



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 12:23 am BST

PDB ID : 9SPI / pdb_00009spi
EMDB ID : EMD-55091
Title : CRYO-EM STRUCTURE OF HUMAN 80S RIBOSOME WITH A/P/E-SITE
TRNA AND MRNA CONTAINING URIDINE
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-09-17
Resolution : 2.40 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:

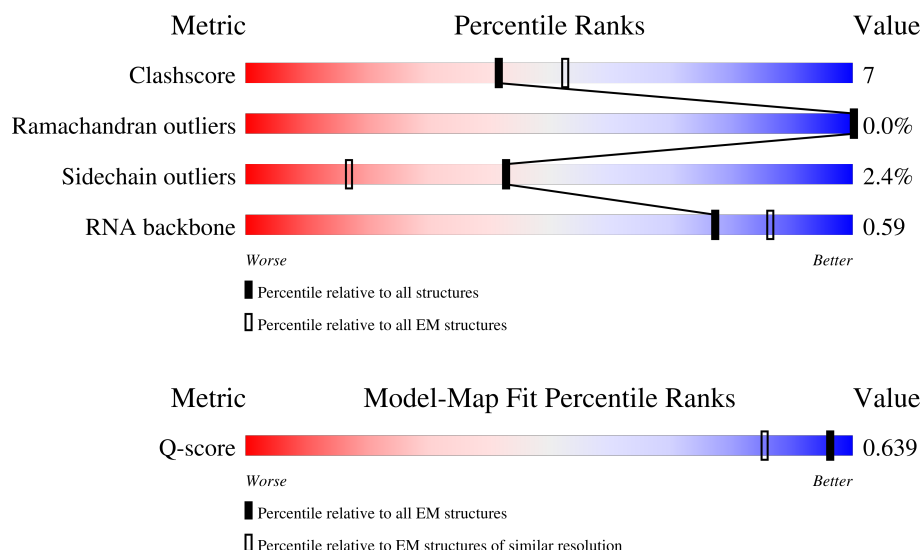
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 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.



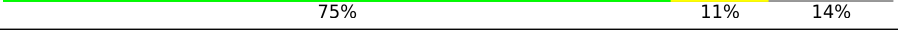
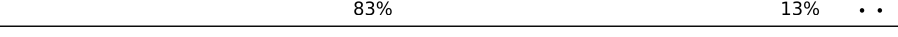
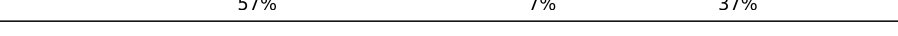
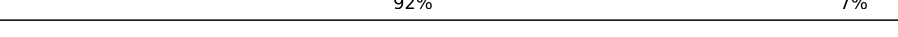
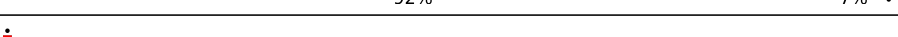
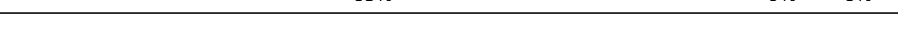
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	At	77	
2	Et	75	
3	L5	5069	

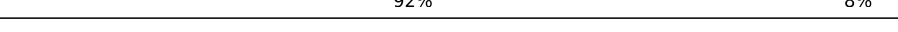
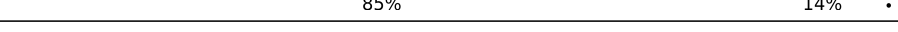
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	257	
7	LB	403	
8	LC	427	
9	LD	297	
10	LE	288	
11	LF	248	
12	LG	266	
13	LH	192	
14	LI	214	
15	LJ	178	
16	LL	211	
17	LM	215	
18	LN	204	
19	LO	203	
20	LP	184	
21	LQ	188	
22	LR	196	
23	LS	176	
24	LT	160	
25	LU	128	
26	LV	140	
27	LW	157	
28	LX	156	

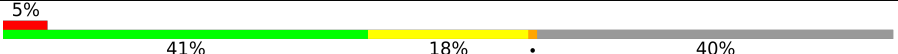
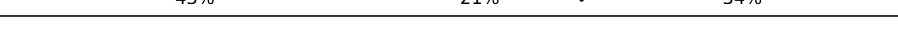
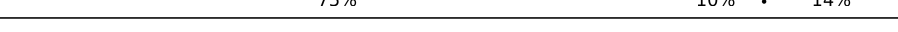
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Mol	Chain	Length	Quality of chain
29	LY	145	
30	LZ	136	
31	La	148	
32	Lb	159	
33	Lc	115	
34	Ld	125	
35	Le	135	
36	Lf	110	
37	Lg	117	
38	Lh	123	
39	Li	105	
40	Lj	97	
41	Lk	70	
42	Ll	51	
43	Lm	128	
44	Ln	25	
45	Lo	106	
46	Lp	92	
47	Lr	137	
48	Mr	7	
49	Pt	76	
50	S2	1869	
51	SA	295	
52	SB	264	
53	SC	293	

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Mol	Chain	Length	Quality of chain
54	SD	243	
55	SE	263	
56	SF	204	
57	SG	249	
58	SH	194	
59	SI	208	
60	SJ	194	
61	SK	165	
62	SL	158	
63	SM	132	
64	SN	151	
65	SO	151	
66	SP	145	
67	SQ	146	
68	SR	135	
69	SS	152	
70	ST	145	
71	SU	119	
72	SV	83	
73	SW	130	
74	SX	143	
75	SY	133	
76	SZ	125	
77	Sa	115	
78	Sb	84	

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Mol	Chain	Length	Quality of chain
79	Sc	69	
80	Sd	56	
81	Se	133	
82	Sf	156	
83	Sg	317	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	HYG	S2	1944	X	-	-	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 216235 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 tRNA-Ile-AAT-9-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	At	73	Total	C	N	O	P	0	0
			1559	697	280	510	72		

- Molecule 2 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Et	54	Total	C	N	O	P	0	0
			1155	516	214	372	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3413	Total	C	N	O	P	0	0
			73250	32661	13401	23776	3412		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	149	Total	C	N	O	P	0	0
			3177	1418	564	1046	149		

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LA	248	Total	C	N	O	S	1	0
			1907	1194	392	315	6		

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LB	397	Total	C	N	O	S	0	0
			3203	2040	602	547	14		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LC	361	Total	C	N	O	S	0	0
			2873	1808	574	477	14		

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LD	294	Total	C	N	O	S	0	0
			2385	1507	436	428	14		

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	223	Total	C	N	O	S	0	0
			1782	1147	338	293	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LF	225	Total	C	N	O	S	0	0
			1856	1193	357	297	9		

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	228	Total	C	N	O	S	0	0
			1824	1162	352	306	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	207	Total	C	N	O	S	0	0
			1672	1062	322	275	13		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LJ	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LO	200	Total	C	N	O	S	0	0
			1640	1058	320	257	5		

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LP	153	Total	C	N	O	S	1	0
			1249	781	243	216	9		

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LR	180	Total	C	N	O	S	0	0
			1449	898	311	231	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LT	159	Total	C	N	O	S	1	0
			1303	828	253	216	6		

- Molecule 25 is a protein called 60S ribosomal protein L22.

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

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LV	133	Total	C	N	O	S	0	0
			988	623	186	174	5		

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	64	Total	C	N	O	S	0	0
			529	338	103	85	3		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LX	118	Total	C	N	O	S	0	0
			966	618	181	166	1		

- Molecule 29 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LY	132	Total	C	N	O	S	0	0
			1098	689	222	184	3		

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lb	104	Total	C	N	O	S	0	0
			841	523	184	130	4		

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	98	Total	C	N	O	S	0	0
			761	482	134	139	6		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	128	Total	C	N	O	S	1	0
			1061	672	219	165	5		

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	110	Total	C	N	O	S	0	0
			880	558	175	144	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lg	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lm	52	Total	C	N	O	S	1	0
			432	269	90	67	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lo	105	Total	C	N	O	S	2	0
			875	548	181	140	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lp	90	Total	C	N	O	S	0	0
			698	440	134	117	7		

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

- Molecule 48 is a RNA chain called Synthetic mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Mr	7	Total	C	N	O	P	0	0
			145	65	23	50	7		

- Molecule 49 is a RNA chain called P site tRNA Arg-ACG.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Pt	72	Total	C	N	O	P	0	0
			1547	692	281	502	72		

- Molecule 50 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	S2	1562	Total	C	N	O	P	0	0
			33424	14950	6020	10893	1561		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SA	214	Total	C	N	O	S	0	0
			1693	1077	297	312	7		

- Molecule 52 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SB	199	Total	C	N	O	S	0	0
			1627	1037	292	285	13		

- Molecule 53 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SC	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 54 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SD	222	Total	C	N	O	S	0	0
			1721	1098	309	307	7		

- Molecule 55 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SE	257	Total	C	N	O	S	0	0
			2041	1305	379	349	8		

- Molecule 56 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SF	180	Total	C	N	O	S	0	0
			1417	890	263	257	7		

- Molecule 57 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SG	205	Total	C	N	O	S	0	0
			1652	1038	329	278	7		

- Molecule 58 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SH	163	Total	C	N	O	S	0	0
			1317	846	243	228			

- Molecule 59 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SI	201	Total	C	N	O	S	0	0
			1651	1035	325	286	5		

- Molecule 60 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SJ	175	Total	C	N	O	S	0	0
			1424	905	284	233	2		

- Molecule 61 is a protein called 40S ribosomal protein S10.

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

- Molecule 62 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SL	142	Total	C	N	O	S	0	0
			1164	741	220	197	6		

- Molecule 63 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SM	79	Total	C	N	O	S	0	0
			556	353	101	99	3		

- Molecule 64 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SN	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 65 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SO	106	Total	C	N	O	S	0	0
			788	482	156	146	4		

- Molecule 66 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SP	128	Total	C	N	O	S	0	0
			1037	656	195	179	7		

- Molecule 67 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SQ	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 68 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SR	127	Total	C	N	O	S	0	0
			1032	648	194	186	4		

- Molecule 69 is a protein called 40S ribosomal protein S18.

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

- Molecule 70 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	ST	140	Total	C	N	O	S	1	0
			1104	697	208	196	3		

- Molecule 71 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SU	95	Total	C	N	O	S	0	0
			755	474	142	135	4		

- Molecule 72 is a protein called 40S ribosomal protein S21.

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

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

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

- Molecule 74 is a protein called 40S ribosomal protein S23.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SY	121	Total	C	N	O	S	0	0
			995	631	195	164	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SZ	82	Total	C	N	O	S	0	0
			661	425	123	112	1		

- Molecule 77 is a protein called 40S ribosomal protein S26.

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

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sb	75	Total	C	N	O	S	0	0
			592	372	111	105	4		

- Molecule 79 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sc	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 80 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 81 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Se	53	Total	C	N	O	S	0	0
			420	258	94	67	1		

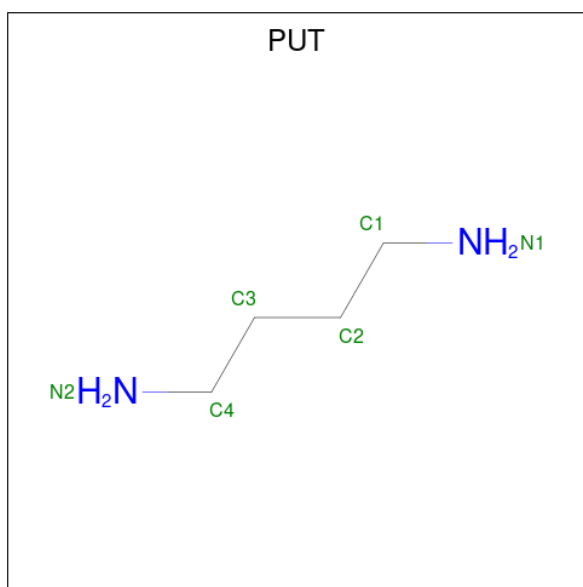
- Molecule 82 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sf	43	Total	C	N	O	S	0	0
			341	217	66	53	5		

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

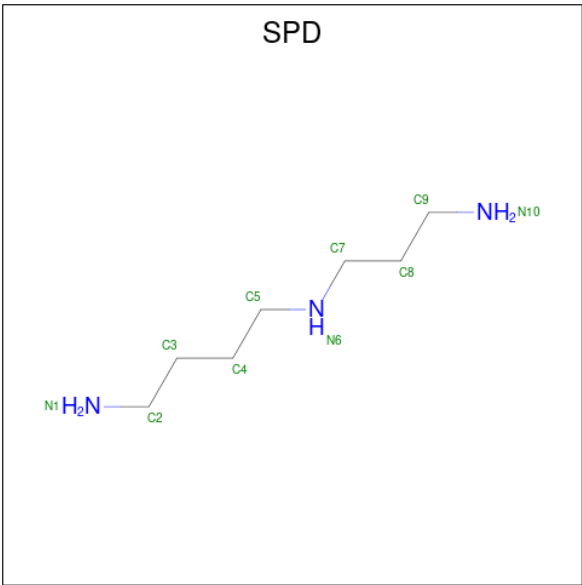
Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sg	282	Total	C	N	O	S	0	0
			2199	1392	386	411	10		

- Molecule 84 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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	S2	1	Total	C	N	0
			6	4	2	
84	S2	1	Total	C	N	0
			6	4	2	

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	L5	159	Total	Mg	0
			159	159	
86	L7	2	Total	Mg	0
			2	2	
86	L8	3	Total	Mg	0
			3	3	
86	LP	1	Total	Mg	0
			1	1	
86	LR	1	Total	Mg	0
			1	1	
86	S2	29	Total	Mg	0
			29	29	

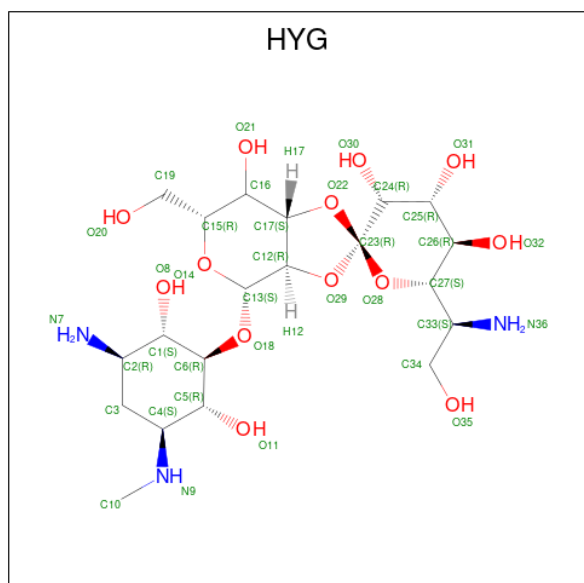
- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
87	L5	60	Total	K	0
			60	60	
87	L8	1	Total	K	0
			1	1	
87	LA	2	Total	K	0
			2	2	
87	LH	1	Total	K	0
			1	1	
87	Lg	1	Total	K	0
			1	1	
87	S2	9	Total	K	0
			9	9	
87	Sd	1	Total	K	0
			1	1	

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula: C₂₀H₃₇N₃O₁₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	At	18	Total 18	O 18	0
90	Et	37	Total 37	O 37	0
90	L5	5891	Total 5891	O 5891	0
90	L7	172	Total 172	O 172	0
90	L8	297	Total 297	O 297	0
90	LA	90	Total 90	O 90	0
90	LB	143	Total 143	O 143	0
90	LC	157	Total 157	O 157	0
90	LD	51	Total 51	O 51	0
90	LE	53	Total 53	O 53	0
90	LF	95	Total 95	O 95	0
90	LG	57	Total 57	O 57	0
90	LH	51	Total 51	O 51	0
90	LI	81	Total 81	O 81	0
90	LJ	16	Total 16	O 16	0
90	LL	81	Total 81	O 81	0
90	LM	35	Total 35	O 35	0
90	LN	106	Total 106	O 106	0
90	LO	81	Total 81	O 81	0
90	LP	56	Total 56	O 56	0
90	LQ	89	Total 89	O 89	0
90	LR	72	Total 72	O 72	0

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Mol	Chain	Residues	Atoms		AltConf
90	LS	89	Total 89	O 89	0
90	LT	59	Total 59	O 59	0
90	LU	5	Total 5	O 5	0
90	LV	42	Total 42	O 42	0
90	LW	22	Total 22	O 22	0
90	LX	32	Total 32	O 32	0
90	LY	40	Total 40	O 40	0
90	LZ	27	Total 27	O 27	0
90	La	72	Total 72	O 72	0
90	Lb	30	Total 30	O 30	0
90	Lc	11	Total 11	O 11	0
90	Ld	34	Total 34	O 34	0
90	Le	77	Total 77	O 77	0
90	Lf	52	Total 52	O 52	0
90	Lg	48	Total 48	O 48	0
90	Lh	43	Total 43	O 43	0
90	Li	38	Total 38	O 38	0
90	Lj	53	Total 53	O 53	0
90	Lk	3	Total 3	O 3	0
90	Ll	34	Total 34	O 34	0
90	Lm	21	Total 21	O 21	0

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Mol	Chain	Residues	Atoms		AltConf
90	Ln	18	Total 18	O 18	0
90	Lo	61	Total 61	O 61	0
90	Lp	38	Total 38	O 38	0
90	Lr	53	Total 53	O 53	0
90	Mr	3	Total 3	O 3	0
90	Pt	34	Total 34	O 34	0
90	S2	974	Total 974	O 974	0
90	SA	3	Total 3	O 3	0
90	SC	12	Total 12	O 12	0
90	SD	4	Total 4	O 4	0
90	SE	10	Total 10	O 10	0
90	SF	3	Total 3	O 3	0
90	SG	2	Total 2	O 2	0
90	SH	1	Total 1	O 1	0
90	SI	28	Total 28	O 28	0
90	SJ	7	Total 7	O 7	0
90	SK	1	Total 1	O 1	0
90	SL	29	Total 29	O 29	0
90	SM	3	Total 3	O 3	0
90	SN	14	Total 14	O 14	0
90	SO	7	Total 7	O 7	0

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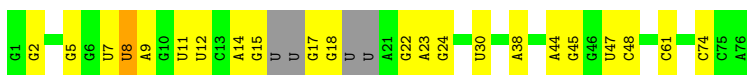
Mol	Chain	Residues	Atoms		AltConf
90	SP	5	Total 5	O 5	0
90	SQ	3	Total 3	O 3	0
90	SR	3	Total 3	O 3	0
90	SS	9	Total 9	O 9	0
90	SU	3	Total 3	O 3	0
90	SV	3	Total 3	O 3	0
90	SW	8	Total 8	O 8	0
90	SX	24	Total 24	O 24	0
90	SY	1	Total 1	O 1	0
90	SZ	1	Total 1	O 1	0
90	Sa	11	Total 11	O 11	0
90	Sb	2	Total 2	O 2	0
90	Sd	4	Total 4	O 4	0
90	Se	3	Total 3	O 3	0

3 Residue-property plots

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

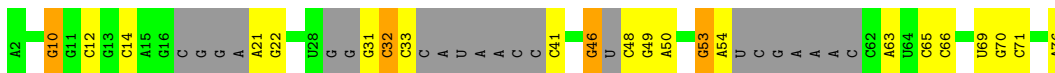
• Molecule 1: tRNA-Ile-AAT-9-1

Chain At: 



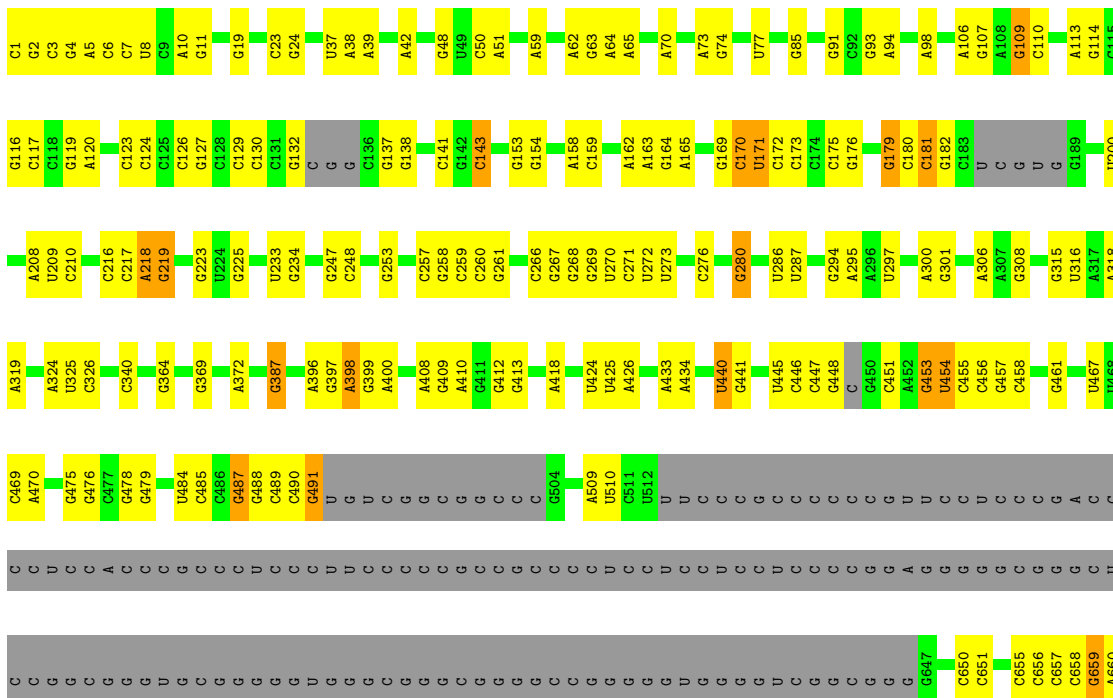
• Molecule 2: E site tRNA

Chain Et: 



• Molecule 3: 28S rRNA

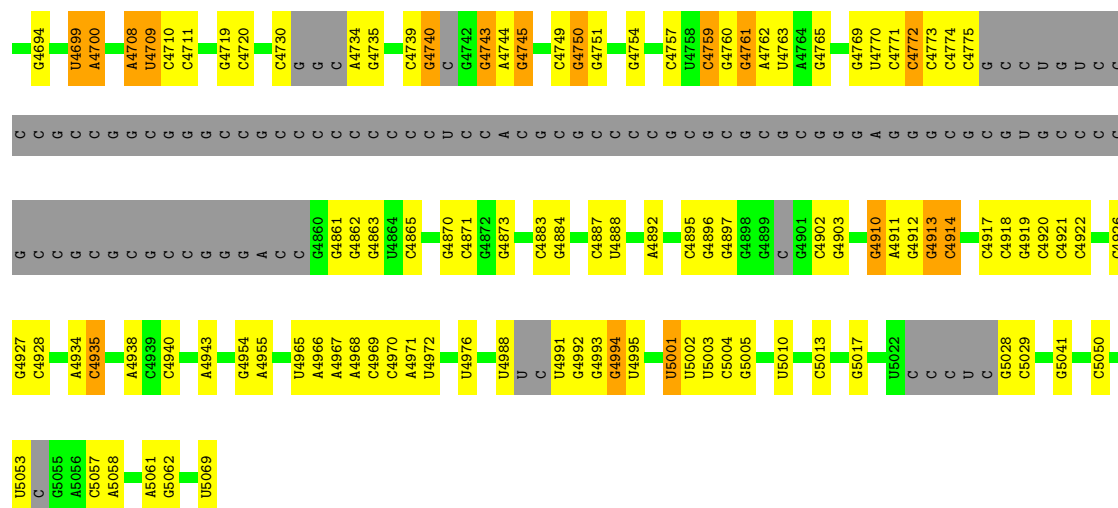
Chain L5: 











