



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 11:46 AM EST

PDB ID : 7LS2
EMDB ID : EMD-23501
Title : 80S ribosome from mouse bound to eEF2 (Class I)
Authors : Loerch, S.; Smith, P.R.; Kunder, N.; Stanowick, A.D.; Lou, T.-F.; Campbell, Z.T.
Deposited on : 2021-02-17
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

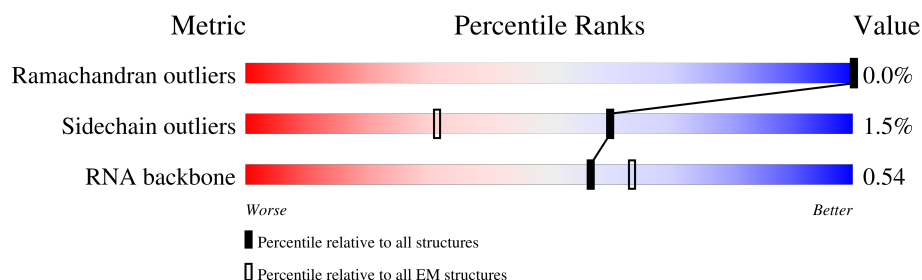
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.





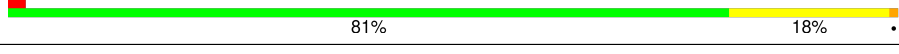
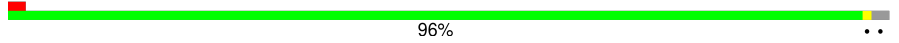
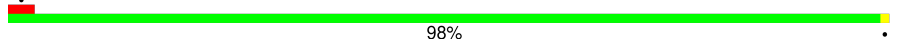

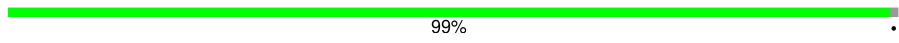
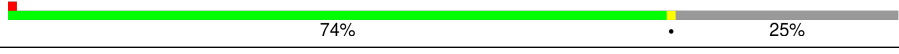
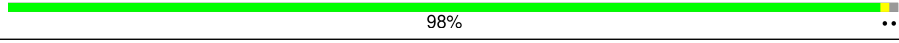

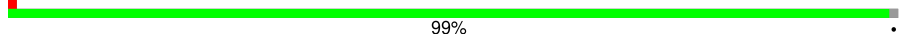
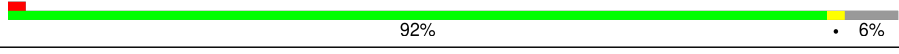
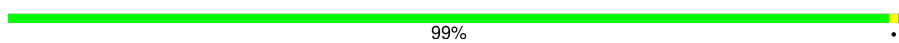
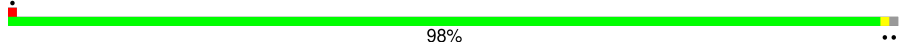





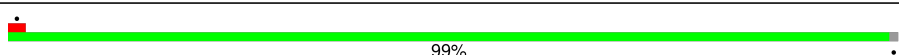
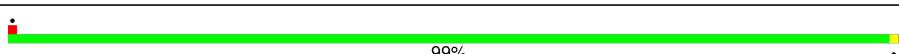
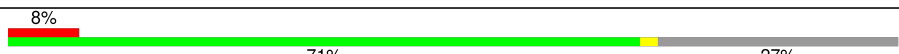



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A1	270	
2	B1	266	
3	C1	192	
4	D1	214	
5	E1	178	
6	F1	211	
7	G1	217	
8	H1	204	

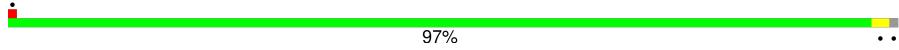
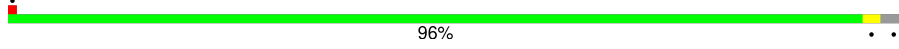
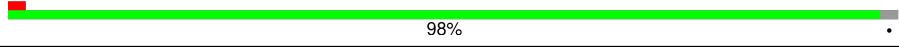
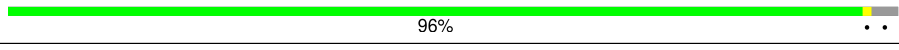

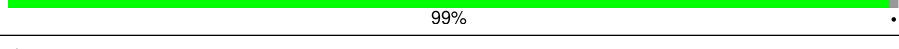
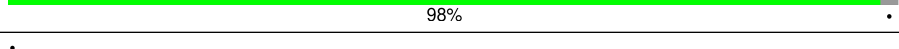
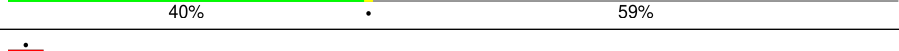
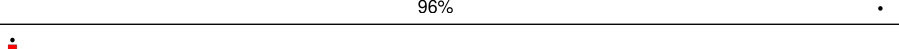
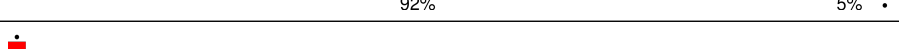
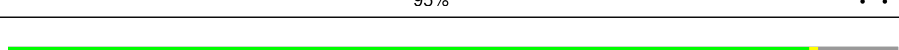

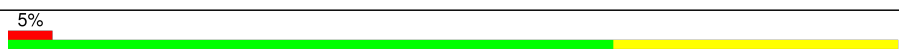

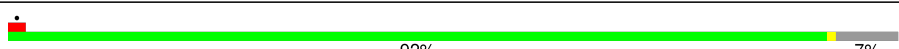
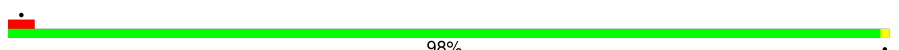
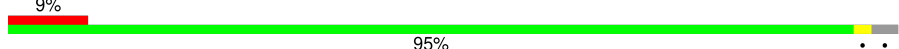
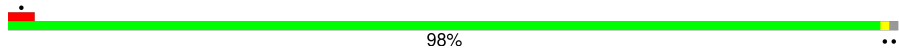

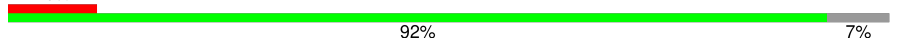
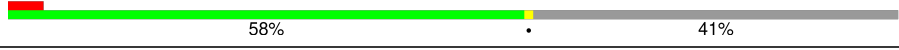
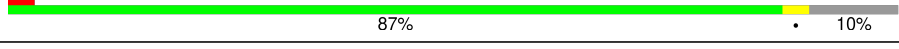
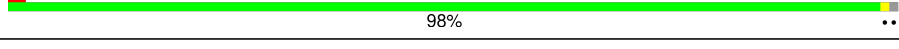
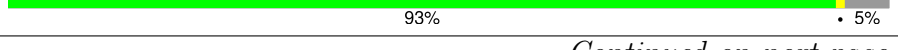

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Mol	Chain	Length	Quality of chain
9	A2	4731	
10	B2	121	
11	C2	156	
12	D2	257	
13	E2	403	
14	F2	419	
15	G2	297	
16	H2	296	
17	I2	203	
18	J2	184	
19	K2	188	
20	L2	196	
21	M2	176	
22	N2	160	
23	O2	128	
24	P2	140	
25	Q2	157	
26	R2	156	
27	S2	145	
28	T2	136	
29	U2	148	
30	V2	160	
31	W2	115	
32	X2	125	
33	Y2	135	

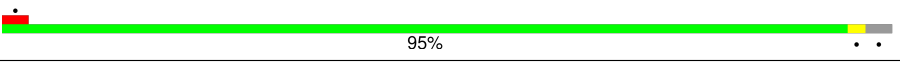

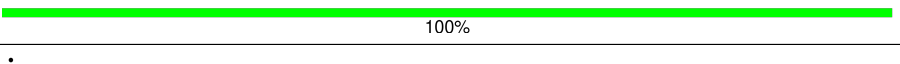
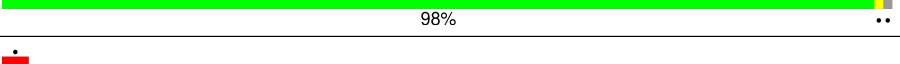

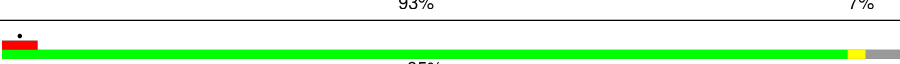
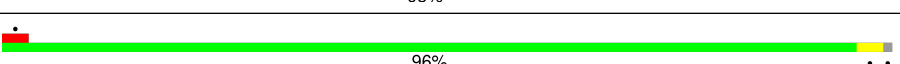
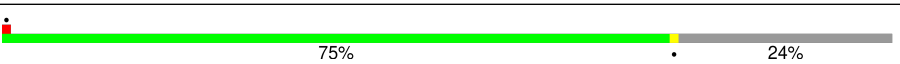

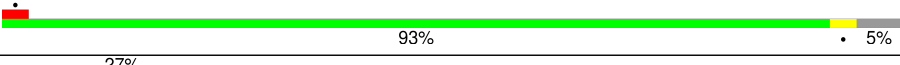
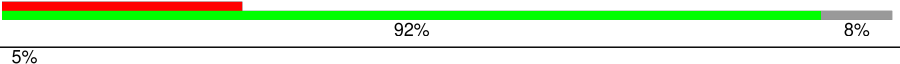
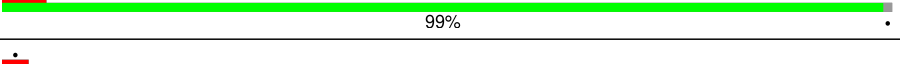

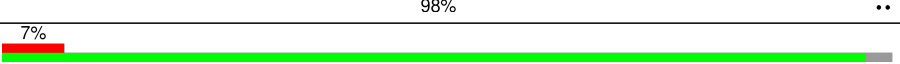
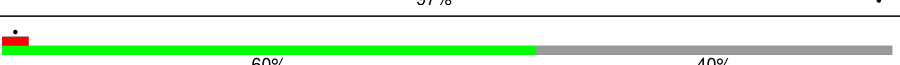
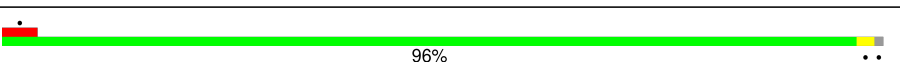


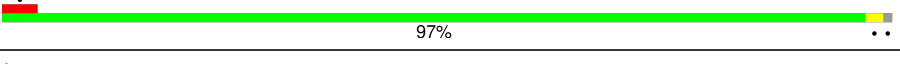

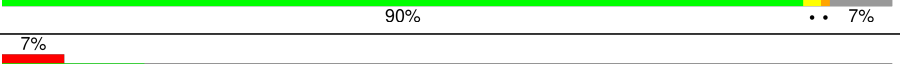

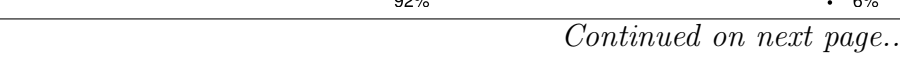


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Mol	Chain	Length	Quality of chain
34	Z2	110	
35	a2	117	
36	b2	123	
37	c2	105	
38	d2	97	
39	e2	70	
40	f2	51	
41	g2	128	
42	h2	25	
43	i2	106	
44	j2	92	
45	k2	137	
46	m2	1871	
47	n2	75	
48	p2	264	
49	q2	243	
50	r2	263	
51	w2	158	
52	z2	135	
53	o2	295	
54	s2	204	
55	v2	165	
56	x2	145	
57	y2	146	
58	A3	152	

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Mol	Chain	Length	Quality of chain
59	B3	145	
60	C3	119	
61	D3	83	
62	E3	143	
63	F3	115	
64	G3	69	
65	H3	56	
66	I3	317	
67	J3	293	
68	K3	249	
69	L3	194	
70	M3	132	
71	N3	151	
72	O3	151	
73	P3	130	
74	Q3	133	
75	R3	125	
76	S3	84	
77	T3	133	
78	U3	156	
79	m	858	
80	j	317	
81	k	165	
82	A	386	
83	t	194	

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Mol	Chain	Length	Quality of chain
84	u	208	<div><div></div><div>7%</div><div>97%</div><div>..</div></div>
85	L1	217	<div><div></div><div>29%</div><div>92%</div><div>• 5%</div></div>

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 227130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	222	Total	C	N	O	S	1	0
			1851	1190	356	297	8		

- Molecule 2 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	230	Total	C	N	O	S	1	0
			1863	1188	359	312	4		

- Molecule 3 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	190	Total	C	N	O	S	0	0
			1519	956	284	273	6		

- Molecule 4 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	208	Total	C	N	O	S	0	0
			1690	1073	327	278	12		

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	174	Total	C	N	O	S	0	0
			1397	880	260	251	6		

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	207	Total	C	N	O	S	0	0
			1676	1048	344	280	4		

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	139	Total	C	N	O	S	0	0
			1143	732	221	183	7		

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 9 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A2	3706	Total	C	N	O	P	0	0
			79519	35463	14497	25854	3705		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B2	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 11 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C2	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 12 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D2	251	Total	C	N	O	S	0	0
			1921	1204	393	318	6		

- Molecule 13 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E2	402	Total	C	N	O	S	0	0
			3238	2060	609	555	14		

- Molecule 14 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F2	367	Total	C	N	O	S	0	0
			2928	1842	583	488	15		

- Molecule 15 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G2	293	Total	C	N	O	S	0	0
			2385	1506	440	425	14		

- Molecule 16 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H2	221	Total	C	N	O	S	0	0
			1789	1145	342	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I2	201	Total	C	N	O	S	0	0
			1640	1055	320	259	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J2	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K2	186	Total	C	N	O	S	0	0
			1511	946	313	248	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L2	184	Total	C	N	O	S	0	0
			1542	955	332	246	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M2	175	Total	C	N	O	S	0	0
			1450	924	283	233	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N2	159	Total	C	N	O	S	0	0
			1298	823	253	216	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O2	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P2	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q2	110	Total	C	N	O	S	0	0
			895	563	180	148	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U2	147	Total	C	N	O	S	0	0
			1164	736	239	185	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V2	117	Total	C	N	O	S	0	0
			945	596	198	146	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W2	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X2	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y2	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z2	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a2	114	Total	C	N	O	S	0	0
			906	565	187	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b2	120	Total	C	N	O	S	0	0
			1001	634	201	165	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c2	102	Total	C	N	O	S	0	0
			827	516	173	133	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e2	69	Total	C	N	O	S	0	0
			568	365	103	99	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f2	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g2	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h2	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i2	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j2	89	Total	C	N	O	S	0	0
			694	436	133	118	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k2	125	Total	C	N	O	S	0	0
			1001	621	207	168	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m2	1724	Total	C	N	O	P	0	0
			36817	16440	6606	12048	1723		

- Molecule 47 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n2	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p2	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q2	226	Total	C	N	O	S	0	0
			1756	1119	316	314	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r2	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 51 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w2	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 52 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z2	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	o2	214	Total	C	N	O	S	0	0
			1694	1077	297	312	8		

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	s2	189	Total	C	N	O	S	0	0
			1496	934	285	270	7		

- Molecule 55 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v2	97	Total	C	N	O	S	0	0
			819	534	147	133	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x2	130	Total	C	N	O	S	0	0
			1073	681	205	180	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y2	144	Total	C	N	O	S	0	0
			1143	726	216	198	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	A3	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 59 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B3	141	Total	C	N	O	S	0	0
			1104	691	215	196	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	C3	102	Total	C	N	O	S	0	0
			807	507	153	143	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	D3	83	Total	C	N	O	S	0	0
			638	392	119	122	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	E3	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	F3	100	Total	C	N	O	S	1	0
			811	506	169	131	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	G3	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	H3	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
66	I3	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
67	J3	222	Total	C	N	O	S	0	0
			1725	1116	298	302	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	K3	227	Total	C	N	O	S	0	0
			1840	1149	367	317	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
69	L3	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	M3	122	Total	C	N	O	S	0	0
			942	593	164	177	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
71	N3	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
72	O3	134	Total	C	N	O	S	0	0
			1002	612	197	187	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
73	P3	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Q3	129	Total	C	N	O	S	0	0
			1049	662	206	176	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	R3	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
76	S3	83	Total	C	N	O	S	0	0
			652	409	121	115	7		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	T3	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
78	U3	62	Total	C	N	O	S	0	0
			505	317	96	85	7		

- Molecule 79 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	m	851	Total	C	N	O	S	0	0
			6649	4217	1146	1242	44		

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	j	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 81 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	k	153	Total	C	N	O	S	0	0
			1159	721	218	217	3		

- Molecule 82 is a protein called Isoform 3 of Plasminogen activator inhibitor 1 RNA-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	A	61	Total	C	N	O	0	0
			486	289	94	103		

- Molecule 83 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	t	183	Total	C	N	O	S	0	0
			1477	944	270	262	1		

- Molecule 84 is a protein called 40S ribosomal protein S8.

