



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2026 – 08:41 AM EDT

PDB ID : 9O3W / pdb_00009o3w
EMDB ID : EMD-70084
Title : Human 80S ribosome bound to IDB-001 stalled on MYC nascent chain
Authors : Sauer, P.V.; Schuller, A.P.; Hamann, L.G.
Deposited on : 2025-04-07
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

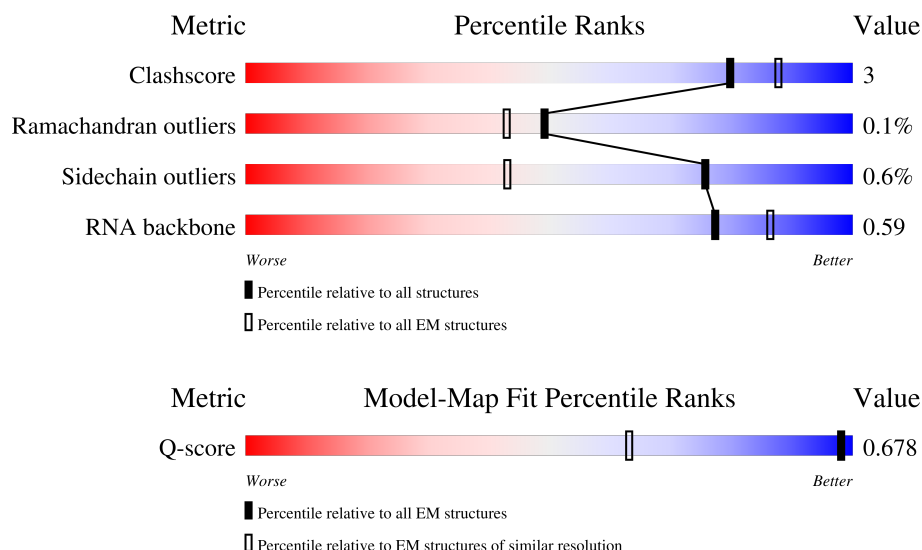
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



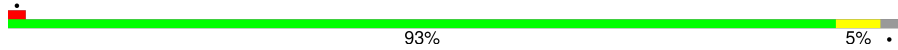
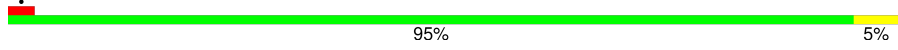
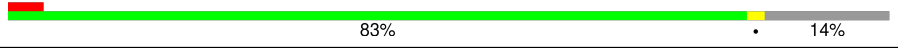
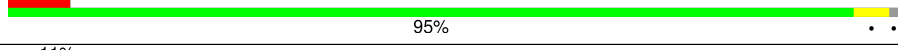
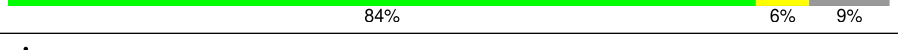
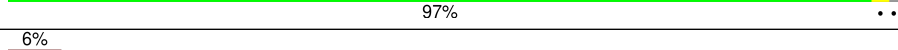
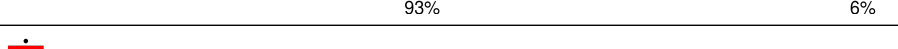
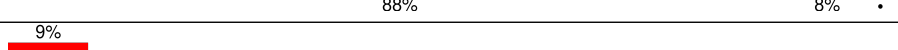
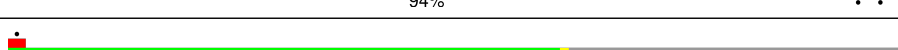
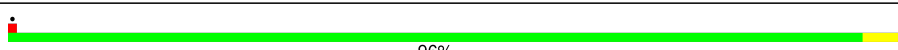
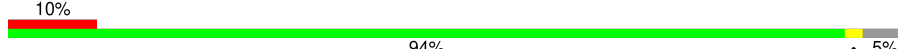
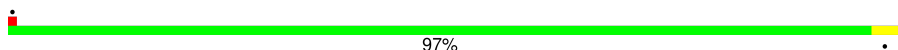
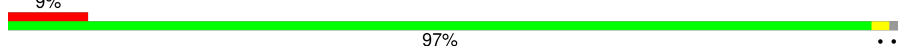
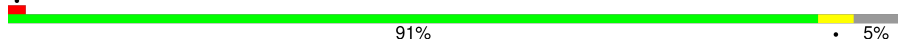
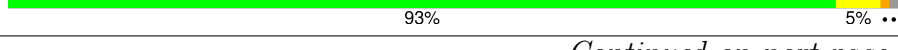
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1185 (1.40 - 2.40)

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

Mol	Chain	Length	Quality of chain
1	L5	5069	9% 51% 17% 30%
2	L7	120	87% 12%
3	L8	156	6% 74% 24%

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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	
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	

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Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	
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	NC	19	
47	Pt	75	
48	S2	1869	
49	SA	295	
50	SB	264	
51	SC	293	
52	SD	243	
53	SE	263	

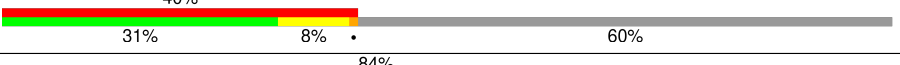
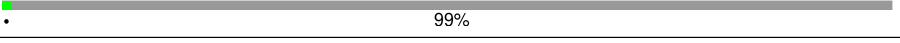
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Mol	Chain	Length	Quality of chain
54	SF	204	
55	SG	249	
56	SH	194	
57	SI	208	
58	SJ	194	
59	SK	165	
60	SL	158	
61	SM	132	
62	SN	151	
63	SO	151	
64	SP	145	
65	SQ	146	
66	SR	135	
67	SS	152	
68	ST	145	
69	SU	119	
70	SV	84	
71	SW	130	
72	SX	143	
73	SY	133	
74	SZ	125	
75	Sa	115	
76	Sb	84	
77	Sc	69	
78	Sd	56	

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Mol	Chain	Length	Quality of chain
79	Se	133	
80	Sf	156	
81	Sg	317	
82	mR	832	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 219527 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3546	Total	C	N	O	P	2	0
			76136	33944	13925	24720	3547		

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	251	Total	C	N	O	S	0	0
			1921	1204	393	318	6		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	223	Total	C	N	O	S	0	0
			1787	1150	339	294	4		

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

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1716	1086	331	285	14		

- Molecule 13 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 14 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 15 is a protein called Large ribosomal subunit protein eL14.

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

- Molecule 16 is a protein called Large ribosomal subunit protein eL15.

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 Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	202	Total	C	N	O	S	0	0
			1655	1066	322	262	5		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

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 Large ribosomal subunit protein eL18.

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 Large ribosomal subunit protein eL19.

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

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 22 is a protein called Large ribosomal subunit protein eL21.

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

- Molecule 23 is a protein called Large ribosomal subunit protein eL22.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	68	Total	C	N	O	S	0	0
			562	356	111	92	3		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 28 is a protein called Large ribosomal subunit protein eL27.

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

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

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

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL31.

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

- Molecule 33 is a protein called Large ribosomal subunit protein eL32.

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 Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	110	Total	C	N	O	S	0	0
			884	560	175	145	4		

- Molecule 35 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 37 is a protein called Large ribosomal subunit protein eL36.

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

- Molecule 38 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL39.

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

- Molecule 41 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	0	0
			864	543	175	140	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

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

- Molecule 45 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	126	Total	C	N	O	S	0	0
			1005	624	207	169	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	2	ACE	-	acetylation	UNP P46779

- Molecule 46 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	NC	19	Total	C	N	O	0	0
			118	68	20	30		

- Molecule 47 is a RNA chain called P-site glutamyl-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Pt	75	Total	C	N	O	P	0	0
			1597	713	275	534	75		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1672	Total	C	N	O	P	0	0
			35736	15981	6403	11681	1671		

- Molecule 49 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	223	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	ACE	-	acetylation	UNP P08865

- Molecule 50 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

- Molecule 51 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 52 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

- Molecule 53 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 55 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 56 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		

- Molecule 57 is a protein called Small ribosomal subunit protein eS8.

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

- Molecule 58 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 59 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 60 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SL	146	Total	C	N	O	S	0	0
			1200	766	226	202	6		

- Molecule 61 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SM	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 62 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 63 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 64 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	131	Total	C	N	O	S	0	0
			1078	684	204	183	7		

- Molecule 65 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 66 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 68 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ST	142	Total	C	N	O	S	0	0
			1103	691	212	197	3		

- Molecule 69 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 70 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SV	84	Total	C	N	O	S	0	0
			640	395	117	123	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 71 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 72 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SX	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 73 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 74 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SZ	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 75 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 77 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sc	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 78 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 79 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Se	50	Total	C	N	O	S	0	0
			395	241	88	65	1		

- Molecule 80 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

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

- Molecule 81 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	mR	6	Total	C	N	O	P	0	0
			133	59	27	41	6		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

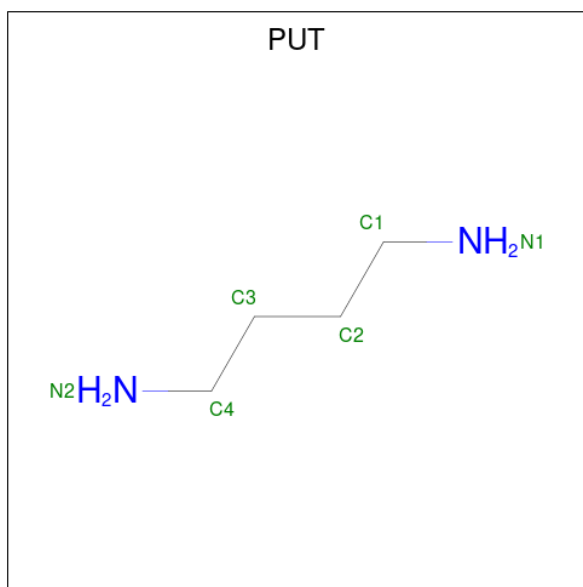
Mol	Chain	Residues	Atoms		AltConf
83	L5	114	Total	K	0
			114	114	
83	L7	3	Total	K	0
			3	3	
83	L8	5	Total	K	0
			5	5	
83	LA	3	Total	K	0
			3	3	
83	LH	1	Total	K	0
			1	1	
83	LI	1	Total	K	0
			1	1	
83	LL	1	Total	K	0
			1	1	
83	LN	1	Total	K	0
			1	1	
83	LQ	1	Total	K	0
			1	1	
83	Lb	1	Total	K	0
			1	1	
83	Le	1	Total	K	0
			1	1	
83	Lf	1	Total	K	0
			1	1	
83	Ll	1	Total	K	0
			1	1	
83	S2	32	Total	K	0
			32	32	
83	SL	1	Total	K	0
			1	1	
83	SO	1	Total	K	0
			1	1	

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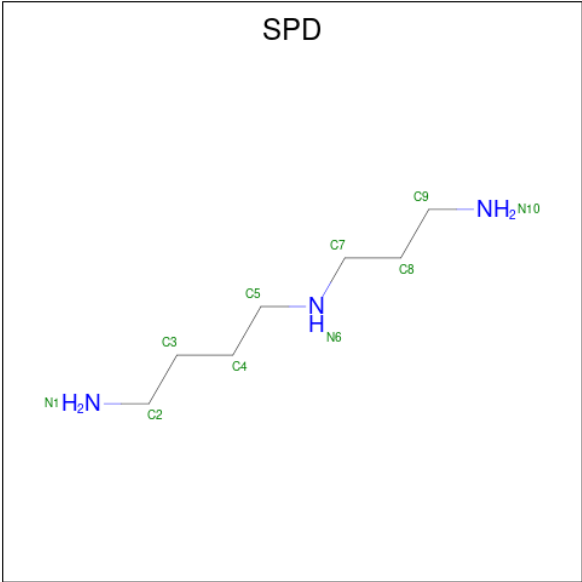
Mol	Chain	Residues	Atoms		AltConf
83	ST	1	Total	K	0
			1	1	
83	Sa	1	Total	K	0
			1	1	

- Molecule 84 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



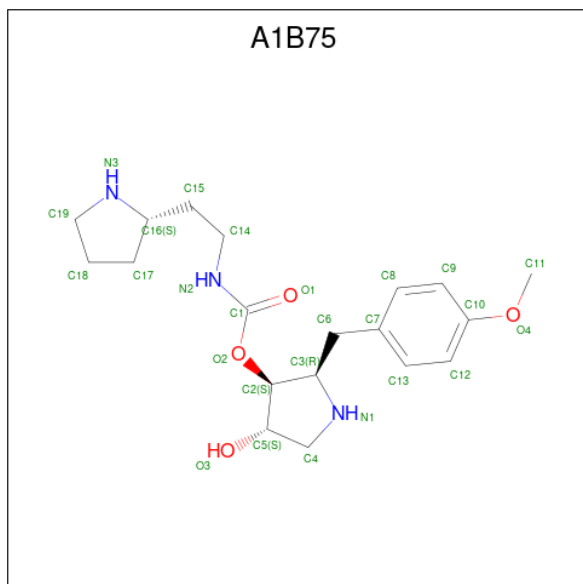
Mol	Chain	Residues	Atoms			AltConf
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	
84	L5	1	Total	C	N	0
			6	4	2	

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



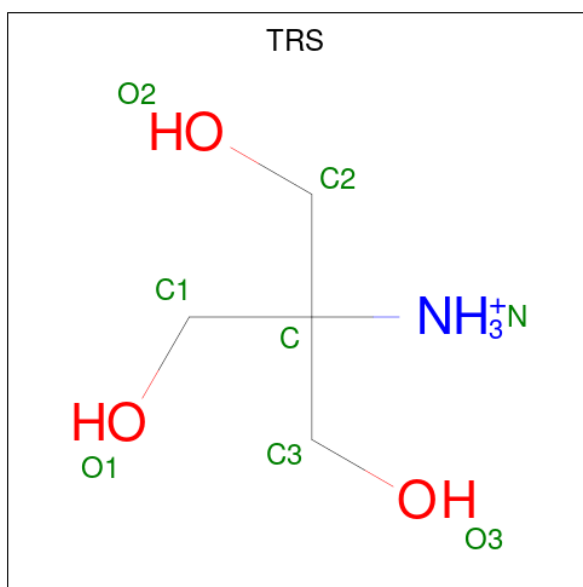
Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N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

- Molecule 86 is (2R,3S,4S)-4-hydroxy-2-[(4-methoxyphenyl)methyl]pyrrolidin-3-yl {2-[(2S)-pyrrolidin-2-yl]ethyl}carbamate (CCD ID: A1B75) (formula: $C_{19}H_{29}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
86	L5	1	26	19	3	4	0

- Molecule 87 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
87	L5	1	Total	C	N	O	0
			8	4	1	3	
87	L5	1	Total	C	N	O	0
			8	4	1	3	

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	L5	271	Total	Mg	0
			271	271	
88	L7	5	Total	Mg	0
			5	5	
88	L8	6	Total	Mg	0
			6	6	
88	LL	1	Total	Mg	0
			1	1	
88	LN	2	Total	Mg	0
			2	2	
88	Lj	1	Total	Mg	0
			1	1	
88	Lo	1	Total	Mg	0
			1	1	
88	S2	83	Total	Mg	0
			83	83	
88	Sd	1	Total	Mg	0
			1	1	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		AltConf
89	Sf	1	Total 1	Zn 1	0

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	L5	337	Total 337	O 337	0
90	L5	60	Total 60	O 60	0
90	L5	1	Total 1	O 1	0
90	L5	1	Total 1	O 1	0
90	L5	1	Total 1	O 1	0
90	L5	42	Total 42	O 42	0
90	L5	1	Total 1	O 1	0
90	L5	24	Total 24	O 24	0
90	L5	3910	Total 3910	O 3910	0
90	L5	65	Total 65	O 65	0
90	L7	33	Total 33	O 33	0
90	L7	48	Total 48	O 48	0
90	L8	1	Total 1	O 1	0
90	L8	11	Total 11	O 11	0
90	L8	3	Total 3	O 3	0
90	LA	90	Total 90	O 90	0
90	LA	40	Total 40	O 40	0
90	LB	142	Total 142	O 142	0

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Mol	Chain	Residues	Atoms		AltConf
90	LC	116	Total 116	O 116	0
90	LD	38	Total 38	O 38	0
90	LE	7	Total 7	O 7	0
90	LF	54	Total 54	O 54	0
90	LG	17	Total 17	O 17	0
90	LH	2	Total 2	O 2	0
90	LH	15	Total 15	O 15	0
90	LI	22	Total 22	O 22	0
90	LI	40	Total 40	O 40	0
90	LJ	3	Total 3	O 3	0
90	LL	28	Total 28	O 28	0
90	LL	11	Total 11	O 11	0
90	LL	18	Total 18	O 18	0
90	LM	11	Total 11	O 11	0
90	LN	7	Total 7	O 7	0
90	LN	92	Total 92	O 92	0
90	LN	22	Total 22	O 22	0
90	LO	79	Total 79	O 79	0
90	LP	62	Total 62	O 62	0
90	LQ	41	Total 41	O 41	0
90	LQ	46	Total 46	O 46	0

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Mol	Chain	Residues	Atoms		AltConf
90	LR	57	Total 57	O 57	0
90	LS	46	Total 46	O 46	0
90	LT	64	Total 64	O 64	0
90	LV	43	Total 43	O 43	0
90	LW	12	Total 12	O 12	0
90	LX	22	Total 22	O 22	0
90	LY	16	Total 16	O 16	0
90	LZ	5	Total 5	O 5	0
90	La	87	Total 87	O 87	0
90	Lb	33	Total 33	O 33	0
90	Lc	8	Total 8	O 8	0
90	Ld	29	Total 29	O 29	0
90	Le	21	Total 21	O 21	0
90	Le	67	Total 67	O 67	0
90	Lf	4	Total 4	O 4	0
90	Lf	34	Total 34	O 34	0
90	Lg	33	Total 33	O 33	0
90	Lg	27	Total 27	O 27	0
90	Lh	15	Total 15	O 15	0
90	Li	11	Total 11	O 11	0
90	Lj	26	Total 26	O 26	0

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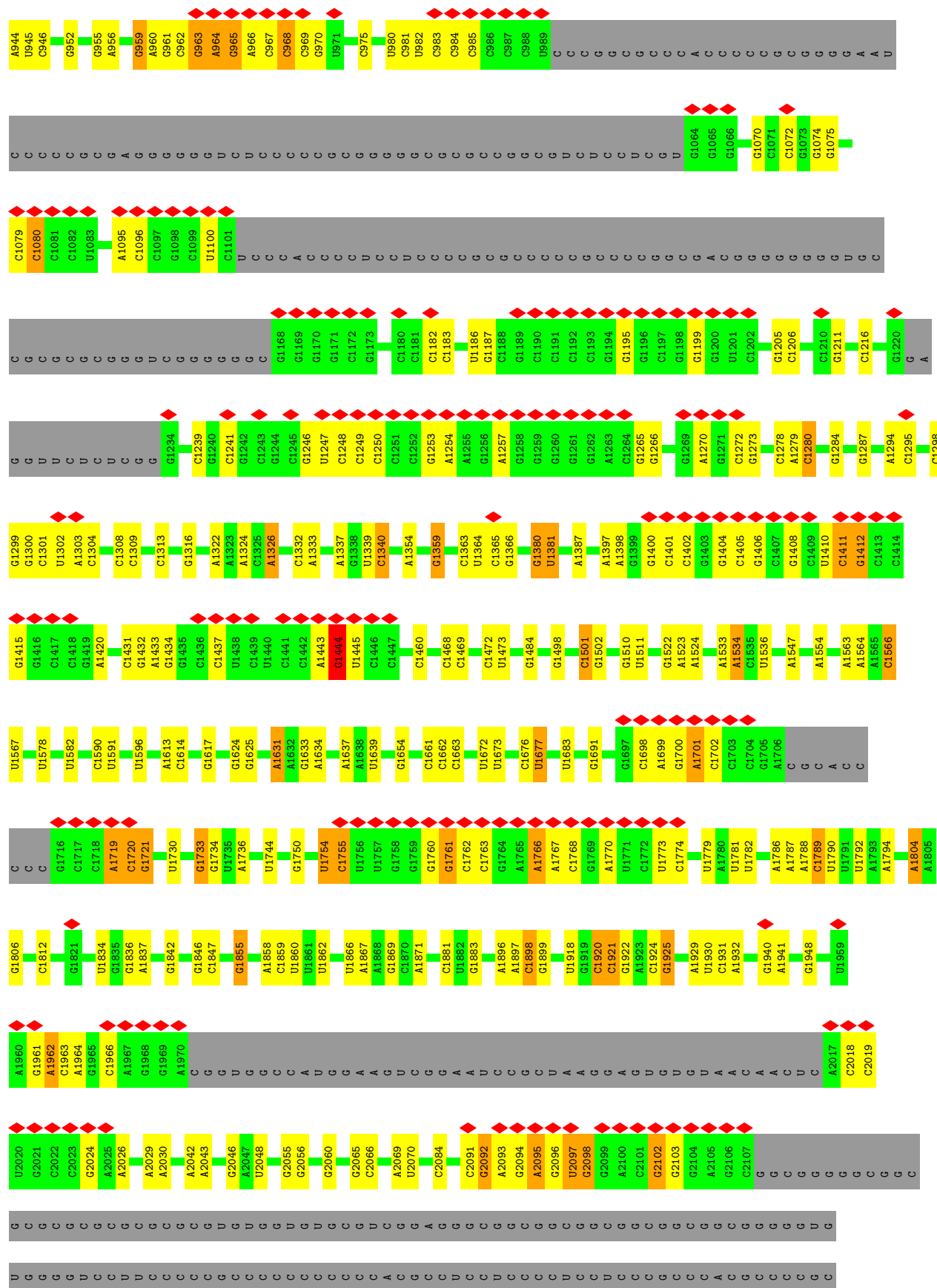
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Mol	Chain	Residues	Atoms		AltConf
90	Lj	19	Total 19	O 19	0
90	Lj	16	Total 16	O 16	0
90	Lk	1	Total 1	O 1	0
90	Ll	33	Total 33	O 33	0
90	Lm	16	Total 16	O 16	0
90	Ln	13	Total 13	O 13	0
90	Lo	28	Total 28	O 28	0
90	Lo	1	Total 1	O 1	0
90	Lo	13	Total 13	O 13	0
90	Lp	29	Total 29	O 29	0
90	Lp	1	Total 1	O 1	0
90	Lr	19	Total 19	O 19	0
90	NC	5	Total 5	O 5	0
90	Pt	3	Total 3	O 3	0
90	S2	80	Total 80	O 80	0
90	S2	111	Total 111	O 111	0
90	S2	10	Total 10	O 10	0
90	S2	105	Total 105	O 105	0
90	S2	76	Total 76	O 76	0
90	S2	23	Total 23	O 23	0
90	S2	2	Total 2	O 2	0

