126.72
3	L5	3867	A2M	C5-C4-N3	-5.69	118.88	126.72
3	L5	4306	OMU	C4-N3-C2	-5.69	119.55	126.61
3	L5	4196	OMG	C5-C4-N3	-5.69	119.34	128.39
3	L5	3944	OMG	C5-C4-N3	-5.68	119.34	128.39
3	L5	1534	A2M	C5-C4-N3	-5.68	118.90	126.72
1	S2	867	OMG	C5-C4-N3	-5.67	119.36	128.39
1	S2	644	OMG	C5-C4-N3	-5.66	119.38	128.39
3	L5	2815	A2M	C5-C4-N3	-5.65	118.94	126.72
3	L5	2364	OMG	C2-N3-C4	5.64	122.01	112.30
3	L5	4523	A2M	C5-C4-N3	-5.61	118.99	126.72
3	L5	1625	OMG	C5-C4-N3	-5.60	119.48	128.39
1	S2	166	A2M	C5-C4-N3	-5.58	119.04	126.72
3	L5	4531	PSU	O2-C2-N1	-5.55	117.06	122.79
3	L5	3825	A2M	C5-C4-N3	-5.54	119.09	126.72
3	L5	3884	PSU	N1-C2-N3	5.53	121.00	115.17
3	L5	1871	A2M	C5-C4-N3	-5.53	119.11	126.72
1	S2	1639	G7M	C5-C4-N3	-5.52	117.72	128.15
3	L5	2401	A2M	C5-C4-N3	-5.44	119.23	126.72
3	L5	4220	6MZ	C5-C4-N3	-5.44	119.23	126.72
3	L5	4637	OMG	C2-N3-C4	5.42	121.63	112.30
1	S2	1383	A2M	C2'-C1'-N9	-5.39	104.88	113.75
3	L5	3792	OMG	C2-N3-C4	5.38	121.58	112.30
3	L5	2837	OMU	N3-C2-N1	5.37	121.88	114.89
3	L5	1322	1MA	C5-C4-N3	-5.34	119.41	127.27
3	L5	3899	OMG	C2-N3-C4	5.32	121.47	112.30
3	L5	4306	OMU	N3-C2-N1	5.32	121.82	114.89
3	L5	3718	A2M	C5-C4-N3	-5.31	119.40	126.72
1	S2	683	OMG	C2-N3-C4	5.31	121.45	112.30
1	S2	1031	A2M	C5-C4-N3	-5.30	119.42	126.72
1	S2	428	OMU	C4-N3-C2	-5.29	120.04	126.61
2	L8	14	OMU	C4-N3-C2	-5.29	120.04	126.61
3	L5	4618	OMG	C2-N3-C4	5.29	121.41	112.30
3	L5	2787	A2M	N3-C4-N9	5.27	136.12	127.17
3	L5	4571	A2M	C5-C4-N3	-5.26	119.47	126.72
3	L5	4392	OMG	C2-N3-C4	5.25	121.35	112.30
3	L5	1326	A2M	C5-C4-N3	-5.24	119.51	126.72
3	L5	3723	A2M	C5-C4-N3	-5.24	119.51	126.72
1	S2	590	A2M	N3-C4-N9	5.20	136.01	127.17
1	S2	1851	MA6	C5-C4-N3	-5.19	119.58	126.72
3	L5	4227	OMU	C4-N3-C2	-5.18	120.18	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4370	OMG	C2-N3-C4	5.17	121.20	112.30
1	S2	644	OMG	C2-N3-C4	5.16	121.19	112.30
3	L5	1522	OMG	C5-C4-N3	-5.16	120.18	128.39
3	L5	2415	OMU	C4-N3-C2	-5.15	120.22	126.61
3	L5	3627	OMG	C2-N3-C4	5.14	121.16	112.30
3	L5	4499	OMG	C2-N3-C4	5.14	121.14	112.30
3	L5	1522	OMG	C2-N3-C4	5.12	121.12	112.30
3	L5	3785	A2M	N3-C4-N9	5.12	135.87	127.17
3	L5	3744	OMG	C2-N3-C4	5.10	121.09	112.30
2	L8	75	OMG	C2-N3-C4	5.09	121.06	112.30
3	L5	4498	OMU	C4-N3-C2	-5.08	120.30	126.61
1	S2	1490	OMG	C2-N3-C4	5.07	121.04	112.30
3	L5	2876	OMG	C2-N3-C4	5.07	121.04	112.30
1	S2	627	OMU	C4-N3-C2	-5.07	120.32	126.61
3	L5	4196	OMG	C2-N3-C4	5.06	121.01	112.30
84	At	46	G7M	C8-N9-C4	5.03	119.55	107.09
3	L5	3825	A2M	N3-C4-N9	5.02	135.71	127.17
1	S2	509	OMG	C2-N3-C4	5.02	120.95	112.30
3	L5	4494	OMG	C2-N3-C4	5.01	120.93	112.30
3	L5	3867	A2M	N3-C4-N9	5.01	135.69	127.17
3	L5	1524	A2M	C5-C4-N3	-5.00	119.83	126.72
3	L5	1316	OMG	C2-N3-C4	4.98	120.89	112.30
3	L5	2424	OMG	C2-N3-C4	4.97	120.86	112.30
1	S2	867	OMG	C2-N3-C4	4.96	120.84	112.30
1	S2	1328	OMG	C2-N3-C4	4.95	120.82	112.30
1	S2	1248	B8N	C4-N3-C2	-4.92	119.56	125.62
1	S2	436	OMG	C2-N3-C4	4.91	120.76	112.30
1	S2	354	OMU	C4-N3-C2	-4.90	120.53	126.61
3	L5	3944	OMG	C2-N3-C4	4.87	120.69	112.30
3	L5	1625	OMG	C2-N3-C4	4.87	120.69	112.30
3	L5	1316	OMG	N9-C4-N3	4.87	135.68	125.95
1	S2	116	OMU	C4-N3-C2	-4.86	120.57	126.61
3	L5	3724	A2M	C5-C4-N3	-4.86	120.02	126.72
3	L5	3627	OMG	N9-C4-N3	4.85	135.65	125.95
3	L5	3899	OMG	N9-C4-N3	4.85	135.65	125.95
3	L5	2837	OMU	C4-N3-C2	-4.83	120.61	126.61
3	L5	4228	OMG	C5-C4-N3	-4.83	120.70	128.39
3	L5	4636	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L5	1522	OMG	N9-C4-N3	4.82	135.60	125.95
1	S2	99	A2M	N3-C4-N9	4.82	135.37	127.17
3	L5	4637	OMG	N9-C4-N3	4.82	135.59	125.95
1	S2	1383	A2M	N3-C4-N9	4.81	135.35	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	159	A2M	N3-C4-N9	4.81	135.35	127.17
3	L5	4227	OMU	N3-C2-N1	4.81	121.15	114.89
1	S2	512	A2M	N3-C4-N9	4.80	135.34	127.17
3	L5	2424	OMG	N9-C4-N3	4.80	135.54	125.95
1	S2	1442	OMU	C4-N3-C2	-4.80	120.66	126.61
3	L5	3760	A2M	C2'-C1'-N9	-4.77	105.90	113.75
1	S2	27	A2M	N3-C4-N9	4.77	135.28	127.17
1	S2	1850	MA6	C2-N1-C6	4.76	123.46	111.83
3	L5	4623	OMG	C2-N3-C4	4.75	120.48	112.30
1	S2	1447	OMG	C2-N3-C4	4.75	120.48	112.30
1	S2	484	A2M	N3-C4-N9	4.74	135.23	127.17
1	S2	172	OMU	C4-N3-C2	-4.73	120.74	126.61
1	S2	1832	6MZ	C5-C4-N3	-4.73	120.20	126.72
3	L5	1792	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	400	A2M	N3-C4-N9	4.72	135.19	127.17
3	L5	4442	PSU	C4-N3-C2	-4.71	119.89	126.37
1	S2	509	OMG	N9-C4-N3	4.70	135.35	125.95
2	L8	55	PSU	C4-N3-C2	-4.70	119.90	126.37
1	S2	105	PSU	C4-N3-C2	-4.69	119.92	126.37
1	S2	1850	MA6	C5-C4-N3	-4.68	120.27	126.72
1	S2	1288	OMU	C4-N3-C2	-4.67	120.81	126.61
1	S2	601	OMG	C2-N3-C4	4.67	120.34	112.30
1	S2	1804	OMU	C4-N3-C2	-4.67	120.82	126.61
3	L5	3760	A2M	N3-C4-N9	4.67	135.10	127.17
3	L5	398	A2M	N3-C4-N9	4.66	135.09	127.17
3	L5	3734	PSU	C4-N3-C2	-4.65	119.97	126.37
1	S2	468	A2M	N3-C4-N9	4.64	135.06	127.17
3	L5	2876	OMG	N9-C4-N3	4.64	135.23	125.95
84	At	8	4SU	C5-C4-S4	-4.62	119.02	124.31
1	S2	1326	UY1	C4-N3-C2	-4.62	120.00	126.37
1	S2	1056	PSU	C4-N3-C2	-4.62	120.01	126.37
3	L5	1625	OMG	N9-C4-N3	4.61	135.18	125.95
3	L5	3830	A2M	N3-C4-N9	4.61	135.00	127.17
3	L5	4228	OMG	C2-N3-C4	4.60	120.23	112.30
3	L5	3818	UY1	C4-N3-C2	-4.60	120.03	126.37
1	S2	1692	PSU	C4-N3-C2	-4.60	120.04	126.37
3	L5	4569	PSU	C4-N3-C2	-4.60	120.04	126.37
3	L5	2815	A2M	N3-C4-N9	4.59	134.97	127.17
3	L5	2843	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L5	1322	1MA	C2-N3-C4	4.58	121.52	112.53
3	L5	4499	OMG	N9-C4-N3	4.58	135.11	125.95
3	L5	3844	PSU	O2-C2-N1	-4.58	118.07	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2363	A2M	N3-C4-N9	4.58	134.95	127.17
3	L5	3944	OMG	C2'-C1'-N9	-4.57	105.56	114.24
1	S2	172	OMU	N3-C2-N1	4.57	120.84	114.89
2	L8	14	OMU	C5-C4-N3	4.57	121.20	114.80
3	L5	4689	PSU	C4-N3-C2	-4.57	120.08	126.37
1	S2	1678	A2M	N3-C4-N9	4.57	134.94	127.17
3	L5	4220	6MZ	N3-C4-N9	4.57	134.93	127.17
3	L5	5001	PSU	C4-N3-C2	-4.56	120.08	126.37
3	L5	1871	A2M	C2'-C1'-N9	-4.56	106.25	113.75
3	L5	4296	PSU	C4-N3-C2	-4.56	120.09	126.37
1	S2	512	A2M	C2'-C1'-N9	-4.53	106.30	113.75
3	L5	1677	PSU	C4-N3-C2	-4.52	120.15	126.37
3	L5	4521	PSU	C4-N3-C2	-4.51	120.15	126.37
1	S2	218	PSU	C4-N3-C2	-4.51	120.16	126.37
3	L5	4306	OMU	C5-C4-N3	4.51	121.12	114.80
3	L5	4590	A2M	N3-C4-N9	4.51	134.83	127.17
1	S2	649	PSU	C4-N3-C2	-4.51	120.17	126.37
3	L5	3785	A2M	C2'-C1'-N9	-4.50	106.34	113.75
1	S2	436	OMG	N9-C4-N3	4.50	134.94	125.95
84	At	46	G7M	C5-C4-N3	-4.49	119.66	128.15
3	L5	3825	A2M	C2'-C1'-N9	-4.49	106.36	113.75
1	S2	166	A2M	N3-C4-N9	4.49	134.80	127.17
1	S2	668	A2M	N3-C4-N9	4.48	134.79	127.17
1	S2	1081	PSU	C4-N3-C2	-4.48	120.20	126.37
3	L5	3637	PSU	C4-N3-C2	-4.47	120.21	126.37
1	S2	918	PSU	C4-N3-C2	-4.47	120.21	126.37
3	L5	3920	PSU	C4-N3-C2	-4.47	120.21	126.37
3	L5	3925	OMU	C4-N3-C2	-4.47	121.06	126.61
1	S2	822	PSU	C4-N3-C2	-4.46	120.22	126.37
3	L5	2415	OMU	C5-C4-N3	4.46	121.05	114.80
1	S2	1243	PSU	C4-N3-C2	-4.46	120.23	126.37
1	S2	681	PSU	C4-N3-C2	-4.46	120.23	126.37
3	L5	3729	PSU	C4-N3-C2	-4.46	120.23	126.37
1	S2	1442	OMU	N3-C2-N1	4.45	120.68	114.89
1	S2	1328	OMG	N9-C4-N3	4.44	134.84	125.95
1	S2	918	PSU	O2-C2-N1	-4.44	118.22	122.79
1	S2	354	OMU	C5-C4-N3	4.43	121.00	114.80
3	L5	1524	A2M	N3-C4-N9	4.42	134.69	127.17
2	L8	14	OMU	N3-C2-N1	4.42	120.64	114.89
3	L5	4361	PSU	C4-N3-C2	-4.42	120.29	126.37
3	L5	2364	OMG	N9-C4-N3	4.41	134.78	125.95
3	L5	3792	OMG	N9-C4-N3	4.41	134.77	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	Pt	47	G7M	N9-C8-N7	-4.41	101.77	112.48
1	S2	1639	G7M	C2-N3-C4	4.41	119.89	112.30
3	L5	4523	A2M	N3-C4-N9	4.40	134.65	127.17
3	L5	4571	A2M	N3-C4-N9	4.39	134.64	127.17
3	L5	2401	A2M	N3-C4-N9	4.39	134.64	127.17
29	SV	1	AME	CT2-CT1-N	-4.39	108.84	116.12
3	L5	4457	PSU	C4-N3-C2	-4.38	120.33	126.37
1	S2	1832	6MZ	C6-C5-N7	4.38	137.20	132.43
3	L5	1326	A2M	N3-C4-N9	4.37	134.61	127.17
1	S2	1238	PSU	C4-N3-C2	-4.37	120.35	126.37
1	S2	119	PSU	C4-N3-C2	-4.37	120.35	126.37
3	L5	4498	OMU	C5-C4-N3	4.36	120.91	114.80
3	L5	1536	PSU	C4-N3-C2	-4.36	120.36	126.37
1	S2	686	PSU	C4-N3-C2	-4.35	120.38	126.37
1	S2	576	A2M	N3-C4-N9	4.35	134.56	127.17
1	S2	1639	G7M	C8-N9-C4	4.35	117.85	107.09
3	L5	3851	PSU	C4-N3-C2	-4.34	120.39	126.37
3	L5	4447	5MC	C5-C6-N1	-4.34	118.59	123.31
3	L5	3762	PSU	O2-C2-N1	-4.34	118.31	122.79
3	L5	4620	OMU	C4-N3-C2	-4.34	121.22	126.61
3	L5	4403	PSU	C4-N3-C2	-4.34	120.39	126.37
1	S2	1031	A2M	N3-C4-N9	4.34	134.54	127.17
3	L5	4498	OMU	N3-C2-N1	4.32	120.52	114.89
1	S2	1851	MA6	C2-N1-C6	4.31	122.37	111.83
1	S2	601	OMG	N9-C4-N3	4.31	134.58	125.95
3	L5	2415	OMU	N3-C2-N1	4.31	120.50	114.89
3	L5	2839	PSU	C4-N3-C2	-4.31	120.43	126.37
3	L5	4623	OMG	N9-C4-N3	4.31	134.57	125.95
1	S2	683	OMG	N9-C4-N3	4.31	134.57	125.95
3	L5	4569	PSU	O2-C2-N1	-4.31	118.35	122.79
3	L5	4431	PSU	C4-N3-C2	-4.31	120.44	126.37
85	Pt	56	PSU	C4-N3-C2	-4.31	120.44	126.37
1	S2	1490	OMG	N9-C4-N3	4.30	134.56	125.95
3	L5	4579	PSU	O2-C2-N1	-4.30	118.35	122.79
3	L5	4228	OMG	C6-C5-N7	4.30	138.12	130.29
1	S2	1447	OMG	N9-C4-N3	4.30	134.55	125.95
3	L5	4493	PSU	C4-N3-C2	-4.29	120.46	126.37
1	S2	814	PSU	C4-N3-C2	-4.29	120.47	126.37
3	L5	4494	OMG	N9-C4-N3	4.29	134.52	125.95
1	S2	354	OMU	N3-C2-N1	4.28	120.47	114.89
2	L8	69	PSU	O2-C2-N1	-4.28	118.38	122.79
1	S2	296	PSU	C4-N3-C2	-4.28	120.48	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	116	OMU	C5-C4-N3	4.28	120.79	114.80
1	S2	34	PSU	C4-N3-C2	-4.27	120.49	126.37
1	S2	109	PSU	C4-N3-C2	-4.27	120.49	126.37
3	L5	4299	PSU	C4-N3-C2	-4.26	120.50	126.37
3	L5	3723	A2M	N3-C4-N9	4.26	134.41	127.17
1	S2	166	A2M	C2'-C1'-N9	-4.26	106.75	113.75
3	L5	3724	A2M	N3-C4-N9	4.26	134.41	127.17
1	S2	1643	PSU	C4-N3-C2	-4.26	120.51	126.37
1	S2	1445	PSU	C4-N3-C2	-4.25	120.51	126.37
1	S2	1851	MA6	C4-C5-N7	-4.25	105.72	110.58
2	L8	75	OMG	N9-C4-N3	4.24	134.42	125.95
3	L5	3695	PSU	C4-N3-C2	-4.24	120.54	126.37
3	L5	3758	PSU	C4-N3-C2	-4.24	120.54	126.37
1	S2	1804	OMU	C5-C4-N3	4.23	120.73	114.80
1	S2	1639	G7M	C1'-N9-C8	-4.23	112.45	126.74
1	S2	1136	PSU	C4-N3-C2	-4.23	120.54	126.37
3	L5	1534	A2M	N3-C4-N9	4.23	134.36	127.17
1	S2	121	OMU	N3-C2-N1	4.22	120.39	114.89
1	S2	651	PSU	C4-N3-C2	-4.22	120.56	126.37
3	L5	4423	PSU	C4-N3-C2	-4.22	120.56	126.37
3	L5	1871	A2M	N3-C4-N9	4.22	134.34	127.17
1	S2	573	PSU	C4-N3-C2	-4.21	120.58	126.37
1	S2	428	OMU	C5-C4-N3	4.21	120.69	114.80
3	L5	3744	OMG	N9-C4-N3	4.20	134.36	125.95
1	S2	428	OMU	N3-C2-N1	4.20	120.36	114.89
1	S2	1288	OMU	N3-C2-N1	4.20	120.36	114.89
3	L5	4392	OMG	N9-C4-N3	4.20	134.34	125.95
1	S2	1244	PSU	C4-N3-C2	-4.19	120.59	126.37
3	L5	4579	PSU	C4-N3-C2	-4.19	120.59	126.37
1	S2	1031	A2M	N3-C2-N1	-4.19	122.24	128.58
1	S2	815	PSU	C4-N3-C2	-4.18	120.61	126.37
3	L5	2839	PSU	O2-C2-N1	-4.18	118.47	122.79
1	S2	406	PSU	C4-N3-C2	-4.18	120.61	126.37
1	S2	801	PSU	C4-N3-C2	-4.18	120.61	126.37
3	L5	3718	A2M	N3-C4-N9	4.18	134.27	127.17
3	L5	1781	PSU	C4-N3-C2	-4.18	120.61	126.37
3	L5	4196	OMG	N9-C4-N3	4.17	134.30	125.95
3	L5	3925	OMU	N3-C2-N1	4.17	120.32	114.89
3	L5	4442	PSU	O2-C2-N1	-4.17	118.49	122.79
3	L5	3715	PSU	C4-N3-C2	-4.17	120.63	126.37
3	L5	4552	PSU	C4-N3-C2	-4.17	120.63	126.37
1	S2	867	OMG	N9-C4-N3	4.16	134.27	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4227	OMU	C5-C4-N3	4.15	120.61	114.80
1	S2	863	PSU	C4-N3-C2	-4.14	120.66	126.37
1	S2	572	PSU	C4-N3-C2	-4.14	120.67	126.37
3	L5	1582	PSU	C4-N3-C2	-4.14	120.67	126.37
1	S2	36	PSU	C4-N3-C2	-4.14	120.67	126.37
3	L5	1683	PSU	C4-N3-C2	-4.14	120.67	126.37
1	S2	1177	PSU	C4-N3-C2	-4.13	120.68	126.37
3	L5	4532	PSU	O2-C2-N1	-4.13	118.53	122.79
1	S2	627	OMU	C5-C4-N3	4.13	120.59	114.80
84	At	39	PSU	C4-N3-C2	-4.13	120.69	126.37
1	S2	609	PSU	C4-N3-C2	-4.11	120.70	126.37
1	S2	1445	PSU	O2-C2-N1	-4.11	118.55	122.79
85	Pt	8	4SU	C5-C4-S4	-4.11	119.61	124.31
3	L5	1779	PSU	C4-N3-C2	-4.11	120.71	126.37
1	S2	1832	6MZ	N1-C2-N3	-4.11	122.36	128.58
1	S2	1625	PSU	O2-C2-N1	-4.10	118.56	122.79
1	S2	109	PSU	O2-C2-N1	-4.10	118.56	122.79
3	L5	4620	OMU	N3-C2-N1	4.10	120.22	114.89
1	S2	1239	PSU	C4-N3-C2	-4.09	120.73	126.37
1	S2	1174	PSU	C4-N3-C2	-4.09	120.73	126.37
3	L5	2632	PSU	C4-N3-C2	-4.09	120.73	126.37
1	S2	116	OMU	N3-C2-N1	4.09	120.21	114.89
3	L5	2787	A2M	C2-N3-C4	4.09	121.81	111.83
3	L5	1744	PSU	O2-C2-N1	-4.09	118.58	122.79
84	At	37	MIA	C6-C5-N7	4.08	136.88	132.43
3	L5	4972	PSU	C4-N3-C2	-4.08	120.75	126.37
3	L5	5010	PSU	C4-N3-C2	-4.08	120.75	126.37
3	L5	3734	PSU	O2-C2-N1	-4.07	118.59	122.79
84	At	32	PSU	C4-N3-C2	-4.07	120.77	126.37
1	S2	406	PSU	O2-C2-N1	-4.07	118.59	122.79
3	L5	1862	PSU	C4-N3-C2	-4.06	120.77	126.37
1	S2	121	OMU	C4-N3-C2	-4.06	121.57	126.61
1	S2	1850	MA6	N3-C4-N9	4.06	134.08	127.17
3	L5	4353	PSU	C4-N3-C2	-4.06	120.78	126.37
3	L5	1782	PSU	C4-N3-C2	-4.05	120.79	126.37
3	L5	1860	PSU	C4-N3-C2	-4.05	120.79	126.37
3	L5	4420	PSU	C4-N3-C2	-4.05	120.79	126.37
1	S2	644	OMG	N9-C4-N3	4.04	134.02	125.95
3	L5	4531	PSU	C4-N3-C2	-4.03	120.82	126.37
3	L5	4620	OMU	C5-C4-N3	4.03	120.44	114.80
3	L5	4431	PSU	O2-C2-N1	-4.01	118.65	122.79
1	S2	1850	MA6	N1-C2-N3	-4.01	122.52	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1347	PSU	C4-N3-C2	-4.00	120.86	126.37
3	L5	3762	PSU	C4-N3-C2	-4.00	120.86	126.37
1	S2	822	PSU	O2-C2-N1	-4.00	118.67	122.79
1	S2	1639	G7M	CN7-N7-C5	4.00	131.78	126.80
1	S2	966	PSU	C4-N3-C2	-4.00	120.87	126.37
3	L5	4628	PSU	C4-N3-C2	-4.00	120.87	126.37
1	S2	590	A2M	C2-N3-C4	3.99	121.58	111.83
1	S2	354	OMU	C2'-C1'-N1	-3.99	106.67	114.24
3	L5	3944	OMG	N9-C4-N3	3.98	133.92	125.95
2	L8	69	PSU	C4-N3-C2	-3.98	120.89	126.37
3	L5	3925	OMU	C5-C4-N3	3.97	120.36	114.80
1	S2	609	PSU	O2-C2-N1	-3.97	118.70	122.79
84	At	46	G7M	C1'-N9-C8	-3.97	113.34	126.74
3	L5	1744	PSU	C4-N3-C2	-3.97	120.91	126.37
3	L5	3770	PSU	C4-N3-C2	-3.96	120.92	126.37
1	S2	172	OMU	C1'-N1-C2	3.95	124.69	117.59
84	At	37	MIA	C15-C14-C13	-3.95	110.81	122.66
3	L5	2508	PSU	C4-N3-C2	-3.95	120.93	126.37
1	S2	36	PSU	O2-C2-N1	-3.95	118.72	122.79
3	L5	4618	OMG	N9-C4-N3	3.94	133.84	125.95
1	S2	93	PSU	C4-N3-C2	-3.94	120.94	126.37
84	At	39	PSU	O2-C2-N1	-3.94	118.73	122.79
3	L5	1536	PSU	O2-C2-N1	-3.93	118.73	122.79
1	S2	1851	MA6	N3-C4-N9	3.93	133.84	127.17
3	L5	3724	A2M	N3-C2-N1	-3.92	122.65	128.58
3	L5	3764	PSU	C4-N3-C2	-3.92	120.97	126.37
3	L5	4370	OMG	N9-C4-N3	3.92	133.79	125.95
1	S2	627	OMU	N3-C2-N1	3.91	119.99	114.89
1	S2	1625	PSU	C4-N3-C2	-3.91	120.98	126.37
1	S2	1232	PSU	C4-N3-C2	-3.91	120.99	126.37
39	LA	216	V5N	CD2-CG-ND1	3.91	111.02	105.76
1	S2	681	PSU	O2-C2-N1	-3.90	118.77	122.79
3	L5	4532	PSU	C4-N3-C2	-3.90	121.00	126.37
3	L5	3884	PSU	C4-N3-C2	-3.90	121.00	126.37
1	S2	1804	OMU	N3-C2-N1	3.89	119.95	114.89
3	L5	400	A2M	C2-N3-C4	3.89	121.32	111.83
3	L5	1871	A2M	C4-C5-N7	-3.88	106.15	110.58
3	L5	2364	OMG	C6-C5-N7	3.87	137.34	130.29
2	L8	55	PSU	O2-C2-N1	-3.86	118.81	122.79
52	La	39	V5N	CD2-CG-ND1	3.86	110.96	105.76
66	Lr	2	SAC	CB-CA-C	-3.86	102.86	111.35
3	L5	4523	A2M	C2'-C1'-N9	-3.85	107.41	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	Pt	8	4SU	N3-C2-N1	3.85	119.91	114.89
3	L5	4618	OMG	C6-C5-N7	3.85	137.30	130.29
1	S2	1288	OMU	C5-C4-N3	3.85	120.19	114.80
3	L5	4423	PSU	O2-C2-N1	-3.85	118.82	122.79
3	L5	3818	UY1	O2-C2-N1	-3.84	118.82	122.79
1	S2	1442	OMU	C5-C4-N3	3.84	120.18	114.80
3	L5	3639	PSU	C4-N3-C2	-3.84	121.08	126.37
1	S2	27	A2M	C2-N3-C4	3.84	121.21	111.83
1	S2	1367	PSU	C4-N3-C2	-3.84	121.08	126.37
1	S2	1177	PSU	O2-C2-N1	-3.83	118.83	122.79
84	At	37	MIA	C16-C14-C13	-3.83	111.16	122.66
1	S2	1243	PSU	O2-C2-N1	-3.83	118.84	122.79
3	L5	4293	PSU	C4-N3-C2	-3.83	121.09	126.37
3	L5	2876	OMG	C6-C5-N7	3.81	137.23	130.29
1	S2	166	A2M	C2-N3-C4	3.81	121.14	111.83
3	L5	4673	PSU	C4-N3-C2	-3.81	121.12	126.37
1	S2	686	PSU	O2-C2-N1	-3.81	118.86	122.79
66	Lr	2	SAC	C2A-C1A-N	-3.80	109.81	116.12
3	L5	4220	6MZ	N1-C2-N3	-3.80	122.84	128.58
1	S2	1678	A2M	C2-N3-C4	3.79	121.08	111.83
3	L5	4370	OMG	C6-C5-N7	3.79	137.18	130.29
1	S2	644	OMG	C2'-C1'-N9	-3.79	107.05	114.24
3	L5	4392	OMG	C6-C5-N7	3.78	137.17	130.29
3	L5	3785	A2M	O4'-C1'-N9	3.78	115.35	108.09
1	S2	119	PSU	O2-C2-N1	-3.77	118.90	122.79
1	S2	468	A2M	C2-N3-C4	3.77	121.04	111.83
1	S2	576	A2M	C4-C5-N7	-3.76	106.28	110.58
3	L5	3920	PSU	O2-C2-N1	-3.76	118.91	122.79
3	L5	3844	PSU	C4-N3-C2	-3.75	121.21	126.37
1	S2	512	A2M	C2-N3-C4	3.74	120.95	111.83
3	L5	3785	A2M	C2-N3-C4	3.74	120.95	111.83
1	S2	159	A2M	C2-N3-C4	3.73	120.95	111.83
3	L5	2363	A2M	C2-N3-C4	3.72	120.93	111.83
1	S2	576	A2M	C2'-C1'-N9	-3.72	107.62	113.75
3	L5	3744	OMG	C2'-C1'-N9	-3.72	107.18	114.24
3	L5	3715	PSU	O2-C2-N1	-3.72	118.95	122.79
1	S2	296	PSU	O2-C2-N1	-3.71	118.96	122.79
3	L5	4220	6MZ	C2-N3-C4	3.71	120.89	111.83
1	S2	468	A2M	C4-C5-N7	-3.71	106.34	110.58
1	S2	1031	A2M	C2-N3-C4	3.71	120.89	111.83
3	L5	4552	PSU	O2-C2-N1	-3.71	118.97	122.79
1	S2	172	OMU	C5-C4-N3	3.70	119.98	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3729	PSU	O2-C2-N1	-3.70	118.97	122.79
3	L5	2815	A2M	C4-C5-N7	-3.70	106.36	110.58
3	L5	4353	PSU	O2-C2-N1	-3.69	118.98	122.79
1	S2	166	A2M	N3-C2-N1	-3.69	123.00	128.58
3	L5	1792	PSU	O2-C2-N1	-3.69	118.99	122.79
84	At	46	G7M	C2-N3-C4	3.68	118.65	112.30
3	L5	1779	PSU	O2-C2-N1	-3.68	119.00	122.79
3	L5	1534	A2M	C2-N3-C4	3.67	120.79	111.83
1	S2	121	OMU	C5-C4-N3	3.67	119.94	114.80
1	S2	484	A2M	C2-N3-C4	3.66	120.78	111.83
1	S2	649	PSU	O2-C2-N1	-3.66	119.01	122.79
3	L5	4196	OMG	C6-C5-N7	3.66	136.95	130.29
3	L5	3764	PSU	O2-C2-N1	-3.65	119.02	122.79
1	S2	1347	PSU	O2-C2-N1	-3.65	119.02	122.79
2	L8	75	OMG	C2'-C1'-N9	-3.65	107.31	114.24
3	L5	3825	A2M	C2-N3-C4	3.65	120.74	111.83
3	L5	3724	A2M	C2'-C1'-N9	-3.65	107.75	113.75
3	L5	4447	5MC	C5-C4-N3	-3.65	118.02	121.75
3	L5	1871	A2M	C2-N3-C4	3.64	120.73	111.83
3	L5	4523	A2M	C4-C5-N7	-3.64	106.42	110.58
1	S2	1832	6MZ	C4-C5-N7	-3.64	106.42	110.58
1	S2	1850	MA6	C4-N9-C8	3.64	109.56	105.74
1	S2	1692	PSU	O2-C2-N1	-3.64	119.04	122.79
3	L5	3785	A2M	C4-N9-C8	3.64	109.56	105.74
1	S2	1832	6MZ	N3-C4-N9	3.63	133.34	127.17
1	S2	1232	PSU	O2-C2-N1	-3.63	119.05	122.79
3	L5	4493	PSU	O2-C2-N1	-3.62	119.05	122.79
1	S2	644	OMG	C6-C5-N7	3.62	136.87	130.29
1	S2	814	PSU	O2-C2-N1	-3.62	119.06	122.79
3	L5	4312	PSU	C4-N3-C2	-3.61	121.39	126.37
3	L5	3899	OMG	C6-C5-N7	3.61	136.86	130.29
1	S2	668	A2M	C2-N3-C4	3.61	120.64	111.83
1	S2	683	OMG	C6-C5-N7	3.61	136.85	130.29
1	S2	1383	A2M	C2-N3-C4	3.61	120.64	111.83
3	L5	4420	PSU	O2-C2-N1	-3.60	119.08	122.79
1	S2	99	A2M	C2-N3-C4	3.60	120.62	111.83
1	S2	576	A2M	C2-N3-C4	3.59	120.61	111.83
3	L5	398	A2M	C2-N3-C4	3.59	120.61	111.83
1	S2	801	PSU	O2-C2-N1	-3.59	119.08	122.79
1	S2	572	PSU	O2-C2-N1	-3.59	119.09	122.79
1	S2	1850	MA6	C2-N3-C4	3.59	120.59	111.83
3	L5	3760	A2M	C2-N3-C4	3.58	120.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4457	PSU	O2-C2-N1	-3.58	119.10	122.79
84	At	8	4SU	N3-C2-N1	3.58	119.55	114.89
3	L5	4590	A2M	C2-N3-C4	3.58	120.57	111.83
3	L5	2401	A2M	C2-N3-C4	3.57	120.56	111.83
3	L5	4296	PSU	O2-C2-N1	-3.57	119.10	122.79
3	L5	3944	OMG	C6-C5-N7	3.57	136.79	130.29
3	L5	1534	A2M	C4-C5-N7	-3.56	106.51	110.58
3	L5	4500	PSU	C4-N3-C2	-3.55	121.48	126.37
1	S2	1832	6MZ	C2-N3-C4	3.54	120.48	111.83
84	At	37	MIA	C4-C5-N7	-3.54	106.53	110.58
1	S2	1643	PSU	O2-C2-N1	-3.53	119.15	122.79
3	L5	3724	A2M	C2-N3-C4	3.53	120.44	111.83
1	S2	93	PSU	O2-C2-N1	-3.53	119.15	122.79
3	L5	3723	A2M	C2-N3-C4	3.52	120.44	111.83
1	S2	1004	PSU	C4-N3-C2	-3.52	121.52	126.37
3	L5	3830	A2M	C2-N3-C4	3.52	120.42	111.83
3	L5	4628	PSU	O2-C2-N1	-3.52	119.16	122.79
3	L5	2401	A2M	N3-C2-N1	-3.52	123.26	128.58
3	L5	4220	6MZ	C6-C5-N7	3.52	136.26	132.43
3	L5	3792	OMG	C6-C5-N7	3.52	136.69	130.29
3	L5	3768	PSU	C4-N3-C2	-3.51	121.53	126.37
3	L5	3770	PSU	O2-C2-N1	-3.51	119.17	122.79
3	L5	3723	A2M	N3-C2-N1	-3.51	123.28	128.58
3	L5	1522	OMG	O6-C6-C5	-3.50	117.29	126.53
1	S2	484	A2M	C4-C5-N7	-3.50	106.58	110.58
1	S2	1850	MA6	C4-C5-N7	-3.50	106.58	110.58
3	L5	1326	A2M	C2-N3-C4	3.50	120.37	111.83
3	L5	3867	A2M	C2-N3-C4	3.49	120.36	111.83
84	At	46	G7M	CN7-N7-C5	3.49	131.15	126.80
1	S2	1239	PSU	O2-C2-N1	-3.49	119.19	122.79
3	L5	4523	A2M	C2-N3-C4	3.48	120.34	111.83
3	L5	1683	PSU	O2-C2-N1	-3.48	119.20	122.79
3	L5	3744	OMG	C6-C5-N7	3.48	136.62	130.29
3	L5	1326	A2M	N3-C2-N1	-3.47	123.32	128.58
3	L5	4623	OMG	C6-C5-N7	3.47	136.61	130.29
1	S2	590	A2M	N3-C2-N1	-3.47	123.33	128.58
3	L5	3782	5MC	C5-C6-N1	-3.47	119.55	123.31
1	S2	159	A2M	C2'-C1'-N9	-3.47	108.05	113.75
3	L5	4571	A2M	C2-N3-C4	3.46	120.29	111.83
3	L5	4590	A2M	C4-C5-N7	-3.46	106.63	110.58
3	L5	2843	PSU	O2-C2-N1	-3.46	119.22	122.79
1	S2	1174	PSU	O2-C2-N1	-3.45	119.23	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1781	PSU	O2-C2-N1	-3.44	119.24	122.79
3	L5	4220	6MZ	C4-C5-N7	-3.44	106.65	110.58
2	L8	75	OMG	C6-C5-N7	3.44	136.55	130.29
3	L5	4530	UR3	C6-N1-C2	-3.44	118.99	121.80
3	L5	3825	A2M	N3-C2-N1	-3.44	123.38	128.58
1	S2	34	PSU	O2-C2-N1	-3.44	119.24	122.79
3	L5	2632	PSU	O2-C2-N1	-3.43	119.25	122.79
1	S2	1326	UY1	O2-C2-N1	-3.43	119.25	122.79
3	L5	2787	A2M	C4-C5-N7	-3.43	106.66	110.58
1	S2	601	OMG	C6-C5-N7	3.43	136.53	130.29
3	L5	4576	PSU	C4-N3-C2	-3.42	121.65	126.37
3	L5	1677	PSU	O2-C2-N1	-3.42	119.26	122.79
3	L5	3724	A2M	C4-N9-C8	3.42	109.33	105.74
3	L5	2363	A2M	C4-C5-N7	-3.40	106.69	110.58
1	S2	512	A2M	C4-C5-N7	-3.40	106.69	110.58
1	S2	1056	PSU	O2-C2-N1	-3.40	119.28	122.79
3	L5	5001	PSU	O2-C2-N1	-3.40	119.28	122.79
1	S2	1678	A2M	C4-C5-N7	-3.40	106.69	110.58
1	S2	99	A2M	N3-C2-N1	-3.40	123.44	128.58
3	L5	1322	1MA	N9-C4-N3	3.40	134.64	126.90
1	S2	159	A2M	C4-C5-N7	-3.40	106.70	110.58
3	L5	3718	A2M	C2'-C1'-N9	-3.40	108.16	113.75
2	L8	69	PSU	C3'-C2'-C1'	3.39	105.69	101.69
1	S2	1804	OMU	O4-C4-C5	-3.39	119.32	125.16
1	S2	1851	MA6	C2-N3-C4	3.39	120.11	111.83
3	L5	2363	A2M	N3-C2-N1	-3.39	123.46	128.58
3	L5	1582	PSU	O2-C2-N1	-3.38	119.30	122.79
1	S2	668	A2M	C4-C5-N7	-3.38	106.72	110.58
3	L5	400	A2M	C4-C5-N7	-3.37	106.72	110.58
3	L5	1522	OMG	C2'-C1'-N9	-3.37	107.84	114.24
3	L5	5010	PSU	O2-C2-N1	-3.37	119.31	122.79
84	At	37	MIA	C2-N3-C4	3.37	121.11	112.29
1	S2	1244	PSU	O2-C2-N1	-3.36	119.32	122.79
1	S2	1238	PSU	O2-C2-N1	-3.36	119.32	122.79
1	S2	218	PSU	O2-C2-N1	-3.36	119.32	122.79
1	S2	1490	OMG	C6-C5-N7	3.36	136.41	130.29
3	L5	1326	A2M	C4-C5-N7	-3.36	106.74	110.58
3	L5	400	A2M	N3-C2-N1	-3.36	123.50	128.58
3	L5	4637	OMG	C6-C5-N7	3.36	136.40	130.29
3	L5	2401	A2M	C4-C5-N7	-3.35	106.75	110.58
1	S2	436	OMG	C6-C5-N7	3.35	136.38	130.29
3	L5	4293	PSU	O2-C2-N1	-3.35	119.34	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	105	PSU	O2-C2-N1	-3.34	119.34	122.79
1	S2	27	A2M	C4-C5-N7	-3.34	106.76	110.58
1	S2	1442	OMU	O4-C4-C5	-3.34	119.41	125.16
3	L5	4494	OMG	C6-C5-N7	3.33	136.36	130.29
3	L5	2787	A2M	N3-C2-N1	-3.33	123.54	128.58
1	S2	1004	PSU	O2-C2-N1	-3.33	119.35	122.79
1	S2	1678	A2M	N3-C2-N1	-3.33	123.55	128.58
1	S2	683	OMG	C2'-C1'-N9	-3.32	107.93	114.24
3	L5	4972	PSU	O2-C2-N1	-3.32	119.37	122.79
1	S2	918	PSU	C3'-C2'-C1'	3.32	105.60	101.69
1	S2	1081	PSU	O2-C2-N1	-3.31	119.37	122.79
3	L5	398	A2M	N3-C2-N1	-3.31	123.56	128.58
3	L5	2815	A2M	C2-N3-C4	3.31	119.92	111.83
1	S2	166	A2M	C4-C5-N7	-3.31	106.80	110.58
3	L5	3825	A2M	C4-N9-C8	3.30	109.21	105.74
3	L5	400	A2M	C2'-C1'-N9	-3.30	108.32	113.75
