



Full wwPDB EM Validation Report ⓘ

Dec 15, 2024 – 08:43 PM EST

PDB ID : 6XA1
EMDB ID : EMD-22085
Title : Structure of a drug-like compound stalled human translation termination complex
Authors : Li, W.; Cate, J.
Deposited on : 2020-06-03
Resolution : 2.80 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:

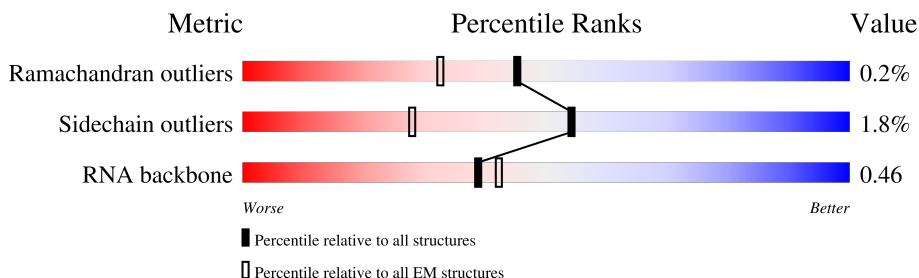
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	LA	248	
2	LB	396	
3	L5	3510	
4	L7	120	
5	L8	155	
6	LC	358	
7	LD	290	
8	LE	247	

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Mol	Chain	Length	Quality of chain
9	LF	225	7% 99%
10	LG	241	36% 98%
11	LH	190	24% 97%
12	LI	213	19% 97%
13	LJ	176	48% 97%
14	LL	204	21% 97%
15	LM	139	17% 99%
16	LN	203	97%
17	LO	201	10% 98%
18	LP	153	9% 99%
19	LQ	187	99%
20	LR	187	25% 94% 6%
21	LS	175	5% 97%
22	LT	159	20% 99%
23	LU	101	72% 99%
24	LV	131	11% 97%
25	LW	124	58% 99%
26	LX	120	23% 99%
27	LY	134	19% 97%
28	LZ	135	30% 96%
29	La	147	7% 98%
30	Lb	121	38% 88% 10%
31	Lc	98	20% 100%
32	Ld	107	16% 98%
33	Le	128	95% 5%

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Mol	Chain	Length	Quality of chain
34	Lf	109	
35	Lg	114	
36	Lh	122	
37	Li	102	
38	Lj	86	
39	Lk	69	
40	Ll	50	
41	Lm	52	
42	Ln	24	
43	Lo	105	
44	Lp	91	
45	Lr	125	
46	S2	1590	
47	SA	216	
48	SB	211	
49	SD	224	
50	SE	258	
51	SF	189	
52	SH	189	
53	SI	205	
54	SK	95	
55	SL	150	
56	SP	131	
57	SQ	140	
58	SR	131	

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Mol	Chain	Length	Quality of chain
59	SS	143	75% 99%
60	ST	141	71% 99%
61	SU	100	77% 99%
62	SV	84	63% 99%
63	SX	139	19% 99%
64	Sa	99	29% 98%
65	Sc	61	80% 98%
66	Sd	55	42% 100%
67	Sg	313	99% 98%
68	SC	220	34% 100%
69	SG	228	82% 98%
70	SJ	180	53% 99%
71	SM	120	93% 92% 7%
72	SN	150	37% 99%
73	SO	135	38% 97%
74	SW	129	19% 98%
75	SY	122	84% 99%
76	SZ	70	93% 99%
77	Sb	82	62% 100%
78	Se	54	52% 94% 6%
79	Sf	63	100% 97%
80	Bv	76	70% 38% 50% 11%
81	j	411	80% 78% 12% 9%
82	k	13	31% 46% 54%
83	NC	25	48% 92% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	B8N	S2	1248	X	-	-	-

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 211887 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 60S ribosomal protein L8.

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

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	LB	396	Total	C	N	O	S	0	0
			3197	2036	601	546	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3510	Total	C	N	O	P	0	0
			75317	33580	13769	24459	3509		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2562	1141	456	845	120		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	155	Total	C	N	O	P	0	0
			3298	1472	582	1089	155		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	358	Total	C	N	O	S	0	0
			2855	1797	570	473	15		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	290	Total	C	N	O	S	0	0
			2357	1493	428	422	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	207	Total	C	N	O	S	0	0
			1677	1064	323	276	14		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	204	Total	C	N	O	S	0	0
			1649	1032	343	270	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called 60S ribosomal protein L18a.

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

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called Heparin-binding protein HBp15.

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

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			882	549	192	137	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lb	89	ALA	VAL	conflict	UNP P47914

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lj	86	Total	C	N	O	S	1	0
			713	439	158	111	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	1	0
			870	547	178	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	1590	Total	C	N	O	P	0	0
			34012	15211	6116	11096	1589		

- Molecule 47 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SA	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 48 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SB	211	Total	C	N	O	S	0	0
			1718	1091	307	306	14		

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SD	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 50 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SE	258	Total	C	N	O	S	0	0
			2050	1311	381	350	8		

- Molecule 51 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 52 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SH	185	Total	C	N	O	S	0	0
			1490	953	272	264	1		

- Molecule 53 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SI	197	Total	C	N	O	S	0	0
			1624	1019	321	279	5		

- Molecule 54 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SK	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 55 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	140	Total	C	N	O	S	0	0
			1144	729	214	195	6		

- Molecule 56 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SP	131	Total	C	N	O	S	0	0
			1075	682	204	182	7		

- Molecule 57 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SQ	140	Total	C	N	O	S	0	0
			1117	710	211	193	3		

- Molecule 58 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SR	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 59 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SS	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 60 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	ST	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 61 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SU	100	Total	C	N	O	S	0	0
			798	501	152	141	4		

- Molecule 62 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SV	84	Total	C	N	O	S	0	0
			639	395	117	122	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SV	0	ACE	-	acetylation	UNP P63220

- Molecule 63 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SX	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 64 is a protein called 40S ribosomal protein S26.

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

- Molecule 65 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sc	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 66 is a protein called 40S ribosomal protein S29.

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

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

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

- Molecule 68 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SC	220	Total	C	N	O	S	1	0
			1715	1109	296	300	10		

- Molecule 69 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SG	228	Total	C	N	O	S	0	0
			1848	1155	368	318	7		

- Molecule 70 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 71 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SM	112	Total	C	N	O	S	0	0
			860	540	149	163	8		

- Molecule 72 is a protein called 40S ribosomal protein S13.

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

- Molecule 73 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SO	138	IAS	ASP	conflict	UNP P62263

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

- Molecule 75 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SY	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 76 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SZ	70	Total	C	N	O	S	0	0
			559	360	102	96	1		

- Molecule 77 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sb	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Se	51	Total	C	N	O	S	0	0
			407	251	90	65	1		

- Molecule 79 is a protein called 40S ribosomal protein S27a.

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

- Molecule 80 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bv	75	Total	C	N	O	P	0	0
			1621	725	289	532	75		

- Molecule 81 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	j	373	Total	C	N	O	S	0	0
			2930	1874	500	547	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	63	UXY	LYS	conflict	UNP P62495

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	k	13	Total	C	N	O	P	0	0
			270	122	44	91	13		

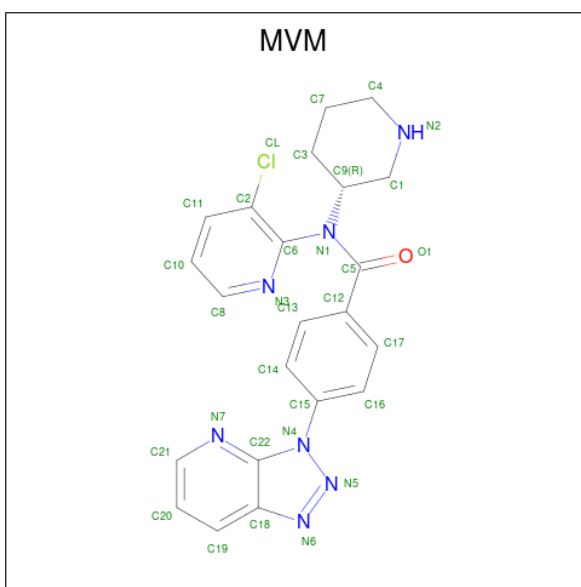
- Molecule 83 is a protein called Stalled Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	NC	25	Total	C	N	O	0	0
			177	121	28	28		

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	L5	145	Total	Mg	0
			145	145	
84	L7	5	Total	Mg	0
			5	5	
84	L8	2	Total	Mg	0
			2	2	
84	S2	35	Total	Mg	0
			35	35	
84	Bv	2	Total	Mg	0
			2	2	
84	k	1	Total	Mg	0
			1	1	

- Molecule 85 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (three-letter code: MVM) (formula: C₂₂H₂₀ClN₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
85	L5	1	Total	C	Cl	N	O	0
			31	22	1	7	1	

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

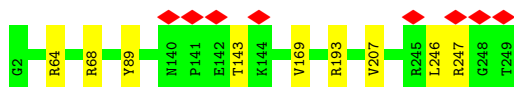
Mol	Chain	Residues	Atoms		AltConf
87	Bv	2	Total	K	0
			2	2	

3 Residue-property plots

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

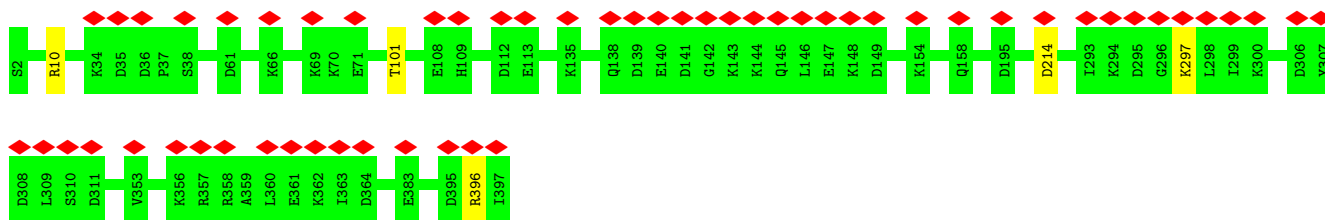
- Molecule 1: 60S ribosomal protein L8

Chain LA:  96%



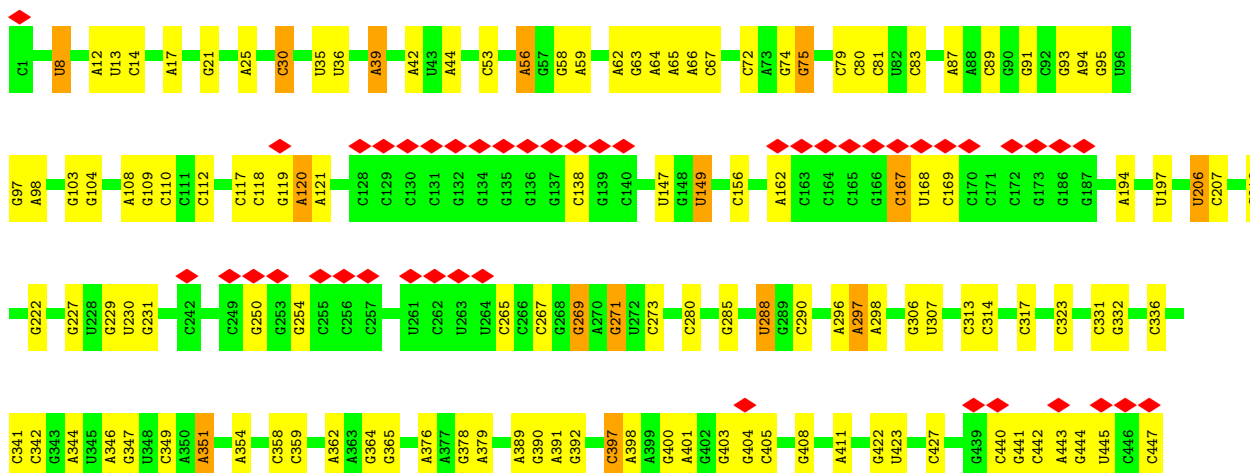
- Molecule 2: 60S ribosomal protein L3

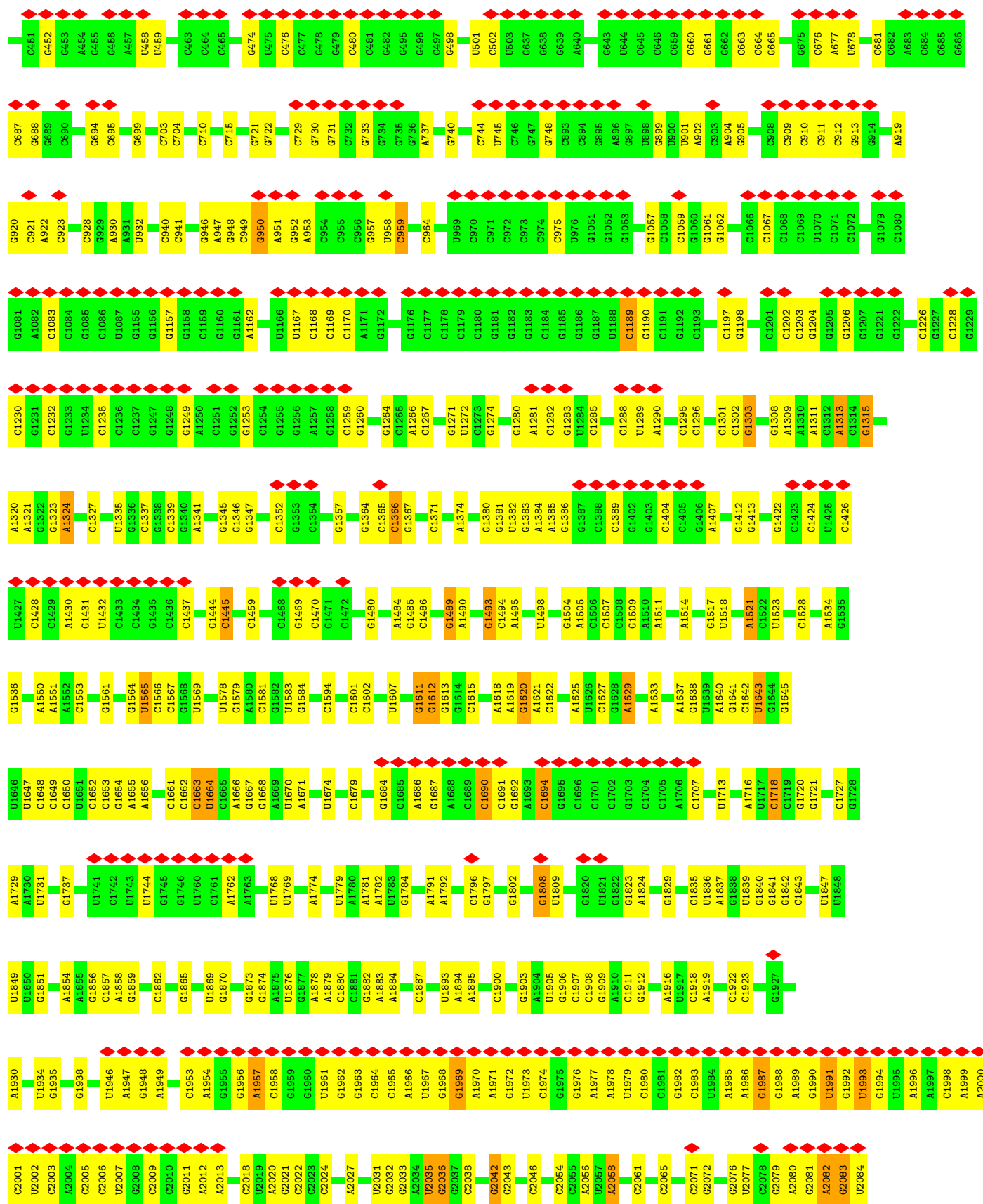
Chain LB:  14% 99%

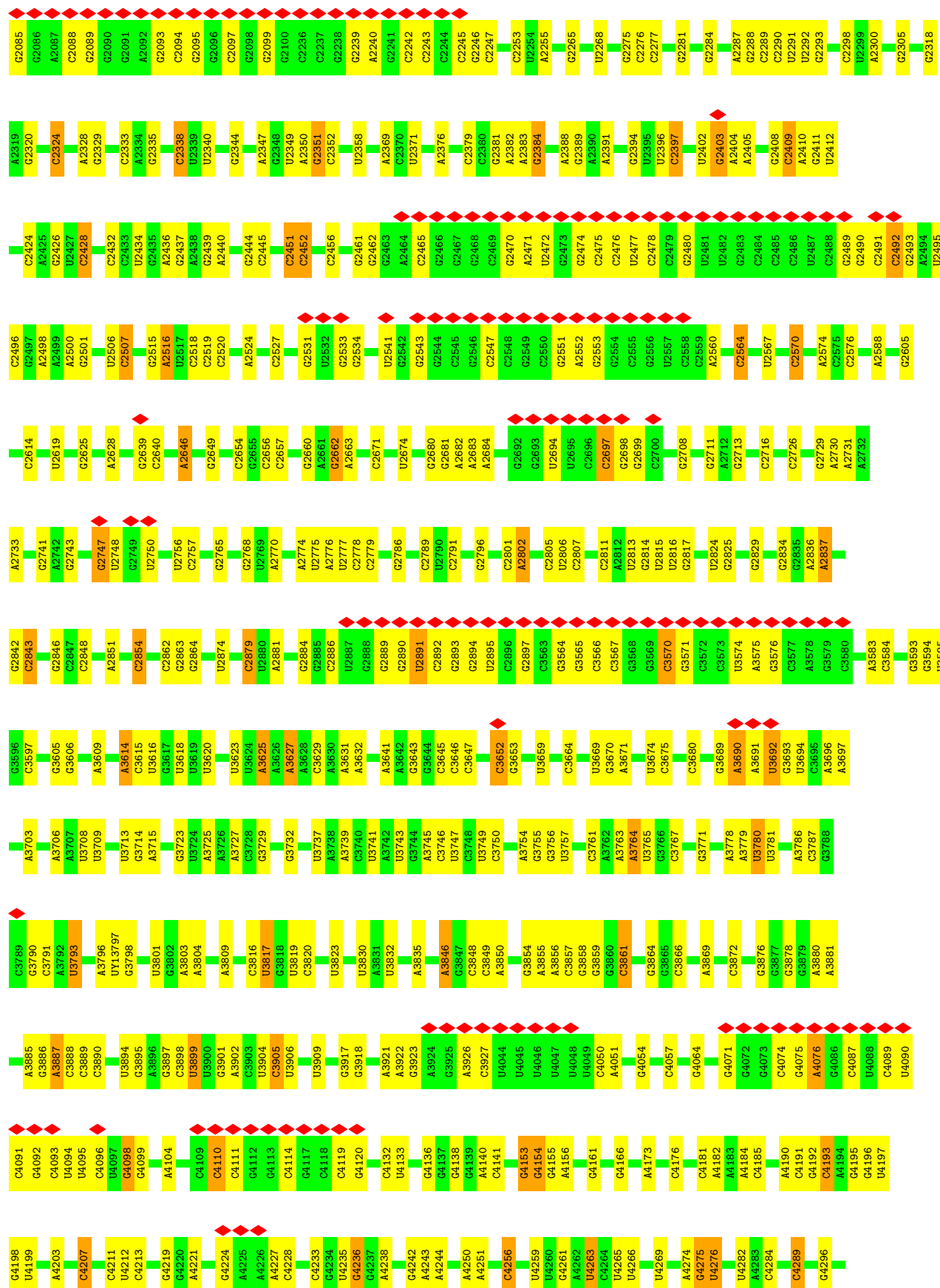


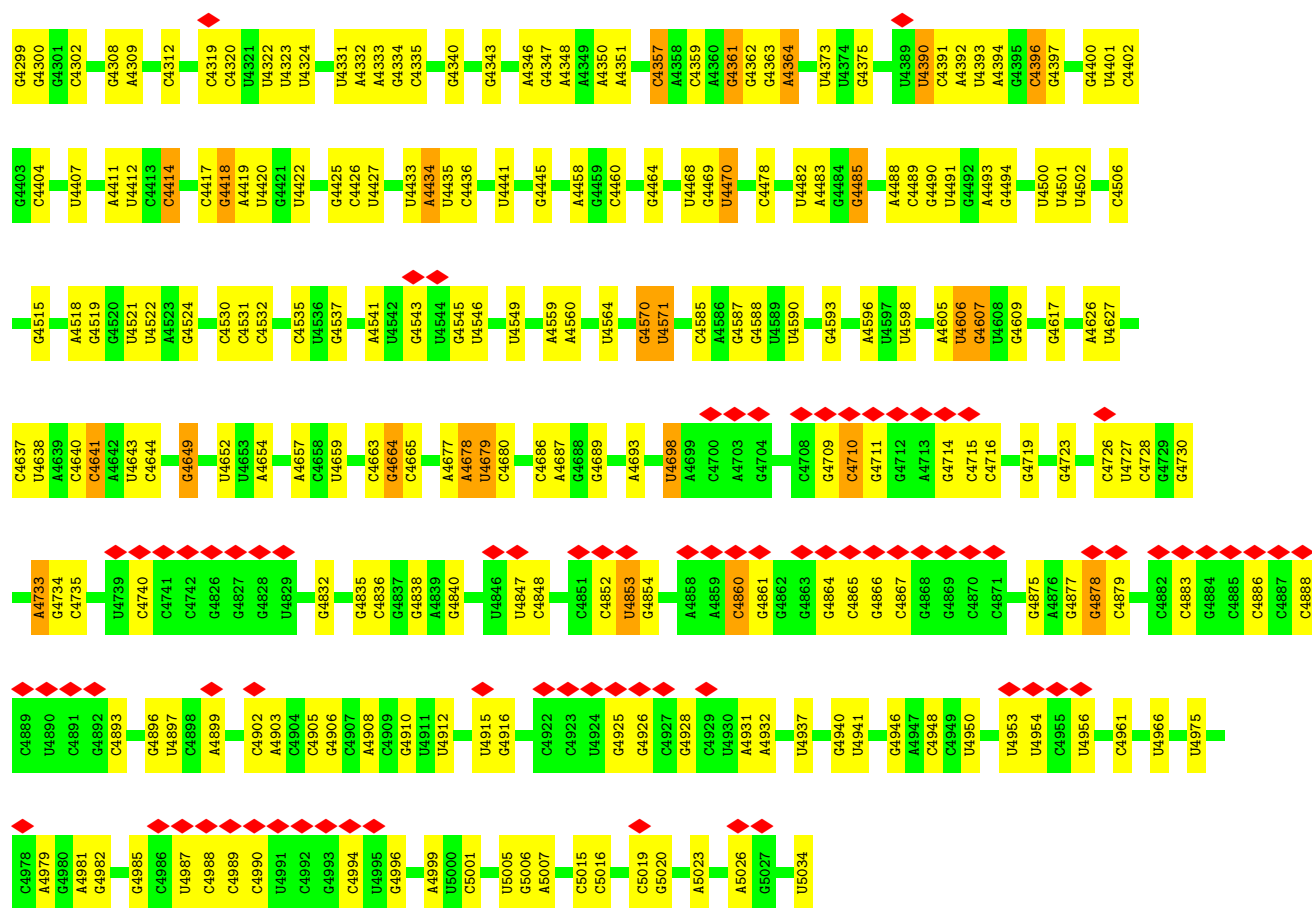
- Molecule 3: 28S rRNA

Chain L5:  17% 65% 32%

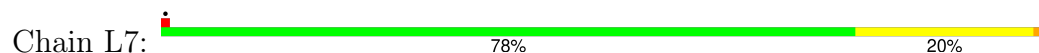




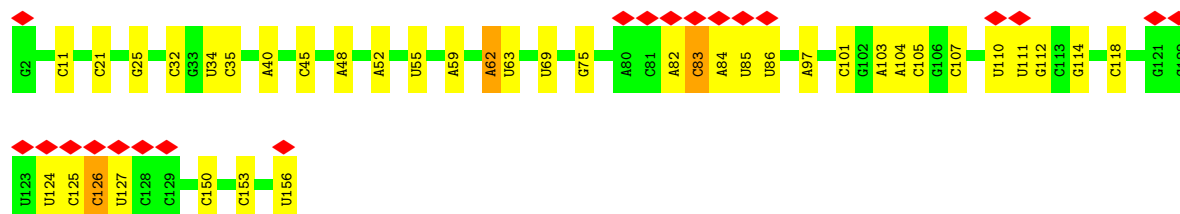
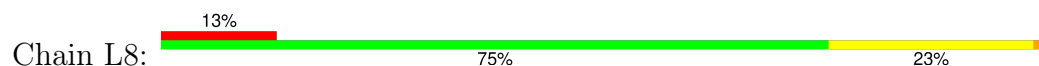




• Molecule 4: 5S rRNA



• Molecule 5: 5.8S rRNA

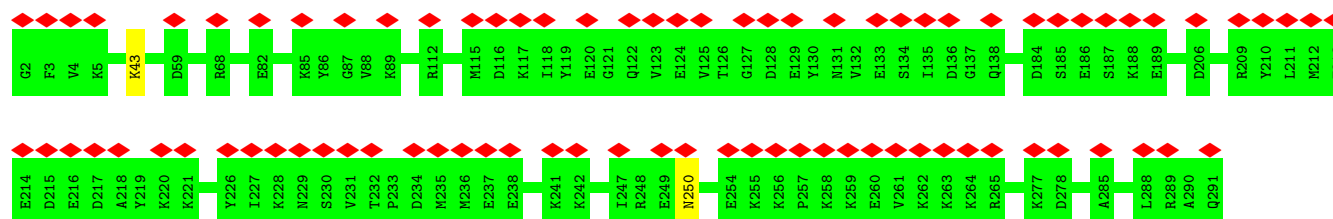


• Molecule 6: 60S ribosomal protein L4





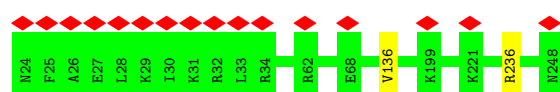
• Molecule 7: 60S ribosomal protein L5



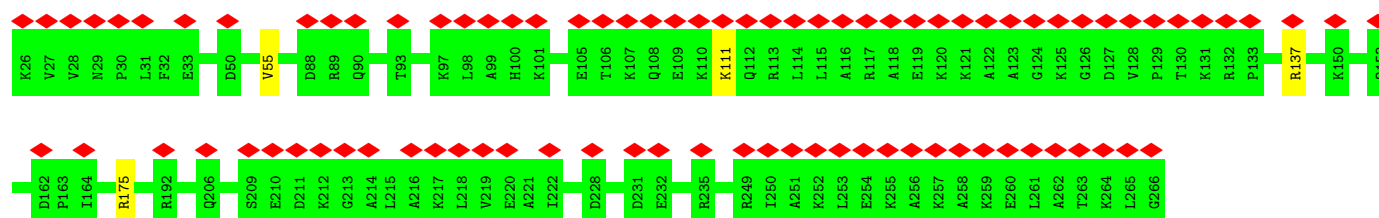
• Molecule 8: 60S ribosomal protein L6



• Molecule 9: 60S ribosomal protein L7

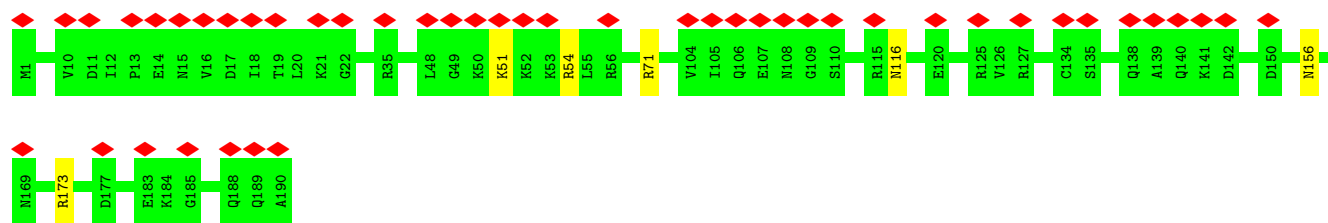


• Molecule 10: 60S ribosomal protein L7a



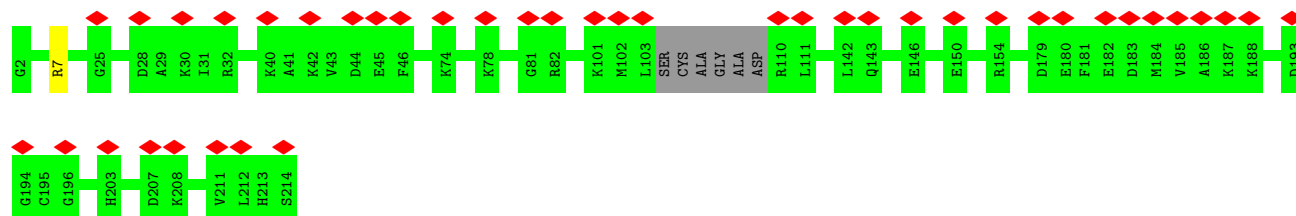
• Molecule 11: 60S ribosomal protein L9





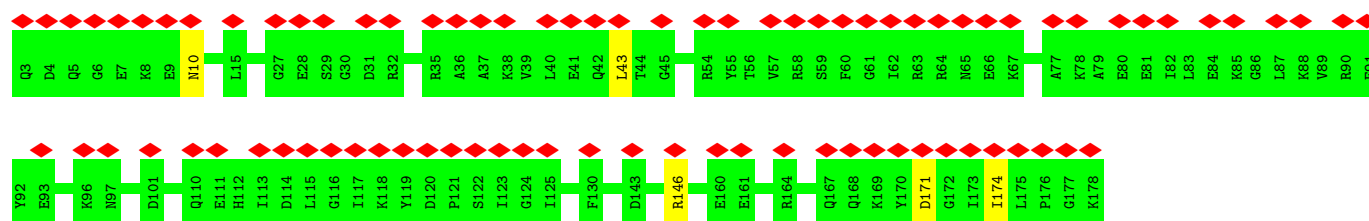
- Molecule 12: 60S ribosomal protein L10-like

Chain LI: 19% 97%



- Molecule 13: 60S ribosomal protein L11

Chain LJ: 48% 97%



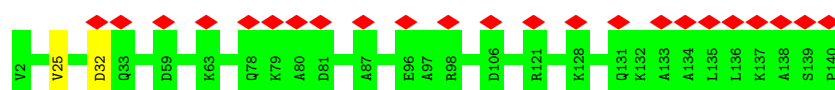
- Molecule 14: 60S ribosomal protein L13

Chain LL: 21% 97%



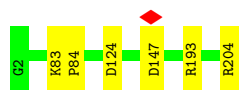
- Molecule 15: 60S ribosomal protein L14

Chain LM: 17% 99%



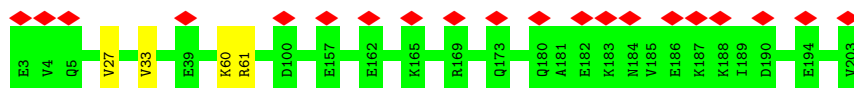
- Molecule 16: 60S ribosomal protein L15

Chain LN:  97%



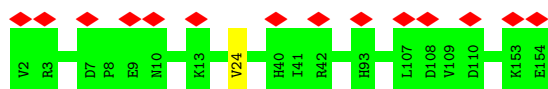
- Molecule 17: 60S ribosomal protein L13a

Chain LO:  98%



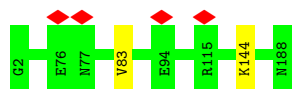
- Molecule 18: 60S ribosomal protein L17

Chain LP:  99%



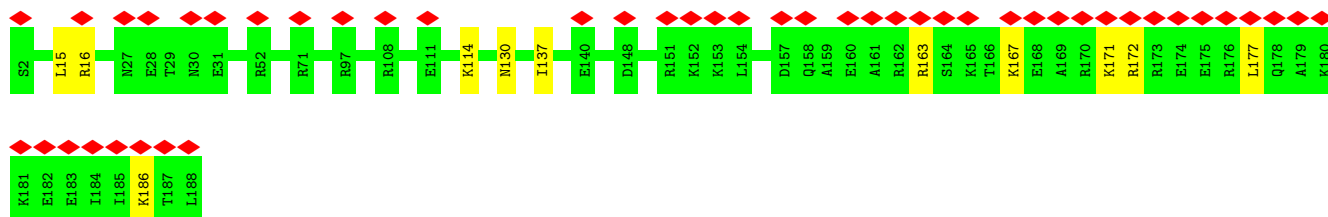
- Molecule 19: 60S ribosomal protein L18

Chain LQ:  99%



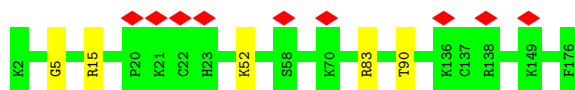
- Molecule 20: 60S ribosomal protein L19

Chain LR:  94%



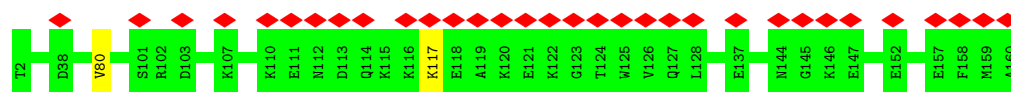
- Molecule 21: 60S ribosomal protein L18a

Chain LS:  97%



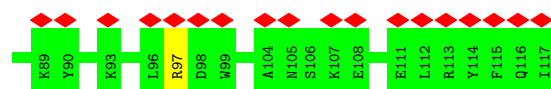
- Molecule 22: 60S ribosomal protein L21

Chain LT:  99%



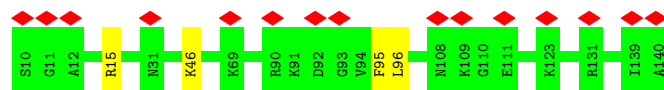
- Molecule 23: Heparin-binding protein HBp15

Chain LU: 72% 99%



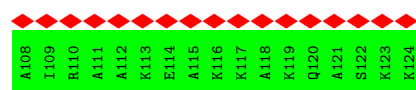
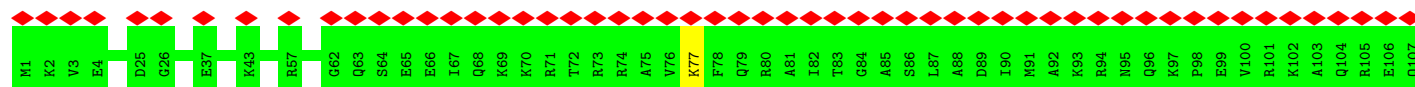
- Molecule 24: 60S ribosomal protein L23

Chain LV: 11% 97%



- Molecule 25: 60S ribosomal protein L24

Chain LW: 58% 99%



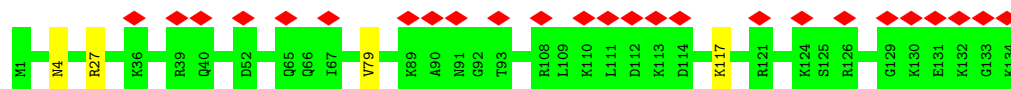
- Molecule 26: 60S ribosomal protein L23a

Chain LX: 23% 99%

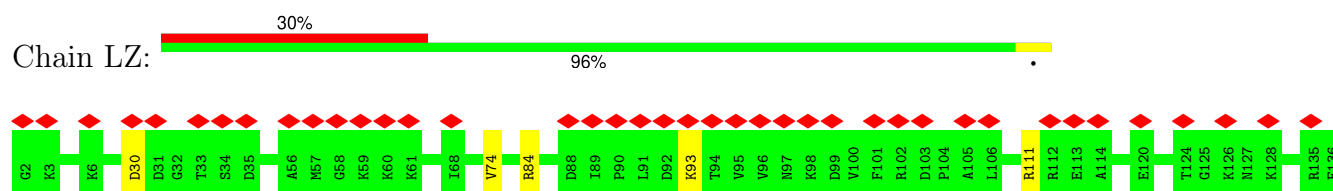


- Molecule 27: 60S ribosomal protein L26

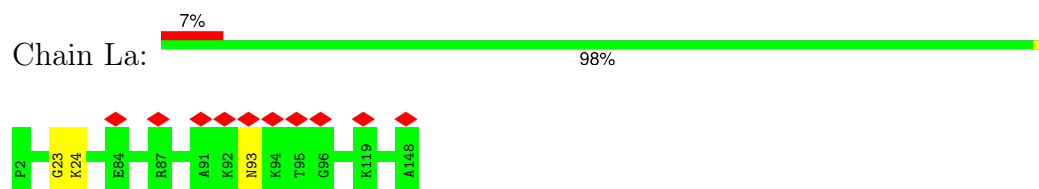
Chain LY: 19% 97%



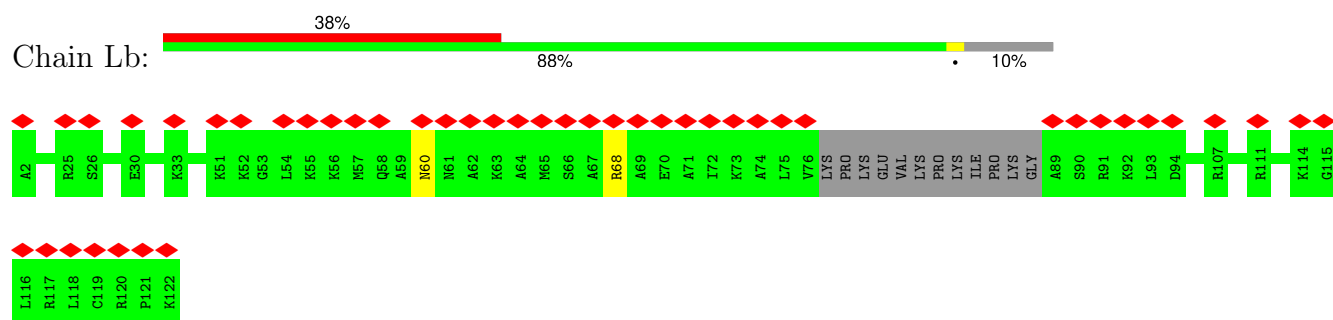
- Molecule 28: 60S ribosomal protein L27



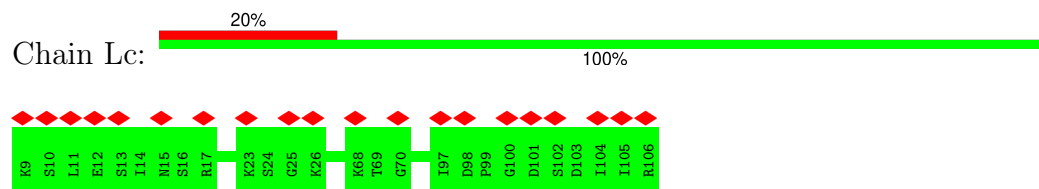
- Molecule 29: 60S ribosomal protein L27a



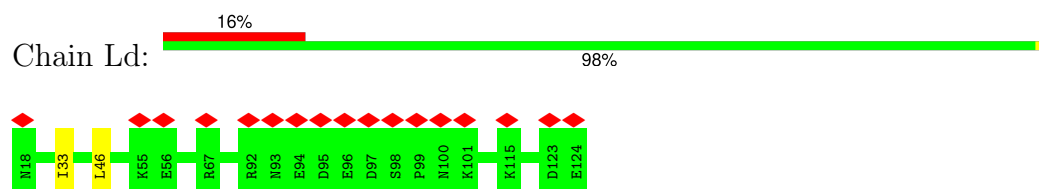
- Molecule 30: 60S ribosomal protein L29



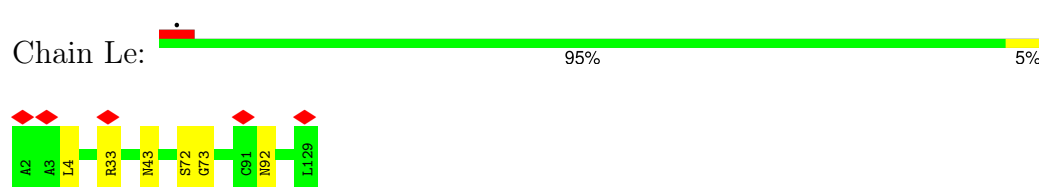
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31

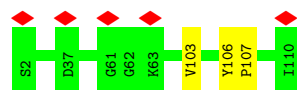


- Molecule 33: 60S ribosomal protein L32

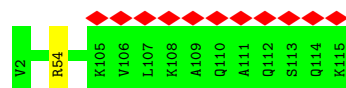


- Molecule 34: 60S ribosomal protein L35a

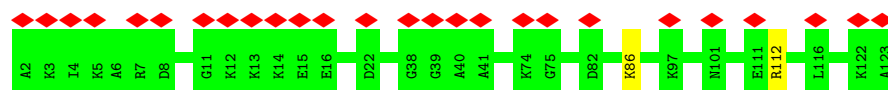




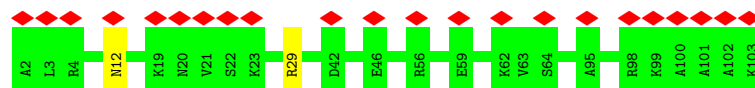
- Molecule 35: 60S ribosomal protein L34



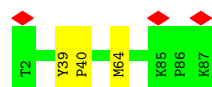
- Molecule 36: 60S ribosomal protein L35



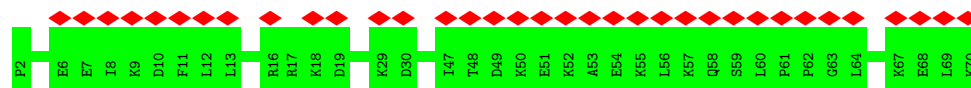
- Molecule 37: 60S ribosomal protein L36



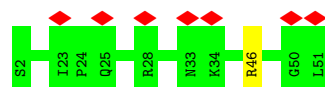
- Molecule 38: 60S ribosomal protein L37



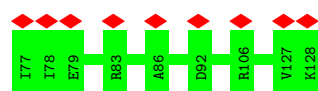
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



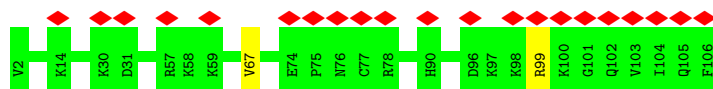
- Molecule 41: 60S ribosomal protein L40



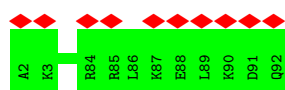
- Molecule 42: 60S ribosomal protein L41



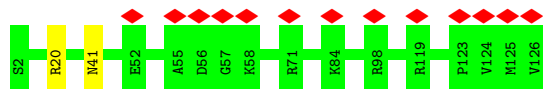
- Molecule 43: 60S ribosomal protein L36a



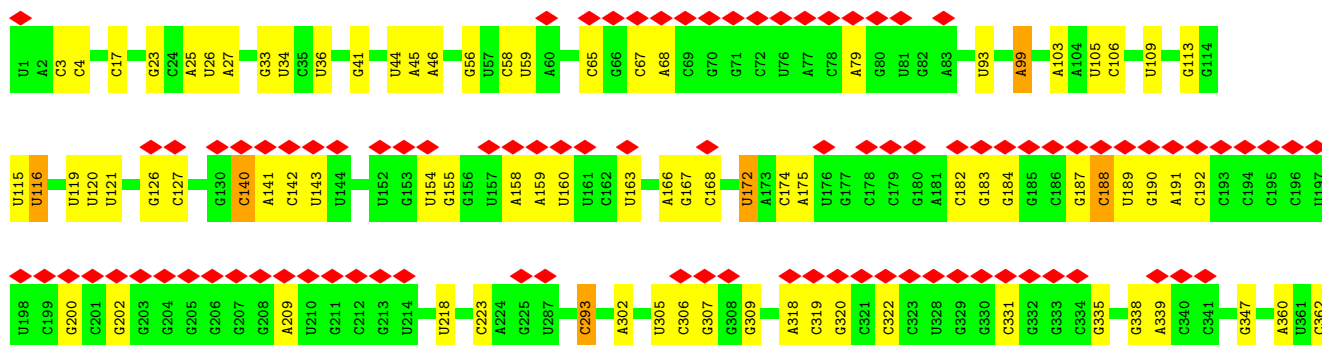
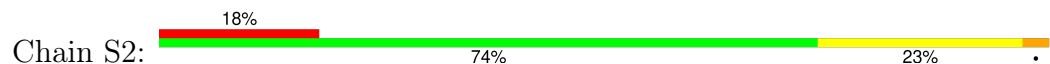
- Molecule 44: 60S ribosomal protein L37a

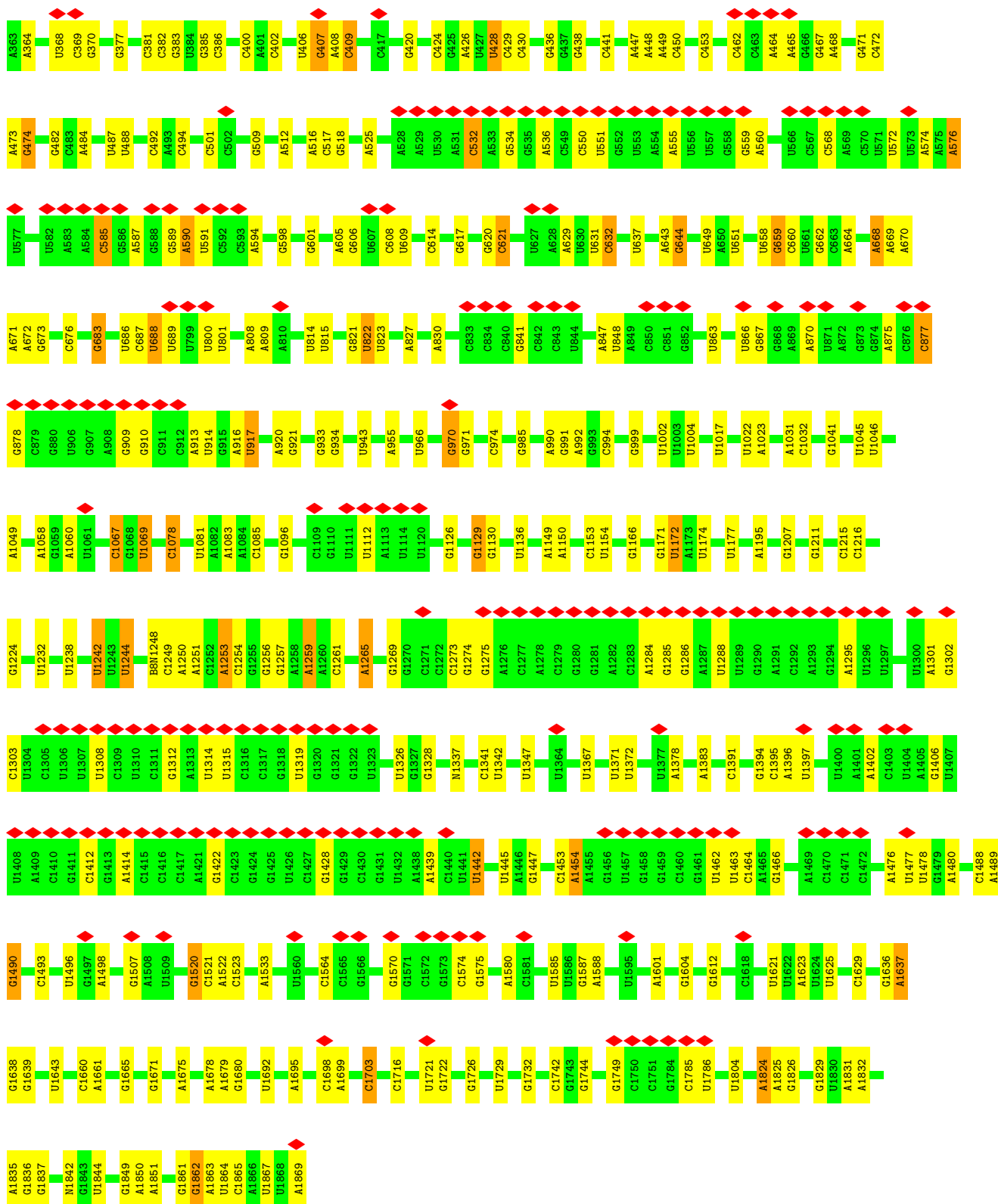


- Molecule 45: 60S ribosomal protein L28



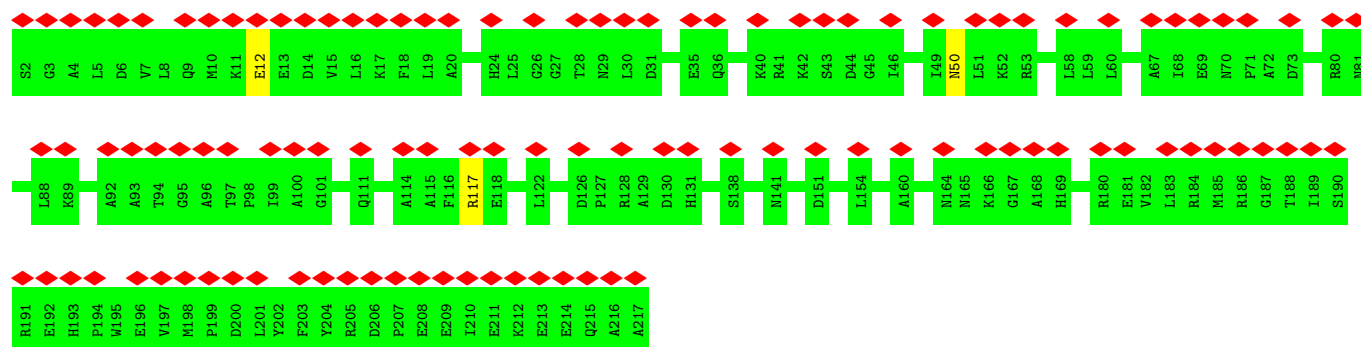
- Molecule 46: 18S rRNA



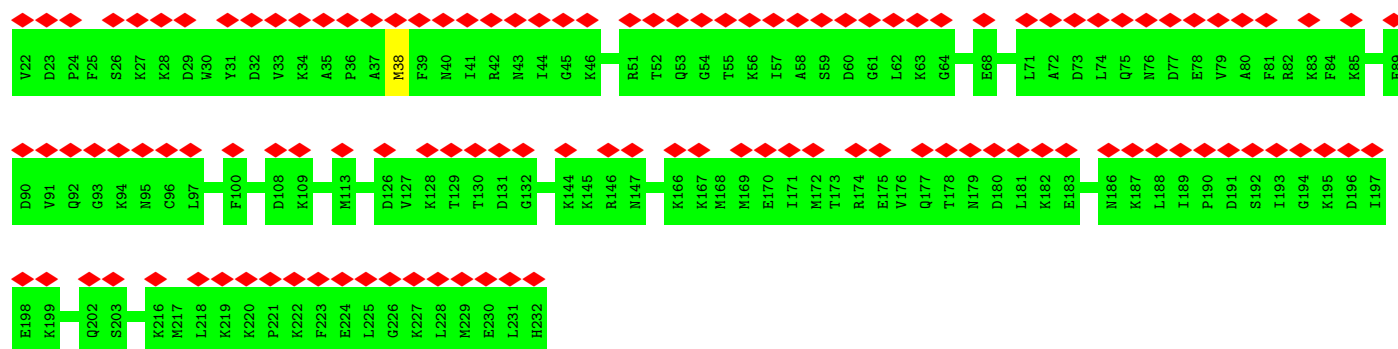


• Molecule 47: 40S ribosomal protein SA

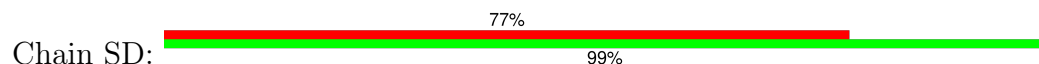




• Molecule 48: 40S ribosomal protein S3a

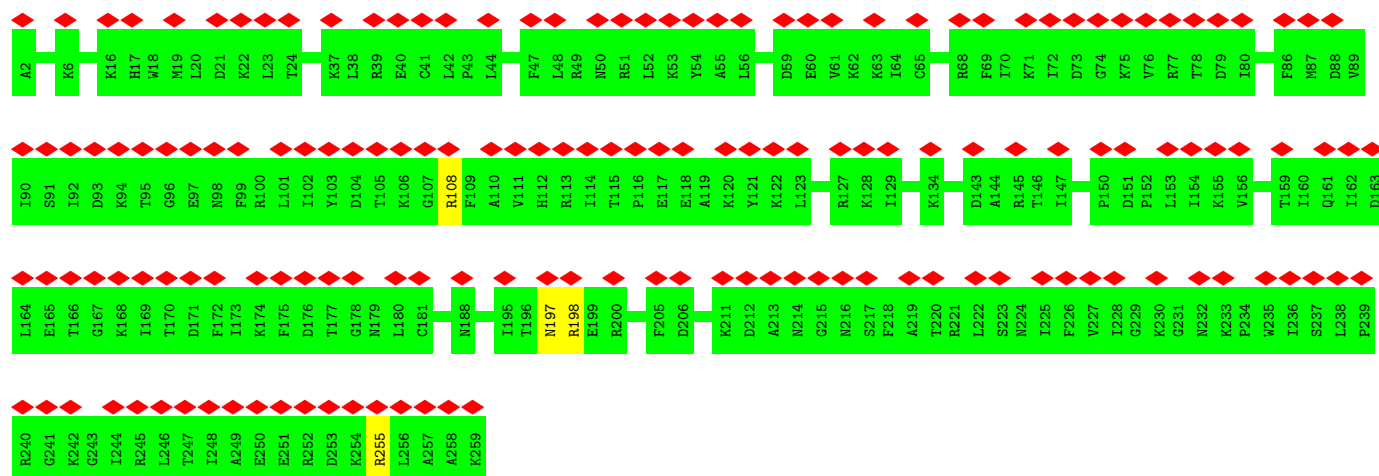


• Molecule 49: 40S ribosomal protein S3



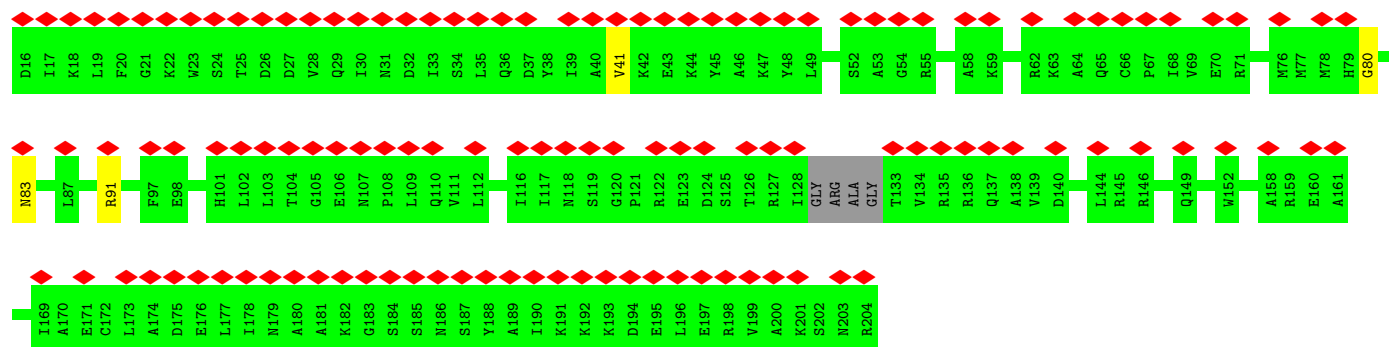
• Molecule 50: 40S ribosomal protein S4, X isoform





