Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 03:37 pm BST

PDB ID	:	9RU8 / pdb_00009ru8
EMDB ID	:	EMD-54266
Title	:	WT-HEK 80S ribosome bound to TISU mRNA (WT-TISU)
Authors	:	Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on	:	2025-07-03
Resolution	:	3.00 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:

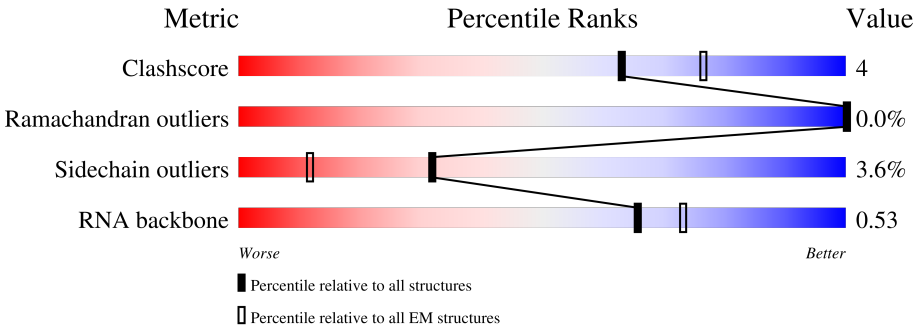
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

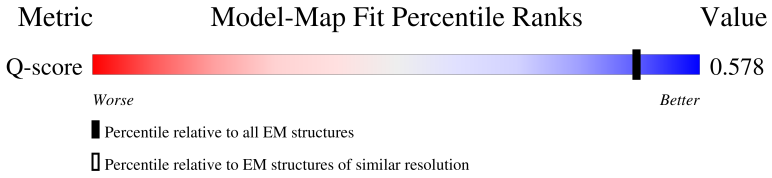
1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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 <=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	Lm	128	35% 5% 60%
2	Ll	51	75% 20%
3	Lo	106	83% 15%

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Mol	Chain	Length	Quality of chain
4	SY	133	77% 14% 8%
5	SX	143	90% 9%
6	SW	130	82% 16%
7	SV	83	87% 13%
8	SR	135	85% 11%
9	SQ	146	92% 5%
10	SO	151	75% 13% 11%
11	SN	151	92% 6%
12	SL	158	80% 9% 10%
13	SK	165	41% 55%
14	SJ	194	81% 10% 8%
15	SH	194	14% 84% 13%
16	Sg	317	13% 72% 24%
17	SF	204	81% 9% 9%
18	SE	263	90% 8%
19	Se	133	35% 62%
20	SD	243	66% 6% 28%
21	Sd	56	71% 27%
22	SC	293	65% 10% 25%
23	Sc	69	81% 7% 12%
24	SB	264	69% 11% 20%
25	Sb	84	5% 89% 8%
26	SA	295	60% 12% 27%
27	LZ	136	77% 18%
28	LY	145	87% 5% 8%

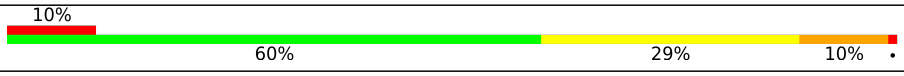
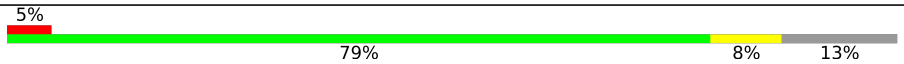
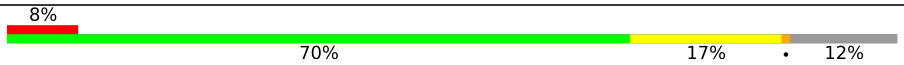
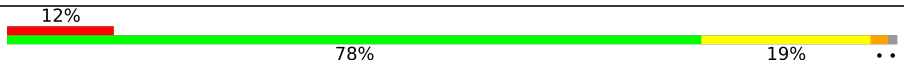
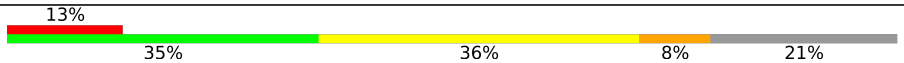
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Mol	Chain	Length	Quality of chain
29	LX	156	64% 12% 24%
30	LW	157	33% 6% 61%
31	LV	140	85% 8% 6%
32	LU	128	8% 59% 17% 23%
33	LT	160	89% 9%
34	LS	176	86% 13%
35	LR	196	5% 85% 7% 8%
36	Lr	137	79% 11% 10%
37	LQ	188	88% 9%
38	LP	154	94% 5%
39	Lp	91	92% 7%
40	LO	203	83% 15%
41	LN	204	88% 11%
42	Ln	25	84% 12%
43	LM	215	53% 10% 37%
44	LL	211	88% 9%
45	Lk	70	67% 27%
46	LJ	178	81% 13% 5%
47	Lj	97	76% 11% 11%
48	LI	214	84% 11% 5%
49	Li	105	84% 13%
50	LH	192	82% 17%
51	Lh	123	89% 11%
52	LG	266	7% 74% 11% 14%
53	Lg	112	89% 8%

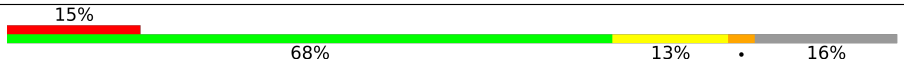
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Mol	Chain	Length	Quality of chain
54	LF	248	
55	Lf	111	
56	LE	288	
57	Le	135	
58	LD	297	
59	Ld	125	
60	LC	427	
61	Lc	115	
62	LB	397	
63	Lb	159	
64	LA	257	
65	La	148	
66	L7	119	
67	Pt	77	
68	Sa	115	
69	L8	156	
70	L5	5069	
71	SZ	125	
72	ST	145	
73	SP	145	
74	S2	1869	
75	SG	249	
76	SI	208	
77	S6	75	
78	SS	152	

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Mol	Chain	Length	Quality of chain
79	mR	27	
80	SU	119	

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 201487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Lm	51	Total	C	N	O	S	0	0
			407	251	87	63	6		

- Molecule 2 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ll	50	Total	C	N	O	S	0	0
			434	275	94	64	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ll	34	ILE	LYS	conflict	UNP P62891

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Lo	105	Total	C	N	O	S	0	0
			822	516	166	134	6		

- Molecule 4 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SY	123	Total	C	N	O	S	0	0
			900	565	181	151	3		

- Molecule 5 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SX	141	Total	C	N	O	S	0	0
			1060	669	214	174	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	62	HIS	PRO	conflict	UNP P62266

- Molecule 6 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SW	129	Total	C	N	O	S	0	0
			1023	653	192	172	6		

- Molecule 7 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SV	83	Total	C	N	O	S	0	0
			623	388	117	113	5		

- Molecule 8 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SR	132	Total	C	N	O	S	0	0
			936	591	173	169	3		

- Molecule 9 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SQ	139	Total	C	N	O	S	0	0
			918	570	181	166	1		

- Molecule 10 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SO	134	Total	C	N	O	S	0	0
			977	600	196	175	6		

- Molecule 11 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SN	150	Total	C	N	O	S	0	0
			1186	761	221	203	1		

- Molecule 12 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SL	142	Total	C	N	O	S	0	0
			1158	737	218	197	6		

- Molecule 13 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SK	74	Total	C	N	O	S	0	0
			468	302	86	79	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SK	68	PHE	TYR	conflict	UNP P46783

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SJ	178	Total	C	N	O	S	0	0
			1430	915	285	228	2		

- Molecule 15 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SH	189	Total	C	N	O	S	0	0
			1408	905	263	239	1		

- Molecule 16 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Sg	241	Total	C	N	O	0	0
			1259	757	255	247		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sg	155	PHE	ARG	conflict	UNP P63244

- Molecule 17 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SF	185	Total	C	N	O	S	0	0
			1327	835	251	238	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SF	15	LYS	PRO	conflict	UNP P46782

- Molecule 18 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SE	260	Total	C	N	O	S	0	0
			2037	1304	383	342	8		

- Molecule 19 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Se	51	Total	C	N	O	S	0	0
			399	243	90	65	1		

- Molecule 20 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SD	175	Total	C	N	O	S	0	0
			1094	689	201	201	3		

- Molecule 21 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sd	55	Total	C	N	O	S	0	0
			430	270	87	68	5		

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SC	220	Total	C	N	O	S	0	0
			1694	1097	292	295	10		

- Molecule 23 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sc	61	Total	C	N	O	S	0	0
			434	264	87	81	2		

- Molecule 24 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SB	212	Total	C	N	O	S	1	0
			1694	1078	306	295	15		

- Molecule 25 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Sb	82	Total	C	N	O	S	0	0
			613	383	113	110	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SA	215	Total	C	N	O	S	0	0
			1658	1056	292	303	7		

- Molecule 27 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LZ	135	Total	C	N	O	S	0	0
			1095	709	207	176	3		

- Molecule 28 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LY	133	Total	C	N	O	S	0	0
			1060	666	215	176	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LY	52	LYS	ASP	conflict	UNP P61254

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 30 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LW	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 31 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LV	131	Total	C	N	O	S	1	0
			987	623	187	172	5		

- Molecule 32 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LU	99	Total	C	N	O	S	0	0
			800	513	140	145	2		

- Molecule 33 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

- Molecule 34 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LS	176	Total	C	N	O	S	0	0
			1456	927	283	235	11		

- Molecule 35 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LR	181	Total	C	N	O	S	0	0
			1458	903	312	234	9		

- Molecule 36 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lr	123	Total	C	N	O	S	0	0
			987	612	205	166	4		

- Molecule 37 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LQ	187	Total	C	N	O	S	0	0
			1505	940	312	248	5		

- Molecule 38 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LP	153	Total	C	N	O	S	0	0
			1230	769	240	212	9		

- Molecule 39 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lp	90	Total	C	N	O	S	0	0
			695	439	134	115	7		

- Molecule 40 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LO	199	Total	C	N	O	S	0	0
			1620	1044	318	253	5		

- Molecule 41 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LN	203	Total	C	N	O	S	0	0
			1694	1069	356	265	4		

- Molecule 42 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			235	142	65	25	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ln	24	ARG	SER	conflict	UNP P62945

- Molecule 43 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LM	136	Total	C	N	O	S	0	0
			1116	716	214	179	7		

- Molecule 44 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LL	205	Total	C	N	O	S	0	0
			1638	1026	342	266	4		

- Molecule 45 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lk	69	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 46 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LJ	169	Total	C	N	O	S	0	0
			1329	843	246	234	6		

- Molecule 47 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lj	86	Total	C	N	O	S	0	0
			701	432	154	110	5		

- Molecule 48 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LI	203	Total	C	N	O	S	0	0
			1632	1038	314	267	13		

- Molecule 49 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Li	102	Total	C	N	O	S	0	0
			812	509	171	127	5		

- Molecule 50 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LH	190	Total	C	N	O	S	0	0
			1499	946	281	266	6		

- Molecule 51 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lh	122	Total	C	N	O	S	0	0
			1010	638	204	167	1		

- Molecule 52 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LG	228	Total	C	N	O	S	0	0
			1791	1142	346	299	4		

- Molecule 53 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lg	110	Total	C	N	O	S	1	0
			871	545	181	139	6		

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LF	225	Total	C	N	O	S	0	0
			1835	1178	350	298	9		

- Molecule 55 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lf	109	Total	C	N	O	S	0	0
			868	549	173	143	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lf	111	LYS	-	expression tag	UNP P18077

- Molecule 56 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LE	217	Total	C	N	O	S	1	0
			1721	1108	327	282	4		

- Molecule 57 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Le	127	Total	C	N	O	S	0	0
			1044	660	215	164	5		

- Molecule 58 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LD	292	Total	C	N	O	S	0	0
			2354	1487	429	424	14		

- Molecule 59 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ld	106	Total	C	N	O	S	0	0
			840	534	165	139	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LC	359	Total	C	N	O	S	0	0
			2862	1802	572	475	13		

- Molecule 61 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lc	98	Total	C	N	O	S	0	0
			760	482	134	138	6		

- Molecule 62 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LB	396	Total	C	N	O	S	0	0
			3174	2022	597	542	13		

- Molecule 63 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lb	101	Total	C	N	O	S	0	0
			815	506	178	127	4		

- Molecule 64 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LA	248	Total	C	N	O	S	1	0
			1899	1190	389	314	6		

- Molecule 65 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	La	147	Total	C	N	O	S	0	0
			1157	732	236	186	3		

- Molecule 66 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	L7	119	Total	C	N	O	P	0	0
			2542	1132	454	837	119		

- Molecule 67 is a RNA chain called P site tRNA.

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

- Molecule 68 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Sa	99	Total	C	N	O	S	0	0
			775	484	159	128	4		

- Molecule 69 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	L8	153	Total	C	N	O	P	0	0
			3256	1453	574	1076	153		

- Molecule 70 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	L5	3446	Total	C	N	O	P	1	0
			73960	32974	13527	24012	3447		

- Molecule 71 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	SZ	63	Total	C	N	O	0	0
			383	245	69	69		

- Molecule 72 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	ST	129	Total	C	N	O	S	0	0
			837	529	163	143	2		

- Molecule 73 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SP	126	Total	C	N	O	S	0	0
			806	504	155	144	3		

- Molecule 74 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	S2	1569	Total	C	N	O	P	0	0
			33557	15003	6040	10945	1569		

- Molecule 75 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SG	220	Total	C	N	O	S	0	0
			1663	1043	329	284	7		

- Molecule 76 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SI	206	Total	C	N	O	S	0	0
			1648	1035	326	282	5		

- Molecule 77 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	S6	59	Total	C	N	O	P	0	0
			1263	565	238	402	58		

- Molecule 78 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	SS	138	Total	C	N	O	0	0
			903	565	178	160		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SS	115	ILE	LYS	conflict	UNP P62269
SS	117	ALA	ILE	conflict	UNP P62269
SS	119	PHE	ALA	conflict	UNP P62269

- Molecule 79 is a RNA chain called TISU mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	mR	7	Total	C	N	O	P	0	0
			152	68	30	47	7		

- Molecule 80 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Lm	1	Total	Zn	0
			1	1	
81	Lo	1	Total	Zn	0
			1	1	
81	Sd	1	Total	Zn	0
			1	1	
81	Lp	1	Total	Zn	0
			1	1	
81	Lg	1	Total	Zn	0
			1	1	

- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
82	SQ	1	Total K 1 1	0
82	Lf	1	Total K 1 1	0
82	LC	1	Total K 1 1	0
82	LB	1	Total K 1 1	0
82	L8	1	Total K 1 1	0
82	L5	60	Total K 60 60	0
82	S2	11	Total K 11 11	0

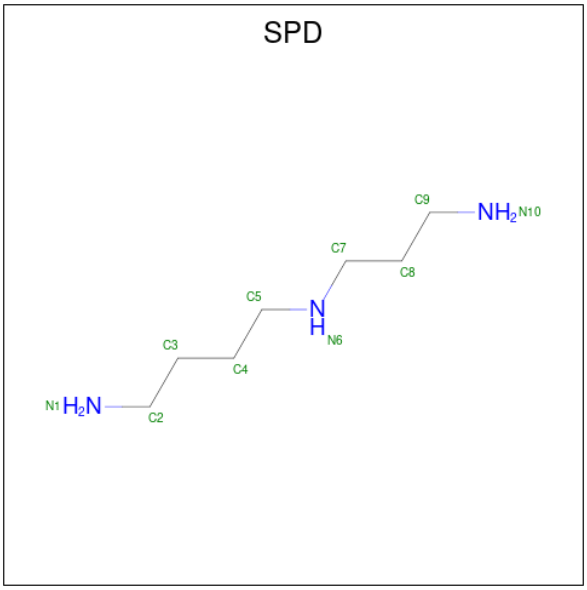
- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	Sd	1	Total Mg 1 1	0
83	LV	1	Total Mg 1 1	0
83	LS	1	Total Mg 1 1	0
83	LP	1	Total Mg 1 1	0
83	LM	1	Total Mg 1 1	0
83	LI	2	Total Mg 2 2	0
83	Le	1	Total Mg 1 1	0
83	LB	1	Total Mg 1 1	0
83	L7	5	Total Mg 5 5	0
83	Pt	1	Total Mg 1 1	0
83	L8	3	Total Mg 3 3	0
83	L5	81	Total Mg 81 81	0
83	S2	21	Total Mg 21 21	0

- Molecule 84 is SODIUM ION (CCD ID: NA) (formula: Na).

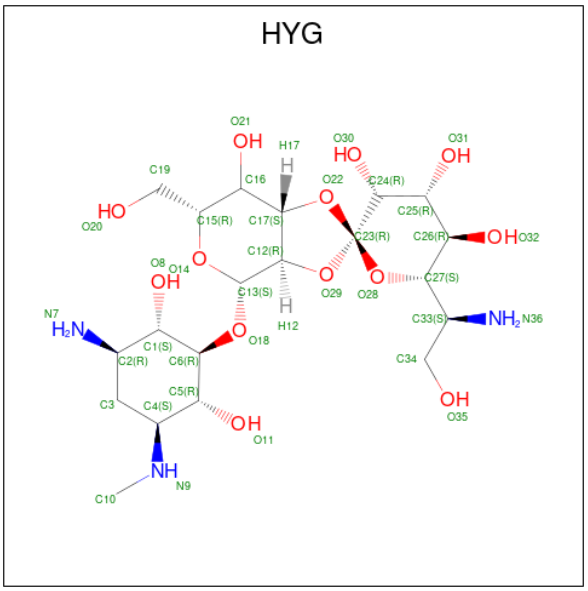
Mol	Chain	Residues	Atoms	AltConf
84	LN	1	Total Na 1 1	0
84	Le	1	Total Na 1 1	0
84	LB	1	Total Na 1 1	0
84	L5	46	Total Na 46 46	0
84	S2	12	Total Na 12 12	0

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

- Molecule 86 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



Mol	Chain	Residues	Atoms	AltConf
86	S2	1	Total C N O 36 20 3 13	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms	AltConf
87	Ll	2	Total O 2 2	0
87	Lo	1	Total O 1 1	0
87	SN	3	Total O 3 3	0
87	SL	1	Total O 1 1	0
87	SF	1	Total O 1 1	0
87	LW	1	Total O 1 1	0
87	LV	2	Total O 2 2	0
87	LT	4	Total O 4 4	0
87	LS	5	Total O 5 5	0
87	LR	3	Total O 3 3	0
87	LQ	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
87	LP	3	Total O 3 3	0
87	Lp	1	Total O 1 1	0
87	LN	5	Total O 5 5	0
87	Ln	2	Total O 2 2	0
87	LM	1	Total O 1 1	0
87	LL	2	Total O 2 2	0
87	Lj	2	Total O 2 2	0
87	LI	1	Total O 1 1	0
87	LH	1	Total O 1 1	0
87	Lh	2	Total O 2 2	0
87	LG	1	Total O 1 1	0
87	Lg	3	Total O 3 3	0
87	LF	3	Total O 3 3	0
87	Le	3	Total O 3 3	0
87	LD	1	Total O 1 1	0
87	LC	1	Total O 1 1	0
87	Lc	2	Total O 2 2	0
87	LB	7	Total O 7 7	0
87	Lb	4	Total O 4 4	0
87	LA	4	Total O 4 4	0
87	La	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
87	L7	9	Total O 9 9	0
87	Pt	1	Total O 1 1	0
87	Sa	1	Total O 1 1	0
87	L8	16	Total O 16 16	0
87	L5	473	Total O 473 473	0
87	S2	101	Total O 101 101	0
87	SI	5	Total O 5 5	0
87	SS	2	Total O 2 2	0

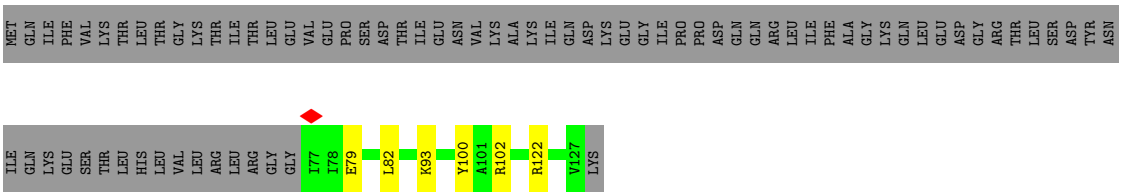
3 Residue-property plots (i)

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

• Molecule 1: Ubiquitin-60S ribosomal protein L40

Chain Lm:

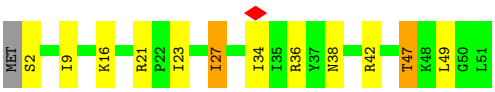




• Molecule 2: Large ribosomal subunit protein eL39

Chain Ll:

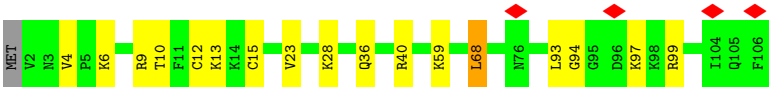




• Molecule 3: Large ribosomal subunit protein eL42

Chain Lo:

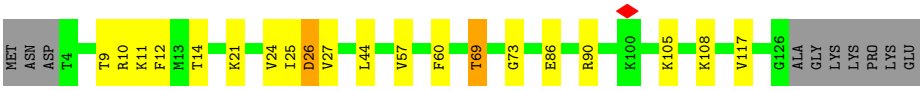




• Molecule 4: 40S ribosomal protein S24

Chain SY:

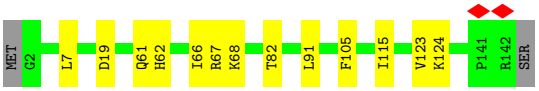




• Molecule 5: Small ribosomal subunit protein uS12

Chain SX:

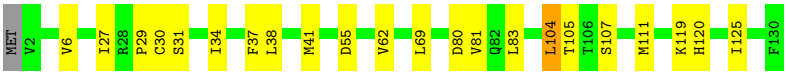




• Molecule 6: 40S ribosomal protein S15a

Chain SW:

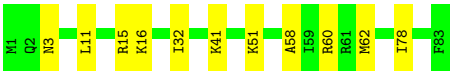




• Molecule 7: 40S ribosomal protein S21

Chain SV:

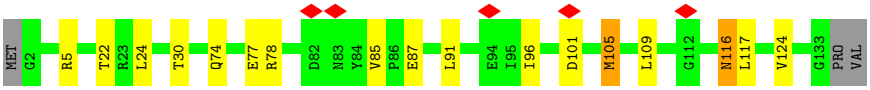




• Molecule 8: 40S ribosomal protein S17

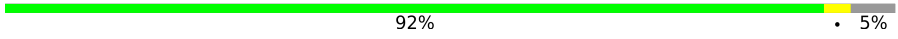
Chain SR:

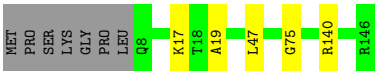




• Molecule 9: 40S ribosomal protein S16

Chain SQ:

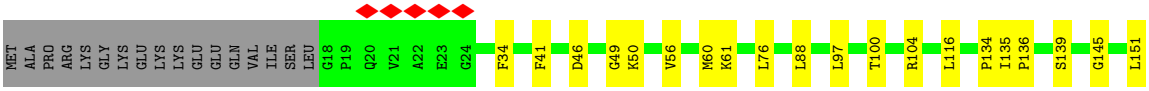




• Molecule 10: 40S ribosomal protein S14

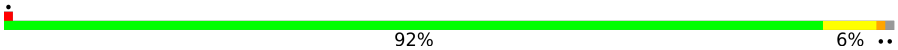
Chain SO:

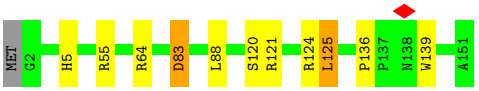




• Molecule 11: 40S ribosomal protein S13

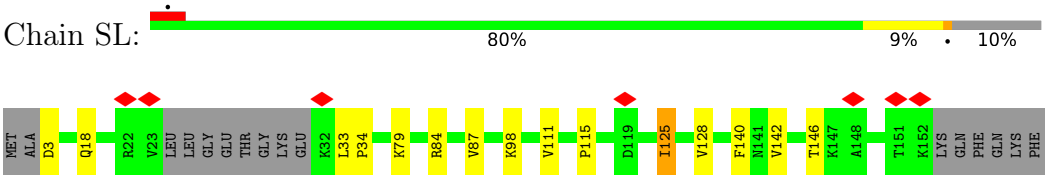
Chain SN:





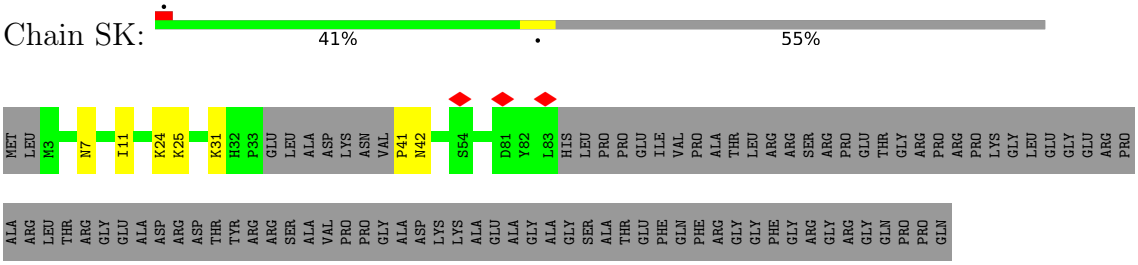
• Molecule 12: Small ribosomal subunit protein uS17

Chain SL:



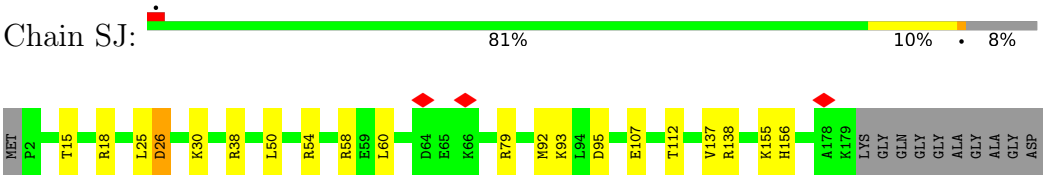
• Molecule 13: Small ribosomal subunit protein eS10

Chain SK:



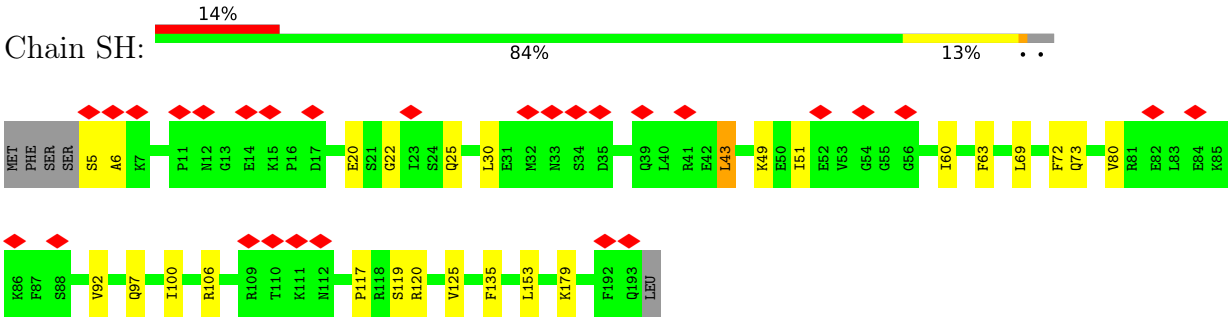
• Molecule 14: 40S ribosomal protein S9

Chain SJ:



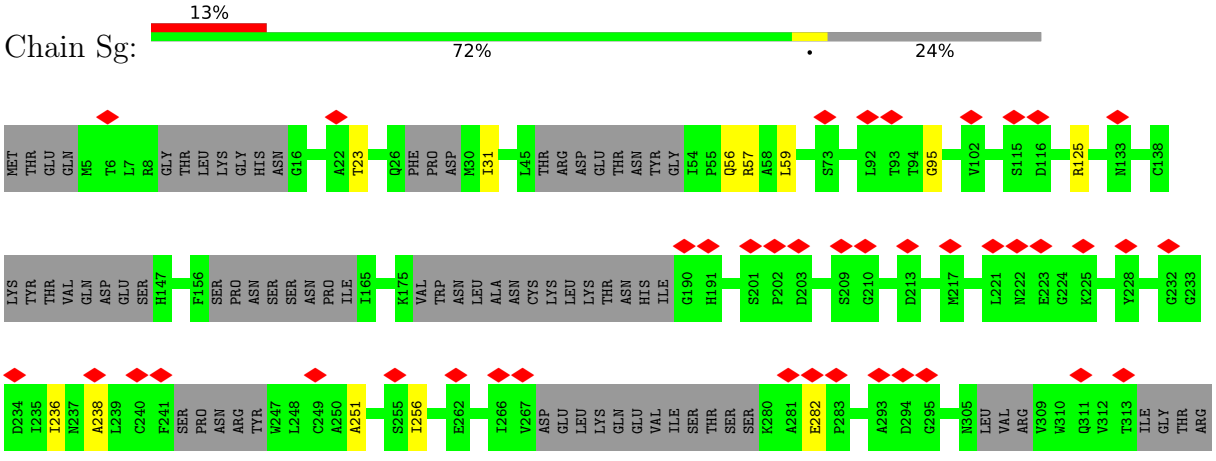
• Molecule 15: 40S ribosomal protein S7

Chain SH:



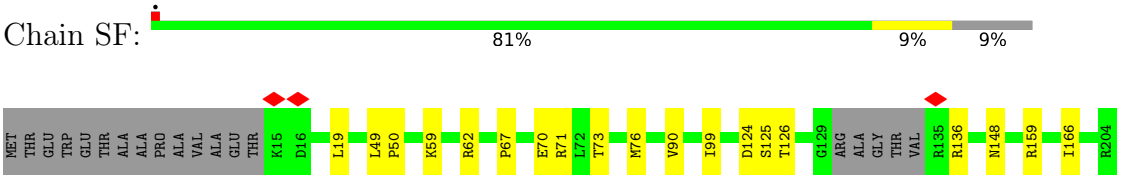
• Molecule 16: Small ribosomal subunit protein RACK1

Chain Sg:



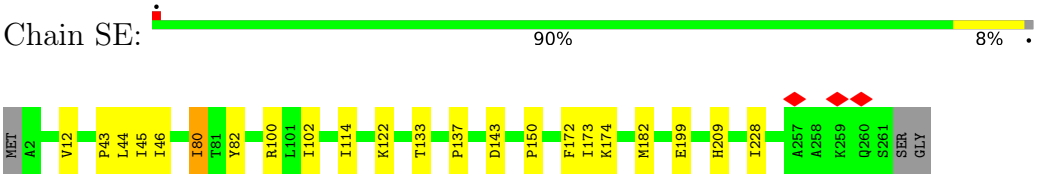
• Molecule 17: Small ribosomal subunit protein uS7

Chain SF:



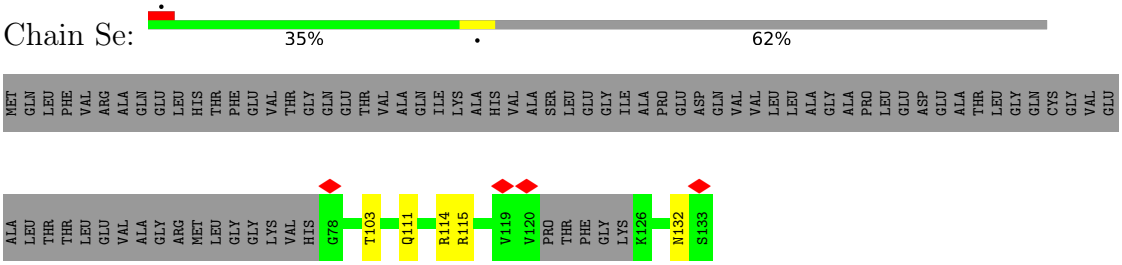
• Molecule 18: Small ribosomal subunit protein eS4, X isoform

Chain SE:



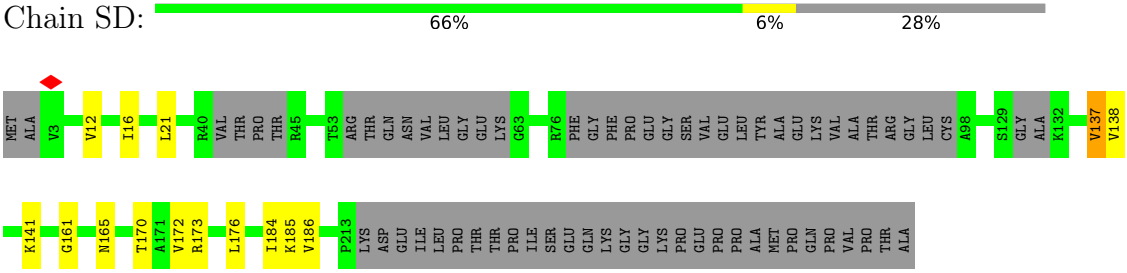
• Molecule 19: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:



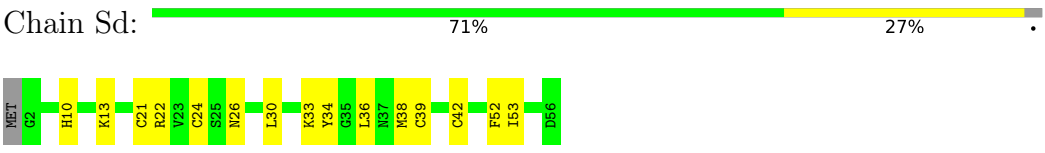
• Molecule 20: 40S ribosomal protein S3

Chain SD:



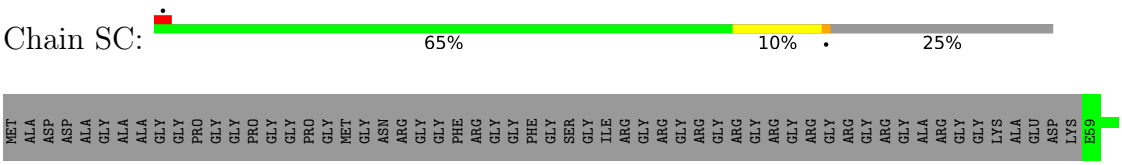
• Molecule 21: 40S ribosomal protein S29

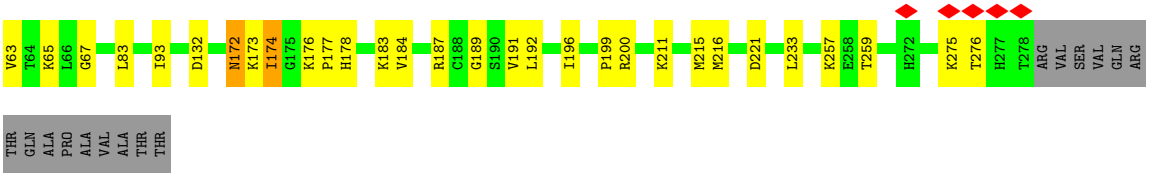
Chain Sd:



• Molecule 22: 40S ribosomal protein S2

Chain SC:

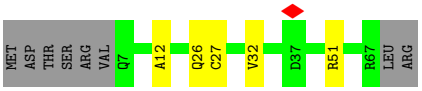




• Molecule 23: 40S ribosomal protein S28

Chain Sc:

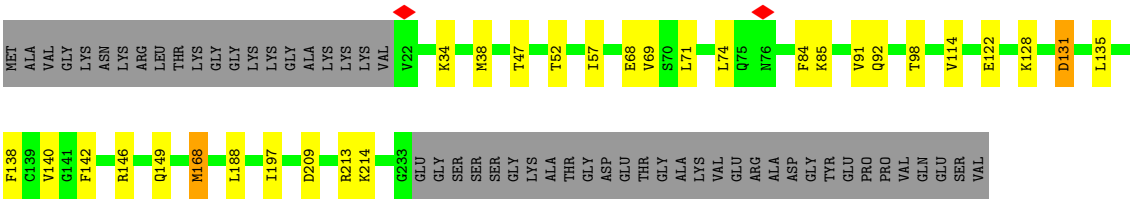




• Molecule 24: 40S ribosomal protein S3a

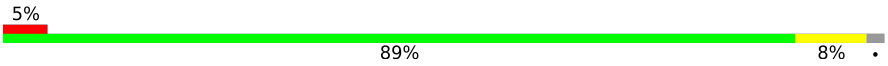
Chain SB:

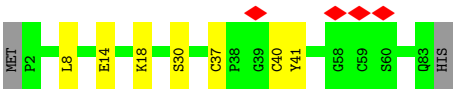




• Molecule 25: 40S ribosomal protein S27

Chain Sb:

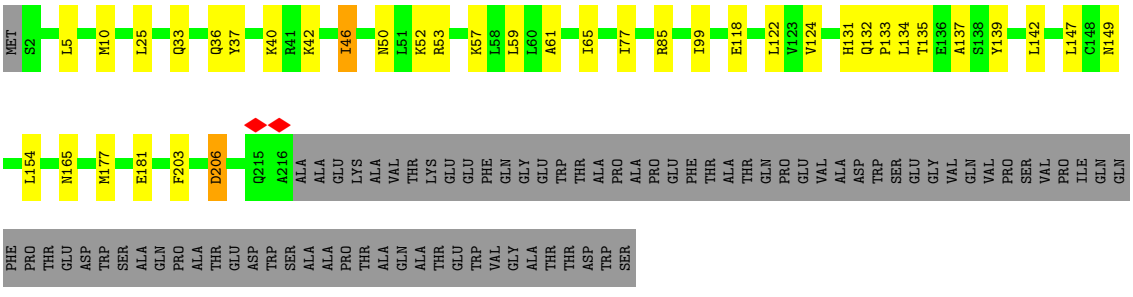




• Molecule 26: 40S ribosomal protein SA

Chain SA:

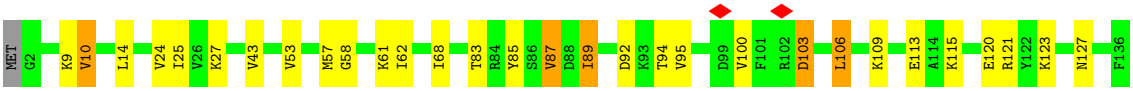




• Molecule 27: 60S ribosomal protein L27

Chain LZ:





• Molecule 28: Large ribosomal subunit protein uL24

Chain LY:

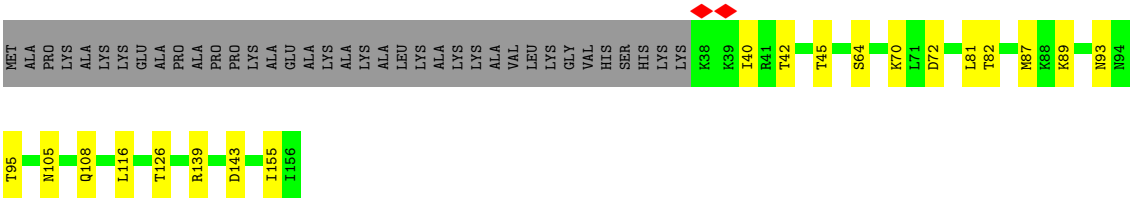




• Molecule 29: 60S ribosomal protein L23a

Chain LX:

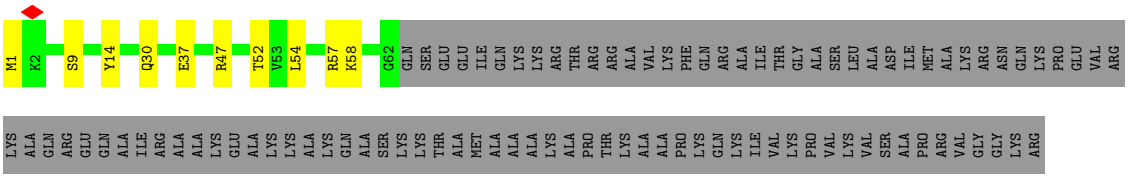




• Molecule 30: 60S ribosomal protein L24

Chain LW:

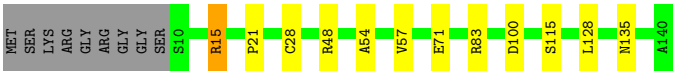




• Molecule 31: 60S ribosomal protein L23

Chain LV:

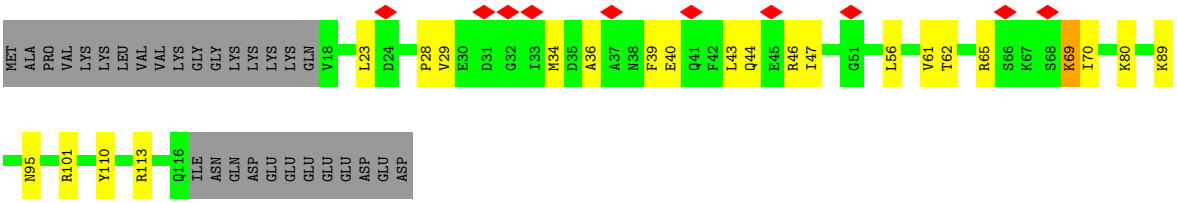




• Molecule 32: 60S ribosomal protein L22

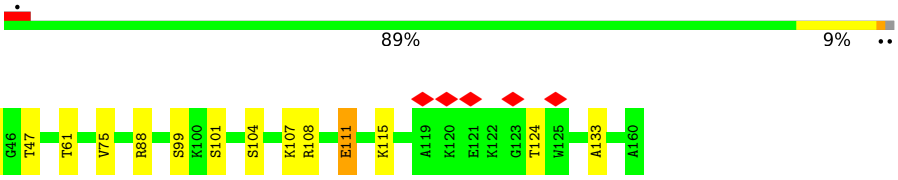
Chain LU:





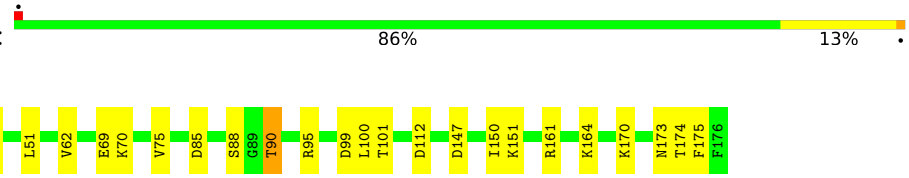
• Molecule 33: 60S ribosomal protein L21

Chain LT:



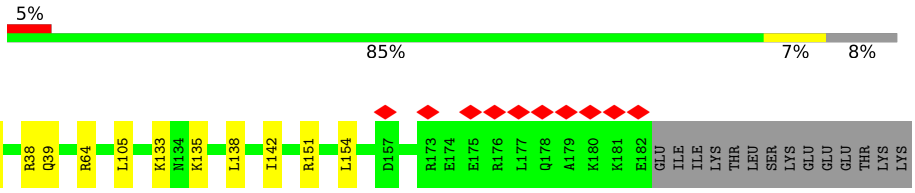
• Molecule 34: 60S ribosomal protein L18a

Chain LS:



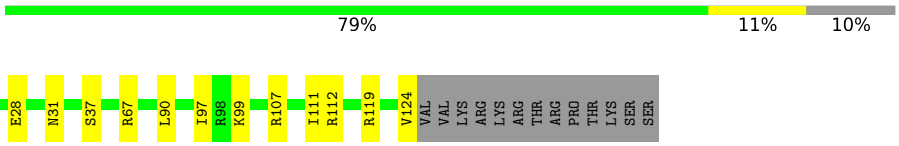
• Molecule 35: 60S ribosomal protein L19

Chain LR:



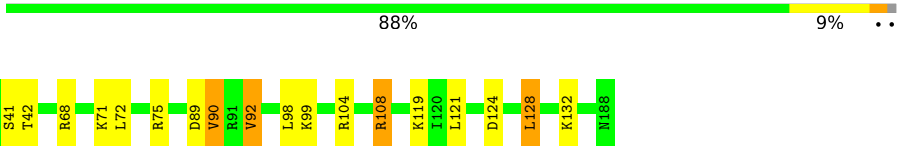
• Molecule 36: Large ribosomal subunit protein eL28

Chain Lr:



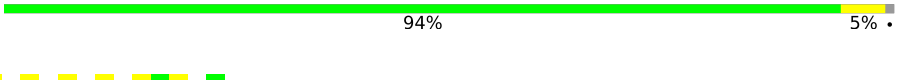
• Molecule 37: 60S ribosomal protein L18

Chain LQ:



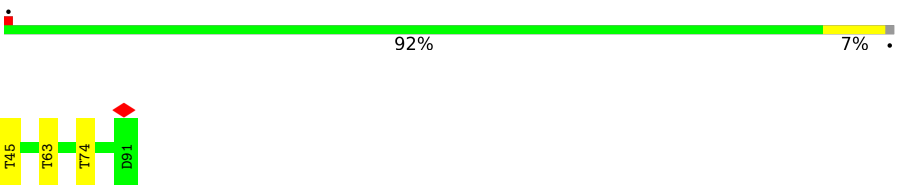
• Molecule 38: Large ribosomal subunit protein uL22

Chain LP:



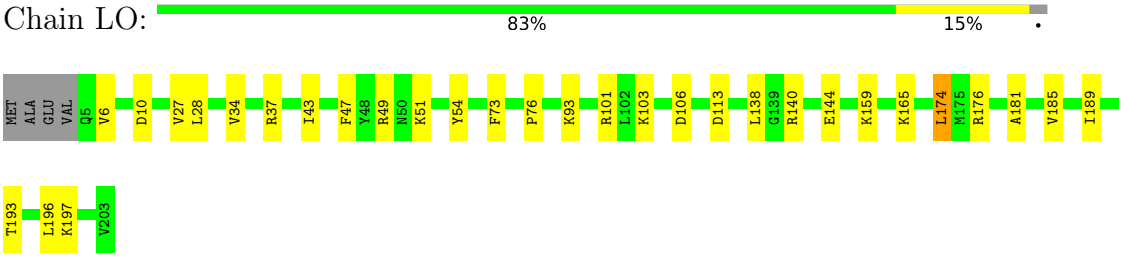
• Molecule 39: Large ribosomal subunit protein eL43

Chain Lp:



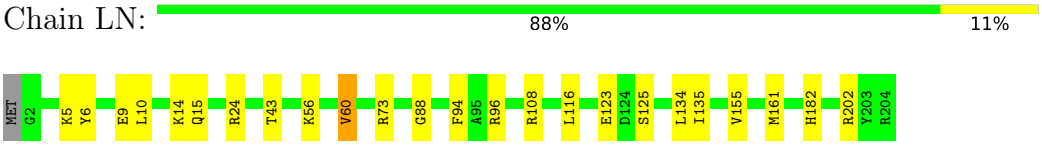
• Molecule 40: 60S ribosomal protein L13a

Chain LO:



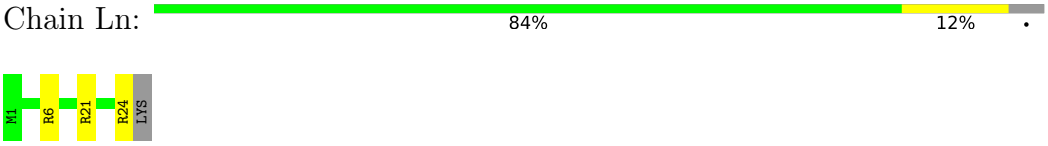
• Molecule 41: 60S ribosomal protein L15

Chain LN:



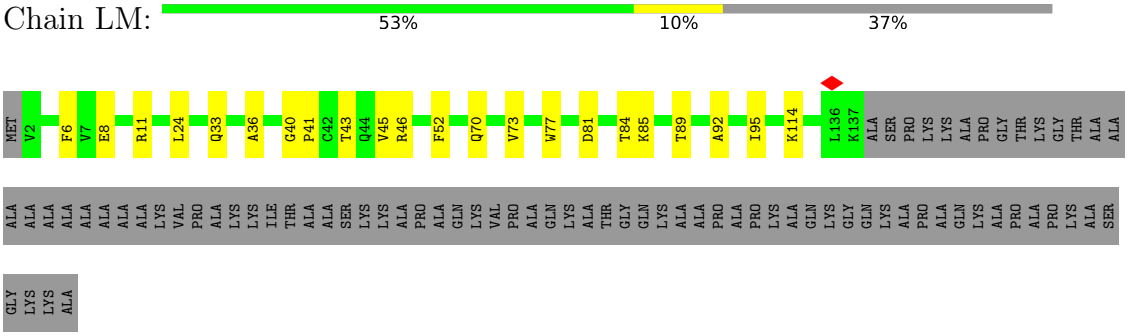
• Molecule 42: Small ribosomal subunit protein eS32

Chain Ln:



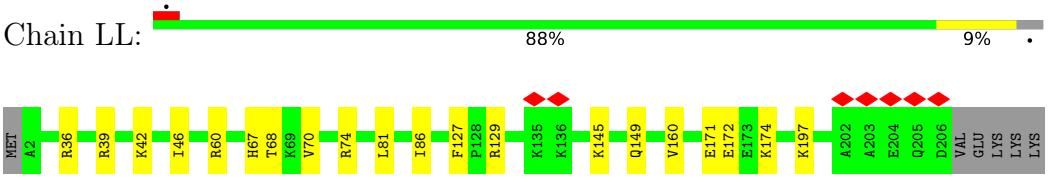
• Molecule 43: 60S ribosomal protein L14

Chain LM:



• Molecule 44: 60S ribosomal protein L13

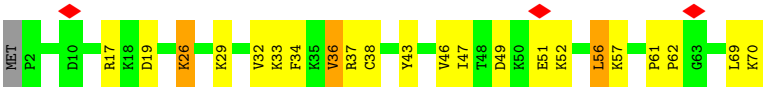
Chain LL:



• Molecule 45: 60S ribosomal protein L38

Chain Lk:

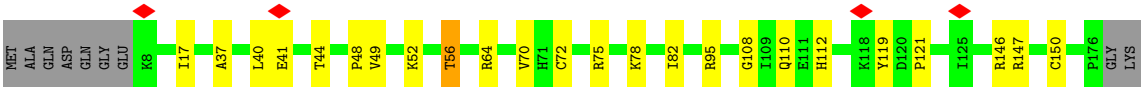




• Molecule 46: 60S ribosomal protein L11

Chain LJ:

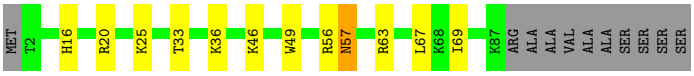




• Molecule 47: Large ribosomal subunit protein eL37

Chain Lj:

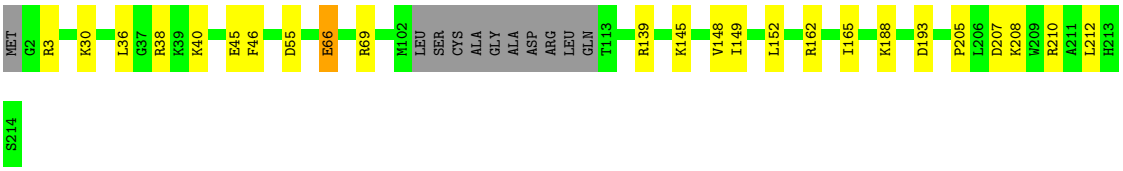




• Molecule 48: 60S ribosomal protein L10

Chain LI:

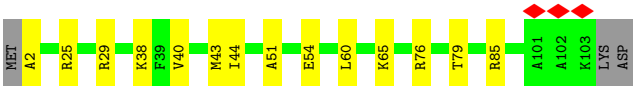




• Molecule 49: 60S ribosomal protein L36

Chain Li:

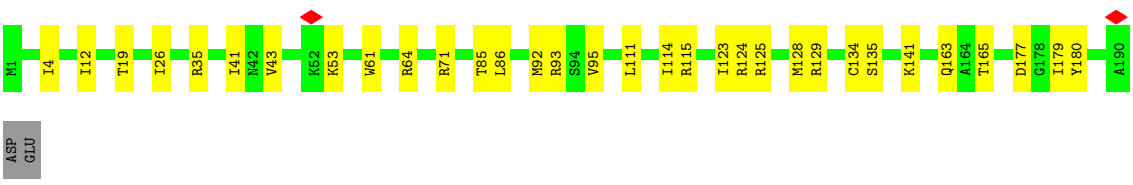




• Molecule 50: 60S ribosomal protein L9

Chain LH:

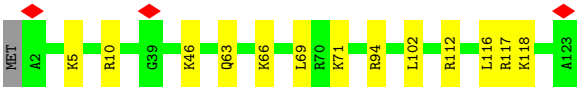




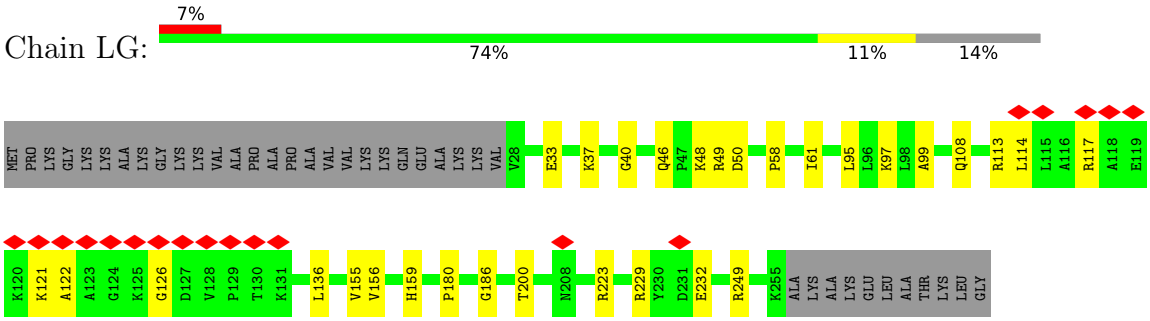
• Molecule 51: 60S ribosomal protein L35

Chain Lh:

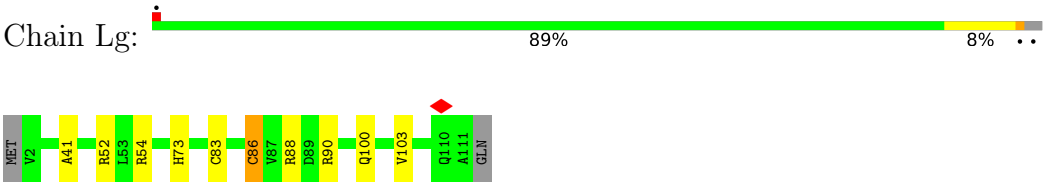




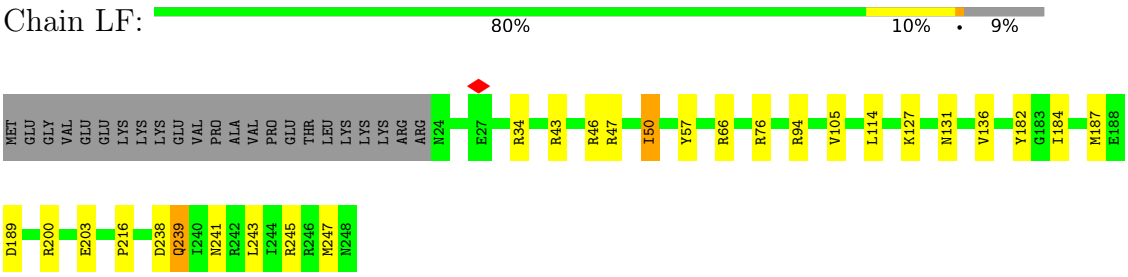
• Molecule 52: 60S ribosomal protein L7a



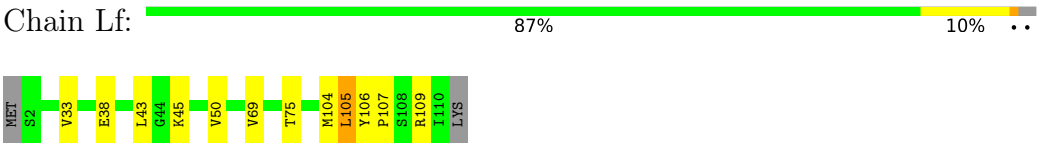
• Molecule 53: Large ribosomal subunit protein eL34



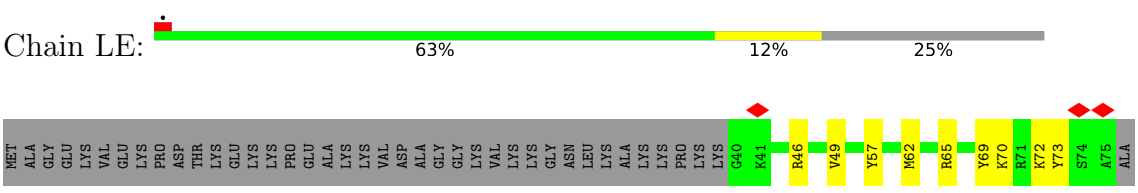
• Molecule 54: Large ribosomal subunit protein uL30

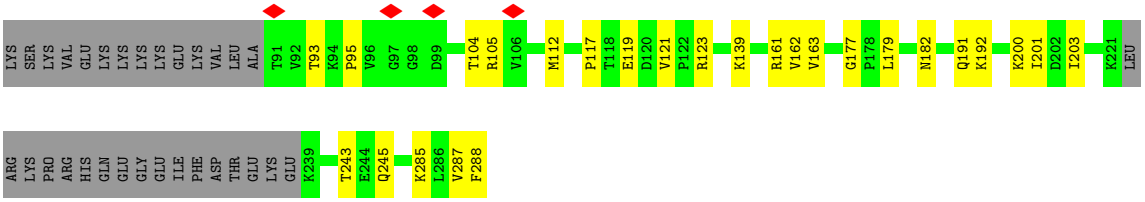


• Molecule 55: Large ribosomal subunit protein eL33

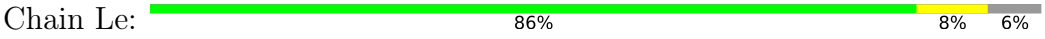


• Molecule 56: Large ribosomal subunit protein eL6



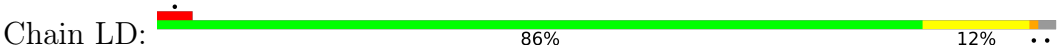


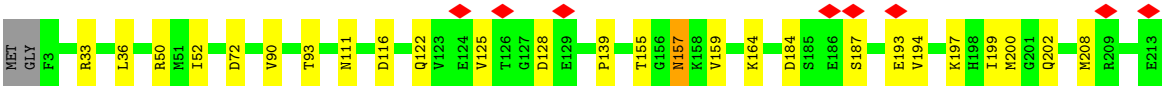
• Molecule 57: 60S ribosomal protein L32

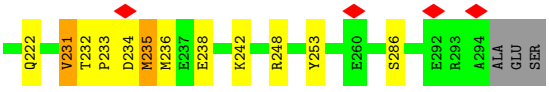




• Molecule 58: 60S ribosomal protein L5

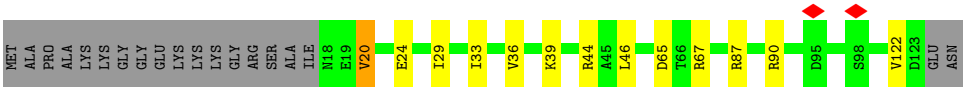




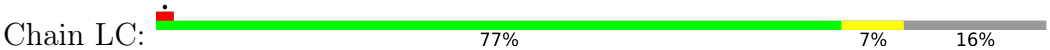


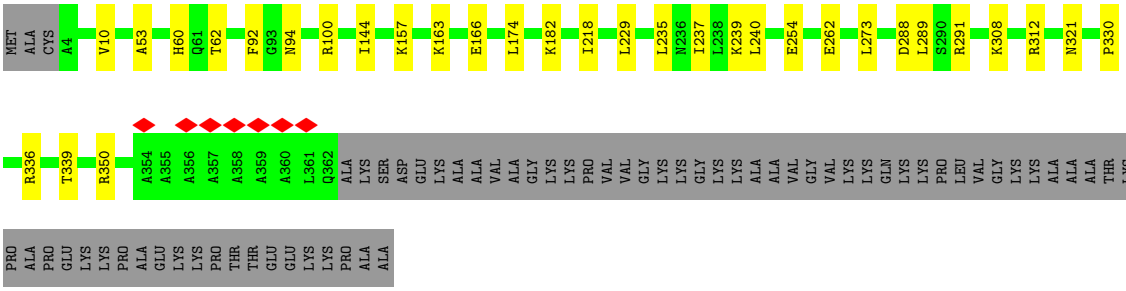
• Molecule 59: 60S ribosomal protein L31





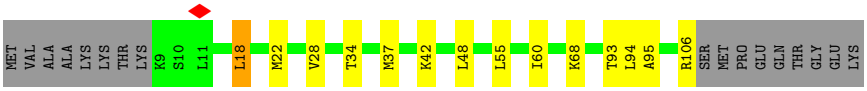
• Molecule 60: 60S ribosomal protein L4





• Molecule 61: 60S ribosomal protein L30

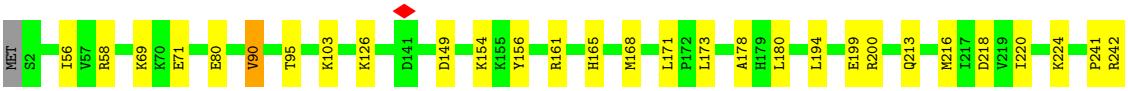




• Molecule 62: Large ribosomal subunit protein uL3

Chain LB:



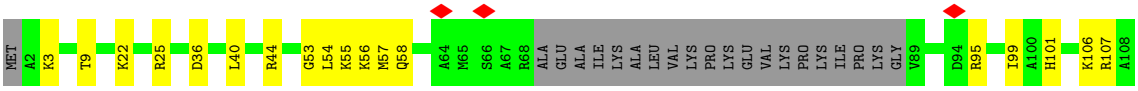


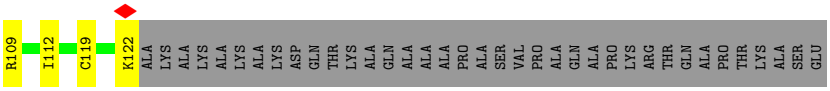


• Molecule 63: Large ribosomal subunit protein eL29

Chain Lb:



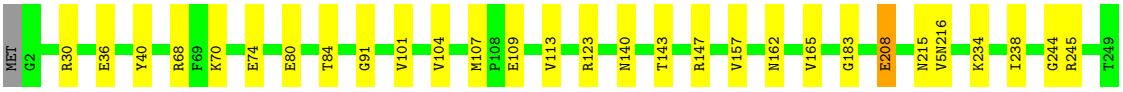


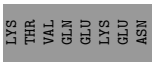


• Molecule 64: Large ribosomal subunit protein uL2

Chain LA:



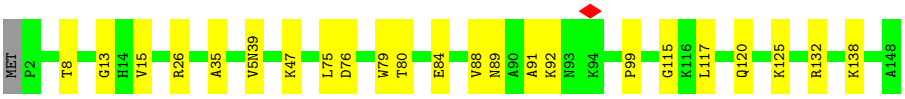




• Molecule 65: Large ribosomal subunit protein uL15

Chain La:

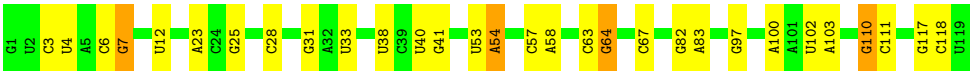




• Molecule 66: 5S rRNA

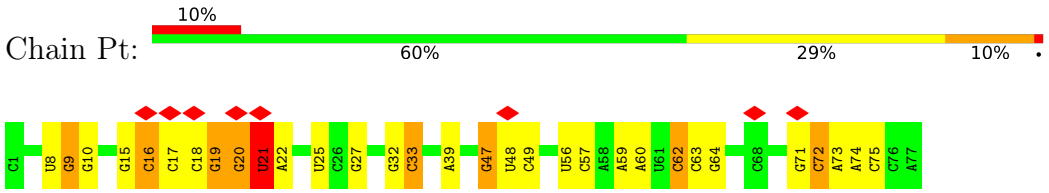
Chain L7:





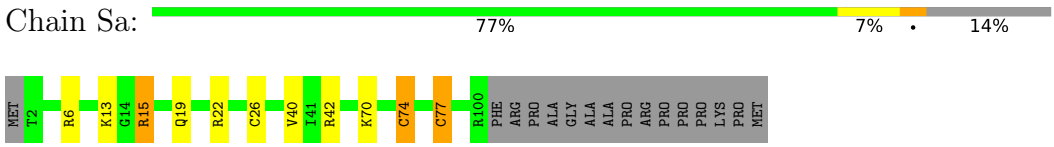
• Molecule 67: P site tRNA

Chain Pt:



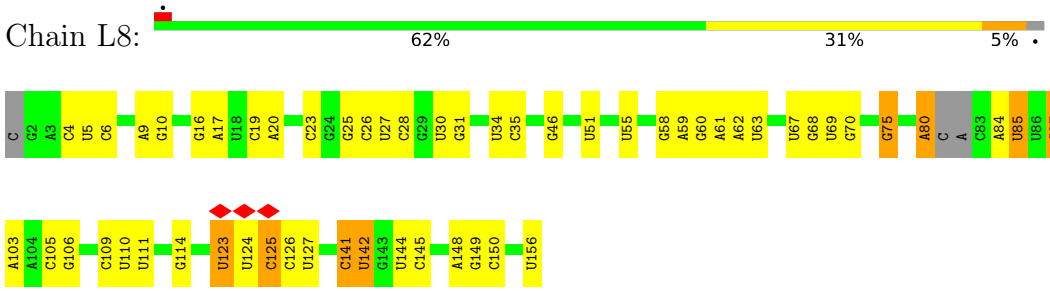
• Molecule 68: 40S ribosomal protein S26

Chain Sa:



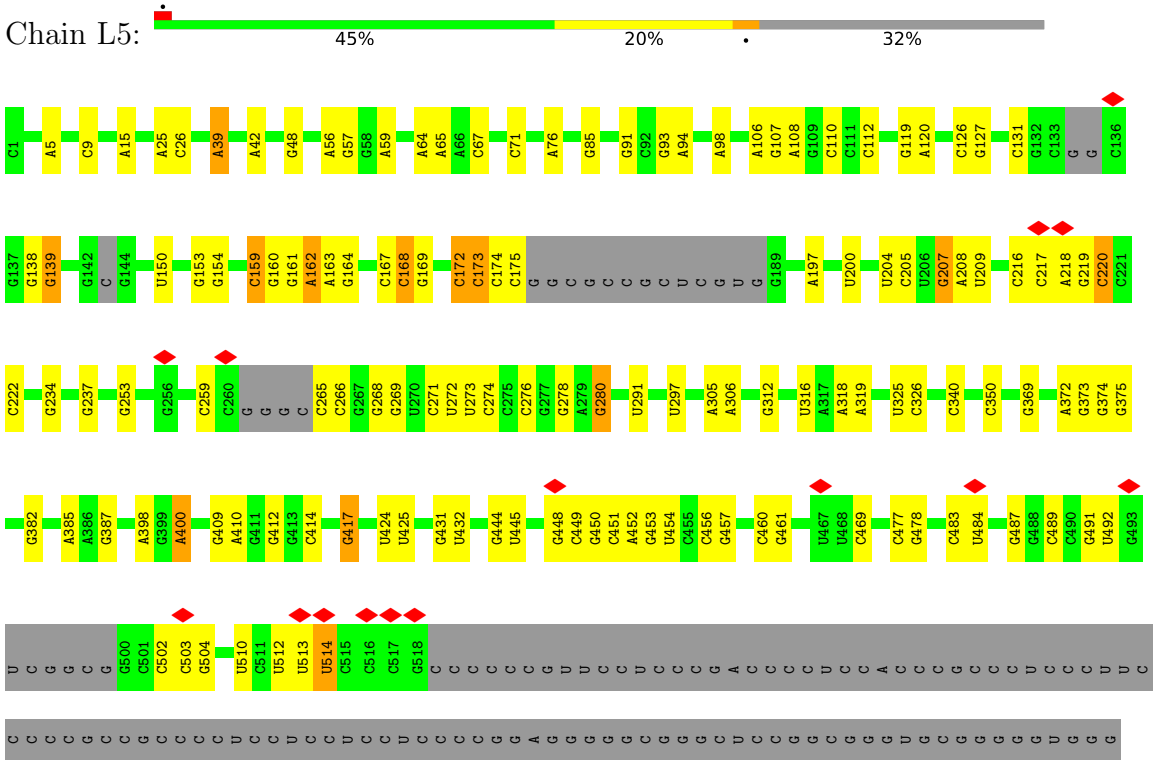
• Molecule 69: 5.8S rRNA

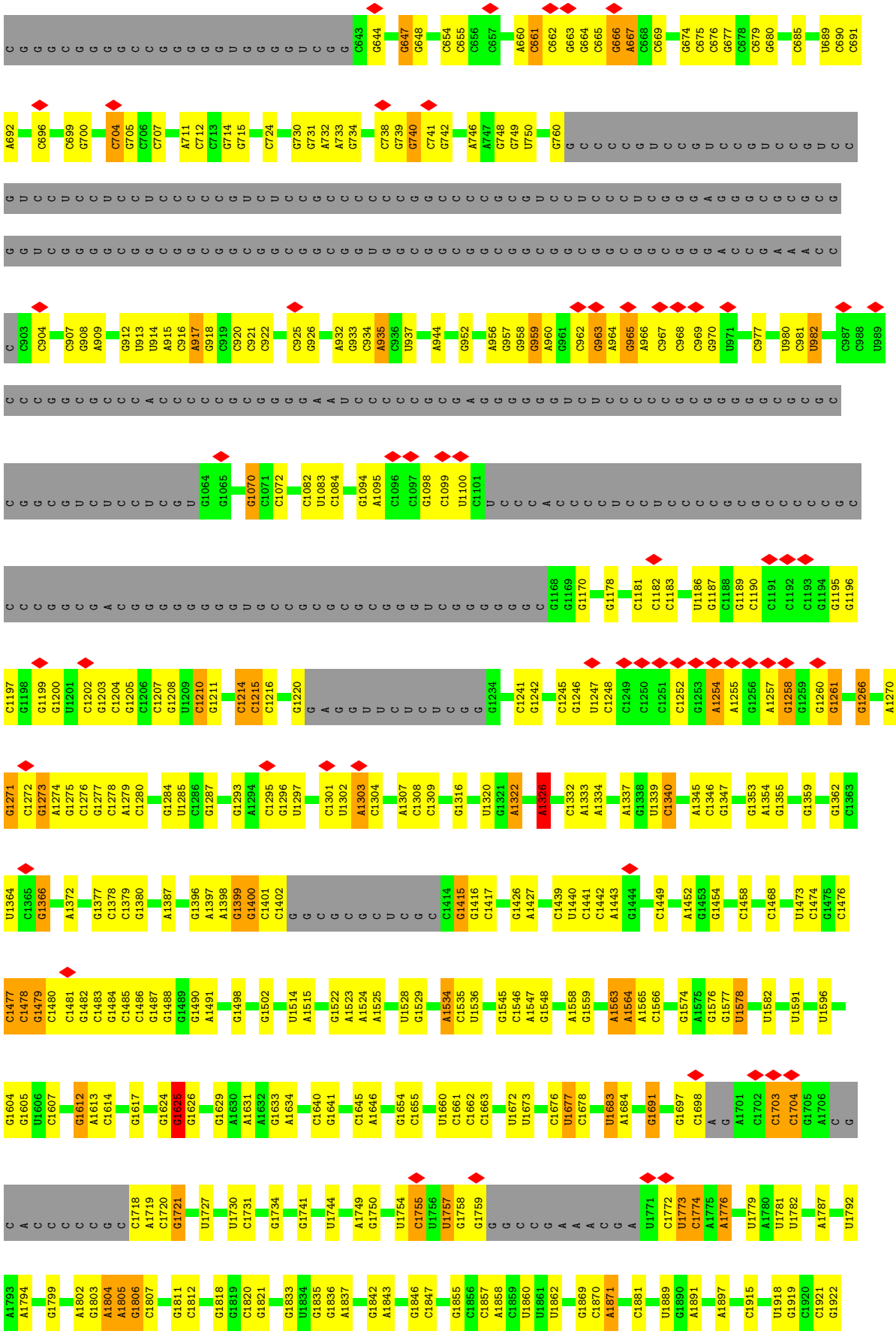
Chain L8:

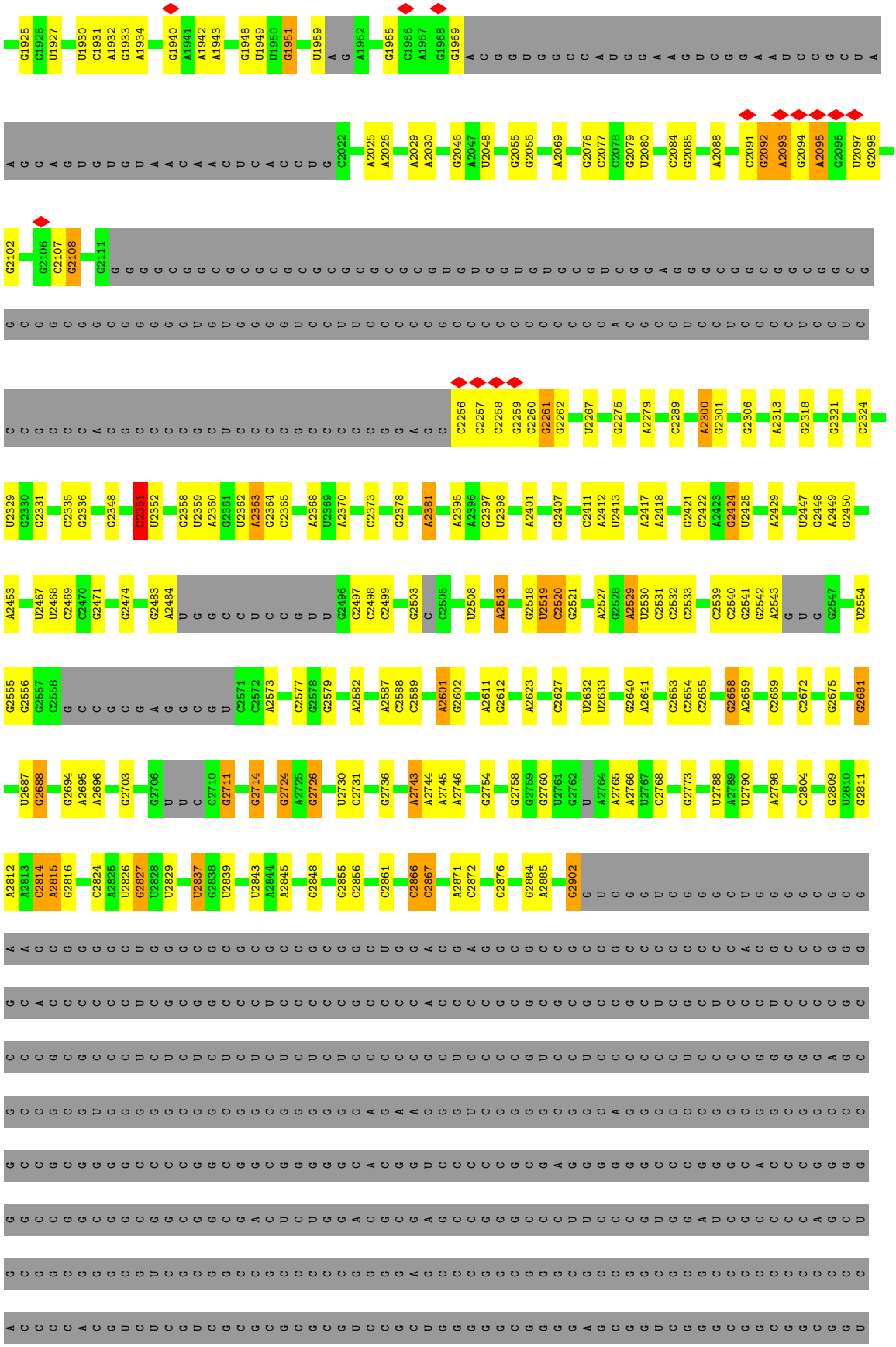


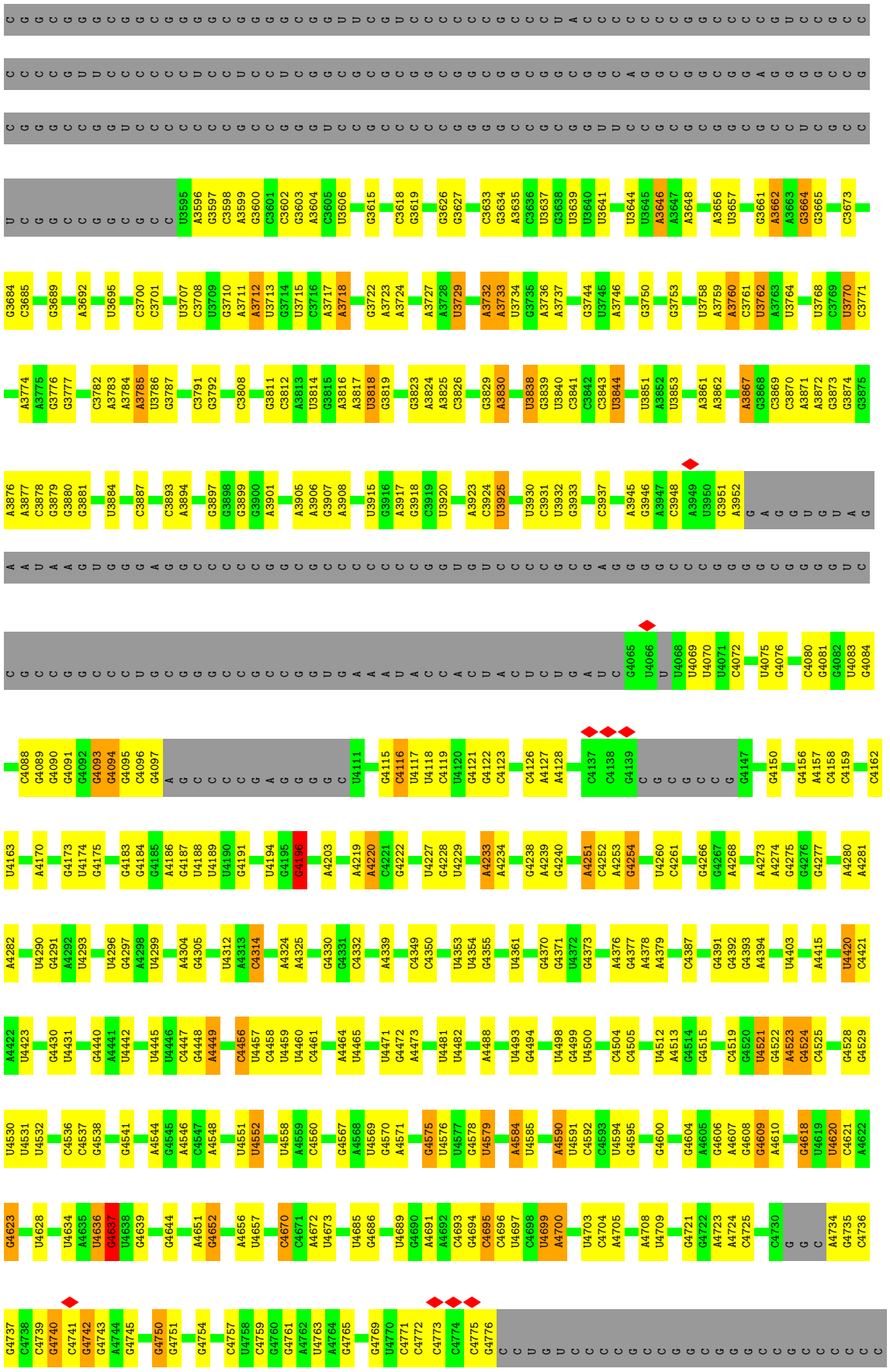
• Molecule 70: 28S rRNA

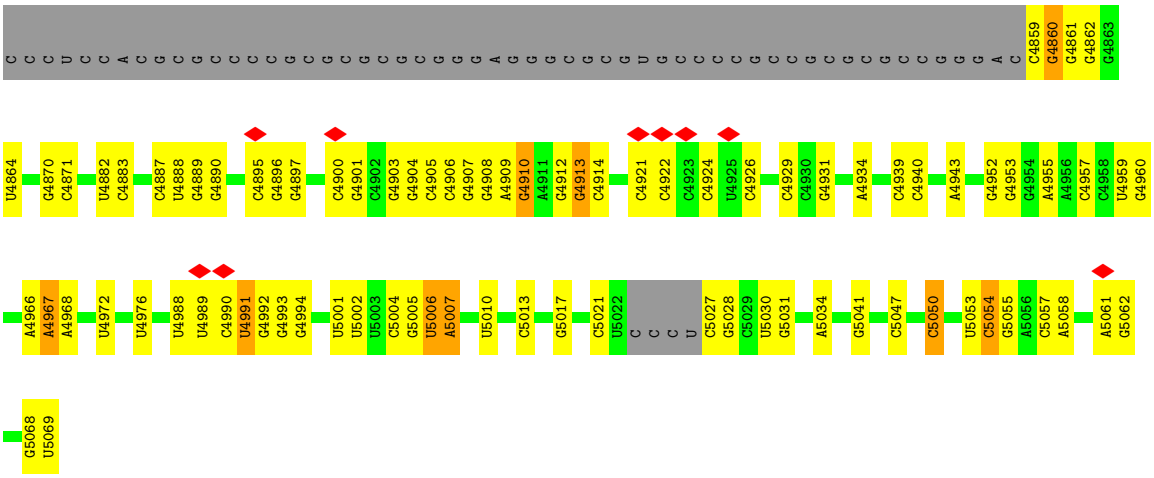
Chain L5:





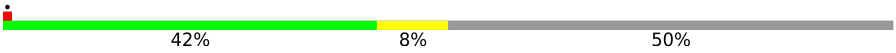


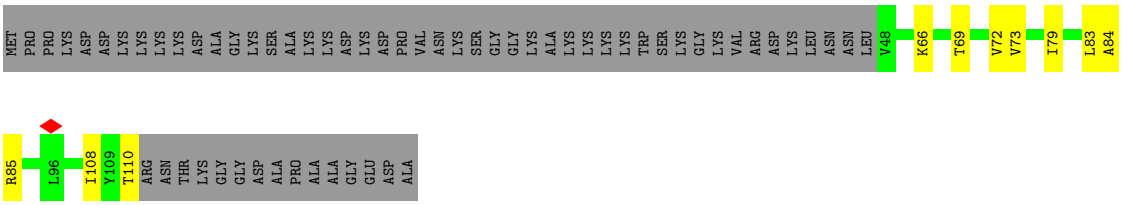




• Molecule 71: Small ribosomal subunit protein eS25

Chain SZ:

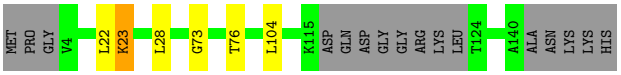




• Molecule 72: 40S ribosomal protein S19

Chain ST:

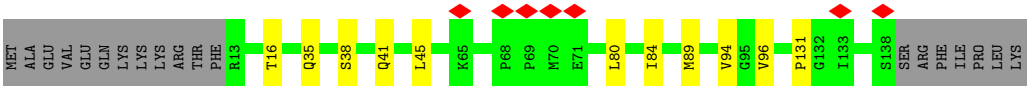




• Molecule 73: 40S ribosomal protein S15

Chain SP:

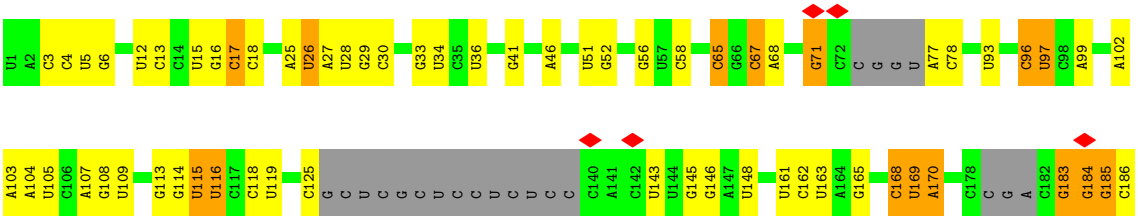


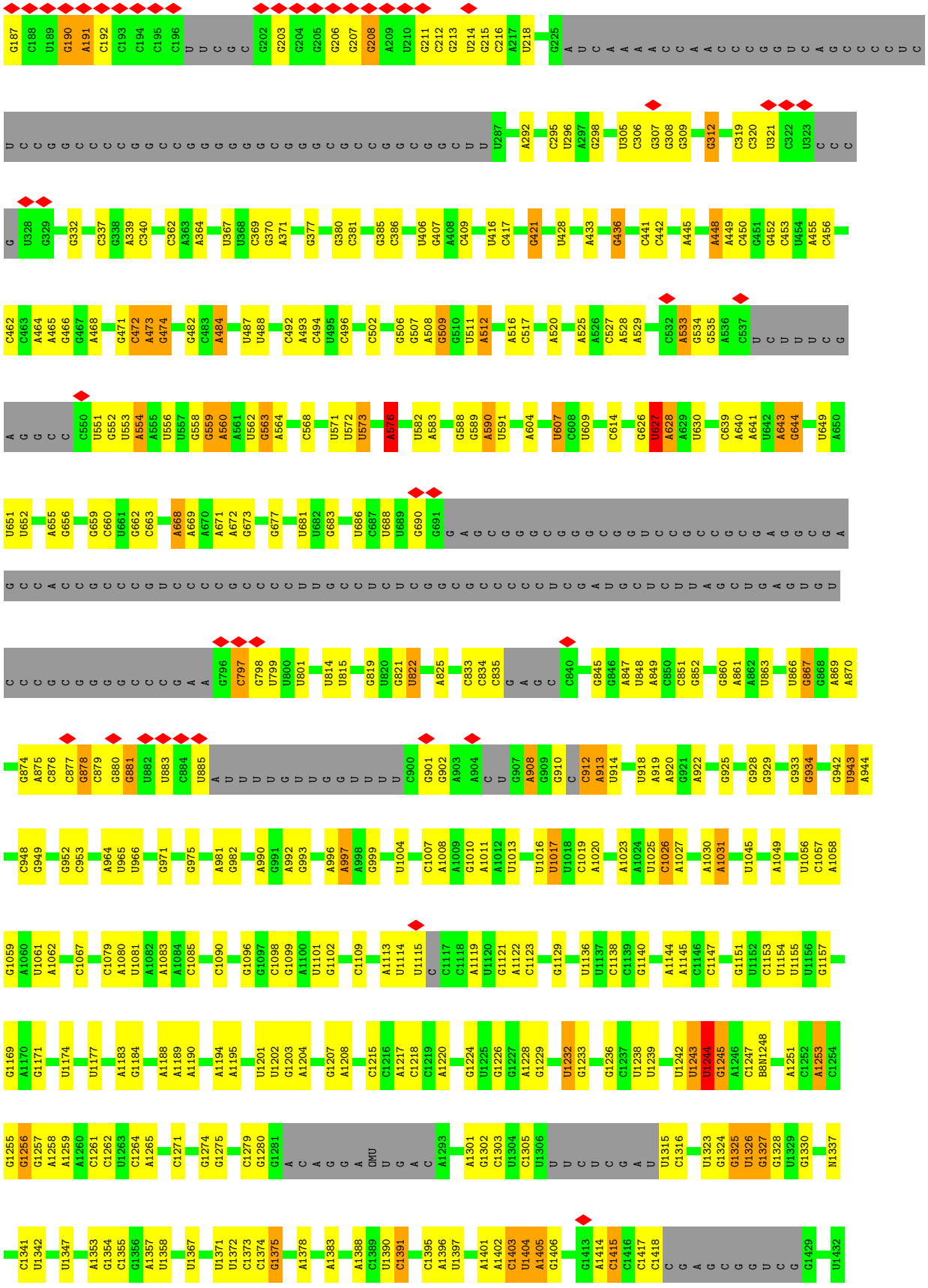


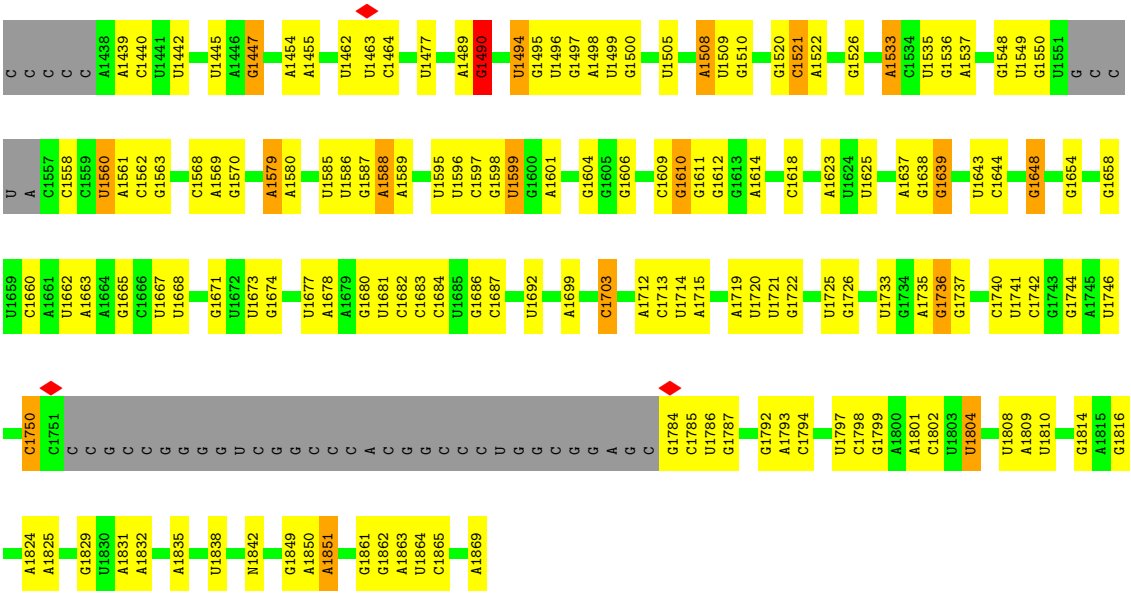
• Molecule 74: 18S rRNA

Chain S2:

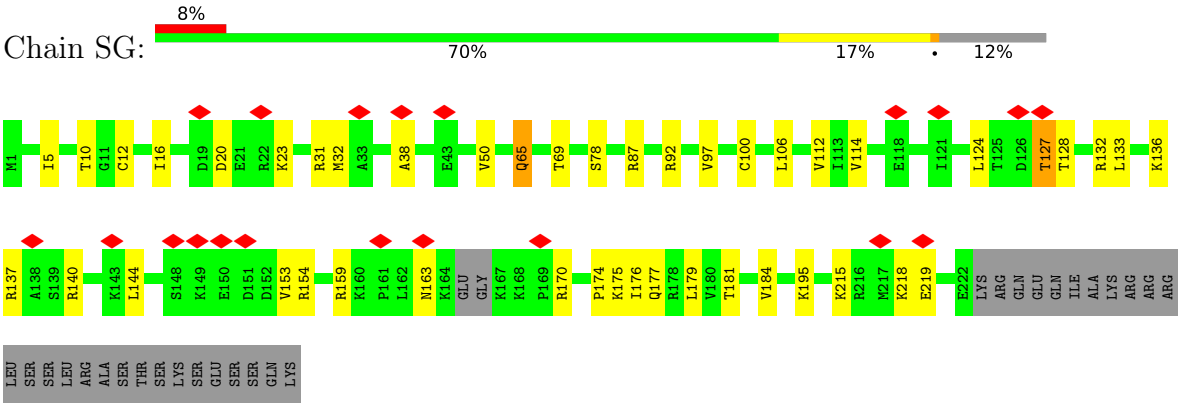




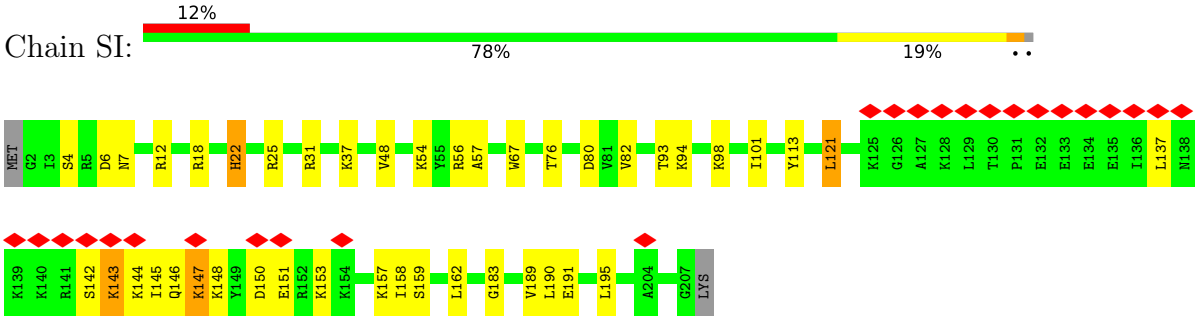




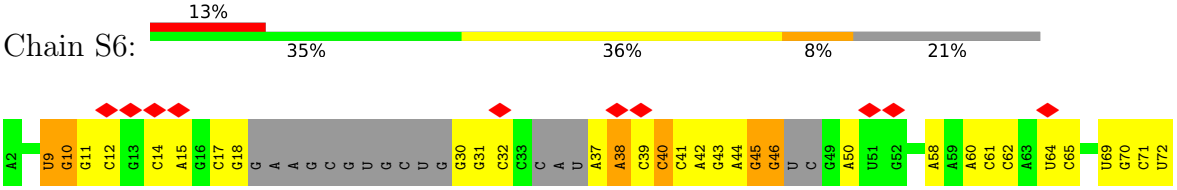
• Molecule 75: 40S ribosomal protein S6



• Molecule 76: 40S ribosomal protein S8

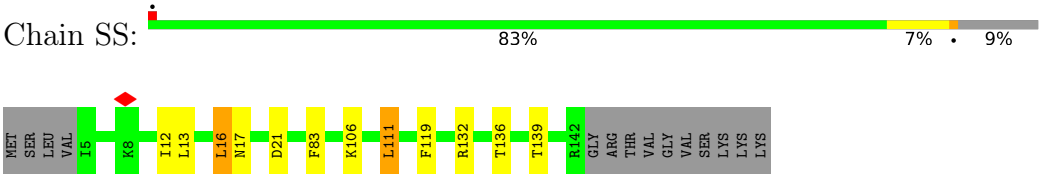


• Molecule 77: E site tRNA





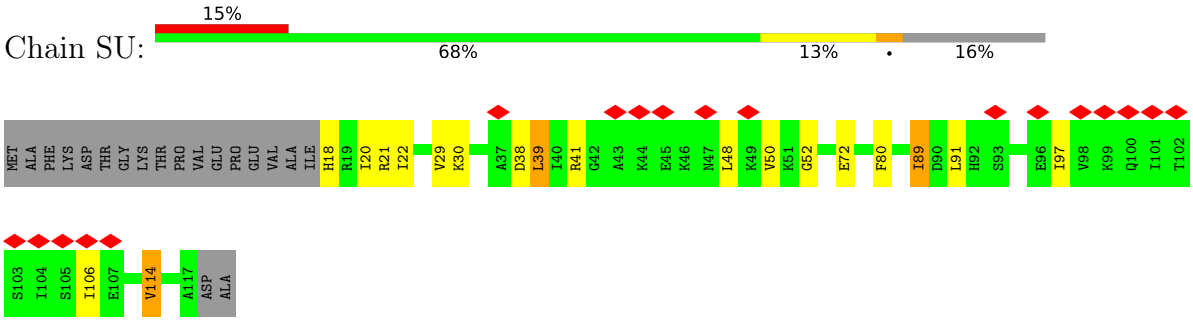
• Molecule 78: Small ribosomal subunit protein uS13



• Molecule 79: TISU mRNA



• Molecule 80: 40S ribosomal protein S20



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	404.16, 404.16, 404.16	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, G7M, ZN, A2M, PSU, SPD, 5MC, OMU, NA, V5N, OMC, MG, B8N, MLZ, K, MA6, 4SU, 6MZ, 1MA, OMG, HYG, 4AC, H2U

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	Lm	0.15	0/413	0.33	0/549
2	Ll	0.17	0/444	0.33	0/588
3	Lo	0.15	0/823	0.31	0/1088
4	SY	0.15	0/917	0.33	0/1234
5	SX	0.15	0/1077	0.33	0/1441
6	SW	0.17	0/1040	0.30	0/1393
7	SV	0.14	0/630	0.32	0/843
8	SR	0.15	0/950	0.35	0/1291
9	SQ	0.15	0/927	0.32	0/1258
10	SO	0.18	0/990	0.37	0/1330
11	SN	0.17	0/1210	0.32	0/1633
12	SL	0.15	0/1178	0.28	0/1578
13	SK	0.14	0/481	0.29	0/662
14	SJ	0.15	0/1455	0.30	0/1954
15	SH	0.15	0/1429	0.33	0/1929
16	Sg	0.14	0/1259	0.38	0/1730
17	SF	0.15	0/1345	0.33	0/1827
18	SE	0.14	0/2079	0.32	0/2801
19	Se	0.13	0/401	0.33	0/524
20	SD	0.14	0/1103	0.29	0/1505
21	Sd	0.15	0/441	0.28	0/589
22	SC	0.16	0/1731	0.34	0/2341
23	Sc	0.14	0/435	0.26	0/587
24	SB	0.16	0/1721	0.34	0/2304
25	Sb	0.14	0/625	0.31	0/842
26	SA	0.16	0/1695	0.31	0/2310
27	LZ	0.15	0/1118	0.30	0/1494
28	LY	0.15	0/1077	0.32	0/1440
29	LX	0.17	0/993	0.34	0/1334
30	LW	0.15	0/532	0.30	0/708
31	LV	0.15	0/1004	0.31	0/1346

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LU	0.15	0/814	0.38	0/1094
33	LT	0.15	0/1325	0.27	0/1770
34	LS	0.16	0/1496	0.30	0/2009
35	LR	0.18	0/1474	0.32	0/1957
36	Lr	0.19	0/1002	0.35	0/1344
37	LQ	0.17	0/1529	0.33	0/2044
38	LP	0.16	0/1256	0.33	0/1687
39	Lp	0.17	0/705	0.34	0/937
40	LO	0.18	0/1652	0.30	0/2211
41	LN	0.17	0/1739	0.34	0/2331
42	Ln	0.21	0/236	0.32	0/300
43	LM	0.17	0/1138	0.34	0/1523
44	LL	0.15	0/1669	0.29	0/2237
45	Lk	0.17	0/563	0.37	0/748
46	LJ	0.15	0/1352	0.32	0/1812
47	Lj	0.15	0/716	0.32	0/947
48	LI	0.16	0/1670	0.29	0/2230
49	Li	0.14	0/823	0.31	0/1092
50	LH	0.16	0/1518	0.31	0/2043
51	Lh	0.17	0/1018	0.34	0/1347
52	LG	0.16	0/1824	0.33	0/2465
53	Lg	0.19	0/884	0.35	0/1179
54	LF	0.18	0/1869	0.33	0/2498
55	Lf	0.17	0/887	0.33	0/1190
56	LE	0.14	0/1758	0.29	0/2360
57	Le	0.17	0/1062	0.31	0/1416
58	LD	0.14	0/2400	0.33	0/3220
59	Ld	0.16	0/854	0.34	0/1153
60	LC	0.16	0/2916	0.31	0/3917
61	Lc	0.18	0/770	0.36	0/1034
62	LB	0.15	0/3242	0.32	0/4343
63	Lb	0.17	0/817	0.37	0/1080
64	LA	0.16	0/1927	0.33	0/2582
65	La	0.16	0/1173	0.32	0/1566
66	L7	0.16	0/2840	0.26	0/4425
67	Pt	0.23	0/1721	0.31	0/2679
68	Sa	0.21	0/788	0.44	1/1059 (0.1%)
69	L8	0.17	0/3564	0.30	0/5550
70	L5	0.19	3/79828 (0.0%)	0.30	0/124490
71	SZ	0.18	0/385	0.33	0/530
72	ST	0.15	0/851	0.28	0/1157
73	SP	0.14	0/814	0.34	0/1109
74	S2	0.21	2/35763 (0.0%)	0.31	0/55704

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	SG	0.13	0/1683	0.29	0/2261
76	SI	0.17	0/1677	0.33	0/2243
77	S6	0.14	0/1411	0.32	0/2192
78	SS	0.14	0/916	0.32	0/1256
79	mR	0.30	0/170	0.66	0/263
80	SU	0.21	0/805	0.43	0/1081
All	All	0.18	5/210817 (0.0%)	0.31	1/310118 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	SA	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	3830	A2M	O3'-P	5.09	1.61	1.56
70	L5	4523	A2M	O3'-P	5.06	1.61	1.56
74	S2	668	A2M	O3'-P	5.05	1.61	1.56
70	L5	3785	A2M	O3'-P	5.02	1.61	1.56
74	S2	512	A2M	O3'-P	5.00	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	Sa	77	CYS	CA-CB-SG	5.08	126.08	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	SA	147	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Lm	407	0	423	4	0
2	Ll	434	0	461	6	0
3	Lo	822	0	856	8	0
4	SY	900	0	831	15	0
5	SX	1060	0	1087	5	0
6	SW	1023	0	1063	11	0
7	SV	623	0	627	8	0
8	SR	936	0	866	8	0
9	SQ	918	0	804	4	0
10	SO	977	0	994	10	0
11	SN	1186	0	1247	8	0
12	SL	1158	0	1214	8	0
13	SK	468	0	317	4	0
14	SJ	1430	0	1498	13	0
15	SH	1408	0	1432	12	0
16	Sg	1259	0	646	6	0
17	SF	1327	0	1251	12	0
18	SE	2037	0	2131	11	0
19	Se	399	0	433	2	0
20	SD	1094	0	910	6	0
21	Sd	430	0	397	9	0
22	SC	1694	0	1769	17	0
23	Sc	434	0	419	3	0
24	SB	1694	0	1744	17	0
25	Sb	613	0	614	4	0
26	SA	1658	0	1630	23	0
27	LZ	1095	0	1164	16	0
28	LY	1060	0	1101	5	0
29	LX	976	0	1053	11	0
30	LW	519	0	533	6	0
31	LV	987	0	1052	5	0
32	LU	800	0	816	13	0
33	LT	1297	0	1366	9	0
34	LS	1456	0	1491	16	0
35	LR	1458	0	1555	8	0
36	Lr	987	0	1050	8	0
37	LQ	1505	0	1613	14	0
38	LP	1230	0	1250	4	0
39	Lp	695	0	746	3	0
40	LO	1620	0	1753	19	0
41	LN	1694	0	1738	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	Ln	235	0	284	2	0
43	LM	1116	0	1176	15	0
44	LL	1638	0	1737	14	0
45	Lk	557	0	611	14	0
46	LJ	1329	0	1346	13	0
47	Lj	701	0	735	9	0
48	LI	1632	0	1675	15	0
49	Li	812	0	870	12	0
50	LH	1499	0	1572	20	0
51	Lh	1010	0	1137	10	0
52	LG	1791	0	1883	19	0
53	Lg	871	0	953	5	0
54	LF	1835	0	1926	19	0
55	Lf	868	0	892	9	0
56	LE	1721	0	1839	22	0
57	Le	1044	0	1132	6	0
58	LD	2354	0	2345	21	0
59	Ld	840	0	859	8	0
60	LC	2862	0	3036	19	0
61	Lc	760	0	793	6	0
62	LB	3174	0	3294	27	0
63	Lb	815	0	869	13	0
64	LA	1899	0	1983	20	0
65	La	1157	0	1190	14	0
66	L7	2542	0	1284	14	0
67	Pt	1645	0	844	15	0
68	Sa	775	0	813	10	0
69	L8	3256	0	1652	30	0
70	L5	73960	0	37478	514	0
71	SZ	383	0	313	7	0
72	ST	837	0	694	3	0
73	SP	806	0	652	3	0
74	S2	33557	0	16987	250	0
75	SG	1663	0	1701	25	0
76	SI	1648	0	1700	28	0
77	S6	1263	0	647	15	0
78	SS	903	0	728	7	0
79	mR	152	0	77	2	0
80	SU	795	0	862	13	0
81	Lg	1	0	0	0	0
81	Lm	1	0	0	0	0
81	Lo	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	Lp	1	0	0	0	0
81	Sd	1	0	0	0	0
82	L5	60	0	0	0	0
82	L8	1	0	0	0	0
82	LB	1	0	0	0	0
82	LC	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	11	0	0	0	0
82	SQ	1	0	0	0	0
83	L5	81	0	0	0	0
83	L7	5	0	0	0	0
83	L8	3	0	0	0	0
83	LB	1	0	0	0	0
83	LI	2	0	0	0	0
83	LM	1	0	0	0	0
83	LP	1	0	0	0	0
83	LS	1	0	0	0	0
83	LV	1	0	0	0	0
83	Le	1	0	0	0	0
83	Pt	1	0	0	0	0
83	S2	21	0	0	0	0
83	Sd	1	0	0	0	0
84	L5	46	0	0	0	0
84	LB	1	0	0	0	0
84	LN	1	0	0	0	0
84	Le	1	0	0	0	0
84	S2	12	0	0	0	0
85	L5	30	0	55	4	0
86	S2	36	0	37	0	0
87	L5	473	0	0	9	0
87	L7	9	0	0	0	0
87	L8	16	0	0	0	0
87	LA	4	0	0	0	0
87	LB	7	0	0	0	0
87	LC	1	0	0	0	0
87	LD	1	0	0	0	0
87	LF	3	0	0	0	0
87	LG	1	0	0	0	0
87	LH	1	0	0	0	0
87	LI	1	0	0	0	0
87	LL	2	0	0	0	0
87	LM	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LN	5	0	0	0	0
87	LP	3	0	0	0	0
87	LQ	3	0	0	0	0
87	LR	3	0	0	1	0
87	LS	5	0	0	0	0
87	LT	4	0	0	0	0
87	LV	2	0	0	0	0
87	LW	1	0	0	0	0
87	La	3	0	0	0	0
87	Lb	4	0	0	0	0
87	Lc	2	0	0	1	0
87	Le	3	0	0	0	0
87	Lg	3	0	0	0	0
87	Lh	2	0	0	0	0
87	Lj	2	0	0	0	0
87	Ll	2	0	0	0	0
87	Ln	2	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Pt	1	0	0	0	0
87	S2	101	0	0	1	0
87	SF	1	0	0	0	0
87	SI	5	0	0	0	0
87	SL	1	0	0	0	0
87	SN	3	0	0	0	0
87	SS	2	0	0	0	0
87	Sa	1	0	0	1	0
All	All	201487	0	144606	1404	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 4.

