wwPDB EM Validation Summary Report

Nov 20, 2022 – 01:28 am GMT

PDB ID	:	6G53
EMDB ID	:	EMD-4351
Title	:	Cryo-EM structure of a late human pre-40S ribosomal subunit - State E
Authors	:	Ameismeier, M.; Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2018-03-28
Resolution	:	4.50 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 (i) 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 (i)) were used in the production of this report:

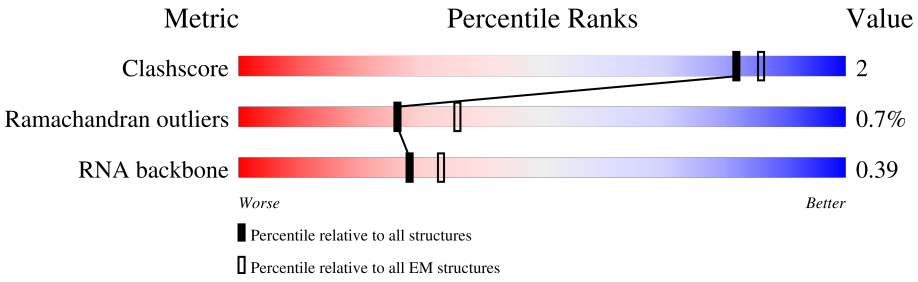
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	1882	6% 52% 32% 12%
2	R	135	23% 85% 10%
3	A	295	73% 27%
4	B	264	9% 80% 19%
5	C	293	5% 73% 26%
6	E	263	11% 98%
7	G	249	7% 91% 8%
8	H	194	12% 95%

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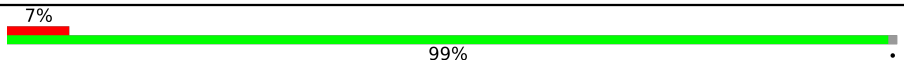
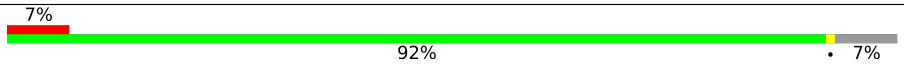
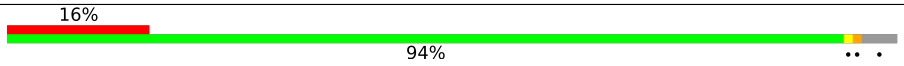
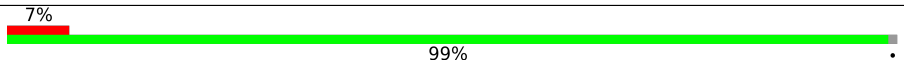
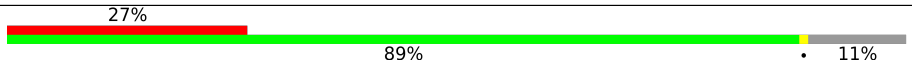
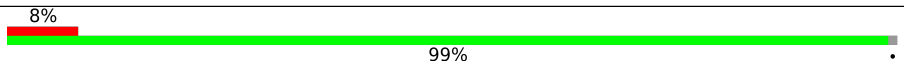
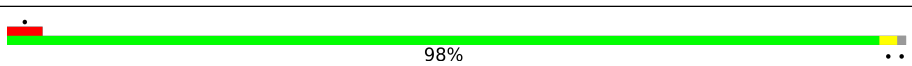
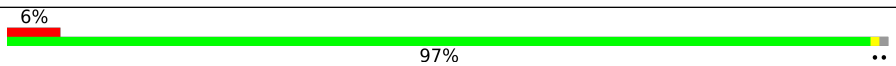
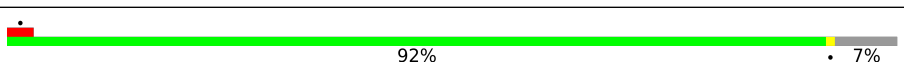
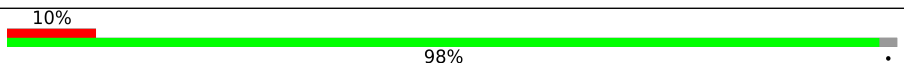
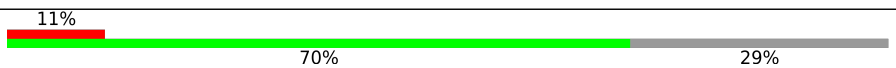
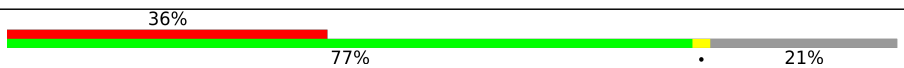
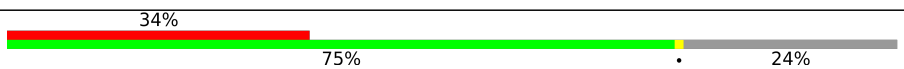
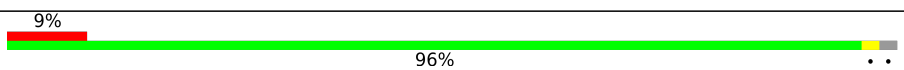
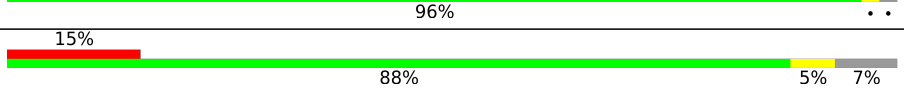
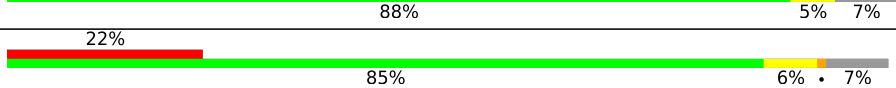
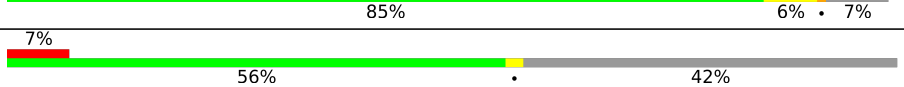
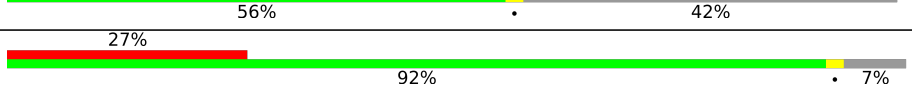
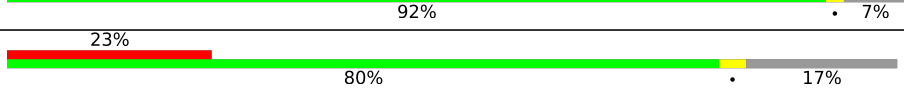
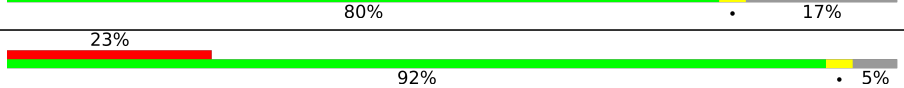
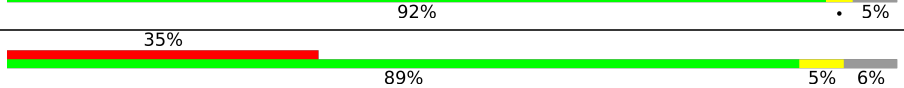
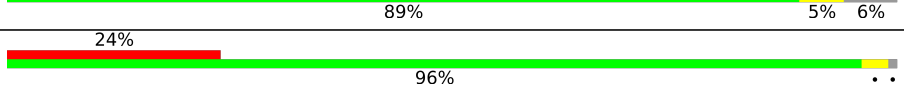
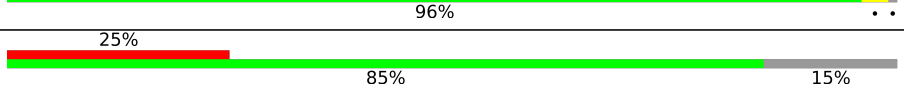
Mol	Chain	Length	Quality of chain
9	I	208	
10	J	194	
11	L	158	
12	N	151	
13	O	151	
14	V	83	
15	W	130	
16	X	143	
17	Y	133	
18	b	84	
19	e	59	
20	x	252	
21	y	412	
22	u	804	
23	t	475	
24	d	56	
25	D	243	
26	F	204	
27	K	165	
28	M	132	
29	P	145	
30	Q	146	
31	S	152	
32	T	145	
33	U	119	

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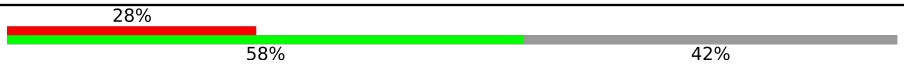
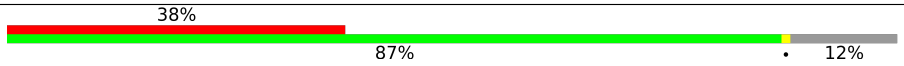
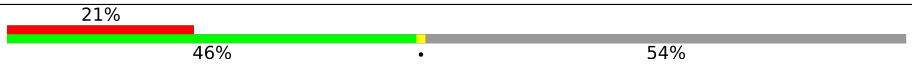
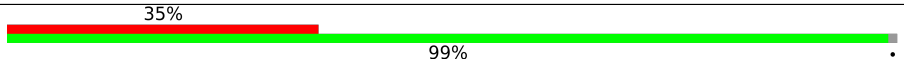
Mol	Chain	Length	Quality of chain
34	Z	125	
35	c	69	
36	f	156	
37	g	317	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 49052 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	O	P		
1	2	1659	19905	8295	9952	1658	0	0

- Molecule 2 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	R	122	604	360	122	122	0	0

- Molecule 3 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	A	216	1068	636	216	216	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	B	213	1054	628	213	213	0	0

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	C	218	1072	636	218	218	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	E	262	1287	763	262	262	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	230	Total 1135	C 675	N 230	O 230	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	186	Total 920	C 548	N 186	O 186	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	205	Total 1009	C 599	N 205	O 205	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	180	Total 888	C 528	N 180	O 180	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	151	Total 744	C 442	N 151	O 151	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	N	149	Total 737	C 439	N 149	O 149	0	0

- Molecule 13 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	135	Total 659	C 389	N 135	O 135	0	0

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	82	Total 403	C 239	N 82	O 82	0	0

- Molecule 15 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	W	129	Total 634	C 376	N 129	O 129	0	0

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	141	Total 690	C 408	N 141	O 141	0	0

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	124	Total 610	C 362	N 124	O 124	0	0

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	b	82	Total 405	C 241	N 82	O 82	0	0

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	e	55	Total 270	C 160	N 55	O 55	0	0

- Molecule 20 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	x	178	Total 880	C 524	N 178	O 178	0	0

- Molecule 21 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	y	325	Total 1606	C 956	N 325	O 325	0	0

- Molecule 22 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	u	615	Total 3042	C 1812	N 615	O 615	0	0

- Molecule 23 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	t	61	Total 304	C 182	N 61	O 61	0	0

- Molecule 24 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	d	55	Total 269	C 159	N 55	O 55	0	0

- Molecule 25 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	D	225	Total 1104	C 654	N 225	O 225	0	0

- Molecule 26 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	F	189	Total 935	C 557	N 189	O 189	0	0

- Molecule 27 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	K	95	Total 472	C 282	N 95	O 95	0	0

- Molecule 28 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	M	123	Total 607	C 361	N 123	O 123	0	0

- Molecule 29 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	P	120	Total 590	C 350	N 120	O 120	0	0

- Molecule 30 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Q	139	Total 683	C 405	N 139	O 139	0	0

- Molecule 31 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	S	143	Total 704	C 418	N 143	O 143	0	0

- Molecule 32 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	T	144	Total 705	C 417	N 144	O 144	0	0

- Molecule 33 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	U	101	Total 500	C 298	N 101	O 101	0	0

- Molecule 34 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Z	72	Total 358	C 214	N 72	O 72	0	0

- Molecule 35 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	61	Total 300	C 178	N 61	O 61	0	0

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	f	72	Total 356	C 212	N 72	O 72	0	0

