Full wwPDB EM Validation Report ⓘ

Aug 17, 2024 – 03:20 pm BST

PDB ID	:	8QOI
EMDB ID	:	EMD-18539
Title	:	Structure of the human 80S ribosome at 1.9 A resolution - the molecular role of chemical modifications and ions in RNA
Authors	:	Holvec, S.; Barchet, C.; Frechin, L.; Hazemann, I.; von Loeffelholz, O.; Klaholz, B.P.
Deposited on	:	2023-09-29
Resolution	:	1.90 Å(reported)
Based on initial model	:	6QZP

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

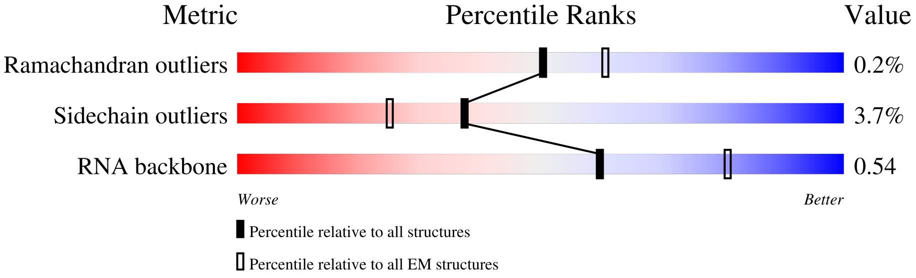
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

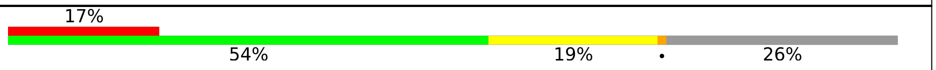
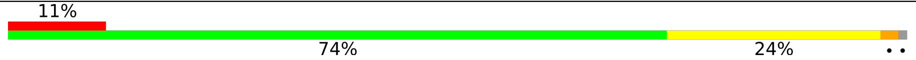
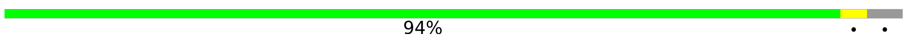
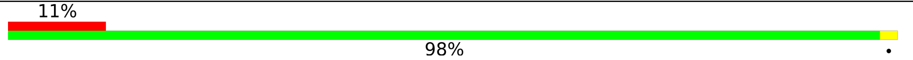
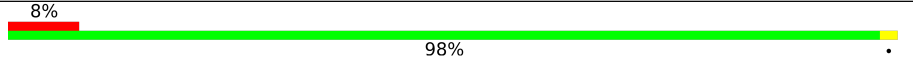
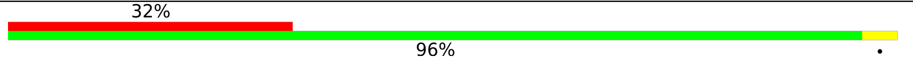
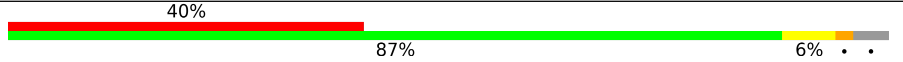
The reported resolution of this entry is 1.90 Å.

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	L5	5069	
2	L7	120	
3	L8	157	
4	LA	257	
5	LB	402	
6	LC	368	
7	LD	293	
8	LE	247	

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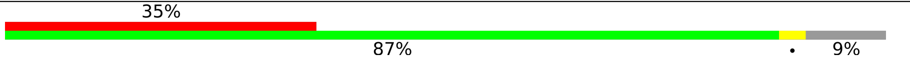
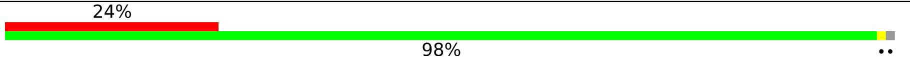
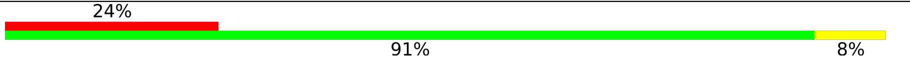
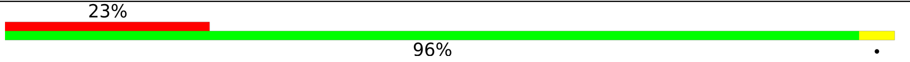
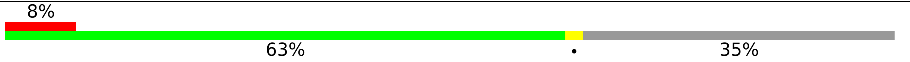
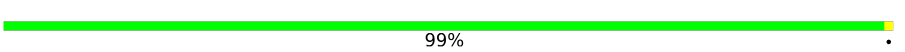
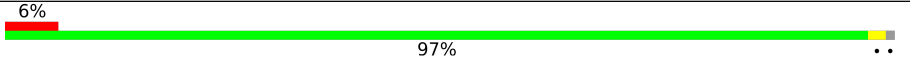
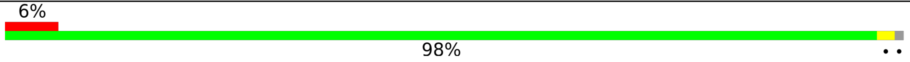
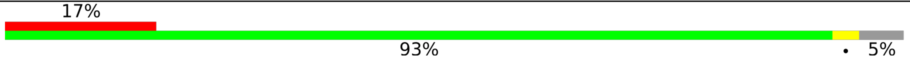
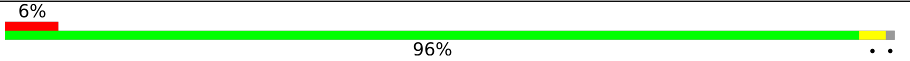
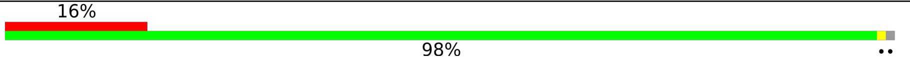
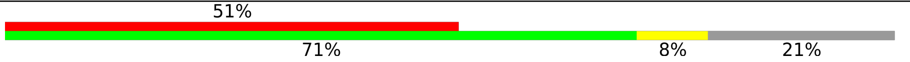
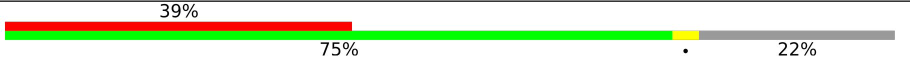
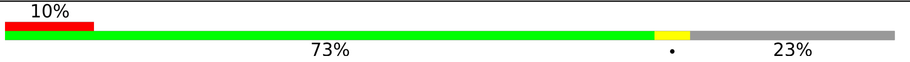
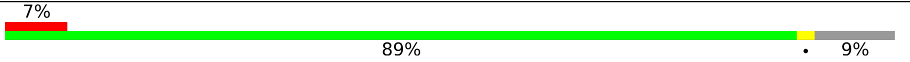
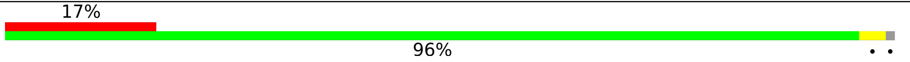
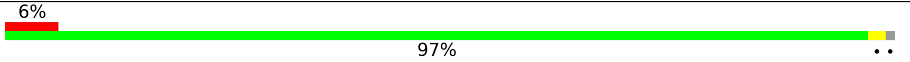
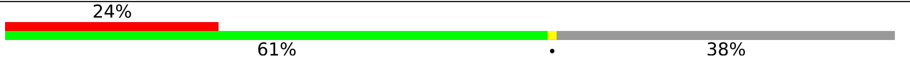
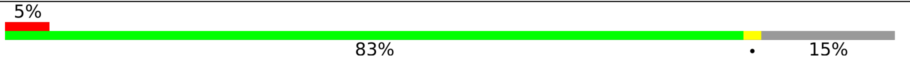
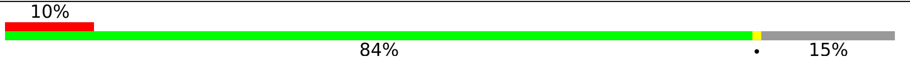
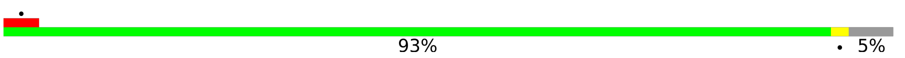
Mol	Chain	Length	Quality of chain
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	

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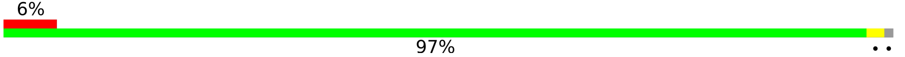
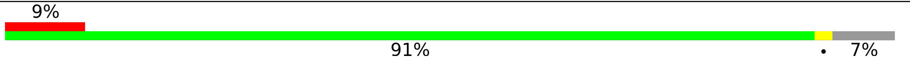
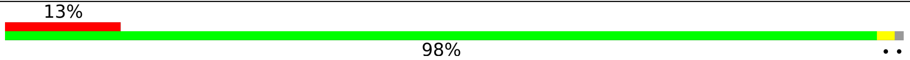
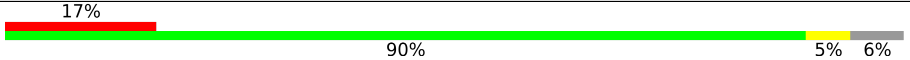
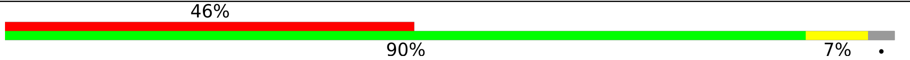
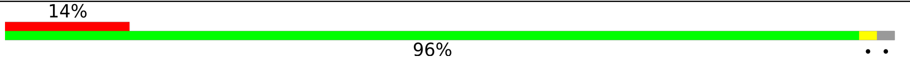
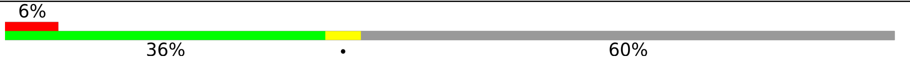
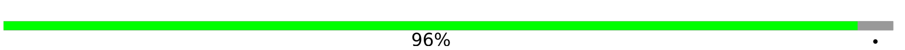
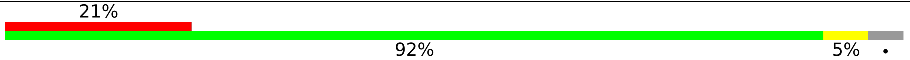
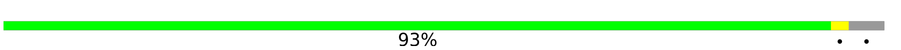
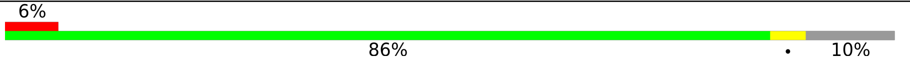
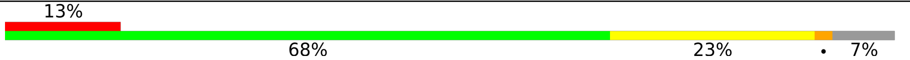
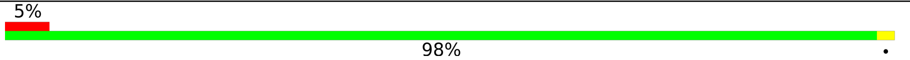
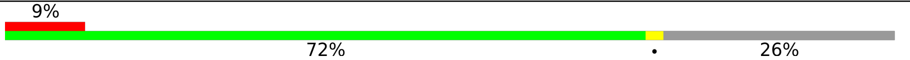
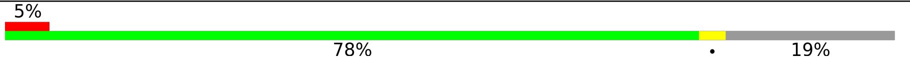
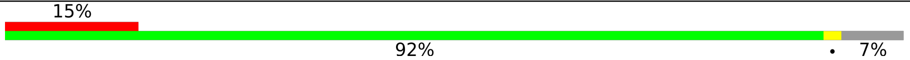
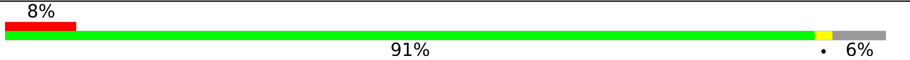
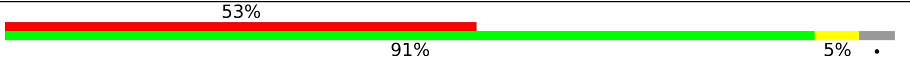
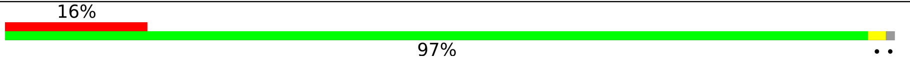
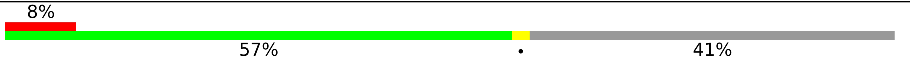
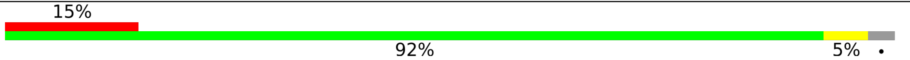
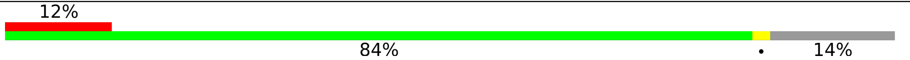
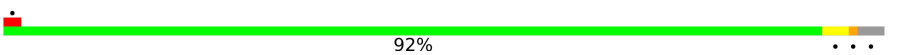
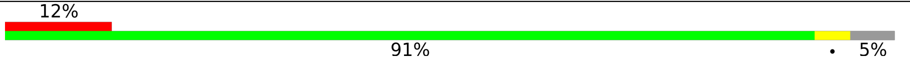
Mol	Chain	Length	Quality of chain
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	S2	1869	
47	SE	263	
48	SA	295	
49	SB	264	
50	SD	243	
51	SF	204	
52	SH	194	
53	SI	208	
54	SK	165	
55	SL	158	
56	SP	145	
57	SQ	146	
58	SS	152	

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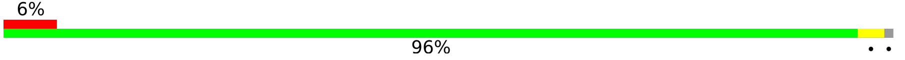
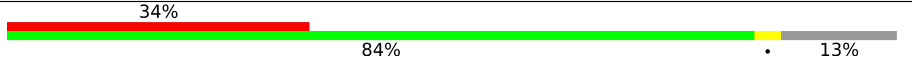
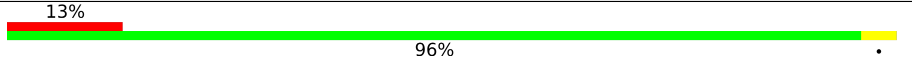
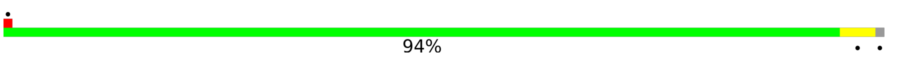
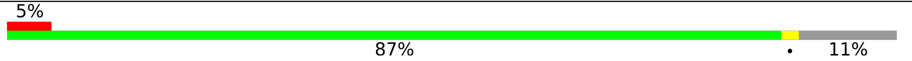
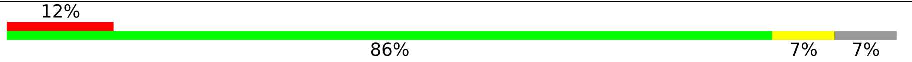
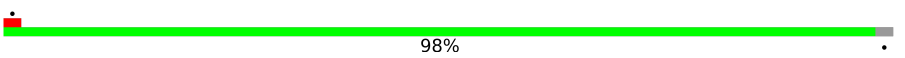
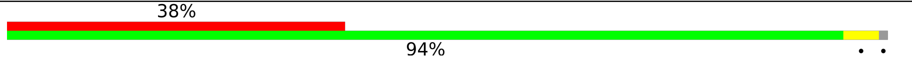
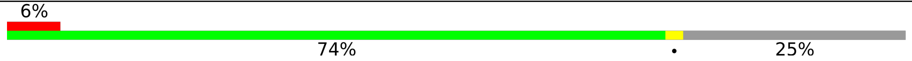
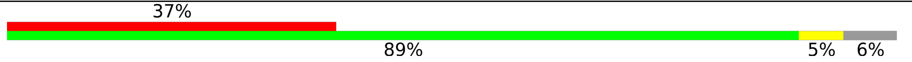
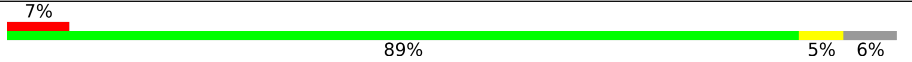
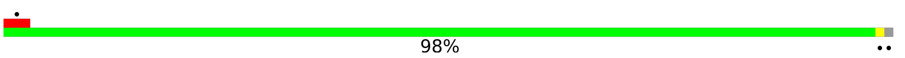
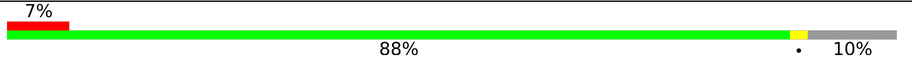
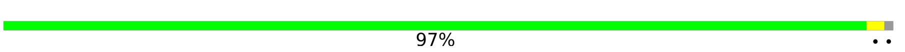
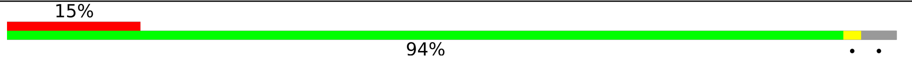
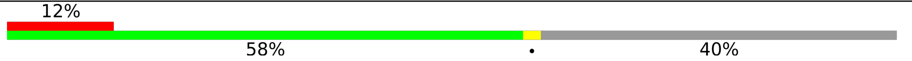
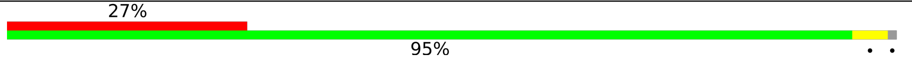
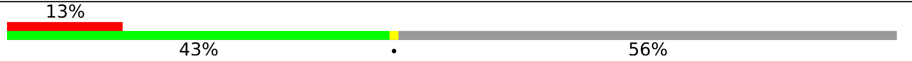
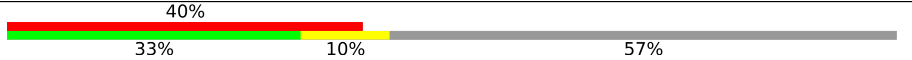
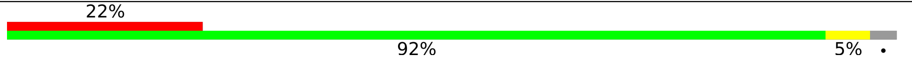
Mol	Chain	Length	Quality of chain
59	ST	145	
60	SU	119	
61	SV	83	
62	SX	143	
63	Sa	115	
64	Sc	69	
65	Sd	56	
66	Sg	317	
67	SC	293	
68	SG	249	
69	SJ	194	
70	SM	132	
71	SN	151	
72	SO	151	
73	SW	130	
74	SY	133	
75	SZ	125	
76	Sb	84	
77	Se	133	
78	Sf	156	
79	SR	135	

2 Entry composition ⓘ

There are 84 unique types of molecules in this entry. The entry contains 233370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA (3773-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3773	80205	35722	14588	26123	3772	0	0

- Molecule 2 is a RNA chain called 5S rRNA (120-MER).

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

- Molecule 3 is a RNA chain called 5.8S rRNA (156-MER).

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

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LD	293	2382	1507	434	427	14	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL30.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LI	213	1713	1083	329	285	16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	49	CYS	GLY	conflict	UNP Q96L21

- 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	210	Total	C	N	O	S	0	0
			1701	1064	352	281	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
			Total	C	N	O	S		
20	LR	187	1566	971	336	250	9	0	0

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

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

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

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LW	122	997	622	203	168	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	132	Total	C	N	O	S	0	0
			1102	692	223	184	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 Large ribosomal subunit protein uL15.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	99	Total	C	N	O	S	0	0
			808	502	177	125	4		

- 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	106	Total	C	N	O	S	0	0
			879	555	170	152	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
			Total	C	N	O	S		
34	Lf	109	876	555	174	144	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Lg	109	868	544	179	139	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Li	99	813	509	173	126	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Lk	68	559	360	101	97	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Lm	51	419	260	88	65	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Lo	102	842	527	174	135	6	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Lp	88	681	430	131	113	7	0	0

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

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

- Molecule 46 is a RNA chain called 18S rRNA (1740-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	S2	1740	36955	16511	6600	12105	1739	0	0

- Molecule 47 is a protein called 40S ribosomal protein S4, X isoform.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	SA	219	1727	1096	302	320	9	0	0

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	SB	215	1747	1109	312	312	14	0	0

- Molecule 50 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SD	227	1765	1125	317	315	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SF	191	1509	943	286	273	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	SH	186	1497	956	274	266	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SK	97	816	533	144	133	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	154	Total	C	N	O	S	0	0
			1258	802	235	215	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SP	125	Total	C	N	O	S	0	0
			1027	653	193	174	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 58 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 59 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	ST	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 60 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SU	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 61 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 62 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SX	141	Total 1098	C 693	N 219	O 183	S 3	0	0

- Molecule 63 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sa	102	Total 829	C 517	N 174	O 133	S 5	1	0

- Molecule 64 is a protein called 40S ribosomal protein S28.

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

- Molecule 65 is a protein called 40S ribosomal protein S29.

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

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SC	221	Total 1724	C 1115	N 298	O 301	S 10	1	0

- Molecule 68 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SG	234	Total 1903	C 1188	N 384	O 324	S 7	0	0

- Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SJ	182	Total 1520	C 967	N 306	O 245	S 2	1	0

- Molecule 70 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SM	118	Total 906	C 568	N 158	O 172	S 8	0	0

- Molecule 71 is a protein called 40S ribosomal protein S13.

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

- Molecule 72 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SO	136	Total 1016	C 621	N 199	O 190	S 6	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SY	128	Total 1048	C 661	N 207	O 175	S 5	1	0

- Molecule 75 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	SZ	75	598	382	111	104	1	0	0

- Molecule 76 is a protein called 40S ribosomal protein S27.

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

- Molecule 77 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Se	58	459	284	100	74	1	0	0

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	Sf	67	548	346	102	93	7	0	0

- Molecule 79 is a protein called 40S ribosomal protein S17.

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

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
80	L5	198	198	198	0
80	L7	2	2	2	0
80	L8	4	4	4	0
80	LI	1	1	1	0
80	LN	1	1	1	0
80	LP	1	1	1	0

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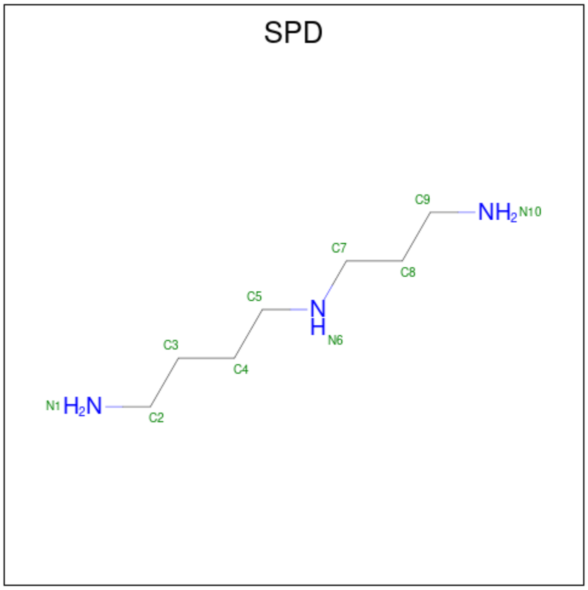
Mol	Chain	Residues	Atoms		AltConf
80	LV	1	Total 1	Mg 1	0
80	S2	84	Total 84	Mg 84	0

- Molecule 81 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
81	L5	78	Total 78	K 78	0
81	L7	1	Total 1	K 1	0
81	LA	1	Total 1	K 1	0
81	LB	1	Total 1	K 1	0
81	LI	1	Total 1	K 1	0
81	Le	1	Total 1	K 1	0
81	Lf	1	Total 1	K 1	0
81	Lo	1	Total 1	K 1	0
81	S2	21	Total 21	K 21	0
81	Sd	1	Total 1	K 1	0
81	SO	1	Total 1	K 1	0

- Molecule 82 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 84 is water.

Mol	Chain	Residues	Atoms	AltConf
84	L5	9116	Total O 9116 9116	0
84	L7	175	Total O 175 175	0
84	L8	376	Total O 376 376	0
84	LA	176	Total O 176 176	0
84	LB	135	Total O 135 135	0
84	LC	149	Total O 149 149	0
84	LD	29	Total O 29 29	0
84	LE	32	Total O 32 32	0
84	LF	83	Total O 83 83	0
84	LG	40	Total O 40 40	0
84	LH	27	Total O 27 27	0
84	LI	36	Total O 36 36	0
84	LJ	5	Total O 5 5	0
84	LL	71	Total O 71 71	0
84	LM	16	Total O 16 16	0
84	LN	131	Total O 131 131	0
84	LO	59	Total O 59 59	0
84	LP	61	Total O 61 61	0
84	LQ	99	Total O 99 99	0
84	LR	103	Total O 103 103	0
84	LS	55	Total O 55 55	0
84	LT	59	Total O 59 59	0

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Mol	Chain	Residues	Atoms	AltConf
84	LU	6	Total O 6 6	0
84	LV	61	Total O 61 61	0
84	LW	49	Total O 49 49	0
84	LX	32	Total O 32 32	0
84	LY	36	Total O 36 36	0
84	LZ	13	Total O 13 13	0
84	La	70	Total O 70 70	0
84	Lb	34	Total O 34 34	0
84	Lc	55	Total O 55 55	0
84	Ld	29	Total O 29 29	0
84	Le	81	Total O 81 81	0
84	Lf	47	Total O 47 47	0
84	Lg	52	Total O 52 52	0
84	Lh	34	Total O 34 34	0
84	Li	24	Total O 24 24	0
84	Lj	55	Total O 55 55	0
84	Lk	6	Total O 6 6	0
84	Ll	22	Total O 22 22	0
84	Lm	17	Total O 17 17	0
84	Ln	39	Total O 39 39	0
84	Lo	22	Total O 22 22	0

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Mol	Chain	Residues	Atoms	AltConf
84	Lp	82	Total O 82 82	0
84	Lr	41	Total O 41 41	0
84	S2	4529	Total O 4529 4529	0
84	SE	85	Total O 85 85	0
84	SA	26	Total O 26 26	0
84	SB	71	Total O 71 71	0
84	SD	53	Total O 53 53	0
84	SF	39	Total O 39 39	0
84	SH	18	Total O 18 18	0
84	SI	96	Total O 96 96	0
84	SK	1	Total O 1 1	0
84	SL	98	Total O 98 98	0
84	SP	8	Total O 8 8	0
84	SQ	29	Total O 29 29	0
84	SS	10	Total O 10 10	0
84	ST	15	Total O 15 15	0
84	SU	8	Total O 8 8	0
84	SV	27	Total O 27 27	0
84	SX	95	Total O 95 95	0
84	Sa	62	Total O 62 62	0
84	Sc	21	Total O 21 21	0

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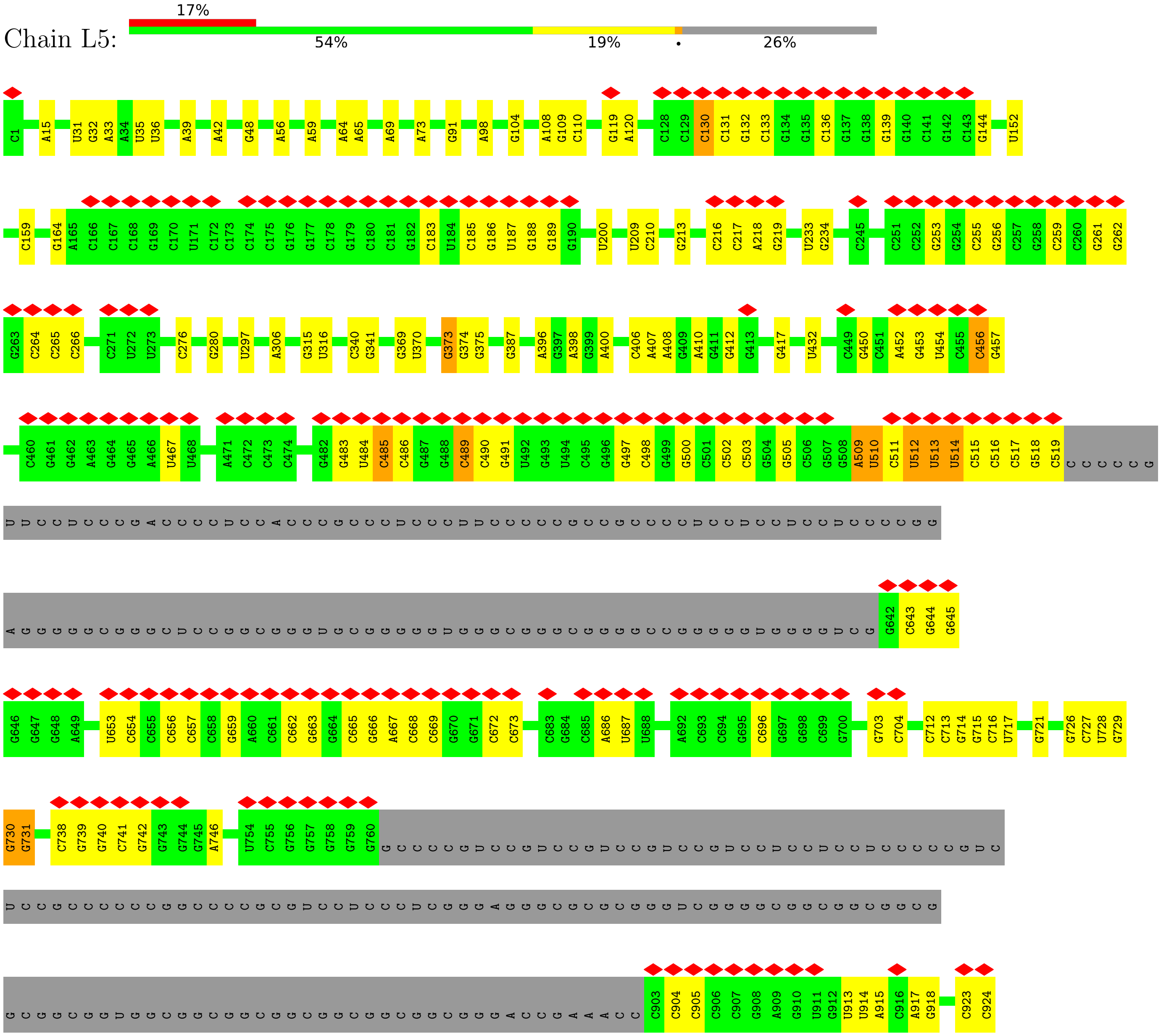
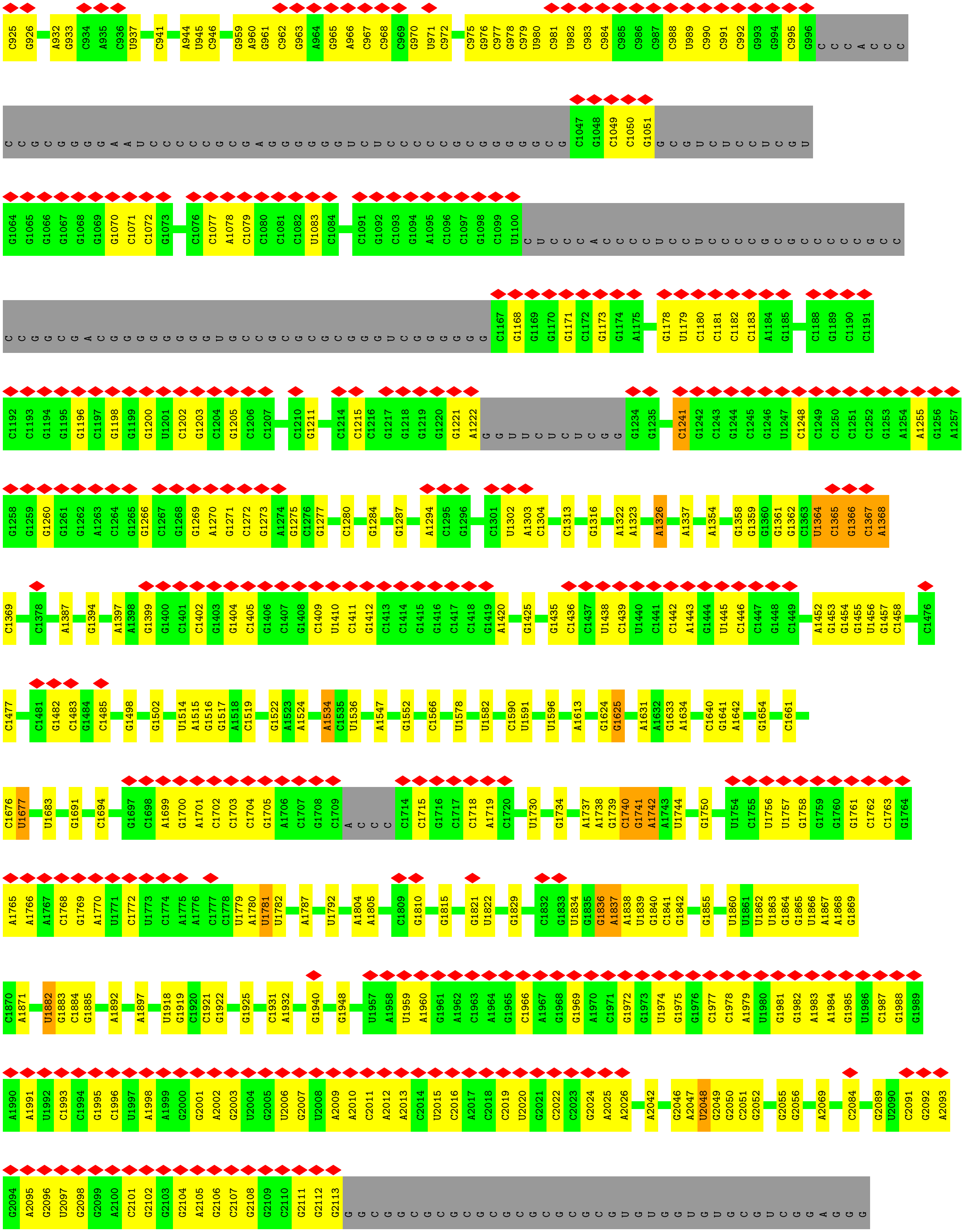
Mol	Chain	Residues	Atoms	AltConf
84	Sd	8	Total O 8 8	0
84	Sg	3	Total O 3 3	0
84	SC	79	Total O 79 79	0
84	SG	28	Total O 28 28	0
84	SJ	76	Total O 76 76	0
84	SN	87	Total O 87 87	0
84	SO	52	Total O 52 52	0
84	SW	64	Total O 64 64	0
84	SY	32	Total O 32 32	0
84	SZ	1	Total O 1 1	0
84	Sb	27	Total O 27 27	0
84	Se	21	Total O 21 21	0
84	SR	29	Total O 29 29	0

3 Residue-property plots ⓘ

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

- Molecule 1: 28S rRNA (3773-MER)

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C C G C G G G G A A U C C C C C C G C G A G G G G G G U C U C C C C C G G G G G G G C G C1047 G1048 C1049 C1050 G1051 G C C G U C U C C U C G U
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C1192 C1193 G1194 G1195 G1196 C1197 G1198 G1199 G1200 U1201 C1202 G1203 C1204 G1205 C1206 C1207 C1210 G1211 C1214 C1215 C1216 G1217 G1218 G1219 G1220 G1221 A1222 G G U U C U C U C G G G1234 G1235 C1241 G1242 C1243 G1244 C1245 G1246 U1247 C1248 C1249 C1250 C1251 C1252 G1253 A1254 A1255 G1256 A1257
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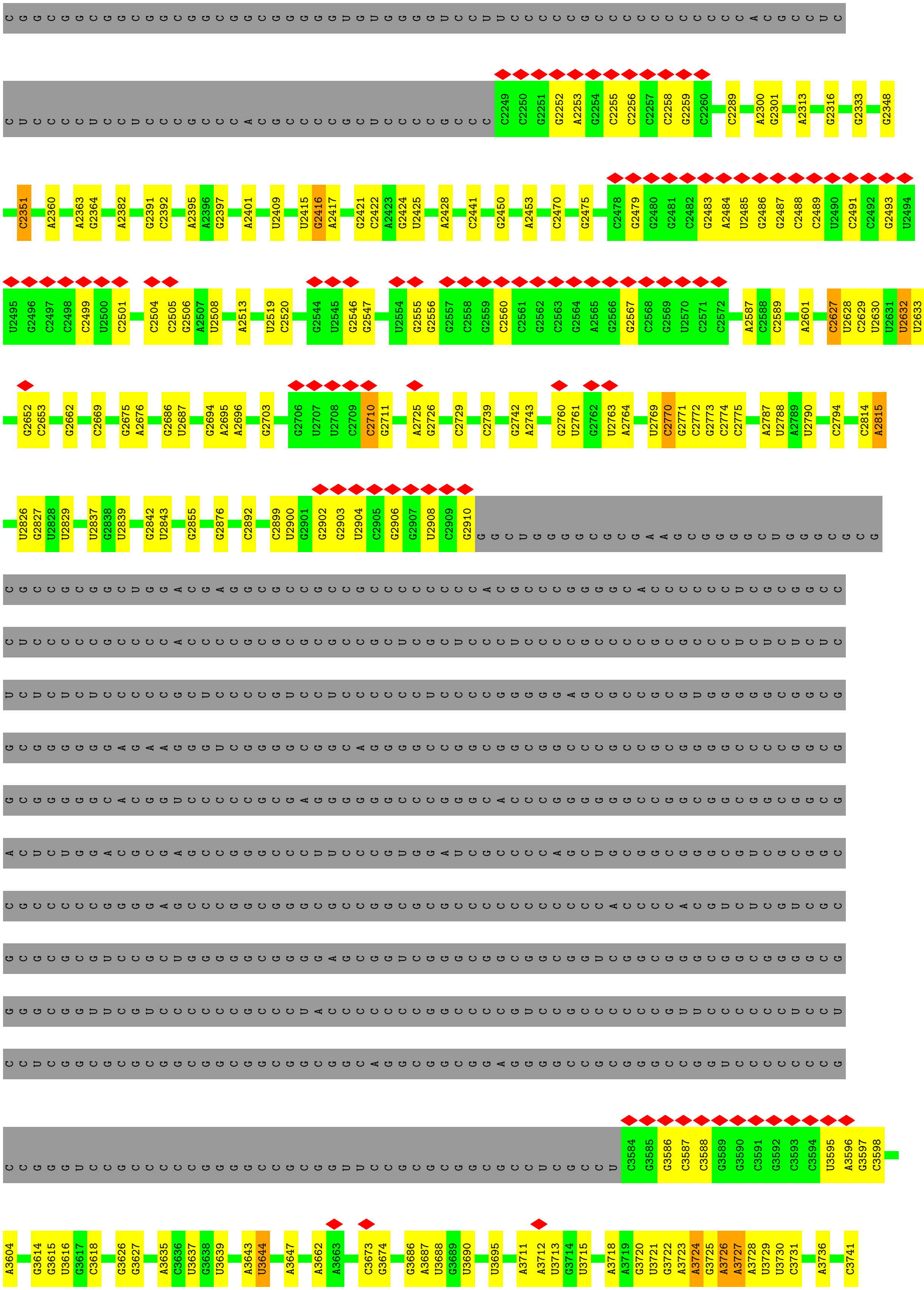
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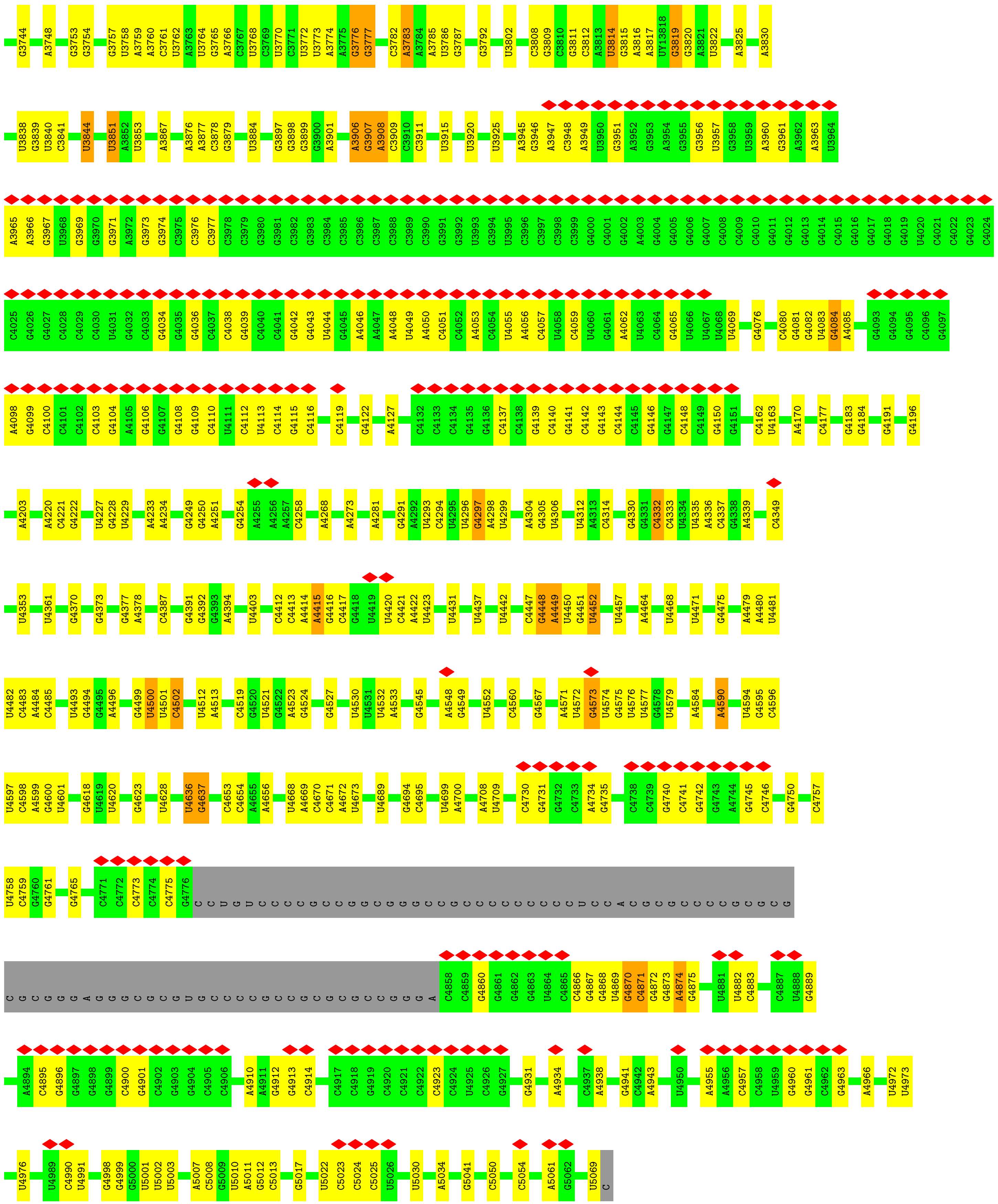
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- Molecule 2: 5S rRNA (120-MER)

