



## wwPDB EM Validation Summary Report ⓘ

Aug 30, 2022 – 02:28 pm BST

PDB ID : 7ZJX  
EMDB ID : EMD-14752  
Title : Rabbit 80S ribosome programmed with SECIS and SBP2  
Authors : Hilal, T.; Simonovic, M.; Spahn, C.M.T.  
Deposited on : 2022-04-12  
Resolution : 3.10 Å (reported)  
Based on initial model : 7O7Y

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

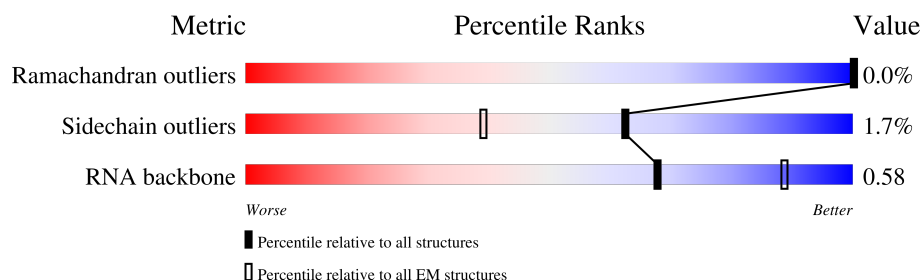
EMDB validation analysis : 0.0.1.dev8  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.30

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



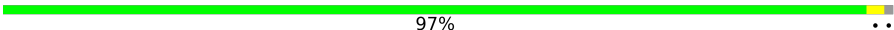



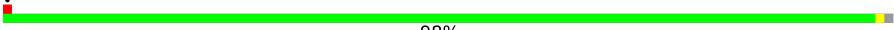
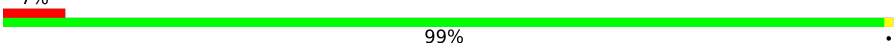
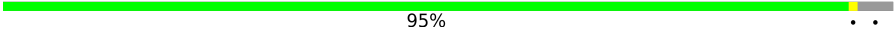
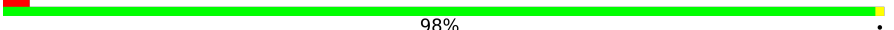
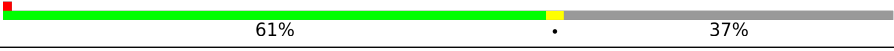

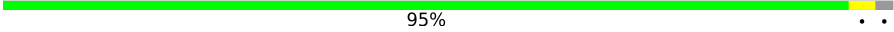

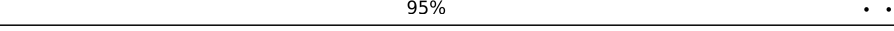
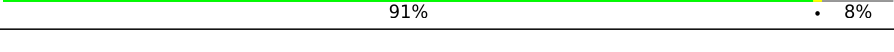
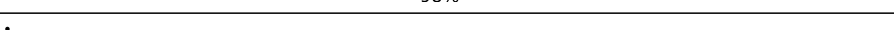
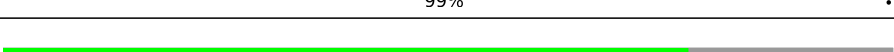




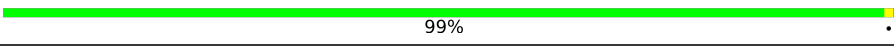
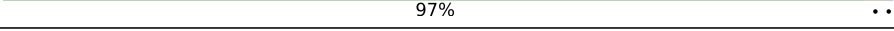

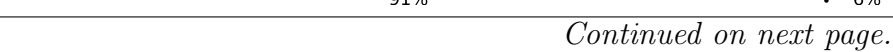

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	854	<div> <div>9%</div> <div>23%</div> <div>76%</div> </div>
2	I	163	<div> <div>22%</div> <div>44%</div> <div>55%</div> <div>.</div> </div>
3	L5	4808	<div> <div>.</div> <div>64%</div> <div>13%</div> <div>22%</div> </div>
4	L7	120	<div> <div>92%</div> <div>8%</div> </div>
5	L8	158	<div> <div>.</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
6	LD	257	<div> <div>.</div> <div>97%</div> <div>..</div> </div>
7	LE	403	<div> <div>97%</div> <div>..</div> </div>
8	LF	413	<div> <div>87%</div> <div>.</div> <div>12%</div> </div>


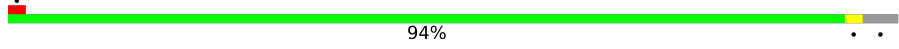
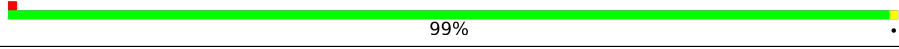
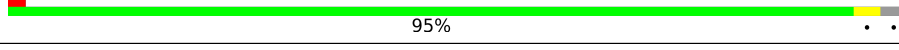
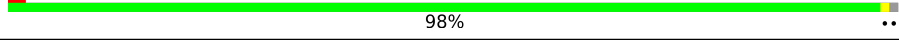
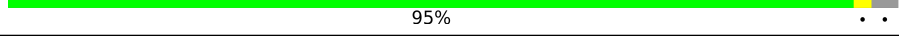
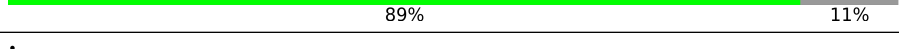
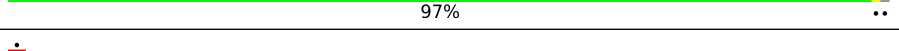
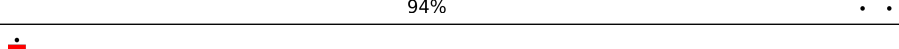
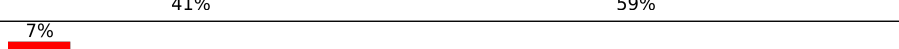
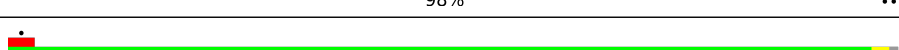
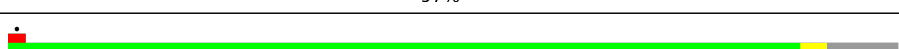
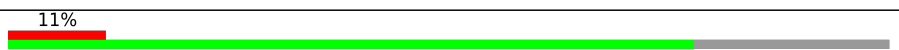
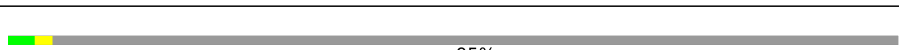
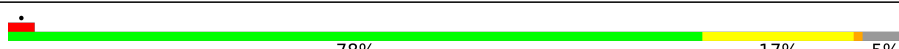

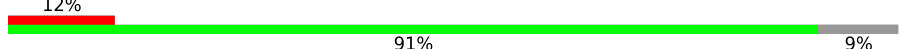



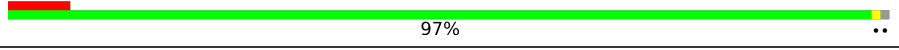
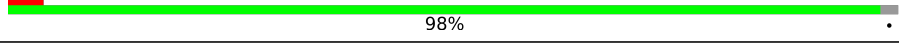



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	LG	297	 97% ..
10	LH	291	 5% 82% 16%
11	LI	247	 91% 9%
12	LJ	266	 86% 12%
13	LK	192	 98% ..
14	LL	214	 7% 99% .
15	LM	178	 95% . .
16	LO	211	 98% .
17	LP	218	 61% 37%
18	LQ	204	 98% .
19	LR	203	 95% . .
20	LS	184	 86% 14%
21	LT	188	 95% . .
22	LU	196	 91% 8%
23	LV	176	 98% .
24	LW	160	 99% .
25	LX	128	 77% 23%
26	LY	140	 7% 99% ..
27	LZ	157	 59% 41%
28	La	156	 76% 24%
29	Lb	145	 91% 8%
30	Lc	136	 99% ..
31	Ld	148	 97% ..
32	Le	245	 42% 56%
33	Lf	115	 9% 91% 6%



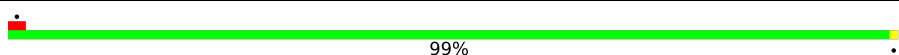
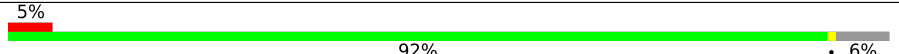
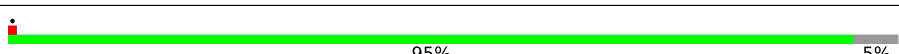
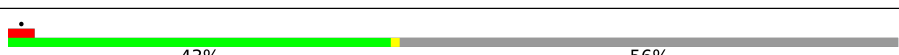
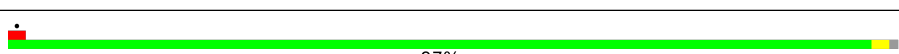
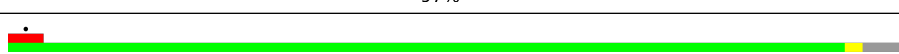
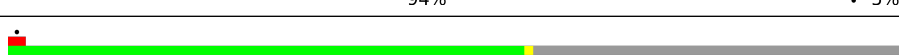
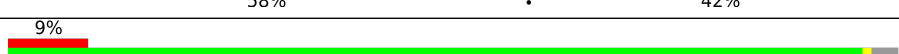
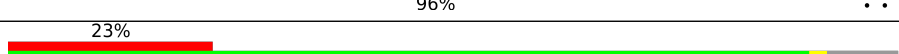
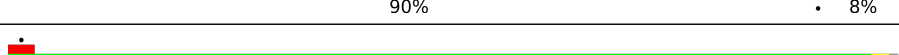
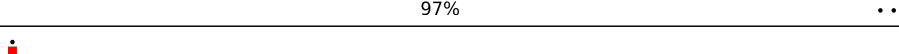
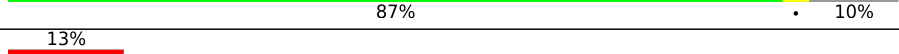


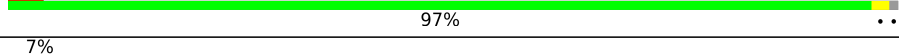
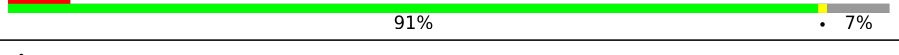
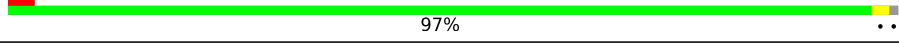
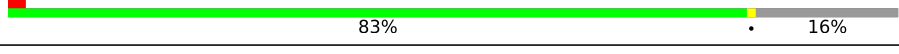
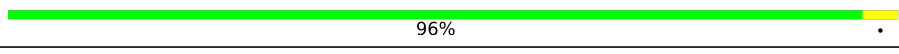
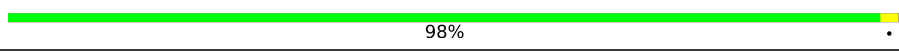
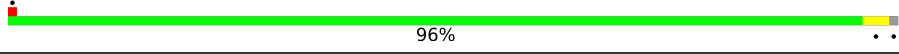
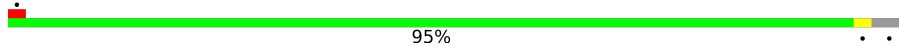

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Lg	125	
35	Lh	135	
36	Li	110	
37	Lj	117	
38	Lk	123	
39	Ll	105	
40	Lm	97	
41	Ln	70	
42	Lo	51	
43	Lp	128	
44	Lq	106	
45	Lr	92	
46	Ls	137	
47	Lx	217	
48	S	855	
49	S2	1870	
50	SB	84	
51	SC	69	
52	SD	156	
53	SE	133	
54	SF	115	
55	SG	317	
56	SH	56	
57	SL	295	
58	SM	264	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	SN	293	
60	SO	281	
61	SP	263	
62	SQ	204	
63	SR	249	
64	SS	432	
65	ST	208	
66	SU	194	
67	SV	165	
68	SW	158	
69	SX	132	
70	SY	151	
71	SZ	151	
72	Sa	145	
73	Sb	172	
74	Sc	135	
75	Sd	152	
76	Se	145	
77	Sf	119	
78	Sg	83	
79	Sh	130	
80	Si	143	
81	Sj	130	
82	Sk	124	
83	Sl	25	

## 2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 222755 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Selenocysteine insertion sequence-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	204	Total	C	N	O	S	0	0
			1379	881	257	238	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	687	ARG	LYS	conflict	UNP Q96T21
B	692	ILE	VAL	conflict	UNP Q96T21

- Molecule 2 is a RNA chain called CrPV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	163	Total	C	N	O	P	0	0
			3447	1544	588	1152	163		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3732	Total	C	N	O	P	0	0
			80089	35700	14644	26013	3732		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 6 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LD	253	Total	C	N	O	S	0	0
			1939	1214	396	323	6		

- Molecule 7 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LE	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LF	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 9 is a protein called Ribosomal\_L18\_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LG	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LG	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LH	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 11 is a protein called 60S ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LI	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	182	ASN	GLY	conflict	UNP A0A7J8C453
LI	199	HIS	ARG	conflict	UNP A0A7J8C453

- Molecule 12 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LJ	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LJ	184	LEU	ILE	conflict	UNP P62424

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LK	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 14 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

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

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

- Molecule 16 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LO	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LO	74	ARG	HIS	conflict	UNP G1TKB3

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
LO	190	ARG	HIS	conflict	UNP G1TKB3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LP	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 18 is a protein called Ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LR	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LR	174	LEU	ILE	conflict	UNP A0A0N8ETI8
LR	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 20 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LS	159	Total	C	N	O	S	0	0
			1288	808	249	222	9		

- Molecule 21 is a protein called 60S ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LT	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LT	134	ARG	CYS	conflict	UNP F6QKI9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LU	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 23 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LV	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LV	36	ASN	ILE	conflict	UNP A0A1Z5LHJ5

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

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

- Molecule 25 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LX	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LX	60	ALA	VAL	conflict	UNP Q4R5I3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LY	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LZ	93	Total	C	N	O	S	0	0
			766	480	153	129	4		

- Molecule 28 is a protein called Ribosomal\_L23eN domain-containing protein.

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

- Molecule 29 is a protein called Ribosomal protein L26.

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

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

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ld	147	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Le	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lf	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

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

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

- Molecule 35 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lh	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Li	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lk	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ll	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 40 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lm	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	Ln	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 42 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lo	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 43 is a protein called 60S ribosomal protein L40.

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

- Molecule 44 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lq	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 45 is a protein called 60S ribosomal protein eL43.

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

- Molecule 46 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ls	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

- Molecule 47 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lx	169	Total	C	N	O		0	0
			840	502	169	169			

- Molecule 48 is a RNA chain called GPX4 SECIS element.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S	46	Total	C	N	O	P	0	0
			983	438	179	320	46		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1118	U	C	conflict	GB 25123295
S	1126	A	C	conflict	GB 25123295
S	1132	A	U	conflict	GB 25123295
S	1133	G	-	insertion	GB 25123295
S	1134	C	-	insertion	GB 25123295
S	1135	C	-	insertion	GB 25123295
S	1136	C	-	insertion	GB 25123295
S	1150	U	A	conflict	GB 25123295

- Molecule 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S2	1770	Total	C	N	O	P	0	0
			37825	16906	6780	12369	1770		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	251	C	U	conflict	GB 37956930
S2	583	U	C	conflict	GB 37956930
S2	584	A	C	conflict	GB 37956930
S2	585	A	G	conflict	GB 37956930
S2	1338	4AC	C	conflict	GB 37956930
S2	1843	4AC	C	conflict	GB 37956930

- Molecule 50 is a protein called 40S ribosomal protein S27.