• Molecule 51: 40S ribosomal protein S5

Chain SF: 66% 96%



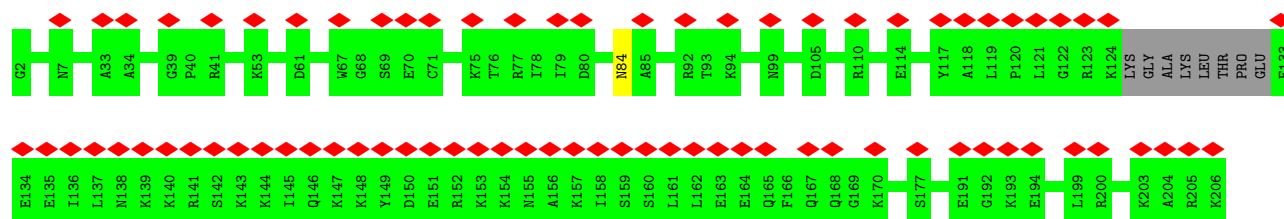
• Molecule 52: 40S ribosomal protein S7

Chain SH: 80% 95%

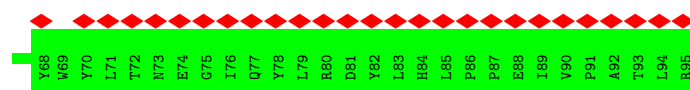
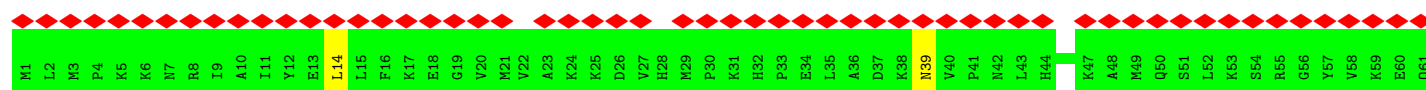


• Molecule 53: 40S ribosomal protein S8

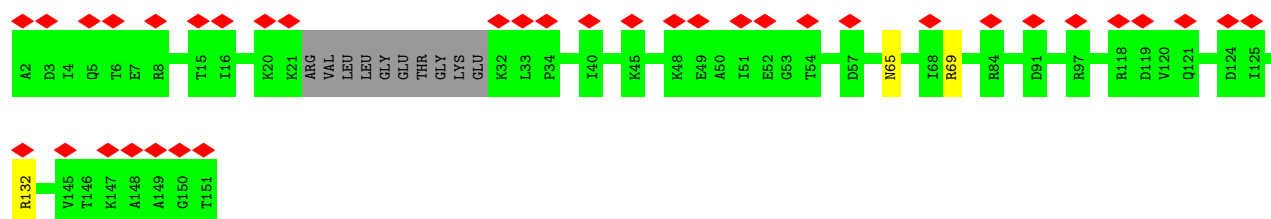
Chain SI: 38% 96%



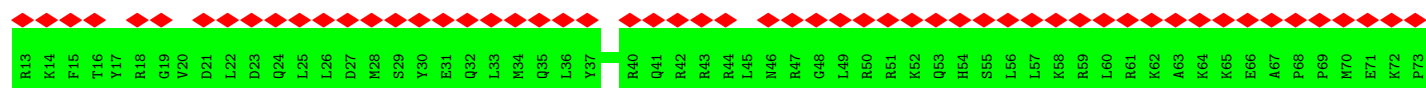
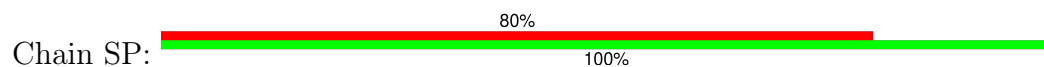
• Molecule 54: 40S ribosomal protein S10



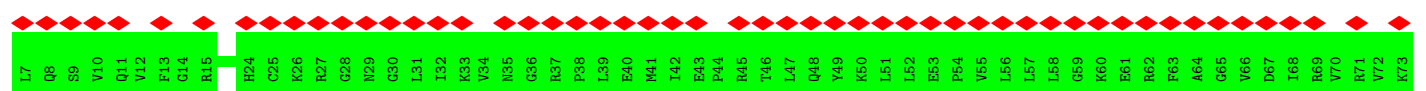
• Molecule 55: 40S ribosomal protein S11

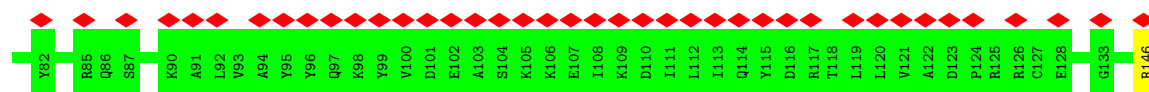


• Molecule 56: 40S ribosomal protein S15

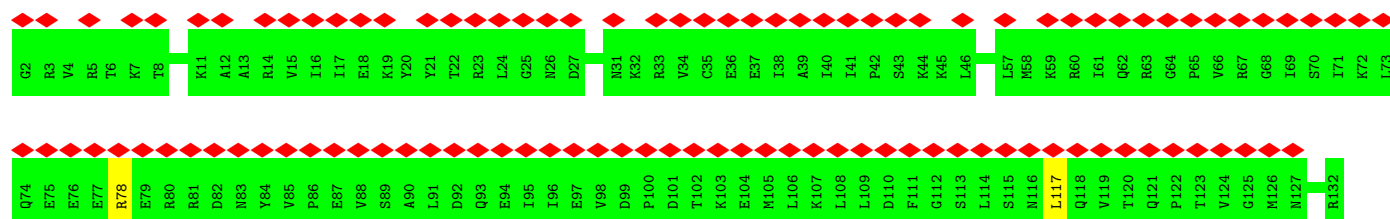
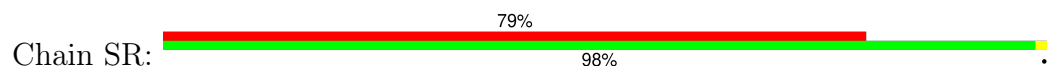


• Molecule 57: 40S ribosomal protein S16

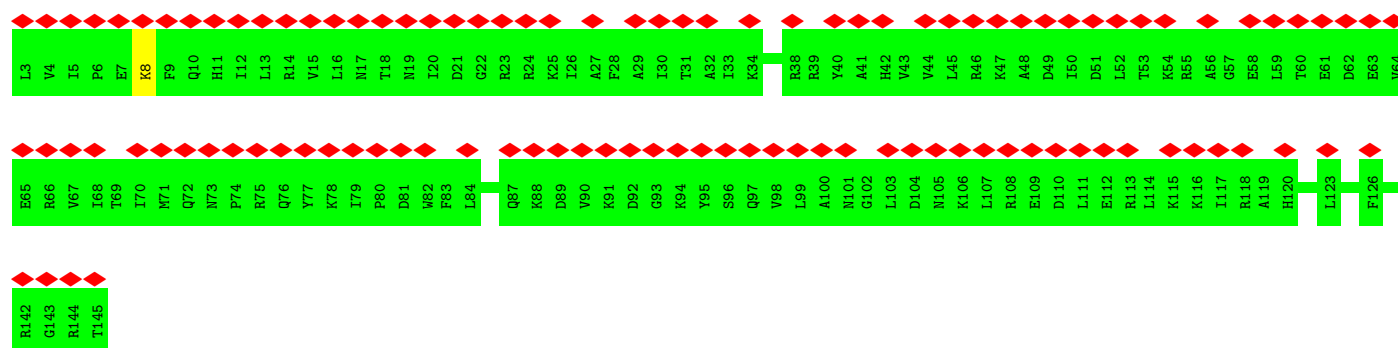
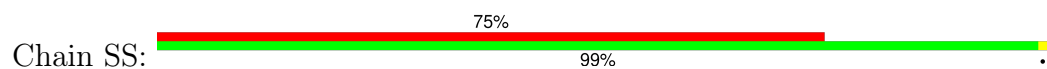




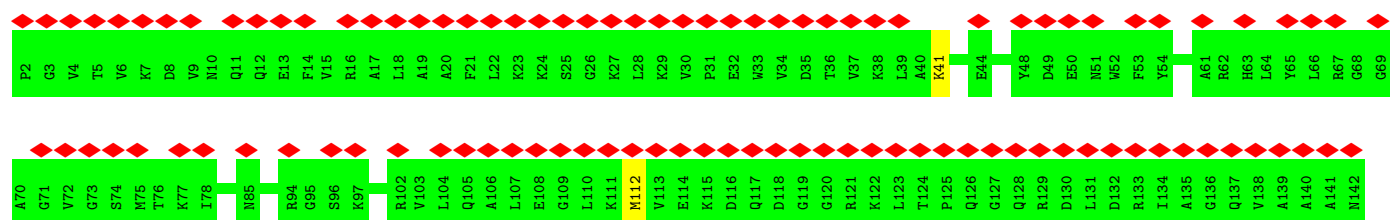
- Molecule 58: 40S ribosomal protein S17



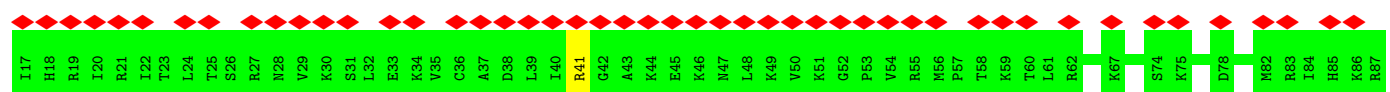
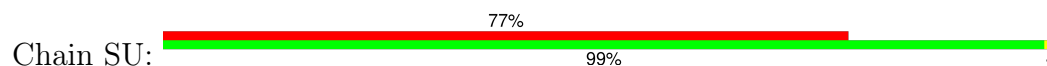
- Molecule 59: 40S ribosomal protein S18



- Molecule 60: 40S ribosomal protein S19



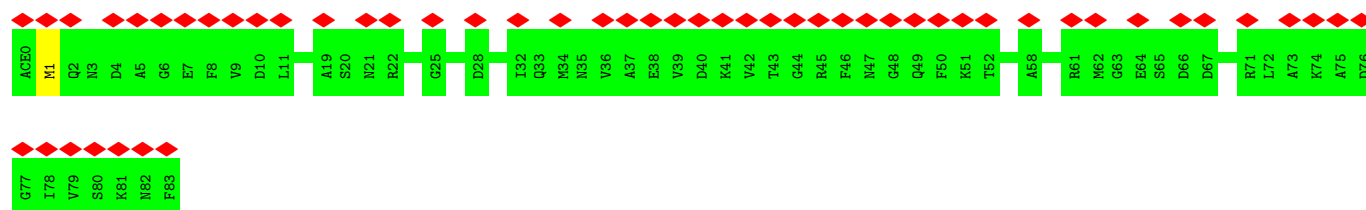
- Molecule 61: 40S ribosomal protein S20





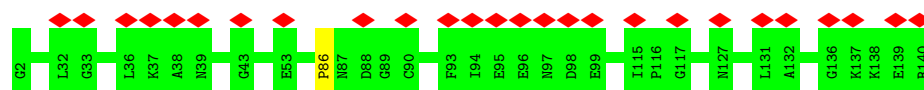
- Molecule 62: 40S ribosomal protein S21

Chain SV: 63% 99%



- Molecule 63: 40S ribosomal protein S23

Chain SX: 19% 99%



- Molecule 64: 40S ribosomal protein S26

Chain Sa: 29% 98%



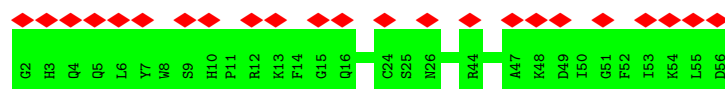
- Molecule 65: 40S ribosomal protein S28

Chain Sc: 80% 98%



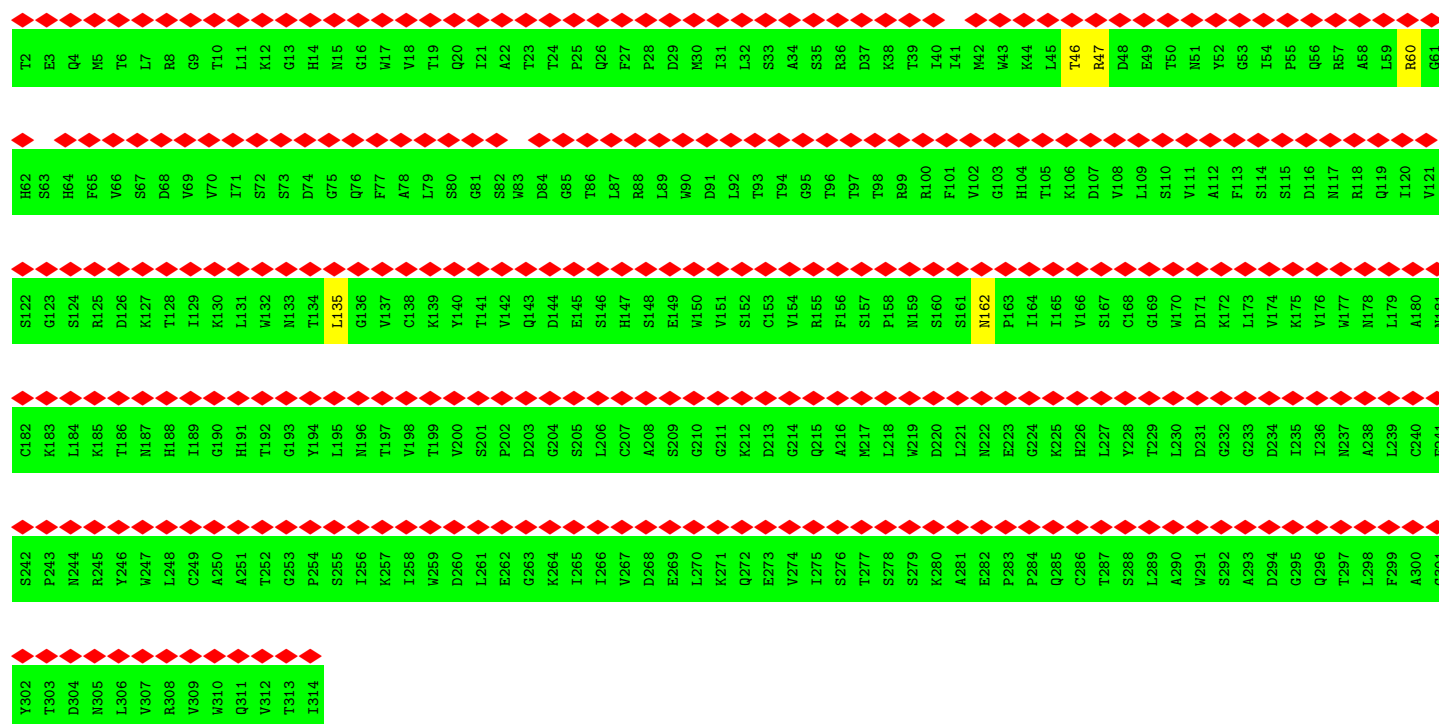
- Molecule 66: 40S ribosomal protein S29

Chain Sd: 42% 100%

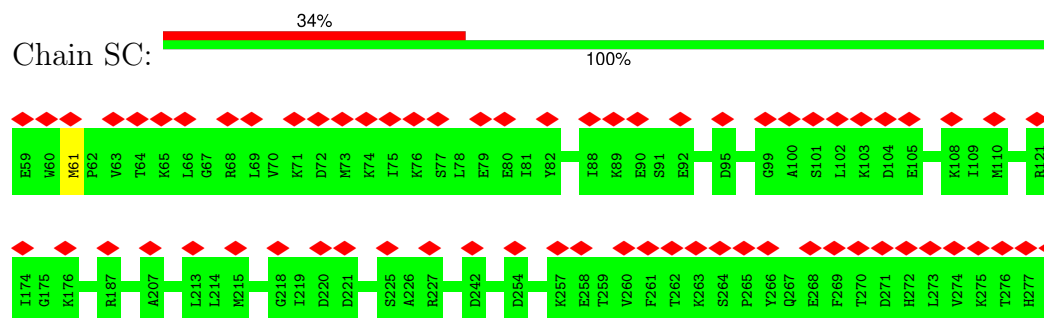


- Molecule 67: Receptor of activated protein C kinase 1

Chain Sg: 99% 98%



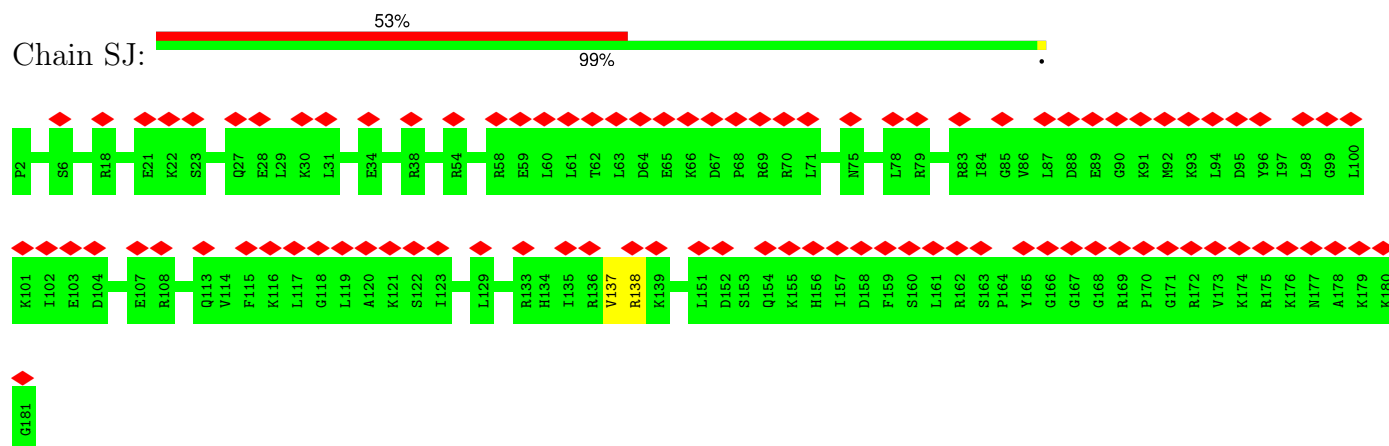
• Molecule 68: 40S ribosomal protein S2



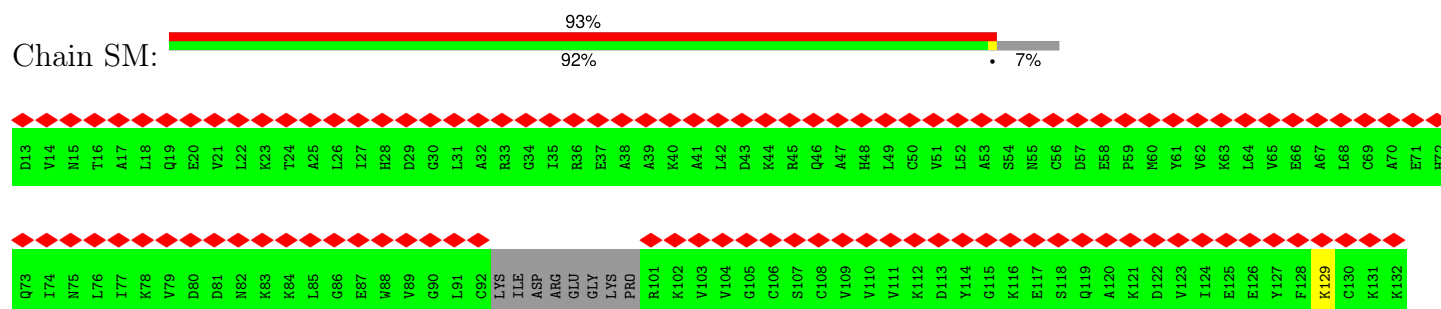
• Molecule 69: 40S ribosomal protein S6



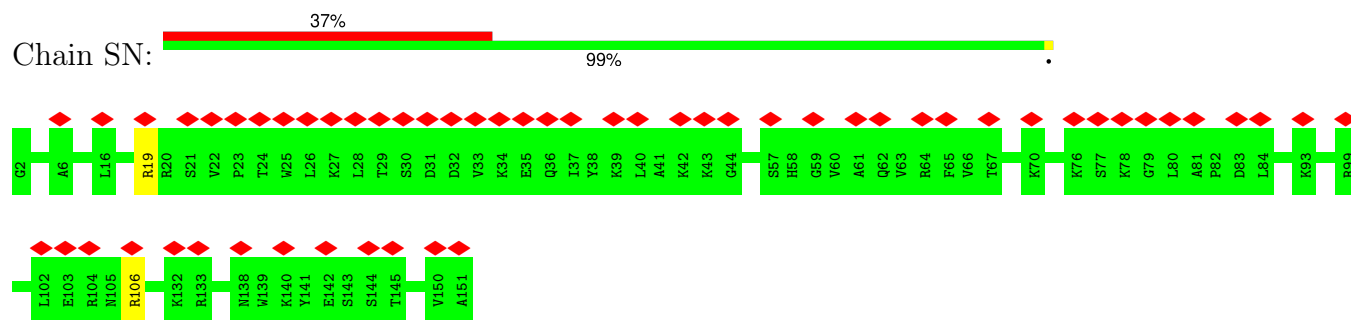
- Molecule 70: 40S ribosomal protein S9



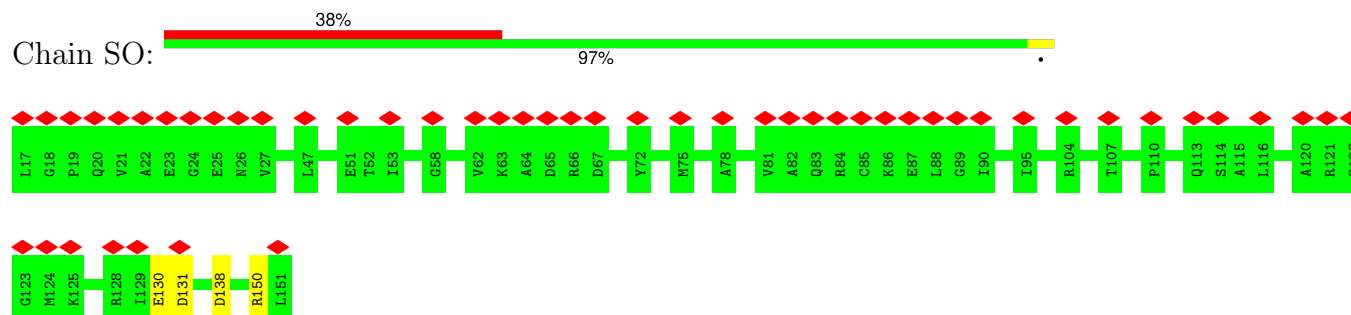
- Molecule 71: 40S ribosomal protein S12



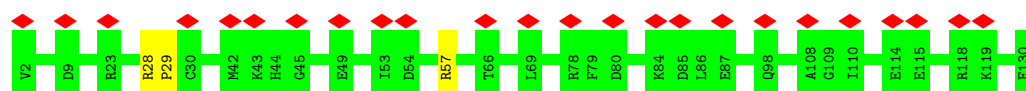
- Molecule 72: 40S ribosomal protein S13



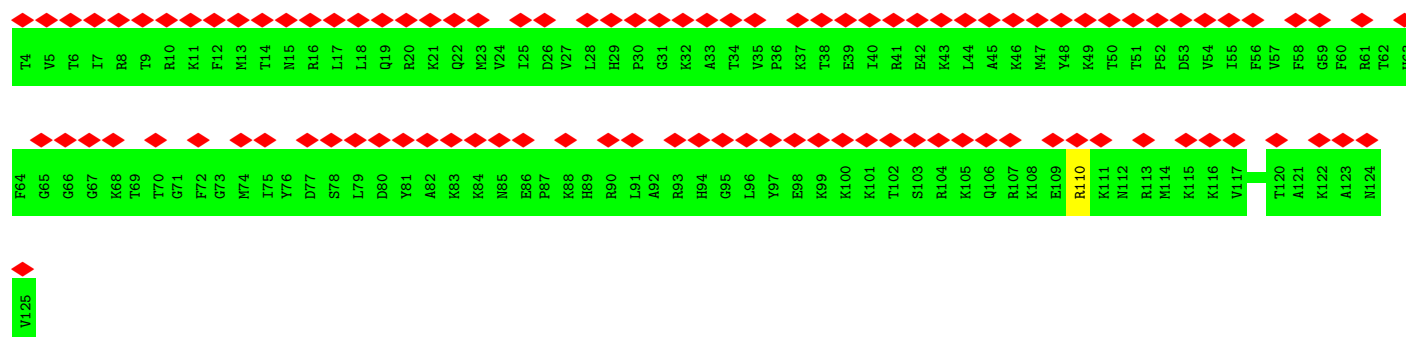
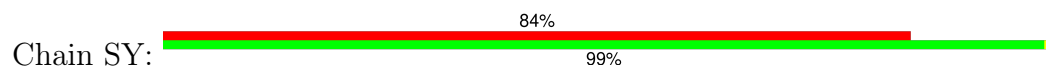
- Molecule 73: 40S ribosomal protein S14



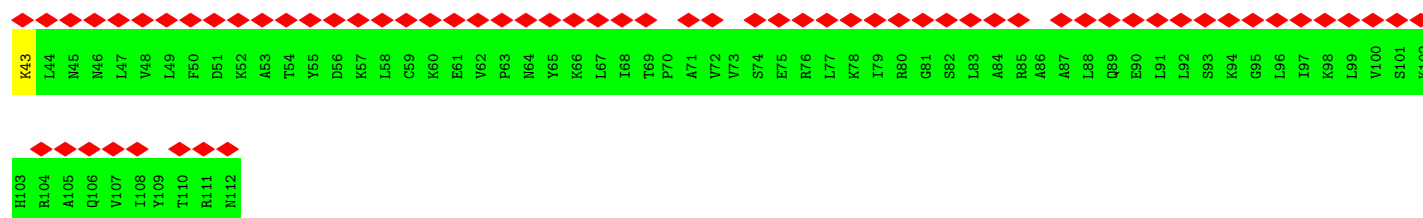
- Molecule 74: 40S ribosomal protein S15a



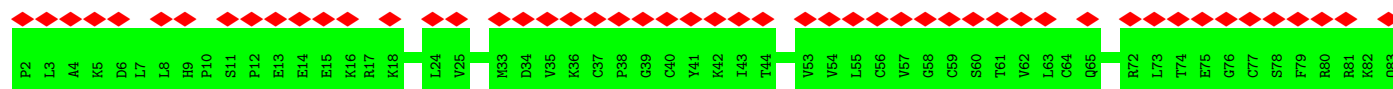
- Molecule 75: 40S ribosomal protein S24



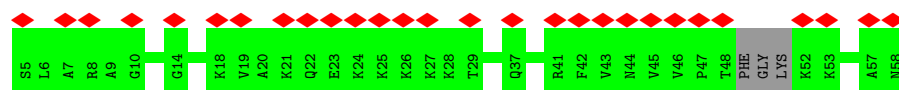
- Molecule 76: 40S ribosomal protein S25



- Molecule 77: 40S ribosomal protein S27

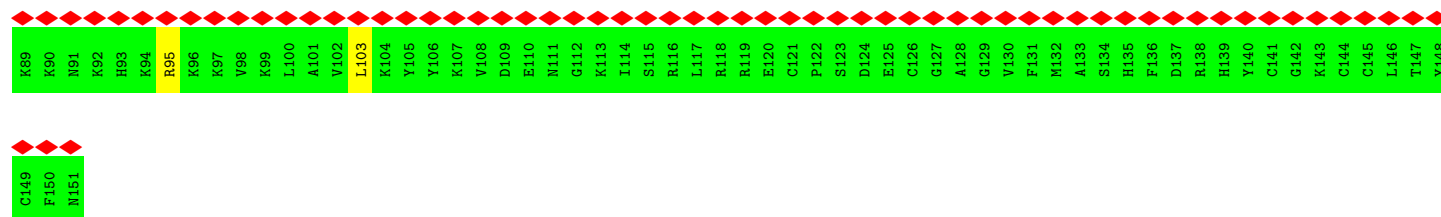


- Molecule 78: 40S ribosomal protein S30



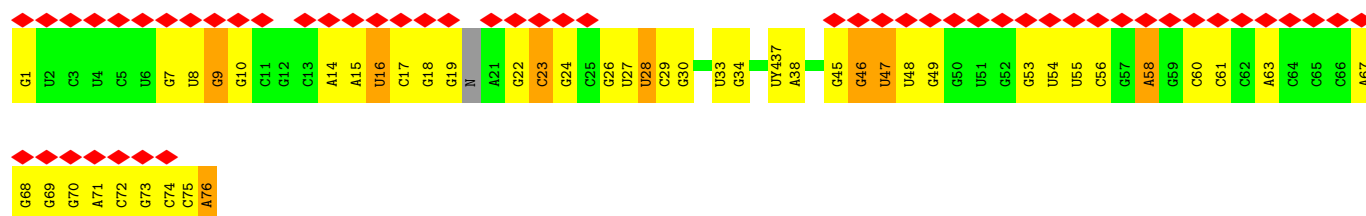
- Molecule 79: 40S ribosomal protein S27a





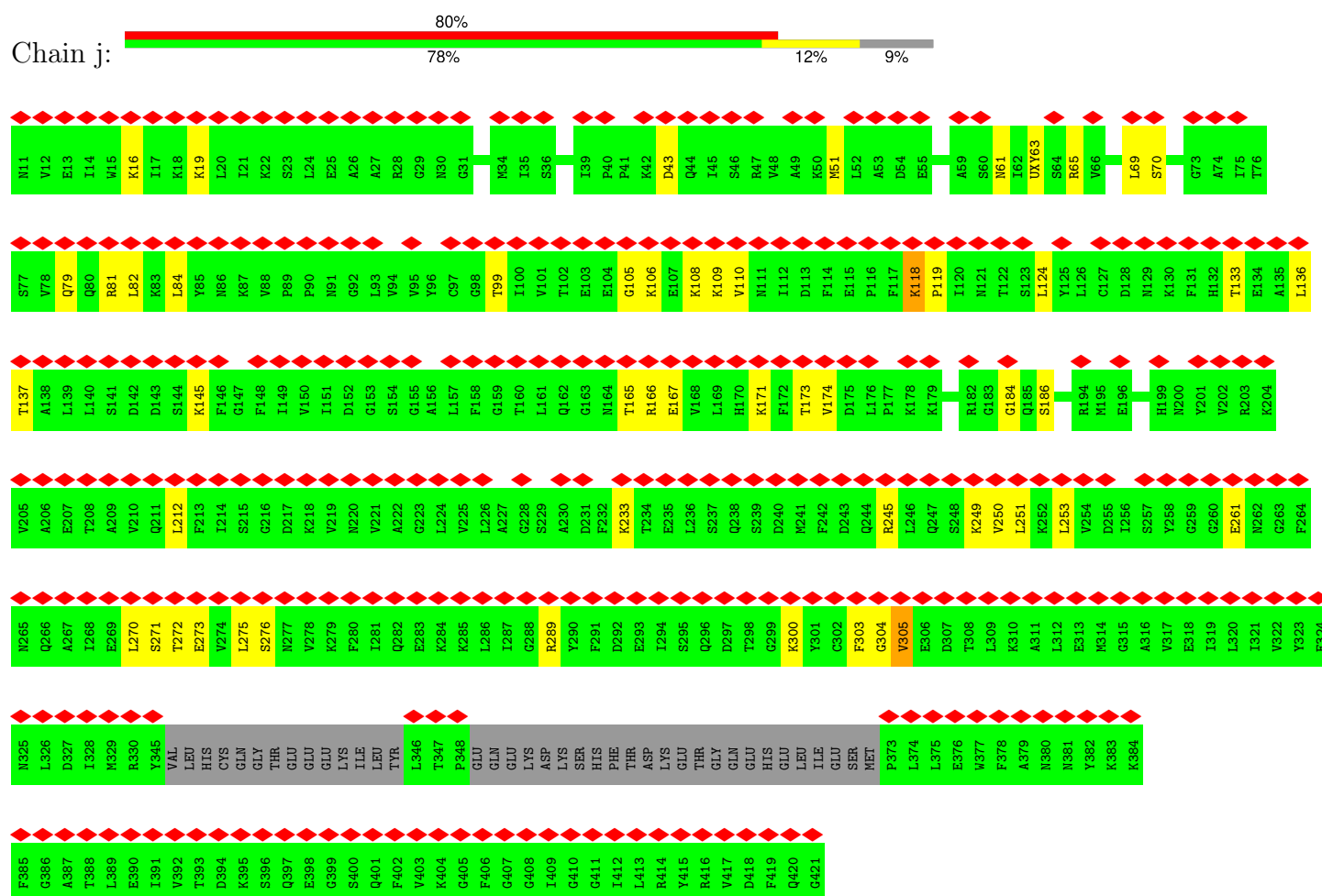
- Molecule 80: P-tRNA

Chain Bv:

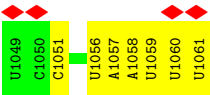


- Molecule 81: Eukaryotic peptide chain release factor subunit 1

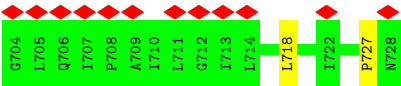
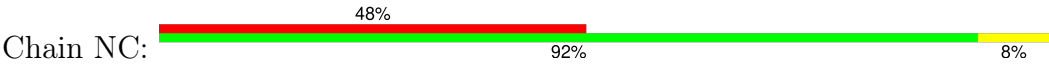
Chain j:



- Molecule 82: mRNA



● Molecule 83: Stalled Nascent chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.260	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	494.5, 494.5, 494.5	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.15, 1.15, 1.15	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, 6MZ, MEQ, UR3, OMC, ZN, ACE, 1MG, OMG, 2MG, M2G, K, MG, A2M, MA6, UY1, B8N, PSU, OMU, H2U, UY4, MVM, 1MA, 4AC, G7M, 5MC, IAS, UXY

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	LA	0.80	1/1936 (0.1%)	0.75	0/2596
2	LB	0.74	0/3265	0.70	1/4370 (0.0%)
3	L5	1.67	159/81383 (0.2%)	1.48	579/126935 (0.5%)
4	L7	1.57	2/2862 (0.1%)	1.17	14/4459 (0.3%)
5	L8	1.55	1/3612 (0.0%)	1.18	17/5627 (0.3%)
6	LC	0.72	0/2898	0.66	0/3891
7	LD	0.67	0/2403	0.61	0/3219
8	LE	0.61	0/1942	0.68	1/2606 (0.0%)
9	LF	0.77	0/1916	0.72	1/2553 (0.0%)
10	LG	0.66	1/1971 (0.1%)	0.70	0/2651
11	LH	0.67	0/1537	0.67	0/2066
12	LI	0.65	0/1716	0.63	0/2291
13	LJ	0.62	0/1433	0.76	2/1915 (0.1%)
14	LL	0.67	0/1680	0.72	1/2249 (0.0%)
15	LM	0.67	0/1161	0.66	0/1554
16	LN	0.86	0/1746	0.78	1/2338 (0.0%)
17	LO	0.80	2/1682 (0.1%)	0.71	0/2250
18	LP	0.75	0/1268	0.68	0/1701
19	LQ	0.77	0/1537	0.71	0/2052
20	LR	0.64	0/1582	0.68	2/2091 (0.1%)
21	LS	0.75	0/1493	0.63	0/2003
22	LT	0.76	0/1326	0.64	0/1770
23	LU	0.54	0/839	0.71	0/1126
24	LV	0.70	0/993	0.75	1/1332 (0.1%)
25	LW	0.61	0/1030	0.65	0/1364
26	LX	0.63	0/1002	0.63	1/1345 (0.1%)
27	LY	0.70	0/1132	0.71	0/1504
28	LZ	0.70	0/1130	0.69	1/1507 (0.1%)
29	La	0.79	0/1191	0.68	0/1591
30	Lb	0.60	0/895	0.64	0/1182
31	Lc	0.71	0/774	0.71	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.71	0/903	0.69	2/1216 (0.2%)
33	Le	0.83	2/1071 (0.2%)	0.68	0/1429
34	Lf	0.82	0/895	0.75	0/1198
35	Lg	0.72	0/916	0.70	0/1220
36	Lh	0.60	0/1023	0.63	0/1351
37	Li	0.57	0/843	0.60	0/1115
38	Lj	0.78	0/731	0.75	1/966 (0.1%)
39	Lk	0.58	0/575	0.66	0/761
40	Ll	0.69	0/454	0.67	0/599
41	Lm	0.65	0/425	0.61	0/561
42	Ln	0.69	0/231	0.92	2/294 (0.7%)
43	Lo	0.72	1/887 (0.1%)	0.71	0/1170
44	Lp	0.75	0/718	0.65	0/953
45	Lr	0.71	0/1017	0.74	0/1364
46	S2	1.97	10/36169 (0.0%)	1.10	107/56356 (0.2%)
47	SA	0.43	0/1742	0.56	0/2367
48	SB	0.49	0/1745	0.58	0/2335
49	SD	0.39	0/1773	0.55	0/2387
50	SE	0.44	0/2092	0.57	0/2816
51	SF	0.41	0/1491	0.55	0/2003
52	SH	0.41	0/1512	0.65	4/2025 (0.2%)
53	SI	0.52	0/1651	0.59	0/2200
54	SK	0.39	0/823	0.59	1/1111 (0.1%)
55	SL	0.59	0/1164	0.61	0/1558
56	SP	0.40	0/1097	0.55	0/1467
57	SQ	0.40	0/1134	0.57	0/1517
58	SR	0.37	0/1078	0.61	1/1447 (0.1%)
59	SS	0.39	0/1202	0.58	0/1610
60	ST	0.41	0/1113	0.56	0/1493
61	SU	0.36	0/808	0.56	0/1085
62	SV	0.45	0/644	0.57	0/862
63	SX	0.51	0/1097	0.61	0/1464
64	Sa	0.52	0/805	0.60	0/1079
65	Sc	0.37	0/481	0.56	0/643
66	Sd	0.49	0/470	0.56	0/623
67	Sg	0.34	0/2493	0.63	1/3394 (0.0%)
68	SC	0.49	0/1755	0.61	0/2371
69	SG	0.38	0/1871	0.58	1/2492 (0.0%)
70	SJ	0.40	0/1524	0.53	0/2035
71	SM	0.29	0/868	0.56	0/1165
72	SN	0.50	0/1232	0.55	0/1656
73	SO	0.51	0/1014	0.60	0/1358
74	SW	0.52	0/1051	0.58	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SY	0.40	0/1019	0.53	0/1354
76	SZ	0.39	0/565	0.59	0/759
77	Sb	0.45	0/653	0.55	0/876
78	Se	0.36	0/410	0.55	0/539
79	Sf	0.38	0/525	0.63	1/695 (0.1%)
80	Bv	0.56	2/1527 (0.1%)	0.76	1/2373 (0.0%)
81	j	0.35	0/2954	0.70	5/3968 (0.1%)
82	k	0.29	0/300	0.67	0/463
83	NC	0.21	0/178	0.47	0/243
All	All	1.37	181/222054 (0.1%)	1.13	749/324968 (0.2%)

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
1	LA	0	1
7	LD	0	1
8	LE	0	1
11	LH	0	1
13	LJ	0	1
21	LS	0	1
22	LT	0	1
23	LU	0	1
29	La	0	1
34	Lf	0	2
36	Lh	0	1
38	Lj	0	1
45	Lr	0	1
46	S2	1	0
52	SH	0	1
63	SX	0	1
70	SJ	0	1
74	SW	0	1
All	All	1	18

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	970	G	C6-N1	171.12	2.59	1.39
46	S2	970	G	N1-C2	140.33	2.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	970	G	N3-C4	134.05	2.29	1.35
46	S2	970	G	C2-N3	117.01	2.26	1.32
46	S2	970	G	C5-C4	116.58	2.19	1.38
46	S2	970	G	C5-C6	91.00	2.33	1.42
3	L5	3690	A	N1-C2	81.45	2.07	1.34
3	L5	3690	A	C2-N3	79.70	2.05	1.33
3	L5	3690	A	N3-C4	68.73	1.76	1.34
3	L5	3690	A	C6-N1	63.97	1.80	1.35
4	L7	1	G	OP3-P	-10.80	1.48	1.61
80	Bv	1	G	OP3-P	-10.27	1.48	1.61
33	Le	72	SER	CA-CB	-9.32	1.39	1.52
3	L5	3690	A	C5-C4	-9.16	1.32	1.38
3	L5	3690	A	N7-C5	-7.97	1.34	1.39
46	S2	970	G	C8-N7	7.88	1.35	1.30
3	L5	3690	A	C5-C6	-7.77	1.34	1.41
3	L5	94	A	N9-C4	-7.67	1.33	1.37
3	L5	4981	A	N9-C4	-7.54	1.33	1.37
3	L5	2452	C	N1-C6	-7.07	1.32	1.37
17	LO	27	VAL	CB-CG1	-6.70	1.38	1.52
3	L5	1640	A	N9-C4	-6.63	1.33	1.37
3	L5	4733	A	N9-C4	-6.63	1.33	1.37
3	L5	1930	A	N9-C4	-6.59	1.33	1.37
3	L5	1883	A	N9-C4	-6.44	1.33	1.37
3	L5	362	A	N9-C4	-6.30	1.34	1.37
3	L5	3854	G	C5-C4	-6.26	1.33	1.38
3	L5	347	G	C5-C4	-6.25	1.33	1.38
10	LG	55	VAL	CB-CG2	-6.23	1.39	1.52
3	L5	1622	C	N3-C4	-6.23	1.29	1.33
3	L5	2410	A	N9-C4	-6.16	1.34	1.37
3	L5	2768	G	C8-N7	-6.12	1.27	1.30
3	L5	1647	U	C2-N3	-6.06	1.33	1.37
3	L5	3632	A	N9-C4	-6.05	1.34	1.37
3	L5	1323	G	N7-C5	-6.01	1.35	1.39
3	L5	120	A	N9-C4	-5.98	1.34	1.37
3	L5	290	C	N3-C4	-5.96	1.29	1.33
3	L5	1324	A	N9-C4	-5.96	1.34	1.37
3	L5	3763	A	N9-C4	-5.92	1.34	1.37
3	L5	3632	A	C8-N7	-5.92	1.27	1.31
46	S2	970	G	N9-C8	5.90	1.42	1.37
3	L5	3625	A	N7-C5	-5.86	1.35	1.39
3	L5	4458	A	N9-C4	-5.86	1.34	1.37
3	L5	1615	C	N3-C4	-5.85	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	298	A	N9-C4	-5.83	1.34	1.37
3	L5	2275	G	C5-C4	-5.80	1.34	1.38
3	L5	3754	A	N9-C4	-5.79	1.34	1.37
3	L5	3632	A	N7-C5	-5.79	1.35	1.39
3	L5	4156	A	N7-C5	-5.78	1.35	1.39
3	L5	2265	G	C6-N1	-5.77	1.35	1.39
1	LA	169	VAL	CB-CG2	-5.76	1.40	1.52
3	L5	1315	G	C5-C4	-5.75	1.34	1.38
3	L5	3754	A	N7-C5	-5.74	1.35	1.39
3	L5	4686	C	N3-C4	-5.73	1.29	1.33
3	L5	2731	A	N9-C4	-5.73	1.34	1.37
3	L5	296	A	N9-C4	-5.70	1.34	1.37
3	L5	3897	G	N7-C5	-5.69	1.35	1.39
3	L5	3850	A	N7-C5	-5.65	1.35	1.39
3	L5	1878	A	N9-C4	-5.64	1.34	1.37
3	L5	1895	A	N7-C5	-5.64	1.35	1.39
3	L5	3786	A	N9-C4	-5.61	1.34	1.37
3	L5	2305	G	C5-C4	-5.60	1.34	1.38
3	L5	1321	A	N9-C4	-5.59	1.34	1.37
3	L5	3779	A	N9-C4	-5.58	1.34	1.37
3	L5	2851	A	N9-C4	-5.57	1.34	1.37
3	L5	341	C	N3-C4	-5.57	1.30	1.33
3	L5	1584	G	C5-C4	-5.57	1.34	1.38
3	L5	1671	A	N9-C4	-5.57	1.34	1.37
3	L5	3889	C	N3-C4	-5.56	1.30	1.33
3	L5	87	A	N7-C5	-5.56	1.35	1.39
3	L5	1645	G	N7-C5	-5.54	1.35	1.39
3	L5	1517	G	C2-N3	-5.53	1.28	1.32
3	L5	1645	G	C6-N1	-5.52	1.35	1.39
3	L5	2628	A	N9-C4	-5.52	1.34	1.37
3	L5	3614	A	N9-C4	-5.50	1.34	1.37
3	L5	1633	A	N9-C4	-5.49	1.34	1.37
3	L5	62	A	N9-C4	-5.49	1.34	1.37
3	L5	4333	A	N9-C4	-5.47	1.34	1.37
3	L5	4359	C	N3-C4	-5.47	1.30	1.33
3	L5	3902	A	N7-C5	-5.47	1.35	1.39
3	L5	4154	G	C6-N1	-5.46	1.35	1.39
3	L5	4637	C	N3-C4	-5.46	1.30	1.33
46	S2	1844	U	C2-N3	-5.46	1.33	1.37
3	L5	2770	A	N7-C5	-5.45	1.35	1.39
3	L5	297	A	N9-C4	-5.45	1.34	1.37
3	L5	2428	C	N3-C4	-5.44	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	56	A	N9-C4	-5.44	1.34	1.37
3	L5	194	A	N9-C4	-5.43	1.34	1.37
3	L5	1667	G	N7-C5	-5.42	1.35	1.39
3	L5	1874	G	C5-C4	-5.42	1.34	1.38
3	L5	2518	C	N1-C6	-5.41	1.33	1.37
3	L5	3627	A	N7-C5	-5.40	1.36	1.39
3	L5	4485	G	N7-C5	-5.40	1.36	1.39
3	L5	1613	G	C5-C4	-5.40	1.34	1.38
3	L5	4418	G	N9-C4	-5.39	1.33	1.38
3	L5	1894	A	N9-C4	-5.38	1.34	1.37
3	L5	3754	A	N3-C4	-5.37	1.31	1.34
4	L7	78	C	N3-C4	-5.36	1.30	1.33
3	L5	2796	G	C5-C4	-5.36	1.34	1.38
3	L5	75	G	N7-C5	-5.34	1.36	1.39
3	L5	1315	G	N1-C2	-5.33	1.33	1.37
3	L5	1638	G	C8-N7	-5.33	1.27	1.30
3	L5	1642	C	N3-C4	-5.32	1.30	1.33
3	L5	2381	G	C6-N1	-5.31	1.35	1.39
3	L5	2516	A	N9-C4	-5.31	1.34	1.37
33	Le	4	LEU	C-N	-5.31	1.21	1.34
3	L5	1308	G	N7-C5	-5.31	1.36	1.39
3	L5	346	A	C5-C4	-5.31	1.35	1.38
3	L5	1883	A	N3-C4	-5.30	1.31	1.34
3	L5	97	G	C5-C4	-5.30	1.34	1.38
5	L8	40	A	N9-C4	-5.27	1.34	1.37
3	L5	1837	A	N7-C5	-5.27	1.36	1.39
3	L5	2456	C	N1-C6	-5.27	1.33	1.37
3	L5	2646	A	N9-C4	-5.26	1.34	1.37
3	L5	4363	G	N9-C4	-5.25	1.33	1.38
46	S2	970	G	N9-C4	-5.25	1.33	1.38
3	L5	4596	A	N7-C5	-5.24	1.36	1.39
17	LO	33	VAL	CB-CG1	-5.23	1.41	1.52
3	L5	2054	C	N3-C4	-5.21	1.30	1.33
3	L5	75	G	C5-C4	-5.21	1.34	1.38
3	L5	4361	G	C6-N1	-5.19	1.35	1.39
3	L5	4193	C	N3-C4	-5.19	1.30	1.33
3	L5	347	G	C8-N7	-5.19	1.27	1.30
3	L5	1781	A	N7-C5	-5.19	1.36	1.39
3	L5	3835	A	N9-C4	-5.18	1.34	1.37
3	L5	2384	G	C5-C4	-5.18	1.34	1.38
3	L5	1835	C	N3-C4	-5.17	1.30	1.33
3	L5	1649	C	N3-C4	-5.16	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1495	A	N9-C4	-5.16	1.34	1.37
3	L5	1518	U	C2-N3	-5.15	1.34	1.37
3	L5	365	G	C5-C4	-5.14	1.34	1.38
3	L5	1320	A	N7-C5	-5.14	1.36	1.39
3	L5	1494	C	N3-C4	-5.13	1.30	1.33
3	L5	1295	C	N3-C4	-5.12	1.30	1.33
3	L5	1894	A	C5-C4	-5.12	1.35	1.38
3	L5	2805	C	N3-C4	-5.12	1.30	1.33
3	L5	4693	A	N9-C4	-5.12	1.34	1.37
3	L5	1619	A	N7-C5	-5.11	1.36	1.39
3	L5	4332	A	N9-C4	-5.11	1.34	1.37
3	L5	4275	G	C5-C4	-5.10	1.34	1.38
3	L5	1611	G	C5-C4	-5.10	1.34	1.38
3	L5	1882	G	C5-C4	-5.10	1.34	1.38
80	Bv	76	A	C5-C4	-5.10	1.35	1.38
3	L5	1413	G	C5-C4	-5.09	1.34	1.38
3	L5	4425	G	C8-N7	-5.09	1.27	1.30
3	L5	2834	G	C5-C4	-5.09	1.34	1.38
3	L5	342	C	N1-C6	-5.09	1.34	1.37
3	L5	2328	A	N7-C5	-5.09	1.36	1.39
3	L5	1654	G	C6-N1	-5.08	1.35	1.39
3	L5	2349	U	C2-N3	-5.08	1.34	1.37
3	L5	2436	A	N9-C4	-5.08	1.34	1.37
3	L5	3780	U	C2-N3	-5.08	1.34	1.37
3	L5	93	G	C5-C4	-5.08	1.34	1.38
3	L5	227	G	N7-C5	-5.08	1.36	1.39
3	L5	1873	G	C6-N1	-5.08	1.35	1.39
3	L5	2036	G	C5-C4	-5.08	1.34	1.38
3	L5	3625	A	C5-C4	-5.07	1.35	1.38
43	Lo	67	VAL	CB-CG2	-5.07	1.42	1.52
3	L5	4155	G	N7-C5	-5.07	1.36	1.39
3	L5	2065	C	N3-C4	-5.06	1.30	1.33
3	L5	1859	G	C5-C4	-5.06	1.34	1.38
3	L5	2807	C	N3-C4	-5.06	1.30	1.33
3	L5	411	A	N7-C5	-5.06	1.36	1.39
3	L5	3631	A	N7-C5	-5.06	1.36	1.39
3	L5	1383	G	N7-C5	-5.05	1.36	1.39
3	L5	1629	A	N9-C4	-5.05	1.34	1.37
3	L5	1851	G	C8-N7	-5.04	1.27	1.30
3	L5	1900	C	N3-C4	-5.04	1.30	1.33
3	L5	1308	G	N9-C8	-5.04	1.34	1.37
3	L5	3906	U	C2-N3	-5.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	271	G	C5-C4	-5.03	1.34	1.38
3	L5	2058	A	N7-C5	-5.03	1.36	1.39
3	L5	3696	A	N9-C4	-5.02	1.34	1.37
3	L5	3778	A	N9-C4	-5.02	1.34	1.37
3	L5	4308	G	C5-C4	-5.02	1.34	1.38
3	L5	63	G	C5-C4	-5.01	1.34	1.38
3	L5	349	C	N3-C4	-5.01	1.30	1.33
3	L5	1493	G	C5-C4	-5.01	1.34	1.38
3	L5	4184	A	N9-C4	-5.01	1.34	1.37
3	L5	3725	A	N9-C4	-5.00	1.34	1.37
3	L5	2021	G	N7-C5	-5.00	1.36	1.39