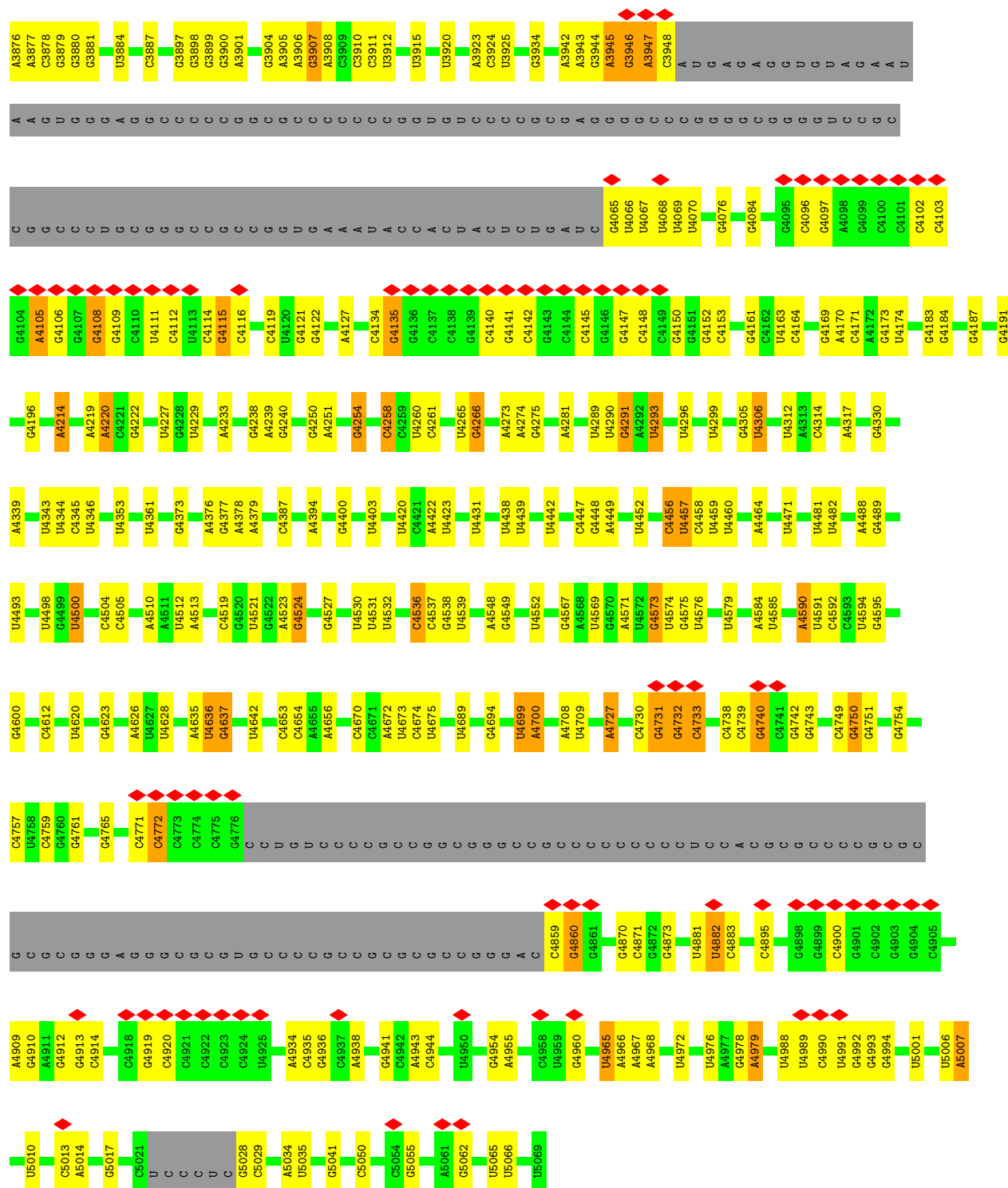
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Mol	Chain	Residues	Atoms		AltConf
90	S2	44	Total 44	O 44	0
90	S2	281	Total 281	O 281	0
90	S2	1	Total 1	O 1	0
90	S2	18	Total 18	O 18	0
90	S2	97	Total 97	O 97	0
90	S2	2	Total 2	O 2	0
90	Sb	6	Total 6	O 6	0
90	Se	2	Total 2	O 2	0
90	mR	3	Total 3	O 3	0





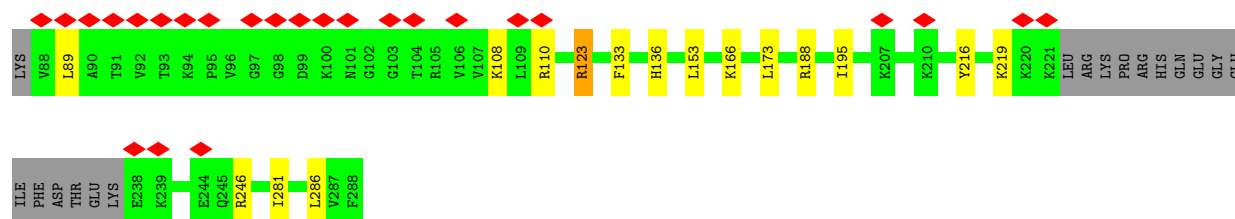


• Molecule 2: 5S rRNA

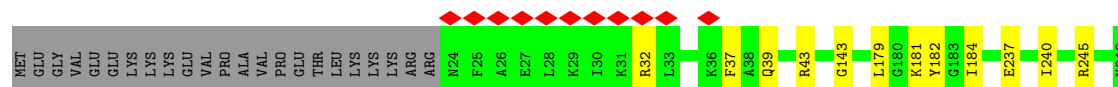
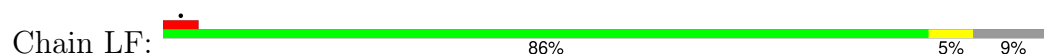
Chain L7: 87% 12%



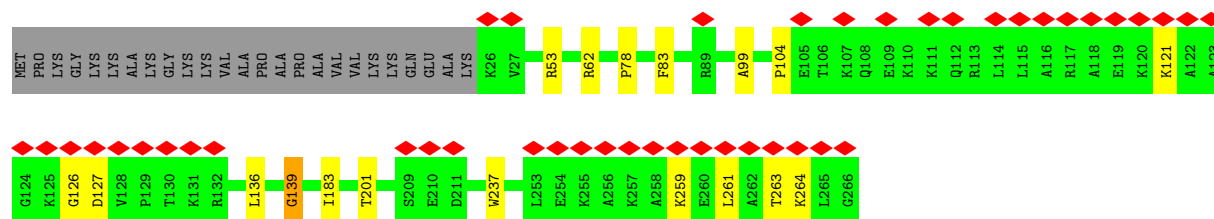
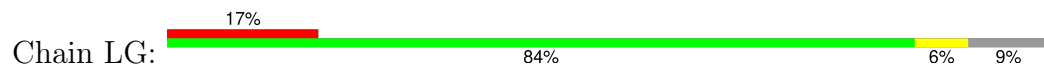
MET
 ALA
 GLY
 GLU
 LYS
 VAL
 GLU
 LYS
 PRO
 ASP
 THR
 LYS
 GLU
 LYS
 LYS
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 GLU
 ALA
 LYS
 LYS
 VAL
 ASP
 ALA
 GLY
 LYS
 VAL
 LYS
 LYS
 GLY
 ASN
 LEU
 LYS
 LYS
 LYS
 LYS
 PRO
 PRO
 LYS
 K39
 G40
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 SER
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 VAL
 GLU
 LYS
 LYS
 LYS
 LYS



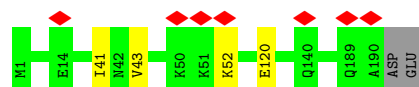
- Molecule 9: 60S ribosomal protein L7



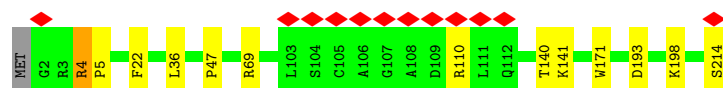
- Molecule 10: Large ribosomal subunit protein eL8



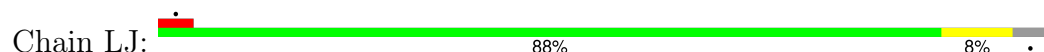
- Molecule 11: Large ribosomal subunit protein uL6



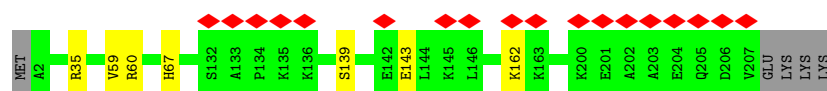
- Molecule 12: Large ribosomal subunit protein uL16

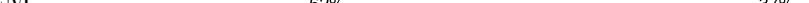


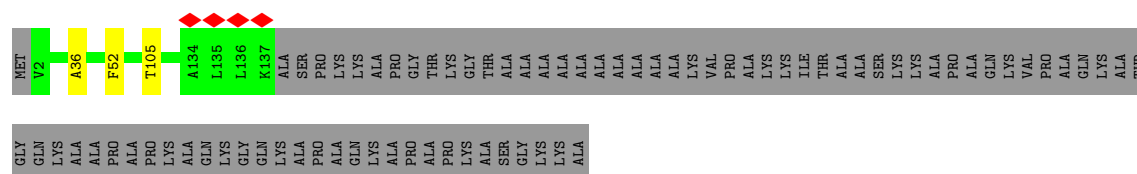
- Molecule 13: Large ribosomal subunit protein uL5

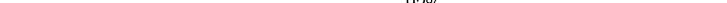


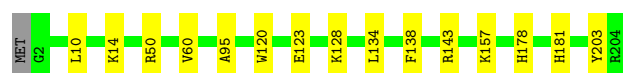
- Molecule 14: Large ribosomal subunit protein eL13

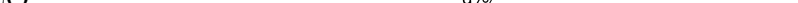


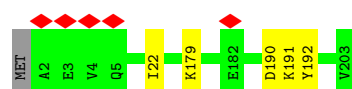
- Chain LM: 

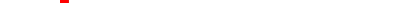


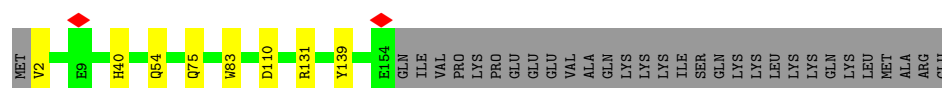
- Chain LN:  92% 7%



- Chain LO:  97%



- Chain LP:  79% 17%

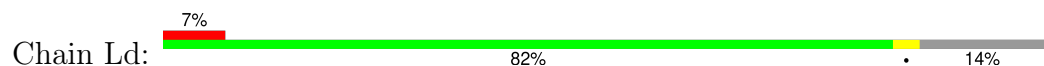


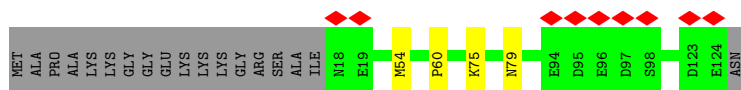
- Chain LQ: 96%



- Chain LB: 10% 94% 5%







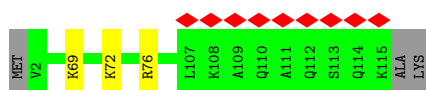
- Molecule 33: Large ribosomal subunit protein eL32



- Molecule 34: Large ribosomal subunit protein eL33



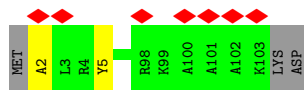
- Molecule 35: Large ribosomal subunit protein eL34



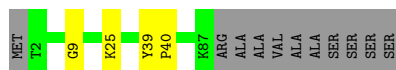
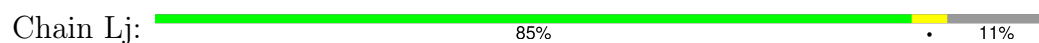
- Molecule 36: Large ribosomal subunit protein uL29



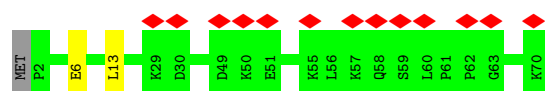
- Molecule 37: Large ribosomal subunit protein eL36



- Molecule 38: Large ribosomal subunit protein eL37



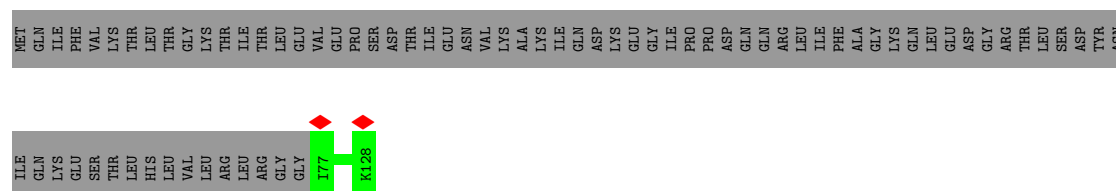
- Molecule 39: Large ribosomal subunit protein eL38



- Molecule 40: Large ribosomal subunit protein eL39



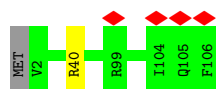
- Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein



- Molecule 42: Small ribosomal subunit protein eS32



- Molecule 43: Large ribosomal subunit protein eL42

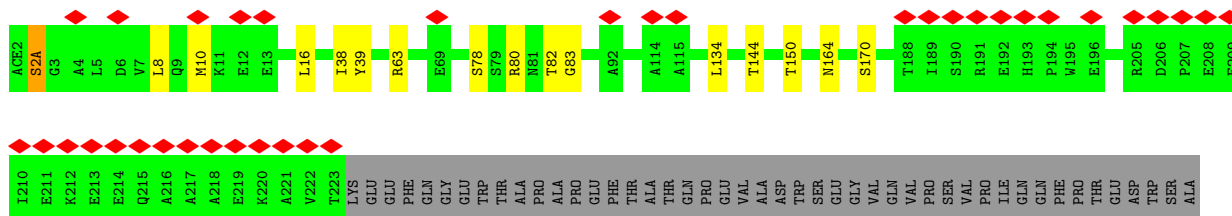


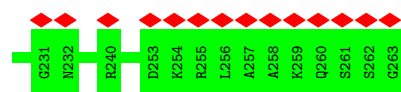
- Molecule 44: Large ribosomal subunit protein eL43



- Molecule 45: Large ribosomal subunit protein eL28

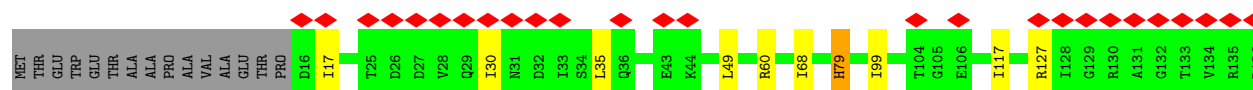






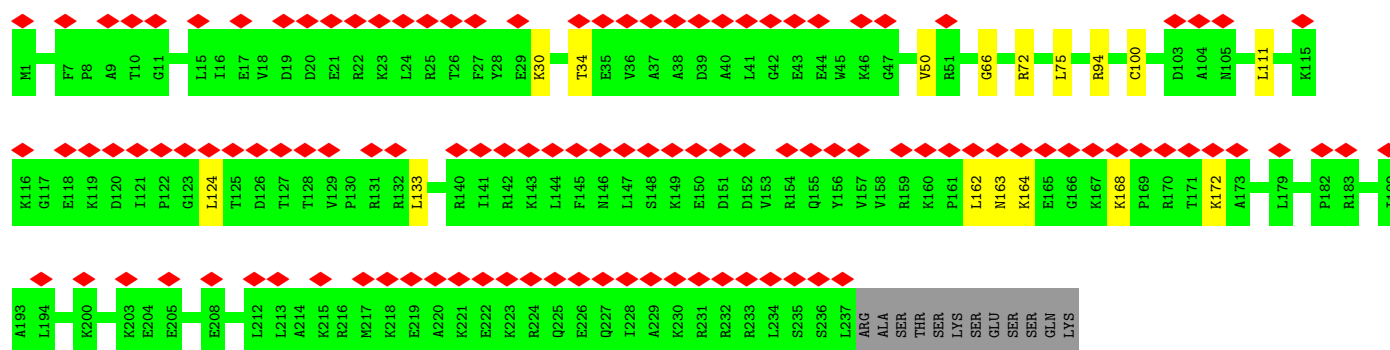
- Molecule 54: Small ribosomal subunit protein uS7

Chain SF:



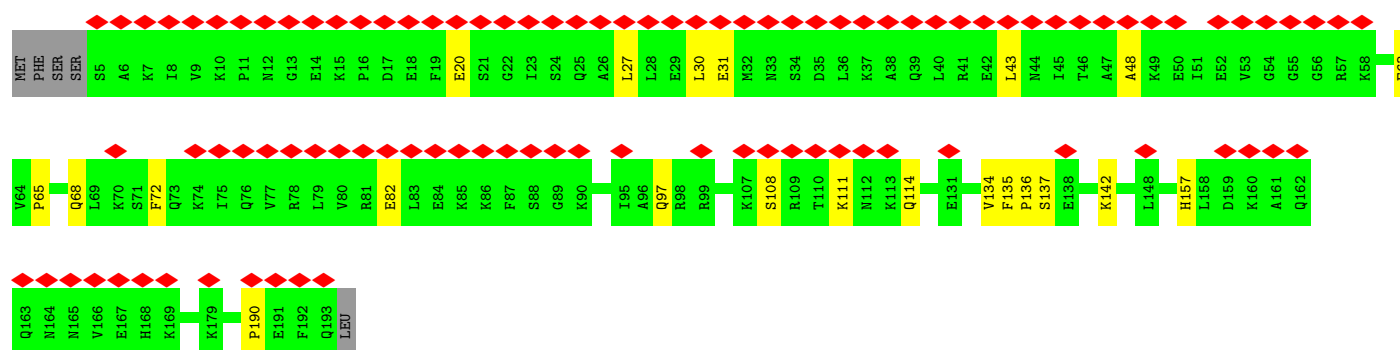
- Molecule 55: Small ribosomal subunit protein eS6

Chain SG:



- Molecule 56: Small ribosomal subunit protein eS7

Chain SH:

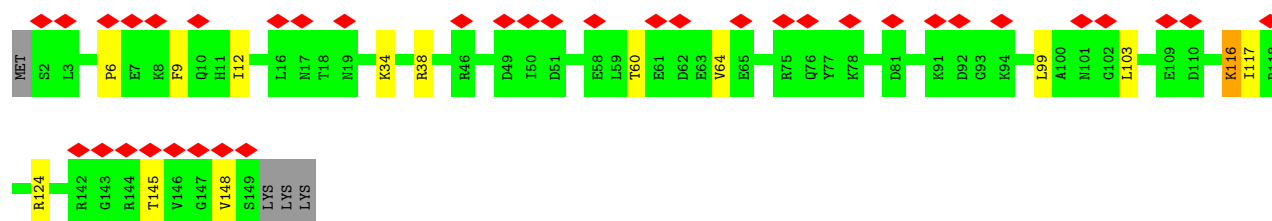


- Molecule 57: Small ribosomal subunit protein eS8

Chain SI:

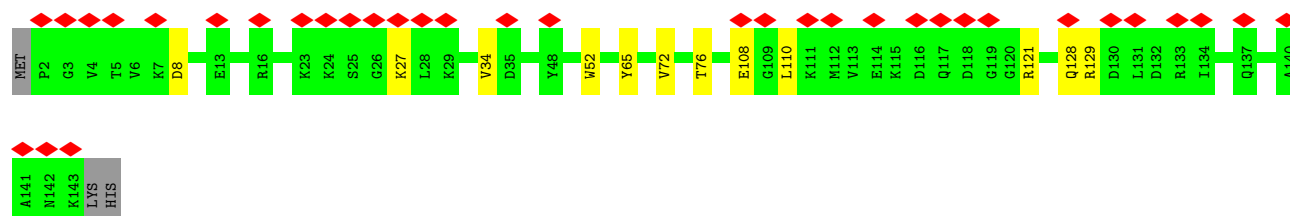


Chain SS: 24% 88% 9% ..



