wwPDB EM Validation Summary Report

Mar 23, 2026 – 10:37 PM UTC

PDB ID	:	9ED0 / pdb_00009ed0
EMDB ID	:	EMD-47929
Title	:	Human LARP1 bound to the 40S small ribosomal subunit
Authors	:	Dong, W.; Kaufhold, R.; Brito Querido, J.
Deposited on	:	2024-11-15
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

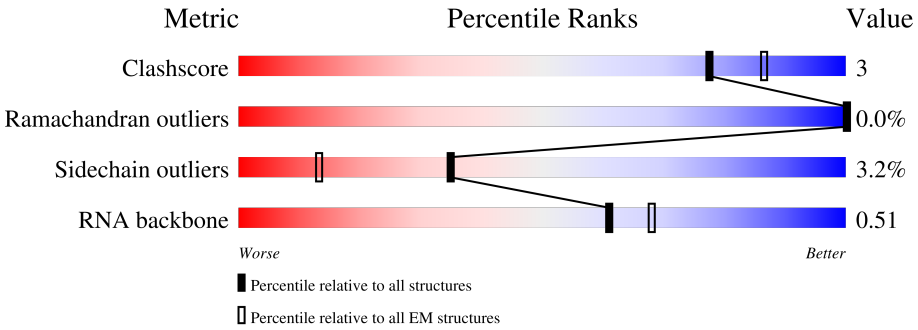
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

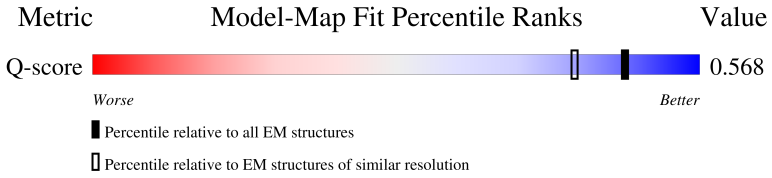
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	2	1869	7% 64% 20% • 13%
2	A	295	7% 59% 11% 30%
3	B	264	16% 71% 8% 20%

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Mol	Chain	Length	Quality of chain
4	C	293	5% 69% 6% 25%
5	D	243	19% 77% 15% 8%
6	E	263	90% 8%
7	F	204	21% 79% 9% 11%
8	G	249	10% 80% 12% 9%
9	H	194	71% 80% 13% 5%
10	I	208	12% 88% 10%
11	J	194	5% 89% 6% 5%
12	K	165	22% 43% 13% 41%
13	L	158	5% 83% 6% 11%
14	M	132	79% 65% 13% 21%
15	N	151	13% 93% 5%
16	O	151	73% 11% 16%
17	P	145	44% 74% 8% 15%
18	Q	146	10% 79% 15% 5%
19	R	135	51% 85% 10%
20	S	152	55% 76% 18% 6%
21	T	145	19% 90% 8%
22	U	119	36% 70% 16% 13%
23	V	83	10% 88% 12%
24	W	130	93% 6%
25	X	143	90% 8%
26	Y	133	87% 8%
27	Z	125	46% 49% 9% 42%
28	a	115	81% 14%

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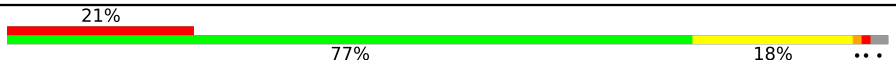
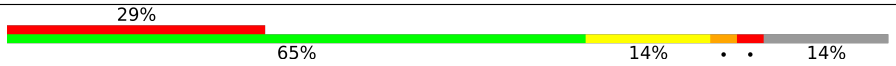
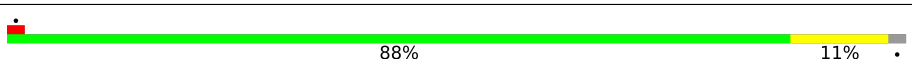
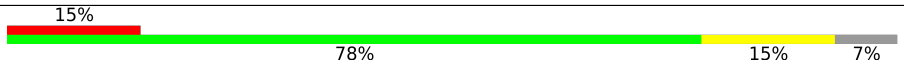
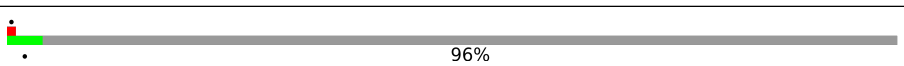
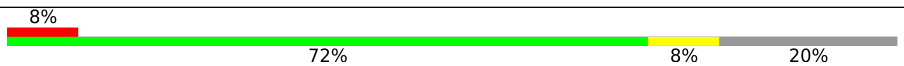
Mol	Chain	Length	Quality of chain
29	b	84	
30	c	69	
31	d	56	
32	e	59	
33	f	156	
34	g	317	
35	h	1096	
36	n	25	

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 73475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1617	34700	15519	6236	11323	1622	6	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1625	1040	287	290	8	1	0

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	210	1711	1086	306	305	14	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	219	1708	1105	295	298	10	1	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	224	1745	1112	314	312	7	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	182	Total	C	N	O	S	0	0
			1445	906	271	261	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

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

- Molecule 9 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	184	Total	C	N	O	S	0	0
			1477	942	271	263	1		

- Molecule 10 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 11 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 12 is a protein called Small ribosomal subunit protein eS10.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	141	Total	C	N	O	S	0	0
			1157	737	217	197	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	104	Total	C	N	O	S	0	0
			790	494	138	151	7		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	127	Total	C	N	O	S	0	0
			957	585	189	177	6		

- Molecule 17 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	123	Total	C	N	O	S	0	0
			998	635	188	169	6		

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1105	704	207	191	3		

- Molecule 19 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	143	Total	C	N	O	S	1	0
			1192	751	240	200	1		

- Molecule 21 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 23 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 27 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	72	Total	C	N	O	S	0	0
			570	366	104	99	1		

- Molecule 28 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	59	Total	C	N	O	S	0	0
			464	281	93	88	2		

- Molecule 31 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 32 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 33 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	64	Total	C	N	O	S	0	0
			522	329	99	87	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	312	Total	C	N	O	S	0	0
			2408	1518	420	458	12		

- Molecule 35 is a protein called La-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	46	Total	C	N	O	S	0	0
			345	214	63	67	1		

- Molecule 36 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	20	Total	C	N	O	S	0	0
			193	119	51	20	3		

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	2	68	Total	K	0
			68	68	
37	S	1	Total	K	0
			1	1	
37	X	1	Total	K	0
			1	1	
37	d	1	Total	K	0
			1	1	

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	2	91	Total	Mg	0
			91	91	
38	G	1	Total	Mg	0
			1	1	

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

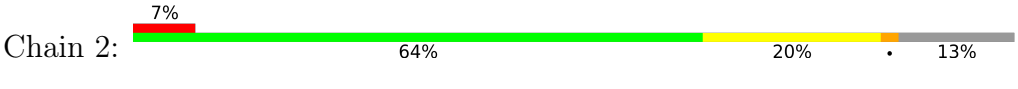
Mol	Chain	Residues	Atoms		AltConf
39	a	1	Total	Zn	0
			1	1	
39	d	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

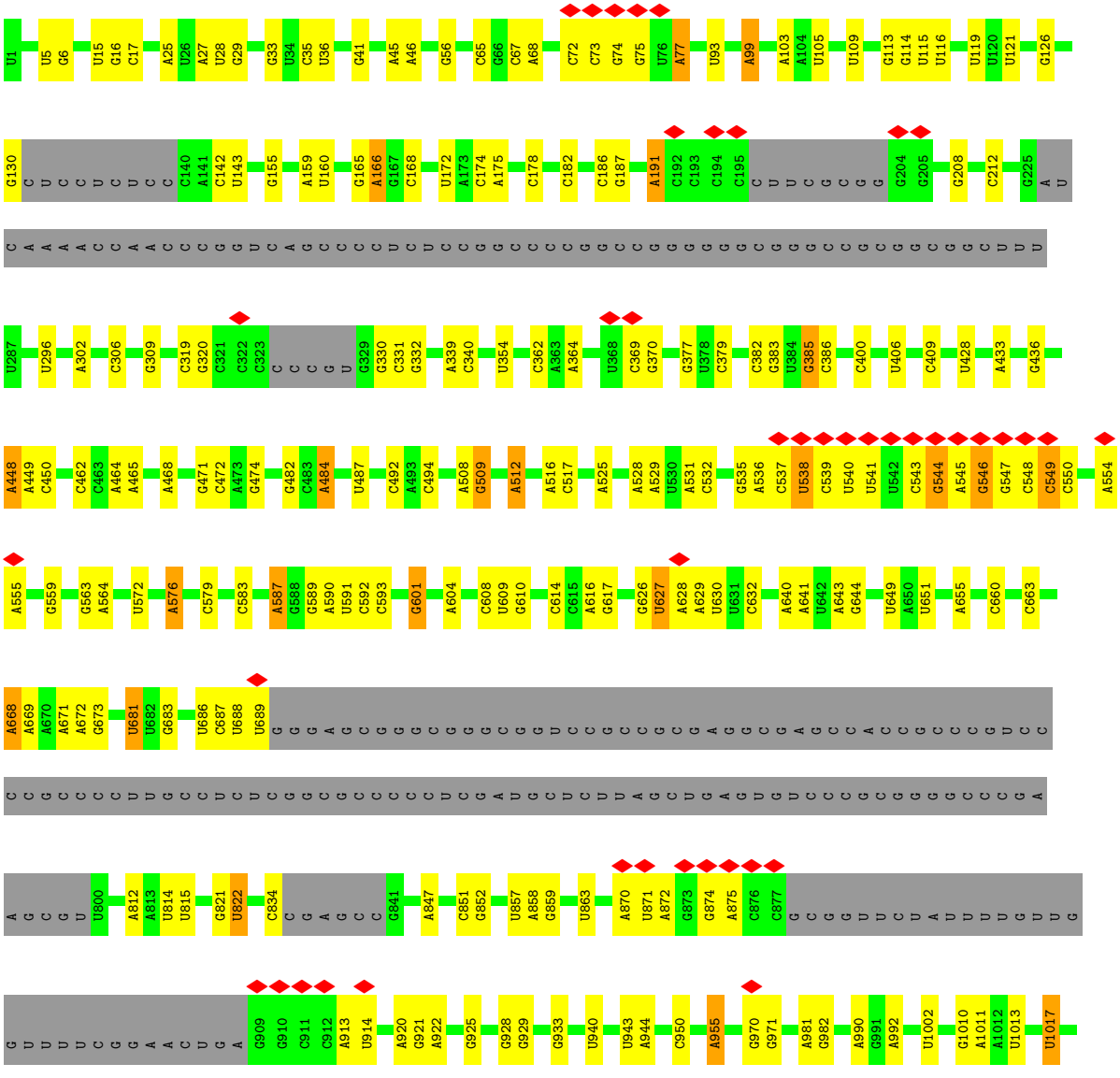
3 Residue-property plots (i)

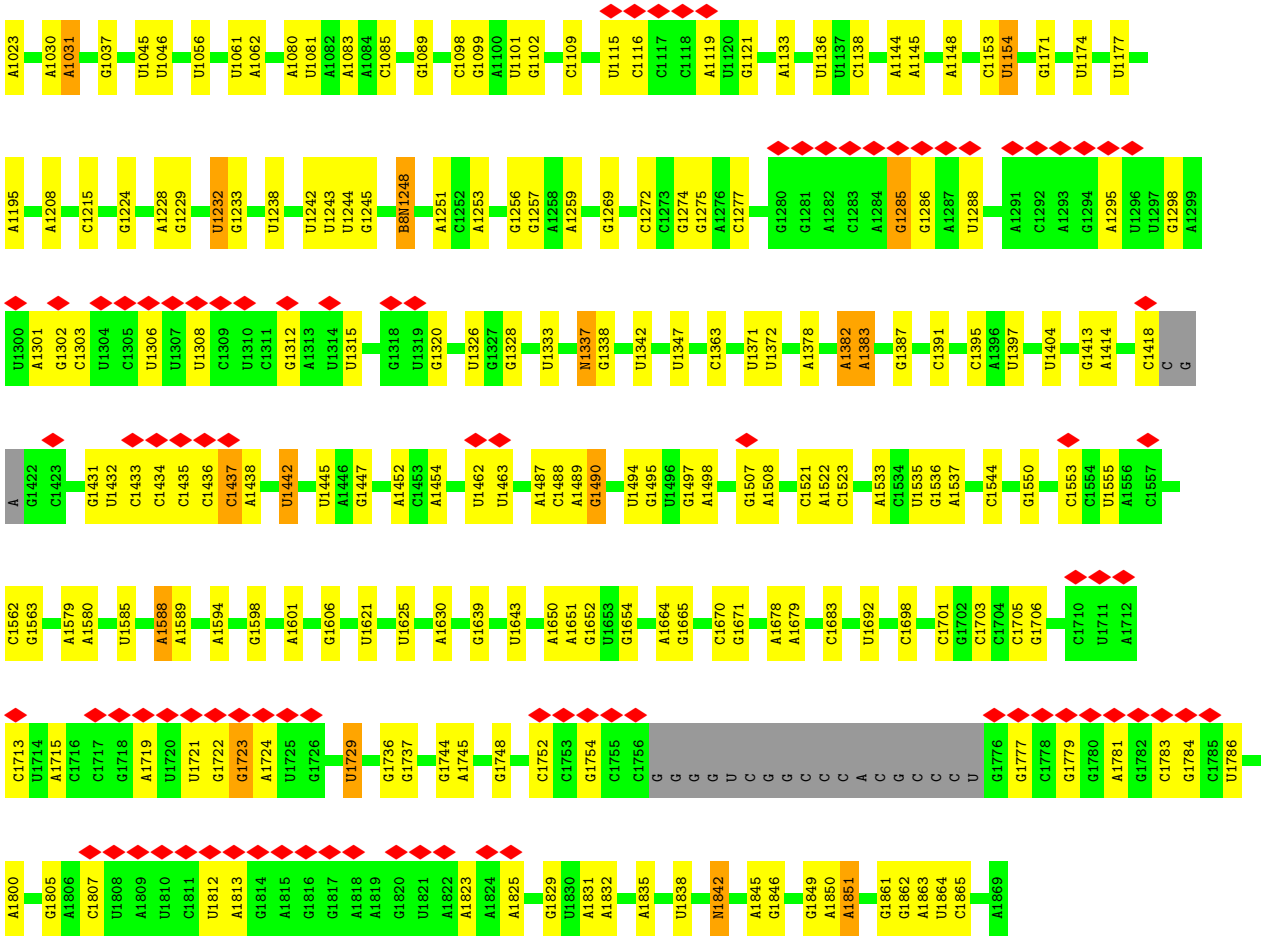
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: rRNA

Chain 2:

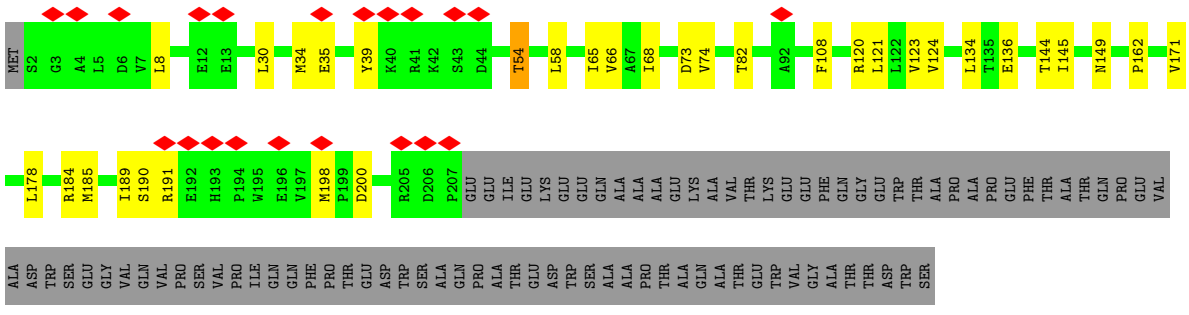






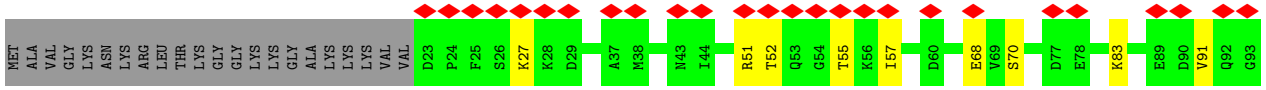
• Molecule 2: Small ribosomal subunit protein uS2

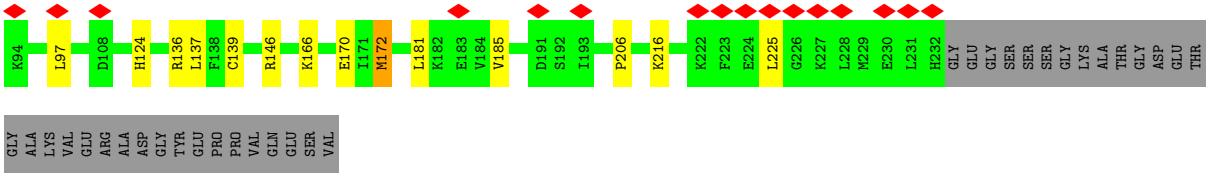
Chain A:



• Molecule 3: Small ribosomal subunit protein eS1

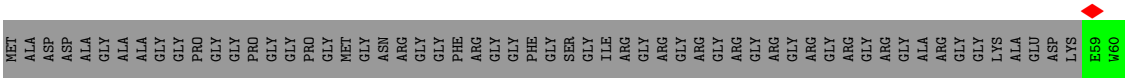
Chain B:

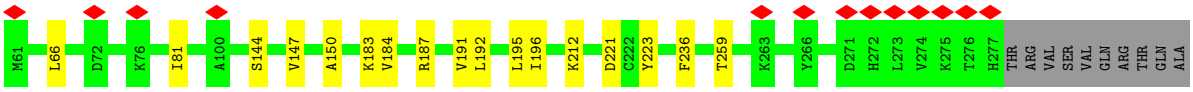




• Molecule 4: Small ribosomal subunit protein uS5

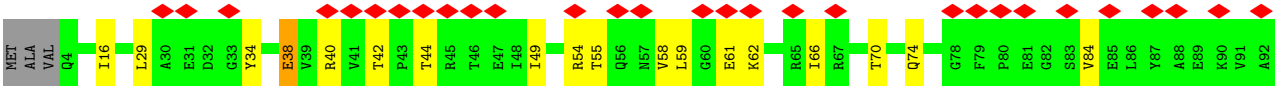
Chain C:

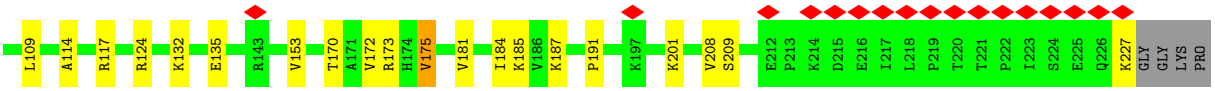




• Molecule 5: Small ribosomal subunit protein uS3

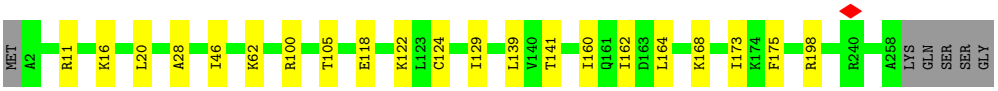
Chain D:





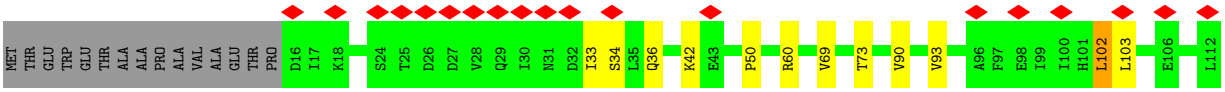
• Molecule 6: Small ribosomal subunit protein eS4, X isoform

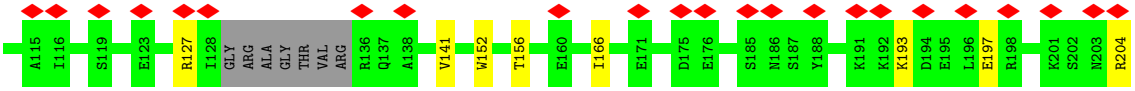
Chain E:



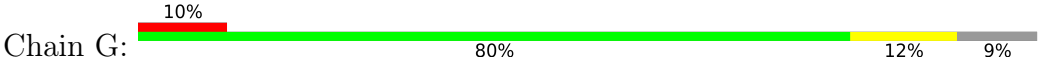
• Molecule 7: Small ribosomal subunit protein uS7

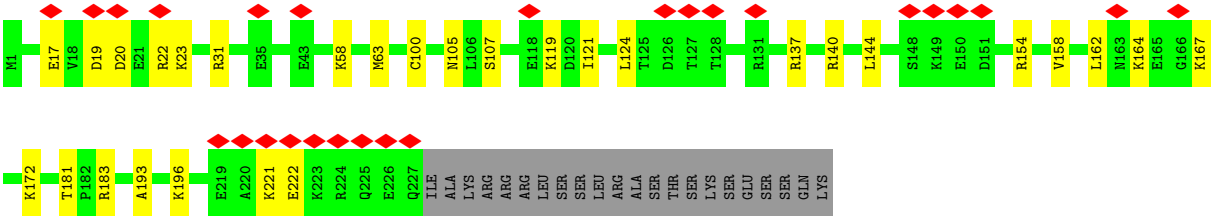
Chain F:



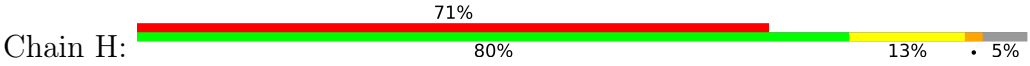


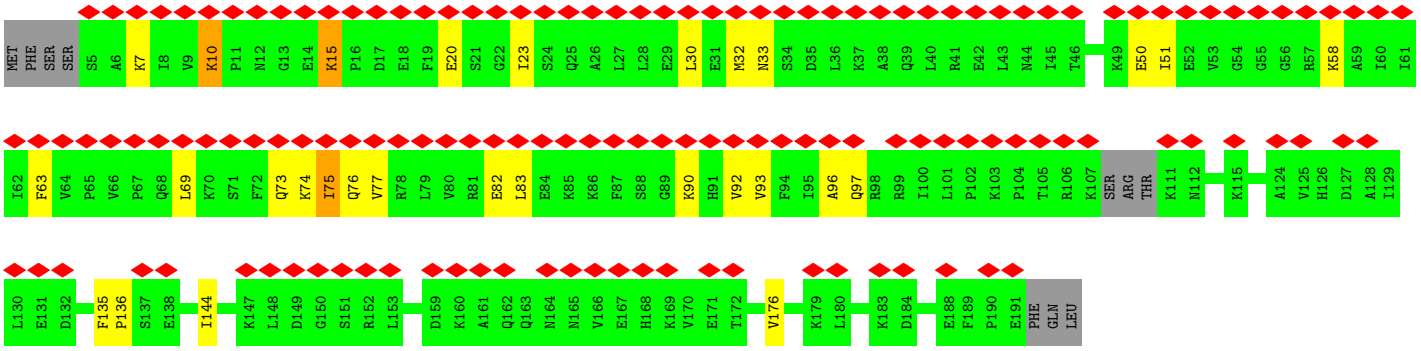
• Molecule 8: Small ribosomal subunit protein eS6



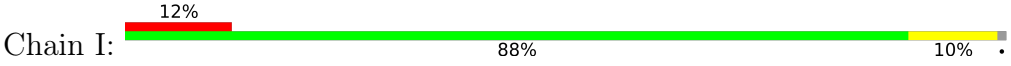


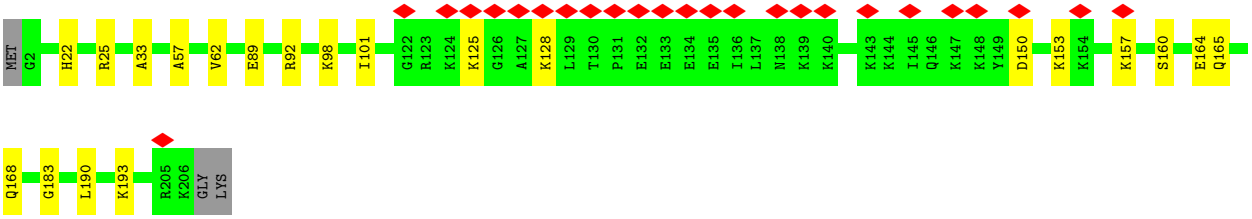
• Molecule 9: Small ribosomal subunit protein eS7



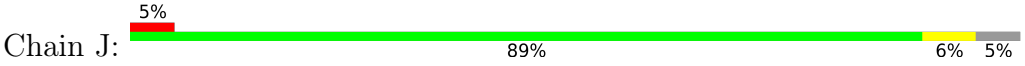


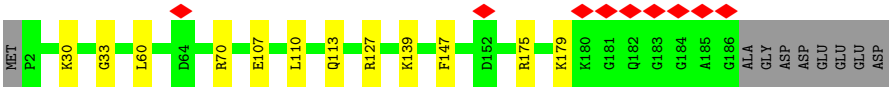
• Molecule 10: Small ribosomal subunit protein eS8





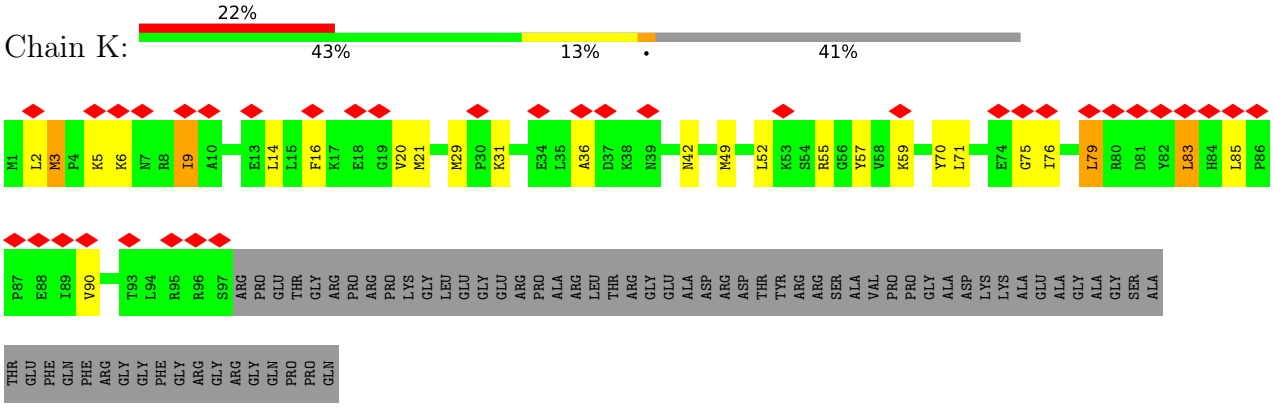
• Molecule 11: Small ribosomal subunit protein uS4





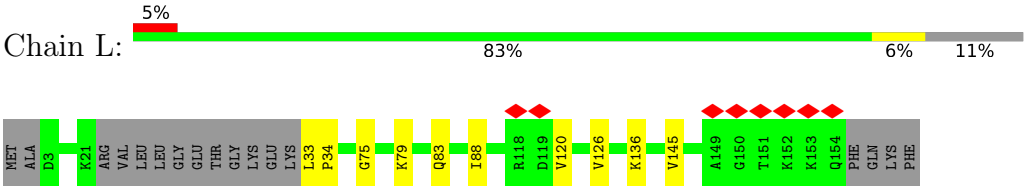
• Molecule 12: Small ribosomal subunit protein eS10

Chain K:



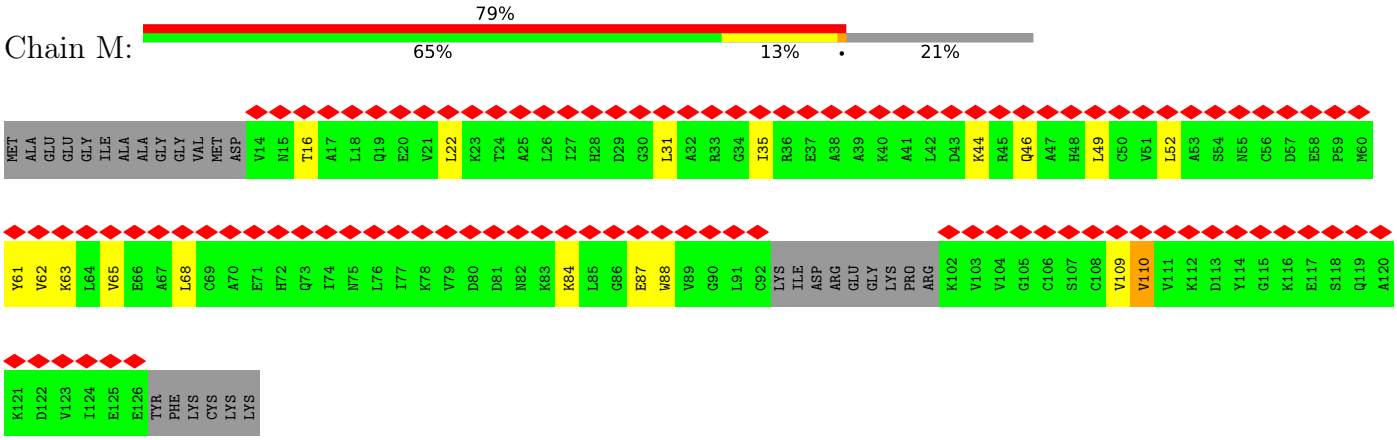
• Molecule 13: Small ribosomal subunit protein uS17

Chain L:



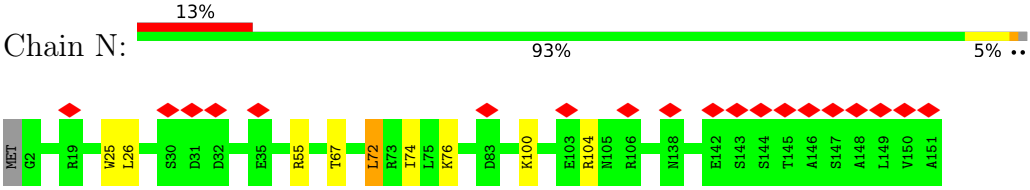
• Molecule 14: Small ribosomal subunit protein eS12

Chain M:



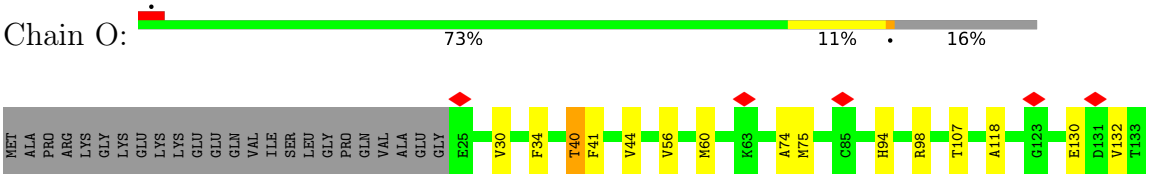
• Molecule 15: Small ribosomal subunit protein uS15

Chain N:



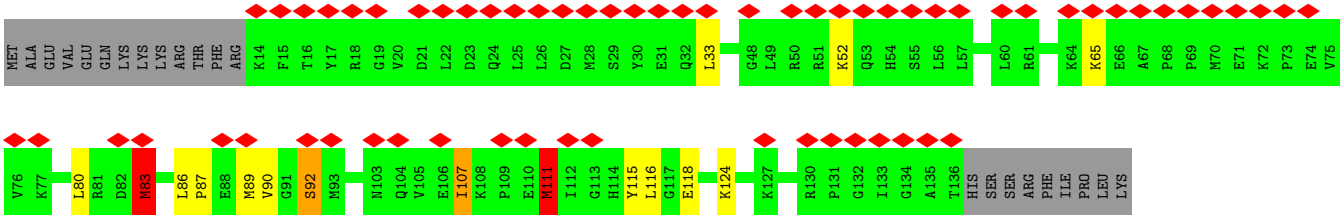
• Molecule 16: Small ribosomal subunit protein uS11

Chain O:



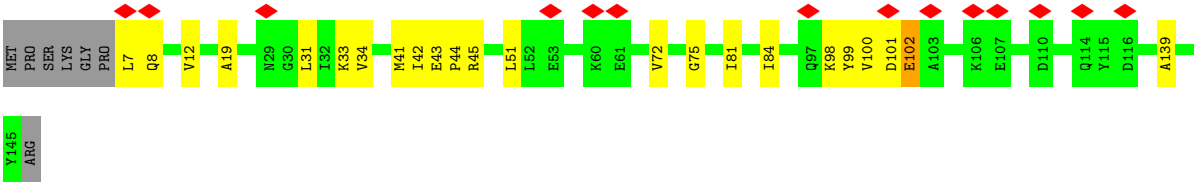
• Molecule 17: Small ribosomal subunit protein uS19

Chain P:



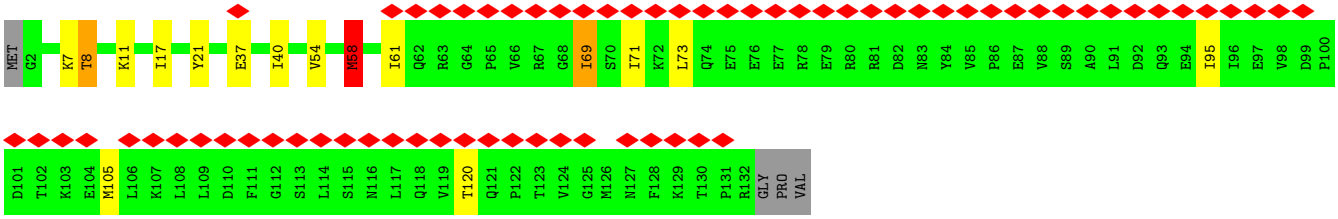
• Molecule 18: Small ribosomal subunit protein uS9

Chain Q:



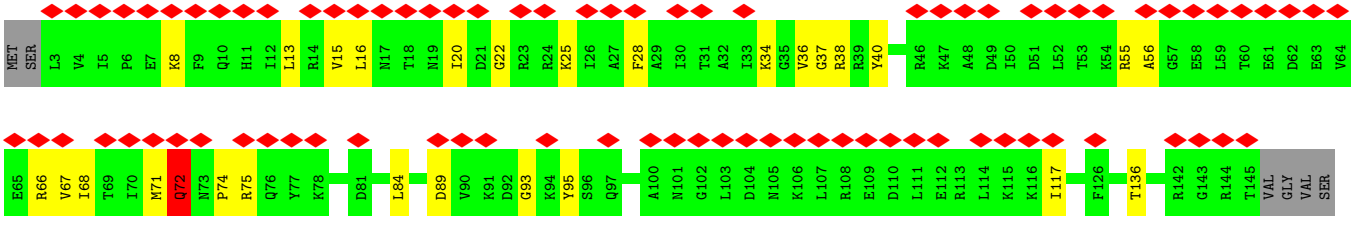
• Molecule 19: Small ribosomal subunit protein eS17

Chain R:



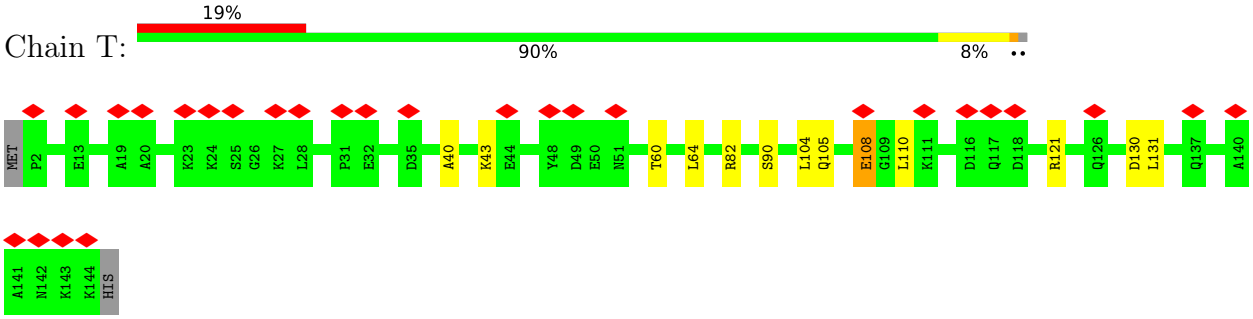
• Molecule 20: Small ribosomal subunit protein uS13

Chain S:



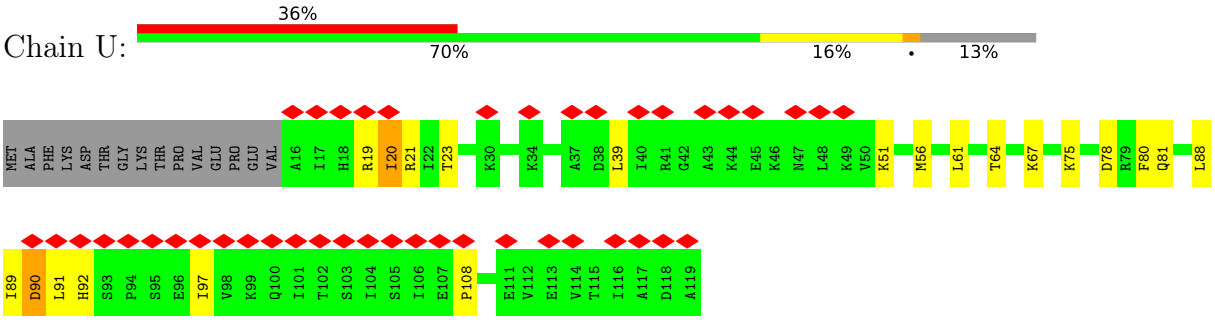
• Molecule 21: Small ribosomal subunit protein eS19

Chain T:



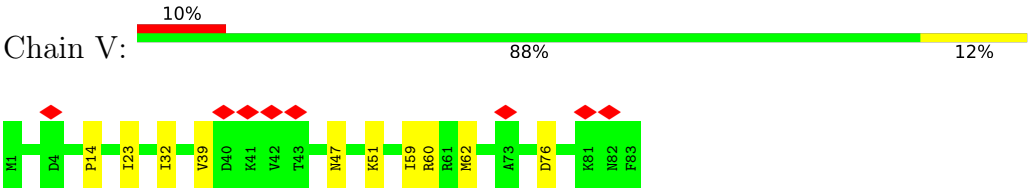
• Molecule 22: Small ribosomal subunit protein uS10

Chain U:



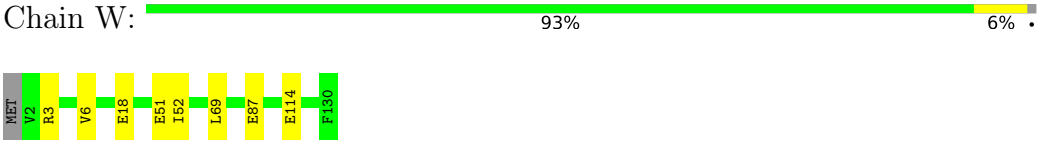
• Molecule 23: Small ribosomal subunit protein eS21

Chain V:



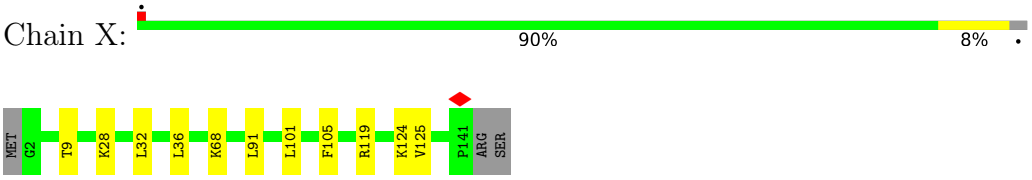
• Molecule 24: Small ribosomal subunit protein uS8

Chain W:



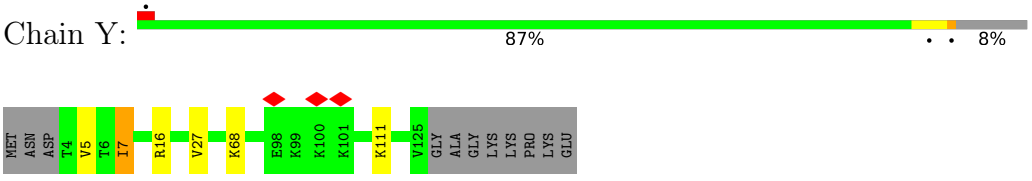
• Molecule 25: 40S ribosomal protein S23

Chain X:



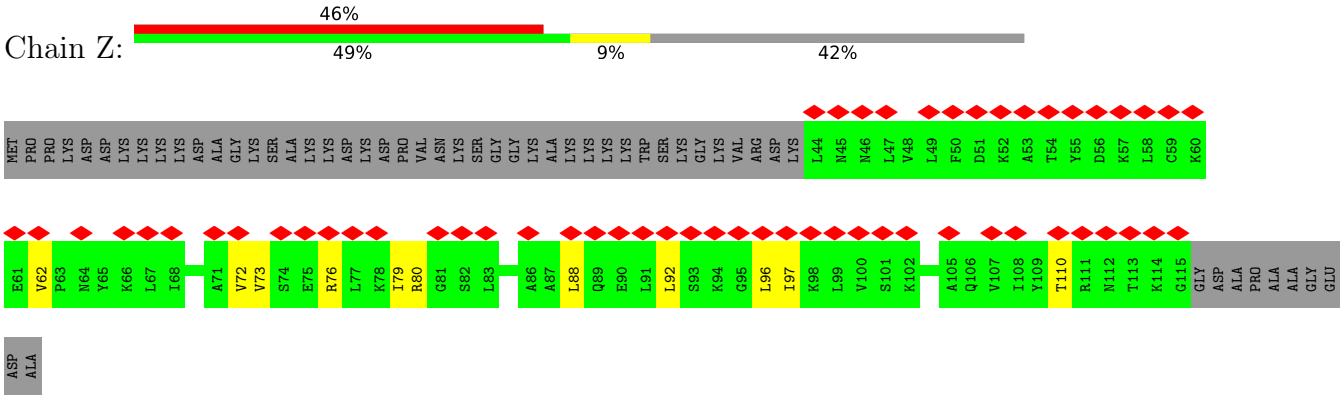
• Molecule 26: 40S ribosomal protein S24

Chain Y:



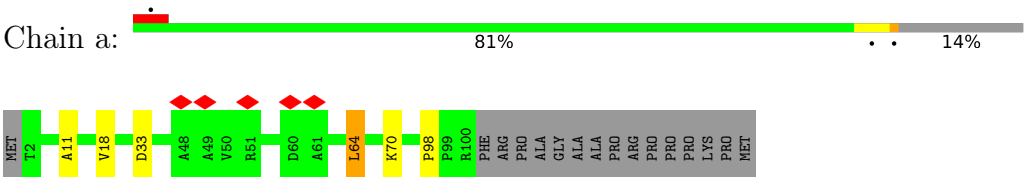
• Molecule 27: Small ribosomal subunit protein eS25

Chain Z:



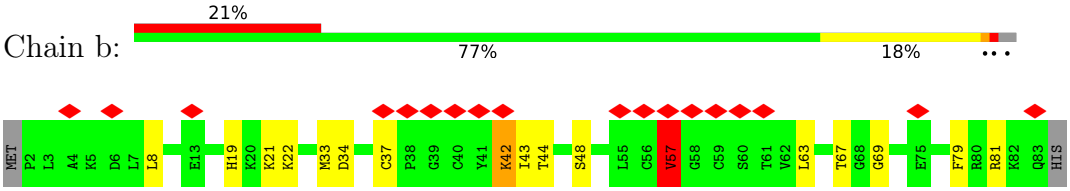
• Molecule 28: Small ribosomal subunit protein eS26

Chain a:



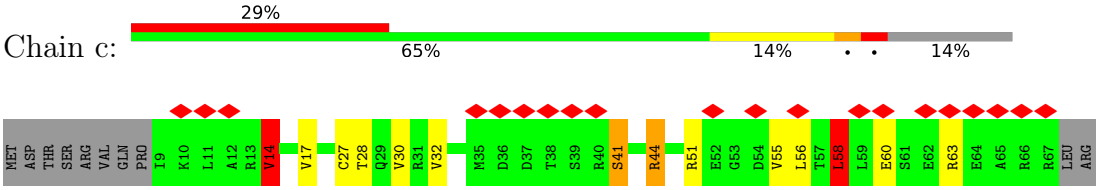
• Molecule 29: Small ribosomal subunit protein eS27

Chain b:



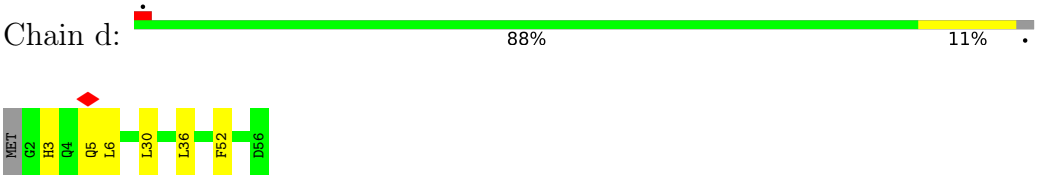
• Molecule 30: Small ribosomal subunit protein eS28

Chain c:



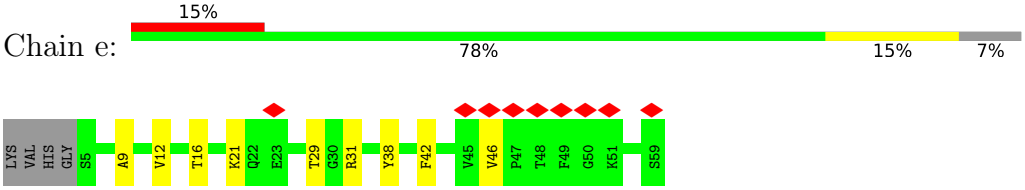
• Molecule 31: Small ribosomal subunit protein uS14

Chain d:



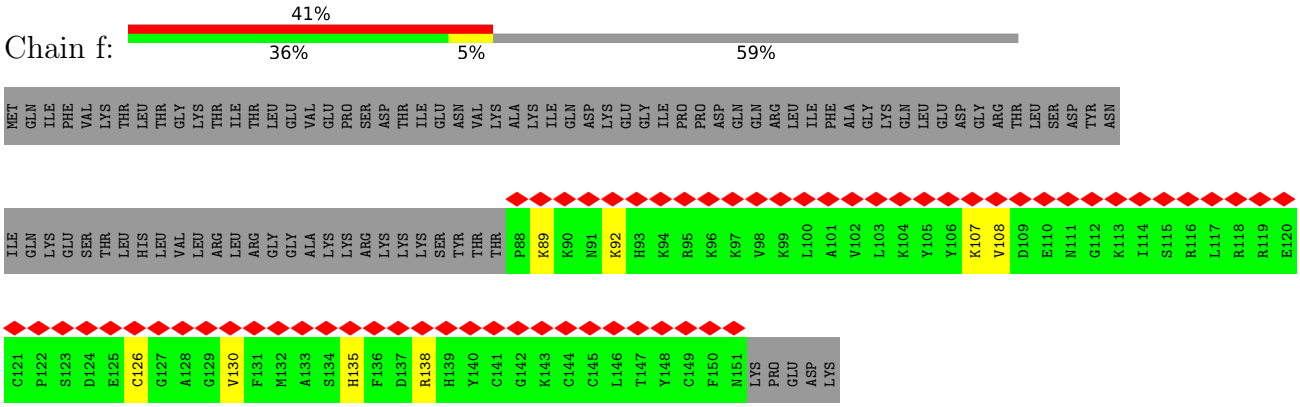
• Molecule 32: Small ribosomal subunit protein eS30

Chain e:



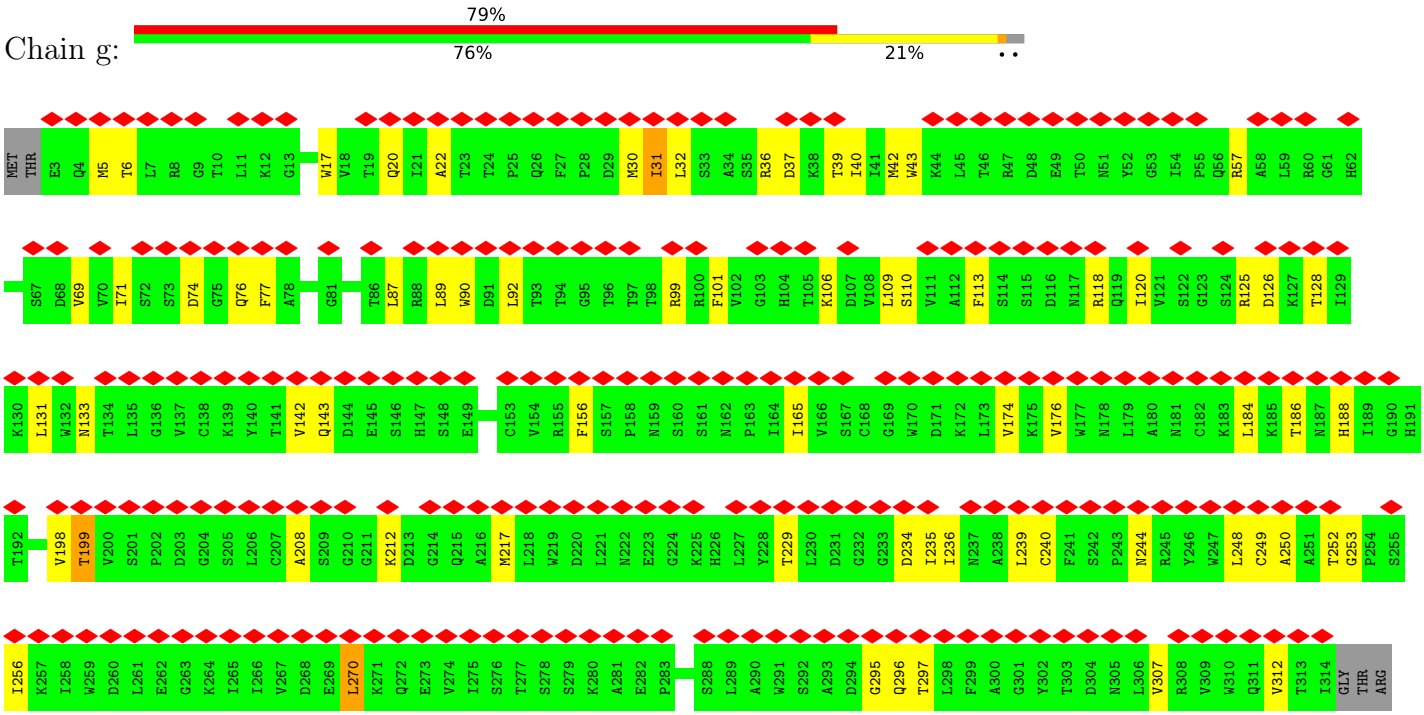
• Molecule 33: Ubiquitin-ribosomal protein eS31 fusion protein

Chain f:



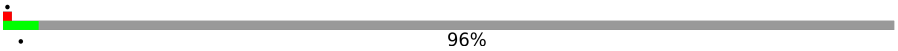
• Molecule 34: Receptor of activated protein C kinase 1

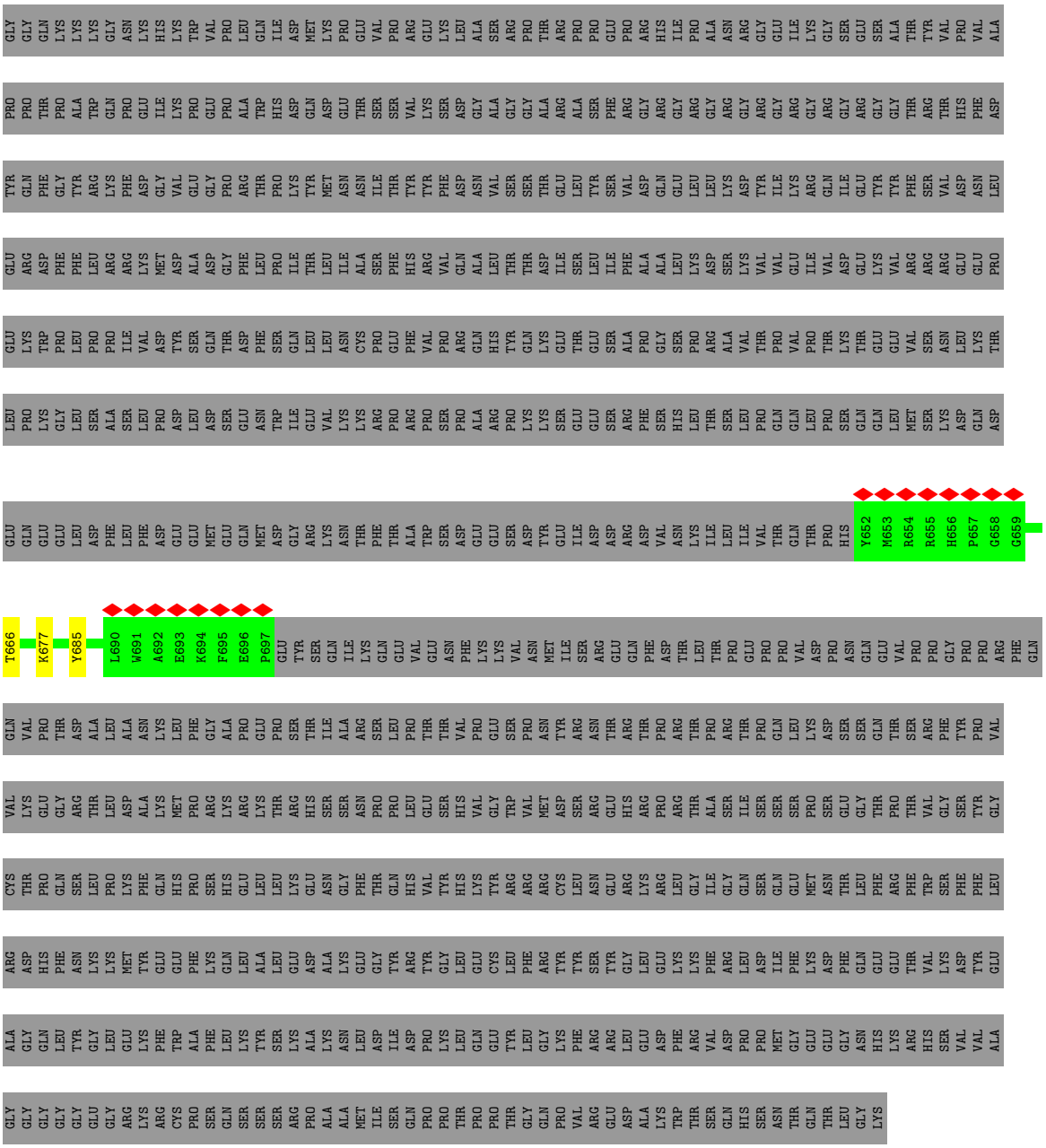
Chain g:



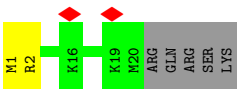
• Molecule 35: La-related protein 1

Chain h:





• Molecule 36: Small ribosomal subunit protein eS32



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124913	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	411.5, 411.5, 411.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.823, 0.823, 0.823	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, ZN, 7MG, OMG, OMU, 6MZ, OMC, MG, K, MA6, A2M, PSU, B8N

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	2	0.27	1/37048 (0.0%)	0.39	1/57731 (0.0%)
2	A	0.33	0/1665	0.56	0/2262
3	B	0.25	0/1738	0.50	1/2325 (0.0%)
4	C	0.28	0/1748	0.49	0/2361
5	D	0.25	0/1773	0.48	0/2387
6	E	0.28	0/2083	0.50	0/2805
7	F	0.37	1/1465 (0.1%)	0.58	0/1969
8	G	0.39	2/1863 (0.1%)	0.57	1/2481 (0.0%)
9	H	0.27	0/1498	0.63	0/2005
10	I	0.36	1/1711 (0.1%)	0.52	0/2282
11	J	0.29	0/1550	0.45	0/2069
12	K	0.60	0/840	0.71	0/1133
13	L	0.31	0/1177	0.47	0/1574
14	M	0.63	1/796 (0.1%)	0.66	0/1072
15	N	0.23	0/1232	0.45	0/1656
16	O	0.32	0/969	0.51	0/1298
17	P	0.39	2/1017 (0.2%)	0.61	1/1361 (0.1%)
18	Q	0.65	6/1122 (0.5%)	0.62	2/1503 (0.1%)
19	R	0.43	1/1078 (0.1%)	0.55	1/1447 (0.1%)
20	S	0.65	3/1214 (0.2%)	1.22	4/1626 (0.2%)
21	T	0.33	1/1131 (0.1%)	0.56	1/1515 (0.1%)
22	U	0.29	0/831	0.60	0/1115
23	V	0.46	1/643 (0.2%)	0.49	0/860
24	W	0.30	0/1051	0.51	0/1406
25	X	0.26	0/1105	0.52	0/1476
26	Y	0.26	0/1019	0.42	0/1354
27	Z	0.36	1/576 (0.2%)	0.54	0/774
28	a	0.32	0/805	0.53	1/1079 (0.1%)
29	b	0.45	2/653 (0.3%)	0.54	1/876 (0.1%)
30	c	0.85	3/465 (0.6%)	0.81	1/621 (0.2%)
31	d	0.27	0/470	0.48	0/623
32	e	0.19	0/443	0.46	0/582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	f	0.18	0/533	0.47	0/706
34	g	0.43	2/2465 (0.1%)	0.66	1/3359 (0.0%)
35	h	0.45	1/352 (0.3%)	0.70	0/475
36	n	0.30	0/194	0.57	0/246
All	All	0.33	29/76323 (0.0%)	0.49	16/110414 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	H	0	1
20	S	0	1
All	All	0	2

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	72	GLN	CD-NE2	14.96	1.64	1.33
14	M	110	VAL	CB-CG1	-11.73	1.13	1.52
30	c	58	LEU	CG-CD2	-11.33	1.15	1.52
18	Q	102	GLU	CD-OE1	-10.08	1.06	1.25
23	V	47	ASN	CG-OD1	-8.91	1.06	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	S	72	GLN	CA-CB-CG	32.95	179.99	114.10
20	S	72	GLN	OE1-CD-NE2	-25.78	96.82	122.60
20	S	72	GLN	N-CA-CB	-6.61	100.49	110.73
20	S	72	GLN	N-CA-C	6.40	121.14	112.88
30	c	44	ARG	CG-CD-NE	6.16	125.54	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	H	15	LYS	Peptide
20	S	72	GLN	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	34700	0	17574	84	0
2	A	1625	0	1645	19	0
3	B	1711	0	1782	9	0
4	C	1708	0	1797	7	0
5	D	1745	0	1839	18	0
6	E	2041	0	2143	10	0
7	F	1445	0	1495	11	0
8	G	1840	0	1989	14	0
9	H	1477	0	1573	16	0
10	I	1682	0	1769	11	0
11	J	1525	0	1640	9	0
12	K	816	0	841	20	0
13	L	1157	0	1222	5	0
14	M	790	0	808	12	0
15	N	1208	0	1293	5	0
16	O	957	0	982	8	0
17	P	998	0	1041	11	0
18	Q	1105	0	1172	11	0
19	R	1064	0	1118	8	0
20	S	1192	0	1253	18	0
21	T	1112	0	1146	4	0
22	U	821	0	883	10	0
23	V	636	0	637	5	0
24	W	1034	0	1080	5	0
25	X	1087	0	1154	6	0
26	Y	1002	0	1075	2	0
27	Z	570	0	626	6	0
28	a	792	0	841	4	0
29	b	640	0	665	9	0
30	c	464	0	488	7	0
31	d	459	0	448	3	0
32	e	438	0	484	5	0
33	f	522	0	529	6	0
34	g	2408	0	2339	36	0
35	h	345	0	303	1	0
36	n	193	0	237	2	0
37	2	68	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	S	1	0	0	0	0
37	X	1	0	0	0	0
37	d	1	0	0	0	0
38	2	91	0	0	0	0
38	G	1	0	0	0	0
39	a	1	0	0	0	0
39	d	1	0	0	0	0
39	f	1	0	0	0	0
All	All	73475	0	57911	372	0