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

- Molecule 85 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	L1	206	Total	C	N	O	S	0	0
			1660	1061	300	291	8		

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

Mol	Chain	Residues	Atoms		AltConf
86	d2	1	Total	Zn	0
			1	1	
86	g2	1	Total	Zn	0
			1	1	
86	i2	1	Total	Zn	0
			1	1	
86	j2	1	Total	Zn	0
			1	1	
86	F3	1	Total	Zn	0
			1	1	
86	H3	1	Total	Zn	0
			1	1	
86	U3	1	Total	Zn	0
			1	1	

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	H3	1	Total	Mg	0
			1	1	

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltCon
88	m	1	Total	C	N	O	P	0
			28	10	5	11	2	

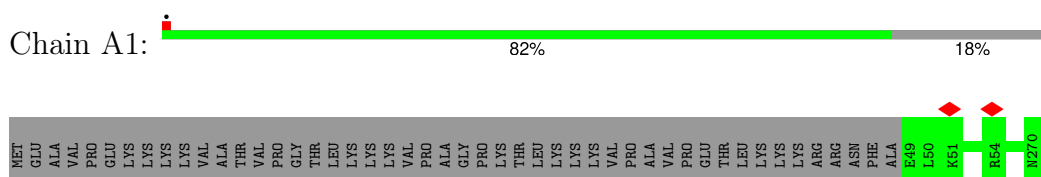
- Molecule 89 is water.

Mol	Chain	Residues	Atoms	AltConf
89	B1	1	Total O 1 1	0
89	A2	1	Total O 1 1	0
89	m2	2	Total O 2 2	0

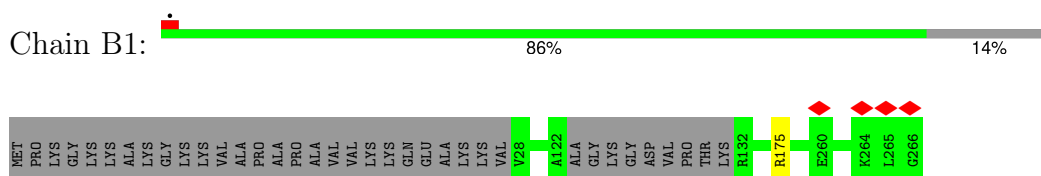
3 Residue-property plots [i](#)

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

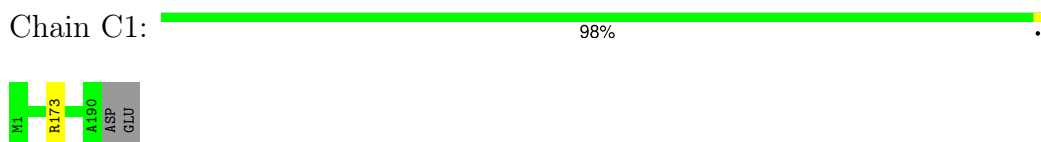
- Molecule 1: 60S ribosomal protein L7



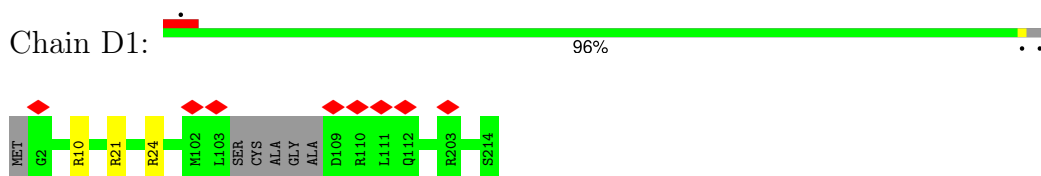
- Molecule 2: 60S ribosomal protein L7a



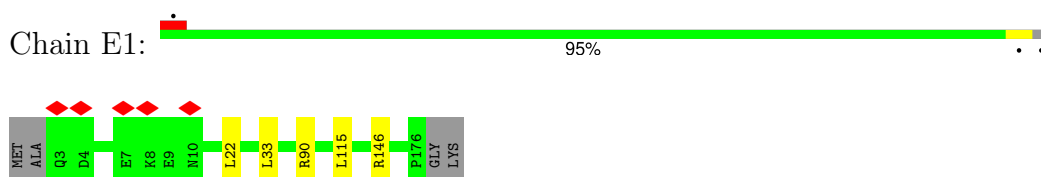
- Molecule 3: 60S ribosomal protein L9



- Molecule 4: 60S ribosomal protein L10-like

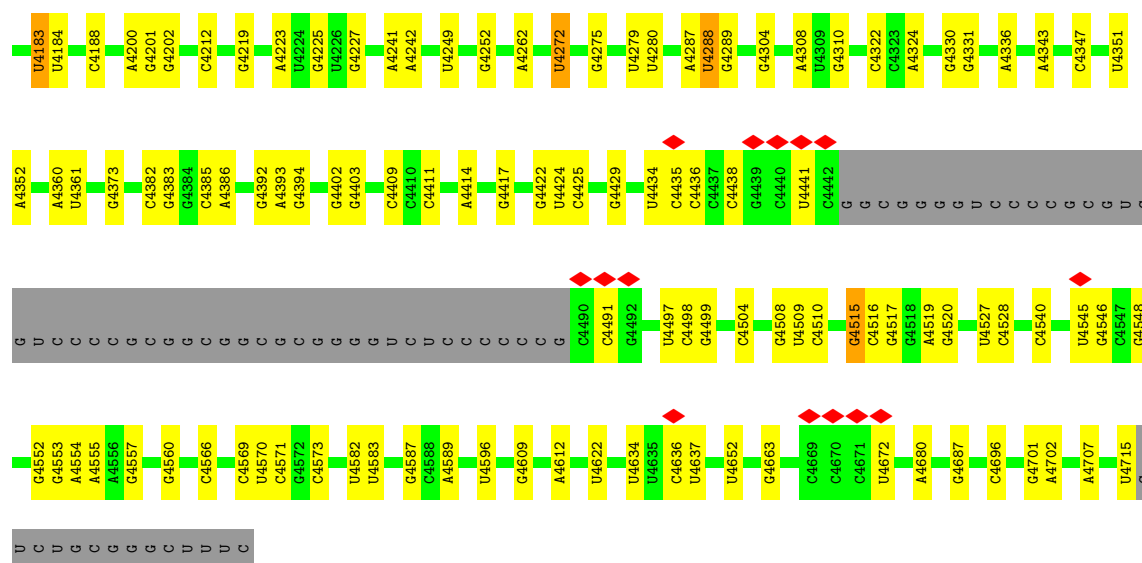


- Molecule 5: 60S ribosomal protein L11

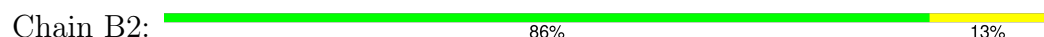




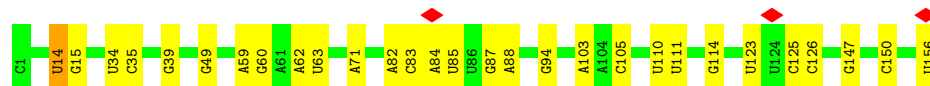
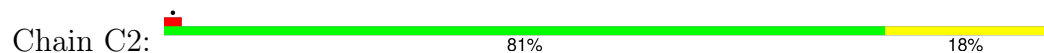




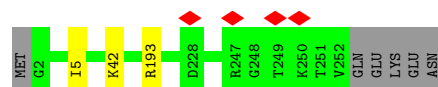
- Molecule 10: 5S rRNA



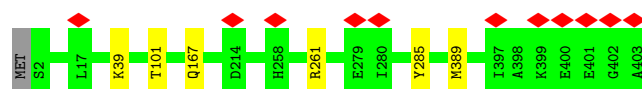
- Molecule 11: 5.8S rRNA



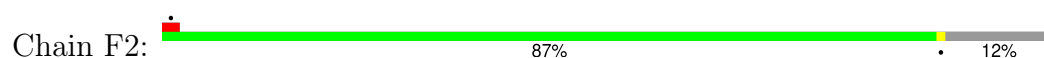
- Molecule 12: 60S ribosomal protein L8

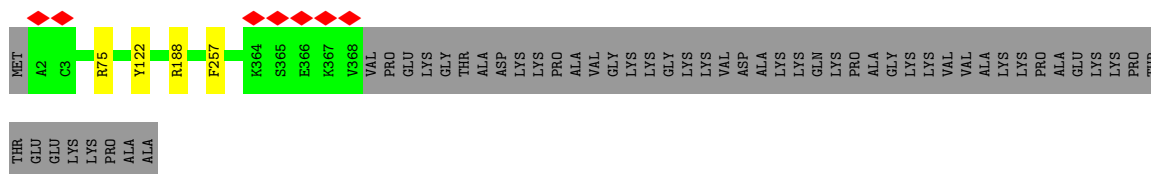


- Molecule 13: 60S ribosomal protein L3



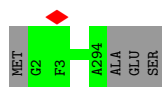
- Molecule 14: 60S ribosomal protein L4






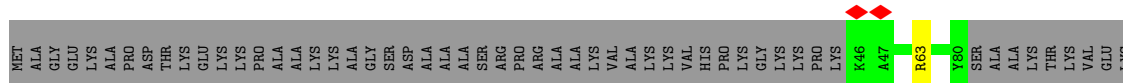
- Molecule 15: 60S ribosomal protein L5

Chain G2:  99%



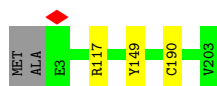
- Molecule 16: 60S ribosomal protein L6

Chain H2:  74%




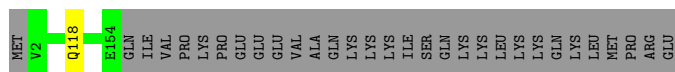
- Molecule 17: 60S ribosomal protein L13a

Chain I2:  98%



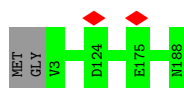
- Molecule 18: 60S ribosomal protein L17

Chain J2:  83%



- Molecule 19: 60S ribosomal protein L18

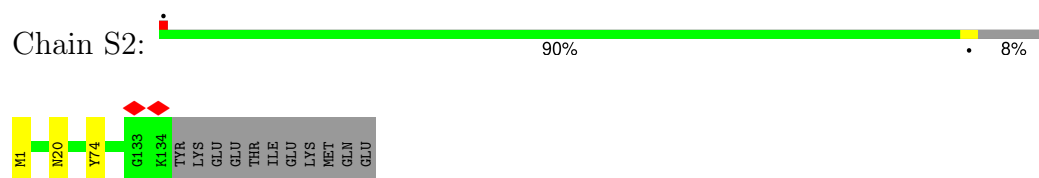
Chain K2:  99%



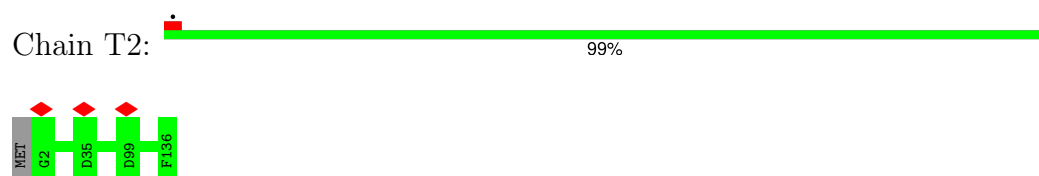
- Molecule 20: 60S ribosomal protein L19

Chain L2:  92%

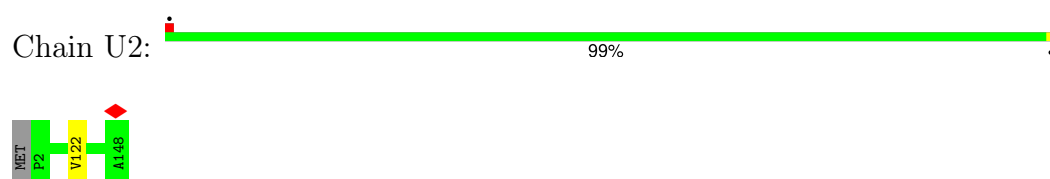
- Molecule 27: 60S ribosomal protein L26



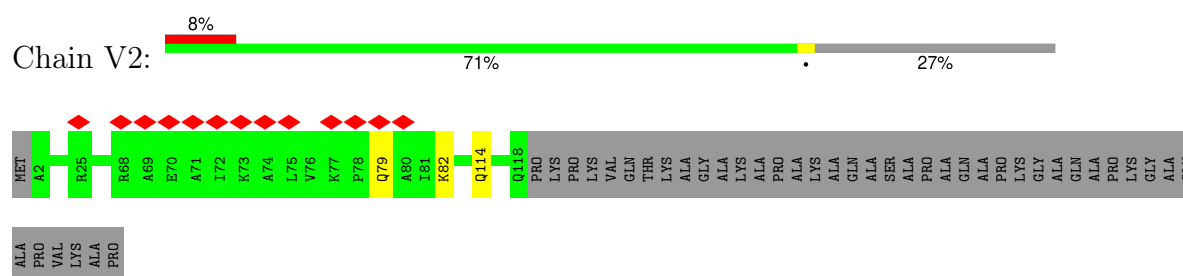
- Molecule 28: 60S ribosomal protein L27



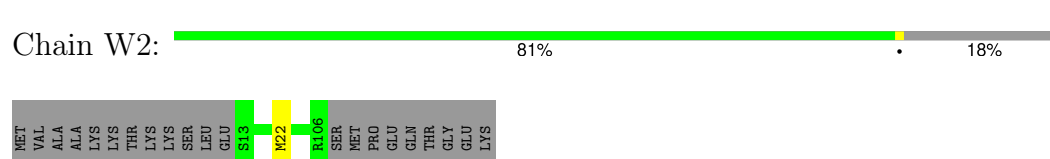
- Molecule 29: 60S ribosomal protein L27a



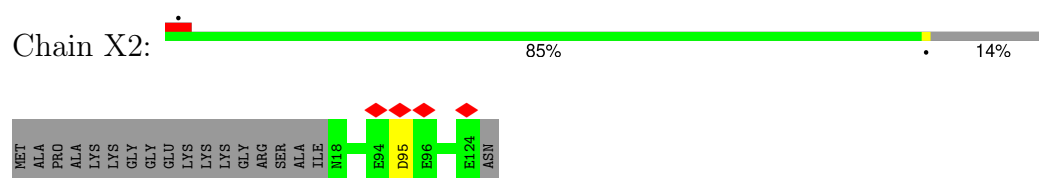
- Molecule 30: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L30

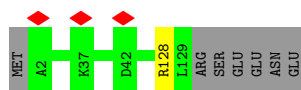


- Molecule 32: 60S ribosomal protein L31



- Molecule 33: 60S ribosomal protein L32

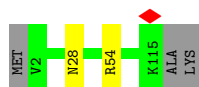




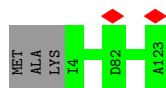
- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



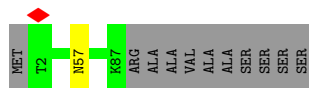
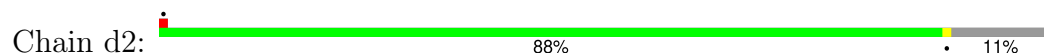
- Molecule 36: 60S ribosomal protein L35



- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37

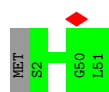


- Molecule 39: 60S ribosomal protein L38



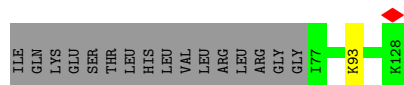
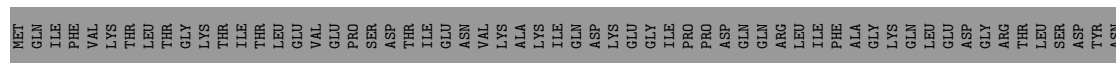
- Molecule 40: 60S ribosomal protein L39

Chain f2:  98%



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain g2:  40% 59%



- Molecule 42: 60S ribosomal protein L41

Chain h2:  96%



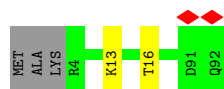
- Molecule 43: 60S ribosomal protein L36a

Chain i2:  92% 5%



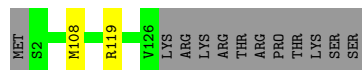
- Molecule 44: 60S ribosomal protein L37a

Chain j2:  95%



- Molecule 45: 60S ribosomal protein L28

Chain k2:  90% 9%



- Molecule 46: 18S rRNA

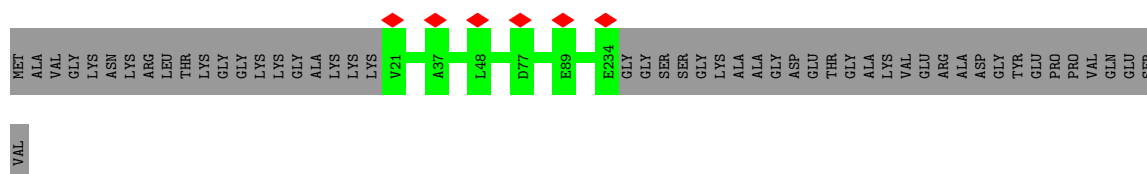
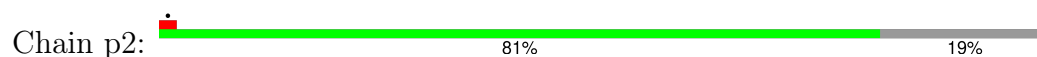
Chain m2:  71% 21% 8%