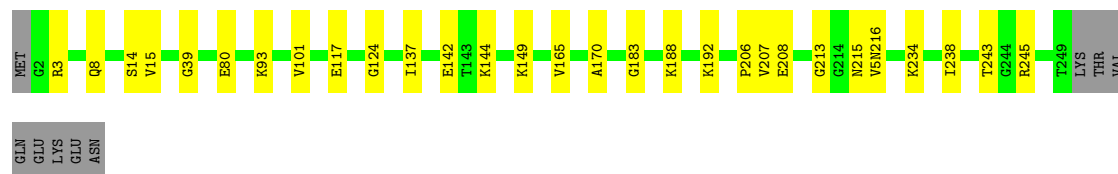
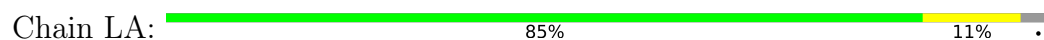
- Molecule 4: 5S rRNA



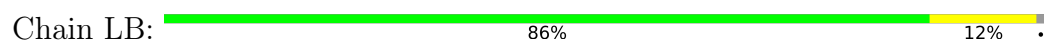
- Molecule 5: 5.8S rRNA



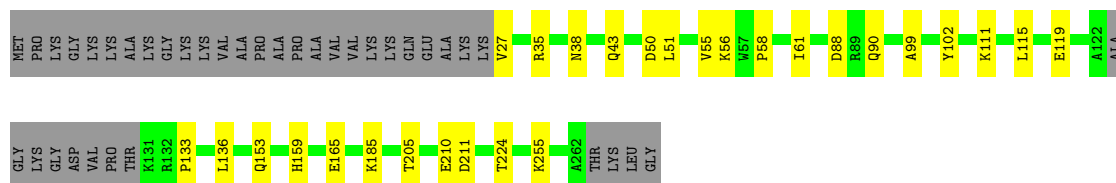
- Molecule 6: Large ribosomal subunit protein uL2



- Molecule 7: Large ribosomal subunit protein uL3



Chain LG:  75% 11% 14%



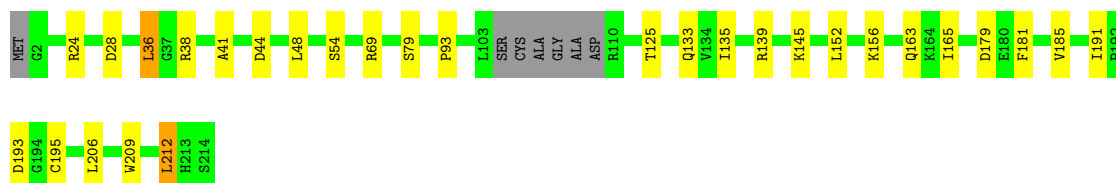
- Molecule 13: 60S ribosomal protein L9

Chain LH:  81% 18% .



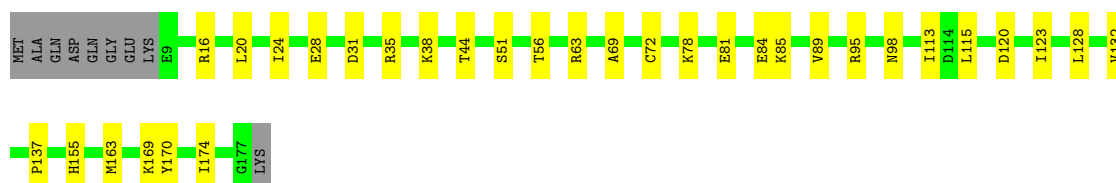
- Molecule 14: 60S ribosomal protein L10

Chain LI:  83% 13% . .



- Molecule 15: 60S ribosomal protein L11

Chain LJ:  77% 18% 5%



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL:  88% 9% .



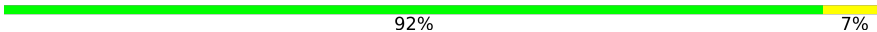
- Molecule 17: 60S ribosomal protein L14

Chain LM:  57% 7% 37%



ALA
ALA
SER
LYS
LYS
LYS
ALA
PRO
PRO
GLN
LYS
VAL
PRO
PRO
ALA
GLN
LYS
ALA
THR
GLY
GLN
LYS
ALA
ALA
PRO
ALA
PRO
LYS
LYS
GLN
LYS
GLY
GLN
LYS
ALA
ALA
PRO
PRO
GLN
LYS
LYS
SER
GLY
LYS
LYS
ALA

• Molecule 18: 60S ribosomal protein L15

Chain LN:  92% 7%

MET G2 R12 R13 K14 Q15 S16 R20 R24 R25 R26 E104 F138 R143 I151 V155 E160 R169 H178 H181 Y203 R204

• Molecule 19: 60S ribosomal protein L13a

Chain LO:  86% 13%

MET ALA GLU V4 R31 V34 R61 P70 R78 L88 P89 G95 L99 K103 D106 K130 R133 A142 V145 E158 E162 Y168 K172 M175 R176 K179 Q180 A181 V185 H199 V203

• Molecule 20: 60S ribosomal protein L17

Chain LP:  74% 9% 17%

MET V2 R3 Y4 S5 S17 S20 A33 R42 Q54 K55 M63 M64 A98 E99 I117 R126 R135 M140 M148 E154 GLN ILE VAL PRO LYS PRO PRO GLU GLU VAL ALA GLN LYS LYS ILE SER GLN LYS LEU LYS LYS LYS

LEU
MET
ALA
ARG
GLU

• Molecule 21: 60S ribosomal protein L18

Chain LQ:  92% 7%

MET G2 V3 D4 I5 R14 R65 R68 R69 M70 A80 V100 R108 K144 R150 A177 R178 R184 R188

• Molecule 22: 60S ribosomal protein L19

Chain LR:  83% 9% 8%

MET S2 R16 K43 P90 V93 M99 R104 R108 S122 V131 F132 K133 I137 K144 D148 R151 A159 R162 K165 A179 K180 K181 GLU GLU ILE LYS THR LEU SER LYS GLU GLU THR LYS

• Molecule 23: 60S ribosomal protein L18a

Chain LS:  85% 13%

M1 R15 T19 P20 K21 T24 L27 Y28 R29 M30 R43 F47 V48 S49 Q50 E69 K70 S71 K76 W81 M83 R98 D99 L100 T101 T107 Q108 R111 E130 V142 K164 T174 F175 F176

• Molecule 24: 60S ribosomal protein L21

MIT
T2
G6
M31
K35
K43
G51
T68
K83
T84
L85
R92
R102
F105
L106
K107
R108
K117
K120
T124
W125
R142
P148
E157
A160

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- MET SER LYS ARG GLY ARG GLY G8 K13 F14 R15 R48 R89 F95 N108 L128 A140

- [illegible]

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| VI49 | VI150 | VI151 | VI152 | VI153 | VI154 | VI155 | VI156 | VI157 | VI158 | VI159 | VI160 | VI161 | VI162 | VI163 | VI164 | VI165 | VI166 | VI167 | VI168 | VI169 | VI170 | VI171 | VI172 | VI173 | VI174 | VI175 | VI176 | VI177 | VI178 | VI179 | VI180 | VI181 | VI182 | VI183 | VI184 | VI185 | VI186 | VI187 | VI188 | VI189 | VI190 | VI191 | VI192 | VI193 | VI194 | VI195 | VI196 | VI197 | VI198 | VI199 | VI200 | VI201 | VI202 | VI203 | VI204 | VI205 | VI206 | VI207 | VI208 | VI209 | VI210 | VI211 | VI212 | VI213 | VI214 | VI215 | VI216 | VI217 | VI218 | VI219 | VI220 | VI221 | VI222 | VI223 | VI224 | VI225 | VI226 | VI227 | VI228 | VI229 | VI230 | VI231 | VI232 | VI233 | VI234 | VI235 | VI236 | VI237 | VI238 | VI239 | VI240 | VI241 | VI242 | VI243 | VI244 | VI245 | VI246 | VI247 | VI248 | VI249 | VI250 | VI251 | VI252 | VI253 | VI254 | VI255 | VI256 | VI257 | VI258 | VI259 | VI260 | VI261 | VI262 | VI263 | VI264 | VI265 | VI266 | VI267 | VI268 | VI269 | VI270 | VI271 | VI272 | VI273 | VI274 | VI275 | VI276 | VI277 | VI278 | VI279 | VI280 | VI281 | VI282 | VI283 | VI284 | VI285 | VI286 | VI287 | VI288 | VI289 | VI290 | VI291 | VI292 | VI293 | VI294 | VI295 | VI296 | VI297 | VI298 | VI299 | VI300 | VI301 | VI302 | VI303 | VI304 | VI305 | VI306 | VI307 | VI308 | VI309 | VI310 | VI311 | VI312 | VI313 | VI314 | VI315 | VI316 | VI317 | VI318 | VI319 | VI320 | VI321 | VI322 | VI323 | VI324 | VI325 | VI326 | VI327 | VI328 | VI329 | VI330 | VI331 | VI332 | VI333 | VI334 | VI335 | VI336 | VI337 | VI338 | VI339 | VI340 | VI341 | VI342 | VI343 | VI344 | VI345 | VI346 | VI347 | VI348 | VI349 | VI350 | VI351 | VI352 | VI353 | VI354 | VI355 | VI356 | VI357 | VI358 | VI359 | VI360 | VI361 | VI362 | VI363 | VI364 | VI365 | VI366 | VI367 | VI368 | VI369 | VI370 | VI371 | VI372 | VI373 | VI374 | VI375 | VI376 | VI377 | VI378 | VI379 | VI380 | VI381 | VI382 | VI383 | VI384 | VI385 | VI386 | VI387 | VI388 | VI389 | VI390 | VI391 | VI392 | VI393 | VI394 | VI395 | VI396 | VI397 | VI398 | VI399 | VI400 | VI401 | VI402 | VI403 | VI404 | VI405 | VI406 | VI407 | VI408 | VI409 | VI410 | VI411 | VI412 | VI413 | VI414 | VI415 | VI416 | VI417 | VI418 | VI419 | VI420 | VI421 | VI422 | VI423 | VI424 | VI425 | VI426 | VI427 | VI428 | VI429 | VI430 | VI431 | VI432 | VI433 | VI434 | VI435 | VI436 | VI437 | VI438 | VI439 | VI440 | VI441 | VI442 | VI443 | VI444 | VI445 | VI446 | VI447 | VI448 | VI449 | VI450 | VI451 | VI452 | VI453 | VI454 | VI455 | VI456 | VI457 | VI458 | VI459 | VI460 | VI461 | VI462 | VI463 | VI464 | VI465 | VI466 | VI467 | VI468 | VI469 | VI470 | VI471 | VI472 | VI473 | VI474 | VI475 | VI476 | VI477 | VI478 | VI479 | VI480 | VI481 | VI482 | VI483 | VI484 | VI485 | VI486 | VI487 | VI488 | VI489 | VI490 | VI491 | VI492 | VI493 | VI494 | VI495 | VI496 | VI497 | VI498 | VI499 | VI500 | VI501 | VI502 | VI503 | VI504 | VI505 | VI506 | VI507 | VI508 | VI509 | VI510 | VI511 | VI512 | VI513 | VI514 | VI515 | VI516 | VI517 | VI518 | VI519 | VI520 | VI521 | VI522 | VI523 | VI524 | VI525 | VI526 | VI527 | VI528 | VI529 | VI530 | VI531 | VI532 | VI533 | VI534 | VI535 | VI536 | VI537 | VI538 | VI539 | VI540 | VI541 | VI542 | VI543 | VI544 | VI545 | VI546 | VI547 | VI548 | VI549 | VI550 | VI551 | VI552 | VI553 | VI554 | VI555 | VI556 | VI557 | VI558 | VI559 | VI560 | VI561 | VI562 | VI563 | VI564 | VI565 | VI566 | VI567 | VI568 | VI569 | VI570 | VI571 | VI572 | VI573 | VI574 | VI575 | VI576 | VI577 | VI578 | VI579 | VI580 | VI581 | VI582 | VI583 | VI584 | VI585 | VI586 | VI587 | VI588 | VI589 | VI590 | VI591 | VI592 | VI593 | VI594 | VI595 | VI596 | VI597 | VI598 | VI599 | VI600 | VI601 | VI602 | VI603</ |
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| R#1 | R26 | R27 | R30 | R31 | R45 | R46 | R47 | R48 | Q66 | Q72 | Y81 | Q86 | R89 | T94 | P101 | R108 | D112 | R113 | D114 | I118 | R126 | Q127 | E131 | R132 | GLY | LYS | TYR | LYS | LYS | GLU | GLU | THR | ILE | GLU | LYS | LYS | MET | CIN | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- 
- WORLDWIDE
PDB
PROTEIN DATA BANK

MET
G2
V11
L14
A15
G16
S19
K27
J28
I29
G32
R48
Y49
P50
R51
X52
V53
X59
I62
F68
K69
H79
P82
V87
D88
I89
P90
L91
D92
X93
T94
V95
D99
R102
K109
A110
R111
R112
K115
E120
R121
T124
F136

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|-------|
| MET |
| P2 |
| K7 |
| VSN39 |
| H49 |
| P50 |
| G51 |
| T72 |
| L75 |
| Q85 |
| V88 |
| K110 |
| K116 |
| A133 |
| E134 |
| E135 |
| A148 |

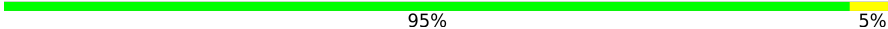
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|------|-----|-----|-----|-----|-----|-----|-----|----|
| NET | VAL | ALA | ALA | LYS | LYS | THR | LYS | LYS | S10 | S13 | R17 | L20 | V21 | V28 | T34 | M37 | I47 | L48 | I60 | N78 | L94 | A95 | I96 | S107 | NET | PRO | GLU | GLN | THR | GLY | GLU | VS |
|------|-----|-----|-----|-----|-----|-----|-----|----|

- | GLU | ASN | Met |
|-----|-----|------|
| | | ALA |
| | | PRO |
| | | ALA |
| | | LYS |
| | | LYS |
| | | GLY |
| | | GLY |
| | | GLU |
| | | LYS |
| | | LYS |
| | | LYS |
| | | GLY |
| | | ARG |
| | | SER |
| | | ALA |
| | | ILE |
| | | N18 |
| | | E19 |
| | | V20 |
| | | V21 |
| | | E24 |
| | | I29 |
| | | I33 |
| | | G37 |
| | | R41 |
| | | R44 |
| | | A45 |
| | | L46 |
| | | K51 |
| | | M54 |
| | | K55 |
| | | F56 |
| | | M57 |
| | | P60 |
| | | I64 |
| | | L68 |
| | | M69 |
| | | K70 |
| | | A71 |
| | | V72 |
| | | R87 |
| | | R90 |
| | | T119 |
| | | R122 |

- | | | | | | | | | | | | | | | | | | |
|-----|----|-----|-----|-----|-----|-----|-----|------------|-----|------|------|-----|-----|-----|-----|-----|-----|
| MET | A2 | K14 | V35 | P56 | K64 | L78 | V82 | E86
V87 | K93 | N107 | L129 | ARG | SER | GLU | GLU | ASN | GLU |
|-----|----|-----|-----|-----|-----|-----|-----|------------|-----|------|------|-----|-----|-----|-----|-----|-----|

- 

Chain Lf:  95% 5%



- Molecule 37: 60S ribosomal protein L34

Chain Lg:  83% 13%



- Molecule 38: 60S ribosomal protein L35

Chain Lh:  81% 18%



- Molecule 39: 60S ribosomal protein L36

Chain Li:  90% 7%



- Molecule 40: Large ribosomal subunit protein eL37

Chain Lj:  79% 9% 11%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  84% 11%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  78% 18%



- Molecule 43: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  35% 5% 59%

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

ILE GLN LYS GLU SER THR LEU HIS VAL LEU ARG LEU ARG GLY I77 P80 S81 L82 R83 Q84 M94 Y100 P105 K125 K128

- Molecule 44: 60S ribosomal protein L41

Chain Ln:  92% 8%

H1 R23 S24 K25

- Molecule 45: Large ribosomal subunit protein eL42

Chain Lo:  85% 14%

MET Y2 K22 Y26 G37 R43 K58 V67 E71 C72 V73 R78 S79 K80 H90 F91 E92 R99 K100 G101 Q102 F106

- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  88% 10%

MET A2 K3 G9 T16 T38 K44 T45 S59 R84 E88 D91 GLN

- Molecule 47: 60S ribosomal protein L28

Chain Lr:  77% 14% 9%

MET S2 R20 S26 T27 E28 S37 M41 E52 P53 A54 V61 R66 R67 S68 R79 R87 L90 I93 I97 R98 K99 R103 I111 S115 V126 LYS ARG LYS ARG THR ARG PRO THR LYS SER

- Molecule 48: Synthetic mRNA

Chain Mr:  71% 29%

C2 A5 C8

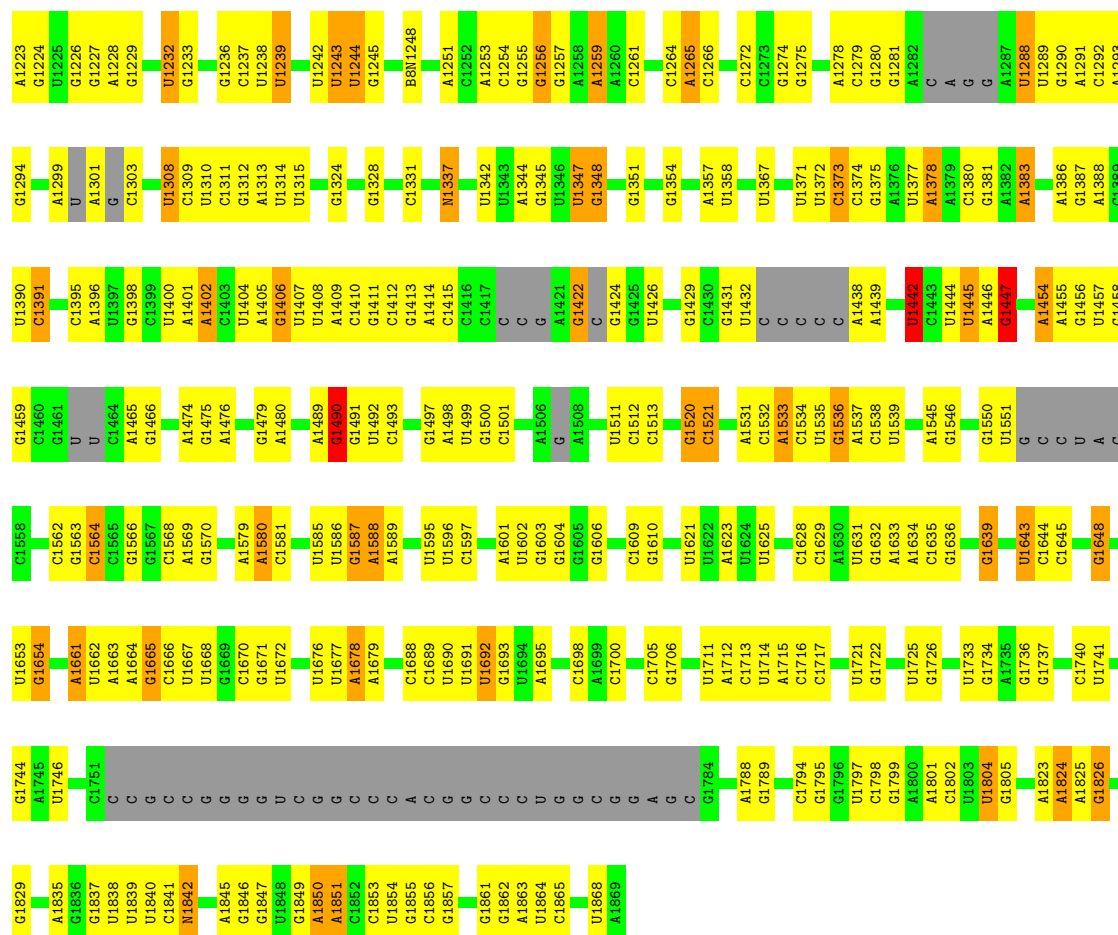
- Molecule 49: P site tRNA Arg-ACG

Chain Pt:  76% 16% 5%

G1 G9 G10 C11 G12 C13 A14 A15 U G17 G18 A A21 G26 G36 G37 A46 U U48 A58 C59 U60 C61 C74 C75 A76

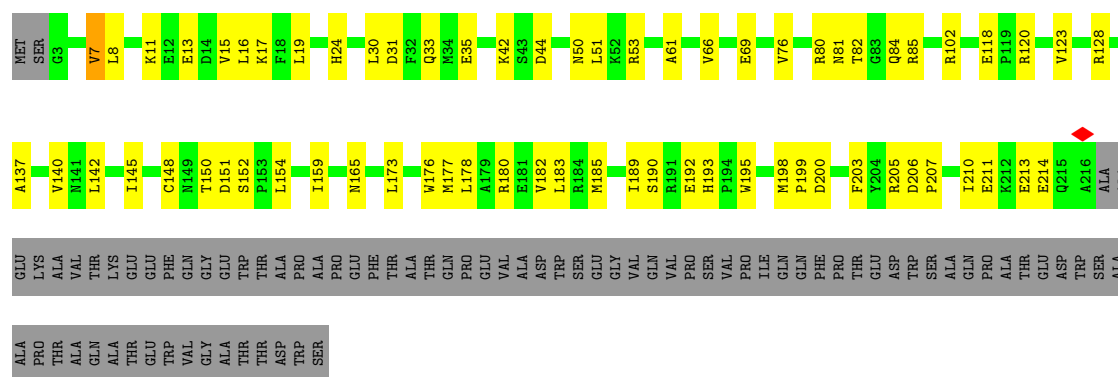
Chain S2:





• Molecule 51: 40S ribosomal protein SA

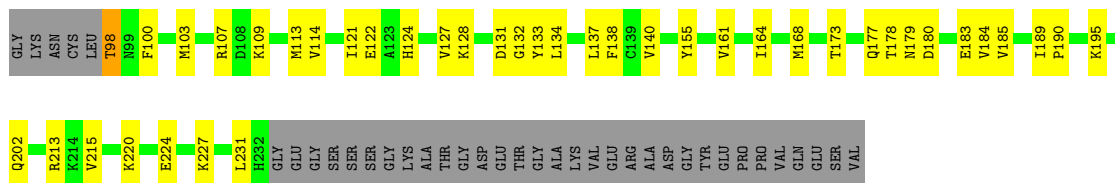
Chain SA: 50% 22% 27%



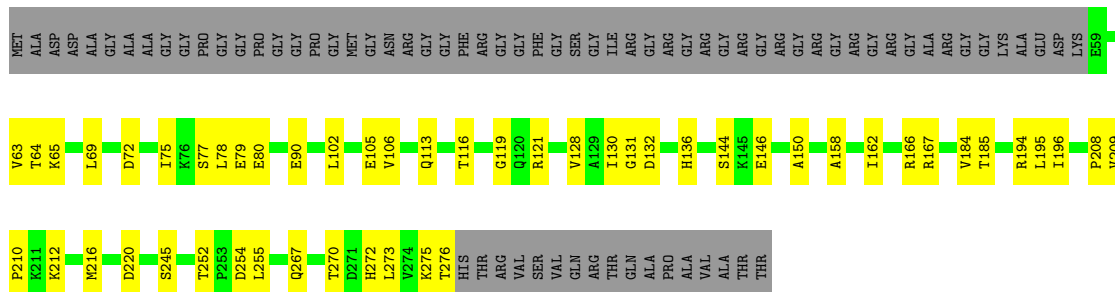
• Molecule 52: 40S ribosomal protein S3a

Chain SB: 53% 22% 25%

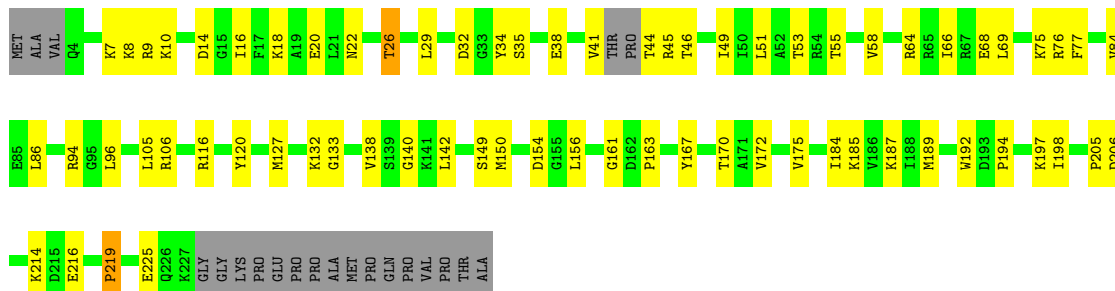




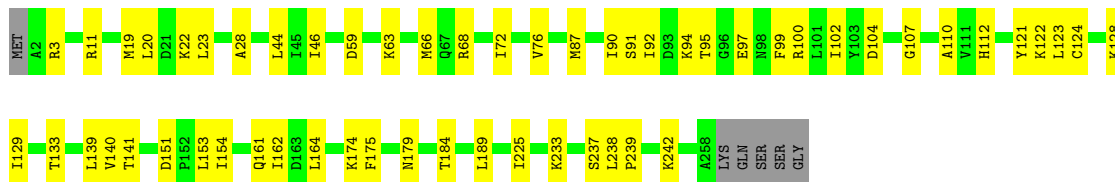
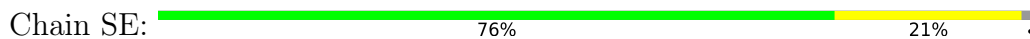
- Molecule 53: 40S ribosomal protein S2



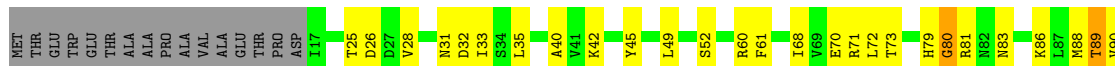
- Molecule 54: 40S ribosomal protein S3

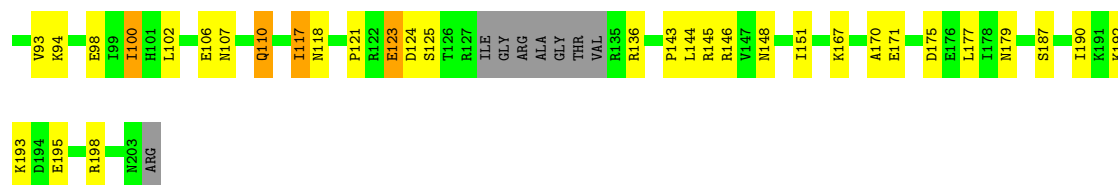


- Molecule 55: Small ribosomal subunit protein eS4, X isoform



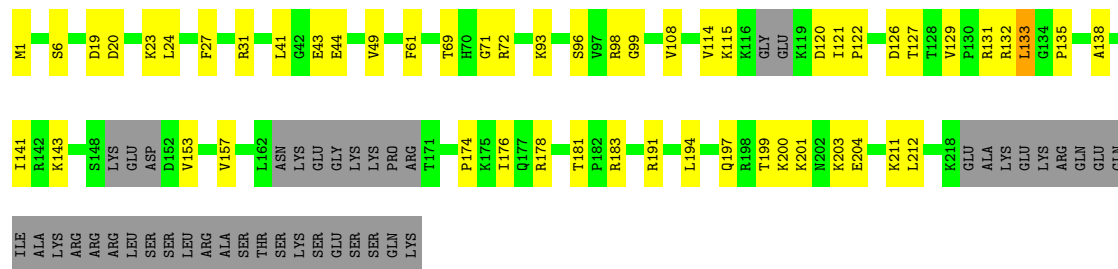
- Molecule 56: 40S ribosomal protein S5





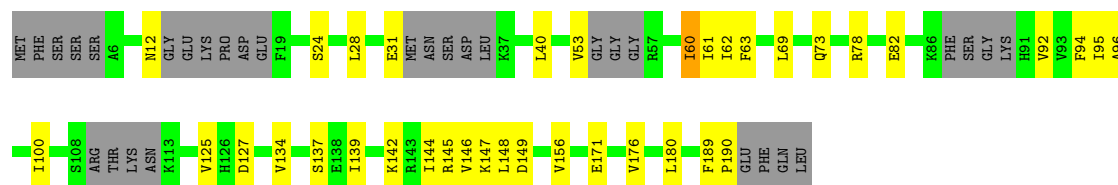
- Molecule 57: 40S ribosomal protein S6

Chain SG: 61% 21% 18%



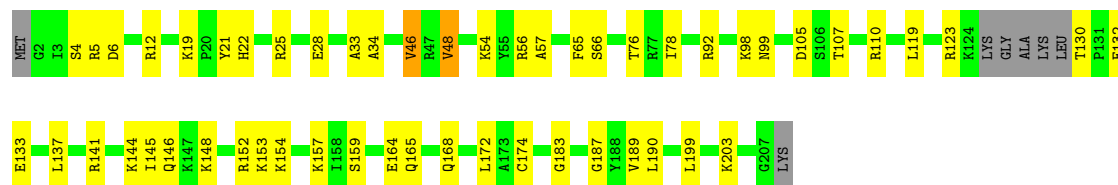
- Molecule 58: 40S ribosomal protein S7

Chain SH: 65% 19% 16%



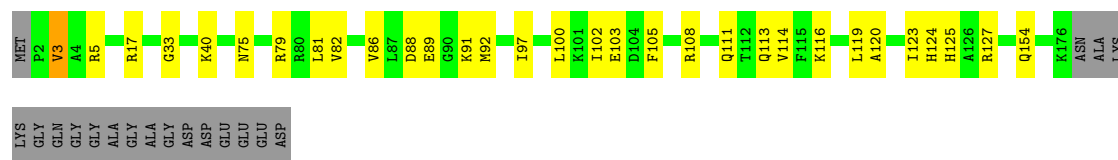
- Molecule 59: 40S ribosomal protein S8

Chain SI: 71% 25% 4%

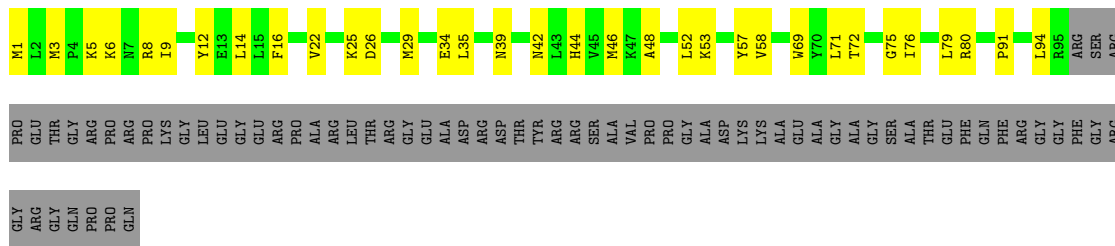


- Molecule 60: 40S ribosomal protein S9

Chain SJ: 74% 15% 10%



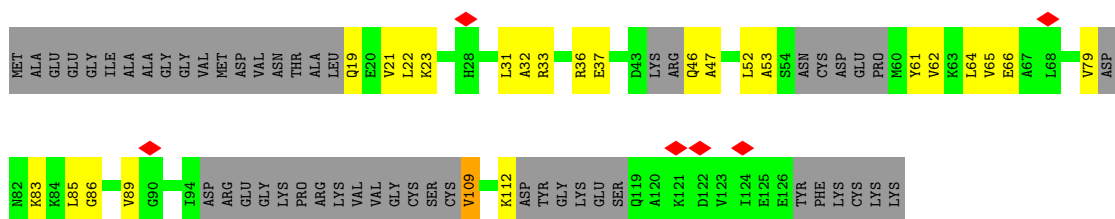
- Molecule 61: 40S ribosomal protein S10



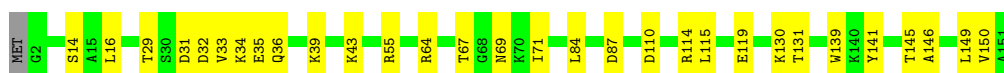
- Molecule 62: 40S ribosomal protein S11



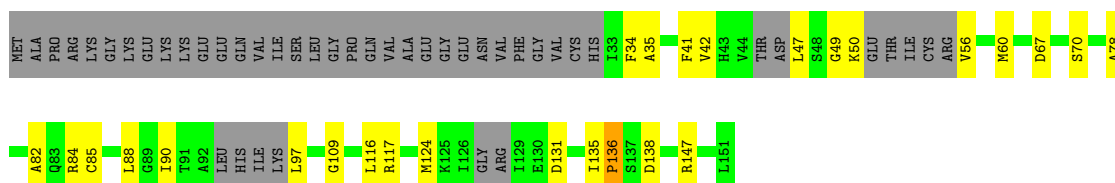
- Molecule 63: 40S ribosomal protein S12



- Molecule 64: 40S ribosomal protein S13

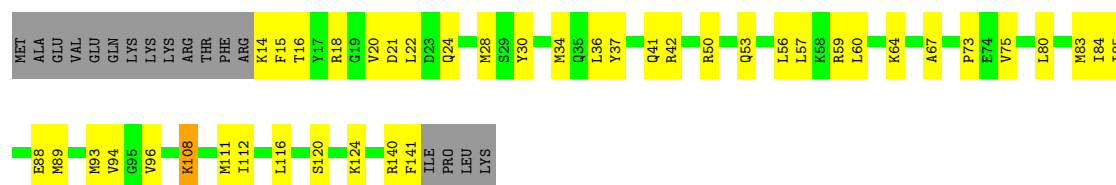


- Molecule 65: 40S ribosomal protein S14



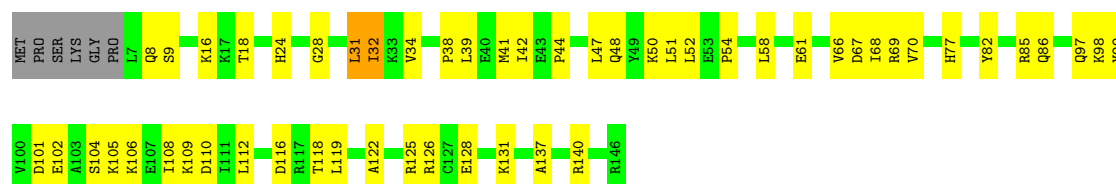
- Molecule 66: 40S ribosomal protein S15

Chain SP:  59% 28% 12%



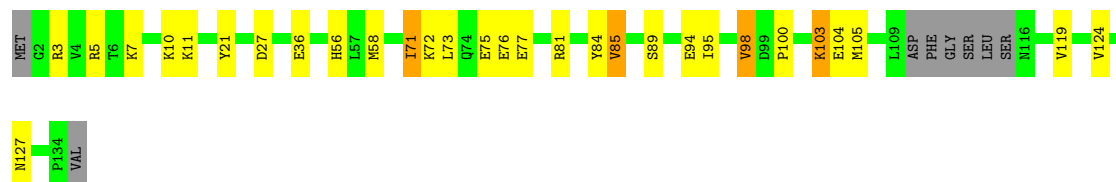
- Molecule 67: 40S ribosomal protein S16

Chain SQ:  60% 35%



- Molecule 68: 40S ribosomal protein S17

Chain SR:  72% 19% 6%



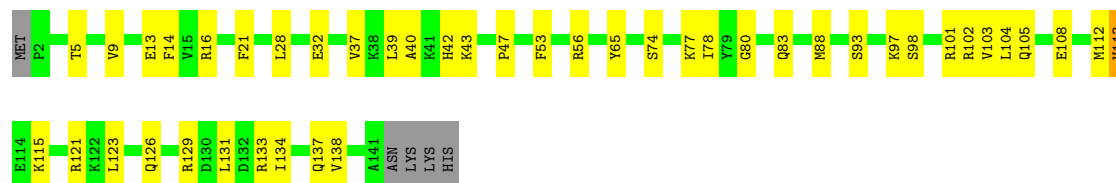
- Molecule 69: 40S ribosomal protein S18

Chain SS:  68% 28%



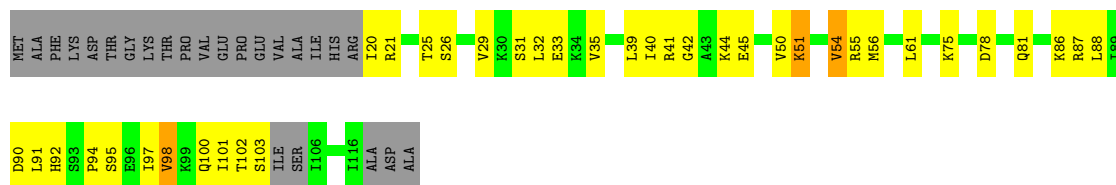
- Molecule 70: 40S ribosomal protein S19

Chain ST:  66% 30%



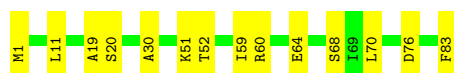
- Molecule 71: 40S ribosomal protein S20

Chain SU:  48% 29% 20%



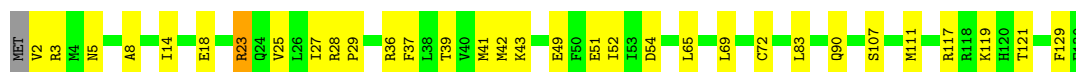
- Molecule 72: 40S ribosomal protein S21

Chain SV:  83% 17%



- Molecule 73: 40S ribosomal protein S15a

Chain SW:  75% 24% ..



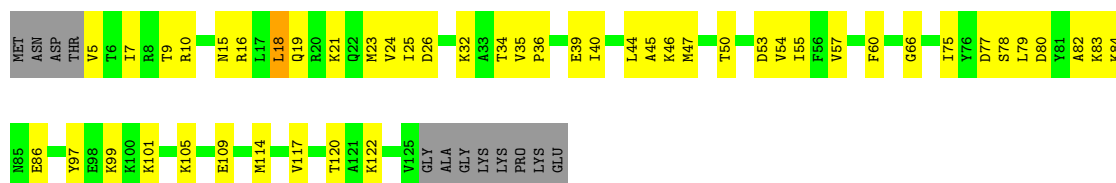
- Molecule 74: 40S ribosomal protein S23

Chain SX:  80% 16% ..



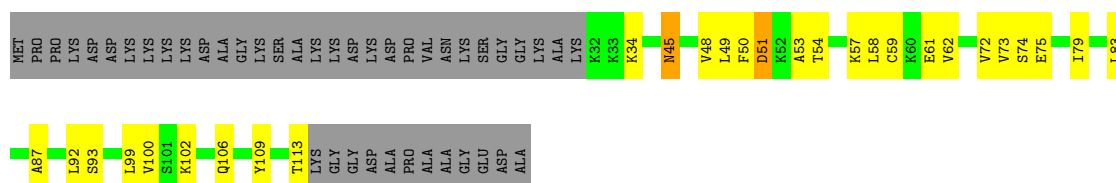
- Molecule 75: 40S ribosomal protein S24

Chain SY:  55% 35% 9%



- Molecule 76: 40S ribosomal protein S25

Chain SZ:  43% 21% 34%



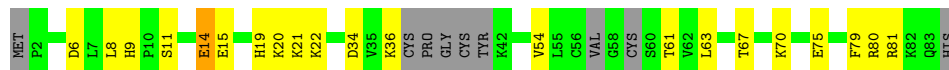
- Molecule 77: 40S ribosomal protein S26

Chain Sa: 



- Molecule 78: 40S ribosomal protein S27

Chain Sb: 



- Molecule 79: 40S ribosomal protein S28

Chain Sc: 



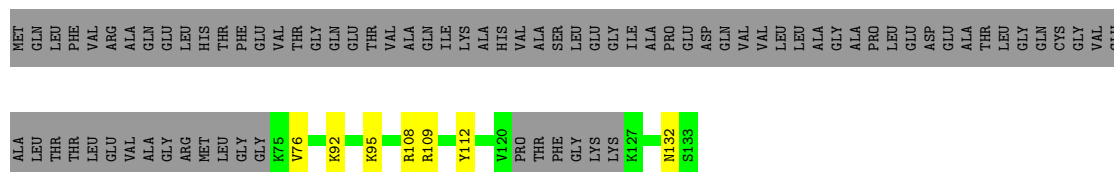
- Molecule 80: 40S ribosomal protein S29

Chain Sd: 



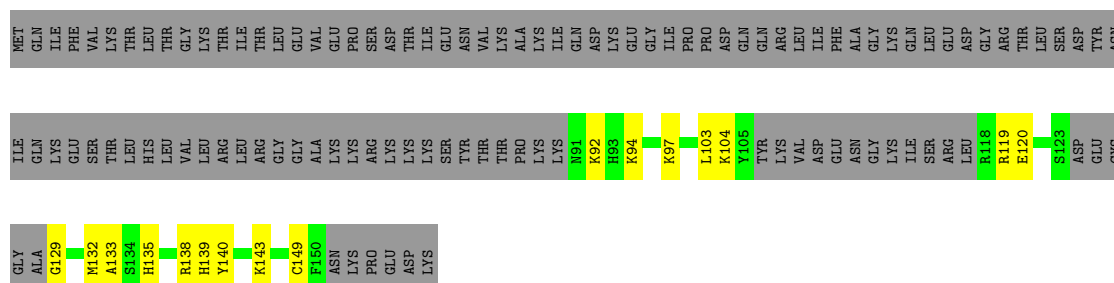
- Molecule 81: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se: 

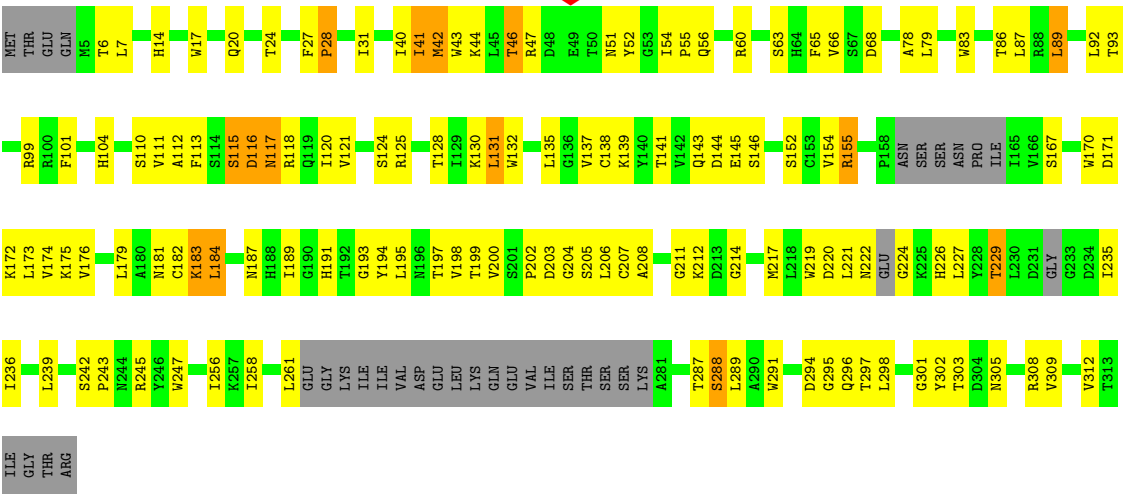


- Molecule 82: Ubiquitin

Chain Sf: 



● Molecule 83: 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	94974	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 ($e^-/\text{\AA}^2$)	1.077	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	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, K, 4AC, V5N, OMU, SPD, MG, UY1, B8N, HY3, OMC, MA7, 5MC, MLZ, M2G, M3L, A2M, 1MG, PUT, 6MZ, PSU, 1MA, HYG, G7M, MA6, OMG, HIC, ZN

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	At	0.70	0/1714	1.00	1/2662 (0.0%)
2	Et	0.11	0/1287	0.27	0/1994
3	L5	0.17	3/78892 (0.0%)	0.30	2/123000 (0.0%)
4	L7	0.13	0/2836	0.26	0/4421
5	L8	0.16	0/3453	0.27	0/5376
6	LA	0.14	0/1935	0.34	0/2592
7	LB	0.12	0/3258	0.30	0/4359
8	LC	0.12	0/2927	0.30	0/3932
9	LD	0.12	0/2430	0.30	0/3254
10	LE	0.13	0/1816	0.29	0/2438
11	LF	0.15	0/1890	0.31	0/2521
12	LG	0.15	0/1855	0.34	1/2501 (0.0%)
13	LH	0.13	0/1537	0.31	0/2066
14	LI	0.13	0/1710	0.30	0/2284
15	LJ	0.13	0/1376	0.35	0/1841
16	LL	0.13	0/1695	0.30	0/2270
17	LM	0.13	0/1142	0.28	0/1527
18	LN	0.14	0/1745	0.33	0/2338
19	LO	0.14	0/1672	0.30	0/2238
20	LP	0.14	0/1279	0.32	0/1716
21	LQ	0.14	0/1536	0.32	0/2052
22	LR	0.13	0/1465	0.28	0/1945
23	LS	0.14	0/1500	0.31	0/2013
24	LT	0.14	0/1334	0.31	0/1781
25	LU	0.15	0/822	0.40	0/1103
26	LV	0.12	0/1002	0.30	0/1345
27	LW	0.13	0/542	0.33	0/722
28	LX	0.12	0/983	0.29	0/1323
29	LY	0.13	0/1115	0.32	0/1484
30	LZ	0.16	0/1130	0.34	0/1507
31	La	0.13	0/1178	0.30	0/1573