All (1404) 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)
70:L5:1100:U:H3	70:L5:1195:G:H1	1.22	0.87
74:S2:885:U:H3	74:S2:901:G:H1	1.21	0.85
70:L5:3634:G:H1	70:L5:3826:C:H5	1.31	0.77
52:LG:180:PRO:HG3	52:LG:223:ARG:HE	1.51	0.76
52:LG:249:ARG:NH2	70:L5:4075:U:OP1	2.19	0.76
49:Li:29:ARG:HH12	70:L5:276:C:H2'	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:4745:G:H1	70:L5:4955:A:H61	1.34	0.76
68:Sa:74:CYS:HB2	68:Sa:77:CYS:H	1.50	0.75
52:LG:40:GLY:HA3	70:L5:4116:C:H1'	1.68	0.75
76:SI:80:ASP:HB2	76:SI:94:LYS:HZ1	1.52	0.73
56:LE:72:LYS:HB2	63:Lb:119:CYS:HB2	1.71	0.72
74:S2:125:C:O3'	75:SG:195:LYS:NZ	2.22	0.72
70:L5:1804:A:H4'	70:L5:1805:A:H5"	1.72	0.72
45:Lk:70:LYS:NZ	70:L5:2714:G:OP1	2.23	0.72
58:LD:232:THR:HG22	58:LD:234:ASP:H	1.54	0.71
70:L5:512:U:H3	70:L5:647:G:H1	1.37	0.71
80:SU:20:ILE:HD11	80:SU:114:VAL:HG13	1.71	0.71
68:Sa:15:ARG:NH1	74:S2:993:G:N7	2.39	0.71
70:L5:2579:G:N2	70:L5:2582:A:OP2	2.23	0.71
58:LD:208:MET:HE2	58:LD:233:PRO:HG3	1.73	0.70
74:S2:535:G:H22	74:S2:551:U:H3	1.39	0.70
27:LZ:89:ILE:HD11	27:LZ:121:ARG:HG2	1.74	0.70
11:SN:64:ARG:NH2	74:S2:919:A:OP2	2.24	0.70
74:S2:878:G:O6	74:S2:908:A:N7	2.25	0.70
74:S2:191:A:H62	74:S2:208:G:H21	1.38	0.70
70:L5:4091:G:H1	70:L5:4158:C:H41	1.37	0.69
47:Lj:56:ARG:NH2	70:L5:374:G:OP2	2.24	0.69
54:LF:43:ARG:NH1	70:L5:1704:C:OP1	2.26	0.69
1:Lm:93:LYS:HG2	1:Lm:102:ARG:HG2	1.73	0.69
70:L5:4620:OMU:OP2	70:L5:4670:C:N4	2.25	0.69
77:S6:9:U:H2'	77:S6:46:G:H21	1.57	0.69
63:Lb:99:ILE:HD11	70:L5:1266:G:H5"	1.73	0.69
74:S2:928:G:H1	74:S2:1013:U:H3	1.41	0.69
56:LE:105:ARG:NH1	70:L5:469:C:O2	2.24	0.69
70:L5:704:C:N4	70:L5:707:C:OP2	2.26	0.69
54:LF:76:ARG:NH1	70:L5:730:G:OP2	2.26	0.69
74:S2:534:G:H22	74:S2:552:G:H1	1.42	0.68
50:LH:114:ILE:HB	50:LH:124:ARG:HG3	1.74	0.68
55:Lf:33:VAL:HG13	55:Lf:38:GLU:HB2	1.74	0.68
27:LZ:68:ILE:O	27:LZ:115:LYS:NZ	2.27	0.68
18:SE:137:PRO:HB2	18:SE:150:PRO:HD2	1.75	0.68
43:LM:41:PRO:HG3	43:LM:73:VAL:HG23	1.76	0.67
60:LC:163:LYS:HB2	60:LC:166:GLU:HG3	1.74	0.67
70:L5:2582:A:H8	70:L5:2681:G:H21	1.42	0.67
74:S2:1750:C:N4	74:S2:1784:G:N7	2.40	0.67
64:LA:215:ASN:ND2	70:L5:4546:A:N7	2.42	0.67
14:SJ:155:LYS:HG3	14:SJ:156:HIS:HD2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:LJ:41:GLU:HG3	46:LJ:48:PRO:HD3	1.77	0.67
64:LA:104:VAL:HA	64:LA:107:MET:HE2	1.77	0.67
54:LF:47:ARG:HH21	60:LC:330:PRO:HG3	1.60	0.66
52:LG:229:ARG:NH1	52:LG:232:GLU:OE2	2.28	0.66
70:L5:4090:G:H1	70:L5:4159:C:H5	1.42	0.66
74:S2:183:G:N7	74:S2:184:G:O2'	2.27	0.66
29:LX:139:ARG:NH1	70:L5:2533:C:OP1	2.28	0.66
69:L8:123:U:O2'	69:L8:125:C:OP1	2.14	0.66
70:L5:2094:G:N2	70:L5:2095:A:O2'	2.28	0.66
74:S2:925:G:H1	74:S2:1017:U:H3	1.44	0.66
14:SJ:26:ASP:OD1	14:SJ:30:LYS:NZ	2.29	0.66
44:LL:172:GLU:HG2	49:Li:2:ALA:HB1	1.78	0.66
52:LG:58:PRO:HD2	52:LG:61:ILE:HD12	1.77	0.65
72:ST:22:LEU:HG	72:ST:28:LEU:HD11	1.77	0.65
64:LA:36:GLU:HG3	64:LA:91:GLY:HA2	1.78	0.65
74:S2:981:A:H2'	74:S2:982:G:C8	2.32	0.65
14:SJ:18:ARG:NH1	74:S2:3:C:O2	2.30	0.64
70:L5:3717:A:H2'	70:L5:3718:A2M:H8	1.78	0.64
15:SH:106:ARG:O	74:S2:798:G:O2'	2.16	0.64
70:L5:1100:U:O2	70:L5:1195:G:N2	2.25	0.64
80:SU:38:ASP:OD1	80:SU:41:ARG:NH2	2.30	0.64
25:Sb:40:CYS:SG	25:Sb:41:TYR:N	2.70	0.64
14:SJ:38:ARG:NH1	74:S2:643:A:OP1	2.31	0.64
26:SA:33:GLN:HB3	26:SA:154:LEU:HD12	1.81	0.63
37:LQ:99:LYS:HE2	37:LQ:121:LEU:HD11	1.80	0.63
76:SI:67:TRP:NE1	76:SI:191:GLU:OE2	2.28	0.63
18:SE:100:ARG:HH12	18:SE:122:LYS:HA	1.64	0.63
70:L5:1203:G:H2'	70:L5:1204:C:H6	1.64	0.63
77:S6:64:U:H2'	77:S6:65:C:H6	1.64	0.63
59:Ld:24:GLU:HG3	59:Ld:87:ARG:HG3	1.81	0.63
21:Sd:52:PHE:HB3	80:SU:80:PHE:HB3	1.81	0.62
77:S6:10:G:H1'	77:S6:45:G:H2'	1.80	0.62
37:LQ:104:ARG:NH2	70:L5:1353:G:N7	2.47	0.62
61:Lc:34:THR:HG23	61:Lc:95:ALA:HB2	1.82	0.62
70:L5:4594:U:H2'	70:L5:4595:G:H8	1.65	0.62
32:LU:28:PRO:HB2	32:LU:34:MET:HG2	1.82	0.62
57:Le:98:GLU:OE2	70:L5:2324:C:O2'	2.17	0.62
70:L5:138:G:H2'	70:L5:139:G:H8	1.64	0.62
70:L5:1870:C:H2'	70:L5:1871:A2M:H8	1.80	0.62
70:L5:3689:G:O2'	70:L5:3818:U:OP2	2.16	0.62
16:Sg:238:ALA:HB3	16:Sg:251:ALA:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:LB:168:MET:HG3	62:LB:178:ALA:HA	1.82	0.62
70:L5:268:G:H2'	70:L5:269:G:H8	1.64	0.61
38:LP:16:LYS:HG2	38:LP:149:ILE:HG12	1.82	0.61
42:Ln:6:ARG:NH2	74:S2:1169:G:OP1	2.32	0.61
70:L5:4091:G:H22	70:L5:4158:C:H5	1.48	0.61
74:S2:1265:A:H8	74:S2:1326:U:H5	1.49	0.61
34:LS:70:LYS:NZ	70:L5:733:A:OP1	2.34	0.61
39:Lp:44:LYS:NZ	70:L5:2672:C:OP1	2.34	0.61
52:LG:159:HIS:HD2	52:LG:186:GLY:H	1.47	0.61
70:L5:2351:OMC:HM22	70:L5:2352:U:H5'	1.81	0.61
74:S2:1326:U:H1'	74:S2:1494:U:H5'	1.83	0.61
27:LZ:103:ASP:N	27:LZ:103:ASP:OD1	2.30	0.61
43:LM:46:ARG:NH1	70:L5:937:U:OP1	2.33	0.61
37:LQ:39:THR:HG22	37:LQ:41:SER:H	1.66	0.61
32:LU:46:ARG:HH21	32:LU:89:LYS:HD3	1.66	0.61
70:L5:3945:A:H2'	70:L5:3946:G:H8	1.65	0.60
77:S6:15:A:H61	77:S6:46:G:H1	1.49	0.60
74:S2:190:G:H5'	76:SI:145:ILE:HD13	1.83	0.60
74:S2:942:G:H2'	74:S2:943:U:C6	2.36	0.60
74:S2:1536:G:H2'	74:S2:1537:A:C8	2.36	0.60
77:S6:40:C:H2'	77:S6:41:C:C6	2.36	0.60
75:SG:32:MET:HG3	75:SG:100:CYS:HB2	1.82	0.60
20:SD:138:VAL:HG22	20:SD:184:ILE:HG22	1.84	0.60
70:L5:1833:G:O2'	70:L5:1835:G:N2	2.34	0.60
21:Sd:13:LYS:NZ	74:S2:1618:C:OP1	2.35	0.60
40:LO:47:PHE:HZ	40:LO:144:GLU:HG3	1.66	0.60
68:Sa:26:CYS:N	68:Sa:77:CYS:SG	2.74	0.60
74:S2:145:G:H2'	74:S2:146:G:C8	2.36	0.60
37:LQ:108:ARG:NH2	70:L5:1355:G:OP1	2.34	0.59
67:Pt:9:G:O2'	67:Pt:10:G:N7	2.30	0.59
70:L5:1399:G:H2'	70:L5:1400:G:C8	2.37	0.59
60:LC:62:THR:OG1	70:L5:375:G:OP1	2.19	0.59
63:Lb:101:HIS:O	63:Lb:109:ARG:NH1	2.34	0.59
24:SB:214:LYS:NZ	74:S2:943:U:OP1	2.35	0.59
62:LB:80:GLU:OE2	62:LB:328:ASN:ND2	2.33	0.59
77:S6:41:C:H2'	77:S6:42:A:C8	2.37	0.59
34:LS:95:ARG:NH2	34:LS:112:ASP:OD1	2.36	0.59
70:L5:2378:G:N2	70:L5:2381:A:OP2	2.35	0.59
35:LR:38:ARG:NH2	70:L5:2527:A:OP1	2.32	0.59
70:L5:3598:C:H2'	70:L5:3599:A:H8	1.66	0.59
6:SW:55:ASP:OD1	6:SW:55:ASP:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LI:38:ARG:NH2	48:LI:45:GLU:OE1	2.35	0.59
52:LG:117:ARG:HE	52:LG:121:LYS:HE2	1.68	0.59
58:LD:125:VAL:HG21	58:LD:200:MET:HE3	1.83	0.59
70:L5:369:G:N2	70:L5:372:A:OP2	2.31	0.59
74:S2:1140:G:HO2'	74:S2:1151:G:HO2'	1.51	0.59
74:S2:71:G:O6	75:SG:170:ARG:NH1	2.35	0.59
4:SY:9:THR:O	74:S2:835:C:N4	2.34	0.59
24:SB:138:PHE:O	24:SB:213:ARG:N	2.36	0.59
26:SA:50:ASN:HB3	26:SA:53:ARG:HG2	1.84	0.58
34:LS:173:ASN:ND2	34:LS:175:PHE:O	2.36	0.58
74:S2:874:G:H2'	74:S2:875:A:H8	1.68	0.58
58:LD:231:VAL:HA	58:LD:235:MET:HE1	1.84	0.58
70:L5:2809:G:O2'	70:L5:4644:G:OP1	2.22	0.58
30:LW:14:TYR:OH	62:LB:384:GLU:OE2	2.21	0.58
64:LA:208:GLU:OE1	70:L5:1629:G:N1	2.30	0.58
70:L5:740:G:H21	70:L5:741:C:H41	1.50	0.58
70:L5:1214:C:H5'	70:L5:1215:C:H5"	1.85	0.58
50:LH:92:MET:HG2	50:LH:179:ILE:HG22	1.84	0.58
74:S2:203:G:OP2	76:SI:143:LYS:NZ	2.32	0.58
1:Lm:100:TYR:O	70:L5:4472:G:O2'	2.20	0.58
15:SH:100:ILE:HG12	15:SH:125:VAL:HG11	1.84	0.58
70:L5:965:G:O2'	70:L5:2256:C:N3	2.34	0.58
70:L5:4634:U:O4	87:L5:5301:HOH:O	2.16	0.58
4:SY:27:VAL:HB	4:SY:69:THR:HG23	1.86	0.58
33:LT:108:ARG:NH2	70:L5:1802:A:O2'	2.37	0.58
62:LB:242:ARG:NH2	70:L5:2856:C:O2	2.35	0.58
58:LD:50:ARG:NH1	58:LD:72:ASP:OD2	2.31	0.58
66:L7:23:A:N3	66:L7:118:C:O2'	2.33	0.58
75:SG:154:ARG:HH21	75:SG:179:LEU:HD21	1.68	0.58
61:Lc:48:LEU:HD11	61:Lc:60:ILE:HG21	1.85	0.58
70:L5:3722:G:H2'	70:L5:3723:A:H8	1.69	0.58
19:Se:111:GLN:O	19:Se:115:ARG:HG2	2.04	0.58
26:SA:36:GLN:O	26:SA:53:ARG:NH1	2.36	0.58
74:S2:1536:G:H2'	74:S2:1537:A:H8	1.68	0.58
74:S2:1265:A:O2'	74:S2:1327:G:OP2	2.19	0.58
80:SU:20:ILE:HG21	80:SU:97:ILE:HD11	1.85	0.58
7:SV:15:ARG:NH1	22:SC:83:LEU:O	2.37	0.57
55:Lf:45:LYS:HD2	55:Lf:105:LEU:HA	1.86	0.57
70:L5:1202:C:H2'	70:L5:1203:G:H8	1.69	0.57
70:L5:5021:C:N4	87:L5:5333:HOH:O	2.33	0.57
62:LB:173:LEU:HD22	62:LB:342:LYS:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:1857:C:H2'	70:L5:1858:A:H8	1.69	0.57
74:S2:527:C:H2'	74:S2:528:A:H8	1.70	0.57
74:S2:1662:U:O4	74:S2:1663:A:N6	2.37	0.57
11:SN:55:ARG:HD3	74:S2:1017:U:H5'	1.86	0.57
53:Lg:83:CYS:SG	53:Lg:86:CYS:HB2	2.44	0.57
38:LP:116:HIS:HB3	38:LP:149:ILE:HB	1.85	0.57
64:LA:123:ARG:NH1	70:L5:4083:U:OP1	2.38	0.57
70:L5:220:C:H5	70:L5:237:G:H1	1.51	0.57
70:L5:1245:C:H2'	70:L5:1246:G:H8	1.70	0.57
80:SU:18:HIS:O	80:SU:18:HIS:ND1	2.32	0.57
22:SC:67:GLY:HA2	22:SC:93:ILE:HD11	1.87	0.57
22:SC:211:LYS:O	22:SC:215:MET:HG2	2.05	0.57
33:LT:75:VAL:HG12	33:LT:88:ARG:HG2	1.87	0.57
44:LL:39:ARG:NH2	70:L5:1362:G:OP1	2.37	0.57
62:LB:103:LYS:NZ	70:L5:4725:C:OP1	2.38	0.57
70:L5:2611:A:H5'	70:L5:2688:G:H4'	1.87	0.57
74:S2:168:C:O2'	75:SG:133:LEU:O	2.22	0.57
48:LI:30:LYS:HG3	48:LI:66:GLU:HG3	1.86	0.57
74:S2:381:C:OP2	76:SI:54:LYS:NZ	2.38	0.57
16:Sg:23:THR:HG21	16:Sg:31:ILE:HA	1.86	0.56
45:Lk:36:VAL:HG23	45:Lk:43:TYR:HB2	1.87	0.56
64:LA:107:MET:HE1	64:LA:113:VAL:HG11	1.87	0.56
29:LX:42:THR:HG21	52:LG:48:LYS:HG3	1.86	0.56
70:L5:268:G:H2'	70:L5:269:G:C8	2.40	0.56
15:SH:119:SER:O	74:S2:913:A:N6	2.37	0.56
43:LM:46:ARG:NH1	70:L5:935:A:O2'	2.38	0.56
44:LL:129:ARG:NH2	70:L5:173:C:O5'	2.38	0.56
54:LF:131:ASN:ND2	70:L5:1727:U:OP1	2.37	0.56
56:LE:161:ARG:O	56:LE:182:ASN:ND2	2.38	0.56
60:LC:53:ALA:O	69:L8:26:C:O2'	2.23	0.56
70:L5:1754:U:H3	70:L5:1776:A:H61	1.53	0.56
74:S2:928:G:H2'	74:S2:929:G:C8	2.39	0.56
2:Ll:2:SER:N	70:L5:2407:G:O6	2.39	0.56
7:SV:58:ALA:O	7:SV:62:MET:HG3	2.05	0.56
28:LY:74:TYR:OH	69:L8:75:OMG:OP2	2.24	0.56
70:L5:1480:C:O2'	70:L5:1482:G:OP2	2.23	0.56
58:LD:157:ASN:HB3	58:LD:159:VAL:HG22	1.86	0.56
70:L5:4173:G:H2'	70:L5:4174:U:C6	2.40	0.56
70:L5:4993:G:H22	70:L5:5058:A:H2	1.53	0.56
37:LQ:68:ARG:HA	37:LQ:71:LYS:HE3	1.87	0.56
43:LM:81:ASP:OD2	43:LM:84:THR:OG1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:L8:126:C:H42	70:L5:2543:A:H4'	1.69	0.56
74:S2:165:G:OP2	74:S2:165:G:N2	2.33	0.56
31:LV:15:ARG:HB2	70:L5:4618:OMG:H5"	1.87	0.56
62:LB:168:MET:HA	62:LB:171:LEU:HD12	1.87	0.56
65:La:47:LYS:NZ	70:L5:1684:A:OP1	2.38	0.56
67:Pt:16:C:H5'	67:Pt:60:A:H2	1.70	0.56
70:L5:711:A:H2'	70:L5:712:C:C6	2.41	0.56
74:S2:1609:C:O2	74:S2:1610:G:N1	2.39	0.56
24:SB:146:ARG:HB2	24:SB:149:GLN:HG3	1.87	0.56
62:LB:213:GLN:NE2	62:LB:285:TYR:O	2.39	0.56
74:S2:797:C:O2'	74:S2:798:G:O4'	2.20	0.56
4:SY:10:ARG:NH2	4:SY:26:ASP:OD1	2.36	0.56
26:SA:77:ILE:HG13	26:SA:122:LEU:HD11	1.88	0.56
35:LR:64:ARG:NH2	70:L5:2633:U:OP1	2.38	0.56
58:LD:116:ASP:OD1	58:LD:116:ASP:N	2.39	0.56
70:L5:4939:C:H5"	70:L5:4940:C:H5'	1.87	0.56
74:S2:1244:PSU:H2'	74:S2:1245:G:H8	1.71	0.56
74:S2:1742:C:H5	74:S2:1792:G:H1	1.52	0.56
26:SA:42:LYS:HD3	26:SA:46:ILE:HG23	1.86	0.55
44:LL:127:PHE:O	51:Lh:117:ARG:NH2	2.34	0.55
56:LE:139:LYS:O	56:LE:191:GLN:NE2	2.35	0.55
27:LZ:100:VAL:HG13	27:LZ:106:LEU:HB3	1.88	0.55
31:LV:115:SER:O	31:LV:135:ASN:ND2	2.38	0.55
41:LN:116:LEU:HD22	41:LN:135:ILE:HD11	1.88	0.55
60:LC:182:LYS:HE3	70:L5:2300:A:H5"	1.88	0.55
62:LB:126:LYS:NZ	70:L5:4966:A:OP2	2.38	0.55
70:L5:1377:G:H21	70:L5:1380:G:H5'	1.71	0.55
70:L5:4274:A:H2'	70:L5:4275:G:C8	2.41	0.55
74:S2:1228:A:H2'	74:S2:1229:G:C8	2.40	0.55
4:SY:105:LYS:NZ	74:S2:52:G:O2'	2.36	0.55
7:SV:41:LYS:HD2	26:SA:5:LEU:HD11	1.87	0.55
40:LO:106:ASP:O	70:L5:4910:G:N2	2.40	0.55
76:SI:142:SER:O	76:SI:146:GLN:HB2	2.06	0.55
41:LN:73:ARG:NH1	41:LN:88:GLY:O	2.40	0.55
41:LN:182:HIS:NE2	70:L5:291:U:O2'	2.33	0.55
56:LE:119:GLU:HG3	57:Le:7:LEU:HD11	1.88	0.55
70:L5:1273:G:H2'	70:L5:1274:A:C8	2.41	0.55
30:LW:1:MET:HE2	62:LB:71:GLU:HB2	1.89	0.55
70:L5:67:C:OP2	70:L5:312:G:N2	2.40	0.55
70:L5:1094:G:H2'	70:L5:1095:A:H8	1.72	0.55
7:SV:32:ILE:HG12	7:SV:60:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LH:12:ILE:HD12	50:LH:53:LYS:HB3	1.89	0.55
54:LF:243:LEU:HD11	54:LF:247:MET:HE3	1.89	0.55
70:L5:1441:C:H2'	70:L5:1442:C:H6	1.72	0.55
4:SY:14:THR:HG23	4:SY:21:LYS:HG2	1.89	0.55
7:SV:3:ASN:HA	22:SC:173:LYS:HG2	1.89	0.55
10:SO:34:PHE:HB3	10:SO:41:PHE:HB2	1.89	0.55
36:Lr:112:ARG:NH1	56:LE:117:PRO:O	2.38	0.55
70:L5:450:G:H1	70:L5:1297:U:H3	1.55	0.55
74:S2:1354:G:N2	74:S2:1357:A:OP2	2.31	0.55
10:SO:50:LYS:O	74:S2:975:G:N2	2.35	0.54
10:SO:56:VAL:HG13	10:SO:60:MET:HE2	1.88	0.54
69:L8:67:U:H2'	69:L8:68:G:H8	1.71	0.54
74:S2:885:U:O2	74:S2:901:G:N2	2.31	0.54
23:Sc:12:ALA:HB1	23:Sc:32:VAL:HB	1.89	0.54
29:LX:93:ASN:ND2	70:L5:2532:C:O2'	2.33	0.54
33:LT:111:GLU:O	33:LT:115:LYS:HG2	2.08	0.54
53:Lg:41:ALA:O	53:Lg:52:ARG:NH1	2.39	0.54
74:S2:1533:A:H2	74:S2:1536:G:N3	2.05	0.54
77:S6:64:U:H2'	77:S6:65:C:C6	2.43	0.54
22:SC:183:LYS:HG2	22:SC:196:ILE:HG12	1.88	0.54
38:LP:37:LYS:NZ	70:L5:425:U:OP1	2.40	0.54
70:L5:2745:A:H2'	70:L5:2746:A:C8	2.42	0.54
73:SP:131:PRO:O	74:S2:1236:G:O2'	2.22	0.54
14:SJ:79:ARG:NH2	74:S2:819:G:OP1	2.40	0.54
8:SR:5:ARG:NH2	74:S2:1455:A:OP1	2.41	0.54
17:SF:125:SER:HB2	17:SF:136:ARG:HH21	1.73	0.54
56:LE:46:ARG:O	56:LE:65:ARG:NH1	2.40	0.54
67:Pt:72:C:H2'	67:Pt:73:A:H8	1.73	0.54
2:Ll:23:ILE:HD12	2:Ll:27:ILE:HD11	1.90	0.54
41:LN:14:LYS:HE2	70:L5:280:G:H5"	1.90	0.54
65:La:26:ARG:NH1	70:L5:1655:C:OP2	2.41	0.54
67:Pt:62:C:H2'	67:Pt:63:C:H6	1.73	0.54
70:L5:2745:A:H2'	70:L5:2746:A:H8	1.73	0.54
74:S2:1490:OMG:N2	80:SU:72:GLU:OE1	2.39	0.54
70:L5:662:C:H2'	70:L5:663:G:H8	1.71	0.54
70:L5:4694:G:N2	70:L5:4694:G:OP1	2.41	0.54
36:Lr:90:LEU:HD22	36:Lr:111:ILE:HG23	1.89	0.54
54:LF:94:ARG:NH1	54:LF:114:LEU:O	2.39	0.54
63:Lb:36:ASP:OD1	70:L5:4314:C:O2'	2.25	0.54
70:L5:4924:C:O2	70:L5:4926:C:N4	2.28	0.54
74:S2:527:C:H2'	74:S2:528:A:C8	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:S2:1253:A:OP2	74:S2:1526:G:N2	2.37	0.54
54:LF:46:ARG:NH1	70:L5:1704:C:O3'	2.41	0.54
70:L5:4734:A:H2'	70:L5:4735:G:C8	2.43	0.53
56:LE:46:ARG:NH2	70:L5:1070:G:O6	2.42	0.53
64:LA:68:ARG:HH11	64:LA:70:LYS:HD2	1.72	0.53
70:L5:2588:C:OP1	70:L5:2768:C:O2'	2.20	0.53
76:SI:150:ASP:HA	76:SI:153:LYS:HG2	1.90	0.53
14:SJ:18:ARG:NH2	74:S2:4:C:O2'	2.38	0.53
59:Ld:46:LEU:HD13	70:L5:2373:C:H5'	1.90	0.53
70:L5:2362:U:H2'	70:L5:2363:A2M:H8	1.89	0.53
70:L5:3598:C:H2'	70:L5:3599:A:C8	2.44	0.53
74:S2:163:U:OP2	75:SG:87:ARG:NH2	2.40	0.53
79:mR:34:A:H2'	79:mR:35:A:H8	1.72	0.53
29:LX:105:ASN:ND2	29:LX:108:GLN:OE1	2.42	0.53
70:L5:660:A:O2'	70:L5:661:C:H5'	2.09	0.53
33:LT:61:THR:HG21	70:L5:1799:G:H21	1.72	0.53
70:L5:4736:C:H2'	70:L5:4737:G:H8	1.74	0.53
18:SE:45:ILE:HB	18:SE:80:ILE:HG23	1.91	0.53
20:SD:161:GLY:HA3	74:S2:1388:A:H61	1.73	0.53
70:L5:4173:G:H2'	70:L5:4174:U:H6	1.73	0.53
56:LE:123:ARG:HG2	70:L5:959:G:C8	2.44	0.53
70:L5:691:C:H2'	70:L5:692:A:C8	2.44	0.53
70:L5:2902:G:O4'	70:L5:3596:A:N6	2.41	0.53
74:S2:1521:C:OP2	78:SS:136:THR:OG1	2.22	0.53
76:SI:121:LEU:HD21	76:SI:158:ILE:HD11	1.91	0.53
66:L7:12:U:OP2	66:L7:67:C:O2'	2.27	0.53
3:Lo:36:GLN:OE1	3:Lo:40:ARG:NH2	2.40	0.53
4:SY:108:LYS:NZ	74:S2:506:G:OP1	2.42	0.53
17:SF:67:PRO:HG2	17:SF:70:GLU:HB2	1.90	0.53
30:LW:47:ARG:HH12	30:LW:54:LEU:HD13	1.73	0.53
70:L5:93:G:H2'	70:L5:94:A:C8	2.44	0.53
70:L5:921:C:H2'	70:L5:922:C:H6	1.73	0.53
70:L5:2866:C:O2'	70:L5:2867:C:O5'	2.21	0.53
74:S2:1228:A:H2'	74:S2:1229:G:H8	1.73	0.53
63:Lb:122:LYS:HA	70:L5:1242:G:H4'	1.89	0.53
27:LZ:14:LEU:HB3	53:Lg:88:ARG:HG3	1.91	0.52
40:LO:34:VAL:HG12	40:LO:103:LYS:HB2	1.90	0.52
65:La:76:ASP:HB3	65:La:115:GLY:HA3	1.92	0.52
70:L5:4449:A:N6	87:L5:5379:HOH:O	2.43	0.52
74:S2:104:A:OP1	76:SI:12:ARG:NH1	2.42	0.52
18:SE:44:LEU:HD13	18:SE:82:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:LL:74:ARG:NH1	70:L5:76:A:OP2	2.42	0.52
62:LB:58:ARG:NH1	62:LB:361:GLU:OE2	2.39	0.52
74:S2:25:A:HO2'	74:S2:26:U:H6	1.56	0.52
39:Lp:38:THR:HA	39:Lp:45:THR:HA	1.91	0.52
53:Lg:90:ARG:NH2	70:L5:4123:C:OP1	2.43	0.52
69:L8:144:U:H2'	69:L8:145:C:C6	2.45	0.52
74:S2:520:A:O2'	74:S2:825:A:N3	2.37	0.52
24:SB:168:MET:HE2	24:SB:197:ILE:HG21	1.92	0.52
47:Lj:63:ARG:NH2	69:L8:58:G:O6	2.42	0.52
50:LH:19:THR:HB	50:LH:26:ILE:HG12	1.90	0.52
70:L5:1252:C:O2	70:L5:1254:A:N6	2.42	0.52
11:SN:120:SER:OG	74:S2:677:G:OP1	2.27	0.52
17:SF:73:THR:HG21	17:SF:90:VAL:HG12	1.92	0.52
58:LD:33:ARG:NH1	66:L7:7:G:OP1	2.42	0.52
34:LS:151:LYS:HG3	43:LM:8:GLU:HB3	1.92	0.52
60:LC:262:GLU:HB3	60:LC:273:LEU:HG	1.92	0.52
70:L5:908:G:H2'	70:L5:909:A:H8	1.75	0.52
70:L5:1479:G:H2'	70:L5:1480:C:C6	2.44	0.52
70:L5:4608:G:O2'	70:L5:4609:G:O5'	2.27	0.52
12:SL:79:LYS:HB2	12:SL:87:VAL:HG22	1.91	0.52
34:LS:95:ARG:NH1	70:L5:1951:G:O2'	2.39	0.52
49:Li:25:ARG:HH21	70:L5:159:C:H5'	1.75	0.52
56:LE:69:TYR:HA	56:LE:72:LYS:HE3	1.92	0.52
70:L5:2658:G:O2'	70:L5:2675:G:N2	2.43	0.52
70:L5:3684:G:H2'	70:L5:3685:C:C6	2.45	0.52
70:L5:3945:A:H2'	70:L5:3946:G:C8	2.45	0.52
74:S2:1447:G:H5'	80:SU:29:VAL:HG11	1.92	0.52
3:Lo:9:ARG:NH1	70:L5:4290:U:OP1	2.43	0.52
70:L5:4860:G:H2'	70:L5:4861:G:H8	1.74	0.52
74:S2:1401:A:H4'	80:SU:52:GLY:HA3	1.90	0.52
10:SO:100:THR:HG21	10:SO:104:ARG:HE	1.75	0.52
62:LB:154:LYS:HG3	62:LB:194:LEU:HD12	1.91	0.52
70:L5:963:G:O6	70:L5:2095:A:N1	2.43	0.52
70:L5:1604:G:H2'	70:L5:1605:G:C8	2.45	0.52
70:L5:1772:C:H2'	70:L5:1773:U:C6	2.45	0.52
73:SP:38:SER:OG	73:SP:41:GLN:OE1	2.27	0.52
6:SW:6:VAL:HG13	6:SW:29:PRO:HD2	1.91	0.51
20:SD:176:LEU:HD13	74:S2:1499:U:H4'	1.92	0.51
35:LR:133:LYS:NZ	87:LR:201:HOH:O	2.42	0.51
50:LH:128:MET:HE2	50:LH:134:CYS:HB2	1.92	0.51
67:Pt:72:C:H2'	67:Pt:73:A:C8	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:2736:G:N7	87:L5:5342:HOH:O	2.34	0.51
70:L5:4115:G:H8	70:L5:4116:C:H5	1.58	0.51
74:S2:534:G:H22	74:S2:552:G:H22	1.57	0.51
75:SG:132:ARG:HG2	75:SG:133:LEU:HG	1.91	0.51
41:LN:60:VAL:HG22	41:LN:134:LEU:HB2	1.92	0.51
61:Lc:106:ARG:NH2	87:Lc:202:HOH:O	2.43	0.51
70:L5:1326:A2M:OP2	70:L5:4445:U:O2'	2.28	0.51
70:L5:2029:A:H2'	70:L5:2030:A:C8	2.45	0.51
70:L5:3700:C:O2'	70:L5:3774:A:N3	2.39	0.51
70:L5:3823:G:C6	85:L5:5102:SPD:H42	2.45	0.51
74:S2:433:A:H5"	76:SI:22:HIS:HB3	1.92	0.51
76:SI:144:LYS:O	76:SI:147:LYS:HG3	2.10	0.51
80:SU:50:VAL:HG22	80:SU:91:LEU:HG	1.92	0.51
14:SJ:107:GLU:HA	14:SJ:112:THR:HG21	1.92	0.51
27:LZ:9:LYS:NZ	27:LZ:83:THR:O	2.43	0.51
74:S2:184:G:H5'	74:S2:185:G:C8	2.46	0.51
75:SG:5:ILE:HD12	75:SG:124:LEU:HD11	1.91	0.51
22:SC:178:HIS:ND1	22:SC:221:ASP:OD2	2.43	0.51
29:LX:40:ILE:HD12	52:LG:50:ASP:HB2	1.91	0.51
58:LD:90:VAL:HG21	58:LD:231:VAL:HG21	1.92	0.51
70:L5:4188:U:H2'	70:L5:4189:U:C6	2.45	0.51
74:S2:312:G:H1	74:S2:337:C:H5	1.57	0.51
74:S2:582:U:H2'	74:S2:583:A:H8	1.75	0.51
74:S2:948:C:H2'	74:S2:949:G:H8	1.76	0.51
51:Lh:10:ARG:NH2	51:Lh:63:GLN:OE1	2.44	0.51
70:L5:1441:C:H2'	70:L5:1442:C:C6	2.45	0.51
70:L5:2407:G:OP2	70:L5:2407:G:N2	2.41	0.51
70:L5:4594:U:H2'	70:L5:4595:G:C8	2.44	0.51
74:S2:107:A:H2'	74:S2:108:G:C8	2.46	0.51
19:Se:114:ARG:NH2	74:S2:639:C:OP1	2.44	0.51
60:LC:321:ASN:OD1	70:L5:1280:C:O2'	2.22	0.51
70:L5:1718:C:H2'	70:L5:1719:A:C4	2.46	0.51
74:S2:528:A:H2'	74:S2:529:A:C8	2.46	0.51
51:Lh:66:LYS:HG2	69:L8:96:C:H5"	1.93	0.51
70:L5:4750:G:H2'	70:L5:4751:G:C8	2.45	0.51
28:LY:54:GLU:HB2	28:LY:108:ARG:HB2	1.93	0.51
70:L5:1094:G:H2'	70:L5:1095:A:C8	2.46	0.51
74:S2:534:G:N2	74:S2:552:G:H22	2.08	0.51
74:S2:1279:C:H2'	74:S2:1280:G:H8	1.76	0.51
70:L5:1703:C:OP2	70:L5:1704:C:N4	2.44	0.51
70:L5:2601:A:N6	70:L5:2744:A:OP2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:3736:A:H2'	70:L5:3737:A:C8	2.46	0.51
18:SE:199:GLU:OE2	18:SE:209:HIS:NE2	2.43	0.50
24:SB:122:GLU:HG2	24:SB:140:VAL:HG23	1.93	0.50
26:SA:59:LEU:HD22	26:SA:181:GLU:HG2	1.93	0.50
56:LE:73:TYR:OH	70:L5:982:U:OP1	2.24	0.50
70:L5:163:A:H2'	70:L5:164:G:H8	1.76	0.50
70:L5:1576:G:O2'	70:L5:1578:U:O2	2.20	0.50
70:L5:4541:G:N2	70:L5:4544:A:OP2	2.37	0.50
22:SC:187:ARG:NH2	22:SC:189:GLY:O	2.43	0.50
33:LT:17:ARG:HG2	70:L5:4277:G:H5"	1.93	0.50
40:LO:49:ARG:NH1	70:L5:1930:U:OP2	2.37	0.50
54:LF:105:VAL:HG13	54:LF:136:VAL:HG12	1.93	0.50
70:L5:3717:A:H2'	70:L5:3718:A2M:C8	2.40	0.50
4:SY:57:VAL:HB	4:SY:60:PHE:HE1	1.75	0.50
8:SR:101:ASP:OD2	26:SA:40:LYS:NZ	2.44	0.50
18:SE:43:PRO:HD2	18:SE:46:ILE:HD12	1.94	0.50
30:LW:9:SER:HA	30:LW:52:THR:HG23	1.92	0.50
70:L5:2411:C:H2'	70:L5:2412:A:H8	1.75	0.50
70:L5:3880:G:H2'	70:L5:3881:G:C8	2.46	0.50
2:Ll:42:ARG:HG3	2:Ll:47:THR:HG23	1.93	0.50
54:LF:57:TYR:OH	54:LF:189:ASP:OD1	2.22	0.50
56:LE:243:THR:HG22	56:LE:245:GLN:H	1.75	0.50
67:Pt:39:A:O2'	74:S2:1058:A:OP1	2.28	0.50
70:L5:1548:G:O2'	70:L5:2812:A:N3	2.40	0.50
74:S2:17:C:O2'	74:S2:1194:A:N1	2.43	0.50
74:S2:1220:A:N3	74:S2:1677:U:O2'	2.43	0.50
74:S2:1714:U:H2'	74:S2:1715:A:C8	2.46	0.50
17:SF:126:THR:OG1	23:Sc:26:GLN:NE2	2.40	0.50
48:LI:207:ASP:OD1	48:LI:210:ARG:NH1	2.43	0.50
70:L5:1933:G:H2'	70:L5:1934:A:C8	2.47	0.50
70:L5:3692:A:OP2	85:L5:5102:SPD:N10	2.42	0.50
70:L5:5047:C:O2'	70:L5:5050:C:OP2	2.27	0.50
73:SP:45:LEU:HD21	73:SP:84:ILE:HD11	1.94	0.50
74:S2:640:A:H2'	74:S2:641:A:C8	2.47	0.50
74:S2:1144:A:H2'	74:S2:1145:A:C8	2.47	0.50
12:SL:125:ILE:HG13	12:SL:146:THR:HB	1.94	0.50
55:Lf:107:PRO:HA	56:LE:192[A]:LYS:HG2	1.94	0.50
70:L5:2411:C:H2'	70:L5:2412:A:C8	2.47	0.50
7:SV:16:LYS:NZ	22:SC:257:LYS:O	2.35	0.50
51:Lh:5:LYS:NZ	69:L8:87:G:OP1	2.39	0.50
61:Lc:18:LEU:O	61:Lc:22:MET:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:163:A:H2'	70:L5:164:G:C8	2.46	0.50
70:L5:1396:G:HO2'	70:L5:1468:C:HO2'	1.57	0.50
70:L5:2765:A:H2'	70:L5:2766:A:C8	2.47	0.50
74:S2:28:U:H2'	74:S2:29:G:H8	1.77	0.50
74:S2:1588:A:H2'	74:S2:1589:A:C8	2.47	0.50
15:SH:51:ILE:HG23	15:SH:179:LYS:HD3	1.93	0.50
29:LX:87:MET:HE1	29:LX:155:ILE:HG22	1.94	0.50
63:Lb:55:LYS:HA	63:Lb:58:GLN:HG3	1.94	0.50
66:L7:103:A:O2'	70:L5:1741:G:O6	2.27	0.50
74:S2:553:U:H2'	74:S2:554:A:C8	2.47	0.50
59:Ld:20:VAL:HA	59:Ld:90:ARG:O	2.12	0.50
74:S2:191:A:H62	74:S2:208:G:N2	2.07	0.50
74:S2:377:G:H5'	76:SI:98:LYS:HB3	1.93	0.50
74:S2:607:U:O2'	74:S2:630:U:O4'	2.30	0.50
75:SG:38:ALA:HB2	75:SG:50:VAL:HG13	1.94	0.50
39:Lp:63:THR:H	64:LA:84:THR:HG22	1.76	0.49
70:L5:679:C:H2'	70:L5:680:G:H8	1.77	0.49
70:L5:2497:C:H2'	70:L5:2498:C:H6	1.77	0.49
74:S2:51:U:H2'	74:S2:52:G:C8	2.47	0.49
74:S2:472:C:O2'	74:S2:474:G:OP1	2.23	0.49
4:SY:12:PHE:HZ	4:SY:21:LYS:HD2	1.77	0.49
5:SX:61:GLN:O	5:SX:62:HIS:ND1	2.45	0.49
70:L5:4745:G:H1	70:L5:4955:A:N6	2.07	0.49
6:SW:6:VAL:HG12	6:SW:34:ILE:HD11	1.94	0.49
48:LI:66:GLU:OE2	48:LI:69:ARG:NH1	2.35	0.49
54:LF:241:ASN:O	54:LF:245:ARG:HG2	2.13	0.49
70:L5:2467:U:H4'	70:L5:2468:U:H5'	1.93	0.49
70:L5:3710:G:O2'	70:L5:3713:U:O4	2.31	0.49
70:L5:5068:G:N2	70:L5:5069:U:O4	2.36	0.49
74:S2:77:A:H2	75:SG:175:LYS:HG3	1.77	0.49
11:SN:83:ASP:OD1	11:SN:83:ASP:N	2.42	0.49
12:SL:111:VAL:HG12	12:SL:140:PHE:HB2	1.92	0.49
62:LB:385:LYS:NZ	70:L5:5002:U:OP2	2.39	0.49
70:L5:1339:U:H2'	70:L5:1340:OMC:C6	2.47	0.49
70:L5:1558:A:H2'	70:L5:1559:G:C8	2.48	0.49
70:L5:4093:G:O2'	70:L5:4094:G:H8	1.95	0.49
70:L5:4861:G:H2'	70:L5:4862:G:H8	1.76	0.49
70:L5:4991:U:H2'	70:L5:4992:G:C8	2.46	0.49
74:S2:416:U:HO2'	74:S2:652:U:HO2'	1.58	0.49
76:SI:113:TYR:CG	76:SI:121:LEU:HD12	2.48	0.49
5:SX:123:VAL:HG12	5:SX:124:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LY:27:ARG:CZ	69:L8:70:G:H5”	2.43	0.49
52:LG:159:HIS:CD2	52:LG:186:GLY:H	2.29	0.49
65:La:13:GLY:HA2	70:L5:1660:U:H3’	1.94	0.49
70:L5:963:G:N2	87:L5:5390:HOH:O	2.46	0.49
70:L5:4504:C:H2’	70:L5:4505:C:C6	2.47	0.49
74:S2:494:C:N4	74:S2:509:OMG:HN22	2.11	0.49
10:SO:135:ILE:O	74:S2:943:U:O2’	2.29	0.49
43:LM:70:GLN:HA	43:LM:73:VAL:HG22	1.95	0.49
60:LC:60:HIS:HA	60:LC:92:PHE:HE1	1.77	0.49
65:La:132:ARG:NH1	70:L5:1468:C:OP1	2.45	0.49
70:L5:689:U:H2’	70:L5:690:C:C6	2.48	0.49
70:L5:2848:G:O2’	70:L5:3838:U:O4	2.24	0.49
74:S2:588:G:OP2	74:S2:588:G:N2	2.45	0.49
74:S2:851:C:H5”	74:S2:852:G:H5’	1.94	0.49
76:SI:37:LYS:HE3	76:SI:93:THR:HG22	1.95	0.49
1:Lm:82:LEU:HB3	50:LH:95:VAL:HG22	1.93	0.49
13:SK:31:LYS:HA	13:SK:41:PRO:HA	1.93	0.49
18:SE:172:PHE:HE2	18:SE:174:LYS:HE3	1.77	0.49
44:LL:129:ARG:HD3	51:Lh:117:ARG:HD2	1.93	0.49
70:L5:920:C:H2’	70:L5:921:C:H6	1.78	0.49
70:L5:4591:U:H2’	70:L5:4592:C:C6	2.48	0.49
74:S2:562:U:H2’	74:S2:563:G:C8	2.48	0.49
27:LZ:24:VAL:HG21	27:LZ:87:VAL:HG12	1.93	0.49
33:LT:45:MET:HE3	33:LT:47:THR:HB	1.95	0.49
52:LG:46:GLN:OE1	52:LG:49:ARG:NH1	2.46	0.49
56:LE:162:VAL:HG12	56:LE:177:GLY:HA2	1.95	0.49
62:LB:246:ARG:NH1	70:L5:4558:U:OP2	2.43	0.49
74:S2:484:A2M:O5’	74:S2:484:A2M:H8	2.13	0.49
31:LV:48:ARG:NH1	70:L5:4621:C:OP1	2.38	0.49
51:Lh:46:LYS:HE2	69:L8:80:A:H1’	1.95	0.49
69:L8:16:G:H22	70:L5:417:G:H2’	1.78	0.49
70:L5:1617:G:H1’	70:L5:2513:A:N6	2.28	0.49
70:L5:4921:C:H2’	70:L5:4922:C:H6	1.78	0.49
9:SQ:140:ARG:HB2	74:S2:1644:C:H4’	1.95	0.49
41:LN:5:LYS:O	41:LN:9:GLU:HG2	2.13	0.49
46:LJ:78:LYS:O	46:LJ:82:ILE:HG12	2.13	0.49
55:Lf:50:VAL:HG22	55:Lf:69:VAL:HG22	1.95	0.49
68:Sa:13:LYS:O	68:Sa:15:ARG:NH2	2.46	0.49
70:L5:1273:G:H2’	70:L5:1274:A:H8	1.78	0.49
35:LR:138:LEU:O	35:LR:142:ILE:HG12	2.13	0.48
47:Lj:57:ASN:O	47:Lj:57:ASN:ND2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LI:36:LEU:HD12	48:LI:69:ARG:HE	1.77	0.48
48:LI:46:PHE:HB2	48:LI:139:ARG:HD2	1.93	0.48
70:L5:4903:G:H2'	70:L5:4904:G:H8	1.78	0.48
45:Lk:34:PHE:HE2	45:Lk:56:LEU:HB3	1.77	0.48
50:LH:93:ARG:NH2	50:LH:141:LYS:O	2.46	0.48
60:LC:235:LEU:HD22	60:LC:240:LEU:HD11	1.95	0.48
62:LB:302:ASN:OD1	62:LB:314:ILE:N	2.45	0.48
74:S2:1203:G:H2'	74:S2:1204:A:C8	2.47	0.48
74:S2:1786:U:H2'	74:S2:1787:G:H8	1.78	0.48
11:SN:5:HIS:HB2	11:SN:121:ARG:HH21	1.79	0.48
14:SJ:58:ARG:HD3	22:SC:199:PRO:HG2	1.94	0.48
45:Lk:26:LYS:HG2	45:Lk:69:LEU:HD12	1.95	0.48
46:LJ:146:ARG:HH21	46:LJ:147:ARG:HH12	1.61	0.48
70:L5:2520:C:H2'	70:L5:2521:G:H8	1.79	0.48
70:L5:4537:C:H2'	70:L5:4538:G:C8	2.48	0.48
45:Lk:29:LYS:H	45:Lk:29:LYS:HD2	1.79	0.48
70:L5:2318:G:N2	70:L5:2321:G:OP2	2.30	0.48
74:S2:559:G:O2'	74:S2:560:A:O5'	2.28	0.48
26:SA:85:ARG:NH1	26:SA:203:PHE:O	2.46	0.48
47:Lj:20:ARG:NH2	69:L8:109:C:O2'	2.36	0.48
70:L5:3861:A:H2'	70:L5:3862:A:C8	2.48	0.48
26:SA:206:ASP:N	26:SA:206:ASP:OD1	2.44	0.48
43:LM:92:ALA:HA	43:LM:95:ILE:HG12	1.95	0.48
55:Lf:43:LEU:O	55:Lf:109:ARG:NH1	2.46	0.48
34:LS:88:SER:HB2	48:LI:162:ARG:HH12	1.78	0.48
52:LG:37:LYS:NZ	70:L5:4126:C:OP1	2.39	0.48
64:LA:234:LYS:HG2	64:LA:238:ILE:HG12	1.96	0.48
70:L5:1942:A:H2'	70:L5:1943:A:C8	2.49	0.48
70:L5:3723:A:H2'	70:L5:3724:A:H8	1.77	0.48
74:S2:627:OMU:H5"	74:S2:627:OMU:H6	1.94	0.48
74:S2:964:A:H2'	74:S2:965:U:H6	1.79	0.48
74:S2:1414:A:H2'	74:S2:1415:C:H6	1.78	0.48
26:SA:137:ALA:HB1	26:SA:142:LEU:HB3	1.96	0.48
34:LS:99:ASP:OD1	34:LS:100:LEU:N	2.46	0.48
70:L5:4521:PSU:OP2	87:L5:5302:HOH:O	2.20	0.48
74:S2:1098:C:H2'	74:S2:1099:G:C8	2.48	0.48
17:SF:159:ARG:NH1	74:S2:1535:U:O4	2.45	0.48
26:SA:37:TYR:OH	26:SA:57:LYS:NZ	2.43	0.48
32:LU:29:VAL:HG11	32:LU:36:ALA:HB2	1.96	0.48
42:Ln:24:ARG:HH12	70:L5:2872:C:H5"	1.79	0.48
56:LE:112:MET:HE1	70:L5:2261:G:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Le:10:PRO:HD2	57:Le:69:MET:HE1	1.96	0.48
59:Ld:36:VAL:HG21	59:Ld:44:ARG:HG2	1.95	0.48
69:L8:141:C:C2	69:L8:142:U:C5	3.01	0.48
70:L5:2543:A:H2	70:L5:2773:G:H22	1.60	0.48
74:S2:1323:U:H2'	74:S2:1324:G:C8	2.49	0.48
50:LH:26:ILE:HG22	50:LH:35:ARG:HG2	1.96	0.48
70:L5:3722:G:H2'	70:L5:3723:A:C8	2.48	0.48
77:S6:10:G:OP2	77:S6:14:C:N4	2.46	0.48
4:SY:10:ARG:HG3	4:SY:24:VAL:HG23	1.96	0.47
61:Lc:37:MET:SD	61:Lc:42:LYS:NZ	2.87	0.47
63:Lb:22:LYS:HD2	63:Lb:25:ARG:HH22	1.79	0.47
64:LA:101:VAL:HG22	64:LA:165:VAL:HG22	1.96	0.47
70:L5:956:A:O2'	70:L5:2077:C:OP1	2.30	0.47
70:L5:1204:C:H2'	70:L5:1205:G:H8	1.78	0.47
71:SZ:69:THR:H	71:SZ:72:VAL:HG22	1.79	0.47
14:SJ:93:LYS:HG2	14:SJ:95:ASP:H	1.80	0.47
27:LZ:83:THR:HG22	27:LZ:85:TYR:H	1.79	0.47
41:LN:108:ARG:HB2	41:LN:161:MET:HE1	1.96	0.47
65:La:35:ALA:HB1	70:L5:39:A:H5"	1.96	0.47
68:Sa:6:ARG:NH1	74:S2:1147:C:OP1	2.47	0.47
69:L8:67:U:H2'	69:L8:68:G:C8	2.48	0.47
74:S2:448:A:H5"	76:SI:25:ARG:HA	1.95	0.47
74:S2:867:OMG:HM23	74:S2:867:OMG:H1'	1.55	0.47
74:S2:1401:A:H2'	74:S2:1402:A:C8	2.48	0.47
31:LV:83:ARG:NH1	31:LV:100:ASP:OD1	2.47	0.47
52:LG:95:LEU:HD11	52:LG:156:VAL:HG21	1.96	0.47
57:Le:67:LYS:O	57:Le:75:ARG:NH2	2.46	0.47
67:Pt:63:C:H2'	67:Pt:64:G:H8	1.79	0.47
69:L8:75:OMG:H1'	69:L8:75:OMG:HM23	1.65	0.47
70:L5:1811:G:H2'	70:L5:1812:C:H6	1.79	0.47
70:L5:4238:G:H2'	70:L5:4239:A:H8	1.80	0.47
74:S2:901:G:H2'	74:S2:902:G:C8	2.49	0.47
74:S2:1719:A:N6	74:S2:1814:G:O2'	2.47	0.47
12:SL:84:ARG:HE	12:SL:115:PRO:HG3	1.78	0.47
14:SJ:155:LYS:HG3	14:SJ:156:HIS:CD2	2.47	0.47
32:LU:47:ILE:HD11	32:LU:56:LEU:HG	1.95	0.47
33:LT:133:ALA:HB3	54:LF:127:LYS:HB2	1.96	0.47
44:LL:60:ARG:NH2	44:LL:68:THR:O	2.47	0.47
70:L5:1332:C:H2'	70:L5:1333:A:H8	1.78	0.47
70:L5:4750:G:H2'	70:L5:4751:G:H8	1.80	0.47
70:L5:4967:A:H2'	70:L5:4968:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:S2:833:C:H2'	74:S2:834:C:C6	2.50	0.47
76:SI:157:LYS:HB3	76:SI:157:LYS:HE3	1.69	0.47
27:LZ:120:GLU:HG2	27:LZ:123:LYS:HE2	1.96	0.47
44:LL:42:LYS:HE3	44:LL:46:ILE:HD13	1.97	0.47
62:LB:224:LYS:HG2	62:LB:340:THR:HB	1.95	0.47
70:L5:3861:A:H2'	70:L5:3862:A:H8	1.79	0.47
74:S2:206:G:H2'	74:S2:207:G:H8	1.79	0.47
74:S2:533:A:H2'	74:S2:534:G:C8	2.48	0.47
75:SG:181:THR:H	75:SG:184:VAL:HG22	1.79	0.47
9:SQ:19:ALA:HB2	9:SQ:75:GLY:HA3	1.96	0.47
24:SB:142:PHE:HD1	24:SB:209:ASP:HB2	1.80	0.47
70:L5:271:C:H2'	70:L5:272:U:C6	2.49	0.47
70:L5:514:U:H5	70:L5:647:G:H21	1.61	0.47
70:L5:908:G:H2'	70:L5:909:A:C8	2.49	0.47
70:L5:4537:C:H2'	70:L5:4538:G:H8	1.79	0.47
7:SV:51:LYS:HG3	7:SV:78:ILE:HD11	1.96	0.47
12:SL:33:LEU:HD12	12:SL:34:PRO:HD2	1.97	0.47
14:SJ:54:ARG:NH1	22:SC:200:ARG:O	2.38	0.47
14:SJ:137:VAL:HG12	14:SJ:138:ARG:HG3	1.96	0.47
18:SE:143:ASP:OD1	18:SE:143:ASP:N	2.44	0.47
29:LX:70:LYS:NZ	69:L8:60:G:OP1	2.46	0.47
40:LO:140:ARG:O	40:LO:144:GLU:HG2	2.15	0.47
64:LA:245:ARG:NH1	70:L5:3657:U:OP1	2.47	0.47
66:L7:63:C:H5'	66:L7:64:G:H5"	1.97	0.47
68:Sa:40:VAL:HG11	68:Sa:42:ARG:HH11	1.80	0.47
70:L5:1271:G:OP2	70:L5:1271:G:N2	2.38	0.47
70:L5:1758:G:N2	70:L5:1773:U:O2	2.48	0.47
70:L5:4174:U:H2'	70:L5:4175:G:H8	1.80	0.47
70:L5:4608:G:O2'	70:L5:4609:G:H8	1.98	0.47
70:L5:4967:A:H2'	70:L5:4968:A:C8	2.50	0.47
74:S2:78:C:OP1	75:SG:159:ARG:NH2	2.41	0.47
74:S2:656:G:N2	74:S2:663:C:H5"	2.30	0.47
76:SI:57:ALA:HB2	76:SI:183:GLY:HA2	1.95	0.47
34:LS:69:GLU:HB2	34:LS:101:THR:HG23	1.95	0.47
70:L5:1846:G:H2'	70:L5:1847:C:C6	2.50	0.47
70:L5:2368:A:N6	70:L5:2827:G:O2'	2.47	0.47
74:S2:17:C:H2'	74:S2:18:C:C6	2.50	0.47
74:S2:1611:G:H8	74:S2:1612:G:C8	2.32	0.47
74:S2:1797:U:H2'	74:S2:1798:C:C6	2.49	0.47
5:SX:68:LYS:HD2	5:SX:91:LEU:HD22	1.96	0.47
8:SR:105:MET:O	8:SR:109:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SK:25:LYS:NZ	74:S2:1497:G:O6	2.47	0.47
41:LN:202:ARG:NH2	70:L5:1372:A:OP1	2.48	0.47
59:Ld:39:LYS:NZ	70:L5:2370:A:N7	2.55	0.47
62:LB:56:ILE:HD13	62:LB:365:LEU:HD22	1.97	0.47
70:L5:4991:U:H2'	70:L5:4992:G:H8	1.79	0.47
74:S2:1505:U:H4'	74:S2:1508:A:H1'	1.97	0.47
45:Lk:17:ARG:NH2	45:Lk:19:ASP:OD2	2.48	0.47
50:LH:111:LEU:HD21	50:LH:125:ARG:HG2	1.96	0.47
44:LL:36:ARG:NH1	70:L5:1366:G:OP2	2.44	0.46
60:LC:350:ARG:HD2	70:L5:724:C:OP1	2.15	0.46
63:Lb:95:ARG:O	63:Lb:99:ILE:HG12	2.14	0.46
67:Pt:20:G:H3'	67:Pt:21:H2U:H52	1.96	0.46
70:L5:162:A:H2'	70:L5:163:A:C8	2.50	0.46
70:L5:654:C:H2'	70:L5:655:C:C6	2.50	0.46
70:L5:2091:C:O2	70:L5:2094:G:O2'	2.22	0.46
74:S2:1562:C:H2'	74:S2:1563:G:H8	1.79	0.46
76:SI:4:SER:OG	76:SI:6:ASP:OD2	2.27	0.46
69:L8:148:A:H2'	69:L8:149:G:C8	2.51	0.46
70:L5:4740:G:C4	70:L5:4742:G:H1'	2.50	0.46
74:S2:5:U:H2'	74:S2:6:G:H8	1.80	0.46
74:S2:211:G:H2'	74:S2:212:C:C6	2.50	0.46
74:S2:212:C:H2'	74:S2:213:G:C8	2.51	0.46
74:S2:1808:U:H2'	74:S2:1809:A:C8	2.51	0.46
2:Ll:16:LYS:HD2	2:Ll:49:LEU:HD22	1.97	0.46
37:LQ:89:ASP:HB3	37:LQ:92:VAL:HG12	1.98	0.46
55:Lf:38:GLU:OE1	56:LE:285:LYS:NZ	2.49	0.46
56:LE:95:PRO:HA	56:LE:104:THR:HA	1.96	0.46
58:LD:122:GLN:O	58:LD:248:ARG:NH2	2.48	0.46
70:L5:382:G:N1	70:L5:385:A:OP2	2.40	0.46
70:L5:1307:A:H2'	70:L5:1308:C:C6	2.50	0.46
70:L5:2092:G:H4'	70:L5:2093:A:H5"	1.97	0.46
70:L5:2539:C:H2'	70:L5:2540:C:C6	2.50	0.46
58:LD:52:ILE:HD13	66:L7:6:C:H4'	1.96	0.46
70:L5:162:A:H2'	70:L5:163:A:H8	1.80	0.46
70:L5:1203:G:H2'	70:L5:1204:C:C6	2.45	0.46
76:SI:148:LYS:O	76:SI:151:GLU:HG3	2.16	0.46
60:LC:157:LYS:HE2	60:LC:157:LYS:HB3	1.73	0.46
70:L5:1754:U:H2'	70:L5:1755:C:C5	2.50	0.46
74:S2:455:A:H2'	74:S2:456:C:C6	2.51	0.46
48:LI:55:ASP:HB2	48:LI:162:ARG:O	2.16	0.46
60:LC:218:ILE:HA	60:LC:229:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Sa:74:CYS:SG	87:Sa:201:HOH:O	2.60	0.46
70:L5:4219:A:H2'	70:L5:4220:6MZ:C8	2.46	0.46
74:S2:12:U:H2'	74:S2:13:C:C6	2.51	0.46
74:S2:1804:OMU:H1'	74:S2:1804:OMU:HM23	1.69	0.46
2:Ll:21:ARG:O	2:Ll:38:ASN:ND2	2.49	0.46
22:SC:275:LYS:HD2	22:SC:276:THR:HG23	1.97	0.46
36:Lr:97:ILE:HD13	36:Lr:107:ARG:HA	1.98	0.46
64:LA:40:TYR:OH	70:L5:4117:U:O2'	2.16	0.46
70:L5:2529:A:O2'	70:L5:2531:C:OP2	2.33	0.46
8:SR:74:GLN:HA	8:SR:77:GLU:HG3	1.97	0.46
21:Sd:10:HIS:NE2	74:S2:1261:C:O2	2.35	0.46
49:Li:76:ARG:HA	49:Li:76:ARG:HD3	1.75	0.46
50:LH:165:THR:HG21	50:LH:179:ILE:HG13	1.97	0.46
62:LB:200:ARG:HA	62:LB:200:ARG:HD3	1.72	0.46
65:La:89:ASN:HA	65:La:92:LYS:HG2	1.97	0.46
65:La:91:ALA:HB2	65:La:120:GLN:HE21	1.81	0.46
70:L5:3873:G:H2'	70:L5:3874:G:C8	2.51	0.46
70:L5:4069:U:H2'	70:L5:4070:U:C6	2.51	0.46
70:L5:5027:C:H4'	70:L5:5028:G:H5'	1.97	0.46
74:S2:1403:C:H41	74:S2:1404:U:H5	1.63	0.46
77:S6:71:C:H2'	77:S6:72:U:H6	1.81	0.46
7:SV:41:LYS:HE2	7:SV:41:LYS:HB3	1.87	0.46
50:LH:71:ARG:HH11	70:L5:4691:A:H5'	1.80	0.46
52:LG:122:ALA:HA	52:LG:126:GLY:HA2	1.97	0.46
58:LD:193:GLU:O	58:LD:197:LYS:HG2	2.15	0.46
66:L7:38:U:N3	66:L7:41:G:OP2	2.39	0.46
70:L5:3917:A:H2'	70:L5:3918:G:H8	1.80	0.46
71:SZ:79:ILE:HB	71:SZ:83:LEU:HD23	1.97	0.46
75:SG:32:MET:HE2	75:SG:65:GLN:HB2	1.98	0.46
18:SE:100:ARG:HB2	18:SE:114:ILE:HD13	1.98	0.46
40:LO:176:ARG:HD2	70:L5:4769:G:H5"	1.97	0.46
48:LI:193:ASP:OD1	48:LI:193:ASP:N	2.49	0.46
64:LA:147:ARG:HG3	64:LA:157:VAL:HG22	1.98	0.46
70:L5:3664:G:H2'	70:L5:3665:G:H8	1.81	0.46
10:SO:134:PRO:HB3	74:S2:944:A:H5"	1.98	0.45
32:LU:40:GLU:O	32:LU:44:GLN:NE2	2.46	0.45
36:Lr:67:ARG:NH2	70:L5:666:G:OP2	2.49	0.45
54:LF:184:ILE:HG23	54:LF:189:ASP:HB3	1.98	0.45
60:LC:94:ASN:ND2	87:L5:5359:HOH:O	2.47	0.45
61:Lc:28:VAL:HG21	61:Lc:37:MET:HG3	1.97	0.45
70:L5:3893:C:H2'	70:L5:3894:A:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:S2:1798:C:H2'	74:S2:1799:G:O4'	2.16	0.45
36:Lr:6:GLN:O	36:Lr:10:VAL:HG22	2.15	0.45
70:L5:444:G:H2'	70:L5:445:U:C6	2.51	0.45
70:L5:699:C:H2'	70:L5:700:G:H8	1.81	0.45
70:L5:907:C:H2'	70:L5:908:G:H8	1.80	0.45
70:L5:3893:C:H2'	70:L5:3894:A:H8	1.80	0.45
2:Ll:23:ILE:HG23	2:Ll:38:ASN:HB2	1.98	0.45
37:LQ:38:ARG:NH1	70:L5:2088:A:OP1	2.50	0.45
40:LO:193:THR:HG22	40:LO:197:LYS:HD3	1.99	0.45
48:LI:188:LYS:HD3	48:LI:212:LEU:HG	1.98	0.45
69:L8:46:G:O2'	69:L8:61:A:N1	2.48	0.45
70:L5:1202:C:H2'	70:L5:1203:G:C8	2.51	0.45
74:S2:96:C:O2	74:S2:473:A:O2'	2.33	0.45
74:S2:848:U:H2'	74:S2:849:A:H8	1.82	0.45
74:S2:1801:A:H2'	74:S2:1802:C:C6	2.52	0.45
8:SR:116:ASN:OD1	8:SR:116:ASN:N	2.40	0.45
17:SF:166:ILE:HG12	74:S2:1599:U:C5	2.52	0.45
20:SD:12:VAL:O	20:SD:16:ILE:HG12	2.16	0.45
20:SD:172:VAL:O	20:SD:173:ARG:NE	2.50	0.45
32:LU:80:LYS:HG2	32:LU:110:TYR:CE2	2.51	0.45
37:LQ:72:LEU:HB2	37:LQ:75:ARG:HD2	1.99	0.45
64:LA:109:GLU:CD	64:LA:109:GLU:H	2.24	0.45
67:Pt:19:G:N2	67:Pt:59:A:O5'	2.49	0.45
74:S2:367:U:H4'	74:S2:371:A:C8	2.52	0.45
74:S2:1740:C:H2'	74:S2:1741:U:C6	2.50	0.45
76:SI:48:VAL:HG11	76:SI:54:LYS:HG3	1.98	0.45
17:SF:71:ARG:NH2	17:SF:148:ASN:OD1	2.50	0.45
38:LP:14:SER:HB3	38:LP:151:THR:HG22	1.98	0.45
52:LG:200:THR:OG1	70:L5:150:U:OP2	2.32	0.45
62:LB:216:MET:HE3	62:LB:283:LYS:HB2	1.98	0.45
62:LB:241:PRO:HD3	70:L5:4456:OMC:HM21	1.99	0.45
70:L5:1662:C:H2'	70:L5:1663:C:C6	2.51	0.45
70:L5:4238:G:H2'	70:L5:4239:A:C8	2.52	0.45
70:L5:4608:G:HO2'	70:L5:4609:G:H8	1.61	0.45
70:L5:4906:C:H2'	70:L5:4907:G:H8	1.81	0.45
74:S2:1007:C:H2'	74:S2:1008:A:C8	2.52	0.45
74:S2:1226:G:N1	74:S2:1639:G7M:OP2	2.39	0.45
24:SB:69:VAL:HG11	24:SB:74:LEU:HD13	1.97	0.45
26:SA:25:LEU:HB3	26:SA:46:ILE:HD11	1.98	0.45
46:LJ:40:LEU:HD12	46:LJ:40:LEU:HA	1.80	0.45
54:LF:182:TYR:HB3	54:LF:200:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:La:84:GLU:O	65:La:88:VAL:HG22	2.16	0.45
70:L5:4861:G:H2'	70:L5:4862:G:C8	2.52	0.45
77:S6:30:G:H2'	77:S6:31:G:C8	2.52	0.45
20:SD:137:VAL:HG13	20:SD:185:LYS:HB2	1.98	0.45
29:LX:72:ASP:OD1	29:LX:72:ASP:N	2.48	0.45
32:LU:101:ARG:HG2	32:LU:113:ARG:HG3	1.99	0.45
65:La:75:LEU:HB3	65:La:117:LEU:HD13	1.99	0.45
70:L5:3707:U:H2'	70:L5:3708:C:C6	2.51	0.45
70:L5:4260:U:H2'	70:L5:4261:C:H6	1.82	0.45
70:L5:4458:C:H2'	70:L5:4459:U:C6	2.52	0.45
70:L5:4584:A:H2'	70:L5:4585:U:O4'	2.16	0.45
70:L5:4908:G:N2	70:L5:4913:G:OP1	2.50	0.45
74:S2:511:U:H2'	74:S2:512:A2M:H8	1.99	0.45
10:SO:49:GLY:O	74:S2:975:G:O2'	2.31	0.45
21:Sd:21:CYS:HB3	21:Sd:26:ASN:H	1.81	0.45
40:LO:10:ASP:OD2	40:LO:37:ARG:NH2	2.48	0.45
70:L5:2498:C:H2'	70:L5:2499:C:H6	1.81	0.45
70:L5:4252:C:OP2	70:L5:4253:A:O2'	2.29	0.45
70:L5:4575:G:N2	87:L5:5402:HOH:O	2.48	0.45
74:S2:934:G:H22	74:S2:1008:A:H2	1.65	0.45
74:S2:1244:PSU:H2'	74:S2:1245:G:C8	2.51	0.45
74:S2:1667:U:H2'	74:S2:1668:U:C6	2.52	0.45
9:SQ:47:LEU:HA	17:SF:49:LEU:HD11	1.98	0.45
16:Sg:251:ALA:HA	16:Sg:256:ILE:HA	1.98	0.45
46:LJ:119:TYR:CZ	46:LJ:121:PRO:HA	2.52	0.45
54:LF:200:ARG:HD2	54:LF:203:GLU:OE1	2.17	0.45
70:L5:676:C:H2'	70:L5:677:G:H8	1.82	0.45
70:L5:1320:U:O2'	70:L5:1891:A:N1	2.47	0.45
70:L5:4992:G:H2'	70:L5:4993:G:C8	2.51	0.45
74:S2:656:G:H5'	74:S2:662:G:N2	2.31	0.45
74:S2:1025:U:OP1	74:S2:1090:C:O2'	2.33	0.45
24:SB:146:ARG:NE	74:S2:1122:A:N3	2.65	0.45
33:LT:104:SER:HA	33:LT:107:LYS:HE3	1.99	0.45
41:LN:6:TYR:HD2	49:Li:44:ILE:HD11	1.82	0.45
43:LM:114:LYS:HD2	70:L5:4929:C:H5"	1.99	0.45
46:LJ:56:THR:HG22	46:LJ:64:ARG:N	2.32	0.45
53:Lg:100:GLN:HA	53:Lg:103:VAL:HG22	1.99	0.45
54:LF:34:ARG:HD2	70:L5:1272:C:H5'	1.98	0.45
59:Ld:65:ASP:OD2	59:Ld:67:ARG:NH1	2.50	0.45
69:L8:17:A:H61	70:L5:417:G:H1'	1.82	0.45
70:L5:138:G:H2'	70:L5:139:G:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:325:U:H2'	70:L5:326:C:C6	2.51	0.45
70:L5:460:C:H2'	70:L5:461:G:H8	1.82	0.45
70:L5:2811:G:N1	70:L5:2814:C:OP2	2.45	0.45
70:L5:4089:G:H2'	70:L5:4090:G:C8	2.52	0.45
70:L5:4239:A:H2'	70:L5:4240:G:C8	2.52	0.45
70:L5:4274:A:H2'	70:L5:4275:G:H8	1.80	0.45
74:S2:952:G:H2'	74:S2:953:C:C6	2.52	0.45
79:mR:34:A:H2'	79:mR:35:A:C8	2.50	0.45
35:LR:4:LEU:HD22	35:LR:7:GLN:HG3	1.97	0.44
70:L5:2724:G:O2'	70:L5:2726:G:OP2	2.35	0.44
70:L5:2744:A:H2'	70:L5:2745:A:C8	2.52	0.44
70:L5:4623:OMG:H1'	70:L5:4623:OMG:HM23	1.68	0.44
71:SZ:66:LYS:O	71:SZ:110:THR:OG1	2.28	0.44
71:SZ:73:VAL:HG23	71:SZ:84:ALA:HB1	1.99	0.44
74:S2:1568:C:H2'	74:S2:1569:A:C8	2.52	0.44
6:SW:111:MET:HE1	6:SW:119:LYS:HE2	1.98	0.44
12:SL:128:VAL:HG12	12:SL:142:VAL:HA	1.98	0.44
26:SA:77:ILE:HD13	26:SA:99:ILE:HB	2.00	0.44
27:LZ:95:VAL:HG21	27:LZ:109:LYS:HG2	1.98	0.44
45:Lk:37:ARG:HD3	45:Lk:38:CYS:O	2.17	0.44
69:L8:9:A:H2'	69:L8:10:G:H8	1.82	0.44
70:L5:956:A:H1'	70:L5:2076:G:H5"	1.98	0.44
70:L5:1082:C:H2'	70:L5:1083:U:O4'	2.17	0.44
70:L5:2519:U:O2'	70:L5:2530:U:O2	2.35	0.44
70:L5:2845:A:H61	70:L5:3843:C:H42	1.65	0.44
70:L5:3692:A:N7	85:L5:5102:SPD:H82	2.32	0.44
70:L5:3871:A:H2'	70:L5:3872:A:C8	2.52	0.44
75:SG:20:ASP:OD1	75:SG:23:LYS:N	2.40	0.44
78:SS:16:LEU:HB3	78:SS:17:ASN:H	1.58	0.44
62:LB:165:HIS:HB3	62:LB:180:LEU:HD12	1.99	0.44
66:L7:82:G:H2'	66:L7:83:A:C8	2.53	0.44
70:L5:3641:U:OP2	70:L5:3646:A:N6	2.44	0.44
74:S2:116:OMU:H6	74:S2:116:OMU:O5'	2.17	0.44
74:S2:1101:U:H2'	74:S2:1102:G:C8	2.52	0.44
76:SI:67:TRP:HA	76:SI:189:VAL:HG22	2.00	0.44
77:S6:69:U:H2'	77:S6:70:G:H8	1.83	0.44
6:SW:37:PHE:HD1	6:SW:41:MET:HE2	1.82	0.44
9:SQ:17:LYS:HE3	74:S2:1648:G:N7	2.33	0.44
21:Sd:39:CYS:HB2	21:Sd:42:CYS:SG	2.58	0.44
32:LU:69:LYS:HE2	32:LU:69:LYS:HB3	1.84	0.44
37:LQ:90:VAL:HG13	65:La:80:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:LM:40:GLY:HA3	43:LM:45:VAL:HB	1.99	0.44
47:Lj:49:TRP:O	70:L5:1646:A:O2'	2.35	0.44
48:LI:40:LYS:HB3	48:LI:40:LYS:HE2	1.80	0.44
58:LD:184:ASP:OD2	58:LD:187:SER:OG	2.35	0.44
70:L5:1186:U:H2'	70:L5:1187:G:N3	2.33	0.44
70:L5:3599:A:H2'	70:L5:3600:G:H8	1.82	0.44
70:L5:4620:OMU:H1'	70:L5:4620:OMU:HM23	1.65	0.44
10:SO:145:GLY:O	68:Sa:22:ARG:NH2	2.50	0.44
30:LW:52:THR:HG22	30:LW:54:LEU:H	1.83	0.44
50:LH:4:ILE:HG12	50:LH:61:TRP:CH2	2.53	0.44
50:LH:85:THR:HG22	50:LH:86:LEU:HD13	2.00	0.44
66:L7:110:G:H2'	66:L7:111:C:C6	2.53	0.44
70:L5:1332:C:H2'	70:L5:1333:A:C8	2.52	0.44
70:L5:3710:G:H1'	70:L5:3712:A:N6	2.32	0.44
74:S2:17:C:H2'	74:S2:18:C:H6	1.82	0.44
4:SY:60:PHE:O	74:S2:571:U:O2'	2.32	0.44
6:SW:107:SER:HB3	74:S2:860:G:H21	1.83	0.44
46:LJ:44:THR:HG21	46:LJ:72:CYS:SG	2.58	0.44
54:LF:66:ARG:NH2	70:L5:1210:C:O2'	2.51	0.44
64:LA:30:ARG:HG3	64:LA:74:GLU:HG2	1.99	0.44
70:L5:456:C:H2'	70:L5:457:G:C8	2.53	0.44
70:L5:2640:G:H2'	70:L5:2641:A:C8	2.52	0.44
70:L5:4723:A:H2'	70:L5:4724:A:C8	2.53	0.44
74:S2:1030:A:H2'	74:S2:1031:A2M:H8	2.00	0.44
26:SA:131:HIS:O	26:SA:135:THR:HG23	2.18	0.44
41:LN:24:ARG:NH2	41:LN:123:GLU:O	2.50	0.44
46:LJ:52:LYS:HE3	46:LJ:52:LYS:HB3	1.84	0.44
50:LH:64:ARG:NH2	70:L5:4693:C:OP1	2.47	0.44
52:LG:48:LYS:HA	52:LG:48:LYS:HD2	1.74	0.44
62:LB:194:LEU:HD23	62:LB:194:LEU:HA	1.84	0.44
70:L5:4905:C:H2'	70:L5:4906:C:H6	1.83	0.44
70:L5:4959:U:H2'	70:L5:4960:G:C8	2.53	0.44
74:S2:453:C:O2'	75:SG:92:ARG:O	2.28	0.44
80:SU:39:LEU:HD13	80:SU:89:ILE:HD12	1.99	0.44
24:SB:34:LYS:O	24:SB:98:THR:OG1	2.35	0.44
24:SB:131:ASP:OD1	24:SB:131:ASP:N	2.50	0.44
32:LU:101:ARG:NH2	70:L5:2623:A:OP1	2.49	0.44
34:LS:32:ILE:HG21	34:LS:40:ALA:HA	2.00	0.44
49:Li:51:ALA:HB3	49:Li:54:GLU:HG3	1.99	0.44
70:L5:456:C:H2'	70:L5:457:G:H8	1.83	0.44
70:L5:3880:G:N7	87:L5:5351:HOH:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:4260:U:H2'	70:L5:4261:C:C6	2.52	0.44
3:Lo:59:LYS:NZ	70:L5:4371:G:OP1	2.50	0.44
18:SE:182:MET:HE2	18:SE:228:ILE:HD13	1.99	0.44
45:Lk:33:LYS:HG2	45:Lk:46:VAL:HG22	1.99	0.44
58:LD:233:PRO:HA	58:LD:236:MET:HE3	2.00	0.44
62:LB:90:VAL:HG13	62:LB:161:ARG:HB2	1.99	0.44
70:L5:1308:C:H2'	70:L5:1309:C:C6	2.53	0.44
70:L5:4905:C:H2'	70:L5:4906:C:C6	2.52	0.44
74:S2:118:C:H1'	74:S2:445:A:C5	2.52	0.44
74:S2:1101:U:H2'	74:S2:1102:G:H8	1.83	0.44
74:S2:1113:A:H2'	74:S2:1114:U:C6	2.53	0.44
16:Sg:59:LEU:HD22	16:Sg:95:GLY:HA2	1.99	0.43
24:SB:142:PHE:CD1	24:SB:209:ASP:HB2	2.53	0.43
41:LN:15:GLN:NE2	70:L5:305:A:OP2	2.49	0.43
46:LJ:56:THR:HG22	46:LJ:64:ARG:H	1.83	0.43
57:Le:33:ARG:NH1	70:L5:1303:A:N7	2.66	0.43
64:LA:104:VAL:N	64:LA:162:ASN:O	2.45	0.43
70:L5:2483:G:H2'	70:L5:2484:A:C8	2.53	0.43
74:S2:115:U:H2'	74:S2:116:OMU:C6	2.48	0.43
74:S2:215:G:H2'	74:S2:216:C:H6	1.82	0.43
74:S2:380:G:OP2	76:SI:56:ARG:NH2	2.48	0.43
4:SY:11:LYS:HB2	4:SY:24:VAL:HG22	2.00	0.43
27:LZ:57:MET:HB3	27:LZ:61:LYS:HB3	1.99	0.43
40:LO:54:TYR:OH	40:LO:73:PHE:O	2.31	0.43
45:Lk:57:LYS:HE2	45:Lk:57:LYS:HB2	1.81	0.43
51:Lh:118:LYS:HB2	51:Lh:118:LYS:HE3	1.79	0.43
70:L5:676:C:H2'	70:L5:677:G:C8	2.52	0.43
70:L5:733:A:H2'	70:L5:734:G:O4'	2.18	0.43
70:L5:1415:G:H2'	70:L5:1416:G:C8	2.53	0.43
70:L5:1416:G:H2'	70:L5:1417:C:C6	2.53	0.43
70:L5:1558:A:H2'	70:L5:1559:G:H8	1.83	0.43
70:L5:2815:A2M:H2'	70:L5:2816:G:C8	2.53	0.43
70:L5:3925:OMU:HM23	70:L5:3925:OMU:H1'	1.72	0.43
74:S2:1324:G:O2'	74:S2:1510:G:O2'	2.34	0.43
74:S2:1725:U:H2'	74:S2:1726:G:H8	1.83	0.43
12:SL:3:ASP:N	12:SL:3:ASP:OD1	2.51	0.43
21:Sd:22:ARG:HB3	21:Sd:38:MET:HG2	1.99	0.43
35:LR:105:LEU:HD12	35:LR:135:LYS:HE3	1.99	0.43
40:LO:181:ALA:O	40:LO:185:VAL:HG22	2.18	0.43
46:LJ:108:GLY:HA3	70:L5:4251:A:H5"	1.99	0.43
47:Lj:46:LYS:HB2	47:Lj:46:LYS:HE3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Lf:104:MET:HG2	55:Lf:106:TYR:CZ	2.53	0.43
67:Pt:25:U:O2'	70:L5:3770:PSU:OP1	2.36	0.43
70:L5:2257:C:O2'	70:L5:2259:G:OP1	2.27	0.43
70:L5:2654:C:H2'	70:L5:2655:C:H6	1.82	0.43
74:S2:1057:C:O2'	74:S2:1059:G:N7	2.46	0.43
34:LS:147:ASP:O	70:L5:748:G:N2	2.51	0.43
44:LL:174:LYS:O	65:La:138:LYS:NZ	2.39	0.43
65:La:79:TRP:HH2	65:La:99:PRO:HG2	1.83	0.43
74:S2:1025:U:H2'	74:S2:1026:C:O4'	2.19	0.43
12:SL:98:LYS:HG3	74:S2:421:G:H5'	1.99	0.43
31:LV:21:PRO:HA	31:LV:54:ALA:HA	2.01	0.43
40:LO:174:LEU:HD13	40:LO:174:LEU:HA	1.83	0.43
54:LF:238:ASP:OD1	54:LF:239:GLN:NE2	2.51	0.43
60:LC:336:ARG:HA	60:LC:339:THR:HG22	2.01	0.43
70:L5:1399:G:O2'	70:L5:1400:G:OP1	2.29	0.43
70:L5:1662:C:H2'	70:L5:1663:C:H6	1.82	0.43
72:ST:73:GLY:O	72:ST:76:THR:OG1	2.27	0.43
22:SC:172:ASN:HB3	22:SC:174:ILE:HG22	2.00	0.43
34:LS:161:ARG:HD2	34:LS:164:LYS:HB3	2.01	0.43
52:LG:121:LYS:O	52:LG:126:GLY:N	2.52	0.43
56:LE:200:LYS:HE3	56:LE:200:LYS:HB2	1.90	0.43
62:LB:156:TYR:OH	70:L5:4909:A:OP2	2.31	0.43
70:L5:167:C:O2'	70:L5:168:C:H5'	2.19	0.43
70:L5:1333:A:H2'	70:L5:1334:A:C8	2.53	0.43
70:L5:1426:G:N1	70:L5:1458:C:OP2	2.32	0.43
70:L5:1473:U:H2'	70:L5:1474:C:C6	2.54	0.43
70:L5:1577:G:O2'	70:L5:1612:G:H4'	2.19	0.43
70:L5:4651:A:H2'	70:L5:4652:G:O4'	2.19	0.43
70:L5:4685:U:H2'	70:L5:4686:G:C8	2.53	0.43
70:L5:4896:G:H2'	70:L5:4897:G:C8	2.54	0.43
74:S2:1144:A:H5'	74:S2:1355:C:H41	1.83	0.43
74:S2:1686:G:H2'	74:S2:1687:C:H6	1.83	0.43
75:SG:78:SER:HB3	75:SG:92:ARG:HG2	2.00	0.43
13:SK:7:ASN:O	13:SK:11:ILE:HG12	2.19	0.43
46:LJ:37:ALA:HB2	46:LJ:70:VAL:HG11	2.00	0.43
49:Li:40:VAL:O	49:Li:44:ILE:HG12	2.18	0.43
70:L5:1440:U:H2'	70:L5:1441:C:C6	2.54	0.43
70:L5:5057:C:H2'	70:L5:5058:A:C8	2.54	0.43
71:SZ:85:ARG:NH1	74:S2:1597:C:OP2	2.44	0.43
74:S2:1560:U:H2'	74:S2:1561:A:H8	1.84	0.43
74:S2:1681:U:H2'	74:S2:1682:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SW:62:VAL:HG11	25:Sb:8:LEU:HG	2.01	0.43
15:SH:117:PRO:HG2	15:SH:120:ARG:HD3	2.00	0.43
17:SF:50:PRO:O	17:SF:70:GLU:HG2	2.18	0.43
40:LO:165:LYS:HD2	40:LO:165:LYS:HA	1.79	0.43
56:LE:201:ILE:HG23	56:LE:203:ILE:HG23	2.00	0.43
66:L7:3:C:H2'	66:L7:4:U:C6	2.54	0.43
70:L5:197:A:N3	70:L5:222:C:O2'	2.46	0.43
70:L5:1257:A:H3'	70:L5:1258:G:H8	1.84	0.43
70:L5:4196:OMG:HM23	70:L5:4196:OMG:H1'	1.59	0.43
70:L5:5053:U:O2'	70:L5:5054:C:OP1	2.36	0.43
74:S2:96:C:H2'	74:S2:97:U:C6	2.53	0.43
74:S2:1079:C:OP2	87:S2:2001:HOH:O	2.20	0.43
74:S2:1232:PSU:H2'	74:S2:1233:G:C8	2.52	0.43
78:SS:111:LEU:HD13	78:SS:111:LEU:HA	1.81	0.43
80:SU:30:LYS:HD2	80:SU:30:LYS:HA	1.63	0.43
60:LC:312:ARG:NH2	70:L5:2275:G:OP2	2.51	0.43
69:L8:16:G:N2	70:L5:417:G:H2'	2.33	0.43
70:L5:1278:C:H2'	70:L5:1279:A:O4'	2.18	0.43
70:L5:1645:C:H2'	70:L5:1646:A:C8	2.53	0.43
74:S2:169:U:O2'	74:S2:170:A:OP1	2.34	0.43
3:Lo:68:LEU:HA	3:Lo:68:LEU:HD12	1.84	0.43
6:SW:30:CYS:SG	6:SW:31:SER:N	2.92	0.43
26:SA:61:ALA:O	26:SA:65:ILE:HG22	2.19	0.43
26:SA:149:ASN:HB2	26:SA:165:ASN:OD1	2.19	0.43
41:LN:155:VAL:HG12	70:L5:57:G:H4'	2.01	0.43
47:Lj:36:LYS:HD3	70:L5:372:A:H5"	2.00	0.43
50:LH:71:ARG:NH1	70:L5:4691:A:H5'	2.33	0.43
50:LH:129:ARG:HH21	70:L5:4704:C:H4'	1.83	0.43
70:L5:1247:U:H2'	70:L5:1248:C:C6	2.54	0.43
70:L5:1625:OMG:H4'	70:L5:1626:G:O5'	2.18	0.43
70:L5:2107:C:H2'	70:L5:2108:G:C8	2.54	0.43
17:SF:99:ILE:HD11	71:SZ:108:ILE:HG12	2.01	0.42
22:SC:216:MET:HE2	22:SC:216:MET:HB3	1.89	0.42
27:LZ:92:ASP:OD2	27:LZ:94:THR:OG1	2.32	0.42
35:LR:39:GLN:NE2	70:L5:2711:G:OP2	2.52	0.42
44:LL:81:LEU:HD22	44:LL:86:ILE:HB	2.01	0.42
63:Lb:53:GLY:HA2	63:Lb:56:LYS:HD2	2.01	0.42
67:Pt:16:C:H5'	67:Pt:60:A:C2	2.52	0.42
67:Pt:33:OMC:H1'	67:Pt:33:OMC:HM23	1.72	0.42
70:L5:25:A:H2'	70:L5:26:C:H6	1.84	0.42
70:L5:1322:1MA:H8	70:L5:1322:1MA:H2'	1.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:1719:A:H1'	70:L5:1721:G:N7	2.34	0.42
70:L5:2884:G:H2'	70:L5:2885:A:H8	1.84	0.42
70:L5:4906:C:H2'	70:L5:4907:G:C8	2.54	0.42
74:S2:16:G:H2'	74:S2:17:C:C6	2.53	0.42
77:S6:37:A:H3'	77:S6:38:A:H2'	2.01	0.42
1:Lm:122:ARG:NH2	70:L5:4473:A:O2'	2.52	0.42
3:Lo:6:LYS:HG3	3:Lo:94:GLY:HA3	2.01	0.42
6:SW:38:LEU:HD23	6:SW:41:MET:HE3	1.99	0.42
40:LO:27:VAL:O	40:LO:101:ARG:NH1	2.52	0.42
48:LI:152:LEU:HB3	48:LI:165:ILE:HD12	1.99	0.42
66:L7:57:C:H2'	66:L7:58:A:H8	1.84	0.42
68:Sa:74:CYS:HB2	68:Sa:77:CYS:N	2.27	0.42
69:L8:19:C:H2'	69:L8:20:A:C8	2.54	0.42
70:L5:1196:G:H2'	70:L5:1197:C:H6	1.84	0.42
70:L5:1477:C:HO2'	70:L5:1478:C:H6	1.65	0.42
70:L5:1806:G:H2'	70:L5:1807:C:C6	2.53	0.42
70:L5:3599:A:H2'	70:L5:3600:G:C8	2.53	0.42
70:L5:3732:A:H3'	70:L5:3733:A:H8	1.84	0.42
74:S2:67:C:H41	75:SG:163:ASN:HA	1.83	0.42
74:S2:880:G:H3'	74:S2:881:G:H8	1.84	0.42
74:S2:1315:U:H2'	74:S2:1316:C:C6	2.54	0.42
74:S2:1325:G:H5'	74:S2:1326:U:OP1	2.19	0.42
74:S2:1405:A:H2'	74:S2:1406:G:O4'	2.19	0.42
74:S2:1609:C:H3'	78:SS:132:ARG:NH1	2.34	0.42
6:SW:104:LEU:HB3	6:SW:125:ILE:HA	2.01	0.42
8:SR:109:LEU:HD22	26:SA:52:LYS:HG3	1.99	0.42
22:SC:65:LYS:HE2	26:SA:118:GLU:HB3	1.99	0.42
28:LY:28:LYS:HE3	28:LY:28:LYS:HB3	1.87	0.42
29:LX:64:SER:HB3	51:Lh:69:LEU:HD13	2.02	0.42
32:LU:95:ASN:O	32:LU:95:ASN:ND2	2.52	0.42
41:LN:9:GLU:HB2	49:Li:44:ILE:HG13	2.01	0.42
56:LE:69:TYR:CD1	56:LE:70:LYS:HG3	2.55	0.42
58:LD:238:GLU:O	58:LD:242:LYS:HD3	2.19	0.42
59:Ld:29:ILE:O	59:Ld:33:ILE:HG12	2.20	0.42
60:LC:60:HIS:NE2	60:LC:100:ARG:HD3	2.34	0.42
70:L5:2261:G:H2'	70:L5:2262:G:C4	2.54	0.42
70:L5:4088:C:H2'	70:L5:4089:G:C8	2.55	0.42
74:S2:1550:G:H3'	74:S2:1579:A:H61	1.85	0.42
75:SG:127:THR:OG1	75:SG:128:THR:N	2.52	0.42
27:LZ:25:ILE:HA	27:LZ:43:VAL:HG12	2.00	0.42
37:LQ:132:LYS:NZ	70:L5:1449:C:OP1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:LA:140:ASN:OD1	64:LA:143:THR:OG1	2.33	0.42
70:L5:1490:G:H2'	70:L5:1491:A:C8	2.53	0.42
74:S2:558:G:H2'	74:S2:559:G:C8	2.54	0.42
74:S2:912:C:H4'	74:S2:913:A:OP2	2.18	0.42
74:S2:1725:U:H2'	74:S2:1726:G:C8	2.54	0.42
3:Lo:13:LYS:HE3	3:Lo:13:LYS:HB3	1.89	0.42
4:SY:86:GLU:OE2	4:SY:90:ARG:NH1	2.38	0.42
10:SO:136:PRO:HG3	10:SO:139:SER:HB3	2.00	0.42
32:LU:113:ARG:NH1	70:L5:2703:G:OP1	2.53	0.42
40:LO:93:LYS:HE2	40:LO:93:LYS:HB2	1.71	0.42
40:LO:113:ASP:OD1	40:LO:113:ASP:N	2.53	0.42
43:LM:6:PHE:H	43:LM:11:ARG:HH21	1.68	0.42
45:Lk:51:GLU:HG2	45:Lk:52:LYS:H	1.85	0.42
46:LJ:64:ARG:HH21	67:Pt:57:C:H4'	1.85	0.42
52:LG:99:ALA:HB1	52:LG:136:LEU:HD11	2.01	0.42
62:LB:95:THR:HG22	70:L5:4910:G:H4'	2.01	0.42
70:L5:1271:G:H21	70:L5:1271:G:P	2.41	0.42
70:L5:1346:C:H2'	70:L5:1347:G:H8	1.83	0.42
70:L5:4859:C:O2'	70:L5:4860:G:N7	2.49	0.42
74:S2:573:PSU:O4	74:S2:576:A2M:H8	2.19	0.42
74:S2:639:C:H2'	74:S2:640:A:H8	1.84	0.42
74:S2:1595:U:H2'	74:S2:1596:U:C6	2.54	0.42
76:SI:142:SER:HB3	76:SI:145:ILE:HG13	2.00	0.42
11:SN:136:PRO:HG2	11:SN:139:TRP:HB2	2.01	0.42
32:LU:23:LEU:HD11	32:LU:39:PHE:HE2	1.83	0.42
58:LD:197:LYS:HE2	58:LD:202:GLN:HG3	2.01	0.42
58:LD:253:TYR:OH	66:L7:117:G:OP1	2.29	0.42
60:LC:237:ILE:HD12	60:LC:237:ILE:HA	1.85	0.42
67:Pt:10:G:N2	67:Pt:27:G:H1'	2.35	0.42
68:Sa:70:LYS:HE3	68:Sa:70:LYS:HB3	1.91	0.42
70:L5:2358:G:H2'	70:L5:2359:U:O4'	2.20	0.42
70:L5:4921:C:C2	70:L5:4922:C:C5	3.07	0.42
70:L5:5030:U:H2'	70:L5:5031:G:H8	1.85	0.42
74:S2:215:G:H2'	74:S2:216:C:C6	2.54	0.42
76:SI:31:ARG:HH12	76:SI:48:VAL:HG12	1.84	0.42
21:Sd:34:TYR:OH	74:S2:1549:U:OP1	2.30	0.42
24:SB:114:VAL:O	74:S2:1869:A:N6	2.53	0.42
26:SA:77:ILE:HB	26:SA:124:VAL:HG12	2.02	0.42
47:Lj:16:HIS:O	47:Lj:25:LYS:NZ	2.50	0.42
64:LA:40:TYR:HA	64:LA:91:GLY:HA3	2.02	0.42
70:L5:1672:U:H2'	70:L5:1673:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:2555:G:H2'	70:L5:2556:G:C8	2.54	0.42
70:L5:4896:G:H2'	70:L5:4897:G:H8	1.83	0.42
74:S2:639:C:H2'	74:S2:640:A:C8	2.55	0.42
32:LU:65:ARG:HG2	32:LU:70:ILE:HG12	2.02	0.42
40:LO:51:LYS:HE3	40:LO:144:GLU:HB3	2.02	0.42
41:LN:56:LYS:NZ	70:L5:153:G:OP1	2.41	0.42
44:LL:145:LYS:HB3	44:LL:145:LYS:HE2	1.77	0.42
50:LH:41:ILE:HG22	50:LH:43:VAL:HG13	2.01	0.42
50:LH:177:ASP:OD1	50:LH:177:ASP:N	2.53	0.42
57:Le:5:ARG:HE	70:L5:454:U:H1'	1.85	0.42
59:Ld:46:LEU:HD23	59:Ld:46:LEU:HA	1.88	0.42
70:L5:172:C:N4	70:L5:265:C:N3	2.49	0.42
70:L5:417:G:OP1	70:L5:2329:U:O2'	2.37	0.42
70:L5:4460:U:H2'	70:L5:4461:C:C6	2.55	0.42
74:S2:1793:A:H2'	74:S2:1794:C:H6	1.85	0.42
75:SG:218:LYS:HB2	75:SG:218:LYS:HE3	1.81	0.42
26:SA:139:TYR:OH	74:S2:1353:A:OP1	2.35	0.42
37:LQ:13:VAL:HG12	70:L5:1691:G:H5"	2.02	0.42
43:LM:24:LEU:HB3	43:LM:77:TRP:HH2	1.84	0.42
63:Lb:54:LEU:HA	63:Lb:57:MET:HG2	2.02	0.42
69:L8:144:U:H2'	69:L8:145:C:H6	1.85	0.42
70:L5:674:G:H2'	70:L5:675:C:C6	2.55	0.42
70:L5:1607:C:H5"	85:L5:5101:SPD:H91	2.02	0.42
70:L5:1927:U:OP1	70:L5:1949:U:O2'	2.30	0.42
70:L5:2418:A:N1	70:L5:2429:A:O2'	2.49	0.42
70:L5:3930:U:H2'	70:L5:3931:C:C6	2.55	0.42
70:L5:4523:A2M:H5"	70:L5:4524:G:H5'	2.01	0.42
74:S2:51:U:H2'	74:S2:52:G:H8	1.84	0.42
74:S2:628:A:N6	74:S2:1500:G:O2'	2.53	0.42
15:SH:22:GLY:O	15:SH:25:GLN:HG2	2.20	0.42
16:Sg:56:GLN:HG3	16:Sg:57:ARG:H	1.84	0.42
62:LB:103:LYS:HD2	62:LB:103:LYS:HA	1.88	0.42
70:L5:207:G:H2'	70:L5:208:A:C8	2.55	0.42
70:L5:1806:G:H2'	70:L5:1807:C:H6	1.85	0.42
74:S2:1673:U:H2'	74:S2:1674:G:O4'	2.20	0.42
74:S2:1703:OMC:HM23	74:S2:1703:OMC:H1'	1.85	0.42
78:SS:106:LYS:HD3	78:SS:106:LYS:HA	1.83	0.42
3:Lo:97:LYS:HD2	70:L5:4233:A:OP2	2.19	0.41
6:SW:31:SER:HB3	6:SW:34:ILE:HG13	2.01	0.41
17:SF:59:LYS:HG2	17:SF:62:ARG:HH21	1.85	0.41
55:Lf:106:TYR:HB2	55:Lf:107:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:1757:U:H3	70:L5:1774:C:N4	2.18	0.41
70:L5:3656:A:H2'	70:L5:3657:U:H6	1.85	0.41
70:L5:4080:C:H2'	70:L5:4081:G:H8	1.85	0.41
70:L5:4174:U:H2'	70:L5:4175:G:C8	2.55	0.41
70:L5:4481:U:H2'	70:L5:4482:U:H6	1.85	0.41
70:L5:4578:G:H2'	70:L5:4579:PSU:C6	2.55	0.41
76:SI:159:SER:HB2	76:SI:162:LEU:HD12	2.01	0.41
4:SY:44:LEU:HD23	4:SY:44:LEU:HA	1.89	0.41
15:SH:43:LEU:HD13	15:SH:72:PHE:CZ	2.55	0.41
15:SH:49:LYS:HB3	15:SH:49:LYS:HE3	1.81	0.41
24:SB:71:LEU:HD22	24:SB:84:PHE:HE2	1.85	0.41
24:SB:74:LEU:HD12	24:SB:74:LEU:HA	1.92	0.41
45:Lk:51:GLU:OE1	45:Lk:51:GLU:N	2.52	0.41
70:L5:1274:A:H2'	70:L5:1275:G:O4'	2.20	0.41
70:L5:1345:A:H2'	70:L5:1346:C:C6	2.55	0.41
70:L5:1942:A:H2'	70:L5:1943:A:H8	1.85	0.41
70:L5:4637:OMG:H1'	70:L5:4637:OMG:HM23	1.86	0.41
70:L5:4699:U:H1'	70:L5:4700:A:H5"	2.02	0.41
74:S2:96:C:H2'	74:S2:97:U:H6	1.84	0.41
76:SI:101:ILE:HD12	76:SI:190:LEU:HD11	2.01	0.41
25:Sb:30:SER:OG	74:S2:1016:U:OP1	2.34	0.41
41:LN:125:SER:HB3	70:L5:3937:C:H1'	2.02	0.41
44:LL:127:PHE:HB2	51:Lh:118:LYS:HG3	2.02	0.41
45:Lk:61:PRO:HA	45:Lk:62:PRO:HD3	1.91	0.41
46:LJ:75:ARG:NH2	66:L7:40:U:O2	2.45	0.41
64:LA:244:GLY:HA3	70:L5:3746:A:H5"	2.01	0.41
70:L5:750:U:H1'	70:L5:917:A:C8	2.55	0.41
70:L5:1528:U:H2'	70:L5:1529:G:C8	2.56	0.41
70:L5:1811:G:H2'	70:L5:1812:C:C6	2.55	0.41
70:L5:2520:C:H2'	70:L5:2521:G:C8	2.55	0.41
70:L5:2601:A:N6	70:L5:2743:A:H3'	2.36	0.41
70:L5:4952:G:H2'	70:L5:4953:G:O4'	2.19	0.41
71:SZ:69:THR:O	71:SZ:73:VAL:HG22	2.20	0.41
74:S2:29:G:H2'	74:S2:30:C:C6	2.55	0.41
74:S2:102:A:H4'	74:S2:104:A:C8	2.56	0.41
74:S2:910:G:OP2	74:S2:910:G:N2	2.42	0.41
74:S2:1189:A:H2'	74:S2:1190:A:C8	2.55	0.41
74:S2:1255:G:OP1	74:S2:1256:G:O2'	2.31	0.41
77:S6:70:G:H2'	77:S6:71:C:C6	2.55	0.41
5:SX:68:LYS:HB3	5:SX:91:LEU:HD13	2.01	0.41
8:SR:96:ILE:HB	8:SR:117:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SE:172:PHE:CE2	18:SE:174:LYS:HE3	2.56	0.41
21:Sd:24:CYS:HB2	74:S2:1496:U:H4'	2.02	0.41
22:SC:257:LYS:HE3	22:SC:257:LYS:HB2	1.88	0.41
34:LS:95:ARG:HH12	70:L5:1951:G:HO2'	1.66	0.41
34:LS:151:LYS:HG2	43:LM:6:PHE:HB3	2.02	0.41
70:L5:153:G:H2'	70:L5:154:G:H8	1.85	0.41
70:L5:424:U:H2'	70:L5:425:U:C6	2.55	0.41
70:L5:1818:G:OP2	70:L5:1818:G:N2	2.37	0.41
70:L5:4156:G:OP2	70:L5:4157:A:O2'	2.30	0.41
21:Sd:33:LYS:HE2	21:Sd:34:TYR:CZ	2.56	0.41
24:SB:149:GLN:HG2	74:S2:1123:C:H4'	2.03	0.41
34:LS:70:LYS:HD2	34:LS:70:LYS:HA	1.83	0.41
35:LR:151:ARG:O	35:LR:154:LEU:HG	2.21	0.41
40:LO:28:LEU:HD23	40:LO:28:LEU:HA	1.93	0.41
43:LM:6:PHE:H	43:LM:11:ARG:NH2	2.18	0.41
43:LM:85:LYS:O	43:LM:89:THR:HG23	2.21	0.41
44:LL:36:ARG:NH2	70:L5:1364:U:OP2	2.32	0.41
45:Lk:47:ILE:HG22	45:Lk:49:ASP:H	1.86	0.41
48:LI:3:ARG:HH12	70:L5:4430:G:H5'	1.86	0.41
63:Lb:3:LYS:HD3	70:L5:4194:U:H3'	2.01	0.41
67:Pt:74:A:H5"	67:Pt:75:C:H5'	2.01	0.41
70:L5:271:C:H2'	70:L5:272:U:H6	1.86	0.41
70:L5:699:C:H2'	70:L5:700:G:C8	2.56	0.41
70:L5:1487:G:H2'	70:L5:1488:G:C8	2.55	0.41
70:L5:2611:A:H2'	70:L5:2612:G:C8	2.55	0.41
70:L5:3684:G:H2'	70:L5:3685:C:H6	1.85	0.41
74:S2:206:G:H2'	74:S2:207:G:C8	2.56	0.41
74:S2:1201:U:H2'	74:S2:1202:U:C6	2.56	0.41
77:S6:69:U:H2'	77:S6:70:G:C8	2.56	0.41
15:SH:63:PHE:HB3	15:SH:97:GLN:HG2	2.00	0.41
33:LT:99:SER:HG	33:LT:101:SER:HG	1.68	0.41
36:Lr:37:SER:OG	70:L5:2267:U:OP1	2.31	0.41
40:LO:76:PRO:HB3	40:LO:138:LEU:HG	2.02	0.41
49:Li:38:LYS:HE3	49:Li:38:LYS:HB3	1.85	0.41
58:LD:199:ILE:HG22	58:LD:200:MET:HE2	2.02	0.41
69:L8:26:C:H2'	69:L8:27:U:C6	2.56	0.41
69:L8:27:U:H2'	69:L8:28:C:C6	2.55	0.41
70:L5:400:A2M:HM'3	70:L5:400:A2M:H1'	1.81	0.41
70:L5:2743:A:H2'	70:L5:2744:A:C8	2.56	0.41
70:L5:3870:C:H2'	70:L5:3871:A:H8	1.85	0.41
74:S2:441:C:H2'	74:S2:442:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:S2:1013:U:OP1	74:S2:1129:G:O2'	2.38	0.41
74:S2:1610:G:OP2	78:SS:132:ARG:NH1	2.51	0.41
74:S2:1712:A:H2'	74:S2:1713:C:C6	2.55	0.41
76:SI:195:LEU:HD12	76:SI:195:LEU:HA	1.90	0.41
37:LQ:124:ASP:OD1	37:LQ:124:ASP:N	2.52	0.41
40:LO:185:VAL:O	40:LO:189:ILE:HG12	2.21	0.41
54:LF:216:PRO:HD3	54:LF:247:MET:HE2	2.02	0.41
70:L5:106:A:H2'	70:L5:107:G:O4'	2.20	0.41
70:L5:1189:G:H2'	70:L5:1190:C:C6	2.56	0.41
70:L5:1545:G:H2'	70:L5:1546:C:C6	2.56	0.41
70:L5:1563:A:H2'	70:L5:1564:A:C8	2.55	0.41
70:L5:2448:G:H2'	70:L5:2449:A:C8	2.56	0.41
70:L5:3661:G:H4'	70:L5:3662:A:H5'	2.02	0.41
70:L5:3867:A2M:HM'3	70:L5:3880:G:N2	2.36	0.41
70:L5:3932:U:H2'	70:L5:3933:G:H8	1.86	0.41
70:L5:4481:U:H2'	70:L5:4482:U:C6	2.56	0.41
70:L5:5004:C:H2'	70:L5:5005:G:O4'	2.20	0.41
72:ST:23:LYS:HD2	72:ST:23:LYS:HA	1.90	0.41
74:S2:1183:A:H2'	74:S2:1184:G:H8	1.86	0.41
77:S6:31:G:H2'	77:S6:32:C:C6	2.56	0.41
15:SH:73:GLN:HB3	15:SH:135:PHE:CE1	2.56	0.41
49:Li:60:LEU:HD23	49:Li:60:LEU:HA	1.94	0.41
54:LF:47:ARG:O	54:LF:50:ILE:HG13	2.21	0.41
69:L8:5:U:H2'	69:L8:6:C:H6	1.86	0.41
70:L5:1098:G:H2'	70:L5:1099:C:C6	2.56	0.41
70:L5:2758:G:O2'	70:L5:2765:A:N3	2.46	0.41
70:L5:3932:U:H2'	70:L5:3933:G:C8	2.55	0.41
70:L5:4254:G:N3	70:L5:4254:G:H2'	2.34	0.41
70:L5:4324:A:H2'	70:L5:4325:A:C8	2.55	0.41
74:S2:416:U:H2'	74:S2:417:C:O4'	2.20	0.41
74:S2:455:A:H2'	74:S2:456:C:H6	1.85	0.41
74:S2:509:OMG:H1'	74:S2:509:OMG:HM23	1.72	0.41
74:S2:1683:C:H2'	74:S2:1684:C:H6	1.86	0.41
75:SG:10:THR:HG23	75:SG:12:CYS:H	1.86	0.41
78:SS:12:ILE:HD13	78:SS:21:ASP:HA	2.02	0.41
80:SU:21:ARG:NH1	80:SU:21:ARG:HB2	2.36	0.41
11:SN:88:LEU:HD13	11:SN:125:LEU:HB3	2.03	0.41
16:Sg:125:ARG:HA	16:Sg:125:ARG:HD3	1.89	0.41
17:SF:126:THR:HG21	23:Sc:27:CYS:SG	2.60	0.41
25:Sb:14:GLU:O	25:Sb:18:LYS:HG3	2.21	0.41
26:SA:132:GLN:HB3	26:SA:133:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LZ:58:GLY:O	27:LZ:62:ILE:HG12	2.20	0.41
29:LX:89:LYS:HG3	29:LX:95:THR:HB	2.02	0.41
29:LX:143:ASP:OD1	29:LX:143:ASP:N	2.52	0.41
36:Lr:28:GLU:OE2	36:Lr:31:ASN:ND2	2.54	0.41
37:LQ:119:LYS:HE2	37:LQ:119:LYS:HB3	1.78	0.41
37:LQ:128:LEU:HA	37:LQ:128:LEU:HD13	1.85	0.41
49:Li:65:LYS:HE2	49:Li:65:LYS:HB3	1.87	0.41
52:LG:33:GLU:O	70:L5:4128:A:O2'	2.34	0.41
56:LE:62:MET:HE1	56:LE:65:ARG:HH11	1.85	0.41
58:LD:128:ASP:O	58:LD:164:LYS:NZ	2.41	0.41
58:LD:139:PRO:HB3	70:L5:1820:C:H5'	2.03	0.41
60:LC:239:LYS:H	60:LC:239:LYS:HG2	1.71	0.41
69:L8:4:C:H2'	69:L8:5:U:H6	1.86	0.41
70:L5:318:A:H2'	70:L5:319:A:H8	1.86	0.41
70:L5:732:A:H2'	70:L5:733:A:O4'	2.21	0.41
70:L5:1260:G:H2'	70:L5:1261:G:O4'	2.21	0.41
70:L5:1857:C:H2'	70:L5:1858:A:C8	2.52	0.41
70:L5:1965:G:H5'	70:L5:4695:C:H1'	2.03	0.41
70:L5:2079:G:H2'	70:L5:2080:U:C6	2.56	0.41
70:L5:2730:U:H2'	70:L5:2731:C:C6	2.56	0.41
70:L5:3602:C:H2'	70:L5:3603:G:H8	1.86	0.41
70:L5:3633:C:H2'	70:L5:3634:G:C8	2.56	0.41
70:L5:4186:A:H2'	70:L5:4187:G:C8	2.55	0.41
70:L5:4522:G:O2'	70:L5:4525:C:OP2	2.32	0.41
70:L5:4551:U:H2'	70:L5:4552:PSU:C6	2.56	0.41
70:L5:4604:G:N2	70:L5:4607:A:OP2	2.37	0.41
70:L5:4903:G:H2'	70:L5:4904:G:C8	2.54	0.41
74:S2:65:C:C6	75:SG:174:PRO:HB3	2.55	0.41
74:S2:553:U:H2'	74:S2:554:A:H8	1.84	0.41
74:S2:948:C:H2'	74:S2:949:G:C8	2.55	0.41
74:S2:1217:A:H2'	74:S2:1218:C:C6	2.55	0.41
74:S2:1417:C:H2'	74:S2:1418:C:C6	2.55	0.41
74:S2:1658:G:OP2	74:S2:1660:C:N4	2.51	0.41
74:S2:1809:A:H2'	74:S2:1810:U:C6	2.56	0.41
75:SG:215:LYS:O	75:SG:219:GLU:HG2	2.21	0.41
5:SX:67:ARG:HD2	5:SX:115:ILE:HG12	2.02	0.41
13:SK:24:LYS:O	13:SK:42:ASN:ND2	2.54	0.41
15:SH:51:ILE:HD12	15:SH:179:LYS:HE2	2.02	0.41
22:SC:132:ASP:OD1	22:SC:132:ASP:N	2.52	0.41
56:LE:57:TYR:HB2	56:LE:62:MET:HE3	2.04	0.41
63:Lb:40:LEU:O	63:Lb:44:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:980:U:H2'	70:L5:981:C:C6	2.56	0.41
70:L5:1514:U:H2'	70:L5:1515:A:C8	2.56	0.41
70:L5:1749:A:H2'	70:L5:1750:G:C8	2.55	0.41
70:L5:4704:C:H2'	70:L5:4705:A:C8	2.55	0.41
74:S2:5:U:H2'	74:S2:6:G:C8	2.55	0.41
74:S2:380:G:P	76:SI:56:ARG:HH22	2.43	0.41
74:S2:1741:U:H2'	74:S2:1742:C:O4'	2.21	0.41
27:LZ:10:VAL:O	27:LZ:83:THR:HB	2.22	0.40
34:LS:174:THR:OG1	70:L5:4763:U:O2'	2.30	0.40
41:LN:94:PHE:CE2	41:LN:96:ARG:HB2	2.56	0.40
48:LI:205:PRO:HD2	48:LI:208:LYS:HG3	2.02	0.40
70:L5:664:G:N2	70:L5:667:A:H62	2.20	0.40
70:L5:1207:C:H2'	70:L5:1208:G:H8	1.86	0.40
70:L5:1564:A:H2'	70:L5:1565:A:C8	2.55	0.40
70:L5:2335:C:H2'	70:L5:2336:G:H8	1.86	0.40
70:L5:2412:A:H2'	70:L5:2413:U:C6	2.56	0.40
70:L5:2497:C:H2'	70:L5:2498:C:C6	2.56	0.40
70:L5:3736:A:H2'	70:L5:3737:A:H8	1.84	0.40
70:L5:3829:G:H2'	70:L5:3830:A2M:H8	2.03	0.40
70:L5:3923:A:H2'	70:L5:3924:C:C6	2.56	0.40
70:L5:4887:C:H2'	70:L5:4888:U:O4'	2.21	0.40
74:S2:15:U:H2'	74:S2:16:G:O4'	2.21	0.40
74:S2:1390:U:H2'	74:S2:1391:OMC:C6	2.57	0.40
75:SG:137:ARG:HB3	75:SG:140:ARG:HB2	2.02	0.40
4:SY:57:VAL:HB	4:SY:60:PHE:CE1	2.56	0.40
30:LW:47:ARG:HG3	30:LW:58:LYS:HD3	2.03	0.40
43:LM:36:ALA:HB2	43:LM:52:PHE:CZ	2.56	0.40
49:Li:25:ARG:HE	70:L5:159:C:H5"	1.86	0.40
50:LH:92:MET:HG3	50:LH:180:TYR:C	2.46	0.40
55:Lf:75:THR:HG22	70:L5:952:G:H4'	2.02	0.40
70:L5:204:U:H2'	70:L5:205:C:C6	2.56	0.40
70:L5:477:C:H2'	70:L5:478:G:C8	2.56	0.40
70:L5:2424:OMG:H1'	70:L5:2424:OMG:HM23	1.80	0.40
70:L5:2837:OMU:H1'	70:L5:2837:OMU:HM23	1.88	0.40
74:S2:996:A:H2'	74:S2:997:A:C8	2.56	0.40
74:S2:1010:G:H2'	74:S2:1011:A:H8	1.85	0.40
74:S2:1374:C:H2'	74:S2:1375:G:O4'	2.21	0.40
74:S2:1395:C:H2'	74:S2:1396:A:N3	2.37	0.40
74:S2:1736:G:H2'	74:S2:1737:G:C8	2.56	0.40
3:Lo:12:CYS:HB3	3:Lo:15:CYS:HB2	2.03	0.40
4:SY:25:ILE:HD11	4:SY:73:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SO:61:LYS:HD2	10:SO:76:LEU:HB3	2.02	0.40
26:SA:10:MET:HE3	26:SA:10:MET:HB2	1.86	0.40
34:LS:85:ASP:OD1	34:LS:90:THR:HB	2.21	0.40
48:LI:145:LYS:O	48:LI:149:ILE:HG12	2.20	0.40
50:LH:115:ARG:HG3	50:LH:123:ILE:HG23	2.03	0.40
51:Lh:102:LEU:HD23	51:Lh:102:LEU:HA	1.94	0.40
63:Lb:54:LEU:O	63:Lb:57:MET:HB2	2.21	0.40
70:L5:1730:U:H2'	70:L5:1731:C:C6	2.57	0.40
70:L5:2555:G:H2'	70:L5:2556:G:H8	1.85	0.40
70:L5:4696:C:H2'	70:L5:4697:U:O4'	2.21	0.40
74:S2:436:OMG:HM23	74:S2:436:OMG:H1'	1.83	0.40
74:S2:1746:U:OP1	75:SG:31:ARG:NH2	2.55	0.40
80:SU:20:ILE:HG23	80:SU:91:LEU:HB2	2.02	0.40
14:SJ:60:LEU:HA	14:SJ:60:LEU:HD23	1.87	0.40
22:SC:176:LYS:HG3	22:SC:177:PRO:HD2	2.04	0.40
60:LC:288:ASP:HB3	60:LC:291:ARG:HB2	2.03	0.40
62:LB:220:ILE:HG12	62:LB:278:THR:HG23	2.03	0.40
66:L7:28:C:H1'	66:L7:54:A:H61	1.86	0.40
69:L8:30:U:H2'	69:L8:31:G:H8	1.86	0.40
70:L5:126:C:H2'	70:L5:127:G:H8	1.86	0.40
70:L5:749:G:N2	70:L5:912:G:O2'	2.51	0.40
70:L5:956:A:H8	70:L5:957:G:C8	2.39	0.40
70:L5:963:G:N7	70:L5:964:A:N6	2.69	0.40
70:L5:1683:PSU:H2'	70:L5:1684:A:C8	2.56	0.40
70:L5:3770:PSU:H2'	70:L5:3771:C:C6	2.55	0.40
70:L5:4088:C:H2'	70:L5:4089:G:H8	1.85	0.40
70:L5:5006:U:H4'	70:L5:5007:A:H5'	2.03	0.40
74:S2:1019:C:H2'	74:S2:1020:A:O4'	2.21	0.40
8:SR:74:GLN:O	8:SR:78:ARG:HG2	2.21	0.40
11:SN:121:ARG:HA	11:SN:124:ARG:HG2	2.04	0.40
15:SH:5:SER:OG	15:SH:6:ALA:N	2.51	0.40
24:SB:38:MET:H	24:SB:38:MET:HG2	1.73	0.40
24:SB:68:GLU:HG3	24:SB:85:LYS:HG2	2.04	0.40
27:LZ:127:ASN:OD1	27:LZ:127:ASN:N	2.54	0.40
28:LY:50:ARG:NH2	69:L8:85:U:O4	2.54	0.40
36:Lr:119:ARG:HA	36:Lr:119:ARG:HD3	1.97	0.40
45:Lk:51:GLU:H	45:Lk:51:GLU:CD	2.27	0.40
47:Lj:67:LEU:HD23	47:Lj:67:LEU:HA	1.89	0.40
58:LD:286:SER:OG	70:L5:1178:G:O2'	2.35	0.40
64:LA:183:GLY:HA2	70:L5:1613:A:H5'	2.04	0.40
65:La:132:ARG:HH21	70:L5:1396:G:H5"	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:L5:512:U:O4	70:L5:647:G:O6	2.40	0.40
70:L5:714:G:H2'	70:L5:715:G:H8	1.86	0.40
70:L5:1207:C:C2	70:L5:1208:G:C8	3.10	0.40
75:SG:153:VAL:HG23	75:SG:176:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
2	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
3	Lo	102/106 (96%)	99 (97%)	3 (3%)	0	100	100
4	SY	121/133 (91%)	118 (98%)	3 (2%)	0	100	100
5	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
6	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
7	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
8	SR	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
9	SQ	137/146 (94%)	127 (93%)	10 (7%)	0	100	100
10	SO	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
11	SN	148/151 (98%)	148 (100%)	0	0	100	100
12	SL	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
13	SK	70/165 (42%)	69 (99%)	1 (1%)	0	100	100
14	SJ	176/194 (91%)	168 (96%)	8 (4%)	0	100	100
15	SH	187/194 (96%)	181 (97%)	6 (3%)	0	100	100
16	Sg	221/317 (70%)	180 (81%)	39 (18%)	2 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	SF	181/204 (89%)	173 (96%)	8 (4%)	0	100	100
18	SE	258/263 (98%)	251 (97%)	7 (3%)	0	100	100
19	Se	47/133 (35%)	47 (100%)	0	0	100	100
20	SD	165/243 (68%)	161 (98%)	4 (2%)	0	100	100
21	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
22	SC	218/293 (74%)	211 (97%)	7 (3%)	0	100	100
23	Sc	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
24	SB	211/264 (80%)	205 (97%)	6 (3%)	0	100	100
25	Sb	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
26	SA	213/295 (72%)	206 (97%)	7 (3%)	0	100	100
27	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
28	LY	131/145 (90%)	128 (98%)	3 (2%)	0	100	100
29	LX	117/156 (75%)	114 (97%)	3 (3%)	0	100	100
30	LW	60/157 (38%)	60 (100%)	0	0	100	100
31	LV	130/140 (93%)	128 (98%)	2 (2%)	0	100	100
32	LU	97/128 (76%)	91 (94%)	6 (6%)	0	100	100
33	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
34	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
35	LR	179/196 (91%)	173 (97%)	6 (3%)	0	100	100
36	Lr	121/137 (88%)	118 (98%)	3 (2%)	0	100	100
37	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
38	LP	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
39	Lp	88/91 (97%)	85 (97%)	3 (3%)	0	100	100
40	LO	197/203 (97%)	193 (98%)	4 (2%)	0	100	100
41	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	LM	134/215 (62%)	133 (99%)	1 (1%)	0	100	100
44	LL	203/211 (96%)	196 (97%)	7 (3%)	0	100	100
45	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
46	LJ	167/178 (94%)	162 (97%)	5 (3%)	0	100	100
47	Lj	84/97 (87%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	LI	199/214 (93%)	197 (99%)	2 (1%)	0	100	100
49	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
50	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
51	Lh	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
52	LG	226/266 (85%)	217 (96%)	9 (4%)	0	100	100
53	Lg	109/112 (97%)	107 (98%)	2 (2%)	0	100	100
54	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
55	Lf	107/111 (96%)	106 (99%)	1 (1%)	0	100	100
56	LE	212/288 (74%)	205 (97%)	7 (3%)	0	100	100
57	Le	125/135 (93%)	122 (98%)	3 (2%)	0	100	100
58	LD	290/297 (98%)	285 (98%)	5 (2%)	0	100	100
59	Ld	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
60	LC	357/427 (84%)	346 (97%)	11 (3%)	0	100	100
61	Lc	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
62	LB	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
63	Lb	96/159 (60%)	92 (96%)	4 (4%)	0	100	100
64	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
65	La	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
68	Sa	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
71	SZ	61/125 (49%)	56 (92%)	5 (8%)	0	100	100
72	ST	125/145 (86%)	122 (98%)	3 (2%)	0	100	100
73	SP	124/145 (86%)	117 (94%)	7 (6%)	0	100	100
75	SG	216/249 (87%)	210 (97%)	6 (3%)	0	100	100
76	SI	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
78	SS	136/152 (90%)	124 (91%)	11 (8%)	1 (1%)	18	53
80	SU	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
All	All	10686/12433 (86%)	10331 (97%)	352 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
78	SS	119	PHE
16	Sg	236	ILE