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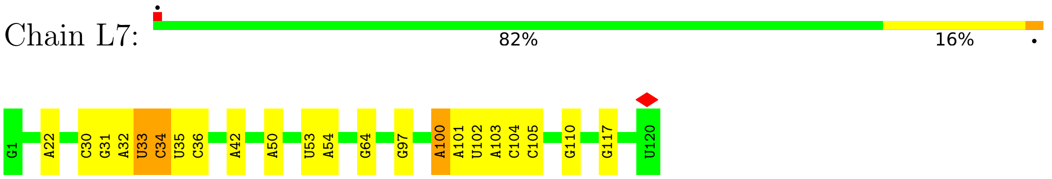
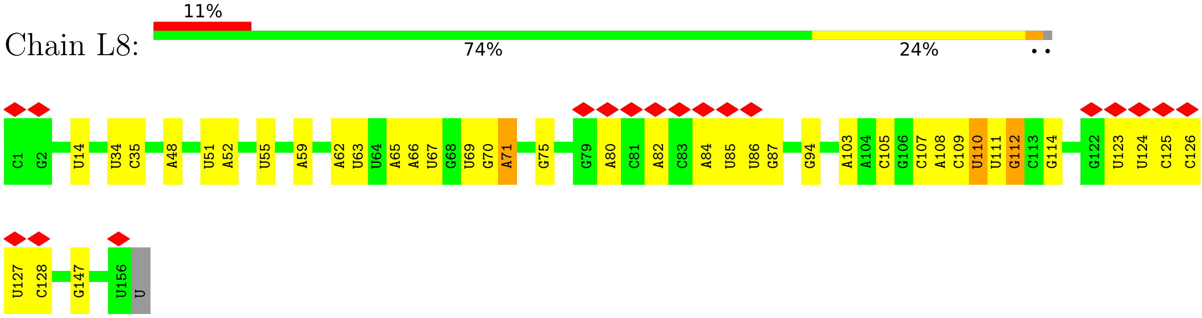


- Molecule 3: 5.8S rRNA (156-MER)

Chain L8:



- Molecule 4: 60S ribosomal protein L8

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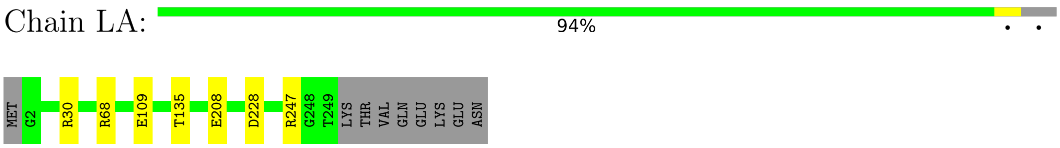
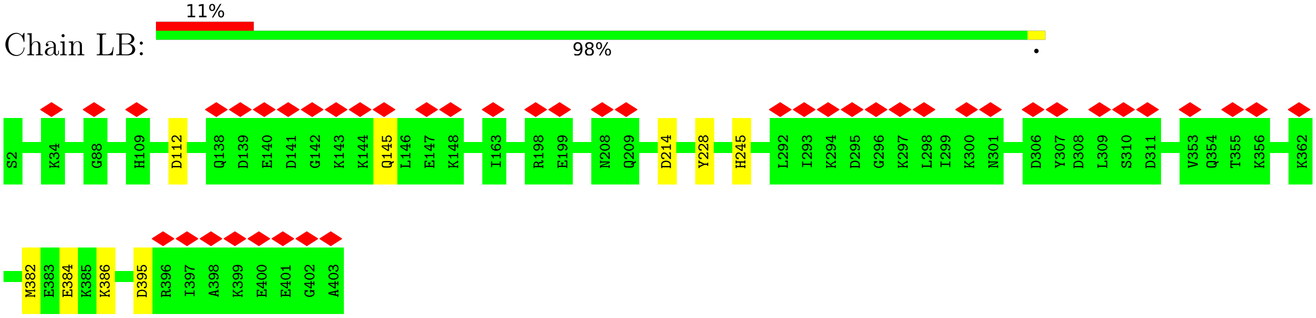


- Molecule 5: Large ribosomal subunit protein uL3

Chain LB:



- Molecule 6: Large ribosomal subunit protein uL4

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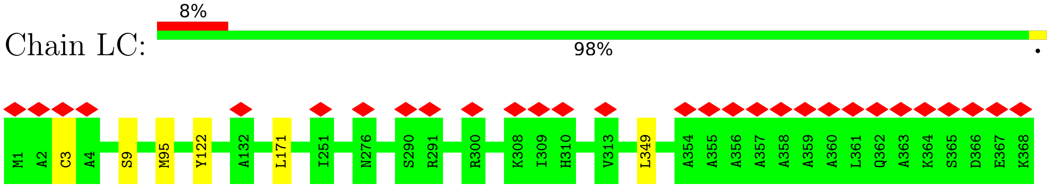
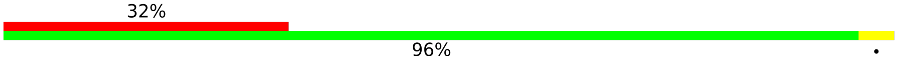
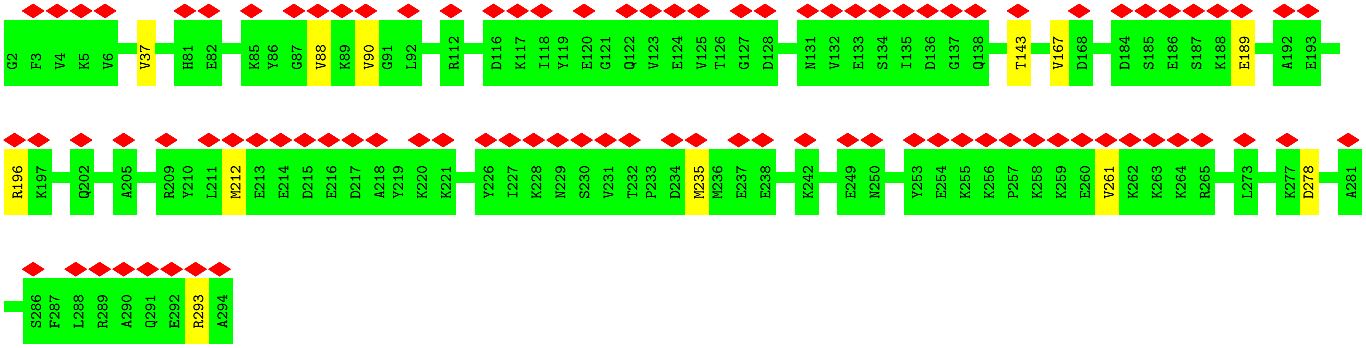


- Molecule 7: Large ribosomal subunit protein uL18

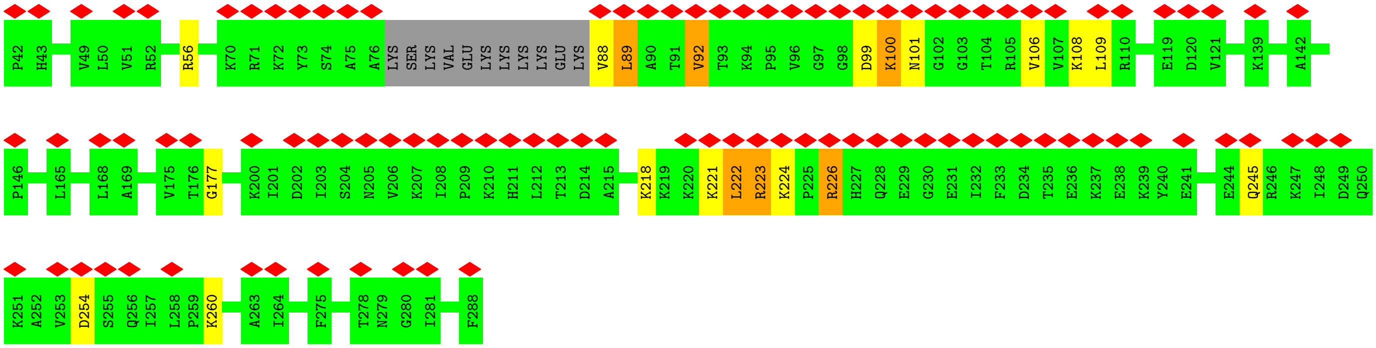
Chain LD:





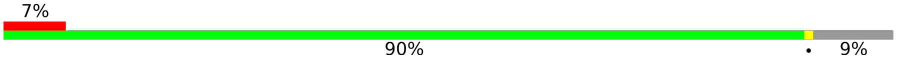
- Molecule 8: Large ribosomal subunit protein eL6

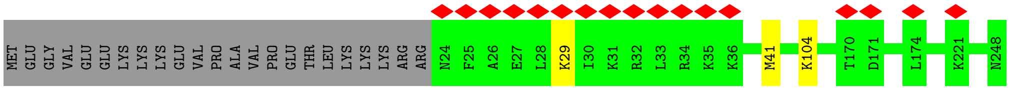
Chain LE:



- Molecule 9: Large ribosomal subunit protein uL30

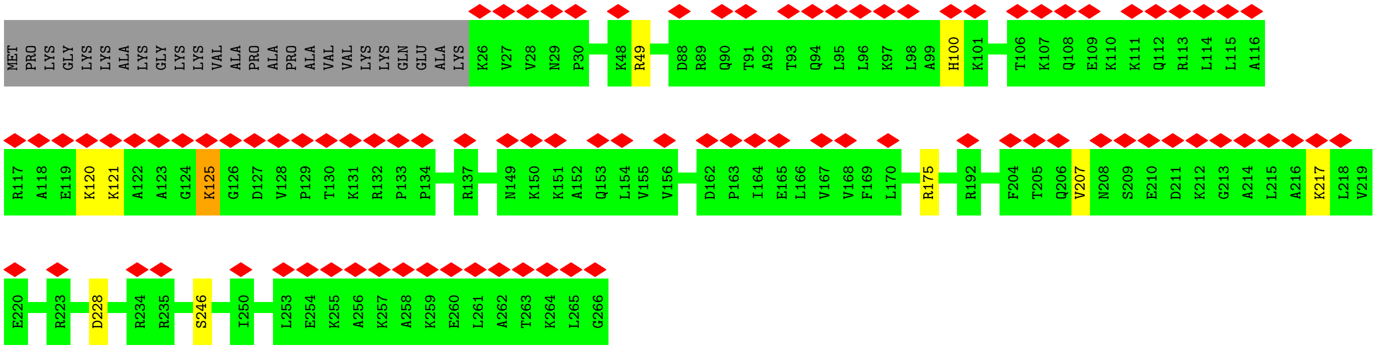
Chain LF:



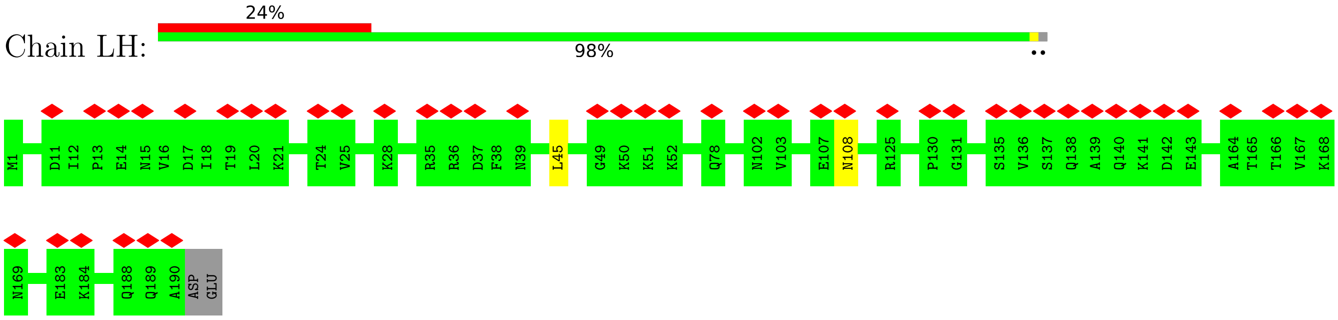


- Molecule 10: 60S ribosomal protein L7a

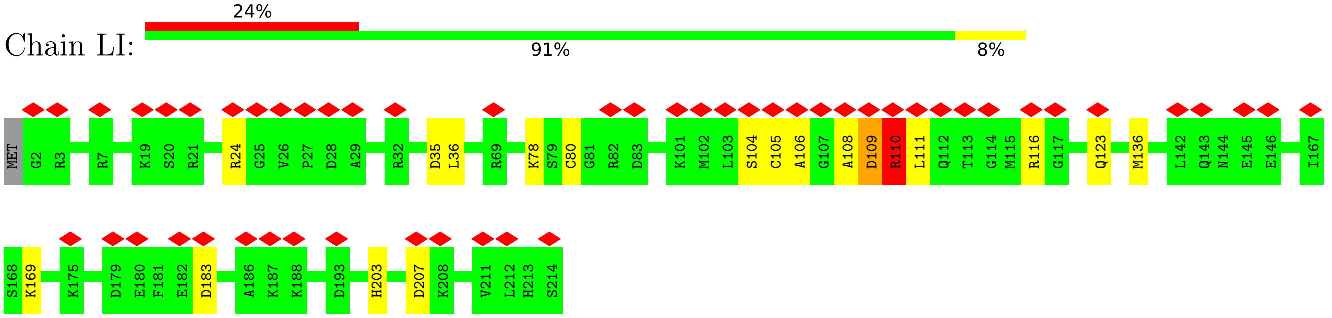
Chain LG:



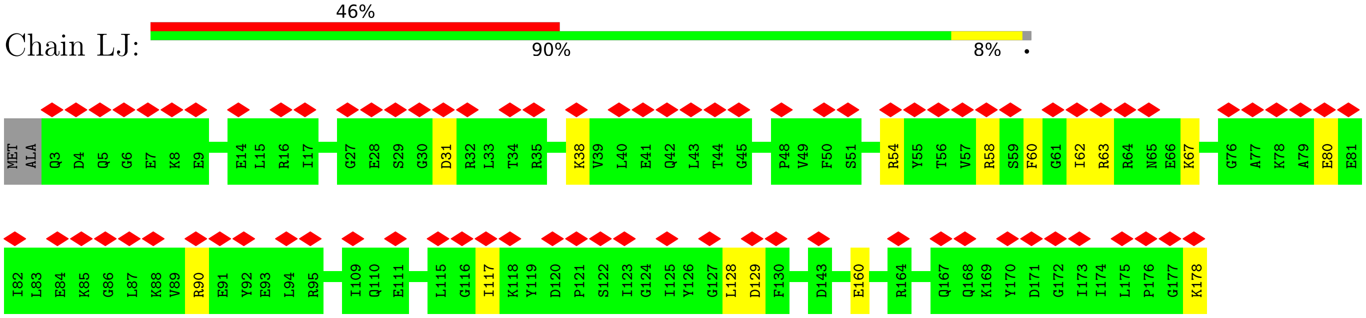
- Molecule 11: 60S ribosomal protein L9



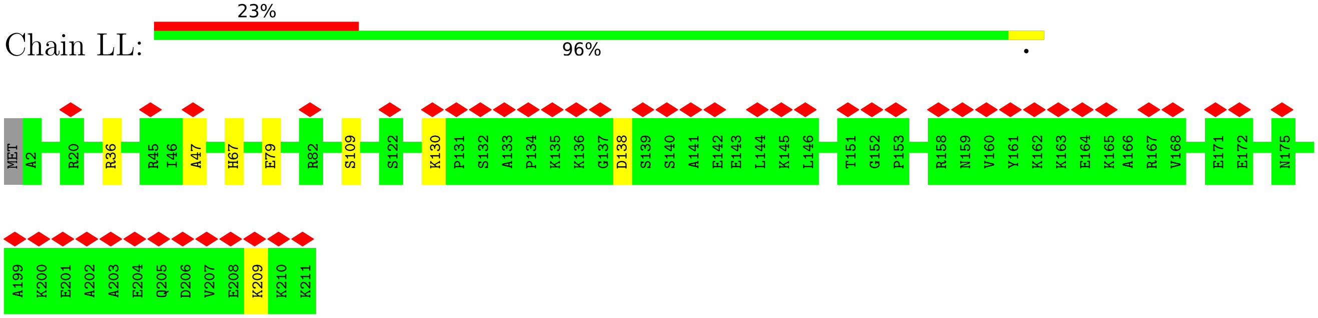
- Molecule 12: 60S ribosomal protein L10-like



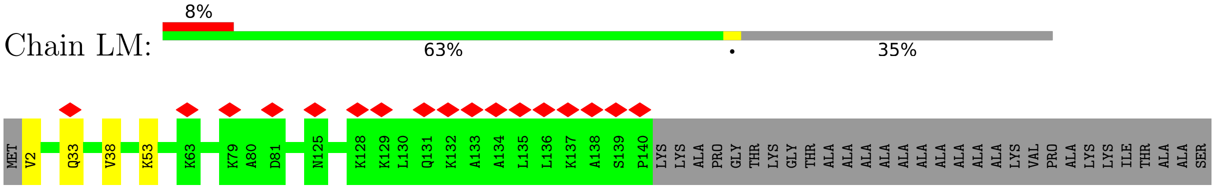
- Molecule 13: 60S ribosomal protein L11



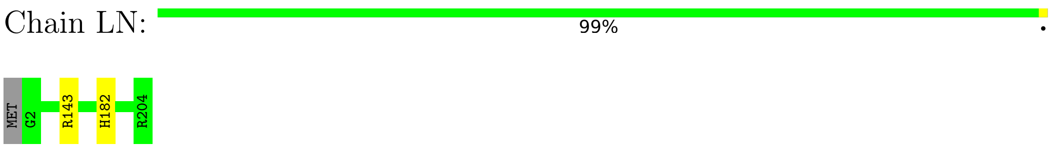
- Molecule 14: 60S ribosomal protein L13



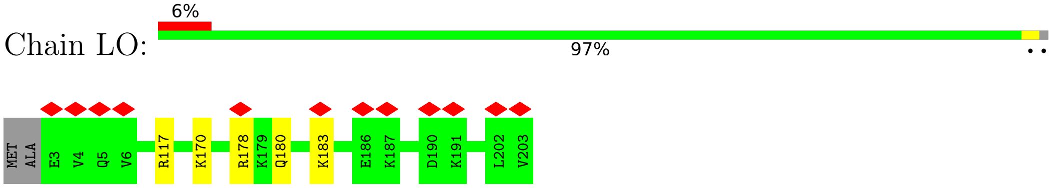
- Molecule 15: 60S ribosomal protein L14



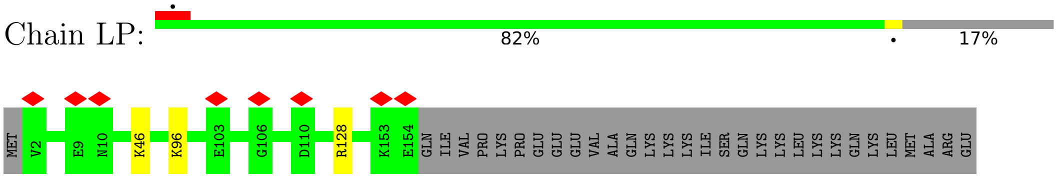
- Molecule 16: 60S ribosomal protein L15



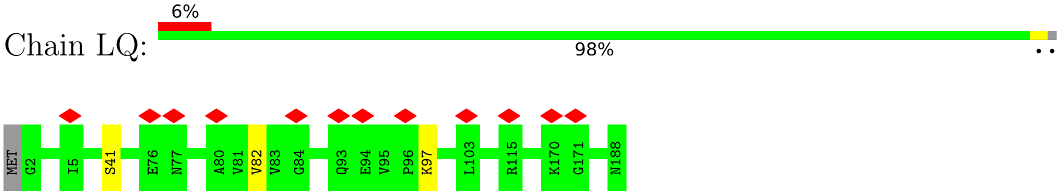
- Molecule 17: 60S ribosomal protein L13a



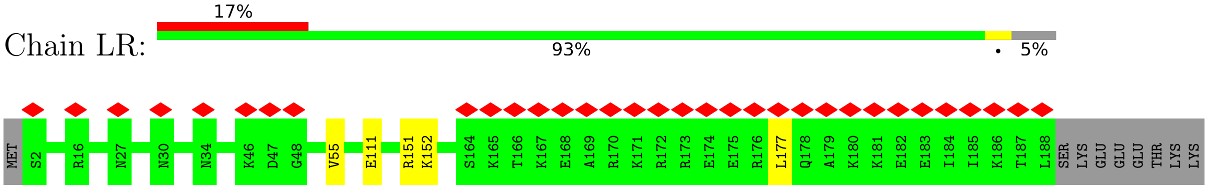
- Molecule 18: 60S ribosomal protein L17



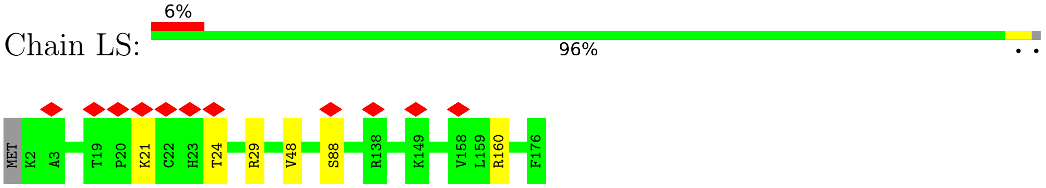
- Molecule 19: 60S ribosomal protein L18



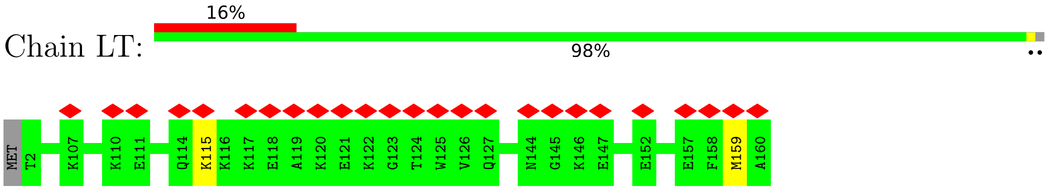
- Molecule 20: 60S ribosomal protein L19



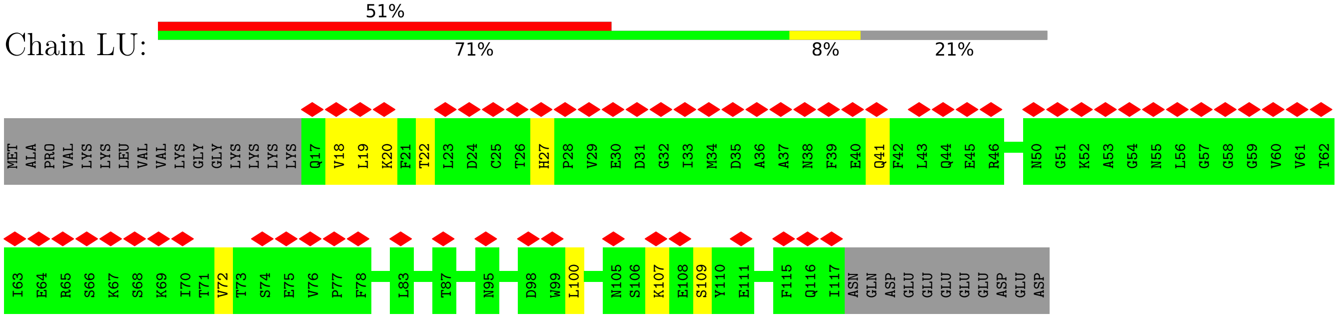
- Molecule 21: 60S ribosomal protein L18a



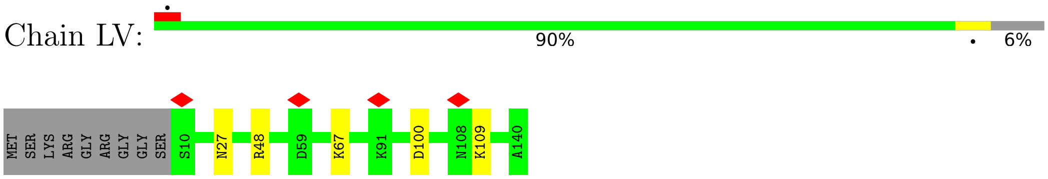
- Molecule 22: 60S ribosomal protein L21



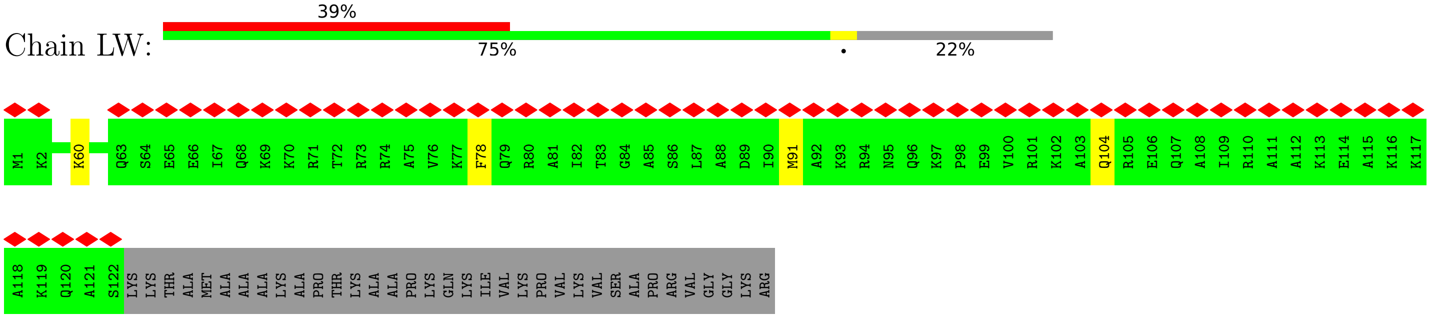
- Molecule 23: 60S ribosomal protein L22



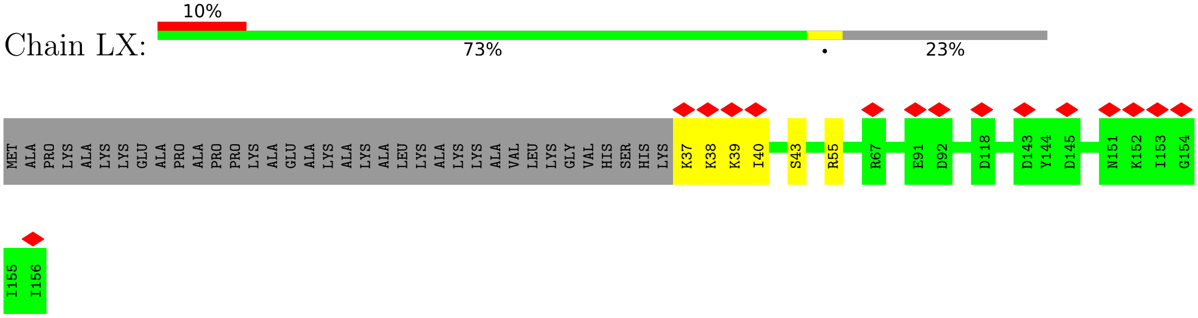
- Molecule 24: 60S ribosomal protein L23



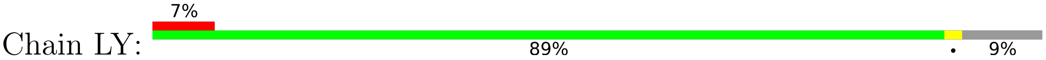
- Molecule 25: 60S ribosomal protein L24

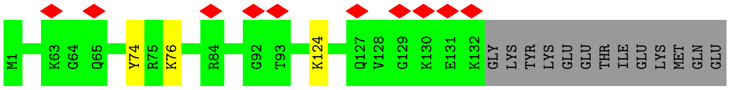


- Molecule 26: 60S ribosomal protein L23a



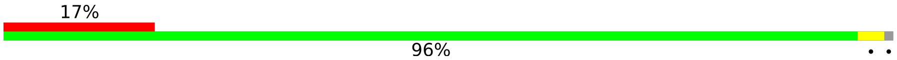
- Molecule 27: 60S ribosomal protein L26

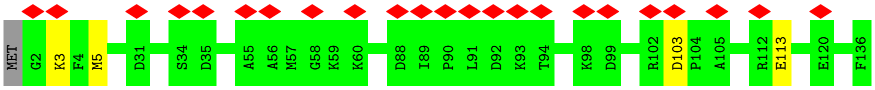




- Molecule 28: 60S ribosomal protein L27

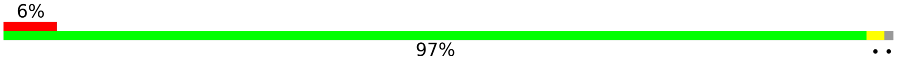
Chain LZ:

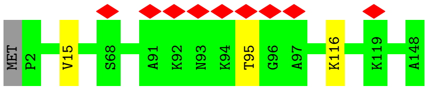




- Molecule 29: Large ribosomal subunit protein uL15

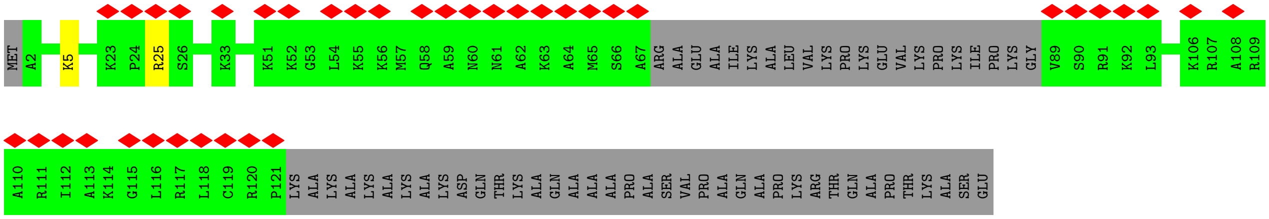
Chain La:





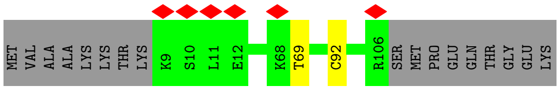
- Molecule 30: 60S ribosomal protein L29

Chain Lb:



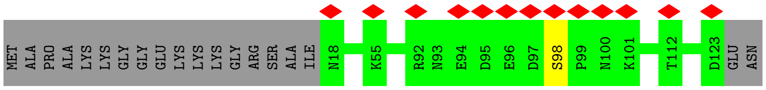
- Molecule 31: 60S ribosomal protein L30

Chain Lc:



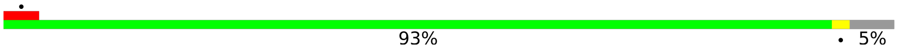
- Molecule 32: 60S ribosomal protein L31

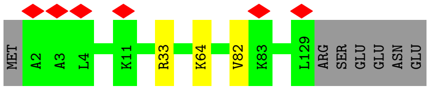
Chain Ld:



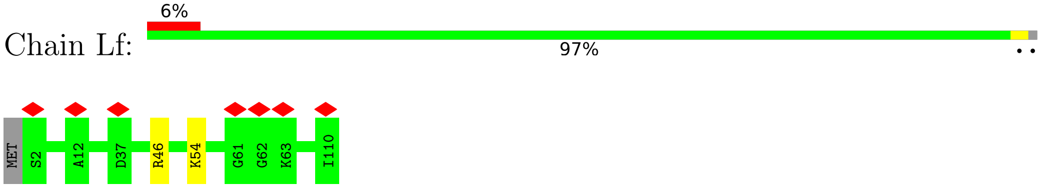
- Molecule 33: 60S ribosomal protein L32

Chain Le:

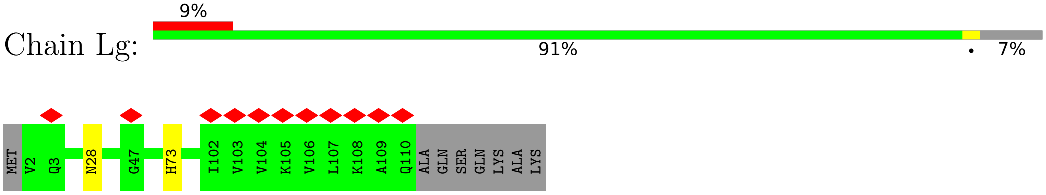




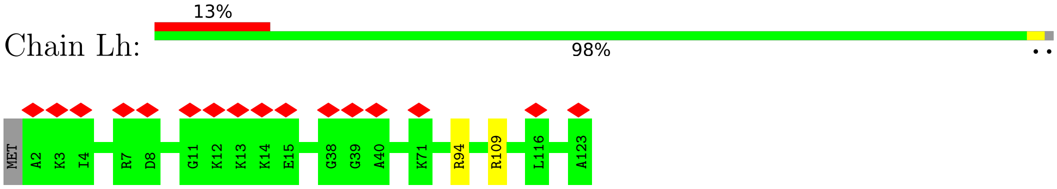
- Molecule 34: 60S ribosomal protein L35a



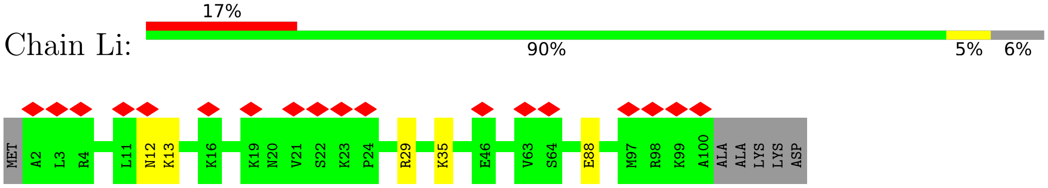
- Molecule 35: 60S ribosomal protein L34



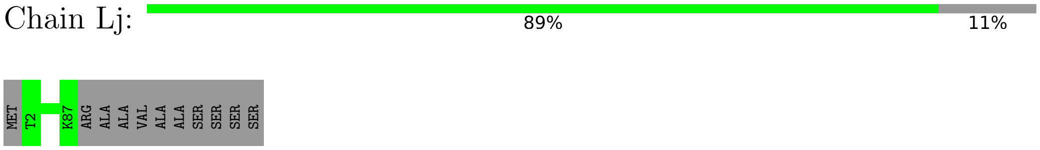
- Molecule 36: 60S ribosomal protein L35



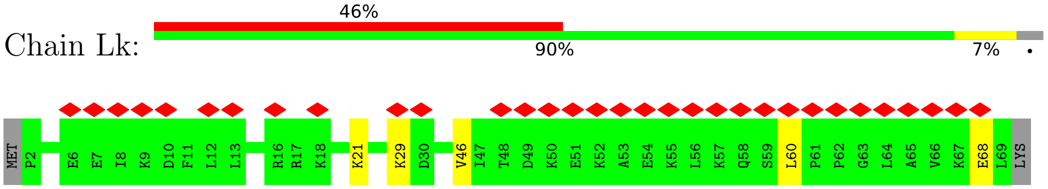
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37

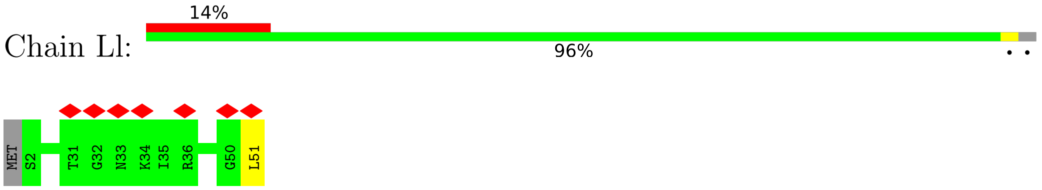


- Molecule 39: 60S ribosomal protein L38



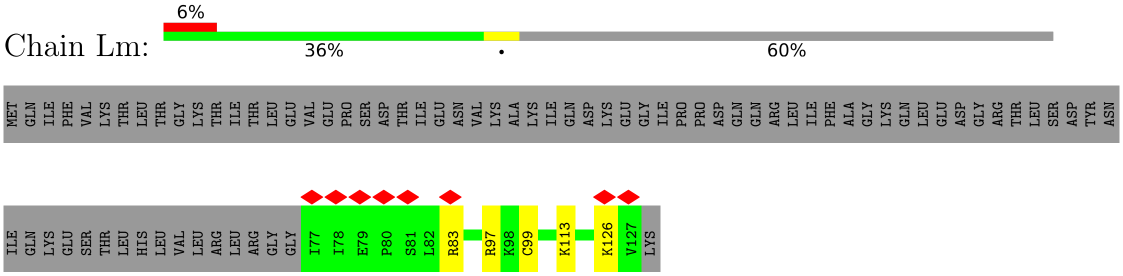
- Molecule 40: 60S ribosomal protein L39

Chain Ll:



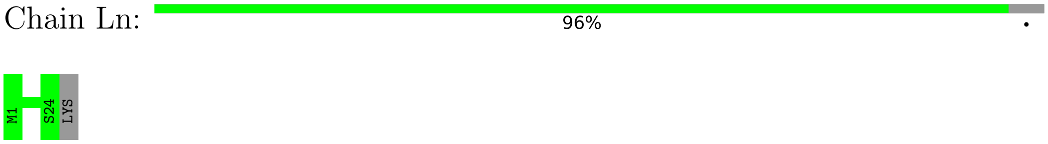
- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:



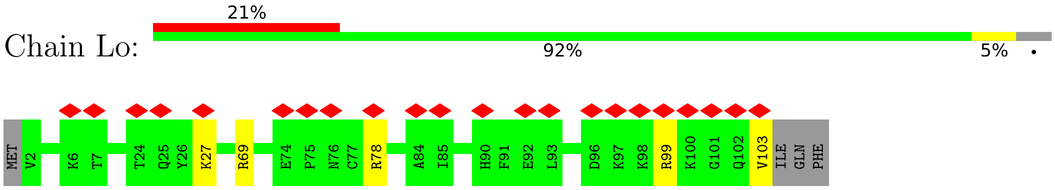
- Molecule 42: 60S ribosomal protein L41

Chain Ln:



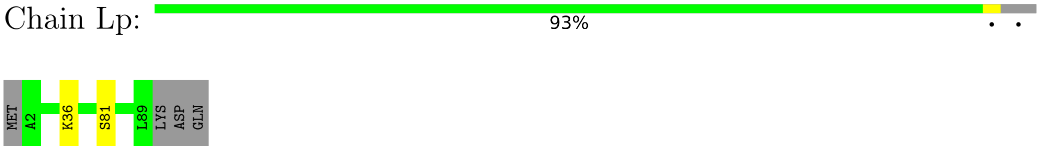
- Molecule 43: 60S ribosomal protein L36a

Chain Lo:



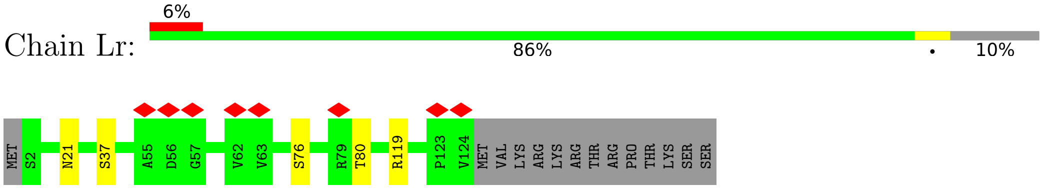
- Molecule 44: 60S ribosomal protein L37a

Chain Lp:



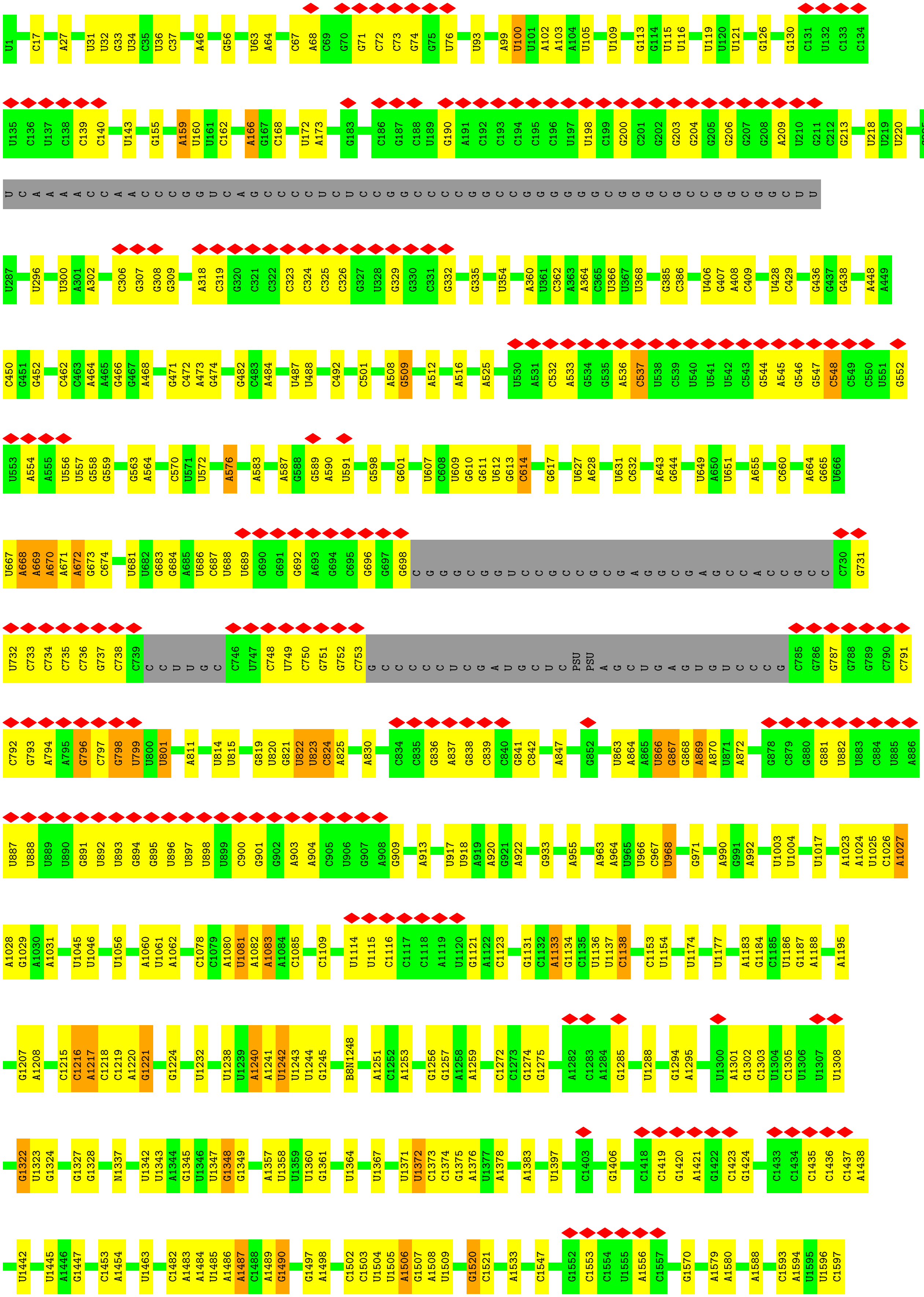
- Molecule 45: 60S ribosomal protein L28

Chain Lr:



- Molecule 46: 18S rRNA (1740-MER)

Chain S2: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U135 C136 U137 C138 C139 C140 U143 G155 A159 U160 U161 C162 A166 G167 C168 U172 A173 G183 C186 G187 C188 U189 G190 A191 C192 C193 C194 C195 C196 U197 U198 C199 G200 C201 G202 G203 G204 G205 G206 G207 G208 A209 U210 G211 C212 G213 U218 U219 U220 G225 A
U C A A A C C A A C C C G G U C A G C C C C U C U C C G G C C C C G G C C G G G G G C G G G C G C C G G C G G C U U
U287 U296 U300 A301 A302 C306 G307 G308 G309 A318 C319 G320 C321 C322 C323 C324 C325 C326 G327 U328 G329 G330 C331 G332 G335 U354 A360 U361 C362 A363 A364 C365 U366 U367 U368 G385 C386 U406 G407 A408 C409 U428 C429 G436 G437 G438 A448 A449
C450 G451 G452 C462 C463 A464 A465 G466 G467 A468 G471 C472 A473 G474 G482 C483 A484 U487 U488 C492 C501 A508 G509 A512 A516 A525 U530 A531 C532 A533 G534 G535 A536 C537 U538 C539 U540 U541 U542 C543 G544 A545 G546 G547 C548 C549 C550 U551 G552
U553 A554 A555 U556 U557 G558 G559 G563 A564 C570 U571 U572 A576 A583 A587 G588 G589 A590 U591 G598 G601 U607 C608 U609 G610 G611 U612 G613 C614 G617 U627 A628 U631 C632 A643 G644 U649 A650 U651 A655 C660 A664 G665 U666
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C792 G793 A794 A795 G796 C797 G798 U799 U800 U801 A811 U814 U815 G819 U820 G821 U822 U823 C824 A825 A830 C834 C835 G836 A837 G838 C839 C840 G841 C842 A847 G852 U863 A864 A865 U866 G867 G868 A869 A870 U871 A872 G878 C879 G880 G881 U882 U883 C884 U885 A886
U887 U888 U889 U890 G891 U892 U893 G894 G895 U896 U897 U898 U899 C900 G901 G902 A903 A904 C905 U906 G907 A908 G909 A913 U917 U918 A919 A920 G921 A922 G933 A955 A963 A964 U965 U966 C967 U968 G971 A990 G991 A992 U1003 U1004 U1017 A1023 A1024 U1025 C1026 A1027
A1028 G1029 A1030 A1031 U1045 U1046 U1056 A1060 U1061 A1062 C1078 C1079 A1080 U1081 A1082 A1083 A1084 C1085 C1109 U1114 U1115 C1116 C1117 C1118 A1119 U1120 G1121 A1122 C1123 G1131 C1132 A1133 G1134 C1135 U1136 U1137 C1138 C1153 U1154 U1174 U1177 A1183 G1184 C1185 U1186 G1187 A1188 A1195
G1207 A1208 C1215 C1216 A1217 C1218 C1219 A1220 G1221 G1224 U1232 U1238 U1239 A1240 A1241 U1242 U1243 U1244 G1245 B8N1248 A1251 C1252 A1253 G1256 G1257 A1258 A1259 C1272 C1273 G1274 G1275 A1282 C1283 A1284 G1285 U1288 G1294 A1295 U1300 A1301 G1302 C1303 U1304 C1305 U1306 U1307 U1308
G1322 U1323 G1324 G1327 G1328 N1337 U1342 U1343 A1344 G1345 U1346 U1347 G1348 G1349 A1357 U1358 U1359 U1360 G1361 U1364 U1367 U1371 U1372 C1373 C1374 G1375 A1376 U1377 A1378 A1383 U1397 C1403 G1406 C1418 C1419 G1420 A1421 G1422 C1423 G1424 C1433 C1434 C1435 C1436 C1437 A1438
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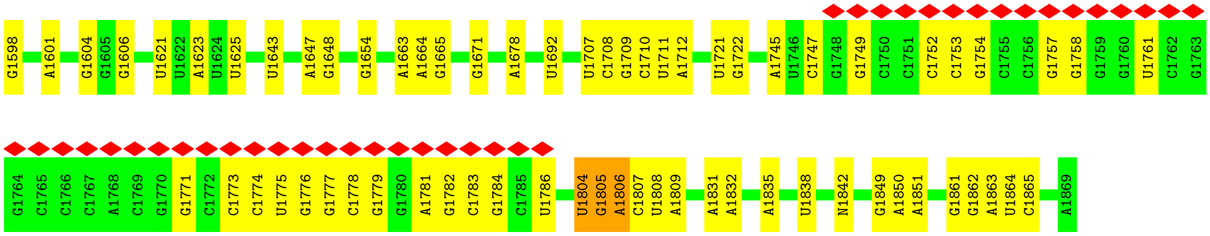
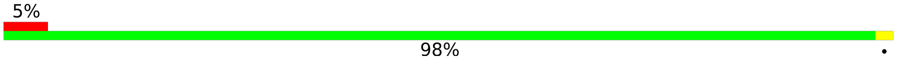
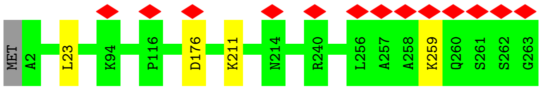


- Molecule 47: 40S ribosomal protein S4, X isoform

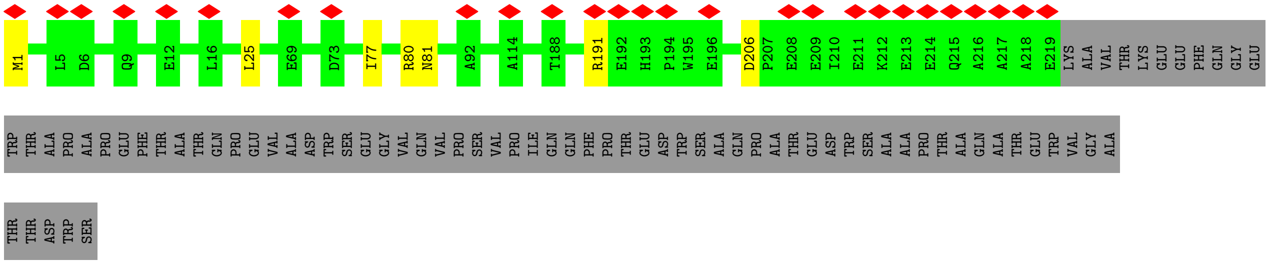
Chain SE:





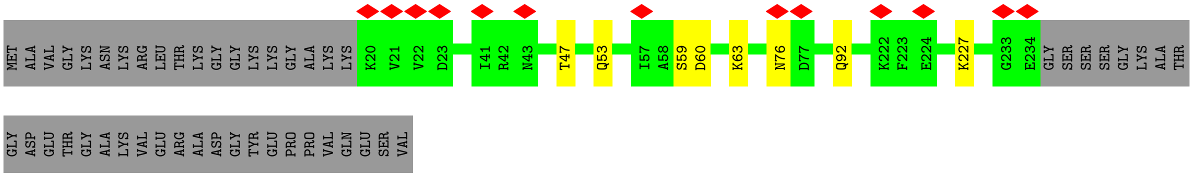
- Molecule 48: 40S ribosomal protein SA

Chain SA:



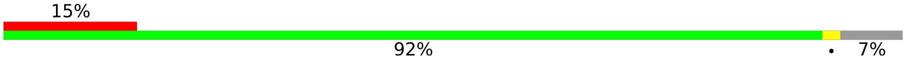
- Molecule 49: 40S ribosomal protein S3a

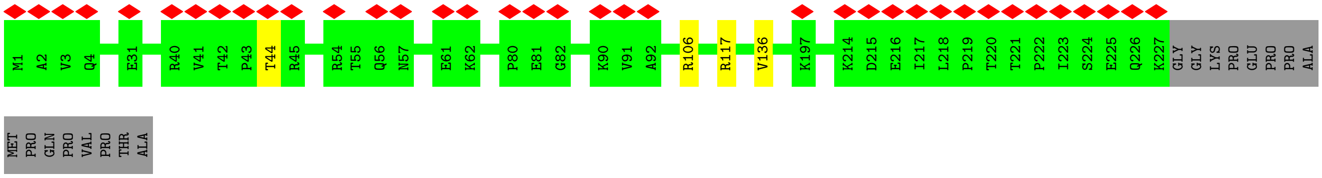
Chain SB:



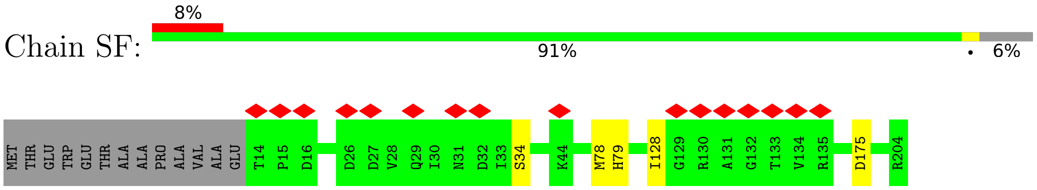
- Molecule 50: 40S ribosomal protein S3

Chain SD:

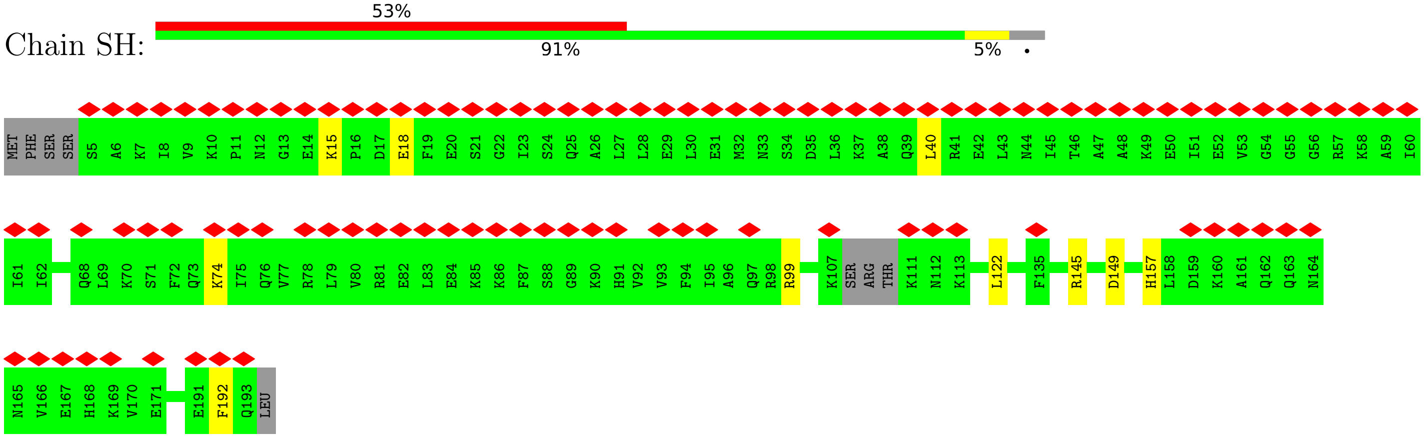




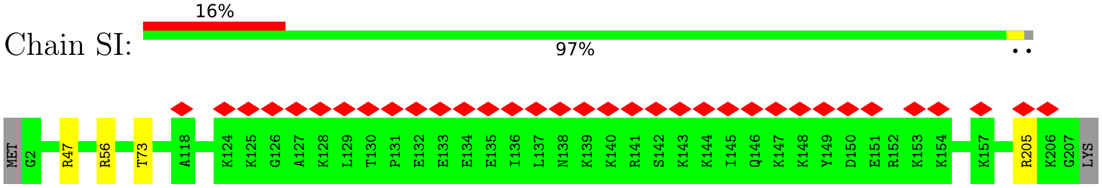
- Molecule 51: 40S ribosomal protein S5



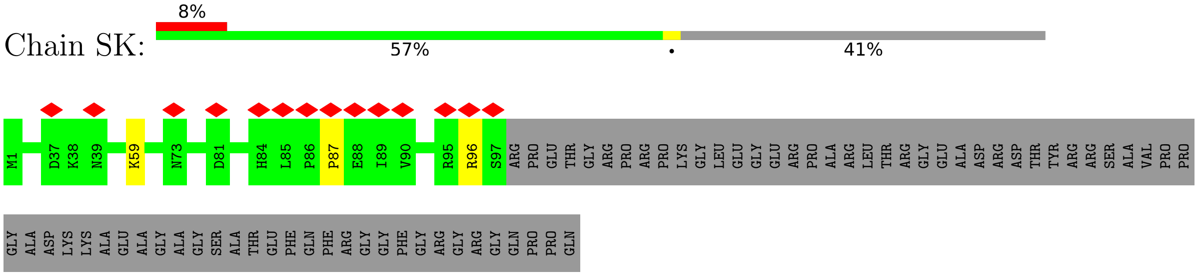
- Molecule 52: 40S ribosomal protein S7



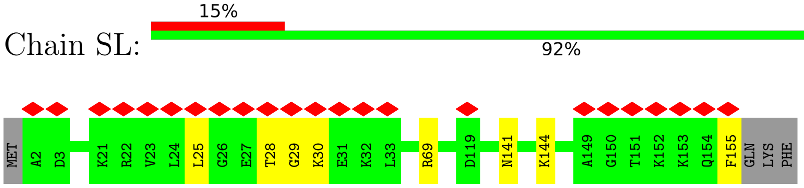
- Molecule 53: 40S ribosomal protein S8



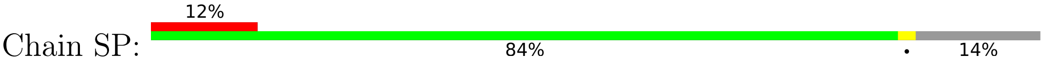
- Molecule 54: 40S ribosomal protein S10

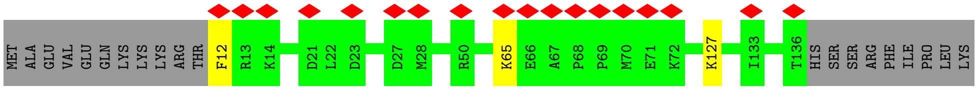


- Molecule 55: 40S ribosomal protein S11



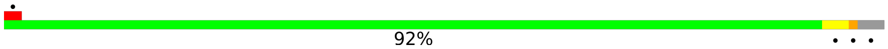
- Molecule 56: 40S ribosomal protein S15

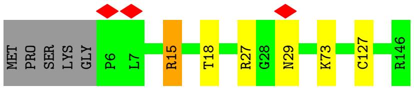




- Molecule 57: 40S ribosomal protein S16

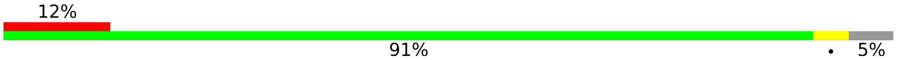
Chain SQ:

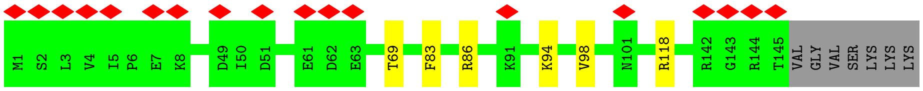




- Molecule 58: 40S ribosomal protein S18

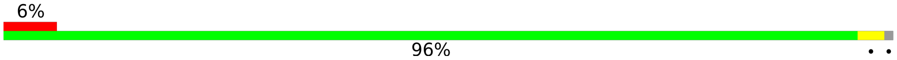
Chain SS:

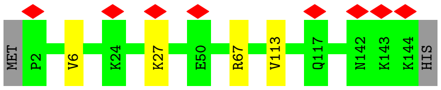




- Molecule 59: Small ribosomal subunit protein eS19

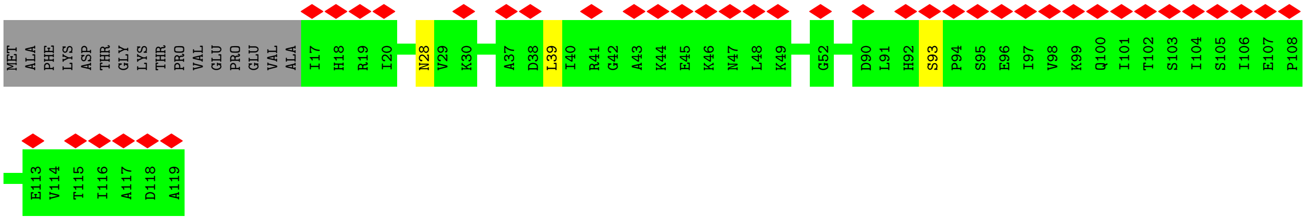
Chain ST:





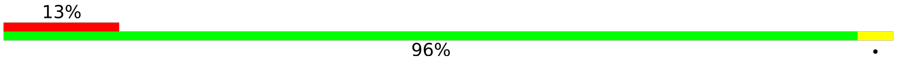
- Molecule 60: 40S ribosomal protein S20

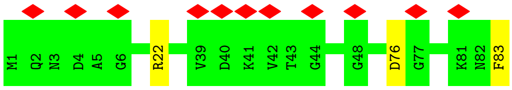
Chain SU:



- Molecule 61: 40S ribosomal protein S21

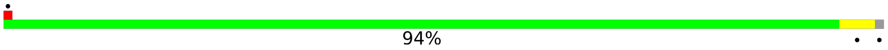
Chain SV:

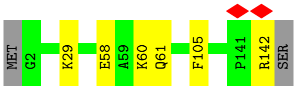




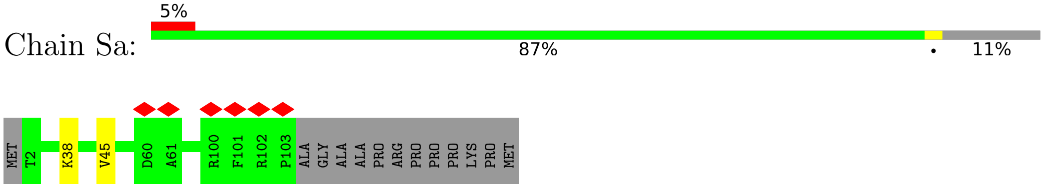
- Molecule 62: 40S ribosomal protein S23

Chain SX:

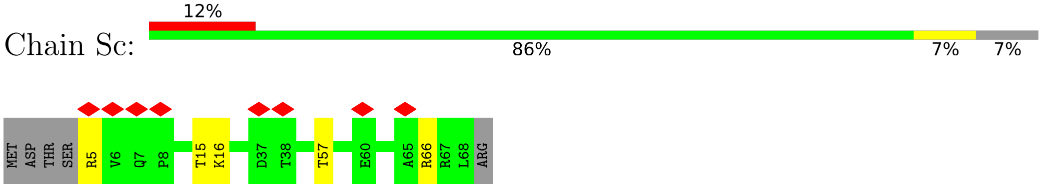




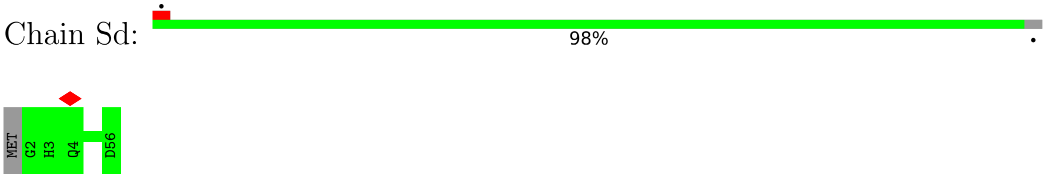
- Molecule 63: 40S ribosomal protein S26



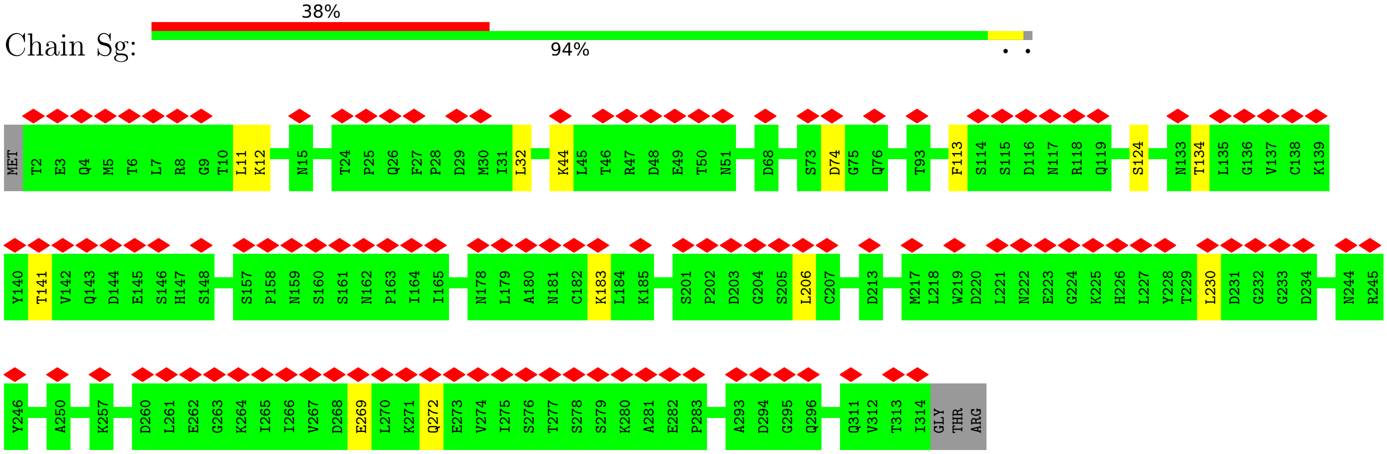
- Molecule 64: 40S ribosomal protein S28



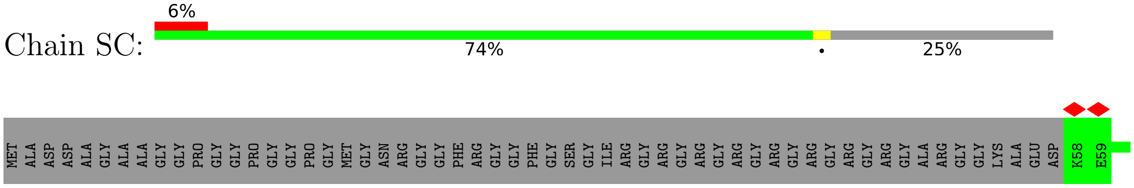
- Molecule 65: 40S ribosomal protein S29

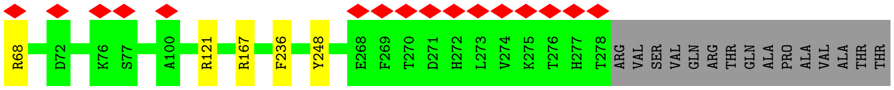


- Molecule 66: Receptor of activated protein C kinase 1



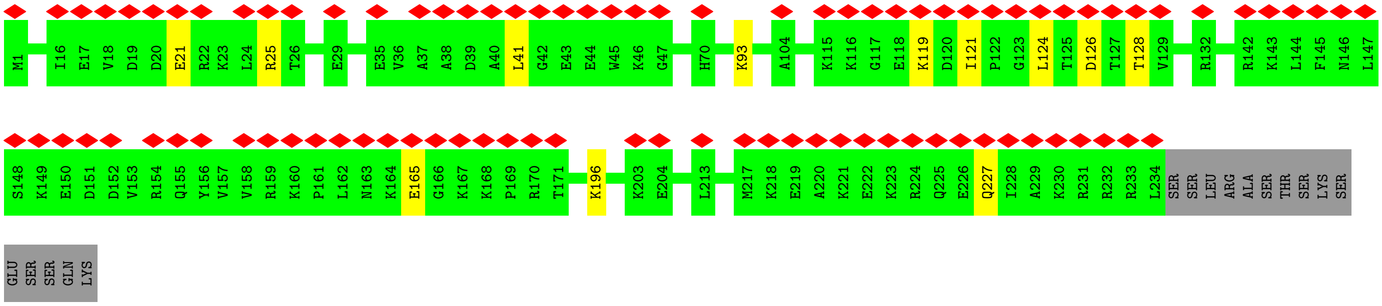
- Molecule 67: 40S ribosomal protein S2





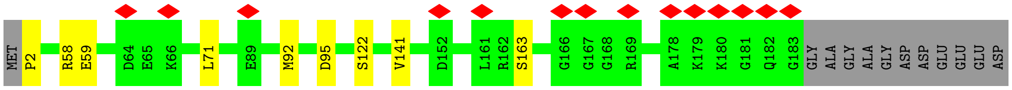
- Molecule 68: 40S ribosomal protein S6

Chain SG:



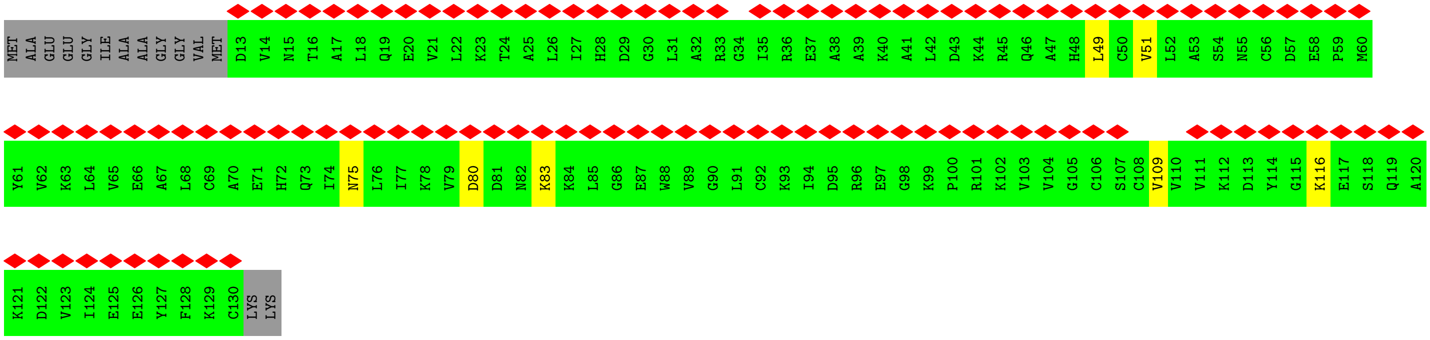
- Molecule 69: 40S ribosomal protein S9

Chain SJ:



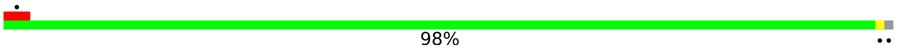
- Molecule 70: 40S ribosomal protein S12

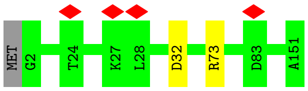
Chain SM:



- Molecule 71: 40S ribosomal protein S13

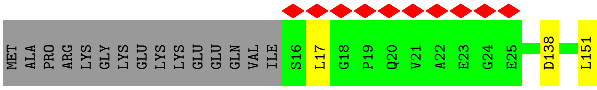
Chain SN:



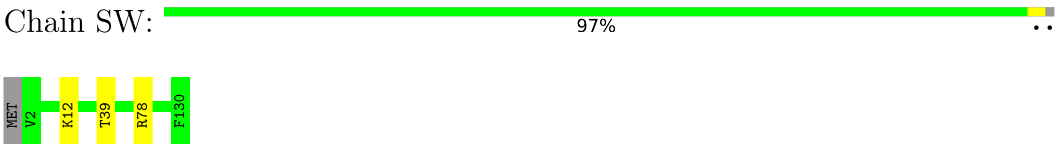


- Molecule 72: 40S ribosomal protein S14

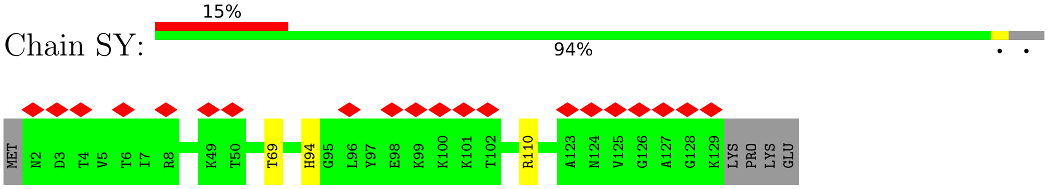
Chain SO:



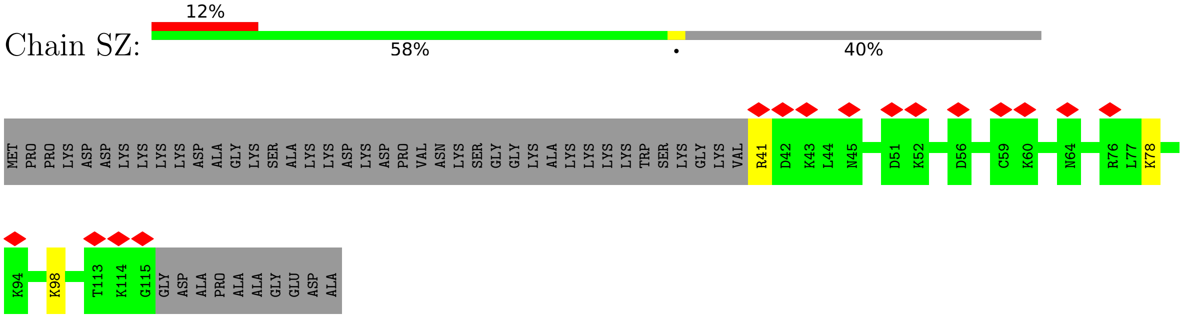
- Molecule 73: 40S ribosomal protein S15a



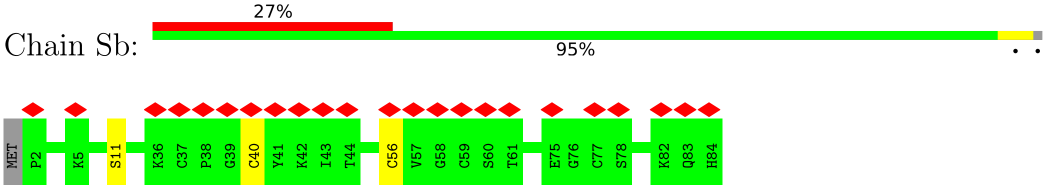
- Molecule 74: 40S ribosomal protein S24



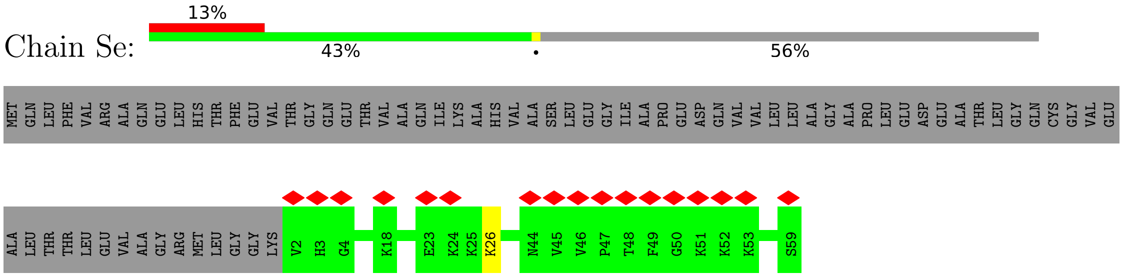
- Molecule 75: 40S ribosomal protein S25



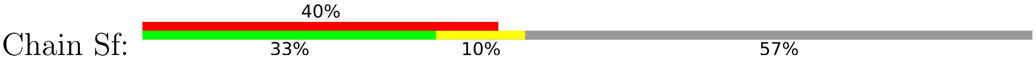
- Molecule 76: 40S ribosomal protein S27

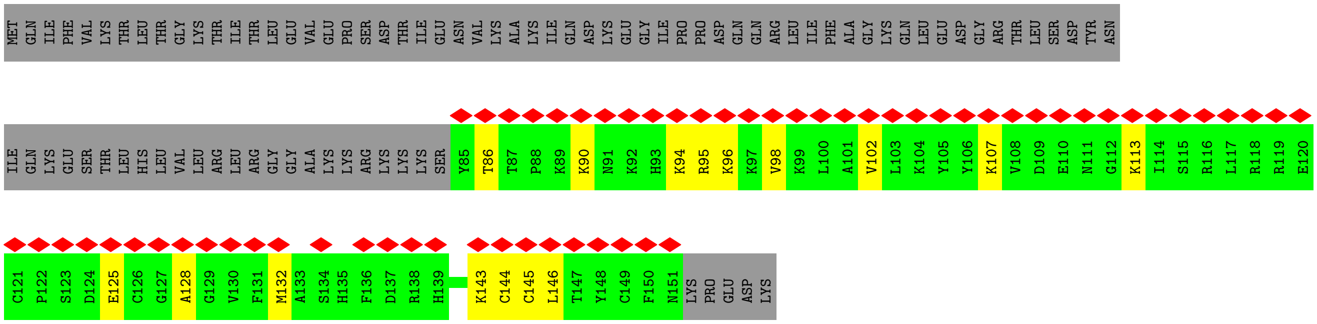


- Molecule 77: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



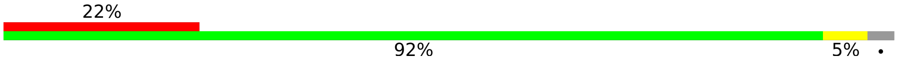
- Molecule 78: Ubiquitin-40S ribosomal protein S27a

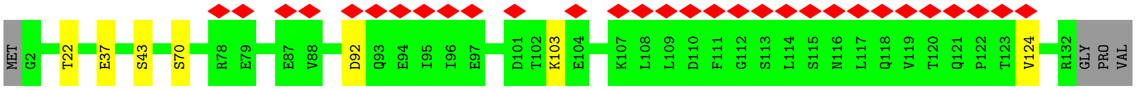




- Molecule 79: 40S ribosomal protein S17

Chain SR:





4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	382016	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, JEOL CRYO ARM 300	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{Å}^2$)	1.0, 1.0	Depositor
Minimum defocus (nm)	500, 1000	Depositor
Maximum defocus (nm)	1100, 2000	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	FEI FALCON IV (4k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.426	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0266	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, OMC, V5N, B8N, PSU, SPD, 1MA, UR3, A2M, MA6, 5MC, IAS, MG, 6MZ, 4AC, M7G, OMG, ZN, HIC, NMM, K, OMU

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	L5	0.43	0/86723	0.90	234/135219 (0.2%)
2	L7	0.41	0/2858	0.93	13/4455 (0.3%)
3	L8	0.41	0/3609	0.88	12/5623 (0.2%)
4	LA	0.32	0/1936	0.61	0/2596
5	LB	0.29	0/3294	0.54	0/4406
6	LC	0.26	0/2981	0.56	1/4002 (0.0%)
7	LD	0.28	0/2428	0.52	0/3252
8	LE	0.33	0/1942	0.55	0/2606
9	LF	0.27	0/1916	0.54	0/2553
10	LG	0.28	0/1971	0.53	0/2651
11	LH	0.26	0/1537	0.53	0/2066
12	LI	0.32	0/1753	0.55	0/2343
13	LJ	0.29	0/1433	0.56	0/1915
14	LL	0.27	0/1732	0.56	0/2315
15	LM	0.27	0/1161	0.52	0/1554
16	LN	0.28	0/1746	0.58	0/2338
17	LO	0.28	0/1682	0.55	0/2250
18	LP	0.28	0/1268	0.54	0/1701
19	LQ	0.27	0/1537	0.61	0/2052
20	LR	0.27	0/1582	0.59	0/2091
21	LS	0.29	0/1493	0.57	0/2003
22	LT	0.28	0/1326	0.53	0/1770
23	LU	0.25	0/839	0.52	0/1126
24	LV	0.32	0/993	0.56	0/1332
25	LW	0.29	0/1012	0.57	0/1342
26	LX	0.29	0/1002	0.53	0/1345
27	LY	0.28	0/1119	0.57	0/1488
28	LZ	0.29	0/1130	0.53	0/1507
29	La	0.27	0/1179	0.54	0/1573
30	Lb	0.25	0/821	0.54	0/1084
31	Lc	0.32	0/774	0.52	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Ld	0.28	0/894	0.57	0/1204
33	Le	0.29	0/1071	0.57	0/1429
34	Lf	0.30	0/895	0.58	0/1198
35	Lg	0.27	0/878	0.58	0/1170
36	Lh	0.26	0/1023	0.53	0/1351
37	Li	0.27	0/824	0.58	0/1090
38	Lj	0.29	0/720	0.60	0/952
39	Lk	0.26	0/565	0.50	0/750
40	Ll	0.26	0/454	0.57	0/599
41	Lm	0.32	0/425	0.54	0/564
42	Ln	0.29	0/231	0.73	0/294
43	Lo	0.28	0/858	0.56	0/1131
44	Lp	0.35	0/691	0.58	0/919
45	Lr	0.30	0/1002	0.60	0/1344
46	S2	0.46	0/39125	0.92	137/60957 (0.2%)
47	SE	0.27	0/2118	0.56	0/2849
48	SA	0.31	0/1764	0.51	0/2396
49	SB	0.27	0/1774	0.50	0/2373
50	SD	0.28	0/1793	0.53	0/2414
51	SF	0.25	0/1531	0.52	0/2059
52	SH	0.27	0/1519	0.51	0/2033
53	SI	0.29	0/1715	0.55	0/2287
54	SK	0.29	0/840	0.57	2/1133 (0.2%)
55	SL	0.34	0/1280	0.58	0/1712
56	SP	0.27	0/1047	0.52	0/1399
57	SQ	0.28	0/1142	0.55	0/1528
58	SS	0.25	0/1216	0.57	0/1628
59	ST	0.26	0/1119	0.49	0/1498
60	SU	0.25	0/827	0.56	0/1110
61	SV	0.28	0/643	0.53	0/860
62	SX	0.31	0/1116	0.56	0/1490
63	Sa	0.30	0/847	0.61	0/1135
64	Sc	0.29	0/508	0.65	0/680
65	Sd	0.27	0/470	0.57	0/623
66	Sg	0.25	0/2493	0.51	0/3394
67	SC	0.28	0/1764	0.50	0/2382
68	SG	0.29	0/1926	0.57	0/2563
69	SJ	0.27	0/1548	0.57	0/2066
70	SM	0.26	0/916	0.50	0/1233
71	SN	0.29	0/1232	0.52	0/1656
72	SO	0.29	0/1020	0.58	0/1366
73	SW	0.30	0/1051	0.56	0/1406
74	SY	0.27	0/1068	0.55	0/1418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
75	SZ	0.27	0/604	0.59	0/810
76	Sb	0.27	0/665	0.53	0/891
77	Se	0.26	0/465	0.58	0/612
78	Sf	0.38	0/560	0.56	0/745
79	SR	0.27	0/1078	0.54	0/1447
All	All	0.38	0/226092	0.79	399/331744 (0.1%)

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
8	LE	0	2
12	LI	0	2
14	LL	0	1
41	Lm	0	1
57	SQ	0	1
73	SW	0	1
All	All	0	8

There are no bond length outliers.