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.14	0/843	0.33	0/1111
33	Lc	0.12	0/771	0.28	0/1035
34	Ld	0.14	0/894	0.33	0/1204
35	Le	0.13	0/1082	0.30	0/1443
36	Lf	0.14	0/899	0.30	0/1205
37	Lg	0.12	0/898	0.29	0/1197
38	Lh	0.12	0/1022	0.26	0/1351
39	Li	0.12	0/843	0.31	0/1115
40	Lj	0.13	0/720	0.32	0/952
41	Lk	0.13	0/565	0.33	0/750
42	Ll	0.15	0/453	0.30	0/599
43	Lm	0.12	0/429	0.30	0/571
44	Ln	0.13	0/240	0.25	0/305
45	Lo	0.13	0/881	0.29	0/1161
46	Lp	0.13	0/708	0.30	0/941
47	Lr	0.14	0/1017	0.29	0/1364
48	Mr	0.62	0/160	0.98	0/246
49	Pt	0.71	0/1617	0.96	0/2509
50	S2	0.20	2/35344 (0.0%)	0.33	2/55048 (0.0%)
51	SA	0.15	0/1730	0.36	0/2351
52	SB	0.15	0/1651	0.38	0/2203
53	SC	0.14	0/1726	0.35	0/2332
54	SD	0.22	1/1747 (0.1%)	0.53	4/2350 (0.2%)
55	SE	0.13	0/2083	0.35	0/2805
56	SF	0.15	0/1437	0.42	0/1933
57	SG	0.17	0/1671	0.45	2/2227 (0.1%)
58	SH	0.14	0/1332	0.38	0/1782
59	SI	0.14	0/1679	0.38	0/2239
60	SJ	0.13	0/1446	0.31	0/1937
61	SK	0.16	0/823	0.42	0/1111
62	SL	0.12	0/1184	0.30	0/1583
63	SM	0.13	0/554	0.36	0/743
64	SN	0.12	0/1231	0.28	0/1656
65	SO	0.18	0/793	0.44	1/1056 (0.1%)
66	SP	0.28	0/1057	0.44	0/1414
67	SQ	0.16	0/1133	0.42	0/1517
68	SR	0.13	0/1045	0.36	0/1402
69	SS	0.13	0/1232	0.38	1/1651 (0.1%)
70	ST	0.16	0/1131	0.39	0/1518
71	SU	0.17	0/763	0.42	0/1023
72	SV	0.12	0/643	0.31	0/860
73	SW	0.15	0/1051	0.35	0/1406
74	SX	0.23	0/1096	0.43	0/1461

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SY	0.15	0/1012	0.42	0/1344
76	SZ	0.18	0/669	0.45	0/895
77	Sa	0.14	0/805	0.33	0/1079
78	Sb	0.15	0/600	0.42	0/798
79	Sc	0.15	0/497	0.39	0/666
80	Sd	0.11	0/469	0.32	0/623
81	Se	0.32	0/423	0.48	0/555
82	Sf	0.12	0/347	0.36	0/457
83	Sg	0.77	3/2251 (0.1%)	0.85	6/3062 (0.2%)
All	All	0.20	9/215753 (0.0%)	0.35	20/316324 (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
83	Sg	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	Sg	28	PRO	CG-CD	-25.69	0.63	1.50
83	Sg	28	PRO	CB-CG	12.98	2.14	1.49
83	Sg	28	PRO	N-CD	9.65	1.61	1.47
54	SD	219	PRO	CG-CD	-5.31	1.32	1.50
50	S2	627	OMU	O3'-P	5.21	1.61	1.56

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	Sg	28	PRO	N-CD-CG	-16.72	78.13	103.20
83	Sg	28	PRO	CA-N-CD	-13.52	93.07	112.00
83	Sg	28	PRO	CB-CG-CD	-12.98	64.57	106.10
54	SD	219	PRO	CA-CB-CG	-11.33	82.98	104.50
54	SD	219	PRO	N-CD-CG	-11.33	86.21	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	Sg	155	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	At	1559	0	793	1	0
2	Et	1155	0	593	14	0
3	L5	73250	0	37111	763	0
4	L7	2538	0	1286	20	0
5	L8	3177	0	1613	41	0
6	LA	1907	0	1999	18	0
7	LB	3203	0	3344	29	0
8	LC	2873	0	3046	23	0
9	LD	2385	0	2419	31	0
10	LE	1782	0	1934	26	0
11	LF	1856	0	1981	16	0
12	LG	1824	0	1938	17	0
13	LH	1518	0	1600	23	0
14	LI	1672	0	1717	17	0
15	LJ	1353	0	1386	23	0
16	LL	1664	0	1773	15	0
17	LM	1120	0	1187	6	0
18	LN	1700	0	1749	14	0
19	LO	1640	0	1788	18	0
20	LP	1249	0	1276	12	0
21	LQ	1512	0	1628	11	0
22	LR	1449	0	1549	14	0
23	LS	1460	0	1502	16	0
24	LT	1303	0	1379	17	0
25	LU	808	0	831	14	0
26	LV	988	0	1047	6	0
27	LW	529	0	537	3	0
28	LX	966	0	1040	13	0
29	LY	1098	0	1178	12	0
30	LZ	1107	0	1182	23	0
31	La	1162	0	1206	8	0
32	Lb	841	0	912	23	0
33	Lc	761	0	796	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Ld	879	0	924	12	0
35	Le	1061	0	1160	8	0
36	Lf	880	0	917	3	0
37	Lg	888	0	977	10	0
38	Lh	1014	0	1148	16	0
39	Li	832	0	917	5	0
40	Lj	705	0	737	8	0
41	Lk	559	0	624	7	0
42	Ll	443	0	483	5	0
43	Lm	432	0	465	5	0
44	Ln	239	0	289	2	0
45	Lo	875	0	941	11	0
46	Lp	698	0	748	7	0
47	Lr	1002	0	1068	14	0
48	Mr	145	0	76	1	0
49	Pt	1547	0	792	4	0
50	S2	33424	0	16927	453	0
51	SA	1693	0	1693	47	0
52	SB	1627	0	1701	35	0
53	SC	1690	0	1777	31	0
54	SD	1721	0	1809	41	0
55	SE	2041	0	2143	34	0
56	SF	1417	0	1458	44	0
57	SG	1652	0	1791	33	0
58	SH	1317	0	1409	24	0
59	SI	1651	0	1726	39	0
60	SJ	1424	0	1499	21	0
61	SK	799	0	823	22	0
62	SL	1164	0	1232	16	0
63	SM	556	0	550	15	0
64	SN	1207	0	1294	19	0
65	SO	788	0	813	22	0
66	SP	1037	0	1074	28	0
67	SQ	1116	0	1185	41	0
68	SR	1032	0	1090	20	0
69	SS	1214	0	1275	32	0
70	ST	1104	0	1132	31	0
71	SU	755	0	820	29	0
72	SV	636	0	637	10	0
73	SW	1034	0	1080	23	0
74	SX	1088	0	1149	13	0
75	SY	995	0	1068	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	SZ	661	0	732	26	0
77	Sa	792	0	841	10	0
78	Sb	592	0	619	13	0
79	Sc	495	0	523	16	0
80	Sd	458	0	448	12	0
81	Se	420	0	463	8	0
82	Sf	341	0	335	15	0
83	Sg	2199	0	2146	76	0
84	L5	36	0	72	2	0
84	S2	12	0	24	3	0
85	L5	140	0	266	9	0
85	LN	10	0	19	0	0
85	S2	30	0	57	0	0
86	L5	159	0	0	0	0
86	L7	2	0	0	0	0
86	L8	3	0	0	0	0
86	LP	1	0	0	0	0
86	LR	1	0	0	0	0
86	S2	29	0	0	0	0
87	L5	60	0	0	0	0
87	L8	1	0	0	0	0
87	LA	2	0	0	0	0
87	LH	1	0	0	0	0
87	Lg	1	0	0	0	0
87	S2	9	0	0	0	0
87	Sd	1	0	0	0	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lm	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	Sa	1	0	0	0	0
88	Sd	1	0	0	0	0
89	S2	36	0	36	1	0
90	At	18	0	0	0	0
90	Et	37	0	0	0	0
90	L5	5891	0	0	9	0
90	L7	172	0	0	0	0
90	L8	297	0	0	0	0
90	LA	90	0	0	0	0
90	LB	143	0	0	0	0
90	LC	157	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	LD	51	0	0	1	0
90	LE	53	0	0	1	0
90	LF	95	0	0	1	0
90	LG	57	0	0	1	0
90	LH	51	0	0	0	0
90	LI	81	0	0	0	0
90	LJ	16	0	0	0	0
90	LL	81	0	0	0	0
90	LM	35	0	0	0	0
90	LN	106	0	0	0	0
90	LO	81	0	0	0	0
90	LP	56	0	0	2	0
90	LQ	89	0	0	0	0
90	LR	72	0	0	1	0
90	LS	89	0	0	2	0
90	LT	59	0	0	0	0
90	LU	5	0	0	0	0
90	LV	42	0	0	0	0
90	LW	22	0	0	0	0
90	LX	32	0	0	1	0
90	LY	40	0	0	1	0
90	LZ	27	0	0	0	0
90	La	72	0	0	0	0
90	Lb	30	0	0	1	0
90	Lc	11	0	0	0	0
90	Ld	34	0	0	0	0
90	Le	77	0	0	0	0
90	Lf	52	0	0	0	0
90	Lg	48	0	0	0	0
90	Lh	43	0	0	1	0
90	Li	38	0	0	1	0
90	Lj	53	0	0	0	0
90	Lk	3	0	0	0	0
90	Ll	34	0	0	0	0
90	Lm	21	0	0	0	0
90	Ln	18	0	0	0	0
90	Lo	61	0	0	1	0
90	Lp	38	0	0	1	0
90	Lr	53	0	0	1	0
90	Mr	3	0	0	0	0
90	Pt	34	0	0	0	0
90	S2	974	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	SA	3	0	0	0	0
90	SC	12	0	0	0	0
90	SD	4	0	0	0	0
90	SE	10	0	0	0	0
90	SF	3	0	0	1	0
90	SG	2	0	0	0	0
90	SH	1	0	0	0	0
90	SI	28	0	0	2	0
90	SJ	7	0	0	0	0
90	SK	1	0	0	0	0
90	SL	29	0	0	2	0
90	SM	3	0	0	0	0
90	SN	14	0	0	0	0
90	SO	7	0	0	0	0
90	SP	5	0	0	0	0
90	SQ	3	0	0	0	0
90	SR	3	0	0	0	0
90	SS	9	0	0	0	0
90	SU	3	0	0	0	0
90	SV	3	0	0	0	0
90	SW	8	0	0	0	0
90	SX	24	0	0	0	0
90	SY	1	0	0	0	0
90	SZ	1	0	0	0	0
90	Sa	11	0	0	0	0
90	Sb	2	0	0	0	0
90	Sd	4	0	0	0	0
90	Se	3	0	0	1	0
All	All	216235	0	153322	2426	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 7.

The worst 5 of 2426 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)
61:SK:91:PRO:HG2	61:SK:94:LEU:HD23	1.52	0.92
76:SZ:45:ASN:O	76:SZ:45:ASN:ND2	2.08	0.85
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.59	0.84
3:L5:4095:G:H1	3:L5:4113:U:H3	1.25	0.82
76:SZ:45:ASN:HD22	76:SZ:45:ASN:C	1.89	0.80

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	
6	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
7	LB	394/403 (98%)	388 (98%)	6 (2%)	0	100	100
8	LC	359/427 (84%)	353 (98%)	6 (2%)	0	100	100
9	LD	292/297 (98%)	284 (97%)	8 (3%)	0	100	100
10	LE	217/288 (75%)	210 (97%)	7 (3%)	0	100	100
11	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
12	LG	224/266 (84%)	222 (99%)	2 (1%)	0	100	100
13	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
14	LI	203/214 (95%)	201 (99%)	2 (1%)	0	100	100
15	LJ	167/178 (94%)	165 (99%)	2 (1%)	0	100	100
16	LL	204/211 (97%)	199 (98%)	5 (2%)	0	100	100
17	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
18	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
19	LO	198/203 (98%)	196 (99%)	2 (1%)	0	100	100
20	LP	152/184 (83%)	150 (99%)	2 (1%)	0	100	100
21	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
22	LR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
24	LT	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
25	LU	97/128 (76%)	94 (97%)	3 (3%)	0	100	100
26	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
27	LW	62/157 (40%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	LX	116/156 (74%)	116 (100%)	0	0	100	100
29	LY	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
30	LZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
31	La	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
32	Lb	99/159 (62%)	97 (98%)	2 (2%)	0	100	100
33	Lc	96/115 (84%)	96 (100%)	0	0	100	100
34	Ld	104/125 (83%)	104 (100%)	0	0	100	100
35	Le	127/135 (94%)	126 (99%)	1 (1%)	0	100	100
36	Lf	108/110 (98%)	108 (100%)	0	0	100	100
37	Lg	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
38	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
40	Lj	84/97 (87%)	84 (100%)	0	0	100	100
41	Lk	66/70 (94%)	66 (100%)	0	0	100	100
42	Ll	48/51 (94%)	48 (100%)	0	0	100	100
43	Lm	50/128 (39%)	50 (100%)	0	0	100	100
44	Ln	23/25 (92%)	23 (100%)	0	0	100	100
45	Lo	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
46	Lp	88/92 (96%)	85 (97%)	3 (3%)	0	100	100
47	Lr	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
51	SA	212/295 (72%)	205 (97%)	7 (3%)	0	100	100
52	SB	191/264 (72%)	185 (97%)	6 (3%)	0	100	100
53	SC	216/293 (74%)	214 (99%)	2 (1%)	0	100	100
54	SD	218/243 (90%)	212 (97%)	6 (3%)	0	100	100
55	SE	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
56	SF	176/204 (86%)	167 (95%)	8 (4%)	1 (1%)	21	32
57	SG	197/249 (79%)	191 (97%)	6 (3%)	0	100	100
58	SH	151/194 (78%)	149 (99%)	2 (1%)	0	100	100
59	SI	197/208 (95%)	194 (98%)	3 (2%)	0	100	100
60	SJ	173/194 (89%)	167 (96%)	6 (4%)	0	100	100
61	SK	93/165 (56%)	89 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	SL	138/158 (87%)	134 (97%)	4 (3%)	0	100	100
63	SM	67/132 (51%)	61 (91%)	6 (9%)	0	100	100
64	SN	148/151 (98%)	148 (100%)	0	0	100	100
65	SO	96/151 (64%)	87 (91%)	9 (9%)	0	100	100
66	SP	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
67	SQ	138/146 (94%)	131 (95%)	7 (5%)	0	100	100
68	SR	123/135 (91%)	121 (98%)	2 (2%)	0	100	100
69	SS	146/152 (96%)	144 (99%)	2 (1%)	0	100	100
70	ST	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
71	SU	91/119 (76%)	86 (94%)	5 (6%)	0	100	100
72	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
73	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
74	SX	137/143 (96%)	136 (99%)	1 (1%)	0	100	100
75	SY	119/133 (90%)	116 (98%)	3 (2%)	0	100	100
76	SZ	80/125 (64%)	77 (96%)	3 (4%)	0	100	100
77	Sa	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
78	Sb	68/84 (81%)	66 (97%)	2 (3%)	0	100	100
79	Sc	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
80	Sd	53/56 (95%)	53 (100%)	0	0	100	100
81	Se	49/133 (37%)	48 (98%)	1 (2%)	0	100	100
82	Sf	37/156 (24%)	35 (95%)	2 (5%)	0	100	100
83	Sg	272/317 (86%)	249 (92%)	19 (7%)	4 (2%)	8	12
All	All	10833/12762 (85%)	10592 (98%)	236 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
56	SF	80	GLY
83	Sg	117	ASN
83	Sg	144	ASP
83	Sg	146	SER
83	Sg	184	LEU

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	
6	LA	190/198 (96%)	189 (100%)	1 (0%)	81	91
7	LB	344/348 (99%)	340 (99%)	4 (1%)	63	81
8	LC	300/348 (86%)	296 (99%)	4 (1%)	61	80
9	LD	246/250 (98%)	240 (98%)	6 (2%)	43	65
10	LE	195/252 (77%)	193 (99%)	2 (1%)	68	84
11	LF	191/215 (89%)	190 (100%)	1 (0%)	81	91
12	LG	191/223 (86%)	190 (100%)	1 (0%)	81	91
13	LH	169/171 (99%)	169 (100%)	0	100	100
14	LI	175/181 (97%)	170 (97%)	5 (3%)	37	60
15	LJ	142/149 (95%)	141 (99%)	1 (1%)	76	88
16	LL	172/177 (97%)	171 (99%)	1 (1%)	78	89
17	LM	116/161 (72%)	113 (97%)	3 (3%)	40	63
18	LN	171/172 (99%)	169 (99%)	2 (1%)	63	81
19	LO	172/174 (99%)	172 (100%)	0	100	100
20	LP	135/163 (83%)	133 (98%)	2 (2%)	57	77
21	LQ	164/165 (99%)	164 (100%)	0	100	100
22	LR	146/175 (83%)	144 (99%)	2 (1%)	59	79
23	LS	157/157 (100%)	151 (96%)	6 (4%)	29	49
24	LT	140/140 (100%)	139 (99%)	1 (1%)	76	88
25	LU	89/115 (77%)	80 (90%)	9 (10%)	7	11
26	LV	102/107 (95%)	102 (100%)	0	100	100
27	LW	54/126 (43%)	53 (98%)	1 (2%)	50	71
28	LX	106/133 (80%)	105 (99%)	1 (1%)	70	85
29	LY	122/135 (90%)	119 (98%)	3 (2%)	42	64
30	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	85
31	La	119/120 (99%)	117 (98%)	2 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Lb	84/125 (67%)	83 (99%)	1 (1%)	63	81
33	Lc	83/97 (86%)	83 (100%)	0	100	100
34	Ld	97/110 (88%)	93 (96%)	4 (4%)	27	46
35	Le	115/121 (95%)	114 (99%)	1 (1%)	70	85
36	Lf	88/89 (99%)	88 (100%)	0	100	100
37	Lg	96/100 (96%)	96 (100%)	0	100	100
38	Lh	109/110 (99%)	109 (100%)	0	100	100
39	Li	86/89 (97%)	84 (98%)	2 (2%)	44	66
40	Lj	73/80 (91%)	73 (100%)	0	100	100
41	Lk	63/65 (97%)	62 (98%)	1 (2%)	55	76
42	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	44
43	Lm	47/115 (41%)	47 (100%)	0	100	100
44	Ln	24/24 (100%)	24 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	73/75 (97%)	73 (100%)	0	100	100
47	Lr	109/121 (90%)	108 (99%)	1 (1%)	70	85
51	SA	178/243 (73%)	174 (98%)	4 (2%)	45	67
52	SB	182/231 (79%)	178 (98%)	4 (2%)	45	67
53	SC	184/225 (82%)	178 (97%)	6 (3%)	33	55
54	SD	184/202 (91%)	172 (94%)	12 (6%)	15	27
55	SE	220/225 (98%)	217 (99%)	3 (1%)	59	79
56	SF	151/170 (89%)	144 (95%)	7 (5%)	24	41
57	SG	178/218 (82%)	173 (97%)	5 (3%)	38	60
58	SH	146/174 (84%)	143 (98%)	3 (2%)	47	69
59	SI	175/180 (97%)	169 (97%)	6 (3%)	32	54
60	SJ	147/168 (88%)	145 (99%)	2 (1%)	59	79
61	SK	86/136 (63%)	84 (98%)	2 (2%)	44	66
62	SL	128/142 (90%)	127 (99%)	1 (1%)	73	86
63	SM	51/108 (47%)	48 (94%)	3 (6%)	18	31
64	SN	130/131 (99%)	127 (98%)	3 (2%)	44	66
65	SO	81/119 (68%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	SP	112/130 (86%)	110 (98%)	2 (2%)	51	73
67	SQ	116/121 (96%)	112 (97%)	4 (3%)	32	54
68	SR	115/122 (94%)	108 (94%)	7 (6%)	17	30
69	SS	128/132 (97%)	125 (98%)	3 (2%)	44	66
70	ST	112/115 (97%)	108 (96%)	4 (4%)	31	52
71	SU	88/107 (82%)	81 (92%)	7 (8%)	11	19
72	SV	67/67 (100%)	66 (98%)	1 (2%)	57	77
73	SW	112/113 (99%)	109 (97%)	3 (3%)	39	62
74	SX	111/114 (97%)	106 (96%)	5 (4%)	24	42
75	SY	106/115 (92%)	100 (94%)	6 (6%)	18	33
76	SZ	73/103 (71%)	68 (93%)	5 (7%)	14	25
77	Sa	86/98 (88%)	82 (95%)	4 (5%)	23	41
78	Sb	68/76 (90%)	64 (94%)	4 (6%)	18	31
79	Sc	56/62 (90%)	52 (93%)	4 (7%)	13	23
80	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	69
81	Se	43/104 (41%)	42 (98%)	1 (2%)	44	66
82	Sf	35/140 (25%)	33 (94%)	2 (6%)	18	33
83	Sg	241/275 (88%)	209 (87%)	32 (13%)	4	5
All	All	9450/10850 (87%)	9223 (98%)	227 (2%)	43	65

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	SI	46	VAL
83	Sg	256	ILE
68	SR	103	LYS
83	Sg	229	THR
83	Sg	86	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
51	SA	141	ASN
65	SO	103	ASN
52	SB	118	GLN

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Mol	Chain	Res	Type
60	SJ	113	GLN
70	ST	63	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	At	66/77 (85%)	20 (30%)	0
2	Et	48/75 (64%)	9 (18%)	0
3	L5	3370/5069 (66%)	394 (11%)	9 (0%)
4	L7	118/120 (98%)	7 (5%)	0
48	Mr	6/7 (85%)	1 (16%)	0
49	Pt	66/76 (86%)	7 (10%)	0
5	L8	146/156 (93%)	12 (8%)	0
50	S2	1539/1869 (82%)	200 (12%)	2 (0%)
All	All	5359/7449 (71%)	650 (12%)	11 (0%)