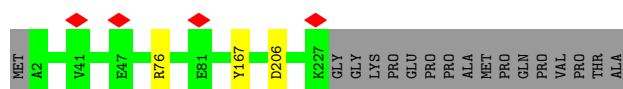
- Molecule 47: tRNA



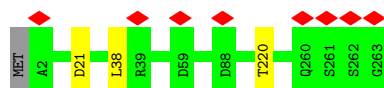
- Molecule 48: 40S ribosomal protein S3a



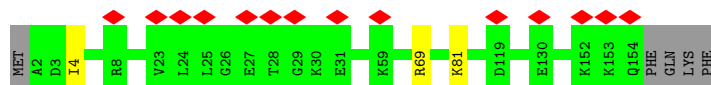
- Molecule 49: 40S ribosomal protein S3



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




- Molecule 51: 40S ribosomal protein S11

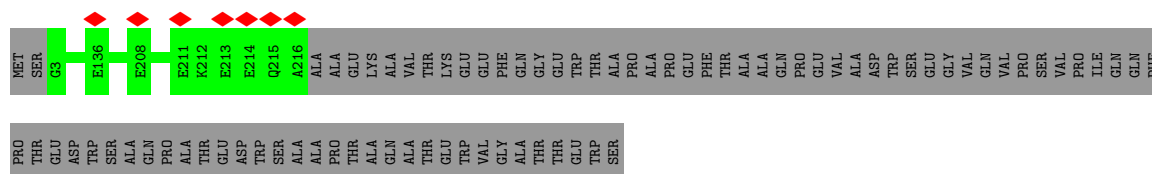


- Molecule 52: 40S ribosomal protein S17



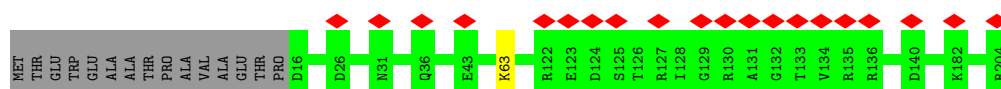
- Molecule 53: 40S ribosomal protein SA

Chain o2:  73% 27%



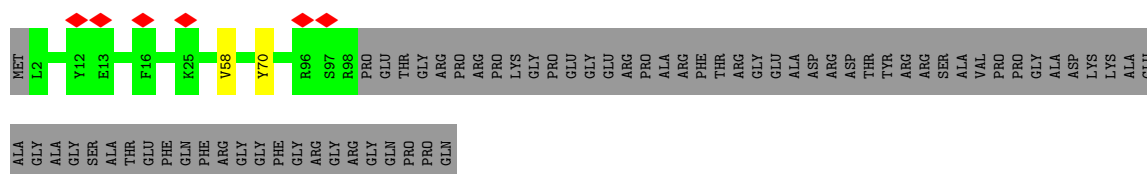
- Molecule 54: 40S ribosomal protein S5

Chain s2:  10% 92% 7%



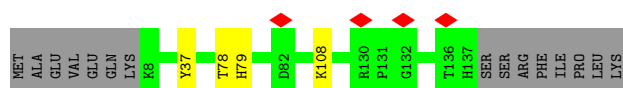
- Molecule 55: 40S ribosomal protein S10

Chain v2:  58% 41%



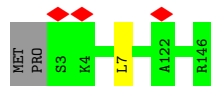
- Molecule 56: 40S ribosomal protein S15

Chain x2:  87% 10%



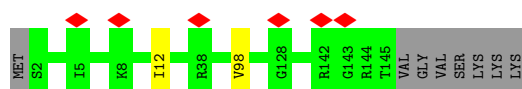
- Molecule 57: 40S ribosomal protein S16

Chain y2:  98% ..



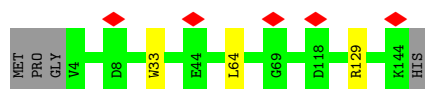
- Molecule 58: 40S ribosomal protein S18

Chain A3:  93% 5%




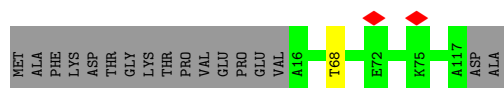
- Molecule 59: 40S ribosomal protein S19

Chain B3:  95%



- Molecule 60: 40S ribosomal protein S20

Chain C3:  85% 14%



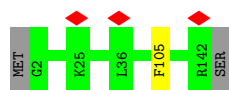
- Molecule 61: 40S ribosomal protein S21

Chain D3:  100%


There are no outlier residues recorded for this chain.

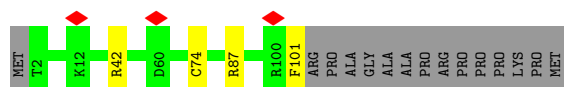
- Molecule 62: 40S ribosomal protein S23

Chain E3:  98%



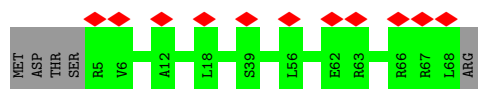
- Molecule 63: 40S ribosomal protein S26

Chain F3:  83% 13%



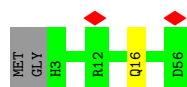
- Molecule 64: 40S ribosomal protein S28

Chain G3:  16% 93% 7%



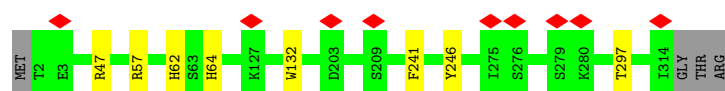
- Molecule 65: 40S ribosomal protein S29

Chain H3:  95%




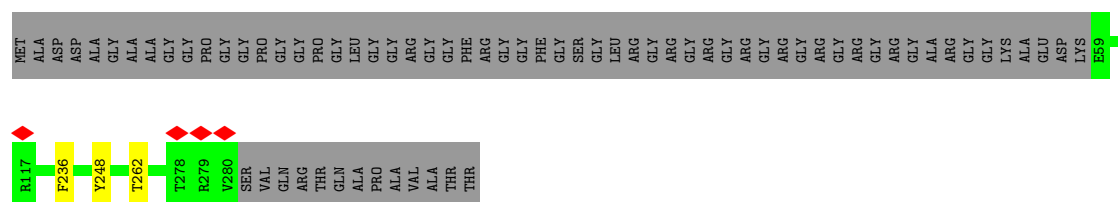
- Molecule 66: Receptor of activated protein C kinase 1

Chain I3:  96%



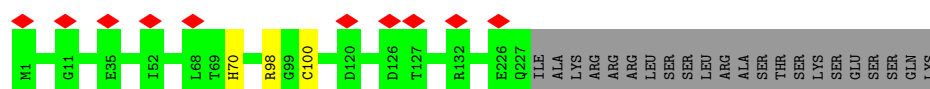
- Molecule 67: 40S ribosomal protein S2

Chain J3:  75% 24%



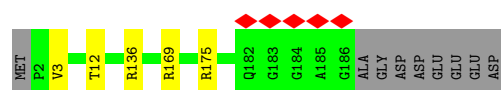
- Molecule 68: 40S ribosomal protein S6

Chain K3:  90% 9%



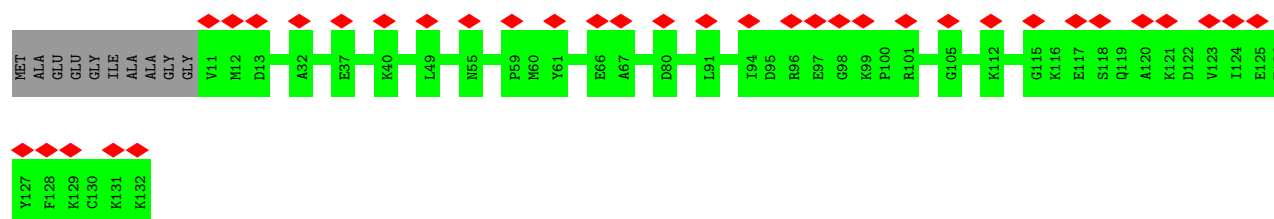
- Molecule 69: 40S ribosomal protein S9

Chain L3:  93% 5%



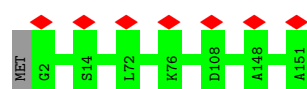
- Molecule 70: 40S ribosomal protein S12

Chain M3:  27% 92% 8%

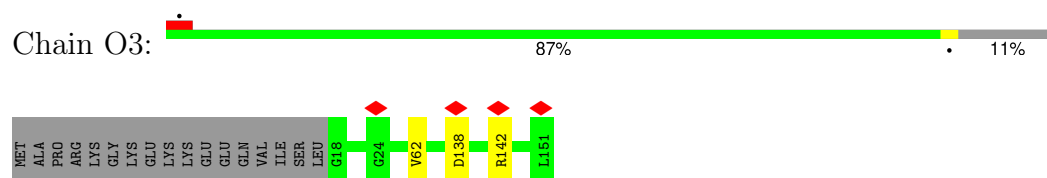


- Molecule 71: 40S ribosomal protein S13

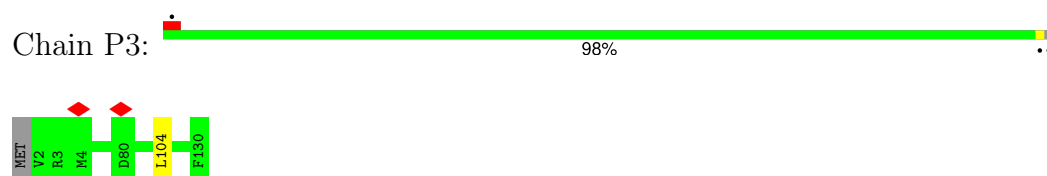
Chain N3:  5% 99%



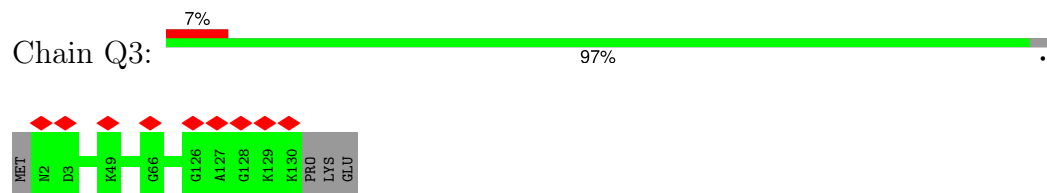
- Molecule 72: 40S ribosomal protein S14



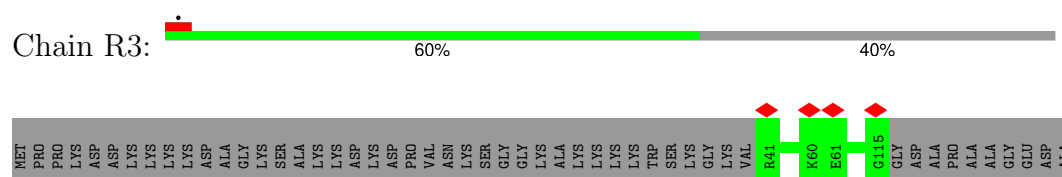
- Molecule 73: 40S ribosomal protein S15a



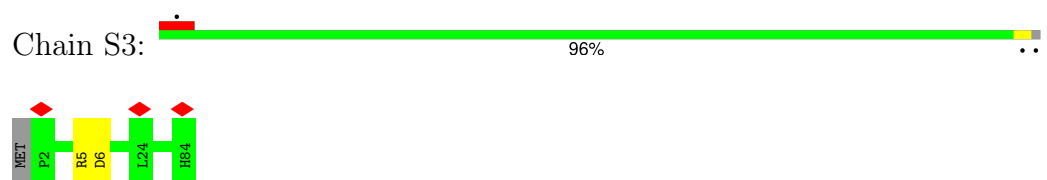
- Molecule 74: 40S ribosomal protein S24



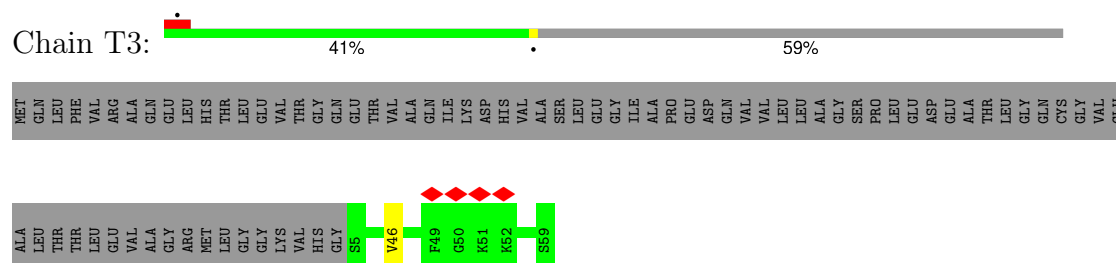
- Molecule 75: 40S ribosomal protein S25



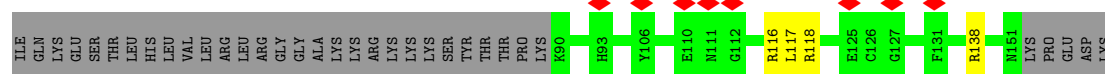
- Molecule 76: 40S ribosomal protein S27-like



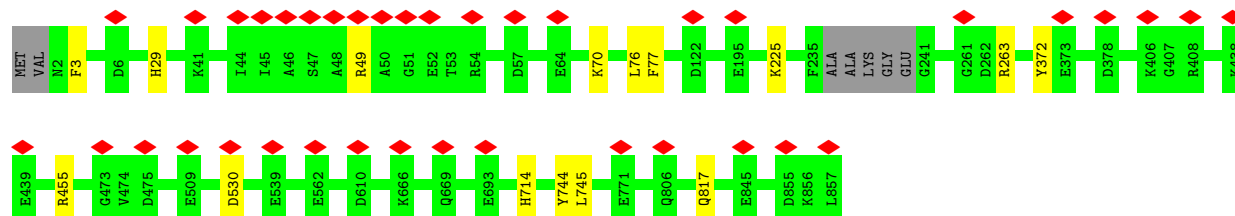
- Molecule 77: 40S ribosomal protein S30



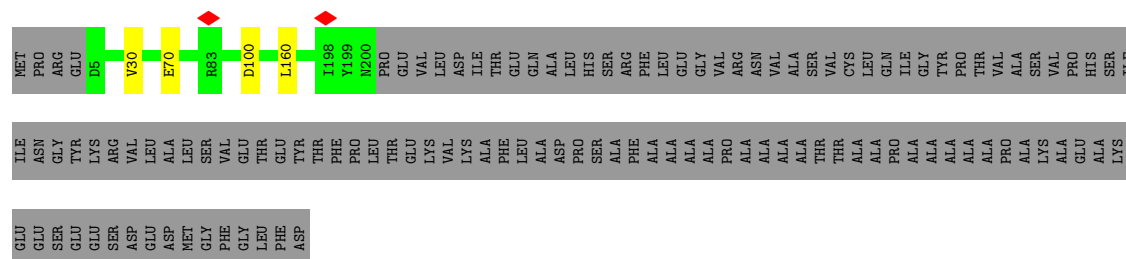
- Molecule 78: Ubiquitin-40S ribosomal protein S27a