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Mol	Chain	Res	Type
16	Sg	282	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Lm	43/116 (37%)	42 (98%)	1 (2%)	44 74
2	Ll	45/48 (94%)	40 (89%)	5 (11%)	6 25
3	Lo	82/93 (88%)	75 (92%)	7 (8%)	10 36
4	SY	75/115 (65%)	72 (96%)	3 (4%)	28 62
5	SX	101/115 (88%)	96 (95%)	5 (5%)	22 56
6	SW	109/113 (96%)	101 (93%)	8 (7%)	13 42
7	SV	63/67 (94%)	62 (98%)	1 (2%)	55 79
8	SR	83/122 (68%)	74 (89%)	9 (11%)	6 26
9	SQ	66/121 (54%)	66 (100%)	0	100 100
10	SO	97/119 (82%)	92 (95%)	5 (5%)	21 55
11	SN	125/131 (95%)	123 (98%)	2 (2%)	55 79
12	SL	127/142 (89%)	125 (98%)	2 (2%)	55 79
13	SK	24/136 (18%)	24 (100%)	0	100 100
14	SJ	145/168 (86%)	140 (97%)	5 (3%)	32 66
15	SH	139/174 (80%)	131 (94%)	8 (6%)	18 51
16	Sg	17/275 (6%)	17 (100%)	0	100 100
17	SF	117/170 (69%)	114 (97%)	3 (3%)	40 72
18	SE	215/225 (96%)	210 (98%)	5 (2%)	44 74
19	Se	39/104 (38%)	37 (95%)	2 (5%)	21 55
20	SD	74/202 (37%)	68 (92%)	6 (8%)	11 38
21	Sd	41/49 (84%)	38 (93%)	3 (7%)	13 42
22	SC	182/225 (81%)	174 (96%)	8 (4%)	25 60
23	Sc	42/62 (68%)	41 (98%)	1 (2%)	43 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	SB	183/231 (79%)	173 (94%)	10 (6%)	19 53
25	Sb	68/76 (90%)	67 (98%)	1 (2%)	57 80
26	SA	169/243 (70%)	165 (98%)	4 (2%)	43 73
27	LZ	113/118 (96%)	105 (93%)	8 (7%)	13 43
28	LY	111/135 (82%)	110 (99%)	1 (1%)	70 85
29	LX	107/133 (80%)	102 (95%)	5 (5%)	23 58
30	LW	54/126 (43%)	51 (94%)	3 (6%)	19 52
31	LV	102/107 (95%)	97 (95%)	5 (5%)	22 56
32	LU	87/115 (76%)	83 (95%)	4 (5%)	24 58
33	LT	139/140 (99%)	136 (98%)	3 (2%)	45 74
34	LS	156/157 (99%)	150 (96%)	6 (4%)	29 63
35	LR	147/175 (84%)	145 (99%)	2 (1%)	59 80
36	Lr	107/121 (88%)	104 (97%)	3 (3%)	38 70
37	LQ	162/165 (98%)	156 (96%)	6 (4%)	30 64
38	LP	131/135 (97%)	129 (98%)	2 (2%)	57 80
39	Lp	72/74 (97%)	70 (97%)	2 (3%)	38 70
40	LO	167/174 (96%)	162 (97%)	5 (3%)	36 69
41	LN	170/172 (99%)	167 (98%)	3 (2%)	51 77
42	Ln	23/24 (96%)	22 (96%)	1 (4%)	26 60
43	LM	115/161 (71%)	113 (98%)	2 (2%)	53 78
44	LL	166/177 (94%)	160 (96%)	6 (4%)	31 65
45	Lk	61/65 (94%)	57 (93%)	4 (7%)	15 46
46	LJ	136/149 (91%)	129 (95%)	7 (5%)	21 55
47	Lj	72/80 (90%)	69 (96%)	3 (4%)	26 61
48	LI	170/181 (94%)	168 (99%)	2 (1%)	63 82
49	Li	80/89 (90%)	77 (96%)	3 (4%)	29 63
50	LH	164/171 (96%)	162 (99%)	2 (1%)	63 82
51	Lh	108/110 (98%)	104 (96%)	4 (4%)	30 64
52	LG	184/223 (82%)	179 (97%)	5 (3%)	39 71
53	Lg	92/96 (96%)	88 (96%)	4 (4%)	26 60
54	LF	186/215 (86%)	183 (98%)	3 (2%)	55 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	Lf	86/90 (96%)	85 (99%)	1 (1%)	63 82
56	LE	184/252 (73%)	177 (96%)	7 (4%)	29 63
57	Le	113/121 (93%)	110 (97%)	3 (3%)	39 71
58	LD	239/250 (96%)	230 (96%)	9 (4%)	29 63
59	Ld	85/110 (77%)	83 (98%)	2 (2%)	43 73
60	LC	299/348 (86%)	293 (98%)	6 (2%)	48 76
61	Lc	82/97 (84%)	77 (94%)	5 (6%)	17 49
62	LB	339/346 (98%)	332 (98%)	7 (2%)	47 75
63	Lb	81/125 (65%)	77 (95%)	4 (5%)	22 56
64	LA	188/198 (95%)	186 (99%)	2 (1%)	65 83
65	La	117/120 (98%)	114 (97%)	3 (3%)	40 72
68	Sa	82/98 (84%)	79 (96%)	3 (4%)	30 64
71	SZ	22/103 (21%)	22 (100%)	0	100 100
72	ST	52/115 (45%)	50 (96%)	2 (4%)	29 63
73	SP	51/130 (39%)	45 (88%)	6 (12%)	5 22
75	SG	163/218 (75%)	152 (93%)	11 (7%)	15 46
76	SI	168/180 (93%)	159 (95%)	9 (5%)	20 53
78	SS	59/132 (45%)	54 (92%)	5 (8%)	10 36
80	SU	92/107 (86%)	86 (94%)	6 (6%)	15 47
All	All	8355/10570 (79%)	8056 (96%)	299 (4%)	32 65

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Lm	79	GLU
2	Ll	9	ILE
2	Ll	27	ILE
2	Ll	34	ILE
2	Ll	36	ARG
2	Ll	47	THR
3	Lo	4	VAL
3	Lo	10	THR
3	Lo	23	VAL
3	Lo	28	LYS
3	Lo	68	LEU

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Mol	Chain	Res	Type
3	Lo	93	LEU
3	Lo	99	ARG
4	SY	26	ASP
4	SY	69	THR
4	SY	117	VAL
5	SX	7	LEU
5	SX	19	ASP
5	SX	66	ILE
5	SX	82	THR
5	SX	105	PHE
6	SW	27	ILE
6	SW	69	LEU
6	SW	80	ASP
6	SW	81	VAL
6	SW	83	LEU
6	SW	104	LEU
6	SW	105	THR
6	SW	120	HIS
7	SV	11	LEU
8	SR	22	THR
8	SR	24	LEU
8	SR	30	THR
8	SR	85	VAL
8	SR	87	GLU
8	SR	91	LEU
8	SR	105	MET
8	SR	116	ASN
8	SR	124	VAL
10	SO	46	ASP
10	SO	88	LEU
10	SO	97	LEU
10	SO	116	LEU
10	SO	151	LEU
11	SN	83	ASP
11	SN	125	LEU
12	SL	18	GLN
12	SL	125	ILE
14	SJ	15	THR
14	SJ	25	LEU
14	SJ	26	ASP
14	SJ	50	LEU
14	SJ	92	MET

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Mol	Chain	Res	Type
15	SH	20	GLU
15	SH	30	LEU
15	SH	43	LEU
15	SH	60	ILE
15	SH	69	LEU
15	SH	80	VAL
15	SH	92	VAL
15	SH	153	LEU
17	SF	19	LEU
17	SF	76	MET
17	SF	124	ASP
18	SE	12	VAL
18	SE	80	ILE
18	SE	102	ILE
18	SE	133	THR
18	SE	173	ILE
19	Se	103	THR
19	Se	132	ASN
20	SD	21	LEU
20	SD	137	VAL
20	SD	141	LYS
20	SD	165	ASN
20	SD	170	THR
20	SD	186	VAL
21	Sd	30	LEU
21	Sd	36	LEU
21	Sd	53	ILE
22	SC	63	VAL
22	SC	172	ASN
22	SC	174	ILE
22	SC	184	VAL
22	SC	191	VAL
22	SC	192	LEU
22	SC	233	LEU
22	SC	259	THR
23	Sc	51	ARG
24	SB	47	THR
24	SB	52	THR
24	SB	57	ILE
24	SB	91	VAL
24	SB	92	GLN
24	SB	128	LYS

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Mol	Chain	Res	Type
24	SB	131	ASP
24	SB	135	LEU
24	SB	168	MET
24	SB	188	LEU
25	Sb	37	CYS
26	SA	46	ILE
26	SA	134	LEU
26	SA	177	MET
26	SA	206	ASP
27	LZ	10	VAL
27	LZ	27	LYS
27	LZ	53	VAL
27	LZ	87	VAL
27	LZ	89	ILE
27	LZ	103	ASP
27	LZ	106	LEU
27	LZ	113	GLU
28	LY	87	ARG
29	LX	45	THR
29	LX	81	LEU
29	LX	82	THR
29	LX	116	LEU
29	LX	126	THR
30	LW	30	GLN
30	LW	37	GLU
30	LW	57	ARG
31	LV	15	ARG
31	LV	28	CYS
31	LV	57	VAL
31	LV	71	GLU
31	LV	128	LEU
32	LU	43	LEU
32	LU	61	VAL
32	LU	62	THR
32	LU	69	LYS
33	LT	38	ASP
33	LT	111	GLU
33	LT	124	THR
34	LS	51	LEU
34	LS	62	VAL
34	LS	75	VAL
34	LS	90	THR

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Mol	Chain	Res	Type
34	LS	150	ILE
34	LS	170	LYS
35	LR	3	MET
35	LR	27	ASN
36	Lr	5	LEU
36	Lr	99	LYS
36	Lr	124	VAL
37	LQ	42	THR
37	LQ	90	VAL
37	LQ	92	VAL
37	LQ	98	LEU
37	LQ	108	ARG
37	LQ	128	LEU
38	LP	75	GLN
38	LP	107	LEU
39	Lp	22	LEU
39	Lp	74	THR
40	LO	6	VAL
40	LO	43	ILE
40	LO	159	LYS
40	LO	174	LEU
40	LO	196	LEU
41	LN	10	LEU
41	LN	43	THR
41	LN	60	VAL
42	Ln	21	ARG
43	LM	33	GLN
43	LM	43	THR
44	LL	67	HIS
44	LL	70	VAL
44	LL	149	GLN
44	LL	160	VAL
44	LL	171	GLU
44	LL	197	LYS
45	Lk	26	LYS
45	Lk	32	VAL
45	Lk	36	VAL
45	Lk	56	LEU
46	LJ	17	ILE
46	LJ	49	VAL
46	LJ	56	THR
46	LJ	95	ARG

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Mol	Chain	Res	Type
46	LJ	110	GLN
46	LJ	112	HIS
46	LJ	150	CYS
47	Lj	33	THR
47	Lj	57	ASN
47	Lj	69	ILE
48	LI	66	GLU
48	LI	148	VAL
49	Li	43	MET
49	Li	79	THR
49	Li	85	ARG
50	LH	135	SER
50	LH	163	GLN
51	Lh	71	LYS
51	Lh	94	ARG
51	Lh	112	ARG
51	Lh	116	LEU
52	LG	97	LYS
52	LG	108	GLN
52	LG	113	ARG
52	LG	114	LEU
52	LG	155	VAL
53	Lg	54[A]	ARG
53	Lg	54[B]	ARG
53	Lg	73	HIS
53	Lg	86	CYS
54	LF	50	ILE
54	LF	187	MET
54	LF	239	GLN
55	Lf	105	LEU
56	LE	49	VAL
56	LE	93	THR
56	LE	121	VAL
56	LE	163	VAL
56	LE	179	LEU
56	LE	287	VAL
56	LE	288	PHE
57	Le	26	ASP
57	Le	78	LEU
57	Le	94	SER
58	LD	36	LEU
58	LD	93	THR

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Mol	Chain	Res	Type
58	LD	111	ASN
58	LD	155	THR
58	LD	157	ASN
58	LD	194	VAL
58	LD	222	GLN
58	LD	231	VAL
58	LD	235	MET
59	Ld	20	VAL
59	Ld	122	VAL
60	LC	10	VAL
60	LC	144	ILE
60	LC	174	LEU
60	LC	254	GLU
60	LC	289	LEU
60	LC	308	LYS
61	Lc	18	LEU
61	Lc	55	LEU
61	Lc	68	LYS
61	Lc	93	THR
61	Lc	94	LEU
62	LB	69	LYS
62	LB	90	VAL
62	LB	149	ASP
62	LB	199	GLU
62	LB	218	ASP
62	LB	348	ARG
62	LB	360	LEU
63	Lb	9	THR
63	Lb	106	LYS
63	Lb	107	ARG
63	Lb	112	ILE
64	LA	80	GLU
64	LA	208	GLU
65	La	8	THR
65	La	15	VAL
65	La	125	LYS
68	Sa	15	ARG
68	Sa	19	GLN
68	Sa	74	CYS
72	ST	23	LYS
72	ST	104	LEU
73	SP	16	THR

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Mol	Chain	Res	Type
73	SP	35	GLN
73	SP	80	LEU
73	SP	89	MET
73	SP	94	VAL
73	SP	96	VAL
75	SG	16	ILE
75	SG	65	GLN
75	SG	69	THR
75	SG	97	VAL
75	SG	106	LEU
75	SG	112	VAL
75	SG	114	VAL
75	SG	127	THR
75	SG	136	LYS
75	SG	144	LEU
75	SG	177	GLN
76	SI	7	ASN
76	SI	18	ARG
76	SI	22	HIS
76	SI	76	THR
76	SI	82	VAL
76	SI	121	LEU
76	SI	137	LEU
76	SI	143	LYS
76	SI	147	LYS
78	SS	13	LEU
78	SS	16	LEU
78	SS	83	PHE
78	SS	111	LEU
78	SS	139	THR
80	SU	22	ILE
80	SU	39	LEU
80	SU	48	LEU
80	SU	89	ILE
80	SU	106	ILE
80	SU	114	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ll	4	HIS
3	Lo	25	GLN

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Mol	Chain	Res	Type
4	SY	22	GLN
5	SX	16	HIS
5	SX	31	HIS
5	SX	63	ASN
7	SV	33	GLN
8	SR	29	HIS
11	SN	49	GLN
11	SN	105	ASN
12	SL	11	GLN
12	SL	94	HIS
12	SL	112	HIS
12	SL	141	ASN
13	SK	28	HIS
13	SK	32	HIS
14	SJ	75	ASN
14	SJ	113	GLN
14	SJ	154	GLN
17	SF	36	GLN
18	SE	17	HIS
18	SE	36	HIS
18	SE	138	HIS
20	SD	159	HIS
21	Sd	3	HIS
25	Sb	9	HIS
25	Sb	51	GLN
26	SA	9	GLN
27	LZ	132	GLN
28	LY	20	ASN
29	LX	105	ASN
29	LX	111	GLN
32	LU	94	ASN
33	LT	66	ASN
33	LT	131	GLN
33	LT	144	ASN
34	LS	108	GLN
36	Lr	4	HIS
36	Lr	6	GLN
36	Lr	31	ASN
36	Lr	41	ASN
37	LQ	7	HIS
37	LQ	162	HIS
38	LP	97	ASN

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Mol	Chain	Res	Type
38	LP	133	HIS
40	LO	63	ASN
40	LO	180	GLN
41	LN	32	GLN
41	LN	109	HIS
43	LM	33	GLN
43	LM	66	HIS
43	LM	70	GLN
44	LL	104	ASN
44	LL	175	ASN
44	LL	188	ASN
46	LJ	71	HIS
47	Lj	13	ASN
50	LH	140	GLN
50	LH	163	GLN
50	LH	188	GLN
52	LG	38	ASN
52	LG	225	ASN
53	Lg	100	GLN
54	LF	80	ASN
54	LF	99	ASN
54	LF	119	ASN
54	LF	126	ASN
55	Lf	99	HIS
56	LE	157	HIS
57	Le	52	GLN
57	Le	81	ASN
58	LD	131	ASN
58	LD	267	ASN
58	LD	282	GLN
59	Ld	34	HIS
60	LC	116	ASN
60	LC	142	HIS
60	LC	212	ASN
60	LC	362	GLN
62	LB	123	HIS
62	LB	138	GLN
62	LB	203	GLN
63	Lb	11	ASN
63	Lb	60	ASN
64	LA	86	GLN
65	La	120	GLN

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Mol	Chain	Res	Type
68	Sa	17	HIS
72	ST	11	GLN
76	SI	167	GLN
78	SS	135	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
66	L7	118/119 (99%)	11 (9%)	0
67	Pt	76/77 (98%)	16 (21%)	0
69	L8	151/156 (96%)	26 (17%)	0
70	L5	3414/5069 (67%)	552 (16%)	10 (0%)
74	S2	1550/1869 (82%)	269 (17%)	6 (0%)
77	S6	55/75 (73%)	18 (32%)	1 (1%)
79	mR	6/27 (22%)	2 (33%)	0
All	All	5370/7392 (72%)	894 (16%)	17 (0%)

All (894) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
66	L7	7	G
66	L7	25	G
66	L7	31	G
66	L7	33	U
66	L7	53	U
66	L7	54	A
66	L7	64	G
66	L7	97	G
66	L7	100	A
66	L7	102	U
66	L7	110	G
67	Pt	9	G
67	Pt	15	G
67	Pt	16	C
67	Pt	17	C
67	Pt	18	C
67	Pt	19	G
67	Pt	20	G
67	Pt	21	H2U
67	Pt	22	A
67	Pt	32	G

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Mol	Chain	Res	Type
67	Pt	47	G7M
67	Pt	48	U
67	Pt	49	C
67	Pt	62	C
67	Pt	71	G
67	Pt	72	C
69	L8	23	C
69	L8	25	G
69	L8	34	U
69	L8	35	C
69	L8	51	U
69	L8	59	A
69	L8	62	A
69	L8	63	U
69	L8	80	A
69	L8	84	A
69	L8	85	U
69	L8	87	G
69	L8	103	A
69	L8	105	C
69	L8	106	G
69	L8	110	U
69	L8	111	U
69	L8	114	G
69	L8	123	U
69	L8	124	U
69	L8	125	C
69	L8	127	U
69	L8	141	C
69	L8	142	U
69	L8	150	C
69	L8	156	U
70	L5	5	A
70	L5	9	C
70	L5	15	A
70	L5	39	A
70	L5	42	A
70	L5	48	G
70	L5	56	A
70	L5	59	A
70	L5	64	A
70	L5	65	A

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Mol	Chain	Res	Type
70	L5	71	C
70	L5	85	G
70	L5	91	G
70	L5	98	A
70	L5	108	A
70	L5	110	C
70	L5	112	C
70	L5	119	G
70	L5	120	A
70	L5	131	C
70	L5	139	G
70	L5	159	C
70	L5	160	G
70	L5	161	G
70	L5	162	A
70	L5	168	C
70	L5	169	G
70	L5	172	C
70	L5	173	C
70	L5	174	C
70	L5	175	C
70	L5	200	U
70	L5	207	G
70	L5	209	U
70	L5	216	C
70	L5	217	C
70	L5	218	A
70	L5	219	G
70	L5	220	C
70	L5	234	G
70	L5	253	G
70	L5	259	C
70	L5	266	C
70	L5	273	U
70	L5	274	C
70	L5	278	G
70	L5	280	G
70	L5	297	U
70	L5	306	A
70	L5	316	U
70	L5	340	C
70	L5	350	C

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Mol	Chain	Res	Type
70	L5	373	G
70	L5	387	G
70	L5	409	G
70	L5	410	A
70	L5	412	G
70	L5	414	C
70	L5	417	G
70	L5	431	G
70	L5	432	U
70	L5	448	G
70	L5	449	C
70	L5	451	C
70	L5	452	A
70	L5	453	G
70	L5	483	C
70	L5	484	U
70	L5	487	G
70	L5	489	C
70	L5	491	G
70	L5	492	U
70	L5	502	C
70	L5	503	C
70	L5	504	G
70	L5	510	U
70	L5	513	U
70	L5	514	U
70	L5	644	G
70	L5	647	G
70	L5	648	G
70	L5	661	C
70	L5	665	C
70	L5	666	G
70	L5	667	A
70	L5	669	C
70	L5	685	C
70	L5	696	C
70	L5	704	C
70	L5	705	G
70	L5	731	G
70	L5	738	C
70	L5	739	G
70	L5	740	G

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Mol	Chain	Res	Type
70	L5	742	G
70	L5	746	A
70	L5	760	G
70	L5	904	C
70	L5	913	U
70	L5	914	U
70	L5	915	A
70	L5	916	C
70	L5	917	A
70	L5	918	G
70	L5	925	C
70	L5	926	G
70	L5	932	A
70	L5	933	G
70	L5	935	A
70	L5	944	A
70	L5	958	G
70	L5	959	G
70	L5	960	A
70	L5	962	C
70	L5	963	G
70	L5	965	G
70	L5	966	A
70	L5	967	C
70	L5	968	C
70	L5	969	C
70	L5	970	G
70	L5	977	C
70	L5	982	U
70	L5	1070	G
70	L5	1072	C
70	L5	1084	C
70	L5	1170	G
70	L5	1181	C
70	L5	1182	C
70	L5	1183	C
70	L5	1199	G
70	L5	1200	G
70	L5	1210	C
70	L5	1211	G
70	L5	1214	C
70	L5	1215	C