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

- Molecule 51 is a protein called 40S ribosomal protein S28.

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

- Molecule 52 is a protein called Ubiquitin carboxyl extension protein 80.

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

- Molecule 53 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SE	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 54 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SF	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 55 is a protein called Guanine nucleotide-binding protein subunit beta-2-like 1.

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

- Molecule 56 is a protein called 40S ribosomal protein S29.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 58 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SM	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 59 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SN	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SN	33	ILE	VAL	conflict	UNP O18789
SN	101	ALA	SER	conflict	UNP O18789

- Molecule 60 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SO	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 61 is a protein called 40S ribosomal protein S4.

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

- Molecule 62 is a protein called Ribosomal protein S5.

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

- Molecule 63 is a protein called 40S ribosomal protein S6.

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

- Molecule 64 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SS	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 65 is a protein called 40S ribosomal protein S8.



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

- Molecule 66 is a protein called 40S ribosomal protein S9.

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

- Molecule 67 is a protein called S10\_ plectin domain-containing protein.

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

- Molecule 68 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SW	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 69 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SX	121	Total	C	N	O	S	0	0
			943	591	167	176	9		

- Molecule 70 is a protein called 40S ribosomal protein S13.

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

- Molecule 71 is a protein called 40S ribosomal protein uS11.

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

- Molecule 72 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sa	127	Total	C	N	O	S	0	0
			1042	662	196	177	7		

- Molecule 73 is a protein called 40S ribosomal protein uS9.

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

- Molecule 74 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sc	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 75 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sd	141	Total	C	N	O	S	0	0
			1171	736	235	199	1		

- Molecule 76 is a protein called 40S Ribosomal protein eS19.

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

- Molecule 77 is a protein called 40S ribosomal protein S20.

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

- Molecule 78 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sg	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 79 is a protein called 40S ribosomal protein S15a.

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

- Molecule 80 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Si	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 81 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sj	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 82 is a protein called 40S ribosomal protein S25.

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

- Molecule 83 is a protein called 60S ribosomal protein L41.

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

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Lj	1	Total	Zn	0
			1	1	
84	Lm	1	Total	Zn	0
			1	1	
84	Lp	1	Total	Zn	0
			1	1	
84	Lq	1	Total	Zn	0
			1	1	
84	Lr	1	Total	Zn	0
			1	1	
84	SD	1	Total	Zn	0
			1	1	

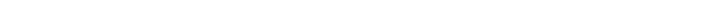
*Continued on next page...*

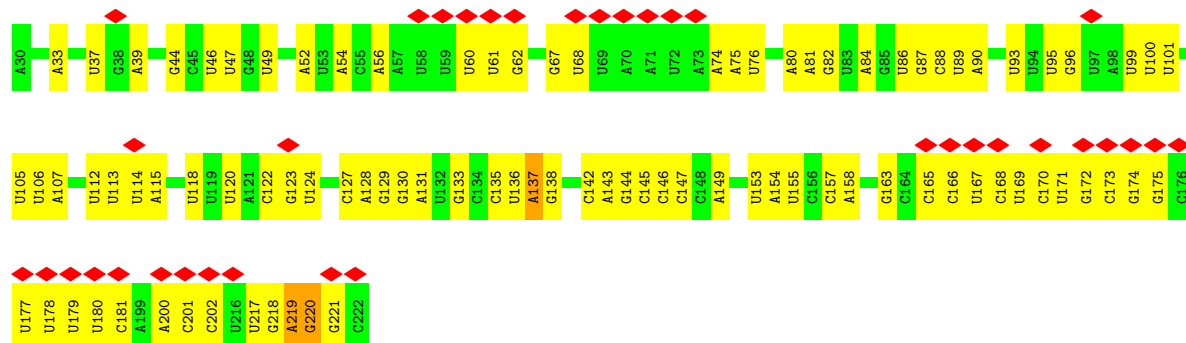
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
84	SF	1	Total 1	Zn 1	0
84	SH	1	Total 1	Zn 1	0



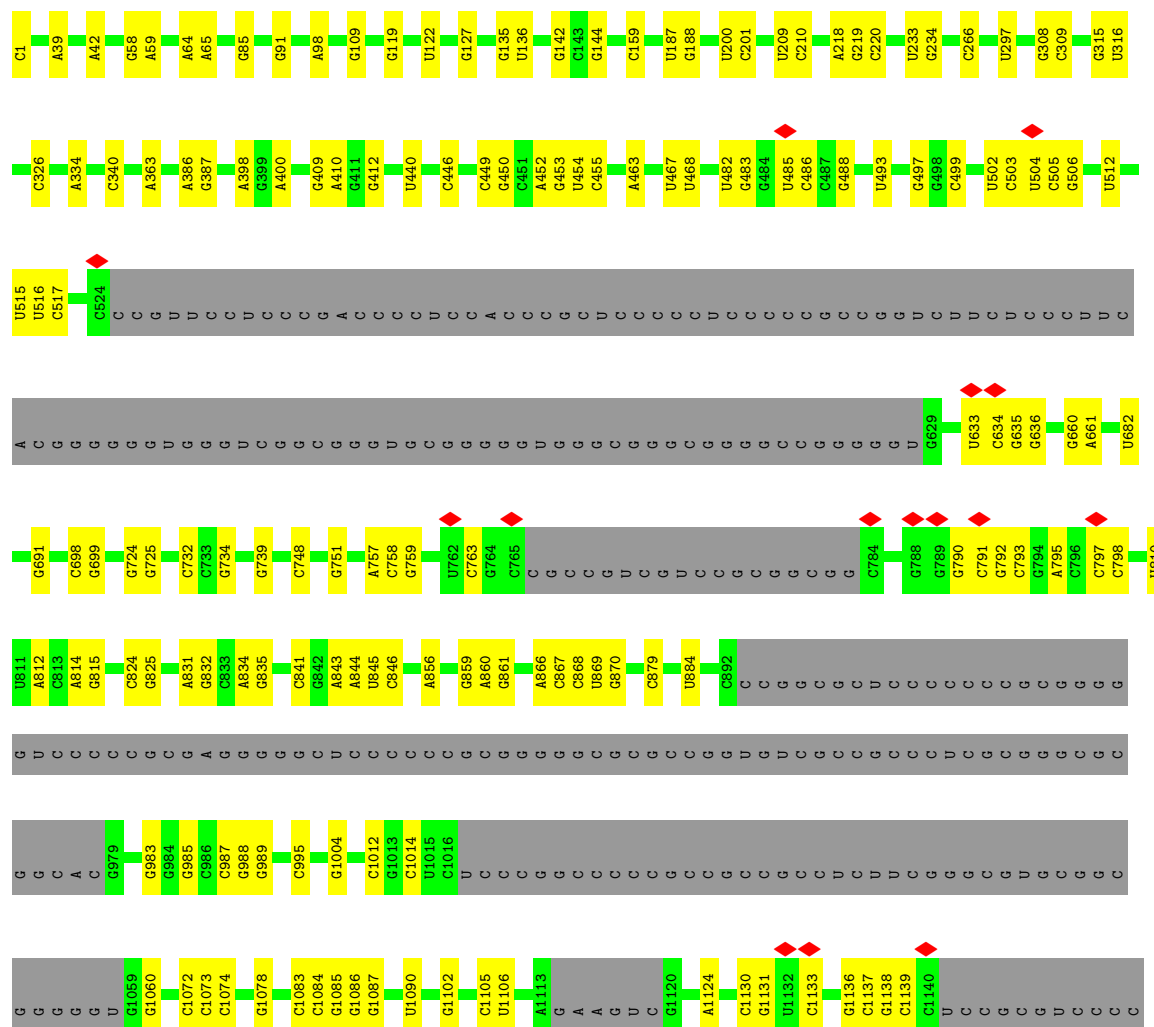
- Molecule 2: CrPV IRES

Chain I:  22% 44% 55%



- Molecule 3: 28S rRNA


Chain L5: 

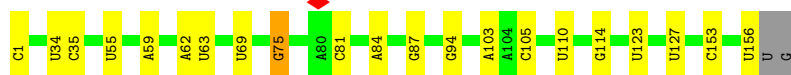








Chain L8:  85% 13% ..



- Molecule 6: 60S ribosomal protein uL2

Chain LD:  97% ..




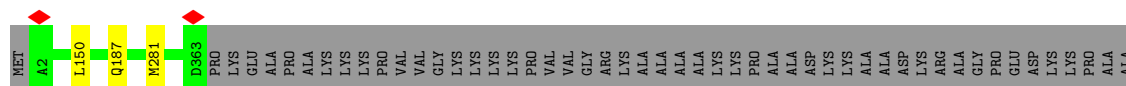
- Molecule 7: 60S ribosomal protein uL3

Chain LE:  97% ..



- Molecule 8: 60S ribosomal protein L4

Chain LF:  87% 12%




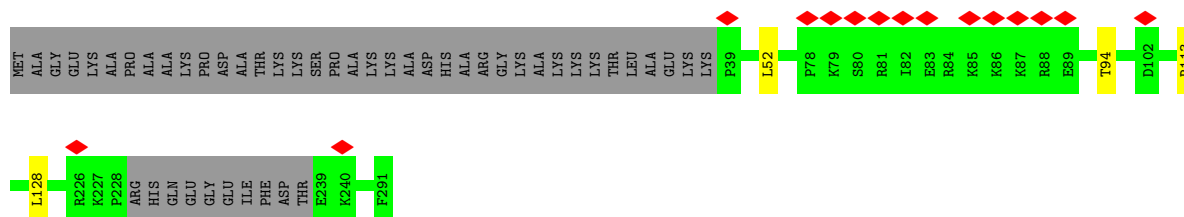
- Molecule 9: Ribosomal\_L18\_c domain-containing protein

Chain LG:  97% ..



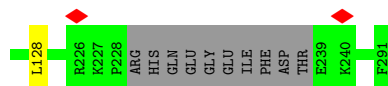
- Molecule 10: 60S ribosomal protein L6

Chain LH:  5% 82% 16%



- Molecule 11: 60S ribosomal Protein uL30

Chain LI:  91% 9%





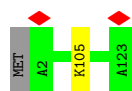
-

- Chain Ld:  97%

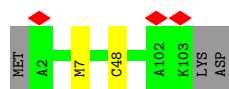




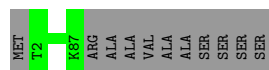
- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36



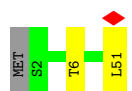
- Molecule 40: Ribosomal protein L37



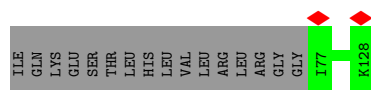
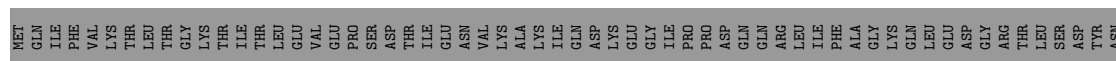
- Molecule 41: 60S ribosomal protein L38



- Molecule 42: 60S ribosomal protein eL39



- Molecule 43: 60S ribosomal protein L40



- 
- Diagram illustrating the protein structure of the R99-K106 region. The structure is shown as a green ribbon. The N-terminus is labeled MET. The C-terminus is labeled V2. The R99-K106 region is highlighted in yellow. The R99-K106 region is labeled with residues R99, K100, G101, Q102, V103, I104, Q105, and F106. Red diamonds are shown above the R99-K106 region.

- 

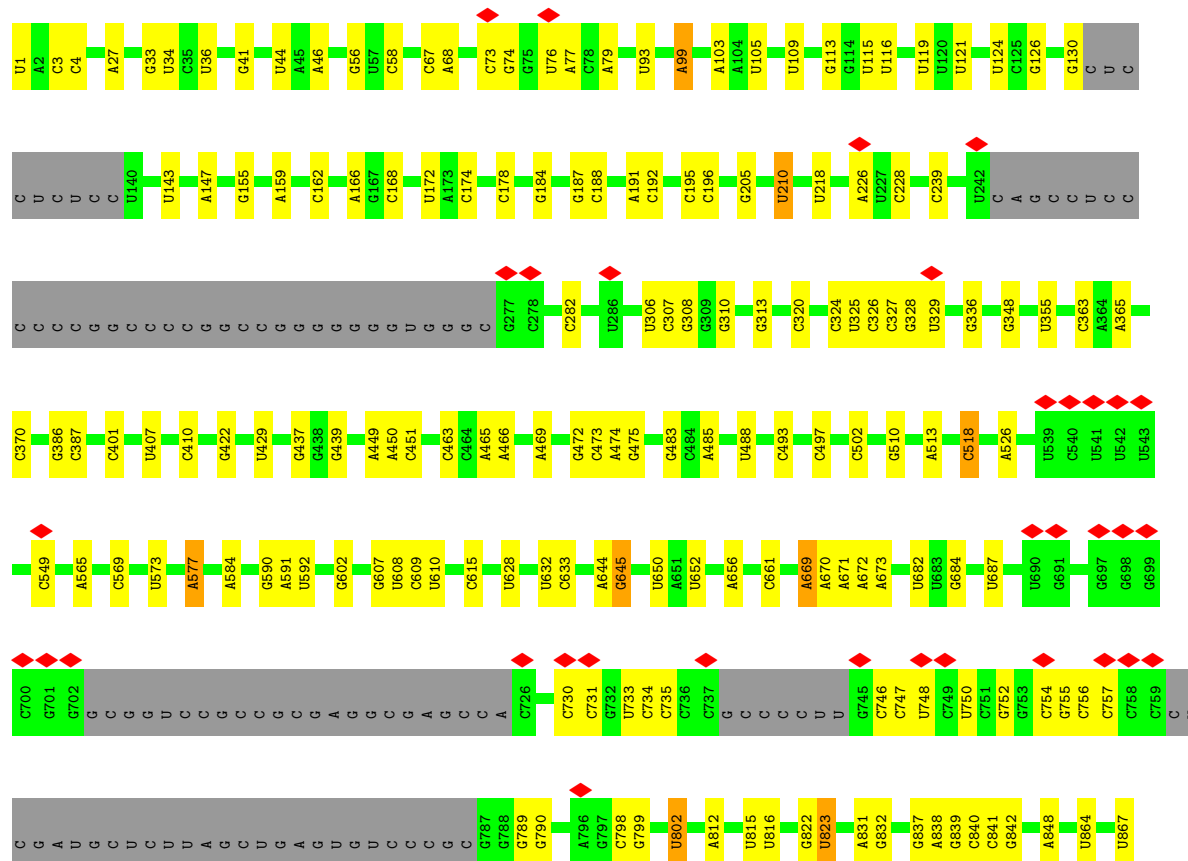
- 
- Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows amino acids: MET, S2, K19, N100, R113, M125, V126, K127, ARG, LYS, ARG, THR, ARG, PRO, THR, LYS, SER, SER. MET, ARG, LYS, ARG, THR, ARG, PRO, THR, LYS, SER, and SER have zero information content. S2, K19, N100, and R113 have low information content (approx. 0.1-0.2 bits). M125, V126, and K127 have high information content (approx. 1.2-1.4 bits) and are marked with red diamonds above them.