All (399) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	S2	609	PSU	P-O3'-C3'	-11.44	105.97	119.70
46	S2	1081	U	P-O3'-C3'	-11.42	105.99	119.70
1	L5	5010	PSU	P-O3'-C3'	-10.99	106.51	119.70
46	S2	798	G	P-O3'-C3'	-10.95	106.56	119.70
1	L5	513	U	P-O3'-C3'	-10.56	107.03	119.70
1	L5	1366	G	P-O3'-C3'	-10.46	107.15	119.70
3	L8	111	U	P-O3'-C3'	-10.40	107.22	119.70
2	L7	36	C	P-O3'-C3'	-10.33	107.30	119.70
1	L5	3730	PSU	P-O3'-C3'	-10.30	107.34	119.70
1	L5	4998	G	P-O3'-C3'	-10.22	107.43	119.70
1	L5	1454	G	P-O3'-C3'	-10.21	107.44	119.70
1	L5	4869	U	P-O3'-C3'	-10.17	107.50	119.70
1	L5	714	G	P-O3'-C3'	-10.09	107.59	119.70
46	S2	1808	U	P-O3'-C3'	-10.06	107.63	119.70
1	L5	4293	PSU	P-O3'-C3'	-9.99	107.71	119.70
1	L5	3764	PSU	P-O3'-C3'	-9.91	107.81	119.70
46	S2	968	U	P-O3'-C3'	-9.89	107.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4415	A	P-O3'-C3'	-9.84	107.89	119.70
3	L8	67	U	P-O3'-C3'	-9.69	108.07	119.70
46	S2	1804	OMU	P-O3'-C3'	-9.64	108.14	119.70
46	S2	672	A	P-O3'-C3'	-9.63	108.14	119.70
1	L5	4867	G	P-O3'-C3'	-9.61	108.17	119.70
1	L5	1741	G	P-O3'-C3'	-9.59	108.20	119.70
46	S2	1345	G	P-O3'-C3'	-9.53	108.26	119.70
1	L5	979	C	P-O3'-C3'	-9.53	108.27	119.70
3	L8	70	G	P-O3'-C3'	-9.53	108.27	119.70
1	L5	1742	A	P-O3'-C3'	-9.51	108.29	119.70
1	L5	1517	G	P-O3'-C3'	-9.50	108.30	119.70
2	L7	35	U	P-O3'-C3'	-9.50	108.31	119.70
54	SK	87	PRO	CA-N-CD	-9.47	98.24	111.50
1	L5	4412	C	P-O3'-C3'	-9.45	108.36	119.70
46	S2	501	C	C2-N1-C1'	9.41	129.15	118.80
46	S2	1216	C	P-O3'-C3'	-9.41	108.41	119.70
1	L5	730	G	P-O3'-C3'	-9.41	108.41	119.70
1	L5	4502	C	P-O3'-C3'	-9.33	108.51	119.70
1	L5	1368	A	P-O3'-C3'	-9.32	108.51	119.70
46	S2	1504	U	P-O3'-C3'	-9.31	108.52	119.70
1	L5	1456	U	P-O3'-C3'	-9.28	108.56	119.70
1	L5	1864	G	P-O3'-C3'	-9.20	108.66	119.70
46	S2	614	C	P-O3'-C3'	-9.20	108.66	119.70
1	L5	4417	C	P-O3'-C3'	-9.18	108.69	119.70
1	L5	2775	C	P-O3'-C3'	-9.16	108.71	119.70
1	L5	4532	PSU	P-O3'-C3'	-9.14	108.74	119.70
46	S2	1807	C	P-O3'-C3'	-9.12	108.75	119.70
1	L5	4597	U	P-O3'-C3'	-9.12	108.75	119.70
1	L5	4082	G	P-O3'-C3'	-9.11	108.77	119.70
1	L5	1863	U	P-O3'-C3'	-9.07	108.81	119.70
46	S2	799	U	P-O3'-C3'	-9.06	108.82	119.70
46	S2	1218	C	P-O3'-C3'	-9.06	108.83	119.70
2	L7	31	G	P-O3'-C3'	-9.05	108.84	119.70
46	S2	610	G	P-O3'-C3'	-9.05	108.84	119.70
1	L5	1453	G	P-O3'-C3'	-9.03	108.86	119.70
1	L5	4080	C	P-O3'-C3'	-8.98	108.92	119.70
1	L5	3814	U	P-O3'-C3'	-8.98	108.92	119.70
1	L5	4500	PSU	P-O3'-C3'	-8.97	108.93	119.70
1	L5	1365	C	P-O3'-C3'	-8.96	108.95	119.70
1	L5	1364	U	P-O3'-C3'	-8.94	108.97	119.70
1	L5	4414	A	P-O3'-C3'	-8.92	108.99	119.70
46	S2	820	U	P-O3'-C3'	-8.90	109.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L7	32	A	P-O3'-C3'	-8.89	109.03	119.70
46	S2	867	OMG	P-O3'-C3'	-8.86	109.07	119.70
1	L5	4297	G	P-O3'-C3'	-8.85	109.09	119.70
1	L5	1739	G	P-O3'-C3'	-8.83	109.10	119.70
2	L7	33	U	P-O3'-C3'	-8.80	109.14	119.70
1	L5	3908	A	P-O3'-C3'	-8.78	109.17	119.70
46	S2	1503	C	P-O3'-C3'	-8.68	109.29	119.70
1	L5	485	C	C2-N1-C1'	8.65	128.31	118.80
1	L5	4452	U	P-O3'-C3'	-8.65	109.32	119.70
3	L8	107	C	P-O3'-C3'	-8.64	109.33	119.70
46	S2	1324	G	P-O3'-C3'	-8.62	109.35	119.70
46	S2	801	PSU	P-O3'-C3'	-8.62	109.35	119.70
46	S2	1322	G	P-O3'-C3'	-8.61	109.37	119.70
46	S2	868	G	P-O3'-C3'	-8.60	109.38	119.70
46	S2	1711	U	P-O3'-C3'	-8.58	109.40	119.70
1	L5	3720	G	P-O3'-C3'	-8.58	109.41	119.70
46	S2	1594	A	P-O3'-C3'	-8.55	109.44	119.70
46	S2	1507	G	P-O3'-C3'	-8.51	109.49	119.70
46	S2	1485	U	P-O3'-C3'	-8.51	109.49	119.70
46	S2	1376	A	P-O3'-C3'	-8.50	109.50	119.70
1	L5	1882	U	P-O3'-C3'	-8.48	109.52	119.70
1	L5	374	G	P-O3'-C3'	-8.48	109.53	119.70
46	S2	34	PSU	P-O3'-C3'	-8.46	109.55	119.70
46	S2	1357	A	P-O3'-C3'	-8.46	109.55	119.70
1	L5	1737	A	P-O3'-C3'	-8.43	109.59	119.70
1	L5	3724	A2M	P-O3'-C3'	-8.43	109.59	119.70
1	L5	4081	G	P-O3'-C3'	-8.41	109.61	119.70
46	S2	686	PSU	P-O3'-C3'	-8.40	109.61	119.70
46	S2	31	U	P-O3'-C3'	-8.40	109.62	119.70
46	S2	613	G	P-O3'-C3'	-8.39	109.63	119.70
1	L5	3762	PSU	P-O3'-C3'	-8.36	109.67	119.70
1	L5	2629	C	P-O3'-C3'	-8.31	109.73	119.70
1	L5	4598	C	P-O3'-C3'	-8.31	109.73	119.70
1	L5	2047	A	P-O3'-C3'	-8.30	109.74	119.70
46	S2	1806	A	P-O3'-C3'	-8.29	109.75	119.70
46	S2	1024	A	P-O3'-C3'	-8.28	109.76	119.70
46	S2	1323	U	P-O3'-C3'	-8.26	109.79	119.70
1	L5	2771	G	P-O3'-C3'	-8.24	109.81	119.70
1	L5	976	G	P-O3'-C3'	-8.24	109.81	119.70
1	L5	417	G	O4'-C1'-N9	8.21	114.77	108.20
1	L5	4416	G	P-O3'-C3'	-8.17	109.90	119.70
46	S2	669	A	P-O3'-C3'	-8.16	109.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	2770	C	P-O3'-C3'	-8.14	109.93	119.70
46	S2	1375	G	P-O3'-C3'	-8.14	109.93	119.70
46	S2	967	C	P-O3'-C3'	-8.13	109.94	119.70
1	L5	2772	C	P-O3'-C3'	-8.13	109.94	119.70
46	S2	863	PSU	P-O3'-C3'	-8.13	109.95	119.70
1	L5	1883	G	P-O3'-C3'	-8.11	109.97	119.70
1	L5	4577	U	P-O3'-C3'	-8.09	110.00	119.70
1	L5	4501	U	P-O3'-C3'	-8.08	110.00	119.70
2	L7	34	C	P-O3'-C3'	-8.07	110.01	119.70
1	L5	512	U	P-O3'-C3'	-8.07	110.02	119.70
1	L5	4594	U	P-O3'-C3'	-8.01	110.09	119.70
1	L5	514	U	P-O3'-C3'	-8.00	110.10	119.70
1	L5	4873	G	P-O3'-C3'	-7.99	110.11	119.70
46	S2	822	PSU	P-O3'-C3'	-7.97	110.13	119.70
1	L5	715	G	P-O3'-C3'	-7.95	110.16	119.70
1	L5	4448	G	P-O3'-C3'	-7.94	110.18	119.70
46	S2	1373	C	P-O3'-C3'	-7.94	110.18	119.70
1	L5	4483	C	P-O3'-C3'	-7.92	110.20	119.70
1	L5	4596	C	P-O3'-C3'	-7.91	110.20	119.70
46	S2	1709	G	P-O3'-C3'	-7.90	110.22	119.70
1	L5	4413	C	P-O3'-C3'	-7.90	110.22	119.70
46	S2	798	G	OP2-P-O3'	7.89	122.56	105.20
46	S2	824	C	P-O3'-C3'	-7.89	110.23	119.70
46	S2	1502	C	P-O3'-C3'	-7.85	110.28	119.70
1	L5	510	U	P-O3'-C3'	-7.85	110.28	119.70
46	S2	1245	G	P-O3'-C3'	-7.85	110.28	119.70
1	L5	3722	G	P-O3'-C3'	-7.85	110.28	119.70
1	L5	4595	G	P-O3'-C3'	-7.83	110.30	119.70
1	L5	5007	A	P-O3'-C3'	-7.82	110.32	119.70
1	L5	3731	C	P-O3'-C3'	-7.82	110.32	119.70
1	L5	1839	U	P-O3'-C3'	-7.79	110.35	119.70
46	S2	1593	C	P-O3'-C3'	-7.76	110.39	119.70
46	S2	1372	U	P-O3'-C3'	-7.73	110.42	119.70
1	L5	4669	A	P-O3'-C3'	-7.72	110.44	119.70
1	L5	4870	G	P-O3'-C3'	-7.72	110.44	119.70
3	L8	69	PSU	P-O3'-C3'	-7.71	110.45	119.70
1	L5	4576	PSU	P-O3'-C3'	-7.71	110.45	119.70
3	L8	112	G	P-O3'-C3'	-7.71	110.45	119.70
1	L5	2774	C	P-O3'-C3'	-7.71	110.45	119.70
1	L5	980	U	P-O3'-C3'	-7.70	110.46	119.70
1	L5	3765	G	P-O3'-C3'	-7.69	110.47	119.70
46	S2	1134	G	P-O3'-C3'	-7.69	110.47	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	35	U	P-O3'-C3'	-7.68	110.48	119.70
46	S2	1244	PSU	P-O3'-C3'	-7.67	110.49	119.70
1	L5	3721	U	P-O3'-C3'	-7.66	110.50	119.70
46	S2	1184	G	P-O3'-C3'	-7.64	110.53	119.70
1	L5	4083	U	P-O3'-C3'	-7.62	110.56	119.70
1	L5	1738	A	P-O3'-C3'	-7.62	110.56	119.70
1	L5	4480	A	P-O3'-C3'	-7.62	110.56	119.70
1	L5	977	C	P-O3'-C3'	-7.61	110.57	119.70
1	L5	1519	C	P-O3'-C3'	-7.61	110.57	119.70
1	L5	3766	A	P-O3'-C3'	-7.58	110.61	119.70
2	L7	105	C	P-O3'-C3'	-7.58	110.61	119.70
46	S2	1188	A	P-O3'-C3'	-7.58	110.61	119.70
1	L5	1455	G	P-O3'-C3'	-7.57	110.61	119.70
3	L8	66	A	P-O3'-C3'	-7.56	110.62	119.70
46	S2	611	G	P-O3'-C3'	-7.56	110.63	119.70
46	S2	1506	A	P-O3'-C3'	-7.54	110.65	119.70
1	L5	4482	U	P-O3'-C3'	-7.53	110.66	119.70
46	S2	1482	C	P-O3'-C3'	-7.53	110.66	119.70
46	S2	1598	G	P-O3'-C3'	-7.52	110.68	119.70
1	L5	2632	PSU	P-O3'-C3'	-7.52	110.68	119.70
1	L5	1866	U	P-O3'-C3'	-7.51	110.68	119.70
1	L5	4484	A	P-O3'-C3'	-7.51	110.68	119.70
46	S2	32	U	P-O3'-C3'	-7.51	110.69	119.70
46	S2	1486	A	P-O3'-C3'	-7.50	110.70	119.70
2	L7	101	A	P-O3'-C3'	-7.49	110.71	119.70
46	S2	797	C	P-O3'-C3'	-7.48	110.72	119.70
1	L5	728	U	P-O3'-C3'	-7.47	110.73	119.70
1	L5	1841	C	P-O3'-C3'	-7.47	110.74	119.70
1	L5	2051	C	P-O3'-C3'	-7.46	110.74	119.70
1	L5	31	U	P-O3'-C3'	-7.45	110.76	119.70
46	S2	1712	A	P-O3'-C3'	-7.45	110.76	119.70
1	L5	4296	PSU	P-O3'-C3'	-7.43	110.78	119.70
1	L5	727	C	P-O3'-C3'	-7.40	110.83	119.70
46	S2	1186	PSU	P-O3'-C3'	-7.40	110.82	119.70
46	S2	1136	PSU	P-O3'-C3'	-7.39	110.83	119.70
46	S2	1133	A	P-O3'-C3'	-7.38	110.84	119.70
1	L5	3909	C	P-O3'-C3'	-7.36	110.87	119.70
46	S2	501	C	N1-C2-O2	7.34	123.30	118.90
1	L5	3637	PSU	P-O3'-C3'	-7.33	110.90	119.70
1	L5	713	C	P-O3'-C3'	-7.33	110.91	119.70
1	L5	4485	C	P-O3'-C3'	-7.33	110.91	119.70
1	L5	4999	G	P-O3'-C3'	-7.33	110.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	S2	36	PSU	P-O3'-C3'	-7.33	110.91	119.70
1	L5	1514	U	P-O3'-C3'	-7.32	110.92	119.70
1	L5	975	C	P-O3'-C3'	-7.30	110.93	119.70
1	L5	4673	PSU	P-O3'-C3'	-7.29	110.95	119.70
1	L5	5002	U	P-O3'-C3'	-7.29	110.95	119.70
1	L5	716	C	P-O3'-C3'	-7.28	110.96	119.70
46	S2	966	PSU	P-O3'-C3'	-7.28	110.96	119.70
46	S2	1240	A	P-O3'-C3'	-7.26	110.99	119.70
2	L7	104	C	P-O3'-C3'	-7.24	111.01	119.70
46	S2	796	G	P-O3'-C3'	-7.22	111.04	119.70
1	L5	978	G	P-O3'-C3'	-7.21	111.04	119.70
46	S2	1487	A	P-O3'-C3'	-7.20	111.07	119.70
46	S2	684	G	P-O3'-C3'	-7.19	111.07	119.70
1	L5	4668	U	P-O3'-C3'	-7.19	111.07	119.70
1	L5	1515	A	P-O3'-C3'	-7.19	111.07	119.70
46	S2	674	C	P-O3'-C3'	-7.18	111.08	119.70
1	L5	1885	G	P-O3'-C3'	-7.17	111.09	119.70
3	L8	71	A	P-O3'-C3'	-7.16	111.11	119.70
46	S2	1349	G	P-O3'-C3'	-7.16	111.11	119.70
1	L5	32	G	P-O3'-C3'	-7.14	111.13	119.70
1	L5	4084	G	P-O3'-C3'	-7.14	111.13	119.70
1	L5	4333	C	P-O3'-C3'	-7.13	111.14	119.70
46	S2	1027	A	P-O3'-C3'	-7.13	111.15	119.70
2	L7	100	A	P-O3'-C3'	-7.12	111.15	119.70
1	L5	511	C	P-O3'-C3'	-7.10	111.18	119.70
1	L5	712	C	P-O3'-C3'	-7.09	111.19	119.70
46	S2	1137	U	P-O3'-C3'	-7.09	111.19	119.70
46	S2	1596	PSU	P-O3'-C3'	-7.07	111.22	119.70
1	L5	233	U	N1-C2-O2	7.04	127.73	122.80
46	S2	1083	A	P-O3'-C3'	-7.03	111.26	119.70
1	L5	2710	C	N3-C2-O2	-7.03	116.98	121.90
1	L5	130	C	N3-C2-O2	-7.02	116.98	121.90
1	L5	2710	C	C2-N1-C1'	7.01	126.51	118.80
46	S2	1505	U	P-O3'-C3'	-7.01	111.29	119.70
1	L5	2773	G	P-O3'-C3'	-7.01	111.29	119.70
1	L5	731	G	P-O3'-C3'	-7.01	111.29	119.70
1	L5	3647	A	P-O3'-C3'	-6.97	111.33	119.70
1	L5	1840	G	P-O3'-C3'	-6.96	111.35	119.70
1	L5	3772	U	P-O3'-C3'	-6.95	111.37	119.70
46	S2	1484	A	P-O3'-C3'	-6.93	111.38	119.70
1	L5	2630	U	P-O3'-C3'	-6.89	111.43	119.70
1	L5	3725	G	P-O3'-C3'	-6.89	111.43	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1552	G	O4'-C1'-N9	6.89	113.71	108.20
1	L5	3688	U	P-O3'-C3'	-6.87	111.46	119.70
46	S2	501	C	C6-N1-C1'	-6.85	112.58	120.80
1	L5	373	G	P-O3'-C3'	-6.83	111.50	119.70
1	L5	1361	G	P-O3'-C3'	-6.83	111.50	119.70
1	L5	4599	A	P-O3'-C3'	-6.82	111.52	119.70
1	L5	2633	U	P-O3'-C3'	-6.80	111.53	119.70
1	L5	2710	C	N1-C2-O2	6.80	122.98	118.90
1	L5	5008	C	P-O3'-C3'	-6.80	111.55	119.70
1	L5	233	U	N3-C2-O2	-6.79	117.44	122.20
1	L5	4874	A	P-O3'-C3'	-6.79	111.55	119.70
1	L5	4530	UR3	P-O3'-C3'	-6.76	111.58	119.70
1	L5	3639	PSU	P-O3'-C3'	-6.74	111.61	119.70
46	S2	864	A	P-O3'-C3'	-6.73	111.62	119.70
46	S2	687	C	P-O3'-C3'	-6.70	111.66	119.70
46	S2	1219	C	P-O3'-C3'	-6.67	111.69	119.70
1	L5	4573	G	P-O3'-C3'	-6.67	111.70	119.70
1	L5	4533	A	P-O3'-C3'	-6.66	111.71	119.70
1	L5	5001	PSU	P-O3'-C3'	-6.64	111.73	119.70
46	S2	1348	G	P-O3'-C3'	-6.64	111.73	119.70
1	L5	33	A	P-O3'-C3'	-6.63	111.74	119.70
1	L5	2634	C	P-O3'-C3'	-6.62	111.75	119.70
1	L5	3727	A	P-O3'-C3'	-6.62	111.75	119.70
46	S2	102	A	P-O3'-C3'	-6.60	111.78	119.70
1	L5	233	U	C2-N1-C1'	6.60	125.62	117.70
1	L5	4872	G	P-O3'-C3'	-6.58	111.81	119.70
46	S2	670	A	P-O3'-C3'	-6.56	111.83	119.70
1	L5	1740	C	P-O3'-C3'	-6.53	111.87	119.70
46	S2	1453	C	C2-N1-C1'	6.51	125.97	118.80
1	L5	3911	C	P-O3'-C3'	-6.49	111.91	119.70
46	S2	1453	C	N1-C2-O2	6.49	122.79	118.90
1	L5	4871	C	P-O3'-C3'	-6.47	111.94	119.70
2	L7	103	A	P-O3'-C3'	-6.46	111.94	119.70
1	L5	375	G	P-O3'-C3'	-6.45	111.97	119.70
46	S2	1220	A	P-O3'-C3'	-6.44	111.97	119.70
46	S2	1029	G	P-O3'-C3'	-6.44	111.97	119.70
1	L5	3783	A	P-O3'-C3'	-6.43	111.99	119.70
46	S2	1187	G	P-O3'-C3'	-6.42	111.99	119.70
46	S2	964	A	P-O3'-C3'	-6.40	112.02	119.70
1	L5	2710	C	C6-N1-C2	-6.40	117.74	120.30
1	L5	1838	A	P-O3'-C3'	-6.39	112.03	119.70
1	L5	3820	G	P-O3'-C3'	-6.38	112.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	509	A	P-O3'-C3'	-6.38	112.05	119.70
46	S2	100	PSU	P-O3'-C3'	-6.37	112.05	119.70
1	L5	3687	A	P-O3'-C3'	-6.37	112.06	119.70
1	L5	1837	A	P-O3'-C3'	-6.37	112.06	119.70
1	L5	2050	G	P-O3'-C3'	-6.37	112.06	119.70
1	L5	1865	G	P-O3'-C3'	-6.36	112.07	119.70
1	L5	4294	C	P-O3'-C3'	-6.33	112.10	119.70
46	S2	1138	C	P-O3'-C3'	-6.33	112.11	119.70
1	L5	3816	A	P-O3'-C3'	-6.33	112.11	119.70
1	L5	369	G	P-O3'-C3'	-6.29	112.15	119.70
1	L5	5003	U	P-O3'-C3'	-6.29	112.15	119.70
1	L5	3809	G	O4'-C1'-N9	6.28	113.23	108.20
1	L5	5012	G	P-O3'-C3'	-6.28	112.16	119.70
1	L5	4337	C	P-O3'-C3'	-6.28	112.17	119.70
46	S2	1221	G	P-O3'-C3'	-6.27	112.17	119.70
1	L5	2048	U	P-O3'-C3'	-6.27	112.18	119.70
46	S2	1078	C	P-O3'-C3'	-6.21	112.25	119.70
1	L5	5011	A	P-O3'-C3'	-6.19	112.27	119.70
1	L5	4450	U	P-O3'-C3'	-6.18	112.28	119.70
1	L5	3690	U	P-O3'-C3'	-6.17	112.30	119.70
1	L5	4332	C	P-O3'-C3'	-6.17	112.29	119.70
3	L8	110	U	P-O3'-C3'	-6.17	112.30	119.70
1	L5	3773	U	P-O3'-C3'	-6.10	112.38	119.70
1	L5	3815	G	P-O3'-C3'	-6.09	112.40	119.70
1	L5	4496	A	P-O3'-C3'	-6.07	112.42	119.70
2	L7	102	U	P-O3'-C3'	-6.07	112.42	119.70
1	L5	485	C	C6-N1-C1'	-6.05	113.54	120.80
46	S2	1028	A	P-O3'-C3'	-6.05	112.44	119.70
46	S2	1080	A	P-O3'-C3'	-6.04	112.46	119.70
1	L5	1369	C	P-O3'-C3'	-5.99	112.51	119.70
46	S2	1026	C	P-O3'-C3'	-5.99	112.52	119.70
46	S2	1597	C	P-O3'-C3'	-5.97	112.53	119.70
3	L8	108	A	P-O3'-C3'	-5.95	112.56	119.70
1	L5	717	U	P-O3'-C3'	-5.92	112.59	119.70
1	L5	4481	U	P-O3'-C3'	-5.88	112.64	119.70
1	L5	3906	A	P-O3'-C3'	-5.88	112.64	119.70
46	S2	559	G	O4'-C1'-N9	5.87	112.90	108.20
46	S2	1374	C	P-O3'-C3'	-5.87	112.65	119.70
46	S2	665	G	P-O3'-C3'	-5.87	112.66	119.70
46	S2	1707	U	P-O3'-C3'	-5.87	112.66	119.70
1	L5	2628	U	P-O3'-C3'	-5.85	112.68	119.70
46	S2	1082	A	P-O3'-C3'	-5.84	112.69	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SK	87	PRO	N-CD-CG	-5.82	94.47	103.20
1	L5	1868	A	P-O3'-C3'	-5.81	112.73	119.70
1	L5	4085	A	P-O3'-C3'	-5.81	112.73	119.70
1	L5	3728	A	P-O3'-C3'	-5.79	112.75	119.70
46	S2	825	A	P-O3'-C3'	-5.79	112.76	119.70
1	L5	1867	A	P-O3'-C3'	-5.77	112.77	119.70
46	S2	1347	PSU	P-O3'-C3'	-5.75	112.80	119.70
46	S2	1520	G	C2-N3-C4	5.75	114.78	111.90
46	S2	1183	A	P-O3'-C3'	-5.75	112.81	119.70
1	L5	4468	U	C5-C4-O4	5.73	129.34	125.90
1	L5	4671	C	P-O3'-C3'	-5.72	112.83	119.70
46	S2	664	A	P-O3'-C3'	-5.72	112.83	119.70
1	L5	2409	U	C2-N1-C1'	5.72	124.56	117.70
1	L5	729	G	P-O3'-C3'	-5.71	112.84	119.70
1	L5	3644	U	P-O3'-C3'	-5.71	112.84	119.70
46	S2	673	G	P-O3'-C3'	-5.71	112.84	119.70
1	L5	2416	G	OP2-P-O3'	5.71	117.77	105.20
1	L5	4479	A	P-O3'-C3'	-5.71	112.84	119.70
1	L5	3643	A	P-O3'-C3'	-5.71	112.85	119.70
46	S2	1358	U	P-O3'-C3'	-5.70	112.86	119.70
46	S2	548	C	C2-N1-C1'	5.67	125.04	118.80
3	L8	109	C	P-O3'-C3'	-5.67	112.90	119.70
1	L5	4449	A	P-O3'-C3'	-5.66	112.91	119.70
1	L5	4335	U	P-O3'-C3'	-5.65	112.92	119.70
46	S2	537	C	C2-N1-C1'	5.65	125.02	118.80
1	L5	485	C	C6-N1-C2	-5.64	118.05	120.30
46	S2	1241	A	P-O3'-C3'	-5.62	112.95	119.70
46	S2	501	C	N3-C2-O2	-5.62	117.97	121.90
1	L5	1458	C	P-O3'-C3'	-5.61	112.97	119.70
46	S2	1805	G	C4'-C3'-C2'	-5.60	97.00	102.60
1	L5	3774	A	P-O3'-C3'	-5.58	113.00	119.70
1	L5	2049	G	P-O3'-C3'	-5.57	113.02	119.70
1	L5	4447	5MC	P-O3'-C3'	-5.57	113.02	119.70
46	S2	1520	G	N3-C4-C5	-5.54	125.83	128.60
1	L5	3819	G	P-O3'-C3'	-5.53	113.06	119.70
1	L5	456	C	O4'-C1'-N1	5.52	112.61	108.20
1	L5	3741	C	N3-C2-O2	-5.51	118.04	121.90
46	S2	1483	A	P-O3'-C3'	-5.50	113.11	119.70
6	LC	171	LEU	CA-CB-CG	5.46	127.85	115.30
1	L5	3686	G	P-O3'-C3'	-5.45	113.16	119.70
1	L5	4336	A	P-O3'-C3'	-5.45	113.17	119.70
46	S2	537	C	N1-C2-O2	5.43	122.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L7	30	C	P-O3'-C3'	-5.43	113.19	119.70
1	L5	4572	U	P-O3'-C3'	-5.42	113.19	119.70
46	S2	612	U	P-O3'-C3'	-5.42	113.20	119.70
46	S2	963	A	P-O3'-C3'	-5.41	113.21	119.70
46	S2	1025	U	P-O3'-C3'	-5.39	113.23	119.70
46	S2	1242	U	P-O3'-C3'	-5.38	113.24	119.70
46	S2	1453	C	N3-C2-O2	-5.38	118.14	121.90
1	L5	4451	G	P-O3'-C3'	-5.37	113.25	119.70
1	L5	1836	G	P-O3'-C3'	-5.35	113.28	119.70
3	L8	65	A	P-O3'-C3'	-5.33	113.31	119.70
1	L5	726	G	P-O3'-C3'	-5.32	113.31	119.70
1	L5	3907	G	P-O3'-C3'	-5.32	113.32	119.70
1	L5	3787	G	P-O3'-C3'	-5.31	113.32	119.70
1	L5	3726	A	P-O3'-C3'	-5.31	113.33	119.70
46	S2	819	G	P-O3'-C3'	-5.30	113.34	119.70
1	L5	3776	G	P-O3'-C3'	-5.30	113.34	119.70
46	S2	869	A	P-O3'-C3'	-5.30	113.34	119.70
1	L5	1884	C	P-O3'-C3'	-5.29	113.36	119.70
1	L5	36	U	P-O3'-C3'	-5.28	113.36	119.70
46	S2	1805	G	C3'-C2'-C1'	-5.28	97.28	101.50
46	S2	1710	C	P-O3'-C3'	-5.28	113.37	119.70
1	L5	4868	G	P-O3'-C3'	-5.26	113.39	119.70
46	S2	1217	A	P-O3'-C3'	-5.25	113.40	119.70
1	L5	1241	C	N1-C2-O2	5.25	122.05	118.90
1	L5	139	G	C5-C6-O6	5.24	131.75	128.60
1	L5	984	C	N3-C2-O2	-5.23	118.24	121.90
1	L5	1367	C	P-O3'-C3'	-5.22	113.44	119.70
46	S2	1360	PSU	P-O3'-C3'	-5.22	113.43	119.70
46	S2	1708	C	P-O3'-C3'	-5.20	113.46	119.70
1	L5	4758	U	N3-C2-O2	-5.19	118.57	122.20
1	L5	4574	U	P-O3'-C3'	-5.18	113.48	119.70
1	L5	1362	G	P-O3'-C3'	-5.16	113.51	119.70
1	L5	4957	C	N3-C2-O2	-5.16	118.29	121.90
46	S2	823	U	P-O3'-C3'	-5.16	113.51	119.70
1	L5	2409	U	N3-C2-O2	-5.15	118.59	122.20
1	L5	4866	C	P-O3'-C3'	-5.15	113.53	119.70
1	L5	489	C	N1-C2-O2	5.12	121.97	118.90
46	S2	501	C	C6-N1-C2	-5.12	118.25	120.30
1	L5	3777	G	C3'-C2'-C1'	-5.11	97.41	101.50
1	L5	4527	G	O4'-C1'-N9	5.10	112.28	108.20
1	L5	1077	C	C2-N1-C1'	5.10	124.41	118.80
1	L5	370	U	P-O3'-C3'	-5.07	113.62	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	S2	37	C	P-O3'-C3'	-5.03	113.66	119.70
46	S2	668	A2M	P-O3'-C3'	-5.02	113.67	119.70
1	L5	2627	C	C2-N1-C1'	5.02	124.32	118.80
46	S2	1361	G	P-O3'-C3'	-5.01	113.69	119.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	LE	223	ARG	Sidechain
8	LE	226	ARG	Sidechain
12	LI	110	ARG	Sidechain
12	LI	116	ARG	Sidechain
14	LL	36	ARG	Sidechain
41	Lm	97	ARG	Sidechain
57	SQ	15	ARG	Sidechain
73	SW	78	ARG	Sidechain

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	
4	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
5	LB	399/402 (99%)	387 (97%)	12 (3%)	0	100	100
6	LC	366/368 (100%)	358 (98%)	8 (2%)	0	100	100
7	LD	291/293 (99%)	279 (96%)	11 (4%)	1 (0%)	41	31
8	LE	232/247 (94%)	213 (92%)	13 (6%)	6 (3%)	5	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LF	224/248 (90%)	219 (98%)	5 (2%)	0	100	100
10	LG	240/266 (90%)	227 (95%)	12 (5%)	1 (0%)	34	24
11	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
12	LI	211/214 (99%)	198 (94%)	9 (4%)	4 (2%)	8	1
13	LJ	174/178 (98%)	161 (92%)	10 (6%)	3 (2%)	9	2
14	LL	208/211 (99%)	194 (93%)	13 (6%)	1 (0%)	29	18
15	LM	137/215 (64%)	135 (98%)	2 (2%)	0	100	100
16	LN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	LO	199/203 (98%)	194 (98%)	5 (2%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
20	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
21	LS	173/176 (98%)	165 (95%)	8 (5%)	0	100	100
22	LT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	LU	99/128 (77%)	88 (89%)	11 (11%)	0	100	100
24	LV	129/140 (92%)	128 (99%)	1 (1%)	0	100	100
25	LW	120/157 (76%)	112 (93%)	8 (7%)	0	100	100
26	LX	118/156 (76%)	116 (98%)	2 (2%)	0	100	100
27	LY	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
28	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
29	La	144/148 (97%)	141 (98%)	2 (1%)	1 (1%)	22	12
30	Lb	95/159 (60%)	91 (96%)	4 (4%)	0	100	100
31	Lc	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
32	Ld	104/125 (83%)	100 (96%)	4 (4%)	0	100	100
33	Le	126/135 (93%)	126 (100%)	0	0	100	100
34	Lf	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
35	Lg	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
36	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	Li	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
38	Lj	84/97 (87%)	84 (100%)	0	0	100	100
39	Lk	66/70 (94%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
44	Lp	86/92 (94%)	83 (96%)	3 (4%)	0	100	100
45	Lr	121/137 (88%)	118 (98%)	3 (2%)	0	100	100
47	SE	260/263 (99%)	259 (100%)	1 (0%)	0	100	100
48	SA	217/295 (74%)	209 (96%)	8 (4%)	0	100	100
49	SB	213/264 (81%)	204 (96%)	9 (4%)	0	100	100
50	SD	225/243 (93%)	219 (97%)	6 (3%)	0	100	100
51	SF	189/204 (93%)	173 (92%)	14 (7%)	2 (1%)	14	5
52	SH	182/194 (94%)	166 (91%)	14 (8%)	2 (1%)	14	5
53	SI	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
54	SK	95/165 (58%)	90 (95%)	5 (5%)	0	100	100
55	SL	152/158 (96%)	140 (92%)	10 (7%)	2 (1%)	12	4
56	SP	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
57	SQ	139/146 (95%)	131 (94%)	8 (6%)	0	100	100
58	SS	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
59	ST	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
60	SU	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
61	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
62	SX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
63	Sa	101/115 (88%)	100 (99%)	1 (1%)	0	100	100
64	Sc	62/69 (90%)	53 (86%)	9 (14%)	0	100	100
65	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
66	Sg	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
67	SC	220/293 (75%)	216 (98%)	4 (2%)	0	100	100
68	SG	232/249 (93%)	223 (96%)	8 (3%)	1 (0%)	34	24
69	SJ	181/194 (93%)	176 (97%)	5 (3%)	0	100	100
70	SM	116/132 (88%)	108 (93%)	7 (6%)	1 (1%)	17	7
71	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	SO	132/151 (87%)	124 (94%)	8 (6%)	0	100	100
73	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
74	SY	127/133 (96%)	125 (98%)	2 (2%)	0	100	100
75	SZ	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
76	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
77	Se	56/133 (42%)	51 (91%)	5 (9%)	0	100	100
78	Sf	65/156 (42%)	52 (80%)	10 (15%)	3 (5%)	2	0
79	SR	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
All	All	11286/12657 (89%)	10866 (96%)	392 (4%)	28 (0%)	50	38

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	LE	99	ASP
10	LG	125	LYS
12	LI	110	ARG
13	LJ	62	ILE
14	LL	47	ALA
52	SH	15	LYS
70	SM	80	ASP
7	LD	88	VAL
8	LE	177	GLY
12	LI	108	ALA
13	LJ	31	ASP
51	SF	128	ILE
78	Sf	125	GLU
8	LE	100	LYS
12	LI	106	ALA
12	LI	109	ASP
52	SH	192	PHE
55	SL	29	GLY
68	SG	124	LEU
8	LE	222	LEU
55	SL	25	LEU
78	Sf	102	VAL
78	Sf	128	ALA
8	LE	89	LEU
13	LJ	117	ILE
29	La	15	VAL

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Mol	Chain	Res	Type
51	SF	79	HIS
8	LE	92	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	
4	LA	190/199 (96%)	183 (96%)	7 (4%)	34	25
5	LB	347/347 (100%)	339 (98%)	8 (2%)	50	45
6	LC	306/306 (100%)	301 (98%)	5 (2%)	62	60
7	LD	246/247 (100%)	235 (96%)	11 (4%)	27	18
8	LE	209/220 (95%)	191 (91%)	18 (9%)	10	4
9	LF	195/215 (91%)	192 (98%)	3 (2%)	65	62
10	LG	204/223 (92%)	194 (95%)	10 (5%)	25	15
11	LH	169/171 (99%)	167 (99%)	2 (1%)	71	70
12	LI	181/182 (100%)	165 (91%)	16 (9%)	10	4
13	LJ	148/149 (99%)	136 (92%)	12 (8%)	11	4
14	LL	176/177 (99%)	170 (97%)	6 (3%)	37	28
15	LM	118/161 (73%)	114 (97%)	4 (3%)	37	28
16	LN	171/172 (99%)	169 (99%)	2 (1%)	71	70
17	LO	173/174 (99%)	168 (97%)	5 (3%)	42	35
18	LP	134/163 (82%)	131 (98%)	3 (2%)	52	47
19	LQ	164/165 (99%)	161 (98%)	3 (2%)	59	55
20	LR	166/175 (95%)	161 (97%)	5 (3%)	41	33
21	LS	156/157 (99%)	150 (96%)	6 (4%)	33	24
22	LT	139/140 (99%)	137 (99%)	2 (1%)	67	65
23	LU	91/115 (79%)	81 (89%)	10 (11%)	6	2
24	LV	101/107 (94%)	96 (95%)	5 (5%)	24	15
25	LW	101/126 (80%)	97 (96%)	4 (4%)	31	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	LX	108/133 (81%)	102 (94%)	6 (6%)	21	11
27	LY	123/135 (91%)	120 (98%)	3 (2%)	49	43
28	LZ	117/118 (99%)	113 (97%)	4 (3%)	37	28
29	La	119/120 (99%)	117 (98%)	2 (2%)	60	57
30	Lb	83/126 (66%)	81 (98%)	2 (2%)	49	43
31	Lc	83/97 (86%)	81 (98%)	2 (2%)	49	43
32	Ld	97/110 (88%)	96 (99%)	1 (1%)	76	76
33	Le	114/121 (94%)	111 (97%)	3 (3%)	46	39
34	Lf	88/89 (99%)	86 (98%)	2 (2%)	50	45
35	Lg	94/100 (94%)	92 (98%)	2 (2%)	53	48
36	Lh	109/110 (99%)	107 (98%)	2 (2%)	59	55
37	Li	85/89 (96%)	80 (94%)	5 (6%)	19	10
38	Lj	73/80 (91%)	73 (100%)	0	100	100
39	Lk	63/65 (97%)	58 (92%)	5 (8%)	12	5
40	Ll	47/48 (98%)	46 (98%)	1 (2%)	53	48
41	Lm	47/116 (40%)	43 (92%)	4 (8%)	10	4
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	91/94 (97%)	86 (94%)	5 (6%)	21	12
44	Lp	71/75 (95%)	69 (97%)	2 (3%)	43	36
45	Lr	107/121 (88%)	102 (95%)	5 (5%)	26	16
47	SE	224/225 (100%)	220 (98%)	4 (2%)	59	55
48	SA	182/243 (75%)	175 (96%)	7 (4%)	33	24
49	SB	196/231 (85%)	188 (96%)	8 (4%)	30	21
50	SD	190/202 (94%)	186 (98%)	4 (2%)	53	48
51	SF	161/170 (95%)	158 (98%)	3 (2%)	57	53
52	SH	166/174 (95%)	158 (95%)	8 (5%)	25	16
53	SI	178/180 (99%)	174 (98%)	4 (2%)	52	47
54	SK	88/136 (65%)	86 (98%)	2 (2%)	50	45
55	SL	138/142 (97%)	132 (96%)	6 (4%)	29	19
56	SP	111/130 (85%)	108 (97%)	3 (3%)	44	38
57	SQ	117/121 (97%)	111 (95%)	6 (5%)	24	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	SS	126/132 (96%)	120 (95%)	6 (5%)	25	16
59	ST	112/114 (98%)	109 (97%)	3 (3%)	44	38
60	SU	94/107 (88%)	91 (97%)	3 (3%)	39	30
61	SV	67/67 (100%)	64 (96%)	3 (4%)	27	18
62	SX	113/115 (98%)	107 (95%)	6 (5%)	22	13
63	Sa	90/98 (92%)	88 (98%)	2 (2%)	52	47
64	Sc	57/62 (92%)	52 (91%)	5 (9%)	10	4
65	Sd	48/49 (98%)	48 (100%)	0	100	100
66	Sg	272/275 (99%)	258 (95%)	14 (5%)	24	14
67	SC	188/225 (84%)	183 (97%)	5 (3%)	44	38
68	SG	204/218 (94%)	193 (95%)	11 (5%)	22	13
69	SJ	162/168 (96%)	153 (94%)	9 (6%)	21	11
70	SM	98/108 (91%)	92 (94%)	6 (6%)	18	9
71	SN	130/131 (99%)	128 (98%)	2 (2%)	65	62
72	SO	105/118 (89%)	103 (98%)	2 (2%)	57	53
73	SW	112/113 (99%)	110 (98%)	2 (2%)	59	55
74	SY	111/115 (96%)	108 (97%)	3 (3%)	44	38
75	SZ	66/103 (64%)	63 (96%)	3 (4%)	27	18
76	Sb	75/76 (99%)	72 (96%)	3 (4%)	31	22
77	Se	47/104 (45%)	46 (98%)	1 (2%)	53	48
78	Sf	60/140 (43%)	47 (78%)	13 (22%)	1	0
79	SR	119/122 (98%)	112 (94%)	7 (6%)	19	10
All	All	9834/10776 (91%)	9467 (96%)	367 (4%)	37	25