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Mol	Chain	Res	Type
70	L5	1216	C
70	L5	1220	G
70	L5	1241	C
70	L5	1254	A
70	L5	1255	A
70	L5	1258	G
70	L5	1261	G
70	L5	1266	G
70	L5	1270	A
70	L5	1271	G
70	L5	1273	G
70	L5	1276	C
70	L5	1277	G
70	L5	1284	G
70	L5	1285	U
70	L5	1287	G
70	L5	1293	G
70	L5	1295	C
70	L5	1296	G
70	L5	1301	C
70	L5	1302	U
70	L5	1303	A
70	L5	1304	C
70	L5	1326	A2M
70	L5	1337	A
70	L5	1354	A
70	L5	1359	G
70	L5	1366	G
70	L5	1378	C
70	L5	1379	C
70	L5	1387	A
70	L5	1397	A
70	L5	1398	A
70	L5	1400	G
70	L5	1401	C
70	L5	1402	C
70	L5	1415	G
70	L5	1427	A
70	L5	1439	C
70	L5	1443	A
70	L5	1452	A
70	L5	1454	G

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Mol	Chain	Res	Type
70	L5	1476	C
70	L5	1477	C
70	L5	1478	C
70	L5	1479	G
70	L5	1481	C
70	L5	1483	C
70	L5	1484	G
70	L5	1485	C
70	L5	1486	C
70	L5	1498	G
70	L5	1502	G
70	L5	1523	A
70	L5	1525	A
70	L5	1534	A2M
70	L5	1535	C
70	L5	1547	A
70	L5	1564	A
70	L5	1566	C
70	L5	1574	G
70	L5	1578	U
70	L5	1591	U
70	L5	1596	U
70	L5	1612	G
70	L5	1614	C
70	L5	1624	G
70	L5	1625	OMG
70	L5	1631	A
70	L5	1633	G
70	L5	1634	A
70	L5	1640	C
70	L5	1641	G
70	L5	1654	G
70	L5	1661	C
70	L5	1676	C
70	L5	1677	PSU
70	L5	1678	C
70	L5	1691	G
70	L5	1697	G
70	L5	1698	C
70	L5	1703	C
70	L5	1704	C
70	L5	1720	C

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Mol	Chain	Res	Type
70	L5	1721	G
70	L5	1734	G
70	L5	1755	C
70	L5	1757	U
70	L5	1759	G
70	L5	1773	U
70	L5	1774	C
70	L5	1776	A
70	L5	1787	A
70	L5	1794	A
70	L5	1803	G
70	L5	1804	A
70	L5	1805	A
70	L5	1806	G
70	L5	1821	G
70	L5	1836	G
70	L5	1837	A
70	L5	1842	G
70	L5	1843	A
70	L5	1855	G
70	L5	1869	G
70	L5	1889	U
70	L5	1897	A
70	L5	1915	C
70	L5	1918	U
70	L5	1919	G
70	L5	1921	C
70	L5	1922	G
70	L5	1925	G
70	L5	1931	C
70	L5	1932	A
70	L5	1940	G
70	L5	1948	G
70	L5	1951	G
70	L5	1959	U
70	L5	1969	G
70	L5	2025	A
70	L5	2026	A
70	L5	2046	G
70	L5	2048	U
70	L5	2055	G
70	L5	2056	G

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Mol	Chain	Res	Type
70	L5	2069	A
70	L5	2084	C
70	L5	2085	G
70	L5	2092	G
70	L5	2093	A
70	L5	2095	A
70	L5	2097	U
70	L5	2098	G
70	L5	2102	G
70	L5	2108	G
70	L5	2258	C
70	L5	2260	C
70	L5	2261	G
70	L5	2279	A
70	L5	2289	C
70	L5	2300	A
70	L5	2301	G
70	L5	2306	G
70	L5	2313	A
70	L5	2331	G
70	L5	2348	G
70	L5	2351	OMC
70	L5	2360	A
70	L5	2381	A
70	L5	2395	A
70	L5	2397	G
70	L5	2398	U
70	L5	2417	A
70	L5	2421	G
70	L5	2425	U
70	L5	2447	U
70	L5	2450	G
70	L5	2453	A
70	L5	2469	C
70	L5	2471	G
70	L5	2474	G
70	L5	2503	G
70	L5	2513	A
70	L5	2518	G
70	L5	2519	U
70	L5	2520	C
70	L5	2529	A

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Mol	Chain	Res	Type
70	L5	2542	G
70	L5	2554	U
70	L5	2573	A
70	L5	2577	C
70	L5	2587	A
70	L5	2589	C
70	L5	2601	A
70	L5	2602	G
70	L5	2627	C
70	L5	2653	C
70	L5	2658	G
70	L5	2659	A
70	L5	2669	C
70	L5	2681	G
70	L5	2687	U
70	L5	2688	G
70	L5	2694	G
70	L5	2695	A
70	L5	2696	A
70	L5	2711	G
70	L5	2714	G
70	L5	2724	G
70	L5	2726	G
70	L5	2743	A
70	L5	2754	G
70	L5	2760	G
70	L5	2788	U
70	L5	2790	U
70	L5	2798	A
70	L5	2814	C
70	L5	2826	U
70	L5	2827	G
70	L5	2829	U
70	L5	2855	G
70	L5	2866	C
70	L5	2867	C
70	L5	2871	A
70	L5	2902	G
70	L5	3597	G
70	L5	3604	A
70	L5	3606	U
70	L5	3615	G

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Mol	Chain	Res	Type
70	L5	3618	C
70	L5	3619	G
70	L5	3626	G
70	L5	3635	A
70	L5	3644	U
70	L5	3646	A
70	L5	3648	A
70	L5	3662	A
70	L5	3664	G
70	L5	3673	C
70	L5	3711	A
70	L5	3712	A
70	L5	3727	A
70	L5	3729	PSU
70	L5	3732	A
70	L5	3733	A
70	L5	3750	G
70	L5	3753	G
70	L5	3759	A
70	L5	3760	A2M
70	L5	3761	C
70	L5	3762	PSU
70	L5	3776	G
70	L5	3777	G
70	L5	3783	A
70	L5	3784	A
70	L5	3785	A2M
70	L5	3786	U
70	L5	3787	G
70	L5	3791	C
70	L5	3811	G
70	L5	3812	C
70	L5	3814	U
70	L5	3816	A
70	L5	3817	A
70	L5	3818	U
70	L5	3819	G
70	L5	3824	A
70	L5	3838	U
70	L5	3839	G
70	L5	3840	U
70	L5	3844	PSU

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Mol	Chain	Res	Type
70	L5	3876	A
70	L5	3877	A
70	L5	3878	C
70	L5	3879	G
70	L5	3897	G
70	L5	3901	A
70	L5	3905	A
70	L5	3906	A
70	L5	3907	G
70	L5	3908	A
70	L5	3915	U
70	L5	3948	C
70	L5	3951	G
70	L5	3952	A
70	L5	4072	C
70	L5	4076	G
70	L5	4084	G
70	L5	4093	G
70	L5	4094	G
70	L5	4095	G
70	L5	4096	C
70	L5	4097	G
70	L5	4116	C
70	L5	4118	U
70	L5	4119	C
70	L5	4121	G
70	L5	4122	G
70	L5	4127	A
70	L5	4150	G
70	L5	4162	C
70	L5	4163	U
70	L5	4170	A
70	L5	4183	G
70	L5	4184	G
70	L5	4191	G
70	L5	4196	OMG
70	L5	4203	A
70	L5	4222	G
70	L5	4229	U
70	L5	4233	A
70	L5	4234	A
70	L5	4251	A

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Mol	Chain	Res	Type
70	L5	4254	G
70	L5	4266	G
70	L5	4268	A
70	L5	4273	A
70	L5	4280	A
70	L5	4281	A
70	L5	4282	A
70	L5	4291	G
70	L5	4297	G
70	L5	4304	A
70	L5	4305	G
70	L5	4314	C
70	L5	4330	G
70	L5	4332	C
70	L5	4339	A
70	L5	4349	C
70	L5	4350	C
70	L5	4354	U
70	L5	4355	G
70	L5	4373	G
70	L5	4376	A
70	L5	4377	G
70	L5	4378	A
70	L5	4379	A
70	L5	4387	C
70	L5	4391	G
70	L5	4393	G
70	L5	4394	A
70	L5	4415	A
70	L5	4420	PSU
70	L5	4421	C
70	L5	4440	G
70	L5	4448	G
70	L5	4449	A
70	L5	4464	A
70	L5	4465	U
70	L5	4488	A
70	L5	4512	U
70	L5	4513	A
70	L5	4515	G
70	L5	4519	C
70	L5	4524	G

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Mol	Chain	Res	Type
70	L5	4528	G
70	L5	4529	G
70	L5	4548	A
70	L5	4560	C
70	L5	4567	G
70	L5	4570	G
70	L5	4575	G
70	L5	4584	A
70	L5	4590	A2M
70	L5	4600	G
70	L5	4606	G
70	L5	4609	G
70	L5	4610	A
70	L5	4636	PSU
70	L5	4637	OMG
70	L5	4639	G
70	L5	4652	G
70	L5	4656	A
70	L5	4657	U
70	L5	4670	C
70	L5	4672	A
70	L5	4695	C
70	L5	4700	A
70	L5	4703	U
70	L5	4708	A
70	L5	4709	U
70	L5	4721	G
70	L5	4739	C
70	L5	4740	G
70	L5	4741	C
70	L5	4742	G
70	L5	4743	G
70	L5	4750	G
70	L5	4754	G
70	L5	4757	C
70	L5	4759	C
70	L5	4761	G
70	L5	4765	G
70	L5	4771	C
70	L5	4772	C
70	L5	4773	C
70	L5	4775	C

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Mol	Chain	Res	Type
70	L5	4776	G
70	L5	4860	G
70	L5	4864	U
70	L5	4870	G
70	L5	4871	C
70	L5	4882	U
70	L5	4883	C
70	L5	4889	G
70	L5	4890	G
70	L5	4895	C
70	L5	4900	C
70	L5	4901	G
70	L5	4910	G
70	L5	4912	G
70	L5	4913	G
70	L5	4914	C
70	L5	4931	G
70	L5	4934	A
70	L5	4943	A
70	L5	4957	C
70	L5	4967	A
70	L5	4976	U
70	L5	4988	U
70	L5	4989	U
70	L5	4990	C
70	L5	4991	U
70	L5	4994	G
70	L5	5006	U
70	L5	5007	A
70	L5	5013	C
70	L5	5017	G
70	L5	5034	A
70	L5	5041	G
70	L5	5050	C
70	L5	5054	C
70	L5	5055	G
70	L5	5061	A
70	L5	5062	G
74	S2	17	C
74	S2	26	U
74	S2	33	G
74	S2	41	G

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Mol	Chain	Res	Type
74	S2	46	A
74	S2	56	G
74	S2	58	C
74	S2	65	C
74	S2	67	C
74	S2	68	A
74	S2	71	G
74	S2	97	U
74	S2	103	A
74	S2	113	G
74	S2	114	G
74	S2	115	U
74	S2	143	U
74	S2	148	U
74	S2	161	U
74	S2	162	C
74	S2	168	C
74	S2	170	A
74	S2	183	G
74	S2	184	G
74	S2	185	G
74	S2	186	C
74	S2	187	G
74	S2	190	G
74	S2	191	A
74	S2	192	C
74	S2	208	G
74	S2	214	U
74	S2	292	A
74	S2	295	C
74	S2	298	G
74	S2	305	U
74	S2	306	C
74	S2	307	G
74	S2	308	G
74	S2	309	G
74	S2	312	G
74	S2	319	C
74	S2	320	C
74	S2	321	U
74	S2	332	G
74	S2	339	A

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Mol	Chain	Res	Type
74	S2	340	C
74	S2	362	C
74	S2	364	A
74	S2	369	C
74	S2	370	G
74	S2	385	G
74	S2	386	C
74	S2	407	G
74	S2	409	C
74	S2	421	G
74	S2	448	A
74	S2	449	A
74	S2	450	C
74	S2	452	G
74	S2	464	A
74	S2	465	A
74	S2	466	G
74	S2	471	G
74	S2	472	C
74	S2	473	A
74	S2	474	G
74	S2	482	G
74	S2	487	U
74	S2	488	U
74	S2	492	C
74	S2	493	A
74	S2	496	C
74	S2	502	C
74	S2	507	G
74	S2	508	A
74	S2	516	A
74	S2	525	A
74	S2	533	A
74	S2	554	A
74	S2	556	U
74	S2	559	G
74	S2	560	A
74	S2	563	G
74	S2	564	A
74	S2	568	C
74	S2	576	A2M
74	S2	589	G

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Mol	Chain	Res	Type
74	S2	590	A2M
74	S2	591	U
74	S2	604	A
74	S2	607	U
74	S2	614	C
74	S2	626	G
74	S2	627	OMU
74	S2	628	A
74	S2	643	A
74	S2	644	OMG
74	S2	655	A
74	S2	659	G
74	S2	660	C
74	S2	668	A2M
74	S2	669	A
74	S2	671	A
74	S2	672	A
74	S2	673	G
74	S2	688	U
74	S2	690	G
74	S2	797	C
74	S2	799	U
74	S2	821	G
74	S2	822	PSU
74	S2	845	G
74	S2	847	A
74	S2	861	A
74	S2	869	A
74	S2	870	A
74	S2	876	C
74	S2	877	C
74	S2	878	G
74	S2	879	C
74	S2	881	G
74	S2	883	U
74	S2	908	A
74	S2	913	A
74	S2	914	U
74	S2	920	A
74	S2	922	A
74	S2	933	G
74	S2	934	G

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Mol	Chain	Res	Type
74	S2	943	U
74	S2	971	G
74	S2	990	A
74	S2	992	A
74	S2	997	A
74	S2	999	G
74	S2	1017	U
74	S2	1023	A
74	S2	1026	C
74	S2	1027	A
74	S2	1045	U
74	S2	1049	A
74	S2	1061	U
74	S2	1062	A
74	S2	1067	C
74	S2	1080	A
74	S2	1083	A
74	S2	1085	C
74	S2	1096	G
74	S2	1109	C
74	S2	1115	U
74	S2	1119	A
74	S2	1121	G
74	S2	1138	C
74	S2	1153	C
74	S2	1154	U
74	S2	1155	U
74	S2	1157	G
74	S2	1171	G
74	S2	1188	A
74	S2	1195	A
74	S2	1207	G
74	S2	1208	A
74	S2	1215	C
74	S2	1224	G
74	S2	1242	U
74	S2	1243	PSU
74	S2	1245	G
74	S2	1247	C
74	S2	1251	A
74	S2	1253	A
74	S2	1256	G

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Mol	Chain	Res	Type
74	S2	1257	G
74	S2	1258	A
74	S2	1259	A
74	S2	1262	C
74	S2	1264	C
74	S2	1271	C
74	S2	1274	G
74	S2	1275	G
74	S2	1301	A
74	S2	1302	G
74	S2	1303	C
74	S2	1305	C
74	S2	1325	G
74	S2	1326	U
74	S2	1327	G
74	S2	1330	G
74	S2	1341	C
74	S2	1342	U
74	S2	1358	U
74	S2	1371	U
74	S2	1372	U
74	S2	1373	C
74	S2	1375	G
74	S2	1378	A
74	S2	1397	U
74	S2	1403	C
74	S2	1404	U
74	S2	1405	A
74	S2	1415	C
74	S2	1439	A
74	S2	1440	C
74	S2	1442	U
74	S2	1447	G
74	S2	1454	A
74	S2	1462	U
74	S2	1463	U
74	S2	1464	C
74	S2	1477	U
74	S2	1489	A
74	S2	1490	OMG
74	S2	1494	U
74	S2	1495	G

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Mol	Chain	Res	Type
74	S2	1498	A
74	S2	1509	U
74	S2	1520	G
74	S2	1521	C
74	S2	1522	A
74	S2	1533	A
74	S2	1548	G
74	S2	1558	C
74	S2	1560	U
74	S2	1570	G
74	S2	1579	A
74	S2	1580	A
74	S2	1585	U
74	S2	1586	U
74	S2	1587	G
74	S2	1588	A
74	S2	1598	G
74	S2	1599	U
74	S2	1601	A
74	S2	1604	G
74	S2	1606	G
74	S2	1610	G
74	S2	1614	A
74	S2	1623	A
74	S2	1637	A
74	S2	1638	G
74	S2	1648	G
74	S2	1654	G
74	S2	1665	G
74	S2	1671	G
74	S2	1680	G
74	S2	1699	A
74	S2	1720	U
74	S2	1721	U
74	S2	1722	G
74	S2	1733	U
74	S2	1735	A
74	S2	1736	G
74	S2	1744	G
74	S2	1750	C
74	S2	1785	C
74	S2	1816	G

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Mol	Chain	Res	Type
74	S2	1824	A
74	S2	1825	A
74	S2	1829	G
74	S2	1831	A
74	S2	1835	A
74	S2	1838	U
74	S2	1849	G
74	S2	1851	MA6
74	S2	1861	G
74	S2	1862	G
74	S2	1863	A
74	S2	1864	U
74	S2	1865	C
77	S6	9	U
77	S6	10	G
77	S6	11	G
77	S6	12	C
77	S6	17	C
77	S6	18	G
77	S6	38	A
77	S6	39	C
77	S6	40	C
77	S6	43	G
77	S6	44	A
77	S6	45	G
77	S6	46	G
77	S6	50	A
77	S6	58	A
77	S6	61	C
77	S6	62	C
77	S6	76	A
79	mR	37	A
79	mR	39	G

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
70	L5	491	G
70	L5	934	C
70	L5	1303	A
70	L5	1399	G
70	L5	1483	C

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Mol	Chain	Res	Type
70	L5	1563	A
70	L5	1633	G
70	L5	2541	G
70	L5	4281	A
70	L5	4699	U
74	S2	96	C
74	S2	169	U
74	S2	912	C
74	S2	1244	PSU
74	S2	1508	A
74	S2	1598	G
77	S6	60	A

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

208 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	$\#\|Z\| > 2$
70	A2M	L5	2815	70	22,25,26	3.42	9 (40%)	31,36,39	2.41	10 (32%)
70	PSU	L5	4636	70	18,21,22	1.06	1 (5%)	22,30,33	1.80	3 (13%)
74	OMG	S2	644	74	23,26,27	2.42	8 (34%)	33,38,41	2.04	10 (30%)
70	OMG	L5	4196	70	23,26,27	2.43	8 (34%)	33,38,41	2.02	10 (30%)
70	OMG	L5	4228	70	23,26,27	2.42	9 (39%)	33,38,41	2.09	10 (30%)
74	PSU	S2	1692	74	18,21,22	1.05	1 (5%)	22,30,33	1.67	4 (18%)
70	PSU	L5	2843	70	18,21,22	1.04	1 (5%)	22,30,33	1.86	4 (18%)
70	PSU	L5	3729	70	18,21,22	1.10	1 (5%)	22,30,33	1.76	4 (18%)
70	PSU	L5	3853	84,70	18,21,22	1.09	1 (5%)	22,30,33	1.69	4 (18%)
70	PSU	L5	3884	70	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
70	PSU	L5	1536	70	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
65	V5N	La	39	65	9,11,12	2.68	2 (22%)	9,14,16	1.27	1 (11%)
70	PSU	L5	4569	70	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	PSU	L5	3762	70	18,21,22	1.09	1 (5%)	22,30,33	1.63	4 (18%)
70	A2M	L5	3718	70	22,25,26	3.42	9 (40%)	31,36,39	2.36	9 (29%)
70	A2M	L5	3825	70	22,25,26	3.43	10 (45%)	31,36,39	2.40	11 (35%)
74	PSU	S2	109	74	18,21,22	1.11	1 (5%)	22,30,33	1.78	4 (18%)
70	OMG	L5	1316	70	23,26,27	2.43	8 (34%)	33,38,41	2.03	10 (30%)
74	PSU	S2	815	74	18,21,22	0.98	1 (5%)	22,30,33	1.65	4 (18%)
70	PSU	L5	3695	70	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
70	PSU	L5	3844	70	18,21,22	1.00	1 (5%)	22,30,33	1.75	4 (18%)
74	OMU	S2	1804	74	19,22,23	3.04	8 (42%)	26,31,34	1.70	4 (15%)
74	MA6	S2	1851	74	23,26,27	1.37	4 (17%)	34,38,41	3.78	11 (32%)
70	OMC	L5	2422	84,70	19,22,23	2.99	8 (42%)	26,31,34	0.78	0
70	PSU	L5	3920	83,70	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
70	OMG	L5	3792	70	23,26,27	2.41	8 (34%)	33,38,41	2.05	9 (27%)
70	PSU	L5	3770	70	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
74	PSU	S2	1174	74	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
74	OMC	S2	517	74	19,22,23	3.00	8 (42%)	26,31,34	0.77	0
70	OMG	L5	4637	70	23,26,27	2.40	8 (34%)	33,38,41	2.07	10 (30%)
74	4AC	S2	1337	74	21,24,25	3.47	9 (42%)	29,34,37	1.03	2 (6%)
70	OMC	L5	1340	70	19,22,23	2.94	8 (42%)	26,31,34	0.76	0
70	OMC	L5	2824	70	19,22,23	3.02	8 (42%)	26,31,34	0.75	0
67	4SU	Pt	8	67	18,21,22	3.51	7 (38%)	26,30,33	2.20	5 (19%)
64	V5N	LA	216	64	9,11,12	2.65	2 (22%)	9,14,16	1.18	1 (11%)
74	OMU	S2	428	74	19,22,23	2.98	8 (42%)	26,31,34	1.73	4 (15%)
63	MLZ	Lb	5	63	8,9,10	0.77	0	4,9,11	0.65	0
70	PSU	L5	1779	70	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
74	A2M	S2	512	74	22,25,26	3.39	10 (45%)	31,36,39	2.47	10 (32%)
74	PSU	S2	651	74	18,21,22	1.03	1 (5%)	22,30,33	1.71	4 (18%)
70	PSU	L5	4353	70	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
70	OMU	L5	4498	70	19,22,23	2.99	8 (42%)	26,31,34	1.70	4 (15%)
70	PSU	L5	4628	70	18,21,22	1.06	1 (5%)	22,30,33	1.87	4 (18%)
74	PSU	S2	1056	74	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
74	A2M	S2	1678	74	22,25,26	3.49	9 (40%)	31,36,39	2.53	11 (35%)
74	A2M	S2	668	83,74	22,25,26	3.40	10 (45%)	31,36,39	2.45	11 (35%)
70	PSU	L5	3764	70	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
70	OMC	L5	2351	70	19,22,23	2.95	8 (42%)	26,31,34	1.08	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	PSU	L5	4552	70	18,21,22	1.02	1 (5%)	22,30,33	1.71	4 (18%)
70	PSU	L5	4493	70	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
70	OMU	L5	2837	70	19,22,23	2.98	8 (42%)	26,31,34	1.77	5 (19%)
70	OMG	L5	4370	70	23,26,27	2.41	8 (34%)	33,38,41	2.06	9 (27%)
70	OMG	L5	2424	70	23,26,27	2.43	8 (34%)	33,38,41	2.03	9 (27%)
70	PSU	L5	1683	70	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
70	PSU	L5	3639	70	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
70	PSU	L5	4689	70	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	S2	296	74	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
70	OMC	L5	2365	83,70	19,22,23	2.94	8 (42%)	26,31,34	0.68	0
74	PSU	S2	866	74	18,21,22	1.11	1 (5%)	22,30,33	1.76	4 (18%)
69	OMG	L8	75	69	23,26,27	2.44	8 (34%)	33,38,41	2.04	10 (30%)
3	MLZ	Lo	53	3	8,9,10	0.73	0	4,9,11	0.61	0
70	A2M	L5	1524	70	22,25,26	3.41	10 (45%)	31,36,39	2.47	11 (35%)
70	OMC	L5	3887	70	19,22,23	2.97	8 (42%)	26,31,34	0.77	0
74	PSU	S2	1232	74	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
70	OMC	L5	3808	70	19,22,23	2.94	8 (42%)	26,31,34	0.85	0
74	4AC	S2	1842	74	21,24,25	3.34	9 (42%)	29,34,37	1.06	3 (10%)
70	PSU	L5	4532	70	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
70	OMG	L5	4618	70	23,26,27	2.41	8 (34%)	33,38,41	2.06	10 (30%)
74	A2M	S2	99	83,74	22,25,26	3.44	9 (40%)	31,36,39	2.35	10 (32%)
70	PSU	L5	4442	70	18,21,22	1.03	1 (5%)	22,30,33	1.73	5 (22%)
74	A2M	S2	1383	74	22,25,26	3.42	9 (40%)	31,36,39	2.38	9 (29%)
74	OMG	S2	867	74	23,26,27	2.41	8 (34%)	33,38,41	2.07	10 (30%)
74	PSU	S2	1239	74	18,21,22	1.05	1 (5%)	22,30,33	1.74	3 (13%)
74	OMC	S2	1703	74	19,22,23	3.00	8 (42%)	26,31,34	0.71	0
74	MA6	S2	1850	74	23,26,27	1.38	4 (17%)	34,38,41	3.66	11 (32%)
67	G7M	Pt	47	67	23,26,27	2.63	9 (39%)	35,39,42	2.46	11 (31%)
74	OMC	S2	1391	74	19,22,23	2.98	8 (42%)	26,31,34	0.79	0
70	PSU	L5	3851	70	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
70	6MZ	L5	4220	70	22,25,26	2.62	4 (18%)	30,36,39	2.30	11 (36%)
70	A2M	L5	3867	70	22,25,26	3.43	9 (40%)	31,36,39	2.43	10 (32%)
70	OMU	L5	4620	70	19,22,23	2.93	8 (42%)	26,31,34	1.67	4 (15%)
74	PSU	S2	105	74	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
74	PSU	S2	649	74	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
74	PSU	S2	1238	74	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
74	OMG	S2	1490	74	23,26,27	2.41	8 (34%)	33,38,41	2.02	10 (30%)
70	OMG	L5	4499	70	23,26,27	2.43	8 (34%)	33,38,41	2.04	10 (30%)
74	A2M	S2	468	74	22,25,26	3.43	9 (40%)	31,36,39	2.32	10 (32%)
74	PSU	S2	1367	74	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
70	PSU	L5	4576	70	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
70	UR3	L5	4530	70	19,22,23	2.77	7 (36%)	26,32,35	1.34	2 (7%)
74	PSU	S2	1081	74	18,21,22	0.96	1 (5%)	22,30,33	1.70	2 (9%)
74	PSU	S2	1243	74	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
70	A2M	L5	1871	70	22,25,26	3.48	9 (40%)	31,36,39	2.39	10 (32%)
70	PSU	L5	1860	70	18,21,22	1.05	1 (5%)	22,30,33	1.69	4 (18%)
70	PSU	L5	4361	70	18,21,22	1.02	1 (5%)	22,30,33	1.73	4 (18%)
70	PSU	L5	4431	70	18,21,22	1.11	1 (5%)	22,30,33	1.71	4 (18%)
74	PSU	S2	36	74	18,21,22	1.03	1 (5%)	22,30,33	1.76	4 (18%)
74	OMU	S2	627	74	19,22,23	3.03	8 (42%)	26,31,34	1.73	5 (19%)
70	A2M	L5	2401	70	22,25,26	3.41	10 (45%)	31,36,39	2.38	10 (32%)
74	PSU	S2	681	74	18,21,22	1.05	1 (5%)	22,30,33	1.71	4 (18%)
70	OMC	L5	2861	70	19,22,23	2.98	8 (42%)	26,31,34	0.78	0
70	A2M	L5	398	70	22,25,26	3.42	9 (40%)	31,36,39	2.37	11 (35%)
70	PSU	L5	1862	70	18,21,22	1.01	1 (5%)	22,30,33	1.80	4 (18%)
74	PSU	S2	801	74	18,21,22	1.11	1 (5%)	22,30,33	1.72	4 (18%)
70	PSU	L5	5001	70	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
70	PSU	L5	1744	70	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
74	PSU	S2	822	74	18,21,22	1.12	2 (11%)	22,30,33	1.83	5 (22%)
74	PSU	S2	686	74	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
69	PSU	L8	69	69	18,21,22	1.03	1 (5%)	22,30,33	1.71	5 (22%)
70	1MA	L5	1322	84,70	21,25,26	2.91	6 (28%)	31,37,40	2.87	8 (25%)
70	A2M	L5	4590	70	22,25,26	3.43	9 (40%)	31,36,39	2.43	9 (29%)
70	PSU	L5	1782	70	18,21,22	1.02	1 (5%)	22,30,33	1.69	3 (13%)
70	OMU	L5	4227	70	19,22,23	2.95	8 (42%)	26,31,34	1.72	4 (15%)
70	PSU	L5	4673	70	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
74	PSU	S2	573	74	18,21,22	1.05	1 (5%)	22,30,33	1.72	3 (13%)
74	PSU	S2	1625	74	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
70	PSU	L5	4312	70	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
74	6MZ	S2	1832	83,74	22,25,26	2.63	4 (18%)	30,36,39	2.33	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	PSU	L5	2632	70	18,21,22	1.02	1 (5%)	22,30,33	1.63	4 (18%)
70	PSU	L5	5010	70	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
74	PSU	S2	93	74	18,21,22	1.00	1 (5%)	22,30,33	1.65	4 (18%)
70	A2M	L5	3760	70	22,25,26	3.41	9 (40%)	31,36,39	2.52	11 (35%)
74	PSU	S2	863	74	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
70	OMG	L5	2876	70	23,26,27	2.44	8 (34%)	33,38,41	2.10	10 (30%)
74	G7M	S2	1639	67,74	23,26,27	2.59	9 (39%)	35,39,42	2.49	11 (31%)
70	OMG	L5	1625	70	23,26,27	2.44	8 (34%)	33,38,41	2.03	10 (30%)
74	PSU	S2	406	74	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
70	PSU	L5	4296	70	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
70	OMC	L5	4536	70	19,22,23	2.98	8 (42%)	26,31,34	0.78	0
70	PSU	L5	2839	70	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
70	OMC	L5	3869	70	19,22,23	2.99	8 (42%)	26,31,34	0.73	0
74	PSU	S2	1445	74	18,21,22	1.08	1 (5%)	22,30,33	1.85	5 (22%)
70	A2M	L5	3830	70	22,25,26	3.40	9 (40%)	31,36,39	2.43	11 (35%)
70	OMC	L5	3701	82,84,70	19,22,23	2.93	8 (42%)	26,31,34	0.73	0
70	A2M	L5	1534	83,70	22,25,26	3.46	9 (40%)	31,36,39	2.36	9 (29%)
70	A2M	L5	2363	84,83,70	22,25,26	3.47	9 (40%)	31,36,39	2.39	10 (32%)
70	PSU	L5	4471	70	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)
74	A2M	S2	484	74	22,25,26	3.42	9 (40%)	31,36,39	2.37	9 (29%)
74	A2M	S2	590	74	22,25,26	3.41	9 (40%)	31,36,39	2.54	11 (35%)
70	OMG	L5	4494	70	23,26,27	2.43	8 (34%)	33,38,41	2.05	9 (27%)
70	OMU	L5	3925	70	19,22,23	2.96	8 (42%)	26,31,34	1.72	5 (19%)
70	PSU	L5	4420	70	18,21,22	1.05	1 (5%)	22,30,33	1.65	5 (22%)
67	OMC	Pt	33	67	19,22,23	3.01	8 (42%)	26,31,34	1.02	2 (7%)
70	PSU	L5	4299	70	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	S2	34	74	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
74	A2M	S2	1031	74	22,25,26	3.46	9 (40%)	31,36,39	2.41	11 (35%)
70	OMG	L5	1522	70	23,26,27	2.42	8 (34%)	33,38,41	2.09	10 (30%)
70	PSU	L5	1781	70	18,21,22	1.08	1 (5%)	22,30,33	1.64	4 (18%)
70	A2M	L5	4523	83,70	22,25,26	3.42	9 (40%)	31,36,39	2.35	9 (29%)
74	OMG	S2	436	74	23,26,27	2.39	8 (34%)	33,38,41	2.06	10 (30%)
74	OMU	S2	116	74	19,22,23	2.99	8 (42%)	26,31,34	1.66	5 (19%)
74	PSU	S2	1347	74	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
70	PSU	L5	4972	70	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	PSU	L5	4293	70	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
70	PSU	L5	4579	70	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
70	OMC	L5	2804	70	19,22,23	2.96	8 (42%)	26,31,34	0.66	0
70	PSU	L5	4403	70	18,21,22	1.04	1 (5%)	22,30,33	1.80	5 (22%)
74	PSU	S2	1136	74	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
70	OMG	L5	4392	70	23,26,27	2.40	8 (34%)	33,38,41	2.06	10 (30%)
74	PSU	S2	1004	74	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
70	OMC	L5	4456	70	19,22,23	2.94	8 (42%)	26,31,34	0.84	1 (3%)
70	A2M	L5	4571	70	22,25,26	3.45	9 (40%)	31,36,39	2.32	10 (32%)
74	PSU	S2	119	74	18,21,22	1.03	1 (5%)	22,30,33	1.58	4 (18%)
74	PSU	S2	218	74	18,21,22	1.06	1 (5%)	22,30,33	1.74	5 (22%)
74	PSU	S2	1244	74	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
74	PSU	S2	814	74	18,21,22	1.02	1 (5%)	22,30,33	1.61	4 (18%)
70	A2M	L5	1326	70	22,25,26	3.41	10 (45%)	31,36,39	2.35	8 (25%)
74	PSU	S2	966	74	18,21,22	0.99	1 (5%)	22,30,33	1.60	3 (13%)
70	PSU	L5	3758	84,70	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
70	PSU	L5	4531	70	18,21,22	1.04	1 (5%)	22,30,33	1.77	5 (22%)
74	B8N	S2	1248	74	24,29,30	3.16	8 (33%)	29,42,45	1.79	7 (24%)
74	PSU	S2	918	74	18,21,22	1.12	2 (11%)	22,30,33	1.83	5 (22%)
69	PSU	L8	55	69	18,21,22	1.07	1 (5%)	22,30,33	1.72	4 (18%)
74	OMG	S2	1328	74	23,26,27	2.43	8 (34%)	33,38,41	2.05	10 (30%)
70	OMG	L5	3627	70	23,26,27	2.43	8 (34%)	33,38,41	2.10	10 (30%)
70	PSU	L5	3768	70	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
74	PSU	S2	1177	74	18,21,22	1.04	1 (5%)	22,30,33	1.68	4 (18%)
70	PSU	L5	3715	70	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
67	PSU	Pt	56	67	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
74	A2M	S2	27	83,74	22,25,26	3.42	10 (45%)	31,36,39	2.38	10 (32%)
70	OMG	L5	4623	70	23,26,27	2.43	8 (34%)	33,38,41	2.05	10 (30%)
70	PSU	L5	2508	70	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
70	OMC	L5	3841	70	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
70	5MC	L5	3782	83,70	18,22,23	3.65	7 (38%)	26,32,35	1.09	2 (7%)
70	PSU	L5	4457	70	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
70	PSU	L5	4500	70	18,21,22	1.11	1 (5%)	22,30,33	1.84	5 (22%)
70	A2M	L5	3785	70	22,25,26	3.35	9 (40%)	31,36,39	2.60	13 (41%)
70	OMG	L5	3899	83,70	23,26,27	2.40	8 (34%)	33,38,41	2.06	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	OMC	L5	1881	82,70	19,22,23	2.97	8 (42%)	26,31,34	0.81	0
74	OMG	S2	683	74	23,26,27	2.44	8 (34%)	33,38,41	2.03	10 (30%)
74	PSU	S2	572	74	18,21,22	1.02	1 (5%)	22,30,33	1.70	5 (22%)
74	OMG	S2	509	74	23,26,27	2.39	8 (34%)	33,38,41	2.00	9 (27%)
70	PSU	L5	3637	70	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
74	A2M	S2	576	74	22,25,26	3.40	9 (40%)	31,36,39	2.31	9 (29%)
70	OMG	L5	3744	70	23,26,27	2.42	8 (34%)	33,38,41	2.03	10 (30%)
74	OMC	S2	462	74	19,22,23	3.00	8 (42%)	26,31,34	0.78	0
74	PSU	S2	609	74	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
74	PSU	S2	1643	83,74	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
70	OMG	L5	2364	70	23,26,27	2.39	8 (34%)	33,38,41	2.05	10 (30%)
70	PSU	L5	1792	82,70	18,21,22	1.03	1 (5%)	22,30,33	1.61	4 (18%)
70	PSU	L5	4423	70	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
70	PSU	L5	1677	70	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
70	5MC	L5	4447	70	18,22,23	3.66	7 (38%)	26,32,35	1.08	1 (3%)
70	PSU	L5	1582	70	18,21,22	1.03	1 (5%)	22,30,33	1.58	4 (18%)
70	PSU	L5	4521	83,70	18,21,22	1.11	1 (5%)	22,30,33	1.79	4 (18%)
70	A2M	L5	400	70	22,25,26	3.42	9 (40%)	31,36,39	2.38	9 (29%)
67	H2U	Pt	21	67	18,21,22	3.04	5 (27%)	21,30,33	1.93	4 (19%)
70	PSU	L5	3734	70	18,21,22	1.00	1 (5%)	22,30,33	1.69	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	A2M	L5	2815	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	4636	70	-	4/7/25/26	0/2/2/2
74	OMG	S2	644	74	-	3/9/27/28	0/3/3/3
70	OMG	L5	4196	70	-	3/9/27/28	0/3/3/3
70	OMG	L5	4228	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	1692	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	2843	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	3729	70	-	2/7/25/26	0/2/2/2
70	PSU	L5	3853	84,70	-	0/7/25/26	0/2/2/2
70	PSU	L5	3884	70	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PSU	L5	1536	70	-	0/7/25/26	0/2/2/2
65	V5N	La	39	65	-	0/9/10/12	0/1/1/1
70	PSU	L5	4569	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	3762	70	-	2/7/25/26	0/2/2/2
70	A2M	L5	3718	70	-	0/9/27/28	0/3/3/3
70	A2M	L5	3825	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	109	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	1316	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	815	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	3695	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	3844	70	-	3/7/25/26	0/2/2/2
74	OMU	S2	1804	74	-	1/9/27/28	0/2/2/2
74	MA6	S2	1851	74	-	1/11/29/30	0/3/3/3
70	OMC	L5	2422	84,70	-	2/9/27/28	0/2/2/2
70	PSU	L5	3920	83,70	-	0/7/25/26	0/2/2/2
70	OMG	L5	3792	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	3770	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1174	74	-	0/7/25/26	0/2/2/2
74	OMC	S2	517	74	-	0/9/27/28	0/2/2/2
70	OMG	L5	4637	70	-	2/9/27/28	0/3/3/3
74	4AC	S2	1337	74	-	0/11/29/30	0/2/2/2
70	OMC	L5	1340	70	-	0/9/27/28	0/2/2/2
70	OMC	L5	2824	70	-	0/9/27/28	0/2/2/2
67	4SU	Pt	8	67	-	0/7/25/26	0/2/2/2
64	V5N	LA	216	64	-	1/9/10/12	0/1/1/1
74	OMU	S2	428	74	-	6/9/27/28	0/2/2/2
63	MLZ	Lb	5	63	-	5/7/8/10	-
70	PSU	L5	1779	70	-	0/7/25/26	0/2/2/2
74	A2M	S2	512	74	-	2/9/27/28	0/3/3/3
74	PSU	S2	651	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4353	70	-	0/7/25/26	0/2/2/2
70	OMU	L5	4498	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	4628	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1056	74	-	0/7/25/26	0/2/2/2
74	A2M	S2	1678	74	-	0/9/27/28	0/3/3/3
74	A2M	S2	668	83,74	-	3/9/27/28	0/3/3/3
70	PSU	L5	3764	70	-	2/7/25/26	0/2/2/2
70	OMC	L5	2351	70	-	3/9/27/28	0/2/2/2
70	PSU	L5	4552	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4493	70	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	OMU	L5	2837	70	-	0/9/27/28	0/2/2/2
70	OMG	L5	4370	70	-	0/9/27/28	0/3/3/3
70	OMG	L5	2424	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	1683	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	3639	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4689	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	296	74	-	0/7/25/26	0/2/2/2
70	OMC	L5	2365	83,70	-	0/9/27/28	0/2/2/2
74	PSU	S2	866	74	-	0/7/25/26	0/2/2/2
69	OMG	L8	75	69	-	1/9/27/28	0/3/3/3
3	MLZ	Lo	53	3	-	4/7/8/10	-
70	A2M	L5	1524	70	-	1/9/27/28	0/3/3/3
70	OMC	L5	3887	70	-	0/9/27/28	0/2/2/2
74	PSU	S2	1232	74	-	0/7/25/26	0/2/2/2
70	OMC	L5	3808	70	-	0/9/27/28	0/2/2/2
74	4AC	S2	1842	74	-	0/11/29/30	0/2/2/2
70	PSU	L5	4532	70	-	0/7/25/26	0/2/2/2
70	OMG	L5	4618	70	-	0/9/27/28	0/3/3/3
74	A2M	S2	99	83,74	-	1/9/27/28	0/3/3/3
70	PSU	L5	4442	70	-	1/7/25/26	0/2/2/2
74	A2M	S2	1383	74	-	0/9/27/28	0/3/3/3
74	OMG	S2	867	74	-	1/9/27/28	0/3/3/3
74	PSU	S2	1239	74	-	0/7/25/26	0/2/2/2
74	OMC	S2	1703	74	-	1/9/27/28	0/2/2/2
74	MA6	S2	1850	74	-	0/11/29/30	0/3/3/3
67	G7M	Pt	47	67	-	1/7/25/26	0/3/3/3
74	OMC	S2	1391	74	-	0/9/27/28	0/2/2/2
70	PSU	L5	3851	70	-	0/7/25/26	0/2/2/2
70	6MZ	L5	4220	70	-	0/9/27/28	0/3/3/3
70	A2M	L5	3867	70	-	1/9/27/28	0/3/3/3
70	OMU	L5	4620	70	-	1/9/27/28	0/2/2/2
74	PSU	S2	105	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	649	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	1238	74	-	0/7/25/26	0/2/2/2
74	OMG	S2	1490	74	-	1/9/27/28	0/3/3/3
70	OMG	L5	4499	70	-	2/9/27/28	0/3/3/3
74	A2M	S2	468	74	-	0/9/27/28	0/3/3/3
74	PSU	S2	1367	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4576	70	-	0/7/25/26	0/2/2/2
70	UR3	L5	4530	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1081	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	1243	74	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	A2M	L5	1871	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	1860	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4361	70	-	1/7/25/26	0/2/2/2
70	PSU	L5	4431	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	36	74	-	0/7/25/26	0/2/2/2
74	OMU	S2	627	74	-	1/9/27/28	0/2/2/2
70	A2M	L5	2401	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	681	74	-	0/7/25/26	0/2/2/2
70	OMC	L5	2861	70	-	0/9/27/28	0/2/2/2
70	A2M	L5	398	70	-	1/9/27/28	0/3/3/3
70	PSU	L5	1862	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	801	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	5001	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	1744	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	822	74	-	2/7/25/26	0/2/2/2
74	PSU	S2	686	74	-	0/7/25/26	0/2/2/2
69	PSU	L8	69	69	-	1/7/25/26	0/2/2/2
70	1MA	L5	1322	84,70	-	0/7/25/26	0/3/3/3
70	A2M	L5	4590	70	-	2/9/27/28	0/3/3/3
70	PSU	L5	1782	70	-	0/7/25/26	0/2/2/2
70	OMU	L5	4227	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	4673	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	573	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	1625	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4312	70	-	0/7/25/26	0/2/2/2
74	6MZ	S2	1832	83,74	-	2/9/27/28	0/3/3/3
70	PSU	L5	2632	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	5010	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	93	74	-	0/7/25/26	0/2/2/2
70	A2M	L5	3760	70	-	3/9/27/28	0/3/3/3
74	PSU	S2	863	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	2876	70	-	1/9/27/28	0/3/3/3
74	G7M	S2	1639	67,74	-	0/7/25/26	0/3/3/3
70	OMG	L5	1625	70	-	2/9/27/28	0/3/3/3
74	PSU	S2	406	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4296	70	-	0/7/25/26	0/2/2/2
70	OMC	L5	4536	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	2839	70	-	0/7/25/26	0/2/2/2
70	OMC	L5	3869	70	-	1/9/27/28	0/2/2/2
74	PSU	S2	1445	74	-	0/7/25/26	0/2/2/2
70	A2M	L5	3830	70	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	OMC	L5	3701	82,84,70	-	4/9/27/28	0/2/2/2
70	A2M	L5	1534	83,70	-	2/9/27/28	0/3/3/3
70	A2M	L5	2363	84,83,70	-	0/9/27/28	0/3/3/3
70	PSU	L5	4471	70	-	0/7/25/26	0/2/2/2
74	A2M	S2	484	74	-	0/9/27/28	0/3/3/3
74	A2M	S2	590	74	-	3/9/27/28	0/3/3/3
70	OMG	L5	4494	70	-	0/9/27/28	0/3/3/3
70	OMU	L5	3925	70	-	1/9/27/28	0/2/2/2
70	PSU	L5	4420	70	-	4/7/25/26	0/2/2/2
67	OMC	Pt	33	67	-	2/9/27/28	0/2/2/2
70	PSU	L5	4299	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	34	74	-	0/7/25/26	0/2/2/2
74	A2M	S2	1031	74	-	0/9/27/28	0/3/3/3
70	OMG	L5	1522	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	1781	70	-	0/7/25/26	0/2/2/2
70	A2M	L5	4523	83,70	-	0/9/27/28	0/3/3/3
74	OMG	S2	436	74	-	0/9/27/28	0/3/3/3
74	OMU	S2	116	74	-	1/9/27/28	0/2/2/2
74	PSU	S2	1347	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	4972	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4293	70	-	2/7/25/26	0/2/2/2
70	PSU	L5	4579	70	-	0/7/25/26	0/2/2/2
70	OMC	L5	2804	70	-	0/9/27/28	0/2/2/2
70	PSU	L5	4403	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1136	74	-	0/7/25/26	0/2/2/2
70	OMG	L5	4392	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	1004	74	-	0/7/25/26	0/2/2/2
70	OMC	L5	4456	70	-	0/9/27/28	0/2/2/2
70	A2M	L5	4571	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	119	74	-	1/7/25/26	0/2/2/2
74	PSU	S2	218	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	1244	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	814	74	-	0/7/25/26	0/2/2/2
70	A2M	L5	1326	70	-	0/9/27/28	0/3/3/3
74	PSU	S2	966	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	3758	84,70	-	1/7/25/26	0/2/2/2
70	PSU	L5	4531	70	-	0/7/25/26	0/2/2/2
74	B8N	S2	1248	74	-	4/16/34/35	0/2/2/2
74	PSU	S2	918	74	-	2/7/25/26	0/2/2/2
69	PSU	L8	55	69	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OMG	S2	1328	74	-	1/9/27/28	0/3/3/3
70	OMG	L5	3627	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	3768	70	-	0/7/25/26	0/2/2/2
74	PSU	S2	1177	74	-	0/7/25/26	0/2/2/2
70	PSU	L5	3715	70	-	0/7/25/26	0/2/2/2
67	PSU	Pt	56	67	-	0/7/25/26	0/2/2/2
74	A2M	S2	27	83,74	-	0/9/27/28	0/3/3/3
70	OMG	L5	4623	70	-	1/9/27/28	0/3/3/3
70	PSU	L5	2508	70	-	2/7/25/26	0/2/2/2
70	OMC	L5	3841	70	-	0/9/27/28	0/2/2/2
70	5MC	L5	3782	83,70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4457	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4500	70	-	1/7/25/26	0/2/2/2
70	A2M	L5	3785	70	-	1/9/27/28	0/3/3/3
70	OMG	L5	3899	83,70	-	0/9/27/28	0/3/3/3
70	OMC	L5	1881	82,70	-	0/9/27/28	0/2/2/2
74	OMG	S2	683	74	-	0/9/27/28	0/3/3/3
74	PSU	S2	572	74	-	0/7/25/26	0/2/2/2
74	OMG	S2	509	74	-	1/9/27/28	0/3/3/3
70	PSU	L5	3637	70	-	0/7/25/26	0/2/2/2
74	A2M	S2	576	74	-	2/9/27/28	0/3/3/3
70	OMG	L5	3744	70	-	0/9/27/28	0/3/3/3
74	OMC	S2	462	74	-	1/9/27/28	0/2/2/2
74	PSU	S2	609	74	-	0/7/25/26	0/2/2/2
74	PSU	S2	1643	83,74	-	1/7/25/26	0/2/2/2
70	OMG	L5	2364	70	-	0/9/27/28	0/3/3/3
70	PSU	L5	1792	82,70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4423	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	1677	70	-	4/7/25/26	0/2/2/2
70	5MC	L5	4447	70	-	4/7/25/26	0/2/2/2
70	PSU	L5	1582	70	-	0/7/25/26	0/2/2/2
70	PSU	L5	4521	83,70	-	1/7/25/26	0/2/2/2
70	A2M	L5	400	70	-	1/9/27/28	0/3/3/3
67	H2U	Pt	21	67	-	4/7/38/39	0/2/2/2
70	PSU	L5	3734	70	-	0/7/25/26	0/2/2/2