- 

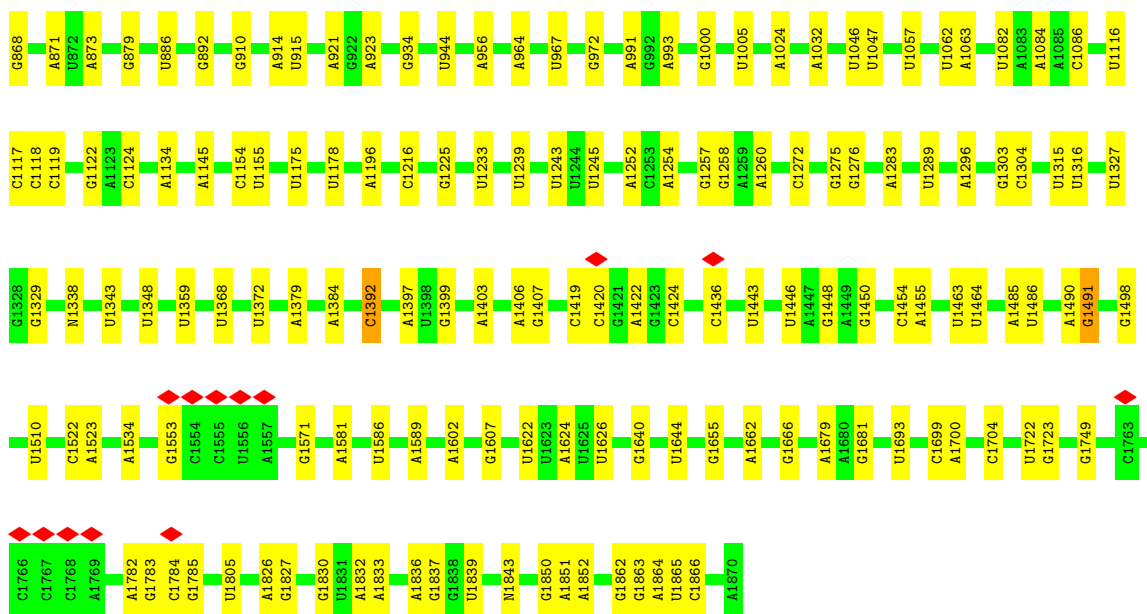
- Chain S: 95%
- A U U U G G U C G G C C G U G G A C G A A G G G G G C C C U G G C U C C C A G G C C C C G C C G A U G A A G C C C G
- G C C G C C C U U U G G C C G A C U G A A A G C C G G C G C U G C U C U G U G G G G C U C U G G G C C G A U G A C C U G C C
- U G G C C G G G A C C A U G U G C G C G G G G A C G A C U G G C U G C U G G C C A U G G C C A C G A C G A C U
- U U U C C C C A A A G A C C A U C G A C C G G C C C A C C A U G G U U A A A C C U G G A A C C A C C G G G C U U C C G U G U
- G C A U C C G U C A C A C A C C G A U G C C C U C C A C C A C C A C C A C C U U A C A C A C C U C C G A C U C C G
- U C C G A A C C U U G G C A C G C C C C G A U A C C G C C U A A G U U U U G C C G G A U U C C C U G G C C C C G U U A A C C

- Molecule 49: 18S rRNA

Chain S2:

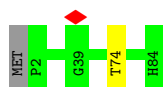






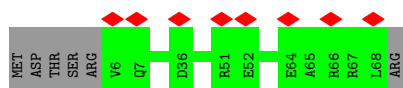
- Molecule 50: 40S ribosomal protein S27

Chain SB: 98%



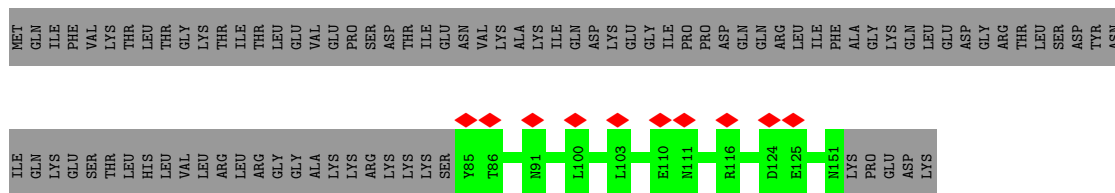
- Molecule 51: 40S ribosomal protein S28

Chain SC: 12% 91% 9%



- Molecule 52: Ubiquitin carboxyl extension protein 80

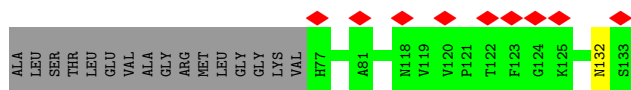
Chain SD: 6% 43% 57%



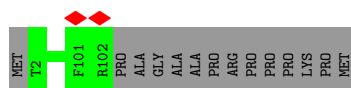
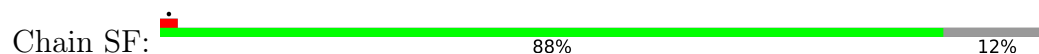
- Molecule 53: 40S ribosomal protein S30

Chain SE: 7% 42% 57%

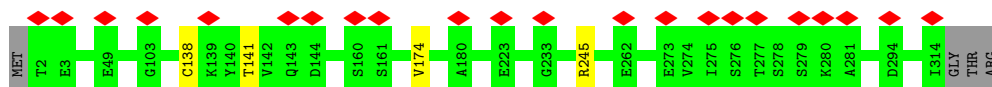




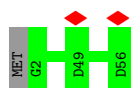
- Molecule 54: 40S ribosomal protein eS26



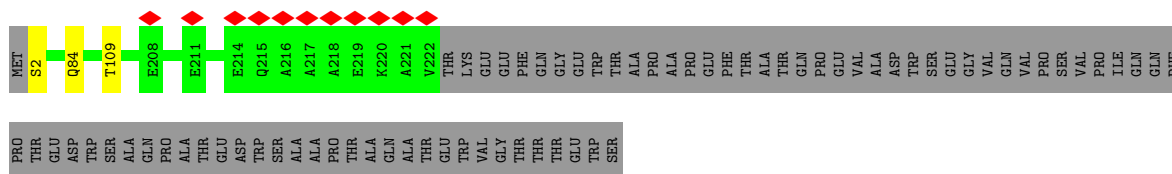
- Molecule 55: Guanine nucleotide-binding protein subunit beta-2-like 1



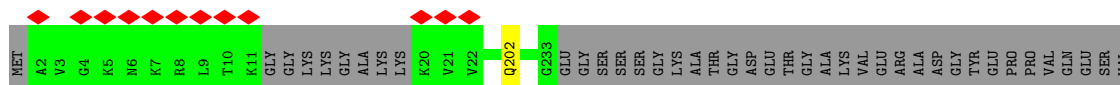
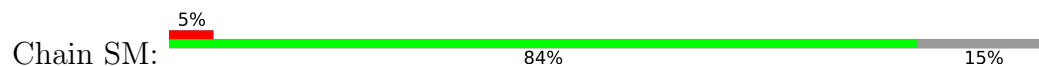
- Molecule 56: 40S ribosomal protein S29



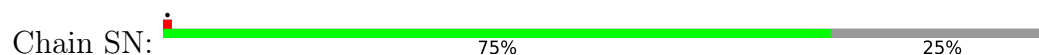
- Molecule 57: 40S ribosomal protein SA

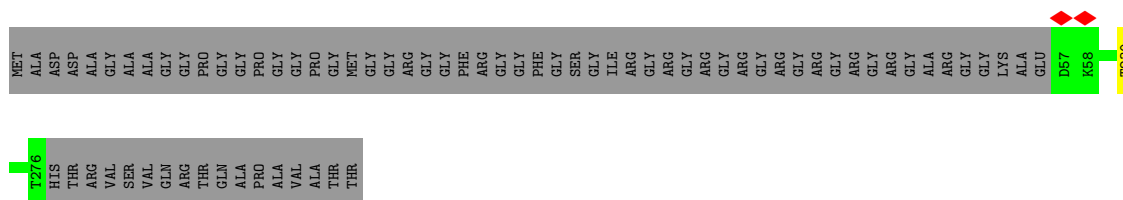


- Molecule 58: 40S ribosomal protein S3a

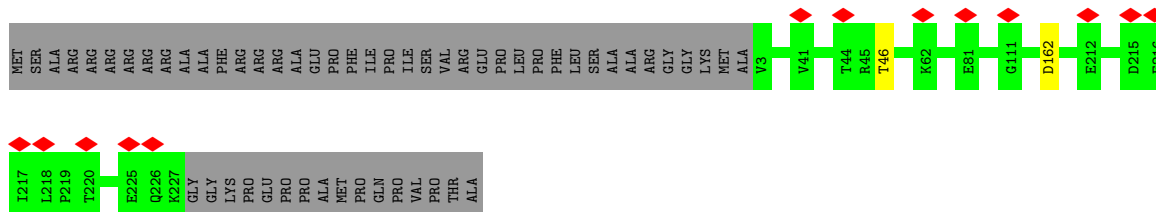
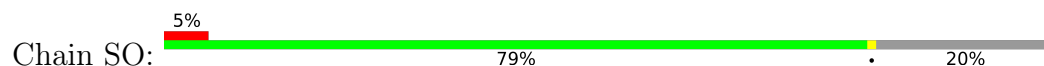


- Molecule 59: 40S ribosomal protein uS5

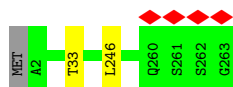




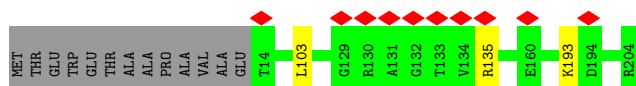
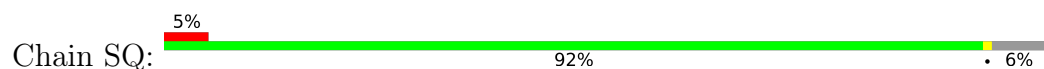
- Molecule 60: 40S ribosomal protein S3



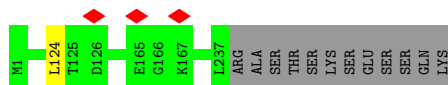
- Molecule 61: 40S ribosomal protein S4



- Molecule 62: Ribosomal protein S5



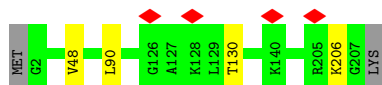
- Molecule 63: 40S ribosomal protein S6



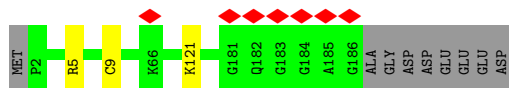
- Molecule 64: 40S ribosomal protein S7



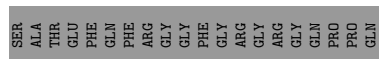
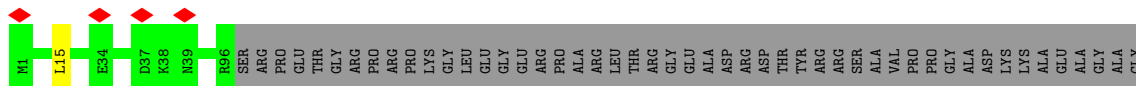
- Molecule 65: 40S ribosomal protein S8



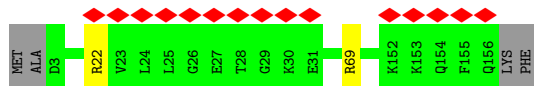
- Molecule 66: 40S ribosomal protein S9



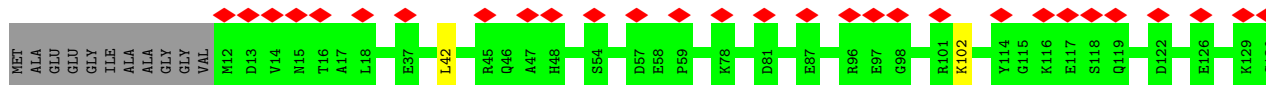
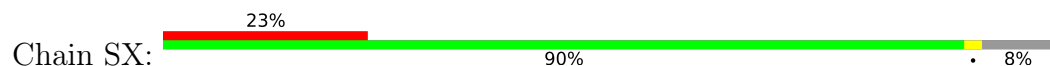
- Molecule 67: S10\_pectin domain-containing protein



- Molecule 68: 40S ribosomal protein S11



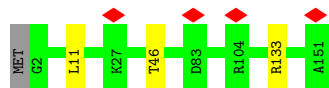
- Molecule 69: 40S ribosomal protein S12





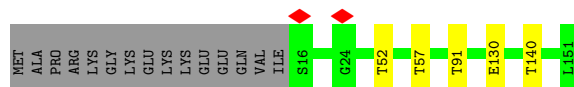
- Molecule 70: 40S ribosomal protein S13

Chain SY: 97%



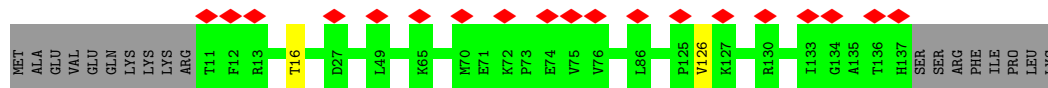
- Molecule 71: 40S ribosomal protein uS11

Chain SZ: 87% 10%



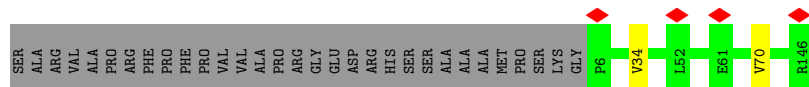
- Molecule 72: 40S ribosomal protein S15

Chain Sa: 13% 86% 12%



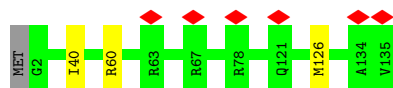
- Molecule 73: 40S ribosomal protein uS9

Chain Sb: 81% 18%



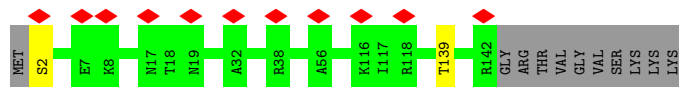
- Molecule 74: 40S ribosomal protein S17

Chain Sc: 97%



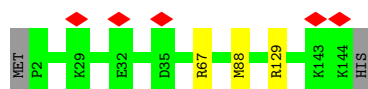
- Molecule 75: 40S ribosomal protein S18

Chain Sd: 7% 91% 7%




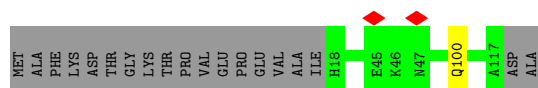
- Molecule 76: 40S Ribosomal protein eS19

Chain Se:  97%



- Molecule 77: 40S ribosomal protein S20

Chain Sf:  83% 16%



- Molecule 78: 40S ribosomal protein eS21

Chain Sg:  96%



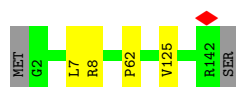
- Molecule 79: 40S ribosomal protein S15a

Chain Sh:  98%



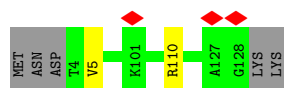
- Molecule 80: 40S ribosomal protein S23

Chain Si:  96%



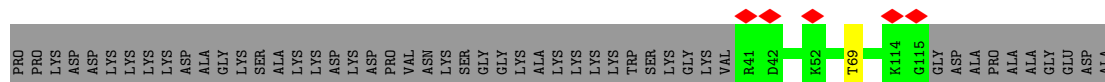
- Molecule 81: 40S ribosomal protein S24

Chain Sj:  95%



- Molecule 82: 40S ribosomal protein S25

Chain Sk:  60% 40%



- Molecule 83: 60S ribosomal protein L41

Chain Sl:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.751	Depositor
Minimum map value	0.000	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	409.2, 409.2, 409.2	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AAC, UR3, 6MZ, MA6, MLZ, OMC, NMM, HY3, M3L, 7MG, SAC, 4AC, PSU, ZN, OMU, OMG, HIC, 1MA, GTP, AYA, 5MC, AME, A2M