5 of 650 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	At	2	G
1	At	5	G
1	At	8	U
1	At	9	A
1	At	11	U

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4699	U
3	L5	4913	G
50	S2	1344	A
50	S2	918	PSU
3	L5	1633	G

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

228 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
50	PSU	S2	119	50	18,21,22	4.50	8 (44%)	22,30,33	1.64	3 (13%)
3	PSU	L5	3768	3	18,21,22	4.49	7 (38%)	22,30,33	1.75	5 (22%)
50	PSU	S2	573	50	18,21,22	4.51	8 (44%)	22,30,33	1.71	5 (22%)
3	PSU	L5	4296	3	18,21,22	4.46	7 (38%)	22,30,33	1.78	5 (22%)
3	A2M	L5	3723	3	22,25,26	3.43	9 (40%)	31,36,39	2.37	10 (32%)
3	OMG	L5	4637	87,3	23,26,27	2.40	9 (39%)	33,38,41	2.47	11 (33%)
50	A2M	S2	99	86,50	22,25,26	3.43	10 (45%)	31,36,39	2.36	12 (38%)
50	OMC	S2	462	50	19,22,23	3.01	8 (42%)	26,31,34	0.71	0
3	PSU	L5	3764	87,3	18,21,22	4.49	7 (38%)	22,30,33	1.76	5 (22%)
3	A2M	L5	3825	3	22,25,26	3.44	9 (40%)	31,36,39	2.35	10 (32%)
50	PSU	S2	105	50	18,21,22	4.48	7 (38%)	22,30,33	1.82	5 (22%)
50	OMG	S2	1328	50	23,26,27	0.30	0	33,38,41	0.37	0
3	OMC	L5	2861	3	19,22,23	3.00	8 (42%)	26,31,34	0.76	0
50	PSU	S2	651	50	18,21,22	4.50	7 (38%)	22,30,33	1.80	5 (22%)
3	PSU	L5	4552	3	18,21,22	4.44	7 (38%)	22,30,33	1.73	5 (22%)
3	OMC	L5	2824	3	19,22,23	2.97	8 (42%)	26,31,34	0.78	0
3	OMU	L5	3925	3	19,22,23	3.03	8 (42%)	26,31,34	1.74	5 (19%)
50	PSU	S2	572	50	18,21,22	4.49	8 (44%)	22,30,33	1.66	4 (18%)
50	OMU	S2	121	50	19,22,23	3.04	8 (42%)	26,31,34	1.70	5 (19%)
3	PSU	L5	4636	3	18,21,22	4.48	8 (44%)	22,30,33	1.79	6 (27%)
50	OMC	S2	517	50	19,22,23	2.99	8 (42%)	26,31,34	0.74	0
3	PSU	L5	3920	3,86	18,21,22	4.43	7 (38%)	22,30,33	1.80	5 (22%)
50	OMG	S2	683	50	23,26,27	2.45	9 (39%)	33,38,41	2.56	10 (30%)
3	OMC	L5	4536	3	19,22,23	2.97	8 (42%)	26,31,34	0.77	0
3	A2M	L5	3830	3	22,25,26	3.41	8 (36%)	31,36,39	2.41	11 (35%)
50	OMU	S2	1804	50	19,22,23	3.07	8 (42%)	26,31,34	1.71	4 (15%)
50	PSU	S2	866	50	18,21,22	4.55	7 (38%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4442	3	18,21,22	4.48	7 (38%)	22,30,33	1.82	6 (27%)
3	OMG	L5	4623	3	23,26,27	2.38	9 (39%)	33,38,41	2.39	11 (33%)
50	PSU	S2	681	50	18,21,22	4.45	7 (38%)	22,30,33	1.77	5 (22%)
50	PSU	S2	1243	50	18,21,22	4.50	7 (38%)	22,30,33	1.71	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	MA6	S2	1850	50	23,26,27	1.41	4 (17%)	34,38,41	2.95	12 (35%)
74	HY3	SX	62	87,74	6,8,9	1.23	0	5,10,12	2.06	2 (40%)
3	PSU	L5	4689	3	18,21,22	4.44	7 (38%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3637	87,3	18,21,22	4.45	7 (38%)	22,30,33	1.82	4 (18%)
3	OMC	L5	3841	3	19,22,23	2.95	8 (42%)	26,31,34	0.71	0
50	MA6	S2	1851	50	23,26,27	1.40	5 (21%)	34,38,41	3.07	13 (38%)
50	A2M	S2	576	50	22,25,26	3.40	9 (40%)	31,36,39	2.40	12 (38%)
5	PSU	L8	55	5	18,21,22	4.46	7 (38%)	22,30,33	1.75	5 (22%)
50	PSU	S2	1232	50	18,21,22	4.52	7 (38%)	22,30,33	1.78	5 (22%)
45	MLZ	Lo	53	45	8,9,10	0.73	0	4,9,11	0.58	0
3	A2M	L5	3718	3	22,25,26	3.42	9 (40%)	31,36,39	2.25	11 (35%)
50	PSU	S2	1136	50	18,21,22	4.50	7 (38%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4521	3,86	18,21,22	4.48	7 (38%)	22,30,33	1.85	6 (27%)
50	PSU	S2	686	50	18,21,22	4.56	7 (38%)	22,30,33	1.82	5 (22%)
50	PSU	S2	1174	50	18,21,22	4.47	7 (38%)	22,30,33	1.71	5 (22%)
50	OMC	S2	1391	50	19,22,23	2.98	8 (42%)	26,31,34	0.69	0
50	A2M	S2	1031	50	22,25,26	3.42	9 (40%)	31,36,39	2.36	10 (32%)
50	A2M	S2	668	86,50	22,25,26	3.40	10 (45%)	31,36,39	2.40	11 (35%)
31	V5N	La	39	31	9,11,12	2.62	2 (22%)	9,14,16	1.30	1 (11%)
3	PSU	L5	1782	3	18,21,22	4.47	7 (38%)	22,30,33	1.82	5 (22%)
3	OMG	L5	3792	3	23,26,27	2.39	9 (39%)	33,38,41	2.48	10 (30%)
50	PSU	S2	1056	50	18,21,22	4.46	7 (38%)	22,30,33	1.82	5 (22%)
50	OMG	S2	867	50	23,26,27	2.44	9 (39%)	33,38,41	2.60	10 (30%)
3	PSU	L5	4312	3	18,21,22	4.49	7 (38%)	22,30,33	1.74	5 (22%)
3	PSU	L5	1792	3	18,21,22	4.47	7 (38%)	22,30,33	1.75	5 (22%)
3	OMC	L5	2351	3	19,22,23	2.96	8 (42%)	26,31,34	0.79	0
3	PSU	L5	2843	3	18,21,22	4.48	7 (38%)	22,30,33	1.77	4 (18%)
3	PSU	L5	3734	3	18,21,22	4.52	7 (38%)	22,30,33	1.82	6 (27%)
3	OMG	L5	4494	3	23,26,27	2.38	9 (39%)	33,38,41	2.45	11 (33%)
3	PSU	L5	4532	3	18,21,22	4.47	7 (38%)	22,30,33	1.75	5 (22%)
7	HIC	LB	245	7	10,11,12	1.52	1 (10%)	8,14,16	1.03	0
3	PSU	L5	1781	3	18,21,22	4.49	7 (38%)	22,30,33	1.71	5 (22%)
3	PSU	L5	4576	3	18,21,22	4.47	7 (38%)	22,30,33	1.81	5 (22%)
3	OMU	L5	4306	3	19,22,23	3.01	8 (42%)	26,31,34	1.69	5 (19%)
3	OMU	L5	4620	3	19,22,23	2.99	8 (42%)	26,31,34	1.62	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	PSU	S2	1445	50	18,21,22	4.52	7 (38%)	22,30,33	1.82	6 (27%)
50	A2M	S2	512	50	22,25,26	3.41	9 (40%)	31,36,39	2.43	11 (35%)
3	PSU	L5	3844	3	18,21,22	4.45	7 (38%)	22,30,33	1.70	4 (18%)
50	OMG	S2	644	50	23,26,27	2.41	9 (39%)	33,38,41	2.51	10 (30%)
3	OMC	L5	2365	3	19,22,23	2.96	8 (42%)	26,31,34	0.71	0
3	UY1	L5	3818	87,3	19,22,23	0.18	0	22,31,34	0.40	0
3	PSU	L5	4361	3	18,21,22	4.45	7 (38%)	22,30,33	1.74	5 (22%)
43	M3L	Lm	98	43	10,11,12	0.51	0	9,14,16	0.48	0
3	OMG	L5	4196	3,49	23,26,27	2.41	9 (39%)	33,38,41	2.55	10 (30%)
3	OMC	L5	1881	3,86	19,22,23	2.96	8 (42%)	26,31,34	0.79	0
3	PSU	L5	4403	3	18,21,22	4.41	7 (38%)	22,30,33	1.89	6 (27%)
3	PSU	L5	4471	3	18,21,22	4.46	7 (38%)	22,30,33	1.71	5 (22%)
3	A2M	L5	4523	3,86	22,25,26	3.40	8 (36%)	31,36,39	2.42	11 (35%)
3	OMC	L5	3887	3	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
5	PSU	L8	69	5	18,21,22	4.51	8 (44%)	22,30,33	1.86	6 (27%)
50	OMC	S2	174	50	19,22,23	3.02	8 (42%)	26,31,34	0.74	0
50	OMU	S2	428	50	19,22,23	3.04	8 (42%)	26,31,34	1.77	5 (19%)
50	PSU	S2	918	50	18,21,22	4.56	8 (44%)	22,30,33	1.89	5 (22%)
3	OMG	L5	3744	3	23,26,27	2.39	9 (39%)	33,38,41	2.47	11 (33%)
50	OMU	S2	627	50	19,22,23	0.26	0	26,31,34	0.45	0
50	PSU	S2	609	50	18,21,22	4.52	7 (38%)	22,30,33	1.81	5 (22%)
3	PSU	L5	2508	3	18,21,22	4.49	7 (38%)	22,30,33	1.73	5 (22%)
3	OMU	L5	4227	3	19,22,23	3.07	8 (42%)	26,31,34	1.76	4 (15%)
50	PSU	S2	649	50	18,21,22	4.48	7 (38%)	22,30,33	1.81	5 (22%)
3	PSU	L5	3851	3	18,21,22	4.45	7 (38%)	22,30,33	1.79	6 (27%)
50	PSU	S2	1244	50	18,21,22	4.49	7 (38%)	22,30,33	1.76	5 (22%)
50	A2M	S2	27	50	22,25,26	3.40	9 (40%)	31,36,39	2.40	11 (35%)
3	OMG	L5	3627	3	23,26,27	2.39	9 (39%)	33,38,41	2.37	13 (39%)
50	PSU	S2	815	50	18,21,22	4.51	7 (38%)	22,30,33	1.77	5 (22%)
50	A2M	S2	468	50	22,25,26	3.43	8 (36%)	31,36,39	2.40	12 (38%)
3	OMC	L5	1340	3	19,22,23	2.92	8 (42%)	26,31,34	0.70	0
50	G7M	S2	1639	50,49	23,26,27	2.62	8 (34%)	35,39,42	2.56	11 (31%)
50	A2M	S2	1383	50	22,25,26	3.42	8 (36%)	31,36,39	2.44	11 (35%)
3	PSU	L5	4293	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
3	PSU	L5	4972	3	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	PSU	S2	296	50	18,21,22	4.52	7 (38%)	22,30,33	1.79	5 (22%)
3	PSU	L5	1744	87,3	18,21,22	4.46	7 (38%)	22,30,33	1.80	5 (22%)
49	M2G	Pt	26	49	24,27,28	0.55	0	35,40,43	0.75	1 (2%)
3	OMC	L5	2422	3,86	19,22,23	2.98	8 (42%)	26,31,34	0.76	0
3	A2M	L5	3785	3	22,25,26	3.36	9 (40%)	31,36,39	2.51	12 (38%)
3	OMU	L5	2837	3	19,22,23	3.01	8 (42%)	26,31,34	1.74	5 (19%)
50	PSU	S2	218	50	18,21,22	4.50	7 (38%)	22,30,33	1.71	4 (18%)
3	OMG	L5	4228	3	23,26,27	2.37	9 (39%)	33,38,41	2.36	12 (36%)
50	4AC	S2	1337	50	21,24,25	3.43	10 (47%)	29,34,37	1.02	2 (6%)
3	A2M	L5	2787	3	22,25,26	3.41	10 (45%)	31,36,39	2.37	11 (35%)
3	PSU	L5	4299	3	18,21,22	4.50	7 (38%)	22,30,33	1.79	5 (22%)
50	PSU	S2	1643	50	18,21,22	4.52	7 (38%)	22,30,33	1.81	6 (27%)
3	OMU	L5	4498	3	19,22,23	3.04	8 (42%)	26,31,34	1.72	5 (19%)
50	OMU	S2	354	50	19,22,23	3.03	8 (42%)	26,31,34	1.75	5 (19%)
50	PSU	S2	863	50	18,21,22	4.53	7 (38%)	22,30,33	1.81	5 (22%)
3	OMG	L5	2876	3	23,26,27	2.41	9 (39%)	33,38,41	2.65	10 (30%)
3	A2M	L5	2363	3,86	22,25,26	3.43	9 (40%)	31,36,39	2.34	10 (32%)
3	PSU	L5	4420	3	18,21,22	4.49	9 (50%)	22,30,33	1.69	4 (18%)
3	OMC	L5	4456	3	19,22,23	2.98	8 (42%)	26,31,34	0.75	0
3	PSU	L5	3729	3	18,21,22	4.49	7 (38%)	22,30,33	1.70	5 (22%)
1	MA7	At	58	1	20,24,25	0.54	0	24,35,38	0.75	0
3	PSU	L5	4431	3	18,21,22	4.47	7 (38%)	22,30,33	1.79	5 (22%)
50	PSU	S2	109	50	18,21,22	4.49	7 (38%)	22,30,33	1.80	5 (22%)
50	PSU	S2	966	50	18,21,22	4.53	7 (38%)	22,30,33	1.85	5 (22%)
50	OMU	S2	1442	50	19,22,23	3.08	8 (42%)	26,31,34	1.66	4 (15%)
50	4AC	S2	1842	50	21,24,25	3.45	9 (42%)	29,34,37	1.06	3 (10%)
3	OMG	L5	3944	3	23,26,27	2.44	9 (39%)	33,38,41	2.54	10 (30%)
50	PSU	S2	1692	50	18,21,22	4.47	7 (38%)	22,30,33	1.78	5 (22%)
3	A2M	L5	1871	3,86	22,25,26	3.44	9 (40%)	31,36,39	2.39	11 (35%)
3	A2M	L5	1326	3	22,25,26	3.43	9 (40%)	31,36,39	2.36	10 (32%)
3	PSU	L5	1862	3	18,21,22	4.50	7 (38%)	22,30,33	1.79	5 (22%)
50	A2M	S2	590	50	22,25,26	3.40	9 (40%)	31,36,39	2.47	12 (38%)
3	PSU	L5	1860	3	18,21,22	4.43	7 (38%)	22,30,33	1.79	5 (22%)
50	OMU	S2	172	50	19,22,23	3.06	8 (42%)	26,31,34	1.74	5 (19%)
3	A2M	L5	398	3	22,25,26	3.41	9 (40%)	31,36,39	2.35	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3899	3,86	23,26,27	2.37	9 (39%)	33,38,41	2.37	13 (39%)
3	A2M	L5	4590	3	22,25,26	3.42	9 (40%)	31,36,39	2.40	10 (32%)
3	PSU	L5	3695	87,3	18,21,22	4.49	7 (38%)	22,30,33	1.90	6 (27%)
50	PSU	S2	822	50	18,21,22	4.55	8 (44%)	22,30,33	1.79	6 (27%)
50	PSU	S2	406	50	18,21,22	4.50	7 (38%)	22,30,33	1.84	5 (22%)
3	A2M	L5	3760	3	22,25,26	0.20	0	31,36,39	0.58	0
3	6MZ	L5	4220	3	22,25,26	2.50	4 (18%)	30,36,39	2.24	9 (30%)
50	PSU	S2	801	50	18,21,22	4.53	7 (38%)	22,30,33	1.82	5 (22%)
3	OMG	L5	4392	3	23,26,27	2.35	9 (39%)	33,38,41	2.36	10 (30%)
6	V5N	LA	216	6	9,11,12	2.61	2 (22%)	9,14,16	1.23	0
50	PSU	S2	1367	50	18,21,22	4.55	7 (38%)	22,30,33	1.85	5 (22%)
3	PSU	L5	3884	3	18,21,22	4.46	7 (38%)	22,30,33	1.79	5 (22%)
3	5MC	L5	4447	3	18,22,23	3.54	7 (38%)	26,32,35	1.07	1 (3%)
3	PSU	L5	5001	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
3	UR3	L5	4530	87,3	19,22,23	2.75	8 (42%)	26,32,35	1.31	2 (7%)
3	PSU	L5	3762	3	18,21,22	4.48	7 (38%)	22,30,33	1.79	5 (22%)
50	OMG	S2	601	50	23,26,27	2.37	9 (39%)	33,38,41	2.48	11 (33%)
3	PSU	L5	4500	3	18,21,22	4.49	7 (38%)	22,30,33	1.87	5 (22%)
3	PSU	L5	1582	3	18,21,22	4.45	7 (38%)	22,30,33	1.74	5 (22%)
3	OMG	L5	2424	3	23,26,27	2.43	8 (34%)	33,38,41	2.58	9 (27%)
50	OMG	S2	1447	50	23,26,27	2.45	9 (39%)	33,38,41	2.58	10 (30%)
50	PSU	S2	1238	50	18,21,22	4.52	7 (38%)	22,30,33	1.85	5 (22%)
50	PSU	S2	814	50	18,21,22	4.47	7 (38%)	22,30,33	1.73	4 (18%)
3	OMG	L5	2364	3	23,26,27	2.35	9 (39%)	33,38,41	2.39	12 (36%)
3	OMG	L5	4499	1,3	23,26,27	2.40	9 (39%)	33,38,41	2.46	10 (30%)
49	1MA	Pt	58	49	21,25,26	0.37	0	31,37,40	0.68	0
3	PSU	L5	2632	3	18,21,22	4.50	7 (38%)	22,30,33	1.74	5 (22%)
3	OMC	L5	2804	3	19,22,23	2.98	8 (42%)	26,31,34	0.70	0
3	A2M	L5	2815	3	22,25,26	3.41	10 (45%)	31,36,39	2.40	10 (32%)
50	A2M	S2	166	50	22,25,26	3.44	9 (40%)	31,36,39	2.43	11 (35%)
50	B8N	S2	1248	50	24,29,30	3.15	8 (33%)	29,42,45	1.73	5 (17%)
3	PSU	L5	4423	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
50	OMG	S2	1490	86,50	23,26,27	2.38	9 (39%)	33,38,41	2.39	11 (33%)
3	PSU	L5	4628	3	18,21,22	4.50	7 (38%)	22,30,33	1.88	5 (22%)
50	PSU	S2	93	50	18,21,22	4.52	7 (38%)	22,30,33	1.68	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3770	3	18,21,22	4.48	7 (38%)	22,30,33	1.80	5 (22%)
3	A2M	L5	3867	3	22,25,26	3.44	10 (45%)	31,36,39	2.37	11 (35%)
3	PSU	L5	3853	3,86	18,21,22	4.45	7 (38%)	22,30,33	1.79	5 (22%)
50	PSU	S2	1081	50	18,21,22	0.93	1 (5%)	22,30,33	0.89	1 (4%)
3	PSU	L5	2839	3	18,21,22	4.48	7 (38%)	22,30,33	1.75	5 (22%)
50	PSU	S2	1004	50	18,21,22	4.54	7 (38%)	22,30,33	1.77	5 (22%)
3	OMG	L5	1522	3	23,26,27	2.38	9 (39%)	33,38,41	2.40	11 (33%)
3	5MC	L5	3782	3,86	18,22,23	3.51	7 (38%)	26,32,35	1.04	2 (7%)
3	PSU	L5	4457	3	18,21,22	4.46	7 (38%)	22,30,33	1.74	5 (22%)
3	PSU	L5	4493	3	18,21,22	4.47	7 (38%)	22,30,33	1.75	5 (22%)
50	OMG	S2	436	50	23,26,27	2.41	9 (39%)	33,38,41	2.47	12 (36%)
50	A2M	S2	159	50	22,25,26	3.43	9 (40%)	31,36,39	2.36	10 (32%)
3	OMC	L5	3808	3	19,22,23	2.93	8 (42%)	26,31,34	0.73	0
3	OMG	L5	4618	3	23,26,27	2.38	9 (39%)	33,38,41	2.39	13 (39%)
50	UY1	S2	1326	50	19,22,23	0.17	0	22,31,34	0.31	0
50	PSU	S2	1239	50	18,21,22	4.53	7 (38%)	22,30,33	1.77	5 (22%)
3	A2M	L5	400	3	22,25,26	3.43	9 (40%)	31,36,39	2.36	10 (32%)
50	PSU	S2	1625	50	18,21,22	4.55	7 (38%)	22,30,33	1.75	5 (22%)
3	PSU	L5	4673	3	18,21,22	4.46	7 (38%)	22,30,33	1.76	5 (22%)
50	PSU	S2	1347	50	18,21,22	4.51	7 (38%)	22,30,33	1.80	5 (22%)
32	MLZ	Lb	5	32	8,9,10	0.76	0	4,9,11	0.61	0
3	OMC	L5	3701	87,3	19,22,23	2.95	8 (42%)	26,31,34	0.73	0
3	PSU	L5	5010	3	18,21,22	4.48	7 (38%)	22,30,33	1.83	4 (18%)
50	OMC	S2	1703	50	19,22,23	0.30	0	26,31,34	0.49	0
50	OMU	S2	116	50	19,22,23	3.02	8 (42%)	26,31,34	1.67	4 (15%)
3	A2M	L5	1534	3,86	22,25,26	3.42	9 (40%)	31,36,39	2.36	11 (35%)
3	PSU	L5	4353	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
50	A2M	S2	484	50	22,25,26	3.38	9 (40%)	31,36,39	2.39	10 (32%)
3	A2M	L5	1524	3	22,25,26	3.41	9 (40%)	31,36,39	2.43	12 (38%)
5	OMU	L8	14	5,3	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
50	PSU	S2	34	50	18,21,22	4.52	7 (38%)	22,30,33	1.79	5 (22%)
3	OMU	L5	2415	3	19,22,23	3.05	8 (42%)	26,31,34	1.70	5 (19%)
3	PSU	L5	3639	3	18,21,22	4.47	7 (38%)	22,30,33	1.81	6 (27%)
3	PSU	L5	4569	3	18,21,22	4.48	7 (38%)	22,30,33	1.72	5 (22%)
3	1MA	L5	1322	3,86	21,25,26	2.89	6 (28%)	31,37,40	2.90	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	1316	3	23,26,27	2.40	9 (39%)	33,38,41	2.42	11 (33%)
3	OMC	L5	3869	3	19,22,23	2.96	8 (42%)	26,31,34	0.74	0
49	1MG	Pt	37	49	22,26,27	0.54	0	33,39,42	0.71	1 (3%)
50	PSU	S2	36	50	18,21,22	4.51	7 (38%)	22,30,33	1.79	5 (22%)
3	A2M	L5	3724	3	22,25,26	3.44	9 (40%)	31,36,39	2.35	10 (32%)
3	PSU	L5	4579	3	18,21,22	4.44	7 (38%)	22,30,33	1.76	5 (22%)
50	OMU	S2	1288	50	19,22,23	3.08	8 (42%)	26,31,34	1.62	5 (19%)
3	PSU	L5	1536	3	18,21,22	4.45	7 (38%)	22,30,33	1.81	5 (22%)
3	PSU	L5	1779	3	18,21,22	4.50	7 (38%)	22,30,33	1.78	5 (22%)
3	PSU	L5	3758	3	18,21,22	4.52	7 (38%)	22,30,33	1.81	5 (22%)
49	1MG	Pt	9	49	22,26,27	0.60	0	33,39,42	0.73	1 (3%)
50	6MZ	S2	1832	86,50	22,25,26	0.14	0	30,36,39	0.40	0
3	A2M	L5	4571	3	22,25,26	3.46	9 (40%)	31,36,39	2.37	11 (35%)
3	PSU	L5	1677	3	18,21,22	4.54	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	L5	1683	87,3	18,21,22	4.50	7 (38%)	22,30,33	1.75	5 (22%)
3	OMG	L5	1625	87,3	23,26,27	2.39	9 (39%)	33,38,41	2.50	10 (30%)
3	OMG	L5	4370	3	23,26,27	2.38	9 (39%)	33,38,41	2.46	10 (30%)
3	A2M	L5	2401	3	22,25,26	3.40	9 (40%)	31,36,39	2.34	9 (29%)
50	OMG	S2	509	50	23,26,27	2.40	9 (39%)	33,38,41	2.51	10 (30%)
50	A2M	S2	1678	50	22,25,26	3.46	9 (40%)	31,36,39	2.43	11 (35%)
5	OMG	L8	75	5	23,26,27	2.39	9 (39%)	33,38,41	2.44	12 (36%)
50	PSU	S2	1177	50	18,21,22	4.50	7 (38%)	22,30,33	1.83	5 (22%)