All (926) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	1832	6MZ	C6-N6	10.79	1.45	1.34
70	L5	4220	6MZ	C6-N6	10.58	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Pt	21	H2U	C2-N1	9.64	1.49	1.35
70	L5	4447	5MC	C6-C5	9.55	1.50	1.34
70	L5	3782	5MC	C6-C5	9.33	1.49	1.34
74	S2	1031	A2M	C2'-C1'	-8.88	1.30	1.53
70	L5	2363	A2M	C2'-C1'	-8.86	1.30	1.53
74	S2	1678	A2M	C2'-C1'	-8.85	1.30	1.53
70	L5	3867	A2M	C2'-C1'	-8.85	1.30	1.53
70	L5	1871	A2M	C2'-C1'	-8.84	1.30	1.53
70	L5	1534	A2M	C2'-C1'	-8.82	1.30	1.53
74	S2	1383	A2M	O4'-C1'	8.73	1.62	1.42
70	L5	1326	A2M	C2'-C1'	-8.69	1.30	1.53
74	S2	468	A2M	C2'-C1'	-8.67	1.30	1.53
74	S2	99	A2M	C2'-C1'	-8.67	1.30	1.53
70	L5	4571	A2M	C2'-C1'	-8.66	1.30	1.53
74	S2	27	A2M	C2'-C1'	-8.65	1.30	1.53
70	L5	4590	A2M	C2'-C1'	-8.64	1.30	1.53
70	L5	1534	A2M	O4'-C1'	8.63	1.62	1.42
70	L5	3830	A2M	C2'-C1'	-8.63	1.30	1.53
70	L5	4590	A2M	O4'-C1'	8.62	1.62	1.42
74	S2	1383	A2M	C2'-C1'	-8.62	1.30	1.53
74	S2	1678	A2M	O4'-C1'	8.62	1.62	1.42
70	L5	398	A2M	C2'-C1'	-8.61	1.30	1.53
70	L5	3825	A2M	C2'-C1'	-8.61	1.30	1.53
70	L5	1871	A2M	O4'-C1'	8.61	1.62	1.42
74	S2	99	A2M	O4'-C1'	8.61	1.62	1.42
70	L5	2401	A2M	O4'-C1'	8.60	1.62	1.42
70	L5	398	A2M	O4'-C1'	8.60	1.62	1.42
70	L5	2815	A2M	C2'-C1'	-8.60	1.30	1.53
70	L5	400	A2M	C2'-C1'	-8.60	1.30	1.53
70	L5	4523	A2M	O4'-C1'	8.58	1.62	1.42
70	L5	3785	A2M	C2'-C1'	-8.58	1.31	1.53
70	L5	4523	A2M	C2'-C1'	-8.58	1.31	1.53
70	L5	3718	A2M	C2'-C1'	-8.58	1.31	1.53
74	S2	468	A2M	O4'-C1'	8.57	1.62	1.42
74	S2	512	A2M	O4'-C1'	8.57	1.62	1.42
70	L5	2363	A2M	O4'-C1'	8.57	1.62	1.42
70	L5	2815	A2M	O4'-C1'	8.56	1.62	1.42
74	S2	590	A2M	O4'-C1'	8.56	1.62	1.42
70	L5	3718	A2M	O4'-C1'	8.56	1.62	1.42
74	S2	484	A2M	C2'-C1'	-8.55	1.31	1.53
70	L5	3760	A2M	C2'-C1'	-8.55	1.31	1.53
70	L5	400	A2M	O4'-C1'	8.55	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	576	A2M	C2'-C1'	-8.54	1.31	1.53
74	S2	27	A2M	O4'-C1'	8.53	1.62	1.42
70	L5	3825	A2M	O4'-C1'	8.51	1.62	1.42
70	L5	2401	A2M	C2'-C1'	-8.50	1.31	1.53
70	L5	4571	A2M	O4'-C1'	8.50	1.62	1.42
70	L5	3830	A2M	O4'-C1'	8.49	1.62	1.42
74	S2	484	A2M	O4'-C1'	8.48	1.62	1.42
74	S2	590	A2M	C2'-C1'	-8.47	1.31	1.53
74	S2	576	A2M	O4'-C1'	8.46	1.62	1.42
70	L5	1524	A2M	O4'-C1'	8.46	1.62	1.42
70	L5	3760	A2M	O4'-C1'	8.43	1.62	1.42
74	S2	512	A2M	C2'-C1'	-8.43	1.31	1.53
74	S2	1031	A2M	O4'-C1'	8.41	1.61	1.42
74	S2	668	A2M	C2'-C1'	-8.40	1.31	1.53
70	L5	1524	A2M	C2'-C1'	-8.39	1.31	1.53
70	L5	3867	A2M	O4'-C1'	8.37	1.61	1.42
70	L5	1326	A2M	O4'-C1'	8.26	1.61	1.42
74	S2	668	A2M	O4'-C1'	8.16	1.61	1.42
70	L5	3785	A2M	O4'-C1'	7.99	1.60	1.42
70	L5	1322	1MA	C2-N3	7.97	1.45	1.30
70	L5	1322	1MA	C4-N3	7.80	1.51	1.35
74	S2	1248	B8N	C4-N3	-7.72	1.26	1.40
74	S2	1248	B8N	C6-N1	7.69	1.55	1.36
67	Pt	8	4SU	C4-N3	7.62	1.45	1.37
74	S2	1804	OMU	C2-N1	7.13	1.49	1.38
70	L5	4530	UR3	C2-N1	7.00	1.48	1.38
70	L5	4498	OMU	C2-N1	6.93	1.49	1.38
74	S2	627	OMU	C2-N1	6.92	1.49	1.38
74	S2	428	OMU	C2-N1	6.89	1.49	1.38
74	S2	116	OMU	C2-N1	6.88	1.49	1.38
74	S2	627	OMU	C2-N3	6.86	1.50	1.38
70	L5	4227	OMU	C2-N1	6.82	1.49	1.38
74	S2	116	OMU	C2-N3	6.81	1.50	1.38
70	L5	3925	OMU	C2-N1	6.79	1.49	1.38
74	S2	1804	OMU	C2-N3	6.78	1.50	1.38
70	L5	2837	OMU	C2-N3	6.78	1.50	1.38
74	S2	1337	4AC	C4-N3	6.77	1.44	1.32
70	L5	2837	OMU	C2-N1	6.76	1.49	1.38
74	S2	428	OMU	C2-N3	6.76	1.50	1.38
74	S2	668	A2M	O4'-C4'	-6.70	1.30	1.45
70	L5	4620	OMU	C2-N1	6.69	1.49	1.38
70	L5	3925	OMU	C2-N3	6.65	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4498	OMU	C2-N3	6.62	1.49	1.38
70	L5	4227	OMU	C2-N3	6.60	1.49	1.38
70	L5	4620	OMU	C2-N3	6.58	1.49	1.38
70	L5	1524	A2M	O4'-C4'	-6.57	1.30	1.45
74	S2	1678	A2M	O4'-C4'	-6.56	1.30	1.45
74	S2	1337	4AC	C6-C5	6.55	1.50	1.35
70	L5	4571	A2M	O4'-C4'	-6.53	1.30	1.45
70	L5	3782	5MC	C4-N3	6.50	1.45	1.34
74	S2	1842	4AC	C4-N3	6.50	1.44	1.32
74	S2	590	A2M	O4'-C4'	-6.49	1.30	1.45
67	Pt	47	G7M	C4-N3	6.47	1.49	1.34
70	L5	3760	A2M	O4'-C4'	-6.46	1.30	1.45
74	S2	683	OMG	C4-N3	6.45	1.49	1.34
70	L5	4196	OMG	C4-N3	6.45	1.49	1.34
74	S2	1328	OMG	C4-N3	6.45	1.49	1.34
70	L5	2363	A2M	O4'-C4'	-6.45	1.30	1.45
70	L5	400	A2M	O4'-C4'	-6.44	1.30	1.45
70	L5	4590	A2M	O4'-C4'	-6.44	1.30	1.45
69	L8	75	OMG	C4-N3	6.43	1.49	1.34
70	L5	1625	OMG	C4-N3	6.43	1.49	1.34
70	L5	1871	A2M	O4'-C4'	-6.43	1.30	1.45
70	L5	3792	OMG	C4-N3	6.42	1.49	1.34
67	Pt	8	4SU	C2-N3	6.41	1.49	1.38
64	LA	216	V5N	CG-ND1	-6.41	1.31	1.37
70	L5	2876	OMG	C4-N3	6.41	1.49	1.34
74	S2	1842	4AC	C6-C5	6.41	1.50	1.35
74	S2	1031	A2M	O4'-C4'	-6.40	1.30	1.45
67	Pt	8	4SU	C2-N1	6.40	1.48	1.38
74	S2	484	A2M	O4'-C4'	-6.40	1.30	1.45
70	L5	4623	OMG	C4-N3	6.39	1.49	1.34
70	L5	1316	OMG	C4-N3	6.39	1.49	1.34
70	L5	4499	OMG	C4-N3	6.39	1.49	1.34
70	L5	3825	A2M	O4'-C4'	-6.38	1.30	1.45
74	S2	1248	B8N	C6-C5	6.38	1.43	1.34
74	S2	462	OMC	C2-N3	6.37	1.49	1.36
70	L5	4392	OMG	C4-N3	6.37	1.49	1.34
70	L5	3627	OMG	C4-N3	6.36	1.49	1.34
65	La	39	V5N	CG-ND1	-6.36	1.31	1.37
70	L5	4370	OMG	C4-N3	6.36	1.49	1.34
70	L5	1326	A2M	O4'-C4'	-6.35	1.30	1.45
70	L5	4523	A2M	O4'-C4'	-6.35	1.30	1.45
74	S2	644	OMG	C4-N3	6.35	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Pt	33	OMC	C2-N3	6.35	1.49	1.36
70	L5	3744	OMG	C4-N3	6.35	1.49	1.34
74	S2	99	A2M	O4'-C4'	-6.35	1.30	1.45
70	L5	1534	A2M	O4'-C4'	-6.35	1.30	1.45
70	L5	4494	OMG	C4-N3	6.34	1.49	1.34
74	S2	867	OMG	C4-N3	6.33	1.49	1.34
74	S2	509	OMG	C4-N3	6.33	1.49	1.34
70	L5	3867	A2M	O4'-C4'	-6.32	1.30	1.45
70	L5	2424	OMG	C4-N3	6.32	1.49	1.34
74	S2	1639	G7M	C4-N3	6.32	1.49	1.34
74	S2	1490	OMG	C4-N3	6.32	1.49	1.34
70	L5	4618	OMG	C4-N3	6.31	1.49	1.34
74	S2	27	A2M	O4'-C4'	-6.31	1.30	1.45
70	L5	3899	OMG	C4-N3	6.31	1.49	1.34
70	L5	1522	OMG	C4-N3	6.31	1.49	1.34
74	S2	517	OMC	C2-N3	6.31	1.49	1.36
70	L5	4637	OMG	C4-N3	6.31	1.49	1.34
70	L5	2364	OMG	C4-N3	6.29	1.49	1.34
70	L5	4228	OMG	C4-N3	6.28	1.49	1.34
70	L5	4536	OMC	C2-N3	6.27	1.49	1.36
74	S2	468	A2M	O4'-C4'	-6.27	1.31	1.45
70	L5	2815	A2M	O4'-C4'	-6.27	1.31	1.45
70	L5	2824	OMC	C2-N3	6.27	1.49	1.36
74	S2	1391	OMC	C2-N3	6.27	1.49	1.36
70	L5	3841	OMC	C2-N3	6.26	1.49	1.36
70	L5	398	A2M	O4'-C4'	-6.25	1.31	1.45
70	L5	3782	5MC	C2-N3	6.25	1.49	1.36
70	L5	3869	OMC	C2-N3	6.25	1.49	1.36
70	L5	2861	OMC	C2-N3	6.24	1.49	1.36
70	L5	1340	OMC	C2-N3	6.24	1.49	1.36
74	S2	436	OMG	C4-N3	6.24	1.49	1.34
70	L5	2804	OMC	C2-N3	6.23	1.49	1.36
70	L5	3785	A2M	O4'-C4'	-6.23	1.31	1.45
70	L5	3718	A2M	O4'-C4'	-6.23	1.31	1.45
74	S2	576	A2M	O4'-C4'	-6.23	1.31	1.45
74	S2	1703	OMC	C2-N3	6.22	1.49	1.36
70	L5	4447	5MC	C4-N3	6.22	1.44	1.34
70	L5	2401	A2M	O4'-C4'	-6.20	1.31	1.45
74	S2	512	A2M	O4'-C4'	-6.19	1.31	1.45
70	L5	3887	OMC	C2-N3	6.18	1.48	1.36
74	S2	1383	A2M	O4'-C4'	-6.17	1.31	1.45
70	L5	2422	OMC	C2-N3	6.15	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4530	UR3	C6-C5	6.15	1.49	1.35
70	L5	2365	OMC	C2-N3	6.15	1.48	1.36
70	L5	4456	OMC	C2-N3	6.14	1.48	1.36
70	L5	3830	A2M	O4'-C4'	-6.14	1.31	1.45
74	S2	1337	4AC	C7-N4	6.14	1.48	1.37
67	Pt	21	H2U	C2-N3	6.09	1.48	1.38
70	L5	1881	OMC	C6-C5	6.08	1.49	1.35
70	L5	1881	OMC	C2-N3	6.06	1.48	1.36
70	L5	3808	OMC	C2-N3	6.05	1.48	1.36
70	L5	3701	OMC	C2-N3	6.05	1.48	1.36
70	L5	2351	OMC	C2-N3	6.04	1.48	1.36
70	L5	4447	5MC	C2-N3	6.04	1.48	1.36
74	S2	1703	OMC	C6-C5	6.04	1.49	1.35
70	L5	2824	OMC	C6-C5	6.02	1.49	1.35
74	S2	1248	B8N	C2-N1	6.00	1.57	1.39
70	L5	3701	OMC	C6-C5	5.98	1.49	1.35
70	L5	2861	OMC	C6-C5	5.98	1.48	1.35
70	L5	4536	OMC	C6-C5	5.97	1.48	1.35
74	S2	517	OMC	C6-C5	5.97	1.48	1.35
70	L5	3887	OMC	C6-C5	5.96	1.48	1.35
74	S2	462	OMC	C6-C5	5.96	1.48	1.35
70	L5	2422	OMC	C6-C5	5.96	1.48	1.35
70	L5	2365	OMC	C6-C5	5.94	1.48	1.35
74	S2	1391	OMC	C6-C5	5.94	1.48	1.35
70	L5	3869	OMC	C6-C5	5.94	1.48	1.35
70	L5	2351	OMC	C6-C5	5.93	1.48	1.35
70	L5	2804	OMC	C6-C5	5.93	1.48	1.35
67	Pt	33	OMC	C6-C5	5.89	1.48	1.35
70	L5	4456	OMC	C6-C5	5.87	1.48	1.35
70	L5	1340	OMC	C6-C5	5.87	1.48	1.35
70	L5	3841	OMC	C6-C5	5.86	1.48	1.35
70	L5	3808	OMC	C6-C5	5.83	1.48	1.35
74	S2	1337	4AC	C2-N3	5.79	1.48	1.36
74	S2	1804	OMU	C6-C5	5.73	1.48	1.35
74	S2	627	OMU	C6-C5	5.72	1.48	1.35
70	L5	4498	OMU	C6-C5	5.65	1.48	1.35
74	S2	116	OMU	C6-C5	5.64	1.48	1.35
70	L5	1625	OMG	C2-N3	5.63	1.46	1.33
70	L5	2837	OMU	C6-C5	5.61	1.48	1.35
74	S2	1842	4AC	C7-N4	5.60	1.47	1.37
70	L5	3925	OMU	C6-C5	5.60	1.48	1.35
70	L5	4620	OMU	C6-C5	5.57	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4227	OMU	C6-C5	5.56	1.48	1.35
70	L5	4499	OMG	C2-N3	5.53	1.46	1.33
74	S2	428	OMU	C6-C5	5.52	1.47	1.35
74	S2	1842	4AC	C2-N3	5.52	1.47	1.36
70	L5	2876	OMG	C2-N3	5.51	1.46	1.33
70	L5	3627	OMG	C2-N3	5.51	1.46	1.33
69	L8	75	OMG	C2-N3	5.50	1.46	1.33
70	L5	2424	OMG	C2-N3	5.50	1.46	1.33
70	L5	4623	OMG	C2-N3	5.49	1.46	1.33
74	S2	644	OMG	C2-N3	5.49	1.46	1.33
70	L5	4637	OMG	C2-N3	5.48	1.46	1.33
70	L5	4494	OMG	C2-N3	5.48	1.46	1.33
70	L5	4196	OMG	C2-N3	5.48	1.46	1.33
70	L5	3744	OMG	C2-N3	5.47	1.46	1.33
74	S2	1328	OMG	C2-N3	5.46	1.46	1.33
74	S2	683	OMG	C2-N3	5.45	1.46	1.33
67	Pt	8	4SU	C6-C5	5.45	1.47	1.35
70	L5	4370	OMG	C2-N3	5.44	1.46	1.33
74	S2	509	OMG	C2-N3	5.43	1.46	1.33
70	L5	4618	OMG	C2-N3	5.43	1.46	1.33
70	L5	4228	OMG	C2-N3	5.41	1.46	1.33
74	S2	867	OMG	C2-N3	5.41	1.46	1.33
70	L5	4392	OMG	C2-N3	5.40	1.46	1.33
70	L5	1522	OMG	C2-N3	5.40	1.46	1.33
70	L5	1316	OMG	C2-N3	5.39	1.46	1.33
74	S2	1639	G7M	C2-N3	5.37	1.46	1.33
74	S2	1490	OMG	C2-N3	5.36	1.46	1.33
70	L5	3899	OMG	C2-N3	5.36	1.46	1.33
70	L5	2364	OMG	C2-N3	5.32	1.46	1.33
67	Pt	47	G7M	C2-N3	5.32	1.46	1.33
70	L5	4530	UR3	C2-N3	5.32	1.49	1.39
74	S2	436	OMG	C2-N3	5.31	1.46	1.33
70	L5	3792	OMG	C2-N3	5.29	1.45	1.33
70	L5	2824	OMC	C4-N3	5.17	1.44	1.34
70	L5	3869	OMC	C4-N3	5.14	1.44	1.34
74	S2	462	OMC	C4-N3	5.13	1.44	1.34
74	S2	1391	OMC	C4-N3	5.10	1.44	1.34
74	S2	517	OMC	C4-N3	5.09	1.44	1.34
67	Pt	33	OMC	C4-N3	5.07	1.44	1.34
70	L5	3841	OMC	C4-N3	5.06	1.44	1.34
74	S2	1703	OMC	C4-N3	5.05	1.44	1.34
70	L5	2422	OMC	C4-N3	5.04	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4536	OMC	C4-N3	5.04	1.44	1.34
67	Pt	33	OMC	C4-N4	5.02	1.45	1.33
70	L5	3808	OMC	C4-N4	5.01	1.45	1.33
70	L5	2804	OMC	C4-N3	5.01	1.44	1.34
70	L5	3887	OMC	C4-N3	5.01	1.44	1.34
70	L5	2365	OMC	C4-N3	5.00	1.44	1.34
70	L5	4447	5MC	C6-N1	4.97	1.46	1.38
74	S2	462	OMC	C4-N4	4.97	1.45	1.33
70	L5	2861	OMC	C4-N3	4.97	1.44	1.34
70	L5	1340	OMC	C4-N3	4.97	1.44	1.34
70	L5	2422	OMC	C4-N4	4.97	1.45	1.33
74	S2	517	OMC	C4-N4	4.94	1.45	1.33
70	L5	3869	OMC	C4-N4	4.94	1.45	1.33
74	S2	1703	OMC	C4-N4	4.94	1.45	1.33
70	L5	3701	OMC	C4-N3	4.93	1.44	1.34
70	L5	2824	OMC	C4-N4	4.93	1.45	1.33
70	L5	3808	OMC	C4-N3	4.92	1.44	1.34
70	L5	3887	OMC	C4-N4	4.92	1.45	1.33
70	L5	2861	OMC	C4-N4	4.91	1.45	1.33
70	L5	4456	OMC	C4-N4	4.90	1.45	1.33
70	L5	1881	OMC	C4-N3	4.89	1.44	1.34
70	L5	3841	OMC	C4-N4	4.89	1.45	1.33
70	L5	2804	OMC	C4-N4	4.89	1.45	1.33
74	S2	1391	OMC	C4-N4	4.89	1.45	1.33
70	L5	4536	OMC	C4-N4	4.89	1.45	1.33
70	L5	1881	OMC	C4-N4	4.88	1.45	1.33
70	L5	3701	OMC	C4-N4	4.87	1.45	1.33
67	Pt	47	G7M	C2-N2	4.87	1.45	1.34
70	L5	4456	OMC	C4-N3	4.87	1.44	1.34
70	L5	1340	OMC	C4-N4	4.86	1.45	1.33
70	L5	2351	OMC	C4-N3	4.83	1.44	1.34
70	L5	2351	OMC	C4-N4	4.82	1.45	1.33
70	L5	2365	OMC	C4-N4	4.81	1.45	1.33
74	S2	1639	G7M	C2-N2	4.80	1.45	1.34
67	Pt	33	OMC	C2-N1	4.80	1.50	1.40
67	Pt	21	H2U	C4-N3	4.79	1.45	1.37
70	L5	3627	OMG	C2-N2	4.79	1.45	1.34
70	L5	3782	5MC	C6-N1	4.78	1.46	1.38
67	Pt	8	4SU	C4-S4	-4.76	1.59	1.68
70	L5	2424	OMG	C2-N2	4.75	1.45	1.34
70	L5	1625	OMG	C2-N2	4.75	1.45	1.34
69	L8	75	OMG	C2-N2	4.75	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	683	OMG	C2-N2	4.74	1.45	1.34
74	S2	867	OMG	C2-N2	4.73	1.45	1.34
70	L5	4499	OMG	C2-N2	4.72	1.45	1.34
74	S2	1328	OMG	C2-N2	4.72	1.45	1.34
70	L5	4370	OMG	C2-N2	4.72	1.45	1.34
74	S2	1490	OMG	C2-N2	4.72	1.45	1.34
70	L5	4618	OMG	C2-N2	4.71	1.45	1.34
74	S2	644	OMG	C2-N2	4.71	1.45	1.34
70	L5	3744	OMG	C2-N2	4.70	1.45	1.34
70	L5	4494	OMG	C2-N2	4.70	1.45	1.34
70	L5	2364	OMG	C2-N2	4.68	1.45	1.34
70	L5	2351	OMC	C2-N1	4.68	1.50	1.40
70	L5	3792	OMG	C2-N2	4.67	1.45	1.34
70	L5	4228	OMG	C2-N2	4.67	1.45	1.34
70	L5	2876	OMG	C2-N2	4.67	1.45	1.34
70	L5	3899	OMG	C2-N2	4.65	1.45	1.34
70	L5	4392	OMG	C2-N2	4.64	1.45	1.34
70	L5	1316	OMG	C2-N2	4.63	1.45	1.34
74	S2	1337	4AC	C5-C4	4.62	1.50	1.40
70	L5	4623	OMG	C2-N2	4.61	1.45	1.34
70	L5	4571	A2M	C6-N6	4.61	1.45	1.34
70	L5	4196	OMG	C2-N2	4.60	1.45	1.34
74	S2	436	OMG	C2-N2	4.60	1.45	1.34
70	L5	1522	OMG	C2-N2	4.60	1.45	1.34
74	S2	509	OMG	C2-N2	4.59	1.45	1.34
74	S2	1639	G7M	C5-N7	-4.58	1.33	1.39
70	L5	3808	OMC	C2-N1	4.57	1.49	1.40
70	L5	4637	OMG	C2-N2	4.56	1.45	1.34
70	L5	3760	A2M	C6-N6	4.53	1.45	1.34
74	S2	1842	4AC	O2-C2	-4.52	1.15	1.23
70	L5	2824	OMC	C2-N1	4.51	1.49	1.40
74	S2	468	A2M	C6-N6	4.51	1.45	1.34
70	L5	3841	OMC	C2-N1	4.51	1.49	1.40
74	S2	517	OMC	C2-N1	4.51	1.49	1.40
70	L5	4456	OMC	C2-N1	4.50	1.49	1.40
70	L5	1524	A2M	C6-N6	4.50	1.45	1.34
74	S2	1678	A2M	C6-N6	4.49	1.45	1.34
74	S2	462	OMC	C2-N1	4.49	1.49	1.40
70	L5	2815	A2M	C6-N6	4.49	1.45	1.34
74	S2	590	A2M	C6-N6	4.48	1.45	1.34
70	L5	2422	OMC	C2-N1	4.48	1.49	1.40
74	S2	1391	OMC	C2-N1	4.47	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4447	5MC	C4-N4	4.47	1.45	1.34
74	S2	668	A2M	C6-N6	4.47	1.45	1.34
70	L5	1881	OMC	C2-N1	4.46	1.49	1.40
70	L5	1871	A2M	C6-N6	4.46	1.45	1.34
70	L5	4590	A2M	C6-N6	4.46	1.45	1.34
70	L5	3869	OMC	C2-N1	4.45	1.49	1.40
74	S2	512	A2M	C6-N6	4.45	1.45	1.34
74	S2	576	A2M	C6-N6	4.45	1.45	1.34
67	Pt	47	G7M	C5-N7	-4.45	1.34	1.39
74	S2	1703	OMC	C2-N1	4.45	1.49	1.40
74	S2	484	A2M	C6-N6	4.45	1.45	1.34
70	L5	398	A2M	C6-N6	4.44	1.45	1.34
74	S2	99	A2M	C6-N6	4.44	1.45	1.34
70	L5	3887	OMC	C2-N1	4.43	1.49	1.40
70	L5	2861	OMC	C2-N1	4.43	1.49	1.40
70	L5	4536	OMC	C2-N1	4.43	1.49	1.40
70	L5	3782	5MC	C4-N4	4.42	1.45	1.34
70	L5	1534	A2M	C6-N6	4.42	1.45	1.34
74	S2	27	A2M	C6-N6	4.41	1.45	1.34
70	L5	4523	A2M	C6-N6	4.40	1.45	1.34
70	L5	2401	A2M	C6-N6	4.40	1.45	1.34
70	L5	400	A2M	C6-N6	4.39	1.45	1.34
67	Pt	8	4SU	C5-C4	4.39	1.48	1.42
70	L5	3718	A2M	C6-N6	4.38	1.45	1.34
70	L5	3867	A2M	C6-N6	4.37	1.45	1.34
70	L5	3825	A2M	C6-N6	4.37	1.45	1.34
74	S2	1842	4AC	C5-C4	4.35	1.50	1.40
74	S2	1842	4AC	C2-N1	4.35	1.49	1.40
70	L5	2363	A2M	C6-N6	4.34	1.45	1.34
70	L5	3782	5MC	C2-N1	4.33	1.49	1.40
70	L5	3830	A2M	C6-N6	4.33	1.45	1.34
70	L5	1340	OMC	C2-N1	4.33	1.49	1.40
74	S2	1383	A2M	C6-N6	4.33	1.45	1.34
74	S2	1031	A2M	C6-N6	4.29	1.44	1.34
70	L5	1326	A2M	C6-N6	4.29	1.44	1.34
74	S2	1337	4AC	O2-C2	-4.29	1.15	1.23
70	L5	3701	OMC	C2-N1	4.27	1.49	1.40
65	La	39	V5N	CD2-NE2	-4.22	1.31	1.37
70	L5	3785	A2M	C6-N6	4.22	1.44	1.34
74	S2	1337	4AC	C2-N1	4.22	1.49	1.40
70	L5	2804	OMC	C2-N1	4.21	1.49	1.40
70	L5	2365	OMC	C2-N1	4.20	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	627	OMU	C4-N3	4.18	1.46	1.38
74	S2	1804	OMU	C4-N3	4.11	1.45	1.38
74	S2	1337	4AC	C4-N4	4.11	1.45	1.39
64	LA	216	V5N	CD2-NE2	-4.10	1.31	1.37
70	L5	4447	5MC	C2-N1	4.07	1.48	1.40
74	S2	428	OMU	C4-N3	4.03	1.45	1.38
74	S2	116	OMU	C4-N3	4.01	1.45	1.38
70	L5	4227	OMU	C4-N3	3.99	1.45	1.38
70	L5	4498	OMU	C4-N3	3.93	1.45	1.38
70	L5	1322	1MA	C2-N1	3.92	1.43	1.35
70	L5	2837	OMU	C4-N3	3.92	1.45	1.38
70	L5	3925	OMU	C4-N3	3.89	1.45	1.38
70	L5	4620	OMU	C4-N3	3.87	1.45	1.38
67	Pt	47	G7M	C5-C6	3.84	1.54	1.43
74	S2	1639	G7M	C5-C6	3.82	1.54	1.43
70	L5	1322	1MA	C5-C6	3.81	1.53	1.43
74	S2	1851	MA6	C6-N6	3.79	1.48	1.36
74	S2	1850	MA6	C6-N6	3.77	1.48	1.36
70	L5	3762	PSU	C6-C5	3.73	1.39	1.35
74	S2	801	PSU	C6-C5	3.70	1.39	1.35
70	L5	4431	PSU	C6-C5	3.63	1.39	1.35
70	L5	3853	PSU	C6-C5	3.62	1.39	1.35
70	L5	1781	PSU	C6-C5	3.62	1.39	1.35
70	L5	4420	PSU	C6-C5	3.61	1.39	1.35
74	S2	866	PSU	C6-C5	3.60	1.39	1.35
74	S2	1842	4AC	C4-N4	3.60	1.45	1.39
74	S2	1248	B8N	C1'-C5	3.57	1.58	1.50
70	L5	5010	PSU	C6-C5	3.56	1.39	1.35
70	L5	4532	PSU	C6-C5	3.55	1.39	1.35
70	L5	4500	PSU	C6-C5	3.52	1.39	1.35
70	L5	3729	PSU	C6-C5	3.51	1.39	1.35
70	L5	4423	PSU	C6-C5	3.51	1.39	1.35
74	S2	1004	PSU	C6-C5	3.50	1.39	1.35
70	L5	4673	PSU	C6-C5	3.50	1.39	1.35
70	L5	1683	PSU	C6-C5	3.49	1.39	1.35
70	L5	4471	PSU	C6-C5	3.48	1.39	1.35
74	S2	109	PSU	C6-C5	3.48	1.39	1.35
74	S2	105	PSU	C6-C5	3.47	1.39	1.35
74	S2	1243	PSU	C6-C5	3.47	1.39	1.35
74	S2	1232	PSU	C6-C5	3.46	1.39	1.35
69	L8	55	PSU	C6-C5	3.46	1.39	1.35
70	L5	4521	PSU	C6-C5	3.46	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Pt	56	PSU	C6-C5	3.45	1.39	1.35
70	L5	3884	PSU	C6-C5	3.45	1.39	1.35
70	L5	4293	PSU	C6-C5	3.44	1.39	1.35
70	L5	3920	PSU	C6-C5	3.44	1.39	1.35
70	L5	3637	PSU	C6-C5	3.44	1.39	1.35
70	L5	1860	PSU	C6-C5	3.43	1.39	1.35
74	S2	1244	PSU	C6-C5	3.43	1.39	1.35
74	S2	119	PSU	C6-C5	3.42	1.39	1.35
74	S2	918	PSU	C6-C5	3.42	1.39	1.35
70	L5	2632	PSU	C6-C5	3.42	1.39	1.35
70	L5	4493	PSU	C6-C5	3.41	1.39	1.35
70	L5	1792	PSU	C6-C5	3.41	1.39	1.35
70	L5	2839	PSU	C6-C5	3.41	1.39	1.35
70	L5	4636	PSU	C6-C5	3.40	1.39	1.35
70	L5	1316	OMG	C5-N7	-3.39	1.32	1.39
70	L5	1536	PSU	C6-C5	3.39	1.39	1.35
70	L5	1744	PSU	C6-C5	3.39	1.39	1.35
70	L5	4689	PSU	C6-C5	3.38	1.39	1.35
74	S2	651	PSU	C6-C5	3.38	1.39	1.35
74	S2	1625	PSU	C6-C5	3.38	1.39	1.35
74	S2	1445	PSU	C6-C5	3.38	1.39	1.35
70	L5	4569	PSU	C6-C5	3.37	1.39	1.35
74	S2	1842	4AC	C6-N1	3.37	1.46	1.38
70	L5	4972	PSU	C6-C5	3.36	1.39	1.35
74	S2	1174	PSU	C6-C5	3.36	1.39	1.35
70	L5	4196	OMG	C5-N7	-3.36	1.32	1.39
74	S2	34	PSU	C6-C5	3.36	1.39	1.35
70	L5	3792	OMG	C5-N7	-3.35	1.32	1.39
74	S2	1337	4AC	C6-N1	3.35	1.46	1.38
70	L5	3715	PSU	C6-C5	3.35	1.39	1.35
70	L5	4299	PSU	C6-C5	3.34	1.39	1.35
70	L5	3695	PSU	C6-C5	3.34	1.39	1.35
74	S2	822	PSU	C6-C5	3.33	1.39	1.35
70	L5	4296	PSU	C6-C5	3.33	1.39	1.35
70	L5	4576	PSU	C6-C5	3.33	1.39	1.35
70	L5	1522	OMG	C5-N7	-3.33	1.32	1.39
70	L5	4623	OMG	C5-N7	-3.33	1.32	1.39
70	L5	1625	OMG	C5-N7	-3.33	1.32	1.39
74	S2	1056	PSU	C6-C5	3.33	1.39	1.35
74	S2	218	PSU	C6-C5	3.32	1.39	1.35
74	S2	814	PSU	C6-C5	3.32	1.39	1.35
74	S2	649	PSU	C6-C5	3.32	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	3851	PSU	C6-C5	3.31	1.39	1.35
74	S2	863	PSU	C6-C5	3.31	1.39	1.35
70	L5	4353	PSU	C6-C5	3.31	1.39	1.35
70	L5	4494	OMG	C5-N7	-3.31	1.32	1.39
70	L5	2876	OMG	C5-N7	-3.30	1.32	1.39
70	L5	4628	PSU	C6-C5	3.30	1.39	1.35
70	L5	2508	PSU	C6-C5	3.30	1.39	1.35
70	L5	2424	OMG	C5-N7	-3.30	1.32	1.39
70	L5	4457	PSU	C6-C5	3.30	1.39	1.35
70	L5	4531	PSU	C6-C5	3.30	1.39	1.35
74	S2	1177	PSU	C6-C5	3.30	1.39	1.35
74	S2	1238	PSU	C6-C5	3.29	1.39	1.35
74	S2	509	OMG	C5-N7	-3.29	1.32	1.39
74	S2	609	PSU	C6-C5	3.29	1.39	1.35
74	S2	1692	PSU	C6-C5	3.29	1.39	1.35
74	S2	1490	OMG	C5-N7	-3.28	1.32	1.39
70	L5	3768	PSU	C6-C5	3.28	1.39	1.35
74	S2	1239	PSU	C6-C5	3.27	1.39	1.35
70	L5	3764	PSU	C6-C5	3.27	1.39	1.35
70	L5	4361	PSU	C6-C5	3.27	1.39	1.35
70	L5	2365	OMC	C6-N1	3.26	1.45	1.38
74	S2	436	OMG	C5-N7	-3.26	1.32	1.39
74	S2	681	PSU	C6-C5	3.26	1.39	1.35
70	L5	1322	1MA	C5-N7	-3.26	1.32	1.39
70	L5	3627	OMG	C5-N7	-3.26	1.32	1.39
74	S2	683	OMG	C5-N7	-3.26	1.32	1.39
70	L5	3899	OMG	C5-N7	-3.25	1.32	1.39
70	L5	1582	PSU	C6-C5	3.25	1.39	1.35
70	L5	1779	PSU	C6-C5	3.25	1.39	1.35
70	L5	1782	PSU	C6-C5	3.25	1.39	1.35
70	L5	2804	OMC	C6-N1	3.25	1.45	1.38
70	L5	3887	OMC	C6-N1	3.25	1.45	1.38
74	S2	93	PSU	C6-C5	3.25	1.39	1.35
74	S2	406	PSU	C6-C5	3.25	1.39	1.35
74	S2	1643	PSU	C6-C5	3.25	1.39	1.35
74	S2	1703	OMC	C6-N1	3.24	1.45	1.38
70	L5	4312	PSU	C6-C5	3.24	1.39	1.35
74	S2	644	OMG	C5-N7	-3.24	1.32	1.39
70	L5	5001	PSU	C6-C5	3.24	1.39	1.35
70	L5	3758	PSU	C6-C5	3.24	1.39	1.35
74	S2	573	PSU	C6-C5	3.24	1.39	1.35
74	S2	1347	PSU	C6-C5	3.23	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	2351	OMC	C6-N1	3.23	1.45	1.38
70	L5	4552	PSU	C6-C5	3.23	1.39	1.35
70	L5	3770	PSU	C6-C5	3.22	1.39	1.35
70	L5	2824	OMC	C6-N1	3.22	1.45	1.38
70	L5	3734	PSU	C6-C5	3.22	1.39	1.35
70	L5	3844	PSU	C6-C5	3.22	1.39	1.35
69	L8	69	PSU	C6-C5	3.22	1.39	1.35
74	S2	1367	PSU	C6-C5	3.21	1.39	1.35
74	S2	686	PSU	C6-C5	3.21	1.39	1.35
70	L5	1871	A2M	O3'-C3'	-3.21	1.35	1.43
70	L5	1881	OMC	C6-N1	3.21	1.45	1.38
70	L5	4579	PSU	C6-C5	3.20	1.39	1.35
70	L5	4618	OMG	C5-N7	-3.20	1.32	1.39
74	S2	1136	PSU	C6-C5	3.20	1.39	1.35
74	S2	296	PSU	C6-C5	3.20	1.39	1.35
70	L5	3785	A2M	C5-C4	-3.19	1.33	1.39
70	L5	1862	PSU	C6-C5	3.19	1.39	1.35
70	L5	2422	OMC	C6-N1	3.19	1.45	1.38
70	L5	3639	PSU	C6-C5	3.19	1.39	1.35
70	L5	2861	OMC	C6-N1	3.19	1.45	1.38
74	S2	572	PSU	C6-C5	3.18	1.39	1.35
70	L5	2843	PSU	C6-C5	3.18	1.39	1.35
74	S2	36	PSU	C6-C5	3.18	1.39	1.35
70	L5	3869	OMC	C6-N1	3.17	1.45	1.38
74	S2	517	OMC	C6-N1	3.17	1.45	1.38
70	L5	4370	OMG	C5-N7	-3.17	1.32	1.39
70	L5	4392	OMG	C5-N7	-3.17	1.32	1.39
69	L8	75	OMG	C5-N7	-3.16	1.32	1.39
70	L5	4228	OMG	C5-N7	-3.16	1.32	1.39
70	L5	4403	PSU	C6-C5	3.16	1.39	1.35
70	L5	2364	OMG	C5-N7	-3.16	1.33	1.39
70	L5	3744	OMG	C5-N7	-3.15	1.33	1.39
70	L5	4637	OMG	C5-N7	-3.15	1.33	1.39
74	S2	1031	A2M	C5-C4	-3.14	1.33	1.39
70	L5	3925	OMU	O4-C4	-3.14	1.18	1.24
70	L5	4536	OMC	C6-N1	3.14	1.45	1.38
74	S2	966	PSU	C6-C5	3.14	1.39	1.35
70	L5	4499	OMG	C5-N7	-3.12	1.33	1.39
70	L5	4442	PSU	C6-C5	3.12	1.39	1.35
70	L5	3841	OMC	C6-N1	3.11	1.45	1.38
74	S2	462	OMC	C6-N1	3.11	1.45	1.38
74	S2	1391	OMC	C6-N1	3.11	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	1677	PSU	C6-C5	3.10	1.38	1.35
70	L5	3760	A2M	O3'-C3'	-3.09	1.35	1.43
70	L5	4530	UR3	C6-N1	3.09	1.45	1.38
70	L5	2837	OMU	O4-C4	-3.09	1.18	1.24
70	L5	3718	A2M	O3'-C3'	-3.09	1.35	1.43
70	L5	3701	OMC	C6-N1	3.09	1.45	1.38
74	S2	1328	OMG	C5-N7	-3.08	1.33	1.39
70	L5	1326	A2M	C5-C4	-3.08	1.33	1.39
74	S2	590	A2M	O3'-C3'	-3.08	1.35	1.43
74	S2	27	A2M	O3'-C3'	-3.07	1.35	1.43
70	L5	4456	OMC	C6-N1	3.07	1.45	1.38
74	S2	428	OMU	O4-C4	-3.06	1.18	1.24
70	L5	3867	A2M	O3'-C3'	-3.06	1.35	1.43
70	L5	4571	A2M	O3'-C3'	-3.06	1.35	1.43
70	L5	1534	A2M	O3'-C3'	-3.06	1.35	1.43
67	Pt	33	OMC	C6-N1	3.05	1.45	1.38
70	L5	4220	6MZ	C5-C4	-3.05	1.33	1.39
74	S2	815	PSU	C6-C5	3.04	1.38	1.35
70	L5	4498	OMU	O4-C4	-3.04	1.18	1.24
70	L5	4620	OMU	O4-C4	-3.04	1.18	1.24
74	S2	668	A2M	C5-C4	-3.03	1.33	1.39
70	L5	3808	OMC	C6-N1	3.03	1.45	1.38
70	L5	1326	A2M	O3'-C3'	-3.03	1.35	1.43
74	S2	867	OMG	C5-N7	-3.03	1.33	1.39
74	S2	1678	A2M	O3'-C3'	-3.03	1.35	1.43
74	S2	1031	A2M	O3'-C3'	-3.02	1.35	1.43
70	L5	4590	A2M	O3'-C3'	-3.02	1.35	1.43
70	L5	2363	A2M	O3'-C3'	-3.02	1.35	1.43
70	L5	400	A2M	O3'-C3'	-3.02	1.35	1.43
74	S2	468	A2M	O3'-C3'	-3.01	1.35	1.43
70	L5	3718	A2M	C5-C4	-3.00	1.33	1.39
70	L5	1871	A2M	C5-C4	-3.00	1.33	1.39
74	S2	1383	A2M	O3'-C3'	-2.99	1.35	1.43
74	S2	1678	A2M	C5-C4	-2.99	1.33	1.39
70	L5	2363	A2M	C5-C4	-2.98	1.33	1.39
70	L5	398	A2M	O3'-C3'	-2.98	1.36	1.43
70	L5	3825	A2M	C5-C4	-2.98	1.33	1.39
70	L5	1340	OMC	C6-N1	2.97	1.45	1.38
70	L5	1524	A2M	O3'-C3'	-2.97	1.36	1.43
70	L5	3830	A2M	C5-C4	-2.97	1.33	1.39
70	L5	3867	A2M	C5-C4	-2.96	1.33	1.39
70	L5	3830	A2M	O3'-C3'	-2.96	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	99	A2M	O3'-C3'	-2.96	1.36	1.43
74	S2	116	OMU	O4-C4	-2.95	1.18	1.24
74	S2	484	A2M	C5-C4	-2.95	1.33	1.39
70	L5	4227	OMU	O4-C4	-2.94	1.18	1.24
70	L5	4220	6MZ	C5-N7	-2.93	1.33	1.39
70	L5	1534	A2M	C5-C4	-2.93	1.33	1.39
70	L5	4523	A2M	C5-C4	-2.93	1.33	1.39
74	S2	27	A2M	C5-C4	-2.92	1.33	1.39
74	S2	468	A2M	C5-C4	-2.92	1.33	1.39
74	S2	512	A2M	C5-C4	-2.92	1.33	1.39
70	L5	1524	A2M	C5-C4	-2.91	1.33	1.39
70	L5	2401	A2M	O3'-C3'	-2.91	1.36	1.43
74	S2	1804	OMU	O4-C4	-2.91	1.18	1.24
70	L5	3825	A2M	O3'-C3'	-2.91	1.36	1.43
70	L5	2815	A2M	O3'-C3'	-2.89	1.36	1.43
74	S2	1804	OMU	C6-N1	2.89	1.45	1.38
70	L5	2815	A2M	C5-C4	-2.89	1.33	1.39
74	S2	627	OMU	O4-C4	-2.88	1.18	1.24
74	S2	576	A2M	O3'-C3'	-2.88	1.36	1.43
74	S2	668	A2M	O2'-C2'	2.88	1.50	1.42
70	L5	400	A2M	C5-C4	-2.88	1.33	1.39
74	S2	1031	A2M	C5-N7	-2.88	1.33	1.39
74	S2	99	A2M	C5-C4	-2.88	1.33	1.39
70	L5	2824	OMC	O2-C2	-2.88	1.18	1.23
70	L5	1326	A2M	O2'-C2'	2.87	1.50	1.42
70	L5	2401	A2M	C5-C4	-2.87	1.33	1.39
67	Pt	47	G7M	C2-N1	2.87	1.44	1.37
74	S2	512	A2M	O3'-C3'	-2.87	1.36	1.43
70	L5	4523	A2M	O3'-C3'	-2.87	1.36	1.43
74	S2	1678	A2M	O2'-C2'	2.86	1.50	1.42
74	S2	1703	OMC	O2-C2	-2.86	1.18	1.23
70	L5	398	A2M	O2'-C2'	2.85	1.49	1.42
74	S2	1832	6MZ	C5-C4	-2.85	1.33	1.39
74	S2	576	A2M	O2'-C2'	2.85	1.49	1.42
74	S2	627	OMU	C6-N1	2.84	1.44	1.38
70	L5	398	A2M	C5-C4	-2.84	1.33	1.39
70	L5	4571	A2M	C5-C4	-2.84	1.33	1.39
74	S2	668	A2M	O3'-C3'	-2.83	1.36	1.43
74	S2	1383	A2M	C5-C4	-2.83	1.33	1.39
70	L5	2861	OMC	O2-C2	-2.83	1.18	1.23
70	L5	4523	A2M	C5-N7	-2.83	1.33	1.39
70	L5	3841	OMC	O2-C2	-2.82	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	484	A2M	O3'-C3'	-2.82	1.36	1.43
70	L5	2815	A2M	O2'-C2'	2.82	1.49	1.42
70	L5	3701	OMC	O2-C2	-2.81	1.18	1.23
70	L5	400	A2M	O2'-C2'	2.81	1.49	1.42
74	S2	1383	A2M	O2'-C2'	2.81	1.49	1.42
74	S2	512	A2M	O2'-C2'	2.81	1.49	1.42
70	L5	4590	A2M	C5-C4	-2.81	1.33	1.39
70	L5	3760	A2M	O2'-C2'	2.80	1.49	1.42
74	S2	99	A2M	O2'-C2'	2.80	1.49	1.42
70	L5	3825	A2M	C5-N7	-2.80	1.33	1.39
70	L5	1881	OMC	O2-C2	-2.80	1.18	1.23
74	S2	576	A2M	C5-N7	-2.79	1.33	1.39
74	S2	484	A2M	C5-N7	-2.79	1.33	1.39
70	L5	2815	A2M	C5-N7	-2.79	1.33	1.39
74	S2	484	A2M	O2'-C2'	2.79	1.49	1.42
74	S2	590	A2M	O2'-C2'	2.78	1.49	1.42
70	L5	3869	OMC	O2-C2	-2.78	1.18	1.23
70	L5	4498	OMU	C6-N1	2.78	1.44	1.38
70	L5	1534	A2M	O2'-C2'	2.78	1.49	1.42
70	L5	3785	A2M	O2'-C2'	2.78	1.49	1.42
70	L5	2804	OMC	O2-C2	-2.78	1.18	1.23
70	L5	3760	A2M	C5-C4	-2.78	1.33	1.39
70	L5	2365	OMC	O2-C2	-2.77	1.18	1.23
70	L5	1340	OMC	O2-C2	-2.77	1.18	1.23
70	L5	2422	OMC	O2-C2	-2.76	1.18	1.23
70	L5	3867	A2M	O2'-C2'	2.76	1.49	1.42
70	L5	2401	A2M	C5-N7	-2.76	1.33	1.39
70	L5	3825	A2M	O2'-C2'	2.76	1.49	1.42
70	L5	2363	A2M	C5-N7	-2.76	1.33	1.39
70	L5	2401	A2M	O2'-C2'	2.76	1.49	1.42
70	L5	4447	5MC	O2-C2	-2.76	1.18	1.23
74	S2	590	A2M	C5-C4	-2.75	1.33	1.39
74	S2	512	A2M	C5-N7	-2.75	1.33	1.39
70	L5	3925	OMU	C6-N1	2.75	1.44	1.38
74	S2	99	A2M	C5-N7	-2.74	1.33	1.39
70	L5	4590	A2M	O2'-C2'	2.73	1.49	1.42
74	S2	468	A2M	O2'-C2'	2.73	1.49	1.42
70	L5	2351	OMC	O2-C2	-2.73	1.18	1.23
74	S2	576	A2M	C5-C4	-2.73	1.33	1.39
74	S2	1639	G7M	C2-N1	2.73	1.44	1.37
70	L5	3785	A2M	O3'-C3'	-2.72	1.36	1.43
74	S2	116	OMU	C6-N1	2.72	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4571	A2M	O2'-C2'	2.72	1.49	1.42
70	L5	2837	OMU	C6-N1	2.72	1.44	1.38
70	L5	2363	A2M	O2'-C2'	2.72	1.49	1.42
70	L5	4227	OMU	C6-N1	2.72	1.44	1.38
74	S2	517	OMC	O2-C2	-2.71	1.18	1.23
70	L5	3830	A2M	O2'-C2'	2.71	1.49	1.42
70	L5	1871	A2M	O2'-C2'	2.71	1.49	1.42
70	L5	3718	A2M	O2'-C2'	2.71	1.49	1.42
70	L5	4392	OMG	O6-C6	-2.71	1.18	1.23
70	L5	1524	A2M	C5-N7	-2.71	1.33	1.39
70	L5	3782	5MC	O2-C2	-2.70	1.18	1.23
70	L5	4523	A2M	O2'-C2'	2.70	1.49	1.42
70	L5	1524	A2M	O2'-C2'	2.70	1.49	1.42
67	Pt	8	4SU	C6-N1	2.70	1.44	1.38
70	L5	4456	OMC	O2-C2	-2.69	1.18	1.23
70	L5	3808	OMC	O2-C2	-2.69	1.18	1.23
70	L5	4571	A2M	C5-N7	-2.69	1.33	1.39
74	S2	1391	OMC	O2-C2	-2.68	1.18	1.23
70	L5	1316	OMG	O6-C6	-2.68	1.18	1.23
74	S2	1383	A2M	C5-N7	-2.68	1.34	1.39
74	S2	428	OMU	C6-N1	2.68	1.44	1.38
70	L5	1326	A2M	C5-N7	-2.68	1.34	1.39
70	L5	3867	A2M	C5-N7	-2.67	1.34	1.39
74	S2	436	OMG	O6-C6	-2.67	1.18	1.23
74	S2	1850	MA6	C5-C4	-2.67	1.34	1.39
74	S2	1851	MA6	C5-C4	-2.67	1.34	1.39
70	L5	4196	OMG	O6-C6	-2.66	1.18	1.23
70	L5	4536	OMC	O2-C2	-2.66	1.18	1.23
74	S2	1081	PSU	C6-C5	2.66	1.38	1.35
70	L5	3785	A2M	C5-N7	-2.66	1.34	1.39
70	L5	3887	OMC	O2-C2	-2.65	1.18	1.23
70	L5	2424	OMG	C2-N1	2.65	1.44	1.37
74	S2	462	OMC	O2-C2	-2.65	1.18	1.23
70	L5	4620	OMU	C6-N1	2.64	1.44	1.38
74	S2	27	A2M	O2'-C2'	2.64	1.49	1.42
74	S2	867	OMG	C2-N1	2.64	1.44	1.37
74	S2	27	A2M	C5-N7	-2.64	1.34	1.39
70	L5	1534	A2M	C5-N7	-2.64	1.34	1.39
70	L5	2364	OMG	O6-C6	-2.63	1.18	1.23
70	L5	1871	A2M	C5-N7	-2.63	1.34	1.39
70	L5	2876	OMG	O6-C6	-2.63	1.18	1.23
70	L5	4494	OMG	O6-C6	-2.63	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4618	OMG	O6-C6	-2.63	1.18	1.23
70	L5	3899	OMG	O6-C6	-2.63	1.18	1.23
70	L5	3627	OMG	O6-C6	-2.62	1.18	1.23
70	L5	2876	OMG	C2-N1	2.62	1.44	1.37
70	L5	3792	OMG	O6-C6	-2.62	1.18	1.23
67	Pt	33	OMC	O2-C2	-2.62	1.18	1.23
74	S2	1678	A2M	C5-N7	-2.62	1.34	1.39
74	S2	1832	6MZ	C5-N7	-2.62	1.34	1.39
70	L5	3744	OMG	C2-N1	2.62	1.44	1.37
74	S2	1328	OMG	O6-C6	-2.62	1.18	1.23
70	L5	3760	A2M	C5-N7	-2.61	1.34	1.39
70	L5	4494	OMG	C2-N1	2.61	1.44	1.37
74	S2	683	OMG	C2-N1	2.61	1.44	1.37
70	L5	4623	OMG	O6-C6	-2.61	1.18	1.23
70	L5	4228	OMG	O6-C6	-2.60	1.18	1.23
74	S2	644	OMG	O6-C6	-2.60	1.18	1.23
70	L5	1522	OMG	O6-C6	-2.60	1.18	1.23
70	L5	4590	A2M	C5-N7	-2.60	1.34	1.39
70	L5	4499	OMG	C2-N1	2.60	1.44	1.37
70	L5	4637	OMG	O6-C6	-2.60	1.18	1.23
74	S2	590	A2M	C5-N7	-2.60	1.34	1.39
69	L8	75	OMG	C2-N1	2.60	1.44	1.37
70	L5	3718	A2M	C5-N7	-2.59	1.34	1.39
70	L5	400	A2M	C5-N7	-2.59	1.34	1.39
70	L5	3627	OMG	C2-N1	2.59	1.44	1.37
74	S2	1328	OMG	C2-N1	2.59	1.44	1.37
70	L5	4499	OMG	O6-C6	-2.59	1.18	1.23
74	S2	683	OMG	O6-C6	-2.59	1.18	1.23
74	S2	1851	MA6	C5-N7	-2.59	1.34	1.39
70	L5	4370	OMG	O6-C6	-2.59	1.18	1.23
74	S2	509	OMG	O6-C6	-2.59	1.18	1.23
74	S2	468	A2M	C5-N7	-2.59	1.34	1.39
70	L5	1625	OMG	C2-N1	2.58	1.44	1.37
70	L5	3830	A2M	C5-N7	-2.58	1.34	1.39
67	Pt	47	G7M	O6-C6	-2.58	1.18	1.23
74	S2	644	OMG	C2-N1	2.58	1.44	1.37
70	L5	4623	OMG	C2-N1	2.58	1.44	1.37
74	S2	1031	A2M	O2'-C2'	2.57	1.49	1.42
74	S2	668	A2M	C5-N7	-2.57	1.34	1.39
70	L5	1316	OMG	C2-N1	2.57	1.44	1.37
70	L5	4618	OMG	C2-N1	2.57	1.44	1.37
74	S2	1850	MA6	C5-N7	-2.56	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	S2	1490	OMG	C2-N1	2.56	1.44	1.37
67	Pt	47	G7M	C6-N1	2.56	1.43	1.38
70	L5	4228	OMG	C2-N1	2.55	1.44	1.37
70	L5	1625	OMG	O6-C6	-2.55	1.18	1.23
74	S2	1490	OMG	O6-C6	-2.55	1.18	1.23
70	L5	3744	OMG	O6-C6	-2.55	1.18	1.23
74	S2	436	OMG	C2-N1	2.55	1.44	1.37
70	L5	1522	OMG	C2-N1	2.54	1.44	1.37
70	L5	4370	OMG	C2-N1	2.53	1.43	1.37
70	L5	2364	OMG	C2-N1	2.53	1.43	1.37
70	L5	2424	OMG	O6-C6	-2.52	1.18	1.23
70	L5	398	A2M	C5-N7	-2.52	1.34	1.39
74	S2	1703	OMC	C5-C4	2.52	1.48	1.42
70	L5	4196	OMG	C2-N1	2.52	1.43	1.37
70	L5	4637	OMG	C5-C6	2.51	1.53	1.44
70	L5	3792	OMG	C2-N1	2.51	1.43	1.37
74	S2	867	OMG	C5-C6	2.51	1.53	1.44
70	L5	4637	OMG	C2-N1	2.50	1.43	1.37
70	L5	3899	OMG	C2-N1	2.50	1.43	1.37
70	L5	4228	OMG	C5-C6	2.49	1.53	1.44
69	L8	75	OMG	O6-C6	-2.49	1.18	1.23
70	L5	2422	OMC	C5-C4	2.49	1.48	1.42
70	L5	1522	OMG	C5-C6	2.48	1.53	1.44
74	S2	1639	G7M	O6-C6	-2.47	1.18	1.23
74	S2	867	OMG	O6-C6	-2.47	1.18	1.23
74	S2	1639	G7M	C6-N1	2.47	1.43	1.38
70	L5	2824	OMC	C5-C4	2.46	1.48	1.42
70	L5	2876	OMG	C5-C6	2.46	1.53	1.44
70	L5	2424	OMG	C5-C6	2.45	1.53	1.44
70	L5	4498	OMU	O2-C2	-2.45	1.18	1.23
70	L5	3701	OMC	C5-C4	2.45	1.48	1.42
70	L5	3925	OMU	O2-C2	-2.45	1.18	1.23
70	L5	4620	OMU	O2-C2	-2.44	1.18	1.23
70	L5	3744	OMG	C5-C6	2.44	1.53	1.44
70	L5	4392	OMG	C5-C6	2.44	1.53	1.44
70	L5	3825	A2M	C8-N9	-2.44	1.33	1.37
69	L8	75	OMG	C5-C6	2.44	1.53	1.44
70	L5	4392	OMG	C2-N1	2.43	1.43	1.37
74	S2	517	OMC	C5-C4	2.43	1.48	1.42
74	S2	509	OMG	C2-N1	2.43	1.43	1.37
70	L5	1881	OMC	C5-C4	2.43	1.48	1.42
74	S2	1031	A2M	C8-N9	-2.42	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	2804	OMC	C5-C4	2.42	1.48	1.42
74	S2	116	OMU	O2-C2	-2.41	1.18	1.23
70	L5	4227	OMU	O2-C2	-2.41	1.18	1.23
74	S2	644	OMG	C5-C6	2.41	1.53	1.44
74	S2	1328	OMG	C5-C6	2.41	1.53	1.44
70	L5	4623	OMG	C5-C6	2.41	1.53	1.44
74	S2	1490	OMG	C5-C6	2.41	1.53	1.44
74	S2	867	OMG	C6-N1	2.40	1.43	1.38
70	L5	4499	OMG	C5-C6	2.40	1.53	1.44
69	L8	75	OMG	C6-N1	2.40	1.43	1.38
70	L5	2364	OMG	C5-C6	2.39	1.53	1.44
70	L5	2861	OMC	C5-C4	2.39	1.48	1.42
70	L5	3627	OMG	C5-C6	2.39	1.53	1.44
70	L5	2837	OMU	O2-C2	-2.38	1.18	1.23
70	L5	1625	OMG	C5-C6	2.38	1.53	1.44
70	L5	2365	OMC	C5-C4	2.37	1.48	1.42
74	S2	462	OMC	C5-C4	2.37	1.48	1.42
70	L5	3899	OMG	C5-C6	2.37	1.53	1.44
74	S2	428	OMU	O2-C2	-2.37	1.18	1.23
70	L5	1316	OMG	C5-C6	2.36	1.53	1.44
74	S2	1804	OMU	O2-C2	-2.36	1.18	1.23
70	L5	4618	OMG	C5-C6	2.36	1.53	1.44
70	L5	3869	OMC	C5-C4	2.35	1.48	1.42
70	L5	3744	OMG	C6-N1	2.35	1.43	1.38
74	S2	627	OMU	C5-C4	2.35	1.48	1.43
74	S2	1248	B8N	O2-C2	-2.35	1.18	1.22
70	L5	4196	OMG	C5-C6	2.34	1.53	1.44
70	L5	4370	OMG	C5-C6	2.34	1.53	1.44
74	S2	509	OMG	C5-C6	2.34	1.53	1.44
74	S2	683	OMG	C6-N1	2.34	1.43	1.38
70	L5	4536	OMC	C5-C4	2.34	1.48	1.42
74	S2	683	OMG	C5-C6	2.34	1.53	1.44
74	S2	436	OMG	C5-C6	2.33	1.53	1.44
70	L5	2424	OMG	C6-N1	2.33	1.43	1.38
70	L5	1522	OMG	C6-N1	2.33	1.43	1.38
74	S2	1248	B8N	O4-C4	-2.33	1.18	1.23
70	L5	2876	OMG	C6-N1	2.33	1.43	1.38
70	L5	4530	UR3	C5-C4	2.33	1.49	1.43
70	L5	4494	OMG	C5-C6	2.32	1.53	1.44
70	L5	4220	6MZ	C8-N9	-2.31	1.33	1.37
70	L5	3887	OMC	C5-C4	2.31	1.48	1.42
70	L5	4456	OMC	C5-C4	2.31	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	4623	OMG	C6-N1	2.31	1.43	1.38
70	L5	3808	OMC	C5-C4	2.30	1.48	1.42
74	S2	627	OMU	O2-C2	-2.30	1.18	1.23
70	L5	3792	OMG	C5-C6	2.30	1.52	1.44
74	S2	1804	OMU	C5-C4	2.30	1.48	1.43
74	S2	1678	A2M	C8-N9	-2.30	1.33	1.37
70	L5	4499	OMG	C6-N1	2.29	1.43	1.38
70	L5	1340	OMC	C5-C4	2.29	1.48	1.42
74	S2	1328	OMG	C6-N1	2.29	1.43	1.38
70	L5	4618	OMG	C6-N1	2.29	1.43	1.38
70	L5	4228	OMG	C6-N1	2.28	1.43	1.38
74	S2	1391	OMC	C5-C4	2.28	1.48	1.42
70	L5	3841	OMC	C5-C4	2.28	1.48	1.42
74	S2	644	OMG	C6-N1	2.27	1.43	1.38
70	L5	4370	OMG	C6-N1	2.27	1.43	1.38
70	L5	1316	OMG	C6-N1	2.27	1.43	1.38
70	L5	1625	OMG	C6-N1	2.27	1.43	1.38
74	S2	484	A2M	C8-N9	-2.27	1.33	1.37
70	L5	4227	OMU	C5-C4	2.27	1.48	1.43
67	Pt	21	H2U	O4-C4	-2.26	1.18	1.23
70	L5	4498	OMU	C5-C4	2.26	1.48	1.43
70	L5	3792	OMG	C6-N1	2.26	1.43	1.38
70	L5	1534	A2M	C8-N9	-2.26	1.33	1.37
70	L5	4494	OMG	C6-N1	2.26	1.43	1.38
70	L5	1322	1MA	C4-N9	-2.25	1.32	1.38
70	L5	2363	A2M	C8-N9	-2.25	1.33	1.37
74	S2	1490	OMG	C6-N1	2.25	1.43	1.38
70	L5	2364	OMG	C6-N1	2.25	1.43	1.38
74	S2	436	OMG	C6-N1	2.24	1.43	1.38
70	L5	2837	OMU	C5-C4	2.23	1.48	1.43
67	Pt	21	H2U	O2-C2	-2.22	1.19	1.23
70	L5	2351	OMC	C5-C4	2.21	1.48	1.42
67	Pt	33	OMC	C5-C4	2.21	1.48	1.42
70	L5	2401	A2M	C8-N9	-2.21	1.33	1.37
70	L5	4196	OMG	C6-N1	2.21	1.42	1.38
70	L5	3830	A2M	C8-N9	-2.21	1.33	1.37
70	L5	3760	A2M	C8-N9	-2.20	1.33	1.37
74	S2	116	OMU	C5-C4	2.20	1.48	1.43
74	S2	99	A2M	C8-N9	-2.20	1.33	1.37
70	L5	4637	OMG	C6-N1	2.20	1.42	1.38
70	L5	3718	A2M	C8-N9	-2.19	1.33	1.37
74	S2	590	A2M	C8-N9	-2.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	L5	3867	A2M	C8-N9	-2.19	1.33	1.37
70	L5	1524	A2M	C8-N9	-2.18	1.33	1.37
70	L5	4523	A2M	C8-N9	-2.18	1.33	1.37
74	S2	668	A2M	C8-N9	-2.18	1.33	1.37
70	L5	3627	OMG	C6-N1	2.17	1.42	1.38
74	S2	27	A2M	C8-N9	-2.17	1.33	1.37
70	L5	2815	A2M	C8-N9	-2.17	1.33	1.37
70	L5	4620	OMU	C5-C4	2.16	1.48	1.43
74	S2	512	A2M	C8-N9	-2.16	1.33	1.37
70	L5	3925	OMU	C5-C4	2.16	1.48	1.43
74	S2	1832	6MZ	C8-N9	-2.16	1.33	1.37
74	S2	1850	MA6	C8-N9	-2.16	1.33	1.37
70	L5	1871	A2M	C8-N9	-2.15	1.33	1.37
70	L5	4590	A2M	C8-N9	-2.15	1.33	1.37
70	L5	3785	A2M	C8-N9	-2.15	1.33	1.37
74	S2	1851	MA6	C8-N9	-2.15	1.33	1.37
67	Pt	47	G7M	C4-N9	-2.14	1.32	1.38
74	S2	1248	B8N	C2-N3	2.14	1.42	1.38
74	S2	822	PSU	O4'-C1'	-2.14	1.40	1.43
74	S2	428	OMU	C5-C4	2.14	1.48	1.43
70	L5	1524	A2M	O5'-C5'	-2.13	1.39	1.44
70	L5	3899	OMG	C6-N1	2.13	1.42	1.38
74	S2	576	A2M	C8-N9	-2.13	1.33	1.37
74	S2	509	OMG	C6-N1	2.12	1.42	1.38
70	L5	4571	A2M	C8-N9	-2.10	1.33	1.37
70	L5	4392	OMG	C6-N1	2.10	1.42	1.38
70	L5	400	A2M	C8-N9	-2.09	1.33	1.37
70	L5	398	A2M	C8-N9	-2.07	1.33	1.37
70	L5	4530	UR3	O4-C4	-2.07	1.19	1.23
74	S2	1383	A2M	O5'-C5'	-2.07	1.39	1.44
70	L5	1326	A2M	C8-N9	-2.07	1.33	1.37
74	S2	918	PSU	O4'-C1'	-2.07	1.41	1.43
70	L5	4530	UR3	O2-C2	-2.07	1.18	1.22
74	S2	668	A2M	O5'-C5'	-2.06	1.39	1.44
70	L5	4228	OMG	C4-N9	-2.05	1.32	1.38
70	L5	1326	A2M	O5'-C5'	-2.05	1.39	1.44
70	L5	2401	A2M	O5'-C5'	-2.03	1.39	1.44
70	L5	3825	A2M	O5'-C5'	-2.02	1.39	1.44
74	S2	27	A2M	O5'-C5'	-2.02	1.39	1.44
74	S2	468	A2M	C8-N9	-2.01	1.33	1.37
74	S2	512	A2M	O5'-C5'	-2.01	1.39	1.44
74	S2	1639	G7M	C4-N9	-2.01	1.32	1.38