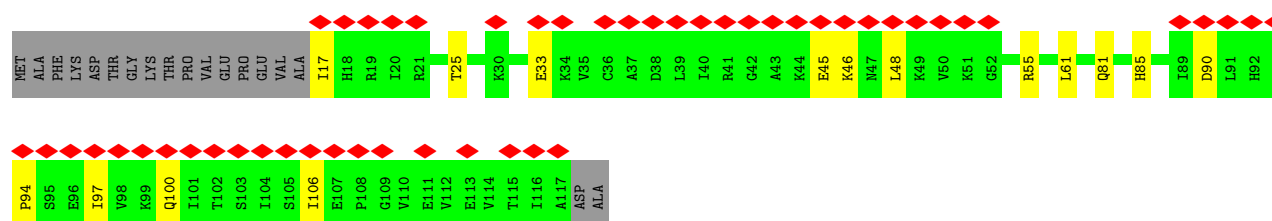
- Molecule 68: Small ribosomal subunit protein eS19

Chain ST: 24% 90% 8% .



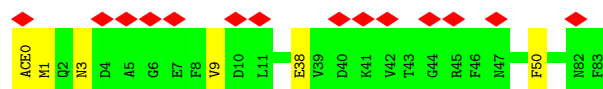
- Molecule 69: Small ribosomal subunit protein uS10

Chain SU: 43% 72% 13% 15%



- Molecule 70: 40S ribosomal protein S21

Chain SV: 17% 93% 7%



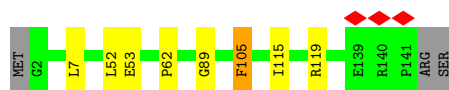
- Molecule 71: Small ribosomal subunit protein uS8

Chain SW: 92% 8%

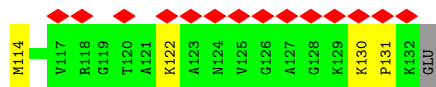
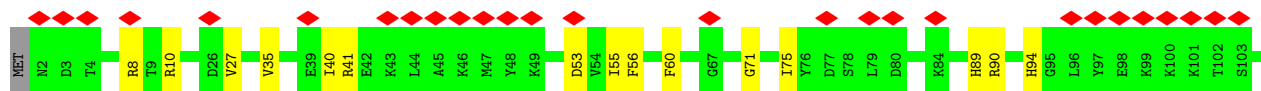
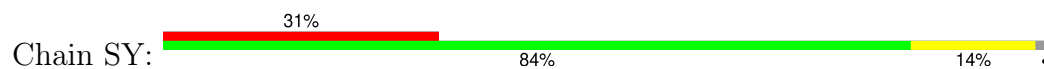


- Molecule 72: Small ribosomal subunit protein uS12

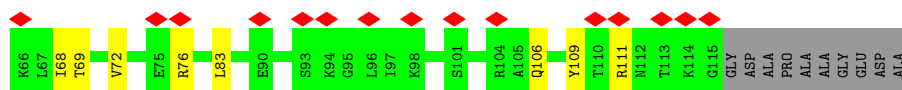
Chain SX: 92% 5% ..



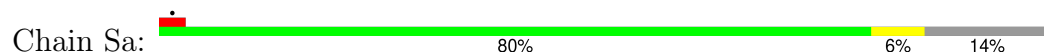
- Molecule 73: 40S ribosomal protein S24



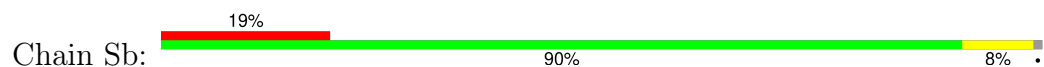
- Molecule 74: Small ribosomal subunit protein eS25



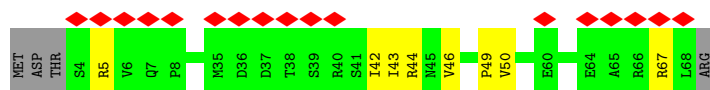
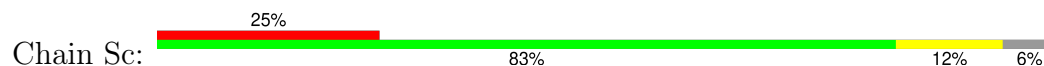
- Molecule 75: Small ribosomal subunit protein eS26



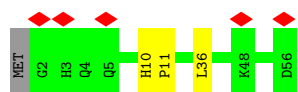
- Molecule 76: Small ribosomal subunit protein eS27



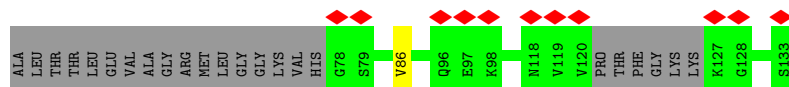
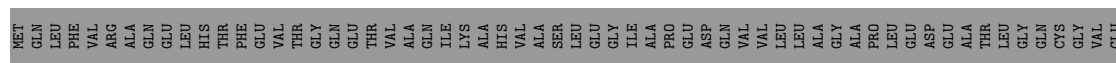
- Molecule 77: Small ribosomal subunit protein eS28



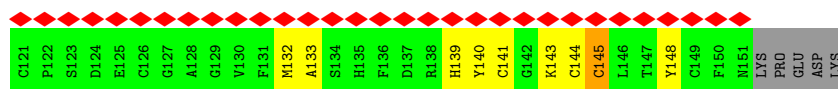
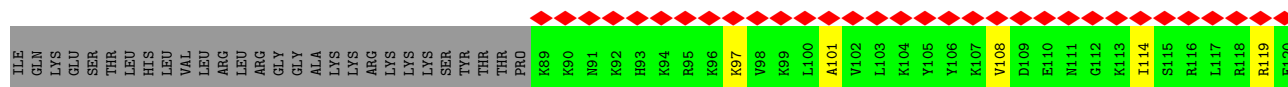
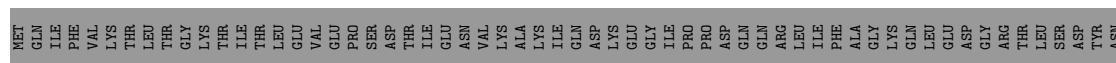
- Molecule 78: Small ribosomal subunit protein uS14



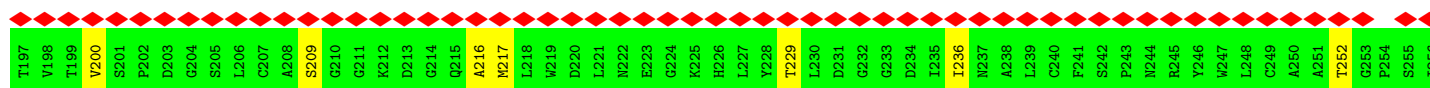
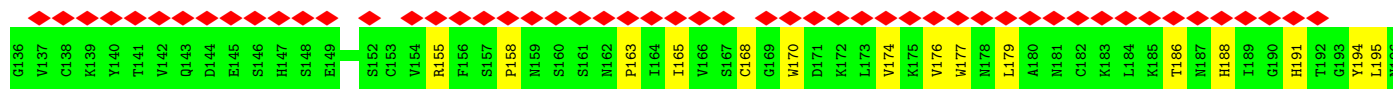
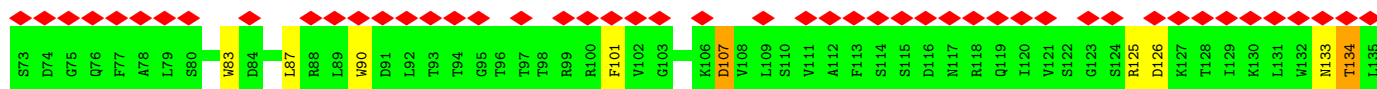
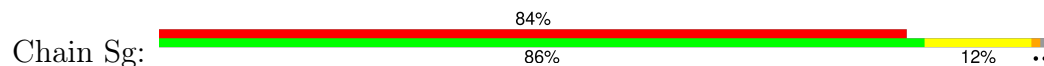
- Molecule 79: FAU ubiquitin-like and ribosomal protein S30

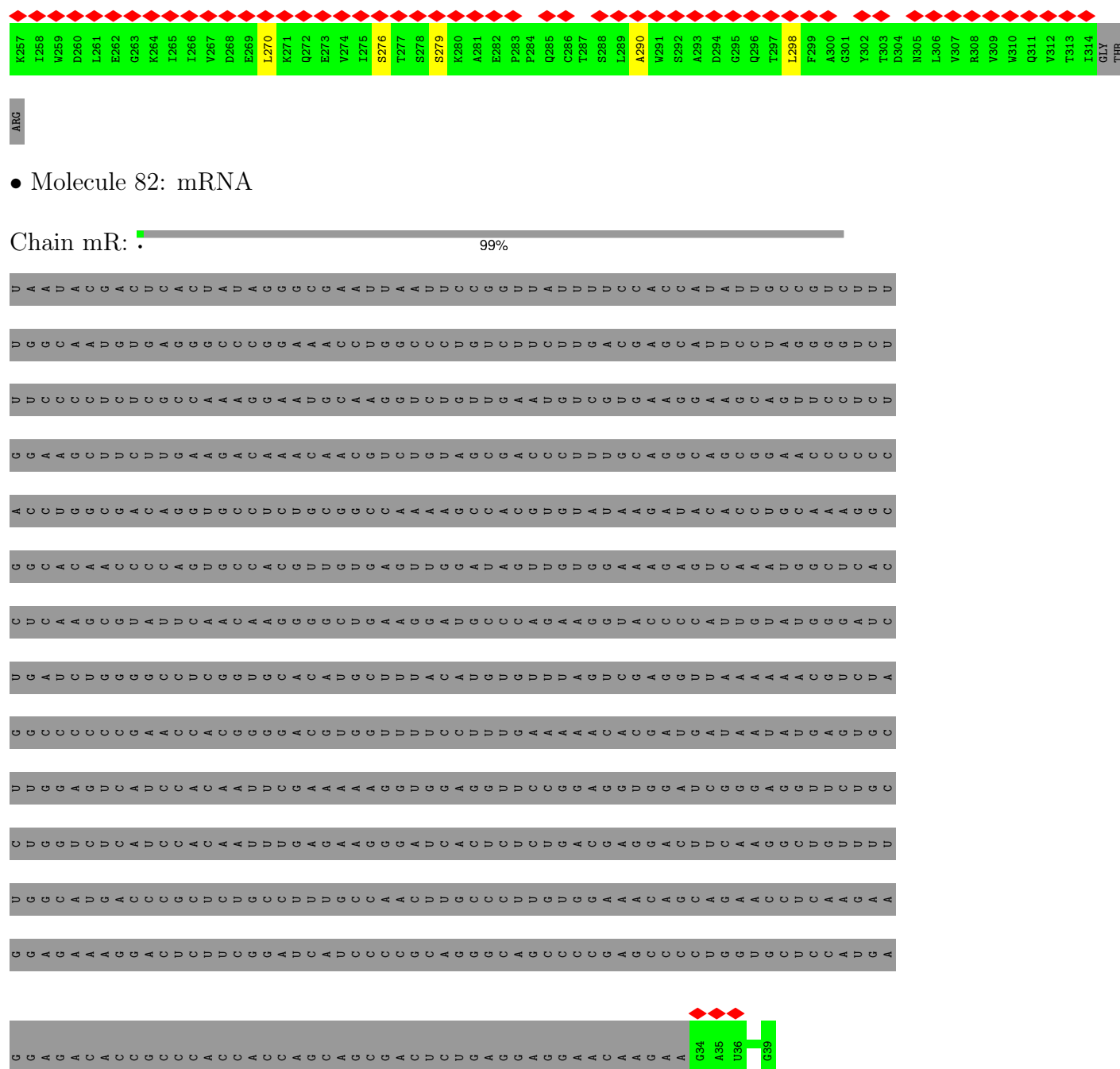


- Molecule 80: Ubiquitin-ribosomal protein eS31 fusion protein



- Molecule 81: Receptor of activated protein C kinase 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	538472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.479	Depositor
Minimum map value	-0.471	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.112	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, OMG, TRS, K, MLZ, MG, ACE, PUT, 4AC, PSU, 6MZ, H2U, ZN, G7M, OMU, A1B75, 5MC, HY3, MA6, B8N, M3L, A2M, 2MU, 1MA, UY1, 2MG, SPD, HIC, OMC

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	0.52	4/82102 (0.0%)	0.65	8/128082 (0.0%)
2	L7	0.51	0/2858	0.63	2/4455 (0.0%)
3	L8	0.52	0/3609	0.63	0/5623
4	LA	0.41	0/1959	0.62	0/2627
5	LB	0.36	0/3295	0.59	0/4406
6	LC	0.37	0/2968	0.56	0/3985
7	LD	0.33	0/2437	0.52	0/3263
8	LE	0.31	0/1821	0.52	0/2442
9	LF	0.37	0/1905	0.53	0/2539
10	LG	0.31	0/1960	0.61	2/2637 (0.1%)
11	LH	0.34	0/1537	0.52	0/2066
12	LI	0.34	0/1755	0.53	0/2344
13	LJ	0.30	0/1385	0.54	0/1852
14	LL	0.31	0/1695	0.51	0/2270
15	LM	0.34	0/1142	0.51	0/1527
16	LN	0.41	0/1746	0.59	0/2338
17	LO	0.37	0/1687	0.54	0/2257
18	LP	0.40	0/1268	0.58	0/1701
19	LQ	0.37	0/1537	0.58	0/2052
20	LR	0.33	0/1582	0.48	0/2091
21	LS	0.36	0/1501	0.51	0/2013
22	LT	0.36	0/1326	0.56	0/1770
23	LU	0.31	0/822	0.53	0/1103
24	LV	0.37	0/1003	0.54	0/1345
25	LW	0.36	0/574	0.55	0/763
26	LX	0.34	0/984	0.54	0/1323
27	LY	0.34	0/1132	0.54	0/1504
28	LZ	0.36	0/1130	0.58	0/1507
29	La	0.41	0/1191	0.59	0/1591
30	Lb	0.33	0/900	0.52	0/1187
31	Lc	0.36	0/780	0.54	0/1046

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.36	0/903	0.54	0/1216
33	Le	0.39	0/1071	0.57	0/1429
34	Lf	0.39	0/903	0.60	0/1208
35	Lg	0.35	0/916	0.52	0/1220
36	Lh	0.32	0/1023	0.49	0/1351
37	Li	0.31	0/843	0.48	0/1115
38	Lj	0.42	0/720	0.65	0/952
39	Lk	0.30	0/575	0.51	0/761
40	Ll	0.38	0/454	0.60	0/599
41	Lm	0.35	0/426	0.52	0/564
42	Ln	0.38	0/241	0.59	0/305
43	Lo	0.37	0/867	0.55	0/1141
44	Lp	0.39	0/718	0.61	0/953
45	Lr	0.36	0/1018	0.49	0/1366
46	NC	0.31	0/52	0.73	0/68
47	Pt	0.37	0/1640	0.71	1/2555 (0.0%)
48	S2	0.45	2/37935 (0.0%)	0.61	4/59125 (0.0%)
49	SA	0.29	0/1785	0.48	0/2426
50	SB	0.33	0/1832	0.50	0/2449
51	SC	0.32	0/1762	0.47	0/2381
52	SD	0.26	0/1784	0.46	0/2403
53	SE	0.31	0/2118	0.53	0/2849
54	SF	0.28	0/1516	0.53	0/2037
55	SG	0.26	0/1946	0.51	0/2590
56	SH	0.27	0/1540	0.51	0/2064
57	SI	0.33	0/1715	0.53	0/2287
58	SJ	0.30	0/1550	0.54	0/2069
59	SK	0.24	0/834	0.47	0/1125
60	SL	0.34	0/1221	0.50	0/1632
61	SM	0.20	0/960	0.50	0/1286
62	SN	0.31	0/1232	0.49	0/1656
63	SO	0.34	0/1023	0.57	0/1372
64	SP	0.25	0/1100	0.54	0/1470
65	SQ	0.29	0/1142	0.51	0/1528
66	SR	0.26	0/1098	0.50	0/1474
67	SS	0.27	0/1232	0.50	0/1651
68	ST	0.27	0/1122	0.49	0/1504
69	SU	0.28	0/813	0.51	0/1092
70	SV	0.38	1/645 (0.2%)	0.54	0/862
71	SW	0.34	0/1051	0.48	0/1406
72	SX	0.34	0/1096	0.57	0/1461
73	SY	0.26	0/1083	0.53	0/1438
74	SZ	0.25	0/691	0.57	0/922

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sa	0.35	0/805	0.54	0/1079
76	Sb	0.30	0/665	0.55	0/891
77	Sc	0.29	0/514	0.59	0/688
78	Sd	0.28	0/470	0.50	0/623
79	Se	0.28	0/397	0.54	0/519
80	Sf	0.21	0/525	0.58	0/695
81	Sg	0.22	0/2493	0.51	0/3394
82	mR	0.37	0/149	0.97	0/231
All	All	0.43	7/221805 (0.0%)	0.60	17/325191 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LC	0	1
8	LE	0	1
9	LF	0	1
10	LG	0	2
12	LI	0	1
13	LJ	0	1
14	LL	0	1
16	LN	0	1
18	LP	0	1
23	LU	0	1
30	Lb	0	1
34	Lf	0	2
43	Lo	0	1
50	SB	0	1
58	SJ	0	1
63	SO	0	2
65	SQ	0	1
67	SS	0	2
72	SX	0	1
All	All	0	23

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	SV	0	ACE	C-N	5.97	1.45	1.33
1	L5	4590	A2M	O3'-P	5.29	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	1871	A2M	O3'-P	5.23	1.61	1.56
1	L5	3718	A2M	O3'-P	5.12	1.61	1.56
48	S2	1804	OMU	O3'-P	5.07	1.61	1.56

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	417	G	O4'-C1'-N9	5.81	116.92	108.20
1	L5	3756	A	O4'-C1'-N9	5.78	116.87	108.20
1	L5	1444	G	N9-C1'-C2'	5.74	120.60	112.00
1	L5	1523	A	N9-C1'-C2'	5.63	120.44	112.00
48	S2	1247	C	C4'-C3'-O3'	5.57	117.75	109.40