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	30	ARG
4	LA	68	ARG
4	LA	109	GLU
4	LA	135	THR
4	LA	208	GLU
4	LA	228	ASP
4	LA	247	ARG

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Mol	Chain	Res	Type
5	LB	112	ASP
5	LB	145	GLN
5	LB	214	ASP
5	LB	228	TYR
5	LB	382	MET
5	LB	384	GLU
5	LB	386	LYS
5	LB	395	ASP
6	LC	3	CYS
6	LC	9	SER
6	LC	95	MET
6	LC	122	TYR
6	LC	349	LEU
7	LD	37	VAL
7	LD	90	VAL
7	LD	143	THR
7	LD	167	VAL
7	LD	189	GLU
7	LD	196	ARG
7	LD	212	MET
7	LD	235	MET
7	LD	261	VAL
7	LD	278	ASP
7	LD	293	ARG
8	LE	56	ARG
8	LE	88	VAL
8	LE	89	LEU
8	LE	92	VAL
8	LE	100	LYS
8	LE	101	ASN
8	LE	106	VAL
8	LE	108	LYS
8	LE	109	LEU
8	LE	218	LYS
8	LE	221	LYS
8	LE	222	LEU
8	LE	223	ARG
8	LE	224	LYS
8	LE	226	ARG
8	LE	245	GLN
8	LE	254	ASP
8	LE	260	LYS

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Mol	Chain	Res	Type
9	LF	29	LYS
9	LF	41	MET
9	LF	104	LYS
10	LG	49	ARG
10	LG	100	HIS
10	LG	120	LYS
10	LG	121	LYS
10	LG	125	LYS
10	LG	175	ARG
10	LG	207	VAL
10	LG	217	LYS
10	LG	228	ASP
10	LG	246	SER
11	LH	45	LEU
11	LH	108	ASN
12	LI	24	ARG
12	LI	35	ASP
12	LI	36	LEU
12	LI	78	LYS
12	LI	80	CYS
12	LI	104	SER
12	LI	105	CYS
12	LI	109	ASP
12	LI	110	ARG
12	LI	111	LEU
12	LI	123	GLN
12	LI	136	MET
12	LI	169	LYS
12	LI	183	ASP
12	LI	203	HIS
12	LI	207	ASP
13	LJ	38	LYS
13	LJ	54	ARG
13	LJ	58	ARG
13	LJ	60	PHE
13	LJ	63	ARG
13	LJ	67	LYS
13	LJ	80	GLU
13	LJ	90	ARG
13	LJ	128	LEU
13	LJ	129	ASP
13	LJ	160	GLU

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Mol	Chain	Res	Type
13	LJ	178	LYS
14	LL	67	HIS
14	LL	79	GLU
14	LL	109	SER
14	LL	130	LYS
14	LL	138	ASP
14	LL	209	LYS
15	LM	2	VAL
15	LM	33	GLN
15	LM	38	VAL
15	LM	53	LYS
16	LN	143	ARG
16	LN	182	HIS
17	LO	117	ARG
17	LO	170	LYS
17	LO	178	ARG
17	LO	180	GLN
17	LO	183	LYS
18	LP	46	LYS
18	LP	96	LYS
18	LP	128	ARG
19	LQ	41	SER
19	LQ	82	VAL
19	LQ	97	LYS
20	LR	55	VAL
20	LR	111	GLU
20	LR	151	ARG
20	LR	152	LYS
20	LR	177	LEU
21	LS	21	LYS
21	LS	24	THR
21	LS	29	ARG
21	LS	48	VAL
21	LS	88	SER
21	LS	160	ARG
22	LT	115	LYS
22	LT	159	MET
23	LU	18	VAL
23	LU	19	LEU
23	LU	20	LYS
23	LU	22	THR
23	LU	27	HIS

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Mol	Chain	Res	Type
23	LU	41	GLN
23	LU	72	VAL
23	LU	100	LEU
23	LU	107	LYS
23	LU	109	SER
24	LV	27	ASN
24	LV	48	ARG
24	LV	67	LYS
24	LV	100	ASP
24	LV	109	LYS
25	LW	60	LYS
25	LW	78	PHE
25	LW	91	MET
25	LW	104	GLN
26	LX	37	LYS
26	LX	38	LYS
26	LX	39	LYS
26	LX	40	ILE
26	LX	43	SER
26	LX	55	ARG
27	LY	74	TYR
27	LY	76	LYS
27	LY	124	LYS
28	LZ	3	LYS
28	LZ	5	MET
28	LZ	103	ASP
28	LZ	113	GLU
29	La	95	THR
29	La	116	LYS
30	Lb	5	LYS
30	Lb	25	ARG
31	Lc	69	THR
31	Lc	92	CYS
32	Ld	98	SER
33	Le	33	ARG
33	Le	64	LYS
33	Le	82	VAL
34	Lf	46	ARG
34	Lf	54	LYS
35	Lg	28	ASN
35	Lg	73	HIS
36	Lh	94	ARG

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Mol	Chain	Res	Type
36	Lh	109	ARG
37	Li	12	ASN
37	Li	13	LYS
37	Li	29	ARG
37	Li	35	LYS
37	Li	88	GLU
39	Lk	21	LYS
39	Lk	29	LYS
39	Lk	46	VAL
39	Lk	60	LEU
39	Lk	68	GLU
40	Ll	51	LEU
41	Lm	83	ARG
41	Lm	99	CYS
41	Lm	113	LYS
41	Lm	126	LYS
43	Lo	27	LYS
43	Lo	69	ARG
43	Lo	78	ARG
43	Lo	99	ARG
43	Lo	103	VAL
44	Lp	36	LYS
44	Lp	81	SER
45	Lr	21	ASN
45	Lr	37	SER
45	Lr	76	SER
45	Lr	80	THR
45	Lr	119	ARG
47	SE	23	LEU
47	SE	176	ASP
47	SE	211	LYS
47	SE	259	LYS
48	SA	1	MET
48	SA	25	LEU
48	SA	77	ILE
48	SA	80	ARG
48	SA	81	ASN
48	SA	191	ARG
48	SA	206	ASP
49	SB	47	THR
49	SB	53	GLN
49	SB	59	SER

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Mol	Chain	Res	Type
49	SB	60	ASP
49	SB	63	LYS
49	SB	76	ASN
49	SB	92	GLN
49	SB	227	LYS
50	SD	44	THR
50	SD	106	ARG
50	SD	117	ARG
50	SD	136	VAL
51	SF	34	SER
51	SF	78	MET
51	SF	175	ASP
52	SH	18	GLU
52	SH	40	LEU
52	SH	74	LYS
52	SH	99	ARG
52	SH	122	LEU
52	SH	145	ARG
52	SH	149	ASP
52	SH	157	HIS
53	SI	47	ARG
53	SI	56	ARG
53	SI	73	THR
53	SI	205	ARG
54	SK	59	LYS
54	SK	96	ARG
55	SL	28	THR
55	SL	30	LYS
55	SL	69	ARG
55	SL	141	ASN
55	SL	144	LYS
55	SL	155	PHE
56	SP	12	PHE
56	SP	65	LYS
56	SP	127	LYS
57	SQ	15	ARG
57	SQ	18	THR
57	SQ	27	ARG
57	SQ	29	ASN
57	SQ	73	LYS
57	SQ	127	CYS
58	SS	69	THR

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Mol	Chain	Res	Type
58	SS	83	PHE
58	SS	86	ARG
58	SS	94	LYS
58	SS	98	VAL
58	SS	118	ARG
59	ST	6	VAL
59	ST	27	LYS
59	ST	113	VAL
60	SU	28	ASN
60	SU	39	LEU
60	SU	93	SER
61	SV	22	ARG
61	SV	76	ASP
61	SV	83	PHE
62	SX	29	LYS
62	SX	58	GLU
62	SX	60	LYS
62	SX	61	GLN
62	SX	105	PHE
62	SX	142	ARG
63	Sa	38	LYS
63	Sa	45	VAL
64	Sc	5	ARG
64	Sc	15	THR
64	Sc	16	LYS
64	Sc	57	THR
64	Sc	66	ARG
66	Sg	11	LEU
66	Sg	12	LYS
66	Sg	32	LEU
66	Sg	44	LYS
66	Sg	74	ASP
66	Sg	113	PHE
66	Sg	124	SER
66	Sg	134	THR
66	Sg	141	THR
66	Sg	183	LYS
66	Sg	206	LEU
66	Sg	230	LEU
66	Sg	269	GLU
66	Sg	272	GLN
67	SC	68	ARG

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Mol	Chain	Res	Type
67	SC	121	ARG
67	SC	167	ARG
67	SC	236	PHE
67	SC	248	TYR
68	SG	21	GLU
68	SG	25	ARG
68	SG	41	LEU
68	SG	93	LYS
68	SG	119	LYS
68	SG	121	ILE
68	SG	126	ASP
68	SG	128	THR
68	SG	165	GLU
68	SG	196	LYS
68	SG	227	GLN
69	SJ	2	PRO
69	SJ	58	ARG
69	SJ	59	GLU
69	SJ	71	LEU
69	SJ	92	MET
69	SJ	95	ASP
69	SJ	122	SER
69	SJ	141	VAL
69	SJ	163	SER
70	SM	49	LEU
70	SM	51	VAL
70	SM	75	ASN
70	SM	83	LYS
70	SM	109	VAL
70	SM	116	LYS
71	SN	32	ASP
71	SN	73	ARG
72	SO	17	LEU
72	SO	151	LEU
73	SW	12	LYS
73	SW	39	THR
74	SY	69	THR
74	SY	94	HIS
74	SY	110	ARG
75	SZ	41	ARG
75	SZ	78	LYS
75	SZ	98	LYS

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Mol	Chain	Res	Type
76	Sb	11	SER
76	Sb	40	CYS
76	Sb	56	CYS
77	Se	26	LYS
78	Sf	86	THR
78	Sf	90	LYS
78	Sf	94	LYS
78	Sf	95	ARG
78	Sf	96	LYS
78	Sf	98	VAL
78	Sf	107	LYS
78	Sf	113	LYS
78	Sf	132	MET
78	Sf	143	LYS
78	Sf	144	CYS
78	Sf	145	CYS
78	Sf	146	LEU
79	SR	22	THR
79	SR	37	GLU
79	SR	43	SER
79	SR	70	SER
79	SR	92	ASP
79	SR	103	LYS
79	SR	124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
8	LE	101	ASN
15	LM	33	GLN
20	LR	158	GLN
24	LV	27	ASN
62	SX	61	GLN
67	SC	267	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3704/5069 (73%)	761 (20%)	21 (0%)
2	L7	119/120 (99%)	12 (10%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L8	155/157 (98%)	28 (18%)	0
46	S2	1708/1869 (91%)	322 (18%)	10 (0%)
All	All	5686/7215 (78%)	1123 (19%)	31 (0%)

All (1123) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	15	A
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	59	A
1	L5	64	A
1	L5	65	A
1	L5	69	A
1	L5	73	A
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	119	G
1	L5	120	A
1	L5	130	C
1	L5	131	C
1	L5	132	G
1	L5	133	C
1	L5	136	C
1	L5	144	G
1	L5	152	U
1	L5	159	C
1	L5	164	G
1	L5	183	C
1	L5	185	C
1	L5	186	G
1	L5	187	U
1	L5	188	G
1	L5	189	G
1	L5	200	U
1	L5	209	U

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Mol	Chain	Res	Type
1	L5	210	C
1	L5	213	G
1	L5	216	C
1	L5	217	C
1	L5	218	A
1	L5	219	G
1	L5	234	G
1	L5	253	G
1	L5	255	C
1	L5	256	G
1	L5	259	C
1	L5	261	G
1	L5	262	G
1	L5	264	C
1	L5	265	C
1	L5	266	C
1	L5	276	C
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	341	G
1	L5	373	G
1	L5	387	G
1	L5	396	A
1	L5	407	A
1	L5	408	A
1	L5	410	A
1	L5	412	G
1	L5	432	U
1	L5	450	G
1	L5	452	A
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	467	U
1	L5	483	G
1	L5	484	U
1	L5	485	C

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Mol	Chain	Res	Type
1	L5	486	C
1	L5	489	C
1	L5	490	C
1	L5	491	G
1	L5	497	G
1	L5	498	C
1	L5	500	G
1	L5	502	C
1	L5	503	C
1	L5	505	G
1	L5	509	A
1	L5	510	U
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	516	C
1	L5	517	C
1	L5	518	G
1	L5	519	C
1	L5	643	C
1	L5	644	G
1	L5	645	G
1	L5	653	U
1	L5	654	C
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	662	C
1	L5	663	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	669	C
1	L5	672	C
1	L5	673	C
1	L5	686	A
1	L5	687	U
1	L5	696	C
1	L5	703	G
1	L5	704	C

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Mol	Chain	Res	Type
1	L5	721	G
1	L5	730	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	740	G
1	L5	741	C
1	L5	742	G
1	L5	746	A
1	L5	904	C
1	L5	905	C
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	925	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	937	U
1	L5	941	C
1	L5	944	A
1	L5	945	U
1	L5	946	C
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	963	G
1	L5	965	G
1	L5	966	A
1	L5	967	C
1	L5	968	C
1	L5	970	G
1	L5	971	U
1	L5	972	C
1	L5	981	C
1	L5	982	U
1	L5	983	C

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Mol	Chain	Res	Type
1	L5	988	C
1	L5	989	U
1	L5	990	C
1	L5	991	C
1	L5	992	C
1	L5	995	C
1	L5	1049	C
1	L5	1050	C
1	L5	1051	G
1	L5	1070	G
1	L5	1071	C
1	L5	1072	C
1	L5	1078	A
1	L5	1079	C
1	L5	1083	U
1	L5	1168	G
1	L5	1171	G
1	L5	1173	G
1	L5	1178	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1196	G
1	L5	1198	G
1	L5	1200	G
1	L5	1202	C
1	L5	1203	G
1	L5	1205	G
1	L5	1211	G
1	L5	1215	C
1	L5	1221	G
1	L5	1222	A
1	L5	1241	C
1	L5	1248	C
1	L5	1255	A
1	L5	1260	G
1	L5	1266	G
1	L5	1269	G
1	L5	1270	A
1	L5	1271	G

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Mol	Chain	Res	Type
1	L5	1272	C
1	L5	1273	G
1	L5	1275	G
1	L5	1277	G
1	L5	1280	C
1	L5	1284	G
1	L5	1287	G
1	L5	1294	A
1	L5	1302	U
1	L5	1303	A
1	L5	1304	C
1	L5	1313	C
1	L5	1326	A2M
1	L5	1337	A
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1364	U
1	L5	1365	C
1	L5	1366	G
1	L5	1367	C
1	L5	1368	A
1	L5	1387	A
1	L5	1394	G
1	L5	1397	A
1	L5	1399	G
1	L5	1402	C
1	L5	1404	G
1	L5	1405	C
1	L5	1409	C
1	L5	1410	U
1	L5	1411	C
1	L5	1412	G
1	L5	1420	A
1	L5	1425	G
1	L5	1435	G
1	L5	1436	C
1	L5	1438	U
1	L5	1439	C
1	L5	1442	C
1	L5	1443	A
1	L5	1445	U

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Mol	Chain	Res	Type
1	L5	1446	C
1	L5	1452	A
1	L5	1457	G
1	L5	1477	C
1	L5	1482	G
1	L5	1483	C
1	L5	1485	C
1	L5	1498	G
1	L5	1502	G
1	L5	1516	G
1	L5	1534	A2M
1	L5	1547	A
1	L5	1566	C
1	L5	1578	U
1	L5	1591	U
1	L5	1596	U
1	L5	1613	A
1	L5	1624	G
1	L5	1625	OMG
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1640	C
1	L5	1641	G
1	L5	1642	A
1	L5	1654	G
1	L5	1661	C
1	L5	1676	C
1	L5	1677	PSU
1	L5	1691	G
1	L5	1694	C
1	L5	1699	A
1	L5	1700	G
1	L5	1701	A
1	L5	1702	C
1	L5	1703	C
1	L5	1704	C
1	L5	1705	G
1	L5	1715	C
1	L5	1718	C
1	L5	1719	A
1	L5	1730	U

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Mol	Chain	Res	Type
1	L5	1734	G
1	L5	1740	C
1	L5	1741	G
1	L5	1742	A
1	L5	1750	G
1	L5	1756	U
1	L5	1757	U
1	L5	1758	G
1	L5	1761	G
1	L5	1762	C
1	L5	1763	C
1	L5	1765	A
1	L5	1766	A
1	L5	1768	C
1	L5	1769	G
1	L5	1770	A
1	L5	1772	C
1	L5	1780	A
1	L5	1781	PSU
1	L5	1787	A
1	L5	1804	A
1	L5	1805	A
1	L5	1810	G
1	L5	1815	G
1	L5	1821	G
1	L5	1822	U
1	L5	1829	G
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1855	G
1	L5	1869	G
1	L5	1882	U
1	L5	1892	A
1	L5	1897	A
1	L5	1918	U
1	L5	1919	G
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C

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Mol	Chain	Res	Type
1	L5	1932	A
1	L5	1940	G
1	L5	1948	G
1	L5	1959	U
1	L5	1960	A
1	L5	1966	C
1	L5	1969	G
1	L5	1972	G
1	L5	1974	U
1	L5	1975	G
1	L5	1977	C
1	L5	1978	C
1	L5	1979	A
1	L5	1981	G
1	L5	1982	G
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1987	C
1	L5	1988	G
1	L5	1991	A
1	L5	1993	C
1	L5	1995	G
1	L5	1996	C
1	L5	1998	A
1	L5	2001	G
1	L5	2002	A
1	L5	2003	G
1	L5	2006	U
1	L5	2007	G
1	L5	2009	A
1	L5	2010	A
1	L5	2011	C
1	L5	2012	A
1	L5	2013	A
1	L5	2015	U
1	L5	2016	C
1	L5	2019	C
1	L5	2020	U
1	L5	2022	C
1	L5	2024	G
1	L5	2025	A

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Mol	Chain	Res	Type
1	L5	2026	A
1	L5	2042	A
1	L5	2046	G
1	L5	2048	U
1	L5	2052	G
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A
1	L5	2084	C
1	L5	2089	G
1	L5	2091	C
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C
1	L5	2102	G
1	L5	2104	G
1	L5	2105	A
1	L5	2106	G
1	L5	2107	C
1	L5	2108	G
1	L5	2111	G
1	L5	2112	G
1	L5	2113	G
1	L5	2252	G
1	L5	2253	A
1	L5	2255	C
1	L5	2256	C
1	L5	2258	C
1	L5	2259	G
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2313	A
1	L5	2316	G
1	L5	2333	G
1	L5	2348	G
1	L5	2351	OMC
1	L5	2360	A

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Mol	Chain	Res	Type
1	L5	2382	A
1	L5	2392	C
1	L5	2395	A
1	L5	2397	G
1	L5	2417	A
1	L5	2421	G
1	L5	2422	OMC
1	L5	2425	U
1	L5	2428	A
1	L5	2441	C
1	L5	2450	G
1	L5	2453	A
1	L5	2470	C
1	L5	2475	G
1	L5	2479	G
1	L5	2483	G
1	L5	2484	A
1	L5	2485	U
1	L5	2486	G
1	L5	2487	G
1	L5	2488	C
1	L5	2489	C
1	L5	2491	C
1	L5	2493	G
1	L5	2499	C
1	L5	2501	C
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2513	A
1	L5	2519	U
1	L5	2520	C
1	L5	2546	G
1	L5	2547	G
1	L5	2555	G
1	L5	2556	G
1	L5	2560	C
1	L5	2567	G
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2627	C

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Mol	Chain	Res	Type
1	L5	2632	PSU
1	L5	2638	G
1	L5	2652	G
1	L5	2653	C
1	L5	2662	G
1	L5	2669	C
1	L5	2676	A
1	L5	2686	G
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2703	G
1	L5	2710	C
1	L5	2711	G
1	L5	2725	A
1	L5	2726	G
1	L5	2729	C
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2769	U
1	L5	2770	C
1	L5	2788	U
1	L5	2790	U
1	L5	2794	C
1	L5	2814	C
1	L5	2815	A2M
1	L5	2826	U
1	L5	2827	G
1	L5	2829	U
1	L5	2842	G
1	L5	2855	G
1	L5	2892	C
1	L5	2899	C
1	L5	2900	U
1	L5	2902	G
1	L5	2903	G
1	L5	2904	U

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Mol	Chain	Res	Type
1	L5	2906	G
1	L5	2908	U
1	L5	2910	G
1	L5	3586	G
1	L5	3587	C
1	L5	3588	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
1	L5	3598	C
1	L5	3604	A
1	L5	3615	G
1	L5	3616	U
1	L5	3618	C
1	L5	3626	G
1	L5	3635	A
1	L5	3644	U
1	L5	3662	A
1	L5	3673	C
1	L5	3674	G
1	L5	3711	A
1	L5	3712	A
1	L5	3713	U
1	L5	3723	A
1	L5	3724	A2M
1	L5	3726	A
1	L5	3727	A
1	L5	3729	U
1	L5	3736	A
1	L5	3748	A
1	L5	3753	G
1	L5	3754	G
1	L5	3757	G
1	L5	3758	U
1	L5	3759	A
1	L5	3760	A
1	L5	3761	C
1	L5	3776	G
1	L5	3777	G
1	L5	3783	A
1	L5	3786	U
1	L5	3802	U

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Mol	Chain	Res	Type
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3819	G
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3844	PSU
1	L5	3851	PSU
1	L5	3876	A
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3897	G
1	L5	3898	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3945	A
1	L5	3946	G
1	L5	3947	A
1	L5	3948	C
1	L5	3949	A
1	L5	3951	G
1	L5	3956	G
1	L5	3957	U
1	L5	3960	A
1	L5	3961	G
1	L5	3963	A
1	L5	3965	A
1	L5	3966	A
1	L5	3967	G
1	L5	3969	G
1	L5	3971	G
1	L5	3973	G
1	L5	3974	G
1	L5	3976	C
1	L5	3977	C
1	L5	4034	G

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Mol	Chain	Res	Type
1	L5	4036	G
1	L5	4038	C
1	L5	4039	G
1	L5	4042	G
1	L5	4043	G
1	L5	4044	U
1	L5	4046	A
1	L5	4048	A
1	L5	4049	U
1	L5	4050	A
1	L5	4051	C
1	L5	4053	A
1	L5	4055	U
1	L5	4056	A
1	L5	4057	C
1	L5	4059	C
1	L5	4062	A
1	L5	4065	G
1	L5	4069	U
1	L5	4076	G
1	L5	4084	G
1	L5	4098	A
1	L5	4099	G
1	L5	4100	C
1	L5	4103	C
1	L5	4104	G
1	L5	4106	G
1	L5	4108	G
1	L5	4109	G
1	L5	4110	C
1	L5	4112	C
1	L5	4113	U
1	L5	4114	C
1	L5	4115	G
1	L5	4116	C
1	L5	4119	C
1	L5	4122	G
1	L5	4127	A
1	L5	4137	C
1	L5	4139	G
1	L5	4140	C
1	L5	4141	G

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Mol	Chain	Res	Type
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4148	C
1	L5	4150	G
1	L5	4162	C
1	L5	4163	U
1	L5	4170	A
1	L5	4177	C
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4203	A
1	L5	4221	C
1	L5	4222	G
1	L5	4229	U
1	L5	4233	A
1	L5	4234	A
1	L5	4249	G
1	L5	4250	G
1	L5	4251	A
1	L5	4254	G
1	L5	4258	C
1	L5	4268	A
1	L5	4273	A
1	L5	4281	A
1	L5	4291	G
1	L5	4297	G
1	L5	4298	A
1	L5	4304	A
1	L5	4305	G
1	L5	4314	C
1	L5	4330	G
1	L5	4332	C
1	L5	4339	A
1	L5	4349	C
1	L5	4373	G
1	L5	4377	G
1	L5	4378	A
1	L5	4387	C
1	L5	4391	G

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Mol	Chain	Res	Type
1	L5	4394	A
1	L5	4415	A
1	L5	4421	C
1	L5	4422	A
1	L5	4437	U
1	L5	4448	G
1	L5	4449	A
1	L5	4452	U
1	L5	4464	A
1	L5	4475	G
1	L5	4500	PSU
1	L5	4502	C
1	L5	4512	U
1	L5	4513	A
1	L5	4519	C
1	L5	4524	G
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4560	C
1	L5	4567	G
1	L5	4573	G
1	L5	4575	G
1	L5	4584	A
1	L5	4590	A2M
1	L5	4600	G
1	L5	4601	U
1	L5	4636	PSU
1	L5	4637	OMG
1	L5	4654	C
1	L5	4656	A
1	L5	4670	C
1	L5	4672	A
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4730	C
1	L5	4731	G
1	L5	4734	A
1	L5	4735	G

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Mol	Chain	Res	Type
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4746	C
1	L5	4750	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4773	C
1	L5	4775	C
1	L5	4860	G
1	L5	4870	G
1	L5	4871	C
1	L5	4874	A
1	L5	4875	G
1	L5	4882	U
1	L5	4883	C
1	L5	4889	G
1	L5	4895	C
1	L5	4896	G
1	L5	4900	C
1	L5	4901	G
1	L5	4910	A
1	L5	4912	G
1	L5	4914	C
1	L5	4923	C
1	L5	4931	G
1	L5	4934	A
1	L5	4938	A
1	L5	4941	G
1	L5	4943	A
1	L5	4955	A
1	L5	4960	G
1	L5	4961	G
1	L5	4963	G
1	L5	4966	A
1	L5	4976	U
1	L5	4990	C
1	L5	4991	U
1	L5	5013	C

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Mol	Chain	Res	Type
1	L5	5017	G
1	L5	5022	U
1	L5	5023	C
1	L5	5024	C
1	L5	5025	C
1	L5	5030	U
1	L5	5034	A
1	L5	5041	G
1	L5	5050	C
1	L5	5054	C
1	L5	5061	A
1	L5	5069	U
2	L7	22	A
2	L7	33	U
2	L7	34	C
2	L7	42	A
2	L7	50	A
2	L7	53	U
2	L7	54	A
2	L7	64	G
2	L7	97	G
2	L7	100	A
2	L7	110	G
2	L7	117	G
3	L8	34	U
3	L8	35	C
3	L8	48	A
3	L8	51	U
3	L8	52	A
3	L8	59	A
3	L8	62	A
3	L8	63	U
3	L8	71	A
3	L8	80	A
3	L8	82	A
3	L8	84	A
3	L8	85	U
3	L8	86	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C

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Mol	Chain	Res	Type
3	L8	110	U
3	L8	112	G
3	L8	114	G
3	L8	123	U
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	128	C
3	L8	147	G
46	S2	17	C
46	S2	33	G
46	S2	46	A
46	S2	56	G
46	S2	64	A
46	S2	67	C
46	S2	68	A
46	S2	71	G
46	S2	72	C
46	S2	73	C
46	S2	74	G
46	S2	76	U
46	S2	100	PSU
46	S2	103	A
46	S2	113	G
46	S2	115	U
46	S2	126	G
46	S2	130	G
46	S2	139	C
46	S2	140	C
46	S2	143	U
46	S2	155	G
46	S2	159	A2M
46	S2	160	U
46	S2	162	C
46	S2	166	A2M
46	S2	168	C
46	S2	173	A
46	S2	190	G
46	S2	198	U
46	S2	200	G
46	S2	203	G

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Mol	Chain	Res	Type
46	S2	204	G
46	S2	206	G
46	S2	209	A
46	S2	213	G
46	S2	220	U
46	S2	302	A
46	S2	306	C
46	S2	307	G
46	S2	308	G
46	S2	309	G
46	S2	318	A
46	S2	319	C
46	S2	323	C
46	S2	324	C
46	S2	325	C
46	S2	326	C
46	S2	329	G
46	S2	332	G
46	S2	335	G
46	S2	360	A
46	S2	362	C
46	S2	364	A
46	S2	368	U
46	S2	385	G
46	S2	386	C
46	S2	407	G
46	S2	408	A
46	S2	409	C
46	S2	429	C
46	S2	438	G
46	S2	448	A
46	S2	450	C
46	S2	452	G
46	S2	462	OMC
46	S2	464	A
46	S2	466	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

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Mol	Chain	Res	Type
46	S2	488	U
46	S2	492	C
46	S2	508	A
46	S2	509	OMG
46	S2	516	A
46	S2	525	A
46	S2	532	C
46	S2	533	A
46	S2	536	A
46	S2	537	C
46	S2	544	G
46	S2	545	A
46	S2	546	G
46	S2	547	G
46	S2	548	C
46	S2	552	G
46	S2	554	A
46	S2	556	U
46	S2	557	U
46	S2	558	G
46	S2	563	G
46	S2	564	A
46	S2	570	C
46	S2	576	A2M
46	S2	583	A
46	S2	587	A
46	S2	589	G
46	S2	591	U
46	S2	598	G
46	S2	607	U
46	S2	614	C
46	S2	617	G
46	S2	627	U
46	S2	628	A
46	S2	631	U
46	S2	632	C
46	S2	643	A
46	S2	655	A
46	S2	660	C
46	S2	668	A2M
46	S2	669	A
46	S2	670	A

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Mol	Chain	Res	Type
46	S2	671	A
46	S2	672	A
46	S2	688	U
46	S2	689	U
46	S2	692	G
46	S2	696	G
46	S2	698	G
46	S2	731	G
46	S2	732	U
46	S2	733	C
46	S2	734	C
46	S2	735	C
46	S2	736	C
46	S2	737	G
46	S2	738	C
46	S2	748	C
46	S2	749	U
46	S2	750	C
46	S2	751	G
46	S2	752	G
46	S2	753	C
46	S2	787	G
46	S2	791	C
46	S2	792	C
46	S2	793	G
46	S2	794	A
46	S2	796	G
46	S2	798	G
46	S2	799	U
46	S2	801	PSU
46	S2	811	A
46	S2	821	G
46	S2	822	PSU
46	S2	823	U
46	S2	824	C
46	S2	830	A
46	S2	836	G
46	S2	837	A
46	S2	838	G
46	S2	839	C
46	S2	841	G
46	S2	842	C

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Mol	Chain	Res	Type
46	S2	847	A
46	S2	867	OMG
46	S2	869	A
46	S2	870	A
46	S2	872	A
46	S2	881	G
46	S2	882	U
46	S2	887	U
46	S2	888	U
46	S2	891	G
46	S2	892	U
46	S2	893	U
46	S2	894	G
46	S2	895	G
46	S2	896	U
46	S2	897	U
46	S2	898	U
46	S2	900	C
46	S2	901	G
46	S2	903	A
46	S2	904	A
46	S2	909	G
46	S2	913	A
46	S2	917	U
46	S2	920	A
46	S2	922	A
46	S2	933	G
46	S2	955	A
46	S2	968	U
46	S2	971	G
46	S2	990	A
46	S2	992	A
46	S2	1017	U
46	S2	1023	A
46	S2	1027	A
46	S2	1060	A
46	S2	1061	U
46	S2	1062	A
46	S2	1081	U
46	S2	1083	A
46	S2	1085	C
46	S2	1109	C

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Mol	Chain	Res	Type
46	S2	1114	U
46	S2	1115	U
46	S2	1116	C
46	S2	1121	G
46	S2	1123	C
46	S2	1131	G
46	S2	1133	A
46	S2	1138	C
46	S2	1153	C
46	S2	1154	U
46	S2	1195	A
46	S2	1207	G
46	S2	1208	A
46	S2	1215	C
46	S2	1216	C
46	S2	1217	A
46	S2	1221	G
46	S2	1224	G
46	S2	1240	A
46	S2	1242	U
46	S2	1243	U
46	S2	1251	A
46	S2	1253	A
46	S2	1256	G
46	S2	1257	G
46	S2	1259	A
46	S2	1274	G
46	S2	1275	G
46	S2	1285	G
46	S2	1294	G
46	S2	1295	A
46	S2	1301	A
46	S2	1302	G
46	S2	1303	C
46	S2	1305	C
46	S2	1308	U
46	S2	1322	G
46	S2	1327	G
46	S2	1343	U
46	S2	1348	G
46	S2	1364	U
46	S2	1371	U

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Mol	Chain	Res	Type
46	S2	1372	U
46	S2	1378	A
46	S2	1397	U
46	S2	1406	G
46	S2	1419	C
46	S2	1420	G
46	S2	1421	A
46	S2	1423	C
46	S2	1424	G
46	S2	1435	C
46	S2	1436	C
46	S2	1437	C
46	S2	1438	A
46	S2	1454	A
46	S2	1463	U
46	S2	1487	A
46	S2	1489	A
46	S2	1490	OMG
46	S2	1497	G
46	S2	1498	A
46	S2	1506	A
46	S2	1508	A
46	S2	1509	U
46	S2	1521	C
46	S2	1533	A
46	S2	1547	C
46	S2	1553	C
46	S2	1556	A
46	S2	1570	G
46	S2	1579	A
46	S2	1580	A
46	S2	1588	A
46	S2	1601	A
46	S2	1604	G
46	S2	1606	G
46	S2	1621	U
46	S2	1623	A
46	S2	1647	A
46	S2	1648	G
46	S2	1654	G
46	S2	1663	A
46	S2	1664	A

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Mol	Chain	Res	Type
46	S2	1665	G
46	S2	1671	G
46	S2	1721	U
46	S2	1722	G
46	S2	1745	A
46	S2	1747	C
46	S2	1749	G
46	S2	1752	C
46	S2	1753	C
46	S2	1754	G
46	S2	1757	G
46	S2	1758	G
46	S2	1761	U
46	S2	1771	G
46	S2	1773	C
46	S2	1774	C
46	S2	1775	U
46	S2	1776	G
46	S2	1777	G
46	S2	1778	C
46	S2	1779	G
46	S2	1781	A
46	S2	1782	G
46	S2	1783	C
46	S2	1784	G
46	S2	1786	U
46	S2	1804	OMU
46	S2	1806	A
46	S2	1809	A
46	S2	1831	A
46	S2	1835	A
46	S2	1838	U
46	S2	1849	G
46	S2	1861	G
46	S2	1862	G
46	S2	1863	A
46	S2	1864	U
46	S2	1865	C

All (31) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type

Mol	Chain	Res	Type
1	L5	406	C
1	L5	509	A
1	L5	914	U
1	L5	1590	C
1	L5	1613	A
1	L5	1633	G
1	L5	1740	C
1	L5	2391	G
1	L5	2416	G
1	L5	2675	G
1	L5	2760	G
1	L5	3614	G
1	L5	3673	C
1	L5	3726	A
1	L5	3786	U
1	L5	3876	A
1	L5	4420	U
1	L5	4600	G
1	L5	4653	C
1	L5	4699	U
1	L5	4913	G
46	S2	563	G
46	S2	688	U
46	S2	823	U
46	S2	866	PSU
46	S2	1081	U
46	S2	1242	U
46	S2	1342	U
46	S2	1508	A
46	S2	1520	G
46	S2	1805	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	L5	3768	1	18,21,22	1.37	3 (16%)	22,30,33	1.97	3 (13%)
1	OMG	L5	4228	1	18,26,27	0.85	1 (5%)	19,38,41	1.22	3 (15%)
46	A2M	S2	1678	46	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
1	OMG	L5	2424	1	18,26,27	0.92	1 (5%)	19,38,41	1.03	2 (10%)
1	A2M	L5	2815	1	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	L5	4500	1	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
46	PSU	S2	34	46	18,21,22	0.86	1 (5%)	22,30,33	0.67	0
1	5MC	L5	4447	1,81	18,22,23	0.36	0	26,32,35	0.61	0
3	OMU	L8	14	1,3	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
46	PSU	S2	1177	46	18,21,22	1.33	2 (11%)	22,30,33	1.97	4 (18%)
46	6MZ	S2	1832	80,46,81	18,25,26	0.84	1 (5%)	16,36,39	2.35	3 (18%)
1	PSU	L5	4299	1	18,21,22	0.86	1 (5%)	22,30,33	0.61	0
1	OMG	L5	3627	1	18,26,27	0.87	1 (5%)	19,38,41	1.28	2 (10%)
1	OMC	L5	1340	1	19,22,23	0.78	0	26,31,34	0.62	0
46	A2M	S2	484	46	18,25,26	0.99	1 (5%)	18,36,39	1.28	2 (11%)
46	OMC	S2	517	46	19,22,23	0.79	0	26,31,34	0.72	0
46	OMC	S2	462	46	19,22,23	0.82	0	26,31,34	0.76	0
46	PSU	S2	1232	46	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	L5	5001	1	18,21,22	0.83	1 (5%)	22,30,33	0.66	0
46	A2M	S2	576	46	18,25,26	0.89	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	L5	2839	1	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
46	OMG	S2	1490	80,46	18,26,27	0.86	1 (5%)	19,38,41	1.13	3 (15%)
46	PSU	S2	119	46	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	L5	3639	1	18,21,22	0.92	1 (5%)	22,30,33	0.63	0
46	A2M	S2	99	80,46	18,25,26	0.60	0	18,36,39	0.77	1 (5%)
46	PSU	S2	801	46	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
1	PSU	L5	1536	1	18,21,22	1.34	2 (11%)	22,30,33	1.79	3 (13%)
1	PSU	L5	4689	1	18,21,22	1.33	2 (11%)	22,30,33	1.99	3 (13%)
5	HIC	LB	245	5	8,11,12	1.66	2 (25%)	6,14,16	0.93	0
46	PSU	S2	918	46	18,21,22	1.41	3 (16%)	22,30,33	1.99	4 (18%)
1	PSU	L5	2508	1	18,21,22	1.34	3 (16%)	22,30,33	1.89	3 (13%)
1	PSU	L5	4312	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
46	PSU	S2	863	46	18,21,22	0.88	1 (5%)	22,30,33	0.59	0
46	UY1	S2	1326	80,46	19,22,23	0.20	0	22,31,34	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	4AC	S2	1337	46	21,24,25	1.03	1 (4%)	29,34,37	1.08	3 (10%)
46	OMU	S2	354	46	19,22,23	1.22	2 (10%)	26,31,34	1.81	5 (19%)
46	A2M	S2	512	46	18,25,26	1.01	1 (5%)	18,36,39	1.29	2 (11%)
46	PSU	S2	93	46	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
46	OMU	S2	428	46	19,22,23	1.21	2 (10%)	26,31,34	1.67	4 (15%)
46	PSU	S2	1003	46	18,21,22	1.38	3 (16%)	22,30,33	1.85	3 (13%)
46	MA6	S2	1850	46	18,26,27	0.92	1 (5%)	19,38,41	1.46	3 (15%)
1	OMC	L5	1881	1,80	19,22,23	0.28	0	26,31,34	0.58	0
1	A2M	L5	3785	1,80	18,25,26	0.63	0	18,36,39	0.84	1 (5%)
1	OMU	L5	2837	1	19,22,23	1.20	2 (10%)	26,31,34	1.82	5 (19%)
46	OMC	S2	1272	46	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
1	A2M	L5	3867	1	18,25,26	0.95	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	L5	3822	1	18,21,22	1.46	3 (16%)	22,30,33	1.93	5 (22%)
46	PSU	S2	218	46	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
3	PSU	L8	69	3	18,21,22	0.88	1 (5%)	22,30,33	0.70	0
1	A2M	L5	1871	1,80	18,25,26	1.00	1 (5%)	18,36,39	1.33	3 (16%)
1	A2M	L5	4523	1,80	18,25,26	1.04	2 (11%)	18,36,39	1.35	3 (16%)
1	A2M	L5	2787	1,80	18,25,26	1.01	1 (5%)	18,36,39	1.45	2 (11%)
1	PSU	L5	4576	1	18,21,22	0.88	1 (5%)	22,30,33	0.61	0
46	PSU	S2	1136	46	18,21,22	0.87	1 (5%)	22,30,33	0.70	0
46	OMU	S2	116	46	19,22,23	1.18	3 (15%)	26,31,34	1.75	5 (19%)
46	PSU	S2	63	46	18,21,22	1.36	2 (11%)	22,30,33	1.95	4 (18%)
46	PSU	S2	296	46	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	5MC	L5	3782	1,80	18,22,23	0.94	2 (11%)	26,32,35	1.15	2 (7%)
1	PSU	L5	1792	1,81	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
46	PSU	S2	1045	46	18,21,22	1.41	3 (16%)	22,30,33	1.83	3 (13%)
59	NMM	ST	67	59	9,11,12	1.54	1 (11%)	6,12,14	3.83	2 (33%)
1	PSU	L5	4442	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
46	PSU	S2	1244	46	18,21,22	0.88	1 (5%)	22,30,33	0.69	0
46	A2M	S2	668	80,46	18,25,26	0.58	0	18,36,39	0.81	1 (5%)
1	UR3	L5	4530	1	19,22,23	0.27	0	26,32,35	0.62	0
46	PSU	S2	651	46	18,21,22	1.33	3 (16%)	22,30,33	1.92	3 (13%)
1	PSU	L5	4636	1	18,21,22	1.36	2 (11%)	22,30,33	2.01	5 (22%)
46	PSU	S2	649	46	18,21,22	1.38	2 (11%)	22,30,33	1.95	3 (13%)
1	OMU	L5	2415	1	19,22,23	1.22	3 (15%)	26,31,34	1.72	5 (19%)