All (1125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1851	MA6	N1-C6-N6	-15.79	99.82	117.08
74	S2	1850	MA6	N1-C6-N6	-15.05	100.62	117.08
70	L5	1322	1MA	C1'-N9-C8	-9.09	100.81	126.70
74	S2	1851	MA6	C5-C6-N6	8.87	140.75	125.30
70	L5	1322	1MA	C1'-N9-C4	8.83	152.73	126.50
74	S2	1850	MA6	C5-C6-N6	8.43	139.98	125.30
67	Pt	8	4SU	C4-N3-C2	-7.71	119.85	127.34
74	S2	1639	G7M	C1'-N9-C4	7.34	148.29	126.50
67	Pt	47	G7M	C1'-N9-C8	-7.31	102.07	126.74
74	S2	1639	G7M	C1'-N9-C8	-7.26	102.24	126.74
67	Pt	47	G7M	C1'-N9-C4	7.04	147.42	126.50
67	Pt	21	H2U	C4-N3-C2	-6.56	120.35	125.79
74	S2	590	A2M	C5-C4-N3	-6.02	118.90	126.75
70	L5	2876	OMG	C5-C4-N3	-6.01	118.71	128.46
70	L5	3830	A2M	N3-C2-N1	-5.83	119.48	128.60
74	S2	512	A2M	N3-C2-N1	-5.79	119.54	128.60
70	L5	4590	A2M	N3-C2-N1	-5.78	119.56	128.60
70	L5	3760	A2M	C5-C4-N3	-5.77	119.22	126.75
70	L5	1322	1MA	N1-C2-N3	-5.75	119.16	126.00
74	S2	512	A2M	C5-C4-N3	-5.75	119.25	126.75
74	S2	1031	A2M	N3-C2-N1	-5.73	119.64	128.60
70	L5	1871	A2M	N3-C2-N1	-5.69	119.70	128.60
70	L5	1625	OMG	C5-C4-N3	-5.68	119.25	128.46
74	S2	668	A2M	N3-C2-N1	-5.67	119.72	128.60
70	L5	4637	OMG	C5-C4-N3	-5.67	119.26	128.46
70	L5	1534	A2M	N3-C2-N1	-5.67	119.74	128.60
70	L5	2815	A2M	C5-C4-N3	-5.67	119.36	126.75
74	S2	1678	A2M	C5-C4-N3	-5.66	119.37	126.75
70	L5	2363	A2M	N3-C2-N1	-5.64	119.78	128.60
74	S2	1850	MA6	N1-C2-N3	-5.62	119.81	128.60
70	L5	400	A2M	N3-C2-N1	-5.59	119.85	128.60
74	S2	1678	A2M	N3-C2-N1	-5.59	119.85	128.60
70	L5	1326	A2M	N3-C2-N1	-5.59	119.86	128.60
74	S2	683	OMG	C5-C4-N3	-5.58	119.40	128.46
70	L5	2401	A2M	C5-C4-N3	-5.58	119.47	126.75
74	S2	644	OMG	C5-C4-N3	-5.58	119.42	128.46
70	L5	3792	OMG	C5-C4-N3	-5.57	119.42	128.46
74	S2	468	A2M	N3-C2-N1	-5.56	119.90	128.60
74	S2	484	A2M	N3-C2-N1	-5.56	119.90	128.60
74	S2	590	A2M	N3-C2-N1	-5.56	119.91	128.60
67	Pt	8	4SU	C5-C4-N3	5.56	119.84	114.69
74	S2	1383	A2M	N3-C2-N1	-5.56	119.91	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	4571	A2M	N3-C2-N1	-5.53	119.95	128.60
74	S2	509	OMG	C5-C4-N3	-5.53	119.50	128.46
74	S2	1851	MA6	N1-C2-N3	-5.52	119.96	128.60
74	S2	27	A2M	N3-C2-N1	-5.52	119.97	128.60
70	L5	3760	A2M	N3-C2-N1	-5.51	119.97	128.60
74	S2	1031	A2M	C5-C4-N3	-5.51	119.56	126.75
74	S2	99	A2M	N3-C2-N1	-5.51	119.98	128.60
70	L5	4618	OMG	C5-C4-N3	-5.51	119.52	128.46
70	L5	3825	A2M	C5-C4-N3	-5.51	119.56	126.75
70	L5	3718	A2M	N3-C2-N1	-5.50	120.00	128.60
70	L5	3825	A2M	N3-C2-N1	-5.50	120.00	128.60
70	L5	1524	A2M	N3-C2-N1	-5.48	120.03	128.60
70	L5	4196	OMG	C5-C4-N3	-5.48	119.58	128.46
74	S2	27	A2M	C5-C4-N3	-5.47	119.61	126.75
74	S2	1851	MA6	C5-C4-N3	-5.46	119.62	126.75
70	L5	4523	A2M	C5-C4-N3	-5.46	119.62	126.75
70	L5	2401	A2M	N3-C2-N1	-5.46	120.07	128.60
70	L5	3830	A2M	C5-C4-N3	-5.45	119.64	126.75
70	L5	4523	A2M	N3-C2-N1	-5.45	120.07	128.60
70	L5	2815	A2M	N3-C2-N1	-5.45	120.08	128.60
70	L5	4392	OMG	C5-C4-N3	-5.43	119.66	128.46
70	L5	3785	A2M	C5-C4-N3	-5.42	119.68	126.75
70	L5	2364	OMG	C5-C4-N3	-5.42	119.67	128.46
70	L5	3785	A2M	N3-C2-N1	-5.42	120.13	128.60
70	L5	4623	OMG	C5-C4-N3	-5.41	119.68	128.46
70	L5	398	A2M	N3-C2-N1	-5.41	120.14	128.60
70	L5	3867	A2M	C5-C4-N3	-5.40	119.70	126.75
74	S2	99	A2M	C5-C4-N3	-5.39	119.71	126.75
70	L5	3899	OMG	C5-C4-N3	-5.38	119.74	128.46
74	S2	1383	A2M	C5-C4-N3	-5.37	119.74	126.75
70	L5	4494	OMG	C5-C4-N3	-5.36	119.76	128.46
74	S2	1490	OMG	C5-C4-N3	-5.36	119.76	128.46
74	S2	484	A2M	C5-C4-N3	-5.36	119.76	126.75
70	L5	3627	OMG	C5-C4-N3	-5.36	119.77	128.46
70	L5	1524	A2M	C5-C4-N3	-5.36	119.76	126.75
74	S2	576	A2M	C5-C4-N3	-5.35	119.77	126.75
70	L5	400	A2M	C5-C4-N3	-5.35	119.78	126.75
70	L5	3744	OMG	C5-C4-N3	-5.34	119.79	128.46
70	L5	3718	A2M	C5-C4-N3	-5.34	119.78	126.75
70	L5	2837	OMU	C4-N3-C2	-5.34	119.54	126.58
70	L5	2424	OMG	C5-C4-N3	-5.34	119.80	128.46
70	L5	398	A2M	C5-C4-N3	-5.33	119.79	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	4227	OMU	C4-N3-C2	-5.33	119.55	126.58
70	L5	4498	OMU	C4-N3-C2	-5.32	119.56	126.58
70	L5	4590	A2M	C5-C4-N3	-5.31	119.83	126.75
70	L5	3867	A2M	N3-C2-N1	-5.30	120.31	128.60
70	L5	3925	OMU	C4-N3-C2	-5.30	119.59	126.58
70	L5	4220	6MZ	N1-C2-N3	-5.30	120.31	128.60
74	S2	627	OMU	C4-N3-C2	-5.30	119.59	126.58
74	S2	428	OMU	C4-N3-C2	-5.30	119.59	126.58
74	S2	576	A2M	N3-C2-N1	-5.29	120.33	128.60
70	L5	4499	OMG	C5-C4-N3	-5.28	119.89	128.46
74	S2	436	OMG	C5-C4-N3	-5.28	119.89	128.46
70	L5	1316	OMG	C5-C4-N3	-5.27	119.91	128.46
74	S2	1850	MA6	C5-C4-N3	-5.27	119.88	126.75
70	L5	1522	OMG	C5-C4-N3	-5.26	119.92	128.46
70	L5	2363	A2M	C5-C4-N3	-5.26	119.89	126.75
74	S2	1328	OMG	C5-C4-N3	-5.24	119.95	128.46
70	L5	1326	A2M	C5-C4-N3	-5.24	119.91	126.75
74	S2	668	A2M	C5-C4-N3	-5.24	119.92	126.75
69	L8	75	OMG	C5-C4-N3	-5.23	119.97	128.46
70	L5	1534	A2M	C5-C4-N3	-5.23	119.93	126.75
74	S2	1832	6MZ	N1-C2-N3	-5.22	120.43	128.60
74	S2	468	A2M	C5-C4-N3	-5.21	119.96	126.75
70	L5	4370	OMG	C5-C4-N3	-5.19	120.04	128.46
70	L5	4571	A2M	C5-C4-N3	-5.18	119.99	126.75
74	S2	1248	B8N	C5-C4-N3	5.18	125.76	116.17
70	L5	3867	A2M	N6-C6-N1	-5.17	107.03	118.35
74	S2	1804	OMU	C4-N3-C2	-5.16	119.78	126.58
74	S2	867	OMG	C5-C4-N3	-5.14	120.13	128.46
74	S2	1678	A2M	N6-C6-N1	-5.13	107.12	118.35
74	S2	512	A2M	N6-C6-N1	-5.08	107.22	118.35
70	L5	1871	A2M	C5-C4-N3	-5.08	120.12	126.75
70	L5	4590	A2M	N6-C6-N1	-5.08	107.23	118.35
74	S2	1832	6MZ	N9-C8-N7	-5.06	107.00	113.91
70	L5	4228	OMG	C5-C4-N3	-5.06	120.26	128.46
74	S2	590	A2M	N6-C6-N1	-5.04	107.32	118.35
70	L5	3785	A2M	N6-C6-N1	-5.03	107.33	118.35
70	L5	4620	OMU	C4-N3-C2	-5.02	119.96	126.58
70	L5	2363	A2M	N6-C6-N1	-4.99	107.41	118.35
70	L5	1524	A2M	N6-C6-N1	-4.98	107.44	118.35
70	L5	3718	A2M	N6-C6-N1	-4.96	107.49	118.35
74	S2	668	A2M	N6-C6-N1	-4.94	107.53	118.35
70	L5	1534	A2M	N6-C6-N1	-4.92	107.57	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	4530	UR3	C4-N3-C2	-4.92	119.93	124.56
70	L5	398	A2M	N6-C6-N1	-4.91	107.59	118.35
70	L5	3830	A2M	N6-C6-N1	-4.91	107.59	118.35
70	L5	400	A2M	N6-C6-N1	-4.90	107.61	118.35
70	L5	4628	PSU	N1-C2-N3	4.90	120.69	115.13
74	S2	116	OMU	C4-N3-C2	-4.90	120.11	126.58
70	L5	2876	OMG	C2-N3-C4	4.89	121.01	112.30
74	S2	27	A2M	N6-C6-N1	-4.88	107.66	118.35
74	S2	1832	6MZ	C5-C4-N3	-4.85	120.43	126.75
70	L5	1326	A2M	N6-C6-N1	-4.84	107.75	118.35
70	L5	3637	PSU	N1-C2-N3	4.83	120.61	115.13
70	L5	3825	A2M	N6-C6-N1	-4.83	107.78	118.35
70	L5	2843	PSU	C4-N3-C2	-4.83	119.39	126.34
74	S2	1383	A2M	N6-C6-N1	-4.81	107.82	118.35
70	L5	2815	A2M	N6-C6-N1	-4.80	107.85	118.35
70	L5	1871	A2M	N6-C6-N1	-4.79	107.85	118.35
70	L5	3760	A2M	N6-C6-N1	-4.79	107.86	118.35
70	L5	2843	PSU	N1-C2-N3	4.79	120.55	115.13
74	S2	576	A2M	N6-C6-N1	-4.78	107.87	118.35
70	L5	4636	PSU	C4-N3-C2	-4.77	119.46	126.34
74	S2	484	A2M	N6-C6-N1	-4.77	107.89	118.35
70	L5	3792	OMG	C2-N3-C4	4.75	120.77	112.30
74	S2	99	A2M	N6-C6-N1	-4.75	107.95	118.35
74	S2	1031	A2M	N6-C6-N1	-4.74	107.97	118.35
74	S2	1367	PSU	C4-N3-C2	-4.71	119.55	126.34
74	S2	1239	PSU	C4-N3-C2	-4.71	119.55	126.34
70	L5	4500	PSU	N1-C2-N3	4.71	120.47	115.13
74	S2	1445	PSU	C4-N3-C2	-4.71	119.56	126.34
74	S2	1445	PSU	N1-C2-N3	4.70	120.46	115.13
70	L5	2401	A2M	N6-C6-N1	-4.70	108.06	118.35
70	L5	4220	6MZ	N9-C8-N7	-4.69	107.49	113.91
74	S2	573	PSU	C4-N3-C2	-4.68	119.60	126.34
74	S2	1136	PSU	C4-N3-C2	-4.68	119.60	126.34
70	L5	1862	PSU	C4-N3-C2	-4.67	119.60	126.34
74	S2	468	A2M	N6-C6-N1	-4.67	108.12	118.35
74	S2	822	PSU	N1-C2-N3	4.67	120.42	115.13
74	S2	683	OMG	C2-N3-C4	4.67	120.62	112.30
70	L5	4521	PSU	C4-N3-C2	-4.67	119.61	126.34
74	S2	649	PSU	N1-C2-N3	4.67	120.42	115.13
70	L5	2364	OMG	C2-N3-C4	4.66	120.61	112.30
70	L5	4457	PSU	N1-C2-N3	4.65	120.40	115.13
70	L5	5001	PSU	N1-C2-N3	4.65	120.39	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	609	PSU	C4-N3-C2	-4.65	119.65	126.34
70	L5	4457	PSU	C4-N3-C2	-4.64	119.65	126.34
74	S2	918	PSU	N1-C2-N3	4.64	120.39	115.13
70	L5	4628	PSU	C4-N3-C2	-4.64	119.65	126.34
74	S2	1081	PSU	C4-N3-C2	-4.63	119.67	126.34
74	S2	1367	PSU	N1-C2-N3	4.63	120.38	115.13
70	L5	4637	OMG	C2-N3-C4	4.62	120.54	112.30
70	L5	4293	PSU	N1-C2-N3	4.62	120.37	115.13
70	L5	4523	A2M	N6-C6-N1	-4.62	108.22	118.35
74	S2	1347	PSU	C4-N3-C2	-4.62	119.68	126.34
70	L5	4500	PSU	C4-N3-C2	-4.62	119.68	126.34
70	L5	3639	PSU	C4-N3-C2	-4.62	119.68	126.34
74	S2	686	PSU	C4-N3-C2	-4.62	119.69	126.34
70	L5	1677	PSU	C4-N3-C2	-4.62	119.69	126.34
74	S2	1244	PSU	C4-N3-C2	-4.62	119.69	126.34
70	L5	3695	PSU	C4-N3-C2	-4.61	119.69	126.34
70	L5	4618	OMG	C2-N3-C4	4.61	120.51	112.30
70	L5	4531	PSU	C4-N3-C2	-4.61	119.70	126.34
70	L5	3770	PSU	N1-C2-N3	4.61	120.35	115.13
70	L5	4673	PSU	N1-C2-N3	4.60	120.35	115.13
70	L5	1683	PSU	N1-C2-N3	4.60	120.34	115.13
74	S2	1056	PSU	C4-N3-C2	-4.60	119.71	126.34
70	L5	1862	PSU	N1-C2-N3	4.60	120.34	115.13
70	L5	4571	A2M	N6-C6-N1	-4.60	108.28	118.35
70	L5	3764	PSU	N1-C2-N3	4.59	120.33	115.13
70	L5	4353	PSU	C4-N3-C2	-4.59	119.73	126.34
74	S2	36	PSU	C4-N3-C2	-4.58	119.73	126.34
74	S2	406	PSU	N1-C2-N3	4.58	120.32	115.13
74	S2	109	PSU	N1-C2-N3	4.58	120.32	115.13
74	S2	1244	PSU	N1-C2-N3	4.58	120.31	115.13
74	S2	406	PSU	C4-N3-C2	-4.58	119.75	126.34
70	L5	3695	PSU	N1-C2-N3	4.57	120.31	115.13
70	L5	4403	PSU	C4-N3-C2	-4.57	119.76	126.34
70	L5	1782	PSU	C4-N3-C2	-4.57	119.76	126.34
70	L5	3844	PSU	C4-N3-C2	-4.57	119.76	126.34
70	L5	1779	PSU	C4-N3-C2	-4.56	119.76	126.34
70	L5	1683	PSU	C4-N3-C2	-4.56	119.77	126.34
70	L5	3770	PSU	C4-N3-C2	-4.56	119.77	126.34
74	S2	644	OMG	C2-N3-C4	4.56	120.42	112.30
70	L5	1625	OMG	C2-N3-C4	4.55	120.41	112.30
74	S2	686	PSU	N1-C2-N3	4.55	120.29	115.13
70	L5	3758	PSU	C4-N3-C2	-4.55	119.78	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	3637	PSU	C4-N3-C2	-4.55	119.78	126.34
74	S2	1490	OMG	C2-N3-C4	4.55	120.40	112.30
74	S2	1347	PSU	N1-C2-N3	4.55	120.28	115.13
70	L5	1779	PSU	N1-C2-N3	4.54	120.28	115.13
70	L5	3853	PSU	N1-C2-N3	4.54	120.27	115.13
70	L5	4636	PSU	N1-C2-N3	4.54	120.27	115.13
70	L5	3920	PSU	N1-C2-N3	4.54	120.27	115.13
70	L5	1744	PSU	C4-N3-C2	-4.54	119.80	126.34
70	L5	4293	PSU	C4-N3-C2	-4.54	119.80	126.34
67	Pt	56	PSU	C4-N3-C2	-4.54	119.80	126.34
74	S2	34	PSU	N1-C2-N3	4.54	120.27	115.13
70	L5	4361	PSU	C4-N3-C2	-4.54	119.80	126.34
70	L5	4220	6MZ	C5-C4-N3	-4.54	120.83	126.75
70	L5	3884	PSU	N1-C2-N3	4.53	120.26	115.13
74	S2	1243	PSU	N1-C2-N3	4.53	120.26	115.13
70	L5	4299	PSU	N1-C2-N3	4.53	120.26	115.13
70	L5	4423	PSU	N1-C2-N3	4.53	120.26	115.13
70	L5	4689	PSU	C4-N3-C2	-4.52	119.82	126.34
74	S2	1248	B8N	C4-N3-C2	-4.52	119.75	125.46
74	S2	1004	PSU	N1-C2-N3	4.52	120.25	115.13
70	L5	4403	PSU	N1-C2-N3	4.52	120.25	115.13
70	L5	3744	OMG	C2-N3-C4	4.52	120.35	112.30
74	S2	918	PSU	C4-N3-C2	-4.52	119.83	126.34
70	L5	3729	PSU	N1-C2-N3	4.52	120.25	115.13
70	L5	4521	PSU	N1-C2-N3	4.51	120.25	115.13
74	S2	1174	PSU	C4-N3-C2	-4.51	119.84	126.34
70	L5	2839	PSU	C4-N3-C2	-4.51	119.84	126.34
74	S2	1238	PSU	C4-N3-C2	-4.51	119.84	126.34
70	L5	4392	OMG	C2-N3-C4	4.51	120.33	112.30
74	S2	866	PSU	N1-C2-N3	4.51	120.24	115.13
74	S2	609	PSU	N1-C2-N3	4.51	120.23	115.13
70	L5	5001	PSU	C4-N3-C2	-4.50	119.85	126.34
70	L5	5010	PSU	N1-C2-N3	4.50	120.23	115.13
74	S2	109	PSU	C4-N3-C2	-4.50	119.85	126.34
70	L5	4493	PSU	C4-N3-C2	-4.50	119.85	126.34
70	L5	4972	PSU	N1-C2-N3	4.50	120.22	115.13
70	L5	3785	A2M	N9-C8-N7	-4.50	107.77	113.91
74	S2	1678	A2M	N9-C8-N7	-4.50	107.77	113.91
70	L5	1677	PSU	N1-C2-N3	4.50	120.22	115.13
74	S2	1238	PSU	N1-C2-N3	4.49	120.22	115.13
70	L5	3884	PSU	C4-N3-C2	-4.49	119.87	126.34
70	L5	3844	PSU	N1-C2-N3	4.49	120.22	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	866	PSU	C4-N3-C2	-4.49	119.87	126.34
70	L5	1744	PSU	N1-C2-N3	4.49	120.22	115.13
70	L5	4361	PSU	N1-C2-N3	4.49	120.22	115.13
70	L5	3851	PSU	C4-N3-C2	-4.49	119.87	126.34
74	S2	681	PSU	C4-N3-C2	-4.49	119.87	126.34
70	L5	4228	OMG	C1'-N9-C4	-4.49	113.18	126.50
70	L5	4493	PSU	N1-C2-N3	4.48	120.21	115.13
70	L5	4370	OMG	C2-N3-C4	4.48	120.29	112.30
70	L5	4531	PSU	N1-C2-N3	4.48	120.21	115.13
74	S2	1136	PSU	N1-C2-N3	4.48	120.21	115.13
70	L5	4312	PSU	N1-C2-N3	4.48	120.20	115.13
74	S2	218	PSU	C4-N3-C2	-4.48	119.89	126.34
70	L5	1522	OMG	C2-N3-C4	4.48	120.28	112.30
70	L5	3729	PSU	C4-N3-C2	-4.47	119.89	126.34
70	L5	3758	PSU	N1-C2-N3	4.47	120.20	115.13
74	S2	1232	PSU	N1-C2-N3	4.47	120.19	115.13
74	S2	1643	PSU	N1-C2-N3	4.47	120.19	115.13
74	S2	1832	6MZ	C5-N7-C8	4.47	109.86	103.51
70	L5	3768	PSU	C4-N3-C2	-4.46	119.91	126.34
70	L5	4196	OMG	C2-N3-C4	4.46	120.25	112.30
70	L5	3734	PSU	C4-N3-C2	-4.46	119.91	126.34
74	S2	1232	PSU	C4-N3-C2	-4.46	119.91	126.34
74	S2	801	PSU	C4-N3-C2	-4.46	119.91	126.34
70	L5	4431	PSU	N1-C2-N3	4.46	120.18	115.13
69	L8	75	OMG	C2-N3-C4	4.46	120.24	112.30
70	L5	4499	OMG	C2-N3-C4	4.46	120.24	112.30
70	L5	3899	OMG	C2-N3-C4	4.46	120.24	112.30
74	S2	436	OMG	C2-N3-C4	4.46	120.24	112.30
74	S2	1056	PSU	N1-C2-N3	4.45	120.18	115.13
70	L5	4312	PSU	C4-N3-C2	-4.45	119.92	126.34
69	L8	55	PSU	C4-N3-C2	-4.45	119.92	126.34
70	L5	4423	PSU	C4-N3-C2	-4.45	119.93	126.34
70	L5	1871	A2M	N9-C8-N7	-4.44	107.84	113.91
74	S2	36	PSU	N1-C2-N3	4.44	120.16	115.13
67	Pt	56	PSU	N1-C2-N3	4.44	120.16	115.13
74	S2	218	PSU	N1-C2-N3	4.44	120.16	115.13
70	L5	4673	PSU	C4-N3-C2	-4.44	119.94	126.34
74	S2	668	A2M	N9-C8-N7	-4.44	107.84	113.91
74	S2	34	PSU	C4-N3-C2	-4.44	119.94	126.34
70	L5	3627	OMG	C2-N3-C4	4.44	120.20	112.30
70	L5	4569	PSU	C4-N3-C2	-4.44	119.95	126.34
70	L5	3851	PSU	N1-C2-N3	4.44	120.16	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	5010	PSU	C4-N3-C2	-4.44	119.95	126.34
70	L5	4296	PSU	N1-C2-N3	4.44	120.16	115.13
74	S2	801	PSU	N1-C2-N3	4.44	120.16	115.13
70	L5	3768	PSU	N1-C2-N3	4.43	120.15	115.13
70	L5	4228	OMG	C2-N3-C4	4.43	120.20	112.30
74	S2	1692	PSU	C4-N3-C2	-4.43	119.95	126.34
70	L5	4579	PSU	N1-C2-N3	4.43	120.15	115.13
74	S2	1328	OMG	C2-N3-C4	4.43	120.19	112.30
70	L5	1536	PSU	C4-N3-C2	-4.43	119.96	126.34
74	S2	105	PSU	C4-N3-C2	-4.43	119.96	126.34
69	L8	55	PSU	N1-C2-N3	4.43	120.15	115.13
70	L5	4689	PSU	N1-C2-N3	4.43	120.14	115.13
70	L5	4552	PSU	N1-C2-N3	4.42	120.14	115.13
74	S2	105	PSU	N1-C2-N3	4.42	120.14	115.13
70	L5	4442	PSU	N1-C2-N3	4.42	120.14	115.13
70	L5	4972	PSU	C4-N3-C2	-4.42	119.97	126.34
74	S2	1625	PSU	C4-N3-C2	-4.42	119.97	126.34
70	L5	4623	OMG	C2-N3-C4	4.42	120.17	112.30
74	S2	296	PSU	C4-N3-C2	-4.42	119.97	126.34
74	S2	651	PSU	N1-C2-N3	4.42	120.13	115.13
74	S2	572	PSU	C4-N3-C2	-4.42	119.98	126.34
69	L8	69	PSU	N1-C2-N3	4.42	120.13	115.13
70	L5	4494	OMG	C2-N3-C4	4.42	120.17	112.30
70	L5	4431	PSU	C4-N3-C2	-4.41	119.98	126.34
70	L5	4296	PSU	C4-N3-C2	-4.41	119.98	126.34
70	L5	3639	PSU	N1-C2-N3	4.41	120.13	115.13
70	L5	3764	PSU	C4-N3-C2	-4.41	119.98	126.34
70	L5	4299	PSU	C4-N3-C2	-4.41	119.98	126.34
74	S2	509	OMG	C2-N3-C4	4.41	120.16	112.30
70	L5	4471	PSU	N1-C2-N3	4.41	120.13	115.13
70	L5	2508	PSU	N1-C2-N3	4.41	120.12	115.13
70	L5	4569	PSU	N1-C2-N3	4.40	120.12	115.13
70	L5	1860	PSU	C4-N3-C2	-4.40	120.00	126.34
70	L5	2839	PSU	N1-C2-N3	4.40	120.12	115.13
70	L5	4579	PSU	C4-N3-C2	-4.40	120.00	126.34
70	L5	3920	PSU	C4-N3-C2	-4.40	120.00	126.34
74	S2	1625	PSU	N1-C2-N3	4.39	120.10	115.13
74	S2	867	OMG	C2-N3-C4	4.39	120.12	112.30
74	S2	822	PSU	C4-N3-C2	-4.39	120.02	126.34
74	S2	1177	PSU	C4-N3-C2	-4.38	120.03	126.34
70	L5	4532	PSU	N1-C2-N3	4.38	120.09	115.13
70	L5	1316	OMG	C2-N3-C4	4.38	120.10	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1174	PSU	N1-C2-N3	4.38	120.09	115.13
74	S2	649	PSU	C4-N3-C2	-4.37	120.04	126.34
70	L5	4353	PSU	N1-C2-N3	4.37	120.08	115.13
74	S2	681	PSU	N1-C2-N3	4.37	120.08	115.13
74	S2	1643	PSU	C4-N3-C2	-4.37	120.05	126.34
70	L5	4552	PSU	C4-N3-C2	-4.36	120.05	126.34
70	L5	4576	PSU	N1-C2-N3	4.36	120.07	115.13
74	S2	93	PSU	C4-N3-C2	-4.36	120.06	126.34
70	L5	4590	A2M	C5-C6-N6	4.36	132.91	123.43
69	L8	69	PSU	C4-N3-C2	-4.36	120.06	126.34
70	L5	4576	PSU	C4-N3-C2	-4.35	120.06	126.34
74	S2	296	PSU	N1-C2-N3	4.35	120.06	115.13
70	L5	2424	OMG	C2-N3-C4	4.35	120.06	112.30
74	S2	1004	PSU	C4-N3-C2	-4.35	120.07	126.34
74	S2	1239	PSU	N1-C2-N3	4.35	120.06	115.13
74	S2	1243	PSU	C4-N3-C2	-4.35	120.07	126.34
74	S2	863	PSU	N1-C2-N3	4.35	120.06	115.13
70	L5	1860	PSU	N1-C2-N3	4.35	120.06	115.13
74	S2	572	PSU	N1-C2-N3	4.33	120.04	115.13
70	L5	3867	A2M	C5-C6-N6	4.33	132.85	123.43
70	L5	3734	PSU	N1-C2-N3	4.33	120.03	115.13
74	S2	651	PSU	C4-N3-C2	-4.33	120.11	126.34
70	L5	4442	PSU	C4-N3-C2	-4.32	120.12	126.34
70	L5	3760	A2M	N9-C8-N7	-4.31	108.01	113.91
70	L5	3762	PSU	N1-C2-N3	4.31	120.02	115.13
70	L5	1781	PSU	N1-C2-N3	4.31	120.01	115.13
74	S2	1850	MA6	N9-C8-N7	-4.31	108.02	113.91
74	S2	867	OMG	C1'-N9-C4	-4.30	113.72	126.50
74	S2	863	PSU	C4-N3-C2	-4.30	120.14	126.34
74	S2	815	PSU	N1-C2-N3	4.30	120.00	115.13
70	L5	1536	PSU	N1-C2-N3	4.30	120.00	115.13
74	S2	93	PSU	N1-C2-N3	4.30	120.00	115.13
74	S2	1081	PSU	N1-C2-N3	4.29	119.99	115.13
70	L5	398	A2M	N9-C8-N7	-4.29	108.05	113.91
74	S2	1678	A2M	C5-C6-N6	4.28	132.75	123.43
70	L5	2363	A2M	N9-C8-N7	-4.28	108.06	113.91
74	S2	1031	A2M	N9-C8-N7	-4.28	108.06	113.91
70	L5	3715	PSU	C4-N3-C2	-4.28	120.18	126.34
70	L5	4420	PSU	N1-C2-N3	4.27	119.97	115.13
70	L5	3715	PSU	N1-C2-N3	4.27	119.97	115.13
70	L5	3830	A2M	N9-C8-N7	-4.26	108.08	113.91
70	L5	4532	PSU	C4-N3-C2	-4.26	120.20	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1692	PSU	N1-C2-N3	4.25	119.95	115.13
70	L5	1782	PSU	N1-C2-N3	4.25	119.94	115.13
70	L5	1524	A2M	N9-C8-N7	-4.25	108.11	113.91
74	S2	1639	G7M	C2-N3-C4	4.24	119.86	112.30
74	S2	1177	PSU	N1-C2-N3	4.24	119.93	115.13
70	L5	1781	PSU	C4-N3-C2	-4.24	120.24	126.34
70	L5	4228	OMG	C1'-N9-C8	4.23	138.75	126.70
74	S2	966	PSU	C4-N3-C2	-4.23	120.24	126.34
74	S2	573	PSU	N1-C2-N3	4.23	119.92	115.13
70	L5	1792	PSU	C4-N3-C2	-4.23	120.25	126.34
74	S2	814	PSU	C4-N3-C2	-4.22	120.26	126.34
70	L5	3853	PSU	C4-N3-C2	-4.22	120.26	126.34
70	L5	1524	A2M	C5-C6-N6	4.22	132.60	123.43
70	L5	2632	PSU	C4-N3-C2	-4.21	120.28	126.34
70	L5	3825	A2M	N9-C8-N7	-4.19	108.18	113.91
74	S2	1832	6MZ	C4-C5-C6	4.18	120.05	116.81
74	S2	512	A2M	C5-C6-N6	4.18	132.53	123.43
70	L5	2508	PSU	C4-N3-C2	-4.18	120.32	126.34
70	L5	4471	PSU	C4-N3-C2	-4.17	120.33	126.34
70	L5	2632	PSU	N1-C2-N3	4.17	119.85	115.13
74	S2	668	A2M	C5-C6-N6	4.17	132.50	123.43
70	L5	1522	OMG	C1'-N9-C4	-4.16	114.13	126.50
67	Pt	47	G7M	C2-N3-C4	4.16	119.72	112.30
70	L5	1792	PSU	N1-C2-N3	4.16	119.84	115.13
74	S2	468	A2M	N9-C8-N7	-4.16	108.23	113.91
70	L5	4590	A2M	N9-C8-N7	-4.15	108.24	113.91
74	S2	815	PSU	C4-N3-C2	-4.15	120.36	126.34
70	L5	2815	A2M	N9-C8-N7	-4.15	108.24	113.91
70	L5	1582	PSU	N1-C2-N3	4.15	119.83	115.13
74	S2	814	PSU	N1-C2-N3	4.14	119.81	115.13
70	L5	400	A2M	N9-C8-N7	-4.13	108.26	113.91
70	L5	3867	A2M	N9-C8-N7	-4.13	108.27	113.91
74	S2	119	PSU	N1-C2-N3	4.13	119.80	115.13
70	L5	2401	A2M	N9-C8-N7	-4.12	108.27	113.91
74	S2	1851	MA6	N9-C8-N7	-4.12	108.28	113.91
70	L5	3718	A2M	C5-C6-N6	4.11	132.37	123.43
70	L5	1534	A2M	C5-C6-N6	4.11	132.37	123.43
70	L5	4370	OMG	C1'-N9-C4	-4.10	114.31	126.50
70	L5	1534	A2M	N9-C8-N7	-4.10	108.31	113.91
74	S2	966	PSU	N1-C2-N3	4.10	119.77	115.13
70	L5	1326	A2M	N9-C8-N7	-4.10	108.31	113.91
74	S2	99	A2M	N9-C8-N7	-4.10	108.31	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	1871	A2M	C5-C6-N6	4.09	132.34	123.43
70	L5	2363	A2M	C5-C6-N6	4.09	132.34	123.43
74	S2	590	A2M	C5-C6-N6	4.09	132.34	123.43
74	S2	590	A2M	N9-C8-N7	-4.08	108.33	113.91
70	L5	4571	A2M	N9-C8-N7	-4.08	108.33	113.91
74	S2	27	A2M	N9-C8-N7	-4.08	108.33	113.91
70	L5	3830	A2M	C5-C6-N6	4.08	132.31	123.43
74	S2	1851	MA6	C4-C5-C6	4.07	120.44	115.88
70	L5	4220	6MZ	C4-C5-C6	4.06	119.96	116.81
74	S2	576	A2M	C5-C6-N6	4.06	132.27	123.43
70	L5	398	A2M	C5-C6-N6	4.05	132.25	123.43
74	S2	1850	MA6	C4-C5-C6	4.05	120.42	115.88
74	S2	27	A2M	C5-C6-N6	4.05	132.25	123.43
70	L5	3762	PSU	C4-N3-C2	-4.05	120.51	126.34
74	S2	1383	A2M	N9-C8-N7	-4.05	108.38	113.91
70	L5	400	A2M	C5-C6-N6	4.04	132.23	123.43
70	L5	3825	A2M	C5-C6-N6	4.04	132.23	123.43
70	L5	3627	OMG	C1'-N9-C4	-4.04	114.50	126.50
70	L5	1522	OMG	C1'-N9-C8	4.02	138.13	126.70
74	S2	1328	OMG	C1'-N9-C4	-4.02	114.57	126.50
70	L5	1326	A2M	C5-C6-N6	4.01	132.16	123.43
69	L8	75	OMG	C1'-N9-C4	-4.01	114.60	126.50
70	L5	4420	PSU	C4-N3-C2	-4.01	120.57	126.34
74	S2	484	A2M	N9-C8-N7	-4.00	108.45	113.91
70	L5	2815	A2M	C5-C6-N6	3.99	132.12	123.43
74	S2	512	A2M	N9-C8-N7	-3.99	108.45	113.91
74	S2	867	OMG	C1'-N9-C8	3.99	138.05	126.70
74	S2	1031	A2M	C5-C6-N6	3.98	132.09	123.43
74	S2	99	A2M	C5-C6-N6	3.98	132.09	123.43
70	L5	4499	OMG	C1'-N9-C4	-3.98	114.69	126.50
70	L5	3718	A2M	N9-C8-N7	-3.96	108.49	113.91
74	S2	1383	A2M	C5-C6-N6	3.96	132.05	123.43
70	L5	3785	A2M	C5-C6-N6	3.96	132.05	123.43
74	S2	484	A2M	C5-C6-N6	3.95	132.02	123.43
70	L5	4392	OMG	C1'-N9-C4	-3.95	114.78	126.50
70	L5	2424	OMG	C1'-N9-C4	-3.94	114.80	126.50
70	L5	3899	OMG	C1'-N9-C4	-3.94	114.81	126.50
70	L5	1322	1MA	C5-C4-N3	-3.93	121.39	127.26
70	L5	4523	A2M	N9-C8-N7	-3.92	108.55	113.91
70	L5	4447	5MC	C5-C6-N1	-3.92	119.31	123.34
70	L5	3760	A2M	C5-C6-N6	3.92	131.95	123.43
74	S2	576	A2M	N9-C8-N7	-3.91	108.56	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1804	OMU	N3-C2-N1	3.90	120.07	114.89
67	Pt	47	G7M	C5-C6-N1	3.89	119.92	111.79
74	S2	1639	G7M	C5-C6-N1	3.89	119.92	111.79
70	L5	2401	A2M	C5-C6-N6	3.89	131.90	123.43
74	S2	468	A2M	C5-C6-N6	3.89	131.90	123.43
74	S2	436	OMG	C1'-N9-C4	-3.89	114.94	126.50
70	L5	4370	OMG	C1'-N9-C8	3.89	137.77	126.70
70	L5	4523	A2M	C5-C6-N6	3.88	131.88	123.43
70	L5	3925	OMU	N3-C2-N1	3.87	120.02	114.89
74	S2	590	A2M	C2-N3-C4	3.86	120.88	111.75
70	L5	4571	A2M	C5-C6-N6	3.86	131.83	123.43
70	L5	2837	OMU	N3-C2-N1	3.85	120.00	114.89
70	L5	4220	6MZ	C5-N7-C8	3.85	108.98	103.51
70	L5	2424	OMG	C1'-N9-C8	3.85	137.66	126.70
70	L5	3627	OMG	C1'-N9-C8	3.84	137.64	126.70
74	S2	512	A2M	C2-N3-C4	3.84	120.83	111.75
70	L5	3785	A2M	C4'-O4'-C1'	-3.84	101.01	109.47
74	S2	119	PSU	C4-N3-C2	-3.83	120.82	126.34
70	L5	4494	OMG	C1'-N9-C4	-3.83	115.14	126.50
70	L5	4227	OMU	N3-C2-N1	3.82	119.96	114.89
74	S2	590	A2M	N3-C4-N9	3.81	133.37	127.08
70	L5	1582	PSU	C4-N3-C2	-3.81	120.85	126.34
70	L5	4392	OMG	C1'-N9-C8	3.80	137.53	126.70
70	L5	3744	OMG	C1'-N9-C4	-3.80	115.23	126.50
70	L5	4623	OMG	C1'-N9-C4	-3.79	115.24	126.50
70	L5	1322	1MA	C2-N3-C4	3.79	119.86	112.41
70	L5	3760	A2M	N3-C4-N9	3.79	133.33	127.08
74	S2	1639	G7M	C5-C4-N3	-3.79	120.89	128.15
70	L5	2364	OMG	C1'-N9-C4	-3.78	115.26	126.50
70	L5	4620	OMU	N3-C2-N1	3.78	119.91	114.89
74	S2	627	OMU	N3-C2-N1	3.78	119.91	114.89
74	S2	1678	A2M	C2-N3-C4	3.77	120.66	111.75
69	L8	75	OMG	C1'-N9-C8	3.77	137.43	126.70
70	L5	4498	OMU	N3-C2-N1	3.77	119.89	114.89
74	S2	116	OMU	N3-C2-N1	3.77	119.89	114.89
70	L5	1316	OMG	C1'-N9-C4	-3.73	115.41	126.50
70	L5	3760	A2M	C2-N3-C4	3.73	120.56	111.75
70	L5	4499	OMG	C1'-N9-C8	3.72	137.30	126.70
74	S2	1490	OMG	C1'-N9-C4	-3.71	115.48	126.50
70	L5	3899	OMG	C1'-N9-C8	3.71	137.25	126.70
70	L5	2876	OMG	N9-C4-N3	3.70	133.37	125.94
74	S2	1850	MA6	C2-N1-C6	3.70	120.49	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1328	OMG	C1'-N9-C8	3.69	137.20	126.70
70	L5	3830	A2M	C2-N3-C4	3.68	120.44	111.75
70	L5	4590	A2M	C2-N3-C4	3.68	120.44	111.75
70	L5	4494	OMG	C1'-N9-C8	3.67	137.14	126.70
70	L5	400	A2M	C2-N3-C4	3.67	120.41	111.75
70	L5	4618	OMG	C1'-N9-C4	-3.67	115.61	126.50
74	S2	436	OMG	C1'-N9-C8	3.66	137.13	126.70
70	L5	2815	A2M	C2-N3-C4	3.65	120.39	111.75
74	S2	1851	MA6	C2-N1-C6	3.65	120.38	111.75
70	L5	4623	OMG	C1'-N9-C8	3.65	137.09	126.70
74	S2	428	OMU	N3-C2-N1	3.64	119.73	114.89
70	L5	1534	A2M	C2-N3-C4	3.64	120.34	111.75
74	S2	668	A2M	C2-N3-C4	3.63	120.34	111.75
70	L5	1625	OMG	N9-C4-N3	3.63	133.22	125.94
70	L5	2364	OMG	C1'-N9-C8	3.63	137.02	126.70
70	L5	2363	A2M	C2-N3-C4	3.62	120.31	111.75
70	L5	3785	A2M	C2-N3-C4	3.62	120.29	111.75
74	S2	27	A2M	C2-N3-C4	3.61	120.28	111.75
70	L5	4196	OMG	C1'-N9-C4	-3.61	115.78	126.50
74	S2	1031	A2M	C2-N3-C4	3.61	120.28	111.75
70	L5	2401	A2M	C2-N3-C4	3.61	120.28	111.75
74	S2	1383	A2M	C2-N3-C4	3.60	120.26	111.75
74	S2	99	A2M	C2-N3-C4	3.60	120.25	111.75
70	L5	3825	A2M	C2-N3-C4	3.60	120.25	111.75
70	L5	1524	A2M	C2-N3-C4	3.60	120.25	111.75
74	S2	484	A2M	C2-N3-C4	3.60	120.25	111.75
67	Pt	8	4SU	N3-C2-N1	3.59	119.65	114.89
70	L5	3744	OMG	C1'-N9-C8	3.58	136.90	126.70
70	L5	1326	A2M	C2-N3-C4	3.58	120.21	111.75
74	S2	1490	OMG	C1'-N9-C8	3.58	136.88	126.70
70	L5	3718	A2M	C2-N3-C4	3.57	120.18	111.75
70	L5	4523	A2M	C2-N3-C4	3.57	120.18	111.75
70	L5	4637	OMG	C1'-N9-C4	-3.57	115.91	126.50
74	S2	1851	MA6	C2-N3-C4	3.57	120.17	111.75
67	Pt	47	G7M	C5-C4-N3	-3.56	121.32	128.15
70	L5	4571	A2M	C2-N3-C4	3.54	120.12	111.75
74	S2	1678	A2M	C5-N7-C8	3.54	108.54	103.51
74	S2	1639	G7M	CN7-N7-C5	3.54	131.16	126.77
74	S2	644	OMG	C1'-N9-C4	-3.54	116.00	126.50
74	S2	683	OMG	N9-C4-N3	3.53	133.04	125.94
74	S2	468	A2M	C2-N3-C4	3.53	120.10	111.75
70	L5	1871	A2M	C2-N3-C4	3.53	120.09	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	3867	A2M	C2-N3-C4	3.53	120.08	111.75
70	L5	4498	OMU	C5-C4-N3	3.51	120.09	114.84
70	L5	2815	A2M	N3-C4-N9	3.51	132.87	127.08
70	L5	1316	OMG	C1'-N9-C8	3.51	136.69	126.70
70	L5	398	A2M	C2-N3-C4	3.51	120.04	111.75
70	L5	4618	OMG	C1'-N9-C8	3.50	136.66	126.70
74	S2	1850	MA6	C2-N3-C4	3.49	120.01	111.75
67	Pt	21	H2U	N3-C2-N1	3.48	120.33	116.65
74	S2	509	OMG	C1'-N9-C4	-3.48	116.17	126.50
74	S2	428	OMU	C5-C4-N3	3.47	120.03	114.84
70	L5	2401	A2M	N3-C4-N9	3.44	132.75	127.08
67	Pt	8	4SU	C5-C4-S4	-3.44	120.04	124.47
70	L5	3792	OMG	N9-C4-N3	3.44	132.84	125.94
74	S2	512	A2M	N3-C4-N9	3.42	132.72	127.08
74	S2	576	A2M	C2-N3-C4	3.42	119.84	111.75
70	L5	4227	OMU	C5-C4-N3	3.42	119.95	114.84
70	L5	4196	OMG	C1'-N9-C8	3.41	136.40	126.70
67	Pt	47	G7M	O6-C6-C5	-3.41	120.37	128.06
70	L5	3792	OMG	C1'-N9-C4	-3.40	116.39	126.50
70	L5	3925	OMU	C5-C4-N3	3.40	119.93	114.84
74	S2	509	OMG	C1'-N9-C8	3.40	136.37	126.70
70	L5	4637	OMG	C1'-N9-C8	3.40	136.37	126.70
74	S2	644	OMG	C1'-N9-C8	3.39	136.35	126.70
74	S2	509	OMG	N9-C4-N3	3.39	132.75	125.94
70	L5	4637	OMG	N9-C4-N3	3.38	132.73	125.94
70	L5	3785	A2M	O4'-C1'-N9	3.38	114.71	108.06
70	L5	3830	A2M	N3-C4-N9	3.38	132.64	127.08
74	S2	1031	A2M	N3-C4-N9	3.37	132.64	127.08
70	L5	3825	A2M	N3-C4-N9	3.37	132.63	127.08
74	S2	644	OMG	N9-C4-N3	3.36	132.69	125.94
70	L5	2876	OMG	C2-N1-C6	-3.36	118.97	125.10
74	S2	1850	MA6	N3-C4-N9	3.36	132.62	127.08
70	L5	3760	A2M	C5-N7-C8	3.35	108.27	103.51
74	S2	627	OMU	C5-C4-N3	3.34	119.84	114.84
74	S2	1678	A2M	N3-C4-N9	3.34	132.58	127.08
70	L5	2837	OMU	C5-C4-N3	3.33	119.83	114.84
70	L5	4618	OMG	N9-C4-N3	3.32	132.60	125.94
70	L5	4196	OMG	N9-C4-N3	3.32	132.60	125.94
74	S2	27	A2M	N3-C4-N9	3.31	132.54	127.08
74	S2	683	OMG	C1'-N9-C4	-3.31	116.67	126.50
70	L5	4523	A2M	N3-C4-N9	3.31	132.53	127.08
74	S2	1851	MA6	N3-C4-N9	3.27	132.47	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1832	6MZ	C4-C5-N7	-3.27	106.63	110.62
74	S2	1832	6MZ	C2-N3-C4	3.27	119.48	111.75
70	L5	4494	OMG	N9-C4-N3	3.27	132.50	125.94
74	S2	1804	OMU	C5-C4-N3	3.26	119.72	114.84
70	L5	1524	A2M	C5-N7-C8	3.25	108.13	103.51
70	L5	4620	OMU	C5-C4-N3	3.25	119.71	114.84
70	L5	4623	OMG	N9-C4-N3	3.25	132.47	125.94
74	S2	1031	A2M	C5-N7-C8	3.24	108.12	103.51
70	L5	2815	A2M	C5-N7-C8	3.24	108.12	103.51
70	L5	4637	OMG	C2-N1-C6	-3.24	119.19	125.10
74	S2	668	A2M	C5-N7-C8	3.24	108.11	103.51
70	L5	1625	OMG	C1'-N9-C4	-3.23	116.90	126.50
70	L5	1316	OMG	N9-C4-N3	3.22	132.41	125.94
74	S2	1328	OMG	N9-C4-N3	3.22	132.40	125.94
70	L5	3792	OMG	C1'-N9-C8	3.21	135.84	126.70
70	L5	4499	OMG	N9-C4-N3	3.21	132.39	125.94
70	L5	3825	A2M	C5-N7-C8	3.21	108.07	103.51
70	L5	3785	A2M	C5-N7-C8	3.21	108.07	103.51
70	L5	3782	5MC	C5-C6-N1	-3.21	120.03	123.34
70	L5	3627	OMG	N9-C4-N3	3.21	132.38	125.94
70	L5	3785	A2M	N3-C4-N9	3.20	132.36	127.08
70	L5	3830	A2M	C5-N7-C8	3.20	108.06	103.51
74	S2	99	A2M	N3-C4-N9	3.20	132.36	127.08
74	S2	1639	G7M	O6-C6-C5	-3.20	120.84	128.06
70	L5	4571	A2M	N3-C4-N9	3.20	132.35	127.08
74	S2	644	OMG	C2-N1-C6	-3.20	119.27	125.10
70	L5	400	A2M	N3-C4-N9	3.19	132.34	127.08
70	L5	3899	OMG	N9-C4-N3	3.19	132.34	125.94
74	S2	484	A2M	N3-C4-N9	3.19	132.33	127.08
74	S2	590	A2M	C5-N7-C8	3.18	108.03	103.51
70	L5	2363	A2M	C5-N7-C8	3.18	108.03	103.51
70	L5	4590	A2M	C5-N7-C8	3.18	108.02	103.51
70	L5	4392	OMG	N9-C4-N3	3.17	132.31	125.94
74	S2	1851	MA6	C5-N7-C8	3.17	108.01	103.51
70	L5	2364	OMG	N9-C4-N3	3.17	132.30	125.94
70	L5	3744	OMG	N9-C4-N3	3.17	132.30	125.94
70	L5	3867	A2M	N3-C4-N9	3.16	132.29	127.08
70	L5	1871	A2M	C5-N7-C8	3.16	108.00	103.51
70	L5	1625	OMG	C2-N1-C6	-3.16	119.34	125.10
74	S2	1383	A2M	N3-C4-N9	3.16	132.29	127.08
74	S2	512	A2M	C5-N7-C8	3.15	107.99	103.51
70	L5	3718	A2M	N3-C4-N9	3.15	132.28	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	4220	6MZ	C2-N3-C4	3.15	119.19	111.75
74	S2	1490	OMG	N9-C4-N3	3.15	132.26	125.94
74	S2	576	A2M	N3-C4-N9	3.15	132.27	127.08
70	L5	398	A2M	C5-N7-C8	3.15	107.98	103.51
74	S2	468	A2M	N3-C4-N9	3.14	132.26	127.08
74	S2	116	OMU	C5-C4-N3	3.14	119.53	114.84
74	S2	99	A2M	C5-N7-C8	3.14	107.96	103.51
70	L5	4618	OMG	C2-N1-C6	-3.13	119.38	125.10
70	L5	2401	A2M	C5-N7-C8	3.12	107.94	103.51
74	S2	1850	MA6	C5-N7-C8	3.12	107.94	103.51
74	S2	436	OMG	N9-C4-N3	3.12	132.19	125.94
70	L5	398	A2M	N3-C4-N9	3.11	132.22	127.08
69	L8	75	OMG	N9-C4-N3	3.11	132.19	125.94
70	L5	3867	A2M	C5-N7-C8	3.11	107.92	103.51
70	L5	4370	OMG	N9-C4-N3	3.10	132.17	125.94
70	L5	1524	A2M	N3-C4-N9	3.10	132.20	127.08
70	L5	2424	OMG	N9-C4-N3	3.10	132.16	125.94
70	L5	1871	A2M	N3-C4-N9	3.09	132.18	127.08
74	S2	683	OMG	C1'-N9-C8	3.09	135.50	126.70
70	L5	2363	A2M	N3-C4-N9	3.09	132.18	127.08
70	L5	1522	OMG	C2-N1-C6	-3.08	119.48	125.10
70	L5	4220	6MZ	C9-N6-C6	-3.08	120.22	122.87
74	S2	683	OMG	C2-N1-C6	-3.08	119.48	125.10
70	L5	2424	OMG	C2-N1-C6	-3.08	119.48	125.10
70	L5	4623	OMG	C2-N1-C6	-3.08	119.49	125.10
74	S2	509	OMG	C2-N1-C6	-3.07	119.50	125.10
70	L5	1779	PSU	O2-C2-N1	-3.07	119.41	122.79
70	L5	4494	OMG	C2-N1-C6	-3.07	119.51	125.10
74	S2	867	OMG	C2-N1-C6	-3.06	119.51	125.10
74	S2	27	A2M	C5-N7-C8	3.06	107.86	103.51
70	L5	3792	OMG	C2-N1-C6	-3.06	119.52	125.10
74	S2	1383	A2M	C5-N7-C8	3.06	107.85	103.51
74	S2	822	PSU	O2-C2-N1	-3.06	119.42	122.79
70	L5	4392	OMG	C2-N1-C6	-3.06	119.53	125.10
70	L5	4590	A2M	N3-C4-N9	3.05	132.12	127.08
74	S2	428	OMU	O4-C4-C5	-3.05	119.80	125.16
70	L5	400	A2M	C5-N7-C8	3.05	107.84	103.51
70	L5	1534	A2M	N3-C4-N9	3.05	132.10	127.08
70	L5	1326	A2M	N3-C4-N9	3.04	132.10	127.08
70	L5	4196	OMG	C2-N1-C6	-3.03	119.57	125.10
70	L5	2837	OMU	O4-C4-C5	-3.03	119.82	125.16
74	S2	436	OMG	C2-N1-C6	-3.03	119.58	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1248	B8N	N3-C2-N1	3.02	121.03	116.76
70	L5	4523	A2M	C5-N7-C8	3.02	107.80	103.51
70	L5	2351	OMC	O2-C2-N3	-3.01	117.43	122.33
70	L5	3627	OMG	C2-N1-C6	-3.01	119.62	125.10
70	L5	1625	OMG	C1'-N9-C8	3.00	135.25	126.70
70	L5	2364	OMG	C2-N1-C6	-3.00	119.63	125.10
70	L5	1534	A2M	C5-N7-C8	3.00	107.77	103.51
74	S2	668	A2M	N3-C4-N9	2.99	132.01	127.08
74	S2	1328	OMG	C2-N1-C6	-2.99	119.65	125.10
69	L8	75	OMG	C2-N1-C6	-2.99	119.65	125.10
74	S2	484	A2M	C5-N7-C8	2.99	107.75	103.51
70	L5	2876	OMG	C1'-N9-C4	-2.99	117.63	126.50
70	L5	1326	A2M	C5-N7-C8	2.98	107.74	103.51
70	L5	1522	OMG	N9-C4-N3	2.98	131.92	125.94
70	L5	4370	OMG	C2-N1-C6	-2.97	119.68	125.10
70	L5	1316	OMG	C2-N1-C6	-2.97	119.68	125.10
70	L5	4499	OMG	C2-N1-C6	-2.97	119.68	125.10
70	L5	4228	OMG	C2-N1-C6	-2.97	119.69	125.10
74	S2	867	OMG	N9-C4-N3	2.94	131.85	125.94
70	L5	4571	A2M	C5-N7-C8	2.94	107.68	103.51
74	S2	468	A2M	C5-N7-C8	2.94	107.68	103.51
70	L5	3744	OMG	C2-N1-C6	-2.93	119.75	125.10
74	S2	1639	G7M	N9-C4-N3	2.93	131.82	125.94
74	S2	576	A2M	C5-N7-C8	2.93	107.67	103.51
70	L5	3899	OMG	C2-N1-C6	-2.92	119.77	125.10
74	S2	867	OMG	N9-C8-N7	-2.92	107.89	113.39
70	L5	4227	OMU	O4-C4-C5	-2.92	120.03	125.16
67	Pt	47	G7M	N9-C4-N3	2.92	131.80	125.94
74	S2	1639	G7M	CN7-N7-C8	-2.90	120.36	124.84
74	S2	1490	OMG	C2-N1-C6	-2.90	119.81	125.10
70	L5	3718	A2M	C5-N7-C8	2.89	107.62	103.51
74	S2	627	OMU	O4-C4-C5	-2.89	120.08	125.16
70	L5	4228	OMG	N9-C8-N7	-2.88	107.96	113.39
74	S2	1238	PSU	O2-C2-N1	-2.88	119.62	122.79
70	L5	2876	OMG	C1'-N9-C8	2.88	134.90	126.70
70	L5	3925	OMU	O4-C4-C5	-2.86	120.13	125.16
67	Pt	47	G7M	CN7-N7-C5	2.85	130.31	126.77
74	S2	1639	G7M	C2-N1-C6	-2.85	119.90	125.10
74	S2	116	OMU	O4-C4-C5	-2.85	120.15	125.16
70	L5	4228	OMG	N9-C4-N3	2.83	131.63	125.94
74	S2	1004	PSU	O2-C2-N1	-2.83	119.67	122.79
70	L5	3899	OMG	N9-C8-N7	-2.83	108.06	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1328	OMG	N9-C8-N7	-2.82	108.07	113.39
70	L5	3627	OMG	N9-C8-N7	-2.82	108.08	113.39
70	L5	1522	OMG	N9-C8-N7	-2.81	108.11	113.39
74	S2	1804	OMU	O4-C4-C5	-2.80	120.24	125.16
70	L5	2876	OMG	C5-C6-N1	2.80	120.29	113.19
70	L5	4531	PSU	O2-C2-N1	-2.79	119.71	122.79
70	L5	3792	OMG	C5-C6-N1	2.79	120.28	113.19
74	S2	822	PSU	C6-N1-C2	-2.79	119.83	122.68
74	S2	436	OMG	N9-C8-N7	-2.79	108.13	113.39
69	L8	75	OMG	N9-C8-N7	-2.79	108.14	113.39
70	L5	3770	PSU	O2-C2-N1	-2.79	119.72	122.79
70	L5	4498	OMU	O4-C4-C5	-2.78	120.27	125.16
70	L5	4620	OMU	O4-C4-C5	-2.77	120.29	125.16
74	S2	1445	PSU	O2-C2-N1	-2.77	119.74	122.79
70	L5	4499	OMG	N9-C8-N7	-2.77	108.18	113.39
74	S2	683	OMG	C5-C6-N1	2.77	120.22	113.19
70	L5	1744	PSU	O2-C2-N1	-2.76	119.75	122.79
70	L5	4370	OMG	C5-C6-N1	2.76	120.21	113.19
70	L5	4579	PSU	O2-C2-N1	-2.76	119.75	122.79
74	S2	649	PSU	O2-C2-N1	-2.76	119.75	122.79
70	L5	4618	OMG	C5-C6-N1	2.75	120.18	113.19
70	L5	4370	OMG	N9-C8-N7	-2.75	108.21	113.39
67	Pt	47	G7M	C2-N1-C6	-2.75	120.09	125.10
74	S2	644	OMG	C5-C6-N1	2.75	120.17	113.19
70	L5	4392	OMG	C5-C6-N1	2.74	120.16	113.19
70	L5	3884	PSU	O2-C2-N1	-2.74	119.77	122.79
70	L5	1316	OMG	N9-C8-N7	-2.74	108.23	113.39
70	L5	4637	OMG	N9-C8-N7	-2.74	108.23	113.39
70	L5	4312	PSU	O2-C2-N1	-2.74	119.78	122.79
74	S2	1174	PSU	O2-C2-N1	-2.74	119.78	122.79
74	S2	1328	OMG	C5-C6-N1	2.74	120.14	113.19
70	L5	4628	PSU	O2-C2-N1	-2.74	119.78	122.79
70	L5	4637	OMG	C5-C6-N1	2.73	120.14	113.19
70	L5	1625	OMG	C5-C6-N1	2.73	120.12	113.19
70	L5	2839	PSU	O2-C2-N1	-2.73	119.79	122.79
70	L5	4423	PSU	O2-C2-N1	-2.72	119.79	122.79
69	L8	75	OMG	C5-C6-N1	2.71	120.08	113.19
70	L5	4499	OMG	C5-C6-N1	2.71	120.07	113.19
70	L5	4228	OMG	C5-C6-N1	2.71	120.06	113.19
70	L5	1677	PSU	O2-C2-N1	-2.71	119.81	122.79
70	L5	3744	OMG	N9-C8-N7	-2.70	108.30	113.39
70	L5	4196	OMG	C5-C6-N1	2.70	120.06	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	4392	OMG	N9-C8-N7	-2.70	108.30	113.39
70	L5	2364	OMG	C5-C6-N1	2.70	120.05	113.19
74	S2	1243	PSU	O2-C2-N1	-2.70	119.81	122.79
70	L5	3792	OMG	O6-C6-C5	-2.70	119.44	126.60
74	S2	406	PSU	O2-C2-N1	-2.70	119.82	122.79
74	S2	686	PSU	O2-C2-N1	-2.70	119.82	122.79
70	L5	4494	OMG	C5-C6-N1	2.69	120.03	113.19
70	L5	1522	OMG	C5-C6-N1	2.69	120.03	113.19
74	S2	649	PSU	C6-N1-C2	-2.69	119.93	122.68
70	L5	2364	OMG	N9-C8-N7	-2.69	108.33	113.39
70	L5	3627	OMG	C5-C6-N1	2.69	120.02	113.19
70	L5	4196	OMG	N9-C8-N7	-2.69	108.33	113.39
70	L5	3758	PSU	O2-C2-N1	-2.68	119.84	122.79
74	S2	1347	PSU	O2-C2-N1	-2.68	119.84	122.79
70	L5	4623	OMG	C5-C6-N1	2.68	119.99	113.19
70	L5	1862	PSU	O2-C2-N1	-2.68	119.84	122.79
74	S2	683	OMG	O6-C6-C5	-2.68	119.50	126.60
70	L5	3764	PSU	O2-C2-N1	-2.68	119.84	122.79
74	S2	436	OMG	C5-C6-N1	2.67	119.98	113.19
74	S2	867	OMG	C5-C6-N1	2.67	119.98	113.19
70	L5	4618	OMG	N9-C8-N7	-2.67	108.36	113.39
70	L5	4500	PSU	O2-C2-N1	-2.67	119.85	122.79
74	S2	1136	PSU	O2-C2-N1	-2.67	119.85	122.79
70	L5	4494	OMG	O6-C6-C5	-2.67	119.52	126.60
67	Pt	56	PSU	O2-C2-N1	-2.67	119.85	122.79
74	S2	509	OMG	C5-C6-N1	2.67	119.97	113.19
74	S2	866	PSU	O2-C2-N1	-2.67	119.85	122.79
74	S2	609	PSU	O2-C2-N1	-2.66	119.86	122.79
70	L5	1625	OMG	N9-C8-N7	-2.66	108.38	113.39
70	L5	4623	OMG	N9-C8-N7	-2.66	108.38	113.39
74	S2	119	PSU	C6-N1-C2	-2.66	119.97	122.68
70	L5	1625	OMG	O6-C6-C5	-2.66	119.55	126.60
74	S2	36	PSU	O2-C2-N1	-2.66	119.87	122.79
70	L5	2508	PSU	O2-C2-N1	-2.65	119.87	122.79
74	S2	1625	PSU	O2-C2-N1	-2.65	119.87	122.79
70	L5	1316	OMG	C5-C6-N1	2.64	119.90	113.19
74	S2	683	OMG	N9-C8-N7	-2.64	108.42	113.39
70	L5	2632	PSU	O2-C2-N1	-2.64	119.89	122.79
74	S2	1248	B8N	O4-C4-N3	-2.63	115.51	119.98
74	S2	34	PSU	O2-C2-N1	-2.63	119.89	122.79
70	L5	3792	OMG	N9-C8-N7	-2.63	108.43	113.39
70	L5	4532	PSU	O2-C2-N1	-2.63	119.89	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	3762	PSU	O2-C2-N1	-2.63	119.89	122.79
74	S2	105	PSU	O2-C2-N1	-2.63	119.89	122.79
67	Pt	21	H2U	C5-C4-N3	2.62	119.60	116.65
70	L5	3744	OMG	C5-C6-N1	2.62	119.84	113.19
74	S2	1490	OMG	N9-C8-N7	-2.62	108.46	113.39
70	L5	2424	OMG	C5-C6-N1	2.62	119.83	113.19
70	L5	2876	OMG	O6-C6-C5	-2.61	119.67	126.60
74	S2	1490	OMG	C5-C6-N1	2.61	119.83	113.19
70	L5	2876	OMG	N9-C8-N7	-2.61	108.47	113.39
70	L5	4628	PSU	C6-N1-C2	-2.61	120.02	122.68
70	L5	4569	PSU	O2-C2-N1	-2.61	119.92	122.79
69	L8	69	PSU	O2-C2-N1	-2.60	119.92	122.79
70	L5	5010	PSU	O2-C2-N1	-2.60	119.92	122.79
70	L5	3899	OMG	C5-C6-N1	2.60	119.80	113.19
70	L5	3768	PSU	O2-C2-N1	-2.60	119.93	122.79
67	Pt	21	H2U	C5-C6-N1	2.60	120.17	111.61
74	S2	644	OMG	N9-C8-N7	-2.60	108.50	113.39
74	S2	1367	PSU	O2-C2-N1	-2.60	119.93	122.79
70	L5	4220	6MZ	N3-C4-N9	2.59	131.36	127.08
70	L5	4494	OMG	N9-C8-N7	-2.59	108.51	113.39
70	L5	4972	PSU	O2-C2-N1	-2.59	119.94	122.79
70	L5	4618	OMG	O6-C6-C5	-2.59	119.73	126.60
74	S2	1328	OMG	O6-C6-C5	-2.58	119.75	126.60
70	L5	4370	OMG	O6-C6-C5	-2.58	119.76	126.60
70	L5	2424	OMG	O6-C6-C5	-2.58	119.77	126.60
74	S2	436	OMG	O6-C6-C5	-2.57	119.77	126.60
74	S2	644	OMG	O6-C6-C5	-2.57	119.77	126.60
70	L5	4299	PSU	O2-C2-N1	-2.57	119.96	122.79
70	L5	4457	PSU	O2-C2-N1	-2.57	119.96	122.79
70	L5	4403	PSU	O2-C2-N1	-2.57	119.96	122.79
74	S2	1244	PSU	O2-C2-N1	-2.57	119.97	122.79
67	Pt	47	G7M	CN7-N7-C8	-2.56	120.88	124.84
70	L5	3762	PSU	C6-N1-C2	-2.56	120.06	122.68
70	L5	3639	PSU	O2-C2-N1	-2.56	119.97	122.79
74	S2	296	PSU	O2-C2-N1	-2.56	119.97	122.79
74	S2	1643	PSU	O2-C2-N1	-2.56	119.98	122.79
74	S2	572	PSU	O2-C2-N1	-2.56	119.98	122.79
70	L5	4420	PSU	C6-N1-C2	-2.56	120.07	122.68
70	L5	4636	PSU	O2-C2-N1	-2.55	119.98	122.79
70	L5	4689	PSU	O2-C2-N1	-2.55	119.98	122.79
74	S2	966	PSU	O2-C2-N1	-2.55	119.98	122.79
70	L5	4623	OMG	O6-C6-C5	-2.55	119.84	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1239	PSU	O2-C2-N1	-2.55	119.99	122.79
70	L5	1683	PSU	O2-C2-N1	-2.54	119.99	122.79
70	L5	4471	PSU	O2-C2-N1	-2.54	119.99	122.79
70	L5	3729	PSU	O2-C2-N1	-2.54	119.99	122.79
70	L5	4420	PSU	O2-C2-N1	-2.54	120.00	122.79
74	S2	651	PSU	O2-C2-N1	-2.53	120.01	122.79
74	S2	863	PSU	O2-C2-N1	-2.53	120.01	122.79
74	S2	1832	6MZ	N3-C4-N9	2.52	131.24	127.08
70	L5	2424	OMG	N9-C8-N7	-2.52	108.64	113.39
70	L5	3785	A2M	O4'-C1'-C2'	-2.52	102.15	106.57
70	L5	1316	OMG	O6-C6-C5	-2.52	119.92	126.60
74	S2	1177	PSU	O2-C2-N1	-2.51	120.02	122.79
69	L8	75	OMG	O6-C6-C5	-2.51	119.94	126.60
70	L5	4220	6MZ	C4-C5-N7	-2.51	107.56	110.62
74	S2	918	PSU	O2-C2-N1	-2.50	120.03	122.79
70	L5	4196	OMG	O6-C6-C5	-2.50	119.96	126.60
74	S2	109	PSU	C6-N1-C2	-2.50	120.12	122.68
67	Pt	47	G7M	N9-C8-N7	-2.50	106.02	112.21
74	S2	918	PSU	C6-N1-C2	-2.50	120.12	122.68
70	L5	2843	PSU	O2-C2-N1	-2.50	120.04	122.79
70	L5	4220	6MZ	C4-N9-C1'	-2.50	120.64	126.59
74	S2	1842	4AC	C6-C5-C4	2.50	120.02	116.96
70	L5	4442	PSU	O2-C2-N1	-2.50	120.04	122.79
70	L5	3884	PSU	C6-N1-C2	-2.49	120.14	122.68
74	S2	1678	A2M	C4-C5-N7	-2.49	107.59	110.62
70	L5	4530	UR3	C6-N1-C2	-2.49	119.56	121.79
70	L5	4552	PSU	O2-C2-N1	-2.49	120.05	122.79
70	L5	4499	OMG	O6-C6-C5	-2.48	120.02	126.60
74	S2	93	PSU	O2-C2-N1	-2.48	120.06	122.79
74	S2	509	OMG	O6-C6-C5	-2.48	120.02	126.60
70	L5	4293	PSU	O2-C2-N1	-2.48	120.06	122.79
70	L5	2508	PSU	C6-N1-C2	-2.47	120.15	122.68
70	L5	2364	OMG	O6-C6-C5	-2.47	120.04	126.60
70	L5	3782	5MC	CM5-C5-C6	-2.47	119.55	122.85
70	L5	4471	PSU	C6-N1-C2	-2.47	120.16	122.68
70	L5	3627	OMG	O6-C6-C5	-2.47	120.06	126.60
70	L5	4576	PSU	O2-C2-N1	-2.46	120.08	122.79
74	S2	1004	PSU	C6-N1-C2	-2.46	120.17	122.68
70	L5	3715	PSU	O2-C2-N1	-2.46	120.08	122.79
70	L5	4673	PSU	O2-C2-N1	-2.46	120.08	122.79
70	L5	3844	PSU	O2-C2-N1	-2.46	120.08	122.79
74	S2	815	PSU	C6-N1-C2	-2.46	120.17	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	1536	PSU	O2-C2-N1	-2.46	120.08	122.79
74	S2	867	OMG	O6-C6-C5	-2.46	120.08	126.60
70	L5	4361	PSU	O2-C2-N1	-2.46	120.09	122.79
74	S2	1243	PSU	C6-N1-C2	-2.45	120.17	122.68
70	L5	3744	OMG	O6-C6-C5	-2.45	120.09	126.60
70	L5	4673	PSU	C6-N1-C2	-2.45	120.17	122.68
74	S2	1490	OMG	O6-C6-C5	-2.45	120.10	126.60
74	S2	109	PSU	O2-C2-N1	-2.45	120.09	122.79
67	Pt	33	OMC	O2-C2-N3	-2.45	118.35	122.33
70	L5	4392	OMG	O6-C6-C5	-2.45	120.11	126.60
70	L5	4228	OMG	O6-C6-C5	-2.44	120.11	126.60
69	L8	55	PSU	O2-C2-N1	-2.44	120.10	122.79
70	L5	3853	PSU	C6-N1-C2	-2.44	120.19	122.68
70	L5	4500	PSU	C6-N1-C2	-2.44	120.19	122.68
74	S2	918	PSU	O4'-C1'-C2'	2.44	108.59	105.14
70	L5	4521	PSU	O2-C2-N1	-2.44	120.10	122.79
74	S2	1238	PSU	C6-N1-C2	-2.44	120.19	122.68
74	S2	801	PSU	O2-C2-N1	-2.44	120.11	122.79
74	S2	509	OMG	N9-C8-N7	-2.44	108.80	113.39
70	L5	4637	OMG	O6-C6-C5	-2.44	120.13	126.60
70	L5	3764	PSU	C6-N1-C2	-2.43	120.20	122.68
70	L5	2351	OMC	C1'-N1-C2	2.42	123.83	118.42
70	L5	1322	1MA	N9-C8-N7	-2.42	108.84	113.39
70	L5	4972	PSU	C6-N1-C2	-2.41	120.21	122.68
70	L5	3899	OMG	O6-C6-C5	-2.41	120.20	126.60
74	S2	1232	PSU	O2-C2-N1	-2.41	120.14	122.79
74	S2	218	PSU	O2-C2-N1	-2.41	120.14	122.79
70	L5	4299	PSU	C6-N1-C2	-2.41	120.22	122.68
70	L5	4493	PSU	O2-C2-N1	-2.41	120.14	122.79
70	L5	4296	PSU	O2-C2-N1	-2.40	120.15	122.79
70	L5	4532	PSU	C6-N1-C2	-2.40	120.23	122.68
70	L5	5001	PSU	O2-C2-N1	-2.40	120.15	122.79
74	S2	863	PSU	C6-N1-C2	-2.40	120.23	122.68
74	S2	1643	PSU	C6-N1-C2	-2.40	120.23	122.68
70	L5	1522	OMG	O6-C6-C5	-2.39	120.25	126.60
70	L5	4531	PSU	C6-C5-C4	2.39	119.87	118.20
70	L5	1782	PSU	O2-C2-N1	-2.39	120.16	122.79
70	L5	3734	PSU	O2-C2-N1	-2.39	120.16	122.79
74	S2	34	PSU	C6-N1-C2	-2.39	120.24	122.68
70	L5	4423	PSU	C6-N1-C2	-2.39	120.24	122.68
70	L5	4689	PSU	C6-N1-C2	-2.39	120.24	122.68
70	L5	3715	PSU	C6-N1-C2	-2.38	120.25	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	1337	4AC	C6-C5-C4	2.38	119.87	116.96
74	S2	866	PSU	C6-N1-C2	-2.38	120.25	122.68
70	L5	3770	PSU	C6-N1-C2	-2.37	120.25	122.68
70	L5	5001	PSU	C6-N1-C2	-2.37	120.26	122.68
70	L5	1582	PSU	C6-N1-C2	-2.37	120.26	122.68
70	L5	1871	A2M	C4-N9-C8	2.37	108.30	105.73
70	L5	3729	PSU	C6-N1-C2	-2.36	120.27	122.68
70	L5	4576	PSU	C6-N1-C2	-2.36	120.27	122.68
74	S2	406	PSU	C6-N1-C2	-2.35	120.28	122.68
70	L5	4293	PSU	C6-N1-C2	-2.34	120.29	122.68
74	S2	1232	PSU	C6-N1-C2	-2.34	120.29	122.68
70	L5	3637	PSU	C6-N1-C2	-2.34	120.29	122.68
70	L5	4579	PSU	C6-N1-C2	-2.34	120.29	122.68
70	L5	2815	A2M	C6-C5-C4	2.33	120.31	117.18
70	L5	3920	PSU	C6-N1-C2	-2.33	120.31	122.68
70	L5	1860	PSU	O2-C2-N1	-2.33	120.23	122.79
74	S2	1850	MA6	C4-N9-C8	2.32	108.25	105.73
70	L5	1744	PSU	C6-N1-C2	-2.32	120.31	122.68
70	L5	4431	PSU	O2-C2-N1	-2.32	120.24	122.79
70	L5	3851	PSU	O2-C2-N1	-2.31	120.24	122.79
70	L5	2401	A2M	C6-C5-C4	2.31	120.29	117.18
74	S2	1692	PSU	O2-C2-N1	-2.31	120.25	122.79
74	S2	1445	PSU	C6-N1-C2	-2.31	120.32	122.68
70	L5	4431	PSU	C6-N1-C2	-2.31	120.32	122.68
74	S2	801	PSU	C6-N1-C2	-2.30	120.33	122.68
70	L5	1792	PSU	O2-C2-N1	-2.30	120.26	122.79
70	L5	3695	PSU	C6-N1-C2	-2.30	120.33	122.68
74	S2	576	A2M	C6-C5-C4	2.30	120.27	117.18
70	L5	3758	PSU	C6-N1-C2	-2.30	120.33	122.68
70	L5	2837	OMU	O2-C2-N1	-2.29	119.74	122.79
70	L5	4353	PSU	O2-C2-N1	-2.29	120.27	122.79
74	S2	668	A2M	C3'-C2'-C1'	2.29	107.20	102.89
74	S2	1056	PSU	O2-C2-N1	-2.29	120.27	122.79
74	S2	1337	4AC	C5-C4-N3	-2.28	118.92	122.59
70	L5	1862	PSU	C6-N1-C2	-2.28	120.35	122.68
74	S2	651	PSU	C6-N1-C2	-2.28	120.36	122.68
74	S2	1031	A2M	C6-C5-C4	2.28	120.24	117.18
70	L5	4442	PSU	C6-N1-C2	-2.28	120.36	122.68
74	S2	814	PSU	O2-C2-N1	-2.27	120.29	122.79
70	L5	1779	PSU	C6-N1-C2	-2.27	120.36	122.68
74	S2	573	PSU	O2-C2-N1	-2.27	120.29	122.79
74	S2	1248	B8N	O4'-C1'-C2'	2.27	108.34	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	3920	PSU	O2-C2-N1	-2.27	120.30	122.79
74	S2	296	PSU	C6-N1-C2	-2.27	120.37	122.68
74	S2	105	PSU	C6-N1-C2	-2.27	120.37	122.68
70	L5	3695	PSU	O2-C2-N1	-2.26	120.30	122.79
74	S2	1625	PSU	C6-N1-C2	-2.26	120.37	122.68
70	L5	4552	PSU	C6-N1-C2	-2.26	120.37	122.68
70	L5	5010	PSU	C6-N1-C2	-2.26	120.37	122.68
70	L5	4523	A2M	C6-C5-C4	2.26	120.22	117.18
74	S2	1832	6MZ	C4-N9-C8	2.26	108.18	105.73
74	S2	590	A2M	C6-C5-C4	2.25	120.21	117.18
70	L5	3760	A2M	C4-N9-C8	2.25	108.16	105.73
74	S2	1174	PSU	C6-N1-C2	-2.25	120.39	122.68
74	S2	681	PSU	O2-C2-N1	-2.24	120.32	122.79
70	L5	3825	A2M	C6-C5-C4	2.24	120.20	117.18
74	S2	668	A2M	C4-C5-N7	-2.24	107.89	110.62
74	S2	814	PSU	C6-N1-C2	-2.24	120.40	122.68
70	L5	1524	A2M	C4-C5-N7	-2.24	107.90	110.62
70	L5	4590	A2M	C4-C5-N7	-2.24	107.90	110.62
70	L5	4220	6MZ	C4-N9-C8	2.23	108.15	105.73
67	Pt	56	PSU	C6-N1-C2	-2.23	120.40	122.68
69	L8	69	PSU	C6-N1-C2	-2.23	120.41	122.68
70	L5	1522	OMG	C8-N7-C5	2.22	108.27	104.24
74	S2	686	PSU	C6-N1-C2	-2.22	120.41	122.68
65	La	39	V5N	O-C-CA	-2.22	118.96	124.78
74	S2	815	PSU	O2-C2-N1	-2.22	120.35	122.79
70	L5	3760	A2M	C6-C5-C4	2.22	120.17	117.18
70	L5	4442	PSU	O4'-C1'-C2'	2.22	108.27	105.14
74	S2	627	OMU	O2-C2-N1	-2.21	119.84	122.79
70	L5	3785	A2M	C4-N9-C8	2.21	108.12	105.73
70	L5	3627	OMG	C8-N7-C5	2.21	108.24	104.24
74	S2	1248	B8N	C31-N3-C2	2.21	120.98	117.67
70	L5	1683	PSU	C6-N1-C2	-2.21	120.43	122.68
70	L5	4296	PSU	C6-N1-C2	-2.21	120.43	122.68
70	L5	4493	PSU	C6-N1-C2	-2.21	120.43	122.68
70	L5	4457	PSU	C6-N1-C2	-2.20	120.43	122.68
74	S2	572	PSU	C6-N1-C2	-2.20	120.43	122.68
74	S2	1244	PSU	C6-N1-C2	-2.20	120.43	122.68
70	L5	1781	PSU	C6-N1-C2	-2.20	120.44	122.68
74	S2	1177	PSU	C6-N1-C2	-2.20	120.44	122.68
74	S2	1347	PSU	C6-N1-C2	-2.20	120.44	122.68
70	L5	4312	PSU	C6-N1-C2	-2.20	120.44	122.68
70	L5	2843	PSU	C6-N1-C2	-2.20	120.44	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	36	PSU	C6-N1-C2	-2.20	120.44	122.68
70	L5	1781	PSU	O2-C2-N1	-2.19	120.38	122.79
74	S2	1832	6MZ	C5-C4-N9	2.19	108.33	105.78
67	Pt	33	OMC	C1'-N1-C2	2.19	123.31	118.42
70	L5	2876	OMG	C8-N7-C5	2.19	108.21	104.24
74	S2	1678	A2M	C6-C5-C4	2.19	120.13	117.18
74	S2	1367	PSU	C6-N1-C2	-2.18	120.45	122.68
70	L5	3899	OMG	C8-N7-C5	2.18	108.19	104.24
74	S2	609	PSU	C6-N1-C2	-2.18	120.45	122.68
74	S2	668	A2M	C4-N9-C8	2.18	108.09	105.73
74	S2	867	OMG	C8-N7-C5	2.18	108.18	104.24
70	L5	1322	1MA	C2'-C1'-N9	2.17	119.38	113.22
70	L5	1536	PSU	C6-N1-C2	-2.17	120.46	122.68
70	L5	3851	PSU	C6-N1-C2	-2.17	120.46	122.68
70	L5	4569	PSU	C6-N1-C2	-2.17	120.46	122.68
74	S2	681	PSU	C6-N1-C2	-2.17	120.47	122.68
70	L5	4403	PSU	C6-N1-C2	-2.17	120.47	122.68
74	S2	1842	4AC	O2-C2-N3	-2.16	118.81	122.33
70	L5	4637	OMG	C8-N7-C5	2.16	108.15	104.24
70	L5	4521	PSU	C6-N1-C2	-2.16	120.48	122.68
74	S2	1842	4AC	C5-C4-N3	-2.16	119.12	122.59
70	L5	1322	1MA	C5-C4-N9	2.16	109.54	105.63
70	L5	3825	A2M	C4-C5-N7	-2.15	107.99	110.62
74	S2	1851	MA6	C4-C5-N7	-2.15	108.00	110.62
70	L5	3768	PSU	C6-N1-C2	-2.15	120.48	122.68
70	L5	398	A2M	C4-C5-N7	-2.15	108.00	110.62
70	L5	2363	A2M	C4-C5-N7	-2.15	108.00	110.62
74	S2	1678	A2M	C4-N9-C8	2.15	108.06	105.73
70	L5	4403	PSU	O4'-C1'-C2'	2.15	108.17	105.14
70	L5	3867	A2M	C4-C5-N7	-2.14	108.01	110.62
74	S2	93	PSU	C6-N1-C2	-2.14	120.49	122.68
70	L5	3853	PSU	O2-C2-N1	-2.14	120.44	122.79
70	L5	2632	PSU	C6-N1-C2	-2.13	120.50	122.68
70	L5	1316	OMG	C8-N7-C5	2.13	108.10	104.24
70	L5	1524	A2M	C4'-O4'-C1'	-2.13	104.78	109.47
70	L5	3639	PSU	C6-N1-C2	-2.13	120.51	122.68
74	S2	99	A2M	C6-C5-C4	2.13	120.04	117.18
69	L8	55	PSU	C6-N1-C2	-2.13	120.51	122.68
74	S2	218	PSU	C6-N1-C2	-2.13	120.51	122.68
70	L5	1677	PSU	C6-N1-C2	-2.12	120.51	122.68
70	L5	4228	OMG	C8-N7-C5	2.12	108.08	104.24
74	S2	572	PSU	O4'-C1'-C2'	2.12	108.13	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	L5	3830	A2M	C4-N9-C8	2.12	108.02	105.73
74	S2	512	A2M	C6-C5-C4	2.12	120.03	117.18
74	S2	99	A2M	C4-C5-N7	-2.12	108.04	110.62
70	L5	2351	OMC	O2-C2-N1	2.11	123.26	118.89
70	L5	4500	PSU	C6-C5-C4	2.11	119.68	118.20
70	L5	1792	PSU	C6-N1-C2	-2.11	120.52	122.68
74	S2	1056	PSU	C6-N1-C2	-2.11	120.52	122.68
70	L5	2839	PSU	C6-N1-C2	-2.11	120.53	122.68
74	S2	1692	PSU	C6-N1-C2	-2.11	120.53	122.68
70	L5	4353	PSU	C6-N1-C2	-2.10	120.53	122.68
70	L5	3695	PSU	O4'-C1'-C2'	2.10	108.11	105.14
70	L5	1860	PSU	C6-N1-C2	-2.10	120.53	122.68
70	L5	4392	OMG	C8-N7-C5	2.10	108.04	104.24
74	S2	484	A2M	C6-C5-C4	2.10	120.01	117.18
69	L8	75	OMG	C8-N7-C5	2.10	108.04	104.24
70	L5	3718	A2M	C6-C5-C4	2.10	120.00	117.18
74	S2	1031	A2M	C4-C5-N7	-2.10	108.06	110.62
74	S2	1639	G7M	N9-C8-N7	-2.10	107.02	112.21
74	S2	218	PSU	O4'-C1'-C2'	2.09	108.10	105.14
74	S2	512	A2M	C4-C5-N7	-2.09	108.07	110.62
70	L5	3785	A2M	C4-C5-N7	-2.09	108.07	110.62
74	S2	1136	PSU	C6-N1-C2	-2.09	120.55	122.68
70	L5	4361	PSU	C6-N1-C2	-2.09	120.55	122.68
74	S2	119	PSU	O2-C2-N1	-2.08	120.50	122.79
70	L5	1625	OMG	C8-N7-C5	2.08	108.01	104.24
70	L5	4196	OMG	C8-N7-C5	2.08	108.01	104.24
70	L5	3925	OMU	O2-C2-N1	-2.08	120.02	122.79
70	L5	1582	PSU	O2-C2-N1	-2.08	120.50	122.79
74	S2	27	A2M	C6-C5-C4	2.08	119.97	117.18
70	L5	398	A2M	C4-N9-C8	2.08	107.98	105.73
74	S2	590	A2M	C4-C5-N7	-2.08	108.09	110.62
70	L5	4623	OMG	C8-N7-C5	2.07	107.99	104.24
70	L5	2363	A2M	C4-N9-C8	2.07	107.97	105.73
70	L5	1534	A2M	C4-C5-N7	-2.07	108.10	110.62
70	L5	2815	A2M	C4-C5-N7	-2.07	108.10	110.62
74	S2	822	PSU	O4'-C1'-C2'	2.07	108.06	105.14
74	S2	1445	PSU	C6-C5-C4	2.07	119.64	118.20
70	L5	398	A2M	C6-C5-C4	2.07	119.96	117.18
74	S2	468	A2M	C6-C5-C4	2.07	119.96	117.18
70	L5	4618	OMG	C8-N7-C5	2.06	107.98	104.24
70	L5	3760	A2M	C4-C5-N7	-2.06	108.11	110.62
70	L5	2364	OMG	C8-N7-C5	2.06	107.97	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
74	S2	436	OMG	C8-N7-C5	2.06	107.97	104.24
70	L5	3744	OMG	C8-N7-C5	2.06	107.97	104.24
70	L5	4456	OMC	O2-C2-N3	-2.06	118.98	122.33
74	S2	468	A2M	C4-N9-C8	2.06	107.96	105.73
74	S2	1328	OMG	C8-N7-C5	2.06	107.96	104.24
70	L5	3830	A2M	C4-C5-N7	-2.05	108.12	110.62
69	L8	69	PSU	O4'-C1'-C2'	2.05	108.04	105.14
74	S2	1031	A2M	C4-N9-C8	2.05	107.95	105.73
70	L5	3844	PSU	C6-N1-C2	-2.05	120.59	122.68
70	L5	4499	OMG	C8-N7-C5	2.05	107.95	104.24
70	L5	3867	A2M	C6-C5-C4	2.05	119.94	117.18
64	LA	216	V5N	O-C-CA	-2.04	119.42	124.78
70	L5	3825	A2M	C4-N9-C8	2.04	107.94	105.73
74	S2	1383	A2M	C6-C5-C4	2.04	119.92	117.18
74	S2	27	A2M	C4-C5-N7	-2.04	108.14	110.62
70	L5	3734	PSU	C6-N1-C2	-2.04	120.60	122.68
74	S2	1248	B8N	O36-C34-C33	2.04	120.32	113.38
70	L5	400	A2M	C4-C5-N7	-2.03	108.14	110.62
70	L5	2401	A2M	C4-C5-N7	-2.03	108.14	110.62
70	L5	1524	A2M	C6-C5-C4	2.03	119.91	117.18
70	L5	4571	A2M	C4-N9-C8	2.03	107.93	105.73
70	L5	3637	PSU	O2-C2-N1	-2.03	120.56	122.79
70	L5	3830	A2M	C6-C5-C4	2.03	119.91	117.18
70	L5	4531	PSU	C6-N1-C2	-2.03	120.61	122.68
74	S2	116	OMU	O2-C2-N1	-2.02	120.11	122.79
70	L5	4571	A2M	C6-C5-C4	2.02	119.89	117.18
67	Pt	8	4SU	O2-C2-N1	-2.01	120.11	122.79
70	L5	1871	A2M	C4-C5-N7	-2.01	108.17	110.62
74	S2	683	OMG	C8-N7-C5	2.01	107.87	104.24
74	S2	590	A2M	C4'-O4'-C1'	-2.01	105.05	109.47
70	L5	4420	PSU	O4'-C1'-C2'	2.00	107.97	105.14
74	S2	1490	OMG	C8-N7-C5	2.00	107.87	104.24
74	S2	644	OMG	C8-N7-C5	2.00	107.86	104.24