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

The worst 5 of 372 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:67:VAL:O	20:S:71:MET:HB2	1.62	1.00
1:2:538:U:H3	1:2:549:C:H42	1.11	0.97
2:A:58:LEU:HD12	2:A:178:LEU:HD23	1.74	0.68
14:M:44:LYS:HG2	14:M:46:GLN:HG3	1.75	0.68
34:g:87:LEU:HB2	34:g:101:PHE:HB2	1.76	0.67

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	205/295 (70%)	199 (97%)	6 (3%)	0	100	100
3	B	208/264 (79%)	207 (100%)	1 (0%)	0	100	100
4	C	218/293 (74%)	212 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	222/243 (91%)	222 (100%)	0	0	100	100
6	E	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
7	F	178/204 (87%)	171 (96%)	7 (4%)	0	100	100
8	G	225/249 (90%)	221 (98%)	4 (2%)	0	100	100
9	H	180/194 (93%)	166 (92%)	14 (8%)	0	100	100
10	I	203/208 (98%)	194 (96%)	9 (4%)	0	100	100
11	J	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
12	K	95/165 (58%)	94 (99%)	1 (1%)	0	100	100
13	L	137/158 (87%)	132 (96%)	5 (4%)	0	100	100
14	M	100/132 (76%)	92 (92%)	8 (8%)	0	100	100
15	N	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
16	O	125/151 (83%)	119 (95%)	5 (4%)	1 (1%)	16	44
17	P	121/145 (83%)	120 (99%)	1 (1%)	0	100	100
18	Q	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
19	R	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
20	S	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
21	T	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
22	U	102/119 (86%)	96 (94%)	6 (6%)	0	100	100
23	V	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
24	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
25	X	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
26	Y	120/133 (90%)	119 (99%)	1 (1%)	0	100	100
27	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
28	a	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
29	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
30	c	57/69 (83%)	55 (96%)	2 (4%)	0	100	100
31	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
32	e	53/59 (90%)	52 (98%)	1 (2%)	0	100	100
33	f	62/156 (40%)	56 (90%)	6 (10%)	0	100	100
34	g	310/317 (98%)	297 (96%)	13 (4%)	0	100	100
35	h	44/1096 (4%)	41 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	n	18/25 (72%)	18 (100%)	0	0	100	100
All	All	4764/6597 (72%)	4626 (97%)	137 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	138	ASP

5.3.2 Protein sidechains (i)

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	
2	A	173/243 (71%)	170 (98%)	3 (2%)	53	83
3	B	192/231 (83%)	187 (97%)	5 (3%)	40	75
4	C	186/225 (83%)	181 (97%)	5 (3%)	39	74
5	D	188/202 (93%)	178 (95%)	10 (5%)	20	52
6	E	220/225 (98%)	217 (99%)	3 (1%)	59	85
7	F	155/170 (91%)	149 (96%)	6 (4%)	28	64
8	G	198/218 (91%)	195 (98%)	3 (2%)	57	84
9	H	164/174 (94%)	157 (96%)	7 (4%)	26	60
10	I	178/180 (99%)	175 (98%)	3 (2%)	53	83
11	J	161/168 (96%)	161 (100%)	0	100	100
12	K	88/136 (65%)	82 (93%)	6 (7%)	14	42
13	L	128/142 (90%)	126 (98%)	2 (2%)	55	83
14	M	86/108 (80%)	83 (96%)	3 (4%)	32	67
15	N	130/131 (99%)	128 (98%)	2 (2%)	57	84
16	O	100/119 (84%)	96 (96%)	4 (4%)	28	63
17	P	106/130 (82%)	100 (94%)	6 (6%)	18	49
18	Q	115/121 (95%)	112 (97%)	3 (3%)	40	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	R	119/122 (98%)	112 (94%)	7 (6%)	18 48
20	S	125/132 (95%)	123 (98%)	2 (2%)	55 83
21	T	113/115 (98%)	109 (96%)	4 (4%)	32 67
22	U	94/107 (88%)	87 (93%)	7 (7%)	13 37
23	V	67/67 (100%)	67 (100%)	0	100 100
24	W	112/113 (99%)	111 (99%)	1 (1%)	70 89
25	X	112/115 (97%)	108 (96%)	4 (4%)	31 66
26	Y	107/115 (93%)	103 (96%)	4 (4%)	30 65
27	Z	63/103 (61%)	62 (98%)	1 (2%)	55 83
28	a	86/98 (88%)	85 (99%)	1 (1%)	63 87
29	b	74/76 (97%)	70 (95%)	4 (5%)	20 51
30	c	52/62 (84%)	45 (86%)	7 (14%)	4 13
31	d	48/49 (98%)	46 (96%)	2 (4%)	26 61
32	e	45/48 (94%)	41 (91%)	4 (9%)	9 29
33	f	57/140 (41%)	56 (98%)	1 (2%)	51 82
34	g	264/275 (96%)	253 (96%)	11 (4%)	26 61
35	h	31/948 (3%)	30 (97%)	1 (3%)	34 70
36	n	19/24 (79%)	19 (100%)	0	100 100
All	All	4156/5632 (74%)	4024 (97%)	132 (3%)	35 70

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	e	16	THR
33	f	89	LYS
34	g	307	VAL
12	K	79	LEU
12	K	21	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
21	T	63	HIS
34	g	215	GLN
24	W	24	GLN

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Mol	Chain	Res	Type
34	g	285	GLN
34	g	15	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1601/1869 (85%)	261 (16%)	4 (0%)

5 of 261 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	17	C
1	2	25	A
1	2	33	G
1	2	41	G
1	2	45	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	331	C
1	2	531	A
1	2	627	U
1	2	871	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	2	686	1	18,21,22	2.39	7 (38%)	21,30,33	2.05	4 (19%)
1	OMG	2	1328	1,37	23,26,27	2.49	3 (13%)	32,38,41	1.93	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2	1045	1	18,21,22	2.42	7 (38%)	21,30,33	2.02	4 (19%)
1	OMG	2	509	38,1	23,26,27	2.43	5 (21%)	32,38,41	1.93	9 (28%)
1	PSU	2	1232	1	18,21,22	2.48	7 (38%)	21,30,33	2.17	4 (19%)
1	A2M	2	484	1	22,25,26	3.45	7 (31%)	30,36,39	2.13	8 (26%)
1	A2M	2	590	1	22,25,26	3.44	7 (31%)	30,36,39	2.39	11 (36%)
1	OMU	2	1326	38,1	19,22,23	2.74	7 (36%)	25,31,34	2.03	6 (24%)
1	OMU	2	354	1	19,22,23	2.76	7 (36%)	25,31,34	1.81	5 (20%)
1	OMC	2	517	1	19,22,23	1.76	5 (26%)	25,31,34	1.11	1 (4%)
1	PSU	2	814	1	18,21,22	2.50	8 (44%)	21,30,33	2.02	3 (14%)
1	OMU	2	172	1	19,22,23	2.77	7 (36%)	25,31,34	1.96	5 (20%)
1	OMG	2	601	1	23,26,27	2.47	4 (17%)	32,38,41	1.92	9 (28%)
1	6MZ	2	1832	38,1,37	22,25,26	2.49	3 (13%)	29,36,39	2.54	11 (37%)
1	A2M	2	1383	1	22,25,26	3.48	7 (31%)	30,36,39	2.09	8 (26%)
1	PSU	2	406	1	18,21,22	2.49	7 (38%)	21,30,33	2.05	4 (19%)
1	PSU	2	1692	1,37	18,21,22	2.47	7 (38%)	21,30,33	2.01	4 (19%)
1	OMG	2	436	1	23,26,27	2.48	4 (17%)	32,38,41	1.96	9 (28%)
1	PSU	2	863	1	18,21,22	2.50	7 (38%)	21,30,33	2.04	4 (19%)
1	PSU	2	1238	1	18,21,22	2.42	7 (38%)	21,30,33	2.00	4 (19%)
1	PSU	2	651	1	18,21,22	2.48	7 (38%)	21,30,33	2.08	4 (19%)
1	OMU	2	1288	1	19,22,23	2.70	6 (31%)	25,31,34	1.91	7 (28%)
1	OMU	2	116	1	19,22,23	2.76	8 (42%)	25,31,34	1.82	4 (16%)
1	A2M	2	1678	1	22,25,26	3.53	6 (27%)	30,36,39	2.17	8 (26%)
1	PSU	2	1347	1	18,21,22	2.47	7 (38%)	21,30,33	2.04	4 (19%)
1	OMU	2	428	1	19,22,23	2.75	7 (36%)	25,31,34	1.96	6 (24%)
1	PSU	2	109	1,37	18,21,22	2.46	7 (38%)	21,30,33	2.12	4 (19%)
1	PSU	2	1081	1	18,21,22	2.58	8 (44%)	21,30,33	2.06	5 (23%)
1	PSU	2	105	1,37	18,21,22	2.48	7 (38%)	21,30,33	2.11	4 (19%)
1	B8N	2	1248	1	25,29,30	2.56	8 (32%)	28,42,45	1.54	5 (17%)
1	OMC	2	174	38,1	19,22,23	1.77	5 (26%)	25,31,34	1.01	1 (4%)
1	A2M	2	468	1	22,25,26	3.46	7 (31%)	30,36,39	2.12	8 (26%)
1	OMG	2	683	1	23,26,27	2.50	3 (13%)	32,38,41	1.94	9 (28%)
1	PSU	2	572	1,37	18,21,22	2.47	7 (38%)	21,30,33	2.08	4 (19%)
1	OMC	2	1703	1	19,22,23	1.77	5 (26%)	25,31,34	1.04	1 (4%)
1	OMU	2	1442	38,1	19,22,23	2.73	7 (36%)	25,31,34	1.90	5 (20%)
1	PSU	2	1244	1	18,21,22	2.42	7 (38%)	21,30,33	2.06	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2	1445	1	18,21,22	2.41	7 (38%)	21,30,33	2.08	5 (23%)
1	PSU	2	1643	38,1	18,21,22	2.44	7 (38%)	21,30,33	2.07	5 (23%)
1	MA6	2	1850	1	23,26,27	1.32	3 (13%)	33,38,41	2.38	10 (30%)
1	A2M	2	1031	1	22,25,26	3.47	7 (31%)	30,36,39	2.04	8 (26%)
1	OMC	2	1391	1	19,22,23	1.78	5 (26%)	25,31,34	1.03	1 (4%)
1	PSU	2	681	1	18,21,22	2.47	8 (44%)	21,30,33	1.99	4 (19%)
1	PSU	2	1136	1	18,21,22	2.46	7 (38%)	21,30,33	2.09	4 (19%)
1	OMU	2	121	1	19,22,23	2.80	7 (36%)	25,31,34	1.75	5 (20%)
1	PSU	2	119	1	18,21,22	2.56	7 (38%)	21,30,33	2.03	4 (19%)
1	OMG	2	1490	38,1	23,26,27	2.45	4 (17%)	32,38,41	1.89	9 (28%)
1	PSU	2	93	1	18,21,22	2.48	7 (38%)	21,30,33	2.00	4 (19%)
1	A2M	2	512	1	22,25,26	3.47	7 (31%)	30,36,39	2.17	10 (33%)
1	A2M	2	159	1	22,25,26	3.48	7 (31%)	30,36,39	2.10	8 (26%)
1	4AC	2	1842	1	21,24,25	1.92	7 (33%)	28,34,37	2.00	8 (28%)
1	A2M	2	668	38,1	22,25,26	3.45	7 (31%)	30,36,39	2.11	9 (30%)
1	PSU	2	296	1	18,21,22	2.46	7 (38%)	21,30,33	2.15	4 (19%)
1	PSU	2	1056	1	18,21,22	2.41	7 (38%)	21,30,33	1.98	4 (19%)
1	OMC	2	1272	1	19,22,23	1.74	4 (21%)	25,31,34	1.08	1 (4%)
1	7MG	2	1639	1	23,26,27	3.55	6 (26%)	27,39,42	2.12	8 (29%)
1	PSU	2	1174	1,37	18,21,22	2.47	7 (38%)	21,30,33	2.08	4 (19%)
1	MA6	2	1851	1	23,26,27	1.35	3 (13%)	33,38,41	2.39	11 (33%)
1	PSU	2	36	1	18,21,22	2.52	7 (38%)	21,30,33	1.93	4 (19%)
1	OMG	2	1447	1	23,26,27	2.49	3 (13%)	32,38,41	1.92	9 (28%)
1	PSU	2	815	1	18,21,22	2.45	7 (38%)	21,30,33	2.10	4 (19%)
1	A2M	2	166	1	22,25,26	3.49	7 (31%)	30,36,39	2.20	8 (26%)
1	A2M	2	576	1,37	22,25,26	3.46	7 (31%)	30,36,39	2.08	9 (30%)
1	PSU	2	1177	1	18,21,22	2.45	7 (38%)	21,30,33	2.04	4 (19%)
1	A2M	2	99	38,1	22,25,26	3.49	7 (31%)	30,36,39	2.12	8 (26%)
1	PSU	2	1046	1	18,21,22	2.48	8 (44%)	21,30,33	2.04	3 (14%)
1	4AC	2	1337	1	21,24,25	1.97	7 (33%)	28,34,37	1.76	5 (17%)
1	OMC	2	462	1	19,22,23	1.79	5 (26%)	25,31,34	1.06	1 (4%)
1	PSU	2	1625	1	18,21,22	2.43	7 (38%)	21,30,33	1.96	4 (19%)
1	PSU	2	649	1	18,21,22	2.50	7 (38%)	21,30,33	2.10	4 (19%)
1	A2M	2	27	38,1	22,25,26	3.46	6 (27%)	30,36,39	2.19	10 (33%)
1	OMG	2	644	1	23,26,27	2.47	4 (17%)	32,38,41	1.93	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2	822	1	18,21,22	2.53	8 (44%)	21,30,33	2.11	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	686	1	-	0/7/25/26	0/2/2/2
1	OMG	2	1328	1,37	-	0/9/27/28	0/3/3/3
1	PSU	2	1045	1	-	2/7/25/26	0/2/2/2
1	OMG	2	509	38,1	-	0/9/27/28	0/3/3/3
1	PSU	2	1232	1	-	0/7/25/26	0/2/2/2
1	A2M	2	484	1	-	0/9/27/28	0/3/3/3
1	A2M	2	590	1	-	1/9/27/28	0/3/3/3
1	OMU	2	1326	38,1	-	0/9/27/28	0/2/2/2
1	OMU	2	354	1	-	0/9/27/28	0/2/2/2
1	OMC	2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	2	814	1	-	0/7/25/26	0/2/2/2
1	OMU	2	172	1	-	0/9/27/28	0/2/2/2
1	OMG	2	601	1	-	1/9/27/28	0/3/3/3
1	6MZ	2	1832	38,1,37	-	0/9/27/28	0/3/3/3
1	A2M	2	1383	1	-	0/9/27/28	0/3/3/3
1	PSU	2	406	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1692	1,37	-	0/7/25/26	0/2/2/2
1	OMG	2	436	1	-	0/9/27/28	0/3/3/3
1	PSU	2	863	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1238	1	-	0/7/25/26	0/2/2/2
1	PSU	2	651	1	-	0/7/25/26	0/2/2/2
1	OMU	2	1288	1	-	0/9/27/28	0/2/2/2
1	OMU	2	116	1	-	0/9/27/28	0/2/2/2
1	A2M	2	1678	1	-	0/9/27/28	0/3/3/3
1	PSU	2	1347	1	-	0/7/25/26	0/2/2/2
1	OMU	2	428	1	-	4/9/27/28	0/2/2/2
1	PSU	2	109	1,37	-	0/7/25/26	0/2/2/2
1	PSU	2	1081	1	-	1/7/25/26	0/2/2/2
1	PSU	2	105	1,37	-	0/7/25/26	0/2/2/2
1	B8N	2	1248	1	-	6/16/34/35	0/2/2/2
1	OMC	2	174	38,1	-	0/9/27/28	0/2/2/2
1	A2M	2	468	1	-	0/9/27/28	0/3/3/3
1	OMG	2	683	1	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	572	1,37	-	0/7/25/26	0/2/2/2
1	OMC	2	1703	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1442	38,1	-	0/9/27/28	0/2/2/2
1	PSU	2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1445	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1643	38,1	-	0/7/25/26	0/2/2/2
1	MA6	2	1850	1	-	3/11/29/30	0/3/3/3
1	A2M	2	1031	1	-	0/9/27/28	0/3/3/3
1	OMC	2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	2	681	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1136	1	-	0/7/25/26	0/2/2/2
1	OMU	2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	2	119	1	-	1/7/25/26	0/2/2/2
1	OMG	2	1490	38,1	-	1/9/27/28	0/3/3/3
1	PSU	2	93	1	-	0/7/25/26	0/2/2/2
1	A2M	2	512	1	-	2/9/27/28	0/3/3/3
1	A2M	2	159	1	-	0/9/27/28	0/3/3/3
1	4AC	2	1842	1	-	2/11/29/30	0/2/2/2
1	A2M	2	668	38,1	-	3/9/27/28	0/3/3/3
1	PSU	2	296	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1056	1	-	0/7/25/26	0/2/2/2
1	OMC	2	1272	1	-	0/9/27/28	0/2/2/2
1	7MG	2	1639	1	-	1/7/37/38	0/3/3/3
1	PSU	2	1174	1,37	-	0/7/25/26	0/2/2/2
1	MA6	2	1851	1	-	5/11/29/30	0/3/3/3
1	PSU	2	36	1	-	0/7/25/26	0/2/2/2
1	OMG	2	1447	1	-	2/9/27/28	0/3/3/3
1	PSU	2	815	1	-	0/7/25/26	0/2/2/2
1	A2M	2	166	1	-	0/9/27/28	0/3/3/3
1	A2M	2	576	1,37	-	2/9/27/28	0/3/3/3
1	PSU	2	1177	1	-	0/7/25/26	0/2/2/2
1	A2M	2	99	38,1	-	2/9/27/28	0/3/3/3
1	PSU	2	1046	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1337	1	-	4/11/29/30	0/2/2/2
1	OMC	2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1625	1	-	0/7/25/26	0/2/2/2
1	PSU	2	649	1	-	0/7/25/26	0/2/2/2
1	A2M	2	27	38,1	-	0/9/27/28	0/3/3/3
1	OMG	2	644	1	-	1/9/27/28	0/3/3/3
1	PSU	2	822	1	-	0/7/25/26	0/2/2/2