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
1	OMG	L5	4196	1,80	18,26,27	0.89	1 (5%)	19,38,41	1.05	2 (10%)
46	PSU	S2	1046	46	18,21,22	1.39	3 (16%)	22,30,33	1.94	4 (18%)
1	PSU	L5	4552	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	L5	1582	1	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
1	A2M	L5	2401	1	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	L5	4618	1	18,26,27	0.90	1 (5%)	19,38,41	1.14	2 (10%)
1	PSU	L5	4628	1	18,21,22	1.36	3 (16%)	22,30,33	1.88	3 (13%)
1	PSU	L5	5010	1	18,21,22	0.87	1 (5%)	22,30,33	0.65	0
46	PSU	S2	1596	46	18,21,22	0.87	1 (5%)	22,30,33	0.62	0
1	PSU	L5	4673	1,81	18,21,22	0.89	1 (5%)	22,30,33	0.56	0
46	A2M	S2	27	80,46	18,25,26	0.95	1 (5%)	18,36,39	1.39	3 (16%)
46	PSU	S2	1174	46	18,21,22	1.37	2 (11%)	22,30,33	2.04	3 (13%)
1	A2M	L5	3718	1	18,25,26	0.97	1 (5%)	18,36,39	1.14	2 (11%)
46	B8N	S2	1248	46	24,29,30	0.95	1 (4%)	29,42,45	1.53	6 (20%)
46	OMG	S2	1447	46	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
1	1MA	L5	1322	1,80	16,25,26	1.55	2 (12%)	18,37,40	1.14	3 (16%)
1	PSU	L5	3920	1,80	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
46	OMU	S2	1288	46	19,22,23	1.20	2 (10%)	26,31,34	1.71	5 (19%)
46	PSU	S2	1625	46	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	L5	1323	1	18,25,26	0.98	1 (5%)	18,36,39	1.28	2 (11%)
1	PSU	L5	3764	1	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
46	PSU	S2	300	46	18,21,22	1.32	2 (11%)	22,30,33	1.90	4 (18%)
1	OMC	L5	2861	1	19,22,23	0.78	0	26,31,34	0.58	0
46	PSU	S2	366	46	18,21,22	1.39	3 (16%)	22,30,33	2.00	4 (18%)
1	OMG	L5	4637	1,81	18,26,27	0.99	1 (5%)	19,38,41	1.01	2 (10%)
1	OMU	L5	4227	1	19,22,23	1.23	2 (10%)	26,31,34	1.72	5 (19%)
1	PSU	L5	1781	1	18,21,22	1.33	2 (11%)	22,30,33	1.97	4 (18%)
1	A2M	L5	3724	1	18,25,26	0.60	0	18,36,39	0.74	1 (5%)
1	PSU	L5	4493	1,81	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
1	OMC	L5	2804	1	19,22,23	0.79	0	26,31,34	0.85	0
1	OMG	L5	4623	1	18,26,27	0.88	1 (5%)	19,38,41	1.14	3 (15%)
46	PSU	S2	822	46	18,21,22	0.87	1 (5%)	22,30,33	0.93	1 (4%)
1	A2M	L5	3825	1	18,25,26	0.93	1 (5%)	18,36,39	1.35	3 (16%)
46	A2M	S2	1383	46	18,25,26	1.00	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	L5	1782	1	18,21,22	1.38	3 (16%)	22,30,33	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	PSU	L5	3637	1,81	18,21,22	0.86	1 (5%)	22,30,33	0.78	0
1	OMU	L5	4620	1	19,22,23	1.20	3 (15%)	26,31,34	1.69	5 (19%)
46	PSU	S2	36	46	18,21,22	0.86	1 (5%)	22,30,33	0.63	0
1	A2M	L5	398	1	18,25,26	1.06	2 (11%)	18,36,39	1.25	2 (11%)
1	OMC	L5	2824	1	19,22,23	0.79	0	26,31,34	0.68	0
1	PSU	L5	3730	1	18,21,22	0.87	1 (5%)	22,30,33	0.66	0
46	A2M	S2	468	46	18,25,26	0.99	1 (5%)	18,36,39	1.35	3 (16%)
46	PSU	S2	572	46	18,21,22	1.36	2 (11%)	22,30,33	1.84	4 (18%)
46	OMG	S2	683	46	18,26,27	1.01	2 (11%)	19,38,41	0.81	0
46	PSU	S2	681	46	18,21,22	1.32	3 (16%)	22,30,33	2.06	4 (18%)
1	OMG	L5	2364	1	18,26,27	0.90	1 (5%)	19,38,41	1.02	2 (10%)
1	OMU	L5	4498	1,80	19,22,23	0.21	0	26,31,34	0.47	0
1	PSU	L5	1779	1	18,21,22	1.37	2 (11%)	22,30,33	1.94	5 (22%)
1	PSU	L5	4293	1	18,21,22	0.88	1 (5%)	22,30,33	0.58	0
1	A2M	L5	1326	1	18,25,26	0.97	1 (5%)	18,36,39	1.15	2 (11%)
46	PSU	S2	966	46	18,21,22	0.86	1 (5%)	22,30,33	0.66	0
1	OMC	L5	2365	1,80	19,22,23	0.78	0	26,31,34	0.75	0
46	PSU	S2	1238	46	18,21,22	1.36	3 (16%)	22,30,33	1.99	5 (22%)
1	PSU	L5	3851	1	18,21,22	1.34	2 (11%)	22,30,33	2.00	3 (13%)
1	OMC	L5	3887	1	19,22,23	0.82	0	26,31,34	0.89	0
1	PSU	L5	4353	1	18,21,22	1.38	3 (16%)	22,30,33	1.97	4 (18%)
1	PSU	L5	4361	1	18,21,22	1.34	2 (11%)	22,30,33	1.98	4 (18%)
46	PSU	S2	1004	46	18,21,22	1.42	3 (16%)	22,30,33	1.91	3 (13%)
1	OMG	L5	1522	1	18,26,27	0.90	1 (5%)	19,38,41	1.20	2 (10%)
3	PSU	L8	55	3	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	L5	1316	1,81	18,26,27	0.87	1 (5%)	19,38,41	1.17	3 (15%)
46	PSU	S2	100	80,46	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
46	OMG	S2	644	46	18,26,27	0.91	1 (5%)	19,38,41	1.06	2 (10%)
1	A2M	L5	400	1	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
1	A2M	L5	1524	1	18,25,26	0.99	1 (5%)	18,36,39	1.23	2 (11%)
1	OMG	L5	3899	1	18,26,27	0.89	0	19,38,41	1.15	2 (10%)
46	OMG	S2	509	80,46	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
29	V5N	La	39	29	4,11,12	1.19	0	5,14,16	1.33	0
1	OMC	L5	3808	1	19,22,23	0.80	0	26,31,34	0.75	1 (3%)
1	PSU	L5	1683	1,81	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	L5	4536	1	19,22,23	0.79	0	26,31,34	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
46	PSU	S2	1186	46	18,21,22	0.88	1 (5%)	22,30,33	0.73	0
1	OMG	L5	2876	1	18,26,27	0.90	1 (5%)	19,38,41	1.25	3 (15%)
1	PSU	L5	4431	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
46	PSU	S2	1347	46	18,21,22	0.87	1 (5%)	22,30,33	0.68	0
46	PSU	S2	1445	46	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
46	OMC	S2	1391	46	19,22,23	0.79	0	26,31,34	0.78	0
46	OMU	S2	172	46	19,22,23	1.17	2 (10%)	26,31,34	1.80	5 (19%)
1	PSU	L5	4973	1	18,21,22	1.31	2 (11%)	22,30,33	1.83	3 (13%)
1	OMG	L5	4370	1	18,26,27	0.86	1 (5%)	19,38,41	1.19	3 (15%)
1	PSU	L5	3770	1	18,21,22	1.44	3 (16%)	22,30,33	1.92	3 (13%)
46	PSU	S2	105	46	18,21,22	1.36	2 (11%)	22,30,33	1.95	3 (13%)
46	OMG	S2	436	46	18,26,27	0.90	1 (5%)	19,38,41	1.15	2 (10%)
1	PSU	L5	4471	1	18,21,22	1.40	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	L5	4296	1	18,21,22	0.89	1 (5%)	22,30,33	0.59	0
1	PSU	L5	3715	1	18,21,22	1.37	3 (16%)	22,30,33	1.97	3 (13%)
1	A2M	L5	4571	1	18,25,26	1.02	1 (5%)	18,36,39	1.26	2 (11%)
46	PSU	S2	686	46	18,21,22	0.86	1 (5%)	22,30,33	0.73	0
46	A2M	S2	590	46	18,25,26	1.01	2 (11%)	18,36,39	1.26	2 (11%)
1	OMC	L5	4456	1	19,22,23	0.78	0	26,31,34	0.67	0
1	PSU	L5	4579	1	18,21,22	0.88	1 (5%)	22,30,33	0.61	0
46	OMU	S2	1804	46	19,22,23	0.21	0	26,31,34	0.43	0
46	MA6	S2	1851	46	18,26,27	0.91	1 (5%)	19,38,41	1.50	3 (15%)
46	A2M	S2	159	46	18,25,26	1.00	1 (5%)	18,36,39	1.47	4 (22%)
1	OMC	L5	3841	1	19,22,23	0.81	1 (5%)	26,31,34	0.88	1 (3%)
1	PSU	L5	4521	1,80,81	18,21,22	1.29	2 (11%)	22,30,33	1.95	4 (18%)
46	OMG	S2	601	46	18,26,27	0.92	1 (5%)	19,38,41	1.04	2 (10%)
46	OMU	S2	1442	80,46	19,22,23	1.20	3 (15%)	26,31,34	1.69	5 (19%)
1	OMG	L5	1625	1,81	18,26,27	0.96	1 (5%)	19,38,41	1.06	3 (15%)
1	OMG	L5	3792	1	18,26,27	0.92	1 (5%)	19,38,41	1.14	3 (15%)
1	OMC	L5	3869	1	19,22,23	0.82	0	26,31,34	0.80	0
1	OMG	L5	4392	1	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
1	PSU	L5	3762	1	18,21,22	0.83	1 (5%)	22,30,33	0.64	0
46	PSU	S2	406	46	18,21,22	1.38	3 (16%)	22,30,33	1.89	3 (13%)
1	PSU	L5	3884	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	L5	2363	1,80	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
46	PSU	S2	1360	80,46,81	18,21,22	0.88	1 (5%)	22,30,33	0.80	1 (4%)
1	PSU	L5	3844	1	18,21,22	1.39	3 (16%)	22,30,33	1.97	3 (13%)
46	OMC	S2	174	46	19,22,23	0.79	0	26,31,34	0.73	0
46	4AC	S2	1842	46	21,24,25	0.94	1 (4%)	29,34,37	1.06	4 (13%)
46	PSU	S2	109	46	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	L5	1744	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
46	A2M	S2	1031	46	18,25,26	0.93	1 (5%)	18,36,39	1.40	3 (16%)
1	PSU	L5	3695	1,81	18,21,22	1.35	3 (16%)	22,30,33	1.98	4 (18%)
72	IAS	SO	138	72	6,7,8	1.04	0	6,8,10	1.66	3 (50%)
1	OMC	L5	2351	1,80	19,22,23	0.79	0	26,31,34	0.90	1 (3%)
1	OMG	L5	4499	1	18,26,27	0.99	2 (11%)	19,38,41	0.72	0
1	PSU	L5	4423	1	18,21,22	1.36	3 (16%)	22,30,33	1.92	3 (13%)
1	PSU	L5	4972	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
1	OMG	L5	4494	1	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
46	PSU	S2	1367	46	18,21,22	1.39	2 (11%)	22,30,33	1.91	4 (18%)
46	OMC	S2	1703	46	19,22,23	0.79	0	26,31,34	0.80	0
1	PSU	L5	3853	1,80	18,21,22	1.33	2 (11%)	22,30,33	1.75	3 (13%)
46	PSU	S2	1692	46	18,21,22	1.42	3 (16%)	22,30,33	1.88	3 (13%)
1	6MZ	L5	4220	1	18,25,26	0.85	1 (5%)	16,36,39	1.98	4 (25%)
1	PSU	L5	1860	1	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
1	OMG	L5	3744	1	18,26,27	0.93	1 (5%)	19,38,41	1.12	2 (10%)
1	A2M	L5	1534	1,80	18,25,26	1.03	1 (5%)	18,36,39	1.40	2 (11%)
1	A2M	L5	3830	1	18,25,26	0.99	1 (5%)	18,36,39	1.19	2 (11%)
1	OMC	L5	2422	1,80	19,22,23	0.83	0	26,31,34	0.76	0
1	PSU	L5	4403	1	18,21,22	1.33	3 (16%)	22,30,33	1.94	4 (18%)
1	OMC	L5	3701	1,81	19,22,23	0.76	0	26,31,34	0.87	0
46	PSU	S2	667	46	18,21,22	0.85	1 (5%)	22,30,33	0.61	0
46	PSU	S2	609	46	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
46	PSU	S2	815	46	18,21,22	1.32	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	L5	4590	1	18,25,26	1.02	1 (5%)	18,36,39	1.34	3 (16%)
1	OMU	L5	3925	1	19,22,23	1.19	2 (10%)	26,31,34	1.70	5 (19%)
46	OMG	S2	867	46	18,26,27	1.00	2 (11%)	19,38,41	0.69	0
46	OMU	S2	121	46	19,22,23	1.20	3 (15%)	26,31,34	1.69	5 (19%)
3	OMG	L8	75	3	18,26,27	0.91	1 (5%)	19,38,41	1.07	2 (10%)
1	OMU	L5	4306	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	PSU	L5	1862	1	18,21,22	1.35	2 (11%)	22,30,33	1.96	4 (18%)
46	PSU	S2	814	46	18,21,22	1.35	3 (16%)	22,30,33	1.84	3 (13%)
1	UY1	L5	3818	1,81	19,22,23	0.22	0	22,31,34	0.50	0
1	PSU	L5	1677	1	18,21,22	1.36	3 (16%)	22,30,33	2.05	5 (22%)
1	PSU	L5	2843	1	18,21,22	1.36	3 (16%)	22,30,33	1.80	4 (18%)
1	PSU	L5	4457	1	18,21,22	1.39	2 (11%)	22,30,33	1.96	3 (13%)
46	PSU	S2	1056	46	18,21,22	1.47	3 (16%)	22,30,33	1.94	4 (18%)
1	PSU	L5	2632	1	18,21,22	0.86	1 (5%)	22,30,33	0.60	0
46	A2M	S2	166	46	18,25,26	1.07	1 (5%)	18,36,39	1.41	3 (16%)
46	PSU	S2	1643	80,46	18,21,22	1.37	2 (11%)	22,30,33	1.88	4 (18%)
46	PSU	S2	866	46	18,21,22	0.89	1 (5%)	22,30,33	0.96	1 (4%)
1	PSU	L5	4532	1	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
46	OMG	S2	1328	46,81	18,26,27	1.02	2 (11%)	19,38,41	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	3768	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4228	1	-	0/5/27/28	0/3/3/3
46	A2M	S2	1678	46	-	1/5/27/28	0/3/3/3
1	OMG	L5	2424	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	2815	1	-	4/5/27/28	0/3/3/3
1	PSU	L5	4500	1	-	5/7/25/26	0/2/2/2
46	PSU	S2	34	46	-	0/7/25/26	0/2/2/2
1	5MC	L5	4447	1,81	-	4/7/25/26	0/2/2/2
3	OMU	L8	14	1,3	-	1/9/27/28	0/2/2/2
46	PSU	S2	1177	46	-	0/7/25/26	0/2/2/2
46	6MZ	S2	1832	80,46,81	-	1/5/27/28	0/3/3/3
1	PSU	L5	4299	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3627	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	1340	1	-	0/9/27/28	0/2/2/2
46	A2M	S2	484	46	-	0/5/27/28	0/3/3/3
46	OMC	S2	517	46	-	0/9/27/28	0/2/2/2
46	OMC	S2	462	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1232	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	5001	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	S2	576	46	-	2/5/27/28	0/3/3/3
1	PSU	L5	2839	1	-	0/7/25/26	0/2/2/2
46	OMG	S2	1490	80,46	-	3/5/27/28	0/3/3/3
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3639	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	99	80,46	-	0/5/27/28	0/3/3/3
46	PSU	S2	801	46	-	2/7/25/26	0/2/2/2
1	PSU	L5	1536	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4689	1	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
46	PSU	S2	918	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4312	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	863	46	-	0/7/25/26	0/2/2/2
46	UY1	S2	1326	80,46	-	2/9/27/28	0/2/2/2
46	4AC	S2	1337	46	-	0/11/29/30	0/2/2/2
46	OMU	S2	354	46	-	0/9/27/28	0/2/2/2
46	A2M	S2	512	46	-	2/5/27/28	0/3/3/3
46	PSU	S2	93	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	428	46	-	6/9/27/28	0/2/2/2
46	PSU	S2	1003	46	-	0/7/25/26	0/2/2/2
46	MA6	S2	1850	46	-	0/7/29/30	0/3/3/3
1	OMC	L5	1881	1,80	-	0/9/27/28	0/2/2/2
1	A2M	L5	3785	1,80	-	1/5/27/28	0/3/3/3
1	OMU	L5	2837	1	-	0/9/27/28	0/2/2/2
46	OMC	S2	1272	46	-	1/9/27/28	0/2/2/2
1	A2M	L5	3867	1	-	1/5/27/28	0/3/3/3
1	PSU	L5	3822	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	218	46	-	0/7/25/26	0/2/2/2
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
1	A2M	L5	1871	1,80	-	0/5/27/28	0/3/3/3
1	A2M	L5	4523	1,80	-	0/5/27/28	0/3/3/3
1	A2M	L5	2787	1,80	-	0/5/27/28	0/3/3/3
1	PSU	L5	4576	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1136	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	116	46	-	1/9/27/28	0/2/2/2
46	PSU	S2	63	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	296	46	-	0/7/25/26	0/2/2/2
1	5MC	L5	3782	1,80	-	0/7/25/26	0/2/2/2
1	PSU	L5	1792	1,81	-	1/7/25/26	0/2/2/2
46	PSU	S2	1045	46	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	NMM	ST	67	59	-	0/9/11/13	-
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1244	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	668	80,46	-	2/5/27/28	0/3/3/3
1	UR3	L5	4530	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	651	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	4/7/25/26	0/2/2/2
46	PSU	S2	649	46	-	0/7/25/26	0/2/2/2
1	OMU	L5	2415	1	-	1/9/27/28	0/2/2/2
1	OMG	L5	4196	1,80	-	1/5/27/28	0/3/3/3
46	PSU	S2	1046	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4552	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1582	1	-	2/7/25/26	0/2/2/2
1	A2M	L5	2401	1	-	0/5/27/28	0/3/3/3
1	OMG	L5	4618	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	5010	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1596	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4673	1,81	-	0/7/25/26	0/2/2/2
46	A2M	S2	27	80,46	-	1/5/27/28	0/3/3/3
46	PSU	S2	1174	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	3718	1	-	1/5/27/28	0/3/3/3
46	B8N	S2	1248	46	-	3/16/34/35	0/2/2/2
46	OMG	S2	1447	46	-	1/5/27/28	0/3/3/3
1	1MA	L5	1322	1,80	-	0/3/25/26	0/3/3/3
1	PSU	L5	3920	1,80	-	0/7/25/26	0/2/2/2
46	OMU	S2	1288	46	-	0/9/27/28	0/2/2/2
46	PSU	S2	1625	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	1323	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	3764	1	-	2/7/25/26	0/2/2/2
46	PSU	S2	300	46	-	0/7/25/26	0/2/2/2
1	OMC	L5	2861	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	366	46	-	0/7/25/26	0/2/2/2
1	OMG	L5	4637	1,81	-	1/5/27/28	0/3/3/3
1	OMU	L5	4227	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	1781	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3724	1	-	3/5/27/28	0/3/3/3
1	PSU	L5	4493	1,81	-	0/7/25/26	0/2/2/2
1	OMC	L5	2804	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	4623	1	-	0/5/27/28	0/3/3/3
46	PSU	S2	822	46	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	L5	3825	1	-	0/5/27/28	0/3/3/3
46	A2M	S2	1383	46	-	3/5/27/28	0/3/3/3
1	PSU	L5	1782	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3637	1,81	-	0/7/25/26	0/2/2/2
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	36	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	398	1	-	1/5/27/28	0/3/3/3
1	OMC	L5	2824	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	3730	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	468	46	-	1/5/27/28	0/3/3/3
46	PSU	S2	572	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	683	46	-	0/5/27/28	0/3/3/3
46	PSU	S2	681	46	-	0/7/25/26	0/2/2/2
1	OMG	L5	2364	1	-	0/5/27/28	0/3/3/3
1	OMU	L5	4498	1,80	-	0/9/27/28	0/2/2/2
1	PSU	L5	1779	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	1326	1	-	1/5/27/28	0/3/3/3
46	PSU	S2	966	46	-	2/7/25/26	0/2/2/2
1	OMC	L5	2365	1,80	-	0/9/27/28	0/2/2/2
46	PSU	S2	1238	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3851	1	-	2/7/25/26	0/2/2/2
1	OMC	L5	3887	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	4353	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4361	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1004	46	-	0/7/25/26	0/2/2/2
1	OMG	L5	1522	1	-	0/5/27/28	0/3/3/3
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2
1	OMG	L5	1316	1,81	-	0/5/27/28	0/3/3/3
46	PSU	S2	100	80,46	-	2/7/25/26	0/2/2/2
46	OMG	S2	644	46	-	1/5/27/28	0/3/3/3
1	A2M	L5	400	1	-	1/5/27/28	0/3/3/3
1	A2M	L5	1524	1	-	1/5/27/28	0/3/3/3
1	OMG	L5	3899	1	-	0/5/27/28	0/3/3/3
46	OMG	S2	509	80,46	-	0/5/27/28	0/3/3/3
29	V5N	La	39	29	-	0/5/10/12	0/1/1/1
1	OMC	L5	3808	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	1683	1,81	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	1186	46	-	0/7/25/26	0/2/2/2
1	OMG	L5	2876	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	4431	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1347	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1445	46	-	0/7/25/26	0/2/2/2
46	OMC	S2	1391	46	-	0/9/27/28	0/2/2/2
46	OMU	S2	172	46	-	0/9/27/28	0/2/2/2
1	PSU	L5	4973	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4370	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	3770	1	-	2/7/25/26	0/2/2/2
46	PSU	S2	105	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	436	46	-	0/5/27/28	0/3/3/3
1	PSU	L5	4471	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4296	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3715	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	4571	1	-	1/5/27/28	0/3/3/3
46	PSU	S2	686	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	590	46	-	1/5/27/28	0/3/3/3
1	OMC	L5	4456	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4579	1	-	0/7/25/26	0/2/2/2
46	OMU	S2	1804	46	-	0/9/27/28	0/2/2/2
46	MA6	S2	1851	46	-	3/7/29/30	0/3/3/3
46	A2M	S2	159	46	-	2/5/27/28	0/3/3/3
1	OMC	L5	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4521	1,80,81	-	0/7/25/26	0/2/2/2
46	OMG	S2	601	46	-	0/5/27/28	0/3/3/3
46	OMU	S2	1442	80,46	-	1/9/27/28	0/2/2/2
1	OMG	L5	1625	1,81	-	1/5/27/28	0/3/3/3
1	OMG	L5	3792	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	3869	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	4392	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	3762	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	406	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3884	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2363	1,80	-	2/5/27/28	0/3/3/3
46	PSU	S2	1360	80,46,81	-	0/7/25/26	0/2/2/2
1	PSU	L5	3844	1	-	2/7/25/26	0/2/2/2
46	OMC	S2	174	46	-	0/9/27/28	0/2/2/2
46	4AC	S2	1842	46	-	0/11/29/30	0/2/2/2
46	PSU	S2	109	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1744	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	1031	46	-	1/5/27/28	0/3/3/3
1	PSU	L5	3695	1,81	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	IAS	SO	138	72	-	1/7/7/8	-
1	OMC	L5	2351	1,80	-	2/9/27/28	0/2/2/2
1	OMG	L5	4499	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	4423	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4972	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4494	1	-	1/5/27/28	0/3/3/3
46	PSU	S2	1367	46	-	0/7/25/26	0/2/2/2
46	OMC	S2	1703	46	-	0/9/27/28	0/2/2/2
1	PSU	L5	3853	1,80	-	0/7/25/26	0/2/2/2
46	PSU	S2	1692	46	-	0/7/25/26	0/2/2/2
1	6MZ	L5	4220	1	-	0/5/27/28	0/3/3/3
1	PSU	L5	1860	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3744	1	-	0/5/27/28	0/3/3/3
1	A2M	L5	1534	1,80	-	2/5/27/28	0/3/3/3
1	A2M	L5	3830	1	-	0/5/27/28	0/3/3/3
1	OMC	L5	2422	1,80	-	1/9/27/28	0/2/2/2
1	PSU	L5	4403	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	3701	1,81	-	4/9/27/28	0/2/2/2
46	PSU	S2	667	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	609	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	815	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	4590	1	-	1/5/27/28	0/3/3/3
1	OMU	L5	3925	1	-	0/9/27/28	0/2/2/2
46	OMG	S2	867	46	-	1/5/27/28	0/3/3/3
46	OMU	S2	121	46	-	1/9/27/28	0/2/2/2
3	OMG	L8	75	3	-	0/5/27/28	0/3/3/3
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	1862	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	814	46	-	0/7/25/26	0/2/2/2
1	UY1	L5	3818	1,81	-	6/9/27/28	0/2/2/2
1	PSU	L5	1677	1	-	2/7/25/26	0/2/2/2
1	PSU	L5	2843	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4457	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1056	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	2632	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	166	46	-	2/5/27/28	0/3/3/3
46	PSU	S2	1643	80,46	-	0/7/25/26	0/2/2/2
46	PSU	S2	866	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4532	1	-	0/7/25/26	0/2/2/2
46	OMG	S2	1328	46,81	-	0/5/27/28	0/3/3/3

All (325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	1322	1MA	C2-N3	4.94	1.35	1.29
59	ST	67	NMM	CZ-NH2	4.14	1.44	1.34
1	L5	3639	PSU	C6-C5	3.60	1.39	1.35
5	LB	245	HIC	CD2-CG	3.49	1.41	1.36
46	S2	866	PSU	C6-C5	3.44	1.39	1.35
1	L5	4296	PSU	C6-C5	3.44	1.39	1.35
3	L8	69	PSU	C6-C5	3.43	1.39	1.35
1	L5	4293	PSU	C6-C5	3.42	1.39	1.35
46	S2	863	PSU	C6-C5	3.41	1.39	1.35
1	L5	4579	PSU	C6-C5	3.41	1.39	1.35
1	L5	4576	PSU	C6-C5	3.41	1.39	1.35
1	L5	4532	PSU	C6-C5	3.40	1.39	1.35
46	S2	1244	PSU	C6-C5	3.40	1.39	1.35
46	S2	1360	PSU	C6-C5	3.39	1.39	1.35
46	S2	1596	PSU	C6-C5	3.38	1.39	1.35
1	L5	3764	PSU	C6-C5	3.38	1.39	1.35
46	S2	609	PSU	C6-C5	3.37	1.39	1.35
46	S2	822	PSU	C6-C5	3.37	1.39	1.35
1	L5	2632	PSU	C6-C5	3.37	1.39	1.35
1	L5	4673	PSU	C6-C5	3.37	1.39	1.35
46	S2	34	PSU	C6-C5	3.36	1.39	1.35
1	L5	3822	PSU	C4-N3	-3.36	1.32	1.38
1	L5	5010	PSU	C6-C5	3.36	1.39	1.35
1	L5	4493	PSU	C6-C5	3.36	1.39	1.35
46	S2	1347	PSU	C6-C5	3.36	1.39	1.35
1	L5	4299	PSU	C6-C5	3.35	1.39	1.35
46	S2	667	PSU	C6-C5	3.35	1.39	1.35
46	S2	1136	PSU	C6-C5	3.35	1.39	1.35
46	S2	100	PSU	C6-C5	3.34	1.39	1.35
1	L5	2839	PSU	C6-C5	3.33	1.39	1.35
46	S2	1056	PSU	C4-N3	-3.33	1.32	1.38
46	S2	801	PSU	C6-C5	3.33	1.39	1.35
46	S2	1186	PSU	C6-C5	3.32	1.39	1.35
1	L5	3884	PSU	C6-C5	3.32	1.39	1.35
1	L5	4500	PSU	C6-C5	3.31	1.39	1.35
1	L5	3730	PSU	C6-C5	3.31	1.39	1.35
46	S2	966	PSU	C6-C5	3.31	1.39	1.35
1	L5	3637	PSU	C6-C5	3.30	1.39	1.35
46	S2	36	PSU	C6-C5	3.29	1.39	1.35
1	L5	4552	PSU	C6-C5	3.29	1.39	1.35
46	S2	1174	PSU	C6-C5	3.25	1.39	1.35
46	S2	686	PSU	C6-C5	3.24	1.39	1.35
1	L5	5001	PSU	C6-C5	3.24	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	296	PSU	C6-C5	3.22	1.39	1.35
46	S2	1232	PSU	C6-C5	3.21	1.39	1.35
1	L5	3762	PSU	C6-C5	3.20	1.39	1.35
1	L5	4457	PSU	C6-C5	3.20	1.39	1.35
1	L5	4353	PSU	C6-C5	3.20	1.39	1.35
46	S2	1692	PSU	C6-C5	3.20	1.39	1.35
46	S2	93	PSU	C6-C5	3.19	1.39	1.35
1	L5	4471	PSU	C6-C5	3.19	1.39	1.35
1	L5	1536	PSU	C6-C5	3.17	1.39	1.35
1	L5	3770	PSU	C6-C5	3.17	1.39	1.35
1	L5	1779	PSU	C6-C5	3.16	1.39	1.35
46	S2	406	PSU	C6-C5	3.15	1.39	1.35
1	L5	1782	PSU	C6-C5	3.15	1.39	1.35
46	S2	109	PSU	C6-C5	3.14	1.39	1.35
1	L5	4423	PSU	C6-C5	3.13	1.39	1.35
46	S2	1238	PSU	C6-C5	3.12	1.39	1.35
1	L5	1792	PSU	C6-C5	3.12	1.39	1.35
1	L5	3920	PSU	C6-C5	3.12	1.39	1.35
3	L8	55	PSU	C6-C5	3.11	1.38	1.35
1	L5	3851	PSU	C6-C5	3.11	1.38	1.35
46	S2	1248	B8N	C6-C5	3.11	1.39	1.34
46	S2	1445	PSU	C6-C5	3.10	1.38	1.35
46	S2	649	PSU	C6-C5	3.10	1.38	1.35
1	L5	4431	PSU	C6-C5	3.10	1.38	1.35
1	L5	4973	PSU	C6-C5	3.06	1.38	1.35
46	S2	1367	PSU	C4-N3	-3.06	1.33	1.38
46	S2	1625	PSU	C6-C5	3.05	1.38	1.35
1	L5	3715	PSU	C4-N3	-3.05	1.33	1.38
1	L5	4636	PSU	C6-C5	3.05	1.38	1.35
1	L5	3844	PSU	C6-C5	3.02	1.38	1.35
1	L5	1683	PSU	C6-C5	3.02	1.38	1.35
1	L5	1322	1MA	C6-N6	3.02	1.35	1.27
1	L5	1862	PSU	C6-C5	3.02	1.38	1.35
1	L5	4628	PSU	C6-C5	3.02	1.38	1.35
46	S2	63	PSU	C6-C5	3.01	1.38	1.35
1	L5	3770	PSU	C4-N3	-3.01	1.33	1.38
46	S2	366	PSU	C4-N3	-3.01	1.33	1.38
46	S2	1045	PSU	C4-N3	-3.00	1.33	1.38
1	L5	4972	PSU	C6-C5	3.00	1.38	1.35
1	L5	2843	PSU	C6-C5	3.00	1.38	1.35
1	L5	1744	PSU	C6-C5	2.99	1.38	1.35
1	L5	4442	PSU	C6-C5	2.99	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	1860	PSU	C6-C5	2.98	1.38	1.35
46	S2	1643	PSU	C6-C5	2.98	1.38	1.35
46	S2	218	PSU	C6-C5	2.97	1.38	1.35
46	S2	300	PSU	C6-C5	2.97	1.38	1.35
1	L5	4493	PSU	C4-N3	-2.96	1.33	1.38
46	S2	572	PSU	C6-C5	2.96	1.38	1.35
46	S2	63	PSU	C4-N3	-2.95	1.33	1.38
46	S2	1238	PSU	C4-N3	-2.95	1.33	1.38
1	L5	4361	PSU	C6-C5	2.95	1.38	1.35
46	S2	1004	PSU	C6-C5	2.94	1.38	1.35
46	S2	1367	PSU	C6-C5	2.94	1.38	1.35
46	S2	1046	PSU	C6-C5	2.93	1.38	1.35
1	L5	1860	PSU	C4-N3	-2.93	1.33	1.38
46	S2	814	PSU	C6-C5	2.92	1.38	1.35
1	L5	1781	PSU	C6-C5	2.91	1.38	1.35
1	L5	3853	PSU	C6-C5	2.91	1.38	1.35
46	S2	815	PSU	C6-C5	2.91	1.38	1.35
1	L5	3768	PSU	C4-N3	-2.91	1.33	1.38
46	S2	1177	PSU	C4-N3	-2.91	1.33	1.38
46	S2	119	PSU	C6-C5	2.91	1.38	1.35
1	L5	3844	PSU	C4-N3	-2.89	1.33	1.38
1	L5	1677	PSU	C6-C5	2.89	1.38	1.35
46	S2	1003	PSU	C6-C5	2.89	1.38	1.35
46	S2	105	PSU	C6-C5	2.88	1.38	1.35
46	S2	918	PSU	C6-C5	2.88	1.38	1.35
1	L5	2839	PSU	C4-N3	-2.88	1.33	1.38
1	L5	1779	PSU	C4-N3	-2.88	1.33	1.38
46	S2	366	PSU	C6-C5	2.87	1.38	1.35
46	S2	1004	PSU	C4-N3	-2.87	1.33	1.38
1	L5	3744	OMG	C6-N1	-2.87	1.33	1.37
46	S2	93	PSU	C4-N3	-2.86	1.33	1.38
1	L5	2508	PSU	C4-N3	-2.86	1.33	1.38
1	L5	2843	PSU	C4-N3	-2.86	1.33	1.38
1	L5	1582	PSU	C6-C5	2.86	1.38	1.35
46	S2	1046	PSU	C4-N3	-2.86	1.33	1.38
1	L5	3792	OMG	C6-N1	-2.86	1.33	1.37
46	S2	1692	PSU	C4-N3	-2.86	1.33	1.38
1	L5	4521	PSU	C6-C5	2.85	1.38	1.35
46	S2	296	PSU	C4-N3	-2.85	1.33	1.38
1	L5	1862	PSU	C4-N3	-2.84	1.33	1.38
1	L5	2508	PSU	C6-C5	2.84	1.38	1.35
46	S2	649	PSU	C4-N3	-2.84	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	651	PSU	C6-C5	2.84	1.38	1.35
46	S2	1445	PSU	C4-N3	-2.83	1.33	1.38
1	L5	4972	PSU	C4-N3	-2.83	1.33	1.38
1	L5	3695	PSU	C6-C5	2.82	1.38	1.35
46	S2	1174	PSU	C4-N3	-2.82	1.33	1.38
46	S2	1003	PSU	C4-N3	-2.82	1.33	1.38
1	L5	4521	PSU	C4-N3	-2.82	1.33	1.38
46	S2	651	PSU	C4-N3	-2.81	1.33	1.38
1	L5	1782	PSU	C4-N3	-2.81	1.33	1.38
1	L5	4312	PSU	C6-C5	2.81	1.38	1.35
3	L8	55	PSU	C4-N3	-2.81	1.33	1.38
1	L5	1781	PSU	C4-N3	-2.81	1.33	1.38
46	S2	1045	PSU	C6-C5	2.80	1.38	1.35
46	S2	918	PSU	C4-N3	-2.80	1.33	1.38
1	L5	3822	PSU	C6-C5	2.80	1.38	1.35
46	S2	814	PSU	C4-N3	-2.79	1.33	1.38
46	S2	105	PSU	C4-N3	-2.79	1.33	1.38
1	L5	3768	PSU	C6-C5	2.79	1.38	1.35
1	L5	4403	PSU	C6-C5	2.78	1.38	1.35
1	L5	4353	PSU	C4-N3	-2.78	1.33	1.38
1	L5	4423	PSU	C4-N3	-2.78	1.33	1.38
1	L5	4637	OMG	C6-N1	-2.78	1.33	1.37
46	S2	681	PSU	C4-N3	-2.78	1.33	1.38
1	L5	1744	PSU	C4-N3	-2.78	1.33	1.38
46	S2	1643	PSU	C4-N3	-2.78	1.33	1.38
46	S2	681	PSU	C6-C5	2.77	1.38	1.35
1	L5	3695	PSU	C4-N3	-2.77	1.33	1.38
46	S2	109	PSU	C4-N3	-2.76	1.33	1.38
1	L5	4689	PSU	C6-C5	2.76	1.38	1.35
1	L5	1582	PSU	C4-N3	-2.76	1.33	1.38
46	S2	354	OMU	C4-N3	-2.75	1.33	1.38
46	S2	300	PSU	C4-N3	-2.75	1.33	1.38
1	L5	1625	OMG	C6-N1	-2.74	1.33	1.37
46	S2	572	PSU	C4-N3	-2.73	1.33	1.38
1	L5	4403	PSU	C4-N3	-2.73	1.33	1.38
1	L5	1536	PSU	C4-N3	-2.72	1.33	1.38
1	L5	4628	PSU	C4-N3	-2.71	1.33	1.38
1	L5	4442	PSU	C4-N3	-2.71	1.33	1.38
1	L5	3920	PSU	C4-N3	-2.71	1.33	1.38
1	L5	3782	5MC	C6-C5	2.71	1.39	1.34
1	L5	4431	PSU	C4-N3	-2.71	1.33	1.38
1	L5	4306	OMU	C4-N3	-2.70	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4552	PSU	C4-N3	-2.70	1.33	1.38
1	L5	4471	PSU	C4-N3	-2.70	1.33	1.38
46	S2	1625	PSU	C4-N3	-2.70	1.33	1.38
1	L5	4361	PSU	C4-N3	-2.70	1.33	1.38
1	L5	4636	PSU	C4-N3	-2.70	1.33	1.38
46	S2	428	OMU	C4-N3	-2.69	1.33	1.38
1	L5	4689	PSU	C4-N3	-2.69	1.33	1.38
1	L5	4457	PSU	C4-N3	-2.69	1.33	1.38
46	S2	406	PSU	C4-N3	-2.69	1.33	1.38
1	L5	4312	PSU	C4-N3	-2.67	1.33	1.38
46	S2	121	OMU	C4-N3	-2.67	1.33	1.38
46	S2	1328	OMG	C5-C6	-2.67	1.42	1.47
46	S2	683	OMG	C5-C6	-2.66	1.42	1.47
1	L5	4227	OMU	C4-N3	-2.66	1.33	1.38
1	L5	2424	OMG	C6-N1	-2.66	1.33	1.37
46	S2	1232	PSU	C4-N3	-2.66	1.33	1.38
1	L5	1792	PSU	C4-N3	-2.65	1.33	1.38
46	S2	218	PSU	C4-N3	-2.64	1.33	1.38
1	L5	4494	OMG	C6-N1	-2.64	1.33	1.37
46	S2	1177	PSU	C6-C5	2.63	1.38	1.35
1	L5	4973	PSU	C4-N3	-2.62	1.34	1.38
1	L5	3884	PSU	C4-N3	-2.62	1.34	1.38
46	S2	119	PSU	C4-N3	-2.61	1.34	1.38
1	L5	3853	PSU	C4-N3	-2.61	1.34	1.38
3	L8	14	OMU	C4-N3	-2.61	1.33	1.38
1	L5	4499	OMG	C5-C6	-2.61	1.42	1.47
1	L5	2837	OMU	C4-N3	-2.60	1.33	1.38
1	L5	1677	PSU	C4-N3	-2.60	1.34	1.38
46	S2	867	OMG	C5-C6	-2.59	1.42	1.47
46	S2	644	OMG	C6-N1	-2.59	1.34	1.37
46	S2	1337	4AC	C4-N4	-2.59	1.36	1.39
46	S2	1442	OMU	C4-N3	-2.59	1.33	1.38
46	S2	601	OMG	C6-N1	-2.59	1.34	1.37
46	S2	509	OMG	C6-N1	-2.58	1.34	1.37
1	L5	1683	PSU	C4-N3	-2.57	1.34	1.38
46	S2	172	OMU	C4-N3	-2.57	1.34	1.38
1	L5	2415	OMU	C4-N3	-2.57	1.34	1.38
46	S2	166	A2M	C5-C4	2.56	1.47	1.40
1	L5	3627	OMG	C6-N1	-2.56	1.34	1.37
46	S2	436	OMG	C6-N1	-2.55	1.34	1.37
1	L5	4392	OMG	C6-N1	-2.55	1.34	1.37
1	L5	4620	OMU	C4-N3	-2.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1056	PSU	C6-C5	2.54	1.38	1.35
46	S2	815	PSU	C4-N3	-2.54	1.34	1.38
46	S2	1288	OMU	C4-N3	-2.53	1.34	1.38
1	L5	2876	OMG	C6-N1	-2.52	1.34	1.37
1	L5	3851	PSU	C4-N3	-2.52	1.34	1.38
1	L5	3715	PSU	C6-C5	2.50	1.38	1.35
46	S2	1832	6MZ	C5-C4	2.49	1.47	1.40
46	S2	354	OMU	C2-N3	-2.49	1.33	1.38
46	S2	918	PSU	O4'-C1'	-2.47	1.40	1.43
46	S2	1447	OMG	C6-N1	-2.47	1.34	1.37
1	L5	3925	OMU	C4-N3	-2.47	1.34	1.38
46	S2	159	A2M	C5-C4	2.47	1.47	1.40
1	L5	2364	OMG	C6-N1	-2.46	1.34	1.37
46	S2	116	OMU	C4-N3	-2.46	1.34	1.38
46	S2	484	A2M	C5-C4	2.45	1.47	1.40
3	L8	75	OMG	C6-N1	-2.44	1.34	1.37
1	L5	1534	A2M	C5-C4	2.44	1.47	1.40
46	S2	1490	OMG	C6-N1	-2.43	1.34	1.37
1	L5	1316	OMG	C6-N1	-2.42	1.34	1.37
1	L5	2815	A2M	C5-C4	2.42	1.47	1.40
1	L5	398	A2M	C5-C4	2.42	1.47	1.40
1	L5	3822	PSU	C2-N3	-2.42	1.33	1.37
46	S2	1056	PSU	C2-N3	-2.42	1.33	1.37
1	L5	2401	A2M	C5-C4	2.41	1.47	1.40
1	L5	3718	A2M	C5-C4	2.41	1.47	1.40
1	L5	4523	A2M	C5-C4	2.40	1.47	1.40
1	L5	400	A2M	C5-C4	2.40	1.47	1.40
1	L5	4590	A2M	C5-C4	2.40	1.47	1.40
1	L5	1522	OMG	C6-N1	-2.40	1.34	1.37
46	S2	1678	A2M	C5-C4	2.39	1.47	1.40
46	S2	1851	MA6	C5-C4	2.38	1.47	1.40
1	L5	1524	A2M	C5-C4	2.38	1.47	1.40
1	L5	4220	6MZ	C5-C4	2.37	1.47	1.40
1	L5	4571	A2M	C5-C4	2.37	1.47	1.40
1	L5	4196	OMG	C6-N1	-2.37	1.34	1.37
1	L5	3867	A2M	C5-C4	2.36	1.47	1.40
46	S2	1383	A2M	C5-C4	2.36	1.47	1.40
1	L5	2787	A2M	C5-C4	2.36	1.47	1.40
46	S2	512	A2M	C5-C4	2.36	1.47	1.40
1	L5	4227	OMU	C2-N3	-2.36	1.33	1.38
1	L5	4306	OMU	C2-N3	-2.35	1.33	1.38
46	S2	590	A2M	C5-C4	2.35	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2363	A2M	C5-C4	2.35	1.47	1.40
1	L5	1871	A2M	C5-C4	2.34	1.47	1.40
1	L5	1323	A2M	C5-C4	2.34	1.47	1.40
1	L5	4618	OMG	C6-N1	-2.34	1.34	1.37
46	S2	468	A2M	C5-C4	2.34	1.47	1.40
46	S2	1842	4AC	C4-N4	-2.33	1.36	1.39
1	L5	1326	A2M	C5-C4	2.32	1.47	1.40
46	S2	1045	PSU	C2-N3	-2.30	1.33	1.37
1	L5	3830	A2M	C5-C4	2.29	1.47	1.40
1	L5	4228	OMG	C6-N1	-2.28	1.34	1.37
1	L5	2415	OMU	C2-N3	-2.28	1.33	1.38
3	L8	14	OMU	C2-N3	-2.28	1.33	1.38
1	L5	1677	PSU	O4'-C1'	-2.28	1.40	1.43
1	L5	3782	5MC	C6-N1	-2.28	1.34	1.38
1	L5	2843	PSU	C2-N3	-2.27	1.33	1.37
1	L5	1582	PSU	C2-N3	-2.26	1.33	1.37
46	S2	1442	OMU	C2-N3	-2.25	1.34	1.38
46	S2	172	OMU	C2-N3	-2.24	1.34	1.38
46	S2	428	OMU	C2-N3	-2.24	1.34	1.38
1	L5	4623	OMG	C6-N1	-2.23	1.34	1.37
1	L5	4493	PSU	C2-N3	-2.23	1.33	1.37
1	L5	2837	OMU	C2-N3	-2.22	1.34	1.38
46	S2	121	OMU	C2-N3	-2.21	1.34	1.38
46	S2	576	A2M	C5-C4	2.21	1.46	1.40
46	S2	27	A2M	C5-C4	2.20	1.46	1.40
46	S2	1850	MA6	C5-C4	2.20	1.46	1.40
46	S2	1328	OMG	C8-N7	-2.20	1.31	1.35
1	L5	4370	OMG	C6-N1	-2.20	1.34	1.37
1	L5	3825	A2M	C5-C4	2.19	1.46	1.40
46	S2	1003	PSU	C2-N3	-2.19	1.33	1.37
46	S2	1004	PSU	C2-N3	-2.17	1.33	1.37
5	LB	245	HIC	CZ-NE2	-2.16	1.42	1.48
46	S2	1238	PSU	C2-N3	-2.15	1.33	1.37
46	S2	1046	PSU	C2-N3	-2.15	1.33	1.37
46	S2	1288	OMU	C2-N3	-2.13	1.34	1.38
46	S2	681	PSU	C2-N3	-2.13	1.33	1.37
1	L5	4620	OMU	C2-N3	-2.12	1.34	1.38
1	L5	3925	OMU	C2-N3	-2.12	1.34	1.38
1	L5	1782	PSU	C2-N3	-2.12	1.33	1.37
46	S2	366	PSU	C2-N3	-2.11	1.33	1.37
46	S2	683	OMG	C8-N7	-2.11	1.31	1.35
46	S2	1031	A2M	C5-C4	2.10	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2415	OMU	C5-C4	-2.09	1.39	1.43
1	L5	398	A2M	O4'-C1'	2.09	1.44	1.41
3	L8	14	OMU	C2-N1	2.09	1.41	1.38
46	S2	1692	PSU	C2-N3	-2.09	1.33	1.37
1	L5	4620	OMU	C5-C4	-2.09	1.39	1.43
46	S2	867	OMG	C8-N7	-2.08	1.31	1.35
1	L5	3841	OMC	C6-C5	2.07	1.39	1.35
1	L5	3768	PSU	C2-N3	-2.07	1.34	1.37
46	S2	93	PSU	C2-N3	-2.07	1.34	1.37
46	S2	121	OMU	C5-C4	-2.06	1.39	1.43
1	L5	3844	PSU	C2-N3	-2.06	1.34	1.37
46	S2	590	A2M	O4'-C1'	2.06	1.44	1.41
1	L5	3770	PSU	C2-N3	-2.06	1.34	1.37
1	L5	3715	PSU	C2-N1	-2.05	1.33	1.36
1	L5	4353	PSU	C2-N3	-2.05	1.34	1.37
1	L5	4423	PSU	C2-N3	-2.05	1.34	1.37
1	L5	2508	PSU	C2-N3	-2.04	1.34	1.37
46	S2	814	PSU	C2-N3	-2.03	1.34	1.37
46	S2	406	PSU	C2-N3	-2.03	1.34	1.37
46	S2	651	PSU	C2-N3	-2.03	1.34	1.37
1	L5	4499	OMG	C8-N7	-2.02	1.31	1.35
1	L5	2839	PSU	C2-N3	-2.02	1.34	1.37
46	S2	116	OMU	C2-N3	-2.01	1.34	1.38
46	S2	116	OMU	C5-C4	-2.01	1.39	1.43
1	L5	4306	OMU	C5-C4	-2.01	1.39	1.43
46	S2	1442	OMU	C5-C4	-2.01	1.39	1.43
1	L5	4403	PSU	C2-N3	-2.01	1.34	1.37
1	L5	3695	PSU	C2-N3	-2.00	1.34	1.37
1	L5	4523	A2M	O4'-C1'	2.00	1.43	1.41
1	L5	4628	PSU	C2-N3	-2.00	1.34	1.37