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
50	PSU	S2	119	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	573	50	-	2/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4637	87,3	-	3/9/27/28	0/3/3/3
50	A2M	S2	99	86,50	-	2/9/27/28	0/3/3/3
50	OMC	S2	462	50	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3764	87,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	105	50	-	0/7/25/26	0/2/2/2
50	OMG	S2	1328	50	-	1/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	651	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	572	50	-	2/7/25/26	0/2/2/2
50	OMU	S2	121	50	-	0/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
50	OMC	S2	517	50	-	0/9/27/28	0/2/2/2
3	PSU	L5	3920	3,86	-	0/7/25/26	0/2/2/2
50	OMG	S2	683	50	-	2/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
50	OMU	S2	1804	50	-	1/9/27/28	0/2/2/2
50	PSU	S2	866	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	681	50	-	0/7/25/26	0/2/2/2
50	PSU	S2	1243	50	-	5/7/25/26	0/2/2/2
50	MA6	S2	1850	50	-	0/11/29/30	0/3/3/3
74	HY3	SX	62	87,74	-	1/1/12/14	0/1/1/1
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	87,3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
50	MA6	S2	1851	50	-	3/11/29/30	0/3/3/3
50	A2M	S2	576	50	-	2/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
50	PSU	S2	1232	50	-	0/7/25/26	0/2/2/2
45	MLZ	Lo	53	45	-	0/7/8/10	-
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	1136	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	3,86	-	0/7/25/26	0/2/2/2
50	PSU	S2	686	50	-	0/7/25/26	0/2/2/2
50	PSU	S2	1174	50	-	0/7/25/26	0/2/2/2
50	OMC	S2	1391	50	-	0/9/27/28	0/2/2/2
50	A2M	S2	1031	50	-	0/9/27/28	0/3/3/3
50	A2M	S2	668	86,50	-	5/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	V5N	La	39	31	-	1/9/10/12	0/1/1/1
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	1056	50	-	0/7/25/26	0/2/2/2
50	OMG	S2	867	50	-	1/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	2/7/25/26	0/2/2/2
7	HIC	LB	245	7	-	0/5/6/8	0/1/1/1
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	1445	50	-	0/7/25/26	0/2/2/2
50	A2M	S2	512	50	-	2/9/27/28	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
50	OMG	S2	644	50	-	4/9/27/28	0/3/3/3
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	UY1	L5	3818	87,3	-	4/9/27/28	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
43	M3L	Lm	98	43	-	2/9/10/12	-
3	OMG	L5	4196	3,49	-	0/9/27/28	0/3/3/3
3	OMC	L5	1881	3,86	-	0/9/27/28	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,86	-	0/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
50	OMC	S2	174	50	-	0/9/27/28	0/2/2/2
50	OMU	S2	428	50	-	6/9/27/28	0/2/2/2
50	PSU	S2	918	50	-	2/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
50	OMU	S2	627	50	-	0/9/27/28	0/2/2/2
50	PSU	S2	609	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PSU	S2	649	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	2/7/25/26	0/2/2/2
50	PSU	S2	1244	50	-	0/7/25/26	0/2/2/2
50	A2M	S2	27	50	-	1/9/27/28	0/3/3/3
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	815	50	-	0/7/25/26	0/2/2/2
50	A2M	S2	468	50	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
50	G7M	S2	1639	50,49	-	0/7/25/26	0/3/3/3
50	A2M	S2	1383	50	-	2/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	296	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
49	M2G	Pt	26	49	-	0/11/29/30	0/3/3/3
3	OMC	L5	2422	3,86	-	2/9/27/28	0/2/2/2
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	218	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
50	4AC	S2	1337	50	-	0/11/29/30	0/2/2/2
3	A2M	L5	2787	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	1643	50	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
50	OMU	S2	354	50	-	0/9/27/28	0/2/2/2
50	PSU	S2	863	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	3,86	-	0/9/27/28	0/3/3/3
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
1	MA7	At	58	1	-	1/7/21/22	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	109	50	-	0/7/25/26	0/2/2/2
50	PSU	S2	966	50	-	0/7/25/26	0/2/2/2
50	OMU	S2	1442	50	-	3/9/27/28	0/2/2/2
50	4AC	S2	1842	50	-	0/11/29/30	0/2/2/2
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
50	PSU	S2	1692	50	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	1871	3,86	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
50	A2M	S2	590	50	-	4/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
50	OMU	S2	172	50	-	0/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	3899	3,86	-	0/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3695	87,3	-	0/7/25/26	0/2/2/2
50	PSU	S2	822	50	-	2/7/25/26	0/2/2/2
50	PSU	S2	406	50	-	0/7/25/26	0/2/2/2
3	A2M	L5	3760	3	-	0/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	801	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
6	V5N	LA	216	6	-	1/9/10/12	0/1/1/1
50	PSU	S2	1367	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
50	OMG	S2	601	50	-	1/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
50	OMG	S2	1447	50	-	2/9/27/28	0/3/3/3
50	PSU	S2	1238	50	-	0/7/25/26	0/2/2/2
50	PSU	S2	814	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4499	1,3	-	0/9/27/28	0/3/3/3
49	1MA	Pt	58	49	-	2/7/25/26	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2815	3	-	3/9/27/28	0/3/3/3
50	A2M	S2	166	50	-	0/9/27/28	0/3/3/3
50	B8N	S2	1248	50	-	2/16/34/35	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	OMG	S2	1490	86,50	-	3/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	93	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3853	3,86	-	0/7/25/26	0/2/2/2
50	PSU	S2	1081	50	-	1/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	1004	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	3782	3,86	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
50	OMG	S2	436	50	-	0/9/27/28	0/3/3/3
50	A2M	S2	159	50	-	0/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
50	UY1	S2	1326	50	-	2/9/27/28	0/2/2/2
50	PSU	S2	1239	50	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	1625	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	1347	50	-	0/7/25/26	0/2/2/2
32	MLZ	Lb	5	32	-	2/7/8/10	-
3	OMC	L5	3701	87,3	-	4/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
50	OMC	S2	1703	50	-	0/9/27/28	0/2/2/2
50	OMU	S2	116	50	-	2/9/27/28	0/2/2/2
3	A2M	L5	1534	3,86	-	3/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
50	A2M	S2	484	50	-	0/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
5	OMU	L8	14	5,3	-	1/9/27/28	0/2/2/2
50	PSU	S2	34	50	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	1MA	L5	1322	3,86	-	1/7/25/26	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	1MG	Pt	37	49	-	0/7/25/26	0/3/3/3
50	PSU	S2	36	50	-	0/7/25/26	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
50	OMU	S2	1288	50	-	1/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
49	1MG	Pt	9	49	-	1/7/25/26	0/3/3/3
50	6MZ	S2	1832	86,50	-	1/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	87,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
50	OMG	S2	509	50	-	2/9/27/28	0/3/3/3
50	A2M	S2	1678	50	-	1/9/27/28	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
50	PSU	S2	1177	50	-	0/7/25/26	0/2/2/2

The worst 5 of 1630 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	1625	PSU	C6-C5	11.83	1.49	1.35
50	S2	1232	PSU	C6-C5	11.82	1.49	1.35
50	S2	93	PSU	C6-C5	11.81	1.49	1.35
3	L5	1683	PSU	C6-C5	11.80	1.49	1.35
50	S2	686	PSU	C6-C5	11.77	1.49	1.35

The worst 5 of 1320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	1851	MA6	N1-C6-N6	-11.53	104.48	117.08
50	S2	1850	MA6	N1-C6-N6	-10.70	105.39	117.08
3	L5	1322	1MA	C1'-N9-C8	-9.31	100.21	126.70
3	L5	1322	1MA	C1'-N9-C4	8.98	153.18	126.50
3	L5	2876	OMG	C1'-N9-C8	-8.63	102.14	126.70

There are no chirality outliers.

5 of 155 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	LA	216	V5N	O-C-CA-CB
32	Lb	5	MLZ	N-CA-CB-CG
32	Lb	5	MLZ	C-CA-CB-CG
43	Lm	98	M3L	C-CA-CB-CG
3	L5	398	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

101 monomers are involved in 140 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	S2	573	PSU	1	0
3	L5	3723	A2M	4	0
3	L5	4637	OMG	2	0
50	S2	99	A2M	1	0
50	S2	462	OMC	2	0
50	S2	1328	OMG	1	0
3	L5	2861	OMC	1	0
3	L5	4552	PSU	1	0
3	L5	3925	OMU	1	0
50	S2	683	OMG	1	0
3	L5	4536	OMC	1	0
50	S2	1804	OMU	1	0
50	S2	681	PSU	3	0
50	S2	1850	MA6	1	0
3	L5	4689	PSU	1	0
3	L5	3637	PSU	1	0
3	L5	3841	OMC	1	0
50	S2	576	A2M	3	0
50	S2	1232	PSU	1	0
3	L5	3718	A2M	4	0
50	S2	1136	PSU	1	0
50	S2	1174	PSU	2	0
50	S2	1391	OMC	1	0
50	S2	1031	A2M	1	0
50	S2	867	OMG	2	0
3	L5	2351	OMC	1	0
3	L5	3734	PSU	1	0
3	L5	4532	PSU	1	0
3	L5	4306	OMU	1	0
3	L5	4620	OMU	4	0
50	S2	1445	PSU	1	0
50	S2	512	A2M	2	0
50	S2	644	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4196	OMG	1	0
50	S2	918	PSU	2	0
50	S2	609	PSU	1	0
3	L5	4227	OMU	1	0
50	S2	1244	PSU	1	0
3	L5	3627	OMG	1	0
50	S2	468	A2M	1	0
3	L5	1340	OMC	1	0
50	S2	1639	G7M	1	0
50	S2	1383	A2M	1	0
3	L5	4228	OMG	1	0
50	S2	1337	4AC	1	0
50	S2	1643	PSU	1	0
50	S2	354	OMU	1	0
3	L5	2876	OMG	3	0
3	L5	2363	A2M	1	0
3	L5	4456	OMC	1	0
50	S2	1442	OMU	1	0
50	S2	1842	4AC	1	0
3	L5	3944	OMG	2	0
50	S2	1692	PSU	1	0
3	L5	1871	A2M	1	0
3	L5	1326	A2M	1	0
3	L5	1860	PSU	1	0
3	L5	398	A2M	2	0
3	L5	3760	A2M	1	0
3	L5	4220	6MZ	1	0
50	S2	801	PSU	2	0
3	L5	4392	OMG	3	0
3	L5	3884	PSU	1	0
3	L5	4447	5MC	1	0
3	L5	5001	PSU	2	0
50	S2	601	OMG	2	0
3	L5	2424	OMG	1	0
50	S2	1447	OMG	2	0
3	L5	2364	OMG	1	0
3	L5	4499	OMG	1	0
49	Pt	58	1MA	1	0
3	L5	2815	A2M	1	0
50	S2	166	A2M	2	0
50	S2	1490	OMG	1	0
50	S2	93	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3770	PSU	1	0
3	L5	3867	A2M	2	0
50	S2	1004	PSU	2	0
3	L5	1522	OMG	1	0
3	L5	3782	5MC	1	0
3	L5	4457	PSU	1	0
50	S2	436	OMG	2	0
50	S2	159	A2M	3	0
3	L5	3808	OMC	1	0
3	L5	4618	OMG	2	0
50	S2	1239	PSU	1	0
50	S2	1347	PSU	1	0
50	S2	116	OMU	3	0
50	S2	484	A2M	1	0
3	L5	2415	OMU	3	0
3	L5	3724	A2M	2	0
3	L5	4579	PSU	2	0
50	S2	1288	OMU	2	0
3	L5	1536	PSU	1	0
3	L5	1779	PSU	1	0
49	Pt	9	1MG	1	0
3	L5	4571	A2M	1	0
3	L5	1683	PSU	1	0
3	L5	1625	OMG	1	0
50	S2	1678	A2M	2	0
5	L8	75	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 304 ligands modelled in this entry, 277 are monoatomic - leaving 27 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
84	PUT	S2	1902	-	5,5,5	0.25	0	4,4,4	0.16	0
84	PUT	L5	5101	-	5,5,5	0.24	0	4,4,4	0.17	0
84	PUT	L5	5106	-	5,5,5	0.23	0	4,4,4	0.20	0
85	SPD	L5	5109	-	9,9,9	0.43	0	8,8,8	0.31	0
84	PUT	L5	5103	-	5,5,5	0.24	0	4,4,4	0.19	0
85	SPD	L5	5112	-	9,9,9	0.43	0	8,8,8	0.36	0
85	SPD	L5	5114	-	9,9,9	0.44	0	8,8,8	0.25	0
85	SPD	L5	5120	-	9,9,9	0.43	0	8,8,8	0.30	0
85	SPD	LN	301	-	9,9,9	0.43	0	8,8,8	0.28	0
85	SPD	S2	1905	-	9,9,9	0.43	0	8,8,8	0.29	0
85	SPD	L5	5107	-	9,9,9	0.43	0	8,8,8	0.38	0
85	SPD	L5	5118	-	9,9,9	0.44	0	8,8,8	0.32	0
84	PUT	L5	5104	-	5,5,5	0.24	0	4,4,4	0.18	0
85	SPD	L5	5111	-	9,9,9	0.45	0	8,8,8	0.30	0
85	SPD	L5	5116	-	9,9,9	0.44	0	8,8,8	0.28	0
84	PUT	S2	1901	-	5,5,5	0.23	0	4,4,4	0.16	0
85	SPD	L5	5108	-	9,9,9	0.44	0	8,8,8	0.23	0
85	SPD	L5	5119	-	9,9,9	0.44	0	8,8,8	0.25	0
84	PUT	L5	5102	-	5,5,5	0.24	0	4,4,4	0.17	0
85	SPD	L5	5113	-	9,9,9	0.43	0	8,8,8	0.41	0
85	SPD	S2	1903	-	9,9,9	0.44	0	8,8,8	0.27	0
85	SPD	S2	1904	-	9,9,9	0.15	0	8,8,8	0.09	0
89	HYG	S2	1944	87	35,39,39	0.46	0	43,60,60	1.56	2 (4%)
85	SPD	L5	5110	-	9,9,9	0.43	0	8,8,8	0.27	0
85	SPD	L5	5117	-	9,9,9	0.44	0	8,8,8	0.26	0
85	SPD	L5	5115	-	9,9,9	0.44	0	8,8,8	0.31	0
84	PUT	L5	5105	-	5,5,5	0.24	0	4,4,4	0.17	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
84	PUT	S2	1902	-	-	0/3/3/3	-
84	PUT	L5	5101	-	-	0/3/3/3	-
84	PUT	L5	5106	-	-	0/3/3/3	-
85	SPD	L5	5109	-	-	2/7/7/7	-
84	PUT	L5	5103	-	-	0/3/3/3	-
85	SPD	L5	5112	-	-	1/7/7/7	-
85	SPD	L5	5114	-	-	0/7/7/7	-
85	SPD	L5	5120	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	LN	301	-	-	0/7/7/7	-
85	SPD	S2	1905	-	-	0/7/7/7	-
85	SPD	L5	5107	-	-	0/7/7/7	-
85	SPD	L5	5118	-	-	0/7/7/7	-
84	PUT	L5	5104	-	-	0/3/3/3	-
85	SPD	L5	5111	-	-	0/7/7/7	-
85	SPD	L5	5116	-	-	0/7/7/7	-
84	PUT	S2	1901	-	-	0/3/3/3	-
85	SPD	L5	5108	-	-	0/7/7/7	-
85	SPD	L5	5119	-	-	0/7/7/7	-
84	PUT	L5	5102	-	-	0/3/3/3	-
85	SPD	L5	5113	-	-	0/7/7/7	-
85	SPD	S2	1903	-	-	0/7/7/7	-
85	SPD	S2	1904	-	-	2/7/7/7	-
89	HYG	S2	1944	87	1/1/16/17	6/12/87/87	0/4/4/4
85	SPD	L5	5110	-	-	0/7/7/7	-
85	SPD	L5	5117	-	-	0/7/7/7	-
85	SPD	L5	5115	-	-	0/7/7/7	-
84	PUT	L5	5105	-	-	0/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	S2	1944	HYG	O29-C12-C13	9.08	134.69	110.86
89	S2	1944	HYG	C23-O28-C27	2.36	116.50	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
89	S2	1944	HYG	C12

5 of 11 torsion outliers are listed below:

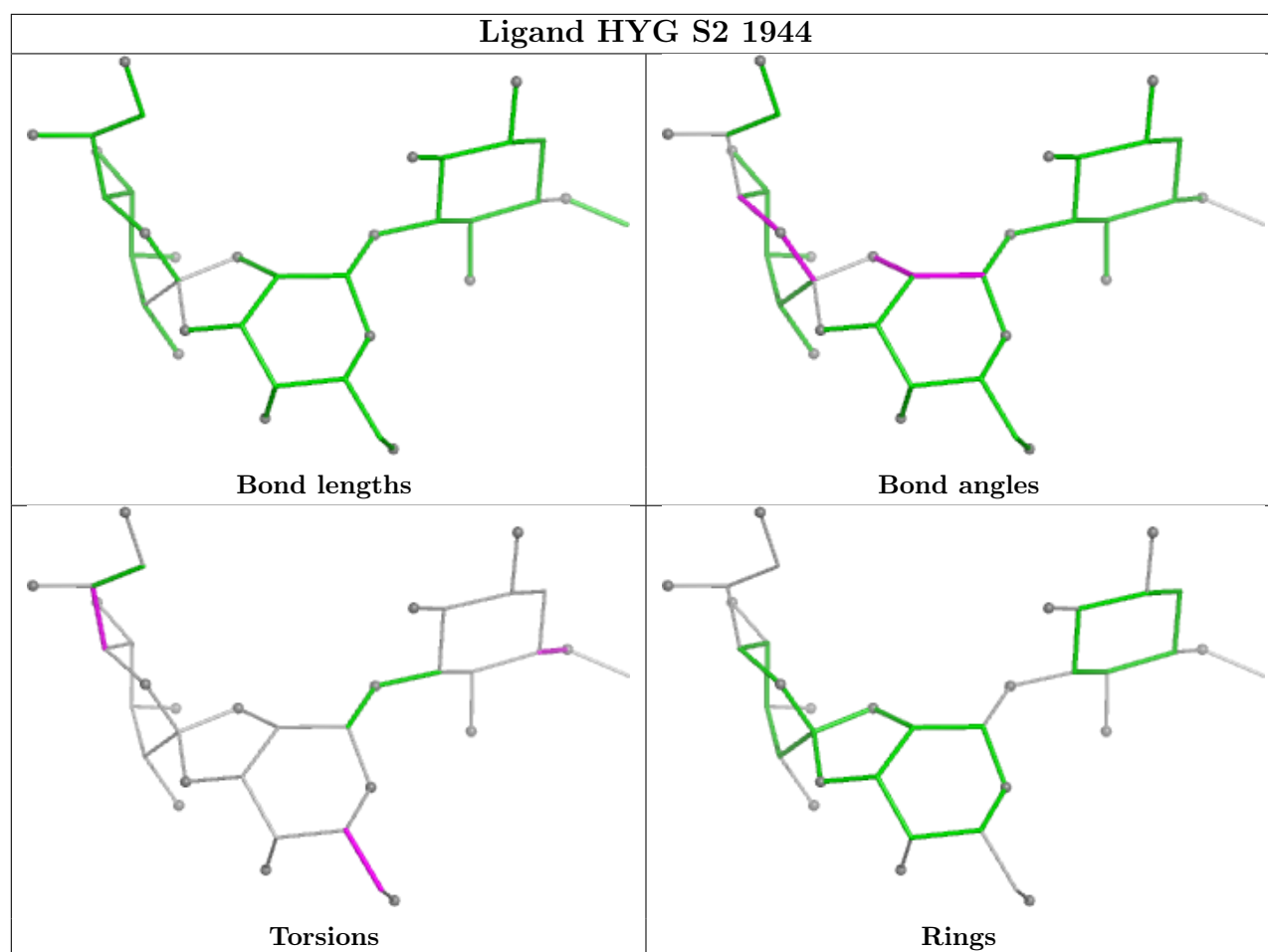
Mol	Chain	Res	Type	Atoms
89	S2	1944	HYG	C5-C4-N9-C10
89	S2	1944	HYG	C26-C27-C33-C34
89	S2	1944	HYG	O28-C27-C33-C34
85	S2	1904	SPD	N6-C7-C8-C9
89	S2	1944	HYG	C16-C15-C19-O20

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	S2	1902	PUT	2	0
84	L5	5106	PUT	1	0
85	L5	5109	SPD	1	0
85	L5	5112	SPD	2	0
85	L5	5120	SPD	1	0
85	L5	5111	SPD	1	0
84	S2	1901	PUT	1	0
84	L5	5102	PUT	1	0
85	L5	5113	SPD	1	0
89	S2	1944	HYG	1	0
85	L5	5110	SPD	1	0
85	L5	5117	SPD	1	0
85	L5	5115	SPD	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

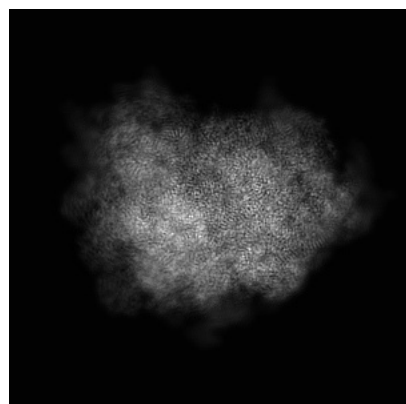
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55091. These allow visual inspection of the internal detail of the map and identification of artifacts.