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LC	201	ARG	Sidechain
8	LE	123	ARG	Sidechain
9	LF	245	ARG	Sidechain
10	LG	139	GLY	Peptide
10	LG	62	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	76136	0	38528	396	0
2	L7	2558	0	1295	8	0
3	L8	3316	0	1687	17	0
4	LA	1921	0	2022	11	0
5	LB	3240	0	3377	16	0
6	LC	2914	0	3087	6	0
7	LD	2391	0	2426	7	0
8	LE	1787	0	1945	12	0
9	LF	1870	0	1996	9	0
10	LG	1927	0	2074	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	LH	1518	0	1600	3	0
12	LI	1716	0	1765	9	0
13	LJ	1362	0	1399	10	0
14	LL	1664	0	1773	3	0
15	LM	1120	0	1187	1	0
16	LN	1701	0	1749	9	0
17	LO	1655	0	1799	3	0
18	LP	1242	0	1269	5	0
19	LQ	1513	0	1628	5	0
20	LR	1566	0	1729	1	0
21	LS	1461	0	1502	4	0
22	LT	1298	0	1366	3	0
23	LU	808	0	831	5	0
24	LV	989	0	1047	3	0
25	LW	562	0	569	1	0
26	LX	967	0	1040	3	0
27	LY	1115	0	1205	3	0
28	LZ	1107	0	1182	5	0
29	La	1162	0	1213	3	0
30	Lb	898	0	983	7	0
31	Lc	770	0	809	5	0
32	Ld	888	0	930	2	0
33	Le	1053	0	1147	3	0
34	Lf	884	0	923	2	0
35	Lg	906	0	998	1	0
36	Lh	1015	0	1148	4	0
37	Li	832	0	917	2	0
38	Lj	705	0	737	2	0
39	Lk	569	0	637	1	0
40	Ll	444	0	482	3	0
41	Lm	432	0	471	0	0
42	Ln	240	0	289	0	0
43	Lo	864	0	929	0	0
44	Lp	708	0	756	5	0
45	Lr	1005	0	1072	2	0
46	NC	118	0	55	2	0
47	Pt	1597	0	817	13	0
48	S2	35736	0	18083	224	0
49	SA	1750	0	1755	11	0
50	SB	1806	0	1888	6	0
51	SC	1725	0	1813	16	0
52	SD	1756	0	1852	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	SE	2076	0	2177	13	0
54	SF	1495	0	1549	12	0
55	SG	1923	0	2089	11	0
56	SH	1517	0	1605	12	0
57	SI	1686	0	1772	10	0
58	SJ	1525	0	1640	6	0
59	SK	810	0	836	3	0
60	SL	1200	0	1271	4	0
61	SM	950	0	987	16	0
62	SN	1208	0	1293	5	0
63	SO	1010	0	1034	3	0
64	SP	1078	0	1121	11	0
65	SQ	1124	0	1193	9	0
66	SR	1083	0	1137	9	0
67	SS	1214	0	1275	9	0
68	ST	1103	0	1133	8	0
69	SU	803	0	873	7	0
70	SV	640	0	638	5	0
71	SW	1034	0	1080	7	0
72	SX	1088	0	1149	3	0
73	SY	1065	0	1142	13	0
74	SZ	683	0	761	7	0
75	Sa	792	0	841	4	0
76	Sb	651	0	672	4	0
77	Sc	512	0	541	6	0
78	Sd	459	0	448	2	0
79	Se	395	0	434	1	0
80	Sf	515	0	521	12	0
81	Sg	2436	0	2393	22	0
82	mR	133	0	66	0	0
83	L5	114	0	0	0	0
83	L7	3	0	0	0	0
83	L8	5	0	0	0	0
83	LA	3	0	0	0	0
83	LH	1	0	0	0	0
83	LI	1	0	0	0	0
83	LL	1	0	0	0	0
83	LN	1	0	0	0	0
83	LQ	1	0	0	0	0
83	Lb	1	0	0	0	0
83	Le	1	0	0	0	0
83	Lf	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	L1	1	0	0	0	0
83	S2	32	0	0	0	0
83	SL	1	0	0	0	0
83	SO	1	0	0	0	0
83	ST	1	0	0	0	0
83	Sa	1	0	0	0	0
84	L5	42	0	84	5	0
85	L5	120	0	228	2	0
85	S2	20	0	38	0	0
86	L5	26	0	0	1	0
87	L5	16	0	24	1	0
88	L5	271	0	0	0	0
88	L7	5	0	0	0	0
88	L8	6	0	0	0	0
88	LL	1	0	0	0	0
88	LN	2	0	0	0	0
88	Lj	1	0	0	0	0
88	Lo	1	0	0	0	0
88	S2	83	0	0	0	0
88	Sd	1	0	0	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	1	0	0	0	0
89	Sf	1	0	0	0	0
90	L5	4442	0	0	1	0
90	L7	81	0	0	0	0
90	L8	15	0	0	0	0
90	LA	130	0	0	0	0
90	LB	142	0	0	1	0
90	LC	116	0	0	0	0
90	LD	38	0	0	0	0
90	LE	7	0	0	0	0
90	LF	54	0	0	0	0
90	LG	17	0	0	0	0
90	LH	17	0	0	0	0
90	LI	62	0	0	0	0
90	LJ	3	0	0	0	0
90	LL	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	LM	11	0	0	0	0
90	LN	121	0	0	0	0
90	LO	79	0	0	0	0
90	LP	62	0	0	0	0
90	LQ	87	0	0	0	0
90	LR	57	0	0	0	0
90	LS	46	0	0	0	0
90	LT	64	0	0	0	0
90	LV	43	0	0	0	0
90	LW	12	0	0	0	0
90	LX	22	0	0	0	0
90	LY	16	0	0	0	0
90	LZ	5	0	0	0	0
90	La	87	0	0	0	0
90	Lb	33	0	0	0	0
90	Lc	8	0	0	0	0
90	Ld	29	0	0	0	0
90	Le	88	0	0	0	0
90	Lf	38	0	0	0	0
90	Lg	60	0	0	0	0
90	Lh	15	0	0	0	0
90	Li	11	0	0	0	0
90	Lj	61	0	0	0	0
90	Lk	1	0	0	0	0
90	Ll	33	0	0	0	0
90	Lm	16	0	0	0	0
90	Ln	13	0	0	0	0
90	Lo	42	0	0	0	0
90	Lp	30	0	0	0	0
90	Lr	19	0	0	0	0
90	NC	5	0	0	0	0
90	Pt	3	0	0	0	0
90	S2	850	0	0	2	0
90	Sb	6	0	0	0	0
90	Se	2	0	0	0	0
90	mR	3	0	0	0	0
All	All	219527	0	157826	989	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 989 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2485:U:H3	1:L5:2493:G:H1	1.09	0.99
1:L5:3946:G:N2	1:L5:4067:U:O2	2.06	0.87
47:Pt:18:G:H1	47:Pt:55:PSU:HN3	1.25	0.84
1:L5:3944:OMG:HM22	1:L5:3945:A:H5''	1.62	0.81
61:SM:52:LEU:HB2	61:SM:78:LYS:HE3	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	249/257 (97%)	241 (97%)	8 (3%)	0	100	100
5	LB	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
6	LC	364/427 (85%)	357 (98%)	7 (2%)	0	100	100
7	LD	292/297 (98%)	284 (97%)	7 (2%)	1 (0%)	36	29
8	LE	217/288 (75%)	205 (94%)	11 (5%)	1 (0%)	24	16
9	LF	223/248 (90%)	218 (98%)	4 (2%)	1 (0%)	30	22
10	LG	239/266 (90%)	231 (97%)	8 (3%)	0	100	100
11	LH	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
12	LI	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
13	LJ	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
14	LL	204/211 (97%)	200 (98%)	4 (2%)	0	100	100
15	LM	134/215 (62%)	133 (99%)	1 (1%)	0	100	100
16	LN	201/204 (98%)	193 (96%)	7 (4%)	1 (0%)	24	16
17	LO	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	LR	185/196 (94%)	185 (100%)	0	0	100	100
21	LS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
22	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
23	LU	97/128 (76%)	97 (100%)	0	0	100	100
24	LV	131/140 (94%)	127 (97%)	4 (3%)	0	100	100
25	LW	64/157 (41%)	63 (98%)	1 (2%)	0	100	100
26	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	LY	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
28	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
29	La	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	18	10
30	Lb	106/159 (67%)	103 (97%)	3 (3%)	0	100	100
31	Lc	97/115 (84%)	97 (100%)	0	0	100	100
32	Ld	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
33	Le	126/135 (93%)	126 (100%)	0	0	100	100
34	Lf	108/110 (98%)	108 (100%)	0	0	100	100
35	Lg	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
38	Lj	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
39	Lk	67/70 (96%)	67 (100%)	0	0	100	100
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	23/25 (92%)	23 (100%)	0	0	100	100
43	Lo	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
44	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
45	Lr	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
46	NC	4/19 (21%)	3 (75%)	1 (25%)	0	100	100
49	SA	221/295 (75%)	219 (99%)	2 (1%)	0	100	100
50	SB	219/264 (83%)	215 (98%)	4 (2%)	0	100	100
51	SC	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
52	SD	224/243 (92%)	223 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
54	SF	187/204 (92%)	177 (95%)	9 (5%)	1 (0%)	24	16
55	SG	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
56	SH	187/194 (96%)	180 (96%)	7 (4%)	0	100	100
57	SI	204/208 (98%)	196 (96%)	7 (3%)	1 (0%)	24	16
58	SJ	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
59	SK	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
60	SL	142/158 (90%)	139 (98%)	3 (2%)	0	100	100
61	SM	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
62	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
63	SO	133/151 (88%)	130 (98%)	3 (2%)	0	100	100
64	SP	129/145 (89%)	126 (98%)	3 (2%)	0	100	100
65	SQ	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
66	SR	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
67	SS	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
68	ST	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
69	SU	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
70	SV	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
71	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
72	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
73	SY	129/133 (97%)	127 (98%)	2 (2%)	0	100	100
74	SZ	83/125 (66%)	81 (98%)	2 (2%)	0	100	100
75	Sa	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
76	Sb	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
77	Sc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
78	Sd	53/56 (95%)	53 (100%)	0	0	100	100
79	Se	46/133 (35%)	45 (98%)	1 (2%)	0	100	100
80	Sf	61/156 (39%)	55 (90%)	6 (10%)	0	100	100
81	Sg	311/317 (98%)	297 (96%)	12 (4%)	2 (1%)	21	13
All	All	11255/12782 (88%)	10989 (98%)	257 (2%)	9 (0%)	49	40

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	LE	166	LYS
57	SI	131	PRO
9	LF	237	GLU
16	LN	157	LYS
7	LD	17	GLN

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	193/199 (97%)	192 (100%)	1 (0%)	81	84
5	LB	347/348 (100%)	346 (100%)	1 (0%)	86	88
6	LC	305/348 (88%)	301 (99%)	4 (1%)	61	61
7	LD	247/250 (99%)	247 (100%)	0	100	100
8	LE	196/252 (78%)	196 (100%)	0	100	100
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	203 (100%)	0	100	100
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	180/181 (99%)	180 (100%)	0	100	100
13	LJ	143/149 (96%)	141 (99%)	2 (1%)	59	59
14	LL	172/177 (97%)	171 (99%)	1 (1%)	78	81
15	LM	116/161 (72%)	115 (99%)	1 (1%)	70	73
16	LN	171/172 (99%)	170 (99%)	1 (1%)	78	81
17	LO	173/174 (99%)	172 (99%)	1 (1%)	78	81
18	LP	134/163 (82%)	133 (99%)	1 (1%)	76	78
19	LQ	164/165 (99%)	163 (99%)	1 (1%)	78	81
20	LR	166/175 (95%)	164 (99%)	2 (1%)	63	63
21	LS	157/157 (100%)	157 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	89/115 (77%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	LV	102/107 (95%)	101 (99%)	1 (1%)	68	70
25	LW	58/126 (46%)	58 (100%)	0	100	100
26	LX	106/133 (80%)	106 (100%)	0	100	100
27	LY	124/135 (92%)	124 (100%)	0	100	100
28	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	73
29	La	120/121 (99%)	120 (100%)	0	100	100
30	Lb	90/125 (72%)	89 (99%)	1 (1%)	65	67
31	Lc	84/97 (87%)	84 (100%)	0	100	100
32	Ld	98/110 (89%)	98 (100%)	0	100	100
33	Le	114/121 (94%)	113 (99%)	1 (1%)	70	73
34	Lf	89/89 (100%)	87 (98%)	2 (2%)	45	42
35	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	70
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	73
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	59
39	Lk	64/65 (98%)	63 (98%)	1 (2%)	55	54
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	47 (100%)	0	100	100
42	Ln	24/24 (100%)	23 (96%)	1 (4%)	26	19
43	Lo	92/93 (99%)	92 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/120 (91%)	109 (100%)	0	100	100
46	NC	6/6 (100%)	5 (83%)	1 (17%)	2	0
49	SA	184/242 (76%)	183 (100%)	1 (0%)	81	84
50	SB	202/231 (87%)	201 (100%)	1 (0%)	81	84
51	SC	188/225 (84%)	186 (99%)	2 (1%)	65	67
52	SD	189/202 (94%)	188 (100%)	1 (0%)	81	84
53	SE	224/225 (100%)	223 (100%)	1 (0%)	84	87
54	SF	159/170 (94%)	158 (99%)	1 (1%)	78	81
55	SG	207/218 (95%)	205 (99%)	2 (1%)	68	70
56	SH	168/174 (97%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	SI	178/180 (99%)	175 (98%)	3 (2%)	53	52
58	SJ	161/168 (96%)	160 (99%)	1 (1%)	78	81
59	SK	87/136 (64%)	87 (100%)	0	100	100
60	SL	132/142 (93%)	132 (100%)	0	100	100
61	SM	104/108 (96%)	98 (94%)	6 (6%)	18	10
62	SN	130/131 (99%)	130 (100%)	0	100	100
63	SO	105/119 (88%)	105 (100%)	0	100	100
64	SP	117/130 (90%)	116 (99%)	1 (1%)	70	73
65	SQ	117/121 (97%)	116 (99%)	1 (1%)	70	73
66	SR	121/122 (99%)	120 (99%)	1 (1%)	73	75
67	SS	128/132 (97%)	126 (98%)	2 (2%)	55	54
68	ST	112/115 (97%)	112 (100%)	0	100	100
69	SU	93/107 (87%)	91 (98%)	2 (2%)	45	42
70	SV	67/67 (100%)	67 (100%)	0	100	100
71	SW	112/113 (99%)	112 (100%)	0	100	100
72	SX	111/114 (97%)	109 (98%)	2 (2%)	51	50
73	SY	113/115 (98%)	113 (100%)	0	100	100
74	SZ	75/103 (73%)	74 (99%)	1 (1%)	61	61
75	Sa	86/98 (88%)	86 (100%)	0	100	100
76	Sb	75/76 (99%)	75 (100%)	0	100	100
77	Sc	58/62 (94%)	58 (100%)	0	100	100
78	Sd	48/49 (98%)	48 (100%)	0	100	100
79	Se	40/104 (38%)	40 (100%)	0	100	100
80	Sf	56/140 (40%)	54 (96%)	2 (4%)	31	23
81	Sg	272/275 (99%)	269 (99%)	3 (1%)	65	67
All	All	9808/10856 (90%)	9746 (99%)	62 (1%)	76	81

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	SA	2(A)	SER
72	SX	115	ILE
55	SG	124	LEU

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Mol	Chain	Res	Type
72	SX	105	PHE
81	Sg	107	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
53	SE	98	ASN
61	SM	46	GLN
53	SE	188	ASN
56	SH	186	ASN
63	SO	83	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3529/5069 (69%)	454 (12%)	76 (2%)
2	L7	119/120 (99%)	6 (5%)	0
3	L8	155/156 (99%)	17 (10%)	4 (2%)
47	Pt	74/75 (98%)	15 (20%)	0
48	S2	1667/1869 (89%)	209 (12%)	31 (1%)
82	mR	5/832 (0%)	0	0
All	All	5549/8121 (68%)	701 (12%)	111 (2%)

5 of 701 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	25	A
1	L5	39	A
1	L5	42	A
1	L5	43	U
1	L5	48	G

5 of 111 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	3904	G
48	S2	1825	A
1	L5	4870	G
48	S2	1784	G
48	S2	1061	U