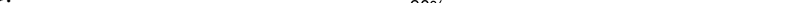


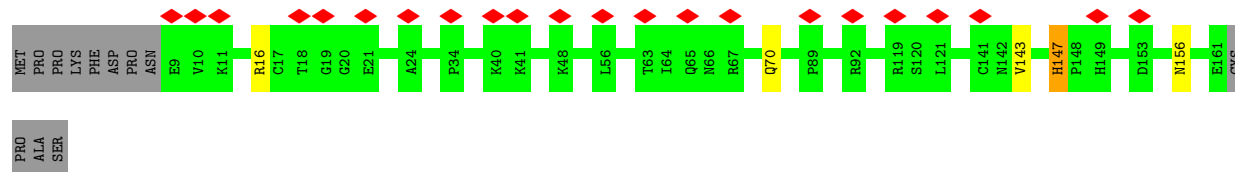
- Chain m:  97%



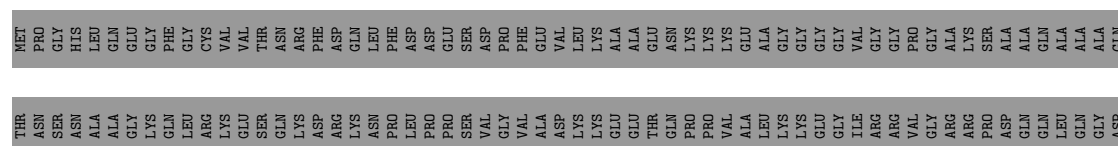
- Chain j:  61% 38%



- Chain k:  13% 90% .. 7%



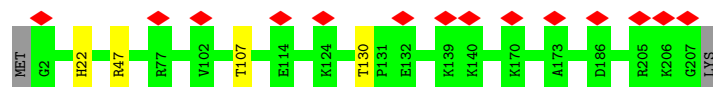
- Chain A:  7% 16% 84%



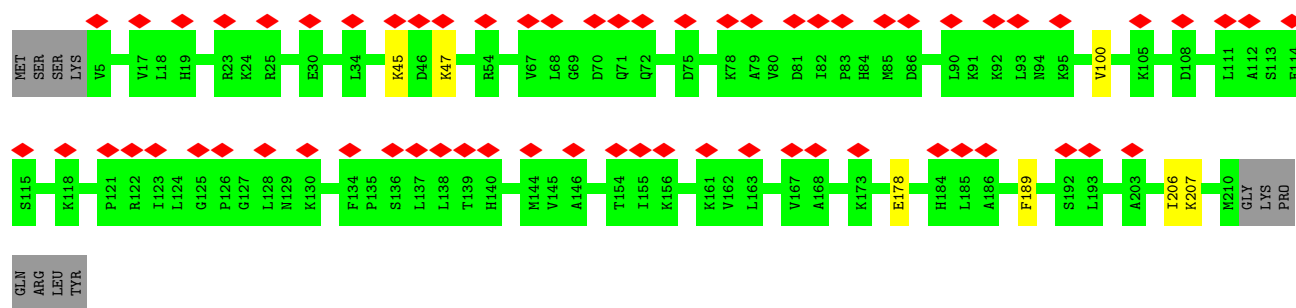
- Molecule 83: 40S ribosomal protein S7



- Molecule 84: 40S ribosomal protein S8



- Molecule 85: 60S ribosomal protein L10a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23297	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.264	Depositor
Minimum map value	-17.005	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.034	Depositor
Recommended contour level	4	Depositor
Map size (Å)	814.07996, 814.07996, 814.07996	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, GDP, A2M, MLZ, 5MC, MHG, ZN, 1MA, I4U, PSU, B9H, MG, G7M, 6MZ, E7G, B8T, P7G, OMG, 2MG, E6G, OMC, B8W, B9B, B8Q, UR3, 4AC, DDE, OMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A1	0.26	0/1888	0.51	0/2516
2	B1	0.24	0/1898	0.50	0/2553
3	C1	0.25	0/1537	0.51	0/2065
4	D1	0.25	0/1728	0.51	0/2306
5	E1	0.25	0/1420	0.53	0/1899
6	F1	0.25	0/1707	0.54	0/2286
7	G1	0.26	0/1165	0.51	0/1558
8	H1	0.25	0/1746	0.54	0/2338
9	A2	0.24	0/86883	0.79	28/135484 (0.0%)
10	B2	0.23	0/2858	0.79	0/4455
11	C2	0.23	0/3679	0.79	0/5732
12	D2	0.26	0/1959	0.55	0/2627
13	E2	0.25	0/3305	0.50	0/4422
14	F2	0.25	0/2971	0.52	0/3987
15	G2	0.25	0/2431	0.49	0/3256
16	H2	0.25	0/1822	0.51	0/2443
17	I2	0.26	0/1670	0.50	0/2232
18	J2	0.25	0/1268	0.51	0/1700
19	K2	0.25	0/1535	0.57	0/2048
20	L2	0.23	0/1558	0.52	0/2059
21	M2	0.26	0/1490	0.53	0/2000
22	N2	0.25	0/1326	0.50	0/1769
23	O2	0.25	0/839	0.49	0/1126
24	P2	0.26	0/983	0.49	0/1319
25	Q2	0.26	0/909	0.51	0/1203
26	R2	0.25	0/984	0.51	0/1323
27	S2	0.24	0/1132	0.52	0/1504
28	T2	0.26	0/1130	0.49	0/1507
29	U2	0.25	0/1193	0.51	0/1593
30	V2	0.24	0/963	0.47	0/1275
31	W2	0.25	0/742	0.46	0/996

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	X2	0.24	0/903	0.53	0/1216
33	Y2	0.24	0/1071	0.51	0/1429
34	Z2	0.26	0/895	0.55	0/1198
35	a2	0.24	0/916	0.55	0/1221
36	b2	0.24	0/1009	0.51	0/1332
37	c2	0.24	0/838	0.53	0/1111
38	d2	0.25	0/720	0.57	0/952
39	e2	0.24	0/574	0.47	0/760
40	f2	0.24	0/454	0.54	0/599
41	g2	0.23	0/425	0.52	0/561
42	h2	0.23	0/231	0.67	0/294
43	i2	0.25	0/855	0.53	0/1128
44	j2	0.25	0/704	0.49	0/935
45	k2	0.24	0/1016	0.54	0/1363
46	m2	0.22	0/40772	0.79	12/63546 (0.0%)
47	n2	0.22	0/1795	0.80	0/2798
48	p2	0.24	0/1765	0.47	0/2362
49	q2	0.25	0/1784	0.50	0/2402
50	r2	0.25	0/2118	0.50	0/2849
51	w2	0.25	0/1268	0.53	0/1696
52	z2	0.23	0/1094	0.49	0/1469
53	o2	0.24	0/1731	0.48	0/2352
54	s2	0.23	0/1517	0.48	0/2038
55	v2	0.24	0/843	0.44	0/1137
56	x2	0.25	0/1094	0.51	0/1460
57	y2	0.25	0/1161	0.52	0/1553
58	A3	0.23	0/1208	0.55	0/1618
59	B3	0.24	0/1122	0.48	0/1503
60	C3	0.23	0/817	0.53	0/1097
61	D3	0.26	0/645	0.50	0/863
62	E3	0.25	0/1116	0.51	0/1490
63	F3	0.25	0/828	0.55	0/1109
64	G3	0.24	0/508	0.59	0/680
65	H3	0.25	0/466	0.51	0/618
66	I3	0.24	0/2493	0.50	0/3394
67	J3	0.25	0/1762	0.47	0/2382
68	K3	0.24	0/1863	0.53	0/2481
69	L3	0.24	0/1550	0.53	0/2069
70	M3	0.23	0/952	0.42	0/1278
71	N3	0.23	0/1232	0.47	0/1656
72	O3	0.25	0/1015	0.53	0/1361
73	P3	0.25	0/1051	0.52	0/1406
74	Q3	0.24	0/1066	0.50	0/1415

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
75	R3	0.24	0/604	0.50	0/810
76	S3	0.24	0/665	0.49	0/890
77	T3	0.25	0/443	0.54	0/582
78	U3	0.25	0/515	0.50	0/682
79	m	0.25	0/6756	0.47	0/9122
80	j	0.24	0/1530	0.46	0/2064
81	k	0.23	0/1173	0.49	0/1581
82	A	0.23	0/493	0.51	0/655
83	t	0.25	0/1499	0.47	0/2007
84	u	0.24	0/1715	0.52	0/2287
85	L1	0.24	0/1686	0.49	0/2262
All	All	0.24	0/241045	0.69	40/352704 (0.0%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	m2	624	C	N3-C2-O2	-8.27	116.11	121.90
46	m2	1149	C	N3-C2-O2	-8.18	116.18	121.90
9	A2	260	C	N3-C2-O2	-7.97	116.32	121.90
9	A2	822	C	N3-C2-O2	-7.77	116.46	121.90
9	A2	1893	C	C2-N1-C1'	7.24	126.77	118.80

There are no chirality outliers.

There are no planarity outliers.

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	A1	221/270 (82%)	214 (97%)	7 (3%)	0	100	100
2	B1	227/266 (85%)	220 (97%)	7 (3%)	0	100	100
3	C1	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
4	D1	204/214 (95%)	201 (98%)	3 (2%)	0	100	100
5	E1	172/178 (97%)	167 (97%)	5 (3%)	0	100	100
6	F1	205/211 (97%)	194 (95%)	11 (5%)	0	100	100
7	G1	137/217 (63%)	133 (97%)	4 (3%)	0	100	100
8	H1	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
12	D2	249/257 (97%)	234 (94%)	15 (6%)	0	100	100
13	E2	400/403 (99%)	397 (99%)	3 (1%)	0	100	100
14	F2	364/419 (87%)	359 (99%)	5 (1%)	0	100	100
15	G2	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
16	H2	215/296 (73%)	208 (97%)	7 (3%)	0	100	100
17	I2	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
18	J2	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
19	K2	184/188 (98%)	181 (98%)	3 (2%)	0	100	100
20	L2	182/196 (93%)	181 (100%)	1 (0%)	0	100	100
21	M2	173/176 (98%)	166 (96%)	7 (4%)	0	100	100
22	N2	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
23	O2	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
24	P2	127/140 (91%)	125 (98%)	2 (2%)	0	100	100
25	Q2	106/157 (68%)	104 (98%)	2 (2%)	0	100	100
26	R2	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	S2	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
28	T2	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	U2	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
30	V2	115/160 (72%)	110 (96%)	5 (4%)	0	100	100
31	W2	92/115 (80%)	86 (94%)	6 (6%)	0	100	100
32	X2	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
33	Y2	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
34	Z2	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
35	a2	112/117 (96%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	b2	118/123 (96%)	115 (98%)	3 (2%)	0	100	100
37	c2	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
38	d2	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
39	e2	67/70 (96%)	67 (100%)	0	0	100	100
40	f2	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
41	g2	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
42	h2	22/25 (88%)	22 (100%)	0	0	100	100
43	i2	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
44	j2	87/92 (95%)	83 (95%)	4 (5%)	0	100	100
45	k2	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
48	p2	212/264 (80%)	210 (99%)	2 (1%)	0	100	100
49	q2	224/243 (92%)	217 (97%)	7 (3%)	0	100	100
50	r2	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
51	w2	151/158 (96%)	144 (95%)	7 (5%)	0	100	100
52	z2	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
53	o2	212/295 (72%)	211 (100%)	1 (0%)	0	100	100
54	s2	187/204 (92%)	182 (97%)	5 (3%)	0	100	100
55	v2	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
56	x2	128/145 (88%)	124 (97%)	3 (2%)	1 (1%)	16	48
57	y2	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
58	A3	142/152 (93%)	138 (97%)	4 (3%)	0	100	100
59	B3	139/145 (96%)	139 (100%)	0	0	100	100
60	C3	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
61	D3	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
62	E3	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
63	F3	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
64	G3	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
65	H3	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
66	I3	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
67	J3	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
68	K3	225/249 (90%)	223 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	L3	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
70	M3	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
71	N3	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
72	O3	132/151 (87%)	126 (96%)	6 (4%)	0	100	100
73	P3	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
74	Q3	127/133 (96%)	122 (96%)	5 (4%)	0	100	100
75	R3	73/125 (58%)	73 (100%)	0	0	100	100
76	S3	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
77	T3	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
78	U3	60/156 (38%)	59 (98%)	1 (2%)	0	100	100
79	m	846/858 (99%)	823 (97%)	23 (3%)	0	100	100
80	j	194/317 (61%)	191 (98%)	3 (2%)	0	100	100
81	k	151/165 (92%)	144 (95%)	6 (4%)	1 (1%)	19	51
82	A	57/386 (15%)	57 (100%)	0	0	100	100
83	t	179/194 (92%)	174 (97%)	5 (3%)	0	100	100
84	u	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
85	L1	204/217 (94%)	187 (92%)	16 (8%)	1 (0%)	25	58
All	All	12686/14730 (86%)	12350 (97%)	333 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
81	k	147	HIS
56	x2	108	LYS
85	L1	207	LYS

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	A1	194/234 (83%)	194 (100%)	0	100	100
2	B1	198/223 (89%)	197 (100%)	1 (0%)	86	92
3	C1	169/171 (99%)	168 (99%)	1 (1%)	84	91
4	D1	177/180 (98%)	174 (98%)	3 (2%)	56	78
5	E1	147/149 (99%)	142 (97%)	5 (3%)	32	62
6	F1	174/178 (98%)	169 (97%)	5 (3%)	37	65
7	G1	118/157 (75%)	118 (100%)	0	100	100
8	H1	171/172 (99%)	168 (98%)	3 (2%)	54	76
12	D2	193/199 (97%)	190 (98%)	3 (2%)	58	79
13	E2	347/348 (100%)	341 (98%)	6 (2%)	56	78
14	F2	307/347 (88%)	303 (99%)	4 (1%)	65	82
15	G2	245/249 (98%)	245 (100%)	0	100	100
16	H2	198/256 (77%)	196 (99%)	2 (1%)	73	86
17	I2	172/173 (99%)	169 (98%)	3 (2%)	56	78
18	J2	134/164 (82%)	133 (99%)	1 (1%)	81	90
19	K2	164/165 (99%)	164 (100%)	0	100	100
20	L2	163/175 (93%)	160 (98%)	3 (2%)	54	76
21	M2	155/156 (99%)	154 (99%)	1 (1%)	84	91
22	N2	138/139 (99%)	136 (99%)	2 (1%)	62	81
23	O2	91/114 (80%)	91 (100%)	0	100	100
24	P2	100/107 (94%)	99 (99%)	1 (1%)	73	86
25	Q2	90/126 (71%)	89 (99%)	1 (1%)	70	84
26	R2	106/133 (80%)	106 (100%)	0	100	100
27	S2	124/135 (92%)	121 (98%)	3 (2%)	44	70
28	T2	117/118 (99%)	117 (100%)	0	100	100
29	U2	120/121 (99%)	119 (99%)	1 (1%)	79	89
30	V2	98/124 (79%)	95 (97%)	3 (3%)	35	63
31	W2	79/97 (81%)	78 (99%)	1 (1%)	65	82
32	X2	98/110 (89%)	97 (99%)	1 (1%)	73	86
33	Y2	114/121 (94%)	113 (99%)	1 (1%)	75	88
34	Z2	88/89 (99%)	86 (98%)	2 (2%)	45	70
35	a2	98/100 (98%)	96 (98%)	2 (2%)	50	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	b2	108/110 (98%)	108 (100%)	0	100	100
37	c2	86/90 (96%)	85 (99%)	1 (1%)	67	83
38	d2	73/80 (91%)	72 (99%)	1 (1%)	62	81
39	e2	64/65 (98%)	64 (100%)	0	100	100
40	f2	47/48 (98%)	47 (100%)	0	100	100
41	g2	47/115 (41%)	46 (98%)	1 (2%)	48	72
42	h2	23/24 (96%)	23 (100%)	0	100	100
43	i2	91/94 (97%)	86 (94%)	5 (6%)	18	47
44	j2	73/75 (97%)	71 (97%)	2 (3%)	40	67
45	k2	109/121 (90%)	107 (98%)	2 (2%)	54	76
48	p2	195/229 (85%)	195 (100%)	0	100	100
49	q2	189/202 (94%)	186 (98%)	3 (2%)	58	79
50	r2	224/225 (100%)	221 (99%)	3 (1%)	65	82
51	w2	137/142 (96%)	134 (98%)	3 (2%)	47	71
52	z2	120/121 (99%)	118 (98%)	2 (2%)	56	78
53	o2	179/242 (74%)	179 (100%)	0	100	100
54	s2	159/170 (94%)	158 (99%)	1 (1%)	84	91
55	v2	88/136 (65%)	86 (98%)	2 (2%)	45	70
56	x2	116/130 (89%)	113 (97%)	3 (3%)	41	68
57	y2	119/121 (98%)	118 (99%)	1 (1%)	79	89
58	A3	125/132 (95%)	123 (98%)	2 (2%)	58	79
59	B3	112/115 (97%)	109 (97%)	3 (3%)	40	67
60	C3	93/107 (87%)	92 (99%)	1 (1%)	70	84
61	D3	67/67 (100%)	67 (100%)	0	100	100
62	E3	113/115 (98%)	112 (99%)	1 (1%)	75	88
63	F3	88/98 (90%)	84 (96%)	4 (4%)	23	53
64	G3	57/62 (92%)	57 (100%)	0	100	100
65	H3	48/49 (98%)	47 (98%)	1 (2%)	48	72
66	I3	272/275 (99%)	264 (97%)	8 (3%)	37	65
67	J3	188/224 (84%)	185 (98%)	3 (2%)	58	79
68	K3	198/218 (91%)	195 (98%)	3 (2%)	60	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	L3	161/168 (96%)	156 (97%)	5 (3%)	35	63
70	M3	102/108 (94%)	102 (100%)	0	100	100
71	N3	130/131 (99%)	130 (100%)	0	100	100
72	O3	104/119 (87%)	101 (97%)	3 (3%)	37	65
73	P3	112/113 (99%)	111 (99%)	1 (1%)	75	88
74	Q3	111/115 (96%)	111 (100%)	0	100	100
75	R3	66/103 (64%)	66 (100%)	0	100	100
76	S3	75/76 (99%)	73 (97%)	2 (3%)	40	67
77	T3	45/106 (42%)	44 (98%)	1 (2%)	47	71
78	U3	55/140 (39%)	51 (93%)	4 (7%)	11	37
79	m	725/729 (100%)	711 (98%)	14 (2%)	52	75
80	j	164/255 (64%)	160 (98%)	4 (2%)	44	70
81	k	126/137 (92%)	121 (96%)	5 (4%)	27	58
82	A	52/304 (17%)	52 (100%)	0	100	100
83	t	164/174 (94%)	160 (98%)	4 (2%)	44	70
84	u	178/180 (99%)	174 (98%)	4 (2%)	47	71
85	L1	187/197 (95%)	181 (97%)	6 (3%)	34	63
All	All	11052/12487 (88%)	10884 (98%)	168 (2%)	60	80