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	B	0.27	0/1398	0.46	0/1905
2	I	0.17	0/3847	0.77	4/5981 (0.1%)
3	L5	0.26	1/86665 (0.0%)	0.69	8/135207 (0.0%)
4	L7	0.27	0/2835	0.68	1/4418 (0.0%)
5	L8	0.31	1/3635 (0.0%)	0.68	0/5661
6	LD	0.27	0/1977	0.55	0/2651
7	LE	0.26	0/3261	0.50	0/4364
8	LF	0.26	0/2932	0.52	0/3939
9	LG	0.26	0/2437	0.48	0/3264
10	LH	0.26	0/1998	0.51	0/2673
11	LI	0.27	0/1922	0.50	0/2563
12	LJ	0.25	0/1908	0.49	0/2566
13	LK	0.26	0/1535	0.50	0/2063
14	LL	0.26	0/1756	0.51	0/2346
15	LM	0.25	0/1385	0.53	0/1852
16	LO	0.25	0/1733	0.55	0/2316
17	LP	0.26	0/1158	0.50	0/1547
18	LQ	0.26	0/1746	0.55	0/2338
19	LR	0.26	0/1662	0.50	0/2222
20	LS	0.26	0/1315	0.49	0/1763
21	LT	0.26	0/1539	0.56	0/2054
22	LU	0.24	0/1524	0.54	0/2013
23	LV	0.27	0/1497	0.54	0/2008
24	LW	0.26	0/1326	0.50	0/1770
25	LX	0.26	0/820	0.48	0/1100
26	LY	0.27	0/1048	0.51	0/1402
27	LZ	0.26	0/779	0.50	0/1034
28	La	0.25	0/984	0.49	0/1323
29	Lb	0.25	0/1132	0.53	0/1504
30	Lc	0.27	0/1130	0.50	0/1507
31	Ld	0.26	0/1188	0.51	0/1587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Le	0.24	0/884	0.52	0/1169
33	Lf	0.25	0/847	0.45	0/1134
34	Lg	0.25	0/903	0.52	0/1216
35	Lh	0.26	0/1088	0.52	0/1451
36	Li	0.28	0/903	0.54	0/1208
37	Lj	0.26	0/916	0.55	0/1220
38	Lk	0.24	0/1021	0.50	0/1348
39	Ll	0.25	0/841	0.53	0/1112
40	Lm	0.25	0/720	0.57	0/952
41	Ln	0.25	0/575	0.46	0/761
42	Lo	0.24	0/459	0.53	0/608
43	Lp	0.24	0/426	0.52	0/564
44	Lq	0.25	0/866	0.51	0/1141
45	Lr	0.25	0/718	0.51	0/953
46	Ls	0.25	0/1020	0.54	0/1366
47	Lx	0.23	0/836	0.40	0/1161
48	S	0.25	0/1098	0.80	1/1710 (0.1%)
49	S2	0.23	1/40365 (0.0%)	0.69	7/62915 (0.0%)
50	SB	0.25	0/665	0.48	0/891
51	SC	0.24	0/497	0.57	0/666
52	SD	0.25	0/560	0.49	0/745
53	SE	0.25	0/462	0.55	0/607
54	SF	0.25	0/828	0.54	0/1109
55	SG	0.24	0/2493	0.48	0/3394
56	SH	0.25	0/470	0.51	0/623
57	SL	0.25	0/1771	0.47	0/2406
58	SM	0.25	0/1841	0.46	0/2459
59	SN	0.26	0/1742	0.47	0/2354
60	SO	0.25	0/1779	0.49	0/2395
61	SP	0.25	0/2118	0.51	0/2849
62	SQ	0.24	0/1531	0.49	0/2059
63	SR	0.25	0/1946	0.54	0/2590
64	SS	0.25	0/1552	0.49	0/2079
65	ST	0.25	0/1715	0.52	0/2287
66	SU	0.24	0/1550	0.53	0/2069
67	SV	0.25	0/834	0.44	0/1125
68	SW	0.26	0/1284	0.52	0/1717
69	SX	0.23	0/953	0.44	0/1276
70	SY	0.24	0/1232	0.49	0/1656
71	SZ	0.26	0/1029	0.54	0/1380
72	Sa	0.25	0/1063	0.49	0/1421
73	Sb	0.24	0/1142	0.52	0/1528
74	Sc	0.23	0/1094	0.48	0/1469

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	Sd	0.23	0/1180	0.54	0/1581
76	Se	0.24	0/1119	0.47	0/1498
77	Sf	0.24	0/805	0.52	0/1081
78	Sg	0.26	0/636	0.50	0/852
79	Sh	0.25	0/1051	0.50	0/1406
80	Si	0.25	0/1107	0.50	0/1475
81	Sj	0.25	0/1032	0.52	0/1371
82	Sk	0.24	0/604	0.49	0/810
83	Sl	0.22	0/240	0.65	0/305
All	All	0.25	3/234483 (0.0%)	0.63	21/344463 (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
47	Lx	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	1	U	OP3-P	-10.60	1.48	1.61
3	L5	1	C	OP3-P	-10.58	1.48	1.61
5	L8	1	C	OP3-P	-10.57	1.48	1.61

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	219	A	OP1-P-O3'	-10.62	81.84	105.20
2	I	219	A	OP2-P-O3'	-10.56	81.96	105.20
49	S2	1454	C	C2-N1-C1'	8.73	128.40	118.80
49	S2	1454	C	N1-C2-O2	8.72	124.13	118.90
2	I	220	G	OP1-P-OP2	7.42	130.73	119.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	Lx	60	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	200/854 (23%)	171 (86%)	28 (14%)	1 (0%)	29	64
6	LD	251/257 (98%)	238 (95%)	13 (5%)	0	100	100
7	LE	395/403 (98%)	386 (98%)	9 (2%)	0	100	100
8	LF	360/413 (87%)	354 (98%)	6 (2%)	0	100	100
9	LG	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
10	LH	239/291 (82%)	231 (97%)	8 (3%)	0	100	100
11	LI	224/247 (91%)	218 (97%)	6 (3%)	0	100	100
12	LJ	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
13	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
14	LL	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
15	LM	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
16	LO	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
17	LP	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
18	LQ	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	LR	197/203 (97%)	197 (100%)	0	0	100	100
20	LS	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
21	LT	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
22	LU	178/196 (91%)	178 (100%)	0	0	100	100
23	LV	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
24	LW	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
25	LX	97/128 (76%)	95 (98%)	2 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LY	137/140 (98%)	137 (100%)	0	0	100	100
27	LZ	89/157 (57%)	89 (100%)	0	0	100	100
28	La	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
29	Lb	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
30	Lc	133/136 (98%)	133 (100%)	0	0	100	100
31	Ld	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	22	57
32	Le	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
33	Lf	106/115 (92%)	106 (100%)	0	0	100	100
34	Lg	105/125 (84%)	105 (100%)	0	0	100	100
35	Lh	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
36	Li	108/110 (98%)	108 (100%)	0	0	100	100
37	Lj	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
38	Lk	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
39	Ll	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
40	Lm	84/97 (87%)	84 (100%)	0	0	100	100
41	Ln	67/70 (96%)	67 (100%)	0	0	100	100
42	Lo	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	Lp	49/128 (38%)	49 (100%)	0	0	100	100
44	Lq	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
45	Lr	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
46	Ls	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
47	Lx	161/217 (74%)	143 (89%)	18 (11%)	0	100	100
50	SB	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
51	SC	61/69 (88%)	61 (100%)	0	0	100	100
52	SD	65/156 (42%)	64 (98%)	1 (2%)	0	100	100
53	SE	55/133 (41%)	55 (100%)	0	0	100	100
54	SF	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
55	SG	311/317 (98%)	300 (96%)	11 (4%)	0	100	100
56	SH	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
57	SL	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
58	SM	220/264 (83%)	216 (98%)	4 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	SN	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
60	SO	223/281 (79%)	220 (99%)	3 (1%)	0	100	100
61	SP	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
62	SQ	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
63	SR	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
64	SS	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
65	ST	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
66	SU	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
67	SV	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
68	SW	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
69	SX	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
70	SY	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
71	SZ	134/151 (89%)	128 (96%)	6 (4%)	0	100	100
72	Sa	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
73	Sb	139/172 (81%)	132 (95%)	7 (5%)	0	100	100
74	Sc	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
75	Sd	139/152 (91%)	136 (98%)	3 (2%)	0	100	100
76	Se	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
77	Sf	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
78	Sg	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
79	Sh	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
80	Si	136/143 (95%)	135 (99%)	1 (1%)	0	100	100
81	Sj	123/130 (95%)	123 (100%)	0	0	100	100
82	Sk	73/124 (59%)	71 (97%)	2 (3%)	0	100	100
83	Sl	23/25 (92%)	23 (100%)	0	0	100	100
All	All	11651/14208 (82%)	11395 (98%)	254 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	703	SER
31	Ld	15	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	102/761 (13%)	99 (97%)	3 (3%)	42	72
6	LD	195/199 (98%)	191 (98%)	4 (2%)	53	79
7	LE	344/347 (99%)	336 (98%)	8 (2%)	50	77
8	LF	302/337 (90%)	299 (99%)	3 (1%)	76	90
9	LG	247/250 (99%)	240 (97%)	7 (3%)	43	73
10	LH	216/251 (86%)	212 (98%)	4 (2%)	57	81
11	LI	197/215 (92%)	195 (99%)	2 (1%)	76	90
12	LJ	199/223 (89%)	196 (98%)	3 (2%)	65	85
13	LK	169/171 (99%)	167 (99%)	2 (1%)	71	88
14	LL	180/181 (99%)	178 (99%)	2 (1%)	73	89
15	LM	143/149 (96%)	142 (99%)	1 (1%)	84	93
16	LO	175/176 (99%)	172 (98%)	3 (2%)	60	83
17	LP	117/161 (73%)	113 (97%)	4 (3%)	37	69
18	LQ	171/172 (99%)	168 (98%)	3 (2%)	59	82
19	LR	171/173 (99%)	164 (96%)	7 (4%)	30	64
20	LS	139/163 (85%)	138 (99%)	1 (1%)	84	93
21	LT	164/165 (99%)	156 (95%)	8 (5%)	25	57
22	LU	159/175 (91%)	158 (99%)	1 (1%)	86	94
23	LV	154/154 (100%)	151 (98%)	3 (2%)	57	81
24	LW	139/140 (99%)	139 (100%)	0	100	100
25	LX	88/113 (78%)	88 (100%)	0	100	100
26	LY	106/107 (99%)	105 (99%)	1 (1%)	78	91
27	LZ	79/126 (63%)	79 (100%)	0	100	100
28	La	106/134 (79%)	106 (100%)	0	100	100
29	Lb	124/135 (92%)	122 (98%)	2 (2%)	62	84
30	Lc	117/118 (99%)	116 (99%)	1 (1%)	78	91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Ld	118/120 (98%)	116 (98%)	2 (2%)	60	83
32	Le	87/183 (48%)	83 (95%)	4 (5%)	27	59
33	Lf	92/98 (94%)	89 (97%)	3 (3%)	38	69
34	Lg	98/110 (89%)	94 (96%)	4 (4%)	30	64
35	Lh	116/121 (96%)	113 (97%)	3 (3%)	46	74
36	Li	89/89 (100%)	88 (99%)	1 (1%)	73	89
37	Lj	98/100 (98%)	95 (97%)	3 (3%)	40	70
38	Lk	109/110 (99%)	108 (99%)	1 (1%)	78	91
39	Ll	86/89 (97%)	84 (98%)	2 (2%)	50	77
40	Lm	73/80 (91%)	73 (100%)	0	100	100
41	Ln	64/65 (98%)	63 (98%)	1 (2%)	62	84
42	Lo	47/48 (98%)	45 (96%)	2 (4%)	29	62
43	Lp	47/115 (41%)	47 (100%)	0	100	100
44	Lq	92/93 (99%)	91 (99%)	1 (1%)	73	89
45	Lr	74/75 (99%)	72 (97%)	2 (3%)	44	74
46	Ls	109/120 (91%)	106 (97%)	3 (3%)	43	73
50	SB	75/76 (99%)	74 (99%)	1 (1%)	69	87
51	SC	56/62 (90%)	56 (100%)	0	100	100
52	SD	60/140 (43%)	60 (100%)	0	100	100
53	SE	47/106 (44%)	46 (98%)	1 (2%)	53	79
54	SF	88/98 (90%)	88 (100%)	0	100	100
55	SG	272/275 (99%)	268 (98%)	4 (2%)	65	85
56	SH	48/49 (98%)	48 (100%)	0	100	100
57	SL	182/243 (75%)	180 (99%)	2 (1%)	73	89
58	SM	203/231 (88%)	202 (100%)	1 (0%)	88	94
59	SN	185/223 (83%)	184 (100%)	1 (0%)	88	94
60	SO	189/232 (82%)	187 (99%)	2 (1%)	73	89
61	SP	224/225 (100%)	222 (99%)	2 (1%)	78	91
62	SQ	161/170 (95%)	158 (98%)	3 (2%)	57	81
63	SR	207/218 (95%)	206 (100%)	1 (0%)	88	94
64	SS	170/360 (47%)	167 (98%)	3 (2%)	59	82

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	ST	178/180 (99%)	174 (98%)	4 (2%)	52	78
66	SU	161/168 (96%)	158 (98%)	3 (2%)	57	81
67	SV	87/136 (64%)	86 (99%)	1 (1%)	73	89
68	SW	139/142 (98%)	137 (99%)	2 (1%)	67	86
69	SX	103/108 (95%)	101 (98%)	2 (2%)	57	81
70	SY	130/131 (99%)	127 (98%)	3 (2%)	50	77
71	SZ	106/119 (89%)	101 (95%)	5 (5%)	26	59
72	Sa	113/130 (87%)	111 (98%)	2 (2%)	59	82
73	Sb	117/140 (84%)	115 (98%)	2 (2%)	60	83
74	Sc	120/121 (99%)	117 (98%)	3 (2%)	47	75
75	Sd	122/131 (93%)	121 (99%)	1 (1%)	81	92
76	Se	112/114 (98%)	110 (98%)	2 (2%)	59	82
77	Sf	92/107 (86%)	91 (99%)	1 (1%)	73	89
78	Sg	67/67 (100%)	65 (97%)	2 (3%)	41	71
79	Sh	112/113 (99%)	110 (98%)	2 (2%)	59	82
80	Si	112/114 (98%)	109 (97%)	3 (3%)	44	74
81	Sj	107/112 (96%)	105 (98%)	2 (2%)	57	81
82	Sk	66/102 (65%)	65 (98%)	1 (2%)	65	85
83	Sl	24/24 (100%)	24 (100%)	0	100	100
All	All	9937/11879 (84%)	9770 (98%)	167 (2%)	62	83

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	SO	46	THR
71	SZ	91	THR
62	SQ	103	LEU
66	SU	5	ARG
74	Sc	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
46	Ls	6	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
58	SM	40	ASN
61	SP	179	ASN
57	SL	50	ASN
58	SM	118	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	160/163 (98%)	90 (56%)	6 (3%)
3	L5	3718/4808 (77%)	532 (14%)	3 (0%)
4	L7	118/120 (98%)	8 (6%)	0
48	S	45/855 (5%)	19 (42%)	4 (8%)
49	S2	1759/1870 (94%)	243 (13%)	2 (0%)
5	L8	155/158 (98%)	18 (11%)	0
All	All	5955/7974 (74%)	910 (15%)	15 (0%)

5 of 910 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	33	A
2	I	37	U
2	I	39	A
2	I	44	G
2	I	46	U