All (749) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3690	A	N1-C2-N3	-237.89	10.36	129.30
3	L5	3690	A	C2-N3-C4	85.13	153.17	110.60
3	L5	3690	A	C6-N1-C2	73.75	162.85	118.60
3	L5	3690	A	C4-C5-C6	-44.98	94.51	117.00
46	S2	970	G	C4-C5-N7	-37.55	95.78	110.80
46	S2	970	G	N7-C8-N9	30.61	128.40	113.10
3	L5	3690	A	N3-C4-N9	29.64	151.11	127.40
46	S2	970	G	C2-N3-C4	29.07	126.44	111.90
3	L5	3690	A	N3-C4-C5	-27.90	107.27	126.80
3	L5	3690	A	C5-C6-N1	-25.01	105.19	117.70
46	S2	970	G	N1-C2-N3	-23.55	109.77	123.90
46	S2	970	G	N3-C4-N9	22.47	139.48	126.00
46	S2	970	G	N9-C4-C5	-21.68	96.73	105.40
3	L5	3690	A	C6-C5-N7	18.97	145.58	132.30
3	L5	3690	A	C4-C5-N7	18.30	119.85	110.70
46	S2	970	G	C6-C5-N7	16.08	140.05	130.40
81	j	303	PHE	N-CA-C	14.67	150.60	111.00
3	L5	3690	A	N1-C6-N6	13.78	126.86	118.60
81	j	305	VAL	N-CA-CB	13.64	141.51	111.50
46	S2	501	C	N1-C2-O2	13.29	126.87	118.90
46	S2	293	C	N1-C2-O2	13.12	126.77	118.90
46	S2	501	C	C2-N1-C1'	13.00	133.10	118.80
81	j	304	GLY	N-CA-C	12.76	145.00	113.10
46	S2	293	C	C2-N1-C1'	12.42	132.46	118.80
3	L5	1366	C	N3-C2-O2	-12.01	113.49	121.90
3	L5	3690	A	C5-N7-C8	-11.96	97.92	103.90
3	L5	1366	C	N1-C2-O2	11.78	125.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1366	C	C6-N1-C2	-11.68	115.63	120.30
3	L5	2396	U	C2-N1-C1'	11.39	131.37	117.70
46	S2	1453	C	N1-C2-O2	11.30	125.68	118.90
3	L5	2396	U	N1-C2-O2	11.29	130.70	122.80
3	L5	4641	C	O4'-C1'-N1	11.04	117.03	108.20
46	S2	501	C	N3-C2-O2	-10.77	114.36	121.90
3	L5	3690	A	N9-C4-C5	-10.68	101.53	105.80
3	L5	2396	U	N3-C2-O2	-10.58	114.80	122.20
46	S2	1453	C	C2-N1-C1'	10.27	130.09	118.80
46	S2	970	G	C5-N7-C8	10.18	109.39	104.30
3	L5	2247	C	N1-C2-O2	10.11	124.96	118.90
3	L5	4641	C	N1-C1'-C2'	9.91	126.89	114.00
3	L5	2397	C	N1-C2-O2	9.81	124.79	118.90
46	S2	293	C	N3-C2-O2	-9.80	115.04	121.90
3	L5	4981	A	C5-N7-C8	-9.76	99.02	103.90
46	S2	970	G	N3-C2-N2	9.64	126.65	119.90
46	S2	970	G	N3-C4-C5	-9.63	123.78	128.60
46	S2	293	C	C6-N1-C1'	-9.16	109.81	120.80
46	S2	501	C	C6-N1-C1'	-9.12	109.85	120.80
3	L5	4733	A	C6-N1-C2	9.11	124.07	118.60
3	L5	1653	C	C6-N1-C2	-9.03	116.69	120.30
3	L5	2697	C	N1-C2-O2	8.98	124.29	118.90
3	L5	2247	C	C2-N1-C1'	8.84	128.52	118.80
81	j	303	PHE	CB-CA-C	-8.82	92.77	110.40
16	LN	147	ASP	CB-CG-OD1	8.79	126.21	118.30
3	L5	4733	A	N1-C2-N3	-8.71	124.95	129.30
46	S2	970	G	C4-C5-C6	8.69	124.02	118.80
3	L5	2697	C	N3-C2-O2	-8.62	115.87	121.90
3	L5	2247	C	N3-C2-O2	-8.55	115.92	121.90
3	L5	4185	C	N1-C2-O2	8.54	124.03	118.90
46	S2	1453	C	N3-C2-O2	-8.53	115.93	121.90
69	SG	180	VAL	C-N-CA	8.51	142.97	121.70
3	L5	1494	C	C6-N1-C2	-8.34	116.97	120.30
46	S2	501	C	C6-N1-C2	-8.30	116.98	120.30
3	L5	3746	C	C6-N1-C2	-8.28	116.99	120.30
3	L5	1808	G	N3-C4-N9	8.28	130.97	126.00
3	L5	2396	U	C6-N1-C1'	-8.16	109.77	121.20
3	L5	2697	C	C2-N1-C1'	8.12	127.73	118.80
46	S2	970	G	N1-C2-N2	8.11	123.50	116.20
5	L8	101	C	N1-C2-O2	8.11	123.76	118.90
3	L5	4727	U	C2-N1-C1'	8.04	127.35	117.70
46	S2	970	G	C8-N9-C4	8.04	109.62	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4981	A	N7-C8-N9	8.02	117.81	113.80
3	L5	3861	C	N1-C2-O2	8.00	123.70	118.90
3	L5	3861	C	N3-C2-O2	-7.99	116.31	121.90
3	L5	3615	C	C6-N1-C2	-7.96	117.11	120.30
28	LZ	30	ASP	CB-CG-OD1	7.95	125.45	118.30
3	L5	1993	U	C5-C6-N1	7.89	126.65	122.70
3	L5	1366	C	C2-N1-C1'	7.82	127.40	118.80
3	L5	4910	G	N3-C4-N9	7.82	130.69	126.00
3	L5	4207	C	N1-C2-O2	7.77	123.56	118.90
3	L5	30	C	C6-N1-C2	-7.77	117.19	120.30
3	L5	2277	C	C6-N1-C2	-7.73	117.21	120.30
3	L5	3690	A	N7-C8-N9	7.72	117.66	113.80
3	L5	2397	C	N3-C2-O2	-7.67	116.53	121.90
3	L5	3754	A	N7-C8-N9	7.66	117.63	113.80
3	L5	118	C	N1-C2-O2	7.62	123.47	118.90
46	S2	532	C	O5'-P-OP1	7.60	119.82	110.70
3	L5	408	G	O4'-C1'-N9	7.59	114.28	108.20
3	L5	3754	A	C5-N7-C8	-7.59	100.11	103.90
3	L5	138	C	N1-C2-O2	7.58	123.45	118.90
3	L5	4532	C	C6-N1-C2	-7.57	117.27	120.30
46	S2	1520	G	C4-N9-C1'	7.54	136.31	126.50
3	L5	4852	C	N1-C2-O2	7.52	123.41	118.90
3	L5	3746	C	N1-C2-O2	7.51	123.40	118.90
3	L5	1694	C	C6-N1-C2	-7.50	117.30	120.30
3	L5	1808	G	C4-N9-C1'	7.48	136.22	126.50
3	L5	2083	G	C4-N9-C1'	7.48	136.22	126.50
3	L5	1445	C	N3-C2-O2	-7.47	116.67	121.90
3	L5	4185	C	N3-C2-O2	-7.47	116.67	121.90
3	L5	4193	C	N1-C2-O2	7.41	123.34	118.90
3	L5	206	U	C2-N1-C1'	7.38	126.56	117.70
46	S2	1022	U	N1-C2-O2	7.37	127.96	122.80
3	L5	4207	C	N3-C2-O2	-7.31	116.78	121.90
3	L5	3690	A	O4'-C1'-N9	7.31	114.05	108.20
3	L5	2671	C	C6-N1-C2	-7.31	117.38	120.30
3	L5	4910	G	C4-C5-N7	7.29	113.72	110.80
3	L5	4181	C	C6-N1-C2	-7.28	117.39	120.30
58	SR	117	LEU	CA-CB-CG	7.28	132.03	115.30
46	S2	1453	C	C6-N1-C1'	-7.24	112.11	120.80
3	L5	3690	A	C8-N9-C4	-7.19	102.92	105.80
3	L5	4110	C	N1-C2-O2	7.19	123.21	118.90
3	L5	1843	C	C6-N1-C2	-7.16	117.44	120.30
3	L5	1445	C	N1-C2-O2	7.16	123.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4532	C	C5-C6-N1	7.15	124.58	121.00
3	L5	3888	C	C6-N1-C2	-7.10	117.46	120.30
46	S2	1078	C	N3-C2-O2	-7.08	116.94	121.90
3	L5	4570	G	C4-N9-C1'	-7.07	117.30	126.50
5	L8	11	C	C6-N1-C2	-7.07	117.47	120.30
3	L5	3664	C	C6-N1-C2	-7.07	117.47	120.30
3	L5	2305	G	C8-N9-C4	7.05	109.22	106.40
3	L5	2662	G	P-O3'-C3'	7.05	128.16	119.70
3	L5	2397	C	C2-N1-C1'	7.03	126.54	118.80
3	L5	30	C	N3-C2-O2	-7.03	116.98	121.90
3	L5	1567	C	C6-N1-C2	-7.02	117.49	120.30
3	L5	4521	U	N3-C2-O2	-7.00	117.30	122.20
3	L5	1880	C	N1-C2-O2	6.99	123.09	118.90
3	L5	4715	C	C2-N1-C1'	6.98	126.48	118.80
46	S2	1022	U	C2-N1-C1'	6.97	126.06	117.70
3	L5	2247	C	C6-N1-C2	-6.97	117.51	120.30
3	L5	3888	C	N3-C2-O2	-6.95	117.04	121.90
3	L5	4396	C	N1-C2-O2	6.94	123.06	118.90
3	L5	4570	G	P-O3'-C3'	6.93	128.02	119.70
3	L5	4727	U	N3-C2-O2	-6.93	117.35	122.20
4	L7	104	C	N1-C2-O2	6.91	123.05	118.90
3	L5	4716	C	N1-C2-O2	6.90	123.04	118.90
3	L5	4905	C	N1-C2-O2	6.90	123.04	118.90
46	S2	688	U	P-O3'-C3'	6.89	127.97	119.70
3	L5	1507	C	C6-N1-C2	-6.89	117.55	120.30
3	L5	4727	U	N1-C2-O2	6.87	127.61	122.80
3	L5	427	C	N1-C2-O2	6.83	123.00	118.90
3	L5	83	C	C6-N1-C2	-6.82	117.57	120.30
4	L7	111	C	C6-N1-C2	-6.78	117.59	120.30
46	S2	453	C	N1-C2-O2	6.77	122.96	118.90
3	L5	4404	C	N1-C2-O2	6.76	122.96	118.90
3	L5	2340	U	N3-C2-O2	-6.76	117.47	122.20
3	L5	3746	C	C5-C6-N1	6.73	124.37	121.00
46	S2	407	G	C4-N9-C1'	6.72	135.24	126.50
3	L5	2061	C	C6-N1-C2	-6.71	117.61	120.30
46	S2	1520	G	C8-N9-C1'	-6.71	118.27	127.00
3	L5	4715	C	N1-C2-O2	6.70	122.92	118.90
3	L5	427	C	N3-C2-O2	-6.70	117.21	121.90
46	S2	532	C	O5'-P-OP2	-6.69	99.68	105.70
3	L5	2397	C	C5-C6-N1	6.67	124.33	121.00
3	L5	4193	C	N3-C2-O2	-6.67	117.23	121.90
3	L5	1690	C	N1-C2-O2	6.66	122.90	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4571	U	N1-C2-O2	6.66	127.46	122.80
3	L5	2807	C	N1-C2-O2	6.66	122.89	118.90
3	L5	1796	C	N1-C2-O2	6.65	122.89	118.90
3	L5	3746	C	N3-C2-O2	-6.65	117.24	121.90
3	L5	1808	G	C8-N9-C1'	-6.64	118.37	127.00
3	L5	1366	C	C5-C6-N1	6.61	124.31	121.00
3	L5	2747	G	P-O3'-C3'	6.61	127.64	119.70
46	S2	407	G	N3-C4-N9	6.59	129.95	126.00
3	L5	4213	C	N1-C2-O2	6.58	122.85	118.90
3	L5	4571	U	N3-C2-O2	-6.58	117.59	122.20
3	L5	167	C	N1-C2-O2	6.58	122.85	118.90
3	L5	4402	C	C5-C6-N1	6.57	124.29	121.00
46	S2	501	C	C5-C6-N1	6.57	124.28	121.00
3	L5	83	C	C5-C6-N1	6.57	124.28	121.00
3	L5	2515	G	C4-N9-C1'	6.57	135.03	126.50
3	L5	4905	C	C2-N1-C1'	6.56	126.02	118.80
14	LL	146	LEU	CA-CB-CG	6.54	130.34	115.30
3	L5	1808	G	N3-C4-C5	-6.53	125.33	128.60
3	L5	206	U	N1-C2-O2	6.53	127.37	122.80
3	L5	3690	A	C4-N9-C1'	6.52	138.04	126.30
3	L5	1490	A	N1-C6-N6	-6.52	114.69	118.60
3	L5	2492	C	N1-C2-O2	6.51	122.81	118.90
3	L5	703	C	C6-N1-C2	-6.51	117.70	120.30
4	L7	68	C	N1-C2-O2	6.50	122.80	118.90
3	L5	2083	G	N3-C4-N9	6.49	129.90	126.00
3	L5	715	C	N3-C2-O2	-6.49	117.36	121.90
3	L5	2507	C	C6-N1-C2	-6.49	117.70	120.30
5	L8	101	C	N3-C2-O2	-6.48	117.36	121.90
3	L5	1991	U	C2-N1-C1'	6.47	125.46	117.70
46	S2	293	C	C6-N1-C2	-6.46	117.72	120.30
46	S2	1078	C	N1-C2-O2	6.46	122.77	118.90
3	L5	1371	C	C6-N1-C2	-6.45	117.72	120.30
3	L5	1489	G	O5'-P-OP2	-6.44	99.91	105.70
46	S2	127	C	N1-C2-O2	6.44	122.76	118.90
3	L5	1880	C	C5-C6-N1	6.44	124.22	121.00
3	L5	2515	G	N3-C4-N9	6.43	129.86	126.00
3	L5	149	U	N1-C2-O2	6.42	127.30	122.80
3	L5	1653	C	C5-C6-N1	6.42	124.21	121.00
3	L5	2381	G	O4'-C1'-N9	6.40	113.32	108.20
3	L5	1594	C	C6-N1-C2	-6.39	117.75	120.30
3	L5	1679	C	N1-C2-O2	6.38	122.73	118.90
3	L5	1601	C	N1-C2-O2	6.38	122.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	149	U	N3-C2-O2	-6.37	117.74	122.20
3	L5	2456	C	C5-C6-N1	-6.37	117.81	121.00
3	L5	1652	C	C4-C5-C6	-6.36	114.22	117.40
3	L5	1652	C	C5-C6-N1	6.36	124.18	121.00
3	L5	4910	G	N9-C4-C5	-6.36	102.86	105.40
3	L5	4275	G	C8-N9-C4	6.35	108.94	106.40
3	L5	4981	A	C4-C5-N7	6.35	113.88	110.70
3	L5	1655	A	N1-C2-N3	-6.34	126.13	129.30
3	L5	4910	G	C6-C5-N7	-6.33	126.60	130.40
4	L7	78	C	N3-C2-O2	-6.33	117.47	121.90
46	S2	1844	U	N3-C4-O4	-6.33	114.97	119.40
46	S2	1022	U	N3-C2-O2	-6.33	117.77	122.20
3	L5	4679	U	C2-N1-C1'	6.32	125.28	117.70
3	L5	2083	G	C8-N9-C1'	-6.31	118.80	127.00
3	L5	4716	C	N3-C2-O2	-6.31	117.48	121.90
46	S2	1060	A	O4'-C1'-N9	6.31	113.25	108.20
3	L5	1638	G	C4-N9-C1'	6.31	134.70	126.50
3	L5	4535	C	C6-N1-C2	-6.30	117.78	120.30
3	L5	663	C	N1-C2-O2	6.30	122.68	118.90
3	L5	2451	C	C5-C6-N1	6.30	124.15	121.00
3	L5	4335	C	C6-N1-C2	-6.29	117.78	120.30
3	L5	1718	C	N1-C2-O2	6.29	122.68	118.90
3	L5	2515	G	C8-N9-C1'	-6.29	118.82	127.00
46	S2	293	C	C5-C6-N1	6.29	124.14	121.00
3	L5	1873	G	C4-C5-N7	6.29	113.31	110.80
3	L5	2765	G	O5'-P-OP2	-6.28	100.05	105.70
3	L5	4570	G	C8-N9-C1'	6.27	135.15	127.00
52	SH	30	LEU	CA-CB-CG	6.26	129.71	115.30
81	j	305	VAL	N-CA-C	-6.26	94.09	111.00
3	L5	2371	U	N3-C2-O2	-6.26	117.82	122.20
3	L5	4910	G	C5-C6-O6	-6.26	124.84	128.60
46	S2	1453	C	C6-N1-C2	-6.25	117.80	120.30
3	L5	4886	C	N1-C2-O2	6.25	122.65	118.90
54	SK	14	LEU	CA-CB-CG	6.24	129.66	115.30
3	L5	3888	C	N1-C2-O2	6.22	122.63	118.90
3	L5	2083	G	N3-C4-C5	-6.20	125.50	128.60
3	L5	2697	C	C6-N1-C2	-6.20	117.82	120.30
5	L8	45	C	C6-N1-C2	-6.19	117.83	120.30
3	L5	397	C	P-O3'-C3'	6.18	127.12	119.70
3	L5	3671	A	N9-C4-C5	-6.18	103.33	105.80
46	S2	659	G	C4-N9-C1'	6.17	134.51	126.50
3	L5	704	C	C6-N1-C2	-6.16	117.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3620	U	C4-C5-C6	6.16	123.40	119.70
3	L5	2397	C	C6-N1-C2	-6.16	117.84	120.30
3	L5	3754	A	C2-N3-C4	-6.16	107.52	110.60
3	L5	1916	A	C2-N3-C4	6.15	113.67	110.60
3	L5	3754	A	C8-N9-C4	-6.15	103.34	105.80
3	L5	1900	C	C6-N1-C2	-6.14	117.84	120.30
3	L5	1916	A	C4-N9-C1'	6.14	137.36	126.30
3	L5	1840	G	C4-N9-C1'	6.14	134.48	126.50
3	L5	4686	C	N3-C2-O2	-6.14	117.61	121.90
3	L5	4570	G	O4'-C1'-N9	6.13	113.11	108.20
3	L5	81	C	C5-C6-N1	6.13	124.07	121.00
3	L5	4878	G	P-O3'-C3'	6.13	127.06	119.70
46	S2	1520	G	N3-C4-N9	6.12	129.67	126.00
46	S2	1253	A	P-O3'-C3'	6.12	127.04	119.70
3	L5	912	C	C5-C6-N1	6.11	124.06	121.00
3	L5	1862	C	C6-N1-C2	-6.11	117.86	120.30
3	L5	715	C	N1-C2-O2	6.11	122.56	118.90
3	L5	4110	C	C2-N1-C1'	6.11	125.52	118.80
3	L5	269	G	O4'-C1'-N9	-6.10	103.32	108.20
3	L5	2879	C	N1-C2-O2	6.10	122.56	118.90
3	L5	4596	A	C8-N9-C4	-6.10	103.36	105.80
3	L5	4679	U	N1-C2-O2	6.10	127.07	122.80
3	L5	1622	C	N1-C2-O2	6.09	122.55	118.90
3	L5	341	C	N3-C2-O2	-6.09	117.64	121.90
46	S2	974	C	C5-C6-N1	6.08	124.04	121.00
3	L5	3620	U	C5-C6-N1	-6.08	119.66	122.70
46	S2	1265	A	N3-C4-N9	6.07	132.26	127.40
5	L8	21	C	N1-C2-O2	6.07	122.54	118.90
3	L5	1649	C	N3-C2-O2	-6.07	117.65	121.90
3	L5	2291	U	N3-C2-O2	-6.06	117.96	122.20
3	L5	4176	C	N1-C2-O2	6.06	122.53	118.90
3	L5	3692	U	C2-N1-C1'	6.05	124.96	117.70
3	L5	4981	A	C2-N3-C4	-6.05	107.58	110.60
3	L5	2275	G	N1-C6-O6	-6.04	116.28	119.90
3	L5	1622	C	N3-C2-O2	-6.04	117.67	121.90
46	S2	974	C	C6-N1-C2	-6.03	117.89	120.30
3	L5	4852	C	C2-N1-C1'	6.03	125.43	118.80
3	L5	4396	C	N3-C2-O2	-6.02	117.69	121.90
3	L5	4404	C	C4-C5-C6	-6.02	114.39	117.40
3	L5	3890	C	C6-N1-C2	-6.02	117.89	120.30
3	L5	1638	G	C8-N9-C1'	-6.02	119.18	127.00
3	L5	80	C	C6-N1-C2	-6.01	117.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3890	C	N3-C2-O2	-6.01	117.69	121.90
3	L5	2654	C	C6-N1-C2	-6.00	117.90	120.30
3	L5	3647	C	N1-C2-O2	6.00	122.50	118.90
3	L5	2817	G	C4-C5-N7	6.00	113.20	110.80
3	L5	2451	C	C6-N1-C2	-5.99	117.90	120.30
3	L5	1507	C	C5-C6-N1	5.99	124.00	121.00
3	L5	2298	C	C6-N1-C2	-5.99	117.91	120.30
3	L5	2349	U	N1-C2-O2	5.99	126.99	122.80
46	S2	877	C	N1-C2-O2	5.99	122.49	118.90
3	L5	4905	C	N3-C2-O2	-5.98	117.71	121.90
3	L5	1230	C	N1-C2-O2	5.98	122.49	118.90
3	L5	1302	C	N1-C2-O2	5.97	122.48	118.90
46	S2	1637	A	P-O3'-C3'	5.97	126.87	119.70
4	L7	78	C	N1-C2-O2	5.97	122.48	118.90
3	L5	3646	C	C6-N1-C2	-5.97	117.91	120.30
3	L5	273	C	N3-C2-O2	-5.97	117.72	121.90
13	LJ	171	ASP	CB-CG-OD1	5.97	123.67	118.30
3	L5	4652	U	N1-C2-O2	5.96	126.98	122.80
3	L5	2891	U	N3-C2-O2	-5.96	118.03	122.20
3	L5	4207	C	C6-N1-C2	-5.96	117.92	120.30
3	L5	2394	G	C4-N9-C1'	5.95	134.23	126.50
3	L5	4852	C	N3-C2-O2	-5.95	117.74	121.90
3	L5	4275	G	O4'-C1'-N9	5.94	112.95	108.20
3	L5	1643	U	C5-C6-N1	5.94	125.67	122.70
3	L5	1339	C	C5-C6-N1	5.94	123.97	121.00
3	L5	1679	C	N3-C2-O2	-5.93	117.75	121.90
3	L5	1620	G	P-O3'-C3'	5.93	126.81	119.70
3	L5	314	C	N3-C2-O2	-5.92	117.76	121.90
46	S2	407	G	C8-N9-C1'	-5.92	119.31	127.00
46	S2	632	C	N1-C2-O2	5.91	122.45	118.90
3	L5	1189	C	C6-N1-C2	-5.91	117.94	120.30
3	L5	3887	A	N9-C1'-C2'	-5.90	105.51	112.00
46	S2	1242	U	C2-N1-C1'	5.90	124.78	117.70
3	L5	3669	U	N3-C2-O2	-5.90	118.07	122.20
3	L5	81	C	C6-N1-C2	-5.90	117.94	120.30
3	L5	1857	C	N3-C2-O2	-5.89	117.78	121.90
46	S2	127	C	C2-N1-C1'	5.89	125.27	118.80
3	L5	1835	C	C6-N1-C2	-5.88	117.95	120.30
5	L8	32	C	C6-N1-C2	-5.88	117.95	120.30
46	S2	970	G	O4'-C1'-N9	5.88	112.91	108.20
3	L5	14	C	C6-N1-C2	-5.88	117.95	120.30
3	L5	2403	G	P-O3'-C3'	5.88	126.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Bv	23	C	C2-N1-C1'	5.87	125.26	118.80
3	L5	2891	U	N1-C2-O2	5.87	126.91	122.80
3	L5	67	C	C6-N1-C2	-5.87	117.95	120.30
3	L5	138	C	N3-C2-O2	-5.86	117.80	121.90
3	L5	1841	G	C8-N9-C4	-5.86	104.06	106.40
3	L5	1720	G	N3-C4-N9	5.85	129.51	126.00
3	L5	940	C	C6-N1-C2	-5.85	117.96	120.30
3	L5	2038	C	C6-N1-C2	-5.85	117.96	120.30
3	L5	4414	C	N1-C2-O2	5.85	122.41	118.90
3	L5	206	U	C6-N1-C1'	-5.85	113.02	121.20
3	L5	4740	C	N1-C2-O2	5.84	122.41	118.90
46	S2	676	C	N1-C2-O2	5.84	122.41	118.90
3	L5	4698	U	N3-C2-O2	-5.84	118.11	122.20
3	L5	2349	U	N3-C2-O2	-5.84	118.11	122.20
4	L7	67	C	C6-N1-C2	-5.82	117.97	120.30
3	L5	2379	C	C6-N1-C2	-5.82	117.97	120.30
3	L5	480	C	N1-C2-O2	5.81	122.39	118.90
3	L5	2082	A	O4'-C1'-N9	5.81	112.85	108.20
4	L7	102	U	N1-C2-O2	5.80	126.86	122.80
3	L5	2046	C	C6-N1-C2	-5.80	117.98	120.30
3	L5	4289	C	N1-C2-O2	5.80	122.38	118.90
3	L5	1987	G	N3-C4-N9	5.79	129.47	126.00
3	L5	4897	U	N1-C2-O2	5.79	126.85	122.80
3	L5	2324	C	C6-N1-C2	-5.78	117.99	120.30
3	L5	2779	C	N3-C2-O2	-5.78	117.85	121.90
3	L5	4948	C	N1-C2-O2	5.78	122.37	118.90
3	L5	4570	G	OP2-P-O3'	5.78	117.91	105.20
3	L5	4686	C	C6-N1-C2	-5.77	117.99	120.30
3	L5	285	G	C4-N9-C1'	5.77	134.00	126.50
3	L5	4478	C	C6-N1-C2	-5.77	117.99	120.30
46	S2	1129	G	P-O3'-C3'	5.77	126.62	119.70
3	L5	267	C	C6-N1-C2	-5.76	117.99	120.30
3	L5	4095	U	N1-C2-O2	5.76	126.83	122.80
3	L5	2836	A	C5-C6-N1	5.76	120.58	117.70
3	L5	2018	C	C6-N1-C2	-5.76	118.00	120.30
3	L5	4710	C	N1-C2-O2	5.76	122.35	118.90
3	L5	4698	U	N1-C2-O2	5.75	126.83	122.80
3	L5	4242	G	C4-N9-C1'	5.75	133.98	126.50
3	L5	2891	U	C2-N1-C1'	5.74	124.59	117.70
5	L8	32	C	N3-C2-O2	-5.74	117.88	121.90
3	L5	3793	U	N3-C2-O2	-5.74	118.18	122.20
3	L5	4644	C	N3-C2-O2	-5.74	117.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4233	C	C6-N1-C2	-5.74	118.01	120.30
3	L5	2371	U	N1-C2-O2	5.73	126.81	122.80
3	L5	4860	C	N1-C2-O2	5.73	122.34	118.90
46	S2	1069	U	N1-C2-O2	5.73	126.81	122.80
3	L5	4571	U	C2-N1-C1'	5.73	124.57	117.70
3	L5	1880	C	C2-N1-C1'	5.73	125.10	118.80
3	L5	928	C	N1-C2-O2	5.72	122.33	118.90
3	L5	2396	U	C5-C6-N1	5.72	125.56	122.70
3	L5	265	C	N1-C2-O2	5.72	122.33	118.90
3	L5	2854	C	N1-C2-O2	5.72	122.33	118.90
3	L5	3625	A	N7-C8-N9	-5.72	110.94	113.80
3	L5	397	C	C6-N1-C2	-5.71	118.01	120.30
5	L8	32	C	N1-C2-O2	5.70	122.32	118.90
3	L5	2247	C	C6-N1-C1'	-5.70	113.96	120.80
3	L5	4181	C	C5-C6-N1	5.70	123.85	121.00
3	L5	358	C	C6-N1-C2	-5.69	118.02	120.30
3	L5	1663	C	O5'-P-OP2	-5.69	100.58	105.70
3	L5	2265	G	N3-C4-N9	5.69	129.42	126.00
3	L5	2289	C	N3-C2-O2	-5.69	117.92	121.90
46	S2	585	C	N1-C2-O2	5.69	122.31	118.90
3	L5	1969	G	C8-N9-C4	-5.69	104.12	106.40
3	L5	3692	U	N3-C2-O2	-5.69	118.22	122.20
3	L5	112	C	C6-N1-C2	-5.68	118.03	120.30
3	L5	2358	U	C5-C6-N1	5.68	125.54	122.70
3	L5	2807	C	N3-C2-O2	-5.68	117.92	121.90
3	L5	4679	U	N3-C2-O2	-5.68	118.22	122.20
5	L8	21	C	N3-C2-O2	-5.68	117.92	121.90
52	SH	36	LEU	CA-CB-CG	5.68	128.36	115.30
3	L5	4686	C	N1-C2-O2	5.68	122.31	118.90
46	S2	331	C	N1-C2-O2	5.68	122.31	118.90
3	L5	2817	G	N9-C4-C5	-5.67	103.13	105.40
3	L5	4391	C	C6-N1-C2	-5.67	118.03	120.30
3	L5	1226	C	N1-C2-O2	5.67	122.30	118.90
3	L5	4641	C	C4'-C3'-O3'	-5.67	97.50	109.40
3	L5	4740	C	C5-C6-N1	5.67	123.83	121.00
5	L8	11	C	N3-C2-O2	-5.66	117.94	121.90
3	L5	2042	G	P-O3'-C3'	5.65	126.48	119.70
3	L5	4141	C	N1-C2-O2	5.65	122.29	118.90
3	L5	4259	U	N1-C2-O2	5.65	126.75	122.80
3	L5	3652	C	P-O3'-C3'	5.64	126.47	119.70
3	L5	35	U	N3-C2-O2	-5.64	118.25	122.20
3	L5	89	C	N3-C4-C5	5.63	124.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2265	G	C4-N9-C1'	5.63	133.82	126.50
3	L5	1489	G	N3-C4-N9	5.63	129.38	126.00
3	L5	2445	C	N3-C2-O2	-5.63	117.96	121.90
3	L5	4564	U	C2-N1-C1'	5.63	124.46	117.70
3	L5	4897	U	N3-C2-O2	-5.63	118.26	122.20
3	L5	4153	G	N3-C4-C5	-5.63	125.79	128.60
3	L5	4259	U	N3-C2-O2	-5.63	118.26	122.20
3	L5	290	C	N3-C2-O2	-5.62	117.96	121.90
3	L5	1584	G	O4'-C1'-N9	5.62	112.70	108.20
3	L5	2846	G	C4-C5-N7	5.62	113.05	110.80
46	S2	1453	C	C5-C6-N1	5.62	123.81	121.00
32	Ld	46	LEU	CA-CB-CG	-5.62	102.37	115.30
3	L5	2837	A	C8-N9-C4	-5.62	103.55	105.80
3	L5	3909	U	N3-C2-O2	-5.62	118.27	122.20
3	L5	2806	U	N3-C2-O2	-5.61	118.27	122.20
3	L5	4596	A	N7-C8-N9	5.61	116.61	113.80
3	L5	2519	C	C6-N1-C2	-5.61	118.06	120.30
3	L5	959	C	N1-C2-O2	5.61	122.26	118.90
3	L5	2291	U	N1-C2-O2	5.60	126.72	122.80
3	L5	1840	G	C8-N9-C1'	-5.60	119.72	127.00
3	L5	4242	G	C8-N9-C1'	-5.60	119.73	127.00
3	L5	4664	G	O4'-C1'-N9	5.60	112.68	108.20
3	L5	1459	C	N1-C2-O2	5.59	122.26	118.90
4	L7	102	U	N3-C2-O2	-5.59	118.28	122.20
3	L5	4050	C	N1-C2-O2	5.59	122.25	118.90
3	L5	4678	A	C2-N3-C4	5.58	113.39	110.60
3	L5	4644	C	N1-C2-O2	5.58	122.25	118.90
46	S2	407	G	N3-C4-C5	-5.58	125.81	128.60
5	L8	107	C	C6-N1-C2	-5.58	118.07	120.30
3	L5	4098	G	O4'-C1'-N9	-5.57	103.74	108.20
3	L5	4727	U	C6-N1-C1'	-5.57	113.40	121.20
46	S2	676	C	N3-C2-O2	-5.57	118.00	121.90
3	L5	1911	C	C6-N1-C2	-5.57	118.07	120.30
52	SH	148	LEU	CA-CB-CG	5.56	128.10	115.30
3	L5	30	C	N1-C2-O2	5.56	122.23	118.90
3	L5	3905	C	N3-C2-O2	-5.56	118.01	121.90
3	L5	1973	U	N3-C2-O2	-5.55	118.31	122.20
3	L5	4213	C	N3-C2-O2	-5.55	118.01	121.90
3	L5	2042	G	OP2-P-O3'	5.55	117.41	105.20
3	L5	4110	C	N3-C2-O2	-5.55	118.02	121.90
3	L5	2886	C	N1-C2-O2	5.54	122.23	118.90
3	L5	36	U	N3-C2-O2	-5.54	118.32	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	317	C	C6-N1-C2	-5.54	118.08	120.30
3	L5	3849	C	C6-N1-C2	-5.54	118.08	120.30
3	L5	118	C	N3-C2-O2	-5.54	118.02	121.90
3	L5	1565	U	C5-C6-N1	5.54	125.47	122.70
24	LV	96	LEU	CA-CB-CG	5.53	128.02	115.30
4	L7	111	C	N3-C2-O2	-5.53	118.03	121.90
3	L5	4153	G	N3-C4-N9	5.53	129.32	126.00
3	L5	1649	C	C6-N1-C2	-5.52	118.09	120.30
3	L5	1232	C	N1-C2-O2	5.52	122.21	118.90
3	L5	3905	C	C6-N1-C2	-5.51	118.09	120.30
3	L5	1957	A	C8-N9-C4	5.51	108.00	105.80
3	L5	4357	C	N1-C2-O2	5.51	122.21	118.90
3	L5	1694	C	C6-N1-C1'	5.51	127.41	120.80
20	LR	15	LEU	CA-CB-CG	5.51	127.97	115.30
3	L5	1653	C	N3-C2-O2	-5.50	118.05	121.90
3	L5	4531	C	N3-C2-O2	-5.50	118.05	121.90
46	S2	407	G	P-O3'-C3'	5.50	126.31	119.70
4	L7	104	C	N3-C2-O2	-5.50	118.05	121.90
3	L5	1987	G	C4-N9-C1'	5.50	133.65	126.50
3	L5	4196	G	C6-C5-N7	-5.50	127.10	130.40
3	L5	4687	A	N9-C4-C5	-5.49	103.61	105.80
46	S2	1069	U	C5-C6-N1	5.48	125.44	122.70
3	L5	4946	G	N3-C4-N9	5.48	129.29	126.00
3	L5	4905	C	C6-N1-C2	-5.48	118.11	120.30
3	L5	1335	U	N3-C2-O2	-5.47	118.37	122.20
3	L5	4948	C	N3-C2-O2	-5.47	118.07	121.90
3	L5	1226	C	N3-C2-O2	-5.47	118.07	121.90
3	L5	1836	U	N3-C2-O2	-5.47	118.37	122.20
3	L5	1067	C	N1-C2-O2	5.46	122.18	118.90
3	L5	3898	C	C6-N1-C2	-5.46	118.11	120.30
79	Sf	103	LEU	CA-CB-CG	5.46	127.86	115.30
3	L5	1837	A	N7-C8-N9	5.46	116.53	113.80
3	L5	1602	C	C6-N1-C2	-5.46	118.12	120.30
3	L5	4402	C	C4-C5-C6	-5.46	114.67	117.40
3	L5	1561	G	P-O3'-C3'	5.46	126.25	119.70
3	L5	912	C	C6-N1-C2	-5.46	118.12	120.30
3	L5	1880	C	C6-N1-C2	-5.46	118.12	120.30
4	L7	78	C	C6-N1-C2	-5.46	118.12	120.30
13	LJ	174	ILE	CG1-CB-CG2	-5.46	99.40	111.40
3	L5	3905	C	N1-C2-O2	5.45	122.17	118.90
3	L5	2570	C	C6-N1-C2	-5.45	118.12	120.30
3	L5	4735	C	C5-C6-N1	5.45	123.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3909	U	N1-C2-O2	5.44	126.61	122.80
3	L5	2265	G	N3-C4-C5	-5.44	125.88	128.60
3	L5	1718	C	N3-C2-O2	-5.44	118.09	121.90
3	L5	3793	U	N1-C2-O2	5.44	126.61	122.80
3	L5	4211	C	N3-C2-O2	-5.43	118.10	121.90
3	L5	4689	G	C4-N9-C1'	5.43	133.56	126.50
3	L5	4434	A	N9-C4-C5	-5.43	103.63	105.80
20	LR	177	LEU	CA-CB-CG	5.43	127.79	115.30
3	L5	167	C	N3-C2-O2	-5.43	118.10	121.90
5	L8	118	C	N1-C2-O2	5.42	122.15	118.90
3	L5	359	C	N3-C2-O2	-5.42	118.11	121.90
3	L5	1916	A	N3-C4-N9	5.42	131.73	127.40
3	L5	288	U	N3-C2-O2	-5.42	118.41	122.20
5	L8	83	C	P-O3'-C3'	5.42	126.20	119.70
3	L5	1528	C	N1-C2-O2	5.42	122.15	118.90
3	L5	909	C	N1-C2-O2	5.41	122.15	118.90
3	L5	1841	G	N3-C4-C5	-5.41	125.89	128.60
3	L5	4364	A	N1-C6-N6	-5.41	115.35	118.60
3	L5	964	C	N1-C2-O2	5.41	122.14	118.90
3	L5	2547	C	N1-C2-O2	5.41	122.14	118.90
46	S2	532	C	N1-C2-O2	5.41	122.14	118.90
3	L5	4652	U	N3-C2-O2	-5.40	118.42	122.20
3	L5	1987	G	N3-C4-C5	-5.40	125.90	128.60
26	LX	116	LEU	CA-CB-CG	5.40	127.73	115.30
3	L5	138	C	C5-C6-N1	5.40	123.70	121.00
3	L5	3817	U	N3-C2-O2	-5.40	118.42	122.20
46	S2	424	C	N1-C2-O2	5.39	122.14	118.90
3	L5	1486	C	N1-C2-O2	5.39	122.13	118.90
3	L5	2789	C	C6-N1-C2	-5.39	118.14	120.30
3	L5	4211	C	N1-C2-O2	5.38	122.13	118.90
3	L5	2426	G	C4-N9-C1'	5.38	133.50	126.50
3	L5	219	C	N1-C2-O2	5.38	122.13	118.90
3	L5	2778	C	N1-C2-O2	5.38	122.13	118.90
3	L5	4176	C	C6-N1-C2	-5.38	118.15	120.30
3	L5	1494	C	N3-C2-O2	-5.37	118.14	121.90
3	L5	4735	C	C6-N1-C2	-5.37	118.15	120.30
3	L5	35	U	C5-C6-N1	5.37	125.39	122.70
3	L5	103	G	N9-C4-C5	-5.37	103.25	105.40
3	L5	4176	C	N3-C2-O2	-5.37	118.14	121.90
3	L5	2290	C	C6-N1-C2	-5.37	118.15	120.30
3	L5	4961	C	C6-N1-C2	-5.37	118.15	120.30
42	Ln	2	ARG	NE-CZ-NH1	5.37	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2874	U	N3-C2-O2	-5.37	118.44	122.20
3	L5	3801	U	C2-N1-C1'	5.36	124.13	117.70
3	L5	2817	G	C6-C5-N7	-5.36	127.19	130.40
3	L5	4057	C	N3-C2-O2	-5.36	118.15	121.90
3	L5	4501	U	C5-C6-N1	5.36	125.38	122.70
3	L5	1661	C	C6-N1-C2	-5.35	118.16	120.30
8	LE	177	GLY	N-CA-C	-5.35	99.72	113.10
3	L5	1565	U	N3-C2-O2	-5.35	118.46	122.20
3	L5	1808	G	C6-C5-N7	-5.34	127.19	130.40
3	L5	3625	A	C5-N7-C8	5.34	106.57	103.90
3	L5	4119	C	N1-C2-O2	5.34	122.11	118.90
67	Sg	135	LEU	CA-CB-CG	5.34	127.59	115.30
3	L5	2003	C	C6-N1-C2	-5.33	118.17	120.30
3	L5	4853	U	N1-C2-O2	5.33	126.53	122.80
3	L5	4715	C	C5-C6-N1	5.33	123.66	121.00
46	S2	1069	U	N3-C2-O2	-5.33	118.47	122.20
3	L5	4322	U	N3-C2-O2	-5.33	118.47	122.20
3	L5	1581	C	N3-C4-N4	-5.33	114.27	118.00
46	S2	1216	C	N3-C4-C5	5.32	124.03	121.90
3	L5	138	C	C6-N1-C2	-5.32	118.17	120.30
3	L5	3817	U	N1-C2-O2	5.32	126.52	122.80
3	L5	336	C	C6-N1-C2	-5.32	118.17	120.30
3	L5	5001	C	N1-C2-O2	5.32	122.09	118.90
3	L5	940	C	N3-C2-O2	-5.31	118.18	121.90
3	L5	2501	G	C4-N9-C1'	5.31	133.41	126.50
3	L5	2268	U	C2-N1-C1'	5.31	124.07	117.70
3	L5	1652	C	N3-C4-C5	5.31	124.02	121.90
3	L5	4649	G	C4-C5-N7	5.31	112.92	110.80
3	L5	4404	C	C5-C6-N1	5.30	123.65	121.00
3	L5	1720	G	C6-C5-N7	-5.30	127.22	130.40
4	L7	68	C	N3-C2-O2	-5.30	118.19	121.90
46	S2	1067	C	N1-C2-O2	5.30	122.08	118.90
3	L5	2492	C	N3-C2-O2	-5.30	118.19	121.90
3	L5	1916	A	C8-N9-C1'	-5.30	118.16	127.70
3	L5	4359	C	N3-C2-O2	-5.29	118.19	121.90
3	L5	2697	C	C6-N1-C1'	-5.29	114.45	120.80
3	L5	3801	U	N1-C2-O2	5.29	126.50	122.80
3	L5	1956	G	C4-N9-C1'	5.29	133.38	126.50
46	S2	1824	A	P-O3'-C3'	5.29	126.05	119.70
3	L5	67	C	N3-C2-O2	-5.29	118.20	121.90
46	S2	188	C	N1-C2-O2	5.28	122.07	118.90
3	L5	2247	C	C5-C6-N1	5.28	123.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3754	A	O4'-C1'-N9	5.28	112.42	108.20
3	L5	4501	U	N3-C2-O2	-5.27	118.51	122.20
46	S2	1742	C	N1-C2-O2	5.27	122.06	118.90
3	L5	4110	C	C5-C6-N1	5.27	123.64	121.00
3	L5	1564	G	C8-N9-C1'	-5.26	120.16	127.00
3	L5	3647	C	N3-C2-O2	-5.26	118.22	121.90
3	L5	4363	G	OP1-P-O3'	5.26	116.78	105.20
3	L5	1873	G	N9-C4-C5	-5.26	103.30	105.40
3	L5	4050	C	N3-C2-O2	-5.26	118.22	121.90
3	L5	219	C	N3-C2-O2	-5.26	118.22	121.90
3	L5	1601	C	N3-C2-O2	-5.26	118.22	121.90
3	L5	1437	C	N1-C2-O2	5.26	122.06	118.90
3	L5	1674	U	N1-C2-O2	5.26	126.48	122.80
3	L5	3632	A	N9-C4-C5	-5.26	103.70	105.80
38	Lj	64	MET	CA-CB-CG	5.26	122.24	113.30
3	L5	941	C	C6-N1-C2	-5.25	118.20	120.30
3	L5	1839	U	N3-C2-O2	-5.25	118.52	122.20
46	S2	1172	U	N1-C2-O2	5.25	126.48	122.80
3	L5	4110	C	C6-N1-C2	-5.25	118.20	120.30
3	L5	1285	C	C6-N1-C2	-5.25	118.20	120.30
3	L5	4076	A	C2-N3-C4	5.25	113.22	110.60
52	SH	28	LEU	CA-CB-CG	5.25	127.36	115.30
3	L5	2289	C	N1-C2-O2	5.24	122.05	118.90
46	S2	1078	C	C6-N1-C2	-5.24	118.20	120.30
5	L8	118	C	N3-C2-O2	-5.24	118.23	121.90
3	L5	39	A	N1-C6-N6	-5.24	115.46	118.60
3	L5	4361	G	N1-C6-O6	-5.24	116.76	119.90
3	L5	1796	C	N3-C2-O2	-5.24	118.23	121.90
3	L5	2035	U	N3-C2-O2	-5.24	118.53	122.20
3	L5	2671	C	C5-C6-N1	5.23	123.61	121.00
3	L5	4716	C	C2-N1-C1'	5.23	124.55	118.80
3	L5	447	C	C6-N1-C2	-5.22	118.21	120.30
3	L5	1230	C	N3-C2-O2	-5.22	118.24	121.90
3	L5	1900	C	N3-C2-O2	-5.22	118.24	121.90
3	L5	1642	C	N1-C2-O2	5.22	122.03	118.90
3	L5	2391	A	C2-N3-C4	5.22	113.21	110.60
3	L5	2432	C	N1-C2-O2	5.22	122.03	118.90
46	S2	1520	G	N3-C4-C5	-5.21	125.99	128.60
3	L5	4649	G	N9-C4-C5	-5.21	103.32	105.40
3	L5	1337	C	N1-C2-O2	5.21	122.02	118.90
46	S2	659	G	C8-N9-C1'	-5.21	120.23	127.00
3	L5	2445	C	N1-C2-O2	5.20	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4236	G	N3-C4-C5	5.20	131.20	128.60
3	L5	4609	G	C4-N9-C1'	5.19	133.25	126.50
3	L5	138	C	C2-N1-C1'	5.19	124.51	118.80
3	L5	5016	C	N3-C2-O2	-5.19	118.27	121.90
3	L5	2570	C	N1-C2-O2	5.19	122.01	118.90
46	S2	1454	A	P-O3'-C3'	5.19	125.92	119.70
3	L5	3675	C	N1-C2-O2	5.19	122.01	118.90
3	L5	5007	A	C2-N3-C4	5.18	113.19	110.60
3	L5	1718	C	C6-N1-C2	-5.17	118.23	120.30
3	L5	950	G	C4-N9-C1'	5.17	133.22	126.50
3	L5	3692	U	N1-C2-O2	5.17	126.42	122.80
3	L5	4460	C	C6-N1-C2	-5.17	118.23	120.30
46	S2	430	C	C6-N1-C2	-5.17	118.23	120.30
3	L5	1656	A	N1-C6-N6	-5.17	115.50	118.60
3	L5	1991	U	C5-C6-N1	5.17	125.28	122.70
3	L5	4071	G	O4'-C1'-N9	5.17	112.33	108.20
5	L8	62	A	C2-N3-C4	5.17	113.18	110.60
3	L5	4531	C	C6-N1-C2	-5.16	118.23	120.30
3	L5	5001	C	N3-C2-O2	-5.16	118.29	121.90
3	L5	2083	G	C6-C5-N7	-5.16	127.31	130.40
3	L5	313	C	N1-C2-O2	5.16	121.99	118.90
3	L5	3690	A	C8-N9-C1'	-5.16	118.42	127.70
2	LB	214	ASP	CB-CG-OD1	5.15	122.94	118.30
3	L5	265	C	N3-C2-O2	-5.15	118.30	121.90
3	L5	2035	U	N1-C2-O2	5.15	126.41	122.80
3	L5	3659	U	N3-C2-O2	-5.15	118.60	122.20
46	S2	994	C	C6-N1-C2	-5.15	118.24	120.30
3	L5	2394	G	O4'-C1'-N9	5.14	112.31	108.20
3	L5	273	C	N1-C2-O2	5.14	121.99	118.90
3	L5	1565	U	N1-C2-O2	5.14	126.40	122.80
3	L5	2324	C	C2-N1-C1'	5.14	124.46	118.80
3	L5	2817	G	N3-C4-N9	5.14	129.08	126.00
46	S2	453	C	N3-C2-O2	-5.14	118.30	121.90
3	L5	1382	U	N3-C2-O2	-5.14	118.60	122.20
3	L5	3816	C	N3-C2-O2	-5.14	118.30	121.90
3	L5	4359	C	C6-N1-C2	-5.14	118.25	120.30
46	S2	453	C	C2-N1-C1'	5.14	124.45	118.80
3	L5	1564	G	C4-N9-C1'	5.13	133.17	126.50
3	L5	3629	C	N3-C2-O2	-5.13	118.31	121.90
3	L5	1235	C	N1-C2-O2	5.13	121.97	118.90
3	L5	1296	C	C6-N1-C2	-5.12	118.25	120.30
3	L5	710	C	C6-N1-C2	-5.12	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2527	C	C6-N1-C2	-5.12	118.25	120.30
46	S2	1242	U	N1-C2-O2	5.12	126.38	122.80
46	S2	402	C	C5-C6-N1	5.12	123.56	121.00
3	L5	4867	C	N1-C2-O2	5.11	121.97	118.90
3	L5	2094	C	N1-C2-O2	5.11	121.97	118.90
46	S2	409	C	C6-N1-C2	-5.11	118.26	120.30
3	L5	975	C	N1-C2-O2	5.11	121.97	118.90
3	L5	1720	G	C8-N9-C1'	-5.11	120.36	127.00
3	L5	4312	C	C6-N1-C2	-5.11	118.26	120.30
46	S2	1002	U	N1-C2-O2	5.11	126.38	122.80
3	L5	2439	G	C6-C5-N7	-5.11	127.34	130.40
3	L5	2439	G	C4-C5-N7	5.10	112.84	110.80
3	L5	4391	C	C5-C6-N1	5.10	123.55	121.00
3	L5	1782	A	N1-C2-N3	-5.10	126.75	129.30
3	L5	4074	C	C6-N1-C2	-5.10	118.26	120.30
3	L5	4244	A	N1-C6-N6	-5.10	115.54	118.60
3	L5	4883	C	N1-C2-O2	5.10	121.96	118.90
46	S2	877	C	N3-C2-O2	-5.10	118.33	121.90
3	L5	1694	C	C5-C6-N1	5.10	123.55	121.00
3	L5	1893	U	C5-C6-N1	5.10	125.25	122.70
3	L5	2570	C	N3-C2-O2	-5.10	118.33	121.90
3	L5	3570	C	C6-N1-C2	-5.09	118.26	120.30
46	S2	402	C	C6-N1-C2	-5.09	118.26	120.30
3	L5	280	C	C6-N1-C2	-5.09	118.26	120.30
3	L5	3859	G	C4-C5-N7	5.09	112.84	110.80
3	L5	1339	C	C4-C5-C6	-5.09	114.85	117.40
3	L5	3757	U	N3-C2-O2	-5.09	118.64	122.20
3	L5	3645	C	C6-N1-C2	-5.09	118.26	120.30
3	L5	4585	C	C6-N1-C2	-5.09	118.26	120.30
46	S2	1716	C	C6-N1-C2	-5.09	118.26	120.30
3	L5	502	C	N1-C2-O2	5.09	121.95	118.90
46	S2	1022	U	C6-N1-C1'	-5.09	114.08	121.20
3	L5	79	C	N1-C2-O2	5.08	121.95	118.90
3	L5	4236	G	C2-N3-C4	-5.08	109.36	111.90
3	L5	89	C	N1-C2-O2	5.08	121.95	118.90
3	L5	950	G	N3-C4-N9	5.08	129.05	126.00
3	L5	2805	C	C6-N1-C2	-5.08	118.27	120.30
46	S2	474	G	C4-N9-C1'	5.08	133.10	126.50
46	S2	494	C	N1-C2-O2	5.08	121.95	118.90
46	S2	970	G	C4-N9-C1'	-5.08	119.90	126.50
3	L5	4680	C	C6-N1-C2	-5.08	118.27	120.30
3	L5	2024	C	N1-C2-O2	5.08	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2843	C	C6-N1-C2	-5.08	118.27	120.30
46	S2	106	C	C6-N1-C2	-5.08	118.27	120.30
46	S2	1032	C	N3-C2-O2	-5.08	118.35	121.90
3	L5	2022	C	C6-N1-C2	-5.07	118.27	120.30
46	S2	1862	G	N1-C6-O6	-5.07	116.86	119.90
3	L5	2680	G	N1-C6-O6	-5.07	116.86	119.90
3	L5	2854	C	N3-C2-O2	-5.07	118.35	121.90
3	L5	2879	C	N3-C2-O2	-5.07	118.35	121.90
5	L8	126	C	O4'-C1'-N1	5.07	112.25	108.20
3	L5	3763	A	C8-N9-C4	5.06	107.83	105.80
3	L5	1911	C	C5-C6-N1	5.06	123.53	121.00
3	L5	1662	C	N3-C2-O2	-5.06	118.36	121.90
3	L5	1498	U	N1-C2-O2	5.06	126.34	122.80
3	L5	660	C	N1-C2-O2	5.06	121.94	118.90
3	L5	1969	G	N7-C8-N9	5.06	115.63	113.10
3	L5	4057	C	N1-C2-O2	5.06	121.93	118.90
46	S2	1172	U	N3-C2-O2	-5.06	118.66	122.20
46	S2	1314	U	C2-N1-C1'	5.06	123.77	117.70
4	L7	2	U	N3-C2-O2	-5.06	118.66	122.20
5	L8	32	C	C5-C6-N1	5.06	123.53	121.00
3	L5	53	C	C6-N1-C2	-5.05	118.28	120.30
3	L5	2054	C	N3-C2-O2	-5.05	118.36	121.90
3	L5	1579	G	C4-N9-C1'	5.05	133.06	126.50
46	S2	1837	G	C4-N9-C1'	-5.05	119.94	126.50
3	L5	2564	C	N1-C2-O2	5.04	121.93	118.90
46	S2	140	C	P-O3'-C3'	5.04	125.75	119.70
3	L5	1607	U	C5-C6-N1	5.04	125.22	122.70
3	L5	2496	C	C6-N1-C2	-5.04	118.29	120.30
3	L5	3872	C	N1-C2-O2	5.04	121.92	118.90
46	S2	1259	A	C2-N3-C4	5.03	113.12	110.60
32	Ld	33	ILE	CG1-CB-CG2	-5.03	100.34	111.40
46	S2	223	C	N1-C2-O2	5.03	121.92	118.90
3	L5	4111	C	N1-C2-O2	5.03	121.92	118.90
42	Ln	10	MET	CA-CB-CG	5.03	121.85	113.30
46	S2	917	U	N1-C2-O2	5.03	126.32	122.80
3	L5	4256	C	N1-C2-O2	5.03	121.92	118.90
3	L5	351	A	N1-C2-N3	-5.02	126.79	129.30
3	L5	663	C	N3-C2-O2	-5.02	118.39	121.90
3	L5	4689	G	C8-N9-C1'	-5.02	120.47	127.00
3	L5	314	C	N1-C2-O2	5.02	121.91	118.90
3	L5	2843	C	N3-C2-O2	-5.02	118.39	121.90
9	LF	136	VAL	CG1-CB-CG2	-5.02	102.88	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	323	C	N1-C2-O2	5.01	121.91	118.90
3	L5	2444	G	C8-N9-C4	-5.01	104.40	106.40
3	L5	4213	C	C6-N1-C2	-5.01	118.30	120.30
3	L5	1566	C	C6-N1-C2	-5.01	118.30	120.30
3	L5	2305	G	N9-C4-C5	-5.01	103.40	105.40
4	L7	43	U	N3-C2-O2	-5.01	118.69	122.20
3	L5	2716	C	N3-C2-O2	-5.00	118.40	121.90
3	L5	8	U	N3-C2-O2	-5.00	118.70	122.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
46	S2	1248	B8N	C33