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	L3	3	VAL
79	m	745	LEU
69	L3	175	ARG
78	U3	138	ARG
81	k	70	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
67	J3	267	GLN
69	L3	111	GLN
74	Q3	94	HIS
73	P3	91	ASN

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Mol	Chain	Res	Type
61	D3	35	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B2	119/121 (98%)	16 (13%)	0
11	C2	155/156 (99%)	28 (18%)	2 (1%)
46	m2	1715/1871 (91%)	385 (22%)	0
47	n2	74/75 (98%)	24 (32%)	0
9	A2	3676/4731 (77%)	784 (21%)	13 (0%)
All	All	5739/6954 (82%)	1237 (21%)	15 (0%)

5 of 1237 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A2	2	G
9	A2	25	A
9	A2	39	A
9	A2	42	A
9	A2	48	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A2	2382	C
11	C2	59	A
9	A2	2430	G
11	C2	83	C
9	A2	4351	U

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

101 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
9	A2M	A2	3441	9	18,25,26	2.82	8 (44%)	20,36,39	2.58	5 (25%)
9	E7G	A2	1599	9	24,27,28	3.35	11 (45%)	28,40,43	2.35	9 (32%)
9	MHG	A2	4023	9	29,32,33	3.64	10 (34%)	34,46,49	2.55	12 (35%)
46	PSU	m2	1083	46	18,21,22	4.52	6 (33%)	21,30,33	3.00	7 (33%)
9	PSU	A2	3945	9	18,21,22	4.49	6 (33%)	21,30,33	3.01	5 (23%)
46	PSU	m2	824	46	18,21,22	4.54	6 (33%)	21,30,33	2.96	5 (23%)
9	OMC	A2	3543	9	19,22,23	3.04	8 (42%)	25,31,34	0.85	0
46	OMG	m2	646	46	19,26,27	2.56	7 (36%)	21,38,41	1.44	4 (19%)
46	UR3	m2	1832	46	19,22,23	3.21	8 (42%)	26,32,35	1.62	3 (11%)
9	OMG	A2	1335	9	19,26,27	2.55	7 (36%)	21,38,41	1.51	4 (19%)
9	A2M	A2	1673	9	18,25,26	2.66	8 (44%)	20,36,39	2.04	4 (20%)
9	OMG	A2	4146	9	19,26,27	2.55	7 (36%)	21,38,41	1.45	4 (19%)
9	A2M	A2	1140	9	18,25,26	2.71	9 (50%)	20,36,39	1.97	4 (20%)
46	B8N	m2	1250	46	25,29,30	2.49	6 (24%)	28,42,45	2.13	7 (25%)
11	OMU	C2	14	11	19,22,23	3.09	8 (42%)	25,31,34	1.81	5 (20%)
9	OMG	A2	1438	9	19,26,27	2.55	7 (36%)	21,38,41	1.52	4 (19%)
46	PSU	m2	1245	46	18,21,22	4.55	6 (33%)	21,30,33	2.95	6 (28%)
9	OMG	A2	4022	9	19,26,27	2.54	7 (36%)	21,38,41	1.44	4 (19%)
9	OMU	A2	3958	9	19,22,23	3.02	8 (42%)	25,31,34	1.81	5 (20%)
9	OMG	A2	373	9	19,26,27	2.54	7 (36%)	21,38,41	1.46	4 (19%)
9	OMG	A2	3848	9	19,26,27	2.55	7 (36%)	21,38,41	1.45	4 (19%)
9	OMG	A2	2528	9	19,26,27	2.56	7 (36%)	21,38,41	1.46	4 (19%)
46	A2M	m2	670	46	18,25,26	2.74	9 (50%)	20,36,39	1.91	3 (15%)
9	1MA	A2	4067	9	17,25,26	3.89	3 (17%)	17,37,40	1.71	3 (17%)
9	G7M	A2	2277	9	20,26,27	3.96	9 (45%)	16,39,42	1.14	1 (6%)
9	5MC	A2	4099	9	19,22,23	3.83	8 (42%)	26,32,35	1.01	1 (3%)
9	G7M	A2	4202	9	20,26,27	3.96	9 (45%)	16,39,42	1.14	1 (6%)
46	A2M	m2	166	46	18,25,26	2.69	8 (44%)	20,36,39	2.02	3 (15%)
9	P7G	A2	3536	9	24,28,29	3.56	10 (41%)	25,41,44	1.29	2 (8%)
9	OMU	A2	4272	9	19,22,23	3.05	8 (42%)	25,31,34	1.76	5 (20%)
9	OMC	A2	4188	9	19,22,23	3.03	8 (42%)	25,31,34	0.79	0
9	A2M	A2	3481	9	18,25,26	2.68	8 (44%)	20,36,39	1.95	3 (15%)
9	PSU	A2	4094	9	18,21,22	4.58	7 (38%)	21,30,33	2.99	6 (28%)
9	OMG	A2	4289	9	19,26,27	2.54	7 (36%)	21,38,41	1.45	3 (14%)
9	OMC	A2	2120	9	19,22,23	3.04	7 (36%)	25,31,34	1.05	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	OMG	A2	3448	9	19,26,27	2.54	7 (36%)	21,38,41	1.45	4 (19%)
46	A2M	m2	27	46	18,25,26	2.69	9 (50%)	20,36,39	1.87	3 (15%)
9	UR3	A2	1668	9	19,22,23	3.25	8 (42%)	26,32,35	1.64	4 (15%)
9	OMG	A2	2179	9	19,26,27	2.56	7 (36%)	21,38,41	1.47	4 (19%)
46	OMG	m2	685	46	19,26,27	2.55	7 (36%)	21,38,41	1.44	4 (19%)
14	MLZ	F2	333	14	8,9,10	0.73	0	4,9,11	0.91	0
9	OMC	A2	2616	9	19,22,23	3.08	8 (42%)	25,31,34	0.92	1 (4%)
9	B8W	A2	3837	9	18,26,27	5.55	8 (44%)	17,38,41	3.25	7 (41%)
9	G7M	A2	1418	9	20,26,27	3.96	9 (45%)	16,39,42	1.14	1 (6%)
9	OMG	A2	4515	9	19,26,27	2.54	7 (36%)	21,38,41	1.57	4 (19%)
9	E6G	A2	4007	9	19,27,28	4.78	7 (36%)	18,39,42	2.21	5 (27%)
9	OMC	A2	3525	9	19,22,23	3.03	8 (42%)	25,31,34	0.76	0
9	OMG	A2	4275	9	19,26,27	2.54	7 (36%)	21,38,41	1.49	4 (19%)
9	A2M	A2	4223	9	18,25,26	2.68	9 (50%)	20,36,39	1.97	3 (15%)
9	OMC	A2	3357	9	19,22,23	3.04	8 (42%)	25,31,34	0.72	0
9	A2M	A2	3374	9	18,25,26	2.67	8 (44%)	20,36,39	1.94	3 (15%)
9	PSU	A2	1490	9	18,21,22	4.53	6 (33%)	21,30,33	3.02	7 (33%)
9	A2M	A2	1347	9	18,25,26	2.78	9 (50%)	20,36,39	2.09	4 (20%)
9	OMC	A2	3565	9	19,22,23	3.06	8 (42%)	25,31,34	0.82	0
46	OMU	m2	116	46	19,22,23	3.05	8 (42%)	25,31,34	1.71	4 (16%)
9	A2M	A2	1337	9	18,25,26	2.66	8 (44%)	20,36,39	2.01	4 (20%)
9	PSU	A2	3371	9	18,21,22	4.51	6 (33%)	21,30,33	2.93	6 (28%)
9	5MC	A2	3438	9	19,22,23	3.92	8 (42%)	26,32,35	0.97	1 (3%)
9	2MG	A2	1330	9	18,26,27	2.20	5 (27%)	16,38,41	1.68	4 (25%)
9	PSU	A2	3420	9	18,21,22	4.52	6 (33%)	21,30,33	2.87	5 (23%)
46	A2M	m2	1033	46	18,25,26	2.68	8 (44%)	20,36,39	1.90	3 (15%)
9	PSU	A2	1496	9	18,21,22	4.51	6 (33%)	21,30,33	3.04	6 (28%)
9	I4U	A2	3846	9	20,24,25	4.77	15 (75%)	27,34,37	1.63	2 (7%)
9	OMG	A2	1685	9	19,26,27	2.55	8 (42%)	21,38,41	1.51	4 (19%)
9	PSU	A2	4288	9	18,21,22	4.53	7 (38%)	21,30,33	2.98	5 (23%)
41	MLZ	g2	98	41	8,9,10	0.72	0	4,9,11	0.90	0
9	5MC	A2	3987	9	19,22,23	3.90	8 (42%)	26,32,35	1.02	2 (7%)
9	I4U	A2	1472	9	20,24,25	4.77	15 (75%)	27,34,37	1.84	3 (11%)
9	2MG	A2	4517	9	18,26,27	2.17	5 (27%)	16,38,41	1.55	5 (31%)
79	DDE	m	714	79	15,20,21	2.16	4 (26%)	11,28,30	0.94	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	6MZ	A2	3872	9	17,25,26	1.33	2 (11%)	15,36,39	2.17	2 (13%)
9	PSU	A2	4183	9	18,21,22	4.54	6 (33%)	21,30,33	3.09	6 (28%)
9	A2M	A2	2156	9	18,25,26	2.70	8 (44%)	20,36,39	1.94	3 (15%)
9	PSU	A2	1395	9	18,21,22	4.54	7 (38%)	21,30,33	2.92	5 (23%)
9	PSU	A2	2263	9	18,21,22	4.56	6 (33%)	21,30,33	2.90	6 (28%)
9	OMG	A2	1852	9	19,26,27	2.53	7 (36%)	21,38,41	1.44	4 (19%)
46	4AC	m2	1844	46	21,24,25	3.67	9 (42%)	28,34,37	1.15	4 (14%)
9	2MG	A2	878	9	18,26,27	2.16	5 (27%)	16,38,41	1.50	4 (25%)
9	B8T	A2	4135	9	19,22,23	3.29	8 (42%)	25,31,34	0.86	1 (4%)
9	PSU	A2	3385	9	18,21,22	4.52	6 (33%)	21,30,33	3.00	5 (23%)
9	A2M	A2	2118	9	18,25,26	2.68	9 (50%)	20,36,39	1.88	3 (15%)
9	B9B	A2	1387	9	20,28,29	4.61	7 (35%)	19,40,43	2.05	5 (26%)
9	PSU	A2	4152	9	18,21,22	4.56	7 (38%)	21,30,33	3.06	6 (28%)
46	PSU	m2	825	46	18,21,22	4.54	6 (33%)	21,30,33	3.02	6 (28%)
9	P7G	A2	1711	9,10	24,28,29	3.61	10 (41%)	25,41,44	1.23	2 (8%)
9	PSU	A2	4102	9	18,21,22	4.51	6 (33%)	21,30,33	2.97	5 (23%)
46	OMC	m2	519	46	19,22,23	3.07	8 (42%)	25,31,34	0.91	1 (4%)
9	OMC	A2	2559	9	19,22,23	3.03	8 (42%)	25,31,34	0.73	0
46	PSU	m2	614	46	18,21,22	4.50	6 (33%)	21,30,33	2.94	6 (28%)
9	B9H	A2	2541	9	21,25,26	2.95	4 (19%)	22,35,38	1.82	5 (22%)
9	A2M	A2	3379	9	18,25,26	2.67	8 (44%)	20,36,39	1.93	3 (15%)
9	A2M	A2	398	9	18,25,26	2.68	9 (50%)	20,36,39	1.96	3 (15%)
9	PSU	A2	4280	9	18,21,22	4.54	6 (33%)	21,30,33	2.99	6 (28%)
9	OMC	A2	2177	9	19,22,23	3.05	8 (42%)	25,31,34	0.98	1 (4%)
9	UR3	A2	4249	9	19,22,23	3.20	8 (42%)	26,32,35	1.57	4 (15%)
9	B8Q	A2	1269	9	18,22,23	3.02	4 (22%)	21,32,35	1.85	6 (28%)
9	B9B	A2	237	9	20,28,29	4.65	6 (30%)	19,40,43	2.01	4 (21%)
9	E7G	A2	2052	9	24,27,28	3.34	11 (45%)	28,40,43	2.33	8 (28%)
9	PSU	A2	4055	9	18,21,22	4.53	6 (33%)	21,30,33	3.00	7 (33%)
9	A2M	A2	3523	9	18,25,26	2.71	9 (50%)	20,36,39	1.93	3 (15%)
9	OMG	A2	2119	9	19,26,27	2.53	7 (36%)	21,38,41	1.48	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A2M	A2	3441	9	-	2/5/27/28	0/3/3/3
9	E7G	A2	1599	9	-	1/9/39/40	0/3/3/3
9	MHG	A2	4023	9	-	4/16/46/47	0/3/3/3
46	PSU	m2	1083	46	-	1/7/25/26	0/2/2/2
9	PSU	A2	3945	9	-	2/7/25/26	0/2/2/2
46	PSU	m2	824	46	-	3/7/25/26	0/2/2/2
9	OMC	A2	3543	9	-	3/9/27/28	0/2/2/2
46	OMG	m2	646	46	-	2/5/27/28	0/3/3/3
46	UR3	m2	1832	46	-	4/7/25/26	0/2/2/2
9	OMG	A2	1335	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	1673	9	-	0/5/27/28	0/3/3/3
9	OMG	A2	4146	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	1140	9	-	1/5/27/28	0/3/3/3
46	B8N	m2	1250	46	-	3/16/34/35	0/2/2/2
11	OMU	C2	14	11	-	1/9/27/28	0/2/2/2
9	OMG	A2	1438	9	-	3/5/27/28	0/3/3/3
46	PSU	m2	1245	46	-	3/7/25/26	0/2/2/2
9	OMG	A2	4022	9	-	0/5/27/28	0/3/3/3
9	OMU	A2	3958	9	-	3/9/27/28	0/2/2/2
9	OMG	A2	373	9	-	1/5/27/28	0/3/3/3
9	OMG	A2	3848	9	-	0/5/27/28	0/3/3/3
9	OMG	A2	2528	9	-	2/5/27/28	0/3/3/3
46	A2M	m2	670	46	-	1/5/27/28	0/3/3/3
9	1MA	A2	4067	9	-	2/3/25/26	0/3/3/3
9	G7M	A2	2277	9	-	0/3/25/26	0/3/3/3
9	5MC	A2	4099	9	-	4/7/25/26	0/2/2/2
9	G7M	A2	4202	9	-	0/3/25/26	0/3/3/3
46	A2M	m2	166	46	-	3/5/27/28	0/3/3/3
9	P7G	A2	3536	9	-	3/10/40/41	0/3/3/3
9	OMU	A2	4272	9	-	1/9/27/28	0/2/2/2
9	OMC	A2	4188	9	-	0/9/27/28	0/2/2/2
9	A2M	A2	3481	9	-	1/5/27/28	0/3/3/3
9	PSU	A2	4094	9	-	0/7/25/26	0/2/2/2
9	OMG	A2	4289	9	-	2/5/27/28	0/3/3/3
9	OMC	A2	2120	9	-	0/9/27/28	0/2/2/2
9	OMG	A2	3448	9	-	0/5/27/28	0/3/3/3
46	A2M	m2	27	46	-	1/5/27/28	0/3/3/3
9	UR3	A2	1668	9	-	2/7/25/26	0/2/2/2
9	OMG	A2	2179	9	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMG	m2	685	46	-	2/5/27/28	0/3/3/3
14	MLZ	F2	333	14	-	1/7/8/10	-
9	OMC	A2	2616	9	-	0/9/27/28	0/2/2/2
9	B8W	A2	3837	9	-	2/5/27/28	0/3/3/3
9	G7M	A2	1418	9	-	0/3/25/26	0/3/3/3
9	OMG	A2	4515	9	-	1/5/27/28	0/3/3/3
9	E6G	A2	4007	9	-	3/6/28/29	0/3/3/3
9	OMC	A2	3525	9	-	0/9/27/28	0/2/2/2
9	OMG	A2	4275	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	4223	9	-	1/5/27/28	0/3/3/3
9	OMC	A2	3357	9	-	5/9/27/28	0/2/2/2
9	A2M	A2	3374	9	-	1/5/27/28	0/3/3/3
9	PSU	A2	1490	9	-	2/7/25/26	0/2/2/2
9	A2M	A2	1347	9	-	2/5/27/28	0/3/3/3
9	OMC	A2	3565	9	-	0/9/27/28	0/2/2/2
46	OMU	m2	116	46	-	1/9/27/28	0/2/2/2
9	A2M	A2	1337	9	-	0/5/27/28	0/3/3/3
9	PSU	A2	3371	9	-	0/7/25/26	0/2/2/2
9	5MC	A2	3438	9	-	2/7/25/26	0/2/2/2
9	2MG	A2	1330	9	-	0/5/27/28	0/3/3/3
9	PSU	A2	3420	9	-	2/7/25/26	0/2/2/2
46	A2M	m2	1033	46	-	1/5/27/28	0/3/3/3
9	PSU	A2	1496	9	-	0/7/25/26	0/2/2/2
9	I4U	A2	3846	9	-	2/9/29/30	0/2/2/2
9	OMG	A2	1685	9	-	2/5/27/28	0/3/3/3
9	PSU	A2	4288	9	-	5/7/25/26	0/2/2/2
41	MLZ	g2	98	41	-	1/7/8/10	-
9	5MC	A2	3987	9	-	1/7/25/26	0/2/2/2
9	I4U	A2	1472	9	-	0/9/29/30	0/2/2/2
9	2MG	A2	4517	9	-	0/5/27/28	0/3/3/3
79	DDE	m	714	79	-	7/20/21/23	0/1/1/1
9	6MZ	A2	3872	9	-	5/5/27/28	0/3/3/3
9	PSU	A2	4183	9	-	2/7/25/26	0/2/2/2
9	A2M	A2	2156	9	-	2/5/27/28	0/3/3/3
9	PSU	A2	1395	9	-	2/7/25/26	0/2/2/2
9	PSU	A2	2263	9	-	0/7/25/26	0/2/2/2
9	OMG	A2	1852	9	-	0/5/27/28	0/3/3/3
46	4AC	m2	1844	46	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	2MG	A2	878	9	-	2/5/27/28	0/3/3/3
9	B8T	A2	4135	9	-	0/7/27/28	0/2/2/2
9	PSU	A2	3385	9	-	2/7/25/26	0/2/2/2
9	A2M	A2	2118	9	-	0/5/27/28	0/3/3/3
9	B9B	A2	1387	9	-	3/7/29/30	0/3/3/3
9	PSU	A2	4152	9	-	4/7/25/26	0/2/2/2
46	PSU	m2	825	46	-	0/7/25/26	0/2/2/2
9	P7G	A2	1711	9,10	-	2/10/40/41	0/3/3/3
9	PSU	A2	4102	9	-	3/7/25/26	0/2/2/2
46	OMC	m2	519	46	-	4/9/27/28	0/2/2/2
9	OMC	A2	2559	9	-	0/9/27/28	0/2/2/2
46	PSU	m2	614	46	-	0/7/25/26	0/2/2/2
9	B9H	A2	2541	9	-	0/12/47/48	0/2/2/2
9	A2M	A2	3379	9	-	1/5/27/28	0/3/3/3
9	A2M	A2	398	9	-	3/5/27/28	0/3/3/3
9	PSU	A2	4280	9	-	0/7/25/26	0/2/2/2
9	OMC	A2	2177	9	-	3/9/27/28	0/2/2/2
9	UR3	A2	4249	9	-	0/7/25/26	0/2/2/2
9	B8Q	A2	1269	9	-	0/7/42/43	0/2/2/2
9	B9B	A2	237	9	-	6/7/29/30	0/3/3/3
9	E7G	A2	2052	9	-	4/9/39/40	0/3/3/3
9	PSU	A2	4055	9	-	0/7/25/26	0/2/2/2
9	A2M	A2	3523	9	-	3/5/27/28	0/3/3/3
9	OMG	A2	2119	9	-	2/5/27/28	0/3/3/3