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	3549	A
49	S2	191	A
3	L5	4445	U
49	S2	1485	A
48	S	1113	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UR3	L5	4276	3	19,22,23	1.29	3 (15%)	26,32,35	1.24	2 (7%)
49	OMU	S2	1805	49	19,22,23	0.99	2 (10%)	26,31,34	1.76	4 (15%)
3	PSU	L5	3652	3	18,21,22	1.37	3 (16%)	22,30,33	1.88	5 (22%)
49	PSU	S2	687	49	18,21,22	1.41	3 (16%)	22,30,33	1.81	5 (22%)
3	OMC	L5	1284	3	19,22,23	1.18	2 (10%)	26,31,34	0.89	0
3	A2M	L5	1489	3	18,25,26	1.95	5 (27%)	18,36,39	2.11	4 (22%)
49	A2M	S2	1384	49	18,25,26	2.02	5 (27%)	18,36,39	2.17	4 (22%)
49	PSU	S2	93	49	18,21,22	1.41	3 (16%)	22,30,33	1.79	4 (18%)
3	A2M	L5	3557	3	18,25,26	1.96	5 (27%)	18,36,39	2.17	4 (22%)
3	PSU	L5	3462	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
49	A2M	S2	27	49	18,25,26	1.93	5 (27%)	18,36,39	2.22	4 (22%)
49	PSU	S2	864	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
7	HIC	LE	245	7	8,11,12	0.89	0	6,14,16	0.84	0
49	PSU	S2	1057	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
49	PSU	S2	1446	49	18,21,22	1.44	3 (16%)	22,30,33	1.81	4 (18%)
5	OMG	L8	75	5	18,26,27	1.99	2 (11%)	19,38,41	1.67	4 (21%)
3	OMG	L5	1580	3	18,26,27	1.95	2 (11%)	19,38,41	1.75	5 (26%)
3	OMU	L5	2680	3	19,22,23	1.01	2 (10%)	26,31,34	1.81	6 (23%)
49	A2M	S2	166	49	18,25,26	2.02	5 (27%)	18,36,39	2.16	5 (27%)
49	OMC	S2	1392	49	19,22,23	1.17	2 (10%)	26,31,34	0.96	1 (3%)
49	A2M	S2	513	49	18,25,26	1.96	5 (27%)	18,36,39	2.17	5 (27%)
3	OMC	L5	2704	3	19,22,23	1.15	2 (10%)	26,31,34	0.87	1 (3%)
3	PSU	L5	4058	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	2351	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	3466	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
80	HY3	Si	62	80	6,8,9	1.30	1 (16%)	5,10,12	1.40	1 (20%)
49	PSU	S2	650	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	105	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)
49	OMC	S2	174	49	19,22,23	1.17	2 (10%)	26,31,34	0.90	0
49	OMU	S2	172	49	19,22,23	0.99	2 (10%)	26,31,34	1.82	4 (15%)
3	PSU	L5	1731	3	18,21,22	1.37	3 (16%)	22,30,33	1.84	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	PSU	S2	109	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	OMU	S2	628	49	19,22,23	1.01	1 (5%)	26,31,34	1.84	5 (19%)
3	OMG	L5	4369	3	18,26,27	1.98	2 (11%)	19,38,41	1.69	4 (21%)
49	OMC	S2	463	49	19,22,23	1.18	2 (10%)	26,31,34	0.88	0
3	OMG	L5	4245	3	18,26,27	1.96	2 (11%)	19,38,41	1.67	4 (21%)
3	PSU	L5	4246	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	5 (22%)
49	PSU	S2	1644	49	18,21,22	1.43	3 (16%)	22,30,33	1.83	4 (18%)
3	A2M	L5	2244	3	18,25,26	2.01	5 (27%)	18,36,39	2.19	5 (27%)
49	PSU	S2	573	49	18,21,22	1.42	3 (16%)	22,30,33	1.81	4 (18%)
3	PSU	L5	1720	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
3	OMC	L5	2194	3	19,22,23	1.15	2 (10%)	26,31,34	0.94	1 (3%)
3	PSU	L5	4045	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	5MC	L5	4193	3	18,22,23	1.29	3 (16%)	26,32,35	1.48	4 (15%)
49	MA6	S2	1852	49	19,26,27	0.98	1 (5%)	18,38,41	1.75	5 (27%)
3	PSU	L5	3369	3	18,21,22	1.35	3 (16%)	22,30,33	1.85	4 (18%)
3	OMG	L5	3676	3	18,26,27	1.94	2 (11%)	19,38,41	1.76	5 (26%)
3	PSU	L5	4740	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
49	PSU	S2	1047	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	PSU	S2	1082	49	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
3	1MA	L5	1266	3	16,25,26	2.58	3 (18%)	18,37,40	2.30	3 (16%)
3	A2M	L5	4317	3	18,25,26	1.98	5 (27%)	18,36,39	2.13	4 (22%)
49	A2M	S2	1032	49	18,25,26	1.97	5 (27%)	18,36,39	2.17	4 (22%)
3	PSU	L5	3616	3	18,21,22	1.38	3 (16%)	22,30,33	1.90	5 (22%)
3	OMC	L5	4282	3	19,22,23	1.16	2 (10%)	26,31,34	0.94	1 (3%)
3	OMG	L5	3524	3	18,26,27	1.97	2 (11%)	19,38,41	1.67	4 (21%)
3	PSU	L5	1491	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
3	OMG	L5	3974	3	18,26,27	1.96	2 (11%)	19,38,41	1.72	5 (26%)
3	PSU	L5	3583	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	4 (18%)
3	PSU	L5	4203	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
49	A2M	S2	469	49	18,25,26	1.98	5 (27%)	18,36,39	2.19	5 (27%)
49	PSU	S2	119	49	18,21,22	1.43	3 (16%)	22,30,33	1.84	4 (18%)
3	OMC	L5	3619	19,3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
3	OMU	L5	3973	3	19,22,23	1.00	2 (10%)	26,31,34	1.83	6 (23%)
3	A2M	L5	3599	3	18,25,26	1.99	5 (27%)	18,36,39	2.21	5 (27%)
49	OMU	S2	1327	49	19,22,23	1.00	2 (10%)	26,31,34	1.81	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	A2M	L5	2206	3	18,25,26	1.97	5 (27%)	18,36,39	2.11	5 (27%)
49	OMC	S2	518	49	19,22,23	1.15	2 (10%)	26,31,34	0.92	1 (3%)
49	7MG	S2	1640	49	22,26,27	1.18	2 (9%)	29,39,42	2.13	9 (31%)
3	OMG	L5	4138	3	18,26,27	1.96	2 (11%)	19,38,41	1.73	5 (26%)
49	A2M	S2	591	49	18,25,26	1.99	5 (27%)	18,36,39	2.30	5 (27%)
3	PSU	L5	1718	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
49	OMG	S2	684	49	18,26,27	1.96	2 (11%)	19,38,41	1.69	5 (26%)
3	OMG	L5	3631	3	18,26,27	2.00	2 (11%)	19,38,41	1.68	4 (21%)
49	PSU	S2	1348	49	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
3	PSU	L5	4099	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	4 (18%)
3	PSU	L5	4166	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	A2M	S2	485	49	18,25,26	1.92	5 (27%)	18,36,39	2.17	5 (27%)
49	OMG	S2	1491	49	18,26,27	1.95	2 (11%)	19,38,41	1.67	4 (21%)
3	PSU	L5	3490	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)
5	PSU	L8	69	5	18,21,22	1.38	3 (16%)	22,30,33	1.85	4 (18%)
3	OMG	L5	2719	3	18,26,27	1.94	2 (11%)	19,38,41	1.69	4 (21%)
49	PSU	S2	652	49	18,21,22	1.42	3 (16%)	22,30,33	1.85	5 (22%)
3	PSU	L5	3500	3	18,21,22	1.42	3 (16%)	22,30,33	1.84	5 (22%)
3	OMC	L5	3540	3	19,22,23	1.14	2 (10%)	26,31,34	0.88	1 (3%)
3	OMU	L5	3657	44,3	19,22,23	0.99	2 (10%)	26,31,34	1.85	5 (19%)
44	MLZ	Lq	53	44	8,9,10	0.48	0	4,9,11	0.16	0
3	PSU	L5	3496	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	3576	3	18,21,22	1.39	3 (16%)	22,30,33	1.71	4 (18%)
49	PSU	S2	823	49	18,21,22	1.39	3 (16%)	22,30,33	1.80	5 (22%)
3	OMC	L5	3573	3	19,22,23	1.14	2 (10%)	26,31,34	0.90	0
57	SAC	SL	2	57	7,8,9	0.52	0	8,9,11	0.89	1 (12%)
49	PSU	S2	1175	49	18,21,22	1.41	3 (16%)	22,30,33	1.80	4 (18%)
3	OMU	L5	4244	3	19,22,23	1.02	2 (10%)	26,31,34	1.79	5 (19%)
78	AME	Sg	1	78	9,10,11	0.67	0	9,11,13	1.07	1 (11%)
32	MLZ	Le	5	32	8,9,10	0.49	0	4,9,11	0.19	0
3	OMC	L5	3433	3	19,22,23	1.17	2 (10%)	26,31,34	0.98	1 (3%)
49	PSU	S2	816	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
49	PSU	S2	1368	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	5MC	L5	3514	3	18,22,23	1.34	3 (16%)	26,32,35	1.24	3 (11%)
3	PSU	L5	4711	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GTP	L7	1	4	26,34,34	0.97	1 (3%)	32,54,54	1.24	2 (6%)
49	OMU	S2	121	49	19,22,23	1.01	2 (10%)	26,31,34	1.77	6 (23%)
49	OMG	S2	868	49	18,26,27	1.95	2 (11%)	19,38,41	1.67	4 (21%)
3	PSU	L5	1632	3	18,21,22	1.44	4 (22%)	22,30,33	1.70	4 (18%)
49	PSU	S2	34	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)
3	OMG	L5	3359	3	18,26,27	1.97	2 (11%)	19,38,41	1.72	5 (26%)
3	OMU	L5	4052	3	19,22,23	0.99	2 (10%)	26,31,34	1.78	4 (15%)
3	PSU	L5	4298	3	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
49	PSU	S2	1005	49	18,21,22	1.43	3 (16%)	22,30,33	1.82	4 (18%)
3	A2M	L5	1479	3	18,25,26	1.97	5 (27%)	18,36,39	2.19	4 (22%)
49	OMG	S2	602	49	18,26,27	1.97	2 (11%)	19,38,41	1.69	4 (21%)
3	PSU	L5	4267	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
49	MA6	S2	1851	49	19,26,27	0.95	1 (5%)	18,38,41	1.78	6 (33%)
49	PSU	S2	1693	49	18,21,22	1.41	3 (16%)	22,30,33	1.84	5 (22%)
3	OMG	L5	3942	3	18,26,27	1.96	2 (11%)	19,38,41	1.69	4 (21%)
3	OMG	L5	4240	3	18,26,27	1.98	2 (11%)	19,38,41	1.69	5 (26%)
75	SAC	Sd	2	75	7,8,9	0.54	0	8,9,11	0.85	1 (12%)
3	OMC	L5	2647	3	19,22,23	1.15	2 (10%)	26,31,34	1.01	1 (3%)
3	A2M	L5	3456	3	18,25,26	2.00	5 (27%)	18,36,39	2.13	4 (22%)
3	OMC	L5	2208	3	19,22,23	1.16	2 (10%)	26,31,34	0.95	1 (3%)
3	PSU	L5	4107	3	18,21,22	1.38	3 (16%)	22,30,33	1.80	4 (18%)
3	OMG	L5	2207	3	18,26,27	1.98	2 (11%)	19,38,41	1.62	4 (21%)
3	PSU	L5	3427	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
49	OMU	S2	116	49	19,22,23	1.00	2 (10%)	26,31,34	1.73	6 (23%)
49	4AC	S2	1338	49	21,24,25	1.10	2 (9%)	29,34,37	1.19	3 (10%)
49	PSU	S2	967	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	4 (18%)
49	PSU	S2	815	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
43	M3L	Lp	98	43	10,11,12	0.51	0	9,14,16	0.47	0
3	OMG	L5	4364	3	18,26,27	1.96	2 (11%)	19,38,41	1.70	4 (21%)
49	OMU	S2	429	49	19,22,23	1.01	2 (10%)	26,31,34	1.82	6 (23%)
3	PSU	L5	4149	3	18,21,22	1.36	3 (16%)	22,30,33	1.90	4 (18%)
3	A2M	L5	3562	3	18,25,26	1.98	5 (27%)	18,36,39	2.18	5 (27%)
3	PSU	L5	1683	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	5 (22%)
49	PSU	S2	1239	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
3	A2M	L5	2630	3	18,25,26	1.99	5 (27%)	18,36,39	2.29	6 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	L5	4169	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4322	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
49	6MZ	S2	1833	49	18,25,26	0.89	1 (5%)	16,36,39	1.79	4 (25%)
49	PSU	S2	682	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)
3	PSU	L5	3371	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	1537	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	OMG	L5	3476	3	18,26,27	1.97	2 (11%)	19,38,41	1.70	4 (21%)
3	A2M	L5	2658	3	18,25,26	1.98	5 (27%)	18,36,39	2.10	3 (16%)
3	PSU	L5	3585	3	18,21,22	1.39	3 (16%)	22,30,33	1.81	5 (22%)
3	A2M	L5	3492	49,3	18,25,26	2.03	5 (27%)	18,36,39	2.55	6 (33%)
3	PSU	L5	4382	3	18,21,22	1.38	3 (16%)	22,30,33	1.76	4 (18%)
3	PSU	L5	3494	3	18,21,22	1.42	3 (16%)	22,30,33	1.80	5 (22%)
3	PSU	L5	4419	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
49	PSU	S2	1626	49	18,21,22	1.42	3 (16%)	22,30,33	1.77	4 (18%)
3	PSU	L5	4177	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
3	PSU	L5	1638	3	18,21,22	1.38	3 (16%)	22,30,33	1.84	5 (22%)
3	PSU	L5	4278	3	18,21,22	1.48	2 (11%)	22,30,33	1.65	3 (13%)
49	4AC	S2	1843	49	21,24,25	1.12	2 (9%)	29,34,37	1.30	3 (10%)
3	6MZ	L5	3966	3	18,25,26	0.85	1 (5%)	16,36,39	2.10	4 (25%)
49	A2M	S2	577	49	18,25,26	1.97	5 (27%)	18,36,39	2.15	5 (27%)
49	PSU	S2	1178	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
3	OMG	L5	1477	3	18,26,27	1.96	2 (11%)	19,38,41	1.72	5 (26%)
49	OMC	S2	1704	49	19,22,23	1.17	2 (10%)	26,31,34	0.88	1 (3%)
3	A2M	L5	1810	3	18,25,26	1.97	5 (27%)	18,36,39	2.20	6 (33%)
49	A2M	S2	99	49	18,25,26	1.99	5 (27%)	18,36,39	2.20	5 (27%)
3	OMC	L5	1820	3	19,22,23	1.16	2 (10%)	26,31,34	0.93	0
3	OMU	L5	4366	3	19,22,23	0.99	2 (10%)	26,31,34	1.80	5 (19%)
8	AYA	LF	2	8	6,7,8	0.73	0	5,8,10	0.33	0
3	OMG	L5	2267	3	18,26,27	1.95	2 (11%)	19,38,41	1.68	4 (21%)
3	PSU	L5	3502	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
3	OMG	L5	4116	3	18,26,27	1.98	2 (11%)	19,38,41	1.70	4 (21%)
3	A2M	L5	400	3	18,25,26	1.99	5 (27%)	18,36,39	2.13	4 (22%)
49	PSU	S2	36	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)
3	OMU	L5	2258	3	19,22,23	1.01	2 (10%)	26,31,34	1.75	5 (19%)
3	A2M	L5	398	3	18,25,26	2.00	5 (27%)	18,36,39	2.15	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	A2M	S2	159	49	18,25,26	1.95	5 (27%)	18,36,39	2.14	5 (27%)
3	A2M	L5	4269	3	18,25,26	1.97	5 (27%)	18,36,39	2.24	6 (33%)
3	A2M	L5	3517	3	18,25,26	1.89	5 (27%)	18,36,39	2.23	5 (27%)
46	SAC	Ls	2	46	7,8,9	0.52	0	8,9,11	0.84	1 (12%)
3	A2M	L5	3450	3	18,25,26	1.94	5 (27%)	18,36,39	2.17	5 (27%)
49	OMU	S2	1443	49	19,22,23	0.99	2 (10%)	26,31,34	1.74	4 (15%)
3	PSU	L5	4042	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	5 (22%)
49	PSU	S2	210	49	18,21,22	1.45	3 (16%)	22,30,33	1.80	5 (22%)
3	OMC	L5	2265	3	19,22,23	1.15	2 (10%)	26,31,34	0.89	0
3	OMC	L5	4202	3	19,22,23	1.16	2 (10%)	26,31,34	0.91	1 (3%)
3	A2M	L5	4336	3	18,25,26	1.98	5 (27%)	18,36,39	2.16	5 (27%)
49	PSU	S2	610	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
76	NMM	Se	67	76	9,11,12	1.57	1 (11%)	6,12,14	3.46	2 (33%)
49	A2M	S2	669	49	18,25,26	1.87	4 (22%)	18,36,39	2.37	5 (27%)
3	PSU	L5	4188	3	18,21,22	1.37	3 (16%)	22,30,33	1.90	4 (18%)
49	PSU	S2	1046	49	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
3	OMG	L5	1260	3	18,26,27	1.98	2 (11%)	19,38,41	1.71	4 (21%)
3	PSU	L5	1721	3	18,21,22	1.41	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	3447	3	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
3	PSU	L5	4039	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	5 (22%)
49	OMU	S2	1289	49	19,22,23	0.98	2 (10%)	26,31,34	1.74	5 (19%)
49	PSU	S2	407	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
49	PSU	S2	218	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
49	OMG	S2	1329	49	18,26,27	1.94	2 (11%)	19,38,41	1.71	4 (21%)
49	PSU	S2	1233	49	18,21,22	1.42	3 (16%)	22,30,33	1.82	5 (22%)
49	OMG	S2	1448	49	18,26,27	1.93	2 (11%)	19,38,41	1.68	4 (21%)
3	OMC	L5	2667	3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
49	OMG	S2	510	49	18,26,27	1.94	2 (11%)	19,38,41	1.73	5 (26%)
3	PSU	L5	3554	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
49	OMU	S2	355	49	19,22,23	0.99	2 (10%)	26,31,34	1.78	5 (19%)
3	OMC	L5	3601	3	19,22,23	1.14	2 (10%)	26,31,34	0.96	2 (7%)
3	PSU	L5	4217	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	4 (18%)
3	OMG	L5	4383	3	18,26,27	1.98	2 (11%)	19,38,41	1.70	4 (21%)
3	PSU	L5	1799	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
49	OMG	S2	645	49	18,26,27	1.96	2 (11%)	19,38,41	1.73	5 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	OMG	S2	437	49	18,26,27	1.94	2 (11%)	19,38,41	1.71	4 (21%)
49	A2M	S2	1679	49	18,25,26	2.01	5 (27%)	18,36,39	2.16	5 (27%)
3	PSU	L5	1801	3	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
49	PSU	S2	1245	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
5	PSU	L8	55	5	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	2475	3	18,21,22	1.41	3 (16%)	22,30,33	1.87	4 (18%)
49	PSU	S2	867	49	18,21,22	1.42	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	4374	3	18,21,22	1.40	3 (16%)	22,30,33	1.88	5 (22%)
3	PSU	L5	4435	3	18,21,22	1.39	3 (16%)	22,30,33	1.89	5 (22%)
3	PSU	L5	4749	3	18,21,22	1.42	3 (16%)	22,30,33	1.82	4 (18%)
3	A2M	L5	1270	3	18,25,26	1.95	5 (27%)	18,36,39	2.20	5 (27%)
3	PSU	L5	4325	3	18,21,22	1.37	3 (16%)	22,30,33	1.85	5 (22%)
49	PSU	S2	802	49	18,21,22	1.43	3 (16%)	22,30,33	1.80	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
3	UR3	L5	4276	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	1805	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	3652	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	687	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	1284	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1489	3	-	3/5/27/28	0/3/3/3
49	A2M	S2	1384	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	93	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	3557	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3462	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	27	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	864	49	-	0/7/25/26	0/2/2/2
7	HIC	LE	245	7	-	2/5/6/8	0/1/1/1
49	PSU	S2	1057	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1446	49	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	0/5/27/28	0/3/3/3
3	OMG	L5	1580	3	-	2/5/27/28	0/3/3/3
3	OMU	L5	2680	3	-	0/9/27/28	0/2/2/2
49	A2M	S2	166	49	-	0/5/27/28	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	OMC	S2	1392	49	-	1/9/27/28	0/2/2/2
49	A2M	S2	513	49	-	0/5/27/28	0/3/3/3
3	OMC	L5	2704	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4058	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2351	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3466	3	-	0/7/25/26	0/2/2/2
80	HY3	Si	62	80	-	0/1/12/14	0/1/1/1
49	PSU	S2	650	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	105	49	-	0/7/25/26	0/2/2/2
49	OMC	S2	174	49	-	0/9/27/28	0/2/2/2
49	OMU	S2	172	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	1731	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	109	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	628	49	-	2/9/27/28	0/2/2/2
3	OMG	L5	4369	3	-	0/5/27/28	0/3/3/3
49	OMC	S2	463	49	-	0/9/27/28	0/2/2/2
3	OMG	L5	4245	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4246	3	-	2/7/25/26	0/2/2/2
49	PSU	S2	1644	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	2244	3	-	0/5/27/28	0/3/3/3
49	PSU	S2	573	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1720	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2194	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4045	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4193	3	-	4/7/25/26	0/2/2/2
49	MA6	S2	1852	49	-	2/7/29/30	0/3/3/3
3	PSU	L5	3369	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3676	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4740	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1047	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1082	49	-	0/7/25/26	0/2/2/2
3	1MA	L5	1266	3	-	0/3/25/26	0/3/3/3
3	A2M	L5	4317	3	-	0/5/27/28	0/3/3/3
49	A2M	S2	1032	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	3616	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4282	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3524	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1491	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3974	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3583	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4203	3	-	0/7/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A2M	S2	469	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	119	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	3619	19,3	-	1/9/27/28	0/2/2/2
3	OMU	L5	3973	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3599	3	-	1/5/27/28	0/3/3/3
49	OMU	S2	1327	49	-	0/9/27/28	0/2/2/2
3	A2M	L5	2206	3	-	0/5/27/28	0/3/3/3
49	OMC	S2	518	49	-	2/9/27/28	0/2/2/2
49	7MG	S2	1640	49	-	0/7/37/38	0/3/3/3
3	OMG	L5	4138	3	-	0/5/27/28	0/3/3/3
49	A2M	S2	591	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	1718	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	684	49	-	2/5/27/28	0/3/3/3
3	OMG	L5	3631	3	-	0/5/27/28	0/3/3/3
49	PSU	S2	1348	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4099	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4166	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	485	49	-	0/5/27/28	0/3/3/3
49	OMG	S2	1491	49	-	1/5/27/28	0/3/3/3
3	PSU	L5	3490	3	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	OMG	L5	2719	3	-	0/5/27/28	0/3/3/3
49	PSU	S2	652	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	3500	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3540	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	3657	44,3	-	0/9/27/28	0/2/2/2
44	MLZ	Lq	53	44	-	0/7/8/10	-
3	PSU	L5	3496	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3576	3	-	2/7/25/26	0/2/2/2
49	PSU	S2	823	49	-	2/7/25/26	0/2/2/2
3	OMC	L5	3573	3	-	0/9/27/28	0/2/2/2
57	SAC	SL	2	57	-	1/7/8/10	-
49	PSU	S2	1175	49	-	0/7/25/26	0/2/2/2
3	OMU	L5	4244	3	-	0/9/27/28	0/2/2/2
78	AME	Sg	1	78	-	2/9/10/12	-
32	MLZ	Le	5	32	-	1/7/8/10	-
3	OMC	L5	3433	3	-	4/9/27/28	0/2/2/2
49	PSU	S2	816	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1368	49	-	0/7/25/26	0/2/2/2
3	5MC	L5	3514	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4711	3	-	0/7/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	L7	1	4	-	0/18/38/38	0/3/3/3
49	OMU	S2	121	49	-	0/9/27/28	0/2/2/2
49	OMG	S2	868	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	1632	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	34	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3359	3	-	0/5/27/28	0/3/3/3
3	OMU	L5	4052	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4298	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1005	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	1479	3	-	0/5/27/28	0/3/3/3
49	OMG	S2	602	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	4267	3	-	2/7/25/26	0/2/2/2
49	MA6	S2	1851	49	-	1/7/29/30	0/3/3/3
49	PSU	S2	1693	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3942	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4240	3	-	0/5/27/28	0/3/3/3
75	SAC	Sd	2	75	-	0/7/8/10	-
3	OMC	L5	2647	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3456	3	-	0/5/27/28	0/3/3/3
3	OMC	L5	2208	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4107	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2207	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3427	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	116	49	-	0/9/27/28	0/2/2/2
49	4AC	S2	1338	49	-	4/11/29/30	0/2/2/2
49	PSU	S2	967	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	815	49	-	0/7/25/26	0/2/2/2
43	M3L	Lp	98	43	-	0/9/10/12	-
3	OMG	L5	4364	3	-	0/5/27/28	0/3/3/3
49	OMU	S2	429	49	-	4/9/27/28	0/2/2/2
3	PSU	L5	4149	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3562	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1239	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	2630	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4169	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4322	3	-	0/7/25/26	0/2/2/2
49	6MZ	S2	1833	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	682	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	3371	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1537	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3476	3	-	0/5/27/28	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	2658	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	3585	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3492	49,3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4382	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	3494	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4419	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1626	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4177	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1638	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4278	3	-	0/7/25/26	0/2/2/2
49	4AC	S2	1843	49	-	2/11/29/30	0/2/2/2
3	6MZ	L5	3966	3	-	0/5/27/28	0/3/3/3
49	A2M	S2	577	49	-	2/5/27/28	0/3/3/3
49	PSU	S2	1178	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	1477	3	-	0/5/27/28	0/3/3/3
49	OMC	S2	1704	49	-	0/9/27/28	0/2/2/2
3	A2M	L5	1810	3	-	0/5/27/28	0/3/3/3
49	A2M	S2	99	49	-	1/5/27/28	0/3/3/3
3	OMC	L5	1820	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4366	3	-	0/9/27/28	0/2/2/2
8	AYA	LF	2	8	-	2/4/6/8	-
3	OMG	L5	2267	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3502	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4116	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/5/27/28	0/3/3/3
49	PSU	S2	36	49	-	0/7/25/26	0/2/2/2
3	OMU	L5	2258	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	1/5/27/28	0/3/3/3
49	A2M	S2	159	49	-	0/5/27/28	0/3/3/3
3	A2M	L5	4269	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	3517	3	-	2/5/27/28	0/3/3/3
46	SAC	Ls	2	46	-	0/7/8/10	-
3	A2M	L5	3450	3	-	0/5/27/28	0/3/3/3
49	OMU	S2	1443	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4042	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	210	49	-	2/7/25/26	0/2/2/2
3	OMC	L5	2265	3	-	2/9/27/28	0/2/2/2
3	OMC	L5	4202	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4336	3	-	1/5/27/28	0/3/3/3
49	PSU	S2	610	49	-	0/7/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	NMM	Se	67	76	-	2/9/11/13	-
49	A2M	S2	669	49	-	3/5/27/28	0/3/3/3
3	PSU	L5	4188	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1046	49	-	2/7/25/26	0/2/2/2
3	OMG	L5	1260	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	1721	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3447	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4039	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	1289	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	407	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	218	49	-	0/7/25/26	0/2/2/2
49	OMG	S2	1329	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	1233	49	-	0/7/25/26	0/2/2/2
49	OMG	S2	1448	49	-	1/5/27/28	0/3/3/3
3	OMC	L5	2667	3	-	0/9/27/28	0/2/2/2
49	OMG	S2	510	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	3554	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	355	49	-	0/9/27/28	0/2/2/2
3	OMC	L5	3601	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4217	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4383	3	-	2/5/27/28	0/3/3/3
3	PSU	L5	1799	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	645	49	-	3/5/27/28	0/3/3/3
49	OMG	S2	437	49	-	0/5/27/28	0/3/3/3
49	A2M	S2	1679	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	1801	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1245	49	-	0/7/25/26	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	2475	3	-	2/7/25/26	0/2/2/2
49	PSU	S2	867	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4374	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4435	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4749	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1270	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	4325	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	802	49	-	2/7/25/26	0/2/2/2