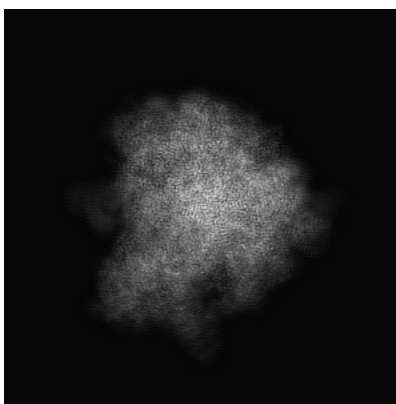
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

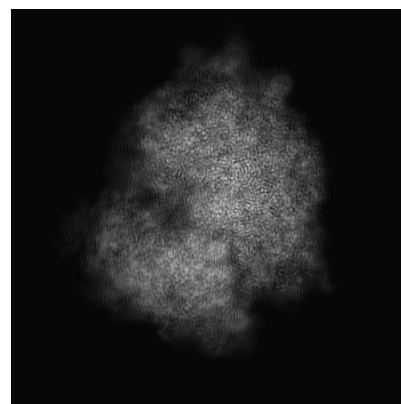
6.1.1 Primary map



X

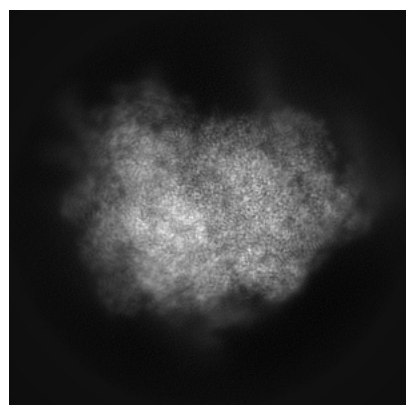


Y

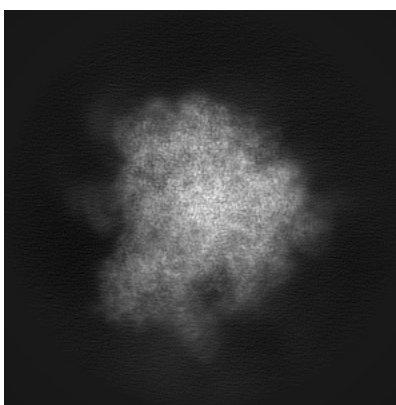


Z

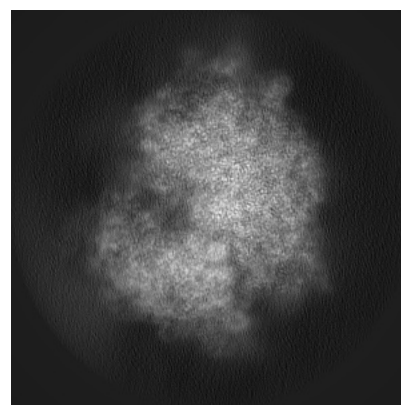
6.1.2 Raw map



X



Y

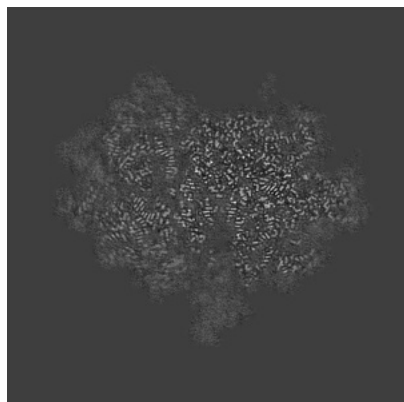


Z

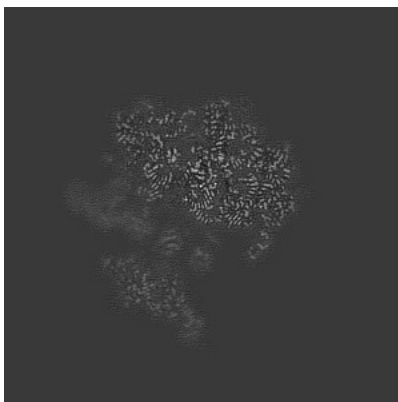
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

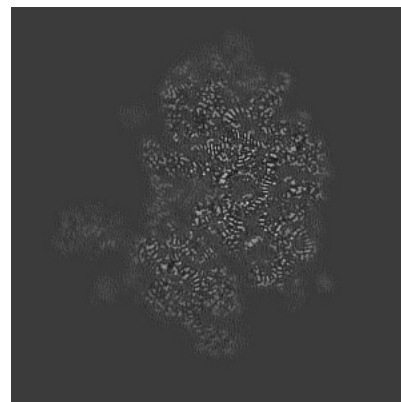
6.2.1 Primary map



X Index: 240

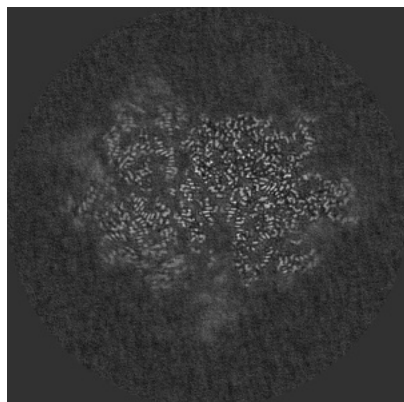


Y Index: 240

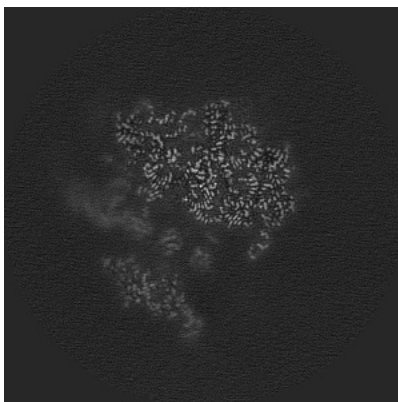


Z Index: 240

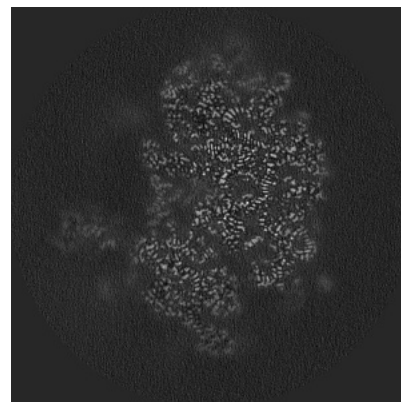
6.2.2 Raw map



X Index: 240



Y Index: 240

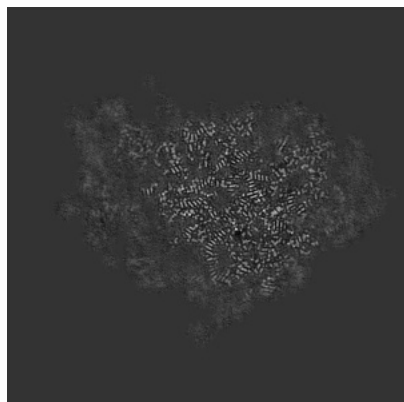


Z Index: 240

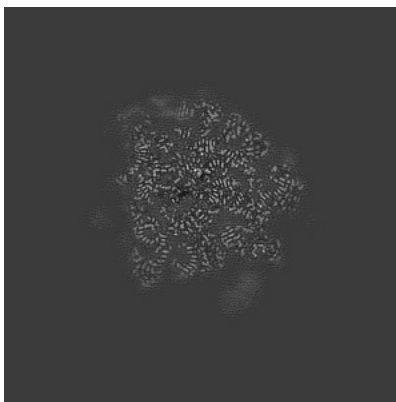
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

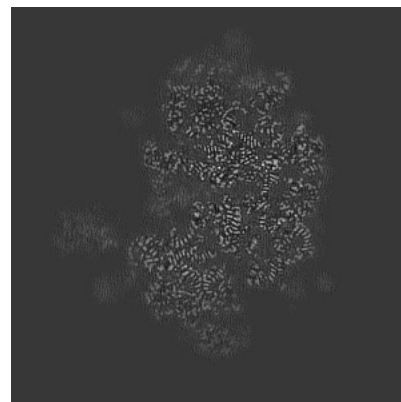
6.3.1 Primary map



X Index: 268

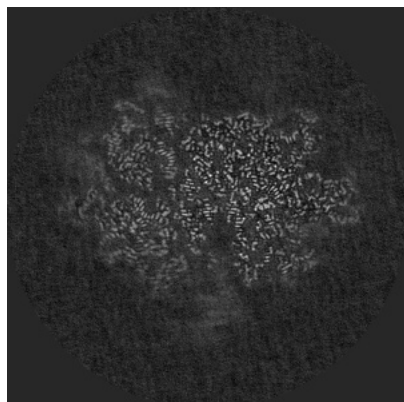


Y Index: 293

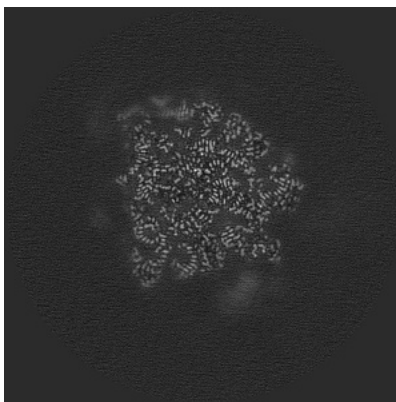


Z Index: 243

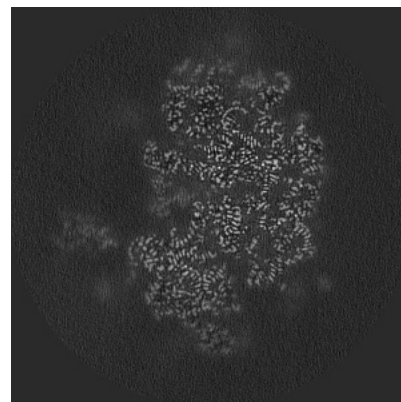
6.3.2 Raw map



X Index: 241



Y Index: 293

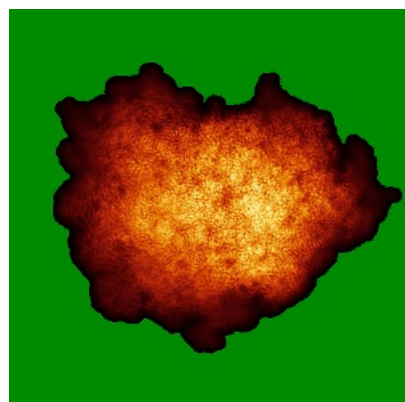


Z Index: 243

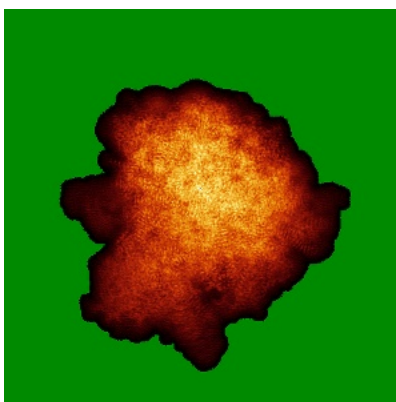
The images above show the largest variance slices of the map in three orthogonal directions.

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

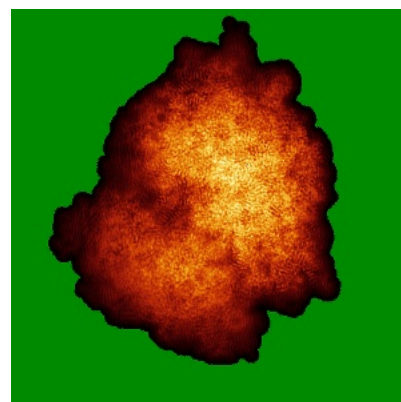
6.4.1 Primary map



X

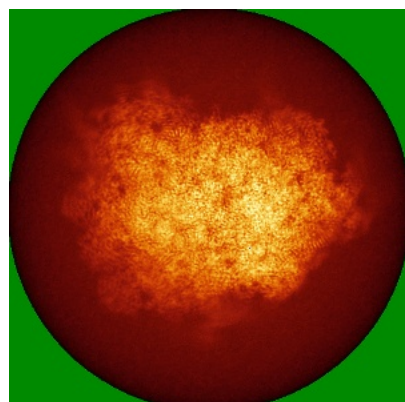


Y

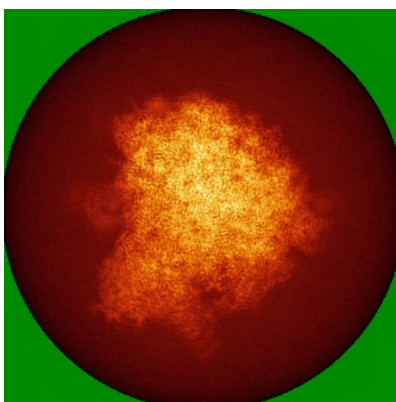


Z

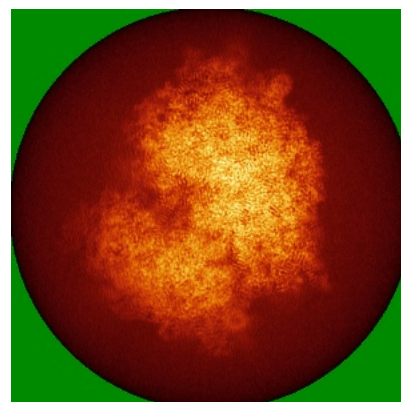
6.4.2 Raw map



X



Y

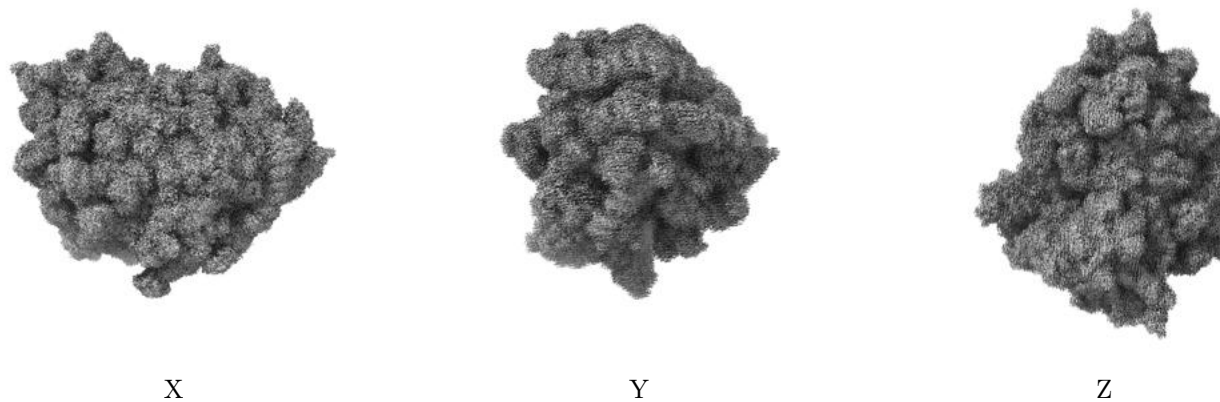


Z

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.

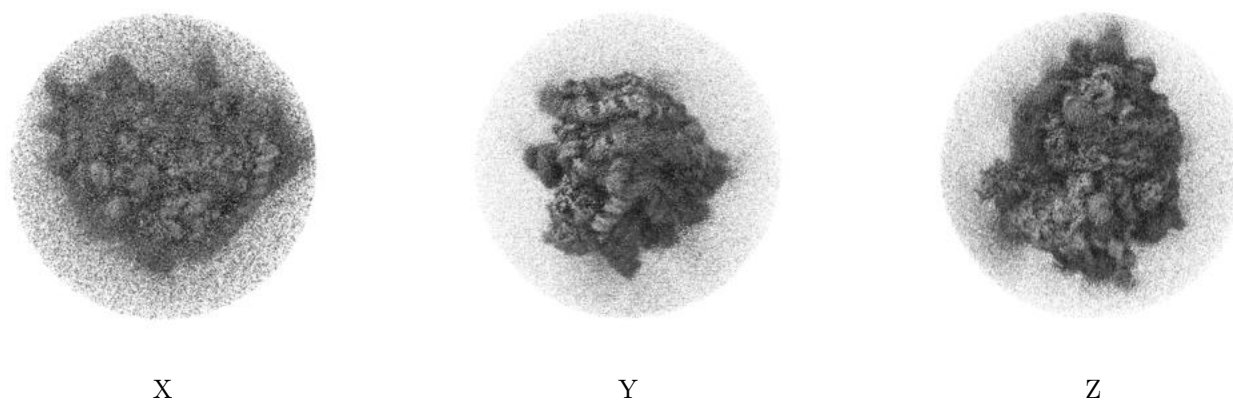
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

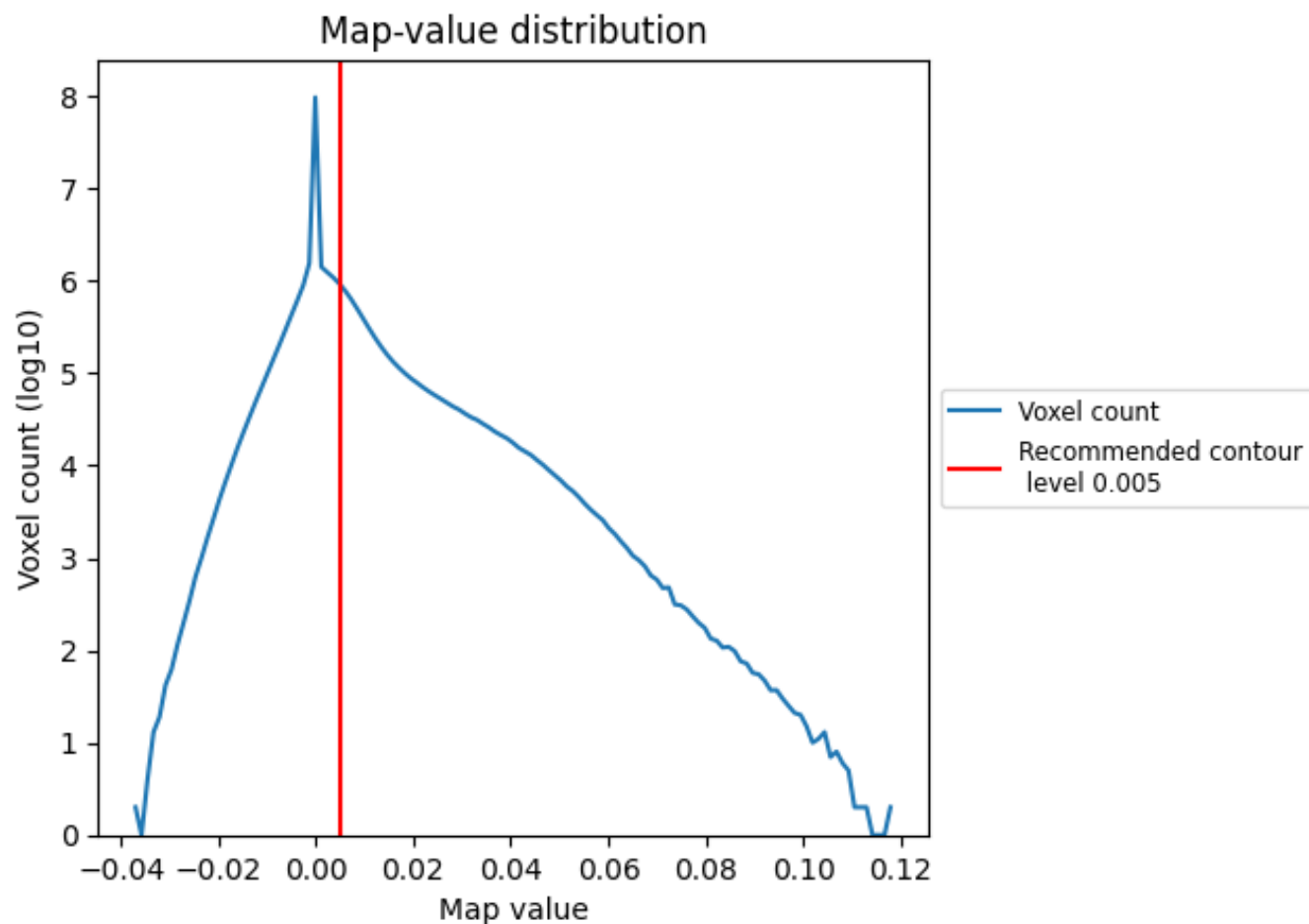
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