3	L5	4498	OMU	O4-C4-C5	-3.30	119.47	125.16
1	S2	27	A2M	N3-C2-N1	-3.30	123.58	128.58
3	L5	4571	A2M	N3-C2-N1	-3.30	123.59	128.58
1	S2	116	OMU	O4-C4-C5	-3.27	119.52	125.16
84	At	32	PSU	O2-C2-N1	-3.27	119.41	122.79
3	L5	4471	PSU	C4-N3-C2	-3.27	121.86	126.37
3	L5	4590	A2M	N3-C2-N1	-3.27	123.64	128.58
3	L5	4299	PSU	O2-C2-N1	-3.27	119.42	122.79
3	L5	1524	A2M	C2-N3-C4	3.26	119.80	111.83
1	S2	1031	A2M	C2-N1-C6	3.26	124.09	118.73
1	S2	573	PSU	O2-C2-N1	-3.26	119.42	122.79
1	S2	512	A2M	N3-C2-N1	-3.26	123.65	128.58
1	S2	867	OMG	C6-C5-N7	3.26	136.22	130.29
3	L5	3851	PSU	O2-C2-N1	-3.25	119.44	122.79
3	L5	3785	A2M	N3-C2-N1	-3.24	123.68	128.58
3	L5	3760	A2M	C4-C5-N7	-3.24	106.88	110.58
3	L5	3830	A2M	C4-C5-N7	-3.24	106.88	110.58
3	L5	4361	PSU	O2-C2-N1	-3.24	119.45	122.79
3	L5	4590	A2M	C2'-C1'-N9	-3.23	108.43	113.75
3	L5	3830	A2M	N3-C2-N1	-3.23	123.69	128.58
1	S2	159	A2M	N3-C2-N1	-3.23	123.70	128.58
1	S2	1248	B8N	N3-C2-N1	3.23	120.66	116.72
1	S2	1842	4AC	C6-C5-C4	3.23	120.89	117.00
3	L5	4530	UR3	C5-C4-N3	3.22	119.28	115.04
1	S2	1136	PSU	O2-C2-N1	-3.22	119.47	122.79
85	Pt	56	PSU	O2-C2-N1	-3.22	119.47	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4521	PSU	O2-C2-N1	-3.22	119.47	122.79
3	L5	4403	PSU	O2-C2-N1	-3.22	119.47	122.79
3	L5	4220	6MZ	C4-N9-C8	3.21	109.11	105.74
3	L5	3853	PSU	C4-N3-C2	-3.21	121.95	126.37
3	L5	2837	OMU	C5-C4-N3	3.21	119.29	114.80
3	L5	4499	OMG	C6-C5-N7	3.21	136.12	130.29
1	S2	1383	A2M	N3-C2-N1	-3.20	123.73	128.58
3	L5	1534	A2M	N3-C2-N1	-3.20	123.73	128.58
1	S2	651	PSU	O2-C2-N1	-3.20	119.49	122.79
1	S2	428	OMU	O4-C4-C5	-3.19	119.65	125.16
3	L5	3627	OMG	C6-C5-N7	3.19	136.10	130.29
3	L5	4312	PSU	O2-C2-N1	-3.19	119.50	122.79
1	S2	1328	OMG	C6-C5-N7	3.18	136.07	130.29
1	S2	1031	A2M	C4-C5-N7	-3.17	106.95	110.58
1	S2	590	A2M	C4-C5-N7	-3.17	106.96	110.58
3	L5	1871	A2M	N3-C2-N1	-3.16	123.79	128.58
3	L5	2364	OMG	C2'-C1'-N9	-3.16	108.24	114.24
3	L5	1326	A2M	C4-N9-C8	3.15	109.04	105.74
3	L5	4296	PSU	C5-C6-N1	-3.14	117.78	122.14
1	S2	1447	OMG	C6-C5-N7	3.14	136.00	130.29
3	L5	4500	PSU	O2-C2-N1	-3.14	119.55	122.79
3	L5	4620	OMU	O4-C4-C5	-3.13	119.76	125.16
1	S2	509	OMG	C6-C5-N7	3.13	135.99	130.29
1	S2	468	A2M	N3-C2-N1	-3.13	123.85	128.58
1	S2	1288	OMU	O4-C4-C5	-3.13	119.77	125.16
3	L5	1524	A2M	N3-C2-N1	-3.12	123.85	128.58
3	L5	3758	PSU	O2-C2-N1	-3.12	119.57	122.79
3	L5	3760	A2M	N3-C2-N1	-3.12	123.86	128.58
3	L5	3723	A2M	C4-C5-N7	-3.12	107.02	110.58
3	L5	3899	OMG	C4-C5-N7	-3.11	105.74	110.67
1	S2	1383	A2M	C4-C5-N7	-3.11	107.03	110.58
3	L5	4689	PSU	O2-C2-N1	-3.11	119.58	122.79
3	L5	1860	PSU	O2-C2-N1	-3.10	119.59	122.79
1	S2	866	PSU	C4-N3-C2	-3.10	122.10	126.37
3	L5	4228	OMG	N9-C4-N3	3.09	132.14	125.95
3	L5	4571	A2M	C4-N9-C8	3.09	108.99	105.74
3	L5	400	A2M	C4-N9-C8	3.09	108.98	105.74
3	L5	3867	A2M	N3-C2-N1	-3.08	123.92	128.58
1	S2	867	OMG	C2'-C1'-N9	-3.08	108.40	114.24
3	L5	3768	PSU	O2-C2-N1	-3.08	119.61	122.79
3	L5	2837	OMU	O2-C2-N1	-3.08	118.79	122.80
3	L5	1316	OMG	C6-C5-N7	3.07	135.88	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2415	OMU	O4-C4-C5	-3.06	119.88	125.16
3	L5	398	A2M	C4-C5-N7	-3.06	107.08	110.58
1	S2	863	PSU	O2-C2-N1	-3.06	119.64	122.79
1	S2	1851	MA6	C5-N7-C8	3.05	108.25	103.45
1	S2	1842	4AC	C5-C4-N3	-3.05	117.83	122.60
3	L5	4571	A2M	C4-C5-N7	-3.04	107.10	110.58
1	S2	627	OMU	O4-C4-C5	-3.04	119.91	125.16
1	S2	1851	MA6	N1-C2-N3	-3.04	123.98	128.58
3	L5	1625	OMG	O6-C6-C5	-3.04	118.52	126.53
1	S2	576	A2M	N3-C2-N1	-3.04	123.99	128.58
3	L5	4523	A2M	N3-C2-N1	-3.03	124.00	128.58
3	L5	3723	A2M	C4-N9-C8	3.01	108.90	105.74
84	At	8	4SU	C2'-C1'-N1	-3.01	104.87	113.25
3	L5	4228	OMG	C4-C5-N7	-3.01	105.90	110.67
3	L5	3867	A2M	C4-N9-C8	3.00	108.89	105.74
3	L5	3718	A2M	C4-C5-N7	-3.00	107.15	110.58
1	S2	99	A2M	C4-C5-N7	-3.00	107.16	110.58
3	L5	1862	PSU	O2-C2-N1	-3.00	119.70	122.79
3	L5	1782	PSU	O2-C2-N1	-2.99	119.70	122.79
3	L5	2804	OMC	O2-C2-N3	-2.99	117.62	122.33
1	S2	1031	A2M	C2'-C1'-N9	-2.98	108.84	113.75
1	S2	484	A2M	N3-C2-N1	-2.98	124.07	128.58
3	L5	4220	6MZ	C5-N7-C8	2.97	108.11	103.45
3	L5	4531	PSU	O3'-C3'-C2'	-2.96	102.32	111.82
1	S2	866	PSU	O2-C2-N1	-2.96	119.74	122.79
3	L5	3718	A2M	C2-N3-C4	2.95	119.05	111.83
3	L5	4620	OMU	C2'-C1'-N1	-2.95	108.64	114.24
3	L5	3639	PSU	O2-C2-N1	-2.94	119.75	122.79
3	L5	4673	PSU	O2-C2-N1	-2.94	119.76	122.79
3	L5	3920	PSU	C5-C6-N1	-2.94	118.06	122.14
1	S2	1678	A2M	C4-N9-C8	2.94	108.82	105.74
1	S2	668	A2M	N3-C2-N1	-2.92	124.16	128.58
3	L5	4536	OMC	C2'-C1'-N1	-2.92	108.70	114.24
3	L5	4523	A2M	C5-N7-C8	2.92	108.03	103.45
3	L5	3637	PSU	C5-C6-N1	-2.91	118.10	122.14
3	L5	1524	A2M	C4-C5-N7	-2.90	107.26	110.58
3	L5	3785	A2M	C4-C5-N7	-2.90	107.26	110.58
3	L5	2401	A2M	C4-N9-C8	2.90	108.78	105.74
1	S2	468	A2M	C2'-C1'-N9	-2.89	108.99	113.75
1	S2	166	A2M	C4-N9-C8	2.89	108.78	105.74
1	S2	815	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	3785	A2M	O4'-C1'-C2'	-2.89	101.62	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	172	OMU	O4-C4-C5	-2.88	120.19	125.16
1	S2	172	OMU	O4'-C1'-N1	2.88	114.88	108.36
3	L5	1871	A2M	C5-N7-C8	2.88	107.97	103.45
1	S2	1447	OMG	C2'-C1'-N9	-2.87	108.78	114.24
3	L5	4306	OMU	O4-C4-C5	-2.87	120.22	125.16
84	At	8	4SU	C1'-N1-C2	2.86	122.74	117.59
3	L5	3782	5MC	O2-C2-N3	-2.85	117.83	122.33
1	S2	428	OMU	O2-C2-N1	-2.85	119.09	122.80
1	S2	1490	OMG	C2'-C1'-N9	-2.85	108.84	114.24
1	S2	1239	PSU	C6-C5-C4	-2.84	116.25	118.17
3	L5	1522	OMG	C6-C5-N7	2.84	135.45	130.29
3	L5	4494	OMG	C4-C5-N7	-2.83	106.18	110.67
1	S2	99	A2M	C4-N9-C8	2.83	108.71	105.74
3	L5	4623	OMG	C2'-C1'-N9	-2.83	108.87	114.24
3	L5	4442	PSU	C5-C6-N1	-2.83	118.21	122.14
84	At	37	MIA	C4-N9-C8	2.83	108.71	105.74
3	L5	3782	5MC	C5-C4-N3	-2.83	118.86	121.75
3	L5	1625	OMG	C6-C5-N7	2.82	135.43	130.29
1	S2	1367	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	3867	A2M	C4-C5-N7	-2.80	107.38	110.58
1	S2	627	OMU	O2-C2-N1	-2.80	119.15	122.80
6	SA	2	SAC	C2A-C1A-N	-2.79	111.49	116.12
3	L5	4637	OMG	C4-C5-N7	-2.79	106.25	110.67
1	S2	966	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	3724	A2M	C4-C5-N7	-2.78	107.41	110.58
3	L5	3825	A2M	C4-C5-N7	-2.78	107.41	110.58
3	L5	1322	1MA	C4-C5-N7	-2.77	106.28	110.67
3	L5	1792	PSU	C5-C6-N1	-2.76	118.31	122.14
3	L5	4636	PSU	C5-C6-N1	-2.76	118.31	122.14
1	S2	1832	6MZ	C4-N9-C8	2.76	108.64	105.74
3	L5	1871	A2M	C4-N9-C8	2.76	108.64	105.74
3	L5	3792	OMG	C4-C5-N7	-2.76	106.30	110.67
84	At	20	H2U	C5-C4-N3	2.76	119.62	116.69
3	L5	3925	OMU	C2'-C1'-N1	-2.75	109.02	114.24
1	S2	1337	4AC	C2'-C1'-N1	-2.75	105.59	113.25
2	L8	55	PSU	C5-C6-N1	-2.75	118.32	122.14
84	At	37	MIA	C11-S10-C2	-2.75	100.19	102.25
1	S2	354	OMU	O4-C4-C5	-2.74	120.43	125.16
3	L5	3695	PSU	O2-C2-N1	-2.74	119.96	122.79
1	S2	512	A2M	C4-N9-C8	2.74	108.61	105.74
3	L5	4523	A2M	C4-N9-C8	2.74	108.61	105.74
3	L5	1524	A2M	C4-N9-C8	2.74	108.61	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1832	6MZ	C2-N1-C6	2.74	124.31	115.24
1	S2	99	A2M	C2'-C1'-N9	-2.73	109.25	113.75
1	S2	517	OMC	C2'-C1'-N1	-2.73	109.06	114.24
3	L5	1326	A2M	C5-N7-C8	2.73	107.74	103.45
3	L5	4636	PSU	O2-C2-N3	-2.71	117.05	121.86
3	L5	4370	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	3944	OMG	C4-C5-N7	-2.70	106.38	110.67
3	L5	4618	OMG	C4-C5-N7	-2.70	106.39	110.67
2	L8	69	PSU	O2'-C2'-C1'	-2.70	104.80	111.21
3	L5	4521	PSU	C5-C6-N1	-2.70	118.39	122.14
3	L5	2401	A2M	C2'-C1'-N9	-2.70	109.31	113.75
3	L5	2787	A2M	C5-N7-C8	2.70	107.69	103.45
3	L5	2815	A2M	N3-C2-N1	-2.70	124.50	128.58
3	L5	3760	A2M	C4-N9-C8	2.70	108.57	105.74
1	S2	1081	PSU	C5-C6-N1	-2.69	118.40	122.14
3	L5	4618	OMG	C2'-C1'-N9	-2.68	109.15	114.24
1	S2	1851	MA6	C4-N9-C8	2.68	108.55	105.74
84	At	8	4SU	C3'-C2'-C1'	2.67	106.52	101.46
3	L5	3825	A2M	C5-N7-C8	2.67	107.65	103.45
3	L5	1677	PSU	C4'-O4'-C1'	-2.66	101.78	108.44
3	L5	3723	A2M	C2'-C1'-N9	-2.66	109.37	113.75
3	L5	4569	PSU	C5-C6-N1	-2.65	118.46	122.14
1	S2	1850	MA6	C5-N7-C8	2.65	107.61	103.45
1	S2	1031	A2M	C4-N9-C8	2.64	108.51	105.74
3	L5	3729	PSU	C5-C6-N1	-2.64	118.48	122.14
3	L5	2365	OMC	C2'-C1'-N1	-2.63	109.24	114.24
3	L5	4521	PSU	O2-C2-N3	-2.63	117.18	121.86
1	S2	468	A2M	C5-N7-C8	2.63	107.59	103.45
1	S2	121	OMU	C2'-C1'-N1	-2.63	109.25	114.24
1	S2	1832	6MZ	C5-N7-C8	2.63	107.58	103.45
3	L5	3637	PSU	O2-C2-N3	-2.63	117.20	121.86
3	L5	4299	PSU	C5-C6-N1	-2.62	118.50	122.14
3	L5	1316	OMG	C2'-C1'-N9	-2.62	109.28	114.24
3	L5	4403	PSU	C5-C6-N1	-2.62	118.51	122.14
1	S2	1056	PSU	C5-C6-N1	-2.61	118.52	122.14
3	L5	400	A2M	C5-N7-C8	2.61	107.55	103.45
3	L5	2815	A2M	C5-N7-C8	2.61	107.55	103.45
1	S2	644	OMG	C4-C5-N7	-2.60	106.55	110.67
6	SA	2	SAC	O-C-CA	-2.59	118.11	124.77
1	S2	601	OMG	C4-C5-N7	-2.59	106.57	110.67
2	L8	14	OMU	O4-C4-C5	-2.58	120.71	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	166	A2M	C5-N7-C8	2.58	107.51	103.45
1	S2	1383	A2M	C4-N9-C8	2.58	108.45	105.74
1	S2	512	A2M	C5-N7-C8	2.58	107.50	103.45
1	S2	1248	B8N	C31-N3-C4	2.58	120.83	117.18
84	At	37	MIA	C2-N1-C6	2.58	122.43	117.54
3	L5	4220	6MZ	N9-C8-N7	-2.57	110.29	113.94
3	L5	2363	A2M	C5-N7-C8	2.57	107.49	103.45
3	L5	1677	PSU	C5-C6-N1	-2.57	118.57	122.14
1	S2	484	A2M	C5-N7-C8	2.56	107.48	103.45
84	At	37	MIA	N3-C2-N1	-2.56	122.32	127.00
3	L5	3637	PSU	O2-C2-N1	-2.56	120.15	122.79
3	L5	3724	A2M	C2-N1-C6	2.56	122.94	118.73
1	S2	1678	A2M	C5-N7-C8	2.56	107.47	103.45
3	L5	2364	OMG	O6-C6-C5	-2.56	119.78	126.53
1	S2	1367	PSU	O2-C2-N3	-2.55	117.32	121.86
3	L5	4196	OMG	C4-C5-N7	-2.55	106.62	110.67
2	L8	75	OMG	C4-C5-N7	-2.55	106.62	110.67
1	S2	159	A2M	C4-N9-C8	2.55	108.41	105.74
3	L5	4532	PSU	C6-C5-C4	-2.55	116.46	118.17
3	L5	3925	OMU	O4-C4-C5	-2.55	120.77	125.16
3	L5	4392	OMG	C4-C5-N7	-2.54	106.64	110.67
3	L5	4447	5MC	O2-C2-N3	-2.54	118.33	122.33
3	L5	2424	OMG	O6-C6-C5	-2.53	119.85	126.53
1	S2	121	OMU	O4-C4-C5	-2.53	120.81	125.16
3	L5	3830	A2M	C4-N9-C8	2.52	108.39	105.74
1	S2	1490	OMG	C4-C5-N7	-2.52	106.68	110.67
3	L5	3899	OMG	C8-N7-C5	2.52	108.75	104.26
3	L5	3695	PSU	C3'-C2'-C1'	2.51	104.66	101.69
1	S2	1326	UY1	C5-C6-N1	-2.51	118.66	122.14
3	L5	3695	PSU	O2-C2-N3	-2.50	117.42	121.86
1	S2	576	A2M	C5-N7-C8	2.50	107.38	103.45
3	L5	3899	OMG	C2'-C1'-N9	-2.50	109.50	114.24
3	L5	3764	PSU	C3'-C2'-C1'	2.50	104.64	101.69
2	L8	14	OMU	C2'-C1'-N1	-2.49	109.51	114.24
3	L5	2843	PSU	C5-C6-N1	-2.49	118.68	122.14
3	L5	3701	OMC	C3'-C2'-C1'	-2.49	98.03	102.81
84	At	37	MIA	C5-N7-C8	2.49	107.37	103.45
3	L5	1534	A2M	O3'-C3'-C4'	-2.49	103.92	111.08
3	L5	4500	PSU	C3'-C2'-C1'	2.49	104.63	101.69
3	L5	3785	A2M	N9-C8-N7	-2.49	110.40	113.94
1	S2	436	OMG	C4-C5-N7	-2.49	106.72	110.67
1	S2	159	A2M	C5-N7-C8	2.49	107.36	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1383	A2M	C5-N7-C8	2.49	107.36	103.45
3	L5	3734	PSU	C5-C6-N1	-2.49	118.69	122.14
1	S2	27	A2M	C4-N9-C8	2.49	108.35	105.74
3	L5	3762	PSU	C3'-C2'-C1'	2.49	104.62	101.69
3	L5	1326	A2M	C2-N1-C6	2.48	122.81	118.73
3	L5	1534	A2M	C2'-C1'-N9	2.48	117.84	113.75
3	L5	2422	OMC	O2-C2-N3	-2.48	118.42	122.33
3	L5	2424	OMG	C6-C5-N7	2.48	134.80	130.29
1	S2	1678	A2M	C2'-C1'-N9	-2.48	109.68	113.75
3	L5	1522	OMG	C5-C6-N1	2.48	119.56	113.25
1	S2	1850	MA6	C6-C5-N7	2.47	137.38	133.43
1	S2	644	OMG	O6-C6-C5	-2.47	120.01	126.53
3	L5	1677	PSU	O2'-C2'-C1'	-2.47	105.36	111.21
3	L5	2837	OMU	O4-C4-C5	-2.47	120.91	125.16
1	S2	1447	OMG	C2'-C3'-C4'	-2.46	96.70	101.99
3	L5	2351	OMC	O2-C2-N3	-2.46	118.45	122.33
3	L5	3627	OMG	C2'-C1'-N9	-2.46	109.58	114.24
1	S2	174	OMC	O2-C2-N3	-2.46	118.46	122.33
3	L5	4623	OMG	C4-C5-N7	-2.46	106.78	110.67
1	S2	1136	PSU	C5-C6-N1	-2.46	118.73	122.14
1	S2	468	A2M	C4-N9-C8	2.45	108.31	105.74
3	L5	4590	A2M	C5-N7-C8	2.45	107.30	103.45
1	S2	1328	OMG	C4-C5-N7	-2.45	106.79	110.67
3	L5	1782	PSU	C6-C5-C4	-2.45	116.52	118.17
40	LB	245	HIC	NE2-CE1-ND1	-2.44	111.73	112.66
3	L5	2876	OMG	C4-C5-N7	-2.44	106.80	110.67
3	L5	3818	UY1	C5-C6-N1	-2.44	118.75	122.14
3	L5	2815	A2M	C4-N9-C8	2.44	108.30	105.74
1	S2	1248	B8N	O36-C34-O35	-2.44	118.55	124.08
3	L5	4530	UR3	C3U-N3-C4	2.43	121.24	117.87
1	S2	683	OMG	C4-C5-N7	-2.43	106.81	110.67
1	S2	1447	OMG	C4-C5-N7	-2.43	106.81	110.67
3	L5	3760	A2M	O4'-C1'-N9	2.43	112.76	108.09
1	S2	27	A2M	C5-N7-C8	2.43	107.27	103.45
3	L5	3853	PSU	O2-C2-N1	-2.43	120.28	122.79
3	L5	2401	A2M	C5-N7-C8	2.42	107.26	103.45
3	L5	3785	A2M	C5-N7-C8	2.42	107.26	103.45
1	S2	1804	OMU	C1'-N1-C2	2.42	121.94	117.59
1	S2	172	OMU	O2-C2-N3	-2.42	117.03	121.49
3	L5	4590	A2M	C4-N9-C8	2.41	108.27	105.74
1	S2	99	A2M	C5-N7-C8	2.41	107.24	103.45
3	L5	3744	OMG	C4-C5-N7	-2.40	106.86	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3825	A2M	N9-C8-N7	-2.40	110.53	113.94
1	S2	1851	MA6	C6-C5-N7	2.40	137.26	133.43
3	L5	4523	A2M	O4'-C1'-N9	2.40	112.69	108.09
3	L5	4293	PSU	C6-C5-C4	-2.39	116.56	118.17
84	At	16	H2U	C5-C6-N1	-2.39	104.29	111.52
3	L5	3884	PSU	C6-C5-C4	-2.38	116.56	118.17
3	L5	1871	A2M	C6-C5-N7	2.38	136.69	132.09
84	At	39	PSU	C3'-C2'-C1'	2.38	104.50	101.69
3	L5	4623	OMG	O6-C6-C5	-2.38	120.25	126.53
3	L5	398	A2M	C4-N9-C8	2.38	108.23	105.74
3	L5	4523	A2M	N9-C8-N7	-2.38	110.57	113.94
3	L5	2508	PSU	O2-C2-N3	-2.37	117.65	121.86
1	S2	590	A2M	C4-N9-C8	2.37	108.23	105.74
3	L5	3760	A2M	C5-N7-C8	2.37	107.17	103.45
1	S2	428	OMU	O2'-C2'-C1'	2.37	113.49	108.99
1	S2	27	A2M	C2'-C1'-N9	-2.37	109.85	113.75
3	L5	3830	A2M	C5-N7-C8	2.37	107.17	103.45
1	S2	576	A2M	C4-N9-C8	2.36	108.22	105.74
1	S2	1850	MA6	N9-C8-N7	-2.36	110.59	113.94
3	L5	1326	A2M	N9-C8-N7	-2.36	110.59	113.94
1	S2	815	PSU	C5-C6-N1	-2.35	118.88	122.14
52	La	39	V5N	O-C-CA	-2.35	118.72	124.77
1	S2	590	A2M	C5-N7-C8	2.35	107.14	103.45
3	L5	1534	A2M	C5-N7-C8	2.35	107.14	103.45
3	L5	4532	PSU	C3'-C2'-C1'	2.35	104.46	101.69
1	S2	1391	OMC	C2'-C1'-N1	-2.35	109.79	114.24
3	L5	1524	A2M	N6-C6-N1	2.35	123.60	118.38
1	S2	867	OMG	C4-C5-N7	-2.34	106.96	110.67
3	L5	3723	A2M	C5-N7-C8	2.34	107.12	103.45
3	L5	3744	OMG	O6-C6-C5	-2.34	120.36	126.53
1	S2	105	PSU	O2-C2-N3	-2.33	117.73	121.86
3	L5	400	A2M	N9-C8-N7	-2.33	110.64	113.94
3	L5	3869	OMC	C2'-C1'-N1	-2.32	109.83	114.24
1	S2	1238	PSU	C5-C6-N1	-2.32	118.92	122.14
3	L5	3853	PSU	C6-C5-C4	-2.32	116.61	118.17
1	S2	509	OMG	C4-C5-N7	-2.32	106.99	110.67
1	S2	484	A2M	C4-N9-C8	2.31	108.17	105.74
3	L5	4498	OMU	O2-C2-N1	-2.31	119.79	122.80
3	L5	4228	OMG	N2-C2-N1	2.31	121.63	116.76
3	L5	3627	OMG	C4-C5-N7	-2.31	107.02	110.67
3	L5	1326	A2M	C2'-C1'-N9	-2.30	109.96	113.75
3	L5	1871	A2M	N9-C8-N7	-2.29	110.68	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	C4-N9-C8	2.29	108.14	105.74
3	L5	2363	A2M	C4-N9-C8	2.29	108.14	105.74
1	S2	1639	G7M	O6-C6-C5	-2.28	122.92	128.01
3	L5	1522	OMG	C8-N9-C4	2.28	110.30	106.03
3	L5	4493	PSU	C5-C6-N1	-2.28	118.97	122.14
84	At	46	G7M	O6-C6-C5	-2.28	122.92	128.01
3	L5	3627	OMG	O6-C6-C5	-2.28	120.52	126.53
84	At	32	PSU	C5-C6-N1	-2.28	118.98	122.14
3	L5	2364	OMG	C5-C6-N1	2.28	119.05	113.25
3	L5	1582	PSU	C5-C6-N1	-2.27	118.98	122.14
1	S2	1383	A2M	O4'-C1'-N9	2.27	112.45	108.09
3	L5	4499	OMG	O6-C6-C5	-2.27	120.54	126.53
3	L5	4499	OMG	C4-C5-N7	-2.27	107.07	110.67
3	L5	4442	PSU	O4'-C1'-C2'	2.27	108.29	105.15
1	S2	668	A2M	C5-N7-C8	2.27	107.01	103.45
3	L5	3724	A2M	N9-C8-N7	-2.26	110.72	113.94
1	S2	966	PSU	C5-C6-N1	-2.26	119.00	122.14
3	L5	3758	PSU	C5-C6-N1	-2.26	119.00	122.14
1	S2	1031	A2M	C5-N7-C8	2.26	107.00	103.45
1	S2	651	PSU	C5-C6-N1	-2.26	119.01	122.14
1	S2	1643	PSU	C5-C6-N1	-2.26	119.01	122.14
3	L5	1781	PSU	C5-C6-N1	-2.25	119.01	122.14
3	L5	1625	OMG	C5-C6-N1	2.25	118.99	113.25
3	L5	398	A2M	C5-N7-C8	2.25	106.98	103.45
3	L5	3851	PSU	O2-C2-N3	-2.25	117.87	121.86
3	L5	3723	A2M	C2-N1-C6	2.25	122.42	118.73
3	L5	4228	OMG	N2-C2-N3	-2.25	115.29	119.67
3	L5	1871	A2M	C2-N1-C6	2.24	122.42	118.73
1	S2	166	A2M	N9-C8-N7	-2.24	110.75	113.94
1	S2	1447	OMG	O6-C6-C5	-2.24	120.61	126.53
3	L5	3884	PSU	O2-C2-N3	-2.24	117.88	121.86
1	S2	1337	4AC	C6-C5-C4	2.24	119.70	117.00
3	L5	3724	A2M	C5-N7-C8	2.24	106.97	103.45
3	L5	4689	PSU	C5-C6-N1	-2.24	119.03	122.14
3	L5	4521	PSU	O4'-C1'-C2'	2.24	108.25	105.15
3	L5	4457	PSU	C3'-C2'-C1'	2.24	104.33	101.69
3	L5	3718	A2M	N3-C2-N1	-2.23	125.20	128.58
1	S2	1678	A2M	N9-C8-N7	-2.23	110.77	113.94
1	S2	1490	OMG	O6-C6-C5	-2.23	120.65	126.53
1	S2	822	PSU	C5-C6-N1	-2.22	119.05	122.14
3	L5	3851	PSU	C5-C6-N1	-2.22	119.05	122.14
1	S2	1442	OMU	C2'-C1'-N1	-2.22	110.02	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4227	OMU	C2'-C1'-N1	-2.22	110.02	114.24
3	L5	4227	OMU	O4-C4-C5	-2.22	121.33	125.16
3	L5	400	A2M	C6-C5-N7	2.22	136.37	132.09
3	L5	2401	A2M	C6-C5-N7	2.22	136.37	132.09
3	L5	3695	PSU	C5-C6-N1	-2.22	119.06	122.14
1	S2	1391	OMC	O2-C2-N3	-2.22	118.83	122.33
3	L5	2861	OMC	O2-C2-N3	-2.22	118.83	122.33
3	L5	4637	OMG	C8-N7-C5	2.22	108.21	104.26
3	L5	3944	OMG	O4'-C4'-C3'	-2.22	100.76	105.15
3	L5	3724	A2M	C6-C5-N7	2.21	136.36	132.09
3	L5	4532	PSU	O2'-C2'-C3'	-2.21	104.73	111.82
1	S2	576	A2M	C6-C5-N7	2.21	136.35	132.09
1	S2	1337	4AC	O7-C7-N4	2.21	125.37	121.90
85	Pt	8	4SU	C1'-N1-C2	2.21	121.56	117.59
3	L5	4471	PSU	O2-C2-N1	-2.21	120.51	122.79
1	S2	1288	OMU	C1'-N1-C2	2.20	121.55	117.59
3	L5	1534	A2M	C6-C5-N7	2.20	136.33	132.09
3	L5	4576	PSU	O2-C2-N1	-2.20	120.52	122.79
3	L5	3762	PSU	C6-C5-C4	-2.20	116.69	118.17
3	L5	3944	OMG	O4'-C1'-N9	2.20	113.34	108.36
1	S2	1842	4AC	O2-C2-N3	-2.19	118.87	122.33
3	L5	2401	A2M	C2-N1-C6	2.19	122.33	118.73
3	L5	4571	A2M	C5-N7-C8	2.19	106.90	103.45
1	S2	1248	B8N	C1'-C5-C4	2.19	120.93	117.61
1	S2	166	A2M	C6-C5-N7	2.19	136.32	132.09
3	L5	4493	PSU	O2-C2-N3	-2.19	117.97	121.86
1	S2	34	PSU	C5-C6-N1	-2.19	119.10	122.14
3	L5	2839	PSU	C5-C6-N1	-2.19	119.10	122.14
3	L5	4456	OMC	C2'-C1'-N1	-2.19	110.09	114.24
1	S2	119	PSU	C3'-C2'-C1'	2.19	104.27	101.69
1	S2	1243	PSU	C5-C6-N1	-2.19	119.11	122.14
3	L5	1534	A2M	C4-N9-C8	2.19	108.03	105.74
1	S2	649	PSU	C5-C6-N1	-2.18	119.11	122.14
3	L5	4590	A2M	C2-N1-C6	2.18	122.31	118.73
1	S2	1328	OMG	O6-C6-C5	-2.18	120.79	126.53
3	L5	4500	PSU	C5-C6-N1	-2.17	119.12	122.14
3	L5	4579	PSU	C5-C6-N1	-2.17	119.12	122.14
2	L8	75	OMG	O6-C6-C5	-2.17	120.80	126.53
3	L5	4618	OMG	O6-C6-C5	-2.17	120.81	126.53
3	L5	3867	A2M	C5-N7-C8	2.17	106.86	103.45
3	L5	4689	PSU	O2-C2-N3	-2.17	118.01	121.86
2	L8	14	OMU	O2-C2-N3	-2.17	117.49	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3723	A2M	N9-C8-N7	-2.16	110.87	113.94
1	S2	1678	A2M	C6-C5-N7	2.16	136.26	132.09
1	S2	668	A2M	C4-N9-C8	2.16	108.01	105.74
3	L5	2815	A2M	C2-N1-C6	2.16	122.28	118.73
3	L5	1322	1MA	C6-C5-N7	2.16	135.97	132.16
1	S2	509	OMG	O6-C6-C5	-2.16	120.84	126.53
3	L5	1326	A2M	C6-C5-N7	2.16	136.25	132.09
3	L5	4392	OMG	C5-C6-N1	2.16	118.74	113.25
3	L5	4536	OMC	O2-C2-N3	-2.15	118.94	122.33
1	S2	918	PSU	C5-C6-N1	-2.15	119.15	122.14
3	L5	4576	PSU	O2-C2-N3	-2.15	118.05	121.86
3	L5	4457	PSU	C6-C5-C4	-2.15	116.72	118.17
3	L5	4628	PSU	C6-C5-C4	-2.15	116.73	118.17
3	L5	4620	OMU	O4'-C1'-N1	2.14	113.22	108.36
40	LB	245	HIC	CB-CG-CD2	-2.14	124.79	129.96
3	L5	4571	A2M	C2-N1-C6	2.14	122.25	118.73
1	S2	572	PSU	O4'-C1'-C2'	2.14	108.11	105.15
3	L5	4228	OMG	O3'-C3'-C4'	-2.14	104.93	111.08
3	L5	2876	OMG	C5-C6-N1	2.14	118.70	113.25
1	S2	1031	A2M	C6-C5-N7	2.14	136.21	132.09
1	S2	1851	MA6	N9-C8-N7	-2.13	110.91	113.94
1	S2	1445	PSU	C5-C6-N1	-2.13	119.18	122.14
3	L5	1316	OMG	O6-C6-C5	-2.13	120.90	126.53
1	S2	105	PSU	C5-C6-N1	-2.13	119.18	122.14
3	L5	3701	OMC	C5-C6-N1	-2.13	118.37	121.84
1	S2	1832	6MZ	N9-C8-N7	-2.13	110.91	113.94
3	L5	4636	PSU	O4'-C1'-C2'	2.13	108.09	105.15
1	S2	172	OMU	O2'-C2'-C1'	2.13	113.03	108.99
3	L5	4403	PSU	O2-C2-N3	-2.13	118.09	121.86
3	L5	398	A2M	C2'-C1'-N9	-2.12	110.26	113.75
1	S2	1842	4AC	N4-C4-N3	2.12	117.31	113.87
1	S2	1248	B8N	O4'-C1'-C2'	2.12	108.08	105.15
3	L5	4403	PSU	O4'-C1'-C2'	2.12	108.08	105.15
1	S2	1081	PSU	O2-C2-N3	-2.12	118.10	121.86
3	L5	1316	OMG	CM2-O2'-C2'	-2.12	109.03	114.47
3	L5	2363	A2M	C6-C5-N7	2.12	136.18	132.09
3	L5	3853	PSU	O2-C2-N3	-2.12	118.10	121.86
1	S2	119	PSU	C6-C5-C4	-2.12	116.75	118.17
3	L5	3723	A2M	C6-C5-N7	2.12	136.17	132.09
3	L5	1862	PSU	C5-C6-N1	-2.12	119.20	122.14
1	S2	573	PSU	C5-C6-N1	-2.11	119.20	122.14
1	S2	814	PSU	C5-C6-N1	-2.11	119.22	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4530	UR3	O4'-C1'-N1	2.10	113.13	108.36
3	L5	2787	A2M	O4'-C1'-C2'	-2.10	102.97	106.59
3	L5	1524	A2M	C2-N1-C6	2.10	122.18	118.73
1	S2	172	OMU	C6-N1-C2	-2.10	118.44	121.00
85	Pt	56	PSU	C5-C6-N1	-2.10	119.23	122.14
3	L5	4392	OMG	O6-C6-C5	-2.10	121.00	126.53
3	L5	4623	OMG	C5-C6-N1	2.10	118.59	113.25
3	L5	2363	A2M	C2-N1-C6	2.10	122.17	118.73
3	L5	4571	A2M	C6-C5-N7	2.09	136.13	132.09
3	L5	4972	PSU	C5-C6-N1	-2.09	119.23	122.14
84	At	32	PSU	C3'-C2'-C1'	2.09	104.16	101.69
1	S2	867	OMG	O6-C6-C5	-2.09	121.02	126.53
1	S2	1174	PSU	C5-C6-N1	-2.09	119.24	122.14
1	S2	166	A2M	C2-N1-C6	2.09	122.16	118.73
3	L5	1860	PSU	O2-C2-N3	-2.09	118.15	121.86
1	S2	1328	OMG	C2'-C1'-N9	-2.08	110.28	114.24
3	L5	4471	PSU	O2-C2-N3	-2.08	118.16	121.86
3	L5	4220	6MZ	C2-N1-C6	2.08	122.14	115.24
1	S2	468	A2M	C6-C5-N7	2.08	136.10	132.09
3	L5	1322	1MA	N1-C2-N3	-2.08	123.52	126.00
3	L5	4228	OMG	O6-C6-C5	-2.08	121.04	126.53
3	L5	4353	PSU	C5-C6-N1	-2.08	119.26	122.14
3	L5	3715	PSU	C5-C6-N1	-2.07	119.26	122.14
3	L5	4637	OMG	C5-C6-N1	2.07	118.53	113.25
39	LA	216	V5N	O-C-CA	-2.07	119.44	124.77
3	L5	4636	PSU	O2-C2-N1	-2.07	120.65	122.79
1	S2	517	OMC	O2-C2-N3	-2.07	119.07	122.33
1	S2	814	PSU	O2'-C2'-C3'	-2.07	105.19	111.82
1	S2	966	PSU	O2-C2-N3	-2.07	118.19	121.86
1	S2	218	PSU	C6-C5-C4	-2.06	116.78	118.17
3	L5	4312	PSU	O2-C2-N3	-2.06	118.20	121.86
3	L5	5001	PSU	C5-C6-N1	-2.06	119.28	122.14
3	L5	2815	A2M	C6-C5-N7	2.06	136.06	132.09
3	L5	3627	OMG	C5-C6-N1	2.06	118.49	113.25
1	S2	436	OMG	O6-C6-C5	-2.06	121.10	126.53
1	S2	1243	PSU	O2-C2-N3	-2.06	118.21	121.86
1	S2	1248	B8N	O2-C2-N3	-2.05	119.22	121.98
84	At	37	MIA	N9-C8-N7	-2.05	111.03	113.94
1	S2	27	A2M	C6-C5-N7	2.05	136.04	132.09
3	L5	4306	OMU	O2-C2-N1	-2.05	120.13	122.80
3	L5	3830	A2M	C2-N1-C6	2.05	122.09	118.73
3	L5	3944	OMG	O6-C6-C5	-2.05	121.13	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5010	PSU	C5-C6-N1	-2.04	119.30	122.14
3	L5	4361	PSU	C5-C6-N1	-2.04	119.31	122.14
1	S2	1703	OMC	O2-C2-N3	-2.04	119.12	122.33
3	L5	1782	PSU	O3'-C3'-C4'	2.04	116.93	111.08
3	L5	3851	PSU	O4'-C1'-C2'	2.03	107.97	105.15
1	S2	1643	PSU	O4'-C1'-C2'	2.03	107.96	105.15
3	L5	3637	PSU	C3'-C2'-C1'	2.03	104.08	101.69
1	S2	296	PSU	C5-C6-N1	-2.03	119.33	122.14
3	L5	1522	OMG	C6-C5-C4	-2.03	115.78	118.83
1	S2	683	OMG	O6-C6-C5	-2.02	121.19	126.53
3	L5	2508	PSU	O2-C2-N1	-2.02	120.70	122.79
1	S2	668	A2M	C6-C5-N7	2.02	135.99	132.09
3	L5	2364	OMG	C2-N1-C6	-2.02	121.45	125.11
3	L5	2401	A2M	N9-C8-N7	-2.02	111.07	113.94
1	S2	99	A2M	C2-N1-C6	2.02	122.04	118.73
3	L5	1536	PSU	C5-C6-N1	-2.01	119.34	122.14
1	S2	1692	PSU	C5-C6-N1	-2.01	119.35	122.14
1	S2	1367	PSU	C5-C6-N1	-2.01	119.35	122.14
1	S2	509	OMG	C5-C6-N1	2.01	118.37	113.25
1	S2	815	PSU	C3'-C2'-C1'	2.01	104.06	101.69
84	At	20	H2U	C5-C6-N1	-2.01	105.45	111.52
3	L5	4523	A2M	C6-C5-N7	2.00	135.95	132.09
3	L5	4590	A2M	C6-C5-N7	2.00	135.95	132.09
3	L5	4420	PSU	C5-C6-N1	-2.00	119.36	122.14
1	S2	512	A2M	N9-C8-N7	-2.00	111.09	113.94
3	L5	4576	PSU	C3'-C2'-C1'	2.00	104.05	101.69