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

229 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	OMC	L5	1881	1,88	19,22,23	0.81	2 (10%)	25,31,34	0.82	0
1	A2M	L5	2787	1	22,25,26	1.27	1 (4%)	30,36,39	1.25	2 (6%)
1	OMC	L5	2804	1	19,22,23	0.77	0	25,31,34	0.50	0
1	A2M	L5	1871	1,88	22,25,26	1.25	1 (4%)	30,36,39	1.33	6 (20%)
1	A2M	L5	2401	1,88	22,25,26	1.25	1 (4%)	30,36,39	1.16	2 (6%)
1	OMG	L5	1522	1	23,26,27	0.69	0	32,38,41	0.80	1 (3%)
48	OMU	S2	116	48	19,22,23	0.70	0	25,31,34	1.11	2 (8%)
1	PSU	L5	5001	1,88	18,21,22	1.00	1 (5%)	21,30,33	1.74	4 (19%)
48	PSU	S2	406	48	18,21,22	1.06	2 (11%)	21,30,33	1.51	4 (19%)
47	2MG	Pt	10	47	23,26,27	1.30	2 (8%)	33,38,41	1.38	4 (12%)
48	PSU	S2	573	48	18,21,22	1.10	1 (5%)	21,30,33	1.59	4 (19%)
1	PSU	L5	3758	1	18,21,22	1.02	1 (5%)	21,30,33	1.47	4 (19%)
1	OMG	L5	1625	1,83	23,26,27	0.57	0	32,38,41	0.55	0
1	PSU	L5	3729	1	18,21,22	1.25	2 (11%)	21,30,33	1.67	4 (19%)
47	2MU	Pt	54	47	20,23,24	1.42	2 (10%)	27,33,36	1.95	7 (25%)
48	PSU	S2	34	48	18,21,22	1.05	2 (11%)	21,30,33	1.50	4 (19%)
1	PSU	L5	3715	1	18,21,22	1.01	1 (5%)	21,30,33	1.64	4 (19%)
48	MA6	S2	1850	48	23,26,27	1.32	3 (13%)	33,38,41	2.94	13 (39%)
1	OMU	L5	4306	1	19,22,23	0.66	0	25,31,34	1.35	5 (20%)
1	OMG	L5	2424	1	23,26,27	0.66	0	32,38,41	0.54	0
1	PSU	L5	3920	1,88	18,21,22	1.28	2 (11%)	21,30,33	1.65	5 (23%)
48	PSU	S2	815	48	18,21,22	1.15	3 (16%)	21,30,33	1.62	4 (19%)
1	PSU	L5	4531	1	18,21,22	1.09	1 (5%)	21,30,33	1.91	3 (14%)
48	A2M	S2	1031	48	22,25,26	1.22	2 (9%)	30,36,39	1.19	4 (13%)
48	OMU	S2	121	48	19,22,23	0.64	0	25,31,34	1.12	2 (8%)
1	A2M	L5	1534	1,88	22,25,26	1.40	2 (9%)	30,36,39	1.31	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L5	3724	1	22,25,26	1.22	2 (9%)	30,36,39	1.40	5 (16%)
48	A2M	S2	1678	48	22,25,26	1.51	3 (13%)	30,36,39	1.50	7 (23%)
1	A2M	L5	3760	1,48	22,25,26	1.50	3 (13%)	30,36,39	1.68	10 (33%)
1	OMG	L5	4494	1	23,26,27	0.66	0	32,38,41	0.71	0
1	OMU	L5	4620	1	19,22,23	0.59	0	25,31,34	1.40	4 (16%)
48	PSU	S2	814	48	18,21,22	0.92	1 (5%)	21,30,33	1.49	3 (14%)
1	PSU	L5	4457	1	18,21,22	1.32	2 (11%)	21,30,33	1.28	4 (19%)
48	OMG	S2	509	48	23,26,27	0.60	0	32,38,41	0.58	0
48	PSU	S2	1243	48	18,21,22	1.20	2 (11%)	21,30,33	1.60	4 (19%)
48	PSU	S2	1232	48	18,21,22	1.08	2 (11%)	21,30,33	1.56	4 (19%)
1	PSU	L5	1744	1,83	18,21,22	1.13	2 (11%)	21,30,33	1.60	4 (19%)
1	OMC	L5	2861	1	19,22,23	0.59	0	25,31,34	0.52	0
1	PSU	L5	3770	1	18,21,22	1.13	2 (11%)	21,30,33	1.59	4 (19%)
1	A2M	L5	3830	1	22,25,26	1.30	3 (13%)	30,36,39	1.36	4 (13%)
1	PSU	L5	1781	1	18,21,22	0.94	1 (5%)	21,30,33	1.47	4 (19%)
1	OMG	L5	3744	1	23,26,27	0.71	0	32,38,41	0.57	0
1	OMC	L5	1340	1	19,22,23	0.86	2 (10%)	25,31,34	0.67	0
48	PSU	S2	609	48	18,21,22	0.99	1 (5%)	21,30,33	1.47	4 (19%)
1	PSU	L5	3639	1	18,21,22	1.39	2 (11%)	21,30,33	1.37	4 (19%)
3	PSU	L8	69	3	18,21,22	1.11	2 (11%)	21,30,33	1.58	5 (23%)
48	PSU	S2	1081	48	18,21,22	1.10	3 (16%)	21,30,33	1.42	4 (19%)
1	PSU	L5	1536	1	18,21,22	1.71	2 (11%)	21,30,33	1.71	6 (28%)
1	OMC	L5	3869	1	19,22,23	0.75	0	25,31,34	0.55	0
48	PSU	S2	1367	48	18,21,22	0.99	1 (5%)	21,30,33	1.63	4 (19%)
48	PSU	S2	1136	48	18,21,22	1.11	2 (11%)	21,30,33	1.67	4 (19%)
1	PSU	L5	4972	1,83	18,21,22	1.15	2 (11%)	21,30,33	1.51	4 (19%)
1	A2M	L5	400	1	22,25,26	1.31	3 (13%)	30,36,39	1.27	3 (10%)
48	OMG	S2	683	48	23,26,27	0.69	0	32,38,41	0.68	0
47	PSU	Pt	13	47	18,21,22	1.06	2 (11%)	21,30,33	1.54	4 (19%)
48	A2M	S2	484	48	22,25,26	1.11	1 (4%)	30,36,39	1.29	5 (16%)
1	OMC	L5	2365	1	19,22,23	0.71	0	25,31,34	0.63	0
1	A2M	L5	3723	1	22,25,26	1.20	2 (9%)	30,36,39	1.48	7 (23%)
1	PSU	L5	4579	1	18,21,22	0.98	1 (5%)	21,30,33	1.68	4 (19%)
1	UR3	L5	4530	1	19,22,23	2.64	7 (36%)	26,32,35	1.76	4 (15%)
1	OMC	L5	2351	1,88	19,22,23	0.76	0	25,31,34	0.88	0
1	PSU	L5	3762	1	18,21,22	0.99	1 (5%)	21,30,33	1.38	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L5	1316	1	23,26,27	0.80	1 (4%)	32,38,41	0.73	1 (3%)
43	MLZ	Lo	53	43	8,9,10	0.66	0	4,9,11	0.70	0
1	1MA	L5	1322	1,88	21,25,26	0.75	0	30,37,40	0.89	1 (3%)
1	PSU	L5	4423	1	18,21,22	0.99	1 (5%)	21,30,33	1.50	4 (19%)
1	PSU	L5	1862	1	18,21,22	1.26	1 (5%)	21,30,33	1.67	4 (19%)
1	OMC	L5	4536	1,88	19,22,23	0.89	1 (5%)	25,31,34	0.68	0
48	PSU	S2	93	48	18,21,22	0.87	1 (5%)	21,30,33	1.52	4 (19%)
48	OMG	S2	644	48	23,26,27	0.63	0	32,38,41	0.65	0
48	6MZ	S2	1832	88,48,83	22,25,26	3.73	13 (59%)	29,36,39	2.79	12 (41%)
48	UY1	S2	1326	48,88	19,22,23	4.10	7 (36%)	21,31,34	2.27	5 (23%)
3	OMU	L8	14	1,83,3	19,22,23	0.65	1 (5%)	25,31,34	1.34	5 (20%)
48	PSU	S2	1239	48	18,21,22	1.23	3 (16%)	21,30,33	1.64	4 (19%)
48	B8N	S2	1248	48	25,29,30	0.64	0	28,42,45	1.14	2 (7%)
1	OMG	L5	4392	1	23,26,27	0.70	0	32,38,41	0.63	0
1	PSU	L5	1582	1	18,21,22	1.18	1 (5%)	21,30,33	1.36	4 (19%)
1	PSU	L5	1792	1,83	18,21,22	1.12	2 (11%)	21,30,33	1.52	4 (19%)
48	PSU	S2	801	48	18,21,22	1.06	1 (5%)	21,30,33	1.71	4 (19%)
48	PSU	S2	1692	48	18,21,22	1.06	2 (11%)	21,30,33	1.49	4 (19%)
48	A2M	S2	159	48	22,25,26	1.28	2 (9%)	30,36,39	1.67	6 (20%)
48	PSU	S2	119	48	18,21,22	1.13	1 (5%)	21,30,33	1.47	4 (19%)
1	A2M	L5	3825	1	22,25,26	1.18	1 (4%)	30,36,39	1.23	3 (10%)
1	PSU	L5	1677	1	18,21,22	1.18	3 (16%)	21,30,33	1.61	5 (23%)
1	PSU	L5	4420	1	18,21,22	1.20	4 (22%)	21,30,33	1.54	4 (19%)
48	A2M	S2	1383	48	22,25,26	1.15	2 (9%)	30,36,39	1.46	6 (20%)
1	OMC	L5	3701	1,83	19,22,23	0.72	1 (5%)	25,31,34	0.73	0
48	OMC	S2	1391	48	19,22,23	0.75	1 (5%)	25,31,34	0.61	0
1	PSU	L5	4576	1	18,21,22	1.03	1 (5%)	21,30,33	1.49	4 (19%)
1	PSU	L5	4442	1	18,21,22	0.99	2 (11%)	21,30,33	1.83	5 (23%)
48	OMU	S2	1288	48	19,22,23	0.70	0	25,31,34	1.39	5 (20%)
48	A2M	S2	590	48	22,25,26	1.41	2 (9%)	30,36,39	1.44	5 (16%)
1	OMG	L5	4228	1	23,26,27	0.64	0	32,38,41	0.72	0
1	6MZ	L5	4220	1	22,25,26	3.82	9 (40%)	29,36,39	2.74	12 (41%)
48	OMG	S2	1490	48,88	23,26,27	0.65	0	32,38,41	0.57	0
1	OMG	L5	2364	1	23,26,27	0.73	0	32,38,41	0.60	0
48	OMC	S2	517	48	19,22,23	0.73	1 (5%)	25,31,34	0.56	0
1	PSU	L5	3637	1,83	18,21,22	1.16	2 (11%)	21,30,33	1.35	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	1174	48,83	18,21,22	1.10	1 (5%)	21,30,33	1.43	4 (19%)
3	PSU	L8	55	3	18,21,22	1.13	2 (11%)	21,30,33	1.54	4 (19%)
1	A2M	L5	4590	1	22,25,26	1.04	1 (4%)	30,36,39	1.21	3 (10%)
1	A2M	L5	3718	1	22,25,26	1.29	2 (9%)	30,36,39	1.27	5 (16%)
1	PSU	L5	3851	1,83	18,21,22	1.48	2 (11%)	21,30,33	1.80	4 (19%)
1	5MC	L5	4447	1,83	19,22,23	3.53	8 (42%)	26,32,35	1.28	3 (11%)
47	H2U	Pt	20	47	18,21,22	0.55	0	19,30,33	1.18	1 (5%)
48	PSU	S2	651	48	18,21,22	0.94	1 (5%)	21,30,33	1.62	4 (19%)
48	PSU	S2	686	48	18,21,22	1.14	2 (11%)	21,30,33	1.53	4 (19%)
48	MA6	S2	1851	48	23,26,27	1.41	4 (17%)	33,38,41	2.95	14 (42%)
1	A2M	L5	3867	1	22,25,26	1.47	3 (13%)	30,36,39	1.26	3 (10%)
1	A2M	L5	398	1	22,25,26	1.20	1 (4%)	30,36,39	1.25	4 (13%)
1	OMG	L5	4499	1	23,26,27	0.56	0	32,38,41	0.62	0
1	PSU	L5	4312	1	18,21,22	0.96	1 (5%)	21,30,33	1.55	5 (23%)
48	PSU	S2	1004	48	18,21,22	1.21	2 (11%)	21,30,33	1.48	4 (19%)
1	PSU	L5	1683	1,83	18,21,22	1.20	1 (5%)	21,30,33	1.41	3 (14%)
1	OMU	L5	4498	1,83	19,22,23	0.72	0	25,31,34	1.34	4 (16%)
48	PSU	S2	105	48	18,21,22	0.92	0	21,30,33	1.71	4 (19%)
48	PSU	S2	1238	48	18,21,22	1.02	1 (5%)	21,30,33	1.58	4 (19%)
1	OMC	L5	2824	1	19,22,23	0.86	1 (5%)	25,31,34	0.56	0
1	PSU	L5	4552	1	18,21,22	1.35	1 (5%)	21,30,33	1.42	4 (19%)
1	OMG	L5	2876	1	23,26,27	0.73	0	32,38,41	0.74	0
48	PSU	S2	681	48	18,21,22	1.28	2 (11%)	21,30,33	1.36	3 (14%)
48	PSU	S2	1445	48	18,21,22	1.07	2 (11%)	21,30,33	1.57	4 (19%)
48	OMG	S2	867	48	23,26,27	0.51	0	32,38,41	0.50	0
1	PSU	L5	4569	1	18,21,22	1.27	4 (22%)	21,30,33	1.30	3 (14%)
48	A2M	S2	668	48,88	22,25,26	1.53	3 (13%)	30,36,39	1.28	4 (13%)
1	PSU	L5	3768	1	18,21,22	1.05	1 (5%)	21,30,33	1.64	4 (19%)
48	PSU	S2	1347	48	18,21,22	1.06	1 (5%)	21,30,33	1.59	4 (19%)
1	PSU	L5	4628	1	18,21,22	1.06	2 (11%)	21,30,33	1.66	4 (19%)
48	A2M	S2	512	48	22,25,26	1.24	2 (9%)	30,36,39	1.32	4 (13%)
48	PSU	S2	109	48	18,21,22	1.00	1 (5%)	21,30,33	1.69	4 (19%)
1	5MC	L5	3782	1,88	19,22,23	3.37	8 (42%)	26,32,35	1.11	2 (7%)
1	OMU	L5	3925	1	19,22,23	0.80	1 (5%)	25,31,34	1.31	4 (16%)
1	PSU	L5	4403	1,83	18,21,22	1.11	1 (5%)	21,30,33	1.60	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L5	4637	1,83	23,26,27	0.72	0	32,38,41	0.48	0
47	5MC	Pt	49	47	19,22,23	3.69	8 (42%)	26,32,35	0.99	1 (3%)
1	A2M	L5	2363	1,88	22,25,26	1.34	2 (9%)	30,36,39	1.39	5 (16%)
1	PSU	L5	4500	1	18,21,22	1.02	2 (11%)	21,30,33	1.77	4 (19%)
48	OMG	S2	1447	48	23,26,27	0.54	0	32,38,41	0.61	0
1	PSU	L5	5010	1	18,21,22	1.19	2 (11%)	21,30,33	1.53	4 (19%)
1	PSU	L5	1782	1	18,21,22	0.98	1 (5%)	21,30,33	1.54	4 (19%)
1	PSU	L5	4493	1,83	18,21,22	1.24	2 (11%)	21,30,33	1.48	4 (19%)
48	A2M	S2	468	48	22,25,26	1.18	2 (9%)	30,36,39	1.42	7 (23%)
48	OMU	S2	1442	48,88	19,22,23	0.62	0	25,31,34	1.31	6 (24%)
1	OMC	L5	3887	1	19,22,23	0.85	1 (5%)	25,31,34	0.72	0
1	OMC	L5	4456	1	19,22,23	0.80	1 (5%)	25,31,34	0.63	0
1	PSU	L5	3844	1	18,21,22	1.32	1 (5%)	21,30,33	1.48	4 (19%)
48	4AC	S2	1337	48	21,24,25	3.06	11 (52%)	28,34,37	1.13	2 (7%)
48	PSU	S2	866	48	18,21,22	1.10	1 (5%)	21,30,33	1.72	4 (19%)
48	PSU	S2	1625	48	18,21,22	0.97	1 (5%)	21,30,33	1.54	4 (19%)
48	4AC	S2	1842	48	21,24,25	2.93	11 (52%)	28,34,37	0.84	1 (3%)
1	OMU	L5	2415	1	19,22,23	0.58	0	25,31,34	1.31	5 (20%)
1	OMC	L5	3841	1	19,22,23	0.84	2 (10%)	25,31,34	0.81	1 (4%)
48	PSU	S2	966	48	18,21,22	0.84	1 (5%)	21,30,33	1.46	4 (19%)
1	OMG	L5	3944	1	23,26,27	0.52	0	32,38,41	0.53	0
1	PSU	L5	3695	1,83	18,21,22	1.00	1 (5%)	21,30,33	1.42	4 (19%)
48	PSU	S2	296	48	18,21,22	0.87	0	21,30,33	1.55	4 (19%)
48	PSU	S2	822	48	18,21,22	1.15	2 (11%)	21,30,33	1.49	5 (23%)
48	OMG	S2	436	48	23,26,27	0.63	0	32,38,41	0.59	0
48	PSU	S2	1177	48	18,21,22	1.08	2 (11%)	21,30,33	1.50	4 (19%)
1	OMC	L5	3808	1	19,22,23	0.75	0	25,31,34	0.67	0
48	PSU	S2	1244	48	18,21,22	1.03	1 (5%)	21,30,33	1.58	4 (19%)
48	PSU	S2	918	48	18,21,22	0.95	2 (11%)	21,30,33	1.72	5 (23%)
1	A2M	L5	1326	1	22,25,26	1.31	3 (13%)	30,36,39	1.27	3 (10%)
48	PSU	S2	572	48	18,21,22	1.01	2 (11%)	21,30,33	1.64	5 (23%)
1	PSU	L5	4296	1	18,21,22	1.24	3 (16%)	21,30,33	1.66	4 (19%)
48	OMU	S2	354	48	19,22,23	0.53	0	25,31,34	1.37	6 (24%)
1	A2M	L5	1524	1	22,25,26	1.34	3 (13%)	30,36,39	1.33	2 (6%)
48	OMU	S2	428	48	19,22,23	0.47	0	25,31,34	1.33	6 (24%)
1	PSU	L5	2839	1	18,21,22	1.24	2 (11%)	21,30,33	1.49	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	1643	48,88	18,21,22	1.00	2 (11%)	21,30,33	1.50	4 (19%)
1	A2M	L5	3785	1	22,25,26	1.50	3 (13%)	30,36,39	1.58	9 (30%)
1	PSU	L5	1779	1	18,21,22	1.10	2 (11%)	21,30,33	1.53	4 (19%)
1	PSU	L5	3764	1	18,21,22	1.66	2 (11%)	21,30,33	1.44	2 (9%)
1	OMG	L5	3899	1,88	23,26,27	0.79	0	32,38,41	0.77	1 (3%)
1	OMG	L5	4623	1	23,26,27	0.66	0	32,38,41	0.79	1 (3%)
48	OMU	S2	627	48	19,22,23	0.59	0	25,31,34	1.40	5 (20%)
41	M3L	Lm	98	41	10,11,12	0.47	0	9,14,16	0.46	0
1	A2M	L5	2815	1,88	22,25,26	1.18	3 (13%)	30,36,39	1.28	5 (16%)
1	PSU	L5	3853	1,88,83	18,21,22	1.38	3 (16%)	21,30,33	1.45	4 (19%)
48	OMC	S2	462	48	19,22,23	0.60	0	25,31,34	0.49	0
1	UY1	L5	3818	1,83	19,22,23	3.85	8 (42%)	21,31,34	2.53	6 (28%)
1	PSU	L5	1860	1	18,21,22	1.13	2 (11%)	21,30,33	1.65	4 (19%)
48	A2M	S2	27	48,88	22,25,26	1.25	1 (4%)	30,36,39	1.35	6 (20%)
1	PSU	L5	4361	1	18,21,22	1.19	2 (11%)	21,30,33	1.54	4 (19%)
48	OMG	S2	601	48	23,26,27	0.61	0	32,38,41	0.60	0
1	OMG	L5	4618	1,83	23,26,27	0.72	0	32,38,41	0.58	0
48	OMU	S2	1804	48	19,22,23	0.67	0	25,31,34	1.49	5 (20%)
30	MLZ	Lb	5	30,83	8,9,10	0.79	0	4,9,11	0.66	0
48	OMC	S2	174	48,88	19,22,23	0.63	0	25,31,34	0.64	0
48	A2M	S2	576	48	22,25,26	1.32	2 (9%)	30,36,39	1.39	6 (20%)
1	PSU	L5	4293	1	18,21,22	1.20	2 (11%)	21,30,33	1.53	4 (19%)
48	PSU	S2	649	48	18,21,22	1.07	2 (11%)	21,30,33	1.60	4 (19%)
3	OMG	L8	75	3	23,26,27	0.63	0	32,38,41	0.66	0
1	PSU	L5	4299	1	18,21,22	0.91	1 (5%)	21,30,33	1.34	3 (14%)
1	PSU	L5	4353	1	18,21,22	1.00	2 (11%)	21,30,33	1.68	4 (19%)
5	HIC	LB	245	5	10,11,12	0.57	0	9,14,16	0.88	0
1	PSU	L5	3734	1	18,21,22	0.91	1 (5%)	21,30,33	1.54	5 (23%)
72	HY3	SX	62	72	7,8,9	6.30	5 (71%)	7,10,12	1.29	1 (14%)
1	A2M	L5	4571	1	22,25,26	1.50	3 (13%)	30,36,39	1.38	6 (20%)
1	A2M	L5	4523	1,88	22,25,26	1.29	3 (13%)	30,36,39	1.31	3 (10%)
48	A2M	S2	166	48	22,25,26	1.32	2 (9%)	30,36,39	1.55	4 (13%)
1	OMU	L5	4227	1	19,22,23	0.84	1 (5%)	25,31,34	1.45	4 (16%)
48	PSU	S2	36	48	18,21,22	0.99	1 (5%)	21,30,33	1.43	3 (14%)
48	OMU	S2	172	48	19,22,23	0.50	0	25,31,34	1.45	6 (24%)
47	PSU	Pt	55	47	18,21,22	1.22	2 (11%)	21,30,33	1.55	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	2632	1	18,21,22	1.09	2 (11%)	21,30,33	1.55	4 (19%)
1	PSU	L5	4471	1	18,21,22	1.20	2 (11%)	21,30,33	1.59	4 (19%)
1	PSU	L5	4521	1,88,83	18,21,22	1.05	2 (11%)	21,30,33	1.62	4 (19%)
1	PSU	L5	3884	1	18,21,22	1.17	2 (11%)	21,30,33	1.62	4 (19%)
48	G7M	S2	1639	47,48	23,26,27	2.56	7 (30%)	34,39,42	2.41	9 (26%)
48	PSU	S2	1056	48	18,21,22	1.06	2 (11%)	21,30,33	1.69	5 (23%)
1	PSU	L5	4636	1	18,21,22	1.23	2 (11%)	21,30,33	1.42	4 (19%)
1	PSU	L5	4689	1	18,21,22	1.13	2 (11%)	21,30,33	1.42	3 (14%)
1	PSU	L5	2508	1	18,21,22	1.26	2 (11%)	21,30,33	1.49	4 (19%)
48	PSU	S2	218	48	18,21,22	0.95	1 (5%)	21,30,33	1.53	4 (19%)
48	A2M	S2	99	48,88	22,25,26	1.09	1 (4%)	30,36,39	1.21	1 (3%)
48	PSU	S2	863	48	18,21,22	0.92	0	21,30,33	1.44	4 (19%)
1	OMG	L5	3627	1	23,26,27	0.77	0	32,38,41	0.77	1 (3%)
1	OMG	L5	3792	1	23,26,27	0.76	1 (4%)	32,38,41	0.58	0
1	OMG	L5	4196	1,47,88	23,26,27	0.74	0	32,38,41	0.80	1 (3%)
1	OMG	L5	4370	1	23,26,27	0.65	0	32,38,41	0.63	0
1	OMC	L5	2422	1,88	19,22,23	0.84	1 (5%)	25,31,34	0.61	0
48	OMG	S2	1328	48	23,26,27	0.58	0	32,38,41	0.45	0
1	PSU	L5	4431	1	18,21,22	1.13	2 (11%)	21,30,33	1.66	4 (19%)
1	PSU	L5	2843	1	18,21,22	1.47	3 (16%)	21,30,33	1.52	4 (19%)
48	OMC	S2	1703	48,83	19,22,23	0.79	1 (5%)	25,31,34	0.58	0
1	PSU	L5	4532	1	18,21,22	0.99	1 (5%)	21,30,33	1.43	4 (19%)
1	OMU	L5	2837	1	19,22,23	0.62	0	25,31,34	1.41	5 (20%)
1	PSU	L5	4673	1,88	18,21,22	1.31	1 (5%)	21,30,33	1.50	4 (19%)