The worst 5 of 610 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1266	1MA	C2-N3	8.88	1.39	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2207	OMG	C5-C6	-7.10	1.33	1.47
3	L5	3631	OMG	C5-C6	-7.06	1.33	1.47
3	L5	3524	OMG	C5-C6	-7.05	1.33	1.47
3	L5	4116	OMG	C5-C6	-7.04	1.33	1.47

The worst 5 of 869 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	Se	67	NMM	NE-CZ-NH2	-7.43	112.67	119.48
3	L5	1266	1MA	N1-C2-N3	-7.18	117.65	126.02
3	L5	4269	A2M	N3-C2-N1	-6.89	117.91	128.68
3	L5	1270	A2M	N3-C2-N1	-6.85	117.97	128.68
3	L5	2630	A2M	N3-C2-N1	-6.85	117.97	128.68

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	LE	245	HIC	CA-CB-CG-ND1
49	S2	429	OMU	C2'-C1'-N1-C2
49	S2	429	OMU	C2'-C1'-N1-C6
49	S2	577	A2M	C3'-C4'-C5'-O5'
49	S2	645	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	181:C	O3'	199:A	P	24.04
1	I	202:C	O3'	216:U	P	23.09



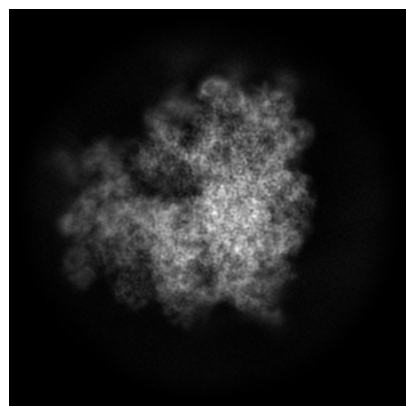
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14752. These allow visual inspection of the internal detail of the map and identification of artifacts.