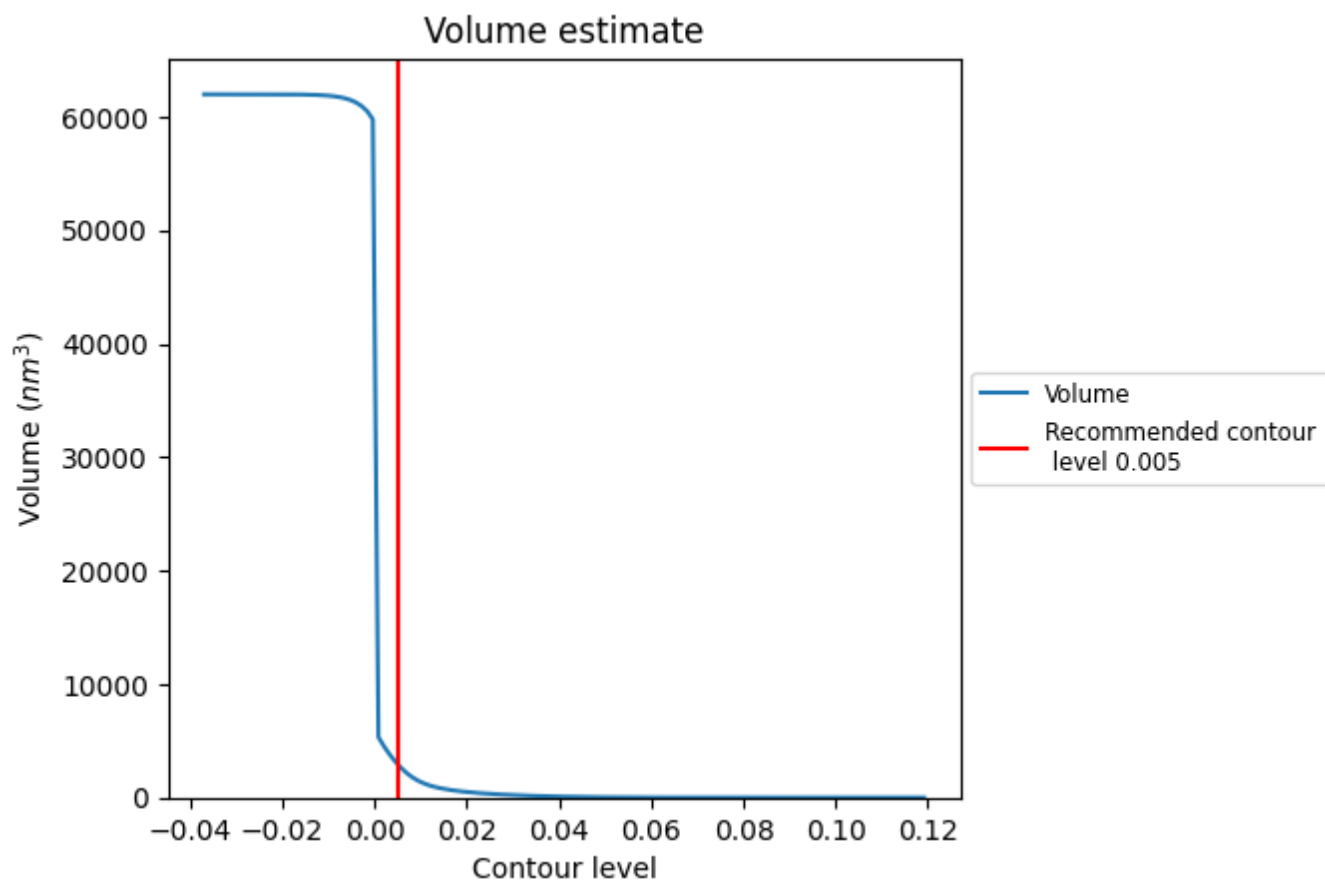
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

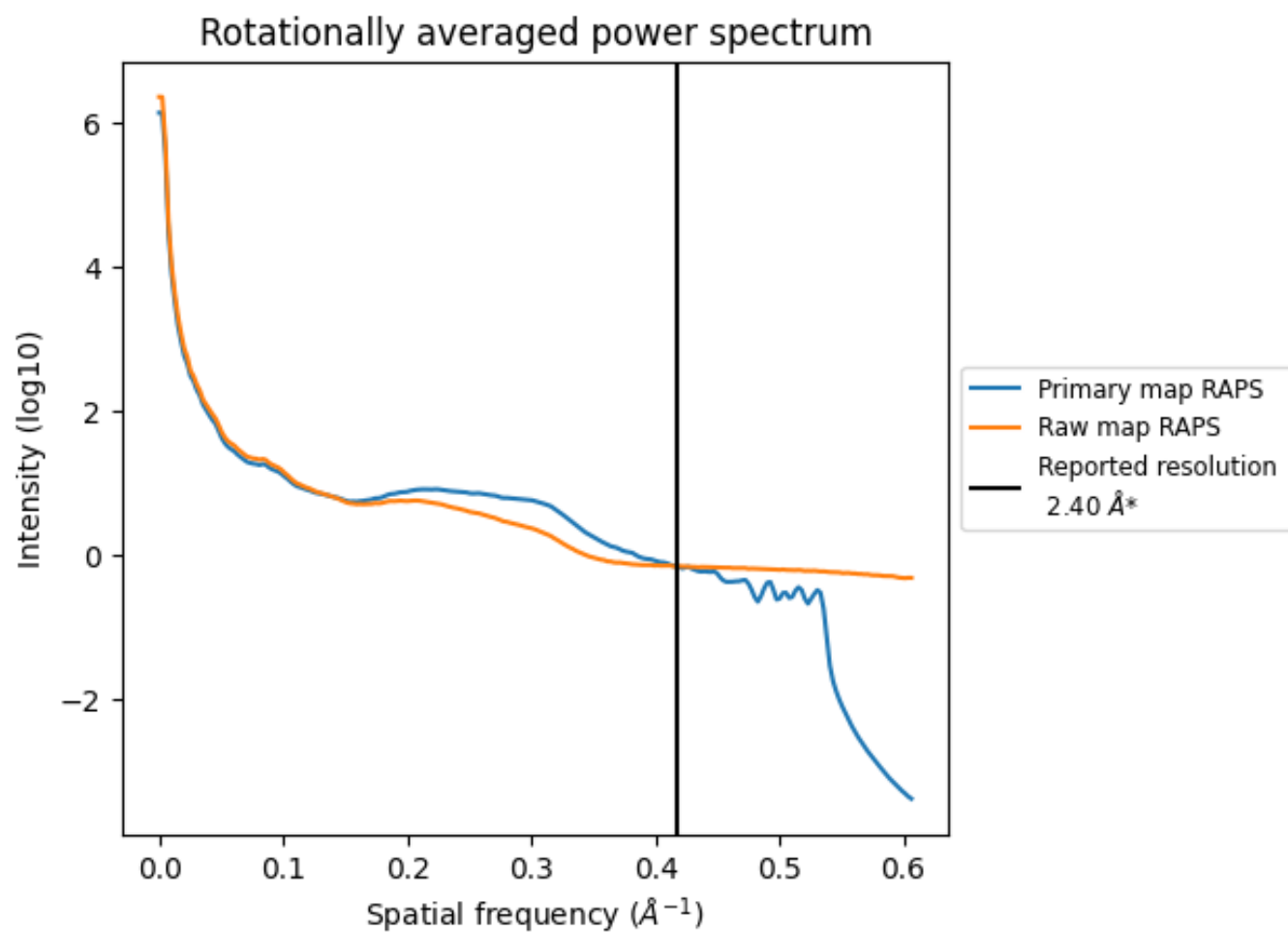
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2936 nm^3 ; this corresponds to an approximate mass of 2653 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 ⓘ

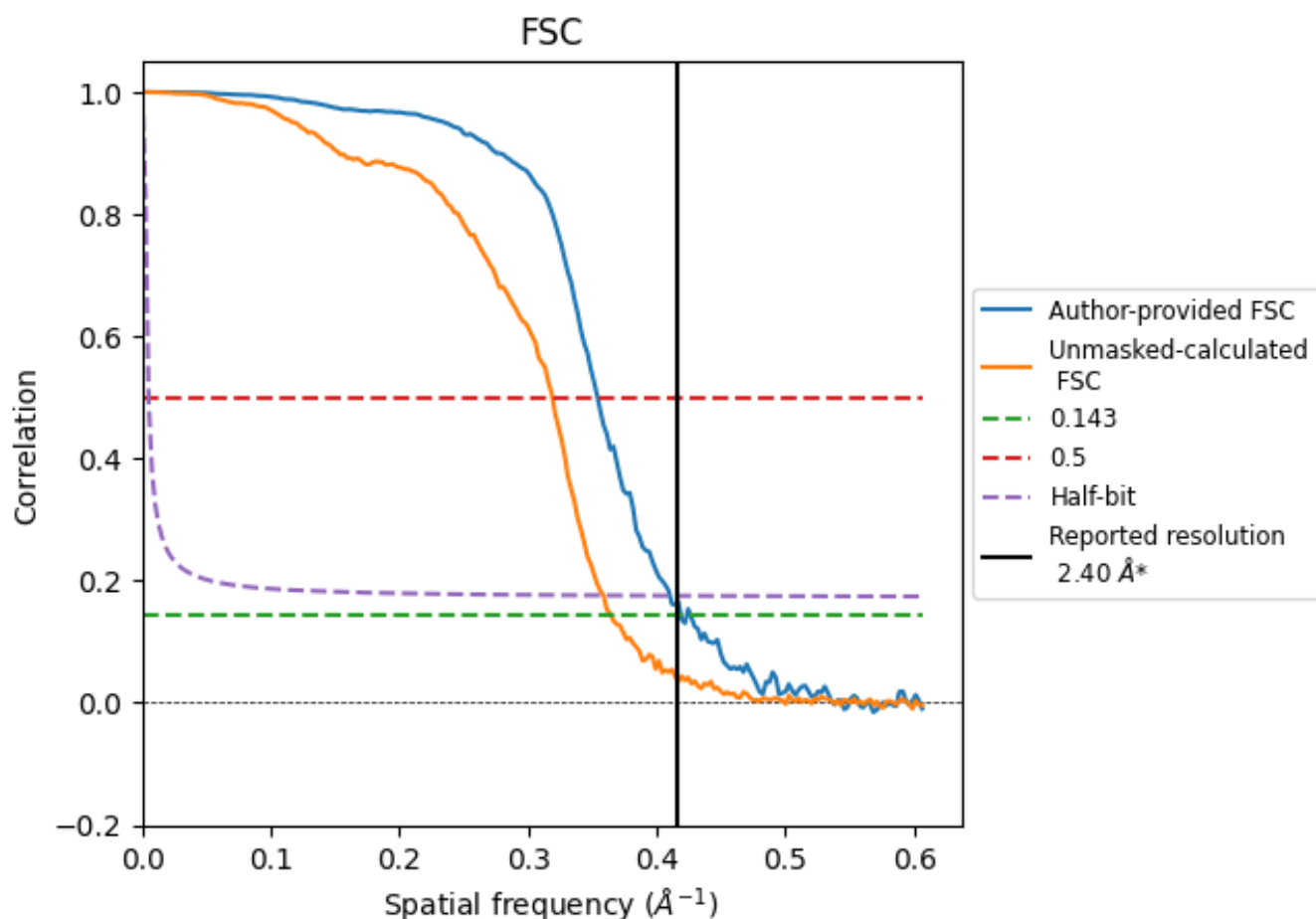


*Reported resolution corresponds to spatial frequency of $0.417 \text{ \AA}^{-1}$

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 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

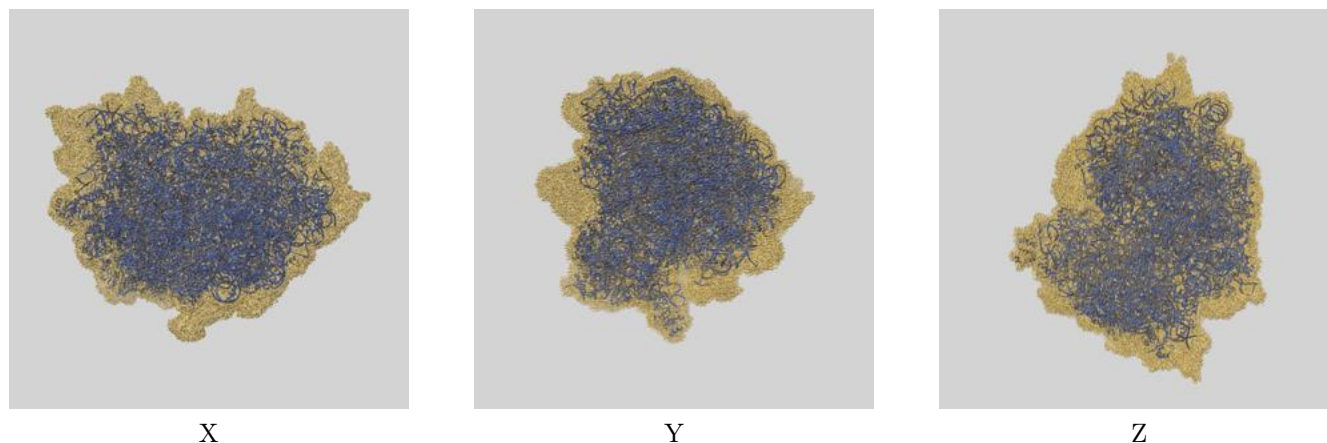
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.39	2.82	2.44
Unmasked-calculated*	2.74	3.14	2.79

*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 2.74 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

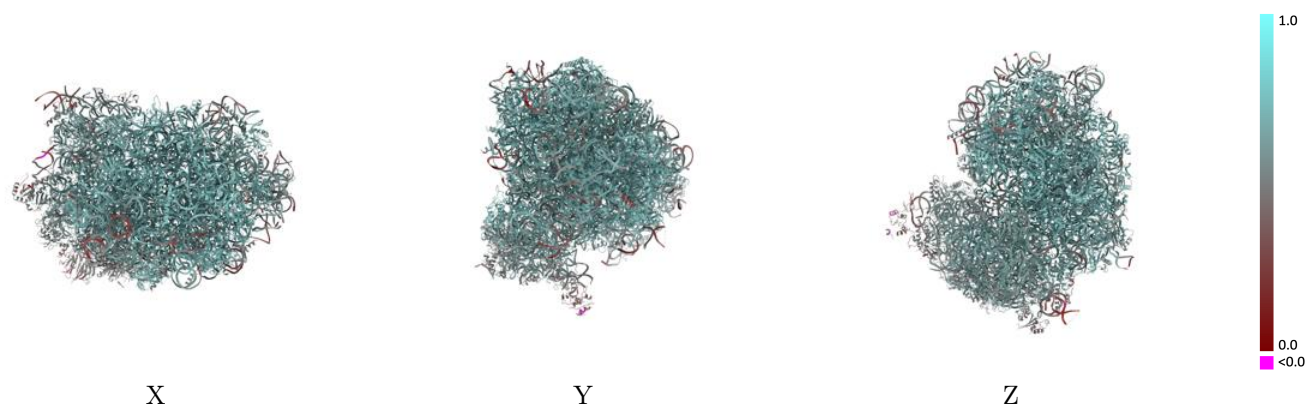
This section contains information regarding the fit between EMDB map EMD-55091 and PDB model 9SPI. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



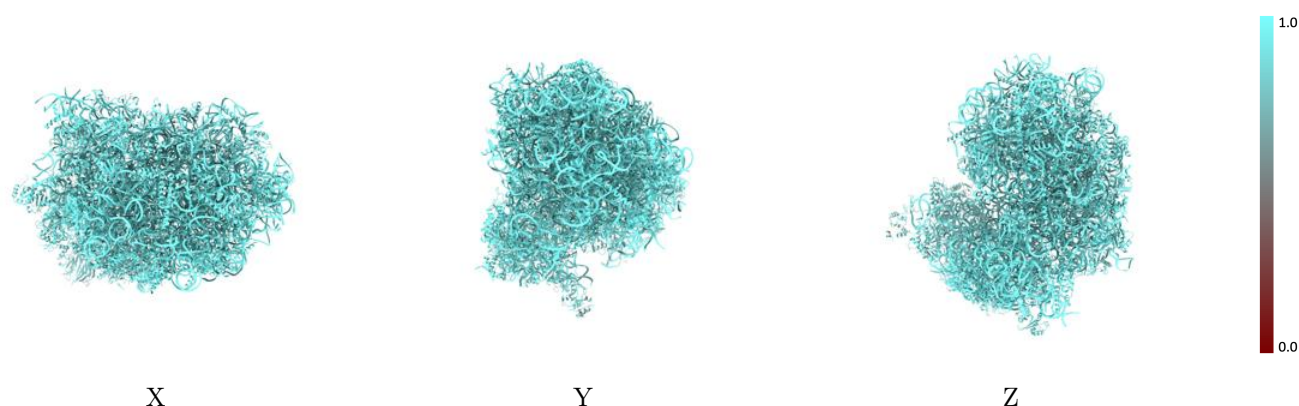
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



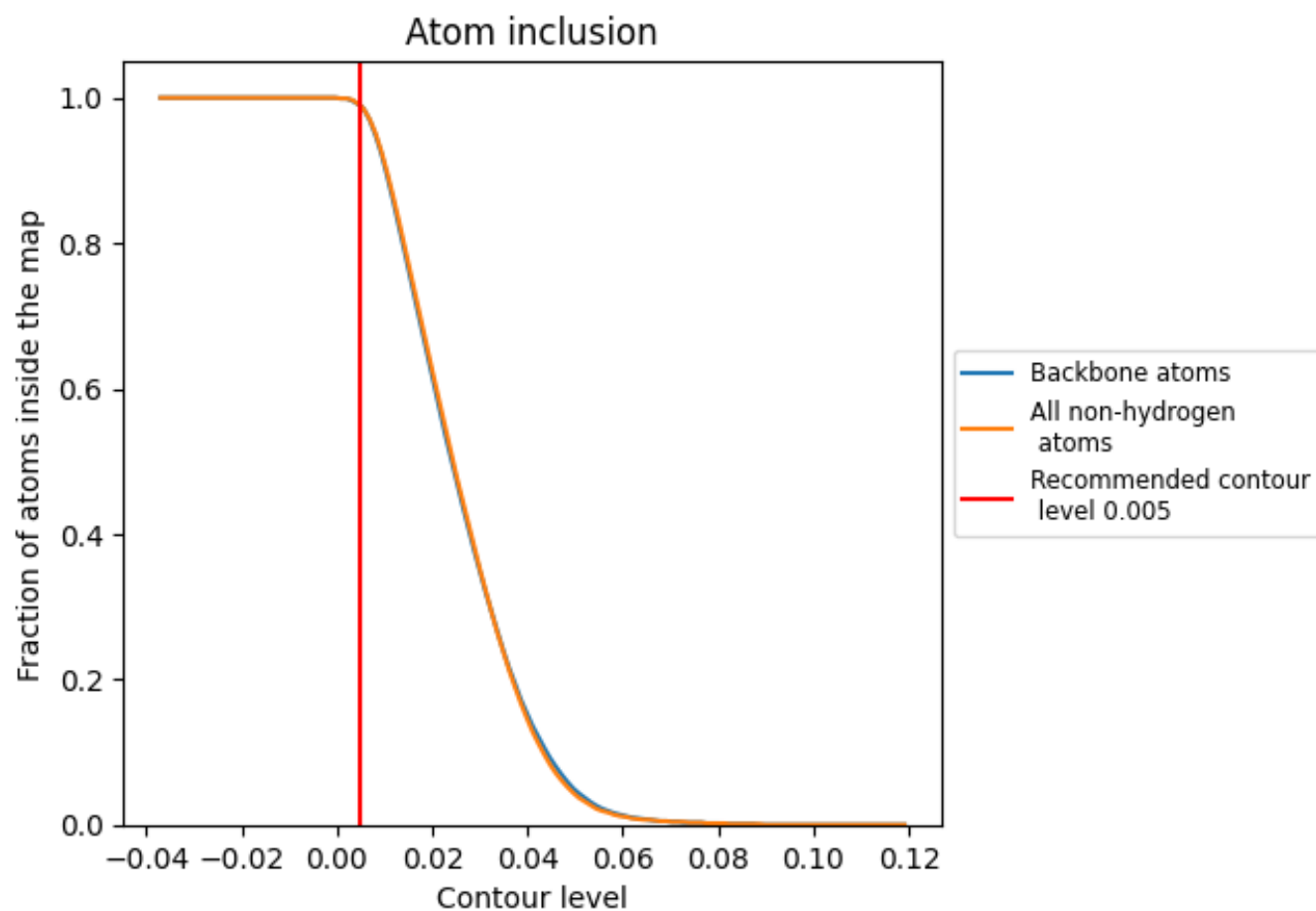
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.6390
At	 0.9700	 0.4980
Et	 0.9620	 0.3690
L5	 0.9940	 0.6590
L7	 1.0000	 0.6730
L8	 0.9980	 0.6830
LA	 1.0000	 0.7340
LB	 0.9970	 0.7180
LC	 0.9960	 0.7120
LD	 0.9920	 0.6570
LE	 0.9940	 0.6590
LF	 0.9940	 0.7170
LG	 0.9890	 0.6570
LH	 0.9950	 0.6800
LI	 0.9960	 0.6920
LJ	 0.9880	 0.5980
LL	 0.9910	 0.6880
LM	 0.9990	 0.6930
LN	 0.9990	 0.7370
LO	 0.9940	 0.7160
LP	 0.9980	 0.7210
LQ	 0.9990	 0.7320
LR	 0.9900	 0.6780
LS	 0.9990	 0.7160
LT	 0.9920	 0.6790
LU	 0.9810	 0.6060
LV	 0.9990	 0.7180
LW	 0.9980	 0.6970
LX	 0.9950	 0.6960
LY	 0.9960	 0.6950
LZ	 0.9980	 0.6760
La	 0.9960	 0.7280
Lb	 0.9900	 0.6500
Lc	 0.9930	 0.6750
Ld	 0.9870	 0.6930



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Chain	Atom inclusion	Q-score
Le	 0.9980	 0.7290
Lf	 0.9990	 0.7320
Lg	 0.9870	 0.6990
Lh	 0.9960	 0.6830
Li	 0.9950	 0.6740
Lj	 1.0000	 0.7350
Lk	 0.9850	 0.6320
Ll	 1.0000	 0.7100
Lm	 0.9980	 0.6990
Ln	 0.9950	 0.6920
Lo	 0.9990	 0.7060
Lp	 0.9960	 0.7120
Lr	 0.9990	 0.7040
Mr	 0.9930	 0.6510
Pt	 0.9790	 0.5270
S2	 0.9940	 0.6130
SA	 0.9730	 0.5510
SB	 0.9620	 0.5170
SC	 0.9860	 0.6320
SD	 0.9670	 0.5520
SE	 0.9940	 0.6000
SF	 0.9810	 0.5560
SG	 0.9770	 0.5610
SH	 0.9540	 0.5010
SI	 0.9810	 0.6150
SJ	 0.9890	 0.6060
SK	 0.9570	 0.5110
SL	 0.9860	 0.6530
SM	 0.7680	 0.3500
SN	 0.9830	 0.6040
SO	 0.9730	 0.5380
SP	 0.9720	 0.5440
SQ	 0.9860	 0.5650
SR	 0.9590	 0.5180
SS	 0.9760	 0.5580
ST	 0.9770	 0.5500
SU	 0.9540	 0.5210
SV	 0.9810	 0.5790
SW	 0.9910	 0.6460
SX	 0.9970	 0.6840
SY	 0.9810	 0.5640
SZ	 0.9460	 0.5070

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Chain	Atom inclusion	Q-score
Sa	 0.9840	 0.6080
Sb	 0.9760	 0.5400
Sc	 0.9600	 0.5290
Sd	 0.9840	 0.6080
Se	 0.9830	 0.5910
Sf	 0.8770	 0.3860
Sg	 0.9230	 0.4070