The worst 5 of 463 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1832	6MZ	C6-N6	10.52	1.46	1.34
1	2	1288	OMU	O4-C4	9.92	1.43	1.24
1	2	172	OMU	O4-C4	9.79	1.43	1.24
1	2	116	OMU	O4-C4	9.76	1.43	1.24
1	2	121	OMU	O4-C4	9.73	1.43	1.24

The worst 5 of 418 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1842	4AC	CM7-C7-N4	7.29	127.03	115.27
1	2	590	A2M	C5-C4-N3	-6.63	117.59	126.72
1	2	1232	PSU	N1-C2-N3	6.44	121.96	115.17
1	2	105	PSU	N1-C2-N3	6.35	121.87	115.17
1	2	1337	4AC	CM7-C7-N4	6.32	125.47	115.27

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	512	A2M	O4'-C4'-C5'-O5'
1	2	601	OMG	C1'-C2'-O2'-CM2
1	2	668	A2M	O4'-C4'-C5'-O5'
1	2	668	A2M	C3'-C4'-C5'-O5'
1	2	1248	B8N	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	509	OMG	2	0
1	2	1232	PSU	1	0
1	2	484	A2M	1	0
1	2	601	OMG	1	0
1	2	1383	A2M	1	0
1	2	1031	A2M	1	0
1	2	681	PSU	1	0
1	2	1842	4AC	1	0
1	2	166	A2M	1	0
1	2	1337	4AC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 166 ligands modelled in this entry, 166 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

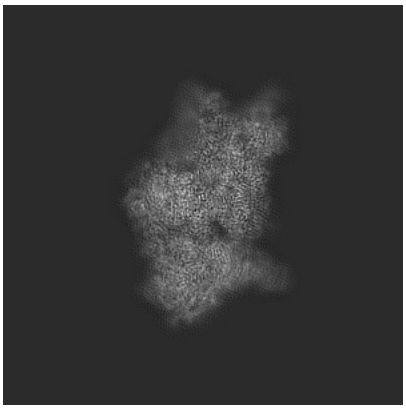
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47929. These allow visual inspection of the internal detail of the map and identification of artifacts.

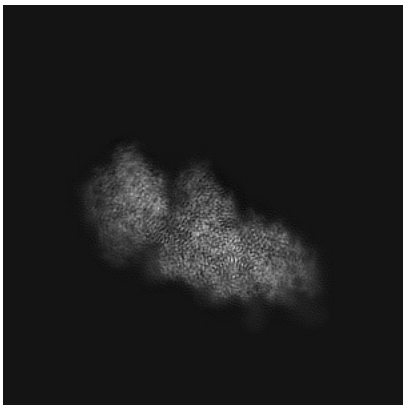
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

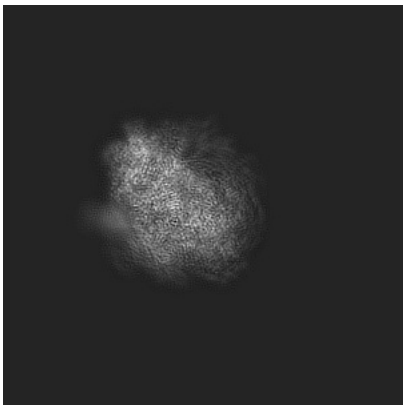
6.1.1 Primary map



X

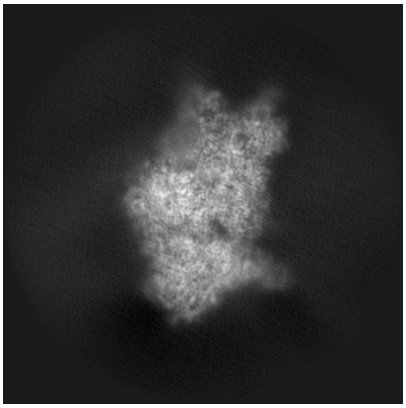


Y

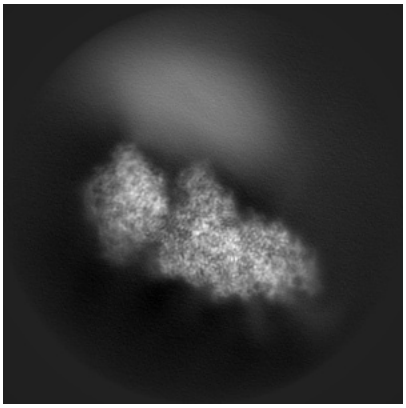


Z

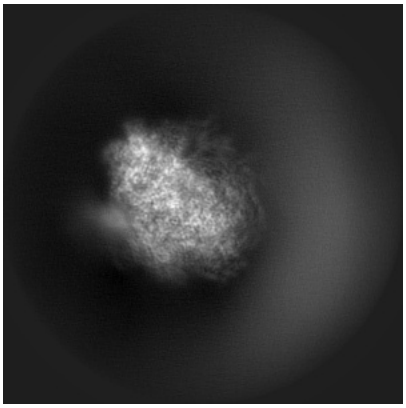
6.1.2 Raw map



X



Y



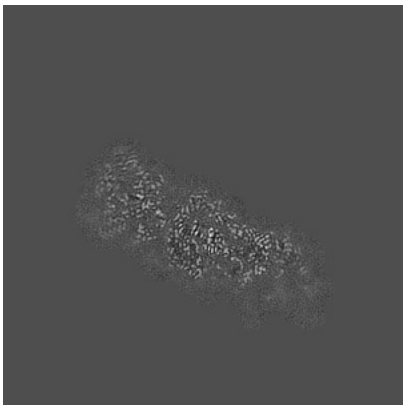
Z

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

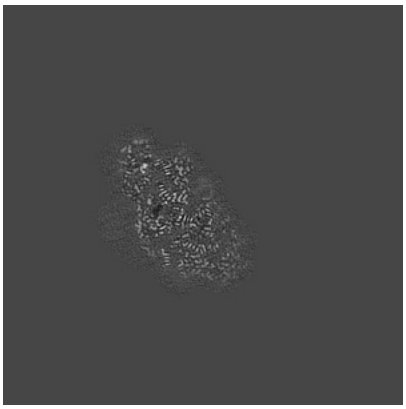
6.2 Central slices (i)

6.2.1 Primary map

X Index: 250

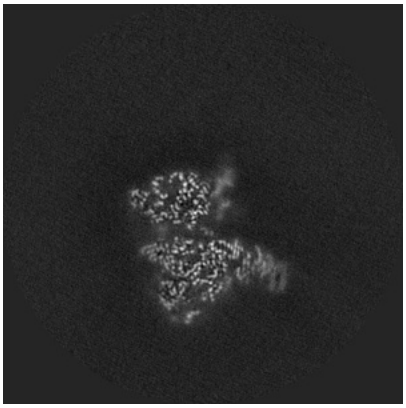


Y Index: 250

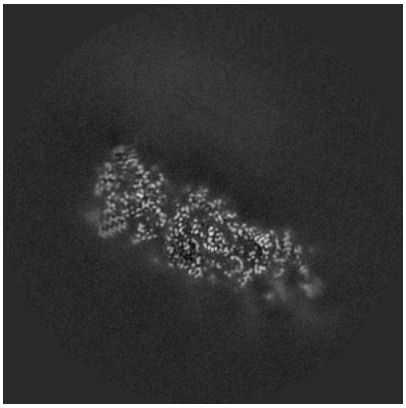


Z Index: 250

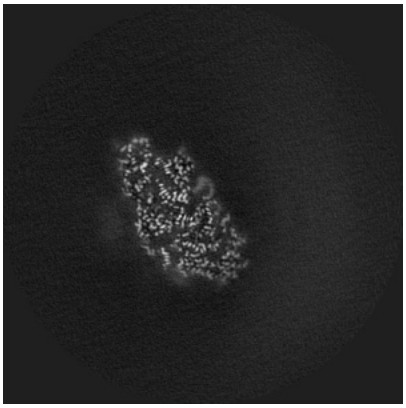
6.2.2 Raw map



X Index: 250



Y Index: 250



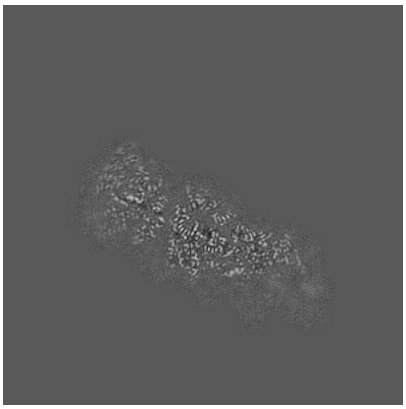
Z Index: 250

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

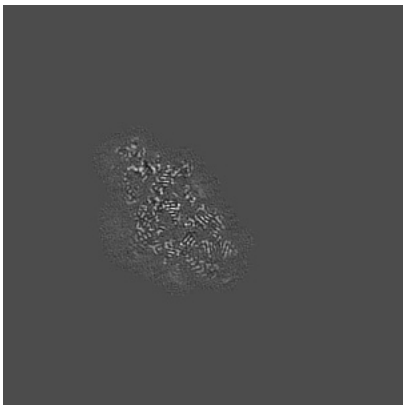
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 214

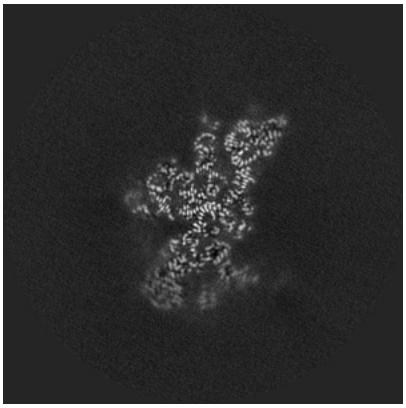


Y Index: 248

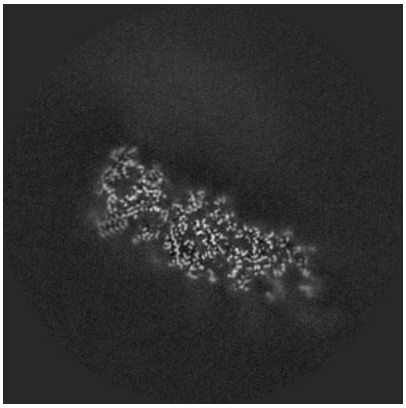


Z Index: 260

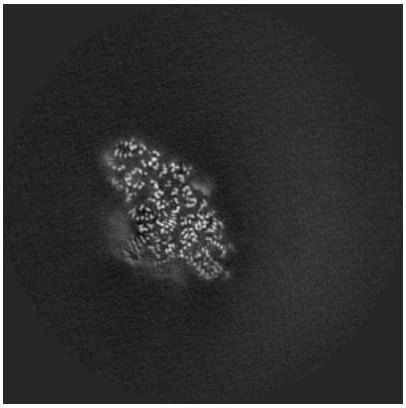
6.3.2 Raw map



X Index: 214



Y Index: 253

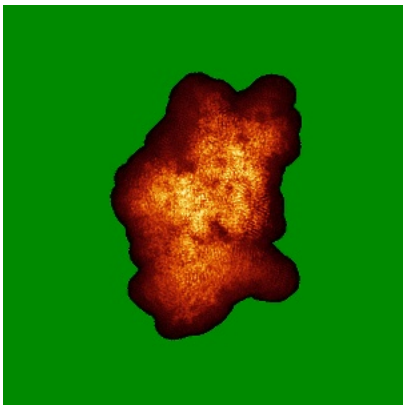


Z Index: 265

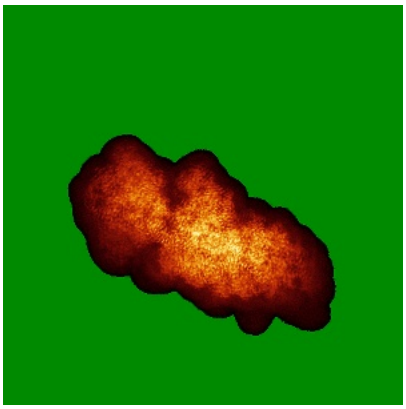
The images above show the largest variance slices of the map in three orthogonal directions.