There are no chirality outliers.

All (165) 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
29	SV	1	AME	OT-CT1-N-CA
66	Lr	2	SAC	C2A-C1A-N-CA
68	Lb	5	MLZ	CD-CE-NZ-CM
86	EF	79	M3L	N-CA-CB-CG
86	EF	79	M3L	C-CA-CB-CG
86	EF	79	M3L	O-C-CA-CB
86	EF	318	M3L	N-CA-CB-CG
86	EF	318	M3L	C-CA-CB-CG
1	S2	27	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
1	S2	172	OMU	O4'-C1'-N1-C2
1	S2	172	OMU	O4'-C1'-N1-C6
1	S2	174	OMC	C1'-C2'-O2'-CM2
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	867	OMG	C1'-C2'-O2'-CM2
1	S2	1248	B8N	N34-C33-C34-O35
1	S2	1288	OMU	O4'-C4'-C5'-O5'
1	S2	1328	OMG	C1'-C2'-O2'-CM2
1	S2	1337	4AC	N3-C4-N4-C7
1	S2	1337	4AC	C5-C4-N4-C7
1	S2	1337	4AC	O7-C7-N4-C4
1	S2	1337	4AC	CM7-C7-N4-C4
1	S2	1447	OMG	C1'-C2'-O2'-CM2
1	S2	1490	OMG	C1'-C2'-O2'-CM2
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1832	6MZ	N1-C6-N6-C9
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	2415	OMU	C1'-C2'-O2'-CM2
3	L5	2424	OMG	C1'-C2'-O2'-CM2
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	2824	OMC	C1'-C2'-O2'-CM2
3	L5	3718	A2M	C1'-C2'-O2'-CM'
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	3760	A2M	C1'-C2'-O2'-CM'
3	L5	3792	OMG	C1'-C2'-O2'-CM2
3	L5	3944	OMG	C1'-C2'-O2'-CM2
3	L5	4420	PSU	O4'-C4'-C5'-O5'
3	L5	4456	OMC	C1'-C2'-O2'-CM2
3	L5	4531	PSU	O4'-C1'-C5-C4
3	L5	4531	PSU	O4'-C1'-C5-C6
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	4618	OMG	C1'-C2'-O2'-CM2
3	L5	4637	OMG	C1'-C2'-O2'-CM2
20	SX	62	HY3	O-C-CA-C3
39	LA	216	V5N	O-C-CA-CB
84	At	16	H2U	O4'-C4'-C5'-O5'
84	At	16	H2U	C3'-C4'-C5'-O5'
84	At	20	H2U	O4'-C1'-N1-C2
84	At	20	H2U	O4'-C1'-N1-C6
84	At	37	MIA	C12-C13-C14-C15
84	At	37	MIA	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
1	S2	644	OMG	O4'-C4'-C5'-O5'
1	S2	1442	OMU	C3'-C4'-C5'-O5'
1	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	4420	PSU	C3'-C4'-C5'-O5'
84	At	46	G7M	C3'-C4'-C5'-O5'
84	At	16	H2U	C4'-C5'-O5'-P
86	EF	318	M3L	CE-CD-CG-CB
66	Lr	2	SAC	OAC-C1A-N-CA
1	S2	683	OMG	O4'-C4'-C5'-O5'
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	3729	PSU	O4'-C4'-C5'-O5'
85	Pt	21	H2U	O4'-C4'-C5'-O5'
85	Pt	21	H2U	C3'-C4'-C5'-O5'
81	Lo	53	MLZ	CG-CD-CE-NZ
3	L5	2787	A2M	C2'-C1'-N9-C4
86	EF	318	M3L	CD-CE-NZ-CM3
86	EF	318	M3L	CG-CD-CE-NZ
1	S2	1248	B8N	N34-C33-C34-O36
86	EF	318	M3L	CD-CE-NZ-CM2
1	S2	172	OMU	C3'-C2'-O2'-CM2
3	L5	1625	OMG	C3'-C2'-O2'-CM2
1	S2	590	A2M	C3'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	1288	OMU	C3'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'
86	EF	318	M3L	CD-CE-NZ-CM1
3	L5	3701	OMC	C2'-C1'-N1-C6
86	EF	55	MLY	CA-CB-CG-CD
1	S2	590	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	O4'-C4'-C5'-O5'
3	L5	2401	A2M	C3'-C4'-C5'-O5'
3	L5	3851	PSU	C3'-C4'-C5'-O5'
84	At	46	G7M	O4'-C4'-C5'-O5'
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
84	At	32	PSU	O4'-C4'-C5'-O5'
1	S2	172	OMU	O4'-C4'-C5'-O5'
3	L5	3760	A2M	O4'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	4637	OMG	O4'-C4'-C5'-O5'
84	At	20	H2U	C4'-C5'-O5'-P
1	S2	1248	B8N	C32-C33-C34-O35
84	At	20	H2U	C3'-C4'-C5'-O5'
84	At	32	PSU	C3'-C4'-C5'-O5'
81	Lo	53	MLZ	CA-CB-CG-CD
1	S2	683	OMG	C3'-C4'-C5'-O5'
3	L5	3729	PSU	C3'-C4'-C5'-O5'
84	At	20	H2U	O4'-C4'-C5'-O5'
3	L5	1792	PSU	O4'-C4'-C5'-O5'
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	3701	OMC	C2'-C1'-N1-C2
1	S2	99	A2M	C1'-C2'-O2'-CM'
1	S2	484	A2M	C1'-C2'-O2'-CM'
3	L5	3744	OMG	C1'-C2'-O2'-CM2
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	3818	UY1	C4'-C5'-O5'-P
1	S2	1248	B8N	C32-C33-C34-O36
29	SV	1	AME	CB-CG-SD-CE
3	L5	4494	OMG	C3'-C2'-O2'-CM2
3	L5	4447	5MC	O4'-C1'-N1-C6
1	S2	1832	6MZ	C5-C6-N6-C9
3	L5	3701	OMC	O4'-C1'-N1-C6
1	S2	576	A2M	O4'-C4'-C5'-O5'
3	L5	2787	A2M	O4'-C4'-C5'-O5'
52	La	39	V5N	O2-CB-CG-CD2
3	L5	4500	PSU	C4'-C5'-O5'-P
3	L5	4447	5MC	O4'-C1'-N1-C2
1	S2	576	A2M	C4'-C5'-O5'-P
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	1534	A2M	C4'-C5'-O5'-P
85	Pt	21	H2U	C4'-C5'-O5'-P
1	S2	1326	UY1	O4'-C1'-C5-C4
3	L5	3818	UY1	O4'-C1'-C5-C4
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	3760	A2M	C2'-C1'-N9-C8
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	1243	PSU	C4'-C5'-O5'-P
1	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
1	S2	822	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
86	EF	55	MLY	CE-CD-CG-CB
1	S2	590	A2M	C4'-C5'-O5'-P
3	L5	1781	PSU	O4'-C4'-C5'-O5'
84	At	8	4SU	O4'-C4'-C5'-O5'
1	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	1322	1MA	C2'-C1'-N9-C8
1	S2	121	OMU	C1'-C2'-O2'-CM2
1	S2	512	A2M	C1'-C2'-O2'-CM'
1	S2	1288	OMU	C1'-C2'-O2'-CM2
1	S2	1383	A2M	C1'-C2'-O2'-CM'
3	L5	3925	OMU	C1'-C2'-O2'-CM2
3	L5	2401	A2M	O4'-C4'-C5'-O5'
3	L5	3851	PSU	O4'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C1'-C5-C6
3	L5	4447	5MC	C2'-C1'-N1-C2
1	S2	590	A2M	O4'-C1'-N9-C8
86	EF	55	MLY	CD-CE-NZ-CH2
84	At	32	PSU	C2'-C1'-C5-C6
3	L5	2787	A2M	O4'-C1'-N9-C8
1	S2	1851	MA6	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
84	At	20	H2U	C2'-C1'-N1-C6
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
1	S2	668	A2M	C2'-C1'-N9-C8
68	Lb	5	MLZ	CA-CB-CG-CD
1	S2	1081	PSU	C4'-C5'-O5'-P
3	L5	1534	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