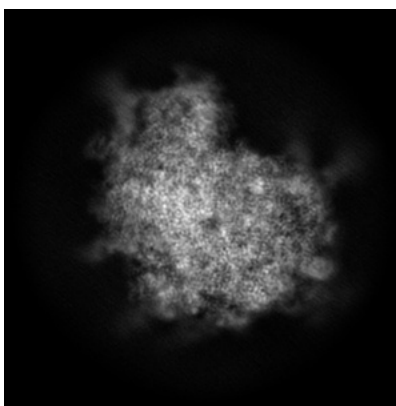
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

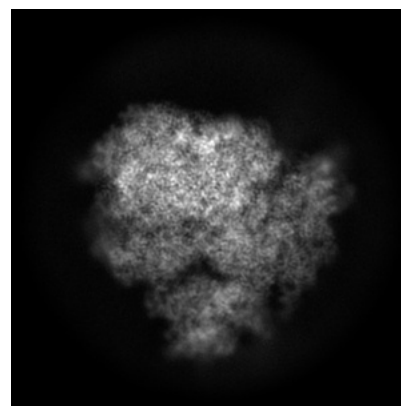
#### 6.1.1 Primary map



X

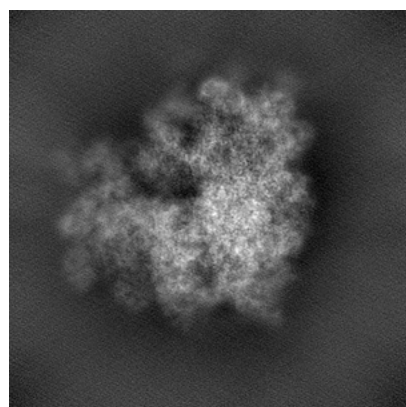


Y

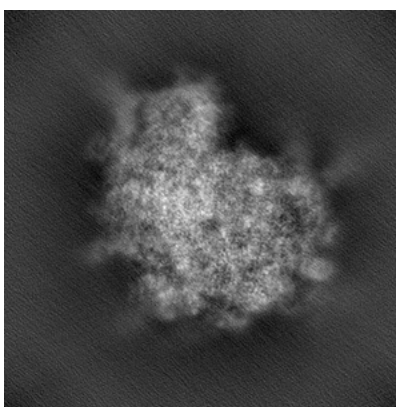


Z

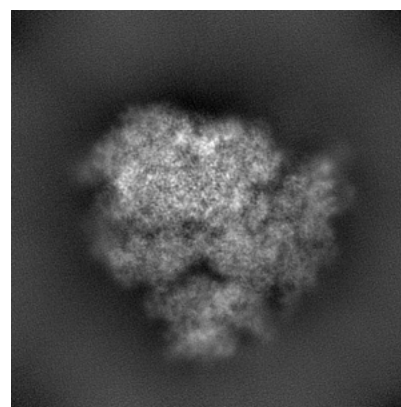
#### 6.1.2 Raw map



X



Y

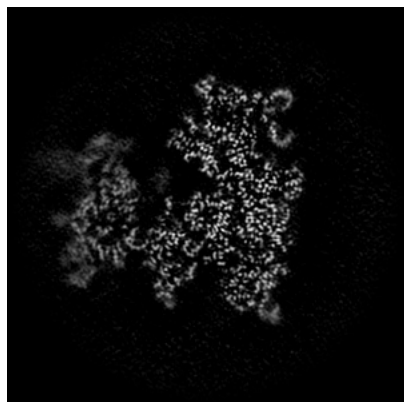


Z

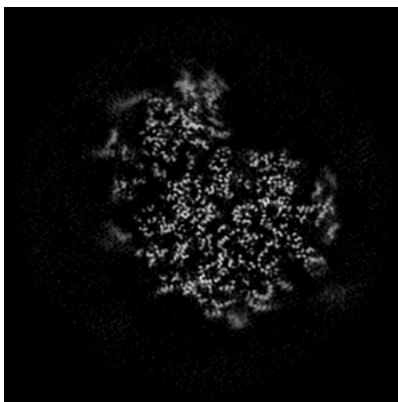
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

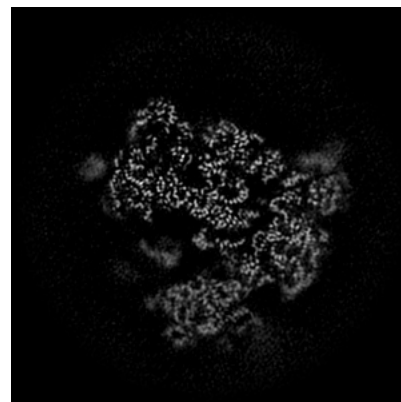
### 6.2.1 Primary map



X Index: 165

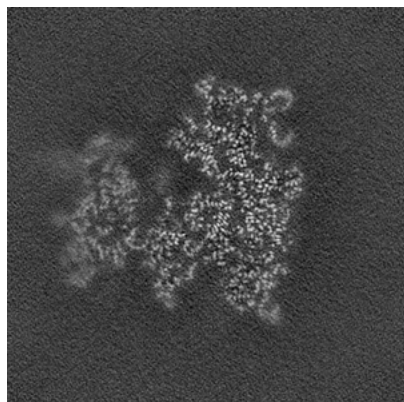


Y Index: 165

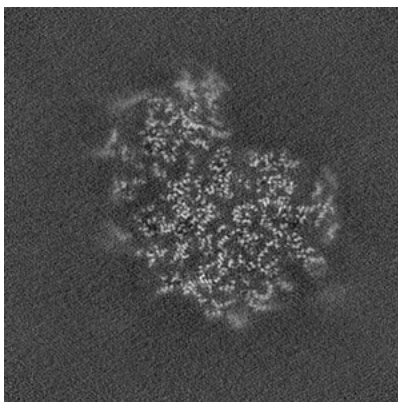


Z Index: 165

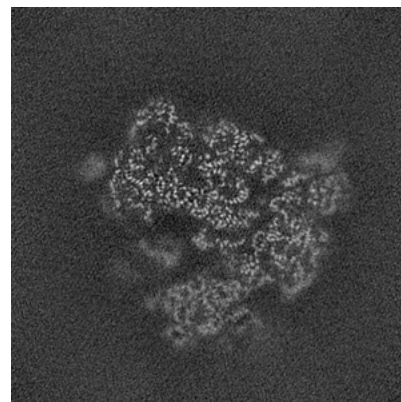
### 6.2.2 Raw map



X Index: 165



Y Index: 165

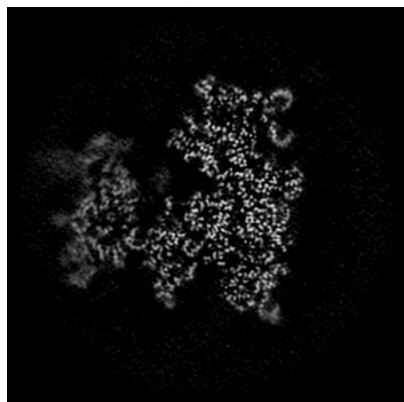


Z Index: 165

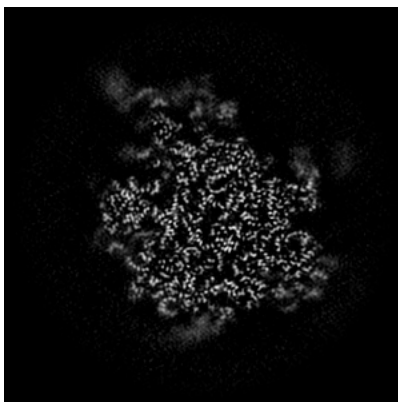
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

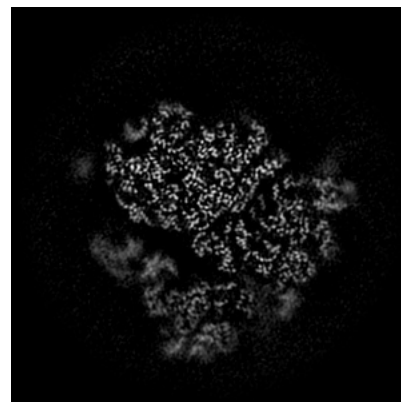
### 6.3.1 Primary map



X Index: 165

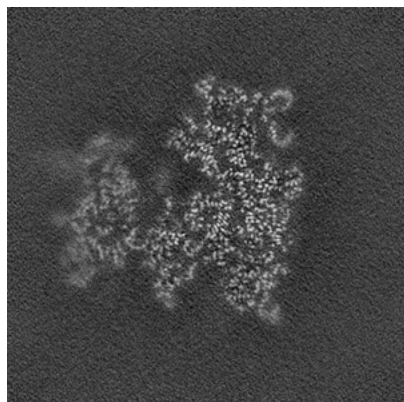


Y Index: 194

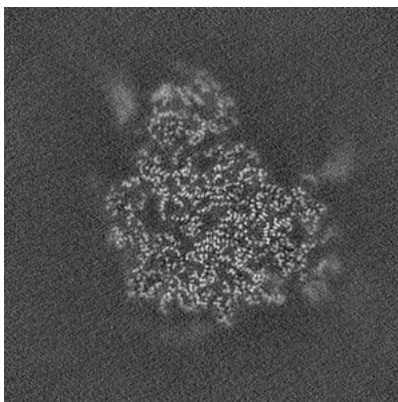


Z Index: 150

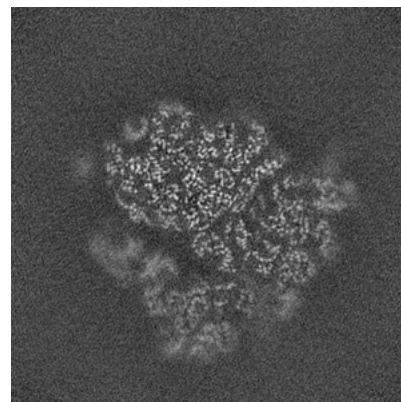
### 6.3.2 Raw map



X Index: 165



Y Index: 186



Z Index: 150

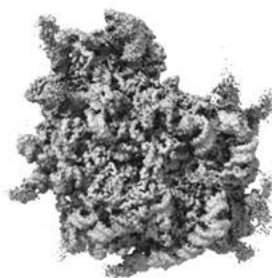
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



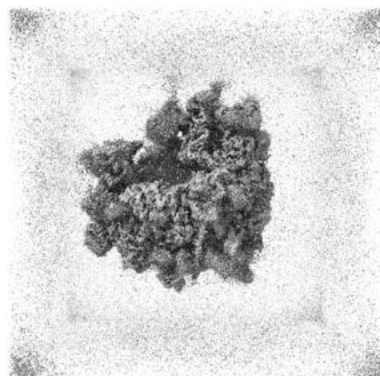
Y



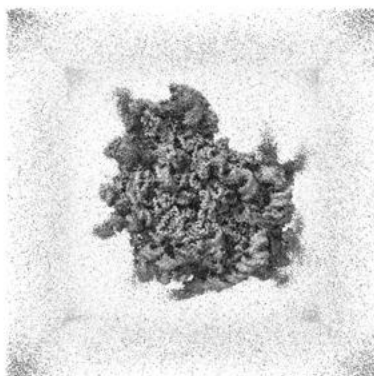
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

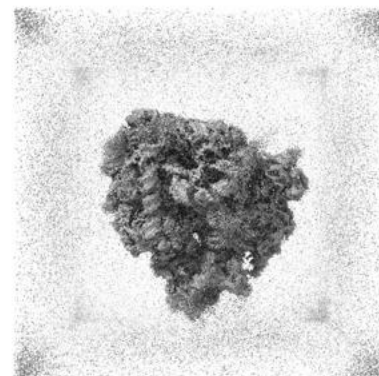
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Mask visualisation [i](#)

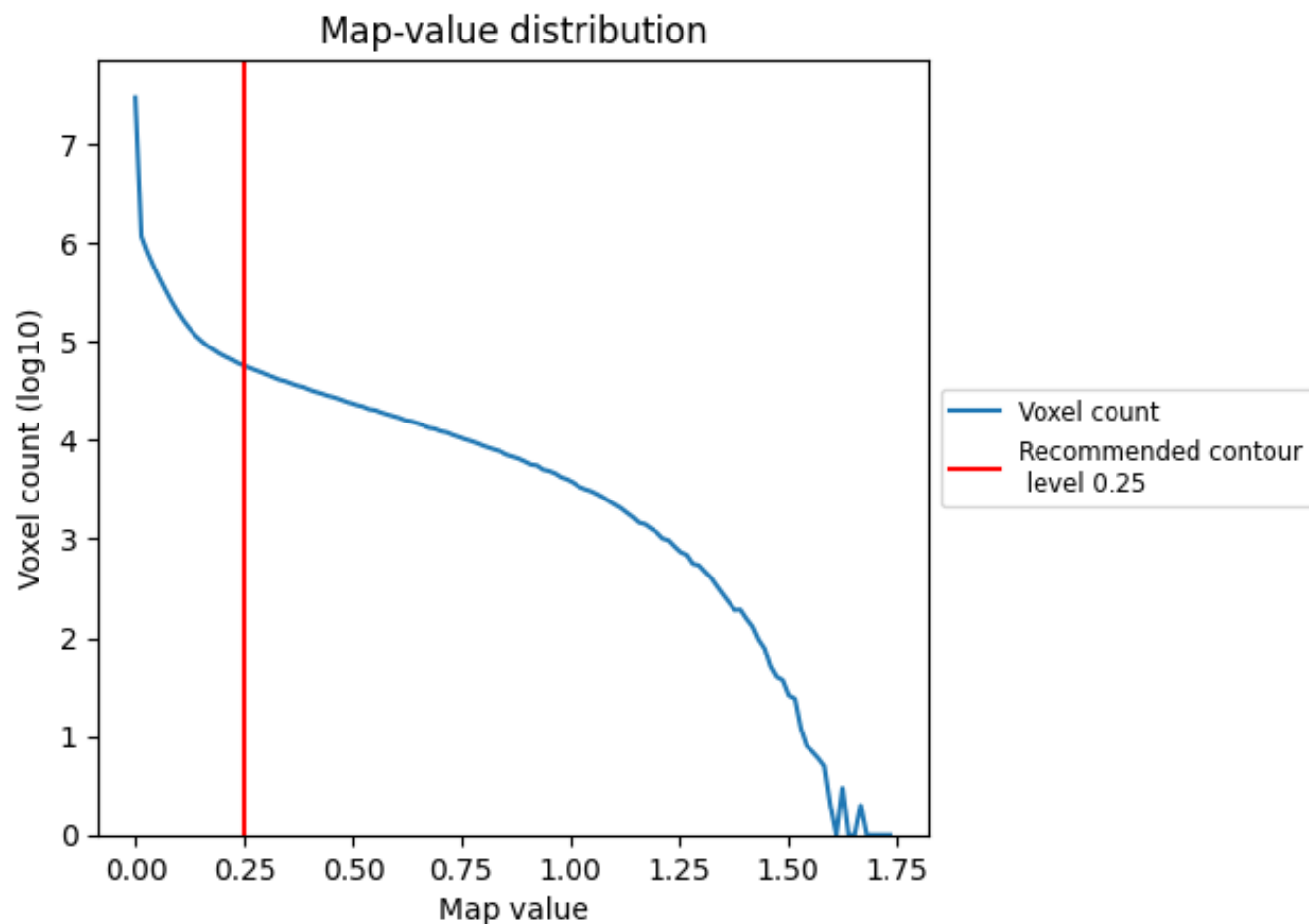
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

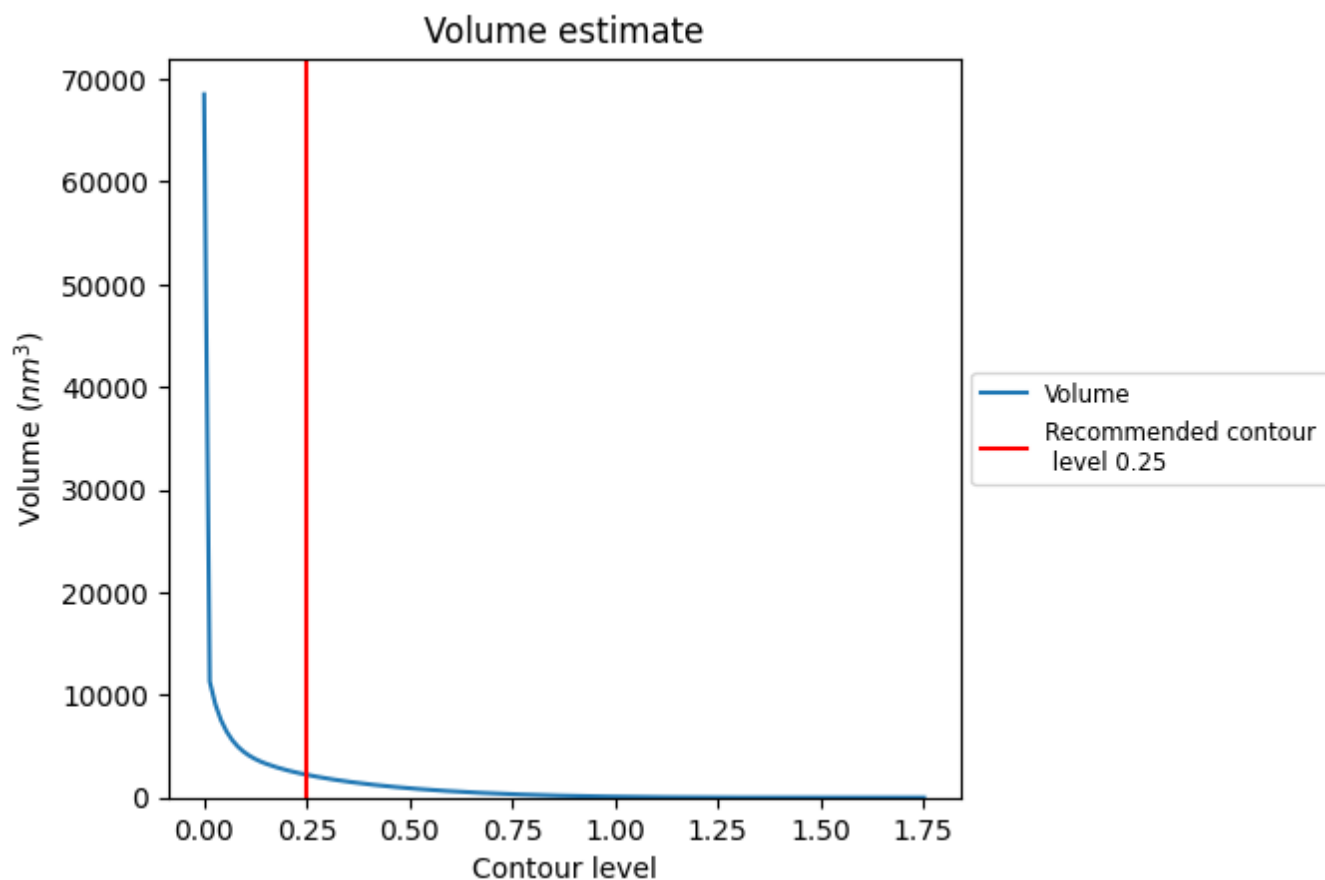
This section contains the results of statistical analysis of the map.