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	LA	246	LEU	Peptide
7	LD	43	LYS	Peptide
8	LE	176	THR	Peptide
11	LH	173	ARG	Peptide
13	LJ	10	ASN	Peptide
21	LS	5	GLY	Peptide
22	LT	80	VAL	Peptide
23	LU	97	ARG	Peptide
29	La	23	GLY	Peptide
34	Lf	103	VAL	Peptide
34	Lf	106	TYR	Peptide
36	Lh	86	LYS	Peptide
38	Lj	39	TYR	Peptide
45	Lr	20	ARG	Peptide
52	SH	11	PRO	Peptide
70	SJ	137	VAL	Peptide
74	SW	28	ARG	Peptide
63	SX	86	PRO	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
2	LB	394/396 (100%)	379 (96%)	15 (4%)	0	100	100
6	LC	355/358 (99%)	340 (96%)	14 (4%)	1 (0%)	37	67
7	LD	288/290 (99%)	275 (96%)	13 (4%)	0	100	100
8	LE	232/247 (94%)	206 (89%)	26 (11%)	0	100	100
9	LF	224/225 (100%)	212 (95%)	12 (5%)	0	100	100
10	LG	240/241 (100%)	223 (93%)	17 (7%)	0	100	100
11	LH	188/190 (99%)	171 (91%)	17 (9%)	0	100	100
12	LI	203/213 (95%)	191 (94%)	12 (6%)	0	100	100
13	LJ	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
14	LL	202/204 (99%)	182 (90%)	20 (10%)	0	100	100
15	LM	137/139 (99%)	127 (93%)	9 (7%)	1 (1%)	19	48
16	LN	201/203 (99%)	193 (96%)	5 (2%)	3 (2%)	8	29
17	LO	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
18	LP	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
19	LQ	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
20	LR	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
21	LS	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
22	LT	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
23	LU	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
24	LV	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
25	LW	122/124 (98%)	108 (88%)	14 (12%)	0	100	100
26	LX	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
27	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
28	LZ	133/135 (98%)	120 (90%)	13 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	La	145/147 (99%)	136 (94%)	8 (6%)	1 (1%)	19	48
30	Lb	105/121 (87%)	95 (90%)	10 (10%)	0	100	100
31	Lc	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
32	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
33	Le	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	16	44
34	Lf	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	42
35	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
38	Lj	85/86 (99%)	78 (92%)	6 (7%)	1 (1%)	11	34
39	Lk	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
40	Ll	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
41	Lm	49/52 (94%)	47 (96%)	2 (4%)	0	100	100
42	Ln	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
43	Lo	104/105 (99%)	99 (95%)	5 (5%)	0	100	100
44	Lp	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
45	Lr	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
47	SA	214/216 (99%)	199 (93%)	14 (6%)	1 (0%)	25	56
48	SB	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
49	SD	222/224 (99%)	210 (95%)	12 (5%)	0	100	100
50	SE	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
51	SF	181/189 (96%)	168 (93%)	12 (7%)	1 (1%)	22	51
52	SH	181/189 (96%)	167 (92%)	14 (8%)	0	100	100
53	SI	193/205 (94%)	185 (96%)	8 (4%)	0	100	100
54	SK	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
55	SL	136/150 (91%)	130 (96%)	6 (4%)	0	100	100
56	SP	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
57	SQ	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
58	SR	129/131 (98%)	119 (92%)	10 (8%)	0	100	100
59	SS	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
60	ST	139/141 (99%)	129 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	SU	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
62	SV	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
63	SX	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
64	Sa	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	13	39
65	Sc	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
66	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
67	Sg	311/313 (99%)	271 (87%)	40 (13%)	0	100	100
68	SC	219/220 (100%)	212 (97%)	7 (3%)	0	100	100
69	SG	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
70	SJ	178/180 (99%)	174 (98%)	3 (2%)	1 (1%)	22	51
71	SM	108/120 (90%)	102 (94%)	6 (6%)	0	100	100
72	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
73	SO	131/135 (97%)	121 (92%)	10 (8%)	0	100	100
74	SW	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	44
75	SY	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
76	SZ	68/70 (97%)	68 (100%)	0	0	100	100
77	Sb	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
78	Se	47/54 (87%)	44 (94%)	3 (6%)	0	100	100
79	Sf	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
81	j	365/411 (89%)	325 (89%)	34 (9%)	6 (2%)	8	27
83	NC	23/25 (92%)	22 (96%)	0	1 (4%)	2	7
All	All	11569/11850 (98%)	10840 (94%)	708 (6%)	21 (0%)	45	73

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	LC	222	ARG
16	LN	124	ASP
29	La	24	LYS
81	j	305	VAL
33	Le	73	GLY
47	SA	12	GLU
51	SF	80	GLY
81	j	105	GLY
15	LM	32	ASP

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Mol	Chain	Res	Type
34	Lf	107	PRO
64	Sa	47	ALA
81	j	118	LYS
38	Lj	40	PRO
81	j	119	PRO
83	NC	727	PRO
70	SJ	138	ARG
16	LN	84	PRO
81	j	184	GLY
74	SW	29	PRO
16	LN	83	LYS
81	j	250	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LA	190/190 (100%)	183 (96%)	7 (4%)	29	63
2	LB	345/345 (100%)	341 (99%)	4 (1%)	67	89
6	LC	298/298 (100%)	293 (98%)	5 (2%)	56	84
7	LD	244/245 (100%)	243 (100%)	1 (0%)	89	96
8	LE	209/220 (95%)	204 (98%)	5 (2%)	44	77
9	LF	195/194 (100%)	194 (100%)	1 (0%)	86	95
10	LG	204/205 (100%)	200 (98%)	4 (2%)	50	81
11	LH	169/169 (100%)	164 (97%)	5 (3%)	36	70
12	LI	177/180 (98%)	176 (99%)	1 (1%)	84	95
13	LJ	148/148 (100%)	146 (99%)	2 (1%)	62	87
14	LL	170/170 (100%)	164 (96%)	6 (4%)	31	65
15	LM	118/118 (100%)	117 (99%)	1 (1%)	79	93
16	LN	171/171 (100%)	169 (99%)	2 (1%)	67	89
17	LO	173/173 (100%)	171 (99%)	2 (1%)	67	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	LP	134/134 (100%)	133 (99%)	1 (1%)	81	94
19	LQ	164/164 (100%)	162 (99%)	2 (1%)	67	89
20	LR	166/166 (100%)	157 (95%)	9 (5%)	18	48
21	LS	156/156 (100%)	152 (97%)	4 (3%)	41	75
22	LT	139/139 (100%)	138 (99%)	1 (1%)	81	94
23	LU	91/91 (100%)	91 (100%)	0	100	100
24	LV	101/101 (100%)	98 (97%)	3 (3%)	36	70
25	LW	103/103 (100%)	102 (99%)	1 (1%)	73	91
26	LX	108/108 (100%)	108 (100%)	0	100	100
27	LY	124/124 (100%)	120 (97%)	4 (3%)	34	68
28	LZ	117/117 (100%)	113 (97%)	4 (3%)	32	66
29	La	120/120 (100%)	119 (99%)	1 (1%)	79	93
30	Lb	89/100 (89%)	87 (98%)	2 (2%)	47	79
31	Lc	83/83 (100%)	83 (100%)	0	100	100
32	Ld	98/98 (100%)	98 (100%)	0	100	100
33	Le	114/114 (100%)	111 (97%)	3 (3%)	41	75
34	Lf	88/88 (100%)	88 (100%)	0	100	100
35	Lg	98/98 (100%)	97 (99%)	1 (1%)	73	91
36	Lh	109/109 (100%)	108 (99%)	1 (1%)	75	92
37	Li	86/86 (100%)	84 (98%)	2 (2%)	45	78
38	Lj	74/73 (101%)	74 (100%)	0	100	100
39	Lk	64/64 (100%)	64 (100%)	0	100	100
40	Ll	47/47 (100%)	46 (98%)	1 (2%)	48	80
41	Lm	47/47 (100%)	47 (100%)	0	100	100
42	Ln	23/23 (100%)	23 (100%)	0	100	100
43	Lo	94/93 (101%)	93 (99%)	1 (1%)	70	90
44	Lp	74/74 (100%)	74 (100%)	0	100	100
45	Lr	109/109 (100%)	108 (99%)	1 (1%)	75	92
47	SA	180/180 (100%)	178 (99%)	2 (1%)	70	90
48	SB	193/193 (100%)	192 (100%)	1 (0%)	86	95
49	SD	188/188 (100%)	186 (99%)	2 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	SE	221/221 (100%)	217 (98%)	4 (2%)	54	83
51	SF	158/159 (99%)	155 (98%)	3 (2%)	52	82
52	SH	165/169 (98%)	164 (99%)	1 (1%)	84	95
53	SI	172/178 (97%)	171 (99%)	1 (1%)	84	95
54	SK	86/86 (100%)	85 (99%)	1 (1%)	67	89
55	SL	126/134 (94%)	123 (98%)	3 (2%)	44	77
56	SP	117/117 (100%)	117 (100%)	0	100	100
57	SQ	116/116 (100%)	115 (99%)	1 (1%)	75	92
58	SR	119/119 (100%)	118 (99%)	1 (1%)	79	93
59	SS	124/124 (100%)	123 (99%)	1 (1%)	79	93
60	ST	111/111 (100%)	109 (98%)	2 (2%)	54	83
61	SU	93/93 (100%)	92 (99%)	1 (1%)	70	90
62	SV	67/67 (100%)	66 (98%)	1 (2%)	60	86
63	SX	111/111 (100%)	111 (100%)	0	100	100
64	Sa	86/86 (100%)	85 (99%)	1 (1%)	67	89
65	Sc	54/54 (100%)	53 (98%)	1 (2%)	52	82
66	Sd	48/48 (100%)	48 (100%)	0	100	100
67	Sg	272/272 (100%)	268 (98%)	4 (2%)	60	86
68	SC	187/186 (100%)	186 (100%)	1 (0%)	86	95
69	SG	199/199 (100%)	196 (98%)	3 (2%)	60	86
70	SJ	160/160 (100%)	160 (100%)	0	100	100
71	SM	93/102 (91%)	92 (99%)	1 (1%)	70	90
72	SN	130/130 (100%)	128 (98%)	2 (2%)	60	86
73	SO	104/104 (100%)	101 (97%)	3 (3%)	37	71
74	SW	112/112 (100%)	111 (99%)	1 (1%)	75	92
75	SY	107/107 (100%)	106 (99%)	1 (1%)	75	92
76	SZ	62/62 (100%)	61 (98%)	1 (2%)	58	85
77	Sb	74/74 (100%)	74 (100%)	0	100	100
78	Se	42/44 (96%)	42 (100%)	0	100	100
79	Sf	56/56 (100%)	55 (98%)	1 (2%)	54	83
81	j	317/353 (90%)	272 (86%)	45 (14%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	NC	19/19 (100%)	18 (95%)	1 (5%)	19	49
All	All	10100/10189 (99%)	9921 (98%)	179 (2%)	54	83

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LA	64	ARG
1	LA	68	ARG
1	LA	89	TYR
1	LA	143	THR
1	LA	193	ARG
1	LA	207	VAL
1	LA	247	ARG
2	LB	10	ARG
2	LB	101	THR
2	LB	297	LYS
2	LB	396	ARG
6	LC	71	ARG
6	LC	95	MET
6	LC	188	ARG
6	LC	317	ASN
6	LC	329	ASN
7	LD	250	ASN
8	LE	56	ARG
8	LE	100	LYS
8	LE	109	LEU
8	LE	210	LYS
8	LE	239	LYS
9	LF	236	ARG
10	LG	111	LYS
10	LG	137[A]	ARG
10	LG	137[B]	ARG
10	LG	175	ARG
11	LH	51	LYS
11	LH	54	ARG
11	LH	71	ARG
11	LH	116	ASN
11	LH	156	ASN
12	LI	7	ARG
13	LJ	43	LEU
13	LJ	146	ARG
14	LL	6	ASN

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Mol	Chain	Res	Type
14	LL	70	VAL
14	LL	124	LEU
14	LL	145	LYS
14	LL	162	LYS
14	LL	165	LYS
15	LM	25	VAL
16	LN	193	ARG
16	LN	204	ARG
17	LO	60	LYS
17	LO	61	ARG
18	LP	24	VAL
19	LQ	83	VAL
19	LQ	144	LYS
20	LR	16	ARG
20	LR	114	LYS
20	LR	130	ASN
20	LR	137	ILE
20	LR	163	ARG
20	LR	167	LYS
20	LR	171	LYS
20	LR	172	ARG
20	LR	186	LYS
21	LS	15	ARG
21	LS	52	LYS
21	LS	83	ARG
21	LS	90	THR
22	LT	117	LYS
24	LV	15	ARG
24	LV	46	LYS
24	LV	95	PHE
25	LW	77	LYS
27	LY	4	ASN
27	LY	27	ARG
27	LY	79	VAL
27	LY	117	LYS
28	LZ	74	VAL
28	LZ	84	ARG
28	LZ	93	LYS
28	LZ	111	ARG
29	La	93	ASN
30	Lb	60	ASN
30	Lb	68	ARG

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Mol	Chain	Res	Type
33	Le	33	ARG
33	Le	43	ASN
33	Le	92	ASN
35	Lg	54	ARG
36	Lh	112	ARG
37	Li	12	ASN
37	Li	29	ARG
40	Ll	46	ARG
43	Lo	99	ARG
45	Lr	41	ASN
47	SA	50	ASN
47	SA	117	ARG
48	SB	38	MET
49	SD	54	ARG
49	SD	76	ARG
50	SE	108	ARG
50	SE	197	ASN
50	SE	198	ARG
50	SE	255	ARG
51	SF	41	VAL
51	SF	83	ASN
51	SF	91	ARG
52	SH	41	ARG
53	SI	84	ASN
54	SK	39	ASN
55	SL	65	ASN
55	SL	69	ARG
55	SL	132	ARG
57	SQ	146	ARG
58	SR	78	ARG
59	SS	8	LYS
60	ST	41	LYS
60	ST	112	MET
61	SU	41	ARG
62	SV	1	MET
64	Sa	15	ARG
65	Sc	40	ARG
67	Sg	46	THR
67	Sg	47	ARG
67	Sg	60	ARG
67	Sg	162	ASN
68	SC	61	MET

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Mol	Chain	Res	Type
69	SG	14	LYS
69	SG	22	ARG
69	SG	98	ARG
71	SM	129	LYS
72	SN	19	ARG
72	SN	106	ARG
73	SO	130	GLU
73	SO	131	ASP
73	SO	150	ARG
74	SW	57	ARG
75	SY	110	ARG
76	SZ	43	LYS
79	Sf	95	ARG
81	j	16	LYS
81	j	19	LYS
81	j	43	ASP
81	j	51	MET
81	j	61	ASN
81	j	65	ARG
81	j	69	LEU
81	j	70	SER
81	j	79	GLN
81	j	81	ARG
81	j	82	LEU
81	j	84	LEU
81	j	99	THR
81	j	106	LYS
81	j	108	LYS
81	j	109	LYS
81	j	110	VAL
81	j	118	LYS
81	j	124	LEU
81	j	133	THR
81	j	136	LEU
81	j	137	THR
81	j	145	LYS
81	j	165	THR
81	j	166	ARG
81	j	167	GLU
81	j	171	LYS
81	j	173	THR
81	j	174	VAL

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Mol	Chain	Res	Type
81	j	186	SER
81	j	212	LEU
81	j	233	LYS
81	j	245	ARG
81	j	249	LYS
81	j	251	LEU
81	j	253	LEU
81	j	261	GLU
81	j	270	LEU
81	j	271	SER
81	j	272	THR
81	j	273	GLU
81	j	275	LEU
81	j	276	SER
81	j	289	ARG
81	j	300	LYS
83	NC	718	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	LA	38	HIS
1	LA	132	ASN
1	LA	139	HIS
2	LB	315	ASN
6	LC	329	ASN
7	LD	63	GLN
7	LD	195	HIS
7	LD	244	HIS
7	LD	250	ASN
8	LE	190	HIS
8	LE	191	GLN
8	LE	268	GLN
9	LF	63	GLN
9	LF	119	ASN
11	LH	42	ASN
11	LH	108	ASN
11	LH	116	ASN
11	LH	156	ASN
12	LI	14	ASN
13	LJ	3	GLN
13	LJ	104	ASN

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Mol	Chain	Res	Type
14	LL	6	ASN
14	LL	205	GLN
15	LM	20	HIS
16	LN	139	HIS
16	LN	196	ASN
18	LP	21	ASN
18	LP	34	GLN
18	LP	97	ASN
18	LP	116	HIS
19	LQ	21	GLN
19	LQ	45	GLN
20	LR	7	GLN
20	LR	130	ASN
21	LS	77	ASN
22	LT	114	GLN
27	LY	4	ASN
27	LY	14	ASN
28	LZ	78	ASN
29	La	28	HIS
29	La	66	ASN
29	La	93	ASN
30	Lb	12	GLN
30	Lb	19	ASN
30	Lb	49	HIS
32	Ld	79	ASN
32	Ld	93	ASN
33	Le	43	ASN
34	Lf	80	ASN
35	Lg	3	GLN
35	Lg	28	ASN
37	Li	12	ASN
37	Li	92	ASN
38	Lj	13	ASN
43	Lo	45	GLN
44	Lp	56	HIS
45	Lr	41	ASN
47	SA	50	ASN
47	SA	193	HIS
48	SB	179	ASN
48	SB	186	ASN
50	SE	98	ASN
50	SE	112	HIS

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Mol	Chain	Res	Type
50	SE	142	HIS
50	SE	157	ASN
50	SE	188	ASN
50	SE	197	ASN
51	SF	83	ASN
52	SH	91	HIS
53	SI	84	ASN
53	SI	181	GLN
54	SK	7	ASN
54	SK	39	ASN
54	SK	73	ASN
55	SL	65	ASN
56	SP	41	GLN
62	SV	35	ASN
65	Sc	24	GLN
65	Sc	29	GLN
67	Sg	64	HIS
67	Sg	162	ASN
69	SG	81	HIS
69	SG	163	ASN
69	SG	202	ASN
70	SJ	154	GLN
71	SM	48	HIS
72	SN	5	HIS
72	SN	49	GLN
73	SO	32	HIS
74	SW	98	GLN
77	Sb	19	HIS
81	j	79	GLN
81	j	80	GLN
81	j	121	ASN
81	j	211	GLN
81	j	265	ASN
83	NC	726	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3484/3510 (99%)	797 (22%)	14 (0%)
4	L7	119/120 (99%)	19 (15%)	0
46	S2	1571/1590 (98%)	324 (20%)	10 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L8	154/155 (99%)	27 (17%)	1 (0%)
80	Bv	72/76 (94%)	40 (55%)	0
82	k	12/13 (92%)	7 (58%)	0
All	All	5412/5464 (99%)	1214 (22%)	25 (0%)

All (1214) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	8	U
3	L5	12	A
3	L5	13	U
3	L5	17	A
3	L5	21	G
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A
3	L5	44	A
3	L5	56	A
3	L5	58	G
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	66	A
3	L5	72	C
3	L5	74	G
3	L5	75	G
3	L5	91	G
3	L5	95	G
3	L5	98	A
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	117	C
3	L5	119	G
3	L5	120	A
3	L5	121	A
3	L5	147	U
3	L5	149	U
3	L5	156	C
3	L5	162	A

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Mol	Chain	Res	Type
3	L5	168	U
3	L5	169	C
3	L5	197	U
3	L5	206	U
3	L5	207	C
3	L5	222	G
3	L5	229	G
3	L5	230	U
3	L5	231	G
3	L5	250	G
3	L5	254	G
3	L5	269	G
3	L5	271	G
3	L5	288	U
3	L5	297	A
3	L5	306	G
3	L5	307	U
3	L5	331	C
3	L5	332	G
3	L5	344	A
3	L5	351	A
3	L5	354	A
3	L5	376	A
3	L5	378	G
3	L5	379	A
3	L5	390	G
3	L5	392	G
3	L5	398	A
3	L5	400	G
3	L5	401	A
3	L5	403	G
3	L5	404	G
3	L5	405	C
3	L5	422	G
3	L5	423	U
3	L5	440	C
3	L5	441	G
3	L5	442	C
3	L5	443	A
3	L5	444	G
3	L5	445	U
3	L5	452	G

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Mol	Chain	Res	Type
3	L5	458	U
3	L5	459	U
3	L5	474	G
3	L5	476	C
3	L5	498	G
3	L5	501	U
3	L5	661	G
3	L5	664	C
3	L5	665	G
3	L5	676	C
3	L5	677	A
3	L5	678	U
3	L5	681	C
3	L5	687	C
3	L5	688	G
3	L5	694	G
3	L5	695	C
3	L5	699	G
3	L5	721	G
3	L5	722	G
3	L5	729	C
3	L5	730	G
3	L5	731	G
3	L5	733	G
3	L5	737	A
3	L5	740	G
3	L5	744	C
3	L5	745	U
3	L5	748	G
3	L5	899	G
3	L5	901	U
3	L5	902	A
3	L5	904	A
3	L5	905	G
3	L5	910	C
3	L5	911	C
3	L5	913	G
3	L5	919	A
3	L5	920	G
3	L5	921	C
3	L5	922	A
3	L5	923	C

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Mol	Chain	Res	Type
3	L5	930	A
3	L5	932	U
3	L5	946	G
3	L5	947	A
3	L5	948	G
3	L5	949	C
3	L5	950	G
3	L5	951	A
3	L5	952	G
3	L5	953	A
3	L5	957	G
3	L5	958	U
3	L5	959	C
3	L5	1057	G
3	L5	1059	C
3	L5	1061	G
3	L5	1062	G
3	L5	1083	C
3	L5	1157	G
3	L5	1162	A
3	L5	1167	U
3	L5	1168	C
3	L5	1169	C
3	L5	1170	C
3	L5	1189	C
3	L5	1190	G
3	L5	1197	C
3	L5	1198	G
3	L5	1202	C
3	L5	1203	C
3	L5	1204	G
3	L5	1206	G
3	L5	1228	C
3	L5	1249	G
3	L5	1253	G
3	L5	1259	C
3	L5	1260	G
3	L5	1264	G
3	L5	1266	A
3	L5	1267	C
3	L5	1271	G
3	L5	1272	U

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Mol	Chain	Res	Type
3	L5	1274	G
3	L5	1280	G
3	L5	1281	A
3	L5	1282	C
3	L5	1283	G
3	L5	1288	C
3	L5	1289	U
3	L5	1290	A
3	L5	1301	C
3	L5	1303	OMG
3	L5	1311	A
3	L5	1313	A2M
3	L5	1315	G
3	L5	1324	A
3	L5	1341	A
3	L5	1345	G
3	L5	1346	G
3	L5	1347	G
3	L5	1352	C
3	L5	1357	G
3	L5	1364	G
3	L5	1365	C
3	L5	1366	C
3	L5	1367	G
3	L5	1374	A
3	L5	1380	G
3	L5	1381	G
3	L5	1384	A
3	L5	1385	A
3	L5	1386	G
3	L5	1389	C
3	L5	1404	C
3	L5	1407	A
3	L5	1412	G
3	L5	1422	G
3	L5	1424	C
3	L5	1426	C
3	L5	1428	C
3	L5	1430	A
3	L5	1431	G
3	L5	1432	U
3	L5	1444	G

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Mol	Chain	Res	Type
3	L5	1445	C
3	L5	1469	G
3	L5	1470	C
3	L5	1480	G
3	L5	1484	A
3	L5	1485	G
3	L5	1489	G
3	L5	1493	G
3	L5	1505	A
3	L5	1514	A
3	L5	1521	A2M
3	L5	1534	A
3	L5	1536	G
3	L5	1550	A
3	L5	1551	A
3	L5	1553	C
3	L5	1565	U
3	L5	1578	U
3	L5	1583	U
3	L5	1611	G
3	L5	1612	OMG
3	L5	1618	A
3	L5	1620	G
3	L5	1621	A
3	L5	1625	A
3	L5	1627	C
3	L5	1629	A
3	L5	1637	A
3	L5	1641	G
3	L5	1643	U
3	L5	1648	C
3	L5	1650	C
3	L5	1663	C
3	L5	1664	PSU
3	L5	1666	A
3	L5	1668	G
3	L5	1684	G
3	L5	1686	A
3	L5	1687	G
3	L5	1690	C
3	L5	1691	C
3	L5	1692	G

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Mol	Chain	Res	Type
3	L5	1694	C
3	L5	1707	C
3	L5	1713	U
3	L5	1716	A
3	L5	1718	C
3	L5	1721	G
3	L5	1727	C
3	L5	1729	A
3	L5	1737	G
3	L5	1744	U
3	L5	1762	A
3	L5	1774	A
3	L5	1784	G
3	L5	1791	A
3	L5	1792	A
3	L5	1797	G
3	L5	1802	G
3	L5	1808	G
3	L5	1809	U
3	L5	1823	G
3	L5	1824	A
3	L5	1829	G
3	L5	1842	G
3	L5	1854	A
3	L5	1856	G
3	L5	1865	G
3	L5	1869	U
3	L5	1870	G
3	L5	1876	U
3	L5	1879	A
3	L5	1884	A
3	L5	1887	C
3	L5	1903	G
3	L5	1905	U
3	L5	1906	G
3	L5	1907	C
3	L5	1908	C
3	L5	1909	G
3	L5	1912	G
3	L5	1918	C
3	L5	1919	A
3	L5	1922	C

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Mol	Chain	Res	Type
3	L5	1923	C
3	L5	1934	U
3	L5	1935	G
3	L5	1938	G
3	L5	1946	U
3	L5	1947	A
3	L5	1948	G
3	L5	1949	A
3	L5	1953	C
3	L5	1954	A
3	L5	1957	A
3	L5	1958	C
3	L5	1961	U
3	L5	1962	G
3	L5	1963	G
3	L5	1964	C
3	L5	1965	C
3	L5	1966	A
3	L5	1967	U
3	L5	1968	G
3	L5	1969	G
3	L5	1970	A
3	L5	1971	A
3	L5	1972	G
3	L5	1974	C
3	L5	1976	G
3	L5	1977	A
3	L5	1978	A
3	L5	1979	U
3	L5	1980	C
3	L5	1982	G
3	L5	1983	C
3	L5	1985	A
3	L5	1986	A
3	L5	1987	G
3	L5	1988	G
3	L5	1989	A
3	L5	1990	G
3	L5	1991	U
3	L5	1992	G
3	L5	1993	U
3	L5	1994	G

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Mol	Chain	Res	Type
3	L5	1996	A
3	L5	1998	C
3	L5	1999	A
3	L5	2000	A
3	L5	2001	C
3	L5	2002	U
3	L5	2005	C
3	L5	2007	U
3	L5	2009	C
3	L5	2011	G
3	L5	2012	A
3	L5	2013	A
3	L5	2020	A
3	L5	2027	A
3	L5	2031	U
3	L5	2032	G
3	L5	2033	G
3	L5	2035	U
3	L5	2036	G
3	L5	2042	G
3	L5	2043	G
3	L5	2056	A
3	L5	2058	A
3	L5	2071	C
3	L5	2072	G
3	L5	2076	G
3	L5	2077	U
3	L5	2079	G
3	L5	2080	A
3	L5	2081	G
3	L5	2082	A
3	L5	2083	G
3	L5	2084	U
3	L5	2085	G
3	L5	2088	C
3	L5	2089	G
3	L5	2093	G
3	L5	2095	G
3	L5	2097	C
3	L5	2099	G
3	L5	2239	G
3	L5	2240	A

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Mol	Chain	Res	Type
3	L5	2242	C
3	L5	2243	C
3	L5	2245	C
3	L5	2246	G
3	L5	2253	C
3	L5	2255	A
3	L5	2276	C
3	L5	2281	G
3	L5	2284	G
3	L5	2287	A
3	L5	2288	G
3	L5	2292	U
3	L5	2293	G
3	L5	2300	A
3	L5	2318	G
3	L5	2320	G
3	L5	2324	C
3	L5	2329	G
3	L5	2333	C
3	L5	2335	G
3	L5	2338	OMC
3	L5	2344	G
3	L5	2347	A
3	L5	2351	OMG
3	L5	2369	A
3	L5	2376	A
3	L5	2382	A
3	L5	2383	A
3	L5	2384	G
3	L5	2389	G
3	L5	2397	C
3	L5	2403	G
3	L5	2404	A
3	L5	2405	A
3	L5	2408	G
3	L5	2409	OMC
3	L5	2412	U
3	L5	2424	C
3	L5	2428	C
3	L5	2434	U
3	L5	2437	G
3	L5	2440	A

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Mol	Chain	Res	Type
3	L5	2451	C
3	L5	2452	C
3	L5	2461	G
3	L5	2462	G
3	L5	2465	C
3	L5	2470	G
3	L5	2471	A
3	L5	2472	U
3	L5	2474	G
3	L5	2475	C
3	L5	2476	C
3	L5	2477	U
3	L5	2478	C
3	L5	2480	G
3	L5	2489	G
3	L5	2490	G
3	L5	2491	C
3	L5	2492	C
3	L5	2493	G
3	L5	2498	A
3	L5	2500	A
3	L5	2506	U
3	L5	2507	C
3	L5	2516	A
3	L5	2520	C
3	L5	2524	A
3	L5	2531	G
3	L5	2533	G
3	L5	2534	G
3	L5	2541	U
3	L5	2543	G
3	L5	2551	G
3	L5	2552	A
3	L5	2553	G
3	L5	2560	A
3	L5	2564	C
3	L5	2567	U
3	L5	2570	C
3	L5	2574	A
3	L5	2576	C
3	L5	2588	A
3	L5	2605	G

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Mol	Chain	Res	Type
3	L5	2614	C
3	L5	2625	G
3	L5	2639	G
3	L5	2640	C
3	L5	2646	A
3	L5	2649	G
3	L5	2656	C
3	L5	2657	C
3	L5	2660	G
3	L5	2663	A
3	L5	2674	U
3	L5	2681	G
3	L5	2682	A
3	L5	2683	A
3	L5	2684	A
3	L5	2694	U
3	L5	2697	C
3	L5	2698	G
3	L5	2699	G
3	L5	2708	G
3	L5	2711	G
3	L5	2713	G
3	L5	2726	C
3	L5	2729	G
3	L5	2730	A
3	L5	2733	A
3	L5	2741	G
3	L5	2743	G
3	L5	2747	G
3	L5	2748	U
3	L5	2750	U
3	L5	2756	U
3	L5	2757	C
3	L5	2775	U
3	L5	2776	A
3	L5	2777	U
3	L5	2786	G
3	L5	2801	C
3	L5	2802	A2M
3	L5	2813	U
3	L5	2814	G
3	L5	2815	U

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Mol	Chain	Res	Type
3	L5	2816	U
3	L5	2825	G
3	L5	2829	G
3	L5	2837	A
3	L5	2842	G
3	L5	2843	C
3	L5	2854	C
3	L5	2862	C
3	L5	2864	G
3	L5	2879	C
3	L5	2881	A
3	L5	2884	G
3	L5	2889	G
3	L5	2890	G
3	L5	2891	U
3	L5	2892	C
3	L5	2893	G
3	L5	2894	G
3	L5	2895	U
3	L5	2897	G
3	L5	3564	G
3	L5	3565	G
3	L5	3566	C
3	L5	3567	C
3	L5	3570	C
3	L5	3571	G
3	L5	3574	U
3	L5	3575	A
3	L5	3576	G
3	L5	3583	A
3	L5	3584	C
3	L5	3594	G
3	L5	3595	U
3	L5	3597	C
3	L5	3605	G
3	L5	3609	A
3	L5	3614	A
3	L5	3623	U
3	L5	3625	A
3	L5	3627	A
3	L5	3641	A
3	L5	3643	G

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Mol	Chain	Res	Type
3	L5	3652	C
3	L5	3653	G
3	L5	3670	G
3	L5	3689	G
3	L5	3690	A
3	L5	3691	A
3	L5	3692	U
3	L5	3693	G
3	L5	3706	A
3	L5	3708	U
3	L5	3714	G
3	L5	3715	A
3	L5	3727	A
3	L5	3729	G
3	L5	3732	G
3	L5	3745	A
3	L5	3750	C
3	L5	3755	G
3	L5	3756	G
3	L5	3764	A2M
3	L5	3765	U
3	L5	3767	C
3	L5	3780	U
3	L5	3781	U
3	L5	3790	G
3	L5	3791	C
3	L5	3793	U
3	L5	3796	A
3	L5	3798	G
3	L5	3803	A
3	L5	3817	U
3	L5	3819	U
3	L5	3846	A2M
3	L5	3855	A
3	L5	3856	A
3	L5	3857	C
3	L5	3858	G
3	L5	3861	C
3	L5	3864	G
3	L5	3869	A
3	L5	3876	G
3	L5	3880	A

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Mol	Chain	Res	Type
3	L5	3881	A
3	L5	3885	A
3	L5	3886	G
3	L5	3887	A
3	L5	3894	U
3	L5	3895	G
3	L5	3899	PSU
3	L5	3901	G
3	L5	3905	C
3	L5	3917	G
3	L5	3918	G
3	L5	3921	A
3	L5	3922	A
3	L5	3923	G
3	L5	3926	A
3	L5	3927	C
3	L5	4051	A
3	L5	4054	G
3	L5	4064	G
3	L5	4075	G
3	L5	4076	A
3	L5	4087	C
3	L5	4089	C
3	L5	4090	U
3	L5	4091	C
3	L5	4092	G
3	L5	4093	C
3	L5	4094	U
3	L5	4096	C
3	L5	4098	G
3	L5	4099	G
3	L5	4104	A
3	L5	4110	C
3	L5	4114	C
3	L5	4120	G
3	L5	4132	C
3	L5	4133	U
3	L5	4136	G
3	L5	4138	G
3	L5	4140	A
3	L5	4153	G
3	L5	4154	G

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Mol	Chain	Res	Type
3	L5	4161	G
3	L5	4173	A
3	L5	4182	A
3	L5	4191	C
3	L5	4192	G
3	L5	4193	C
3	L5	4195	G
3	L5	4199	U
3	L5	4203	A
3	L5	4207	C
3	L5	4212	U
3	L5	4219	G
3	L5	4221	A
3	L5	4224	G
3	L5	4227	A
3	L5	4228	C
3	L5	4235	U
3	L5	4236	G
3	L5	4238	A
3	L5	4243	A
3	L5	4250	A
3	L5	4251	A
3	L5	4256	C
3	L5	4261	G
3	L5	4263	PSU
3	L5	4265	U
3	L5	4274	A
3	L5	4275	G
3	L5	4276	OMU
3	L5	4284	C
3	L5	4289	C
3	L5	4296	G
3	L5	4299	G
3	L5	4300	G
3	L5	4302	C
3	L5	4309	A
3	L5	4319	C
3	L5	4320	C
3	L5	4324	U
3	L5	4334	G
3	L5	4343	G
3	L5	4346	A

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Mol	Chain	Res	Type
3	L5	4347	G
3	L5	4348	A
3	L5	4350	A
3	L5	4351	A
3	L5	4357	C
3	L5	4361	G
3	L5	4364	A
3	L5	4375	G
3	L5	4390	PSU
3	L5	4392	A
3	L5	4394	A
3	L5	4396	C
3	L5	4397	G
3	L5	4400	G
3	L5	4407	U
3	L5	4411	A
3	L5	4414	C
3	L5	4418	G
3	L5	4419	A
3	L5	4420	U
3	L5	4422	U
3	L5	4433	U
3	L5	4434	A
3	L5	4435	U
3	L5	4436	C
3	L5	4445	G
3	L5	4470	PSU
3	L5	4482	U
3	L5	4483	A
3	L5	4485	G
3	L5	4488	A
3	L5	4489	C
3	L5	4490	G
3	L5	4494	G
3	L5	4515	G
3	L5	4518	A
3	L5	4519	G
3	L5	4524	G
3	L5	4530	C
3	L5	4537	G
3	L5	4543	G
3	L5	4545	G

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Mol	Chain	Res	Type
3	L5	4559	A
3	L5	4560	A
3	L5	4570	G
3	L5	4571	U
3	L5	4587	G
3	L5	4605	A
3	L5	4606	PSU
3	L5	4607	OMG
3	L5	4617	G
3	L5	4626	A
3	L5	4627	U
3	L5	4638	U
3	L5	4640	C
3	L5	4649	G
3	L5	4654	A
3	L5	4657	A
3	L5	4663	C
3	L5	4664	G
3	L5	4665	C
3	L5	4677	A
3	L5	4678	A
3	L5	4679	U
3	L5	4698	U
3	L5	4709	G
3	L5	4710	C
3	L5	4711	G
3	L5	4714	G
3	L5	4719	G
3	L5	4723	G
3	L5	4726	C
3	L5	4728	C
3	L5	4730	G
3	L5	4733	A
3	L5	4734	G
3	L5	4832	G
3	L5	4835	G
3	L5	4836	C
3	L5	4838	G
3	L5	4840	G
3	L5	4847	U
3	L5	4848	C
3	L5	4853	U

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Mol	Chain	Res	Type
3	L5	4854	G
3	L5	4860	C
3	L5	4861	G
3	L5	4864	G
3	L5	4865	C
3	L5	4866	G
3	L5	4875	G
3	L5	4877	G
3	L5	4879	C
3	L5	4888	C
3	L5	4893	C
3	L5	4896	G
3	L5	4899	A
3	L5	4902	C
3	L5	4903	A
3	L5	4906	G
3	L5	4908	A
3	L5	4912	U
3	L5	4915	U
3	L5	4916	G
3	L5	4925	G
3	L5	4926	G
3	L5	4928	G
3	L5	4931	A
3	L5	4932	A
3	L5	4940	G
3	L5	4941	U
3	L5	4950	U
3	L5	4953	U
3	L5	4954	U
3	L5	4956	U
3	L5	4979	A
3	L5	4982	G
3	L5	4985	G
3	L5	4987	U
3	L5	4988	C
3	L5	4989	C
3	L5	4990	C
3	L5	4994	C
3	L5	4996	G
3	L5	4999	A
3	L5	5005	U

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Mol	Chain	Res	Type
3	L5	5006	G
3	L5	5015	C
3	L5	5019	C
3	L5	5020	G
3	L5	5023	A
3	L5	5026	A
3	L5	5034	U
4	L7	10	C
4	L7	13	A
4	L7	22	A
4	L7	25	G
4	L7	33	U
4	L7	38	U
4	L7	42	A
4	L7	43	U
4	L7	49	A
4	L7	50	A
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	76	U
4	L7	97	G
4	L7	98	G
4	L7	100	A
4	L7	110	G
4	L7	111	C
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	48	A
5	L8	52	A
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	82	A
5	L8	84	A
5	L8	85	U
5	L8	86	U
5	L8	97	A
5	L8	103	A
5	L8	104	A
5	L8	105	C

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Mol	Chain	Res	Type
5	L8	110	U
5	L8	111	U
5	L8	112	G
5	L8	114	G
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U
5	L8	150	C
5	L8	153	C
5	L8	156	U
46	S2	3	C
46	S2	4	C
46	S2	17	C
46	S2	23	G
46	S2	25	A
46	S2	26	U
46	S2	33	G
46	S2	41	G
46	S2	44	U
46	S2	45	A
46	S2	46	A
46	S2	56	G
46	S2	58	C
46	S2	59	U
46	S2	65	C
46	S2	67	C
46	S2	68	A
46	S2	79	A
46	S2	99	A2M
46	S2	103	A
46	S2	113	G
46	S2	115	U
46	S2	116	OMU
46	S2	120	U
46	S2	126	G
46	S2	141	A
46	S2	142	C
46	S2	143	U
46	S2	154	U
46	S2	155	G
46	S2	158	A

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Mol	Chain	Res	Type
46	S2	160	U
46	S2	163	U
46	S2	167	G
46	S2	168	C
46	S2	172	OMU
46	S2	175	A
46	S2	182	C
46	S2	183	G
46	S2	184	G
46	S2	187	G
46	S2	188	C
46	S2	189	U
46	S2	190	G
46	S2	191	A
46	S2	192	C
46	S2	200	G
46	S2	202	G
46	S2	209	A
46	S2	293	C
46	S2	302	A
46	S2	305	U
46	S2	306	C
46	S2	307	G
46	S2	309	G
46	S2	318	A
46	S2	319	C
46	S2	320	G
46	S2	322	C
46	S2	335	G
46	S2	338	G
46	S2	339	A
46	S2	347	G
46	S2	360	A
46	S2	362	C
46	S2	364	A
46	S2	368	U
46	S2	369	C
46	S2	370	G
46	S2	377	G
46	S2	381	C
46	S2	382	C
46	S2	383	G