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	OMC	L5	1881	1,88	-	0/9/27/28	0/2/2/2
1	A2M	L5	2787	1	-	3/9/27/28	0/3/3/3
1	OMC	L5	2804	1	-	1/9/27/28	0/2/2/2
1	A2M	L5	1871	1,88	-	0/9/27/28	0/3/3/3
1	A2M	L5	2401	1,88	-	1/9/27/28	0/3/3/3
1	OMG	L5	1522	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
1	PSU	L5	5001	1,88	-	0/7/25/26	0/2/2/2
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
47	2MG	Pt	10	47	-	0/9/27/28	0/3/3/3
48	PSU	S2	573	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	3758	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	1625	1,83	-	1/9/27/28	0/3/3/3
1	PSU	L5	3729	1	-	0/7/25/26	0/2/2/2
47	2MU	Pt	54	47	-	1/9/27/28	0/2/2/2
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	3715	1	-	0/7/25/26	0/2/2/2
48	MA6	S2	1850	48	-	0/11/29/30	0/3/3/3
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	2424	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3920	1,88	-	0/7/25/26	0/2/2/2
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4531	1	-	1/7/25/26	0/2/2/2
48	A2M	S2	1031	48	-	0/9/27/28	0/3/3/3
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2
1	A2M	L5	1534	1,88	-	1/9/27/28	0/3/3/3
1	A2M	L5	3724	1	-	0/9/27/28	0/3/3/3
48	A2M	S2	1678	48	-	1/9/27/28	0/3/3/3
1	A2M	L5	3760	1,48	-	4/9/27/28	0/3/3/3
1	OMG	L5	4494	1	-	0/9/27/28	0/3/3/3
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4457	1	-	0/7/25/26	0/2/2/2
48	OMG	S2	509	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	1243	48	-	3/7/25/26	0/2/2/2
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	1744	1,83	-	0/7/25/26	0/2/2/2
1	OMC	L5	2861	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	3770	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1781	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3744	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	1340	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	609	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	3639	1	-	0/7/25/26	0/2/2/2
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
1	PSU	L5	1536	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	L5	3869	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	1367	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1136	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4972	1,83	-	0/7/25/26	0/2/2/2
1	A2M	L5	400	1	-	0/9/27/28	0/3/3/3
48	OMG	S2	683	48	-	0/9/27/28	0/3/3/3
47	PSU	Pt	13	47	-	1/7/25/26	0/2/2/2
48	A2M	S2	484	48	-	0/9/27/28	0/3/3/3
1	OMC	L5	2365	1	-	1/9/27/28	0/2/2/2
1	A2M	L5	3723	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	4579	1	-	0/7/25/26	0/2/2/2
1	UR3	L5	4530	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2351	1,88	-	1/9/27/28	0/2/2/2
1	PSU	L5	3762	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	1316	1	-	0/9/27/28	0/3/3/3
43	MLZ	Lo	53	43	-	0/7/8/10	-
1	1MA	L5	1322	1,88	-	2/7/25/26	0/3/3/3
1	PSU	L5	4423	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1862	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1,88	-	1/9/27/28	0/2/2/2
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	644	48	-	3/9/27/28	0/3/3/3
48	6MZ	S2	1832	88,48,83	-	0/9/27/28	0/3/3/3
48	UY1	S2	1326	48,88	-	2/9/27/28	0/2/2/2
3	OMU	L8	14	1,83,3	-	1/9/27/28	0/2/2/2
48	PSU	S2	1239	48	-	0/7/25/26	0/2/2/2
48	B8N	S2	1248	48	-	5/16/34/35	0/2/2/2
1	OMG	L5	4392	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1582	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1792	1,83	-	0/7/25/26	0/2/2/2
48	PSU	S2	801	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	159	48	-	1/9/27/28	0/3/3/3
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
1	A2M	L5	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1677	1	-	3/7/25/26	0/2/2/2
1	PSU	L5	4420	1	-	2/7/25/26	0/2/2/2
48	A2M	S2	1383	48	-	0/9/27/28	0/3/3/3
1	OMC	L5	3701	1,83	-	4/9/27/28	0/2/2/2
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
1	PSU	L5	4576	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
48	OMU	S2	1288	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	590	48	-	3/9/27/28	0/3/3/3
1	OMG	L5	4228	1	-	0/9/27/28	0/3/3/3
1	6MZ	L5	4220	1	-	0/9/27/28	0/3/3/3
48	OMG	S2	1490	48,88	-	4/9/27/28	0/3/3/3
1	OMG	L5	2364	1	-	1/9/27/28	0/3/3/3
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
1	PSU	L5	3637	1,83	-	0/7/25/26	0/2/2/2
48	PSU	S2	1174	48,83	-	0/7/25/26	0/2/2/2
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2
1	A2M	L5	4590	1	-	1/9/27/28	0/3/3/3
1	A2M	L5	3718	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	3851	1,83	-	1/7/25/26	0/2/2/2
1	5MC	L5	4447	1,83	-	4/7/25/26	0/2/2/2
47	H2U	Pt	20	47	-	3/7/38/39	0/2/2/2
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
48	MA6	S2	1851	48	-	3/11/29/30	0/3/3/3
1	A2M	L5	3867	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	398	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	4499	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4312	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	1683	1,83	-	0/7/25/26	0/2/2/2
1	OMU	L5	4498	1,83	-	0/9/27/28	0/2/2/2
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
1	OMC	L5	2824	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4552	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2876	1	-	0/9/27/28	0/3/3/3
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	867	48	-	1/9/27/28	0/3/3/3
1	PSU	L5	4569	1	-	0/7/25/26	0/2/2/2
48	A2M	S2	668	48,88	-	2/9/27/28	0/3/3/3
1	PSU	L5	3768	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
48	A2M	S2	512	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	L5	3782	1,88	-	0/7/25/26	0/2/2/2
1	OMU	L5	3925	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4403	1,83	-	0/7/25/26	0/2/2/2
1	OMG	L5	4637	1,83	-	1/9/27/28	0/3/3/3
47	5MC	Pt	49	47	-	0/7/25/26	0/2/2/2
1	A2M	L5	2363	1,88	-	0/9/27/28	0/3/3/3
1	PSU	L5	4500	1	-	1/7/25/26	0/2/2/2
48	OMG	S2	1447	48	-	1/9/27/28	0/3/3/3
1	PSU	L5	5010	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1782	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4493	1,83	-	0/7/25/26	0/2/2/2
48	A2M	S2	468	48	-	0/9/27/28	0/3/3/3
48	OMU	S2	1442	48,88	-	0/9/27/28	0/2/2/2
1	OMC	L5	3887	1	-	1/9/27/28	0/2/2/2
1	OMC	L5	4456	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	3844	1	-	1/7/25/26	0/2/2/2
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
48	4AC	S2	1842	48	-	0/11/29/30	0/2/2/2
1	OMU	L5	2415	1	-	0/9/27/28	0/2/2/2
1	OMC	L5	3841	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2
1	OMG	L5	3944	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3695	1,83	-	0/7/25/26	0/2/2/2
48	PSU	S2	296	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	822	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	436	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
1	OMC	L5	3808	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	918	48	-	0/7/25/26	0/2/2/2
1	A2M	L5	1326	1	-	2/9/27/28	0/3/3/3
48	PSU	S2	572	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4296	1	-	0/7/25/26	0/2/2/2
48	OMU	S2	354	48	-	0/9/27/28	0/2/2/2
1	A2M	L5	1524	1	-	1/9/27/28	0/3/3/3
48	OMU	S2	428	48	-	5/9/27/28	0/2/2/2
1	PSU	L5	2839	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	1643	48,88	-	0/7/25/26	0/2/2/2
1	A2M	L5	3785	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	1779	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	3764	1	-	2/7/25/26	0/2/2/2
1	OMG	L5	3899	1,88	-	0/9/27/28	0/3/3/3
1	OMG	L5	4623	1	-	0/9/27/28	0/3/3/3
48	OMU	S2	627	48	-	0/9/27/28	0/2/2/2
41	M3L	Lm	98	41	-	0/9/10/12	-
1	A2M	L5	2815	1,88	-	2/9/27/28	0/3/3/3
1	PSU	L5	3853	1,88,83	-	0/7/25/26	0/2/2/2
48	OMC	S2	462	48	-	1/9/27/28	0/2/2/2
1	UY1	L5	3818	1,83	-	2/9/27/28	0/2/2/2
1	PSU	L5	1860	1	-	0/7/25/26	0/2/2/2
48	A2M	S2	27	48,88	-	0/9/27/28	0/3/3/3
1	PSU	L5	4361	1	-	0/7/25/26	0/2/2/2
48	OMG	S2	601	48	-	1/9/27/28	0/3/3/3
1	OMG	L5	4618	1,83	-	0/9/27/28	0/3/3/3
48	OMU	S2	1804	48	-	1/9/27/28	0/2/2/2
30	MLZ	Lb	5	30,83	-	2/7/8/10	-
48	OMC	S2	174	48,88	-	0/9/27/28	0/2/2/2
48	A2M	S2	576	48	-	1/9/27/28	0/3/3/3
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
3	OMG	L8	75	3	-	0/9/27/28	0/3/3/3
1	PSU	L5	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4353	1	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
1	PSU	L5	3734	1	-	0/7/25/26	0/2/2/2
72	HY3	SX	62	72	-	0/1/12/14	0/1/1/1
1	A2M	L5	4571	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	4523	1,88	-	0/9/27/28	0/3/3/3
48	A2M	S2	166	48	-	0/9/27/28	0/3/3/3
1	OMU	L5	4227	1	-	0/9/27/28	0/2/2/2
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	172	48	-	1/9/27/28	0/2/2/2
47	PSU	Pt	55	47	-	0/7/25/26	0/2/2/2
1	PSU	L5	2632	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4471	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4521	1,88,83	-	0/7/25/26	0/2/2/2
1	PSU	L5	3884	1	-	0/7/25/26	0/2/2/2
48	G7M	S2	1639	47,48	-	0/7/25/26	0/3/3/3
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	2/7/25/26	0/2/2/2
1	PSU	L5	4689	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	99	48,88	-	1/9/27/28	0/3/3/3
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
1	OMG	L5	3627	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	3792	1	-	1/9/27/28	0/3/3/3
1	OMG	L5	4196	1,47,88	-	1/9/27/28	0/3/3/3
1	OMG	L5	4370	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	2422	1,88	-	2/9/27/28	0/2/2/2
48	OMG	S2	1328	48	-	0/9/27/28	0/3/3/3
1	PSU	L5	4431	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	2843	1	-	0/7/25/26	0/2/2/2
48	OMC	S2	1703	48,83	-	0/9/27/28	0/2/2/2
1	PSU	L5	4532	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	2837	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4673	1,88	-	0/7/25/26	0/2/2/2

The worst 5 of 378 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1326	UY1	C6-C5	11.04	1.47	1.35
72	SX	62	HY3	C4-C3	-10.57	1.33	1.52
1	L5	4220	6MZ	C6-N6	10.16	1.45	1.34
1	L5	3818	UY1	C6-C5	9.56	1.45	1.35
48	S2	1326	UY1	C2-N1	9.39	1.48	1.36

The worst 5 of 765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1850	MA6	N1-C6-N6	-8.62	106.35	116.86
48	S2	1851	MA6	N1-C6-N6	-8.39	106.64	116.86
48	S2	1832	6MZ	C9-N6-C6	-7.92	115.51	122.85
1	L5	4531	PSU	C6-C5-C4	6.51	122.57	118.17
48	S2	1639	G7M	C1'-N9-C4	-6.40	107.59	126.49

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	14	OMU	C1'-C2'-O2'-CM2
30	Lb	5	MLZ	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	L5	1677	PSU	C2'-C1'-C5-C4
1	L5	1677	PSU	O4'-C1'-C5-C4
1	L5	1677	PSU	C2'-C1'-C5-C6

There are no ring outliers.

51 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	2787	A2M	1	0
1	L5	2804	OMC	1	0
48	S2	116	OMU	2	0
48	S2	1850	MA6	3	0
1	L5	2424	OMG	1	0
48	S2	121	OMU	1	0
1	L5	4457	PSU	1	0
48	S2	509	OMG	1	0
48	S2	1232	PSU	1	0
1	L5	1340	OMC	1	0
47	Pt	13	PSU	1	0
48	S2	484	A2M	1	0
1	L5	2351	OMC	3	0
1	L5	3762	PSU	1	0
1	L5	4536	OMC	1	0
48	S2	1832	6MZ	1	0
3	L8	14	OMU	1	0
48	S2	1692	PSU	1	0
48	S2	159	A2M	2	0
48	S2	1391	OMC	2	0
1	L5	4220	6MZ	2	0
1	L5	2364	OMG	1	0
1	L5	3718	A2M	3	0
47	Pt	20	H2U	1	0
1	L5	3867	A2M	1	0
1	L5	2876	OMG	1	0
48	S2	867	OMG	1	0
48	S2	1347	PSU	1	0
1	L5	3782	5MC	1	0
1	L5	4637	OMG	1	0
48	S2	468	A2M	1	0
1	L5	4456	OMC	1	0
48	S2	1842	4AC	1	0
1	L5	2415	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	3944	OMG	1	0
48	S2	572	PSU	1	0
48	S2	354	OMU	1	0
1	L5	2815	A2M	2	0
48	S2	462	OMC	1	0
48	S2	27	A2M	1	0
48	S2	1804	OMU	1	0
48	S2	576	A2M	1	0
1	L5	4293	PSU	1	0
3	L8	75	OMG	1	0
5	LB	245	HIC	2	0
48	S2	166	A2M	1	0
48	S2	172	OMU	1	0
47	Pt	55	PSU	1	0
1	L5	2632	PSU	1	0
48	S2	99	A2M	1	0
1	L5	3792	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 573 ligands modelled in this entry, 549 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
85	SPD	L5	5600	-	9,9,9	0.30	0	8,8,8	0.73	0
84	PUT	L5	5621	-	5,5,5	0.18	0	4,4,4	0.28	0
84	PUT	L5	5614	-	5,5,5	0.12	0	4,4,4	0.24	0
85	SPD	L5	5603	-	9,9,9	0.25	0	8,8,8	0.24	0
85	SPD	L5	5607	-	9,9,9	0.29	0	8,8,8	0.70	0
85	SPD	S2	1902	-	9,9,9	0.26	0	8,8,8	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	TRS	L5	5618	-	7,7,7	0.47	0	9,9,9	0.63	0
85	SPD	L5	5608	-	9,9,9	0.25	0	8,8,8	0.24	0
85	SPD	L5	5606	-	9,9,9	0.26	0	8,8,8	0.61	0
84	PUT	L5	5616	-	5,5,5	0.11	0	4,4,4	0.27	0
84	PUT	L5	5611	-	5,5,5	0.09	0	4,4,4	0.18	0
84	PUT	L5	5612	-	5,5,5	0.18	0	4,4,4	0.17	0
84	PUT	L5	5613	-	5,5,5	0.20	0	4,4,4	0.18	0
85	SPD	L5	5604	-	9,9,9	0.28	0	8,8,8	0.64	0
85	SPD	L5	5602	-	9,9,9	0.29	0	8,8,8	0.96	0
84	PUT	L5	5615	-	5,5,5	0.15	0	4,4,4	0.21	0
85	SPD	L5	5609	-	9,9,9	0.26	0	8,8,8	0.31	0
85	SPD	L5	5605	-	9,9,9	0.31	0	8,8,8	0.43	0
85	SPD	L5	5610	-	9,9,9	0.29	0	8,8,8	0.41	0
85	SPD	L5	5620	-	9,9,9	0.22	0	8,8,8	0.49	0
85	SPD	L5	5601	-	9,9,9	0.31	0	8,8,8	0.68	0
86	A1B75	L5	5700	83	28,28,28	1.65	4 (14%)	30,37,37	1.39	5 (16%)
85	SPD	S2	1901	-	9,9,9	0.25	0	8,8,8	0.59	0
87	TRS	L5	5617	-	7,7,7	0.79	0	9,9,9	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	L5	5600	-	-	0/7/7/7	-
84	PUT	L5	5621	-	-	0/3/3/3	-
84	PUT	L5	5614	-	-	0/3/3/3	-
85	SPD	L5	5603	-	-	1/7/7/7	-
85	SPD	L5	5607	-	-	3/7/7/7	-
85	SPD	S2	1902	-	-	0/7/7/7	-
87	TRS	L5	5618	-	-	2/9/9/9	-
85	SPD	L5	5608	-	-	2/7/7/7	-
85	SPD	L5	5606	-	-	1/7/7/7	-
84	PUT	L5	5616	-	-	3/3/3/3	-
84	PUT	L5	5611	-	-	1/3/3/3	-
84	PUT	L5	5612	-	-	1/3/3/3	-
84	PUT	L5	5613	-	-	2/3/3/3	-
85	SPD	L5	5604	-	-	2/7/7/7	-
85	SPD	L5	5602	-	-	1/7/7/7	-
84	PUT	L5	5615	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	L5	5609	-	-	1/7/7/7	-
85	SPD	L5	5605	-	-	2/7/7/7	-
85	SPD	L5	5610	-	-	0/7/7/7	-
85	SPD	L5	5620	-	-	2/7/7/7	-
85	SPD	L5	5601	-	-	1/7/7/7	-
86	A1B75	L5	5700	83	-	1/16/36/36	0/3/3/3
85	SPD	S2	1901	-	-	2/7/7/7	-
87	TRS	L5	5617	-	-	3/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	L5	5700	A1B75	C3-N1	6.49	1.60	1.47
86	L5	5700	A1B75	O3-C5	-2.75	1.37	1.43
86	L5	5700	A1B75	C1-N2	2.60	1.39	1.34
86	L5	5700	A1B75	C4-N1	2.23	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	L5	5700	A1B75	C2-O2-C1	3.43	122.08	117.04
86	L5	5700	A1B75	O2-C1-O1	-3.26	119.76	124.55
86	L5	5700	A1B75	C4-C5-C2	2.62	106.68	103.32
86	L5	5700	A1B75	O2-C1-N2	2.37	114.87	111.01
86	L5	5700	A1B75	C7-C6-C3	2.14	117.03	113.40

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

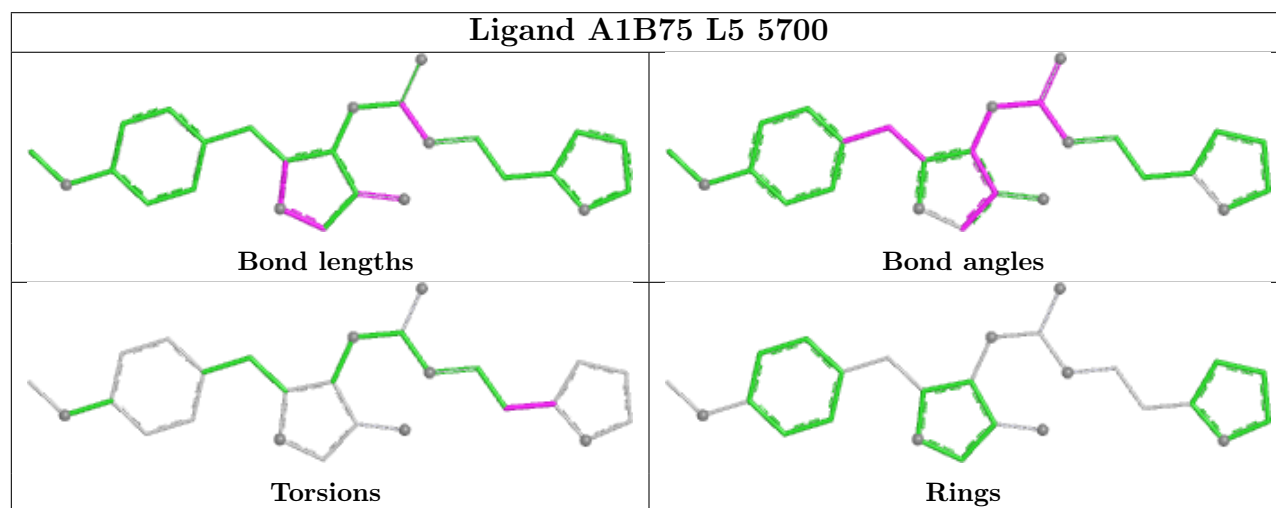
Mol	Chain	Res	Type	Atoms
87	L5	5618	TRS	N-C-C2-O2
87	L5	5617	TRS	N-C-C3-O3
85	L5	5620	SPD	C3-C4-C5-N6
85	L5	5608	SPD	C3-C4-C5-N6
85	L5	5607	SPD	N6-C7-C8-C9

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	L5	5621	PUT	1	0
85	L5	5607	SPD	1	0
87	L5	5618	TRS	1	0
84	L5	5616	PUT	3	0
84	L5	5615	PUT	1	0
85	L5	5610	SPD	1	0
86	L5	5700	A1B75	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	NC	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	NC	20:UNK	C	26:GLU	N	16.32

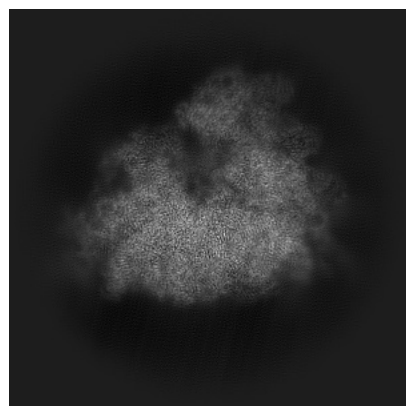
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70084. These allow visual inspection of the internal detail of the map and identification of artifacts.