### 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.

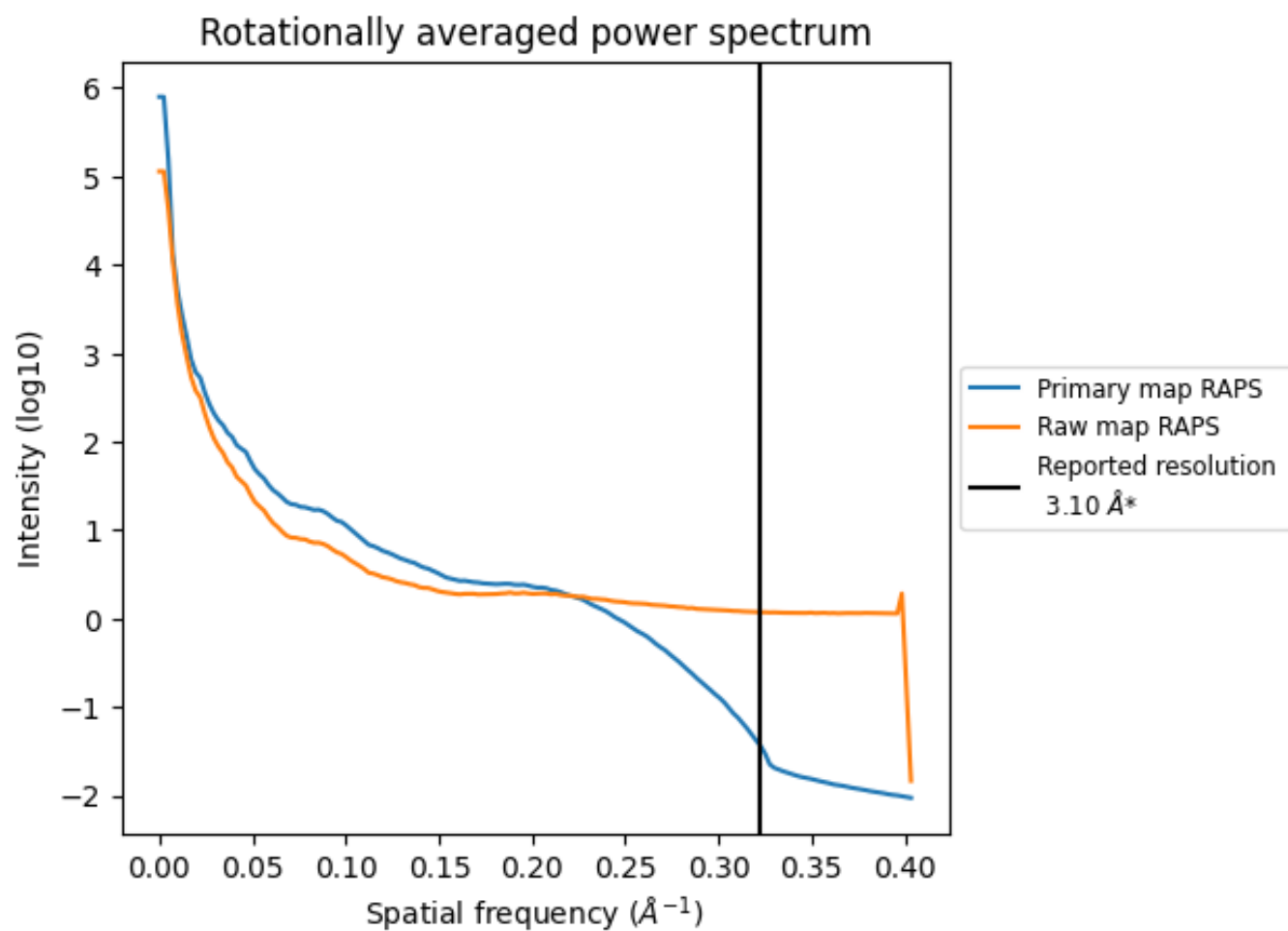
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2219 nm<sup>3</sup>; this corresponds to an approximate mass of 2005 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 ⓘ

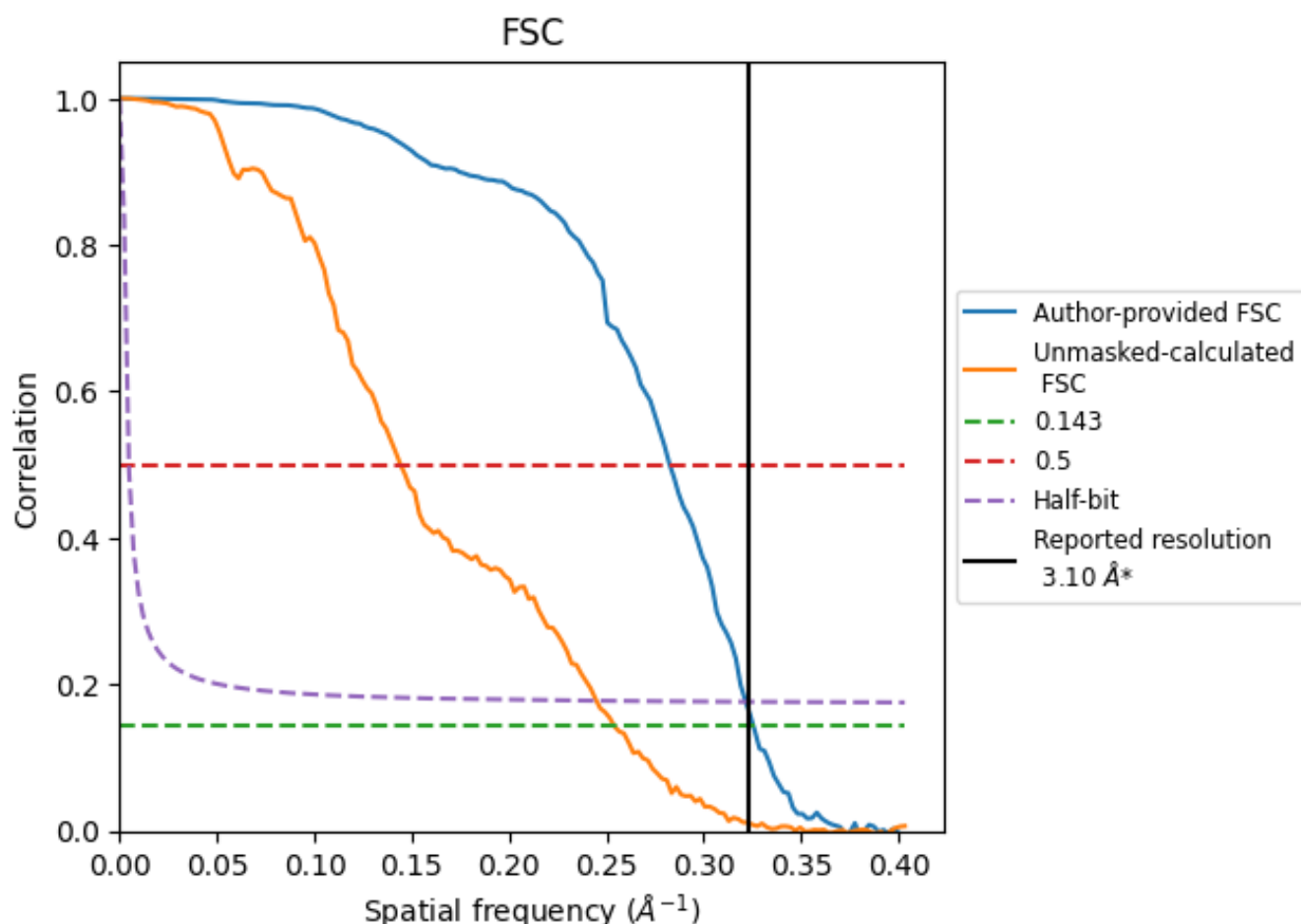


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

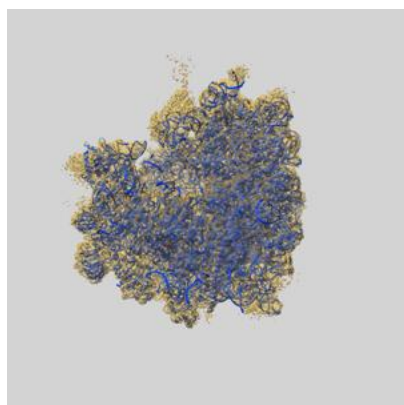
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.54	3.11
Unmasked-calculated*	3.94	6.93	4.08

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.1 by more than 10 %

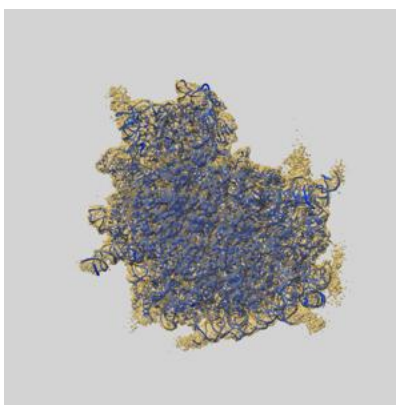
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14752 and PDB model 7ZJX. Per-residue inclusion information can be found in section [3](#) on page [21](#).

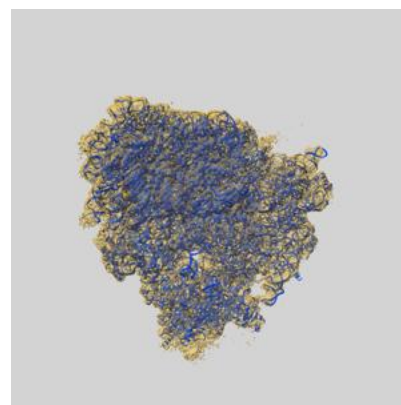
### 9.1 Map-model overlay [i](#)



X



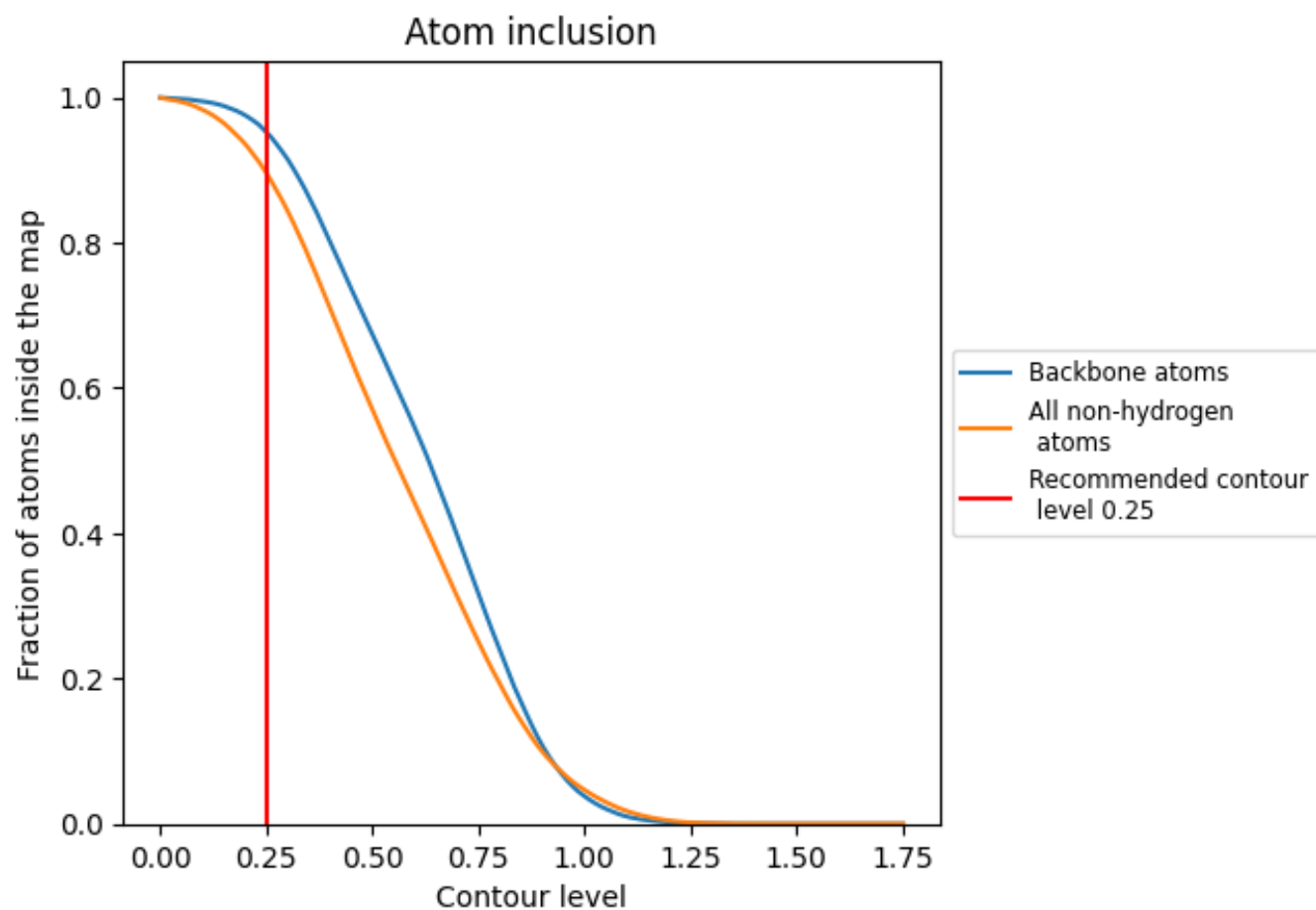
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.