80 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2632	PSU	1	0
3	L5	4456	OMC	1	0
3	L5	4637	OMG	1	0
85	Pt	47	G7M	1	0
3	L5	1326	A2M	1	0
3	L5	4220	6MZ	2	0
1	S2	573	PSU	1	0
1	S2	468	A2M	1	0
86	EF	318	M3L	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	601	OMG	1	0
1	S2	681	PSU	1	0
1	S2	121	OMU	1	0
3	L5	3762	PSU	1	0
86	EF	55	MLY	2	0
1	S2	649	PSU	2	0
1	S2	436	OMG	1	0
3	L5	2363	A2M	2	0
3	L5	2861	OMC	1	0
1	S2	116	OMU	2	0
1	S2	1678	A2M	1	0
1	S2	686	PSU	1	0
1	S2	36	PSU	2	0
1	S2	509	OMG	2	0
3	L5	4420	PSU	1	0
85	Pt	21	H2U	1	0
3	L5	3760	A2M	3	0
3	L5	1534	A2M	1	0
1	S2	1639	G7M	1	0
84	At	39	PSU	1	0
3	L5	4571	A2M	1	0
1	S2	1643	PSU	1	0
1	S2	1490	OMG	1	0
1	S2	1832	6MZ	1	0
1	S2	576	A2M	2	0
3	L5	2364	OMG	2	0
3	L5	1881	OMC	1	0
66	Lr	2	SAC	1	0
1	S2	1328	OMG	1	0
3	L5	3701	OMC	1	0
1	S2	1804	OMU	1	0
3	L5	2876	OMG	1	0
1	S2	1447	OMG	1	0
3	L5	1625	OMG	1	0
3	L5	4370	OMG	1	0
3	L5	1871	A2M	1	0
3	L5	3884	PSU	1	0
3	L5	4228	OMG	1	0
3	L5	4628	PSU	1	0
84	At	32	PSU	2	0
3	L5	3724	A2M	1	0
84	At	8	4SU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	172	OMU	1	0
1	S2	1248	B8N	2	0
3	L5	2351	OMC	2	0
1	S2	119	PSU	1	0
3	L5	4620	OMU	1	0
1	S2	174	OMC	1	0
3	L5	2804	OMC	1	0
1	S2	159	A2M	2	0
3	L5	1524	A2M	1	0
3	L5	3867	A2M	1	0
3	L5	4521	PSU	1	0
1	S2	1850	MA6	1	0
3	L5	3723	A2M	1	0
3	L5	2415	OMU	1	0
86	EF	79	M3L	1	0
1	S2	644	OMG	1	0
1	S2	99	A2M	1	0
3	L5	2424	OMG	2	0
3	L5	1340	OMC	1	0
3	L5	4196	OMG	2	0
1	S2	354	OMU	1	0
1	S2	1851	MA6	2	0
1	S2	512	A2M	2	0
1	S2	484	A2M	1	0
3	L5	3718	A2M	3	0
1	S2	867	OMG	1	0
84	At	16	H2U	2	0
3	L5	4618	OMG	2	0
84	At	46	G7M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 478 are monoatomic - leaving 24 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
94	PHE	At	77	84	10,11,12	0.36	0	8,13,15	0.72	0
95	MET	Pt	78	85	6,7,8	0.57	0	2,7,9	1.28	0
88	PUT	L5	5115	-	5,5,5	0.14	0	4,4,4	0.21	0
87	SPD	L5	5102	-	9,9,9	0.40	0	8,8,8	0.82	0
87	SPD	L5	5103	-	9,9,9	0.40	0	8,8,8	0.97	1 (12%)
88	PUT	L5	5109	-	5,5,5	0.14	0	4,4,4	0.25	0
88	PUT	L5	5113	-	5,5,5	0.13	0	4,4,4	0.26	0
87	SPD	L5	5108	-	9,9,9	0.33	0	8,8,8	1.03	1 (12%)
96	GSP	EF	501	89	33,34,34	0.63	0	47,54,54	0.60	0
88	PUT	L5	5110	-	5,5,5	0.07	0	4,4,4	0.17	0
90	ANM	L5	5101	-	20,20,20	1.20	1 (5%)	24,27,27	1.34	3 (12%)
87	SPD	L5	5106	-	9,9,9	0.35	0	8,8,8	0.70	0
88	PUT	L5	5114	-	5,5,5	0.16	0	4,4,4	0.28	0
88	PUT	L5	5112	-	5,5,5	0.19	0	4,4,4	0.24	0
87	SPD	L5	5105	-	9,9,9	0.31	0	8,8,8	0.75	0
88	PUT	S2	1902	-	5,5,5	0.15	0	4,4,4	0.14	0
88	PUT	L5	5111	-	5,5,5	0.12	0	4,4,4	0.18	0
91	3H3	L5	5117	-	34,34,34	3.30	13 (38%)	36,45,45	3.67	18 (50%)
97	ZIY	EF	502	-	81,82,82	1.02	4 (4%)	111,117,117	1.42	14 (12%)
87	SPD	S2	1901	-	9,9,9	0.14	0	8,8,8	0.23	0
88	PUT	L5	5116	-	5,5,5	0.13	0	4,4,4	0.21	0
88	PUT	S2	1903	-	5,5,5	0.13	0	4,4,4	0.23	0
87	SPD	L5	5104	-	9,9,9	0.33	0	8,8,8	0.78	0
87	SPD	L5	5107	-	9,9,9	0.43	0	8,8,8	0.93	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
94	PHE	At	77	84	-	4/5/6/8	0/1/1/1
95	MET	Pt	78	85	-	3/5/6/8	-
88	PUT	L5	5115	-	-	1/3/3/3	-
87	SPD	L5	5102	-	-	0/7/7/7	-
87	SPD	L5	5103	-	-	5/7/7/7	-
88	PUT	L5	5109	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	PUT	L5	5113	-	-	2/3/3/3	-
87	SPD	L5	5108	-	-	2/7/7/7	-
96	GSP	EF	501	89	-	0/21/38/38	0/3/3/3
88	PUT	L5	5110	-	-	3/3/3/3	-
90	ANM	L5	5101	-	-	4/10/23/23	0/2/2/2
87	SPD	L5	5106	-	-	6/7/7/7	-
88	PUT	L5	5114	-	-	0/3/3/3	-
88	PUT	L5	5112	-	-	0/3/3/3	-
87	SPD	L5	5105	-	-	2/7/7/7	-
88	PUT	S2	1902	-	-	1/3/3/3	-
88	PUT	L5	5111	-	-	0/3/3/3	-
91	3H3	L5	5117	-	-	15/39/51/51	0/1/2/2
97	ZIY	EF	502	-	-	11/120/140/140	0/3/4/4
87	SPD	S2	1901	-	-	0/7/7/7	-
88	PUT	L5	5116	-	-	0/3/3/3	-
88	PUT	S2	1903	-	-	0/3/3/3	-
87	SPD	L5	5104	-	-	4/7/7/7	-
87	SPD	L5	5107	-	-	3/7/7/7	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	L5	5117	3H3	C13-C12	8.93	1.53	1.33
91	L5	5117	3H3	O3-C22	7.72	1.38	1.23
91	L5	5117	3H3	O4-C23	7.24	1.37	1.23
91	L5	5117	3H3	C23-N	6.68	1.48	1.37
91	L5	5117	3H3	C22-N	5.57	1.46	1.37
91	L5	5117	3H3	C3-C2	5.54	1.53	1.33
97	EF	502	ZIY	C72-C71	-4.71	1.32	1.51
90	L5	5101	ANM	O2-C5	4.71	1.45	1.35
91	L5	5117	3H3	C19-C20	3.36	1.58	1.53
91	L5	5117	3H3	O1-C11	-3.11	1.39	1.44
91	L5	5117	3H3	C4-C3	2.79	1.53	1.44
97	EF	502	ZIY	C54-C55	-2.52	1.50	1.53
91	L5	5117	3H3	O-C10	-2.31	1.16	1.21
91	L5	5117	3H3	O1-C10	2.24	1.39	1.34
91	L5	5117	3H3	O2-C16	-2.21	1.18	1.21
91	L5	5117	3H3	C24-C20	-2.15	1.49	1.53
97	EF	502	ZIY	C45-C47	2.08	1.55	1.52
97	EF	502	ZIY	C53-C54	2.06	1.56	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	L5	5117	3H3	O3-C22-N	-10.22	104.55	120.30
91	L5	5117	3H3	C22-N-C23	-9.58	114.32	125.87
91	L5	5117	3H3	O4-C23-N	-8.78	106.76	120.30
97	EF	502	ZIY	O33-C75-C74	6.80	126.68	118.96
91	L5	5117	3H3	O3-C22-C21	-6.57	110.08	122.62
91	L5	5117	3H3	C15-C14-C13	-5.96	105.02	110.73
91	L5	5117	3H3	O4-C23-C24	-5.18	112.74	122.62
90	L5	5101	ANM	O2-C5-C6	4.35	118.84	111.09
97	EF	502	ZIY	O35-C79-C01	3.66	118.40	110.80
91	L5	5117	3H3	C25-C12-C13	-3.60	114.31	123.56
91	L5	5117	3H3	C21-C22-N	-3.40	111.79	115.92
97	EF	502	ZIY	C70-C69-N17	3.33	124.94	118.87
91	L5	5117	3H3	C11-C12-C13	-3.16	108.64	119.78
97	EF	502	ZIY	C36-N05-C30	-3.06	107.20	112.01
91	L5	5117	3H3	C7-C8-C9	-2.96	119.76	125.92
91	L5	5117	3H3	O1-C10-C9	2.94	117.78	111.39
97	EF	502	ZIY	C30-C28-N02	2.78	123.93	118.87
91	L5	5117	3H3	C4-C3-C2	-2.73	106.08	124.25
97	EF	502	ZIY	C73-N20-C70	-2.71	107.76	112.01
97	EF	502	ZIY	C45-C44-N08	2.70	119.63	116.13
91	L5	5117	3H3	C8-C9-C10	-2.68	116.38	122.78
91	L5	5117	3H3	C1-C2-C3	-2.40	121.15	126.11
97	EF	502	ZIY	O37-C79-C01	-2.34	119.30	124.46
97	EF	502	ZIY	C77-O35-C79	2.29	120.93	117.55
97	EF	502	ZIY	O29-C69-C70	-2.25	115.57	120.28
97	EF	502	ZIY	C71-C70-C69	2.24	115.23	110.83
91	L5	5117	3H3	C6-C7-C8	-2.24	107.10	112.73
87	L5	5108	SPD	C7-C8-C9	-2.21	106.29	114.17
90	L5	5101	ANM	O2-C5-O3	-2.20	118.75	122.99
97	EF	502	ZIY	C32-C30-C28	-2.18	106.54	110.83
91	L5	5117	3H3	C24-C23-N	-2.17	113.28	115.92
91	L5	5117	3H3	C25-C12-C11	-2.13	111.75	115.96
90	L5	5101	ANM	C14-O1-C9	2.12	122.05	117.50
87	L5	5103	SPD	C8-C7-N6	-2.08	106.49	112.07
91	L5	5117	3H3	C19-C18-C17	-2.07	108.72	112.96
97	EF	502	ZIY	C71-C72-C73	2.03	110.56	104.90
97	EF	502	ZIY	C53-C54-C55	-2.00	110.25	113.00