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

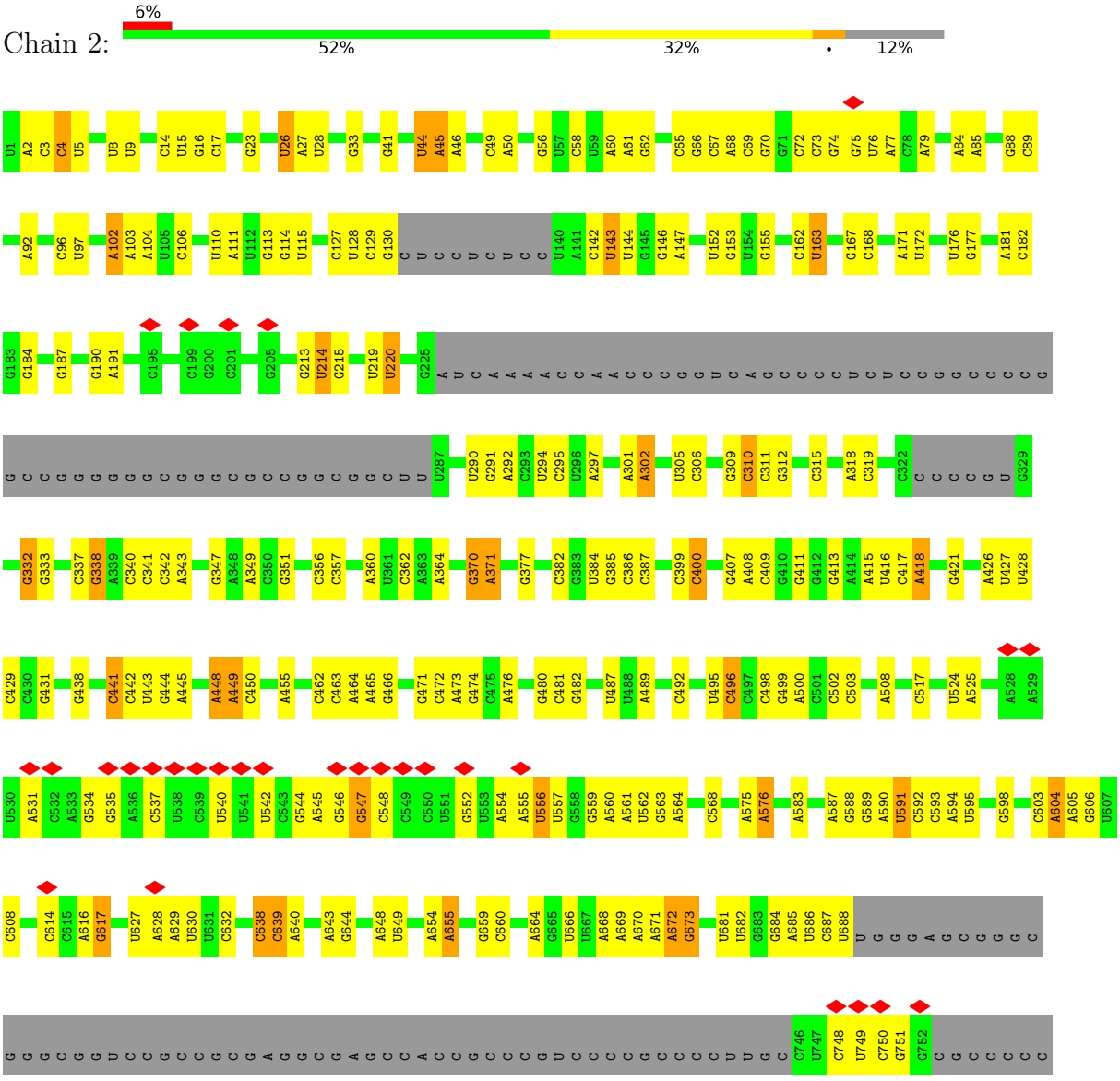
Mol	Chain	Residues	Atoms				AltConf	Trace
37	g	314	Total 1543	C 915	N 314	O 314	0	0

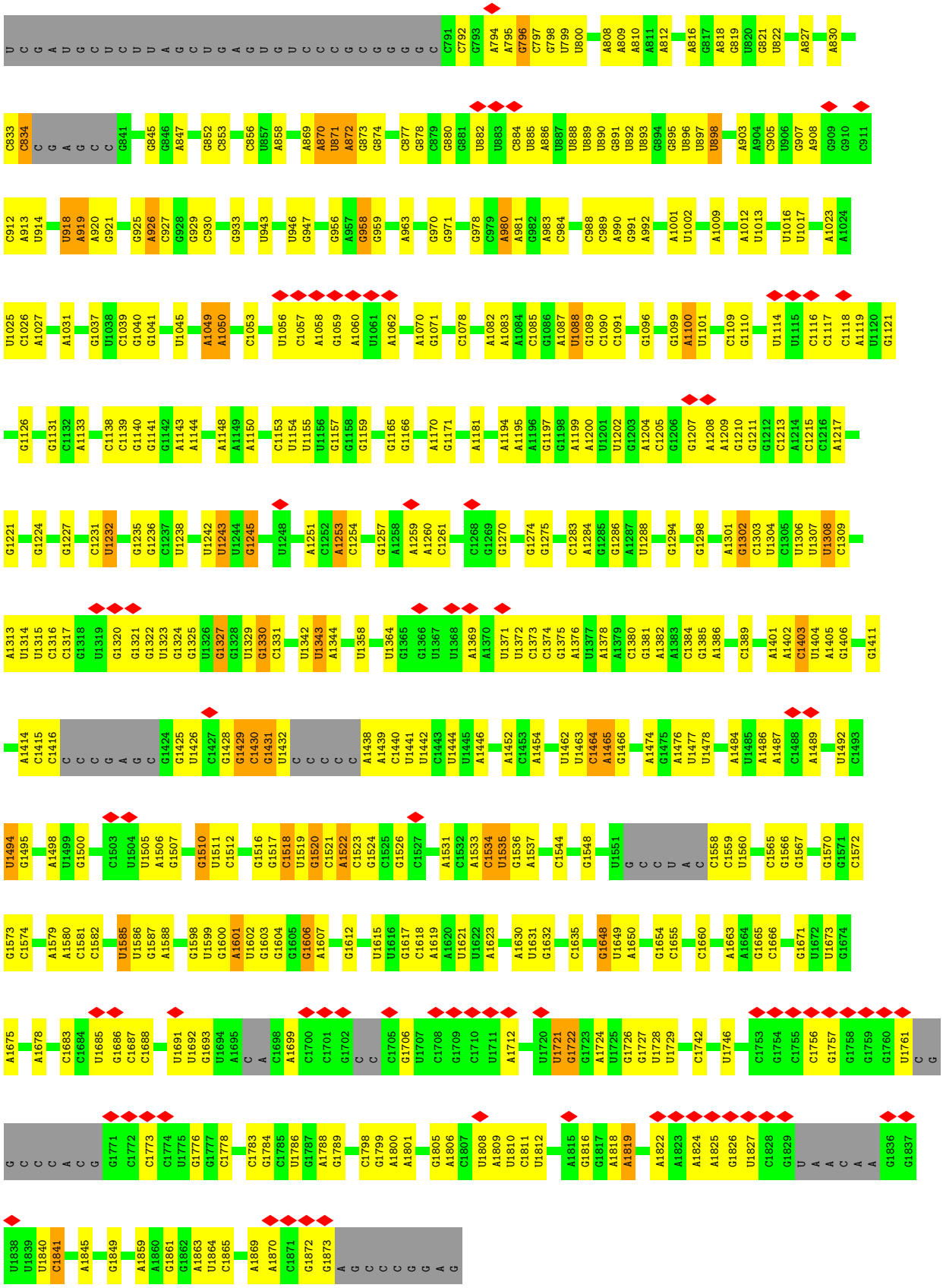
3 Residue-property plots (i)

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: 18S ribosomal RNA

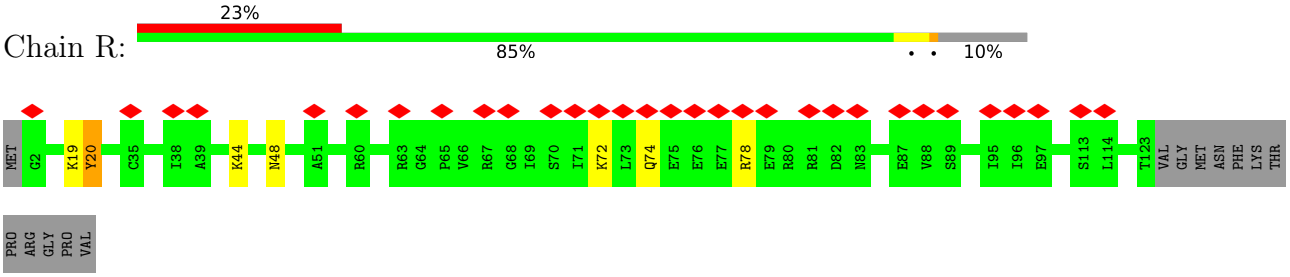
Chain 2:





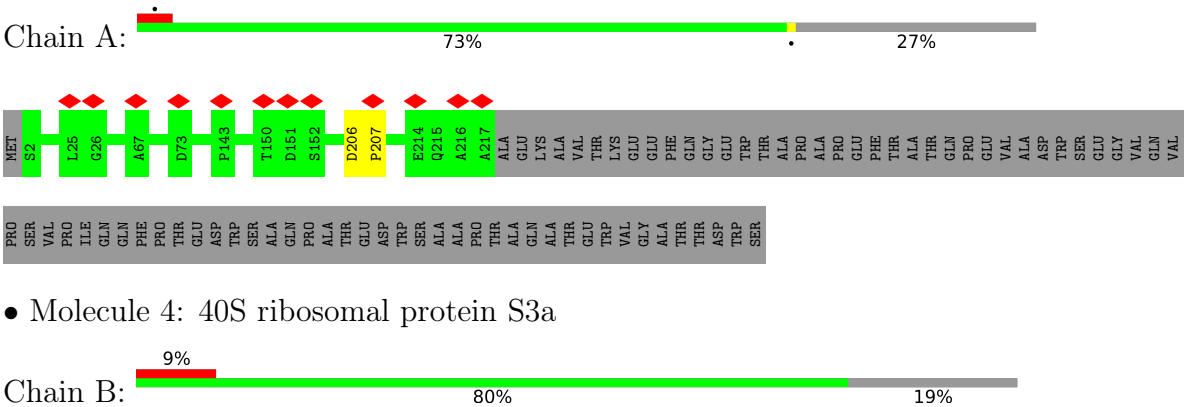
• Molecule 2: 40S ribosomal protein S17

Chain R:



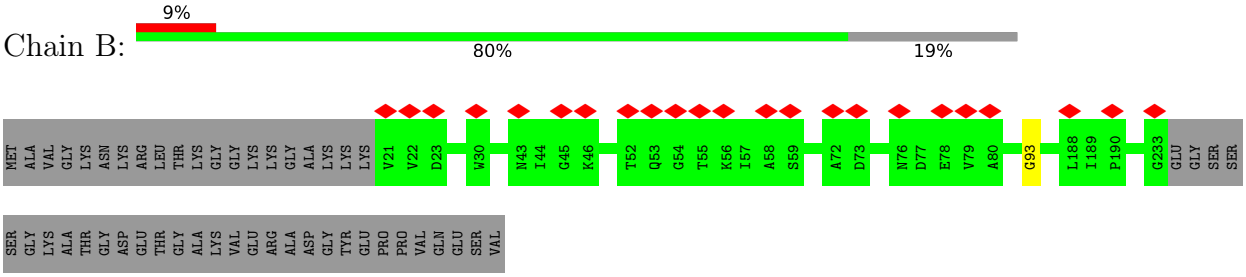
• Molecule 3: 40S ribosomal protein SA

Chain A:



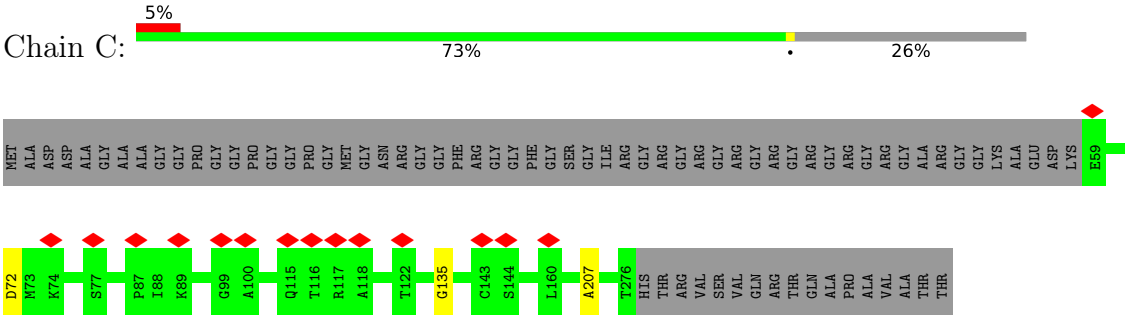
• Molecule 4: 40S ribosomal protein S3a

Chain B:



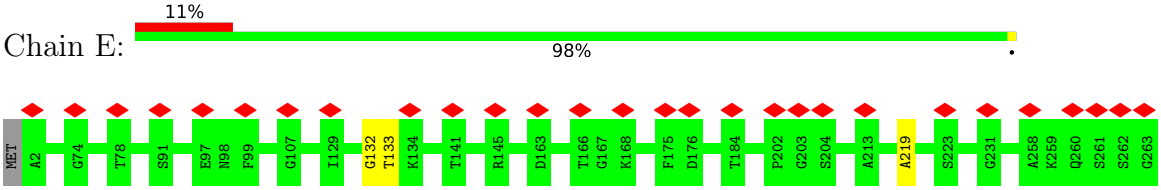
• Molecule 5: 40S ribosomal protein S2

Chain C:



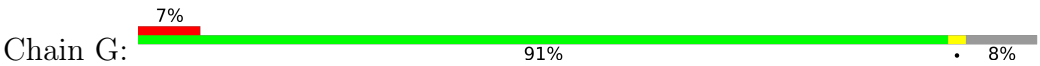
• Molecule 6: 40S ribosomal protein S4, X isoform

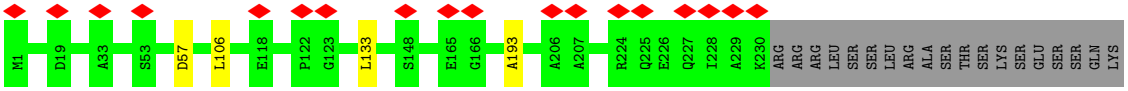
Chain E:



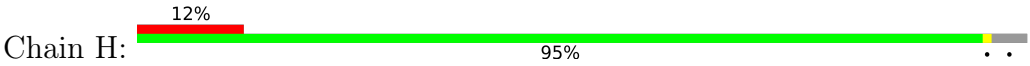
• Molecule 7: 40S ribosomal protein S6

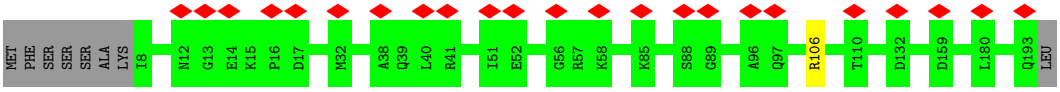
Chain G:



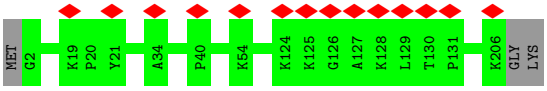


• Molecule 8: 40S ribosomal protein S7

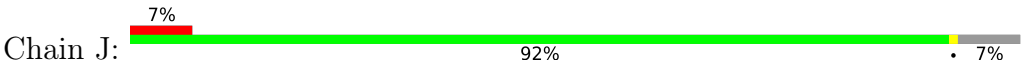


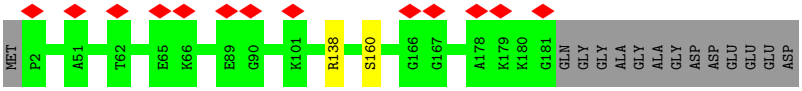


• Molecule 9: 40S ribosomal protein S8

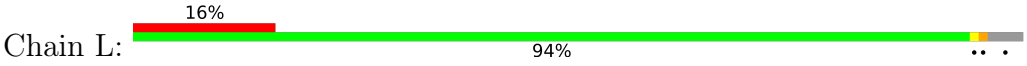


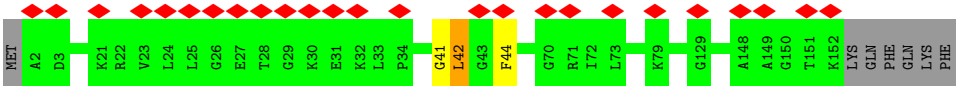
• Molecule 10: 40S ribosomal protein S9



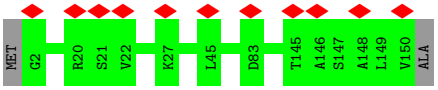


• Molecule 11: 40S ribosomal protein S11

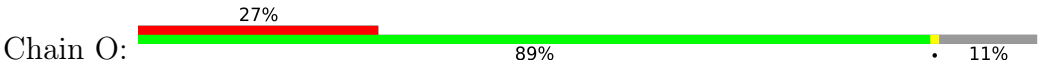


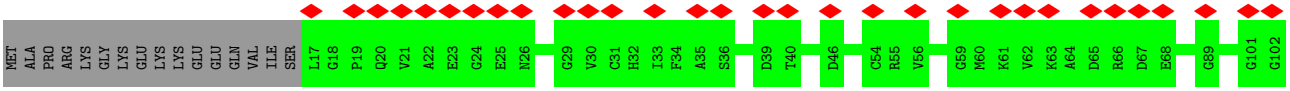


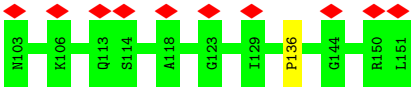
• Molecule 12: 40S ribosomal protein S13



• Molecule 13: 40S ribosomal protein S14

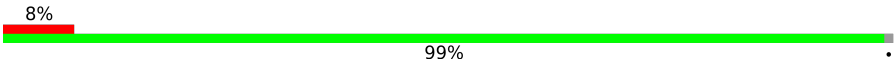


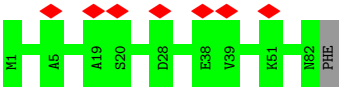




• Molecule 14: 40S ribosomal protein S21

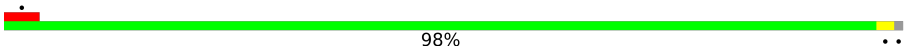
Chain V:

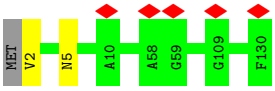




• Molecule 15: 40S ribosomal protein S15a

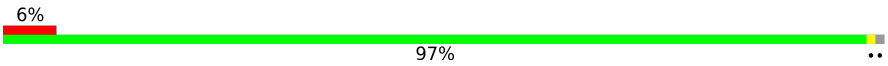
Chain W:

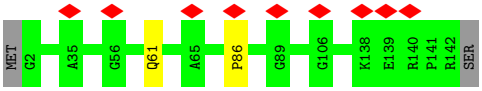




• Molecule 16: 40S ribosomal protein S23

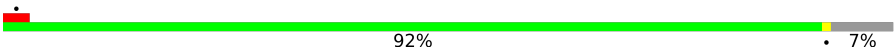
Chain X:

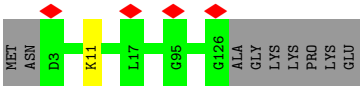




• Molecule 17: 40S ribosomal protein S24

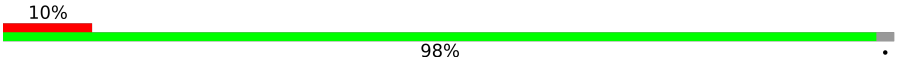
Chain Y:

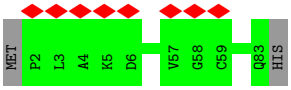




• Molecule 18: 40S ribosomal protein S27

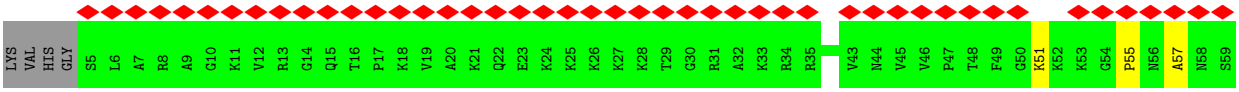
Chain b:





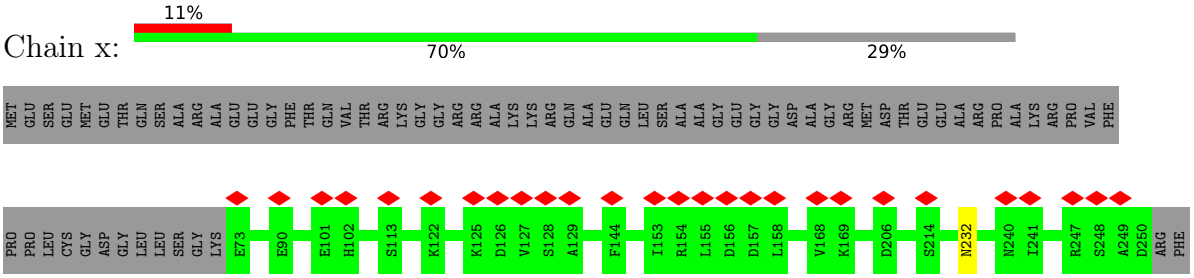
• Molecule 19: 40S ribosomal protein S30

Chain e:



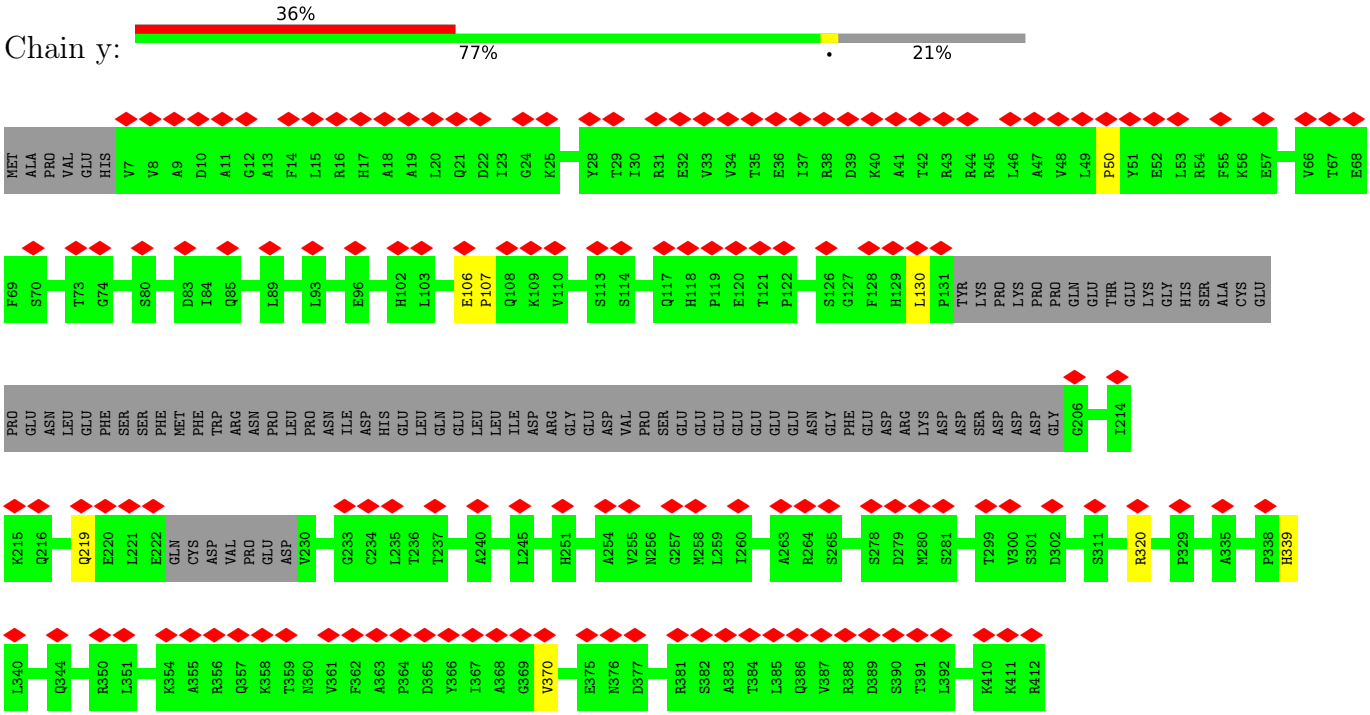
• Molecule 20: RNA-binding protein PNO1

Chain x:



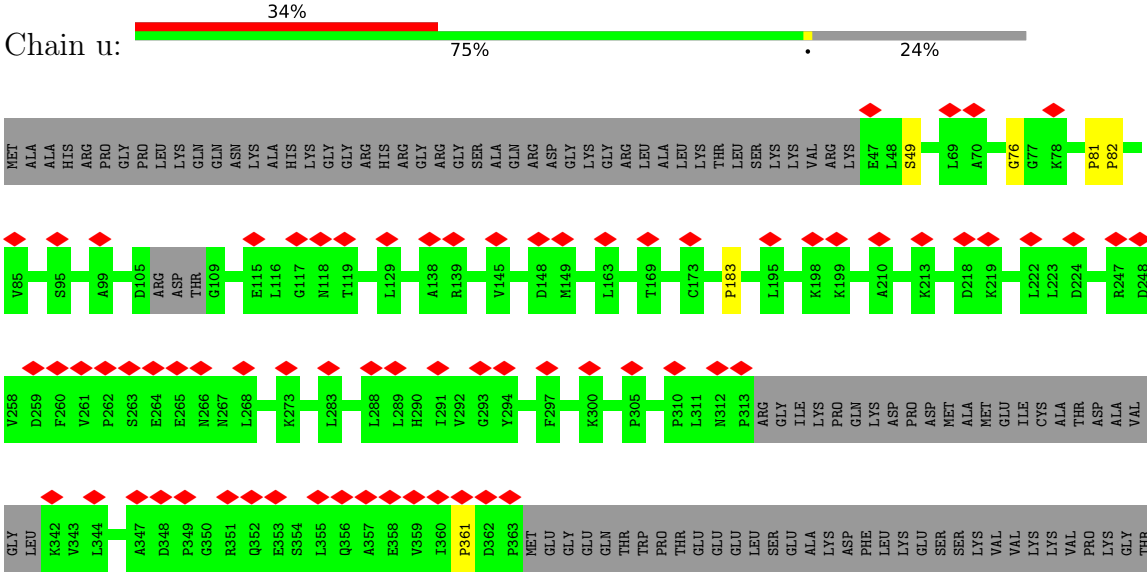
• Molecule 21: RNA-binding protein NOB1

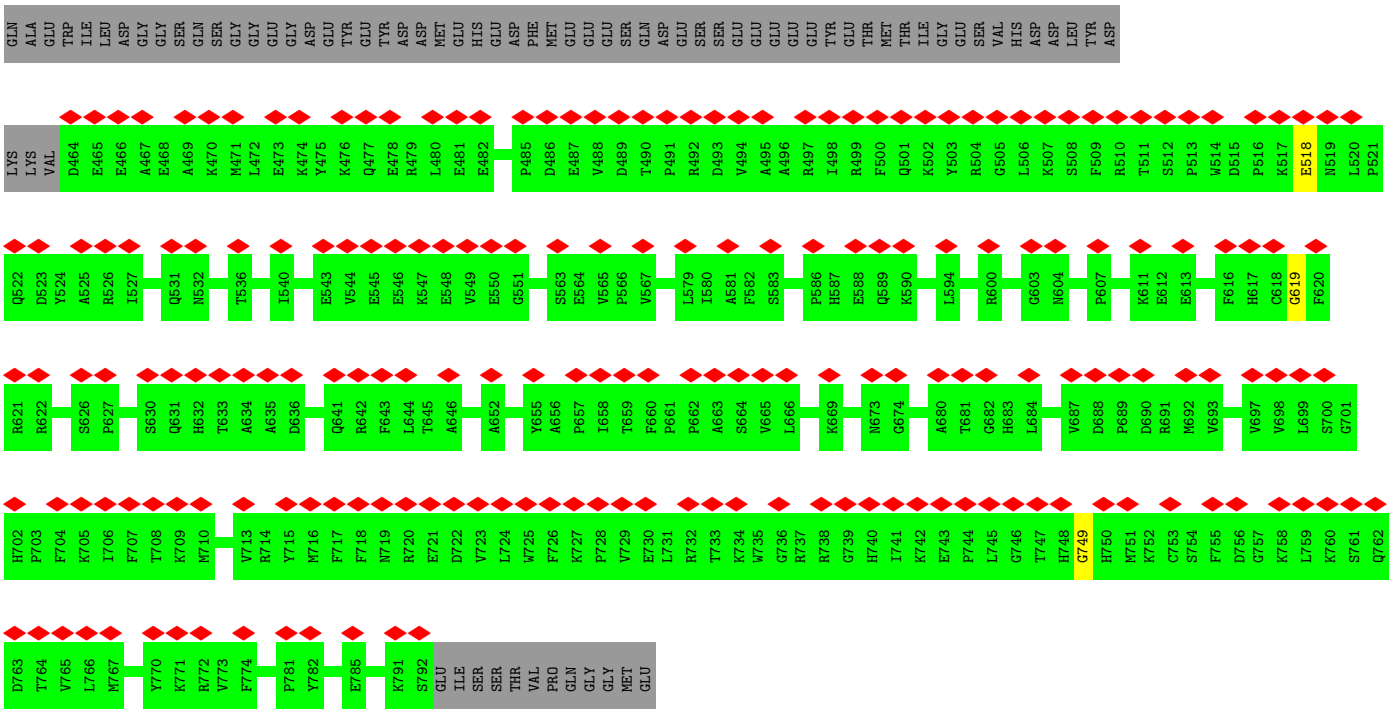
Chain y:



• Molecule 22: Pre-rRNA-processing protein TSR1 homolog

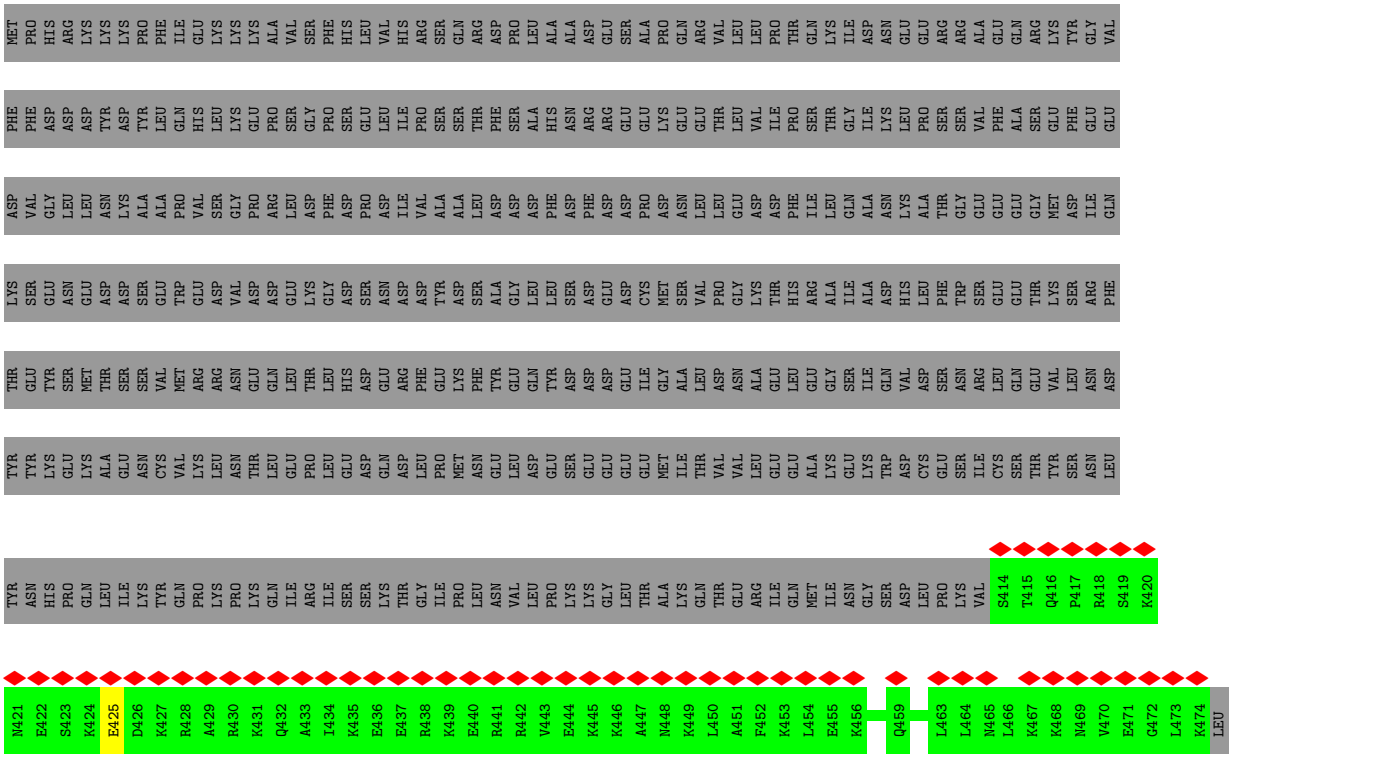
Chain u:





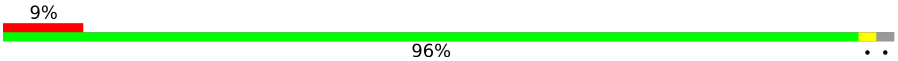
• Molecule 23: Protein LTV1 homolog

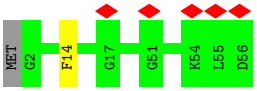
Chain t:



• Molecule 24: 40S ribosomal protein S29

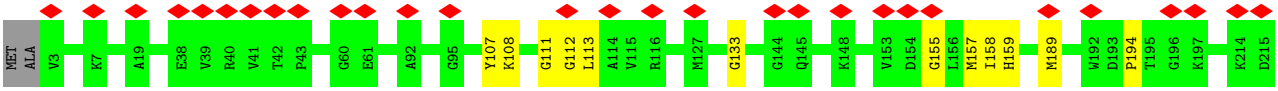
Chain d:

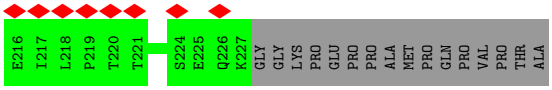




• Molecule 25: 40S ribosomal protein S3

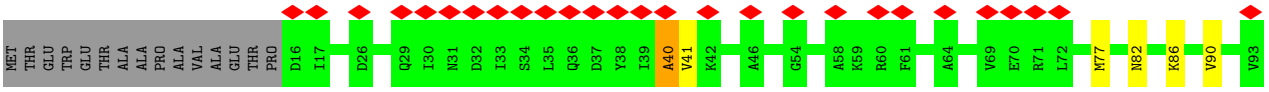
Chain D:

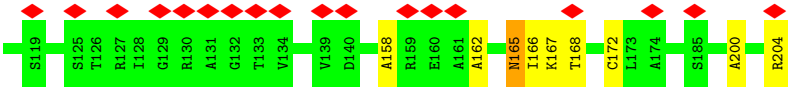




• Molecule 26: 40S ribosomal protein S5

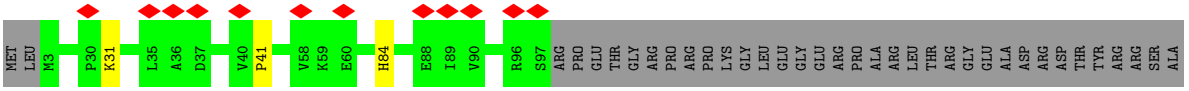
Chain F:





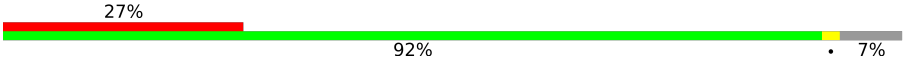
• Molecule 27: 40S ribosomal protein S10

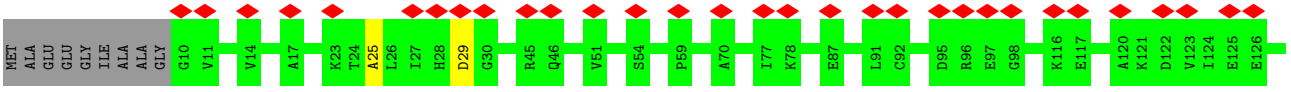
Chain K:

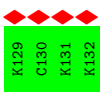


• Molecule 28: 40S ribosomal protein S12

Chain M:

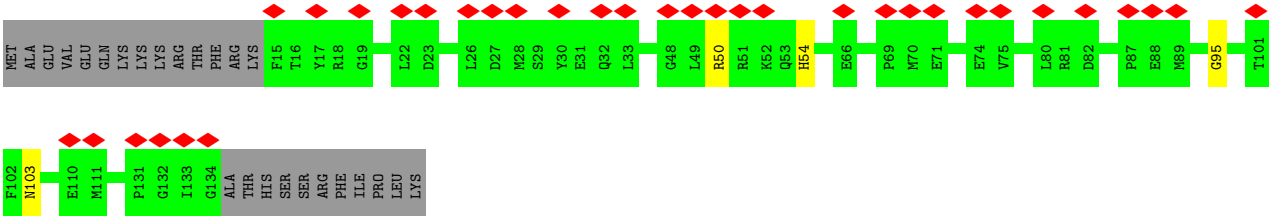




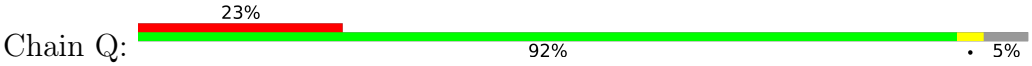


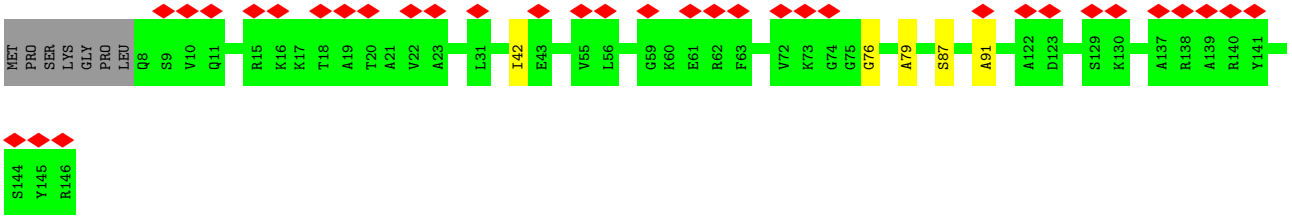
• Molecule 29: 40S ribosomal protein S15

Chain P:

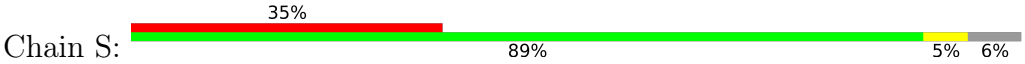


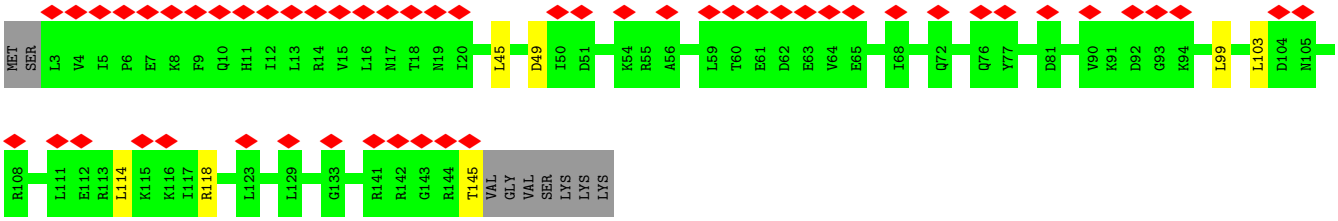
• Molecule 30: 40S ribosomal protein S16



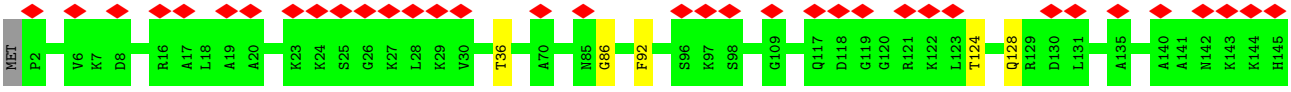


• Molecule 31: 40S ribosomal protein S18

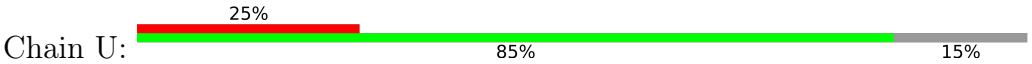


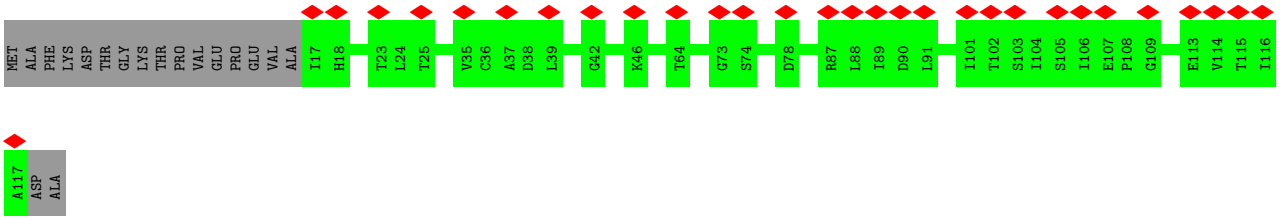


• Molecule 32: 40S ribosomal protein S19



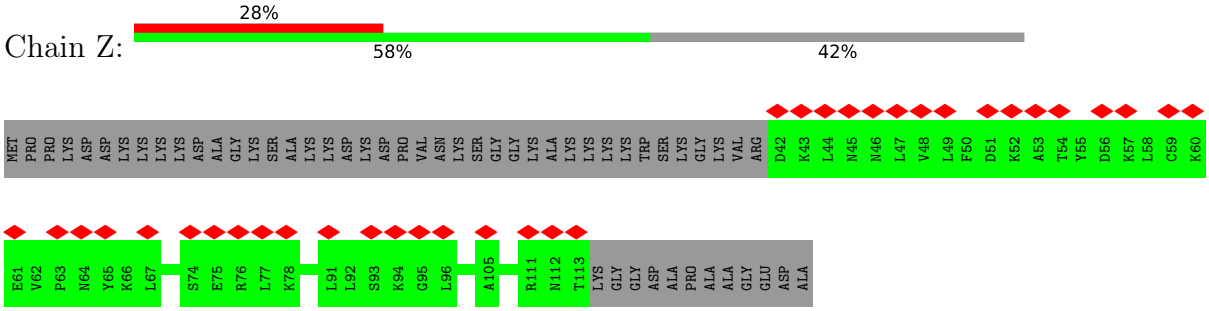
• Molecule 33: 40S ribosomal protein S20





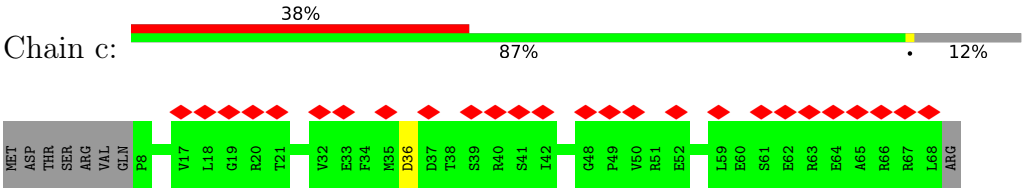
• Molecule 34: 40S ribosomal protein S25

Chain Z:



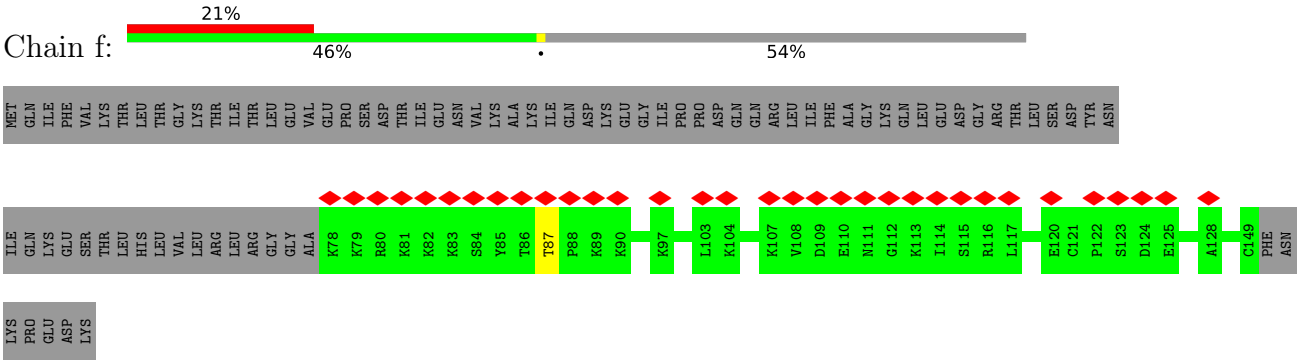
• Molecule 35: 40S ribosomal protein S28

Chain c:



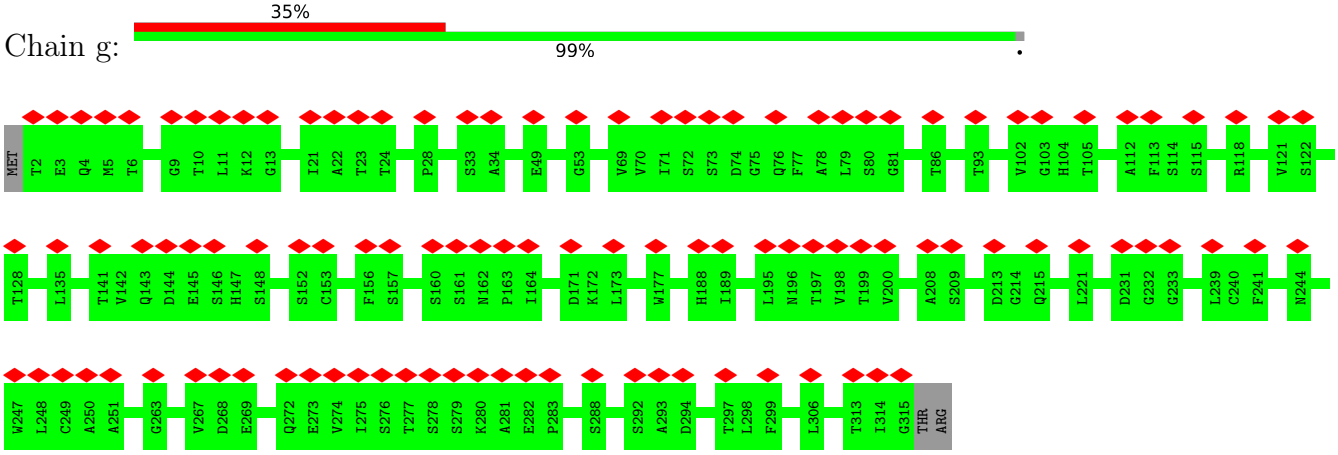
• Molecule 36: Ubiquitin-40S ribosomal protein S27a

Chain f:



• Molecule 37: Receptor of activated protein C kinase 1

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36446	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 ($e^-/Å^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.39	0/21550	0.90	32/33120 (0.1%)
2	R	0.37	0/603	0.65	0/839
3	A	0.40	0/1067	0.65	0/1485
4	B	0.35	0/1053	0.62	0/1466
5	C	0.41	0/1071	0.63	0/1487
6	E	0.34	0/1286	0.61	0/1785
7	G	0.40	0/1134	0.65	0/1577
8	H	0.36	0/919	0.60	0/1279
9	I	0.35	0/1008	0.63	0/1400
10	J	0.40	0/887	0.67	0/1233
11	L	0.35	0/743	0.61	0/1032
12	N	0.42	0/736	0.65	0/1024
13	O	0.38	0/658	0.67	0/910
14	V	0.36	0/402	0.63	0/557
15	W	0.37	0/633	0.66	0/878
16	X	0.38	0/689	0.66	0/954
17	Y	0.37	0/609	0.63	0/845
18	b	0.35	0/404	0.60	0/561
19	e	0.40	0/269	0.61	0/372
20	x	0.33	0/879	0.59	0/1223
21	y	0.35	0/1603	0.60	0/2228
22	u	0.34	0/3038	0.58	0/4227
23	t	0.30	0/303	0.53	0/422
24	d	0.39	0/268	0.64	0/370
25	D	0.39	1/1103 (0.1%)	0.63	0/1530
26	F	0.33	0/934	0.63	0/1300
27	K	0.32	0/471	0.64	1/656 (0.2%)
28	M	0.27	0/606	0.56	0/842
29	P	0.32	0/589	0.57	0/817
30	Q	0.36	0/682	0.65	0/946
31	S	0.30	0/703	0.59	0/976
32	T	0.38	0/704	0.58	0/975
33	U	0.35	0/499	0.64	0/694
34	Z	0.29	0/357	0.61	0/497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	c	0.33	0/299	0.67	1/414 (0.2%)
36	f	0.28	0/355	0.57	0/493
37	g	0.33	0/1542	0.61	0/2141
All	All	0.37	1/50656 (0.0%)	0.76	34/73555 (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
25	D	0	1
26	F	0	4
30	Q	0	1
32	T	0	1
36	f	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	189	MET	C-N	-5.93	1.20	1.34