The worst 5 of 739 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3837	B8W	O4'-C1'	20.40	1.67	1.40
9	A2	4007	E6G	O4'-C1'	16.96	1.63	1.40
9	A2	237	B9B	O4'-C1'	16.83	1.63	1.40
9	A2	1387	B9B	O4'-C1'	16.66	1.62	1.40
9	A2	4067	1MA	C2-N3	15.06	1.47	1.28

The worst 5 of 384 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	4183	PSU	N1-C2-N3	8.07	123.68	115.17
9	A2	4152	PSU	N1-C2-N3	7.93	123.53	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	4023	MHG	C2-N3-C4	7.92	121.90	112.00
9	A2	1496	PSU	N1-C2-N3	7.90	123.50	115.17
9	A2	3837	B8W	N2-C2-N3	7.87	130.08	117.79

There are no chirality outliers.

5 of 159 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	F2	333	MLZ	CD-CE-NZ-CM
41	g2	98	MLZ	C-CA-CB-CG
79	m	714	DDE	O-C-CA-CB
79	m	714	DDE	CA-CB-CG-ND1
79	m	714	DDE	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	GDP	m	900	-	25,30,30	3.73	14 (56%)	30,47,47	1.42	5 (16%)

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
88	GDP	m	900	-	-	4/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	m	900	GDP	O4'-C1'	8.36	1.51	1.40
88	m	900	GDP	C1'-N9	-6.40	1.32	1.50
88	m	900	GDP	O4'-C4'	-6.03	1.31	1.45
88	m	900	GDP	C2-N3	5.54	1.46	1.33
88	m	900	GDP	C3'-C4'	5.48	1.66	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	m	900	GDP	C8-N7-C5	3.87	109.14	102.55
88	m	900	GDP	C5-C6-N1	3.06	119.90	114.07
88	m	900	GDP	C2-N1-C6	-2.87	119.85	125.11
88	m	900	GDP	O6-C6-C5	-2.18	120.00	124.32
88	m	900	GDP	O4'-C4'-C3'	2.16	109.45	105.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

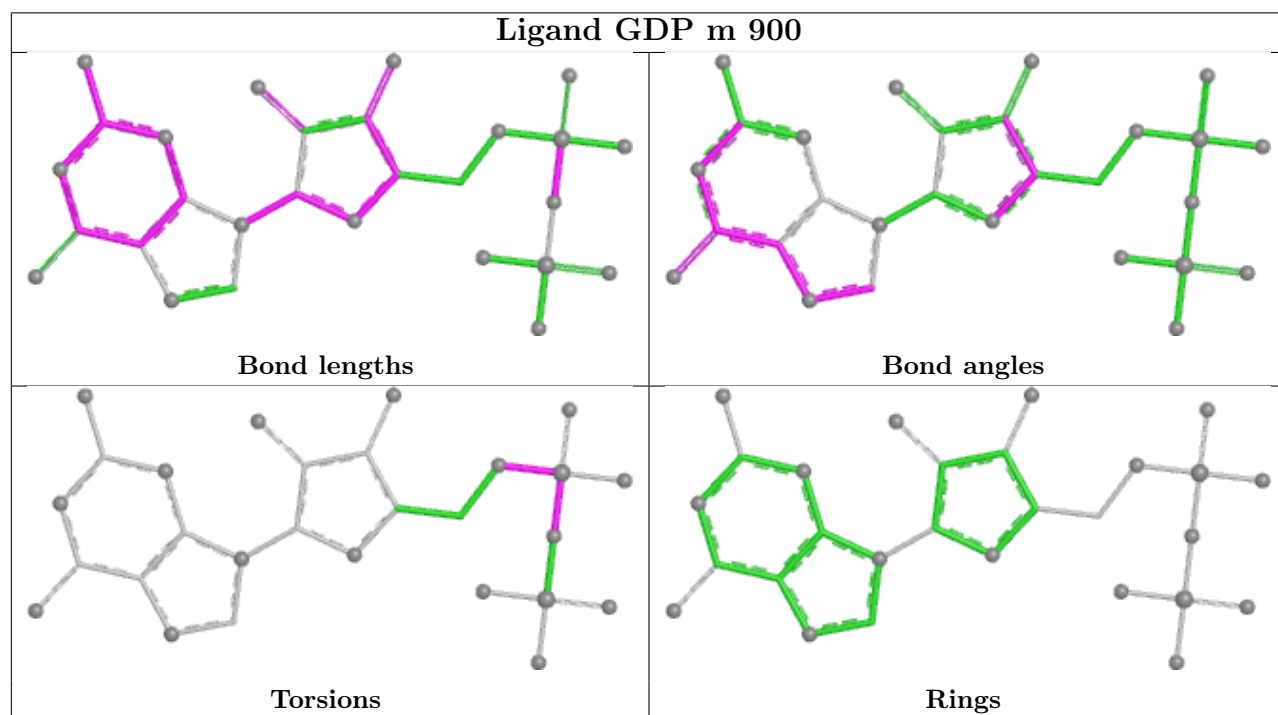
Mol	Chain	Res	Type	Atoms
88	m	900	GDP	C5'-O5'-PA-O3A
88	m	900	GDP	C5'-O5'-PA-O1A
88	m	900	GDP	C5'-O5'-PA-O2A
88	m	900	GDP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

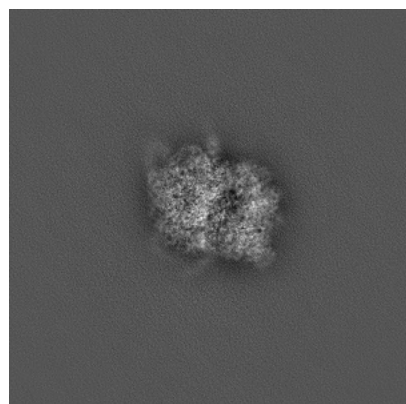
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23501. These allow visual inspection of the internal detail of the map and identification of artifacts.

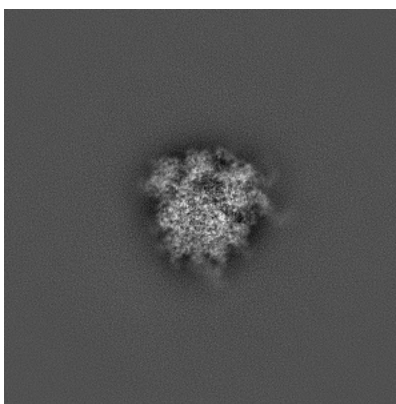
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

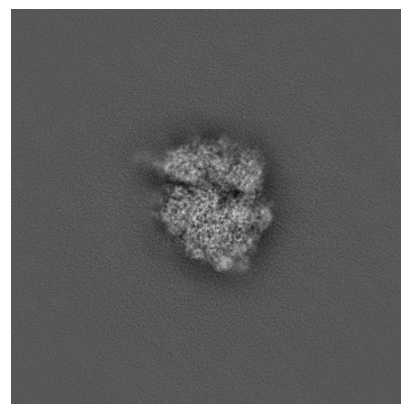
6.1.1 Primary map



X

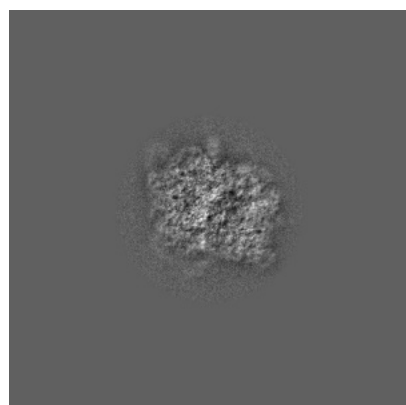


Y

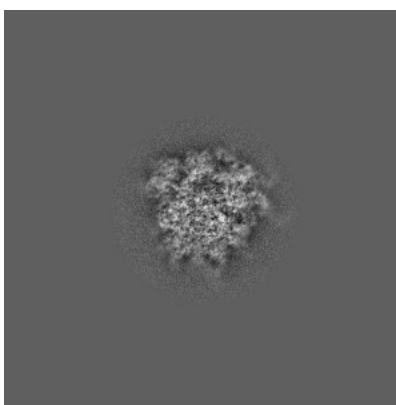


Z

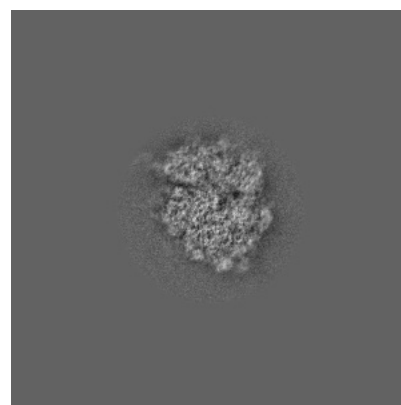
6.1.2 Raw map



X



Y

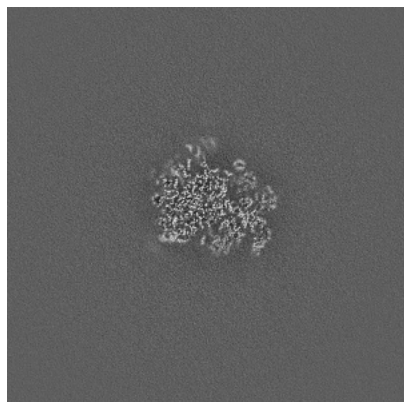


Z

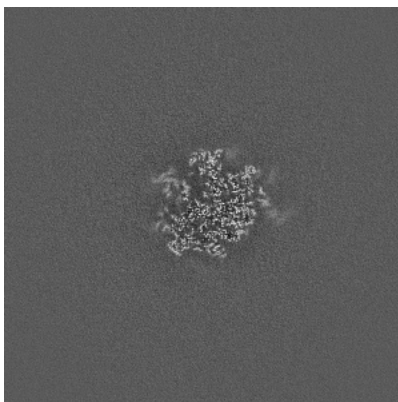
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

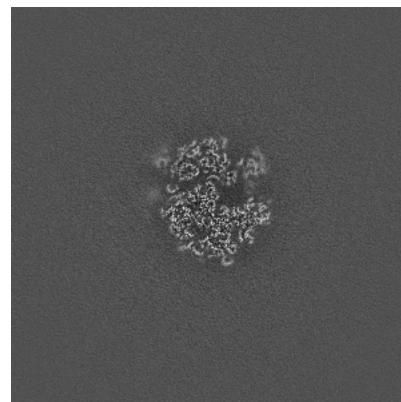
6.2.1 Primary map



X Index: 384

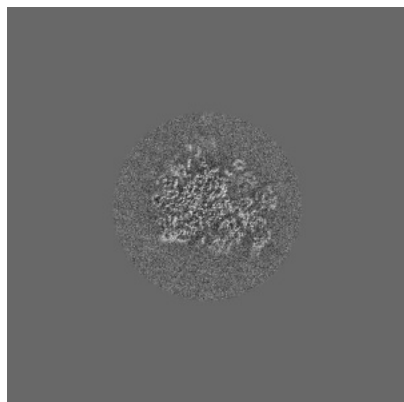


Y Index: 384

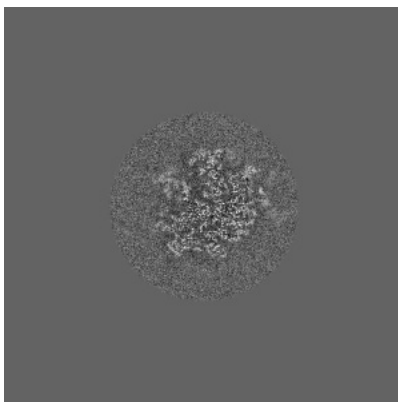


Z Index: 384

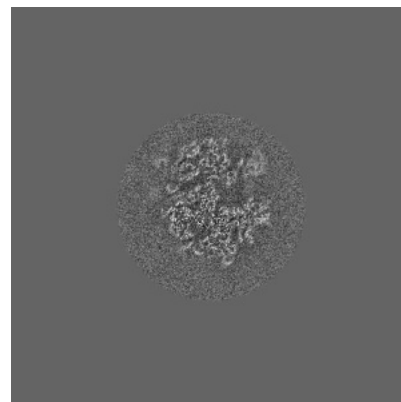
6.2.2 Raw map



X Index: 384



Y Index: 384

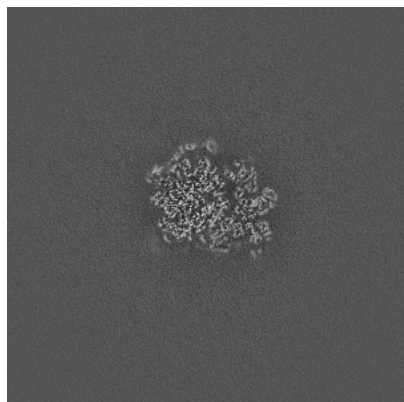


Z Index: 384

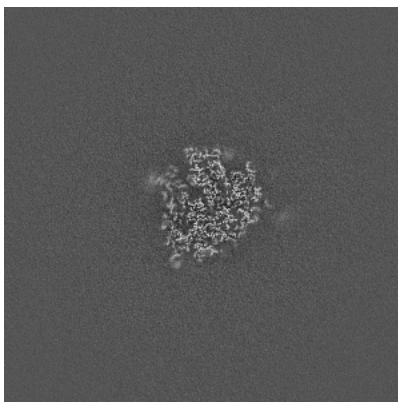
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