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

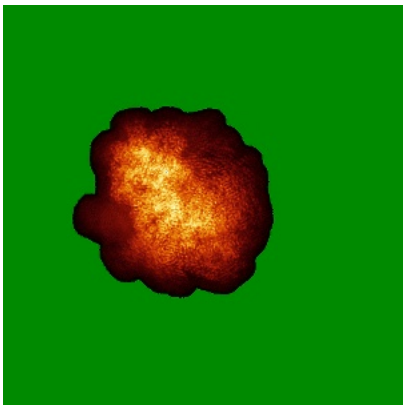
6.4.1 Primary map



X

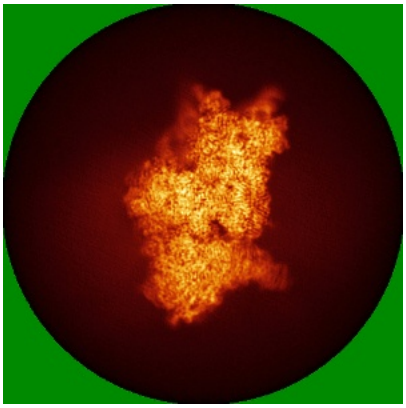


Y

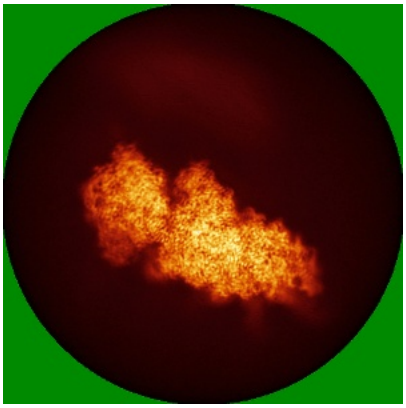


Z

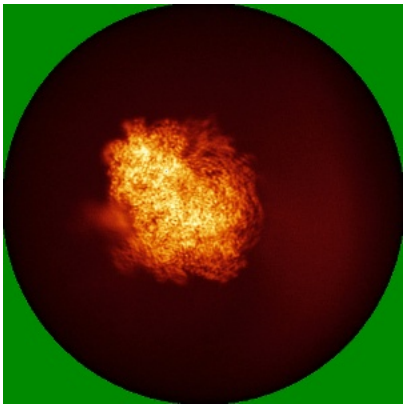
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

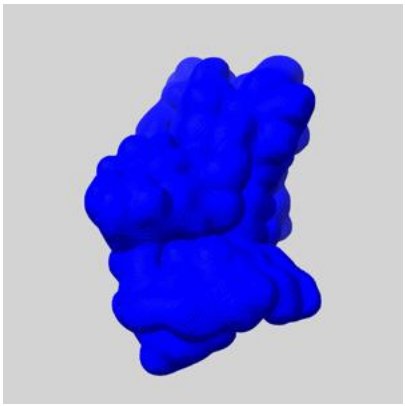
6.6 Mask visualisation

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

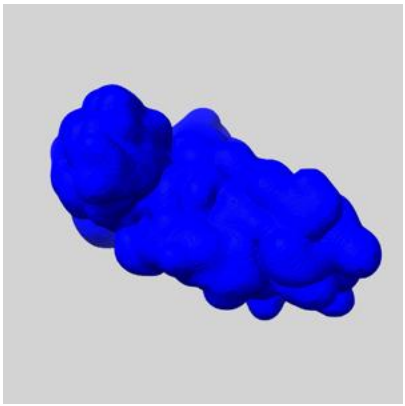
A mask typically either:

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

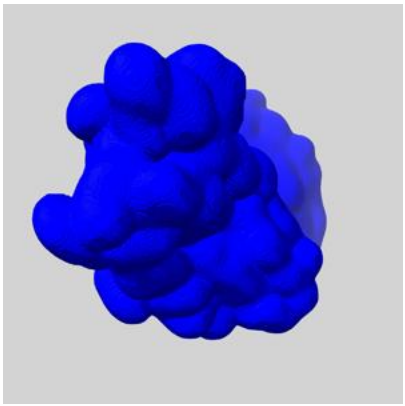
6.6.1 emd_47929_msk_1.map



X



Y

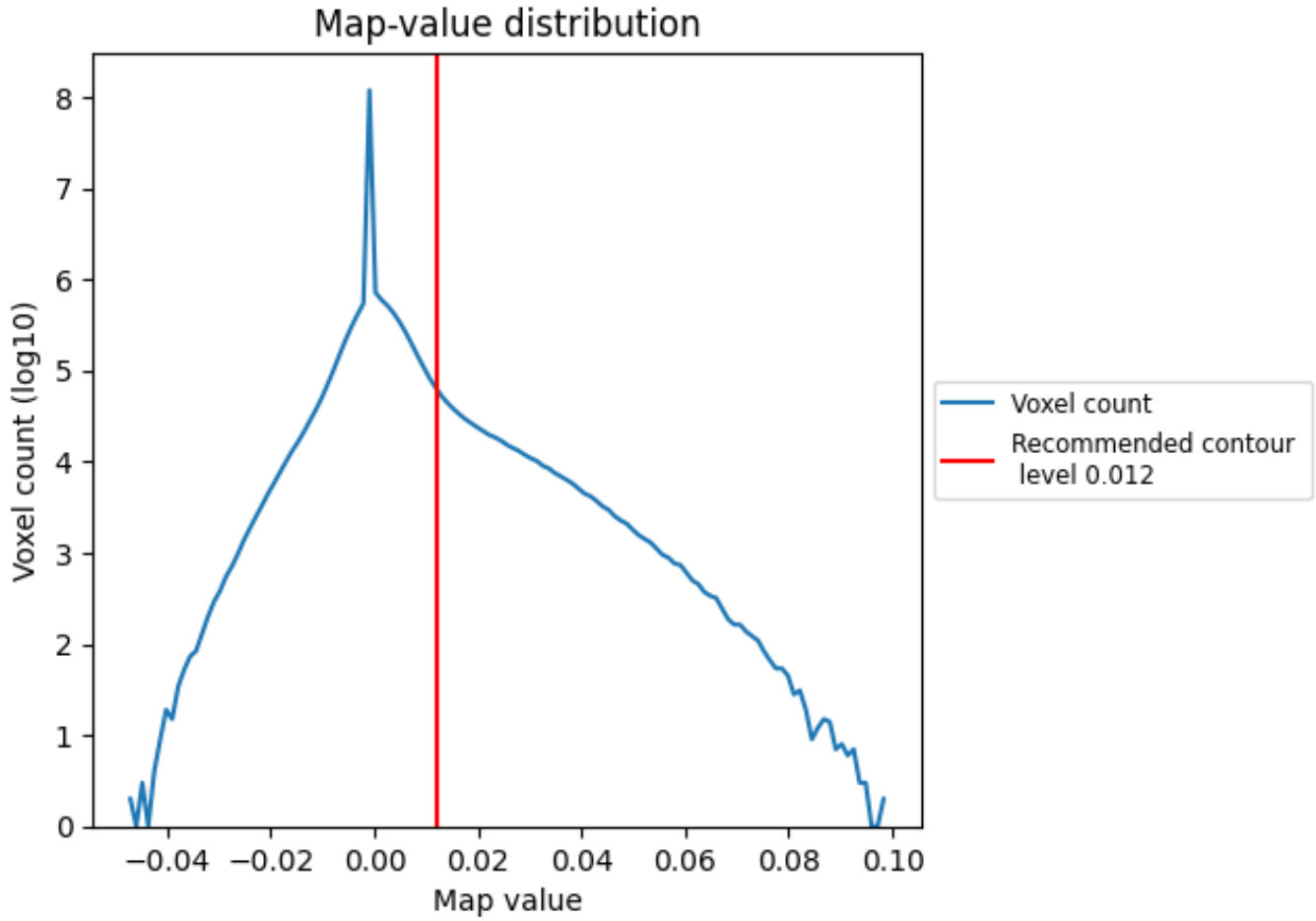


Z

7 Map analysis

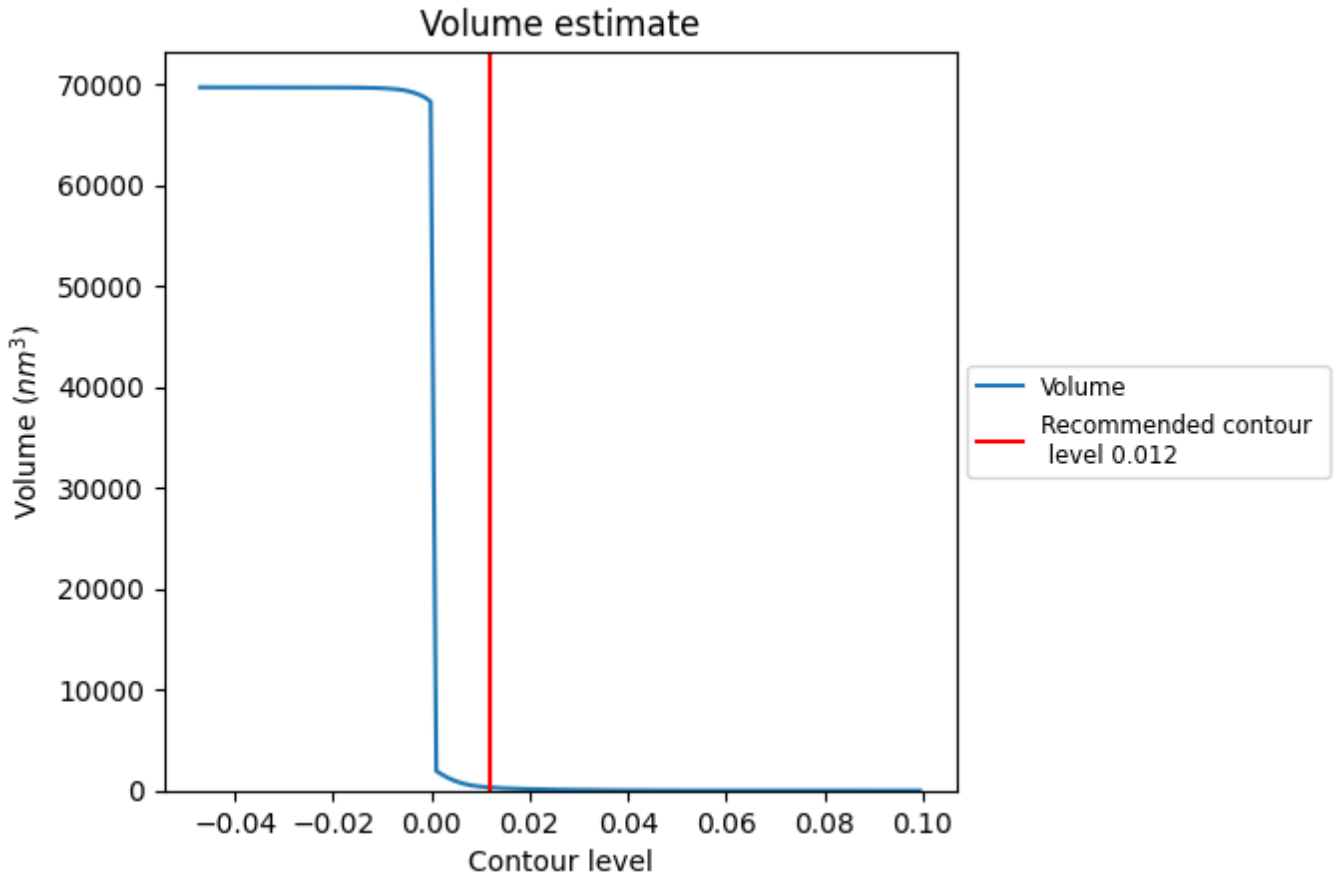
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

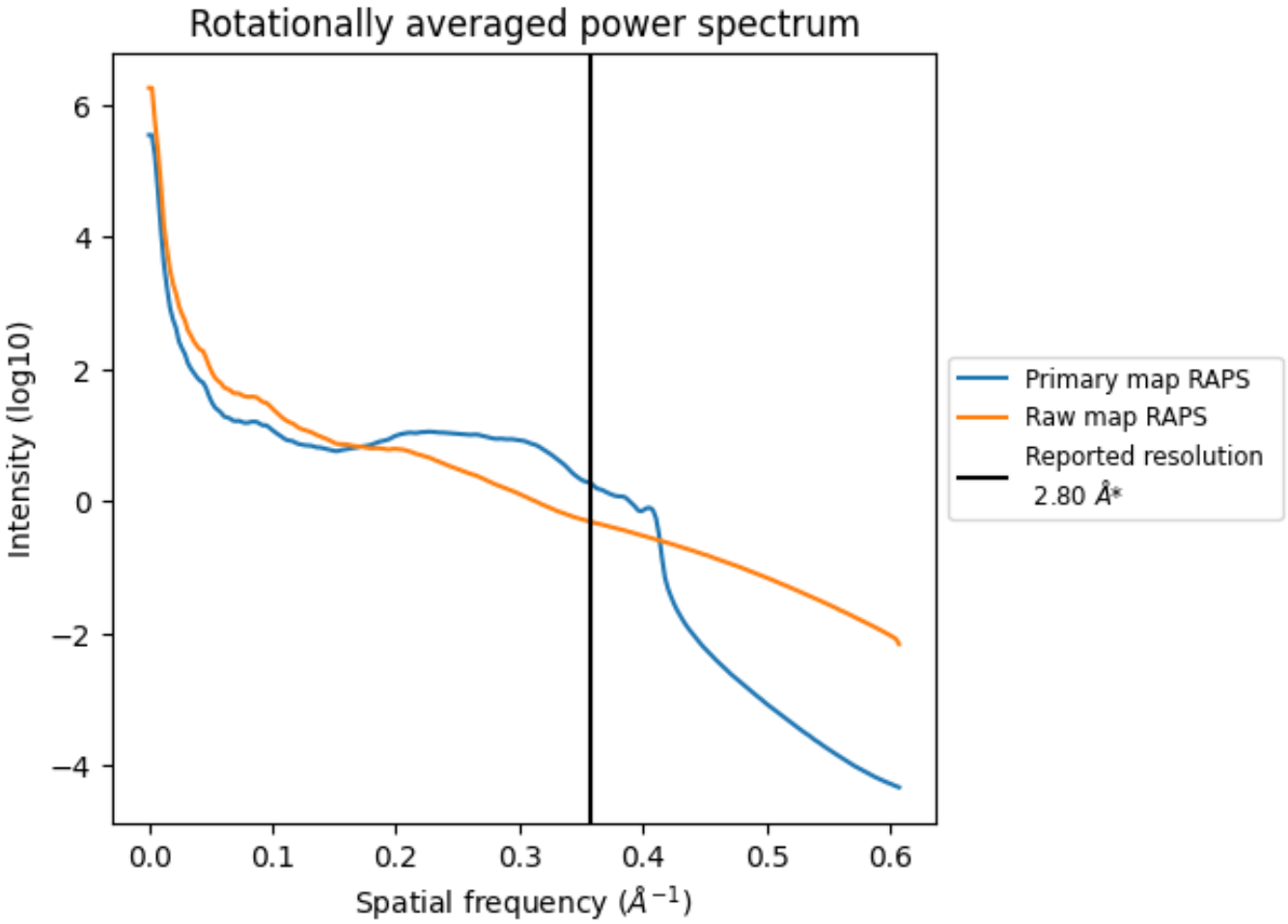
7.2 Volume estimate (i)