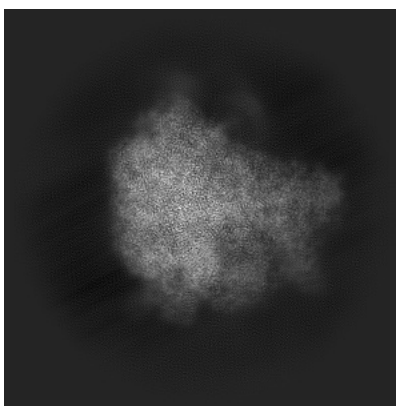
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

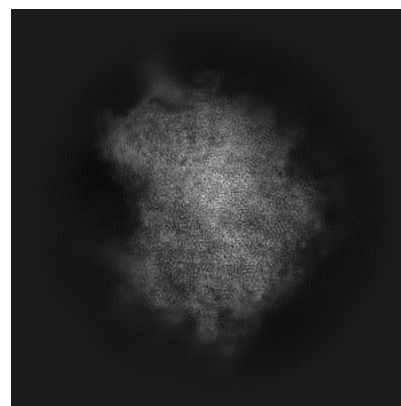
6.1.1 Primary map



X

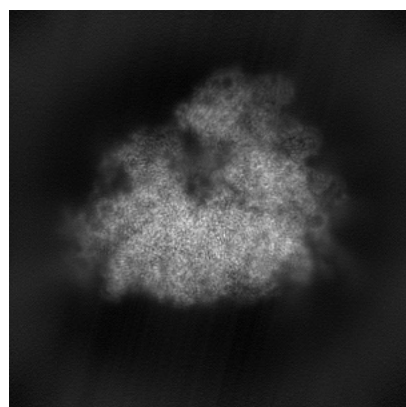


Y

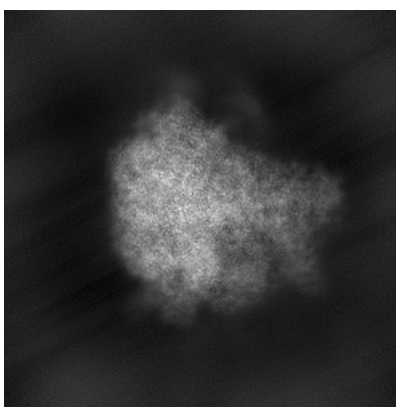


Z

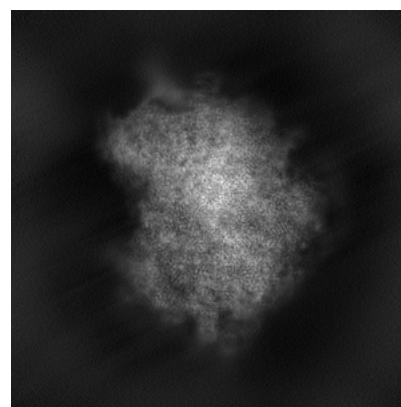
6.1.2 Raw map



X



Y

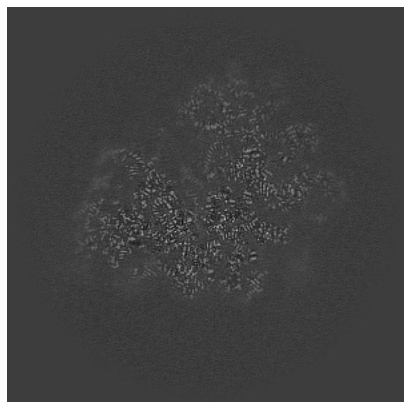


Z

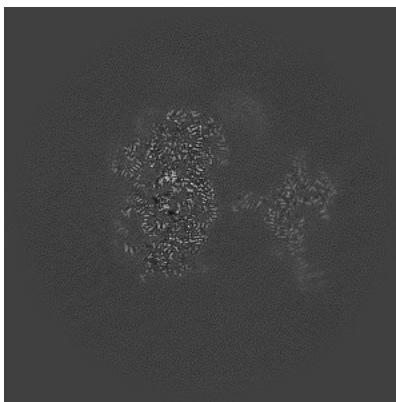
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

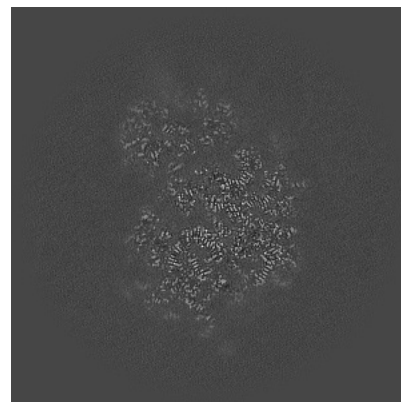
6.2.1 Primary map



X Index: 256

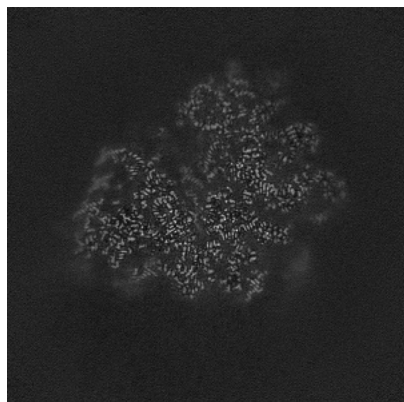


Y Index: 256

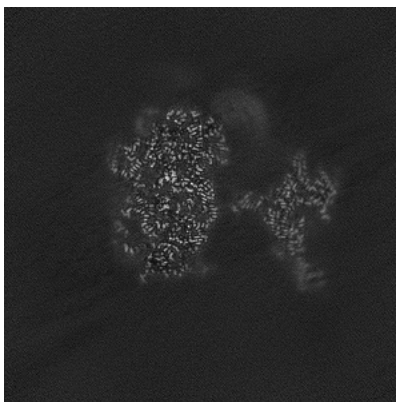


Z Index: 256

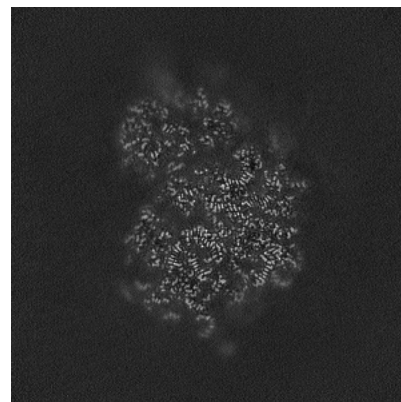
6.2.2 Raw map



X Index: 256



Y Index: 256

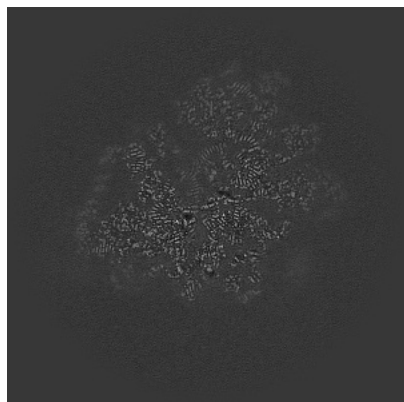


Z Index: 256

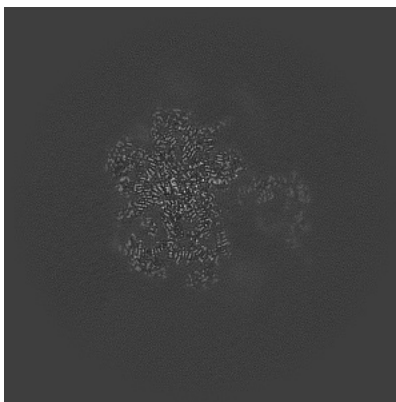
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

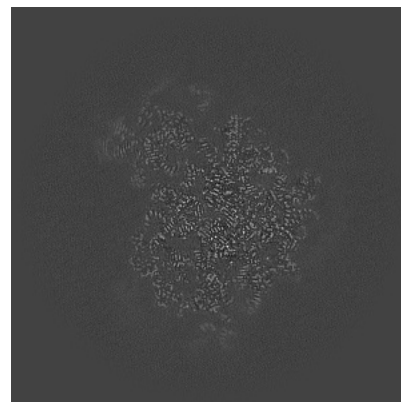
6.3.1 Primary map



X Index: 261

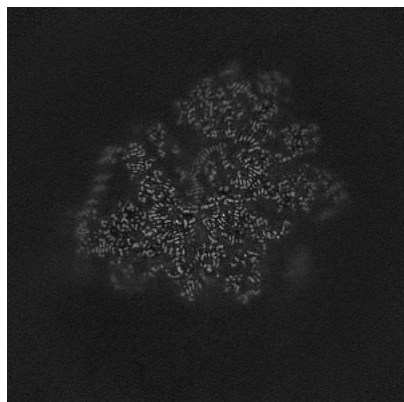


Y Index: 218

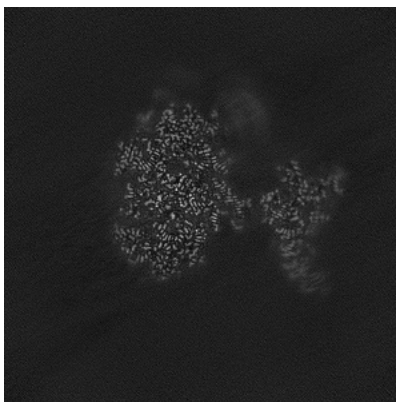


Z Index: 237

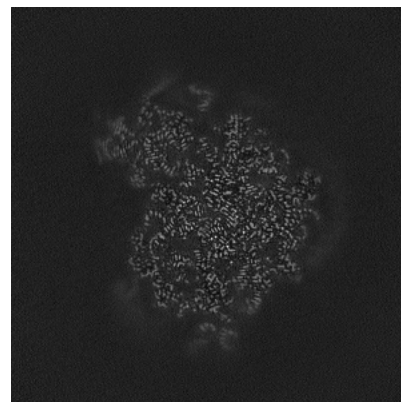
6.3.2 Raw map



X Index: 261



Y Index: 265

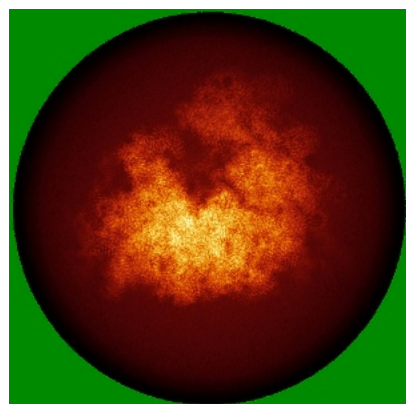


Z Index: 237

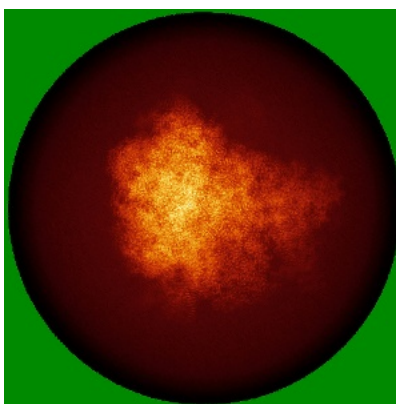
The images above show the largest variance slices of the map in three orthogonal directions.

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

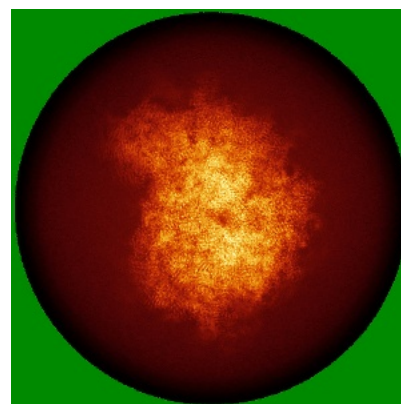
6.4.1 Primary map



X

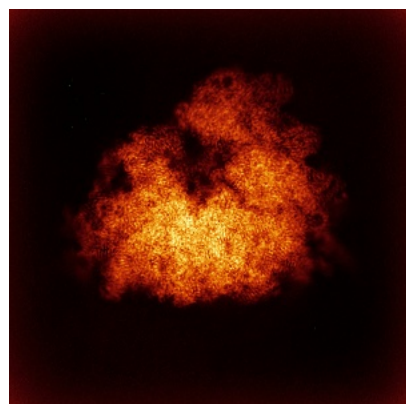


Y

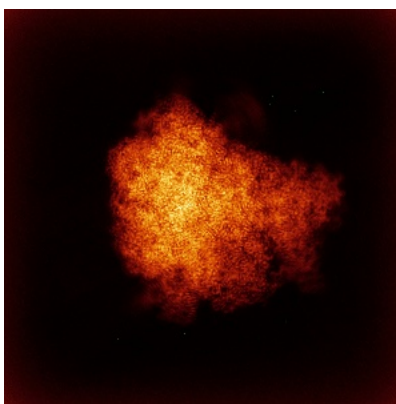


Z

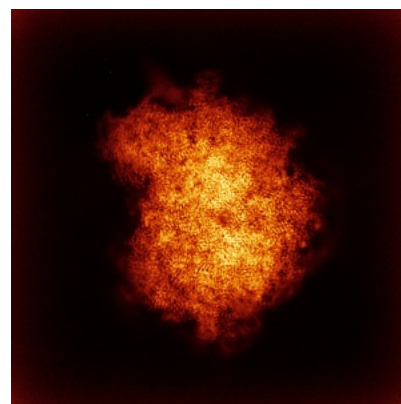
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

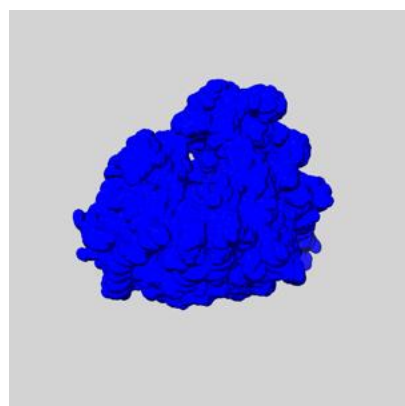
6.6 Mask visualisation [i](#)

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

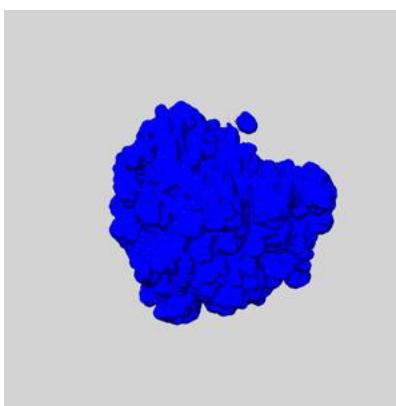
A mask typically either:

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

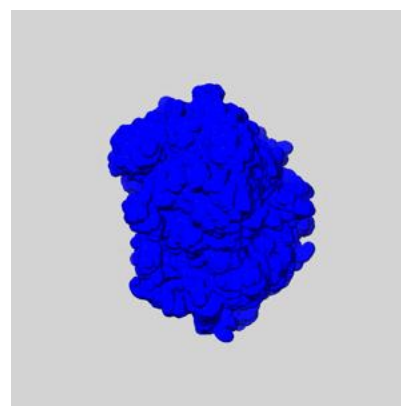
6.6.1 emd_70084_msk_1.map [i](#)



X



Y

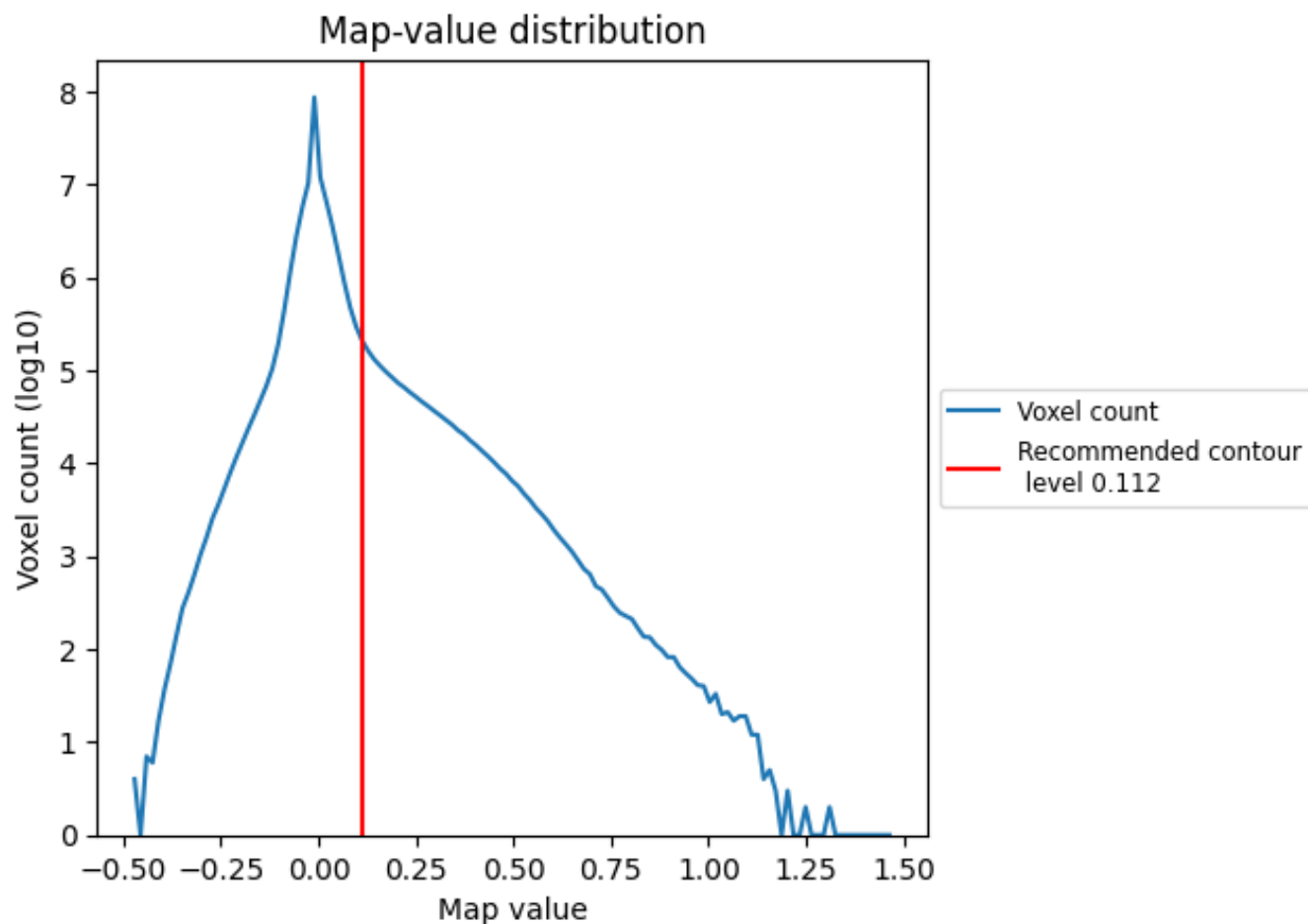


Z

7 Map analysis [i](#)

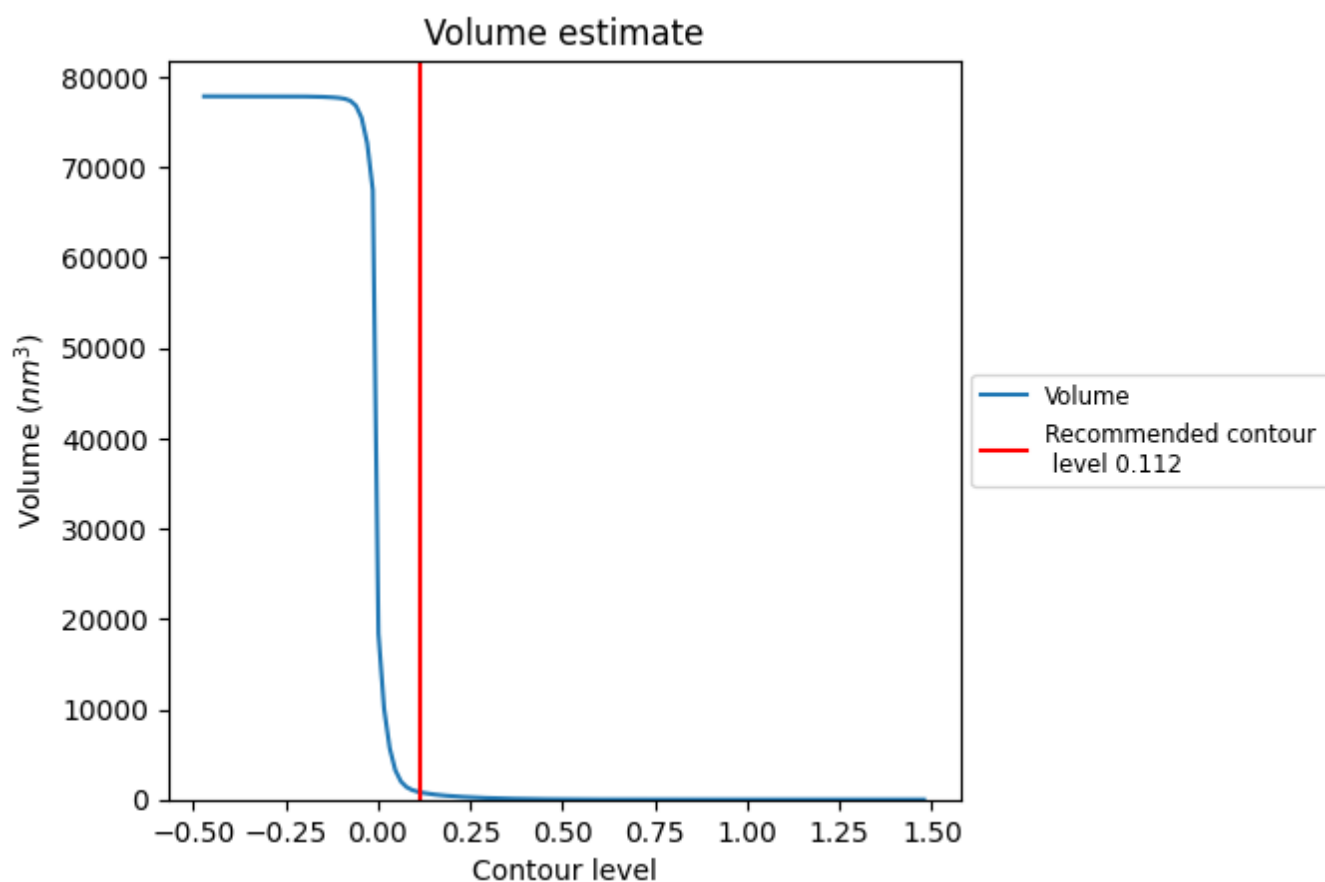
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