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1565	C	P-O3'-C3'	7.66	128.89	119.70
1	2	958	G	C2'-C3'-O3'	7.45	125.89	109.50
1	2	1403	C	P-O3'-C3'	7.42	128.61	119.70
1	2	1330	G	P-O3'-C3'	7.11	128.24	119.70
1	2	1585	U	P-O3'-C3'	6.91	127.99	119.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	D	194	PRO	Peptide
26	F	165	ASN	Peptide
26	F	40	ALA	Peptide
26	F	77	MET	Peptide
26	F	82	ASN	Peptide

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	19905	0	9965	129	0
2	R	604	0	259	3	0
3	A	1068	0	503	0	0
4	B	1054	0	455	0	0
5	C	1072	0	489	1	0
6	E	1287	0	577	2	0
7	G	1135	0	512	2	0
8	H	920	0	399	1	0
9	I	1009	0	451	0	0
10	J	888	0	389	0	0
11	L	744	0	321	1	0
12	N	737	0	330	0	0
13	O	659	0	321	2	0
14	V	403	0	199	0	0
15	W	634	0	283	1	0
16	X	690	0	330	0	0
17	Y	610	0	271	0	0
18	b	405	0	172	0	0
19	e	270	0	126	0	0
20	x	880	0	403	0	0
21	y	1606	0	708	0	0
22	u	3042	0	1329	0	0
23	t	304	0	133	0	0
24	d	269	0	117	0	0
25	D	1104	0	503	10	0
26	F	935	0	442	5	0
27	K	472	0	203	1	0
28	M	607	0	284	1	0
29	P	590	0	251	2	0
30	Q	683	0	320	4	0
31	S	704	0	317	4	0
32	T	705	0	343	3	0
33	U	500	0	210	0	0
34	Z	358	0	161	0	0
35	c	300	0	131	0	0
36	f	356	0	154	0	0
37	g	1543	0	689	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49052	0	23050	154	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 2.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1374:C:H4'	1:2:1464:C:O2'	1.35	1.20
1:2:1374:C:H5'	1:2:1465:A:C4'	1.75	1.16
1:2:1374:C:H5'	1:2:1465:A:H4'	1.28	1.14
1:2:1385:G:OP1	25:D:158:ILE:HA	1.46	1.13
1:2:1374:C:C4'	1:2:1464:C:O2'	2.20	0.90

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	R	120/135 (89%)	99 (82%)	19 (16%)	2 (2%)	9 43
3	A	214/295 (72%)	200 (94%)	12 (6%)	2 (1%)	17 56
4	B	211/264 (80%)	195 (92%)	15 (7%)	1 (0%)	29 68
5	C	216/293 (74%)	202 (94%)	12 (6%)	2 (1%)	17 56
6	E	260/263 (99%)	245 (94%)	14 (5%)	1 (0%)	34 72
7	G	228/249 (92%)	215 (94%)	12 (5%)	1 (0%)	34 72
8	H	184/194 (95%)	174 (95%)	10 (5%)	0	100 100
9	I	203/208 (98%)	191 (94%)	12 (6%)	0	100 100
10	J	178/194 (92%)	159 (89%)	17 (10%)	2 (1%)	14 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	L	149/158 (94%)	143 (96%)	4 (3%)	2 (1%)	12 48
12	N	147/151 (97%)	137 (93%)	10 (7%)	0	100 100
13	O	133/151 (88%)	125 (94%)	8 (6%)	0	100 100
14	V	80/83 (96%)	76 (95%)	4 (5%)	0	100 100
15	W	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19 60
16	X	139/143 (97%)	134 (96%)	3 (2%)	2 (1%)	11 47
17	Y	122/133 (92%)	113 (93%)	8 (7%)	1 (1%)	19 60
18	b	80/84 (95%)	73 (91%)	7 (9%)	0	100 100
19	e	53/59 (90%)	46 (87%)	4 (8%)	3 (6%)	1 20
20	x	176/252 (70%)	169 (96%)	6 (3%)	1 (1%)	25 65
21	y	319/412 (77%)	290 (91%)	21 (7%)	8 (2%)	5 35
22	u	607/804 (76%)	549 (90%)	49 (8%)	9 (2%)	10 46
23	t	59/475 (12%)	52 (88%)	6 (10%)	1 (2%)	9 43
24	d	53/56 (95%)	50 (94%)	2 (4%)	1 (2%)	8 41
25	D	223/243 (92%)	198 (89%)	25 (11%)	0	100 100
26	F	187/204 (92%)	172 (92%)	12 (6%)	3 (2%)	9 45
27	K	93/165 (56%)	85 (91%)	8 (9%)	0	100 100
28	M	121/132 (92%)	114 (94%)	7 (6%)	0	100 100
29	P	118/145 (81%)	115 (98%)	3 (2%)	0	100 100
30	Q	137/146 (94%)	122 (89%)	15 (11%)	0	100 100
31	S	141/152 (93%)	130 (92%)	11 (8%)	0	100 100
32	T	142/145 (98%)	133 (94%)	9 (6%)	0	100 100
33	U	99/119 (83%)	89 (90%)	10 (10%)	0	100 100
34	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100 100
35	c	59/69 (86%)	52 (88%)	7 (12%)	0	100 100
36	f	70/156 (45%)	60 (86%)	10 (14%)	0	100 100
37	g	312/317 (98%)	278 (89%)	34 (11%)	0	100 100
All	All	5830/7304 (80%)	5374 (92%)	413 (7%)	43 (1%)	26 62

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	20	TYR

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Mol	Chain	Res	Type
10	J	160	SER
11	L	42	LEU
16	X	61	GLN
16	X	86	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1645/1882 (87%)	552 (33%)	0

5 of 552 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C
1	2	5	U
1	2	8	U

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	189:MET	C	190:LEU	N	1.20

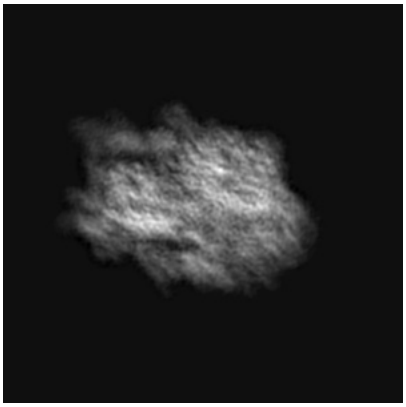
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4351. These allow visual inspection of the internal detail of the map and identification of artifacts.

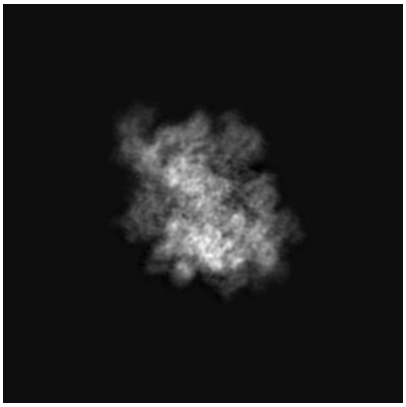
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

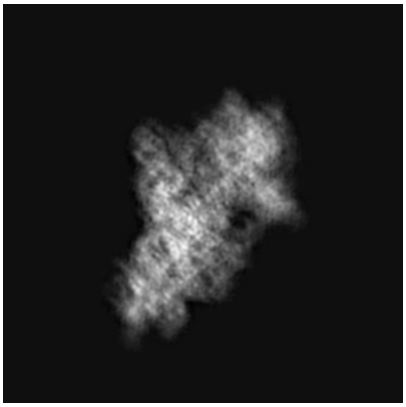
6.1.1 Primary map



X



Y

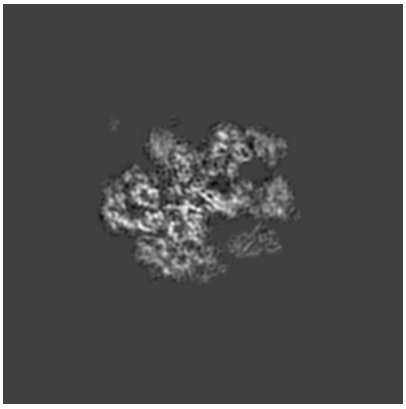


Z

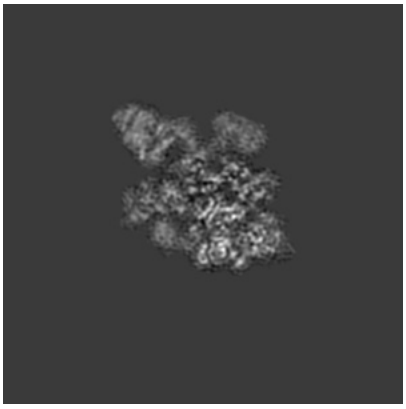
The images above show the map projected in three orthogonal directions.

6.2 Central slices

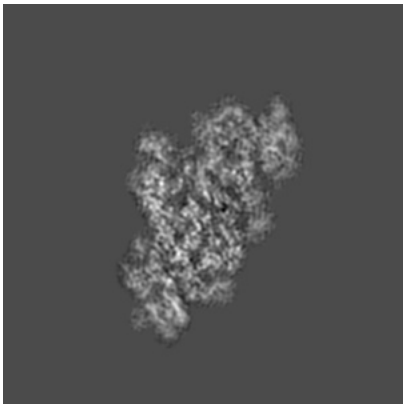
6.2.1 Primary map



X Index: 180



Y Index: 180

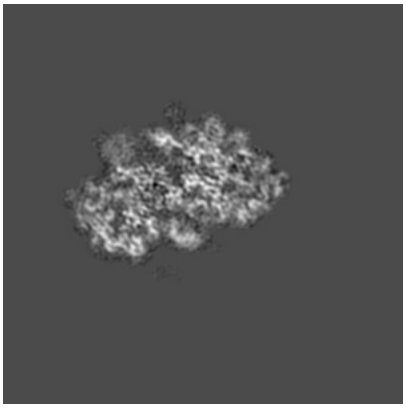


Z Index: 180

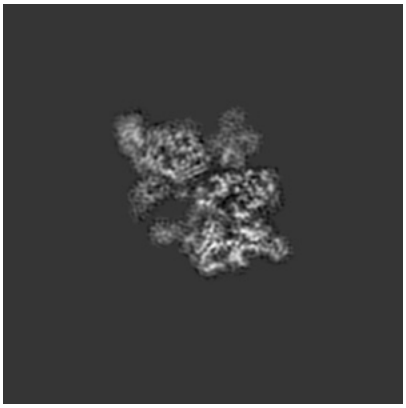
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

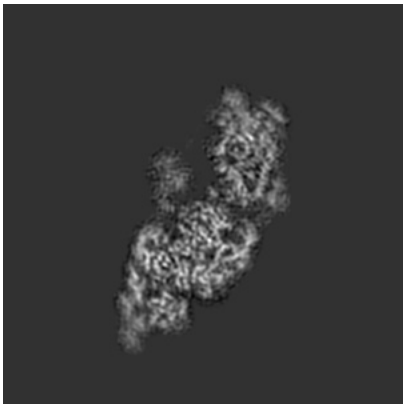
6.3.1 Primary map



X Index: 140



Y Index: 191

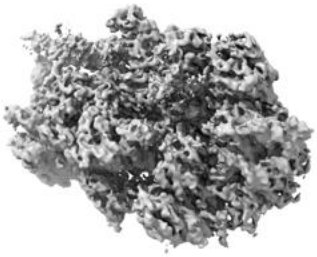


Z Index: 162

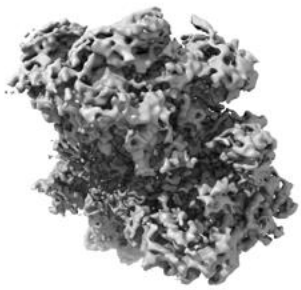
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