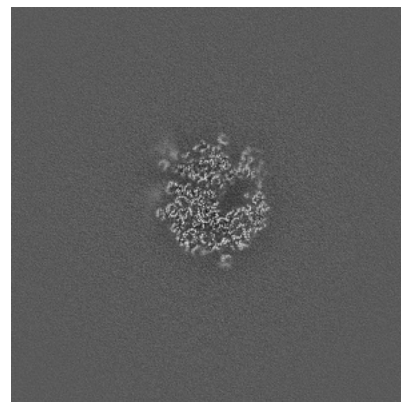
6.3.1 Primary map



X Index: 390

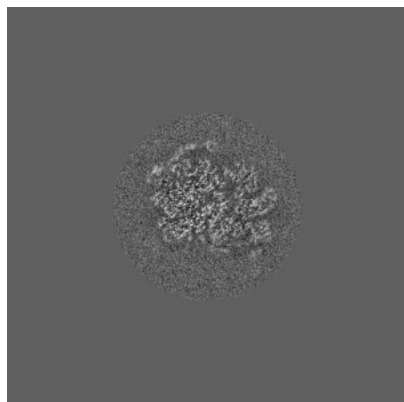


Y Index: 376

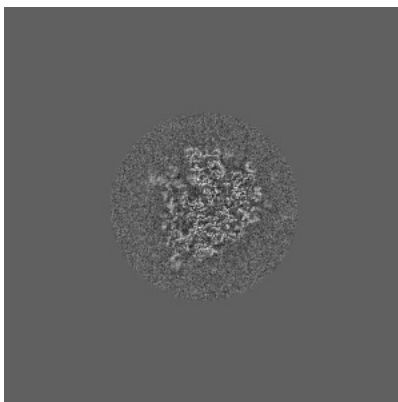


Z Index: 375

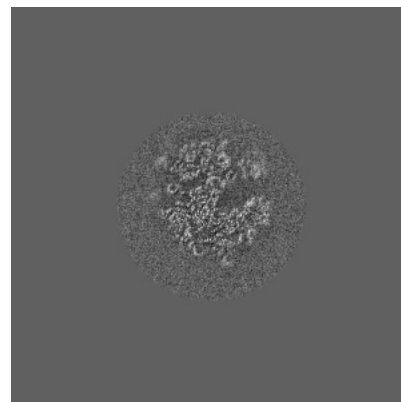
6.3.2 Raw map



X Index: 390



Y Index: 376

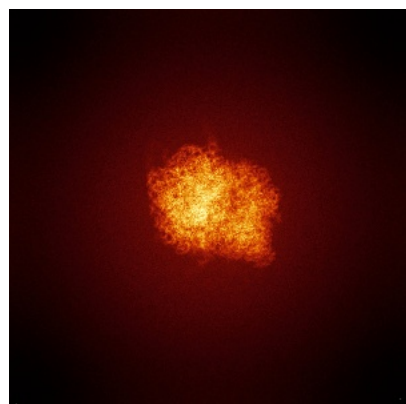


Z Index: 381

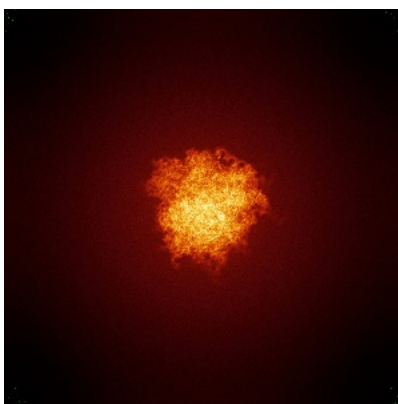
The images above show the largest variance slices of the map in three orthogonal directions.

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

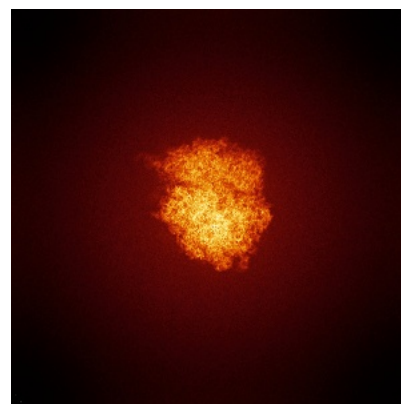
6.4.1 Primary map



X

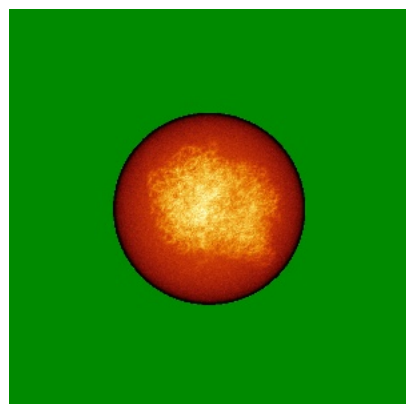


Y

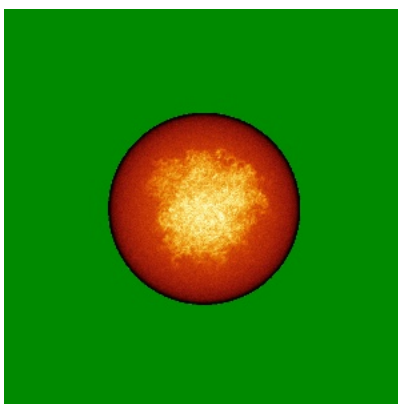


Z

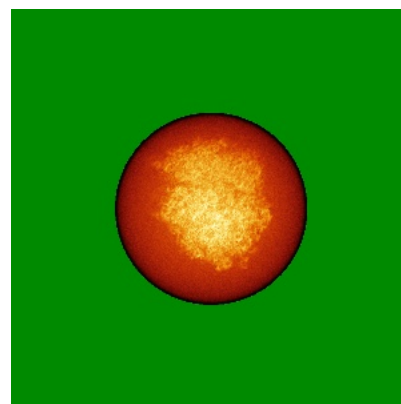
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



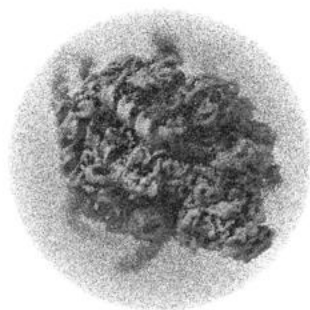
Y



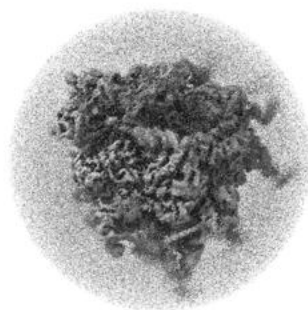
Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

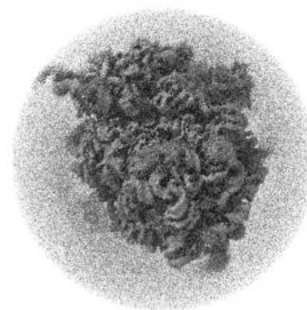
6.5.2 Raw map



X



Y



Z

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

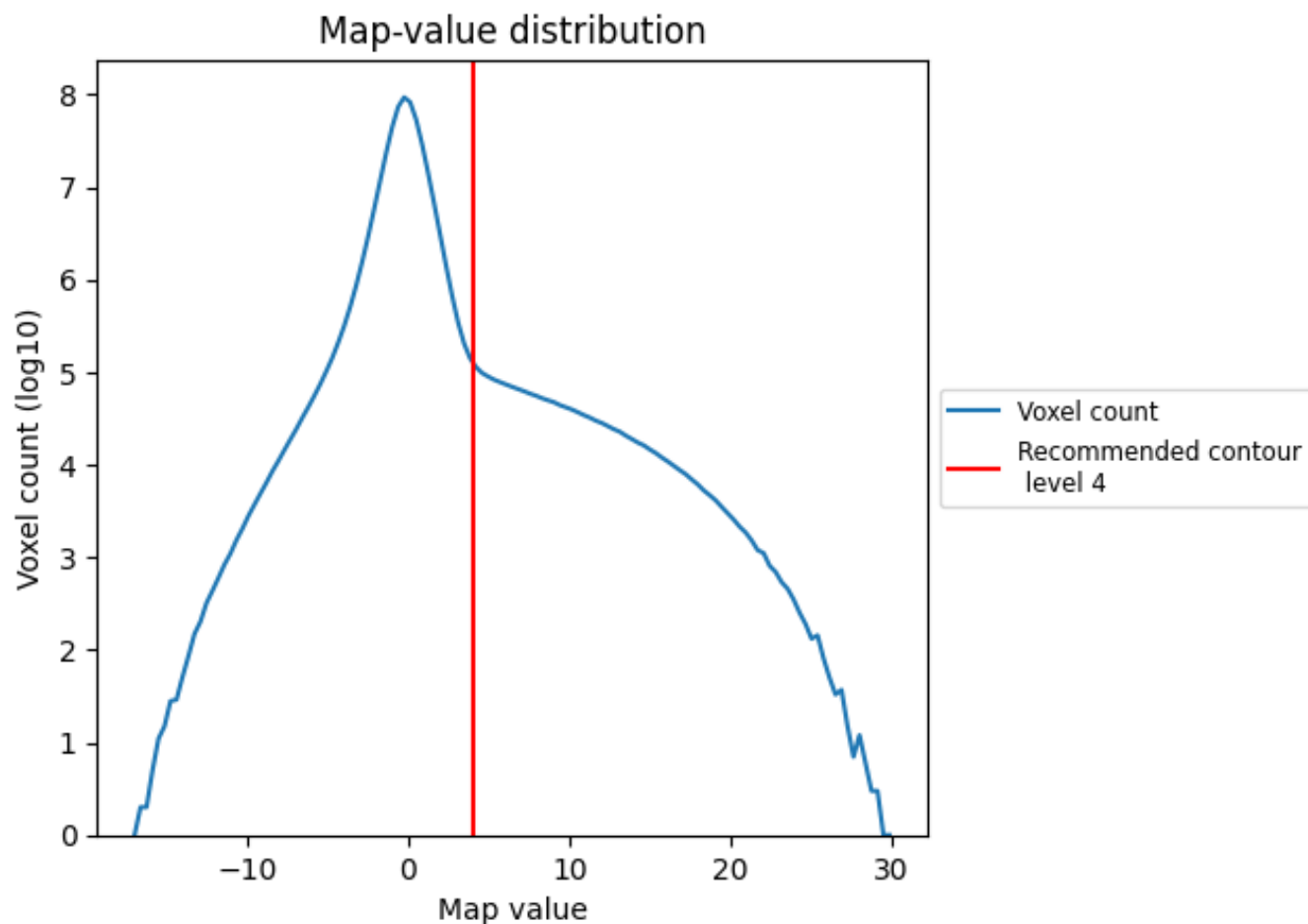
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

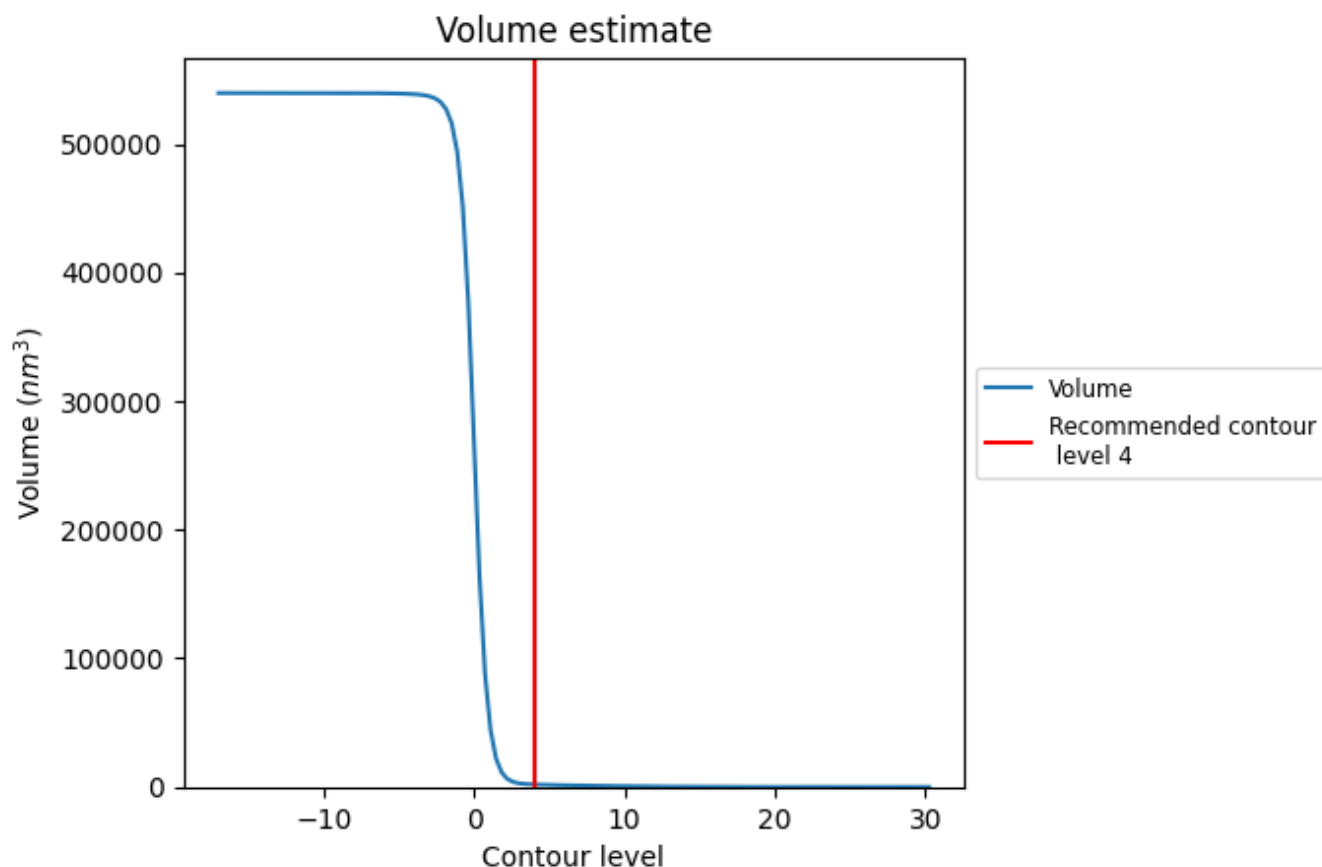
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

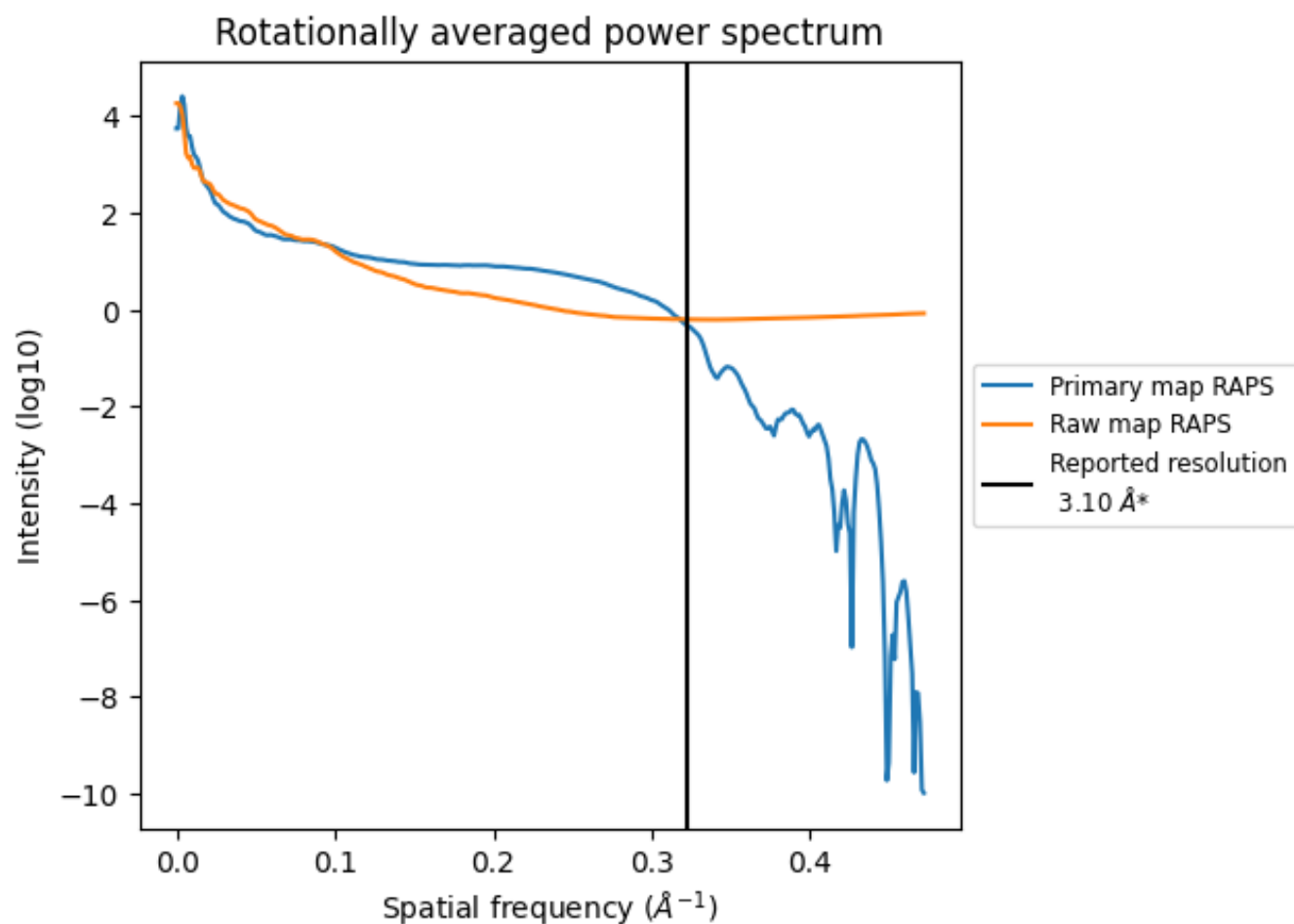
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1947 nm³; this corresponds to an approximate mass of 1759 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 ⓘ