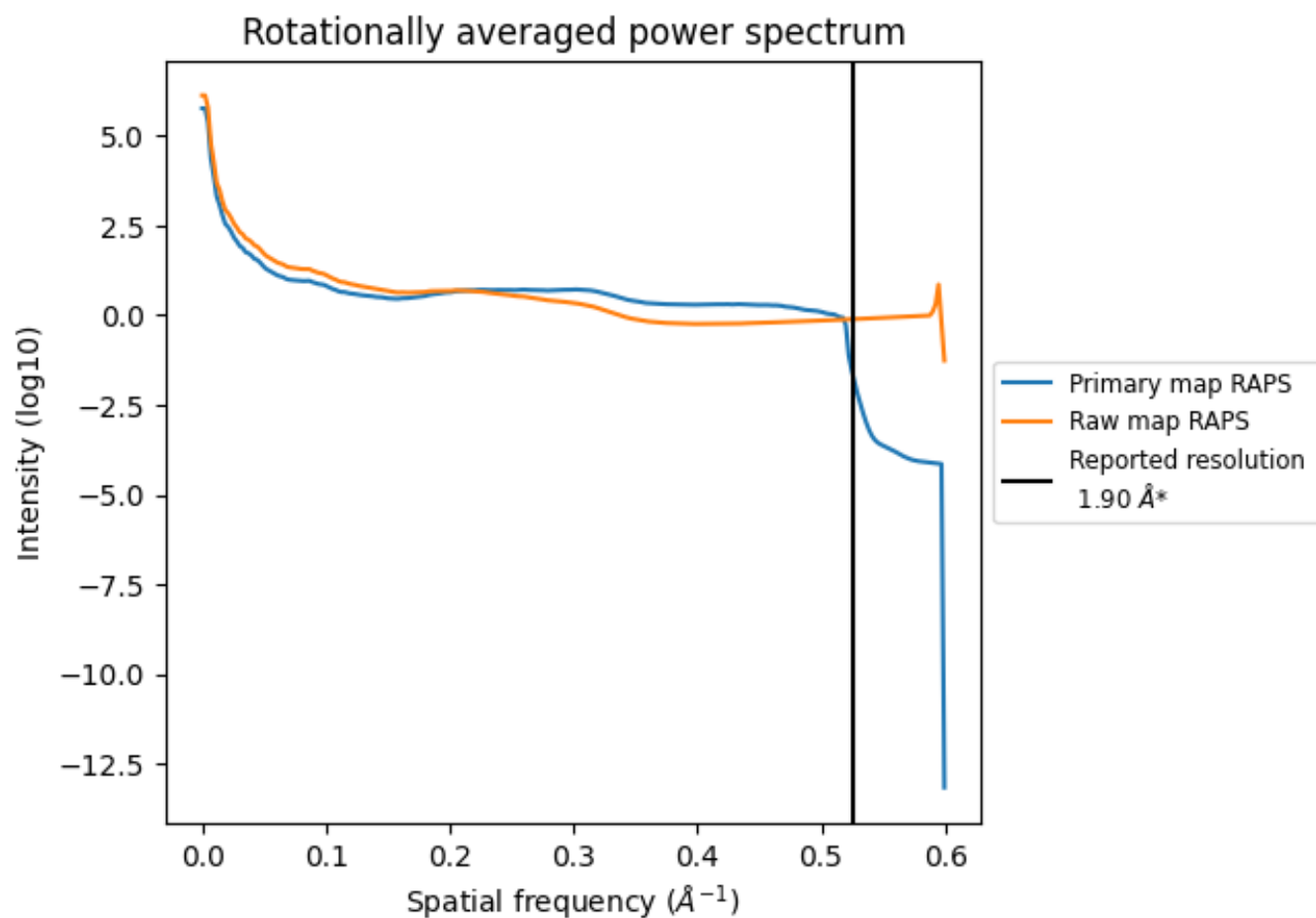
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 834 nm³; this corresponds to an approximate mass of 753 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 ⓘ

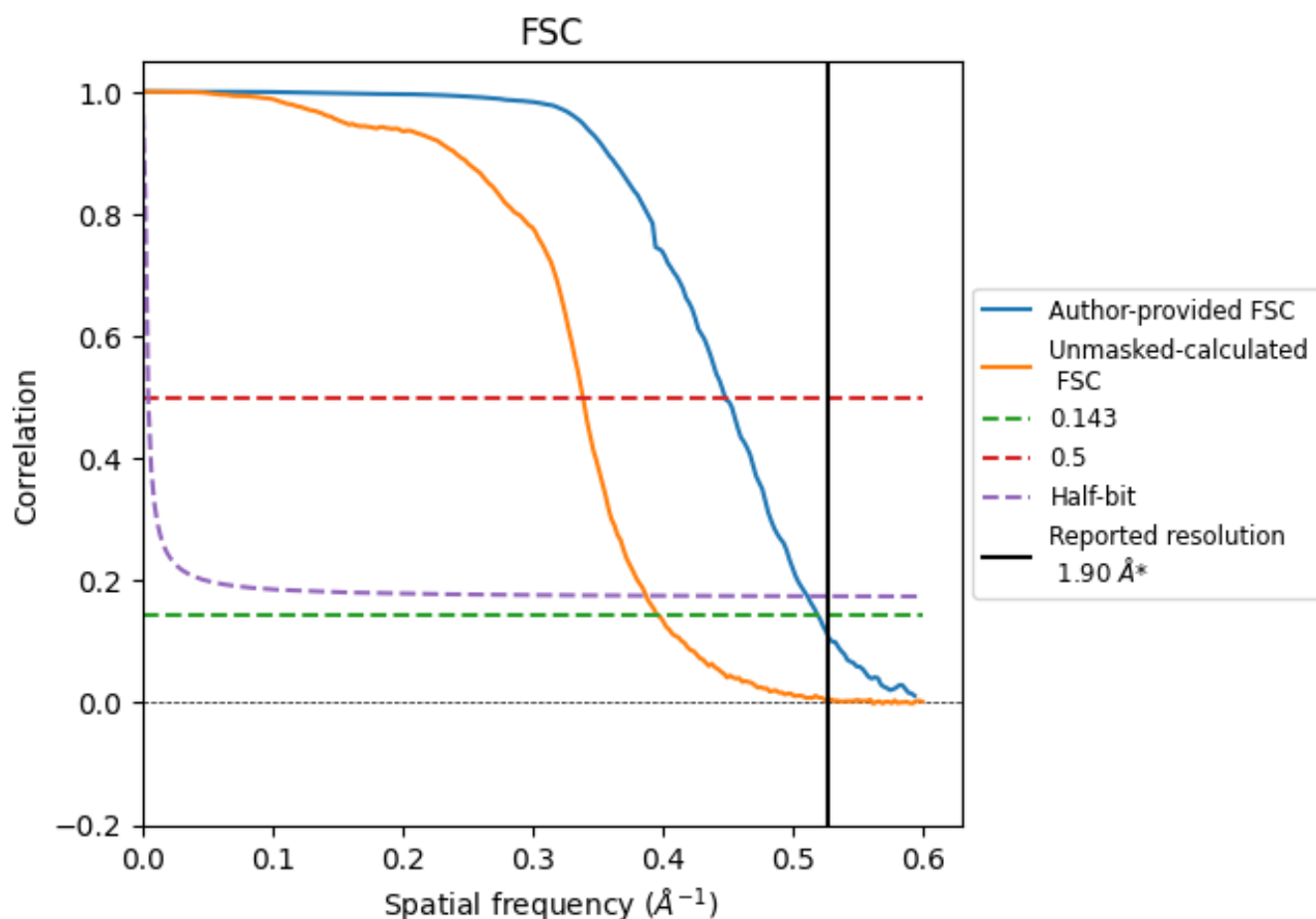


*Reported resolution corresponds to spatial frequency of 0.526 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.526 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

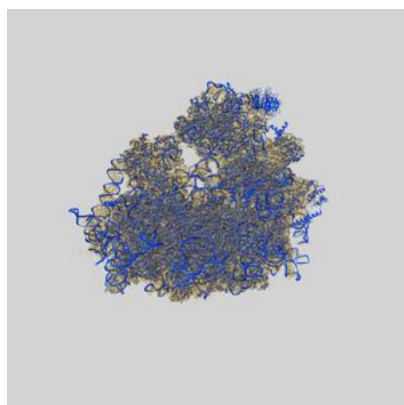
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.90	-	-
Author-provided FSC curve	1.93	2.23	1.96
Unmasked-calculated*	2.53	2.95	2.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.53 differs from the reported value 1.9 by more than 10 %

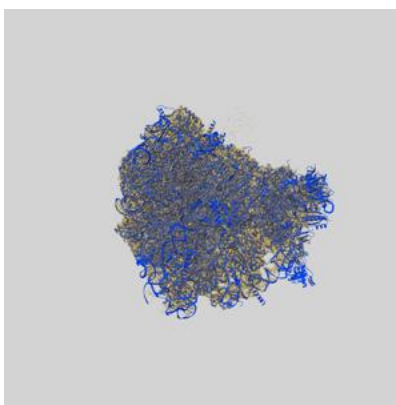
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70084 and PDB model 9O3W. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

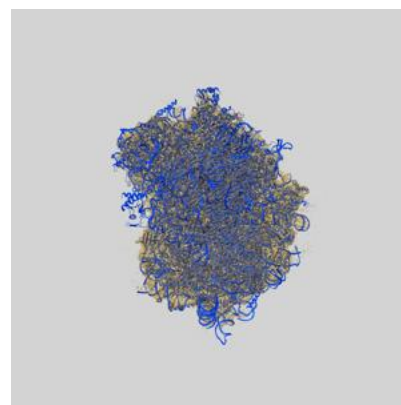
9.1 Map-model overlay [i](#)



X



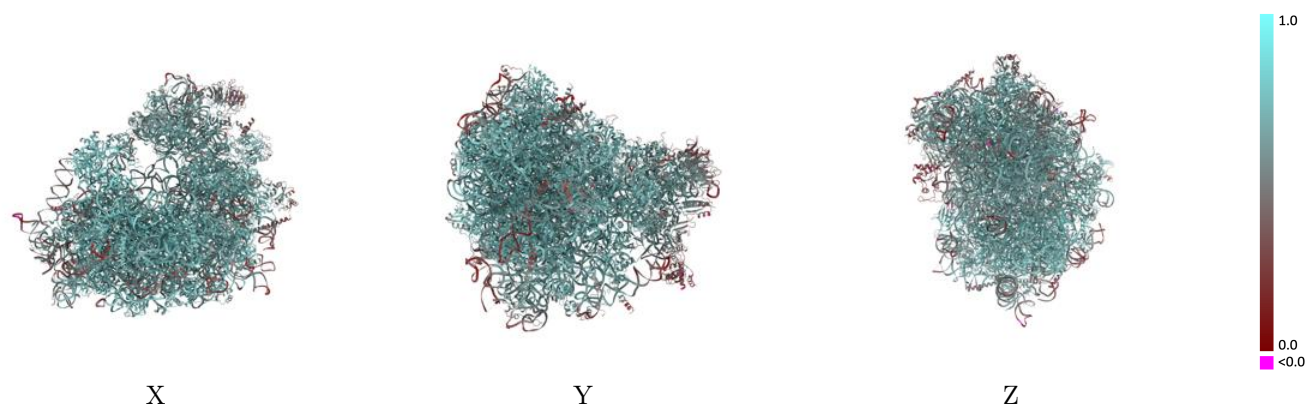
Y



Z

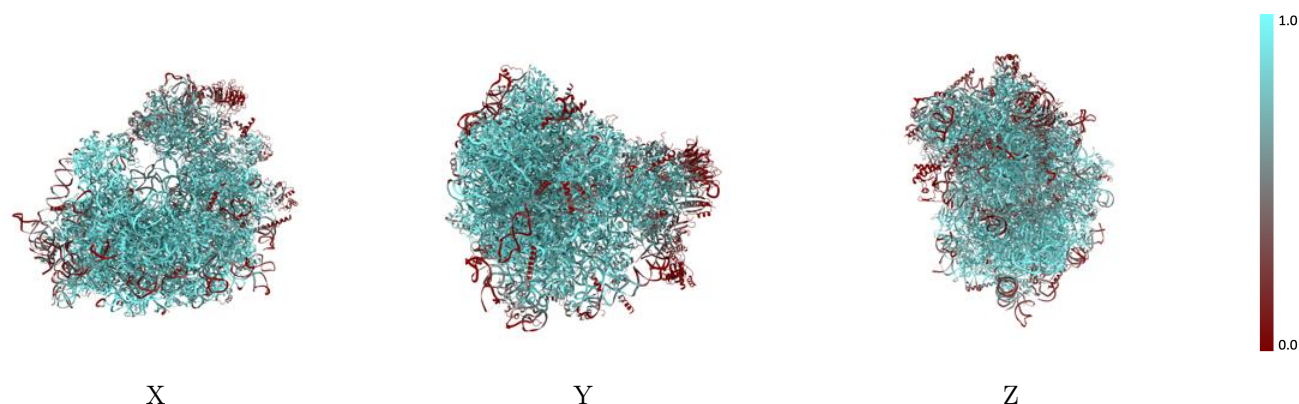
The images above show the 3D surface view of the map at the recommended contour level 0.112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



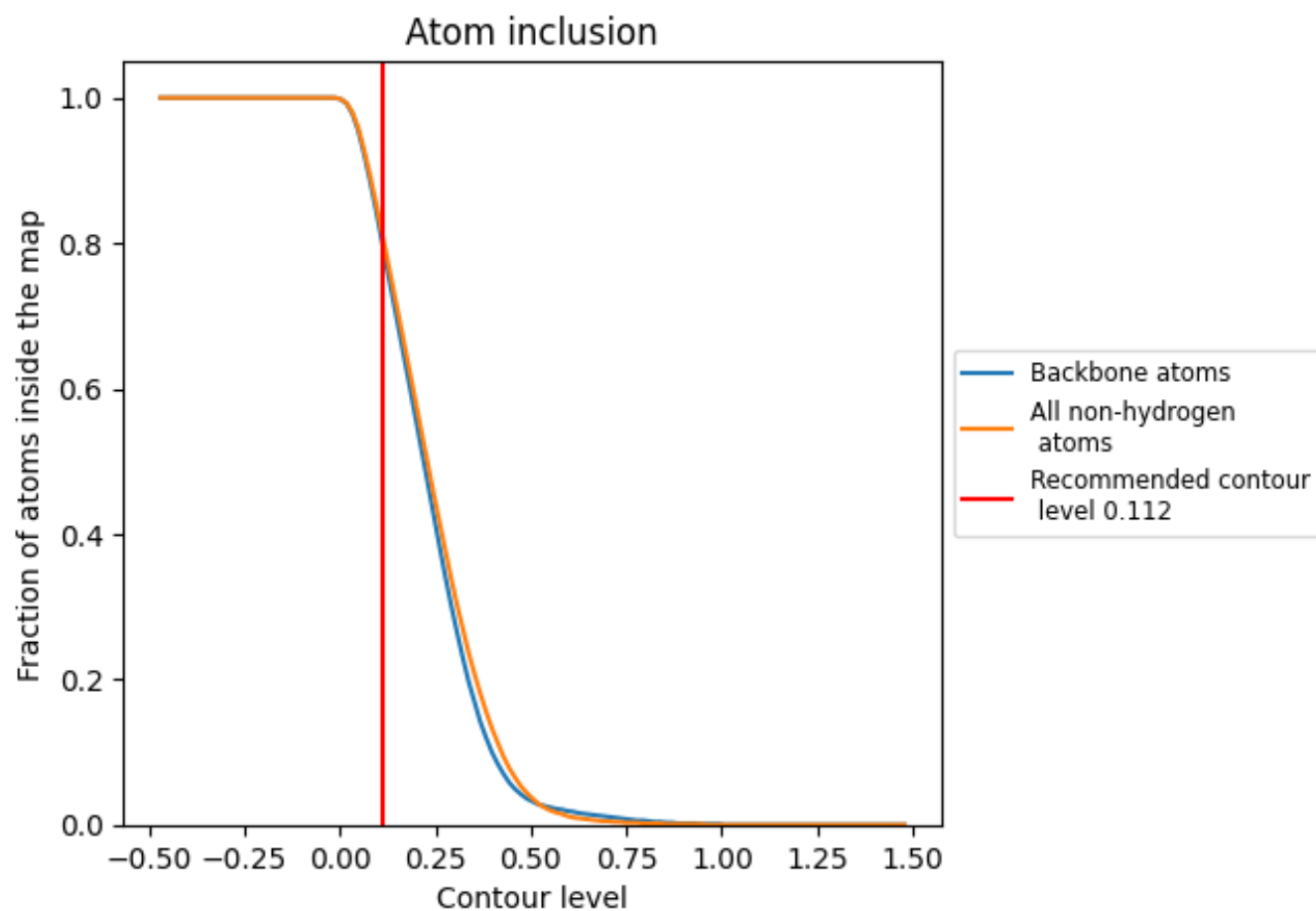
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.112).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.6780
L5	 0.8520	 0.6900
L7	 0.9830	 0.7430
L8	 0.9050	 0.7100
LA	 0.9610	 0.7770
LB	 0.9100	 0.7510
LC	 0.9120	 0.7390
LD	 0.8570	 0.7120
LE	 0.7770	 0.6670
LF	 0.9140	 0.7530
LG	 0.7500	 0.6580
LH	 0.8760	 0.7170
LI	 0.8760	 0.7240
LJ	 0.8060	 0.6790
LL	 0.8590	 0.7120
LM	 0.8900	 0.7140
LN	 0.9830	 0.7820
LO	 0.9140	 0.7500
LP	 0.9280	 0.7570
LQ	 0.9570	 0.7670
LR	 0.8060	 0.6910
LS	 0.9500	 0.7630
LT	 0.8560	 0.7220
LU	 0.7220	 0.6350
LV	 0.9330	 0.7630
LW	 0.8520	 0.7140
LX	 0.8880	 0.7240
LY	 0.8600	 0.7100
LZ	 0.8740	 0.7130
La	 0.9440	 0.7640
Lb	 0.6690	 0.6440
Lc	 0.8750	 0.7170
Ld	 0.8600	 0.7270
Le	 0.9550	 0.7640
Lf	 0.9440	 0.7590



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Chain	Atom inclusion	Q-score
Lg	 0.8870	 0.7360
Lh	 0.8550	 0.7110
Li	 0.8420	 0.7100
Lj	 0.9730	 0.7730
Lk	 0.6910	 0.6390
Ll	 0.9320	 0.7420
Lm	 0.8900	 0.7340
Ln	 0.8860	 0.7430
Lo	 0.8820	 0.7450
Lp	 0.9170	 0.7600
Lr	 0.9150	 0.7320
NC	 0.3640	 0.4800
Pt	 0.7330	 0.6350
S2	 0.8300	 0.6590
SA	 0.7140	 0.6450
SB	 0.7980	 0.6760
SC	 0.7690	 0.6780
SD	 0.4760	 0.5530
SE	 0.7220	 0.6490
SF	 0.6950	 0.6380
SG	 0.4100	 0.5190
SH	 0.4200	 0.5270
SI	 0.7770	 0.6740
SJ	 0.6850	 0.6220
SK	 0.3250	 0.4850
SL	 0.8520	 0.7120
SM	 0.0030	 0.2580
SN	 0.8800	 0.7230
SO	 0.8680	 0.7130
SP	 0.4640	 0.5450
SQ	 0.6170	 0.6330
SR	 0.4650	 0.5620
SS	 0.6000	 0.6190
ST	 0.6140	 0.6180
SU	 0.4280	 0.5280
SV	 0.7020	 0.6590
SW	 0.9090	 0.7250
SX	 0.8810	 0.7190
SY	 0.5120	 0.5500
SZ	 0.4660	 0.5570
Sa	 0.8810	 0.7200
Sb	 0.7000	 0.6520

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Chain	Atom inclusion	Q-score
Sc	 0.5870	 0.5880
Sd	 0.7880	 0.6730
Se	 0.6130	 0.6020
Sf	 0.0180	 0.2740
Sg	 0.1770	 0.4600
mR	 0.3530	 0.5920