All (498) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	ST	67	NMM	NE-CZ-NH2	-8.35	111.82	119.48
46	S2	1832	6MZ	C2-N1-C6	8.01	123.46	116.59
46	S2	1174	PSU	N1-C2-N3	6.41	122.39	115.13
46	S2	1056	PSU	N1-C2-N3	6.39	122.37	115.13
1	L5	1677	PSU	N1-C2-N3	6.37	122.35	115.13
46	S2	366	PSU	N1-C2-N3	6.34	122.31	115.13
1	L5	3770	PSU	N1-C2-N3	6.30	122.27	115.13
1	L5	3822	PSU	N1-C2-N3	6.29	122.25	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3715	PSU	N1-C2-N3	6.28	122.25	115.13
46	S2	105	PSU	N1-C2-N3	6.27	122.23	115.13
1	L5	3851	PSU	N1-C2-N3	6.24	122.20	115.13
1	L5	4353	PSU	N1-C2-N3	6.24	122.20	115.13
1	L5	4361	PSU	N1-C2-N3	6.21	122.16	115.13
1	L5	1860	PSU	N1-C2-N3	6.20	122.16	115.13
1	L5	1862	PSU	N1-C2-N3	6.20	122.15	115.13
1	L5	4636	PSU	N1-C2-N3	6.20	122.15	115.13
1	L5	4220	6MZ	C2-N1-C6	6.18	121.89	116.59
46	S2	109	PSU	N1-C2-N3	6.18	122.13	115.13
1	L5	4403	PSU	N1-C2-N3	6.18	122.13	115.13
46	S2	296	PSU	N1-C2-N3	6.17	122.12	115.13
1	L5	4457	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	1779	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	3768	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	4689	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	3920	PSU	N1-C2-N3	6.15	122.10	115.13
1	L5	3844	PSU	N1-C2-N3	6.15	122.10	115.13
46	S2	406	PSU	N1-C2-N3	6.13	122.08	115.13
46	S2	1367	PSU	N1-C2-N3	6.13	122.07	115.13
46	S2	63	PSU	N1-C2-N3	6.12	122.07	115.13
1	L5	1781	PSU	N1-C2-N3	6.12	122.06	115.13
1	L5	4423	PSU	N1-C2-N3	6.10	122.05	115.13
1	L5	4521	PSU	N1-C2-N3	6.10	122.04	115.13
46	S2	1177	PSU	N1-C2-N3	6.10	122.04	115.13
1	L5	1744	PSU	N1-C2-N3	6.09	122.03	115.13
46	S2	681	PSU	N1-C2-N3	6.08	122.02	115.13
3	L8	55	PSU	N1-C2-N3	6.07	122.01	115.13
1	L5	2839	PSU	N1-C2-N3	6.06	122.00	115.13
46	S2	1445	PSU	N1-C2-N3	6.05	121.99	115.13
46	S2	300	PSU	N1-C2-N3	6.05	121.98	115.13
46	S2	649	PSU	N1-C2-N3	6.04	121.97	115.13
1	L5	2508	PSU	N1-C2-N3	6.03	121.97	115.13
46	S2	1692	PSU	N1-C2-N3	6.03	121.96	115.13
46	S2	918	PSU	N1-C2-N3	6.03	121.96	115.13
46	S2	1004	PSU	N1-C2-N3	6.02	121.95	115.13
1	L5	3884	PSU	N1-C2-N3	6.02	121.95	115.13
46	S2	1046	PSU	N1-C2-N3	5.99	121.92	115.13
1	L5	3695	PSU	N1-C2-N3	5.98	121.91	115.13
46	S2	1643	PSU	N1-C2-N3	5.97	121.89	115.13
1	L5	4628	PSU	N1-C2-N3	5.95	121.87	115.13
1	L5	1782	PSU	N1-C2-N3	5.95	121.87	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	93	PSU	N1-C2-N3	5.94	121.86	115.13
1	L5	1792	PSU	N1-C2-N3	5.93	121.85	115.13
46	S2	651	PSU	N1-C2-N3	5.92	121.84	115.13
1	L5	4972	PSU	N1-C2-N3	5.91	121.83	115.13
46	S2	814	PSU	N1-C2-N3	5.90	121.82	115.13
46	S2	1232	PSU	N1-C2-N3	5.90	121.81	115.13
1	L5	4471	PSU	N1-C2-N3	5.90	121.81	115.13
1	L5	4442	PSU	N1-C2-N3	5.89	121.81	115.13
1	L5	4552	PSU	N1-C2-N3	5.88	121.79	115.13
46	S2	1238	PSU	N1-C2-N3	5.87	121.78	115.13
46	S2	218	PSU	N1-C2-N3	5.86	121.77	115.13
46	S2	572	PSU	N1-C2-N3	5.85	121.76	115.13
1	L5	4431	PSU	N1-C2-N3	5.85	121.76	115.13
46	S2	1625	PSU	N1-C2-N3	5.84	121.75	115.13
46	S2	1045	PSU	N1-C2-N3	5.84	121.75	115.13
1	L5	4493	PSU	N1-C2-N3	5.83	121.73	115.13
1	L5	1683	PSU	N1-C2-N3	5.81	121.72	115.13
46	S2	119	PSU	N1-C2-N3	5.78	121.67	115.13
1	L5	4312	PSU	N1-C2-N3	5.75	121.65	115.13
46	S2	815	PSU	N1-C2-N3	5.69	121.57	115.13
46	S2	1003	PSU	N1-C2-N3	5.68	121.57	115.13
1	L5	4973	PSU	N1-C2-N3	5.65	121.54	115.13
1	L5	1536	PSU	N1-C2-N3	5.61	121.49	115.13
1	L5	1582	PSU	N1-C2-N3	5.56	121.42	115.13
1	L5	2843	PSU	N1-C2-N3	5.55	121.42	115.13
1	L5	3853	PSU	N1-C2-N3	5.43	121.28	115.13
46	S2	1248	B8N	C4-N3-C2	-5.11	118.99	125.46
46	S2	172	OMU	C4-N3-C2	-4.88	120.14	126.58
1	L5	2837	OMU	C4-N3-C2	-4.71	120.37	126.58
46	S2	681	PSU	C4-N3-C2	-4.68	119.60	126.34
46	S2	354	OMU	C4-N3-C2	-4.68	120.41	126.58
1	L5	4227	OMU	C4-N3-C2	-4.64	120.45	126.58
46	S2	116	OMU	C4-N3-C2	-4.60	120.51	126.58
46	S2	1238	PSU	C4-N3-C2	-4.58	119.74	126.34
46	S2	1442	OMU	C4-N3-C2	-4.57	120.55	126.58
46	S2	1288	OMU	C4-N3-C2	-4.53	120.61	126.58
1	L5	4306	OMU	C4-N3-C2	-4.50	120.64	126.58
1	L5	1677	PSU	C4-N3-C2	-4.48	119.89	126.34
1	L5	3925	OMU	C4-N3-C2	-4.46	120.70	126.58
1	L5	2415	OMU	C4-N3-C2	-4.42	120.75	126.58
46	S2	428	OMU	C4-N3-C2	-4.41	120.76	126.58
46	S2	116	OMU	N3-C2-N1	4.40	120.74	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1177	PSU	C4-N3-C2	-4.39	120.01	126.34
46	S2	354	OMU	N3-C2-N1	4.38	120.70	114.89
1	L5	2837	OMU	N3-C2-N1	4.38	120.70	114.89
1	L5	4636	PSU	C4-N3-C2	-4.36	120.05	126.34
46	S2	172	OMU	N3-C2-N1	4.36	120.68	114.89
46	S2	121	OMU	C4-N3-C2	-4.35	120.84	126.58
1	L5	3925	OMU	N3-C2-N1	4.34	120.65	114.89
1	L5	1781	PSU	C4-N3-C2	-4.34	120.09	126.34
1	L5	3851	PSU	C4-N3-C2	-4.33	120.09	126.34
3	L8	14	OMU	C4-N3-C2	-4.33	120.87	126.58
1	L5	4227	OMU	N3-C2-N1	4.32	120.62	114.89
46	S2	1046	PSU	C4-N3-C2	-4.32	120.12	126.34
1	L5	4306	OMU	N3-C2-N1	4.30	120.59	114.89
1	L5	4361	PSU	C4-N3-C2	-4.25	120.22	126.34
46	S2	366	PSU	C4-N3-C2	-4.24	120.22	126.34
1	L5	4353	PSU	C4-N3-C2	-4.24	120.23	126.34
46	S2	649	PSU	C4-N3-C2	-4.23	120.25	126.34
59	ST	67	NMM	NE-CZ-NH1	4.22	128.18	120.26
46	S2	1174	PSU	C4-N3-C2	-4.21	120.27	126.34
1	L5	4689	PSU	C4-N3-C2	-4.20	120.29	126.34
46	S2	121	OMU	N3-C2-N1	4.16	120.41	114.89
1	L5	4620	OMU	C4-N3-C2	-4.15	121.11	126.58
46	S2	1442	OMU	N3-C2-N1	4.13	120.38	114.89
1	L5	3695	PSU	C4-N3-C2	-4.13	120.38	126.34
1	L5	4972	PSU	C4-N3-C2	-4.12	120.40	126.34
46	S2	63	PSU	C4-N3-C2	-4.12	120.41	126.34
1	L5	1862	PSU	C4-N3-C2	-4.11	120.42	126.34
1	L5	4493	PSU	C4-N3-C2	-4.11	120.42	126.34
1	L5	4521	PSU	C4-N3-C2	-4.11	120.42	126.34
1	L5	4620	OMU	N3-C2-N1	4.10	120.33	114.89
46	S2	1288	OMU	N3-C2-N1	4.08	120.31	114.89
46	S2	296	PSU	C4-N3-C2	-4.08	120.46	126.34
46	S2	815	PSU	C4-N3-C2	-4.06	120.49	126.34
46	S2	651	PSU	C4-N3-C2	-4.06	120.49	126.34
1	L5	1744	PSU	C4-N3-C2	-4.04	120.52	126.34
46	S2	105	PSU	C4-N3-C2	-4.04	120.52	126.34
1	L5	2508	PSU	C4-N3-C2	-4.04	120.52	126.34
1	L5	3768	PSU	C4-N3-C2	-4.04	120.52	126.34
46	S2	300	PSU	C4-N3-C2	-4.04	120.52	126.34
1	L5	2415	OMU	N3-C2-N1	4.03	120.25	114.89
1	L5	3920	PSU	C4-N3-C2	-4.03	120.53	126.34
1	L5	1779	PSU	C4-N3-C2	-4.03	120.53	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4403	PSU	C4-N3-C2	-4.00	120.58	126.34
46	S2	1004	PSU	C4-N3-C2	-3.99	120.58	126.34
1	L5	4423	PSU	C4-N3-C2	-3.99	120.59	126.34
46	S2	1851	MA6	C4-C5-N7	-3.98	105.25	109.40
1	L5	1782	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L5	3822	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L5	3884	PSU	C4-N3-C2	-3.97	120.62	126.34
46	S2	218	PSU	C4-N3-C2	-3.96	120.63	126.34
1	L5	4552	PSU	C4-N3-C2	-3.96	120.63	126.34
3	L8	55	PSU	C4-N3-C2	-3.96	120.64	126.34
1	L5	3715	PSU	C4-N3-C2	-3.96	120.64	126.34
1	L5	3695	PSU	O2-C2-N1	-3.96	118.43	122.79
46	S2	1056	PSU	C4-N3-C2	-3.95	120.64	126.34
1	L5	4457	PSU	C4-N3-C2	-3.95	120.65	126.34
1	L5	4312	PSU	C4-N3-C2	-3.94	120.66	126.34
3	L8	14	OMU	C5-C4-N3	3.94	120.73	114.84
1	L5	4442	PSU	C4-N3-C2	-3.93	120.67	126.34
1	L5	3844	PSU	C4-N3-C2	-3.92	120.69	126.34
46	S2	1031	A2M	N3-C2-N1	-3.92	122.55	128.68
1	L5	4431	PSU	C4-N3-C2	-3.92	120.70	126.34
1	L5	1582	PSU	C4-N3-C2	-3.91	120.70	126.34
46	S2	1232	PSU	C4-N3-C2	-3.91	120.71	126.34
1	L5	1683	PSU	C4-N3-C2	-3.90	120.73	126.34
46	S2	93	PSU	C4-N3-C2	-3.89	120.73	126.34
46	S2	1445	PSU	C4-N3-C2	-3.89	120.74	126.34
46	S2	428	OMU	N3-C2-N1	3.89	120.05	114.89
46	S2	918	PSU	C4-N3-C2	-3.88	120.75	126.34
46	S2	109	PSU	C4-N3-C2	-3.88	120.75	126.34
1	L5	1860	PSU	C4-N3-C2	-3.87	120.76	126.34
46	S2	1367	PSU	C4-N3-C2	-3.86	120.77	126.34
46	S2	1643	PSU	C4-N3-C2	-3.86	120.78	126.34
46	S2	1003	PSU	C4-N3-C2	-3.86	120.78	126.34
1	L5	1792	PSU	C4-N3-C2	-3.85	120.79	126.34
1	L5	4628	PSU	C4-N3-C2	-3.85	120.80	126.34
1	L5	2843	PSU	C4-N3-C2	-3.84	120.81	126.34
46	S2	814	PSU	C4-N3-C2	-3.82	120.83	126.34
46	S2	1625	PSU	C4-N3-C2	-3.80	120.86	126.34
1	L5	4689	PSU	O2-C2-N1	-3.80	118.61	122.79
1	L5	3770	PSU	C4-N3-C2	-3.79	120.88	126.34
1	L5	2839	PSU	C4-N3-C2	-3.78	120.89	126.34
46	S2	428	OMU	C5-C4-N3	3.78	120.50	114.84
46	S2	27	A2M	N3-C2-N1	-3.78	122.77	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4973	PSU	C4-N3-C2	-3.78	120.90	126.34
46	S2	354	OMU	C5-C4-N3	3.77	120.48	114.84
1	L5	3768	PSU	O2-C2-N1	-3.77	118.64	122.79
1	L5	1683	PSU	O2-C2-N1	-3.76	118.65	122.79
46	S2	119	PSU	C4-N3-C2	-3.76	120.92	126.34
1	L5	1792	PSU	O2-C2-N1	-3.75	118.67	122.79
1	L5	4471	PSU	C4-N3-C2	-3.74	120.95	126.34
1	L5	3782	5MC	C5-C6-N1	-3.73	119.50	123.34
46	S2	1692	PSU	C4-N3-C2	-3.73	120.96	126.34
1	L5	4312	PSU	O2-C2-N1	-3.72	118.69	122.79
46	S2	572	PSU	C4-N3-C2	-3.72	120.98	126.34
1	L5	2837	OMU	C5-C4-N3	3.71	120.40	114.84
46	S2	1174	PSU	O2-C2-N1	-3.71	118.71	122.79
46	S2	406	PSU	C4-N3-C2	-3.69	121.03	126.34
46	S2	1442	OMU	C5-C4-N3	3.68	120.34	114.84
1	L5	1860	PSU	O2-C2-N1	-3.67	118.75	122.79
46	S2	1288	OMU	C5-C4-N3	3.67	120.33	114.84
1	L5	4636	PSU	O2-C2-N1	-3.67	118.75	122.79
46	S2	1832	6MZ	N3-C2-N1	-3.66	122.96	128.68
46	S2	172	OMU	C5-C4-N3	3.66	120.31	114.84
1	L5	2415	OMU	C5-C4-N3	3.64	120.28	114.84
1	L5	3715	PSU	O2-C2-N1	-3.63	118.80	122.79
1	L5	4227	OMU	C5-C4-N3	3.61	120.25	114.84
1	L5	1536	PSU	C4-N3-C2	-3.61	121.14	126.34
46	S2	1850	MA6	N3-C2-N1	-3.60	123.05	128.68
1	L5	1862	PSU	O2-C2-N1	-3.60	118.82	122.79
1	L5	4457	PSU	O2-C2-N1	-3.60	118.83	122.79
46	S2	116	OMU	C5-C4-N3	3.60	120.22	114.84
46	S2	822	PSU	C3'-C2'-C1'	3.59	105.81	101.64
1	L5	4620	OMU	C5-C4-N3	3.59	120.20	114.84
1	L5	4306	OMU	C5-C4-N3	3.58	120.19	114.84
46	S2	406	PSU	O2-C2-N1	-3.57	118.86	122.79
46	S2	651	PSU	O2-C2-N1	-3.56	118.87	122.79
1	L5	4361	PSU	O2-C2-N1	-3.56	118.88	122.79
46	S2	218	PSU	O2-C2-N1	-3.56	118.88	122.79
46	S2	121	OMU	C5-C4-N3	3.55	120.16	114.84
46	S2	105	PSU	O2-C2-N1	-3.55	118.88	122.79
1	L5	3851	PSU	O2-C2-N1	-3.54	118.89	122.79
3	L8	14	OMU	N3-C2-N1	3.52	119.56	114.89
1	L5	2787	A2M	N3-C2-N1	-3.52	123.18	128.68
46	S2	1850	MA6	C4-C5-N7	-3.50	105.75	109.40
46	S2	681	PSU	O2-C2-N1	-3.50	118.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1045	PSU	C4-N3-C2	-3.49	121.30	126.34
1	L5	4972	PSU	O2-C2-N1	-3.49	118.95	122.79
1	L5	3844	PSU	O2-C2-N1	-3.49	118.95	122.79
1	L5	1677	PSU	O2-C2-N1	-3.49	118.95	122.79
1	L5	3853	PSU	C4-N3-C2	-3.48	121.32	126.34
1	L5	4628	PSU	O2-C2-N1	-3.48	118.96	122.79
1	L5	4973	PSU	O2-C2-N1	-3.48	118.96	122.79
1	L5	4403	PSU	O2-C2-N1	-3.43	119.01	122.79
1	L5	4220	6MZ	N3-C2-N1	-3.42	123.33	128.68
1	L5	4471	PSU	O2-C2-N1	-3.42	119.02	122.79
1	L5	1779	PSU	O2-C2-N1	-3.42	119.03	122.79
1	L5	4521	PSU	O2-C2-N1	-3.42	119.03	122.79
46	S2	1367	PSU	O2-C2-N1	-3.41	119.03	122.79
1	L5	3925	OMU	C5-C4-N3	3.41	119.94	114.84
46	S2	1003	PSU	O2-C2-N1	-3.41	119.04	122.79
1	L5	1871	A2M	N3-C2-N1	-3.40	123.36	128.68
1	L5	1323	A2M	N3-C2-N1	-3.39	123.38	128.68
46	S2	512	A2M	N3-C2-N1	-3.39	123.38	128.68
46	S2	119	PSU	O2-C2-N1	-3.39	119.06	122.79
46	S2	918	PSU	O2-C2-N1	-3.38	119.07	122.79
46	S2	1445	PSU	O2-C2-N1	-3.38	119.07	122.79
46	S2	1177	PSU	O2-C2-N1	-3.38	119.07	122.79
46	S2	296	PSU	O2-C2-N1	-3.38	119.07	122.79
46	S2	1625	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L5	4552	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L5	4431	PSU	O2-C2-N1	-3.37	119.08	122.79
46	S2	1232	PSU	O2-C2-N1	-3.37	119.08	122.79
46	S2	468	A2M	N3-C2-N1	-3.36	123.43	128.68
1	L5	1781	PSU	O2-C2-N1	-3.35	119.11	122.79
46	S2	109	PSU	O2-C2-N1	-3.34	119.11	122.79
46	S2	1004	PSU	O2-C2-N1	-3.34	119.11	122.79
1	L5	3770	PSU	O2-C2-N1	-3.33	119.12	122.79
1	L5	4353	PSU	O2-C2-N1	-3.33	119.12	122.79
1	L5	400	A2M	N3-C2-N1	-3.31	123.51	128.68
1	L5	1326	A2M	N3-C2-N1	-3.30	123.52	128.68
46	S2	815	PSU	O2-C2-N1	-3.29	119.17	122.79
1	L5	4523	A2M	N3-C2-N1	-3.28	123.55	128.68
46	S2	1643	PSU	O2-C2-N1	-3.28	119.18	122.79
1	L5	4590	A2M	N3-C2-N1	-3.28	123.55	128.68
46	S2	590	A2M	N3-C2-N1	-3.26	123.58	128.68
46	S2	1851	MA6	N3-C2-N1	-3.26	123.58	128.68
1	L5	3825	A2M	N3-C2-N1	-3.26	123.59	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4571	A2M	N3-C2-N1	-3.25	123.59	128.68
1	L5	4442	PSU	O2-C2-N1	-3.25	119.21	122.79
1	L5	4423	PSU	O2-C2-N1	-3.25	119.22	122.79
46	S2	649	PSU	O2-C2-N1	-3.25	119.22	122.79
1	L5	2415	OMU	O4-C4-C5	-3.24	119.46	125.16
46	S2	1692	PSU	O2-C2-N1	-3.22	119.24	122.79
46	S2	572	PSU	O2-C2-N1	-3.22	119.25	122.79
1	L5	3867	A2M	N3-C2-N1	-3.21	123.66	128.68
3	L8	55	PSU	O2-C2-N1	-3.21	119.26	122.79
46	S2	1678	A2M	N3-C2-N1	-3.20	123.67	128.68
1	L5	1744	PSU	O2-C2-N1	-3.20	119.26	122.79
1	L5	3884	PSU	O2-C2-N1	-3.20	119.27	122.79
46	S2	366	PSU	O2-C2-N1	-3.17	119.30	122.79
1	L5	2401	A2M	N3-C2-N1	-3.16	123.74	128.68
1	L5	3853	PSU	O2-C2-N1	-3.16	119.31	122.79
1	L5	2815	A2M	N3-C2-N1	-3.16	123.74	128.68
1	L5	2837	OMU	O4-C4-C5	-3.16	119.61	125.16
1	L5	1524	A2M	N3-C2-N1	-3.15	123.75	128.68
46	S2	63	PSU	O2-C2-N1	-3.15	119.32	122.79
46	S2	166	A2M	N3-C2-N1	-3.14	123.77	128.68
46	S2	484	A2M	N3-C2-N1	-3.14	123.77	128.68
46	S2	1046	PSU	O2-C2-N1	-3.13	119.34	122.79
1	L5	3920	PSU	O2-C2-N1	-3.13	119.35	122.79
46	S2	484	A2M	C4-C5-N7	-3.09	106.17	109.40
1	L5	2787	A2M	C4-C5-N7	-3.09	106.18	109.40
3	L8	14	OMU	O4-C4-C5	-3.08	119.75	125.16
1	L5	1582	PSU	O2-C2-N1	-3.05	119.43	122.79
46	S2	300	PSU	O2-C2-N1	-3.05	119.44	122.79
46	S2	116	OMU	O4-C4-C5	-3.04	119.81	125.16
1	L5	398	A2M	N3-C2-N1	-3.04	123.93	128.68
46	S2	1288	OMU	O4-C4-C5	-3.03	119.83	125.16
1	L5	1782	PSU	O2-C2-N1	-3.01	119.47	122.79
46	S2	814	PSU	O2-C2-N1	-3.00	119.48	122.79
1	L5	1536	PSU	O2-C2-N1	-2.99	119.50	122.79
46	S2	1442	OMU	O4-C4-C5	-2.97	119.94	125.16
46	S2	121	OMU	O4-C4-C5	-2.97	119.94	125.16
1	L5	2508	PSU	O2-C2-N1	-2.96	119.53	122.79
46	S2	1056	PSU	O2-C2-N1	-2.95	119.54	122.79
1	L5	2363	A2M	C4-C5-N7	-2.95	106.33	109.40
1	L5	4306	OMU	O4-C4-C5	-2.94	119.98	125.16
1	L5	4620	OMU	O4-C4-C5	-2.94	120.00	125.16
46	S2	172	OMU	O4-C4-C5	-2.93	120.01	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1534	A2M	C4-C5-N7	-2.92	106.36	109.40
46	S2	354	OMU	O4-C4-C5	-2.91	120.04	125.16
46	S2	468	A2M	C4-C5-N7	-2.91	106.37	109.40
46	S2	1850	MA6	C1'-N9-C4	-2.90	121.54	126.64
1	L5	398	A2M	C4-C5-N7	-2.90	106.38	109.40
1	L5	4227	OMU	O4-C4-C5	-2.88	120.09	125.16
46	S2	1832	6MZ	C4-C5-N7	-2.88	106.40	109.40
46	S2	428	OMU	O4-C4-C5	-2.88	120.10	125.16
46	S2	27	A2M	C4-C5-N7	-2.87	106.41	109.40
46	S2	576	A2M	N3-C2-N1	-2.86	124.21	128.68
1	L5	2837	OMU	O2-C2-N1	-2.86	118.99	122.79
46	S2	576	A2M	C4-C5-N7	-2.85	106.42	109.40
1	L5	3925	OMU	O4-C4-C5	-2.84	120.17	125.16
1	L5	2363	A2M	N3-C2-N1	-2.84	124.25	128.68
1	L5	3830	A2M	N3-C2-N1	-2.82	124.27	128.68
46	S2	93	PSU	O2-C2-N1	-2.81	119.69	122.79
46	S2	1238	PSU	O2-C2-N1	-2.81	119.69	122.79
1	L5	1323	A2M	C4-C5-N7	-2.81	106.47	109.40
46	S2	159	A2M	N3-C2-N1	-2.80	124.30	128.68
1	L5	2839	PSU	O2-C2-N1	-2.80	119.71	122.79
46	S2	1337	4AC	C6-C5-C4	2.79	120.38	116.96
1	L5	4571	A2M	C4-C5-N7	-2.79	106.50	109.40
1	L5	1534	A2M	N3-C2-N1	-2.77	124.34	128.68
46	S2	1383	A2M	N3-C2-N1	-2.77	124.35	128.68
1	L5	3718	A2M	C4-C5-N7	-2.77	106.52	109.40
1	L5	3718	A2M	N3-C2-N1	-2.76	124.36	128.68
1	L5	3792	OMG	C5-C6-N1	2.74	118.80	113.95
1	L5	3830	A2M	C4-C5-N7	-2.73	106.56	109.40
46	S2	172	OMU	O2-C2-N1	-2.72	119.16	122.79
1	L5	4590	A2M	C4-C5-N7	-2.70	106.58	109.40
1	L5	1871	A2M	C4-C5-N7	-2.70	106.58	109.40
46	S2	1248	B8N	N3-C2-N1	2.70	120.57	116.76
46	S2	159	A2M	C4-C5-N7	-2.70	106.59	109.40
1	L5	3867	A2M	C4-C5-N7	-2.70	106.59	109.40
46	S2	354	OMU	O2-C2-N1	-2.69	119.20	122.79
46	S2	1045	PSU	O2-C2-N1	-2.69	119.82	122.79
1	L5	3782	5MC	C5-C4-N3	-2.69	118.77	121.67
46	S2	1851	MA6	N1-C6-N6	2.67	119.87	117.06
46	S2	1383	A2M	C4-C5-N7	-2.67	106.62	109.40
46	S2	1842	4AC	C6-C5-C4	2.65	120.20	116.96
1	L5	2876	OMG	C5-C6-N1	2.63	118.60	113.95
46	S2	918	PSU	O4'-C1'-C2'	2.63	108.85	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	512	A2M	C4-C5-N7	-2.62	106.67	109.40
1	L5	1522	OMG	C8-N7-C5	2.61	107.96	102.99
1	L5	2401	A2M	C4-C5-N7	-2.59	106.70	109.40
1	L5	400	A2M	C4-C5-N7	-2.58	106.71	109.40
46	S2	1031	A2M	C2-N1-C6	2.57	123.14	118.75
1	L5	3825	A2M	C4-C5-N7	-2.56	106.73	109.40
1	L5	4392	OMG	C5-C6-N1	2.56	118.47	113.95
1	L5	1524	A2M	C4-C5-N7	-2.55	106.75	109.40
46	S2	116	OMU	O2-C2-N1	-2.54	119.42	122.79
46	S2	436	OMG	C5-C6-N1	2.52	118.40	113.95
46	S2	1490	OMG	C5-C6-N1	2.51	118.39	113.95
1	L5	2815	A2M	C4-C5-N7	-2.51	106.79	109.40
46	S2	590	A2M	C4-C5-N7	-2.50	106.79	109.40
46	S2	166	A2M	C4-C5-N7	-2.49	106.80	109.40
1	L5	4220	6MZ	C9-N6-C6	-2.48	120.73	122.87
1	L5	2364	OMG	C8-N7-C5	2.48	107.71	102.99
1	L5	4392	OMG	C8-N7-C5	2.47	107.70	102.99
1	L5	3899	OMG	C5-C6-N1	2.46	118.30	113.95
46	S2	1678	A2M	C4-C5-N7	-2.46	106.84	109.40
46	S2	1238	PSU	C5-C6-N1	-2.45	118.43	122.11
1	L5	4618	OMG	C8-N7-C5	2.45	107.66	102.99
1	L5	2415	OMU	C1'-N1-C2	2.45	122.01	117.57
1	L5	3627	OMG	C5-C6-N1	2.44	118.27	113.95
1	L5	1522	OMG	C5-C6-N1	2.43	118.24	113.95
46	S2	644	OMG	C5-C6-N1	2.43	118.24	113.95
1	L5	4523	A2M	C4-C5-N7	-2.42	106.88	109.40
1	L5	2876	OMG	C8-N7-C5	2.42	107.60	102.99
1	L5	1322	1MA	N1-C2-N3	-2.42	123.20	126.02
46	S2	1842	4AC	C5-C4-N3	-2.41	118.71	122.59
1	L5	4493	PSU	O2-C2-N1	-2.41	120.14	122.79
1	L5	3822	PSU	C5-C6-N1	-2.40	118.50	122.11
1	L5	3627	OMG	C8-N7-C5	2.40	107.56	102.99
46	S2	436	OMG	C8-N7-C5	2.40	107.55	102.99
1	L5	4306	OMU	O2-C2-N1	-2.39	119.61	122.79
46	S2	121	OMU	O2-C2-N1	-2.39	119.61	122.79
46	S2	366	PSU	C5-C6-N1	-2.39	118.53	122.11
1	L5	1781	PSU	C5-C6-N1	-2.38	118.53	122.11
1	L5	3825	A2M	C2-N1-C6	2.38	122.82	118.75
1	L5	2351	OMC	O2-C2-N3	-2.37	118.48	122.33
1	L5	3744	OMG	C5-C6-N1	2.37	118.13	113.95
3	L8	14	OMU	C1'-N1-C2	2.37	121.85	117.57
46	S2	1337	4AC	C5-C4-N3	-2.36	118.79	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	509	OMG	C5-C6-N1	2.35	118.10	113.95
46	S2	509	OMG	C8-N7-C5	2.35	107.47	102.99
1	L5	4370	OMG	C8-N7-C5	2.35	107.46	102.99
1	L5	1625	OMG	C8-N7-C5	2.34	107.45	102.99
1	L5	2843	PSU	O2-C2-N1	-2.34	120.22	122.79
1	L5	4228	OMG	C8-N7-C5	2.34	107.44	102.99
46	S2	601	OMG	C8-N7-C5	2.34	107.44	102.99
1	L5	3822	PSU	O2-C2-N1	-2.34	120.22	122.79
46	S2	1360	PSU	C3'-C2'-C1'	2.34	104.36	101.64
1	L5	3841	OMC	O2-C2-N3	-2.33	118.54	122.33
1	L5	4623	OMG	C8-N7-C5	2.33	107.43	102.99
1	L5	4636	PSU	C5-C6-N1	-2.33	118.62	122.11
46	S2	1447	OMG	C8-N7-C5	2.33	107.42	102.99
3	L8	75	OMG	C8-N7-C5	2.33	107.42	102.99
1	L5	2876	OMG	O6-C6-C5	-2.32	119.84	124.37
46	S2	668	A2M	C5-C6-N6	2.32	123.88	120.35
1	L5	4623	OMG	C5-C6-N1	2.32	118.04	113.95
1	L5	1326	A2M	C4-C5-N7	-2.31	106.99	109.40
1	L5	4494	OMG	C5-C6-N1	2.30	118.02	113.95
1	L5	4618	OMG	C5-C6-N1	2.30	118.01	113.95
72	SO	138	IAS	OD1-CG-CB	-2.30	118.74	125.43
46	S2	1031	A2M	C4-C5-N7	-2.29	107.01	109.40
1	L5	4620	OMU	O2-C2-N1	-2.29	119.74	122.79
46	S2	99	A2M	C5-C6-N6	2.29	123.83	120.35
46	S2	1337	4AC	O7-C7-N4	2.28	125.52	121.82
1	L5	2424	OMG	C5-C6-N1	2.28	117.99	113.95
1	L5	1322	1MA	C5-C6-N1	2.28	117.30	113.90
1	L5	3744	OMG	C8-N7-C5	2.28	107.34	102.99
1	L5	4227	OMU	O2-C2-N1	-2.28	119.75	122.79
1	L5	1316	OMG	C5-C6-N1	2.28	117.97	113.95
1	L5	3822	PSU	O2-C2-N3	-2.27	117.53	121.82
1	L5	3724	A2M	C5-C6-N6	2.27	123.80	120.35
1	L5	4637	OMG	C8-N7-C5	2.27	107.31	102.99
1	L5	4370	OMG	C5-C6-N1	2.26	117.94	113.95
1	L5	4196	OMG	C8-N7-C5	2.26	107.29	102.99
46	S2	866	PSU	C2'-C3'-C4'	-2.26	98.26	102.64
1	L5	4196	OMG	C5-C6-N1	2.25	117.93	113.95
46	S2	1442	OMU	O2-C2-N1	-2.25	119.79	122.79
1	L5	4228	OMG	C5-C6-N1	2.25	117.93	113.95
3	L8	75	OMG	C5-C6-N1	2.25	117.93	113.95
46	S2	1046	PSU	C5-C6-N1	-2.25	118.74	122.11
46	S2	1490	OMG	C8-N7-C5	2.25	107.27	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	166	A2M	C5'-C4'-C3'	-2.24	106.78	115.18
1	L5	4353	PSU	C5-C6-N1	-2.24	118.75	122.11
1	L5	1582	PSU	C6-C5-C4	-2.23	116.64	118.20
1	L5	1677	PSU	C5-C6-N1	-2.23	118.77	122.11
46	S2	681	PSU	C5-C6-N1	-2.23	118.77	122.11
1	L5	3792	OMG	C8-N7-C5	2.23	107.23	102.99
46	S2	159	A2M	C5'-C4'-C3'	-2.22	106.84	115.18
1	L5	4493	PSU	C5-C6-N1	-2.22	118.77	122.11
46	S2	63	PSU	C5-C6-N1	-2.21	118.79	122.11
46	S2	1177	PSU	C5-C6-N1	-2.21	118.80	122.11
46	S2	1447	OMG	C5-C6-N1	2.20	117.84	113.95
1	L5	4442	PSU	O4'-C1'-C2'	2.19	108.23	105.14
1	L5	1862	PSU	C5-C6-N1	-2.19	118.83	122.11
1	L5	1782	PSU	C5-C6-N1	-2.18	118.84	122.11
1	L5	4403	PSU	O4'-C1'-C2'	2.18	108.21	105.14
1	L5	4637	OMG	C5-C6-N1	2.17	117.78	113.95
46	S2	601	OMG	C5-C6-N1	2.17	117.78	113.95
1	L5	3785	A2M	C5-C6-N6	2.17	123.65	120.35
72	SO	138	IAS	OXT-C-O	-2.17	119.17	124.09
46	S2	644	OMG	C8-N7-C5	2.16	107.11	102.99
46	S2	1272	OMC	O2-C2-N3	-2.16	118.81	122.33
1	L5	4361	PSU	C5-C6-N1	-2.16	118.87	122.11
1	L5	1316	OMG	O6-C6-C5	-2.16	120.16	124.37
1	L5	1316	OMG	C8-N7-C5	2.15	107.09	102.99
1	L5	3695	PSU	C5-C6-N1	-2.14	118.90	122.11
1	L5	3808	OMC	O2-C2-N3	-2.14	118.85	122.33
1	L5	2364	OMG	C5-C6-N1	2.14	117.73	113.95
1	L5	1779	PSU	C5-C6-N1	-2.13	118.91	122.11
1	L5	1625	OMG	C5-C6-N1	2.13	117.71	113.95
1	L5	4972	PSU	C5-C6-N1	-2.13	118.92	122.11
46	S2	1490	OMG	O6-C6-C5	-2.13	120.22	124.37
1	L5	4523	A2M	C2-N1-C6	2.12	122.38	118.75
1	L5	1677	PSU	O4'-C1'-C2'	2.11	108.12	105.14
46	S2	1056	PSU	O4'-C1'-C2'	2.11	108.12	105.14
1	L5	4521	PSU	C5-C6-N1	-2.11	118.95	122.11
46	S2	1288	OMU	C1'-N1-C2	2.11	121.38	117.57
1	L5	3792	OMG	O6-C6-C5	-2.10	120.27	124.37
1	L5	4370	OMG	O6-C6-C5	-2.10	120.27	124.37
1	L5	1871	A2M	C2-N1-C6	2.10	122.34	118.75
1	L5	4220	6MZ	C4-C5-N7	-2.10	107.21	109.40
46	S2	572	PSU	O4'-C1'-C2'	2.10	108.10	105.14
46	S2	468	A2M	C2-N1-C6	2.09	122.33	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1842	4AC	N4-C4-N3	2.09	117.36	113.85
46	S2	300	PSU	C5-C6-N1	-2.09	118.98	122.11
1	L5	2843	PSU	C5-C6-N1	-2.09	118.98	122.11
46	S2	1248	B8N	O4'-C1'-C2'	2.08	108.08	105.14
1	L5	1625	OMG	O6-C6-C5	-2.08	120.31	124.37
46	S2	1248	B8N	C31-N3-C2	2.08	120.78	117.67
46	S2	1248	B8N	O36-C34-O35	-2.07	119.38	124.09
1	L5	1779	PSU	O4'-C1'-C2'	2.07	108.06	105.14
1	L5	4590	A2M	C2-N1-C6	2.06	122.29	118.75
46	S2	1238	PSU	O4-C4-C5	-2.06	118.65	124.05
1	L5	1322	1MA	C8-N7-C5	2.06	106.91	102.99
1	L5	4494	OMG	C8-N7-C5	2.06	106.91	102.99
46	S2	1367	PSU	C5-C6-N1	-2.05	119.03	122.11
1	L5	3925	OMU	O2-C2-N1	-2.05	120.06	122.79
46	S2	1842	4AC	O7-C7-N4	2.04	125.12	121.82
72	SO	138	IAS	OXT-C-CA	2.04	120.33	113.38
46	S2	27	A2M	C2-N1-C6	2.04	122.24	118.75
46	S2	296	PSU	C5-C6-N1	-2.04	119.05	122.11
1	L5	3899	OMG	O6-C6-C5	-2.03	120.40	124.37
46	S2	159	A2M	C2'-C3'-C4'	2.03	106.40	101.99
1	L5	2424	OMG	O6-C6-C5	-2.02	120.42	124.37
1	L5	4228	OMG	O6-C6-C5	-2.02	120.42	124.37
1	L5	2839	PSU	C5-C6-N1	-2.02	119.08	122.11
1	L5	4623	OMG	O6-C6-C5	-2.02	120.42	124.37
1	L5	4636	PSU	O4'-C1'-C2'	2.01	107.98	105.14
46	S2	93	PSU	C5-C6-N1	-2.01	119.10	122.11
46	S2	1643	PSU	O4'-C1'-C2'	2.01	107.97	105.14
46	S2	1248	B8N	O36-C34-C33	2.00	120.20	113.38