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	L5	5117	3H3	C2-C1-C11-O1
91	L5	5117	3H3	C2-C1-C11-C12
91	L5	5117	3H3	C-C1-C11-O1
91	L5	5117	3H3	C-C1-C11-C12
91	L5	5117	3H3	C1-C11-O1-C10
91	L5	5117	3H3	C12-C11-O1-C10
91	L5	5117	3H3	C9-C10-O1-C11
91	L5	5117	3H3	C12-C13-C14-C16
91	L5	5117	3H3	C25-C12-C13-C14
91	L5	5117	3H3	C1-C11-C12-C25
95	Pt	78	MET	C-CA-CB-CG
97	EF	502	ZIY	C47-C48-O18-C52
97	EF	502	ZIY	C62-C63-C64-C65
97	EF	502	ZIY	N20-C74-C75-O33
97	EF	502	ZIY	O31-C74-C75-O33
88	L5	5115	PUT	C1-C2-C3-C4
97	EF	502	ZIY	C22-C14-O03-C19
97	EF	502	ZIY	C13-C14-O03-C19
91	L5	5117	3H3	O-C10-O1-C11
87	L5	5105	SPD	C3-C4-C5-N6
91	L5	5117	3H3	C2-C3-C4-C5
87	L5	5103	SPD	C3-C4-C5-N6
97	EF	502	ZIY	N17-C63-C64-C65
95	Pt	78	MET	CA-CB-CG-SD
87	L5	5106	SPD	N6-C7-C8-C9
97	EF	502	ZIY	C49-C48-O18-C52
87	L5	5108	SPD	N6-C7-C8-C9
91	L5	5117	3H3	O1-C10-C9-C8
87	L5	5106	SPD	C3-C4-C5-N6
87	L5	5106	SPD	C2-C3-C4-C5
90	L5	5101	ANM	C10-C9-O1-C14
90	L5	5101	ANM	C1-C9-O1-C14
87	L5	5103	SPD	C4-C5-N6-C7
87	L5	5106	SPD	C7-C8-C9-N10
87	L5	5104	SPD	C3-C4-C5-N6
94	At	77	PHE	N-CA-CB-CG
88	L5	5110	PUT	C1-C2-C3-C4
87	L5	5104	SPD	N6-C7-C8-C9
87	L5	5103	SPD	C8-C7-N6-C5
87	L5	5108	SPD	C2-C3-C4-C5
87	L5	5103	SPD	N6-C7-C8-C9
88	L5	5110	PUT	N1-C1-C2-C3
88	S2	1902	PUT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
91	L5	5117	3H3	O-C10-C9-C8
87	L5	5104	SPD	C4-C5-N6-C7
94	At	77	PHE	C-CA-CB-CG
97	EF	502	ZIY	C63-C64-C65-C66
87	L5	5107	SPD	N6-C7-C8-C9
87	L5	5104	SPD	C7-C8-C9-N10
87	L5	5105	SPD	C7-C8-C9-N10
87	L5	5106	SPD	N1-C2-C3-C4
88	L5	5113	PUT	C1-C2-C3-C4
94	At	77	PHE	CA-CB-CG-CD2
88	L5	5110	PUT	C2-C3-C4-N2
97	EF	502	ZIY	C63-C64-C65-C67
94	At	77	PHE	CA-CB-CG-CD1
87	L5	5107	SPD	N1-C2-C3-C4
88	L5	5113	PUT	C2-C3-C4-N2
87	L5	5106	SPD	C8-C7-N6-C5
87	L5	5107	SPD	C4-C5-N6-C7
90	L5	5101	ANM	C11-C12-C15-C16
90	L5	5101	ANM	C13-C12-C15-C16
91	L5	5117	3H3	C12-C13-C14-C15
97	EF	502	ZIY	N02-C01-C79-O35
95	Pt	78	MET	CB-CG-SD-CE
87	L5	5103	SPD	N1-C2-C3-C4