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Mol	Chain	Res	Type
46	S2	385	G
46	S2	386	C
46	S2	400	C
46	S2	408	A
46	S2	409	C
46	S2	420	G
46	S2	426	A
46	S2	428	OMU
46	S2	429	C
46	S2	438	G
46	S2	441	C
46	S2	447	A
46	S2	448	A
46	S2	449	A
46	S2	450	C
46	S2	464	A
46	S2	465	A
46	S2	467	G
46	S2	471	G
46	S2	472	C
46	S2	473	A
46	S2	474	G
46	S2	482	G
46	S2	487	U
46	S2	488	U
46	S2	492	C
46	S2	516	A
46	S2	518	G
46	S2	525	A
46	S2	532	C
46	S2	534	G
46	S2	536	A
46	S2	550	C
46	S2	551	U
46	S2	555	A
46	S2	559	G
46	S2	560	A
46	S2	568	C
46	S2	574	A
46	S2	576	A2M
46	S2	585	C
46	S2	587	A

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Mol	Chain	Res	Type
46	S2	589	G
46	S2	590	A2M
46	S2	591	U
46	S2	594	A
46	S2	598	G
46	S2	605	A
46	S2	606	G
46	S2	608	C
46	S2	614	C
46	S2	617	G
46	S2	620	G
46	S2	621	OMC
46	S2	629	A
46	S2	631	U
46	S2	632	C
46	S2	637	U
46	S2	643	A
46	S2	644	OMG
46	S2	658	U
46	S2	659	G
46	S2	660	C
46	S2	662	G
46	S2	664	A
46	S2	668	A2M
46	S2	669	A
46	S2	670	A
46	S2	671	A
46	S2	672	A
46	S2	673	G
46	S2	683	OMG
46	S2	687	C
46	S2	688	U
46	S2	689	U
46	S2	800	U
46	S2	808	A
46	S2	809	A
46	S2	821	G
46	S2	822	PSU
46	S2	823	U
46	S2	827	A
46	S2	830	A
46	S2	841	G

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Mol	Chain	Res	Type
46	S2	847	A
46	S2	848	U
46	S2	870	A
46	S2	875	A
46	S2	877	C
46	S2	878	G
46	S2	909	G
46	S2	910	G
46	S2	913	A
46	S2	914	U
46	S2	916	A
46	S2	917	U
46	S2	920	A
46	S2	921	G
46	S2	933	G
46	S2	934	G
46	S2	943	U
46	S2	955	A
46	S2	970	G
46	S2	971	G
46	S2	985	G
46	S2	990	A
46	S2	991	G
46	S2	992	A
46	S2	999	G
46	S2	1017	U
46	S2	1023	A
46	S2	1041	G
46	S2	1049	A
46	S2	1058	A
46	S2	1067	C
46	S2	1069	U
46	S2	1078	C
46	S2	1083	A
46	S2	1085	C
46	S2	1096	G
46	S2	1112	U
46	S2	1126	G
46	S2	1130	G
46	S2	1149	A
46	S2	1150	A
46	S2	1153	C

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Mol	Chain	Res	Type
46	S2	1154	U
46	S2	1166	G
46	S2	1171	G
46	S2	1172	U
46	S2	1195	A
46	S2	1207	G
46	S2	1211	G
46	S2	1215	C
46	S2	1224	G
46	S2	1242	U
46	S2	1244	PSU
46	S2	1249	C
46	S2	1250	A
46	S2	1251	A
46	S2	1253	A
46	S2	1254	C
46	S2	1256	G
46	S2	1257	G
46	S2	1259	A
46	S2	1261	C
46	S2	1265	A
46	S2	1269	G
46	S2	1273	C
46	S2	1274	G
46	S2	1275	G
46	S2	1284	A
46	S2	1285	G
46	S2	1286	G
46	S2	1295	A
46	S2	1301	A
46	S2	1302	G
46	S2	1303	C
46	S2	1308	U
46	S2	1312	G
46	S2	1315	U
46	S2	1319	U
46	S2	1341	C
46	S2	1342	U
46	S2	1371	U
46	S2	1372	U
46	S2	1378	A
46	S2	1395	C

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Mol	Chain	Res	Type
46	S2	1396	A
46	S2	1397	U
46	S2	1402	A
46	S2	1406	G
46	S2	1412	C
46	S2	1414	A
46	S2	1422	G
46	S2	1428	G
46	S2	1439	A
46	S2	1442	OMU
46	S2	1447	G
46	S2	1454	A
46	S2	1462	U
46	S2	1463	U
46	S2	1464	C
46	S2	1466	G
46	S2	1476	A
46	S2	1477	U
46	S2	1478	U
46	S2	1480	A
46	S2	1488	C
46	S2	1489	A
46	S2	1490	OMG
46	S2	1493	C
46	S2	1496	U
46	S2	1498	A
46	S2	1507	G
46	S2	1520	G
46	S2	1521	C
46	S2	1522	A
46	S2	1523	C
46	S2	1533	A
46	S2	1564	C
46	S2	1570	G
46	S2	1574	C
46	S2	1575	G
46	S2	1580	A
46	S2	1585	U
46	S2	1587	G
46	S2	1588	A
46	S2	1601	A
46	S2	1604	G

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Mol	Chain	Res	Type
46	S2	1612	G
46	S2	1621	U
46	S2	1623	A
46	S2	1629	C
46	S2	1636	G
46	S2	1637	A
46	S2	1638	G
46	S2	1660	C
46	S2	1661	A
46	S2	1665	G
46	S2	1671	G
46	S2	1675	A
46	S2	1680	G
46	S2	1695	A
46	S2	1698	C
46	S2	1699	A
46	S2	1703	OMC
46	S2	1721	U
46	S2	1722	G
46	S2	1726	G
46	S2	1729	U
46	S2	1732	G
46	S2	1744	G
46	S2	1749	G
46	S2	1785	C
46	S2	1786	U
46	S2	1824	A
46	S2	1825	A
46	S2	1826	G
46	S2	1829	G
46	S2	1831	A
46	S2	1835	A
46	S2	1836	G
46	S2	1849	G
46	S2	1861	G
46	S2	1862	G
46	S2	1863	A
46	S2	1864	U
46	S2	1865	C
46	S2	1867	U
46	S2	1869	A
80	Bv	7	G

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Mol	Chain	Res	Type
80	Bv	8	U
80	Bv	9	1MG
80	Bv	14	A
80	Bv	15	A
80	Bv	16	H2U
80	Bv	17	C
80	Bv	18	G
80	Bv	19	G
80	Bv	22	G
80	Bv	23	C
80	Bv	24	G
80	Bv	28	PSU
80	Bv	29	C
80	Bv	30	G
80	Bv	33	U
80	Bv	34	G
80	Bv	38	A
80	Bv	45	G
80	Bv	46	G7M
80	Bv	47	H2U
80	Bv	48	U
80	Bv	49	G
80	Bv	53	G
80	Bv	54	U
80	Bv	56	C
80	Bv	58	1MA
80	Bv	60	C
80	Bv	61	C
80	Bv	63	A
80	Bv	67	A
80	Bv	68	G
80	Bv	69	G
80	Bv	70	G
80	Bv	71	A
80	Bv	72	C
80	Bv	73	G
80	Bv	74	C
80	Bv	75	C
80	Bv	76	A
82	k	1051	C
82	k	1056	U
82	k	1057	A

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Mol	Chain	Res	Type
82	k	1058	A
82	k	1059	U
82	k	1060	U
82	k	1061	U

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	167	C
3	L5	397	C
3	L5	1620	G
3	L5	1908	C
3	L5	2006	C
3	L5	2403	G
3	L5	2662	G
3	L5	2747	G
3	L5	3593	G
3	L5	3652	C
3	L5	4348	A
3	L5	4570	G
3	L5	4641	C
3	L5	4878	G
5	L8	83	C
46	S2	140	C
46	S2	407	G
46	S2	688	U
46	S2	1129	G
46	S2	1253	A
46	S2	1394	G
46	S2	1395	C
46	S2	1637	A
46	S2	1679	A
46	S2	1824	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	2802	3	18,25,26	0.66	0	20,36,39	1.11	2 (10%)
81	UXY	j	63	81	7,9,10	0.75	0	7,10,12	1.36	1 (14%)
46	OMG	S2	1328	46	19,26,27	0.98	1 (5%)	21,38,41	1.09	2 (9%)
3	A2M	L5	1313	3	18,25,26	1.06	1 (5%)	20,36,39	1.63	3 (15%)
3	PSU	L5	4470	3	18,21,22	1.60	6 (33%)	21,30,33	2.33	3 (14%)
3	OMG	L5	4607	3	19,26,27	1.29	2 (10%)	21,38,41	1.23	4 (19%)
80	H2U	Bv	47	80	18,21,22	1.02	2 (11%)	19,30,33	1.35	3 (15%)
46	OMU	S2	121	46	19,22,23	1.35	3 (15%)	25,31,34	1.92	4 (16%)
3	OMU	L5	4468	3	19,22,23	1.53	4 (21%)	25,31,34	1.96	5 (20%)
46	PSU	S2	866	46	18,21,22	1.47	4 (22%)	21,30,33	2.08	4 (19%)
46	4AC	S2	1842	46	21,24,25	1.12	3 (14%)	28,34,37	2.93	7 (25%)
3	UR3	L5	4500	3	19,22,23	1.07	1 (5%)	26,32,35	2.00	6 (23%)
3	OMC	L5	3820	3	19,22,23	1.16	2 (10%)	25,31,34	1.45	4 (16%)
3	OMC	L5	4506	3	19,22,23	1.00	2 (10%)	25,31,34	1.03	1 (4%)
3	OMG	L5	4588	3	19,26,27	1.11	1 (5%)	21,38,41	1.25	4 (19%)
3	PSU	L5	3709	3	18,21,22	1.47	4 (22%)	21,30,33	2.17	4 (19%)
46	OMG	S2	683	46	19,26,27	1.04	1 (5%)	21,38,41	1.13	3 (14%)
3	PSU	L5	2402	3	18,21,22	1.62	4 (22%)	21,30,33	2.45	5 (23%)
3	PSU	L5	3899	3,84	18,21,22	1.88	5 (27%)	21,30,33	2.48	5 (23%)
46	PSU	S2	863	46	18,21,22	1.58	5 (27%)	21,30,33	2.13	4 (19%)
46	PSU	S2	1244	46	18,21,22	1.43	4 (22%)	21,30,33	2.08	4 (19%)
46	PSU	S2	1367	46	18,21,22	1.51	4 (22%)	21,30,33	2.14	3 (14%)
3	PSU	L5	1779	3	18,21,22	1.65	4 (22%)	21,30,33	1.97	4 (19%)
46	PSU	S2	814	46	18,21,22	1.54	4 (22%)	21,30,33	2.12	4 (19%)
3	OMC	L5	3848	3	19,22,23	0.96	1 (5%)	25,31,34	0.95	1 (4%)
80	2MG	Bv	10	80	18,26,27	0.96	1 (5%)	16,38,41	1.47	3 (18%)
3	OMG	L5	1612	3,84	19,26,27	1.16	1 (5%)	21,38,41	1.23	3 (14%)
3	OMC	L5	3866	3	19,22,23	0.93	1 (5%)	25,31,34	0.94	1 (4%)
46	A2M	S2	99	46	18,25,26	0.68	0	20,36,39	0.90	1 (5%)
46	G7M	S2	1639	46,80	20,26,27	1.15	2 (10%)	16,39,42	0.56	0
80	PSU	Bv	27	80	18,21,22	1.36	2 (11%)	21,30,33	2.09	4 (19%)
46	PSU	S2	1692	46	18,21,22	1.67	5 (27%)	21,30,33	2.25	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	649	46	18,21,22	1.60	4 (22%)	21,30,33	2.16	4 (19%)
3	2MG	L5	1504	3	18,26,27	1.25	2 (11%)	16,38,41	1.66	5 (31%)
80	PSU	Bv	55	80	18,21,22	1.34	2 (11%)	21,30,33	2.14	5 (23%)
3	PSU	L5	4263	3	18,21,22	1.77	6 (33%)	21,30,33	2.21	4 (19%)
46	PSU	S2	406	46	18,21,22	1.64	5 (27%)	21,30,33	2.23	5 (23%)
3	OMC	L5	2338	3	19,22,23	1.07	2 (10%)	25,31,34	1.47	3 (12%)
3	PSU	L5	4266	3	18,21,22	1.57	4 (22%)	21,30,33	2.19	4 (19%)
3	PSU	L5	3741	3	18,21,22	1.55	5 (27%)	21,30,33	2.36	5 (23%)
46	PSU	S2	1004	46	18,21,22	1.56	5 (27%)	21,30,33	2.24	3 (14%)
3	PSU	L5	4549	3	18,21,22	1.70	5 (27%)	21,30,33	2.39	6 (28%)
3	PSU	L5	4606	3	18,21,22	1.59	4 (22%)	21,30,33	1.98	4 (19%)
46	PSU	S2	1643	46	18,21,22	1.51	5 (27%)	21,30,33	2.07	4 (19%)
3	OMC	L5	2811	3	19,22,23	0.93	2 (10%)	25,31,34	0.88	1 (4%)
80	UY4	Bv	37	80	26,34,35	1.77	3 (11%)	28,49,52	2.06	8 (28%)
3	PSU	L5	4659	3	18,21,22	1.82	5 (27%)	21,30,33	2.34	6 (28%)
46	A2M	S2	27	46,84	18,25,26	0.68	0	20,36,39	0.82	1 (5%)
46	PSU	S2	218	46	18,21,22	1.47	4 (22%)	21,30,33	2.14	5 (23%)
46	PSU	S2	1174	46	18,21,22	1.60	5 (27%)	21,30,33	2.32	4 (19%)
3	PSU	L5	4966	3	18,21,22	1.80	5 (27%)	21,30,33	2.16	4 (19%)
46	OMG	S2	867	46	19,26,27	0.95	1 (5%)	21,38,41	1.08	2 (9%)
3	OMG	L5	1303	3	19,26,27	1.43	2 (10%)	21,38,41	1.04	1 (4%)
3	OMC	L5	4426	3	19,22,23	1.01	2 (10%)	25,31,34	0.96	1 (4%)
46	A2M	S2	576	46	18,25,26	0.64	0	20,36,39	0.85	1 (5%)
46	B8N	S2	1248	46	25,29,30	1.44	4 (16%)	28,42,45	1.64	6 (21%)
46	OMG	S2	644	46	19,26,27	1.00	1 (5%)	21,38,41	1.11	2 (9%)
3	OMC	L5	2352	3	19,22,23	0.88	2 (10%)	25,31,34	0.73	0
3	PSU	L5	3737	3	18,21,22	1.63	4 (22%)	21,30,33	2.06	4 (19%)
3	PSU	L5	3823	3	18,21,22	1.74	5 (27%)	21,30,33	2.48	4 (19%)
46	OMG	S2	601	46	19,26,27	1.10	1 (5%)	21,38,41	0.91	1 (4%)
3	PSU	L5	4373	3	18,21,22	1.67	5 (27%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1670	3	18,21,22	1.97	4 (22%)	21,30,33	2.15	3 (14%)
46	OMC	S2	174	46	19,22,23	0.87	1 (5%)	25,31,34	0.96	1 (4%)
3	PSU	L5	3743	3	18,21,22	1.60	4 (22%)	21,30,33	2.13	4 (19%)
3	OMG	L5	3878	3	19,26,27	1.25	1 (5%)	21,38,41	1.30	4 (19%)
3	OMG	L5	4464	3	19,26,27	1.32	2 (10%)	21,38,41	1.11	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	L8	69	5	18,21,22	1.60	5 (27%)	21,30,33	2.39	4 (19%)
46	OMU	S2	172	46	19,22,23	1.31	4 (21%)	25,31,34	1.96	5 (20%)
3	PSU	L5	4331	3	18,21,22	1.80	5 (27%)	21,30,33	2.14	5 (23%)
3	PSU	L5	4502	3	18,21,22	1.78	6 (33%)	21,30,33	2.01	5 (23%)
3	PSU	L5	1523	3	18,21,22	1.94	5 (27%)	21,30,33	2.26	4 (19%)
3	A2M	L5	391	3	18,25,26	0.73	0	20,36,39	0.96	1 (5%)
3	OMG	L5	3606	3	19,26,27	1.27	2 (10%)	21,38,41	1.14	2 (9%)
3	PSU	L5	4282	3	18,21,22	1.69	4 (22%)	21,30,33	2.34	5 (23%)
3	PSU	L5	1664	3	18,21,22	1.74	5 (27%)	21,30,33	2.44	6 (28%)
3	PSU	L5	4390	3	18,21,22	1.35	3 (16%)	21,30,33	2.02	4 (19%)
3	PSU	L5	4937	3	18,21,22	1.60	5 (27%)	21,30,33	2.03	5 (23%)
80	H2U	Bv	16	80	18,21,22	1.01	2 (11%)	19,30,33	1.26	3 (15%)
3	PSU	L5	4491	3,84	18,21,22	1.85	5 (27%)	21,30,33	2.40	6 (28%)
81	MEQ	j	185	81	8,9,10	0.47	0	5,10,12	0.48	0
3	PSU	L5	3694	3	18,21,22	1.52	4 (22%)	21,30,33	2.07	4 (19%)
3	PSU	L5	3749	3	18,21,22	1.64	4 (22%)	21,30,33	2.13	3 (14%)
3	PSU	L5	3616	3	18,21,22	2.02	5 (27%)	21,30,33	2.38	5 (23%)
3	OMC	L5	3787	3	19,22,23	0.99	2 (10%)	25,31,34	1.08	2 (8%)
3	OMG	L5	364	3	19,26,27	1.34	2 (10%)	21,38,41	1.37	4 (19%)
3	A2M	L5	2388	3,84	18,25,26	0.73	1 (5%)	20,36,39	0.80	1 (5%)
3	A2M	L5	4541	3	18,25,26	0.72	0	20,36,39	0.81	1 (5%)
3	A2M	L5	3739	3	18,25,26	0.70	0	20,36,39	0.92	1 (5%)
3	PSU	L5	4401	3	18,21,22	1.72	5 (27%)	21,30,33	2.25	4 (19%)
46	OMU	S2	1326	46	19,22,23	1.31	4 (21%)	25,31,34	2.03	7 (28%)
46	PSU	S2	1177	46	18,21,22	1.61	4 (22%)	21,30,33	1.95	4 (19%)
46	OMG	S2	509	46,84	19,26,27	0.97	1 (5%)	21,38,41	1.07	1 (4%)
80	PSU	Bv	28	80	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
3	OMG	L5	3771	3	19,26,27	1.08	1 (5%)	21,38,41	1.51	5 (23%)
3	5MC	L5	4417	3	19,22,23	1.22	1 (5%)	26,32,35	2.09	7 (26%)
80	G7M	Bv	46	80	20,26,27	1.27	3 (15%)	16,39,42	1.42	1 (6%)
3	A2M	L5	1511	3	18,25,26	0.70	0	20,36,39	1.11	1 (5%)
3	A2M	L5	3703	3	18,25,26	0.67	0	20,36,39	0.83	1 (5%)
3	PSU	L5	4598	3	18,21,22	1.78	5 (27%)	21,30,33	2.38	4 (19%)
3	PSU	L5	4269	3	18,21,22	1.75	4 (22%)	21,30,33	1.97	4 (19%)
3	OMG	L5	4593	3	19,26,27	1.17	1 (5%)	21,38,41	1.23	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	1238	46	18,21,22	1.55	4 (22%)	21,30,33	2.09	3 (14%)
46	A2M	S2	1383	46	18,25,26	0.68	0	20,36,39	0.98	1 (5%)
3	A2M	L5	2350	3,84	18,25,26	0.76	0	20,36,39	0.90	1 (5%)
3	PSU	L5	4441	3	18,21,22	1.71	5 (27%)	21,30,33	2.35	4 (19%)
3	OMC	L5	1327	3	19,22,23	0.95	2 (10%)	25,31,34	0.88	1 (4%)
46	OMC	S2	462	46	19,22,23	0.83	0	25,31,34	1.06	2 (8%)
3	PSU	L5	3830	3	18,21,22	1.77	5 (27%)	21,30,33	2.17	6 (28%)
3	A2M	L5	2774	3,84	18,25,26	0.68	0	20,36,39	1.12	2 (10%)
80	M2G	Bv	26	80	20,27,28	1.40	4 (20%)	19,40,43	1.22	3 (15%)
3	PSU	L5	3674	3	18,21,22	1.84	5 (27%)	21,30,33	2.24	5 (23%)
3	OMG	L5	4198	3	19,26,27	1.00	1 (5%)	21,38,41	1.20	2 (9%)
6	MLZ	LC	333	6	8,9,10	0.94	0	4,9,11	0.68	0
3	A2M	L5	3804	3	18,25,26	0.71	0	20,36,39	0.86	1 (5%)
3	OMG	L5	4166	80,3	19,26,27	1.18	2 (10%)	21,38,41	1.31	5 (23%)
46	OMU	S2	428	46	19,22,23	1.24	3 (15%)	25,31,34	1.82	5 (20%)
3	OMG	L5	4469	3	19,26,27	1.08	1 (5%)	21,38,41	1.06	2 (9%)
46	A2M	S2	166	46	18,25,26	0.71	0	20,36,39	0.93	1 (5%)
3	OMC	L5	2409	3,84	19,22,23	1.00	2 (10%)	25,31,34	1.15	2 (8%)
3	A2M	L5	3809	3	18,25,26	0.72	0	20,36,39	0.88	1 (5%)
3	PSU	L5	4412	3	18,21,22	1.66	5 (27%)	21,30,33	2.28	4 (19%)
46	PSU	S2	1136	46	18,21,22	1.50	3 (16%)	21,30,33	2.16	5 (23%)
3	1MA	L5	1309	3,84	17,25,26	1.36	4 (23%)	17,37,40	1.29	3 (17%)
3	OMG	L5	4362	3	19,26,27	1.30	2 (10%)	21,38,41	1.15	2 (9%)
3	PSU	L5	3747	3	18,21,22	1.65	5 (27%)	21,30,33	2.19	4 (19%)
46	MA6	S2	1851	46	19,26,27	0.96	1 (5%)	18,38,41	2.12	3 (16%)
46	PSU	S2	1045	46	18,21,22	1.51	3 (16%)	21,30,33	2.26	4 (19%)
46	A2M	S2	512	46	18,25,26	0.67	0	20,36,39	0.95	1 (5%)
3	A2M	L5	3764	3	18,25,26	0.79	0	20,36,39	1.26	4 (20%)
3	PSU	L5	1849	3	18,21,22	1.75	4 (22%)	21,30,33	2.14	5 (23%)
3	OMU	L5	3904	3	19,22,23	1.81	4 (21%)	25,31,34	2.12	8 (32%)
3	OMU	L5	4197	3	19,22,23	1.48	4 (21%)	25,31,34	2.00	6 (24%)
46	PSU	S2	651	46	18,21,22	1.51	4 (22%)	21,30,33	2.16	4 (19%)
46	A2M	S2	668	46,84	18,25,26	0.76	0	20,36,39	1.16	2 (10%)
3	OMC	L5	2791	3	19,22,23	1.03	2 (10%)	25,31,34	0.91	1 (4%)
46	PSU	S2	815	46	18,21,22	1.50	4 (22%)	21,30,33	2.11	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	105	46	18,21,22	1.57	4 (22%)	21,30,33	2.13	4 (19%)
46	PSU	S2	36	46	18,21,22	1.52	4 (22%)	21,30,33	2.24	3 (14%)
46	A2M	S2	159	46	18,25,26	0.63	0	20,36,39	0.76	1 (5%)
3	PSU	L5	4643	3	18,21,22	1.82	5 (27%)	21,30,33	2.11	3 (14%)
46	OMU	S2	1442	46	19,22,23	1.36	4 (21%)	25,31,34	1.87	4 (16%)
3	PSU	L5	4975	3	18,21,22	1.65	4 (22%)	21,30,33	2.30	3 (14%)
3	OMG	L5	1509	3	19,26,27	1.27	2 (10%)	21,38,41	1.43	4 (19%)
46	PSU	S2	572	46	18,21,22	1.44	4 (22%)	21,30,33	2.21	5 (23%)
46	PSU	S2	1232	46	18,21,22	1.62	4 (22%)	21,30,33	2.16	3 (14%)
3	PSU	L5	1731	3	18,21,22	1.70	4 (22%)	21,30,33	2.31	3 (14%)
46	PSU	S2	1445	46	18,21,22	1.44	4 (22%)	21,30,33	2.00	4 (19%)
3	PSU	L5	4427	3	18,21,22	1.71	5 (27%)	21,30,33	2.44	5 (23%)
3	PSU	L5	2619	3	18,21,22	1.67	5 (27%)	21,30,33	2.27	5 (23%)
3	PSU	L5	4323	3	18,21,22	1.78	5 (27%)	21,30,33	2.43	5 (23%)
3	PSU	L5	3713	3	18,21,22	1.46	5 (27%)	21,30,33	2.25	5 (23%)
46	PSU	S2	1046	46	18,21,22	1.59	5 (27%)	21,30,33	2.03	4 (19%)
3	OMG	L5	2351	3	19,26,27	1.14	1 (5%)	21,38,41	1.36	4 (19%)
80	1MA	Bv	58	80	17,25,26	1.61	2 (11%)	17,37,40	1.30	3 (17%)
46	A2M	S2	468	46	18,25,26	0.65	0	20,36,39	0.89	1 (5%)
3	PSU	L5	3832	3,84	18,21,22	1.82	4 (22%)	21,30,33	2.09	4 (19%)
46	MA6	S2	1850	46	19,26,27	0.85	0	18,38,41	2.08	4 (22%)
5	OMG	L8	75	5	19,26,27	1.06	1 (5%)	21,38,41	1.09	2 (9%)
46	OMC	S2	517	46	19,22,23	0.84	1 (5%)	25,31,34	0.80	1 (4%)
3	PSU	L5	4393	3	18,21,22	1.62	4 (22%)	21,30,33	2.06	4 (19%)
46	6MZ	S2	1832	46	17,25,26	0.87	1 (5%)	15,36,39	2.85	4 (26%)
41	MLZ	Lm	98	41	8,9,10	0.89	0	4,9,11	0.75	0
3	OMG	L5	2411	3	19,26,27	1.10	1 (5%)	21,38,41	1.15	2 (9%)
46	PSU	S2	109	46	18,21,22	1.52	4 (22%)	21,30,33	2.17	4 (19%)
80	1MG	Bv	9	80	19,26,27	1.06	1 (5%)	18,39,42	1.45	4 (22%)
3	UY1	L5	3797	3,84	19,22,23	1.58	5 (26%)	21,31,34	2.01	4 (19%)
46	A2M	S2	590	46	18,25,26	0.62	0	20,36,39	1.06	2 (10%)
3	OMG	L5	2863	3	19,26,27	1.13	2 (10%)	21,38,41	1.24	4 (19%)
5	PSU	L8	55	5	18,21,22	1.55	5 (27%)	21,30,33	2.26	4 (19%)
46	PSU	S2	34	46	18,21,22	1.49	4 (22%)	21,30,33	2.15	5 (23%)
3	PSU	L5	3618	3	18,21,22	2.02	5 (27%)	21,30,33	2.32	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	3680	3	19,22,23	1.03	2 (10%)	25,31,34	0.80	0
46	OMC	S2	1391	46	19,22,23	0.84	0	25,31,34	1.03	1 (4%)
46	OMU	S2	1288	46	19,22,23	1.31	4 (21%)	25,31,34	1.79	4 (16%)
3	PSU	L5	4546	3	18,21,22	1.59	5 (27%)	21,30,33	2.27	3 (14%)
46	4AC	S2	1337	46	21,24,25	1.21	2 (9%)	28,34,37	2.60	9 (32%)
46	A2M	S2	1031	46	18,25,26	0.71	0	20,36,39	0.87	1 (5%)
3	OMG	L5	4340	3	19,26,27	1.16	2 (10%)	21,38,41	1.25	3 (14%)
46	OMU	S2	1804	46	19,22,23	1.35	4 (21%)	25,31,34	1.93	6 (24%)
3	PSU	L5	2495	3	18,21,22	1.61	4 (22%)	21,30,33	2.10	4 (19%)
46	PSU	S2	1625	46	18,21,22	1.44	4 (22%)	21,30,33	2.01	4 (19%)
3	OMU	L5	4590	3	19,22,23	1.64	3 (15%)	25,31,34	1.80	6 (24%)
46	PSU	S2	966	46	18,21,22	1.51	4 (22%)	21,30,33	2.19	5 (23%)
3	PSU	L5	1768	3	18,21,22	1.59	5 (27%)	21,30,33	2.22	3 (14%)
46	OMC	S2	1703	46	19,22,23	0.88	2 (10%)	25,31,34	1.21	2 (8%)
3	OMU	L5	2824	3	19,22,23	1.47	4 (21%)	25,31,34	2.14	4 (16%)
46	PSU	S2	93	46	18,21,22	1.47	4 (22%)	21,30,33	2.07	4 (19%)
46	OMG	S2	436	46	19,26,27	1.00	1 (5%)	21,38,41	1.24	3 (14%)
46	OMG	S2	1490	46	19,26,27	1.08	2 (10%)	21,38,41	1.32	4 (19%)
3	A2M	L5	1521	3	18,25,26	0.79	0	20,36,39	0.91	1 (5%)
46	PSU	S2	1347	46	18,21,22	1.44	4 (22%)	21,30,33	2.05	4 (19%)
73	IAS	SO	138	73	6,7,8	1.30	1 (16%)	3,8,10	1.21	0
3	PSU	L5	1569	3	18,21,22	1.71	5 (27%)	21,30,33	2.19	4 (19%)
3	PSU	L5	4522	3	18,21,22	1.86	5 (27%)	21,30,33	2.47	5 (23%)
46	PSU	S2	609	46	18,21,22	1.45	4 (22%)	21,30,33	2.14	3 (14%)
3	A2M	L5	389	3	18,25,26	0.73	0	20,36,39	1.01	2 (10%)
3	A2M	L5	1858	3,84	18,25,26	0.84	0	20,36,39	0.97	1 (5%)
46	OMC	S2	621	46	19,22,23	0.96	2 (10%)	25,31,34	1.62	5 (20%)
46	PSU	S2	822	46	18,21,22	1.52	5 (27%)	21,30,33	2.16	4 (19%)
46	A2M	S2	1678	46	18,25,26	0.65	0	20,36,39	0.79	1 (5%)
3	OMU	L5	4276	3	19,22,23	1.58	4 (21%)	25,31,34	1.92	6 (24%)
46	PSU	S2	801	46	18,21,22	1.52	4 (22%)	21,30,33	2.08	4 (19%)
3	5MC	L5	3761	3	19,22,23	1.24	2 (10%)	26,32,35	1.71	6 (23%)
3	A2M	L5	3846	3	18,25,26	0.68	0	20,36,39	1.10	2 (10%)
3	A2M	L5	4493	3,84	18,25,26	0.68	0	20,36,39	0.97	2 (10%)
46	PSU	S2	119	46	18,21,22	1.49	5 (27%)	21,30,33	2.04	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	S2	1081	46	18,21,22	1.62	5 (27%)	21,30,33	2.26	5 (23%)
3	A2M	L5	3697	3	18,25,26	0.65	0	20,36,39	0.87	1 (5%)
3	PSU	L5	1847	3	18,21,22	1.70	5 (27%)	21,30,33	2.30	5 (23%)
3	6MZ	L5	4190	3	17,25,26	0.88	1 (5%)	15,36,39	2.40	4 (26%)
46	PSU	S2	686	46	18,21,22	1.56	5 (27%)	21,30,33	2.27	5 (23%)
3	OMC	L5	2848	3	19,22,23	0.97	2 (10%)	25,31,34	0.61	0
46	OMU	S2	116	46	19,22,23	1.29	3 (15%)	25,31,34	1.84	6 (24%)
46	A2M	S2	484	46	18,25,26	0.66	0	20,36,39	0.91	1 (5%)
3	PSU	L5	1769	3	18,21,22	1.65	5 (27%)	21,30,33	2.39	4 (19%)
3	OMG	L5	3723	3	19,26,27	1.14	1 (5%)	21,38,41	1.20	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	2802	3	-	4/5/27/28	0/3/3/3
81	UXY	j	63	81	-	3/8/9/11	-
46	OMG	S2	1328	46	-	0/5/27/28	0/3/3/3
3	A2M	L5	1313	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4470	3	-	3/7/25/26	0/2/2/2
3	OMG	L5	4607	3	-	0/5/27/28	0/3/3/3
80	H2U	Bv	47	80	-	1/7/38/39	0/2/2/2
46	OMU	S2	121	46	-	0/9/27/28	0/2/2/2
3	OMU	L5	4468	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	866	46	-	0/7/25/26	0/2/2/2
46	4AC	S2	1842	46	-	2/11/29/30	0/2/2/2
3	UR3	L5	4500	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3820	3	-	2/9/27/28	0/2/2/2
3	OMC	L5	4506	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4588	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	3709	3	-	0/7/25/26	0/2/2/2
46	OMG	S2	683	46	-	2/5/27/28	0/3/3/3
3	PSU	L5	2402	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3899	3,84	-	2/7/25/26	0/2/2/2
46	PSU	S2	863	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1244	46	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PSU	S2	1367	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	1779	3	-	2/7/25/26	0/2/2/2
46	PSU	S2	814	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	3848	3	-	0/9/27/28	0/2/2/2
80	2MG	Bv	10	80	-	0/5/27/28	0/3/3/3
3	OMG	L5	1612	3,84	-	0/5/27/28	0/3/3/3
3	OMC	L5	3866	3	-	1/9/27/28	0/2/2/2
46	A2M	S2	99	46	-	2/5/27/28	0/3/3/3
46	G7M	S2	1639	46,80	-	0/3/25/26	0/3/3/3
80	PSU	Bv	27	80	-	0/7/25/26	0/2/2/2
46	PSU	S2	1692	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	649	46	-	0/7/25/26	0/2/2/2
3	2MG	L5	1504	3	-	0/5/27/28	0/3/3/3
80	PSU	Bv	55	80	-	1/7/25/26	0/2/2/2
3	PSU	L5	4263	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	406	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	2338	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4266	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3741	3	-	1/7/25/26	0/2/2/2
46	PSU	S2	1004	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	4549	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4606	3	-	3/7/25/26	0/2/2/2
46	PSU	S2	1643	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	2811	3	-	0/9/27/28	0/2/2/2
80	UY4	Bv	37	80	-	3/19/50/51	0/3/3/3
3	PSU	L5	4659	3	-	0/7/25/26	0/2/2/2
46	A2M	S2	27	46,84	-	0/5/27/28	0/3/3/3
46	PSU	S2	218	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1174	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	4966	3	-	0/7/25/26	0/2/2/2
46	OMG	S2	867	46	-	0/5/27/28	0/3/3/3
46	B8N	S2	1248	46	1/1/7/7	1/16/34/35	0/2/2/2
3	OMG	L5	1303	3	-	2/5/27/28	0/3/3/3
3	OMC	L5	4426	3	-	0/9/27/28	0/2/2/2
46	A2M	S2	576	46	-	3/5/27/28	0/3/3/3
46	OMG	S2	644	46	-	3/5/27/28	0/3/3/3
3	OMC	L5	2352	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3737	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3823	3	-	1/7/25/26	0/2/2/2
46	OMG	S2	601	46	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4373	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1670	3	-	0/7/25/26	0/2/2/2
46	OMC	S2	174	46	-	1/9/27/28	0/2/2/2
3	PSU	L5	3743	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	3878	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	4464	3	-	0/5/27/28	0/3/3/3
5	PSU	L8	69	5	-	1/7/25/26	0/2/2/2
46	OMU	S2	172	46	-	2/9/27/28	0/2/2/2
3	PSU	L5	4331	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4502	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1523	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	391	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	3606	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	4282	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1664	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4390	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4937	3	-	0/7/25/26	0/2/2/2
80	H2U	Bv	16	80	-	2/7/38/39	0/2/2/2
3	PSU	L5	4491	3,84	-	0/7/25/26	0/2/2/2
81	MEQ	j	185	81	-	0/8/9/11	-
3	PSU	L5	3694	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3749	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3616	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3787	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	364	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	2388	3,84	-	1/5/27/28	0/3/3/3
3	A2M	L5	4541	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	3739	3	-	2/5/27/28	0/3/3/3
3	PSU	L5	4401	3	-	0/7/25/26	0/2/2/2
46	OMU	S2	1326	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1177	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	509	46,84	-	0/5/27/28	0/3/3/3
80	PSU	Bv	28	80	-	2/7/25/26	0/2/2/2
3	OMG	L5	3771	3	-	0/5/27/28	0/3/3/3
3	5MC	L5	4417	3	-	3/7/25/26	0/2/2/2
80	G7M	Bv	46	80	-	3/3/25/26	0/3/3/3
3	A2M	L5	1511	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	3703	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4598	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4269	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4593	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	1238	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	1383	46	-	0/5/27/28	0/3/3/3
3	A2M	L5	2350	3,84	-	1/5/27/28	0/3/3/3
3	PSU	L5	4441	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	1327	3	-	0/9/27/28	0/2/2/2
46	OMC	S2	462	46	-	0/9/27/28	0/2/2/2
3	PSU	L5	3830	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	2774	3,84	-	1/5/27/28	0/3/3/3
80	M2G	Bv	26	80	-	0/7/29/30	0/3/3/3
3	PSU	L5	3674	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4198	3	-	0/5/27/28	0/3/3/3
6	MLZ	LC	333	6	-	4/7/8/10	-
3	A2M	L5	3804	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4166	80,3	-	0/5/27/28	0/3/3/3
46	OMU	S2	428	46	-	6/9/27/28	0/2/2/2
3	OMG	L5	4469	3	-	0/5/27/28	0/3/3/3
46	A2M	S2	166	46	-	0/5/27/28	0/3/3/3
3	OMC	L5	2409	3,84	-	0/9/27/28	0/2/2/2
3	A2M	L5	3809	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4412	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	1136	46	-	2/7/25/26	0/2/2/2
3	1MA	L5	1309	3,84	-	0/3/25/26	0/3/3/3
3	OMG	L5	4362	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3747	3	-	0/7/25/26	0/2/2/2
46	MA6	S2	1851	46	-	2/7/29/30	0/3/3/3
46	PSU	S2	1045	46	-	2/7/25/26	0/2/2/2
46	A2M	S2	512	46	-	2/5/27/28	0/3/3/3
3	A2M	L5	3764	3	-	2/5/27/28	0/3/3/3
3	PSU	L5	1849	3	-	2/7/25/26	0/2/2/2
3	OMU	L5	3904	3	-	2/9/27/28	0/2/2/2
3	OMU	L5	4197	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	651	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	668	46,84	-	3/5/27/28	0/3/3/3
3	OMC	L5	2791	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	815	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	105	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	36	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	159	46	-	0/5/27/28	0/3/3/3
3	PSU	L5	4643	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMU	S2	1442	46	-	2/9/27/28	0/2/2/2
3	PSU	L5	4975	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1509	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	572	46	-	1/7/25/26	0/2/2/2
46	PSU	S2	1232	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	1731	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	1445	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	4427	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2619	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4323	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3713	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	1046	46	-	0/7/25/26	0/2/2/2
3	OMG	L5	2351	3	-	2/5/27/28	0/3/3/3
80	1MA	Bv	58	80	-	2/3/25/26	0/3/3/3
46	A2M	S2	468	46	-	1/5/27/28	0/3/3/3
3	PSU	L5	3832	3,84	-	0/7/25/26	0/2/2/2
46	MA6	S2	1850	46	-	2/7/29/30	0/3/3/3
5	OMG	L8	75	5	-	0/5/27/28	0/3/3/3
46	OMC	S2	517	46	-	1/9/27/28	0/2/2/2
3	PSU	L5	4393	3	-	0/7/25/26	0/2/2/2
46	6MZ	S2	1832	46	-	0/5/27/28	0/3/3/3
41	MLZ	Lm	98	41	-	1/7/8/10	-
3	OMG	L5	2411	3	-	2/5/27/28	0/3/3/3
46	PSU	S2	109	46	-	0/7/25/26	0/2/2/2
80	1MG	Bv	9	80	-	1/3/25/26	0/3/3/3
3	UY1	L5	3797	3,84	-	7/9/27/28	0/2/2/2
46	A2M	S2	590	46	-	3/5/27/28	0/3/3/3
3	OMG	L5	2863	3	-	0/5/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
46	PSU	S2	34	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	3618	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3680	3	-	4/9/27/28	0/2/2/2
46	OMC	S2	1391	46	-	2/9/27/28	0/2/2/2
46	OMU	S2	1288	46	-	0/9/27/28	0/2/2/2
3	PSU	L5	4546	3	-	0/7/25/26	0/2/2/2
46	4AC	S2	1337	46	-	1/11/29/30	0/2/2/2
46	A2M	S2	1031	46	-	0/5/27/28	0/3/3/3
3	OMG	L5	4340	3	-	0/5/27/28	0/3/3/3
46	OMU	S2	1804	46	-	2/9/27/28	0/2/2/2
3	PSU	L5	2495	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PSU	S2	1625	46	-	2/7/25/26	0/2/2/2
3	OMU	L5	4590	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	966	46	-	0/7/25/26	0/2/2/2
3	PSU	L5	1768	3	-	2/7/25/26	0/2/2/2
46	OMC	S2	1703	46	-	2/9/27/28	0/2/2/2
3	OMU	L5	2824	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	93	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	436	46	-	2/5/27/28	0/3/3/3
46	OMG	S2	1490	46	-	3/5/27/28	0/3/3/3
3	A2M	L5	1521	3	-	1/5/27/28	0/3/3/3
46	PSU	S2	1347	46	-	0/7/25/26	0/2/2/2
73	IAS	SO	138	73	-	3/7/7/8	-
3	PSU	L5	1569	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4522	3	-	0/7/25/26	0/2/2/2
46	PSU	S2	609	46	-	0/7/25/26	0/2/2/2
3	A2M	L5	389	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1858	3,84	-	0/5/27/28	0/3/3/3
46	OMC	S2	621	46	-	4/9/27/28	0/2/2/2
46	PSU	S2	822	46	-	2/7/25/26	0/2/2/2
46	A2M	S2	1678	46	-	0/5/27/28	0/3/3/3
3	OMU	L5	4276	3	-	0/9/27/28	0/2/2/2
46	PSU	S2	801	46	-	1/7/25/26	0/2/2/2
3	5MC	L5	3761	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3846	3	-	2/5/27/28	0/3/3/3
3	A2M	L5	4493	3,84	-	0/5/27/28	0/3/3/3
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1081	46	-	2/7/25/26	0/2/2/2
3	A2M	L5	3697	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1847	3	-	1/7/25/26	0/2/2/2
3	6MZ	L5	4190	3	-	0/5/27/28	0/3/3/3
46	PSU	S2	686	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	2848	3	-	0/9/27/28	0/2/2/2
46	OMU	S2	116	46	-	3/9/27/28	0/2/2/2
46	A2M	S2	484	46	-	0/5/27/28	0/3/3/3
3	PSU	L5	1769	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3723	3	-	0/5/27/28	0/3/3/3