The volume at the recommended contour level is 304 nm^3; this corresponds to an approximate mass of 274 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 (i)

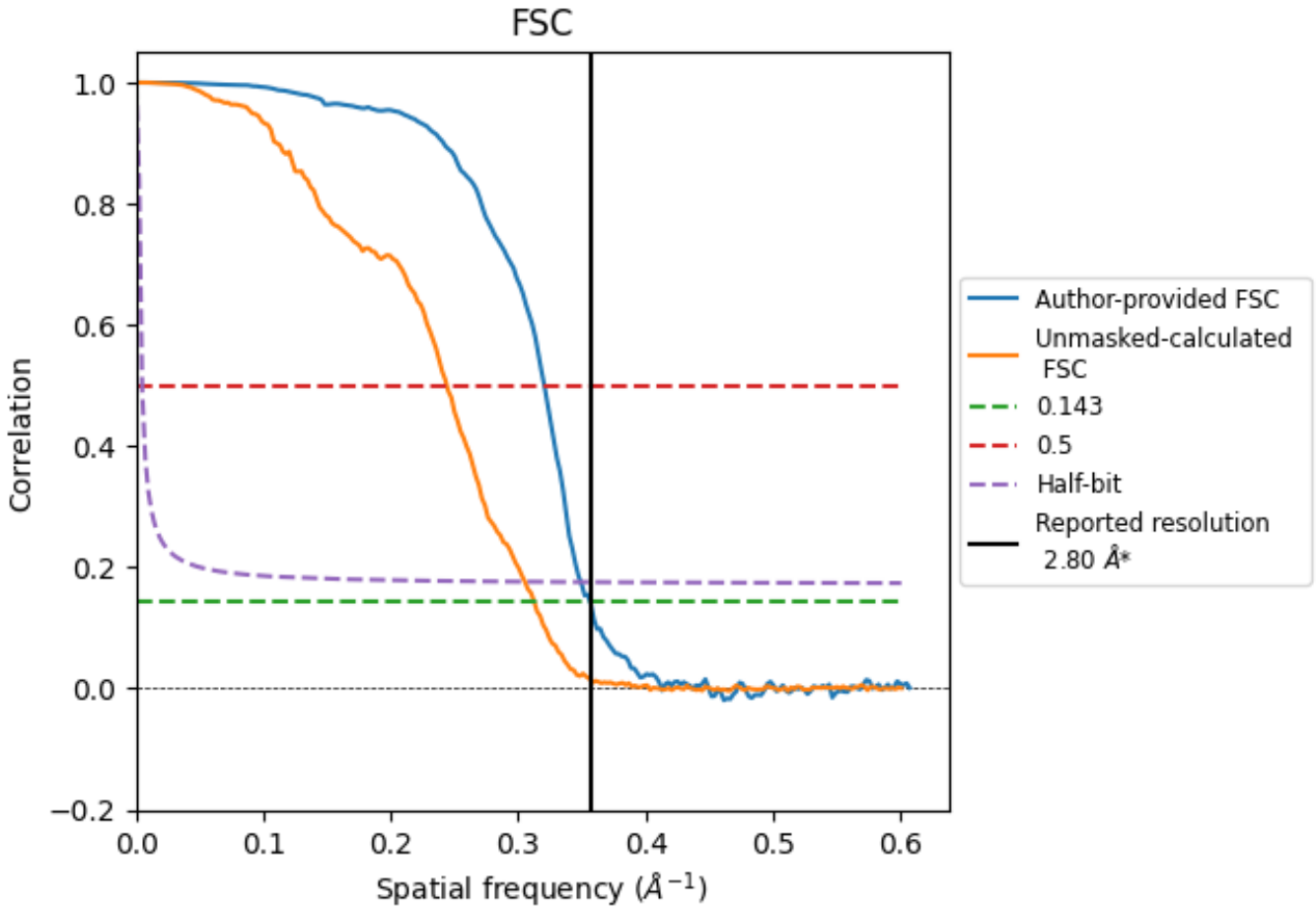


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

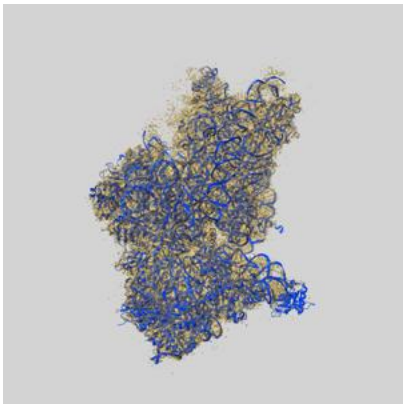
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.12	2.86
Unmasked-calculated*	3.20	4.10	3.28

*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 3.20 differs from the reported value 2.8 by more than 10 %

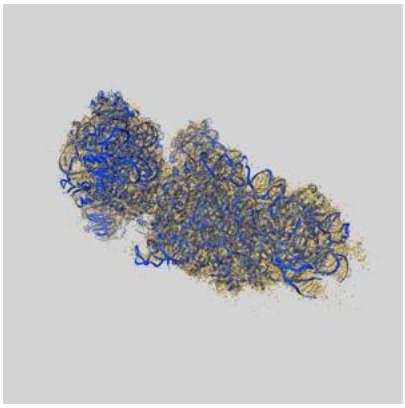
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47929 and PDB model 9ED0. Per-residue inclusion information can be found in section 3 on page 11.

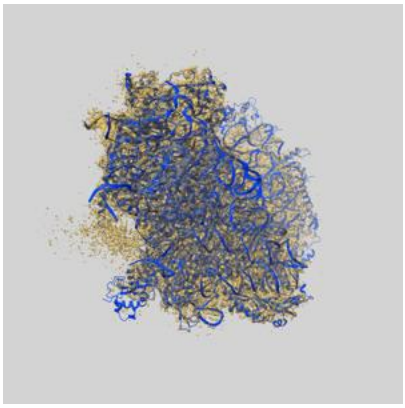
9.1 Map-model overlay



X



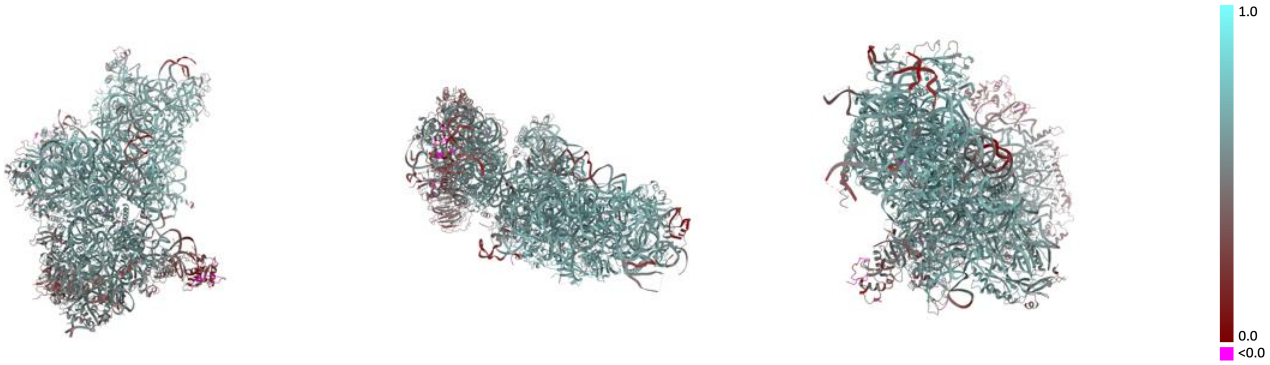
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

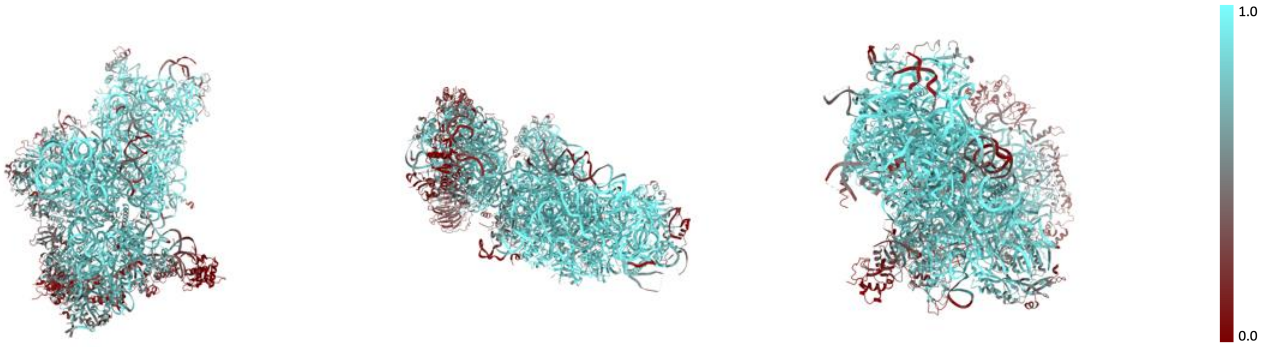
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

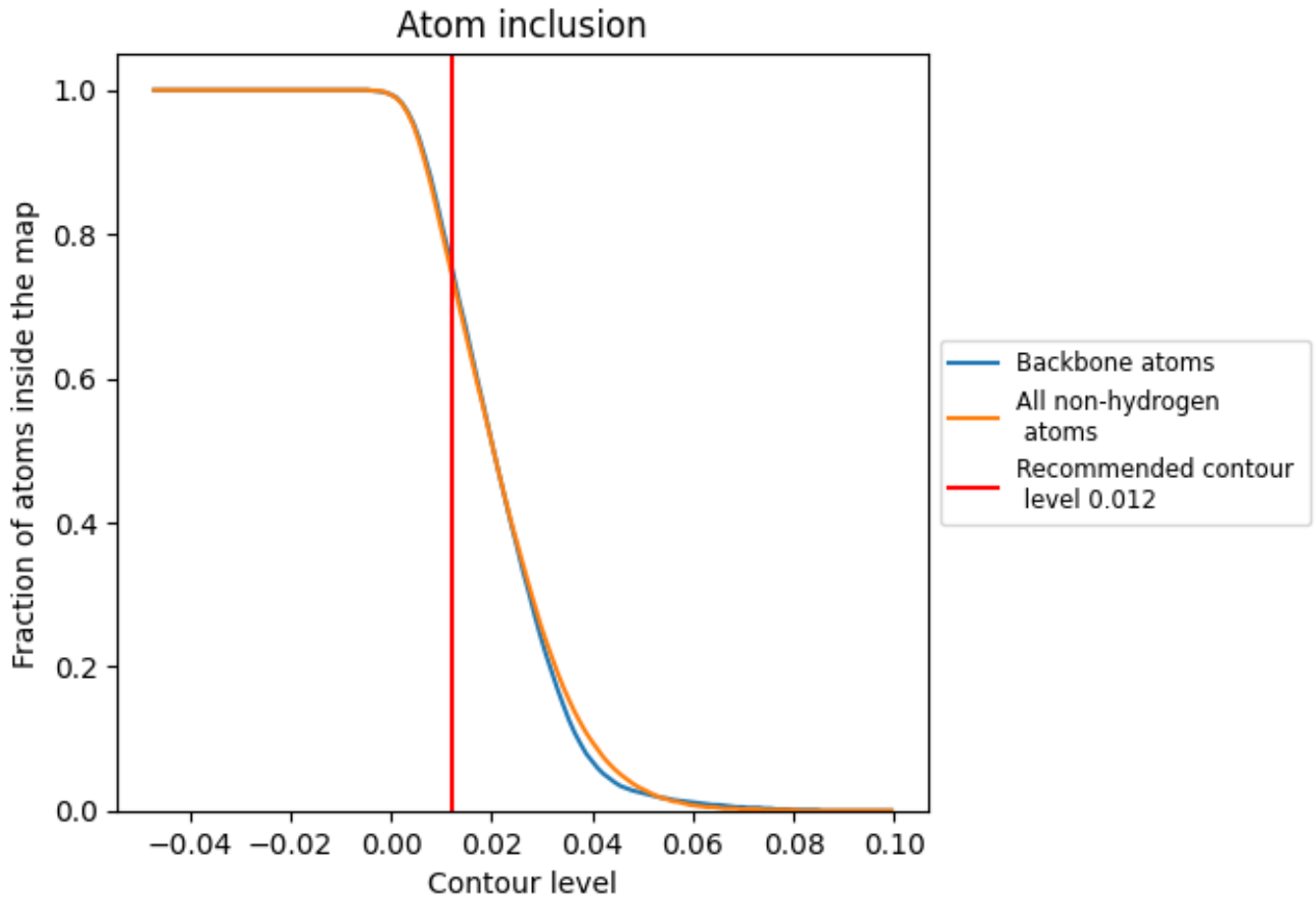
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.5680
2	0.8600	0.5950
A	0.7230	0.5860
B	0.6680	0.5740
C	0.8410	0.6360
D	0.6570	0.5460
E	0.9180	0.6560
F	0.6060	0.5270
G	0.7500	0.5790
H	0.2550	0.3970
I	0.7950	0.6030
J	0.8870	0.6410
K	0.5330	0.5000
L	0.8770	0.6390
M	0.0190	0.2210
N	0.7560	0.6030
O	0.7600	0.5990
P	0.4110	0.4450
Q	0.7390	0.5770
R	0.4100	0.4580
S	0.3830	0.4280
T	0.6550	0.5410
U	0.5270	0.5000
V	0.7440	0.6010
W	0.9260	0.6570
X	0.9150	0.6560
Y	0.8680	0.6400
Z	0.1940	0.3970
a	0.8280	0.6190
b	0.6160	0.5500
c	0.5020	0.4980
d	0.8530	0.6280
e	0.7260	0.5900
f	0.0250	0.1880
g	0.2270	0.3680

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	0.5560	0.5080
n	0.7900	0.6090