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	14	OMU	C1'-C2'-O2'-CM2
1	L5	1582	PSU	O4'-C1'-C5-C4
1	L5	1582	PSU	O4'-C1'-C5-C6
1	L5	1677	PSU	C2'-C1'-C5-C6
1	L5	2824	OMC	C1'-C2'-O2'-CM2
1	L5	3701	OMC	C2'-C1'-N1-C6
1	L5	3724	A2M	C1'-C2'-O2'-CM'
1	L5	3770	PSU	C3'-C4'-C5'-O5'
1	L5	3818	UY1	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	L5	3851	PSU	C3'-C4'-C5'-O5'
1	L5	4196	OMG	C1'-C2'-O2'-CM2
1	L5	4500	PSU	C3'-C4'-C5'-O5'
1	L5	4500	PSU	O4'-C4'-C5'-O5'
1	L5	4571	A2M	C1'-C2'-O2'-CM'
1	L5	4590	A2M	C4'-C5'-O5'-P
1	L5	4636	PSU	C2'-C1'-C5-C6
1	L5	4636	PSU	C3'-C4'-C5'-O5'
1	L5	4637	OMG	C1'-C2'-O2'-CM2
46	S2	121	OMU	C1'-C2'-O2'-CM2
46	S2	166	A2M	C3'-C4'-C5'-O5'
46	S2	468	A2M	C1'-C2'-O2'-CM'
46	S2	576	A2M	C3'-C4'-C5'-O5'
46	S2	801	PSU	C3'-C4'-C5'-O5'
46	S2	822	PSU	C3'-C4'-C5'-O5'
46	S2	1031	A2M	C1'-C2'-O2'-CM'
46	S2	1272	OMC	C1'-C2'-O2'-CM2
46	S2	1326	UY1	C2'-C1'-C5-C4
46	S2	1383	A2M	C1'-C2'-O2'-CM'
46	S2	1442	OMU	C1'-C2'-O2'-CM2
46	S2	1490	OMG	O4'-C4'-C5'-O5'
46	S2	1678	A2M	C1'-C2'-O2'-CM'
46	S2	1851	MA6	O4'-C4'-C5'-O5'
72	SO	138	IAS	CA-CB-CG-OD1
1	L5	2815	A2M	O4'-C4'-C5'-O5'
1	L5	2815	A2M	C3'-C4'-C5'-O5'
1	L5	3770	PSU	O4'-C4'-C5'-O5'
1	L5	3818	UY1	O4'-C4'-C5'-O5'
46	S2	100	PSU	O4'-C4'-C5'-O5'
46	S2	668	A2M	O4'-C4'-C5'-O5'
46	S2	668	A2M	C3'-C4'-C5'-O5'
46	S2	1851	MA6	C3'-C4'-C5'-O5'
1	L5	3818	UY1	C3'-C4'-C5'-O5'
1	L5	4636	PSU	O4'-C4'-C5'-O5'
46	S2	100	PSU	C3'-C4'-C5'-O5'
46	S2	159	A2M	C3'-C4'-C5'-O5'
46	S2	166	A2M	O4'-C4'-C5'-O5'
46	S2	576	A2M	O4'-C4'-C5'-O5'
46	S2	801	PSU	O4'-C4'-C5'-O5'
46	S2	822	PSU	O4'-C4'-C5'-O5'
1	L5	1625	OMG	C3'-C2'-O2'-CM2
1	L5	3701	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	L5	3867	A2M	C3'-C4'-C5'-O5'
1	L5	3851	PSU	O4'-C4'-C5'-O5'
46	S2	159	A2M	O4'-C4'-C5'-O5'
1	L5	4447	5MC	C2'-C1'-N1-C6
46	S2	1248	B8N	N34-C33-C34-O36
46	S2	1248	B8N	N34-C33-C34-O35
1	L5	3818	UY1	C4'-C5'-O5'-P
46	S2	512	A2M	O4'-C4'-C5'-O5'
1	L5	400	A2M	C1'-C2'-O2'-CM'
46	S2	116	OMU	C1'-C2'-O2'-CM2
1	L5	1326	A2M	C4'-C5'-O5'-P
46	S2	1490	OMG	C4'-C5'-O5'-P
46	S2	590	A2M	C3'-C4'-C5'-O5'
46	S2	1248	B8N	C31-C32-C33-C34
1	L5	4500	PSU	C4'-C5'-O5'-P
1	L5	3764	PSU	C3'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C4'-C5'-O5'
46	S2	1447	OMG	C3'-C4'-C5'-O5'
1	L5	3701	OMC	O4'-C1'-N1-C6
1	L5	4447	5MC	O4'-C1'-N1-C6
1	L5	1534	A2M	C4'-C5'-O5'-P
1	L5	3701	OMC	O4'-C1'-N1-C2
1	L5	3764	PSU	O4'-C4'-C5'-O5'
46	S2	512	A2M	C3'-C4'-C5'-O5'
1	L5	4447	5MC	C2'-C1'-N1-C2
46	S2	428	OMU	C2'-C1'-N1-C6
46	S2	644	OMG	C4'-C5'-O5'-P
1	L5	3724	A2M	O4'-C4'-C5'-O5'
46	S2	966	PSU	O4'-C4'-C5'-O5'
1	L5	4494	OMG	C3'-C2'-O2'-CM2
1	L5	2815	A2M	C4'-C5'-O5'-P
1	L5	4447	5MC	O4'-C1'-N1-C2
1	L5	3844	PSU	C4'-C5'-O5'-P
46	S2	1851	MA6	C4'-C5'-O5'-P
46	S2	1383	A2M	C3'-C4'-C5'-O5'
46	S2	1490	OMG	C3'-C4'-C5'-O5'
1	L5	3818	UY1	O4'-C1'-C5-C4
1	L5	4500	PSU	O4'-C1'-C5-C4
46	S2	1326	UY1	O4'-C1'-C5-C4
46	S2	1383	A2M	O4'-C4'-C5'-O5'
46	S2	1832	6MZ	N1-C6-N6-C9
46	S2	428	OMU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
46	S2	867	OMG	O4'-C4'-C5'-O5'
1	L5	398	A2M	C1'-C2'-O2'-CM'
1	L5	2363	A2M	C1'-C2'-O2'-CM'
1	L5	2415	OMU	C1'-C2'-O2'-CM2
1	L5	2815	A2M	C1'-C2'-O2'-CM'
1	L5	3718	A2M	C1'-C2'-O2'-CM'
46	S2	27	A2M	C1'-C2'-O2'-CM'
1	L5	1524	A2M	C3'-C2'-O2'-CM'
1	L5	2363	A2M	C3'-C2'-O2'-CM'
1	L5	3724	A2M	C3'-C4'-C5'-O5'
46	S2	428	OMU	C3'-C4'-C5'-O5'
1	L5	1677	PSU	O4'-C1'-C5-C6
1	L5	3818	UY1	O4'-C1'-C5-C6
1	L5	4500	PSU	O4'-C1'-C5-C6
1	L5	4636	PSU	O4'-C1'-C5-C6
1	L5	2351	OMC	C2'-C1'-N1-C2
1	L5	1534	A2M	O4'-C4'-C5'-O5'
1	L5	1792	PSU	C3'-C4'-C5'-O5'
1	L5	2351	OMC	O4'-C4'-C5'-O5'
1	L5	2422	OMC	O4'-C4'-C5'-O5'
1	L5	3785	A2M	O4'-C4'-C5'-O5'
1	L5	3844	PSU	O4'-C4'-C5'-O5'
46	S2	966	PSU	C3'-C4'-C5'-O5'
1	L5	3887	OMC	C4'-C5'-O5'-P
46	S2	428	OMU	C3'-C2'-O2'-CM2
46	S2	428	OMU	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 410 ligands modelled in this entry, 408 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
82	SPD	L5	5378	-	9,9,9	0.34	0	8,8,8	0.92	0
82	SPD	L5	5377	-	9,9,9	0.33	0	8,8,8	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	SPD	L5	5378	-	-	4/7/7/7	-
82	SPD	L5	5377	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	L5	5378	SPD	N6-C7-C8-C9
82	L5	5377	SPD	C3-C4-C5-N6
82	L5	5378	SPD	C8-C7-N6-C5
82	L5	5378	SPD	C2-C3-C4-C5
82	L5	5377	SPD	N6-C7-C8-C9
82	L5	5377	SPD	N1-C2-C3-C4
82	L5	5378	SPD	C3-C4-C5-N6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

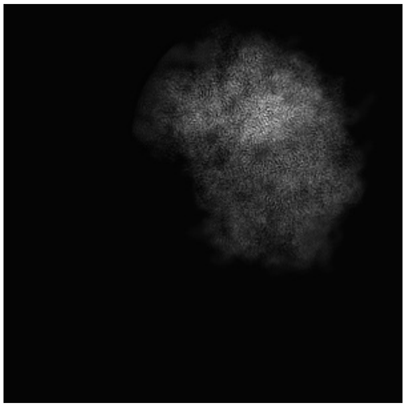
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-18539. These allow visual inspection of the internal detail of the map and identification of artifacts.

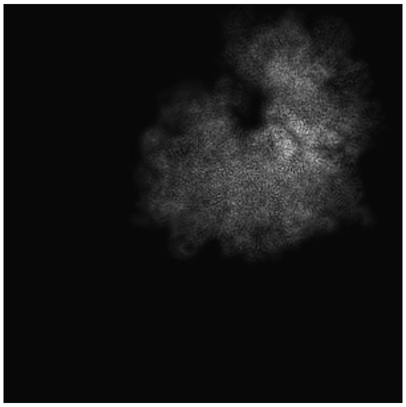
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

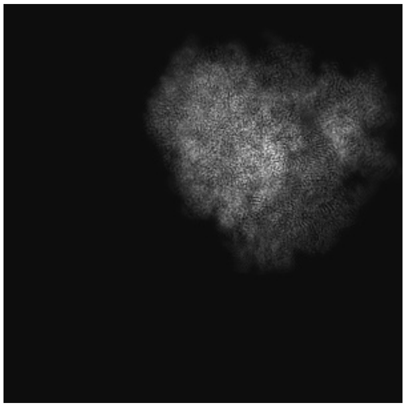
6.1.1 Primary map



X



Y

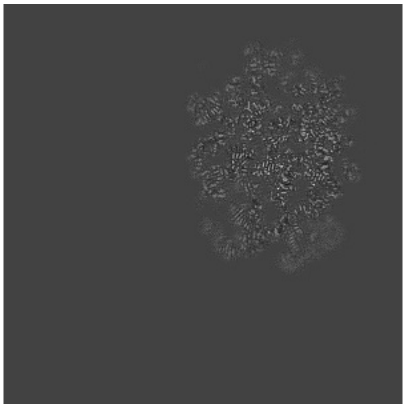


Z

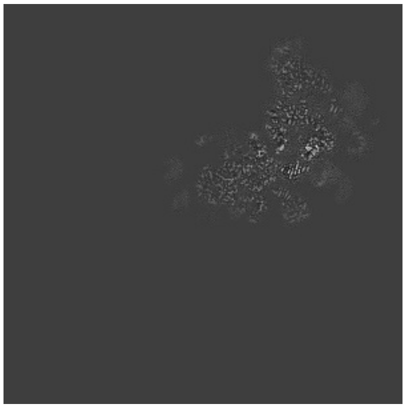
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

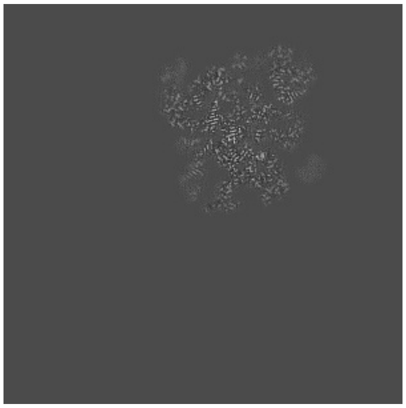
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices ⓘ

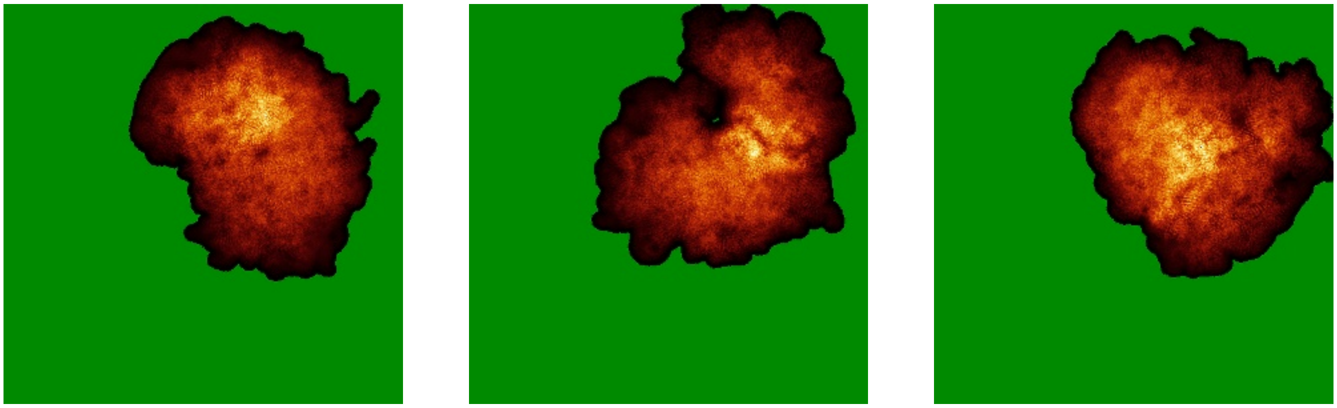
6.3.1 Primary map

X Index: 306 Y Index: 326 Z Index: 363

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

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

6.4.1 Primary map

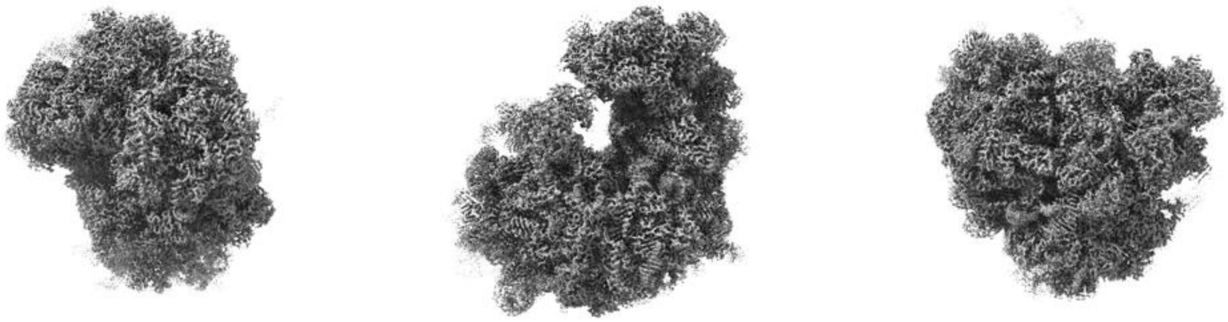


X Y Z

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

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0266. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

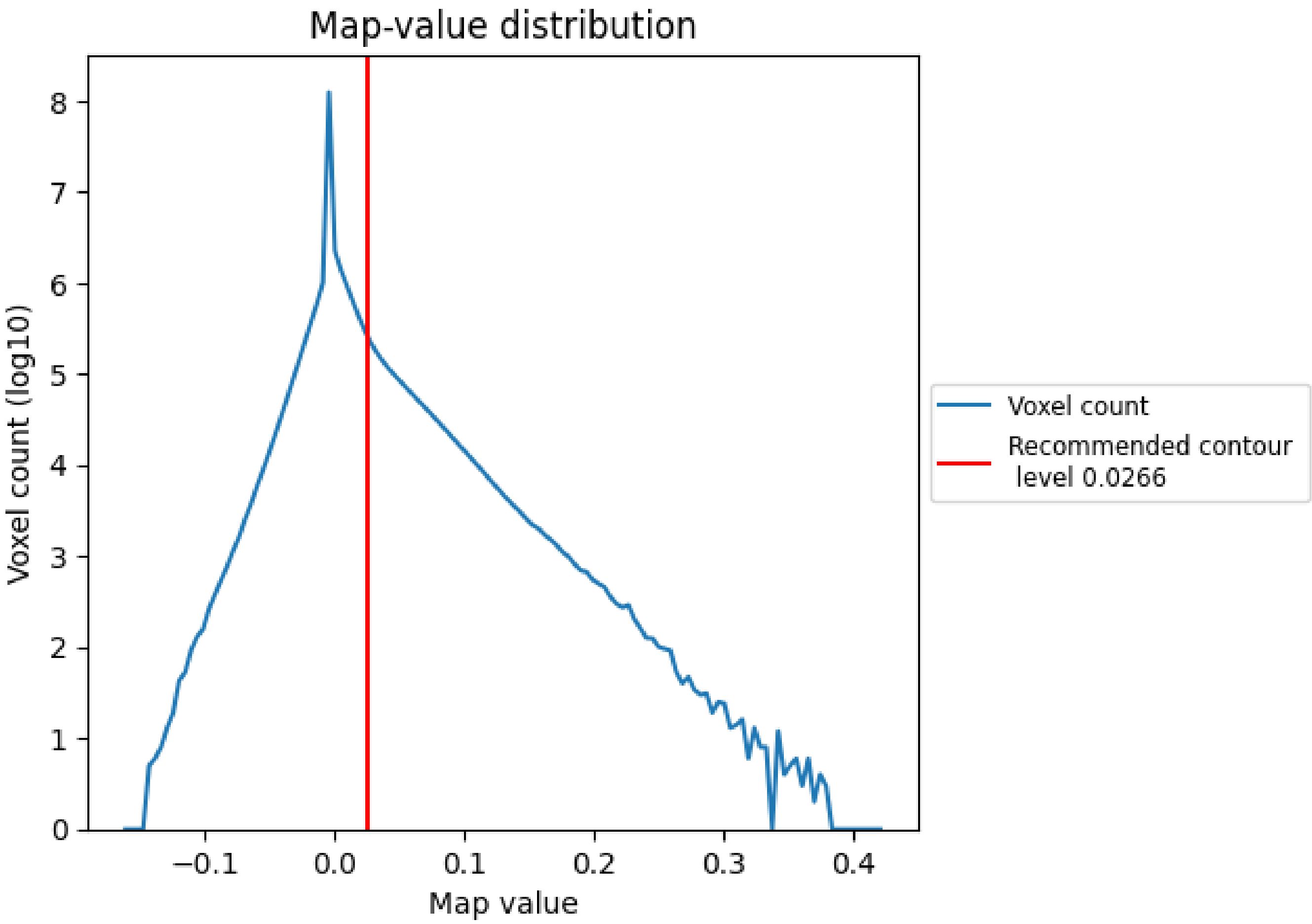
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

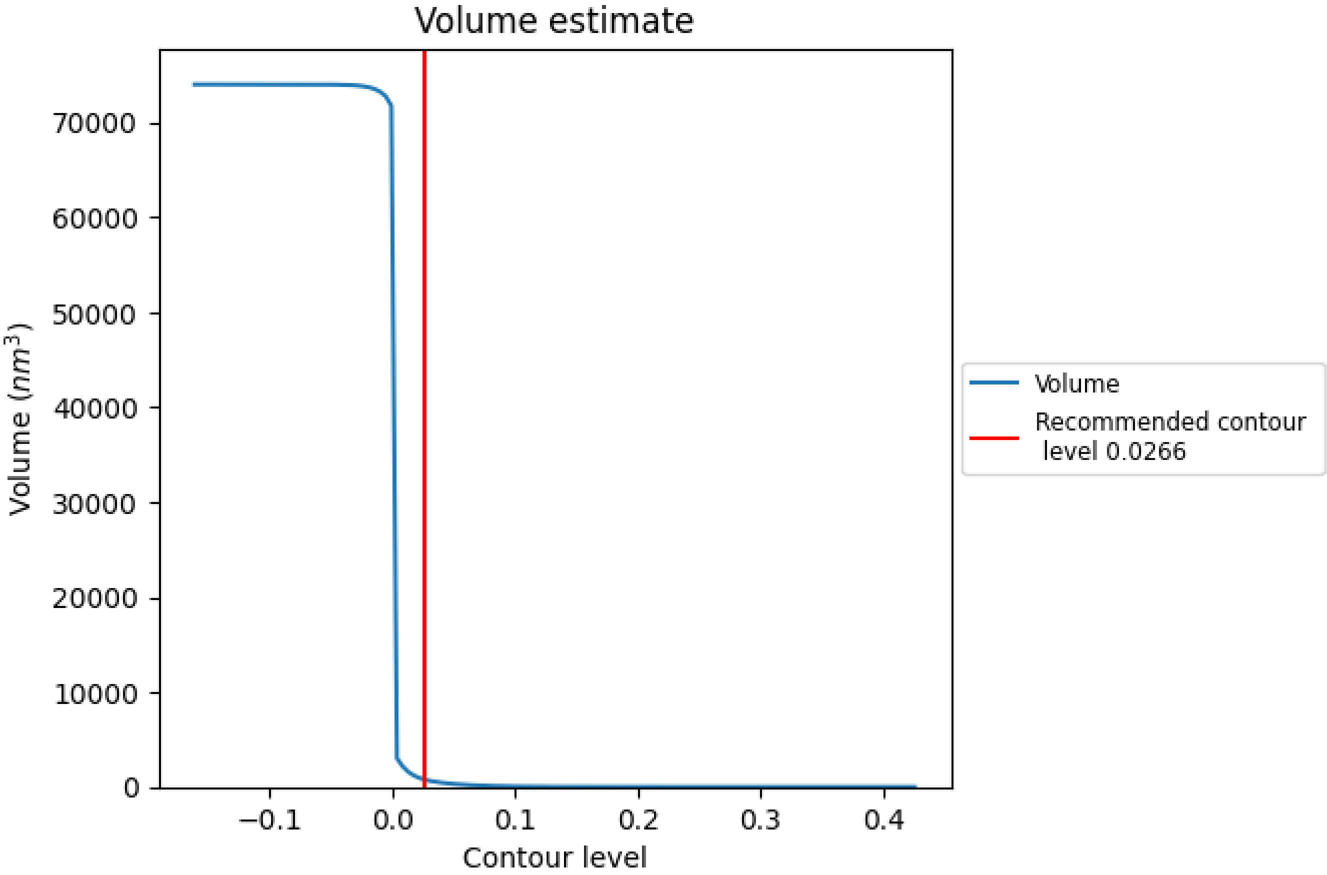
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

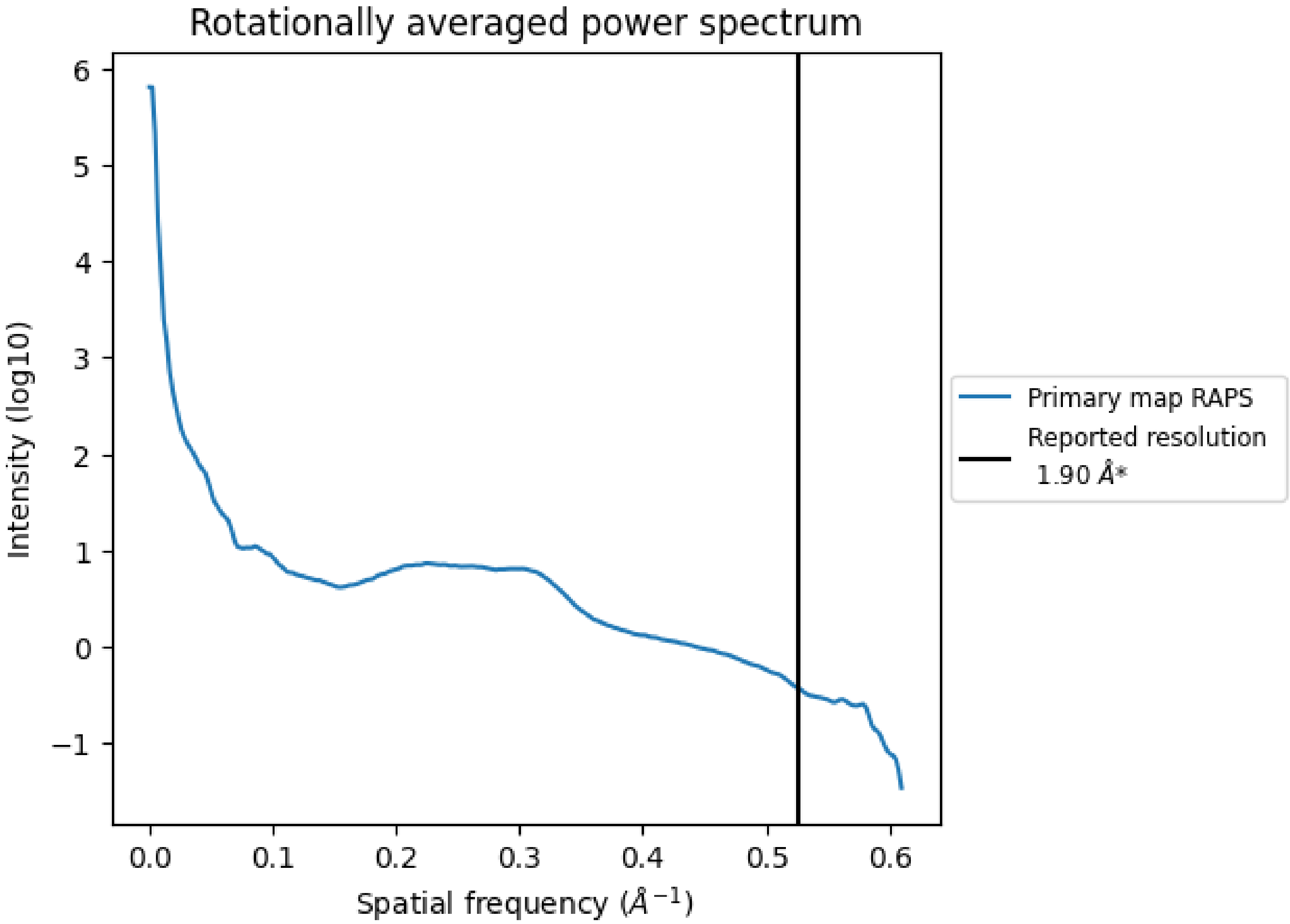
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 776 nm^3; this corresponds to an approximate mass of 701 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 0.526 Å^{-1}

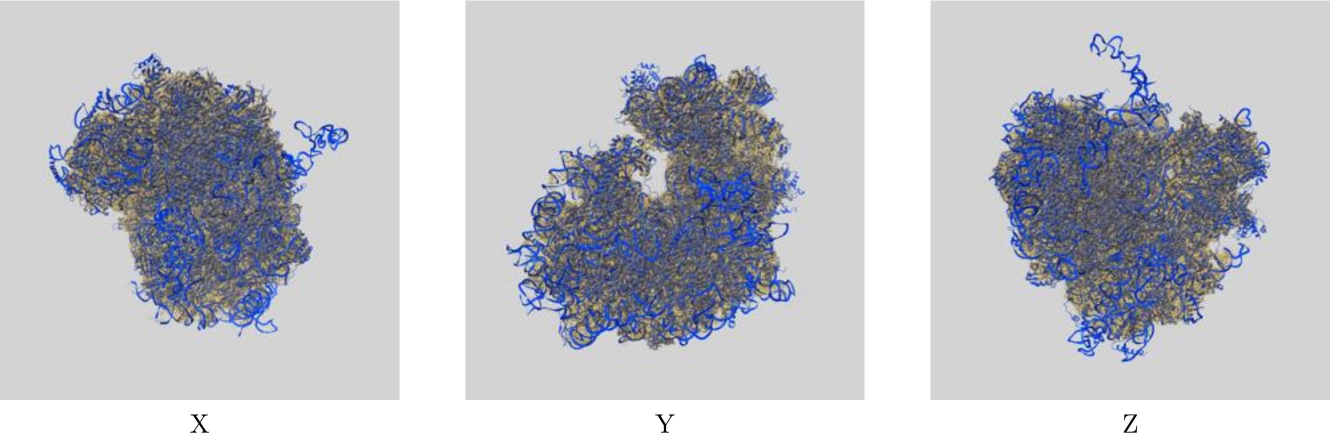
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-18539 and PDB model 8QOI. Per-residue inclusion information can be found in section 3 on page 24.

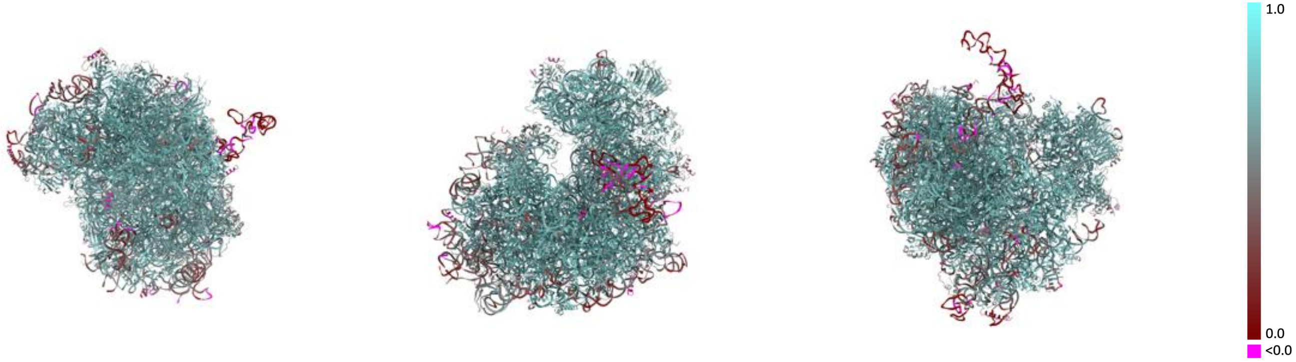
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0266 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.

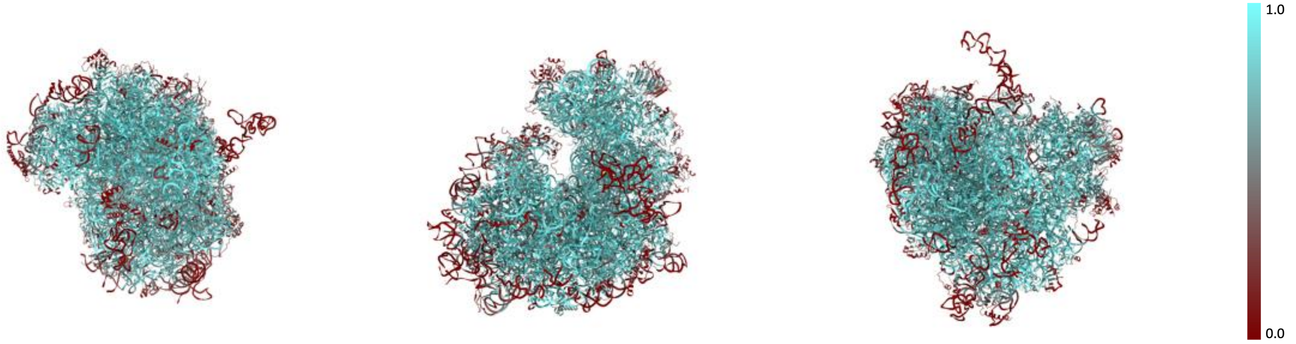
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

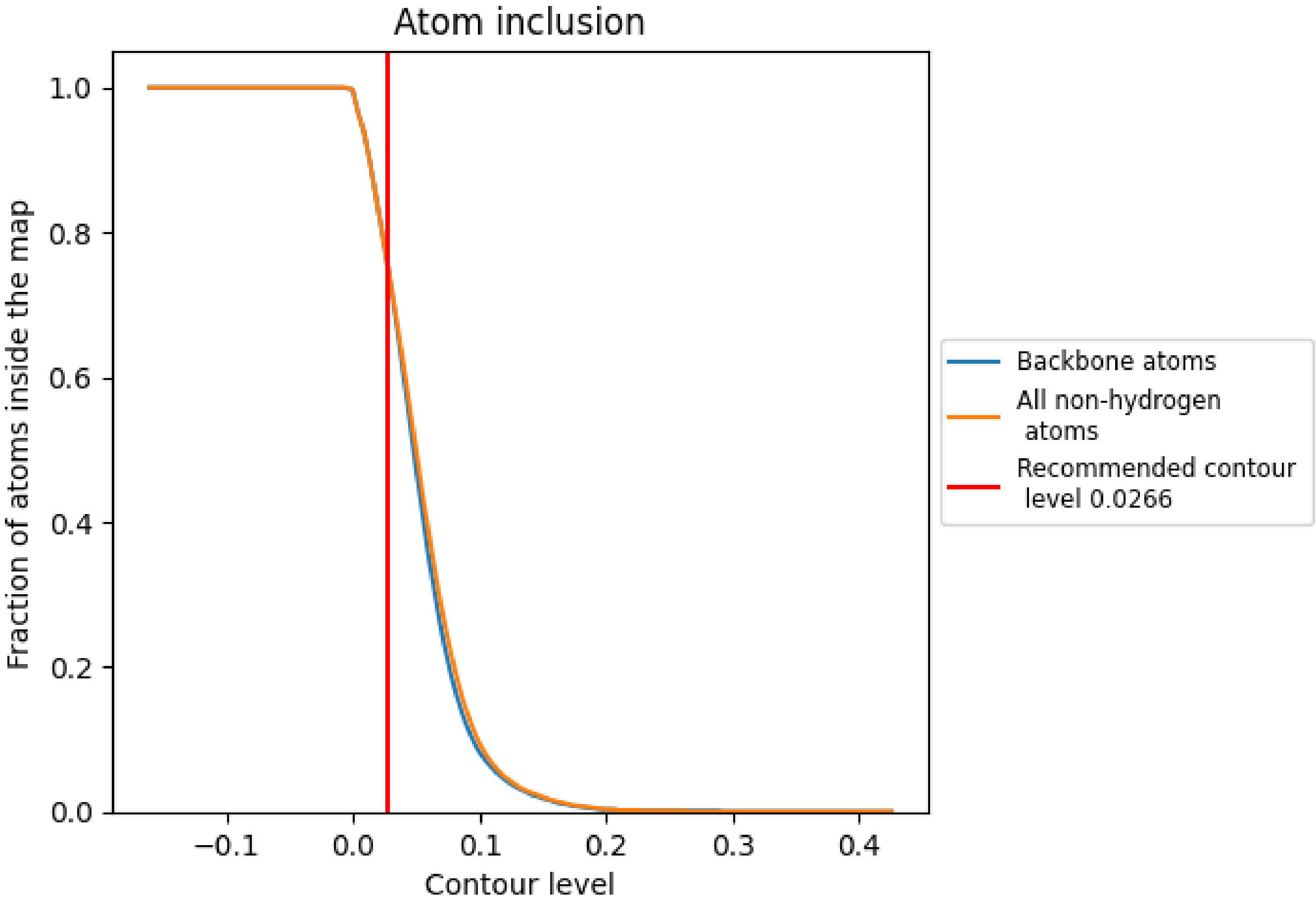
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0266).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.0266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.6690
L5	0.7500	0.6420
L7	0.8910	0.7000
L8	0.8520	0.6880
LA	0.9720	0.7900
LB	0.8180	0.7300
LC	0.8300	0.7310
LD	0.5970	0.6380
LE	0.5300	0.5970
LF	0.8590	0.7570
LG	0.5650	0.6050
LH	0.6550	0.6850
LI	0.6850	0.6830
LJ	0.4600	0.5790
LL	0.7000	0.6660
LM	0.7880	0.6920
LN	0.9670	0.7880
LO	0.8460	0.7410
LP	0.8700	0.7660
LQ	0.8760	0.7740
LR	0.7860	0.6910
LS	0.8670	0.7480
LT	0.7820	0.7160
LU	0.3610	0.5570
LV	0.9200	0.7640
LW	0.5050	0.5020
LX	0.7840	0.7180
LY	0.7960	0.7250
LZ	0.7110	0.6750
La	0.8820	0.7630
Lb	0.5640	0.6440
Lc	0.8720	0.7000
Ld	0.7720	0.7060
Le	0.8720	0.7690
Lf	0.9190	0.7720

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Chain	Atom inclusion	Q-score
Lg	0.8470	0.7210
Lh	0.7700	0.7160
Li	0.6880	0.6900
Lj	0.9540	0.7920
Lk	0.4920	0.5970
Ll	0.8320	0.7400
Lm	0.7810	0.7290
Ln	0.9950	0.7810
Lo	0.7210	0.7220
Lp	0.9740	0.7810
Lr	0.8270	0.7330
S2	0.8310	0.6640
SA	0.7790	0.6830
SB	0.8420	0.7050
SC	0.8400	0.7280
SD	0.7260	0.6640
SE	0.8430	0.7180
SF	0.8190	0.7090
SG	0.5280	0.6140
SH	0.3970	0.5370
SI	0.7950	0.6850
SJ	0.8150	0.7130
SK	0.6960	0.6760
SL	0.8230	0.7070
SM	0.0380	0.4540
SN	0.8920	0.7300
SO	0.8730	0.7040
SP	0.7340	0.6990
SQ	0.8360	0.7240
SR	0.6830	0.6390
SS	0.7530	0.7050
ST	0.8210	0.7210
SU	0.5530	0.6430
SV	0.7480	0.6930
SW	0.9450	0.7600
SX	0.9250	0.7620
SY	0.7100	0.6700
SZ	0.6230	0.6660
Sa	0.8580	0.7170
Sb	0.6450	0.6570
Sc	0.7860	0.6150
Sd	0.8870	0.7390

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Chain	Atom inclusion	Q-score
Se	0.6280	0.6400
Sf	0.1090	0.5240
Sg	0.5000	0.6450