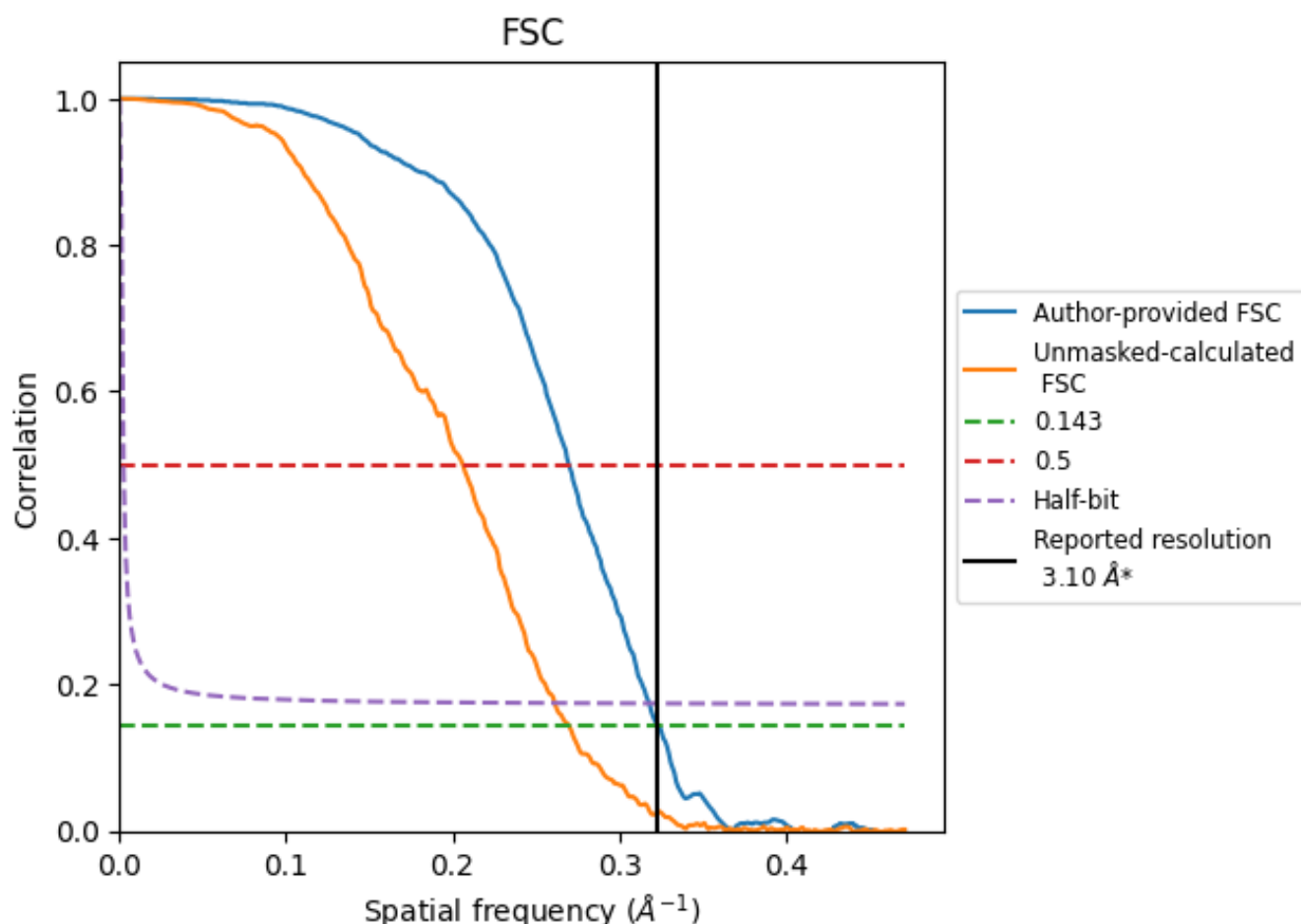


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

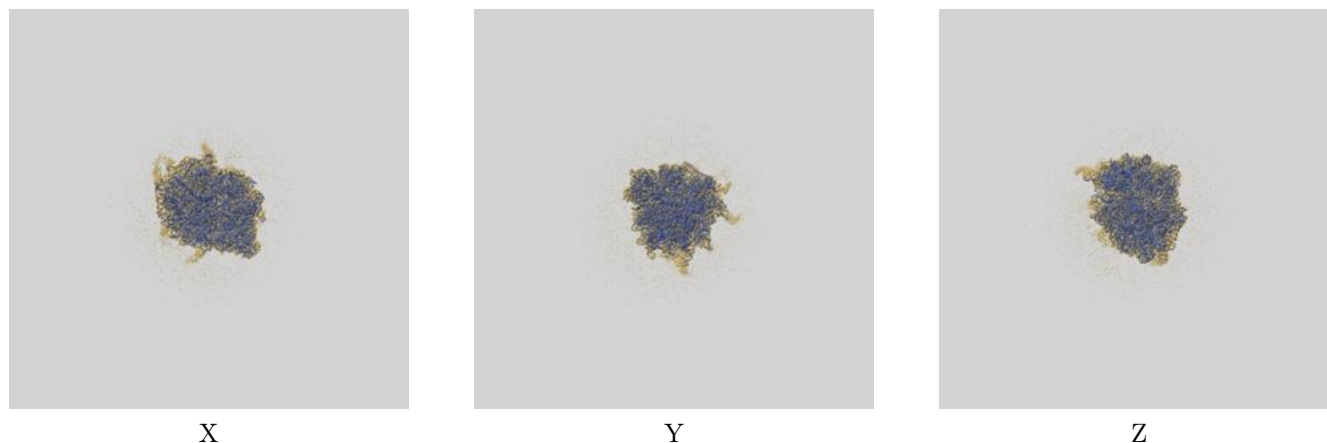
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.71	3.14
Unmasked-calculated*	3.70	4.85	3.82

*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 3.70 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

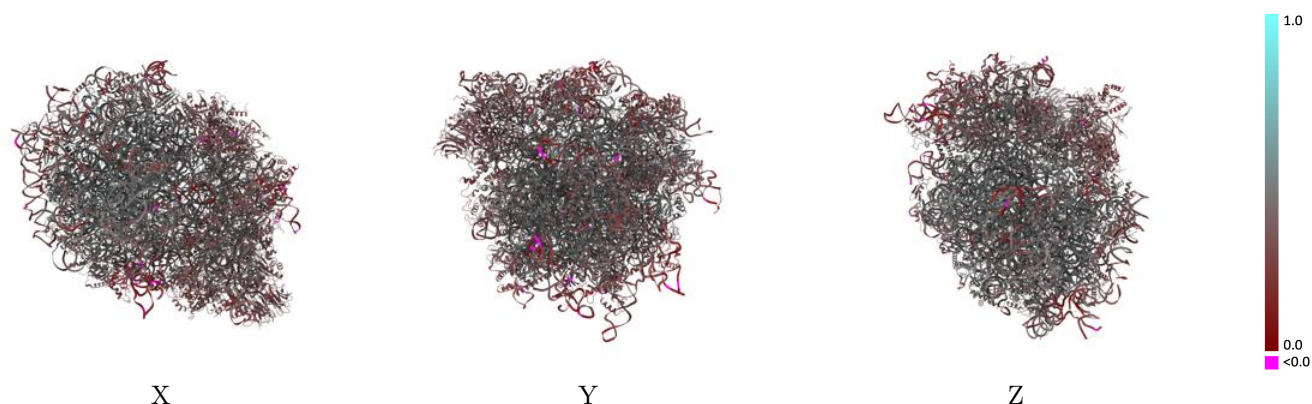
This section contains information regarding the fit between EMDB map EMD-23501 and PDB model 7LS2. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



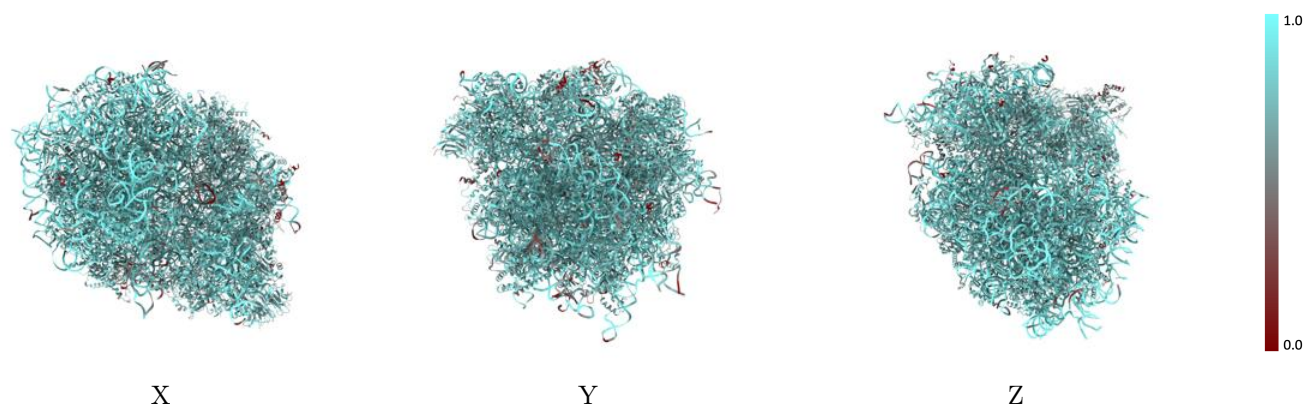
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



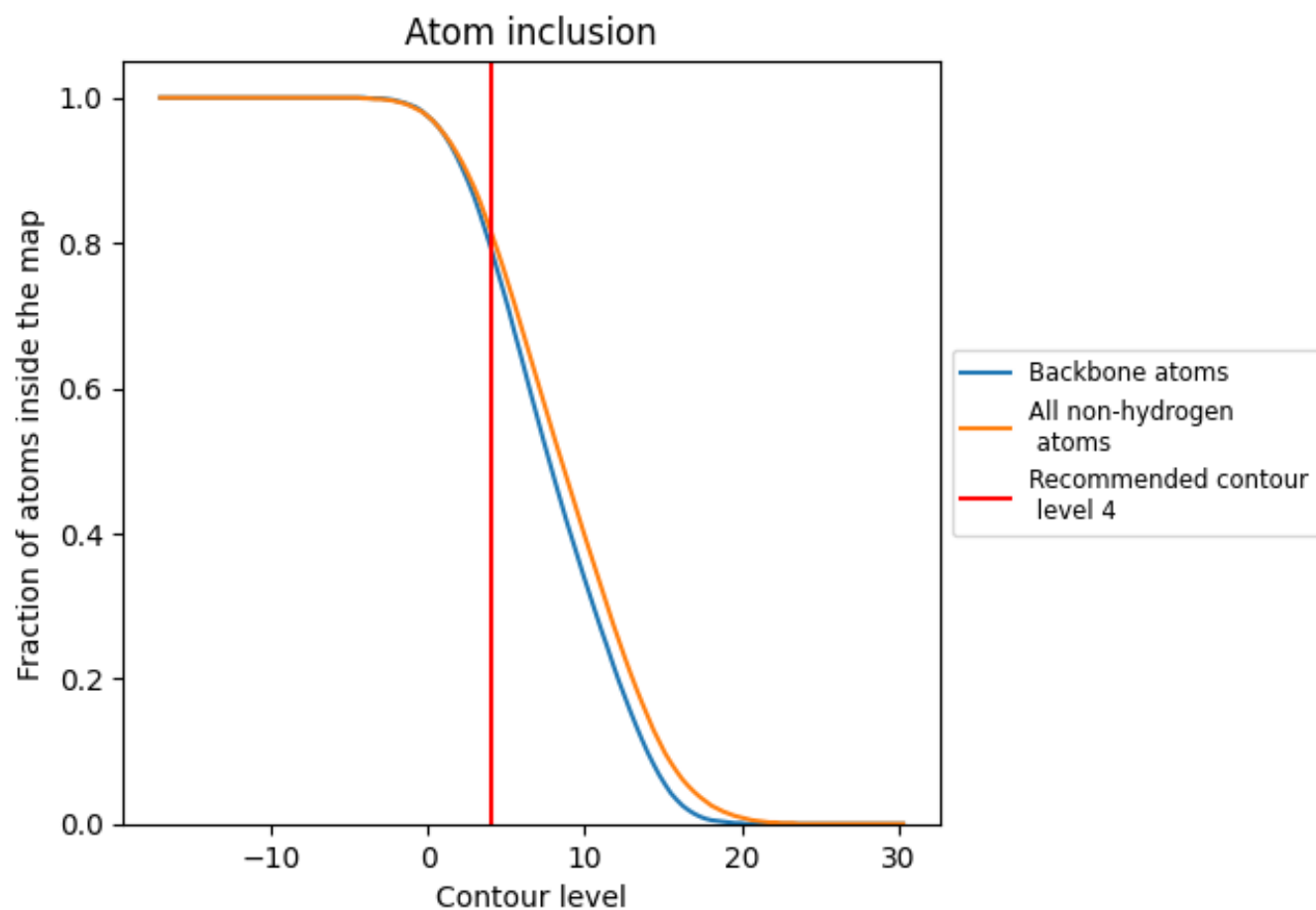
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.4180
A	 0.4700	 0.3630
A1	 0.7780	 0.4580
A2	 0.8970	 0.4300
A3	 0.7120	 0.3420
B1	 0.7880	 0.4240
B2	 0.9540	 0.4720
B3	 0.7440	 0.3570
C1	 0.7800	 0.4590
C2	 0.9040	 0.4380
C3	 0.7140	 0.3830
D1	 0.7730	 0.4580
D2	 0.7590	 0.4860
D3	 0.7780	 0.4410
E1	 0.7680	 0.4040
E2	 0.7830	 0.4710
E3	 0.6950	 0.4540
F1	 0.8060	 0.4500
F2	 0.7790	 0.4700
F3	 0.7430	 0.4340
G1	 0.8210	 0.4530
G2	 0.8280	 0.4350
G3	 0.5950	 0.3320
H1	 0.8020	 0.4830
H2	 0.8040	 0.4460
H3	 0.7470	 0.4140
I2	 0.7930	 0.4640
I3	 0.7380	 0.3410
J2	 0.8090	 0.4840
J3	 0.7490	 0.4370
K2	 0.7850	 0.4790
K3	 0.6940	 0.3330
L1	 0.5420	 0.2240
L2	 0.7780	 0.4350
L3	 0.7300	 0.3840





















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Chain	Atom inclusion	Q-score
M2	 0.8200	 0.4820
M3	 0.5300	 0.2310
N2	 0.7910	 0.4700
N3	 0.7250	 0.4080
O2	 0.7560	 0.3970
O3	 0.7060	 0.3950
P2	 0.7270	 0.4840
P3	 0.7230	 0.4420
Q2	 0.7210	 0.3850
Q3	 0.6740	 0.3340
R2	 0.7830	 0.4460
R3	 0.6790	 0.3080
S2	 0.8010	 0.4570
S3	 0.7300	 0.4000
T2	 0.8160	 0.4530
T3	 0.6970	 0.4040
U2	 0.8140	 0.4920
U3	 0.6830	 0.2920
V2	 0.7270	 0.4210
W2	 0.7940	 0.4470
X2	 0.7890	 0.4580
Y2	 0.7800	 0.4850
Z2	 0.8150	 0.4950
a2	 0.7790	 0.4630
b2	 0.7760	 0.4260
c2	 0.8060	 0.4400
d2	 0.7870	 0.4870
e2	 0.7230	 0.4070
f2	 0.7610	 0.4530
g2	 0.7890	 0.4750
h2	 0.7030	 0.4520
i2	 0.7770	 0.4710
j	 0.7270	 0.3390
j2	 0.7560	 0.4500
k	 0.6280	 0.2890
k2	 0.8350	 0.4750
m	 0.7040	 0.3900
m2	 0.8860	 0.3980
n2	 0.8430	 0.3610
o2	 0.7720	 0.4090
p2	 0.7020	 0.3900
q2	 0.7120	 0.3860

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Chain	Atom inclusion	Q-score
r2	 0.7160	 0.4040
s2	 0.6480	 0.3140
t	 0.7170	 0.3620
u	 0.6780	 0.3720
v2	 0.7150	 0.3530
w2	 0.6800	 0.4210
x2	 0.7060	 0.3510
y2	 0.7120	 0.3540
z2	 0.7150	 0.3830