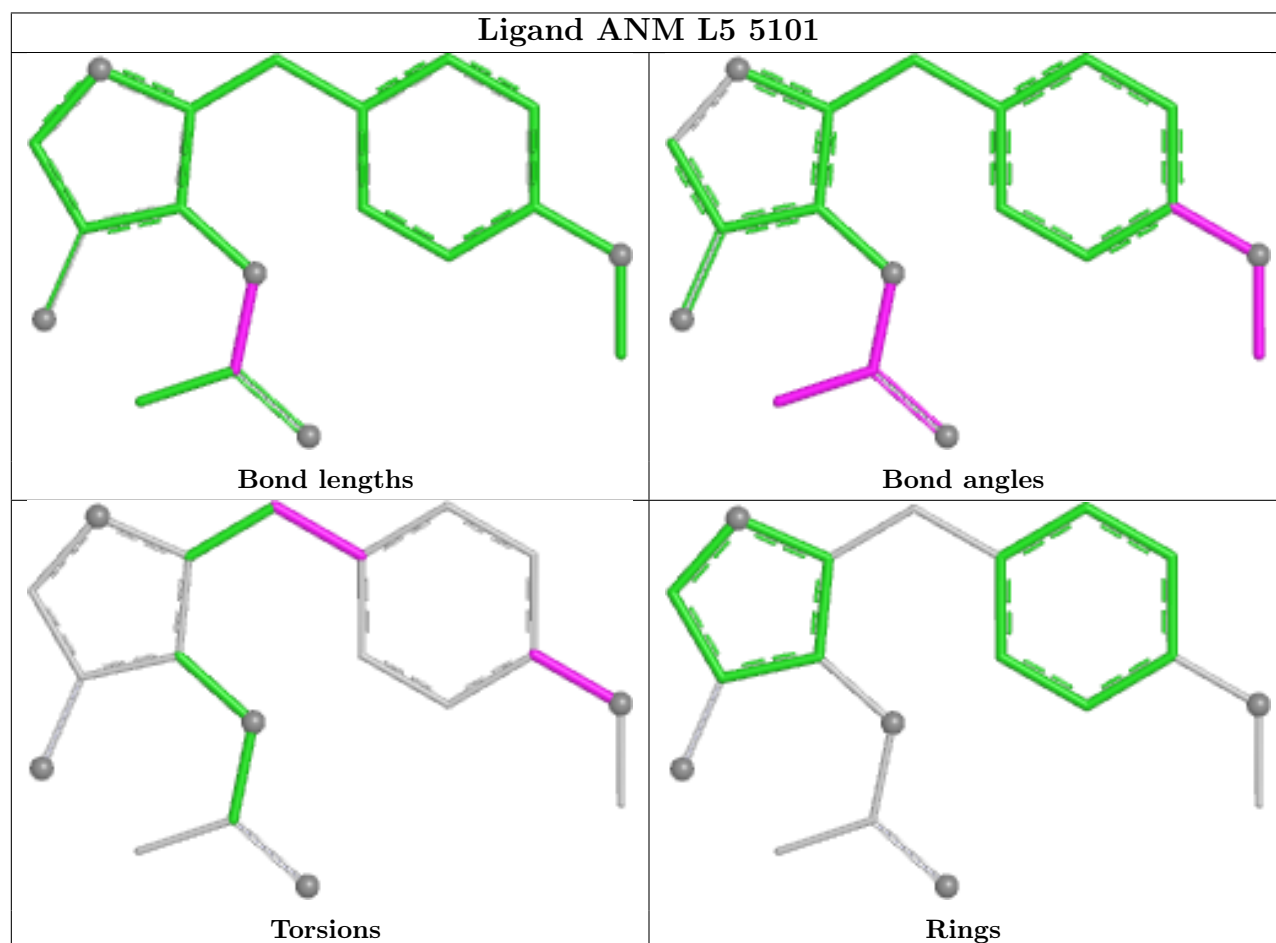
There are no ring outliers.

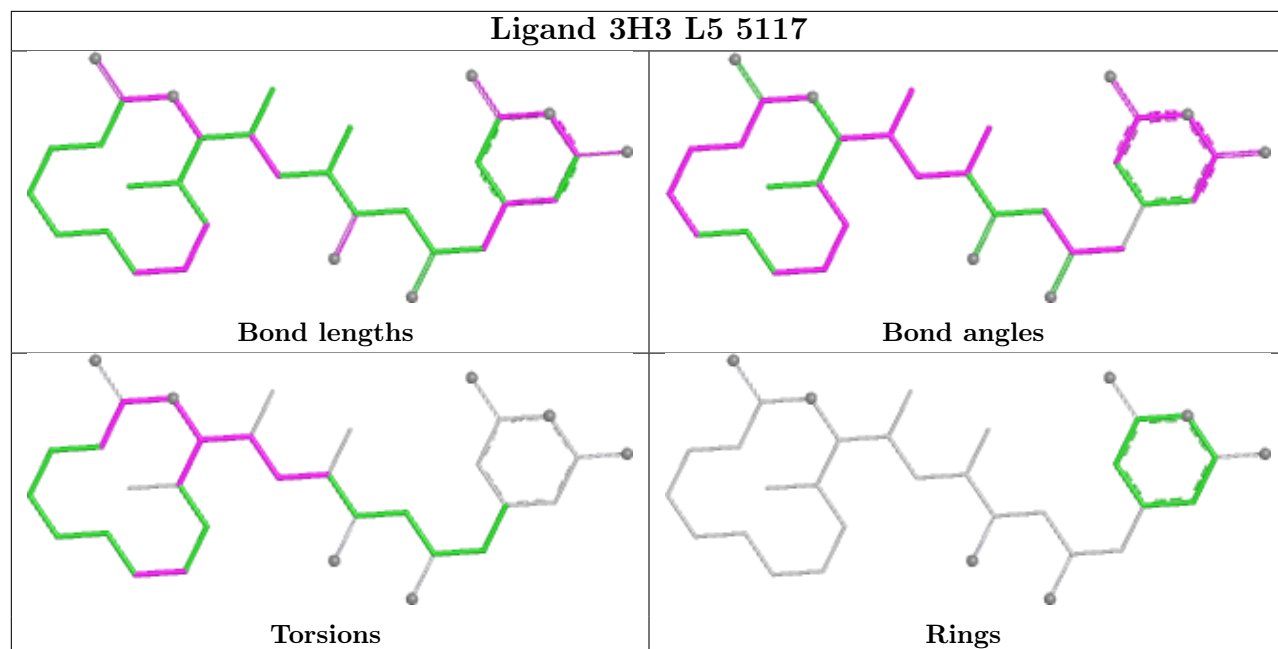
7 monomers are involved in 11 short contacts:

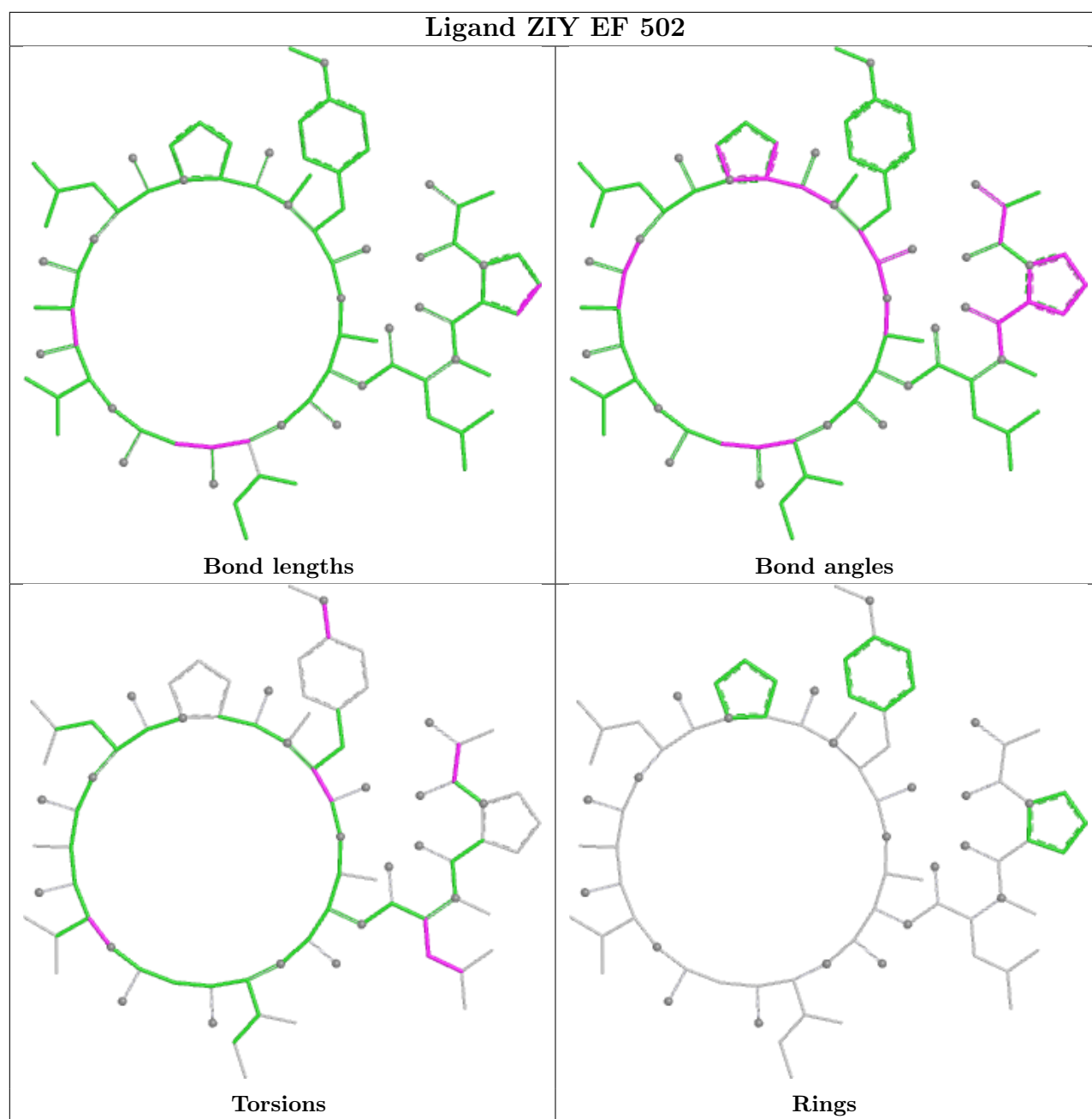
Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	At	77	PHE	2	0
87	L5	5103	SPD	1	0
96	EF	501	GSP	1	0
87	L5	5106	SPD	1	0
91	L5	5117	3H3	4	0
97	EF	502	ZIY	1	0
88	L5	5116	PUT	1	0

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.

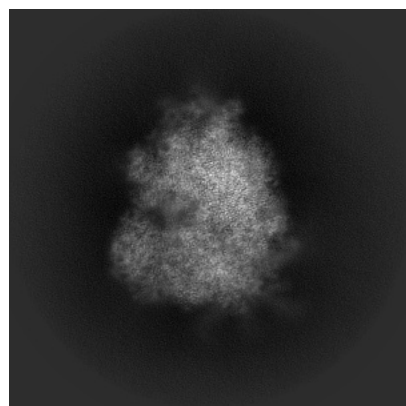
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29759. These allow visual inspection of the internal detail of the map and identification of artifacts.

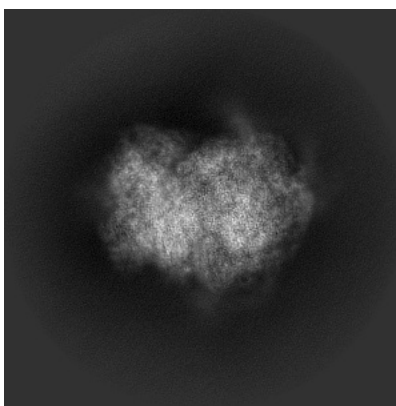
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

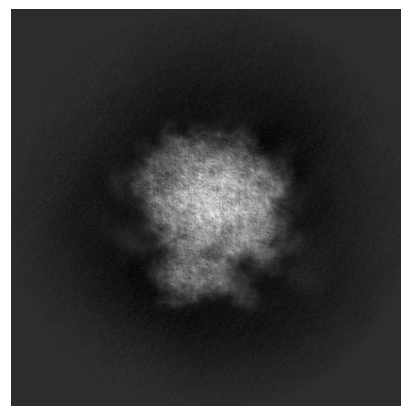
6.1.1 Primary map



X

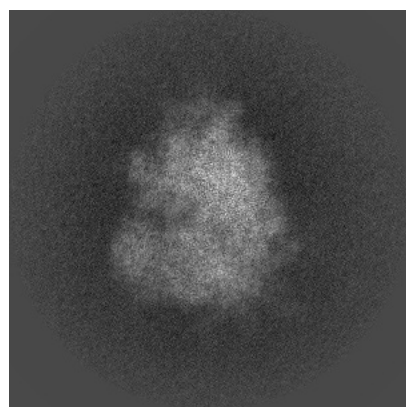


Y

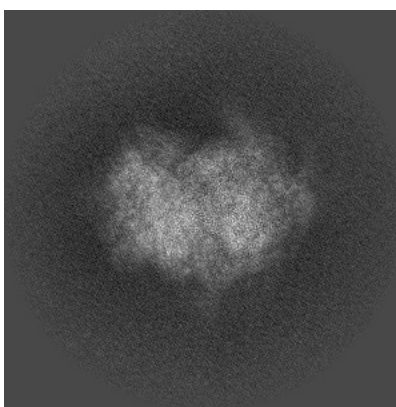


Z

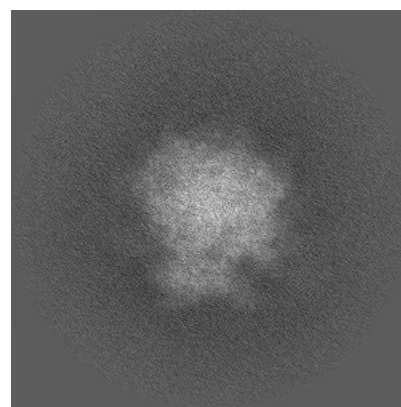
6.1.2 Raw map



X



Y

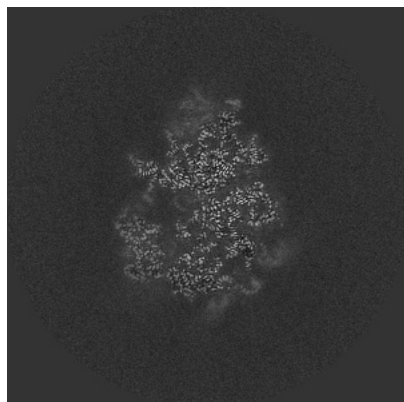


Z

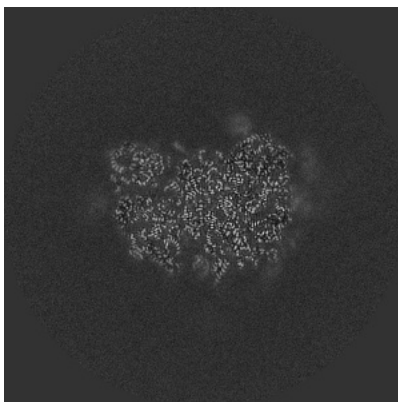
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