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Lo	53	MLZ	N-CA-CB-CG
3	Lo	53	MLZ	C-CA-CB-CG
63	Lb	5	MLZ	N-CA-CB-CG
63	Lb	5	MLZ	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
64	LA	216	V5N	O-C-CA-CB
67	Pt	33	OMC	C1'-C2'-O2'-CM2
69	L8	75	OMG	C1'-C2'-O2'-CM2
70	L5	1625	OMG	O4'-C4'-C5'-O5'
70	L5	1677	PSU	C2'-C1'-C5-C6
70	L5	3701	OMC	C2'-C1'-N1-C2
70	L5	3701	OMC	C2'-C1'-N1-C6
70	L5	3729	PSU	O4'-C4'-C5'-O5'
70	L5	3762	PSU	O4'-C4'-C5'-O5'
70	L5	3867	A2M	C1'-C2'-O2'-CM'
70	L5	3925	OMU	C1'-C2'-O2'-CM2
70	L5	4196	OMG	C1'-C2'-O2'-CM2
70	L5	4420	PSU	C2'-C1'-C5-C4
70	L5	4420	PSU	C2'-C1'-C5-C6
70	L5	4420	PSU	O4'-C4'-C5'-O5'
70	L5	4590	A2M	C4'-C5'-O5'-P
70	L5	4620	OMU	C1'-C2'-O2'-CM2
70	L5	4623	OMG	C1'-C2'-O2'-CM2
70	L5	4636	PSU	C2'-C1'-C5-C6
70	L5	4637	OMG	O4'-C4'-C5'-O5'
74	S2	116	OMU	C1'-C2'-O2'-CM2
74	S2	428	OMU	C2'-C1'-N1-C2
74	S2	428	OMU	C2'-C1'-N1-C6
74	S2	509	OMG	C1'-C2'-O2'-CM2
74	S2	576	A2M	C3'-C4'-C5'-O5'
74	S2	644	OMG	O4'-C4'-C5'-O5'
74	S2	867	OMG	C1'-C2'-O2'-CM2
74	S2	1243	PSU	C3'-C4'-C5'-O5'
74	S2	1243	PSU	O4'-C4'-C5'-O5'
74	S2	1248	B8N	C31-C32-C33-C34
74	S2	1248	B8N	C31-C32-C33-N34
74	S2	1328	OMG	C1'-C2'-O2'-CM2
74	S2	1804	OMU	C1'-C2'-O2'-CM2
74	S2	1832	6MZ	C5-C6-N6-C9
74	S2	1832	6MZ	N1-C6-N6-C9
67	Pt	21	H2U	O4'-C4'-C5'-O5'
70	L5	1625	OMG	C3'-C4'-C5'-O5'
70	L5	3729	PSU	C3'-C4'-C5'-O5'
70	L5	3760	A2M	O4'-C4'-C5'-O5'
70	L5	3760	A2M	C3'-C4'-C5'-O5'
70	L5	3762	PSU	C3'-C4'-C5'-O5'
70	L5	3844	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
70	L5	3844	PSU	O4'-C4'-C5'-O5'
70	L5	4420	PSU	C3'-C4'-C5'-O5'
74	S2	512	A2M	O4'-C4'-C5'-O5'
74	S2	590	A2M	O4'-C4'-C5'-O5'
74	S2	590	A2M	C3'-C4'-C5'-O5'
74	S2	644	OMG	C3'-C4'-C5'-O5'
74	S2	668	A2M	O4'-C4'-C5'-O5'
74	S2	668	A2M	C3'-C4'-C5'-O5'
74	S2	822	PSU	C3'-C4'-C5'-O5'
74	S2	822	PSU	O4'-C4'-C5'-O5'
3	Lo	53	MLZ	CD-CE-NZ-CM
67	Pt	21	H2U	C3'-C4'-C5'-O5'
70	L5	1677	PSU	C3'-C4'-C5'-O5'
70	L5	1677	PSU	O4'-C4'-C5'-O5'
70	L5	4196	OMG	O4'-C4'-C5'-O5'
70	L5	4196	OMG	C3'-C4'-C5'-O5'
70	L5	4637	OMG	C3'-C4'-C5'-O5'
74	S2	576	A2M	O4'-C4'-C5'-O5'
74	S2	918	PSU	O4'-C4'-C5'-O5'
3	Lo	53	MLZ	CG-CD-CE-NZ
70	L5	3764	PSU	O4'-C4'-C5'-O5'
70	L5	4447	5MC	C2'-C1'-N1-C6
74	S2	512	A2M	C3'-C4'-C5'-O5'
63	Lb	5	MLZ	CE-CD-CG-CB
70	L5	4293	PSU	O4'-C4'-C5'-O5'
70	L5	2508	PSU	C3'-C4'-C5'-O5'
70	L5	3760	A2M	C4'-C5'-O5'-P
74	S2	590	A2M	C4'-C5'-O5'-P
74	S2	428	OMU	O4'-C4'-C5'-O5'
63	Lb	5	MLZ	CG-CD-CE-NZ
70	L5	400	A2M	C1'-C2'-O2'-CM'
70	L5	4447	5MC	O4'-C1'-N1-C6
70	L5	4447	5MC	C2'-C1'-N1-C2
70	L5	4500	PSU	C4'-C5'-O5'-P
74	S2	644	OMG	C4'-C5'-O5'-P
74	S2	1490	OMG	C4'-C5'-O5'-P
70	L5	398	A2M	O4'-C4'-C5'-O5'
74	S2	627	OMU	O4'-C4'-C5'-O5'
74	S2	428	OMU	C3'-C4'-C5'-O5'
70	L5	1534	A2M	C4'-C5'-O5'-P
70	L5	2508	PSU	O4'-C4'-C5'-O5'
70	L5	4590	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
74	S2	119	PSU	O4'-C4'-C5'-O5'
74	S2	1703	OMC	O4'-C4'-C5'-O5'
70	L5	4447	5MC	O4'-C1'-N1-C2
67	Pt	21	H2U	C4'-C5'-O5'-P
70	L5	3701	OMC	O4'-C1'-N1-C6
74	S2	428	OMU	O4'-C1'-N1-C6
69	L8	69	PSU	C3'-C4'-C5'-O5'
74	S2	918	PSU	C3'-C4'-C5'-O5'
70	L5	2876	OMG	C3'-C2'-O2'-CM2
70	L5	3785	A2M	C3'-C2'-O2'-CM'
70	L5	3764	PSU	C3'-C4'-C5'-O5'
70	L5	3844	PSU	C4'-C5'-O5'-P
70	L5	4636	PSU	O4'-C4'-C5'-O5'
70	L5	4521	PSU	O4'-C1'-C5-C4
70	L5	3869	OMC	C3'-C2'-O2'-CM2
70	L5	3701	OMC	O4'-C1'-N1-C2
74	S2	428	OMU	O4'-C1'-N1-C2
70	L5	2351	OMC	C2'-C1'-N1-C6
70	L5	1524	A2M	O4'-C1'-N9-C8
74	S2	1248	B8N	N34-C33-C34-O35
70	L5	2422	OMC	C3'-C4'-C5'-O5'
70	L5	4293	PSU	C3'-C4'-C5'-O5'
63	Lb	5	MLZ	CD-CE-NZ-CM
70	L5	2351	OMC	C2'-C1'-N1-C2
70	L5	4442	PSU	O4'-C4'-C5'-O5'
74	S2	99	A2M	O4'-C4'-C5'-O5'
74	S2	462	OMC	C1'-C2'-O2'-CM2
67	Pt	33	OMC	C2'-C1'-N1-C2
70	L5	1534	A2M	O4'-C4'-C5'-O5'
70	L5	2422	OMC	O4'-C4'-C5'-O5'
70	L5	4499	OMG	O4'-C4'-C5'-O5'
70	L5	4499	OMG	C3'-C4'-C5'-O5'
70	L5	1677	PSU	O4'-C1'-C5-C6
70	L5	4636	PSU	O4'-C1'-C5-C6
67	Pt	47	G7M	C4'-C5'-O5'-P
74	S2	1248	B8N	N34-C33-C34-O36
70	L5	2351	OMC	O4'-C4'-C5'-O5'
70	L5	3758	PSU	C3'-C4'-C5'-O5'
70	L5	4361	PSU	O4'-C4'-C5'-O5'
74	S2	668	A2M	C2'-C1'-N9-C8
67	Pt	21	H2U	C2'-C1'-N1-C2
74	S2	1851	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
70	L5	4636	PSU	C4'-C5'-O5'-P
74	S2	1643	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

48 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	L5	2815	A2M	1	0
70	L5	4196	OMG	1	0
70	L5	3718	A2M	2	0
74	S2	1804	OMU	1	0
70	L5	3770	PSU	2	0
70	L5	4637	OMG	1	0
70	L5	1340	OMC	1	0
74	S2	512	A2M	1	0
70	L5	2351	OMC	1	0
70	L5	4552	PSU	1	0
70	L5	2837	OMU	1	0
70	L5	2424	OMG	1	0
70	L5	1683	PSU	1	0
69	L8	75	OMG	2	0
74	S2	1232	PSU	1	0
70	L5	4618	OMG	1	0
74	S2	867	OMG	1	0
74	S2	1703	OMC	1	0
74	S2	1391	OMC	1	0
70	L5	4220	6MZ	1	0
70	L5	3867	A2M	1	0
70	L5	4620	OMU	2	0
74	S2	1490	OMG	1	0
70	L5	1871	A2M	1	0
74	S2	627	OMU	1	0
70	L5	1322	1MA	1	0
74	S2	573	PSU	1	0
74	S2	1639	G7M	1	0
70	L5	1625	OMG	1	0
70	L5	3830	A2M	1	0
70	L5	2363	A2M	1	0
74	S2	484	A2M	1	0
70	L5	3925	OMU	1	0
67	Pt	33	OMC	1	0
74	S2	1031	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	L5	4523	A2M	1	0
74	S2	436	OMG	1	0
74	S2	116	OMU	2	0
70	L5	4579	PSU	1	0
70	L5	4456	OMC	1	0
74	S2	1244	PSU	2	0
70	L5	1326	A2M	1	0
70	L5	4623	OMG	1	0
74	S2	509	OMG	2	0
74	S2	576	A2M	1	0
70	L5	4521	PSU	1	0
70	L5	400	A2M	1	0
67	Pt	21	H2U	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 266 ligands modelled in this entry, 262 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
85	SPD	L5	5103	70	9,9,9	0.28	0	8,8,8	0.23	0
86	HYG	S2	1901	-	35,39,39	3.13	12 (34%)	43,60,60	1.88	8 (18%)
85	SPD	L5	5102	-	9,9,9	0.28	0	8,8,8	0.22	0
85	SPD	L5	5101	-	9,9,9	0.28	0	8,8,8	0.19	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
85	SPD	L5	5103	70	-	4/7/7/7	-
86	HYG	S2	1901	-	-	2/12/87/87	0/4/4/4
85	SPD	L5	5102	-	-	4/7/7/7	-
85	SPD	L5	5101	-	-	2/7/7/7	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	1901	HYG	O29-C12	11.00	1.61	1.43
86	S2	1901	HYG	O22-C17	6.65	1.54	1.43
86	S2	1901	HYG	O14-C13	6.47	1.58	1.41
86	S2	1901	HYG	O28-C23	6.07	1.47	1.40
86	S2	1901	HYG	C16-C15	4.31	1.62	1.53
86	S2	1901	HYG	C17-C12	-4.06	1.44	1.53
86	S2	1901	HYG	O28-C27	3.73	1.49	1.44
86	S2	1901	HYG	C25-C24	-3.26	1.47	1.53
86	S2	1901	HYG	O18-C13	-2.64	1.34	1.41
86	S2	1901	HYG	O30-C24	2.39	1.47	1.42
86	S2	1901	HYG	C26-C25	-2.17	1.46	1.52
86	S2	1901	HYG	O31-C25	2.07	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	S2	1901	HYG	O28-C27-C26	6.61	117.91	108.52
86	S2	1901	HYG	O29-C12-C13	4.84	123.57	110.86
86	S2	1901	HYG	O22-C17-C16	4.08	121.16	111.22
86	S2	1901	HYG	C23-O28-C27	3.91	119.44	112.00
86	S2	1901	HYG	O22-C17-C12	2.75	107.97	103.58
86	S2	1901	HYG	O14-C15-C16	2.72	114.63	109.69
86	S2	1901	HYG	C13-O18-C6	-2.48	111.81	117.96
86	S2	1901	HYG	C19-C15-C16	-2.24	107.76	113.00

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	L5	5103	SPD	C3-C4-C5-N6
85	L5	5102	SPD	C3-C4-C5-N6
86	S2	1901	HYG	O14-C13-O18-C6
85	L5	5103	SPD	C7-C8-C9-N10

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Mol	Chain	Res	Type	Atoms
85	L5	5103	SPD	N6-C7-C8-C9
85	L5	5101	SPD	C8-C7-N6-C5
86	S2	1901	HYG	N36-C33-C34-O35
85	L5	5101	SPD	C7-C8-C9-N10
85	L5	5102	SPD	C7-C8-C9-N10
85	L5	5102	SPD	C2-C3-C4-C5
85	L5	5102	SPD	C4-C5-N6-C7
85	L5	5103	SPD	C2-C3-C4-C5

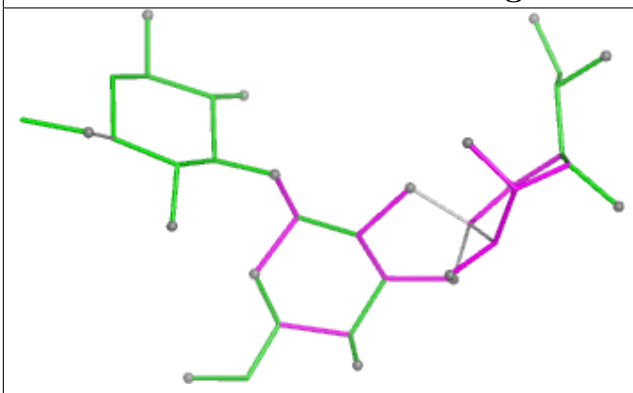
There are no ring outliers.

2 monomers are involved in 4 short contacts:

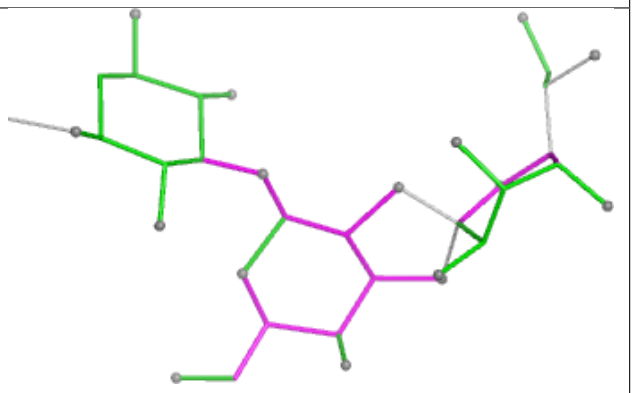
Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	L5	5102	SPD	3	0
85	L5	5101	SPD	1	0

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

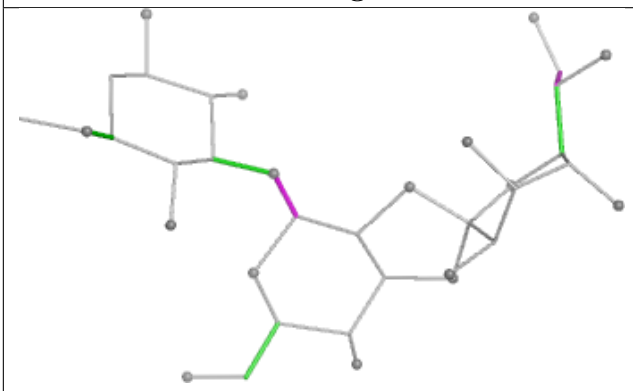
Ligand HYG S2 1901



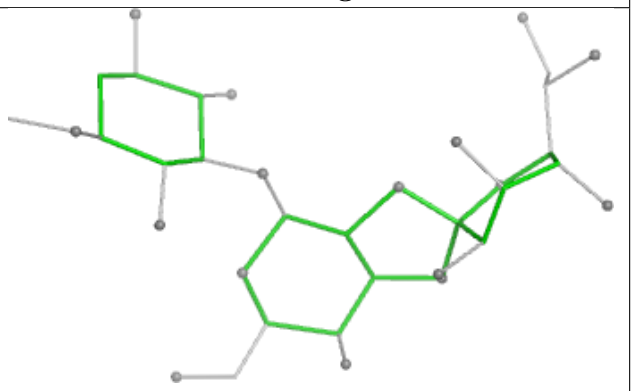
Bond lengths



Bond angles



Torsions



Rings

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.

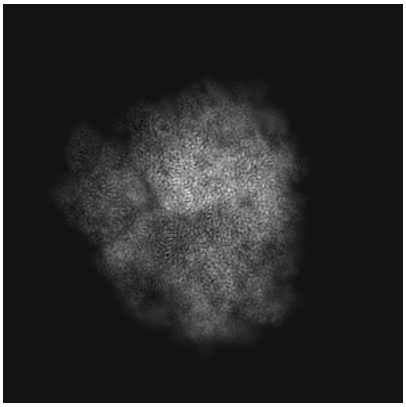
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54266. These allow visual inspection of the internal detail of the map and identification of artifacts.

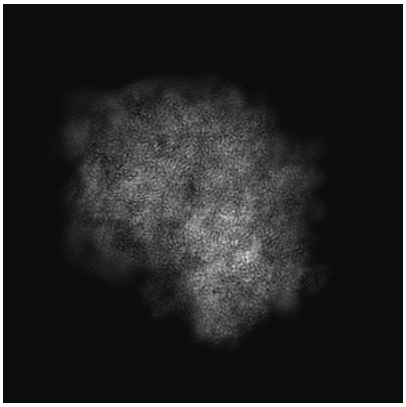
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

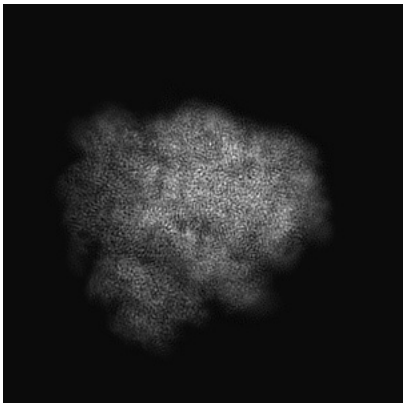
6.1.1 Primary map



X



Y

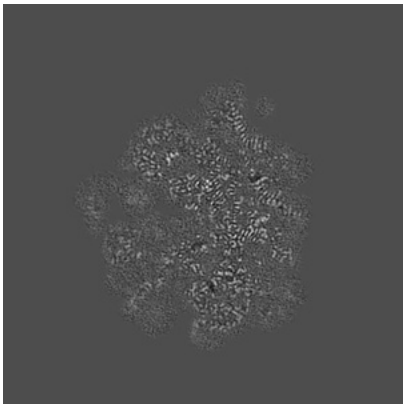


Z

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

6.2 Central slices

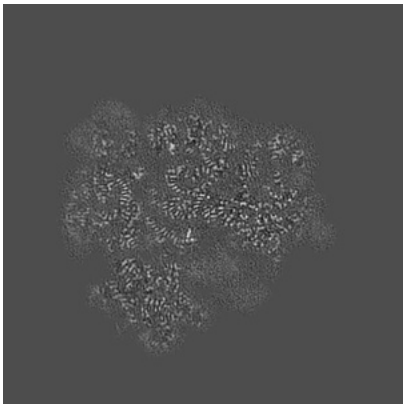
6.2.1 Primary map



X Index: 240



Y Index: 240

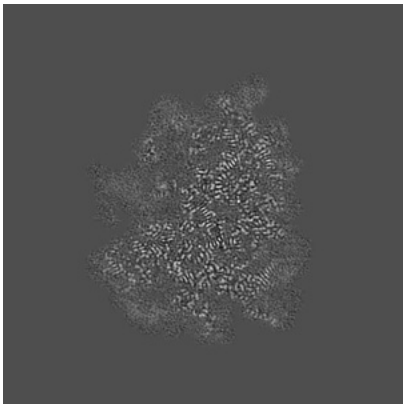


Z Index: 240

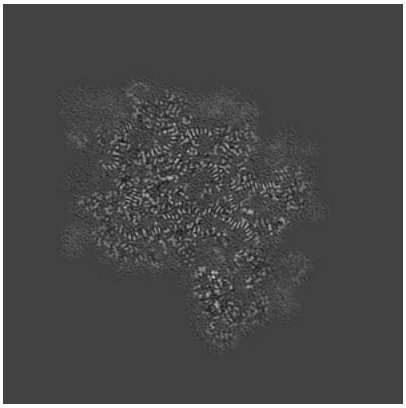
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

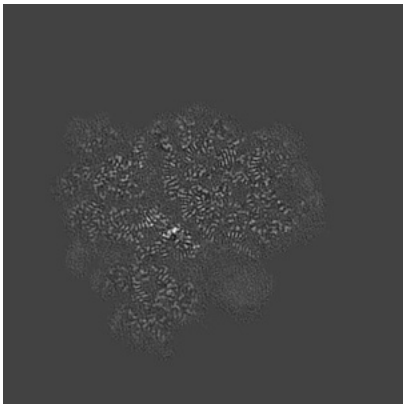
6.3.1 Primary map



X Index: 265



Y Index: 271

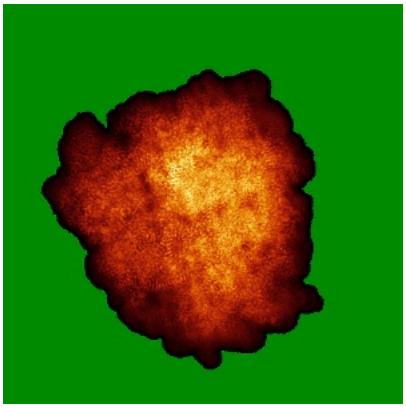


Z Index: 265

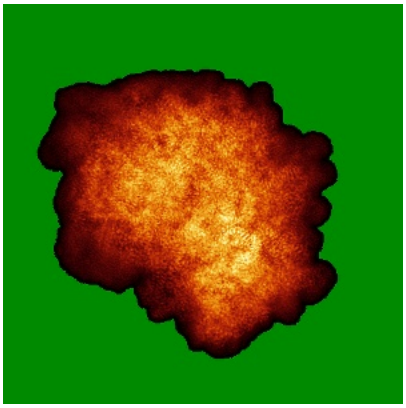
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

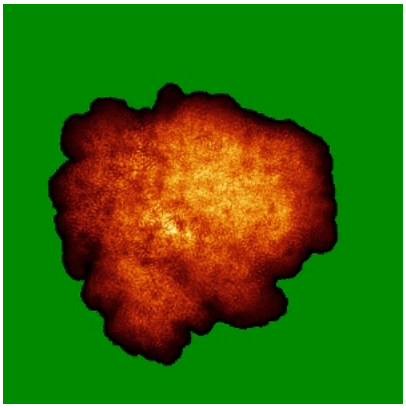
6.4.1 Primary map



X



Y



Z

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.

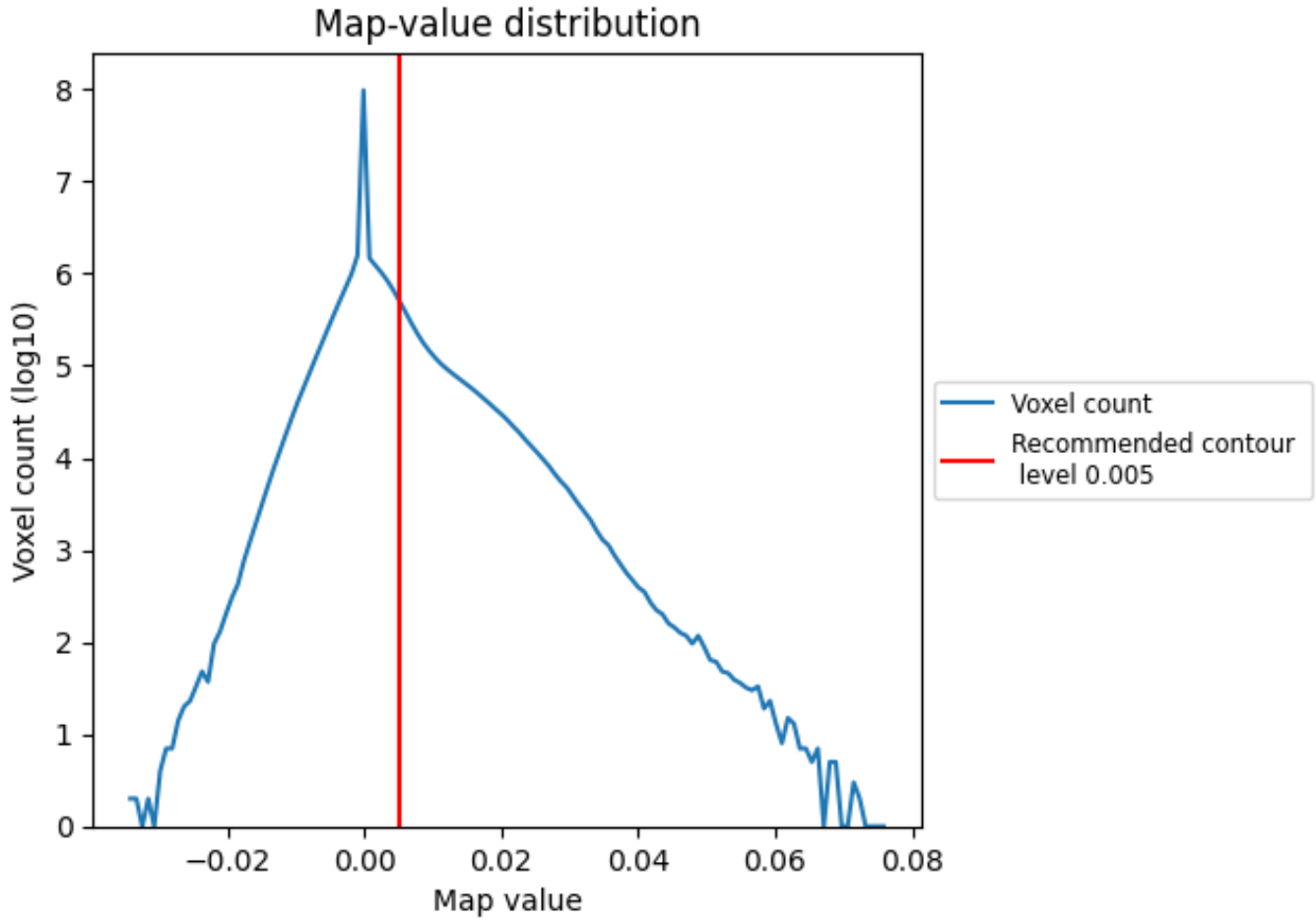
6.6 Mask visualisation (i)

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

7 Map analysis

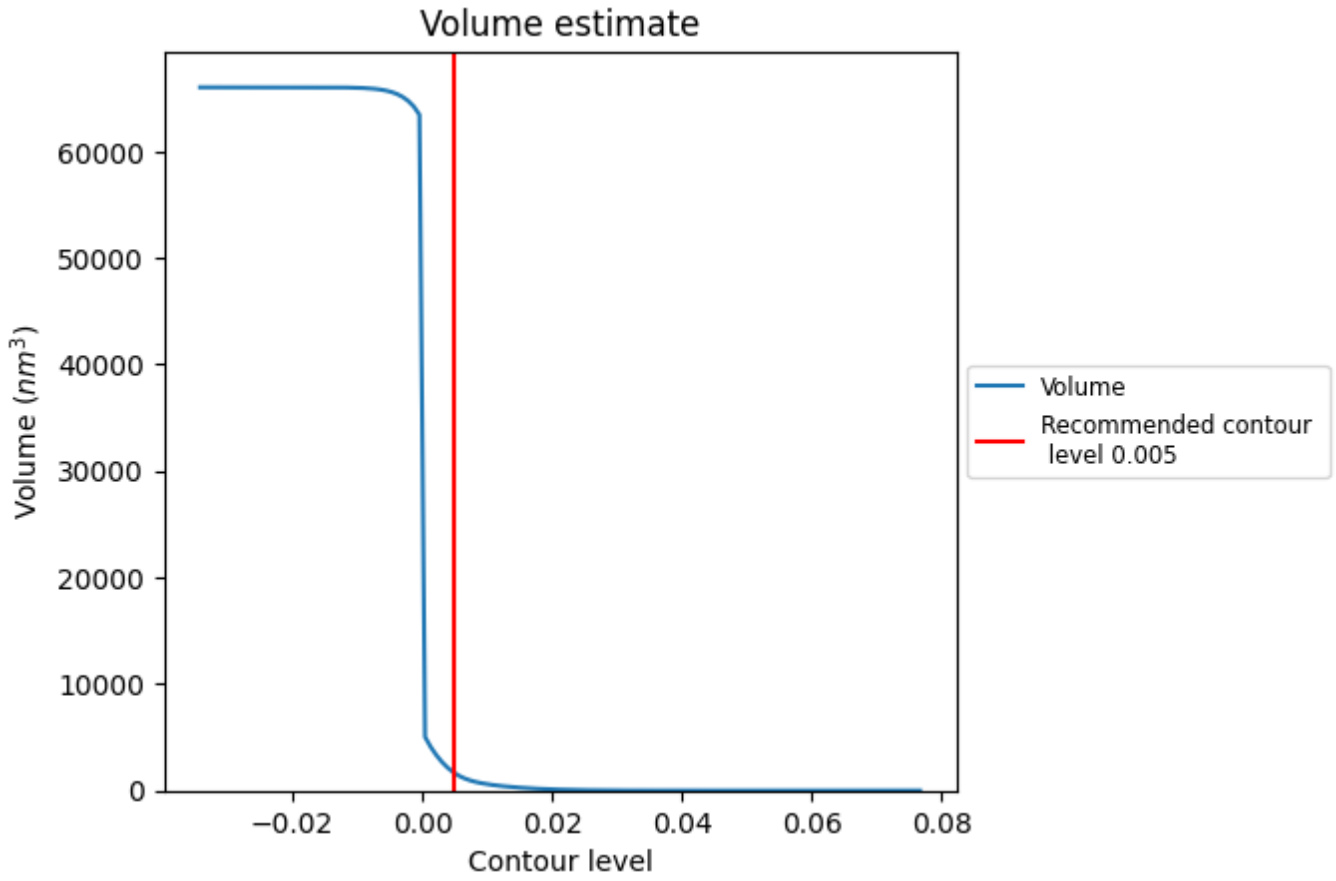
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

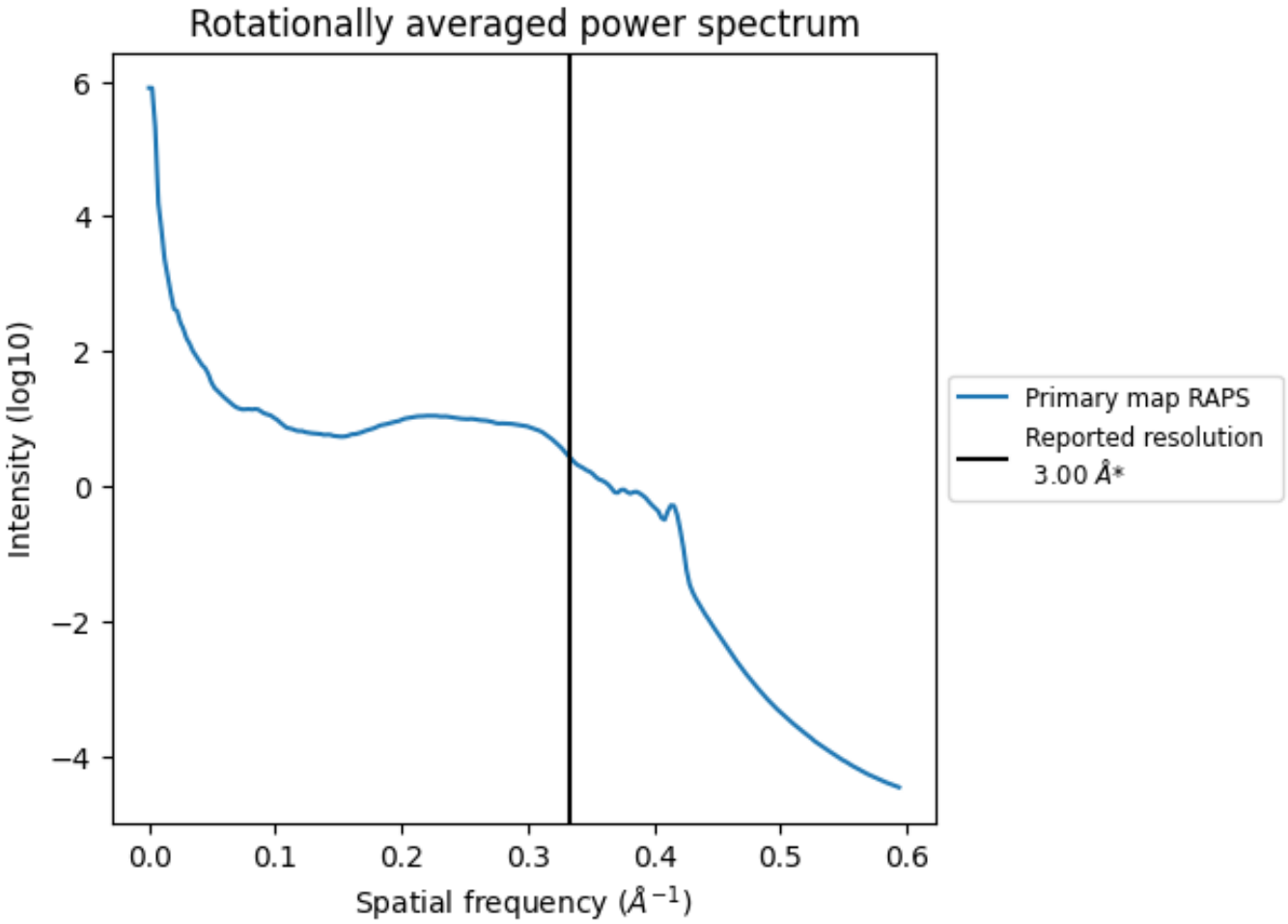
7.2 Volume estimate



The volume at the recommended contour level is 1649 nm^3; this corresponds to an approximate mass of 1489 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 (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

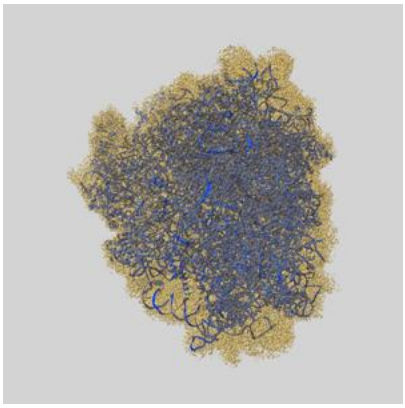
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

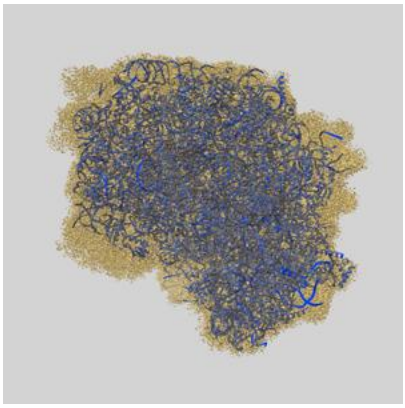
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54266 and PDB model 9RU8. Per-residue inclusion information can be found in section 3 on page 25.

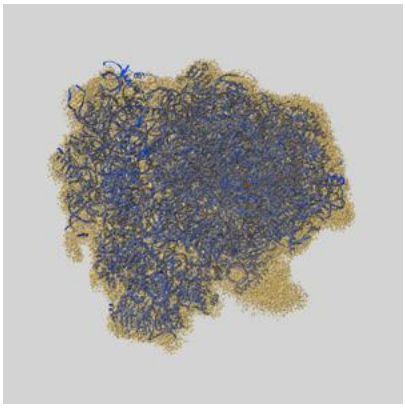
9.1 Map-model overlay



X



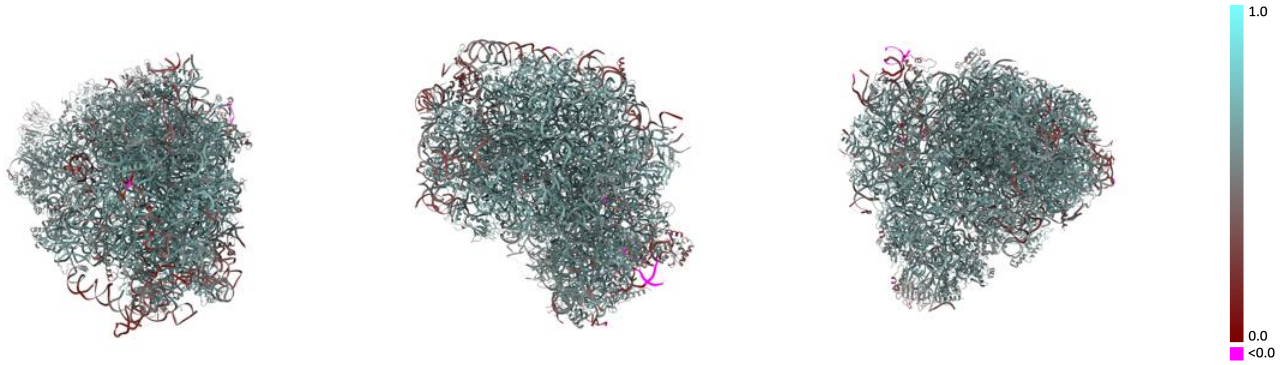
Y



Z

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

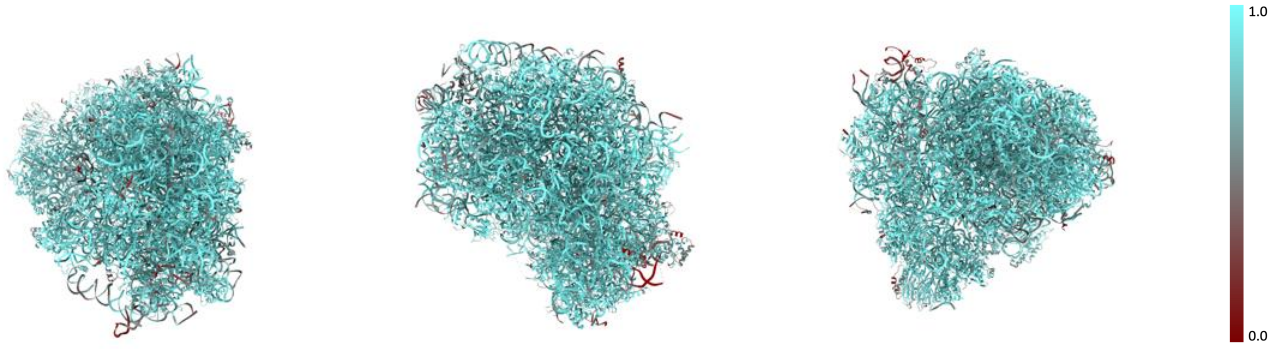
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

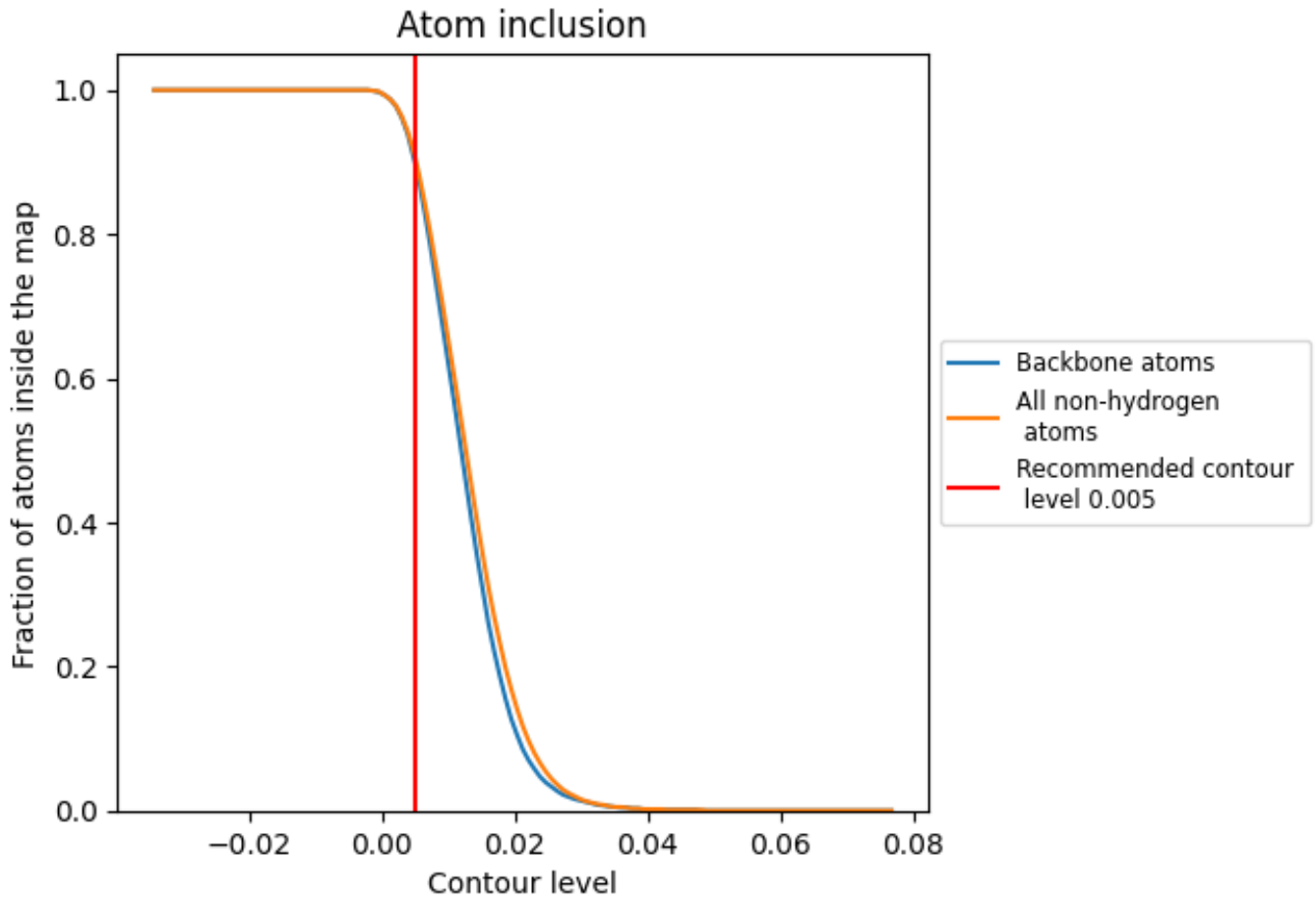
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% 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	0.9090	0.5780
L5	0.9140	0.5720
L7	0.9750	0.6100
L8	0.9410	0.5860
LA	0.9690	0.6410
LB	0.9470	0.6230
LC	0.9460	0.6210
LD	0.8770	0.5690
LE	0.8870	0.5750
LF	0.9540	0.6310
LG	0.8670	0.5620
LH	0.9040	0.5880
LI	0.9310	0.6130
LJ	0.8270	0.5380
LL	0.9120	0.5950
LM	0.9200	0.6000
LN	0.9780	0.6450
LO	0.9600	0.6320
LP	0.9670	0.6320
LQ	0.9540	0.6300
LR	0.8940	0.5860
LS	0.9510	0.6290
LT	0.8990	0.5950
LU	0.7430	0.4810
LV	0.9320	0.6190
LW	0.9400	0.6140
LX	0.9000	0.5840
LY	0.9510	0.6130
LZ	0.9180	0.5850
La	0.9560	0.6310
Lb	0.8280	0.5510
Lc	0.9270	0.5910
Ld	0.9330	0.5980
Le	0.9540	0.6350
Lf	0.9650	0.6410



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Chain	Atom inclusion	Q-score
Lg	0.9490	0.6180
Lh	0.9300	0.5980
Li	0.8900	0.5760
Lj	0.9640	0.6400
Lk	0.8590	0.5500
Ll	0.9450	0.6250
Lm	0.9470	0.6170
Ln	0.9200	0.6000
Lo	0.9170	0.6130
Lp	0.9560	0.6190
Lr	0.9470	0.6180
Pt	0.7240	0.4580
S2	0.9220	0.5740
S6	0.6020	0.3170
SA	0.9020	0.5890
SB	0.9210	0.5860
SC	0.8860	0.5890
SD	0.8630	0.5640
SE	0.9090	0.5910
SF	0.9030	0.5740
SG	0.7860	0.5220
SH	0.7330	0.4950
SI	0.8250	0.5530
SJ	0.9020	0.5850
SK	0.8710	0.5440
SL	0.9020	0.6060
SN	0.9250	0.5940
SO	0.9260	0.5980
SP	0.8690	0.5390
SQ	0.9140	0.5910
SR	0.7880	0.5280
SS	0.9210	0.5730
ST	0.9280	0.5890
SU	0.6930	0.5030
SV	0.8800	0.5800
SW	0.9510	0.6230
SX	0.9320	0.6060
SY	0.9000	0.5760
SZ	0.8630	0.5290
Sa	0.9390	0.5950
Sb	0.8410	0.5560
Sc	0.8740	0.5630

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Chain	Atom inclusion	Q-score
Sd	0.9590	0.6120
Se	0.8520	0.5610
Sg	0.7270	0.4590
mR	0.7960	0.4980