All (597) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	Bv	37	UY4	C04-C02	5.17	1.60	1.52
80	Bv	58	1MA	C2-N3	5.03	1.34	1.28
80	Bv	37	UY4	C6-N1	5.00	1.40	1.34
3	L5	3904	OMU	C4-N3	-4.73	1.30	1.38
3	L5	1303	OMG	C6-N1	-4.67	1.30	1.37
3	L5	3616	PSU	C4-N3	-4.67	1.30	1.38
3	L5	3674	PSU	C4-N3	-4.54	1.30	1.38
3	L5	4362	OMG	C6-N1	-4.52	1.30	1.37
3	L5	3618	PSU	C4-N3	-4.48	1.30	1.38
3	L5	4491	PSU	C4-N3	-4.47	1.30	1.38
3	L5	1523	PSU	C4-N3	-4.36	1.30	1.38
3	L5	4464	OMG	C6-N1	-4.36	1.31	1.37
3	L5	3606	OMG	C6-N1	-4.29	1.31	1.37
3	L5	4522	PSU	C4-N3	-4.28	1.30	1.38
3	L5	4607	OMG	C6-N1	-4.24	1.31	1.37
3	L5	4590	OMU	C4-N3	-4.21	1.31	1.38
3	L5	1670	PSU	C2-N1	-4.19	1.31	1.36
46	S2	1248	B8N	C4-N3	-4.18	1.32	1.40
3	L5	1509	OMG	C6-N1	-4.18	1.31	1.37
3	L5	364	OMG	C6-N1	-4.17	1.31	1.37
3	L5	1670	PSU	C4-N3	-4.12	1.31	1.38
3	L5	3899	PSU	C4-N3	-4.10	1.31	1.38
3	L5	3832	PSU	C4-N3	-4.02	1.31	1.38
3	L5	4323	PSU	C4-N3	-4.02	1.31	1.38
3	L5	3618	PSU	C2-N3	-4.01	1.30	1.37
3	L5	4643	PSU	C4-N3	-4.00	1.31	1.38
3	L5	4659	PSU	C4-N3	-3.99	1.31	1.38
3	L5	3616	PSU	C2-N3	-3.97	1.30	1.37
3	L5	4276	OMU	C4-N3	-3.97	1.31	1.38
3	L5	3830	PSU	C4-N3	-3.97	1.31	1.38
3	L5	4966	PSU	C4-N3	-3.95	1.31	1.38
3	L5	1523	PSU	C2-N1	-3.95	1.31	1.36
3	L5	4263	PSU	C4-N3	-3.94	1.31	1.38
80	Bv	26	M2G	C2-N3	3.88	1.36	1.30
3	L5	3618	PSU	C2-N1	-3.87	1.31	1.36
3	L5	4593	OMG	C6-N1	-3.87	1.31	1.37
3	L5	1849	PSU	C4-N3	-3.86	1.31	1.38
3	L5	4331	PSU	C4-N3	-3.82	1.31	1.38
3	L5	4598	PSU	C4-N3	-3.82	1.31	1.38
3	L5	4340	OMG	C6-N1	-3.82	1.32	1.37
3	L5	4373	PSU	C4-N3	-3.82	1.31	1.38
46	S2	1081	PSU	C4-N3	-3.81	1.31	1.38
3	L5	2351	OMG	C6-N1	-3.81	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1664	PSU	C4-N3	-3.81	1.31	1.38
3	L5	4166	OMG	C6-N1	-3.81	1.32	1.37
3	L5	4393	PSU	C4-N3	-3.79	1.31	1.38
3	L5	1769	PSU	C4-N3	-3.79	1.31	1.38
3	L5	3616	PSU	C2-N1	-3.78	1.31	1.36
3	L5	4197	OMU	C4-N3	-3.77	1.32	1.38
3	L5	1569	PSU	C4-N3	-3.77	1.31	1.38
3	L5	1779	PSU	C4-N3	-3.76	1.31	1.38
46	S2	1692	PSU	C4-N3	-3.76	1.31	1.38
3	L5	4590	OMU	C2-N3	-3.74	1.31	1.38
3	L5	1504	2MG	C6-N1	-3.73	1.32	1.37
3	L5	1523	PSU	C2-N3	-3.73	1.31	1.37
3	L5	3904	OMU	C2-N3	-3.73	1.31	1.38
3	L5	4282	PSU	C4-N3	-3.73	1.31	1.38
3	L5	4468	OMU	C4-N3	-3.72	1.32	1.38
3	L5	4598	PSU	C2-N1	-3.72	1.31	1.36
3	L5	4427	PSU	C4-N3	-3.72	1.31	1.38
3	L5	4659	PSU	C2-N1	-3.71	1.31	1.36
3	L5	4269	PSU	C4-N3	-3.71	1.31	1.38
3	L5	4401	PSU	C4-N3	-3.70	1.31	1.38
3	L5	4502	PSU	C4-N3	-3.70	1.31	1.38
46	S2	406	PSU	C4-N3	-3.69	1.31	1.38
3	L5	4975	PSU	C4-N3	-3.66	1.32	1.38
3	L5	4937	PSU	C4-N3	-3.66	1.32	1.38
3	L5	3899	PSU	C2-N3	-3.65	1.31	1.37
3	L5	4331	PSU	C2-N3	-3.65	1.31	1.37
3	L5	4468	OMU	C2-N3	-3.65	1.31	1.38
3	L5	2619	PSU	C4-N3	-3.64	1.32	1.38
3	L5	4441	PSU	C4-N3	-3.63	1.32	1.38
3	L5	1731	PSU	C4-N3	-3.62	1.32	1.38
3	L5	3737	PSU	C4-N3	-3.61	1.32	1.38
3	L5	2863	OMG	C6-N1	-3.61	1.32	1.37
3	L5	1670	PSU	C2-N3	-3.60	1.31	1.37
3	L5	3723	OMG	C6-N1	-3.60	1.32	1.37
3	L5	3832	PSU	C2-N3	-3.60	1.31	1.37
3	L5	4331	PSU	C2-N1	-3.59	1.32	1.36
46	S2	601	OMG	C6-N1	-3.58	1.32	1.37
46	S2	1174	PSU	C4-N3	-3.58	1.32	1.38
3	L5	1612	OMG	C6-N1	-3.57	1.32	1.37
46	S2	1248	B8N	C2-N3	-3.57	1.32	1.38
3	L5	2402	PSU	C4-N3	-3.57	1.32	1.38
3	L5	4643	PSU	C2-N1	-3.57	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3747	PSU	C4-N3	-3.56	1.32	1.38
3	L5	4491	PSU	C2-N3	-3.56	1.31	1.37
3	L5	4469	OMG	C6-N1	-3.56	1.32	1.37
80	Bv	46	G7M	C5-C4	3.55	1.46	1.39
3	L5	2495	PSU	C4-N3	-3.55	1.32	1.38
46	S2	651	PSU	C4-N3	-3.53	1.32	1.38
3	L5	4549	PSU	C4-N3	-3.53	1.32	1.38
46	S2	686	PSU	C4-N3	-3.53	1.32	1.38
3	L5	4549	PSU	C2-N3	-3.53	1.31	1.37
3	L5	4412	PSU	C4-N3	-3.52	1.32	1.38
3	L5	4643	PSU	C2-N3	-3.52	1.31	1.37
3	L5	3749	PSU	C4-N3	-3.52	1.32	1.38
5	L8	55	PSU	C4-N3	-3.51	1.32	1.38
3	L5	4269	PSU	C2-N1	-3.50	1.32	1.36
3	L5	4588	OMG	C6-N1	-3.50	1.32	1.37
3	L5	3743	PSU	C4-N3	-3.49	1.32	1.38
3	L5	3797	UY1	C4-N3	-3.48	1.32	1.38
3	L5	4417	5MC	C6-N1	-3.48	1.32	1.38
3	L5	3878	OMG	C6-N1	-3.48	1.32	1.37
3	L5	1847	PSU	C2-N1	-3.47	1.32	1.36
3	L5	3674	PSU	C2-N3	-3.47	1.31	1.37
3	L5	1731	PSU	C2-N1	-3.47	1.32	1.36
3	L5	3823	PSU	C4-N3	-3.47	1.32	1.38
46	S2	1490	OMG	C6-N1	-3.47	1.32	1.37
3	L5	4263	PSU	C2-N3	-3.46	1.31	1.37
3	L5	1779	PSU	C2-N3	-3.45	1.31	1.37
3	L5	2824	OMU	C4-N3	-3.44	1.32	1.38
46	S2	109	PSU	C4-N3	-3.44	1.32	1.38
3	L5	3823	PSU	C2-N1	-3.42	1.32	1.36
3	L5	3830	PSU	C2-N1	-3.42	1.32	1.36
46	S2	1004	PSU	C4-N3	-3.42	1.32	1.38
3	L5	4522	PSU	C2-N1	-3.42	1.32	1.36
5	L8	69	PSU	C4-N3	-3.41	1.32	1.38
3	L5	4966	PSU	C2-N3	-3.41	1.31	1.37
46	S2	1177	PSU	C4-N3	-3.40	1.32	1.38
46	S2	1232	PSU	C4-N3	-3.40	1.32	1.38
46	S2	1136	PSU	C4-N3	-3.39	1.32	1.38
3	L5	3832	PSU	C2-N1	-3.38	1.32	1.36
46	S2	649	PSU	C4-N3	-3.38	1.32	1.38
3	L5	4546	PSU	C4-N3	-3.37	1.32	1.38
3	L5	3904	OMU	C5-C4	-3.37	1.36	1.43
3	L5	4323	PSU	C2-N3	-3.37	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1670	PSU	C6-N1	-3.37	1.30	1.36
46	S2	1238	PSU	C4-N3	-3.37	1.32	1.38
3	L5	2411	OMG	C6-N1	-3.36	1.32	1.37
3	L5	4502	PSU	C2-N3	-3.36	1.31	1.37
3	L5	1768	PSU	C4-N3	-3.36	1.32	1.38
3	L5	4470	PSU	C4-N3	-3.35	1.32	1.38
3	L5	4412	PSU	C2-N1	-3.35	1.32	1.36
46	S2	815	PSU	C4-N3	-3.34	1.32	1.38
3	L5	4441	PSU	C2-N1	-3.33	1.32	1.36
3	L5	4427	PSU	C2-N3	-3.31	1.32	1.37
3	L5	3761	5MC	C6-N1	-3.30	1.32	1.38
3	L5	1847	PSU	C4-N3	-3.30	1.32	1.38
3	L5	4606	PSU	C4-N3	-3.30	1.32	1.38
46	S2	1326	OMU	C4-N3	-3.30	1.33	1.38
3	L5	1849	PSU	C2-N3	-3.29	1.32	1.37
46	S2	966	PSU	C4-N3	-3.29	1.32	1.38
46	S2	1045	PSU	C4-N3	-3.29	1.32	1.38
3	L5	4266	PSU	C4-N3	-3.29	1.32	1.38
3	L5	3674	PSU	C2-N1	-3.29	1.32	1.36
46	S2	121	OMU	C4-N3	-3.28	1.33	1.38
3	L5	3694	PSU	C4-N3	-3.28	1.32	1.38
46	S2	801	PSU	C4-N3	-3.27	1.32	1.38
3	L5	1847	PSU	C2-N3	-3.27	1.32	1.37
46	S2	863	PSU	C4-N3	-3.27	1.32	1.38
3	L5	2619	PSU	C2-N3	-3.26	1.32	1.37
3	L5	4659	PSU	C2-N3	-3.26	1.32	1.37
3	L5	4373	PSU	C2-N3	-3.25	1.32	1.37
3	L5	3899	PSU	C2-N1	-3.25	1.32	1.36
3	L5	3741	PSU	C4-N3	-3.25	1.32	1.38
3	L5	4522	PSU	C2-N3	-3.25	1.32	1.37
46	S2	1643	PSU	C4-N3	-3.25	1.32	1.38
3	L5	1731	PSU	C2-N3	-3.25	1.32	1.37
3	L5	3737	PSU	C2-N3	-3.24	1.32	1.37
46	S2	36	PSU	C4-N3	-3.24	1.32	1.38
3	L5	3830	PSU	C2-N3	-3.24	1.32	1.37
3	L5	4276	OMU	C2-N3	-3.24	1.32	1.38
46	S2	105	PSU	C4-N3	-3.24	1.32	1.38
3	L5	3709	PSU	C4-N3	-3.23	1.32	1.38
46	S2	683	OMG	C6-N1	-3.23	1.32	1.37
46	S2	814	PSU	C4-N3	-3.23	1.32	1.38
46	S2	119	PSU	C4-N3	-3.23	1.32	1.38
3	L5	2824	OMU	C5-C4	-3.22	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L8	75	OMG	C6-N1	-3.22	1.32	1.37
3	L5	3771	OMG	C6-N1	-3.21	1.32	1.37
80	Bv	55	PSU	C6-C5	3.21	1.38	1.35
3	L5	4282	PSU	C2-N3	-3.21	1.32	1.37
3	L5	4546	PSU	C2-N1	-3.20	1.32	1.36
46	S2	218	PSU	C4-N3	-3.20	1.32	1.38
3	L5	4590	OMU	C5-C4	-3.19	1.36	1.43
3	L5	1569	PSU	C2-N1	-3.18	1.32	1.36
46	S2	1046	PSU	C4-N3	-3.17	1.32	1.38
80	Bv	27	PSU	C6-C5	3.16	1.38	1.35
46	S2	1367	PSU	C4-N3	-3.16	1.32	1.38
46	S2	1081	PSU	C2-N3	-3.16	1.32	1.37
46	S2	1442	OMU	C4-N3	-3.16	1.33	1.38
46	S2	1347	PSU	C4-N3	-3.15	1.32	1.38
3	L5	1569	PSU	C2-N3	-3.15	1.32	1.37
3	L5	4276	OMU	C5-C4	-3.15	1.36	1.43
46	S2	34	PSU	C4-N3	-3.15	1.33	1.38
46	S2	644	OMG	C6-N1	-3.14	1.33	1.37
80	Bv	58	1MA	C6-N6	3.14	1.35	1.27
3	L5	4269	PSU	C2-N3	-3.13	1.32	1.37
3	L5	2495	PSU	C2-N1	-3.13	1.32	1.36
3	L5	4263	PSU	C2-N1	-3.12	1.32	1.36
3	L5	4323	PSU	C2-N1	-3.12	1.32	1.36
3	L5	3713	PSU	C4-N3	-3.12	1.33	1.38
46	S2	866	PSU	C4-N3	-3.11	1.33	1.38
3	L5	1769	PSU	C2-N3	-3.11	1.32	1.37
3	L5	4502	PSU	C2-N1	-3.11	1.32	1.36
3	L5	3747	PSU	C2-N3	-3.10	1.32	1.37
46	S2	436	OMG	C6-N1	-3.09	1.33	1.37
46	S2	1328	OMG	C6-N1	-3.09	1.33	1.37
3	L5	3747	PSU	C2-N1	-3.08	1.32	1.36
46	S2	572	PSU	C4-N3	-3.08	1.33	1.38
46	S2	1692	PSU	C2-N3	-3.07	1.32	1.37
3	L5	4966	PSU	C2-N1	-3.07	1.32	1.36
80	Bv	37	UY4	C09-N6	3.07	1.44	1.37
46	S2	1174	PSU	C2-N1	-3.07	1.32	1.36
46	S2	1639	G7M	C5-C4	3.07	1.45	1.39
46	S2	609	PSU	C4-N3	-3.06	1.33	1.38
3	L5	4606	PSU	C2-N3	-3.06	1.32	1.37
46	S2	1136	PSU	C2-N3	-3.06	1.32	1.37
46	S2	866	PSU	C6-C5	3.06	1.38	1.35
3	L5	4198	OMG	C6-N1	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1445	PSU	C4-N3	-3.05	1.33	1.38
3	L5	2495	PSU	C2-N3	-3.04	1.32	1.37
46	S2	121	OMU	C2-N3	-3.04	1.32	1.38
46	S2	172	OMU	C4-N3	-3.04	1.33	1.38
3	L5	2402	PSU	C2-N3	-3.03	1.32	1.37
46	S2	822	PSU	C4-N3	-3.03	1.33	1.38
46	S2	1337	4AC	C4-N4	-3.03	1.35	1.39
3	L5	3743	PSU	C2-N3	-3.03	1.32	1.37
3	L5	4598	PSU	C2-N3	-3.02	1.32	1.37
3	L5	4937	PSU	C2-N3	-3.02	1.32	1.37
46	S2	1046	PSU	C2-N1	-3.02	1.32	1.36
3	L5	2824	OMU	C2-N3	-3.02	1.32	1.38
46	S2	1232	PSU	C6-C5	3.02	1.38	1.35
3	L5	4549	PSU	C2-N1	-3.01	1.32	1.36
3	L5	4401	PSU	C2-N1	-3.01	1.32	1.36
46	S2	509	OMG	C6-N1	-3.01	1.33	1.37
3	L5	4197	OMU	C2-N3	-3.01	1.32	1.38
3	L5	1664	PSU	C2-N3	-3.00	1.32	1.37
46	S2	1177	PSU	C2-N1	-3.00	1.32	1.36
3	L5	3761	5MC	C5-C4	2.99	1.46	1.44
3	L5	1664	PSU	O4'-C1'	-2.99	1.39	1.43
3	L5	4401	PSU	C2-N3	-2.99	1.32	1.37
46	S2	105	PSU	C6-C5	2.98	1.38	1.35
3	L5	3820	OMC	C5-C4	-2.97	1.36	1.42
46	S2	93	PSU	C4-N3	-2.97	1.33	1.38
46	S2	1288	OMU	C4-N3	-2.96	1.33	1.38
46	S2	572	PSU	C6-C5	2.96	1.38	1.35
3	L5	4598	PSU	C6-N1	-2.96	1.31	1.36
3	L5	4975	PSU	C2-N1	-2.96	1.32	1.36
3	L5	4412	PSU	C2-N3	-2.96	1.32	1.37
3	L5	4427	PSU	C2-N1	-2.95	1.32	1.36
80	Bv	28	PSU	C4-N3	-2.94	1.33	1.38
3	L5	4975	PSU	C6-C5	2.93	1.38	1.35
3	L5	4468	OMU	C5-C4	-2.93	1.37	1.43
3	L5	1849	PSU	C2-N1	-2.92	1.32	1.36
3	L5	1309	1MA	C2-N3	2.91	1.32	1.28
46	S2	1625	PSU	C4-N3	-2.90	1.33	1.38
46	S2	1804	OMU	C4-N3	-2.90	1.33	1.38
46	S2	649	PSU	C2-N3	-2.88	1.32	1.37
3	L5	1664	PSU	C2-N1	-2.88	1.32	1.36
46	S2	1244	PSU	C4-N3	-2.87	1.33	1.38
46	S2	406	PSU	C2-N3	-2.87	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2338	OMC	C5-C4	-2.87	1.36	1.42
5	L8	69	PSU	C2-N3	-2.87	1.32	1.37
46	S2	1177	PSU	C2-N3	-2.86	1.32	1.37
80	Bv	28	PSU	C6-C5	2.86	1.38	1.35
3	L5	3743	PSU	C2-N1	-2.86	1.32	1.36
46	S2	867	OMG	C6-N1	-2.86	1.33	1.37
3	L5	3694	PSU	C2-N3	-2.86	1.32	1.37
46	S2	686	PSU	C2-N3	-2.86	1.32	1.37
46	S2	109	PSU	C2-N3	-2.84	1.32	1.37
3	L5	4197	OMU	C5-C4	-2.84	1.37	1.43
46	S2	649	PSU	C6-C5	2.84	1.38	1.35
3	L5	4266	PSU	C2-N3	-2.84	1.32	1.37
3	L5	3797	UY1	C2-N3	-2.84	1.32	1.37
3	L5	3823	PSU	C2-N3	-2.83	1.32	1.37
3	L5	2619	PSU	C2-N1	-2.83	1.33	1.36
3	L5	4606	PSU	C2-N1	-2.82	1.33	1.36
46	S2	863	PSU	C2-N1	-2.82	1.33	1.36
3	L5	3741	PSU	C6-C5	2.82	1.38	1.35
3	L5	1768	PSU	C2-N1	-2.81	1.33	1.36
5	L8	55	PSU	C2-N1	-2.81	1.33	1.36
46	S2	1842	4AC	C6-N1	-2.81	1.31	1.38
46	S2	863	PSU	C6-C5	2.81	1.38	1.35
3	L5	4441	PSU	C2-N3	-2.81	1.32	1.37
46	S2	1326	OMU	C2-N3	-2.80	1.33	1.38
3	L5	4282	PSU	C2-N1	-2.80	1.33	1.36
3	L5	1768	PSU	C2-N3	-2.80	1.32	1.37
46	S2	1238	PSU	C2-N1	-2.79	1.33	1.36
3	L5	4491	PSU	O4'-C1'	-2.79	1.40	1.43
46	S2	116	OMU	C5-C4	-2.79	1.37	1.43
3	L5	4373	PSU	C2-N1	-2.79	1.33	1.36
3	L5	1769	PSU	C2-N1	-2.79	1.33	1.36
46	S2	1842	4AC	C4-N4	-2.78	1.35	1.39
46	S2	1232	PSU	C2-N3	-2.78	1.32	1.37
3	L5	4500	UR3	C5-C4	-2.78	1.36	1.43
3	L5	3749	PSU	C2-N3	-2.78	1.32	1.37
46	S2	814	PSU	C2-N3	-2.77	1.32	1.37
3	L5	3823	PSU	C6-N1	-2.77	1.31	1.36
46	S2	1639	G7M	C6-N1	-2.76	1.33	1.37
46	S2	428	OMU	C4-N3	-2.76	1.33	1.38
46	S2	822	PSU	C6-C5	2.76	1.38	1.35
3	L5	4546	PSU	C2-N3	-2.75	1.32	1.37
3	L5	3737	PSU	C2-N1	-2.75	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	172	OMU	C2-N3	-2.75	1.33	1.38
3	L5	2791	OMC	C5-C4	-2.74	1.36	1.42
3	L5	4393	PSU	C2-N3	-2.74	1.33	1.37
46	S2	1445	PSU	C6-C5	2.74	1.38	1.35
46	S2	649	PSU	C2-N1	-2.74	1.33	1.36
3	L5	2402	PSU	C2-N1	-2.73	1.33	1.36
46	S2	93	PSU	C2-N3	-2.73	1.33	1.37
46	S2	1177	PSU	C6-C5	2.73	1.38	1.35
80	Bv	26	M2G	C2-N2	2.73	1.40	1.35
46	S2	966	PSU	C6-C5	2.73	1.38	1.35
3	L5	3616	PSU	C6-N1	-2.73	1.31	1.36
3	L5	4975	PSU	C2-N3	-2.72	1.33	1.37
3	L5	4393	PSU	C6-C5	2.72	1.38	1.35
46	S2	1045	PSU	C2-N3	-2.72	1.33	1.37
46	S2	218	PSU	C6-C5	2.71	1.38	1.35
46	S2	1692	PSU	C2-N1	-2.71	1.33	1.36
46	S2	609	PSU	C6-C5	2.71	1.38	1.35
46	S2	116	OMU	C4-N3	-2.71	1.34	1.38
3	L5	2409	OMC	C5-C4	-2.71	1.36	1.42
46	S2	119	PSU	C2-N3	-2.71	1.33	1.37
3	L5	1779	PSU	C2-N1	-2.71	1.33	1.36
80	Bv	27	PSU	C4-N3	-2.71	1.33	1.38
46	S2	1004	PSU	C2-N1	-2.70	1.33	1.36
5	L8	55	PSU	C2-N3	-2.70	1.33	1.37
3	L5	3709	PSU	C2-N3	-2.70	1.33	1.37
46	S2	34	PSU	C6-C5	2.69	1.38	1.35
3	L5	4266	PSU	C6-C5	2.69	1.38	1.35
46	S2	1046	PSU	C2-N3	-2.69	1.33	1.37
46	S2	1625	PSU	C6-C5	2.69	1.38	1.35
46	S2	218	PSU	C2-N3	-2.69	1.33	1.37
46	S2	1442	OMU	C5-C4	-2.67	1.37	1.43
80	Bv	55	PSU	C4-N3	-2.67	1.33	1.38
46	S2	1442	OMU	C2-N3	-2.67	1.33	1.38
3	L5	1303	OMG	C2-N1	-2.66	1.31	1.37
3	L5	4470	PSU	C2-N1	-2.66	1.33	1.36
3	L5	1327	OMC	C5-C4	-2.66	1.36	1.42
46	S2	651	PSU	C6-C5	2.65	1.38	1.35
3	L5	3848	OMC	C5-C4	-2.65	1.36	1.42
3	L5	4937	PSU	C2-N1	-2.65	1.33	1.36
3	L5	3749	PSU	C2-N1	-2.65	1.33	1.36
3	L5	4390	PSU	C4-N3	-2.64	1.33	1.38
46	S2	1045	PSU	C2-N1	-2.64	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4522	PSU	C6-N1	-2.64	1.32	1.36
46	S2	815	PSU	C2-N3	-2.64	1.33	1.37
3	L5	3797	UY1	O4'-C1'	-2.64	1.40	1.43
3	L5	3694	PSU	C2-N1	-2.64	1.33	1.36
46	S2	105	PSU	C2-N3	-2.64	1.33	1.37
46	S2	116	OMU	C2-N3	-2.64	1.33	1.38
3	L5	4966	PSU	C6-C5	2.63	1.38	1.35
3	L5	4643	PSU	C6-N1	-2.63	1.32	1.36
3	L5	4470	PSU	C2-N3	-2.63	1.33	1.37
46	S2	36	PSU	C6-C5	2.63	1.38	1.35
46	S2	801	PSU	C2-N3	-2.62	1.33	1.37
3	L5	4426	OMC	C5-C4	-2.62	1.36	1.42
46	S2	1174	PSU	C2-N3	-2.62	1.33	1.37
3	L5	4266	PSU	C2-N1	-2.62	1.33	1.36
46	S2	801	PSU	C6-C5	2.61	1.38	1.35
46	S2	406	PSU	C2-N1	-2.60	1.33	1.36
3	L5	2791	OMC	C6-N1	-2.60	1.31	1.38
46	S2	815	PSU	C6-C5	2.60	1.38	1.35
3	L5	1847	PSU	C6-C5	2.59	1.38	1.35
46	S2	1804	OMU	C5-C4	-2.59	1.38	1.43
80	Bv	47	H2U	C2-N3	-2.59	1.33	1.38
3	L5	4606	PSU	O4'-C1'	-2.58	1.40	1.43
80	Bv	16	H2U	C2-N3	-2.58	1.33	1.38
46	S2	966	PSU	C2-N3	-2.58	1.33	1.37
46	S2	1232	PSU	C2-N1	-2.57	1.33	1.36
3	L5	4491	PSU	C2-N1	-2.57	1.33	1.36
46	S2	119	PSU	C6-C5	2.57	1.38	1.35
5	L8	69	PSU	C6-N1	-2.57	1.32	1.36
46	S2	1004	PSU	C2-N3	-2.57	1.33	1.37
46	S2	1804	OMU	C2-N3	-2.57	1.33	1.38
3	L5	4412	PSU	O4'-C1'	-2.56	1.40	1.43
46	S2	34	PSU	C2-N3	-2.56	1.33	1.37
46	S2	428	OMU	C2-N3	-2.56	1.33	1.38
46	S2	1288	OMU	C2-N3	-2.56	1.33	1.38
46	S2	1367	PSU	C6-C5	2.55	1.38	1.35
46	S2	1081	PSU	C2-N1	-2.55	1.33	1.36
3	L5	3680	OMC	C6-N1	-2.55	1.32	1.38
3	L5	4393	PSU	C2-N1	-2.55	1.33	1.36
3	L5	4522	PSU	C6-C5	2.54	1.38	1.35
46	S2	814	PSU	C6-C5	2.54	1.38	1.35
46	S2	1643	PSU	C2-N3	-2.54	1.33	1.37
3	L5	3820	OMC	C6-N1	-2.54	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	822	PSU	C2-N1	-2.53	1.33	1.36
3	L5	1523	PSU	C6-N1	-2.53	1.32	1.36
46	S2	1136	PSU	C2-N1	-2.53	1.33	1.36
3	L5	3713	PSU	C2-N3	-2.53	1.33	1.37
46	S2	93	PSU	C2-N1	-2.53	1.33	1.36
3	L5	3787	OMC	C6-N1	-2.52	1.32	1.38
46	S2	1643	PSU	C2-N1	-2.52	1.33	1.36
3	L5	3797	UY1	C2-N1	-2.51	1.33	1.36
46	S2	109	PSU	C2-N1	-2.50	1.33	1.36
46	S2	36	PSU	C2-N3	-2.50	1.33	1.37
46	S2	651	PSU	C2-N3	-2.50	1.33	1.37
3	L5	4276	OMU	C6-N1	-2.49	1.32	1.38
3	L5	4426	OMC	C6-N1	-2.49	1.32	1.38
3	L5	4506	OMC	C6-N1	-2.48	1.32	1.38
3	L5	4323	PSU	O4'-C1'	-2.48	1.40	1.43
46	S2	1244	PSU	C2-N1	-2.48	1.33	1.36
46	S2	814	PSU	C2-N1	-2.48	1.33	1.36
3	L5	4441	PSU	C6-N1	-2.47	1.32	1.36
46	S2	36	PSU	C2-N1	-2.47	1.33	1.36
80	Bv	9	1MG	C2-N1	2.47	1.41	1.37
46	S2	1625	PSU	C2-N3	-2.46	1.33	1.37
3	L5	4390	PSU	C2-N1	-2.46	1.33	1.36
3	L5	2848	OMC	C6-N1	-2.46	1.32	1.38
46	S2	815	PSU	C2-N1	-2.45	1.33	1.36
3	L5	4659	PSU	C6-N1	-2.44	1.32	1.36
3	L5	3618	PSU	C6-N1	-2.43	1.32	1.36
3	L5	3899	PSU	C6-N1	-2.43	1.32	1.36
3	L5	4323	PSU	C6-N1	-2.43	1.32	1.36
3	L5	4269	PSU	C6-N1	-2.43	1.32	1.36
46	S2	1238	PSU	C6-C5	2.42	1.38	1.35
46	S2	1367	PSU	C2-N1	-2.42	1.33	1.36
46	S2	801	PSU	C2-N1	-2.42	1.33	1.36
3	L5	1849	PSU	C6-C5	2.42	1.38	1.35
46	S2	1244	PSU	C2-N3	-2.42	1.33	1.37
46	S2	686	PSU	C2-N1	-2.41	1.33	1.36
46	S2	1347	PSU	C2-N3	-2.41	1.33	1.37
46	S2	1004	PSU	C6-C5	2.41	1.38	1.35
46	S2	621	OMC	C6-N1	-2.41	1.32	1.38
46	S2	609	PSU	C2-N1	-2.41	1.33	1.36
46	S2	863	PSU	C2-N3	-2.40	1.33	1.37
3	L5	4362	OMG	C2-N1	-2.40	1.31	1.37
46	S2	406	PSU	C6-C5	2.40	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4441	PSU	C6-C5	2.40	1.37	1.35
3	L5	3741	PSU	C2-N3	-2.40	1.33	1.37
80	Bv	47	H2U	C4-N3	-2.39	1.33	1.37
3	L5	4401	PSU	C6-N1	-2.39	1.32	1.36
3	L5	4470	PSU	O4'-C1'	-2.39	1.40	1.43
3	L5	1569	PSU	C6-N1	-2.39	1.32	1.36
3	L5	3618	PSU	O4'-C1'	-2.39	1.40	1.43
5	L8	69	PSU	C2-N1	-2.38	1.33	1.36
46	S2	1347	PSU	C6-C5	2.38	1.37	1.35
46	S2	1238	PSU	C2-N3	-2.37	1.33	1.37
46	S2	105	PSU	C2-N1	-2.37	1.33	1.36
3	L5	3797	UY1	C6-N1	-2.36	1.32	1.36
46	S2	1046	PSU	C6-C5	2.36	1.37	1.35
3	L5	2352	OMC	C5-C4	-2.36	1.37	1.42
3	L5	1847	PSU	C6-N1	-2.36	1.32	1.36
3	L5	3904	OMU	C6-N1	-2.35	1.32	1.38
3	L5	3787	OMC	C5-C4	-2.35	1.37	1.42
46	S2	428	OMU	C5-C4	-2.35	1.38	1.43
3	L5	1504	2MG	C2-N1	-2.35	1.33	1.36
46	S2	1367	PSU	C2-N3	-2.35	1.33	1.37
80	Bv	16	H2U	C4-N3	-2.34	1.33	1.37
3	L5	4502	PSU	C6-N1	-2.34	1.32	1.36
3	L5	2848	OMC	C5-C4	-2.34	1.37	1.42
3	L5	3674	PSU	C6-N1	-2.33	1.32	1.36
46	S2	1625	PSU	C2-N1	-2.33	1.33	1.36
3	L5	4282	PSU	C6-N1	-2.33	1.32	1.36
46	S2	93	PSU	C6-C5	2.32	1.37	1.35
3	L5	2409	OMC	C6-N1	-2.32	1.32	1.38
3	L5	364	OMG	C2-N1	-2.32	1.32	1.37
3	L5	2811	OMC	C5-C4	-2.32	1.37	1.42
46	S2	1244	PSU	C6-C5	2.31	1.37	1.35
46	S2	1445	PSU	C2-N3	-2.31	1.33	1.37
3	L5	3830	PSU	O4'-C1'	-2.31	1.40	1.43
3	L5	2402	PSU	O4'-C1'	-2.31	1.40	1.43
46	S2	1692	PSU	C6-C5	2.31	1.37	1.35
3	L5	4427	PSU	C6-N1	-2.30	1.32	1.36
46	S2	1347	PSU	C2-N1	-2.30	1.33	1.36
46	S2	572	PSU	C2-N3	-2.30	1.33	1.37
46	S2	1337	4AC	C7-N4	-2.30	1.32	1.37
46	S2	609	PSU	C2-N3	-2.29	1.33	1.37
46	S2	172	OMU	C6-N1	-2.29	1.32	1.38
3	L5	4491	PSU	C6-N1	-2.29	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	Bv	26	M2G	C6-N1	-2.29	1.34	1.37
3	L5	2338	OMC	C6-N1	-2.29	1.32	1.38
3	L5	3899	PSU	C6-C5	2.29	1.37	1.35
3	L5	3823	PSU	C6-C5	2.29	1.37	1.35
46	S2	1046	PSU	O4'-C1'	-2.29	1.40	1.43
46	S2	121	OMU	C5-C4	-2.28	1.38	1.43
3	L5	4506	OMC	C5-C4	-2.28	1.37	1.42
46	S2	1643	PSU	C6-C5	2.28	1.37	1.35
3	L5	3866	OMC	C5-C4	-2.28	1.37	1.42
5	L8	69	PSU	O4'-C1'	-2.27	1.40	1.43
3	L5	2811	OMC	C6-N1	-2.27	1.32	1.38
46	S2	863	PSU	C6-N1	-2.27	1.32	1.36
3	L5	4401	PSU	C6-C5	2.26	1.37	1.35
80	Bv	10	2MG	C6-N1	-2.26	1.34	1.37
46	S2	1703	OMC	C5-C4	-2.26	1.37	1.42
3	L5	3741	PSU	O4'-C1'	-2.25	1.40	1.43
3	L5	4546	PSU	C6-N1	-2.25	1.32	1.36
46	S2	1081	PSU	C6-C5	2.25	1.37	1.35
46	S2	866	PSU	C2-N3	-2.25	1.33	1.37
3	L5	4390	PSU	C2-N3	-2.24	1.33	1.37
3	L5	4373	PSU	O4'-C1'	-2.24	1.40	1.43
3	L5	2619	PSU	C6-N1	-2.23	1.32	1.36
3	L5	3741	PSU	C2-N1	-2.23	1.33	1.36
46	S2	406	PSU	O4'-C1'	-2.23	1.40	1.43
46	S2	172	OMU	C5-C4	-2.23	1.38	1.43
3	L5	1327	OMC	C6-N1	-2.23	1.32	1.38
80	Bv	46	G7M	C6-N1	-2.23	1.34	1.37
3	L5	4502	PSU	C6-C5	2.23	1.37	1.35
3	L5	2863	OMG	C2-N1	-2.22	1.32	1.37
3	L5	1309	1MA	C6-N1	-2.22	1.38	1.41
3	L5	1768	PSU	C6-N1	-2.22	1.32	1.36
3	L5	4263	PSU	C6-N1	-2.21	1.32	1.36
46	S2	1832	6MZ	C6-C5	2.21	1.48	1.44
46	S2	1081	PSU	O4'-C1'	-2.21	1.40	1.43
46	S2	218	PSU	C2-N1	-2.21	1.33	1.36
3	L5	3606	OMG	C2-N1	-2.20	1.32	1.37
3	L5	4470	PSU	C6-N1	-2.20	1.32	1.36
46	S2	621	OMC	C5-C4	-2.20	1.37	1.42
3	L5	2824	OMU	C6-N1	-2.20	1.32	1.38
46	S2	1643	PSU	O4'-C1'	-2.20	1.40	1.43
3	L5	2495	PSU	C6-N1	-2.19	1.32	1.36
46	S2	822	PSU	C2-N3	-2.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1174	PSU	C6-N1	-2.19	1.32	1.36
3	L5	3709	PSU	C2-N1	-2.19	1.33	1.36
3	L5	4197	OMU	C6-N1	-2.19	1.32	1.38
3	L5	4427	PSU	O4'-C1'	-2.19	1.40	1.43
80	Bv	26	M2G	O4'-C1'	2.19	1.43	1.40
3	L5	3713	PSU	O4'-C1'	-2.19	1.40	1.43
3	L5	1309	1MA	C6-N6	2.18	1.33	1.27
3	L5	4549	PSU	C6-C5	2.18	1.37	1.35
3	L5	3832	PSU	C6-N1	-2.18	1.32	1.36
46	S2	866	PSU	C2-N1	-2.18	1.33	1.36
46	S2	109	PSU	C6-C5	2.18	1.37	1.35
46	S2	686	PSU	C6-C5	2.17	1.37	1.35
3	L5	1313	A2M	C5-N7	-2.17	1.32	1.39
3	L5	3737	PSU	C6-C5	2.17	1.37	1.35
3	L5	2619	PSU	O4'-C1'	-2.17	1.40	1.43
3	L5	3694	PSU	C6-C5	2.17	1.37	1.35
46	S2	1804	OMU	C2-N1	2.16	1.41	1.38
3	L5	1664	PSU	C6-N1	-2.16	1.32	1.36
46	S2	1851	MA6	C6-C5	2.16	1.48	1.44
3	L5	3680	OMC	C5-C4	-2.15	1.37	1.42
46	S2	822	PSU	O4'-C1'	-2.15	1.40	1.43
3	L5	4502	PSU	O4'-C1'	-2.15	1.40	1.43
80	Bv	28	PSU	C2-N3	-2.15	1.33	1.37
3	L5	3747	PSU	C6-N1	-2.15	1.32	1.36
3	L5	1769	PSU	C6-N1	-2.14	1.32	1.36
3	L5	3743	PSU	C6-C5	2.14	1.37	1.35
3	L5	4263	PSU	C6-C5	2.13	1.37	1.35
3	L5	1769	PSU	C6-C5	2.13	1.37	1.35
3	L5	2352	OMC	C6-N1	-2.13	1.33	1.38
3	L5	3830	PSU	C6-N1	-2.13	1.32	1.36
46	S2	1703	OMC	C6-N1	-2.13	1.33	1.38
46	S2	572	PSU	O4'-C1'	-2.13	1.40	1.43
3	L5	1731	PSU	C6-N1	-2.13	1.32	1.36
3	L5	4464	OMG	C2-N1	-2.13	1.32	1.37
46	S2	119	PSU	C2-N1	-2.13	1.33	1.36
3	L5	4331	PSU	C6-N1	-2.12	1.32	1.36
3	L5	1569	PSU	C6-C5	2.12	1.37	1.35
46	S2	966	PSU	C2-N1	-2.12	1.33	1.36
3	L5	3713	PSU	C6-C5	2.12	1.37	1.35
3	L5	4966	PSU	O4'-C1'	-2.12	1.40	1.43
3	L5	3709	PSU	C6-C5	2.12	1.37	1.35
46	S2	1288	OMU	C2-N1	2.12	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1248	B8N	C6-C5	2.11	1.38	1.35
3	L5	1779	PSU	C6-N1	-2.11	1.32	1.36
46	S2	1174	PSU	C6-C5	2.11	1.37	1.35
3	L5	4470	PSU	C6-C5	2.10	1.37	1.35
3	L5	4937	PSU	C6-N1	-2.10	1.32	1.36
46	S2	1442	OMU	C6-N1	-2.10	1.33	1.38
3	L5	4549	PSU	C6-N1	-2.10	1.32	1.36
46	S2	1288	OMU	C5-C4	-2.10	1.39	1.43
3	L5	1523	PSU	O4'-C1'	-2.10	1.40	1.43
3	L5	2388	A2M	C8-N7	-2.10	1.30	1.34
3	L5	3713	PSU	C2-N1	-2.10	1.33	1.36
46	S2	34	PSU	C2-N1	-2.10	1.33	1.36
3	L5	3674	PSU	O4'-C1'	-2.10	1.40	1.43
3	L5	4607	OMG	C2-N1	-2.10	1.32	1.37
3	L5	4373	PSU	C6-N1	-2.09	1.32	1.36
46	S2	651	PSU	C2-N1	-2.08	1.33	1.36
46	S2	1445	PSU	C2-N1	-2.08	1.33	1.36
3	L5	3747	PSU	C6-C5	2.08	1.37	1.35
3	L5	1509	OMG	C2-N1	-2.08	1.32	1.37
3	L5	4412	PSU	C6-N1	-2.08	1.32	1.36
73	SO	138	IAS	CB-CG	2.07	1.55	1.50
3	L5	3749	PSU	C6-N1	-2.07	1.32	1.36
3	L5	4937	PSU	C6-C5	2.07	1.37	1.35
46	S2	1490	OMG	C2-N1	-2.07	1.32	1.37
46	S2	1004	PSU	C6-N1	-2.07	1.32	1.36
3	L5	4263	PSU	O4'-C1'	-2.07	1.41	1.43
3	L5	4468	OMU	C6-N1	-2.07	1.33	1.38
3	L5	1309	1MA	C2-N1	-2.06	1.31	1.35
3	L5	4598	PSU	O4'-C1'	-2.06	1.41	1.43
3	L5	3616	PSU	O4'-C1'	-2.06	1.41	1.43
3	L5	4659	PSU	O4'-C1'	-2.05	1.41	1.43
3	L5	4190	6MZ	C4-N3	-2.05	1.32	1.35
46	S2	174	OMC	C6-N1	-2.05	1.33	1.38
5	L8	55	PSU	C6-N1	-2.04	1.33	1.36
3	L5	4331	PSU	O4'-C1'	-2.03	1.41	1.43
3	L5	4643	PSU	O4'-C1'	-2.03	1.41	1.43
5	L8	55	PSU	C6-C5	2.03	1.37	1.35
46	S2	1326	OMU	C6-N1	-2.02	1.33	1.38
46	S2	1326	OMU	C5-C4	-2.02	1.39	1.43
46	S2	517	OMC	C5-C4	-2.02	1.38	1.42
46	S2	1692	PSU	C6-N1	-2.02	1.33	1.36
3	L5	4340	OMG	C2-N1	-2.02	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	Bv	46	G7M	O4'-C1'	2.01	1.43	1.40
46	S2	1248	B8N	O4'-C1'	-2.01	1.41	1.43
46	S2	686	PSU	C6-N1	-2.01	1.33	1.36
3	L5	4546	PSU	O4'-C1'	-2.01	1.41	1.43
46	S2	1842	4AC	C5-C4	-2.01	1.36	1.41
3	L5	4166	OMG	C2-N1	-2.01	1.32	1.37
46	S2	119	PSU	O4'-C1'	-2.00	1.41	1.43
3	L5	1768	PSU	O4'-C1'	-2.00	1.41	1.43