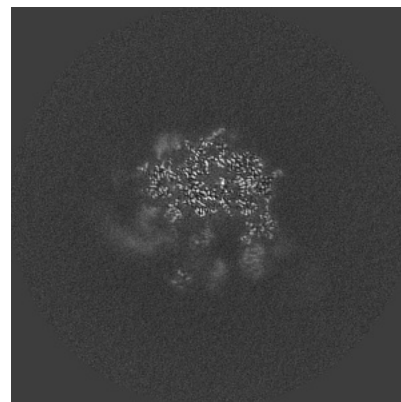
6.2.1 Primary map



X Index: 320

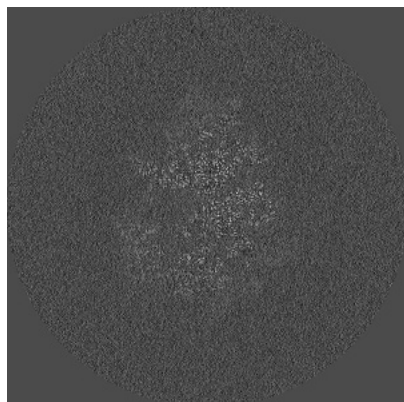


Y Index: 320

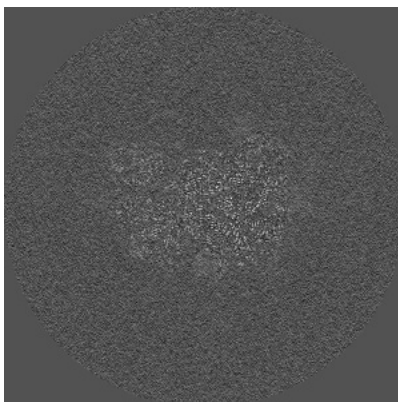


Z Index: 320

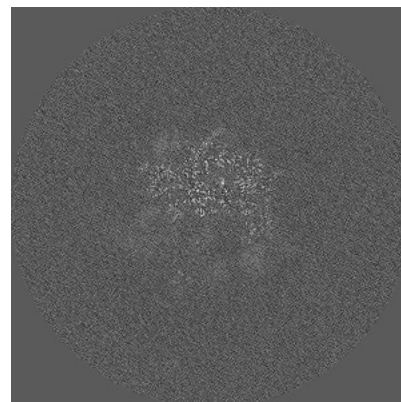
6.2.2 Raw map



X Index: 320



Y Index: 320

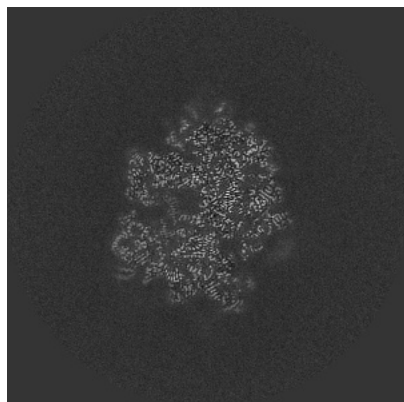


Z Index: 320

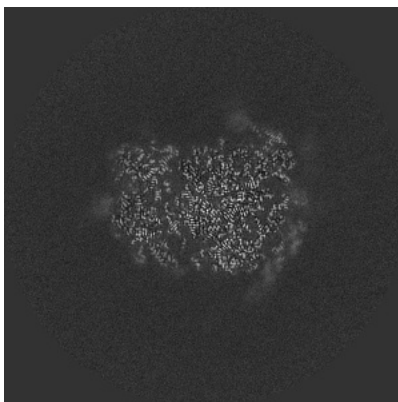
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

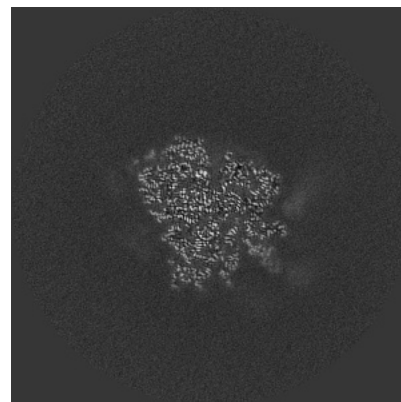
6.3.1 Primary map



X Index: 297

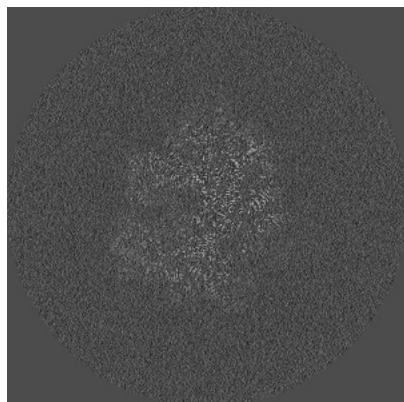


Y Index: 332

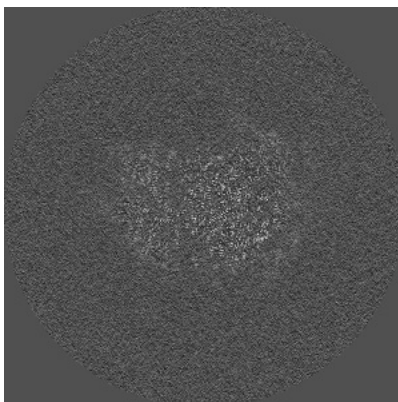


Z Index: 366

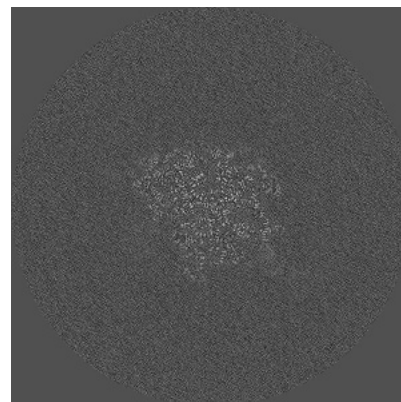
6.3.2 Raw map



X Index: 297



Y Index: 327

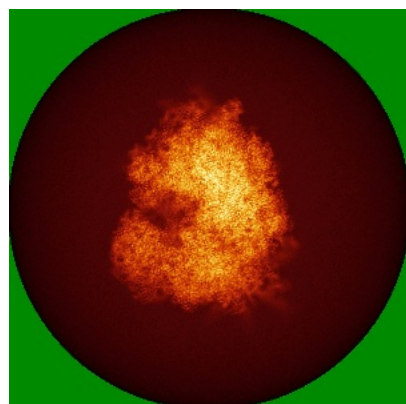


Z Index: 354

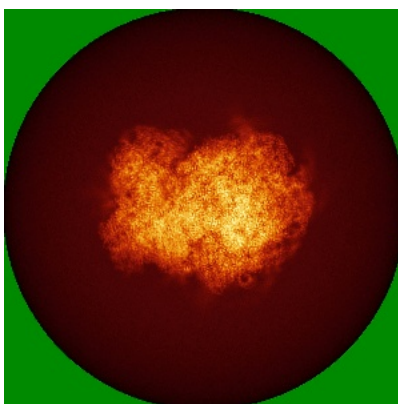
The images above show the largest variance slices of the map in three orthogonal directions.

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

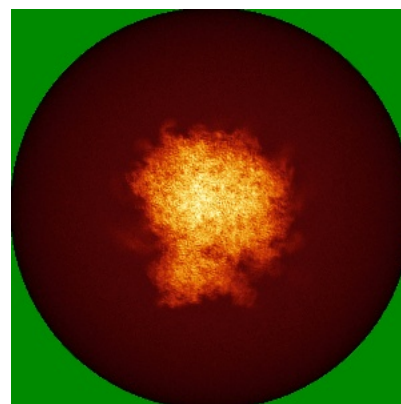
6.4.1 Primary map



X

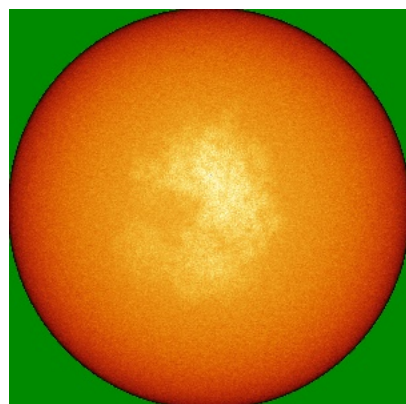


Y

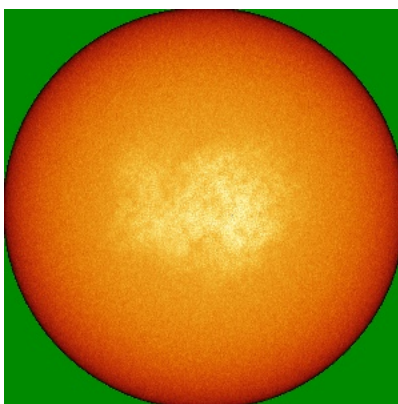


Z

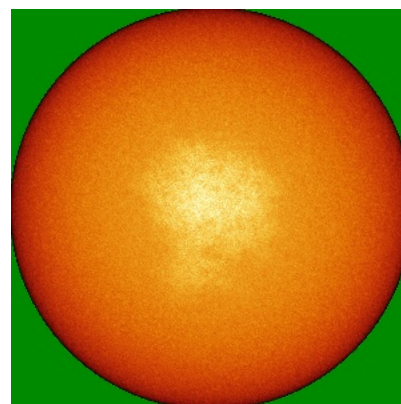
6.4.2 Raw map



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



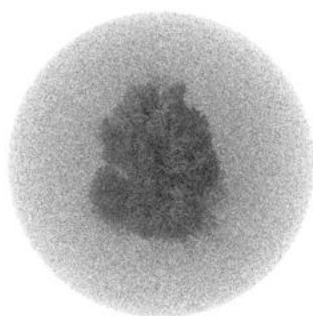
Y



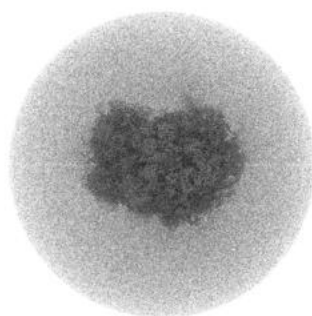
Z

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.

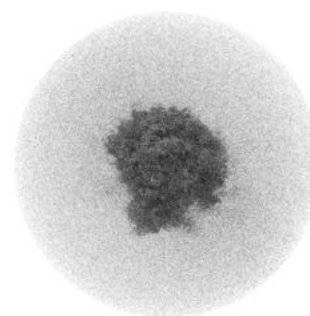
6.5.2 Raw map



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.

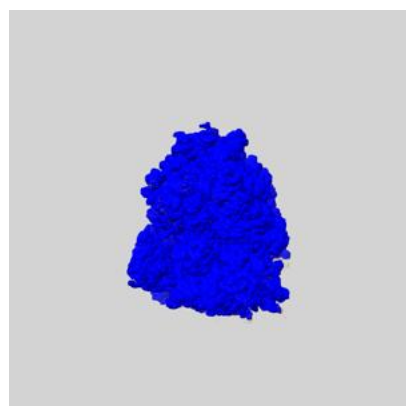
6.6 Mask visualisation [i](#)

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

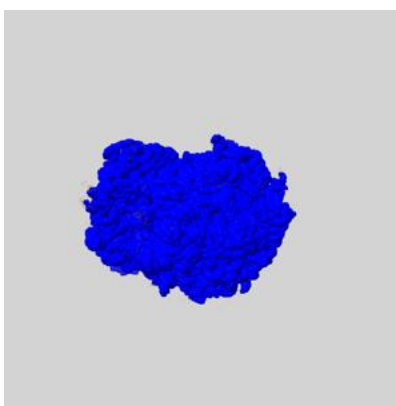
A mask typically either:

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

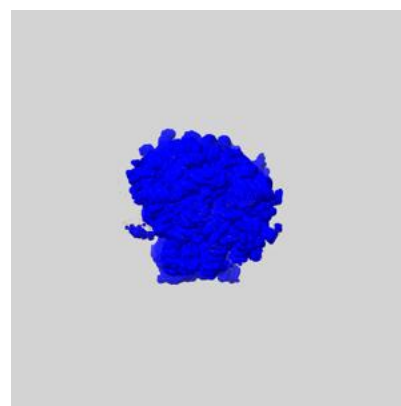
6.6.1 emd_29759_msk_1.map [i](#)



X



Y

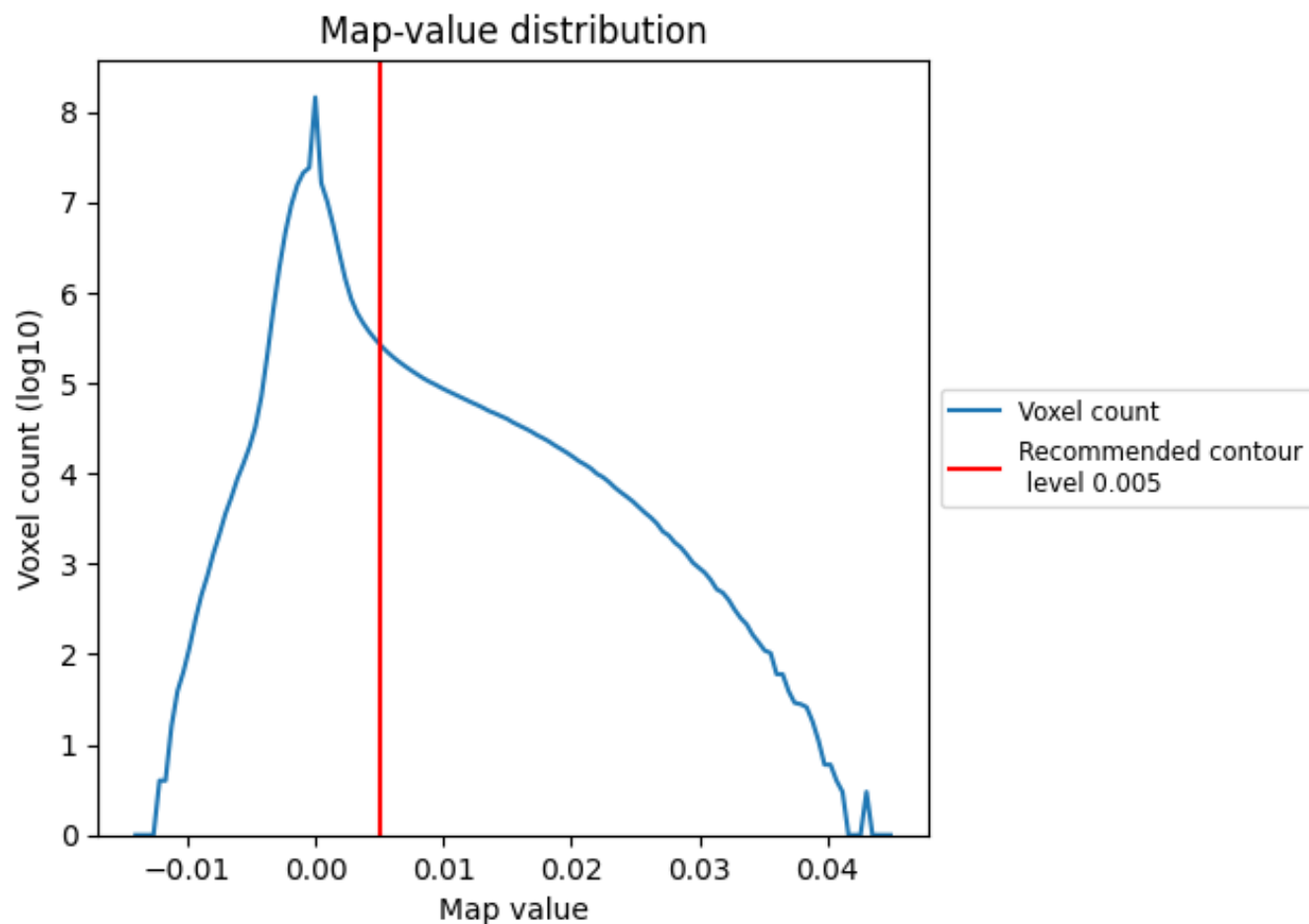


Z

7 Map analysis [i](#)

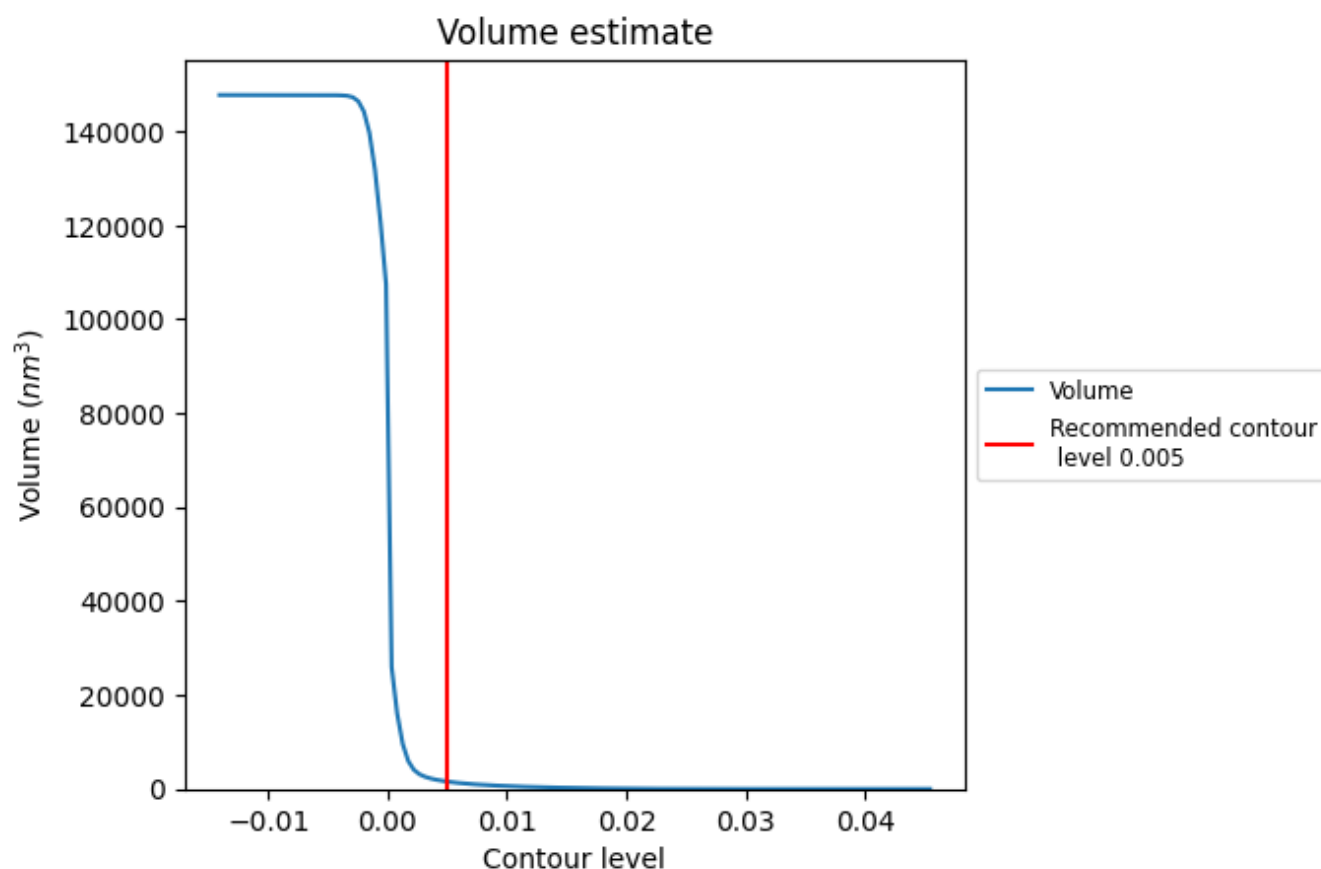
This section contains the results of statistical analysis of the map.

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.