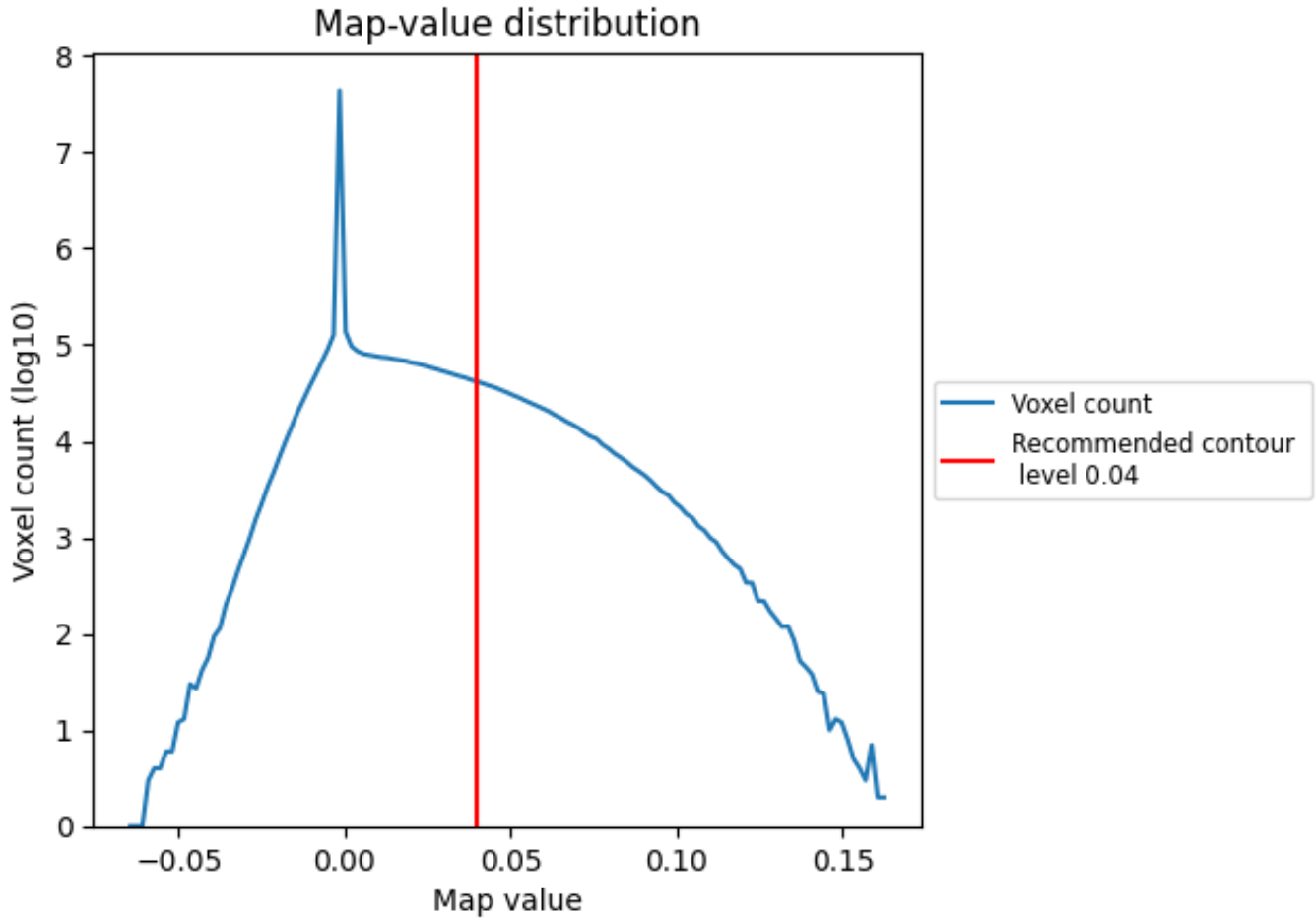
6.5 Mask visualisation (i)

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

7 Map analysis

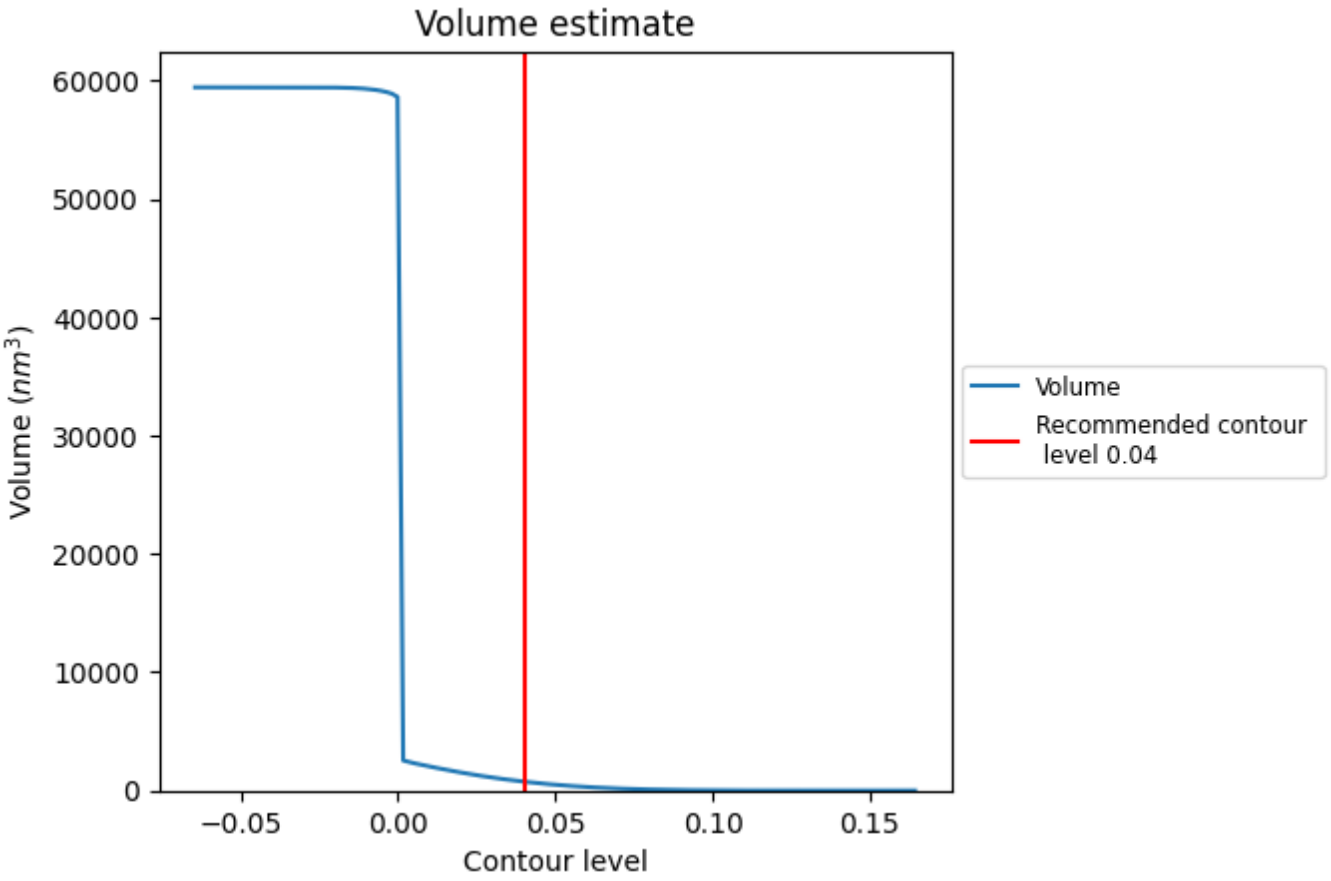
This section contains the results of statistical analysis of the map.

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.

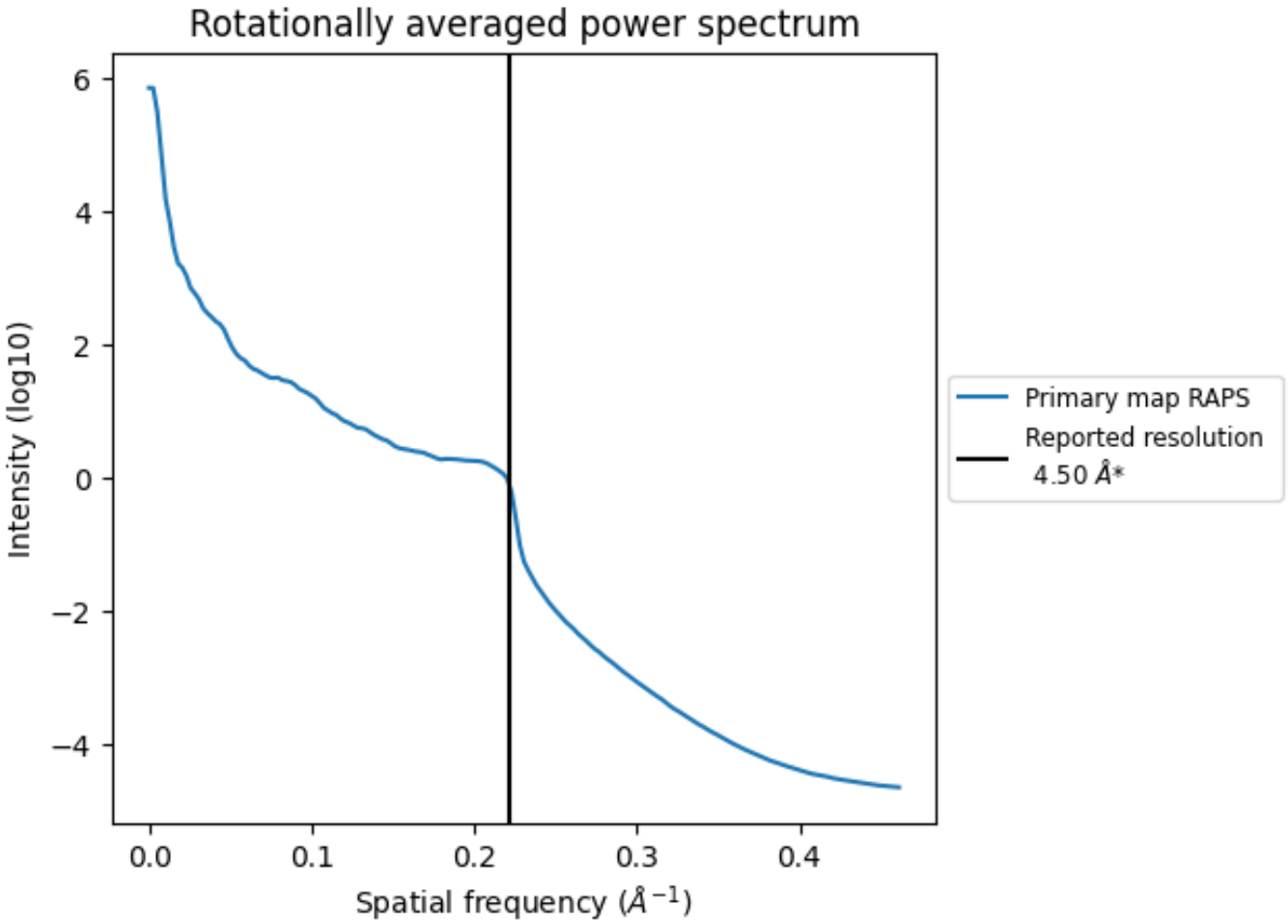
7.2 Volume estimate (i)



The volume at the recommended contour level is 755 nm^3; this corresponds to an approximate mass of 682 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)