All (733) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1842	4AC	CM7-C7-N4	11.26	133.45	115.27
46	S2	1337	4AC	N4-C4-N3	9.21	128.82	113.87
46	S2	1832	6MZ	C2-N1-C6	8.42	123.13	116.60
3	L5	3899	PSU	N1-C2-N3	7.90	123.50	115.17
3	L5	4522	PSU	N1-C2-N3	7.89	123.49	115.17
3	L5	1769	PSU	N1-C2-N3	7.77	123.36	115.17
3	L5	4323	PSU	N1-C2-N3	7.75	123.34	115.17
3	L5	3616	PSU	N1-C2-N3	7.68	123.27	115.17
3	L5	4441	PSU	N1-C2-N3	7.61	123.20	115.17
3	L5	2402	PSU	N1-C2-N3	7.59	123.18	115.17
3	L5	3741	PSU	N1-C2-N3	7.57	123.16	115.17
3	L5	4598	PSU	N1-C2-N3	7.56	123.14	115.17
5	L8	69	PSU	N1-C2-N3	7.56	123.14	115.17
3	L5	3823	PSU	N1-C2-N3	7.53	123.11	115.17
46	S2	1842	4AC	O7-C7-N4	-7.49	110.11	121.90
3	L5	3618	PSU	N1-C2-N3	7.48	123.06	115.17
3	L5	4659	PSU	N1-C2-N3	7.43	123.00	115.17
3	L5	4282	PSU	N1-C2-N3	7.42	123.00	115.17
3	L5	4427	PSU	N1-C2-N3	7.42	123.00	115.17
3	L5	4491	PSU	N1-C2-N3	7.36	122.93	115.17
3	L5	4975	PSU	N1-C2-N3	7.35	122.92	115.17
46	S2	1692	PSU	N1-C2-N3	7.30	122.87	115.17
3	L5	1664	PSU	N1-C2-N3	7.29	122.85	115.17
3	L5	4549	PSU	N1-C2-N3	7.27	122.84	115.17
3	L5	4470	PSU	N1-C2-N3	7.24	122.81	115.17
3	L5	2619	PSU	N1-C2-N3	7.23	122.79	115.17
3	L5	1731	PSU	N1-C2-N3	7.22	122.78	115.17
3	L5	4401	PSU	N1-C2-N3	7.21	122.78	115.17
46	S2	686	PSU	N1-C2-N3	7.19	122.75	115.17
46	S2	1174	PSU	N1-C2-N3	7.18	122.75	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	406	PSU	N1-C2-N3	7.11	122.67	115.17
46	S2	966	PSU	N1-C2-N3	7.09	122.64	115.17
46	S2	1004	PSU	N1-C2-N3	7.05	122.61	115.17
46	S2	1045	PSU	N1-C2-N3	7.03	122.58	115.17
46	S2	36	PSU	N1-C2-N3	7.02	122.57	115.17
3	L5	3830	PSU	N1-C2-N3	7.00	122.56	115.17
3	L5	4263	PSU	N1-C2-N3	6.97	122.52	115.17
3	L5	3713	PSU	N1-C2-N3	6.95	122.50	115.17
3	L5	1670	PSU	N1-C2-N3	6.95	122.50	115.17
46	S2	105	PSU	N1-C2-N3	6.94	122.49	115.17
46	S2	1081	PSU	N1-C2-N3	6.94	122.49	115.17
5	L8	55	PSU	N1-C2-N3	6.92	122.47	115.17
46	S2	1232	PSU	N1-C2-N3	6.92	122.47	115.17
46	S2	34	PSU	N1-C2-N3	6.90	122.45	115.17
3	L5	3674	PSU	N1-C2-N3	6.89	122.44	115.17
3	L5	1847	PSU	N1-C2-N3	6.88	122.43	115.17
46	S2	815	PSU	N1-C2-N3	6.85	122.39	115.17
46	S2	1367	PSU	N1-C2-N3	6.84	122.38	115.17
3	L5	1569	PSU	N1-C2-N3	6.83	122.38	115.17
3	L5	4412	PSU	N1-C2-N3	6.81	122.35	115.17
46	S2	651	PSU	N1-C2-N3	6.81	122.35	115.17
46	S2	822	PSU	N1-C2-N3	6.80	122.34	115.17
3	L5	4546	PSU	N1-C2-N3	6.79	122.33	115.17
46	S2	609	PSU	N1-C2-N3	6.78	122.32	115.17
3	L5	1523	PSU	N1-C2-N3	6.74	122.28	115.17
46	S2	649	PSU	N1-C2-N3	6.74	122.28	115.17
46	S2	109	PSU	N1-C2-N3	6.70	122.24	115.17
46	S2	572	PSU	N1-C2-N3	6.70	122.24	115.17
46	S2	1337	4AC	C5-C4-N4	-6.70	111.66	122.94
3	L5	3737	PSU	N1-C2-N3	6.69	122.23	115.17
3	L5	3747	PSU	N1-C2-N3	6.68	122.22	115.17
3	L5	4190	6MZ	C2-N1-C6	6.68	121.78	116.60
46	S2	218	PSU	N1-C2-N3	6.67	122.20	115.17
3	L5	1768	PSU	N1-C2-N3	6.66	122.20	115.17
3	L5	1849	PSU	N1-C2-N3	6.66	122.19	115.17
3	L5	4266	PSU	N1-C2-N3	6.66	122.19	115.17
3	L5	3749	PSU	N1-C2-N3	6.65	122.19	115.17
46	S2	814	PSU	N1-C2-N3	6.63	122.16	115.17
46	S2	863	PSU	N1-C2-N3	6.63	122.16	115.17
3	L5	3832	PSU	N1-C2-N3	6.62	122.15	115.17
3	L5	4643	PSU	N1-C2-N3	6.62	122.15	115.17
3	L5	4937	PSU	N1-C2-N3	6.62	122.15	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2495	PSU	N1-C2-N3	6.59	122.12	115.17
46	S2	1238	PSU	N1-C2-N3	6.56	122.09	115.17
46	S2	866	PSU	N1-C2-N3	6.55	122.08	115.17
46	S2	1136	PSU	N1-C2-N3	6.54	122.07	115.17
3	L5	3709	PSU	N1-C2-N3	6.52	122.04	115.17
3	L5	3743	PSU	N1-C2-N3	6.50	122.03	115.17
3	L5	4373	PSU	N1-C2-N3	6.50	122.02	115.17
80	Bv	28	PSU	N1-C2-N3	6.49	122.01	115.17
46	S2	801	PSU	N1-C2-N3	6.48	122.01	115.17
80	Bv	27	PSU	N1-C2-N3	6.48	122.00	115.17
46	S2	119	PSU	N1-C2-N3	6.47	122.00	115.17
3	L5	4502	PSU	N1-C2-N3	6.47	122.00	115.17
3	L5	3694	PSU	N1-C2-N3	6.46	121.98	115.17
46	S2	1244	PSU	N1-C2-N3	6.45	121.97	115.17
46	S2	1347	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	4966	PSU	N1-C2-N3	6.37	121.89	115.17
80	Bv	55	PSU	N1-C2-N3	6.37	121.88	115.17
3	L5	4331	PSU	N1-C2-N3	6.35	121.86	115.17
46	S2	1850	MA6	C2-N1-C6	6.32	123.04	116.84
46	S2	1643	PSU	N1-C2-N3	6.31	121.83	115.17
46	S2	1445	PSU	N1-C2-N3	6.23	121.75	115.17
3	L5	4393	PSU	N1-C2-N3	6.21	121.72	115.17
46	S2	1625	PSU	N1-C2-N3	6.20	121.71	115.17
3	L5	4390	PSU	N1-C2-N3	6.14	121.64	115.17
46	S2	1046	PSU	N1-C2-N3	6.11	121.61	115.17
46	S2	1851	MA6	C2-N1-C6	6.08	122.80	116.84
3	L5	4269	PSU	N1-C2-N3	6.07	121.57	115.17
3	L5	3797	UY1	N1-C2-N3	6.01	121.51	115.17
46	S2	93	PSU	N1-C2-N3	6.00	121.50	115.17
3	L5	1779	PSU	N1-C2-N3	5.94	121.43	115.17
46	S2	1177	PSU	N1-C2-N3	5.89	121.38	115.17
3	L5	4606	PSU	N1-C2-N3	5.77	121.25	115.17
3	L5	4417	5MC	C5-C6-N1	-5.75	117.07	123.31
80	Bv	37	UY4	C2-N1-C6	5.59	120.94	116.60
3	L5	2824	OMU	C4-N3-C2	-5.55	119.72	126.61
3	L5	1664	PSU	C4-N3-C2	-5.51	118.78	126.37
46	S2	1326	OMU	C4-N3-C2	-5.51	119.78	126.61
46	S2	172	OMU	C4-N3-C2	-5.39	119.92	126.61
3	L5	4500	UR3	C4-N3-C2	-5.39	120.25	124.58
3	L5	4197	OMU	C4-N3-C2	-5.16	120.20	126.61
80	Bv	37	UY4	N6-C09-N08	5.14	120.83	113.77
3	L5	2402	PSU	C4-N3-C2	-5.13	119.31	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4549	PSU	C4-N3-C2	-5.08	119.37	126.37
5	L8	69	PSU	C4-N3-C2	-5.08	119.38	126.37
3	L5	4598	PSU	O2-C2-N1	-5.07	117.56	122.79
3	L5	4468	OMU	C4-N3-C2	-5.03	120.36	126.61
3	L5	3823	PSU	O2-C2-N1	-5.02	117.61	122.79
3	L5	4323	PSU	C4-N3-C2	-5.02	119.45	126.37
3	L5	4197	OMU	N3-C2-N1	5.01	121.41	114.89
3	L5	3899	PSU	C4-N3-C2	-4.98	119.51	126.37
3	L5	4427	PSU	C4-N3-C2	-4.94	119.56	126.37
46	S2	1442	OMU	C4-N3-C2	-4.93	120.50	126.61
3	L5	3823	PSU	C4-N3-C2	-4.92	119.59	126.37
3	L5	3674	PSU	C4-N3-C2	-4.87	119.66	126.37
46	S2	428	OMU	C4-N3-C2	-4.85	120.59	126.61
46	S2	121	OMU	C4-N3-C2	-4.85	120.59	126.61
3	L5	4276	OMU	C4-N3-C2	-4.84	120.60	126.61
3	L5	2619	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L5	4491	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L5	2824	OMU	N3-C2-N1	4.81	121.15	114.89
46	S2	1045	PSU	C4-N3-C2	-4.79	119.78	126.37
46	S2	121	OMU	N3-C2-N1	4.78	121.11	114.89
3	L5	4412	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	3904	OMU	C5-C4-N3	4.75	121.46	114.80
3	L5	3741	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	4522	PSU	C4-N3-C2	-4.73	119.85	126.37
3	L5	3713	PSU	C4-N3-C2	-4.73	119.86	126.37
3	L5	4470	PSU	C4-N3-C2	-4.73	119.86	126.37
3	L5	3904	OMU	C4-N3-C2	-4.73	120.74	126.61
46	S2	572	PSU	C4-N3-C2	-4.73	119.86	126.37
3	L5	3761	5MC	O2-C2-N3	-4.71	114.90	122.33
3	L5	2338	OMC	O2-C2-N3	-4.70	114.92	122.33
3	L5	3709	PSU	C4-N3-C2	-4.69	119.91	126.37
5	L8	55	PSU	C4-N3-C2	-4.69	119.91	126.37
46	S2	1288	OMU	C4-N3-C2	-4.68	120.80	126.61
46	S2	1248	B8N	N3-C2-N1	4.68	122.43	116.72
3	L5	3618	PSU	C4-N3-C2	-4.67	119.94	126.37
3	L5	4468	OMU	C5-C4-N3	4.67	121.34	114.80
3	L5	1768	PSU	O2-C2-N1	-4.66	117.98	122.79
3	L5	4282	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	1769	PSU	C4-N3-C2	-4.66	119.96	126.37
46	S2	1174	PSU	C4-N3-C2	-4.64	119.98	126.37
46	S2	686	PSU	C4-N3-C2	-4.63	119.99	126.37
3	L5	4546	PSU	C4-N3-C2	-4.63	119.99	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1081	PSU	C4-N3-C2	-4.59	120.05	126.37
46	S2	621	OMC	O2-C2-N3	-4.59	115.10	122.33
3	L5	3616	PSU	C4-N3-C2	-4.58	120.06	126.37
46	S2	109	PSU	C4-N3-C2	-4.58	120.07	126.37
3	L5	4546	PSU	O2-C2-N1	-4.57	118.08	122.79
3	L5	1523	PSU	O2-C2-N1	-4.56	118.08	122.79
46	S2	1326	OMU	N3-C2-N1	4.56	120.83	114.89
3	L5	1731	PSU	C4-N3-C2	-4.56	120.09	126.37
46	S2	406	PSU	C4-N3-C2	-4.56	120.09	126.37
80	Bv	46	G7M	O4'-C1'-N9	4.54	114.76	108.75
3	L5	4500	UR3	C1'-N1-C2	4.54	124.47	117.04
3	L5	4470	PSU	O2-C2-N1	-4.52	118.13	122.79
46	S2	1136	PSU	C4-N3-C2	-4.51	120.16	126.37
3	L5	1731	PSU	O2-C2-N1	-4.50	118.15	122.79
3	L5	2402	PSU	O2-C2-N1	-4.50	118.15	122.79
3	L5	1847	PSU	O2-C2-N1	-4.49	118.16	122.79
46	S2	1804	OMU	C4-N3-C2	-4.49	121.04	126.61
3	L5	4266	PSU	C4-N3-C2	-4.48	120.20	126.37
46	S2	651	PSU	C4-N3-C2	-4.47	120.21	126.37
46	S2	218	PSU	C4-N3-C2	-4.47	120.22	126.37
46	S2	1692	PSU	C4-N3-C2	-4.47	120.22	126.37
3	L5	4468	OMU	N3-C2-N1	4.44	120.67	114.89
3	L5	4975	PSU	C4-N3-C2	-4.43	120.26	126.37
46	S2	34	PSU	C4-N3-C2	-4.42	120.28	126.37
3	L5	2824	OMU	C5-C4-N3	4.41	120.98	114.80
46	S2	966	PSU	C4-N3-C2	-4.40	120.31	126.37
46	S2	36	PSU	C4-N3-C2	-4.39	120.32	126.37
3	L5	1768	PSU	C4-N3-C2	-4.37	120.35	126.37
3	L5	1849	PSU	C4-N3-C2	-4.37	120.35	126.37
5	L8	55	PSU	O2-C2-N1	-4.35	118.30	122.79
46	S2	1326	OMU	C5-C4-N3	4.35	120.89	114.80
46	S2	1004	PSU	C4-N3-C2	-4.34	120.39	126.37
3	L5	4590	OMU	N3-C2-N1	4.34	120.55	114.89
46	S2	172	OMU	N3-C2-N1	4.34	120.54	114.89
46	S2	1804	OMU	C5-C4-N3	4.33	120.86	114.80
3	L5	4373	PSU	C4-N3-C2	-4.31	120.44	126.37
3	L5	3904	OMU	N3-C2-N1	4.31	120.50	114.89
3	L5	4263	PSU	C4-N3-C2	-4.31	120.44	126.37
3	L5	4606	PSU	C4-N3-C2	-4.30	120.45	126.37
46	S2	866	PSU	C4-N3-C2	-4.30	120.45	126.37
46	S2	1367	PSU	C4-N3-C2	-4.29	120.45	126.37
3	L5	4441	PSU	O2-C2-N1	-4.29	118.36	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4276	OMU	C5-C4-N3	4.29	120.80	114.80
3	L5	3797	UY1	C4-N3-C2	-4.29	120.47	126.37
3	L5	3747	PSU	O2-C2-N1	-4.28	118.38	122.79
46	S2	1832	6MZ	C9-N6-C6	4.27	126.81	122.85
5	L8	69	PSU	O2-C2-N1	-4.27	118.39	122.79
80	Bv	55	PSU	C4-N3-C2	-4.26	120.50	126.37
80	Bv	28	PSU	C4-N3-C2	-4.25	120.52	126.37
46	S2	1174	PSU	O2-C2-N1	-4.25	118.41	122.79
3	L5	3749	PSU	C4-N3-C2	-4.25	120.52	126.37
46	S2	1832	6MZ	N3-C2-N1	-4.24	122.92	128.67
46	S2	814	PSU	C4-N3-C2	-4.24	120.54	126.37
46	S2	1442	OMU	N3-C2-N1	4.23	120.40	114.89
3	L5	4401	PSU	O2-C2-N1	-4.23	118.43	122.79
3	L5	4598	PSU	C4-N3-C2	-4.22	120.55	126.37
46	S2	1288	OMU	C5-C4-N3	4.22	120.71	114.80
46	S2	1643	PSU	C4-N3-C2	-4.22	120.56	126.37
3	L5	4966	PSU	C4-N3-C2	-4.22	120.56	126.37
46	S2	801	PSU	C4-N3-C2	-4.21	120.56	126.37
46	S2	119	PSU	C4-N3-C2	-4.21	120.57	126.37
3	L5	4331	PSU	C4-N3-C2	-4.21	120.57	126.37
80	Bv	27	PSU	C4-N3-C2	-4.21	120.57	126.37
46	S2	36	PSU	O2-C2-N1	-4.20	118.46	122.79
3	L5	4659	PSU	C4-N3-C2	-4.19	120.59	126.37
3	L5	3694	PSU	C4-N3-C2	-4.19	120.60	126.37
46	S2	822	PSU	O2-C2-N1	-4.17	118.48	122.79
46	S2	116	OMU	C4-N3-C2	-4.17	121.43	126.61
46	S2	1851	MA6	C4-C5-N7	-4.17	104.93	109.34
46	S2	172	OMU	C5-C4-N3	4.17	120.64	114.80
46	S2	609	PSU	C4-N3-C2	-4.17	120.63	126.37
46	S2	863	PSU	C4-N3-C2	-4.16	120.64	126.37
46	S2	1851	MA6	N3-C2-N1	-4.15	123.04	128.67
46	S2	428	OMU	C5-C4-N3	4.15	120.61	114.80
46	S2	1046	PSU	C4-N3-C2	-4.15	120.66	126.37
3	L5	4500	UR3	C6-N1-C2	-4.15	118.41	121.80
3	L5	4417	5MC	CM5-C5-C4	-4.14	113.70	120.51
3	L5	4276	OMU	N3-C2-N1	4.14	120.28	114.89
3	L5	1779	PSU	C4-N3-C2	-4.14	120.67	126.37
46	S2	1232	PSU	C4-N3-C2	-4.13	120.68	126.37
46	S2	93	PSU	C4-N3-C2	-4.12	120.69	126.37
3	L5	4441	PSU	C4-N3-C2	-4.10	120.72	126.37
46	S2	1347	PSU	C4-N3-C2	-4.10	120.73	126.37
3	L5	1569	PSU	O2-C2-N1	-4.09	118.57	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4190	6MZ	C9-N6-C6	-4.09	119.06	122.85
46	S2	1337	4AC	C1'-N1-C2	4.08	127.45	118.44
46	S2	1004	PSU	O2-C2-N1	-4.07	118.59	122.79
3	L5	4390	PSU	C4-N3-C2	-4.06	120.77	126.37
3	L5	4269	PSU	C4-N3-C2	-4.06	120.78	126.37
46	S2	1238	PSU	C4-N3-C2	-4.06	120.78	126.37
3	L5	4401	PSU	C4-N3-C2	-4.06	120.78	126.37
3	L5	3820	OMC	O2-C2-N3	-4.05	115.94	122.33
3	L5	1569	PSU	C4-N3-C2	-4.05	120.79	126.37
46	S2	1244	PSU	C4-N3-C2	-4.05	120.79	126.37
3	L5	4412	PSU	O2-C2-N1	-4.04	118.62	122.79
46	S2	1445	PSU	C4-N3-C2	-4.03	120.81	126.37
3	L5	3832	PSU	C4-N3-C2	-4.03	120.82	126.37
3	L5	3741	PSU	O2-C2-N1	-4.03	118.63	122.79
3	L5	4323	PSU	O2-C2-N1	-4.03	118.63	122.79
3	L5	3709	PSU	O2-C2-N1	-4.01	118.65	122.79
3	L5	4975	PSU	O2-C2-N1	-4.01	118.65	122.79
46	S2	121	OMU	C5-C4-N3	4.00	120.41	114.80
3	L5	3747	PSU	C4-N3-C2	-4.00	120.86	126.37
46	S2	105	PSU	C4-N3-C2	-3.99	120.87	126.37
46	S2	1625	PSU	C4-N3-C2	-3.98	120.88	126.37
46	S2	609	PSU	O2-C2-N1	-3.98	118.69	122.79
46	S2	428	OMU	N3-C2-N1	3.97	120.06	114.89
3	L5	1670	PSU	C4-N3-C2	-3.97	120.90	126.37
3	L5	4197	OMU	C5-C4-N3	3.97	120.36	114.80
3	L5	3737	PSU	C4-N3-C2	-3.96	120.92	126.37
46	S2	116	OMU	C5-C4-N3	3.96	120.34	114.80
3	L5	1523	PSU	C4-N3-C2	-3.96	120.92	126.37
3	L5	2495	PSU	C4-N3-C2	-3.96	120.92	126.37
46	S2	1244	PSU	O2-C2-N1	-3.95	118.71	122.79
46	S2	1045	PSU	O2-C2-N1	-3.95	118.71	122.79
46	S2	1288	OMU	N3-C2-N1	3.95	120.03	114.89
3	L5	4522	PSU	O2-C2-N1	-3.94	118.72	122.79
46	S2	815	PSU	C4-N3-C2	-3.94	120.94	126.37
3	L5	3743	PSU	O2-C2-N1	-3.93	118.74	122.79
3	L5	3830	PSU	C4-N3-C2	-3.92	120.97	126.37
46	S2	649	PSU	C4-N3-C2	-3.91	120.98	126.37
3	L5	4282	PSU	O2-C2-N1	-3.91	118.76	122.79
3	L5	1670	PSU	O2-C2-N1	-3.91	118.76	122.79
46	S2	1442	OMU	C5-C4-N3	3.90	120.27	114.80
3	L5	4393	PSU	C4-N3-C2	-3.90	120.99	126.37
46	S2	1238	PSU	O2-C2-N1	-3.90	118.76	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1769	PSU	O2-C2-N1	-3.90	118.77	122.79
3	L5	3743	PSU	C4-N3-C2	-3.89	121.01	126.37
46	S2	822	PSU	C4-N3-C2	-3.88	121.03	126.37
80	Bv	28	PSU	O2-C2-N1	-3.86	118.81	122.79
3	L5	1313	A2M	N3-C2-N1	-3.86	123.44	128.67
3	L5	4502	PSU	C4-N3-C2	-3.86	121.06	126.37
3	L5	4643	PSU	C4-N3-C2	-3.85	121.06	126.37
3	L5	2824	OMU	O4-C4-C5	-3.85	118.53	125.16
3	L5	4643	PSU	O2-C2-N1	-3.84	118.83	122.79
46	S2	116	OMU	N3-C2-N1	3.84	119.88	114.89
46	S2	1248	B8N	C4-N3-C2	-3.83	120.91	125.62
3	L5	1313	A2M	O3'-C3'-C2'	-3.82	100.50	111.19
46	S2	686	PSU	O2-C2-N1	-3.82	118.85	122.79
46	S2	1850	MA6	N3-C2-N1	-3.81	123.50	128.67
46	S2	1850	MA6	C4-C5-N7	-3.80	105.32	109.34
80	Bv	37	UY4	N3-C2-N1	-3.80	123.52	128.67
46	S2	1347	PSU	O2-C2-N1	-3.79	118.88	122.79
3	L5	1847	PSU	C6-C5-C4	-3.78	115.62	118.17
3	L5	4427	PSU	C6-C5-C4	-3.78	115.63	118.17
3	L5	4937	PSU	C4-N3-C2	-3.77	121.17	126.37
3	L5	1664	PSU	O2-C2-N1	-3.77	118.90	122.79
46	S2	1367	PSU	O2-C2-N1	-3.76	118.91	122.79
3	L5	4491	PSU	O2-C2-N1	-3.76	118.92	122.79
3	L5	4190	6MZ	N3-C2-N1	-3.75	123.58	128.67
46	S2	1703	OMC	O2-C2-N3	-3.75	116.42	122.33
3	L5	4263	PSU	O2-C2-N1	-3.74	118.93	122.79
46	S2	1177	PSU	C4-N3-C2	-3.73	121.23	126.37
46	S2	863	PSU	O2-C2-N1	-3.73	118.94	122.79
46	S2	649	PSU	O2-C2-N1	-3.71	118.96	122.79
80	Bv	27	PSU	O2-C2-N1	-3.70	118.97	122.79
80	Bv	55	PSU	O2-C2-N1	-3.69	118.98	122.79
3	L5	1847	PSU	C4-N3-C2	-3.69	121.29	126.37
3	L5	4549	PSU	O2-C2-N1	-3.67	119.00	122.79
46	S2	1804	OMU	N3-C2-N1	3.65	119.64	114.89
46	S2	406	PSU	O2-C2-N1	-3.62	119.06	122.79
3	L5	3749	PSU	O2-C2-N1	-3.62	119.06	122.79
3	L5	3694	PSU	O2-C2-N1	-3.62	119.06	122.79
46	S2	815	PSU	O2-C2-N1	-3.62	119.06	122.79
46	S2	1842	4AC	C6-C5-C4	3.61	121.35	117.00
46	S2	801	PSU	O2-C2-N1	-3.61	119.06	122.79
3	L5	3713	PSU	O2-C2-N1	-3.60	119.08	122.79
3	L5	4390	PSU	O2-C2-N1	-3.59	119.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4417	5MC	O2-C2-N3	-3.59	116.67	122.33
3	L5	3771	OMG	CM2-O2'-C2'	-3.58	105.28	114.47
46	S2	1232	PSU	O2-C2-N1	-3.58	119.10	122.79
46	S2	1625	PSU	O2-C2-N1	-3.57	119.11	122.79
46	S2	116	OMU	O4-C4-C5	-3.56	119.02	125.16
3	L5	4590	OMU	C5-C4-N3	3.55	119.78	114.80
46	S2	1643	PSU	O2-C2-N1	-3.55	119.13	122.79
46	S2	814	PSU	O2-C2-N1	-3.54	119.14	122.79
46	S2	109	PSU	O2-C2-N1	-3.54	119.14	122.79
3	L5	4500	UR3	C5-C4-N3	3.53	119.69	115.04
46	S2	1442	OMU	O4-C4-C5	-3.51	119.10	125.16
46	S2	1804	OMU	C1'-N1-C2	3.51	123.90	117.59
3	L5	4331	PSU	C6-C5-C4	-3.50	115.81	118.17
3	L5	2338	OMC	O2-C2-N1	3.46	125.68	118.90
46	S2	1804	OMU	O4-C4-C5	-3.44	119.23	125.16
46	S2	572	PSU	O2-C2-N1	-3.43	119.25	122.79
3	L5	3832	PSU	O2-C2-N1	-3.42	119.26	122.79
46	S2	966	PSU	O2-C2-N1	-3.42	119.26	122.79
46	S2	93	PSU	C6-C5-C4	-3.41	115.87	118.17
46	S2	428	OMU	O4-C4-C5	-3.41	119.28	125.16
3	L5	4966	PSU	C6-C5-C4	-3.40	115.88	118.17
3	L5	2495	PSU	O2-C2-N1	-3.38	119.30	122.79
3	L5	2802	A2M	C1'-N9-C4	3.37	132.57	126.64
46	S2	1490	OMG	C5-C6-N1	3.37	120.49	114.07
46	S2	1692	PSU	O2-C2-N1	-3.36	119.32	122.79
46	S2	34	PSU	O2-C2-N1	-3.36	119.32	122.79
46	S2	651	PSU	O2-C2-N1	-3.35	119.33	122.79
3	L5	2619	PSU	O2-C2-N1	-3.31	119.38	122.79
46	S2	1832	6MZ	C4-C5-N7	-3.29	105.86	109.34
3	L5	4500	UR3	O2-C2-N3	-3.29	116.78	121.33
3	L5	2409	OMC	O2-C2-N3	-3.29	117.14	122.33
3	L5	4266	PSU	O2-C2-N1	-3.27	119.41	122.79
46	S2	436	OMG	C8-N7-C5	3.25	108.09	102.55
3	L5	4198	OMG	C8-N7-C5	3.25	108.09	102.55
3	L5	4393	PSU	O2-C2-N1	-3.24	119.45	122.79
46	S2	866	PSU	O2-C2-N1	-3.24	119.45	122.79
3	L5	3904	OMU	O2-C2-N3	-3.23	115.53	121.49
46	S2	621	OMC	C1'-N1-C2	3.23	125.57	118.44
46	S2	462	OMC	O2-C2-N3	-3.22	117.25	122.33
3	L5	4659	PSU	O2-C2-N1	-3.22	119.47	122.79
3	L5	3830	PSU	O2-C2-N1	-3.19	119.50	122.79
46	S2	1046	PSU	O2-C2-N1	-3.19	119.50	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1391	OMC	O2-C2-N3	-3.18	117.32	122.33
46	S2	1445	PSU	O2-C2-N1	-3.17	119.52	122.79
3	L5	1509	OMG	CM2-O2'-C2'	-3.17	106.33	114.47
3	L5	4590	OMU	C4-N3-C2	-3.16	122.69	126.61
3	L5	4607	OMG	C8-N7-C5	3.16	107.92	102.55
46	S2	1842	4AC	O7-C7-CM7	-3.16	116.44	122.05
46	S2	218	PSU	O2-C2-N1	-3.15	119.53	122.79
3	L5	4417	5MC	N1-C2-N3	3.14	124.25	118.80
3	L5	4966	PSU	O2-C2-N1	-3.13	119.56	122.79
3	L5	3761	5MC	C1'-N1-C6	-3.13	116.00	121.15
80	Bv	55	PSU	C3'-C2'-C1'	3.12	105.37	101.69
80	Bv	37	UY4	N6-C6-N1	3.12	122.22	118.71
46	S2	93	PSU	O2-C2-N1	-3.12	119.57	122.79
3	L5	4427	PSU	O2-C2-N1	-3.10	119.59	122.79
3	L5	4276	OMU	O4-C4-C5	-3.09	119.84	125.16
3	L5	3674	PSU	C5-C6-N1	-3.08	117.86	122.14
3	L5	4937	PSU	O2-C2-N1	-3.08	119.61	122.79
46	S2	105	PSU	O2-C2-N1	-3.08	119.61	122.79
80	Bv	9	1MG	O4'-C1'-N9	3.07	112.82	108.75
46	S2	1248	B8N	C1'-C5-C4	3.06	122.25	117.61
3	L5	4340	OMG	C8-N7-C5	3.06	107.75	102.55
3	L5	3616	PSU	O2-C2-N1	-3.05	119.64	122.79
3	L5	3761	5MC	C5-C4-N3	-3.05	118.63	121.75
3	L5	4468	OMU	O4-C4-C5	-3.05	119.90	125.16
3	L5	4590	OMU	C6-N1-C2	-3.04	117.29	121.00
3	L5	4417	5MC	C5-C4-N3	-3.04	118.64	121.75
46	S2	1177	PSU	O2-C2-N1	-3.04	119.66	122.79
3	L5	3904	OMU	C1'-N1-C2	3.03	123.03	117.59
3	L5	1523	PSU	C6-C5-C4	-3.02	116.14	118.17
3	L5	4593	OMG	C8-N7-C5	3.02	107.69	102.55
46	S2	172	OMU	O4-C4-C5	-3.01	119.98	125.16
3	L5	2351	OMG	C8-N7-C5	3.00	107.66	102.55
3	L5	3866	OMC	O2-C2-N3	-3.00	117.61	122.33
3	L5	364	OMG	CM2-O2'-C2'	-2.99	106.79	114.47
80	Bv	26	M2G	C8-N7-C5	2.99	107.64	102.55
46	S2	668	A2M	C1'-N9-C4	-2.99	121.39	126.64
3	L5	3899	PSU	O2-C2-N1	-2.99	119.71	122.79
3	L5	4506	OMC	O2-C2-N3	-2.98	117.62	122.33
3	L5	1303	OMG	C8-N7-C5	2.98	107.62	102.55
3	L5	4197	OMU	O4-C4-C5	-2.98	120.03	125.16
3	L5	1664	PSU	C5-C6-N1	-2.96	118.03	122.14
3	L5	2863	OMG	C8-N7-C5	2.96	107.58	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1849	PSU	O2-C2-N1	-2.95	119.74	122.79
80	Bv	58	1MA	C8-N7-C5	2.93	107.54	102.55
3	L5	3848	OMC	O2-C2-N3	-2.93	117.72	122.33
46	S2	119	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L5	3737	PSU	O2-C2-N1	-2.92	119.78	122.79
80	Bv	47	H2U	O4'-C1'-N1	2.91	113.27	109.30
3	L5	1612	OMG	C8-N7-C5	2.91	107.50	102.55
80	Bv	9	1MG	C8-N7-C5	2.90	107.49	102.55
3	L5	364	OMG	C5-C6-N1	2.90	119.60	114.07
46	S2	174	OMC	O2-C2-N3	-2.89	117.78	122.33
46	S2	172	OMU	O2-C2-N1	-2.89	119.04	122.80
80	Bv	10	2MG	C8-N7-C5	2.88	107.46	102.55
3	L5	4190	6MZ	C4-C5-N7	-2.88	106.29	109.34
46	S2	1288	OMU	O4-C4-C5	-2.88	120.20	125.16
3	L5	3899	PSU	O2-C2-N3	-2.87	116.76	121.86
46	S2	1842	4AC	C5-C4-N3	-2.87	118.11	122.60
80	Bv	16	H2U	O4'-C1'-N1	2.87	113.20	109.30
46	S2	1328	OMG	C8-N7-C5	2.87	107.43	102.55
3	L5	2774	A2M	CM'-O2'-C2'	-2.86	107.13	114.47
3	L5	3761	5MC	C5-C6-N1	-2.86	120.21	123.31
3	L5	4426	OMC	O2-C2-N3	-2.86	117.82	122.33
3	L5	3904	OMU	O4-C4-C5	-2.86	120.23	125.16
46	S2	1136	PSU	O2-C2-N1	-2.86	119.84	122.79
3	L5	3771	OMG	C8-N7-C5	2.85	107.40	102.55
46	S2	121	OMU	O4-C4-C5	-2.84	120.26	125.16
3	L5	3674	PSU	O2-C2-N1	-2.84	119.86	122.79
46	S2	1177	PSU	C6-C5-C4	-2.83	116.26	118.17
3	L5	2338	OMC	C1'-N1-C2	2.82	124.67	118.44
3	L5	4331	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	3823	PSU	C6-C5-C4	-2.81	116.28	118.17
3	L5	1511	A2M	C5-C6-N6	2.80	124.58	120.31
46	S2	509	OMG	C8-N7-C5	2.80	107.31	102.55
3	L5	3618	PSU	O2-C2-N1	-2.80	119.90	122.79
3	L5	2351	OMG	O6-C6-C5	-2.79	118.79	124.32
3	L5	3771	OMG	O6-C6-C5	-2.79	118.79	124.32
3	L5	3846	A2M	C1'-N9-C4	2.79	131.54	126.64
3	L5	4417	5MC	C1'-N1-C6	2.77	125.72	121.15
46	S2	1842	4AC	N4-C4-N3	2.76	118.35	113.87
3	L5	2402	PSU	C5-C6-N1	-2.76	118.31	122.14
46	S2	1326	OMU	O4-C4-C5	-2.75	120.42	125.16
3	L5	3618	PSU	O2-C2-N3	-2.74	117.00	121.86
3	L5	3713	PSU	C5-C6-N1	-2.73	118.35	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	590	A2M	C1'-N9-C4	2.72	131.42	126.64
3	L5	4269	PSU	O2-C2-N1	-2.71	119.99	122.79
46	S2	1136	PSU	C6-C5-C4	-2.71	116.34	118.17
3	L5	4166	OMG	C2-N1-C6	-2.71	120.14	125.11
3	L5	1313	A2M	C4-C5-N7	-2.71	106.48	109.34
3	L5	3743	PSU	C6-C5-C4	-2.70	116.35	118.17
3	L5	3761	5MC	O2-C2-N1	2.70	124.19	118.90
3	L5	3616	PSU	O2-C2-N3	-2.70	117.06	121.86
3	L5	3787	OMC	O2-C2-N3	-2.68	118.10	122.33
46	S2	1046	PSU	C6-C5-C4	-2.68	116.37	118.17
46	S2	1081	PSU	O2-C2-N1	-2.67	120.04	122.79
46	S2	644	OMG	C8-N7-C5	2.66	107.09	102.55
3	L5	1504	2MG	C8-N7-C5	2.66	107.08	102.55
3	L5	4468	OMU	O2-C2-N1	-2.66	119.34	122.80
46	S2	686	PSU	C5-C6-N1	-2.65	118.46	122.14
46	S2	1081	PSU	C6-C5-C4	-2.65	116.39	118.17
3	L5	3797	UY1	O2-C2-N1	-2.64	120.06	122.79
46	S2	116	OMU	C1'-N1-C2	2.64	122.33	117.59
46	S2	572	PSU	C5-C6-N1	-2.64	118.48	122.14
3	L5	4588	OMG	C5-C6-N1	2.63	119.09	114.07
3	L5	1309	1MA	N1-C2-N3	-2.63	122.61	125.90
3	L5	1504	2MG	C5-C6-N1	2.63	119.09	114.07
3	L5	4606	PSU	O2-C2-N1	-2.63	120.08	122.79
3	L5	364	OMG	C8-N7-C5	2.62	107.01	102.55
46	S2	621	OMC	C1'-N1-C6	-2.62	115.19	120.78
3	L5	3899	PSU	C6-C5-C4	-2.62	116.41	118.17
46	S2	1490	OMG	O6-C6-C5	-2.61	119.14	124.32
3	L5	3820	OMC	CM2-O2'-C2'	-2.61	107.77	114.47
46	S2	1326	OMU	CM2-O2'-C2'	-2.61	107.79	114.47
3	L5	1779	PSU	O2-C2-N3	-2.60	117.23	121.86
3	L5	2351	OMG	C5-C6-N1	2.60	119.03	114.07
3	L5	4393	PSU	C6-C5-C4	-2.60	116.42	118.17
3	L5	4588	OMG	C8-N7-C5	2.60	106.97	102.55
46	S2	1337	4AC	C6-N1-C2	-2.60	116.08	120.46
46	S2	867	OMG	C8-N7-C5	2.59	106.96	102.55
3	L5	1504	2MG	O6-C6-C5	-2.59	119.19	124.32
3	L5	2411	OMG	O6-C6-C5	-2.59	119.19	124.32
46	S2	1842	4AC	C1'-N1-C2	2.56	124.09	118.44
3	L5	4323	PSU	C5-C6-N1	-2.56	118.59	122.14
3	L5	4491	PSU	O4'-C1'-C2'	2.56	108.69	105.15
3	L5	4659	PSU	C6-N1-C2	-2.55	120.32	122.69
3	L5	4362	OMG	C8-N7-C5	2.55	106.89	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1504	2MG	CM2-N2-C2	-2.55	118.17	123.65
3	L5	1509	OMG	C8-N7-C5	2.55	106.89	102.55
3	L5	4362	OMG	C5-C6-N1	2.55	118.93	114.07
80	Bv	47	H2U	C5-C6-N1	-2.54	103.83	111.52
3	L5	3761	5MC	C1'-N1-C2	2.54	124.05	118.44
80	Bv	16	H2U	C5-C6-N1	-2.53	103.85	111.52
46	S2	1337	4AC	O2-C2-N3	-2.53	118.34	122.33
46	S2	621	OMC	O2-C2-N1	2.53	123.86	118.90
3	L5	1509	OMG	C5-C6-N1	2.53	118.90	114.07
3	L5	4491	PSU	C5-C6-N1	-2.53	118.63	122.14
80	Bv	47	H2U	C3'-C2'-C1'	2.52	106.23	101.46
3	L5	2811	OMC	O2-C2-N3	-2.52	118.36	122.33
3	L5	3723	OMG	O6-C6-C5	-2.51	119.35	124.32
3	L5	4427	PSU	O2-C2-N3	-2.50	117.41	121.86
3	L5	1612	OMG	C5-C6-N1	2.50	118.84	114.07
3	L5	4593	OMG	C5-C6-N1	2.50	118.84	114.07
3	L5	1504	2MG	O4'-C1'-N9	-2.49	105.44	108.75
3	L5	3878	OMG	C5-C6-N1	2.49	118.82	114.07
3	L5	4464	OMG	C8-N7-C5	2.48	106.78	102.55
3	L5	4441	PSU	C6-N1-C2	-2.48	120.39	122.69
46	S2	1081	PSU	O2-C2-N3	-2.47	117.47	121.86
3	L5	4166	OMG	C8-N7-C5	2.46	106.75	102.55
3	L5	4549	PSU	C6-C5-C4	-2.46	116.51	118.17
3	L5	4502	PSU	O2-C2-N1	-2.45	120.26	122.79
3	L5	4659	PSU	O2-C2-N3	-2.45	117.51	121.86
3	L5	1309	1MA	C8-N7-C5	2.45	106.72	102.55
3	L5	3747	PSU	C6-C5-C4	-2.45	116.52	118.17
80	Bv	9	1MG	C5-C6-N1	2.45	117.50	113.96
3	L5	3904	OMU	CM2-O2'-C2'	-2.44	108.20	114.47
46	S2	651	PSU	C5-C6-N1	-2.44	118.75	122.14
3	L5	3618	PSU	C5-C6-N1	-2.44	118.76	122.14
80	Bv	26	M2G	O4'-C1'-N9	2.44	111.97	108.75
46	S2	683	OMG	C8-N7-C5	2.43	106.69	102.55
3	L5	4469	OMG	C8-N7-C5	2.43	106.69	102.55
3	L5	4373	PSU	O2-C2-N3	-2.43	117.55	121.86
3	L5	4659	PSU	C6-C5-C4	-2.42	116.54	118.17
3	L5	3723	OMG	C5-C6-N1	2.42	118.69	114.07
3	L5	3606	OMG	C8-N7-C5	2.42	106.67	102.55
5	L8	75	OMG	C8-N7-C5	2.42	106.67	102.55
3	L5	3764	A2M	C4'-O4'-C1'	-2.41	107.72	109.92
3	L5	4166	OMG	C5-C6-N1	2.41	118.66	114.07
3	L5	2411	OMG	C5-C6-N1	2.40	118.65	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1490	OMG	C8-N7-C5	2.40	106.63	102.55
3	L5	3771	OMG	C5-C6-N1	2.40	118.64	114.07
3	L5	2619	PSU	C5-C6-N1	-2.39	118.82	122.14
3	L5	4276	OMU	C1'-N1-C2	2.39	121.89	117.59
46	S2	116	OMU	C6-N1-C2	-2.39	118.09	121.00
46	S2	1703	OMC	C1'-N1-C2	2.38	123.70	118.44
3	L5	4412	PSU	C6-C5-C4	-2.38	116.57	118.17
5	L8	75	OMG	C5-C6-N1	2.38	118.61	114.07
46	S2	601	OMG	C8-N7-C5	2.38	106.60	102.55
46	S2	863	PSU	C6-C5-C4	-2.38	116.57	118.17
3	L5	3904	OMU	C6-N1-C2	-2.37	118.11	121.00
3	L5	4266	PSU	C6-C5-C4	-2.37	116.58	118.17
3	L5	3674	PSU	O2-C2-N3	-2.36	117.66	121.86
3	L5	1509	OMG	O6-C6-C5	-2.36	119.64	124.32
3	L5	2351	OMG	C2-N1-C6	-2.36	120.79	125.11
46	S2	1337	4AC	O7-C7-CM7	-2.36	117.85	122.05
46	S2	966	PSU	C5-C6-N1	-2.36	118.87	122.14
3	L5	4598	PSU	C6-N1-C2	-2.35	120.51	122.69
3	L5	4590	OMU	O4-C4-C5	-2.35	121.11	125.16
80	Bv	58	1MA	C5-C6-N1	2.35	117.33	113.95
3	L5	1779	PSU	C5-C6-N1	-2.35	118.88	122.14
3	L5	3616	PSU	C5-C6-N1	-2.35	118.88	122.14
46	S2	1337	4AC	C6-C5-C4	2.35	119.83	117.00
46	S2	406	PSU	C5-C6-N1	-2.34	118.89	122.14
46	S2	1692	PSU	C5-C6-N1	-2.34	118.89	122.14
3	L5	2495	PSU	C6-C5-C4	-2.33	116.60	118.17
3	L5	4464	OMG	C5-C6-N1	2.33	118.52	114.07
3	L5	4588	OMG	C2-N1-C6	-2.33	120.85	125.11
80	Bv	28	PSU	C5-C6-N1	-2.32	118.92	122.14
3	L5	4607	OMG	CM2-O2'-C2'	-2.32	108.52	114.47
3	L5	2350	A2M	C5-C6-N6	2.32	123.85	120.31
3	L5	2863	OMG	C2-N1-C6	-2.32	120.86	125.11
3	L5	4502	PSU	O2-C2-N3	-2.32	117.74	121.86
3	L5	4522	PSU	O2-C2-N3	-2.32	117.74	121.86
3	L5	3709	PSU	C5-C6-N1	-2.31	118.93	122.14
3	L5	4373	PSU	O2-C2-N1	-2.31	120.40	122.79
3	L5	3878	OMG	C8-N7-C5	2.31	106.49	102.55
3	L5	4606	PSU	C5-C6-N1	-2.31	118.94	122.14
3	L5	4340	OMG	C5-C6-N1	2.31	118.47	114.07
3	L5	3820	OMC	C1'-N1-C2	2.31	123.53	118.44
46	S2	649	PSU	C6-C5-C4	-2.31	116.62	118.17
46	S2	119	PSU	C5-C6-N1	-2.30	118.95	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1248	B8N	O2-C2-N3	-2.30	118.89	121.98
3	L5	2863	OMG	C5-C6-N1	2.29	118.45	114.07
46	S2	866	PSU	C5-C6-N1	-2.29	118.96	122.14
3	L5	1569	PSU	C6-C5-C4	-2.29	116.63	118.17
3	L5	389	A2M	CM'-O2'-C2'	-2.29	108.59	114.47
80	Bv	10	2MG	N1-C2-N2	2.29	118.90	116.56
46	S2	428	OMU	O2-C2-N1	-2.29	119.82	122.80
3	L5	4607	OMG	C2-N1-C6	-2.29	120.92	125.11
3	L5	364	OMG	O6-C6-C5	-2.29	119.79	124.32
46	S2	1692	PSU	O2-C2-N3	-2.28	117.80	121.86
3	L5	4590	OMU	C1'-N1-C6	2.28	125.66	120.78
46	S2	1490	OMG	C2-N1-C6	-2.28	120.93	125.11
46	S2	1045	PSU	C5-C6-N1	-2.28	118.97	122.14
3	L5	3723	OMG	C8-N7-C5	2.28	106.43	102.55
80	Bv	16	H2U	C3'-C2'-C1'	2.28	105.77	101.46
3	L5	3820	OMC	O2-C2-N1	2.28	123.36	118.90
3	L5	4282	PSU	C5-C6-N1	-2.28	118.98	122.14
3	L5	2619	PSU	O2-C2-N3	-2.27	117.83	121.86
3	L5	2802	A2M	C5-C6-N6	2.27	123.77	120.31
46	S2	436	OMG	C5-C6-N1	2.26	118.39	114.07
80	Bv	37	UY4	O29-C09-N6	-2.26	119.62	123.64
3	L5	4417	5MC	N4-C4-N3	2.26	122.60	118.51
46	S2	576	A2M	C5-C6-N6	2.26	123.75	120.31
3	L5	3832	PSU	C5-C6-N1	-2.26	119.00	122.14
3	L5	3697	A2M	C5-C6-N6	2.25	123.74	120.31
3	L5	3809	A2M	C5-C6-N6	2.25	123.74	120.31
3	L5	3606	OMG	C5-C6-N1	2.25	118.36	114.07
3	L5	1769	PSU	O2-C2-N3	-2.25	117.87	121.86
46	S2	159	A2M	C5-C6-N6	2.24	123.73	120.31
46	S2	572	PSU	O4'-C1'-C2'	2.24	108.25	105.15
3	L5	3830	PSU	C6-N1-C2	-2.24	120.61	122.69
3	L5	4340	OMG	CM2-O2'-C2'	-2.24	108.72	114.47
3	L5	4493	A2M	CM'-O2'-C2'	-2.24	108.72	114.47
46	S2	218	PSU	C5-C6-N1	-2.24	119.03	122.14
3	L5	3703	A2M	C5-C6-N6	2.24	123.72	120.31
80	Bv	58	1MA	O4'-C1'-N9	2.24	111.71	108.75
46	S2	105	PSU	O2-C2-N3	-2.24	117.89	121.86
3	L5	3764	A2M	O4'-C1'-N9	2.24	111.71	108.75
46	S2	27	A2M	C5-C6-N6	2.23	123.71	120.31
46	S2	166	A2M	C5-C6-N6	2.23	123.71	120.31
46	S2	1678	A2M	C5-C6-N6	2.23	123.71	120.31
3	L5	4197	OMU	O2-C2-N1	-2.23	119.89	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1031	A2M	C5-C6-N6	2.23	123.71	120.31
46	S2	484	A2M	C5-C6-N6	2.23	123.70	120.31
3	L5	1309	1MA	C5-C6-N1	2.23	117.15	113.95
3	L5	1849	PSU	C5-C6-N1	-2.23	119.05	122.14
46	S2	1174	PSU	C6-C5-C4	-2.22	116.67	118.17
46	S2	1850	MA6	C10-N6-C6	2.22	125.52	119.40
3	L5	3830	PSU	C6-C5-C4	-2.21	116.68	118.17
3	L5	4522	PSU	C6-C5-C4	-2.21	116.68	118.17
80	Bv	55	PSU	C5-C6-N1	-2.21	119.08	122.14
3	L5	3830	PSU	O2-C2-N3	-2.21	117.94	121.86
46	S2	99	A2M	C5-C6-N6	2.21	123.67	120.31
3	L5	4502	PSU	C6-C5-C4	-2.20	116.69	118.17
3	L5	3694	PSU	C5-C6-N1	-2.20	119.09	122.14
46	S2	468	A2M	C5-C6-N6	2.20	123.66	120.31
3	L5	4198	OMG	C5-C6-N1	2.20	118.26	114.07
46	S2	814	PSU	C6-C5-C4	-2.20	116.69	118.17
46	S2	1383	A2M	C5-C6-N6	2.20	123.66	120.31
3	L5	3739	A2M	C5-C6-N6	2.20	123.66	120.31
3	L5	3846	A2M	C5-C6-N6	2.19	123.65	120.31
3	L5	4401	PSU	C5-C6-N1	-2.19	119.10	122.14
46	S2	1244	PSU	C6-C5-C4	-2.19	116.70	118.17
46	S2	512	A2M	C5-C6-N6	2.19	123.65	120.31
3	L5	4588	OMG	O6-C6-C5	-2.19	119.98	124.32
5	L8	69	PSU	C5-C6-N1	-2.19	119.11	122.14
46	S2	822	PSU	O4'-C1'-C2'	2.18	108.17	105.15
3	L5	3737	PSU	O2-C2-N3	-2.18	117.99	121.86
46	S2	590	A2M	C5-C6-N6	2.17	123.62	120.31
3	L5	391	A2M	C5-C6-N6	2.17	123.61	120.31
46	S2	109	PSU	C5-C6-N1	-2.17	119.13	122.14
46	S2	1326	OMU	C5-C6-N1	-2.16	118.32	121.84
3	L5	2863	OMG	O6-C6-C5	-2.16	120.03	124.32
3	L5	4323	PSU	O2-C2-N3	-2.16	118.02	121.86
3	L5	2402	PSU	O4'-C1'-C2'	2.16	108.14	105.15
46	S2	1328	OMG	C5-C6-N1	2.15	118.18	114.07
46	S2	517	OMC	O2-C2-N3	-2.15	118.94	122.33
46	S2	1326	OMU	O2-C2-N1	-2.15	120.00	122.80
3	L5	4390	PSU	O4'-C1'-C2'	2.15	108.12	105.15
3	L5	3878	OMG	C2-N1-C6	-2.15	121.18	125.11
3	L5	1521	A2M	C5-C6-N6	2.15	123.58	120.31
3	L5	4493	A2M	C5-C6-N6	2.14	123.57	120.31
3	L5	4541	A2M	C5-C6-N6	2.14	123.57	120.31
3	L5	1849	PSU	O2-C2-N3	-2.14	118.06	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3741	PSU	C5-C6-N1	-2.14	119.17	122.14
3	L5	3764	A2M	C1'-N9-C4	2.14	130.40	126.64
3	L5	4469	OMG	C5-C6-N1	2.14	118.15	114.07
3	L5	389	A2M	C5-C6-N6	2.14	123.56	120.31
46	S2	668	A2M	C5-C6-N6	2.13	123.56	120.31
3	L5	2774	A2M	C5-C6-N6	2.13	123.55	120.31
46	S2	1136	PSU	O2-C2-N3	-2.12	118.09	121.86
46	S2	966	PSU	O2-C2-N3	-2.12	118.09	121.86
5	L8	55	PSU	C5-C6-N1	-2.12	119.20	122.14
3	L5	3787	OMC	C6-C5-C4	2.12	121.00	117.53
3	L5	4464	OMG	C2-N1-C6	-2.12	121.23	125.11
3	L5	1858	A2M	C5-C6-N6	2.12	123.53	120.31
80	Bv	27	PSU	C5-C6-N1	-2.12	119.20	122.14
80	Bv	26	M2G	C5-C6-N1	2.11	118.10	114.07
3	L5	4197	OMU	C1'-N1-C2	2.11	121.38	117.59
3	L5	4166	OMG	O6-C6-C5	-2.11	120.14	124.32
3	L5	4491	PSU	O2-C2-N3	-2.10	118.12	121.86
46	S2	683	OMG	C5-C6-N1	2.10	118.08	114.07
3	L5	4276	OMU	O2-C2-N3	-2.10	117.61	121.49
80	Bv	37	UY4	C4-C5-N7	-2.10	107.12	109.34
46	S2	1804	OMU	O2-C2-N3	-2.10	117.62	121.49
3	L5	2791	OMC	C1'-N1-C2	2.09	123.06	118.44
46	S2	683	OMG	C2-N1-C6	-2.09	121.28	125.11
3	L5	4549	PSU	O2-C2-N3	-2.09	118.15	121.86
3	L5	4549	PSU	C5-C6-N1	-2.09	119.25	122.14
3	L5	1847	PSU	C6-N1-C2	-2.08	120.76	122.69
81	j	63	UXY	C07-C06-C04	-2.08	109.09	113.47
46	S2	462	OMC	O2-C2-N1	2.08	122.97	118.90
3	L5	3771	OMG	C2-N1-C6	-2.07	121.32	125.11
46	S2	867	OMG	C5-C6-N1	2.07	118.02	114.07
46	S2	34	PSU	C5-C6-N1	-2.07	119.27	122.14
3	L5	4500	UR3	C3U-N3-C2	2.07	120.94	117.33
3	L5	1612	OMG	C2-N1-C6	-2.07	121.33	125.11
3	L5	4269	PSU	C5-C6-N1	-2.07	119.27	122.14
46	S2	1445	PSU	C5-C6-N1	-2.06	119.28	122.14
46	S2	1643	PSU	C6-C5-C4	-2.06	116.78	118.17
46	S2	1337	4AC	CM7-C7-N4	2.06	118.59	115.27
46	S2	644	OMG	C5-C6-N1	2.06	118.00	114.07
3	L5	4282	PSU	O2-C2-N3	-2.06	118.20	121.86
3	L5	3741	PSU	O2-C2-N3	-2.06	118.21	121.86
80	Bv	10	2MG	C5-C6-N1	2.06	117.99	114.07
3	L5	1664	PSU	O4'-C1'-C2'	2.05	107.99	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3878	OMG	O6-C6-C5	-2.05	120.26	124.32
46	S2	1248	B8N	C31-N3-C4	2.05	120.08	117.18
46	S2	119	PSU	O2-C2-N3	-2.05	118.23	121.86
46	S2	1248	B8N	C32-C33-C34	-2.04	105.03	110.45
46	S2	34	PSU	O2-C2-N3	-2.04	118.23	121.86
3	L5	2388	A2M	C5-C6-N6	2.04	123.42	120.31
3	L5	3804	A2M	C5-C6-N6	2.04	123.42	120.31
80	Bv	37	UY4	O03-C02-C04	2.04	121.22	114.15
3	L5	4937	PSU	O2-C2-N3	-2.04	118.24	121.86
3	L5	1664	PSU	O2-C2-N3	-2.04	118.24	121.86
3	L5	4331	PSU	O2-C2-N3	-2.03	118.25	121.86
3	L5	1327	OMC	O2-C2-N3	-2.03	119.12	122.33
80	Bv	9	1MG	O6-C6-C5	-2.03	120.84	124.18
46	S2	436	OMG	C2-N1-C6	-2.03	121.39	125.11
3	L5	4263	PSU	C5-C6-N1	-2.03	119.32	122.14
46	S2	1347	PSU	C5-C6-N1	-2.03	119.32	122.14
46	S2	621	OMC	CM2-O2'-C2'	-2.03	109.27	114.47
46	S2	218	PSU	O2-C2-N3	-2.03	118.26	121.86
3	L5	3764	A2M	C5-C6-N6	2.03	123.40	120.31
3	L5	3797	UY1	C5-C6-N1	-2.02	119.33	122.14
3	L5	4166	OMG	CM2-O2'-C2'	-2.02	109.28	114.47
46	S2	1337	4AC	C1'-N1-C6	-2.02	116.46	120.78
46	S2	406	PSU	O2-C2-N3	-2.02	118.28	121.86
46	S2	686	PSU	O4'-C1'-C2'	2.02	107.94	105.15
3	L5	2409	OMC	C1'-N1-C2	2.02	122.89	118.44
46	S2	801	PSU	C5-C6-N1	-2.01	119.35	122.14
46	S2	1625	PSU	C6-C5-C4	-2.01	116.82	118.17
3	L5	4607	OMG	C5-C6-N1	2.01	117.90	114.07
3	L5	4937	PSU	C5-C6-N1	-2.01	119.36	122.14
80	Bv	37	UY4	O03-C02-O01	-2.00	119.53	124.08
3	L5	3713	PSU	O4'-C1'-C2'	2.00	107.92	105.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
46	S2	1248	B8N	C33

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	LC	333	MLZ	N-CA-CB-CG
6	LC	333	MLZ	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
6	LC	333	MLZ	O-C-CA-CB
6	LC	333	MLZ	CD-CE-NZ-CM
3	L5	2351	OMG	O4'-C4'-C5'-O5'
3	L5	2802	A2M	O4'-C4'-C5'-O5'
3	L5	2802	A2M	C3'-C4'-C5'-O5'
3	L5	3680	OMC	C2'-C1'-N1-C6
3	L5	3764	A2M	O4'-C4'-C5'-O5'
3	L5	4390	PSU	O4'-C4'-C5'-O5'
3	L5	4470	PSU	O4'-C4'-C5'-O5'
46	S2	428	OMU	C2'-C1'-N1-C2
46	S2	428	OMU	C2'-C1'-N1-C6
46	S2	621	OMC	O4'-C1'-N1-C2
46	S2	621	OMC	O4'-C1'-N1-C6
46	S2	621	OMC	O4'-C4'-C5'-O5'
46	S2	644	OMG	O4'-C4'-C5'-O5'
46	S2	644	OMG	C3'-C4'-C5'-O5'
46	S2	683	OMG	O4'-C4'-C5'-O5'
46	S2	683	OMG	C3'-C4'-C5'-O5'
46	S2	822	PSU	O4'-C4'-C5'-O5'
46	S2	1136	PSU	O4'-C1'-C5-C4
46	S2	1136	PSU	O4'-C1'-C5-C6
46	S2	1337	4AC	N3-C4-N4-C7
46	S2	1442	OMU	O4'-C4'-C5'-O5'
46	S2	1850	MA6	O4'-C4'-C5'-O5'
46	S2	1850	MA6	C3'-C4'-C5'-O5'
80	Bv	58	1MA	O4'-C4'-C5'-O5'
81	j	63	UXY	O-C-CA-C03
81	j	63	UXY	O05-C04-C06-C07
3	L5	1303	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMG	C3'-C4'-C5'-O5'
3	L5	3764	A2M	C3'-C4'-C5'-O5'
3	L5	3846	A2M	O4'-C4'-C5'-O5'
3	L5	3899	PSU	C3'-C4'-C5'-O5'
3	L5	3899	PSU	O4'-C4'-C5'-O5'
3	L5	4470	PSU	C3'-C4'-C5'-O5'
3	L5	4606	PSU	C3'-C4'-C5'-O5'
46	S2	99	A2M	O4'-C4'-C5'-O5'
46	S2	116	OMU	C3'-C4'-C5'-O5'
46	S2	116	OMU	O4'-C4'-C5'-O5'
46	S2	172	OMU	O4'-C4'-C5'-O5'
46	S2	822	PSU	C3'-C4'-C5'-O5'
46	S2	1244	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
46	S2	1625	PSU	C3'-C4'-C5'-O5'
46	S2	1703	OMC	O4'-C4'-C5'-O5'
46	S2	1804	OMU	C3'-C4'-C5'-O5'
46	S2	1804	OMU	O4'-C4'-C5'-O5'
80	Bv	28	PSU	C3'-C4'-C5'-O5'
3	L5	1779	PSU	O4'-C4'-C5'-O5'
3	L5	2411	OMG	O4'-C4'-C5'-O5'
3	L5	2411	OMG	C3'-C4'-C5'-O5'
3	L5	3846	A2M	C3'-C4'-C5'-O5'
3	L5	4606	PSU	O4'-C4'-C5'-O5'
46	S2	172	OMU	C3'-C4'-C5'-O5'
46	S2	428	OMU	C3'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C4'-C5'-O5'
46	S2	668	A2M	O4'-C4'-C5'-O5'
46	S2	1442	OMU	C3'-C4'-C5'-O5'
46	S2	1490	OMG	C3'-C4'-C5'-O5'
46	S2	1625	PSU	O4'-C4'-C5'-O5'
80	Bv	28	PSU	O4'-C4'-C5'-O5'
3	L5	3680	OMC	C2'-C1'-N1-C2
3	L5	3820	OMC	C3'-C4'-C5'-O5'
46	S2	590	A2M	C3'-C4'-C5'-O5'
46	S2	621	OMC	C3'-C4'-C5'-O5'
46	S2	668	A2M	C3'-C4'-C5'-O5'
80	Bv	58	1MA	C3'-C4'-C5'-O5'
81	j	63	UXY	C03-C04-C06-C07
3	L5	3743	PSU	C3'-C4'-C5'-O5'
3	L5	4390	PSU	C3'-C4'-C5'-O5'
46	S2	590	A2M	O4'-C4'-C5'-O5'
46	S2	1490	OMG	O4'-C4'-C5'-O5'
80	Bv	37	UY4	C3'-C4'-C5'-O5'
73	SO	138	IAS	N-CA-CB-CG
3	L5	1849	PSU	O4'-C4'-C5'-O5'
3	L5	3797	UY1	C3'-C4'-C5'-O5'
3	L5	3797	UY1	O4'-C4'-C5'-O5'
3	L5	4331	PSU	O4'-C4'-C5'-O5'
46	S2	1244	PSU	C3'-C4'-C5'-O5'
46	S2	1703	OMC	C3'-C4'-C5'-O5'
3	L5	1768	PSU	C3'-C4'-C5'-O5'
3	L5	3830	PSU	C3'-C4'-C5'-O5'
46	S2	512	A2M	C3'-C4'-C5'-O5'
46	S2	1045	PSU	O4'-C4'-C5'-O5'
80	Bv	37	UY4	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	3739	A2M	O4'-C4'-C5'-O5'
46	S2	576	A2M	C3'-C4'-C5'-O5'
46	S2	1045	PSU	C3'-C4'-C5'-O5'
3	L5	1303	OMG	C3'-C4'-C5'-O5'
3	L5	3743	PSU	O4'-C4'-C5'-O5'
3	L5	3820	OMC	O4'-C4'-C5'-O5'
46	S2	99	A2M	C3'-C4'-C5'-O5'
46	S2	1081	PSU	O4'-C4'-C5'-O5'
46	S2	1842	4AC	O7-C7-N4-C4
46	S2	1842	4AC	CM7-C7-N4-C4
3	L5	1779	PSU	C3'-C4'-C5'-O5'
46	S2	644	OMG	C4'-C5'-O5'-P
3	L5	3739	A2M	C3'-C4'-C5'-O5'
3	L5	3878	OMG	C3'-C4'-C5'-O5'
3	L5	3904	OMU	C3'-C4'-C5'-O5'
3	L5	4266	PSU	C3'-C4'-C5'-O5'
80	Bv	46	G7M	O4'-C4'-C5'-O5'
80	Bv	9	1MG	O4'-C4'-C5'-O5'
73	SO	138	IAS	C-CA-CB-CG
46	S2	1248	B8N	N3-C31-C32-C33
73	SO	138	IAS	CA-CB-CG-OD1
3	L5	4588	OMG	O4'-C4'-C5'-O5'
46	S2	468	A2M	O4'-C4'-C5'-O5'
80	Bv	46	G7M	C4'-C5'-O5'-P
3	L5	4441	PSU	C3'-C4'-C5'-O5'
80	Bv	55	PSU	O4'-C4'-C5'-O5'
3	L5	4417	5MC	O4'-C1'-N1-C6
3	L5	2388	A2M	C3'-C2'-O2'-CM'
3	L5	3797	UY1	C1'-C2'-O2'-CM2
3	L5	3797	UY1	C3'-C2'-O2'-CM2
46	S2	174	OMC	C3'-C2'-O2'-CM2
3	L5	364	OMG	C4'-C5'-O5'-P
3	L5	4470	PSU	C4'-C5'-O5'-P
46	S2	1490	OMG	C4'-C5'-O5'-P
46	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	4417	5MC	C2'-C1'-N1-C6
3	L5	1664	PSU	O4'-C1'-C5-C4
3	L5	3797	UY1	O4'-C1'-C5-C4
46	S2	572	PSU	O4'-C1'-C5-C4
3	L5	3680	OMC	O4'-C1'-N1-C2
3	L5	1768	PSU	O4'-C4'-C5'-O5'
41	Lm	98	MLZ	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
3	L5	2802	A2M	C4'-C5'-O5'-P
46	S2	576	A2M	O4'-C4'-C5'-O5'
3	L5	3680	OMC	O4'-C1'-N1-C6
3	L5	3606	OMG	O4'-C4'-C5'-O5'
46	S2	512	A2M	O4'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C1'-N1-C6
3	L5	2802	A2M	C3'-C2'-O2'-CM'
3	L5	3904	OMU	C3'-C2'-O2'-CM2
46	S2	436	OMG	C3'-C2'-O2'-CM2
46	S2	668	A2M	C3'-C2'-O2'-CM'
3	L5	3797	UY1	C4'-C5'-O5'-P
46	S2	576	A2M	C4'-C5'-O5'-P
46	S2	590	A2M	C4'-C5'-O5'-P
3	L5	1847	PSU	O4'-C4'-C5'-O5'
5	L8	69	PSU	O4'-C4'-C5'-O5'
46	S2	1081	PSU	C4'-C5'-O5'-P
80	Bv	16	H2U	C4'-C5'-O5'-P
46	S2	1391	OMC	C1'-C2'-O2'-CM2
3	L5	3823	PSU	C4'-C5'-O5'-P
3	L5	3866	OMC	C4'-C5'-O5'-P
3	L5	3830	PSU	O4'-C4'-C5'-O5'
46	S2	436	OMG	C3'-C4'-C5'-O5'
3	L5	1664	PSU	O4'-C1'-C5-C6
3	L5	3797	UY1	O4'-C1'-C5-C6
3	L5	4606	PSU	O4'-C1'-C5-C6
3	L5	2338	OMC	C3'-C2'-O2'-CM2
3	L5	2774	A2M	C3'-C2'-O2'-CM'
46	S2	116	OMU	C3'-C2'-O2'-CM2
46	S2	517	OMC	C3'-C2'-O2'-CM2
46	S2	1391	OMC	C3'-C2'-O2'-CM2
46	S2	428	OMU	O4'-C1'-N1-C2
3	L5	4417	5MC	O4'-C1'-N1-C2
80	Bv	46	G7M	C3'-C4'-C5'-O5'
80	Bv	37	UY4	C02-C04-C05-C07
3	L5	1521	A2M	O4'-C4'-C5'-O5'
3	L5	4266	PSU	O4'-C4'-C5'-O5'
46	S2	801	PSU	C3'-C4'-C5'-O5'
46	S2	1851	MA6	C3'-C4'-C5'-O5'
3	L5	2338	OMC	C2'-C1'-N1-C2
3	L5	391	A2M	C3'-C2'-O2'-CM'
3	L5	2350	A2M	C3'-C2'-O2'-CM'
3	L5	3741	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
80	Bv	16	H2U	O4'-C1'-N1-C6
80	Bv	47	H2U	O4'-C1'-N1-C6
3	L5	1849	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 201 ligands modelled in this entry, 200 are monoatomic - leaving 1 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	MVM	L5	5246	-	32,35,35	1.09	1 (3%)	39,49,49	1.41	6 (15%)