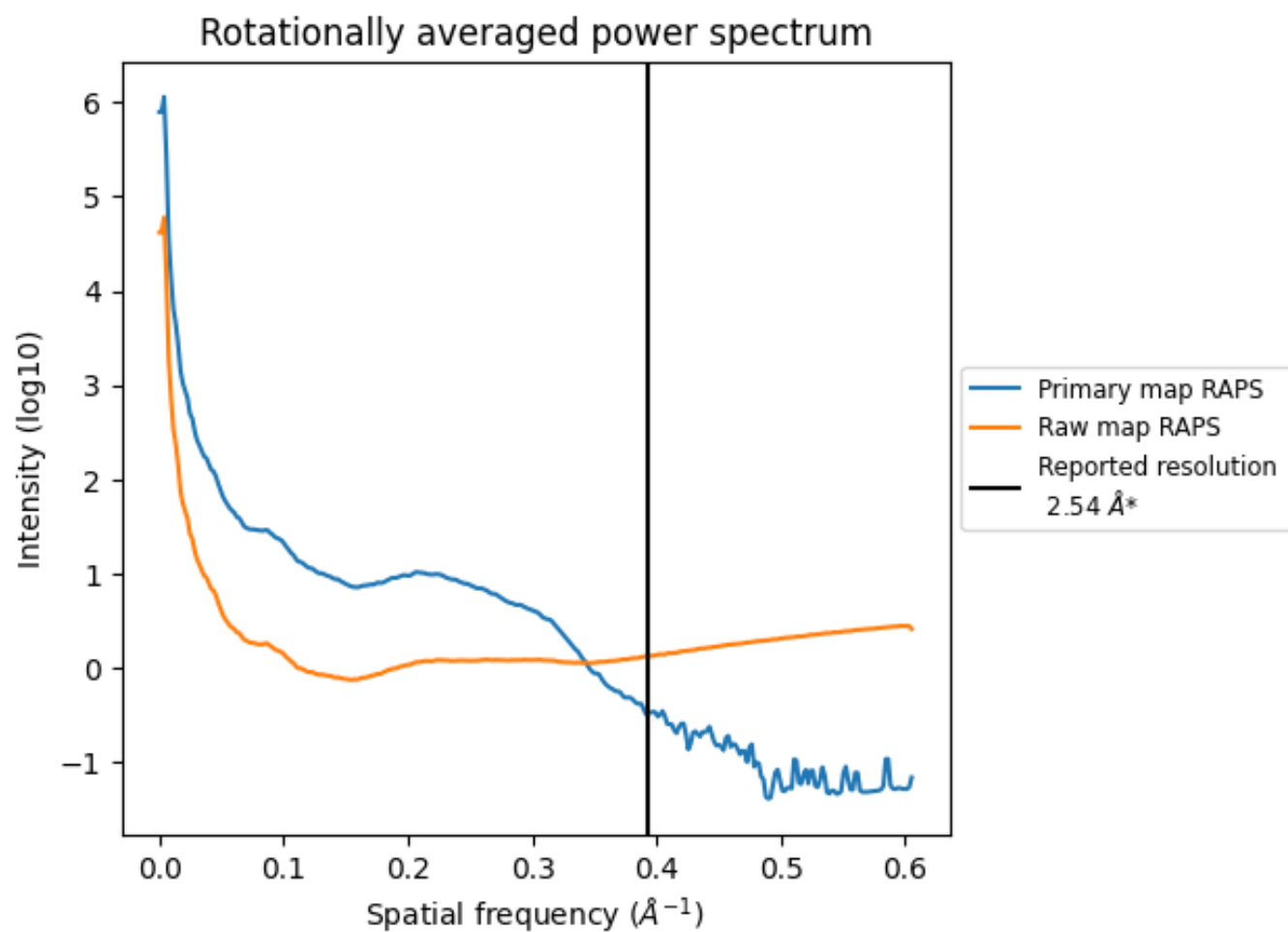
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1563 nm^3 ; this corresponds to an approximate mass of 1412 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 ⓘ

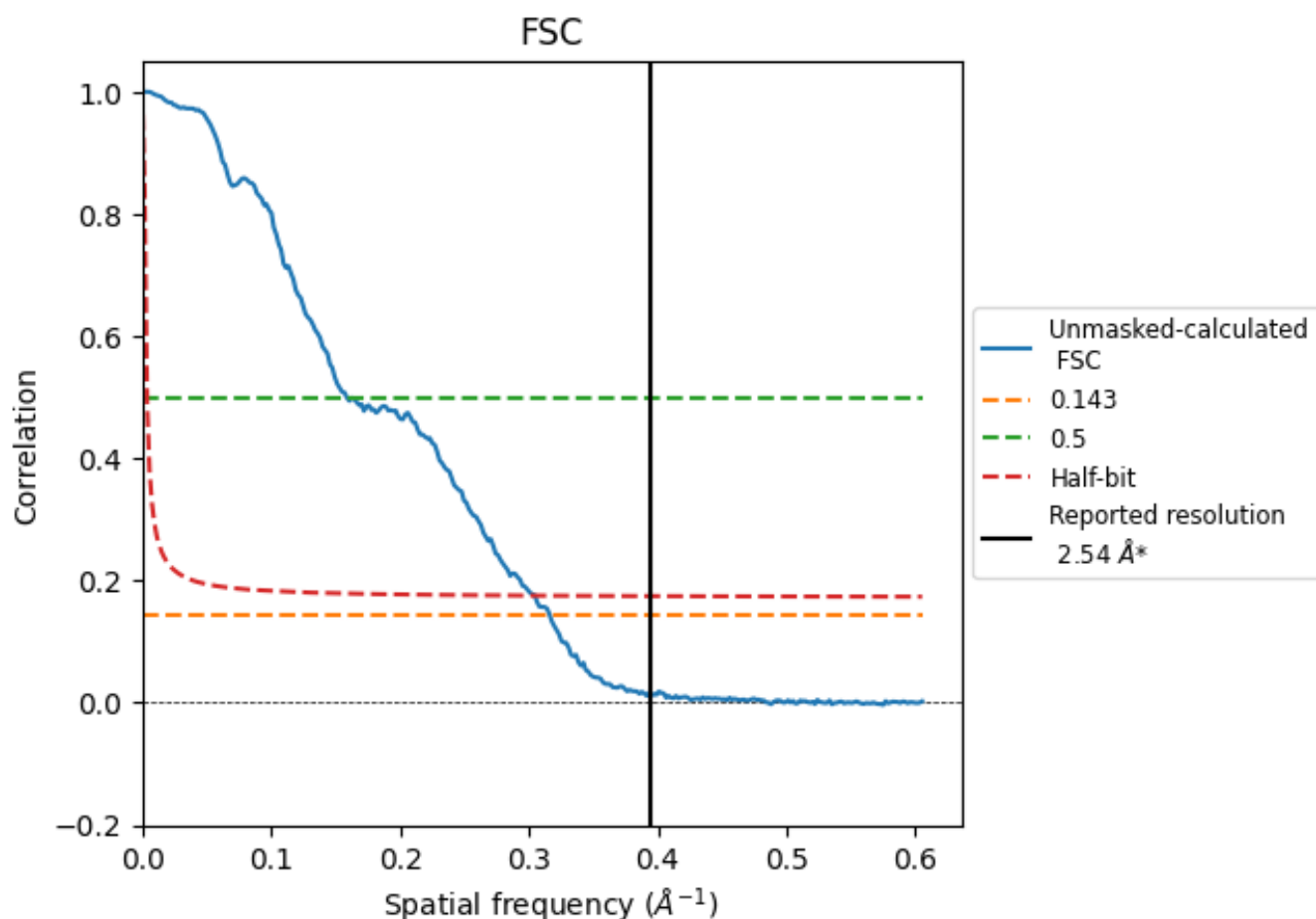


*Reported resolution corresponds to spatial frequency of $0.394 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.394 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

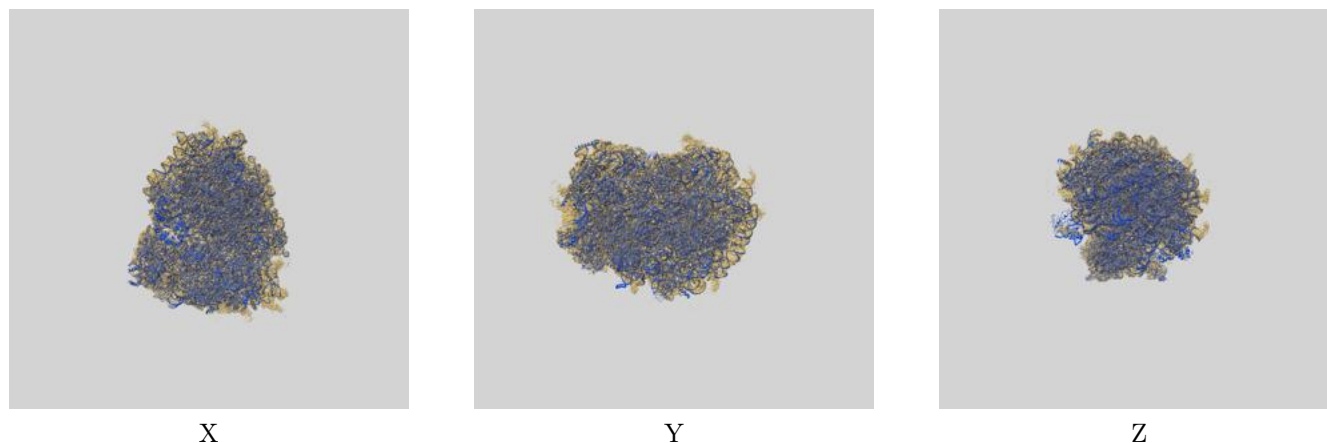
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	6.30	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

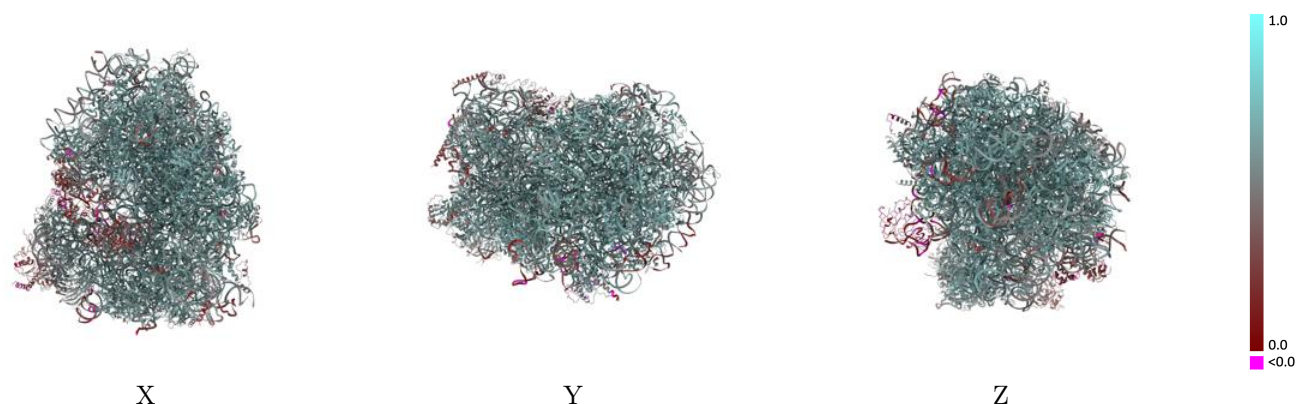
This section contains information regarding the fit between EMDB map EMD-29759 and PDB model 8G60. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



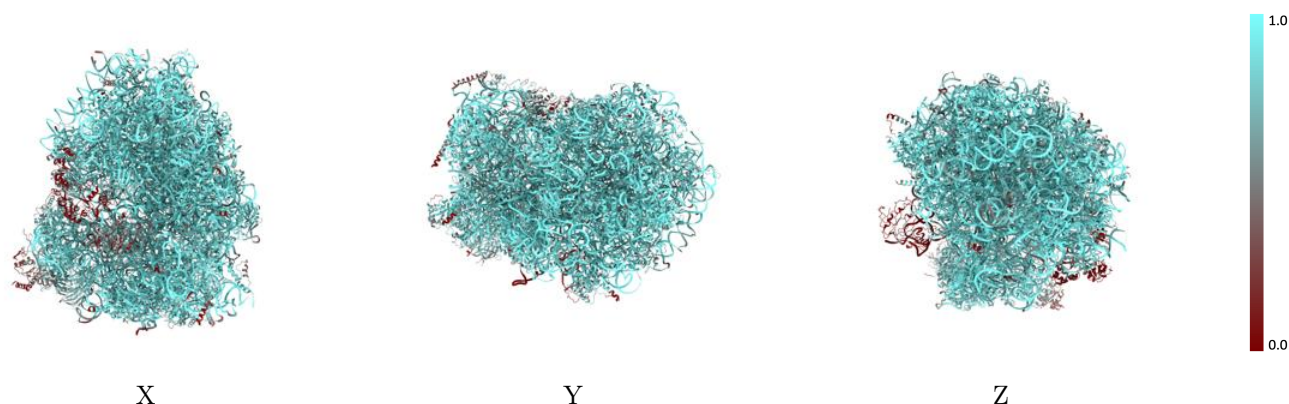
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



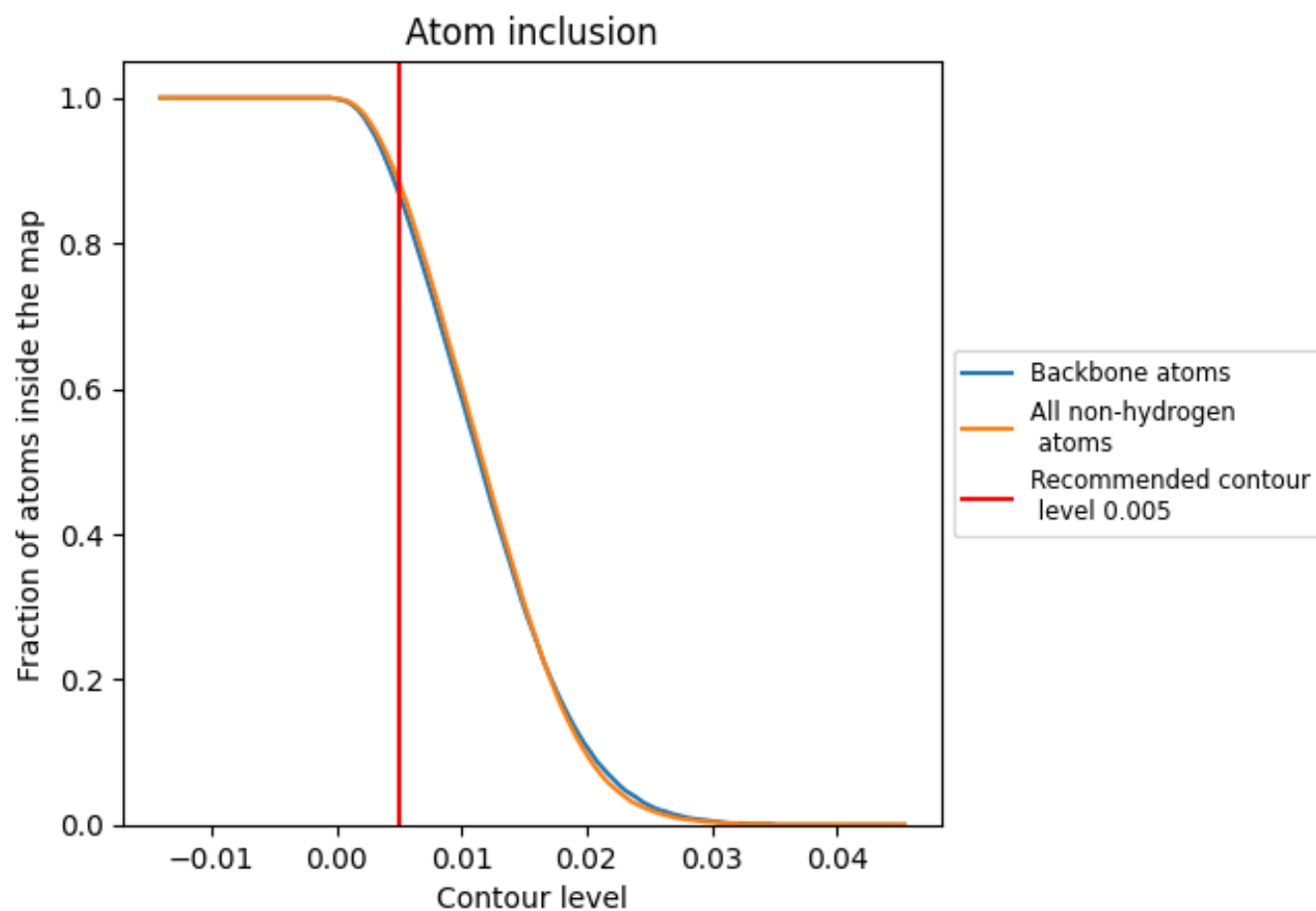
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 88% 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	 0.8840	 0.5760
At	 0.6780	 0.3340
EF	 0.5180	 0.3890
L5	 0.9380	 0.5890
L7	 0.9940	 0.6390
L8	 0.9760	 0.6170
LA	 0.9690	 0.6560
LB	 0.9230	 0.6330
LC	 0.9400	 0.6360
LD	 0.9010	 0.6030
LE	 0.8940	 0.6050
LF	 0.9450	 0.6380
LG	 0.8220	 0.5570
LH	 0.8990	 0.6110
LI	 0.9130	 0.6190
LJ	 0.8600	 0.5920
LK	 0.1030	 0.2140
LL	 0.8950	 0.6090
LM	 0.9250	 0.6150
LN	 0.9820	 0.6550
LO	 0.9440	 0.6370
LP	 0.9460	 0.6470
LQ	 0.9680	 0.6570
LR	 0.8550	 0.5960
LS	 0.9650	 0.6420
LT	 0.9190	 0.6270
LU	 0.8150	 0.5430
LV	 0.9200	 0.6360
LW	 0.6960	 0.4990
LX	 0.9100	 0.6220
LY	 0.9140	 0.6170
LZ	 0.9100	 0.6060
La	 0.9670	 0.6550
Lb	 0.7950	 0.5640
Lc	 0.8940	 0.6130



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Chain	Atom inclusion	Q-score
Ld	 0.8910	 0.6080
Le	 0.9670	 0.6570
Lf	 0.9680	 0.6530
Lg	 0.8990	 0.6190
Lh	 0.9130	 0.6160
Li	 0.8880	 0.5980
Lj	 0.9690	 0.6560
Lk	 0.8220	 0.5690
Ll	 0.9460	 0.6250
Lm	 0.9020	 0.6150
Ln	 0.9080	 0.6230
Lo	 0.9290	 0.6310
Lp	 0.9380	 0.6420
Lq	 0.1600	 0.2630
Lr	 0.9420	 0.6360
Lz	 0.0050	 0.1450
Pt	 0.6650	 0.5440
S2	 0.9600	 0.5840
SA	 0.8660	 0.5840
SB	 0.8560	 0.5930
SC	 0.8940	 0.6050
SD	 0.7650	 0.5270
SE	 0.8670	 0.5900
SF	 0.8350	 0.5640
SG	 0.7440	 0.5050
SH	 0.7420	 0.5270
SI	 0.8670	 0.5860
SJ	 0.8620	 0.5750
SK	 0.7540	 0.4870
SL	 0.8960	 0.6160
SM	 0.2280	 0.2260
SN	 0.9140	 0.6160
SO	 0.8940	 0.6080
SP	 0.7440	 0.5070
SQ	 0.8610	 0.5710
SR	 0.7820	 0.5340
SS	 0.8040	 0.5500
ST	 0.8300	 0.5530
SU	 0.7190	 0.4980
SV	 0.8800	 0.6000
SW	 0.9430	 0.6310
SX	 0.9160	 0.6100

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Chain	Atom inclusion	Q-score
SY	 0.7630	 0.5130
SZ	 0.6950	 0.5130
Sa	 0.9240	 0.6160
Sb	 0.8210	 0.5810
Sc	 0.7330	 0.5380
Sd	 0.9410	 0.5890
Se	 0.7800	 0.5510
Sf	 0.4130	 0.3250
Sg	 0.6850	 0.4910
mR	 0.4470	 0.4820