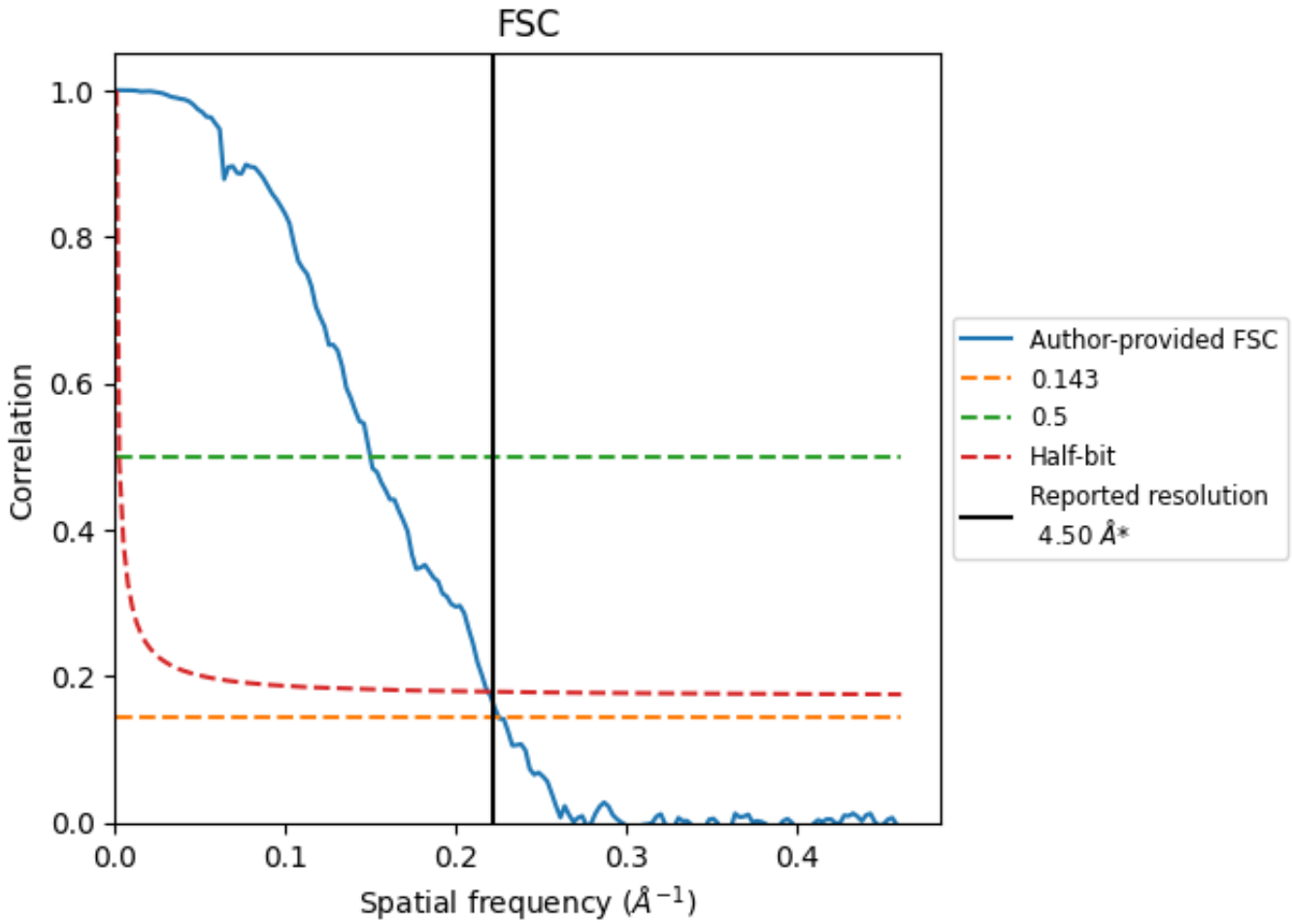


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

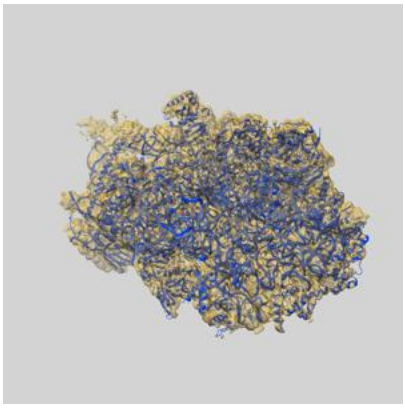
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.44	6.68	4.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

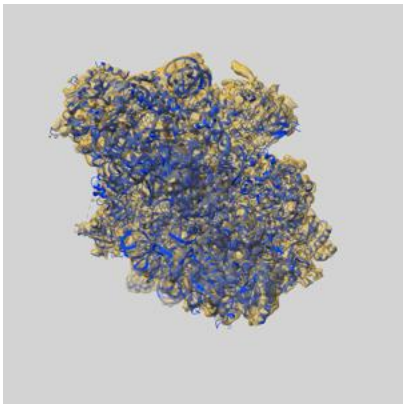
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4351 and PDB model 6G53. Per-residue inclusion information can be found in section 3 on page 11.

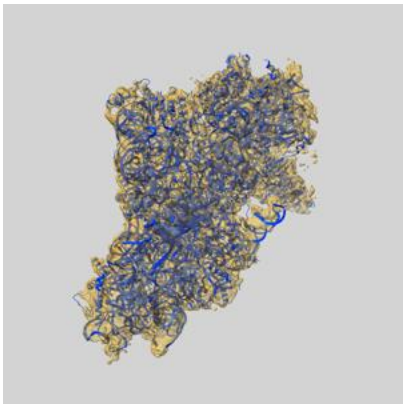
9.1 Map-model overlay



X



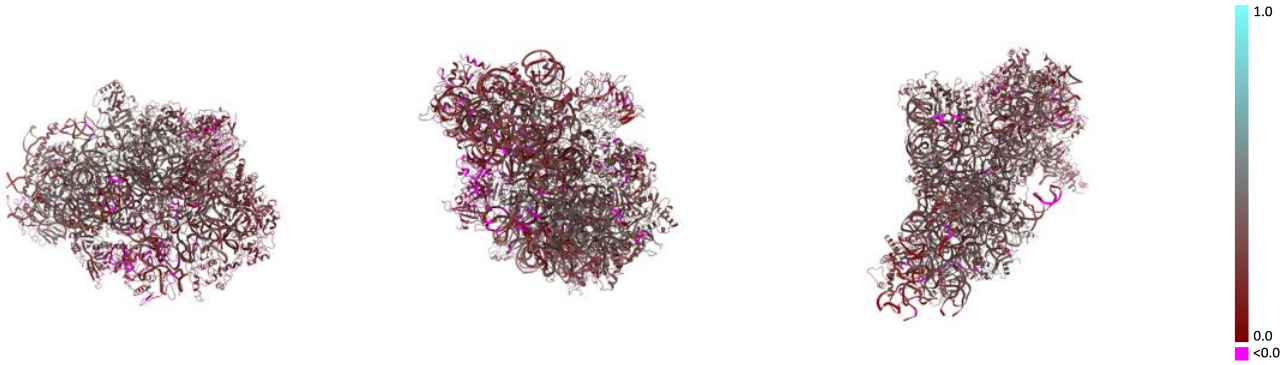
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

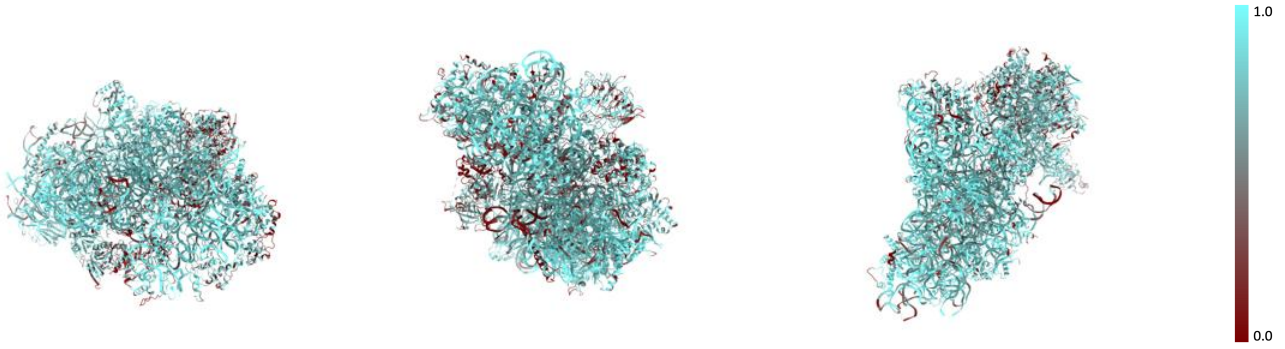
9.2 Q-score mapped to coordinate model (i)



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.

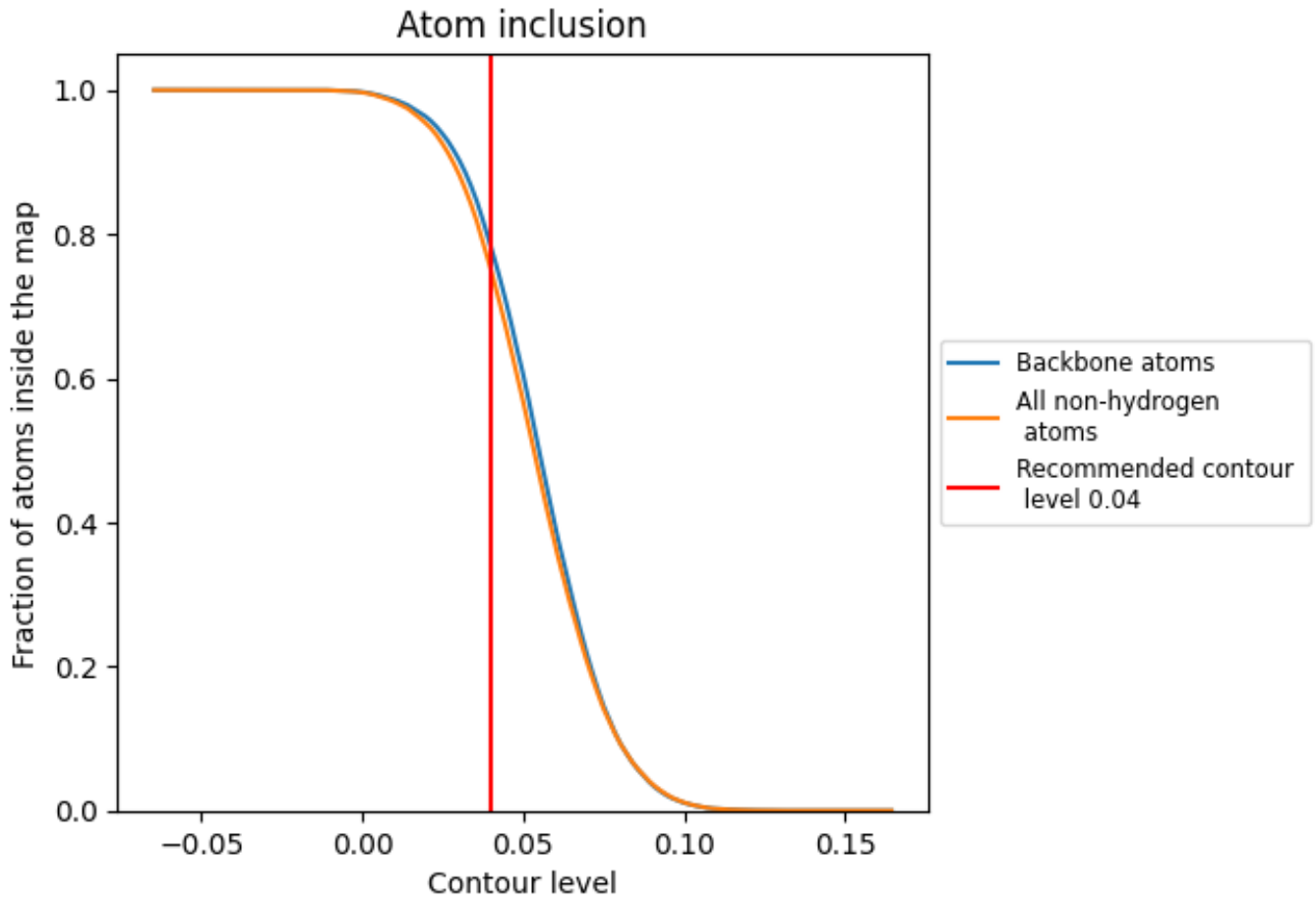
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 78% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7504	0.2790
2	0.8212	0.2830
A	0.8436	0.3510
B	0.8245	0.3270
C	0.8106	0.3590
D	0.7301	0.3120
E	0.8003	0.3400
F	0.7027	0.2540
G	0.8493	0.3130
H	0.8130	0.3090
I	0.8563	0.3150
J	0.8345	0.3430
K	0.8030	0.2870
L	0.7567	0.3630
M	0.6458	0.1930
N	0.8657	0.3330
O	0.5948	0.2950
P	0.6678	0.2340
Q	0.6896	0.2790
R	0.6738	0.3030
S	0.5994	0.1890
T	0.6837	0.2350
U	0.6120	0.2650
V	0.8114	0.3520
W	0.8801	0.3720
X	0.8667	0.3530
Y	0.8902	0.3390
Z	0.4777	0.1400
b	0.8272	0.3440
c	0.5600	0.2590
d	0.7807	0.2910
e	0.1370	0.0240
f	0.5000	0.1120
g	0.6099	0.2300
t	0.1184	0.2220

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Chain	Atom inclusion	Q-score
u	0.5381	0.1480
x	0.7307	0.3180
y	0.4907	0.2560