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	MVM	L5	5246	-	-	0/20/28/28	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	L5	5246	MVM	N6-N5	-3.30	1.28	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	L5	5246	MVM	C1-C9-N1	-3.54	107.27	116.16
85	L5	5246	MVM	C6-N1-C9	3.30	123.30	118.40
85	L5	5246	MVM	C20-C19-C18	-3.11	115.84	120.09
85	L5	5246	MVM	N6-N5-N4	2.90	109.59	106.37
85	L5	5246	MVM	C21-N7-C22	-2.83	113.42	116.81
85	L5	5246	MVM	C9-N1-C5	-2.08	115.51	118.64

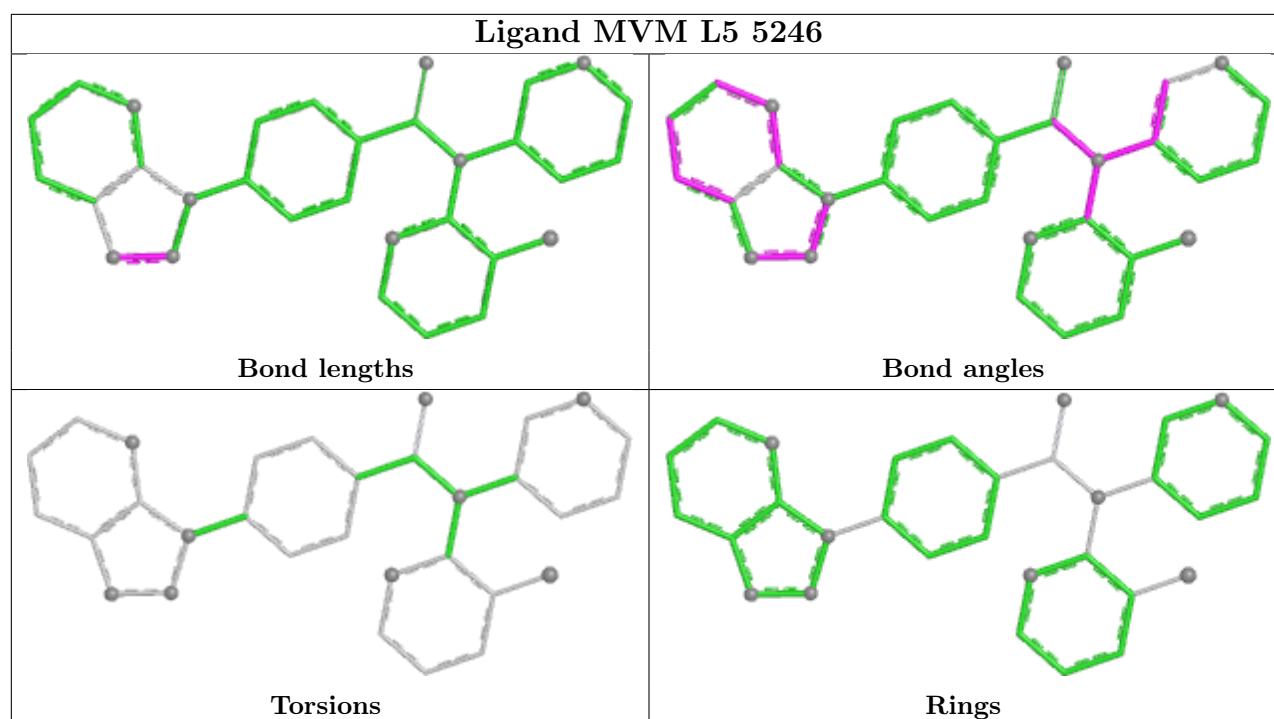
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	L5	22
46	S2	13
81	j	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	482:G	O3'	495:G	P	26.99
1	L5	173:G	O3'	186:G	P	24.85
1	S2	689:U	O3'	799:U	P	24.17
1	L5	250:G	O3'	253:G	P	24.06
1	L5	646:C	O3'	659:C	P	21.79
1	L5	2897:G	O3'	3563:C	P	20.78
1	S2	834:C	O3'	840:C	P	18.34
1	L5	4076:A	O3'	4086:G	P	17.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	130:G	O3'	140:C	P	17.44
1	S2	536:A	O3'	549:C	P	17.41
1	L5	4742:C	O3'	4826:G	P	17.30
1	S2	323:C	O3'	328:U	P	16.97
1	S2	880:G	O3'	906:U	P	16.72
1	L5	1746:G	O3'	1760:U	P	16.64
1	L5	976:U	O3'	1051:G	P	16.02
1	L5	4114:C	O3'	4117:G	P	16.02
1	L5	1389:C	O3'	1402:G	P	15.89
1	L5	1237:C	O3'	1247:G	P	15.86
1	L5	503:U	O3'	637:G	P	15.77
1	L5	748:G	O3'	893:C	P	15.72
1	S2	72:C	O3'	76:U	P	15.38
1	L5	132:G	O3'	134:G	P	14.76
1	L5	1207:G	O3'	1221:G	P	14.33
1	S2	1114:U	O3'	1120:U	P	14.12
1	S2	1751:C	O3'	1784:G	P	13.97
1	L5	2100:G	O3'	2236:C	P	12.67
1	S2	1417:C	O3'	1421:A	P	10.12
1	L5	3927:C	O3'	4044:U	P	9.76
1	L5	4700:C	O3'	4703:A	P	9.72
1	S2	1551:U	O3'	1558:C	P	9.16
1	S2	225:G	O3'	287:U	P	7.98
1	L5	1696:C	O3'	1701:C	P	6.69
1	L5	1087:U	O3'	1155:G	P	6.26
1	L5	212:C	O3'	217:C	P	5.87
1	S2	1432:U	O3'	1438:A	P	4.96
1	j	330:ARG	C	345:TYR	N	4.65
1	j	185:MEQ	C	186:SER	N	1.16

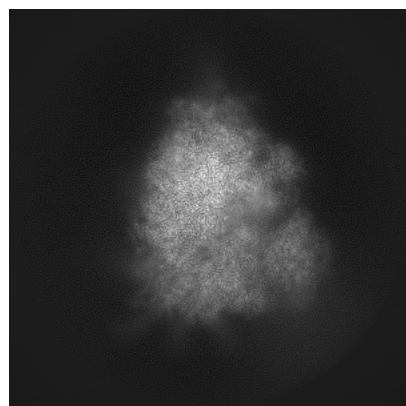
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22085. These allow visual inspection of the internal detail of the map and identification of artifacts.

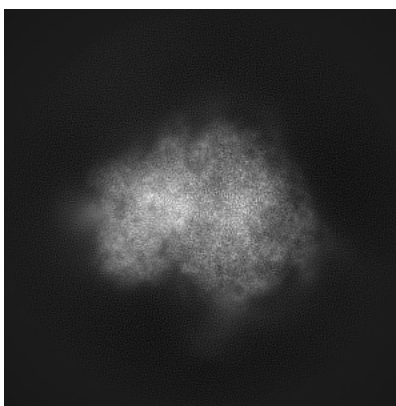
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

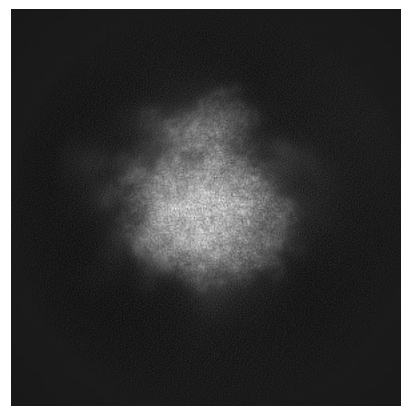
6.1.1 Primary map



X

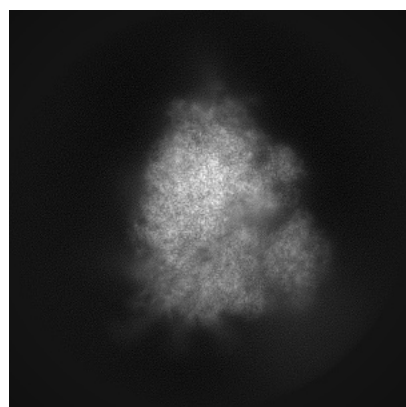


Y

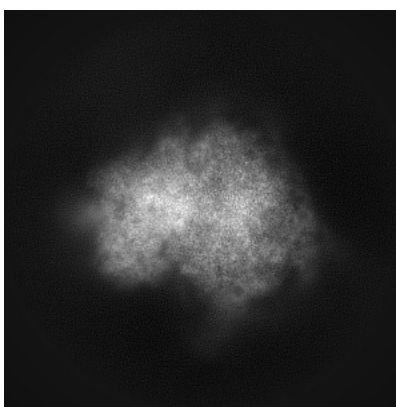


Z

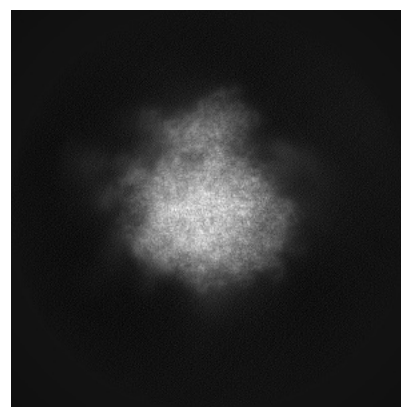
6.1.2 Raw map



X



Y

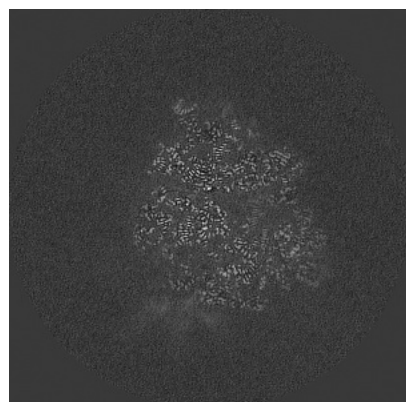


Z

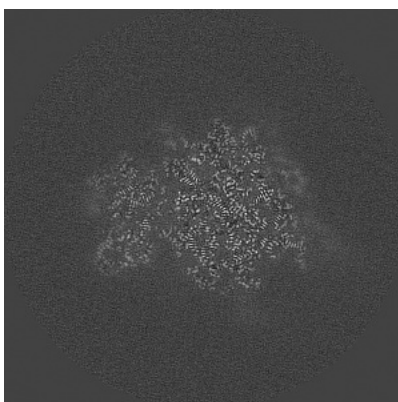
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

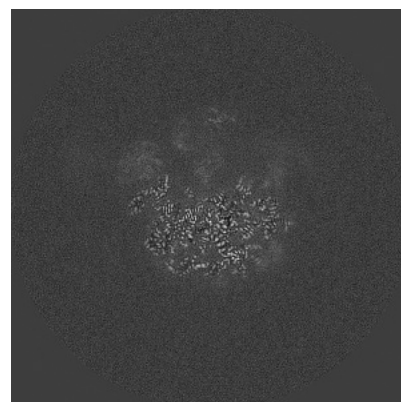
6.2.1 Primary map



X Index: 215

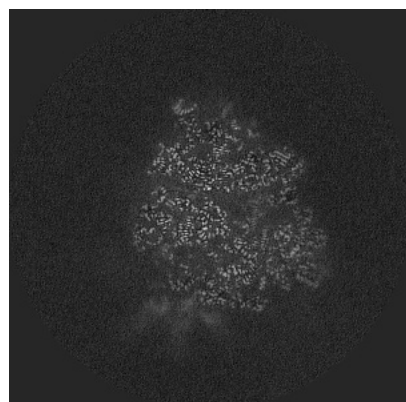


Y Index: 215

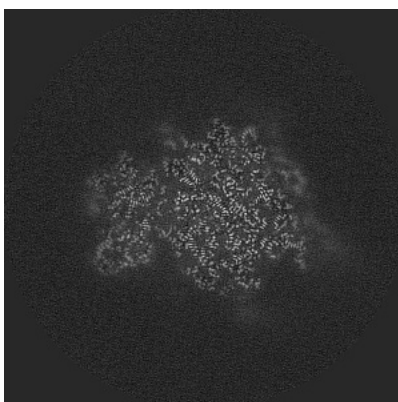


Z Index: 215

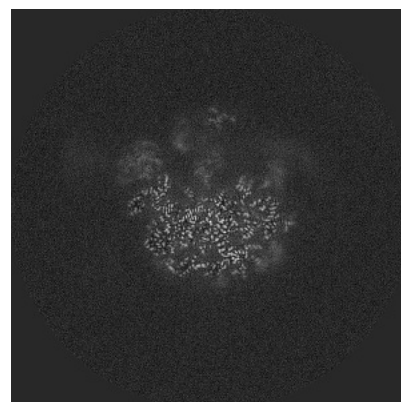
6.2.2 Raw map



X Index: 215



Y Index: 215

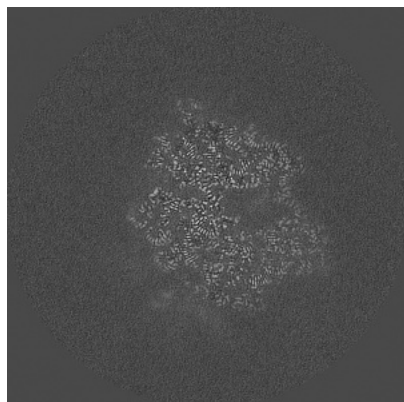


Z Index: 215

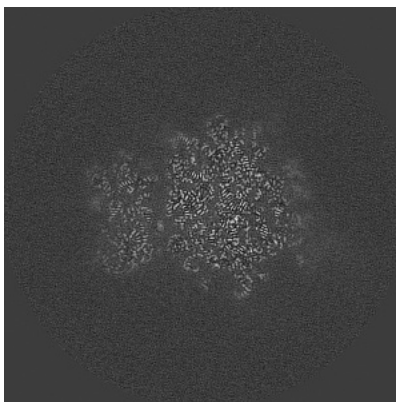
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

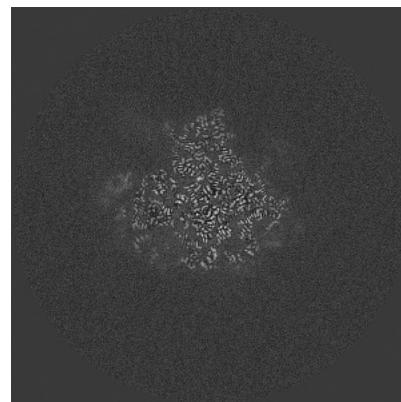
6.3.1 Primary map



X Index: 222

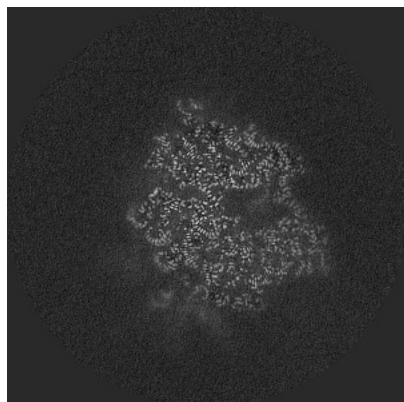


Y Index: 210

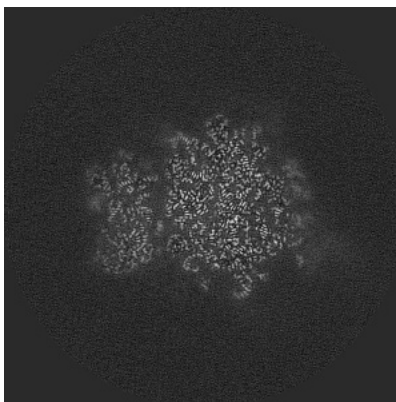


Z Index: 255

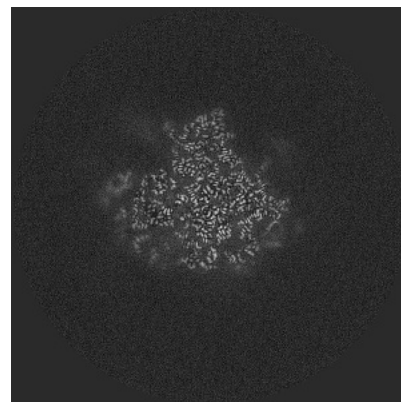
6.3.2 Raw map



X Index: 222



Y Index: 210

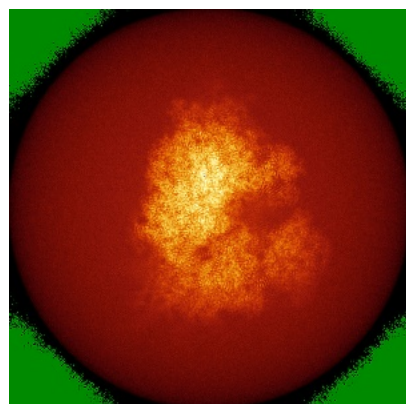


Z Index: 255

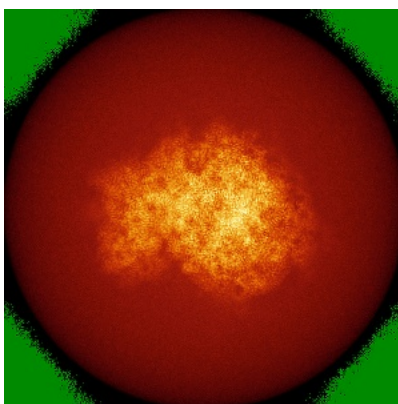
The images above show the largest variance slices of the map in three orthogonal directions.

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

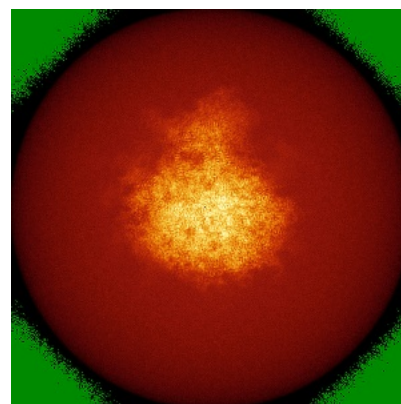
6.4.1 Primary map



X

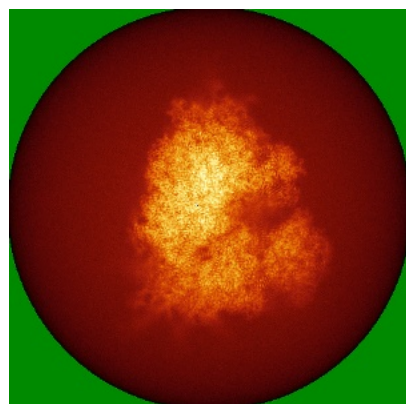


Y

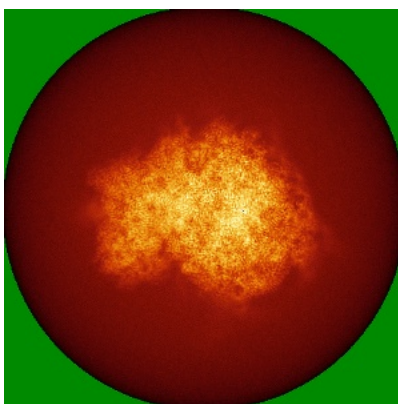


Z

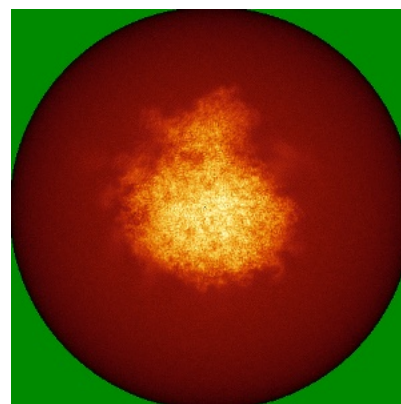
6.4.2 Raw map



X



Y

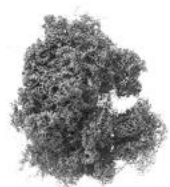


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



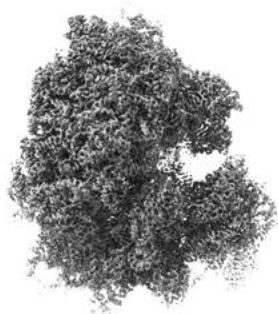
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

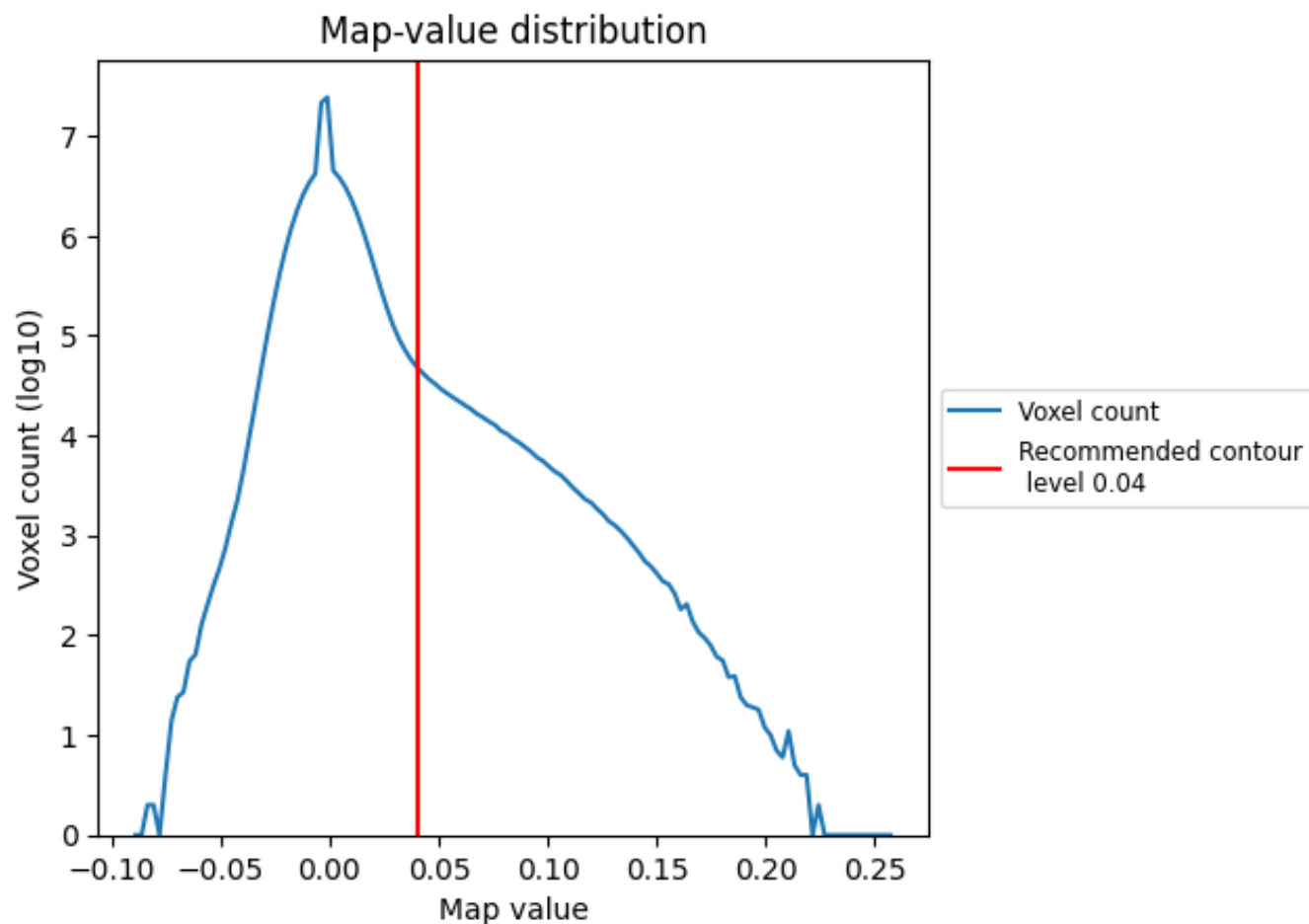
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

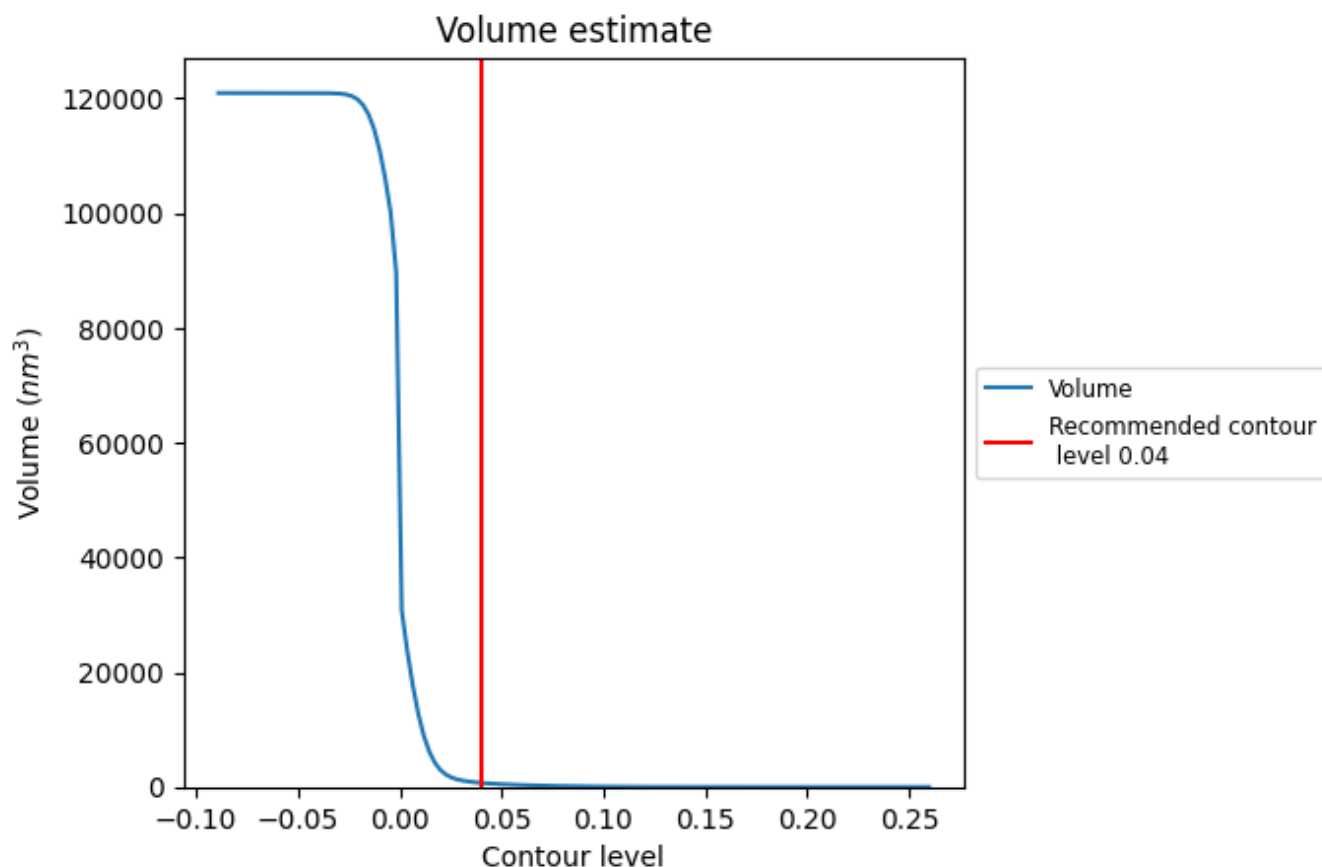
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

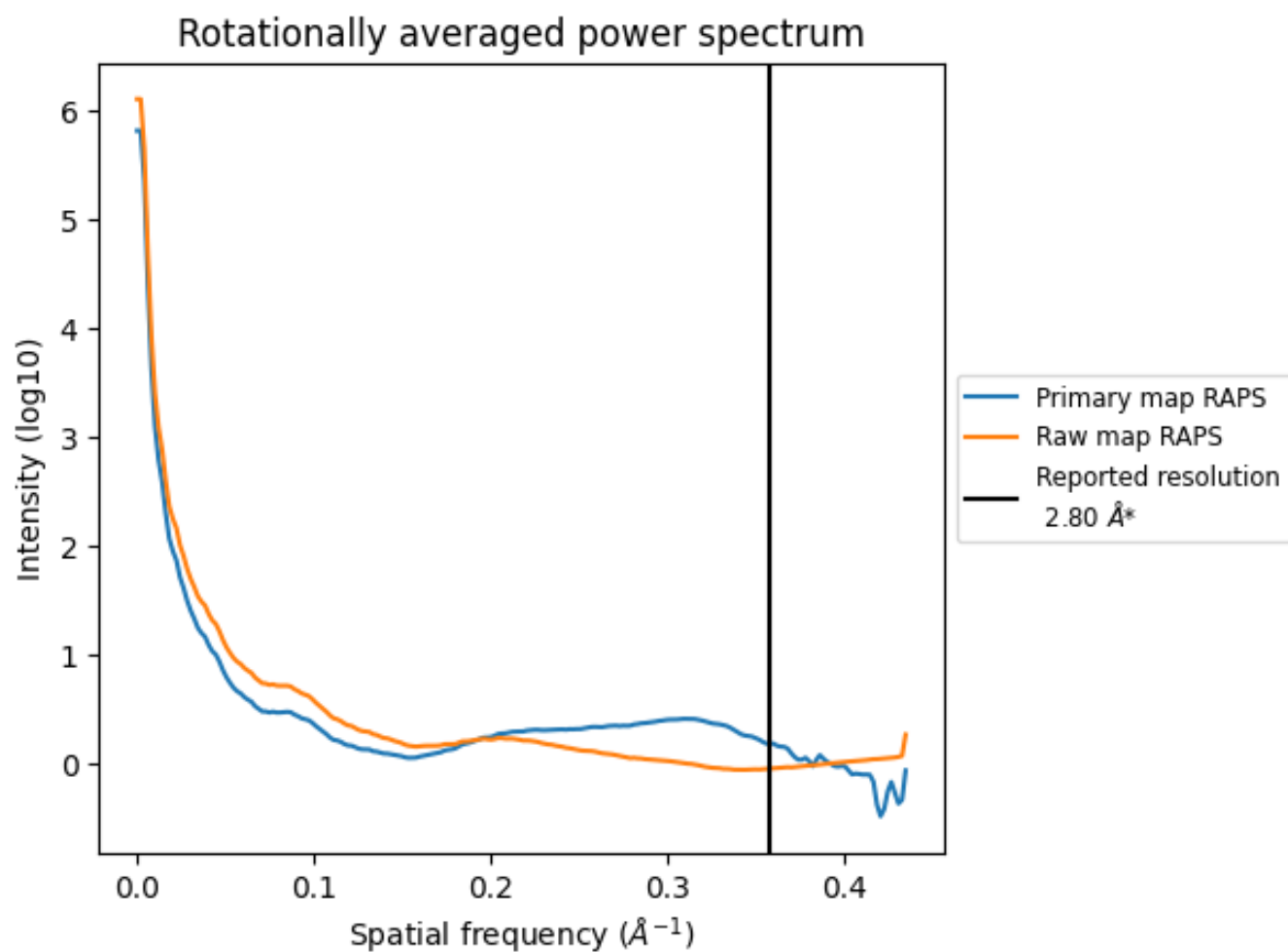
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 709 nm^3 ; this corresponds to an approximate mass of 641 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

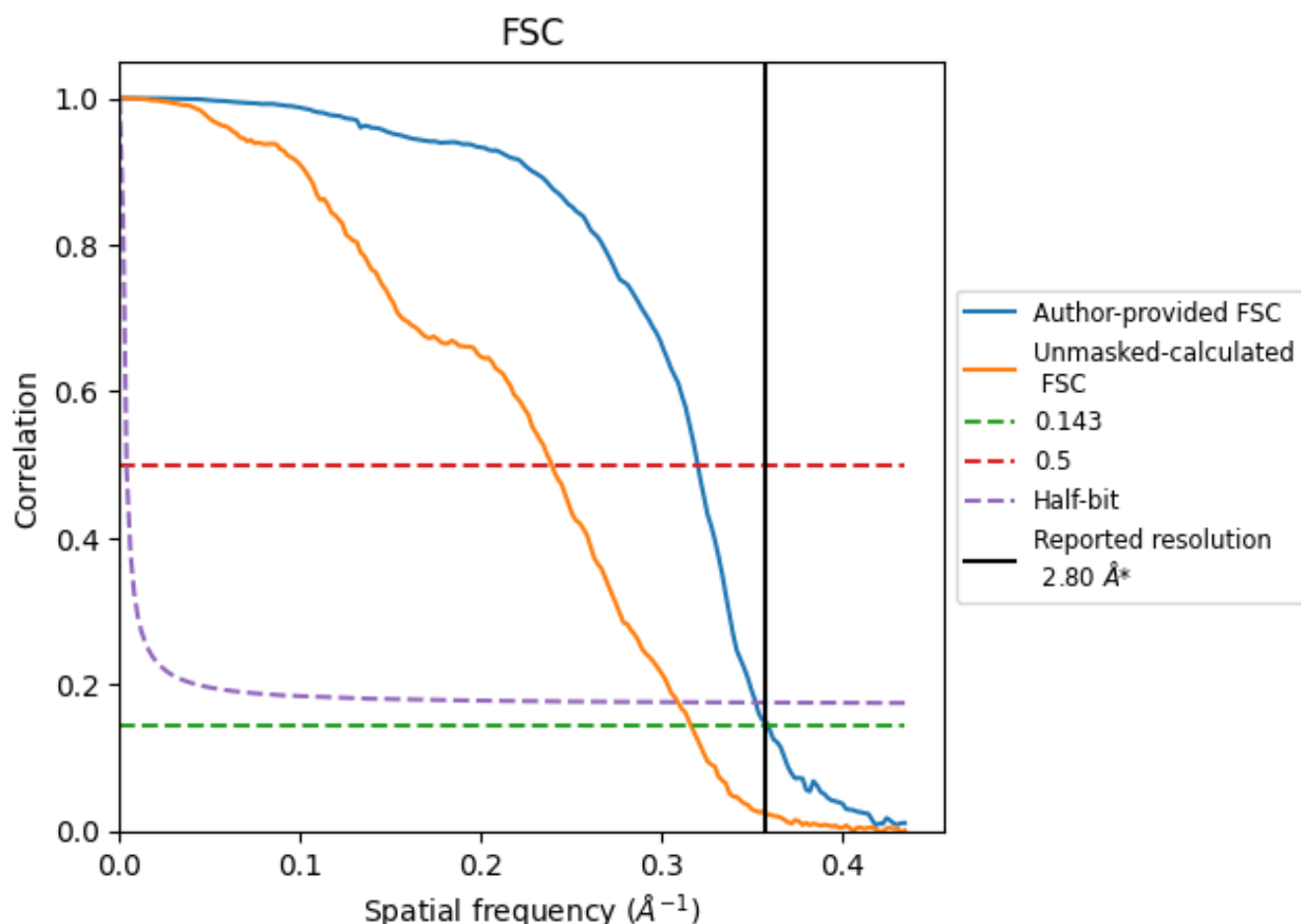


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

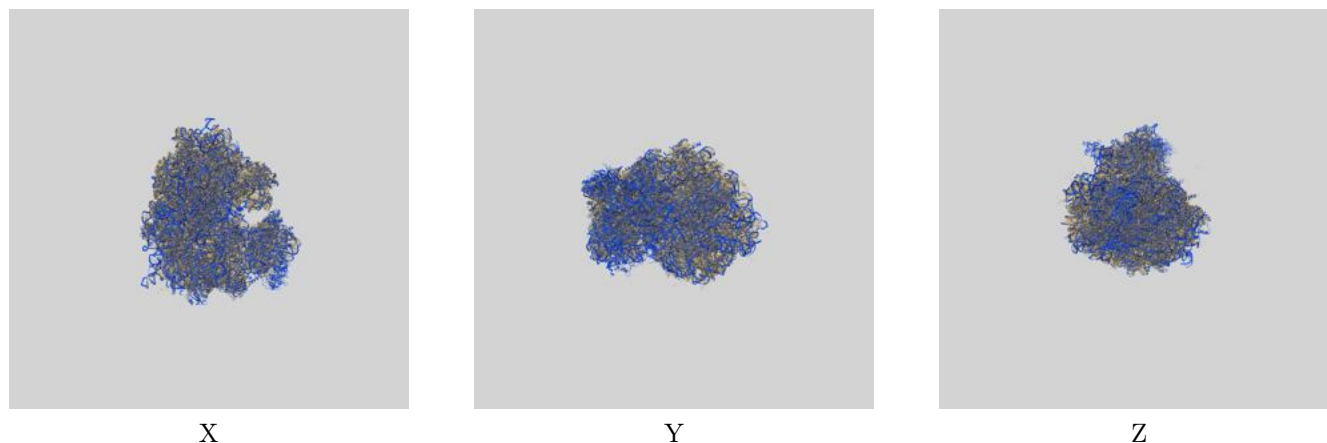
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.12	2.84
Unmasked-calculated*	3.16	4.18	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

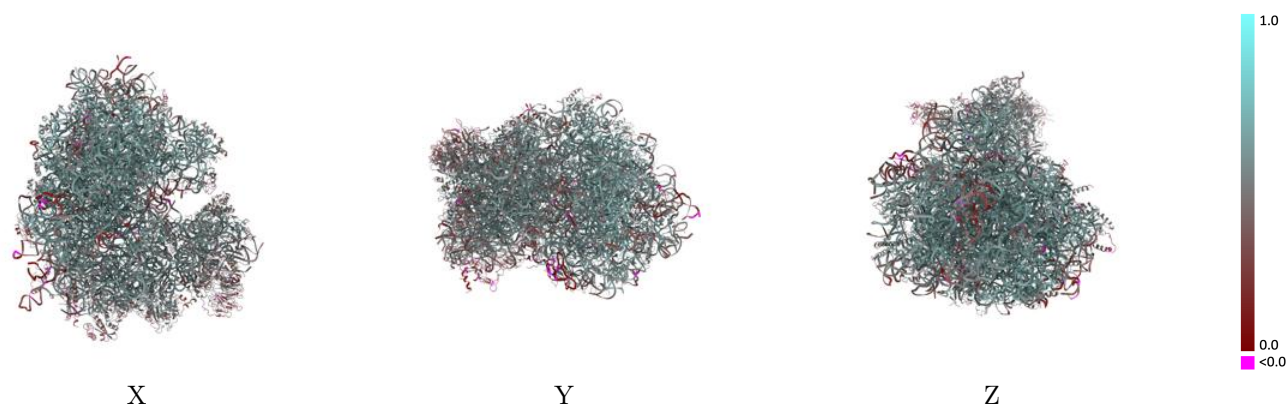
This section contains information regarding the fit between EMDB map EMD-22085 and PDB model 6XA1. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



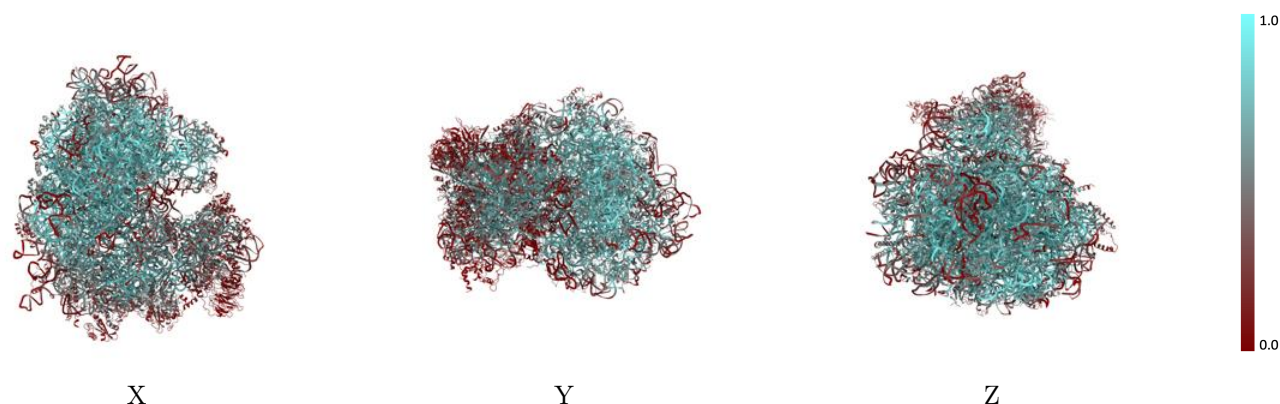
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



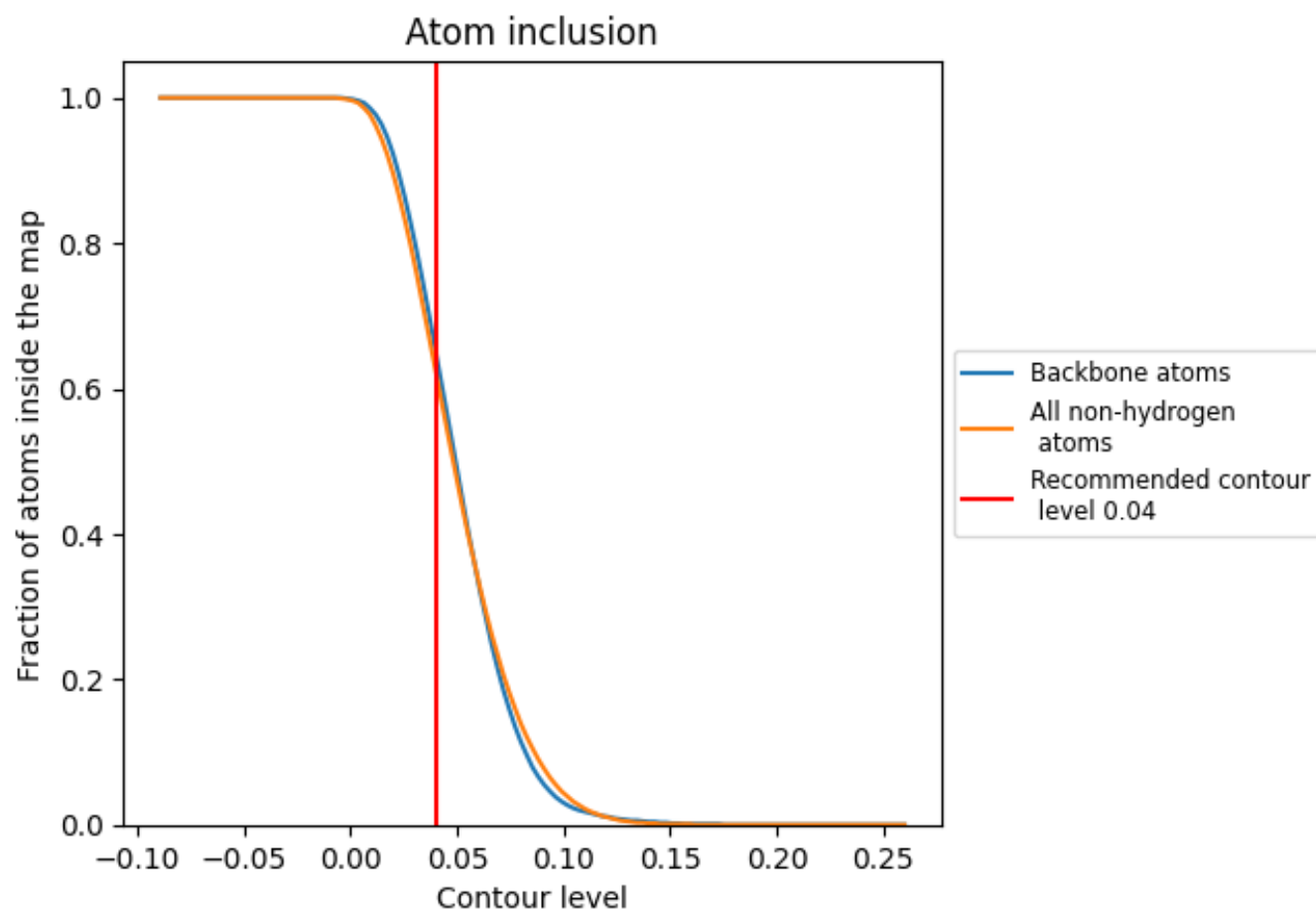
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 62% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6240	 0.5350
Bv	 0.2910	 0.4180
L5	 0.7530	 0.5620
L7	 0.8360	 0.6110
L8	 0.7940	 0.5730
LA	 0.8070	 0.6000
LB	 0.6830	 0.5690
LC	 0.7420	 0.6000
LD	 0.5550	 0.5440
LE	 0.4890	 0.4950
LF	 0.7550	 0.5880
LG	 0.5150	 0.4920
LH	 0.5370	 0.5200
LI	 0.6450	 0.5490
LJ	 0.4100	 0.4390
LL	 0.6300	 0.5520
LM	 0.6120	 0.5480
LN	 0.8590	 0.6190
LO	 0.7330	 0.5730
LP	 0.7380	 0.5870
LQ	 0.7760	 0.6090
LR	 0.5960	 0.4970
LS	 0.7360	 0.5900
LT	 0.6650	 0.5430
LU	 0.2970	 0.4320
LV	 0.7030	 0.5660
LW	 0.3300	 0.3420
LX	 0.6140	 0.5400
LY	 0.6460	 0.5600
LZ	 0.5640	 0.5300
La	 0.8010	 0.6140
Lb	 0.5350	 0.5060
Lc	 0.5860	 0.5160
Ld	 0.6310	 0.5330
Le	 0.7680	 0.6030

















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Chain	Atom inclusion	Q-score
Lf	 0.7920	 0.5980
Lg	 0.6950	 0.5600
Lh	 0.6000	 0.5500
Li	 0.5830	 0.5370
Lj	 0.8380	 0.6010
Lk	 0.4090	 0.4600
Ll	 0.7520	 0.5630
Lm	 0.6550	 0.5470
Ln	 0.7750	 0.5660
Lo	 0.6370	 0.5440
Lp	 0.6910	 0.5640
Lr	 0.6990	 0.5760
NC	 0.4180	 0.5180
S2	 0.6580	 0.5500
SA	 0.3770	 0.4910
SB	 0.3680	 0.5050
SC	 0.4780	 0.5110
SD	 0.2190	 0.4090
SE	 0.3620	 0.4870
SF	 0.3380	 0.4960
SG	 0.1820	 0.3930
SH	 0.1890	 0.3800
SI	 0.4680	 0.5040
SJ	 0.3930	 0.4920
SK	 0.1590	 0.4240
SL	 0.5810	 0.5350
SM	 0.0010	 0.1650
SN	 0.5010	 0.5230
SO	 0.4830	 0.5300
SP	 0.2320	 0.4310
SQ	 0.3280	 0.4820
SR	 0.2120	 0.4120
SS	 0.2500	 0.4570
ST	 0.2730	 0.4870
SU	 0.2330	 0.3680
SV	 0.3480	 0.4750
SW	 0.5670	 0.5380
SX	 0.5870	 0.5430
SY	 0.2360	 0.4300
SZ	 0.1560	 0.4540
Sa	 0.5560	 0.5290
Sb	 0.3190	 0.4510

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Chain	Atom inclusion	Q-score
Sc	 0.2130	 0.4180
Sd	 0.4590	 0.5040
Se	 0.3370	 0.4500
Sf	 0.0120	 0.2590
Sg	 0.0600	 0.3550
j	 0.1570	 0.4010
k	 0.4940	 0.5190