wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 09:05 AM EST

PDB ID	:	7JQB
EMDB ID	:	EMD-22432
Title	:	SARS-CoV-2 Nsp1 and rabbit 40S ribosome complex
Authors	:	Yuan, S.; Xiong, Y.
Deposited on	:	2020-08-10
Resolution	:	2.70 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:

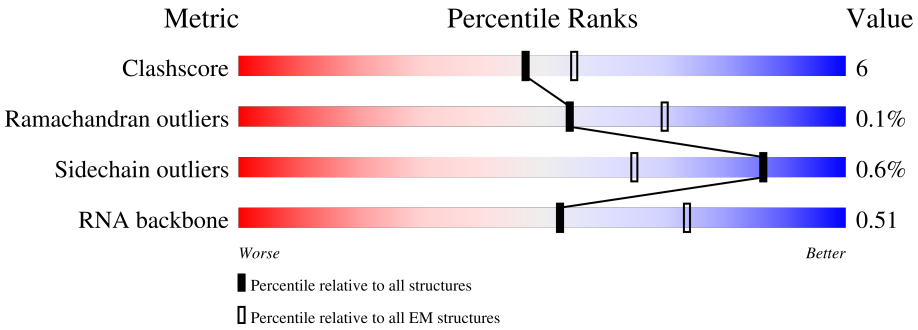
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	A	1869	60% 25% 6% 9%
2	a	125	32% 59% 40%
3	B	295	66% 8% 26%
4	b	115	87% 12%
5	C	264	64% 16% 19%
6	D	293	66% 10% 25%
7	d	69	20% 88% 10%

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Mol	Chain	Length	Quality of chain
8	E	243	14% 80% 14% 6%
9	f	133	6% 42% 57%
10	G	204	25% 66% 25% 9%
11	g	156	40% 43% 56%
12	H	249	80% 14% 5%
13	h	317	34% 98%
14	I	194	82% 13% 5%
15	J	208	82% 17%
16	K	194	83% 12% 5%
17	L	165	13% 46% 12% 42%
18	N	132	87% 66% 23% 11%
19	Q	145	50% 56% 32% 11%
20	R	146	13% 69% 28%
21	S	135	7% 82% 16%
22	T	152	57% 63% 32% 5%
23	U	145	20% 70% 27%
24	V	119	37% 73% 11% 16%
25	W	83	83% 17%
26	Z	130	82% 13% 5%
27	F	36	11% 86% 14%
28	M	263	80% 20%
29	O	158	15% 87% 13%
30	P	151	85% 15%
31	X	168	66% 15% 19%
32	Y	130	87% 12%

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Mol	Chain	Length	Quality of chain
33	c	143	97%
34	e	84	5% 98%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 74976 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	A	1697	36229	16171	6507	11855	1696	0	0

- Molecule 2 is a protein called eS25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	217	1710	1086	300	316	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 4 is a protein called 40S ribosomal protein S26.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8
b	56	ALA	VAL	conflict	UNP G1TFE8
b	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 7 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 8 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 9 is a protein called eS30.

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

- Molecule 10 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 11 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 12 is a protein called eS6.

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

- Molecule 13 is a protein called RACK1.

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

- Molecule 14 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 15 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 16 is a protein called uS4.

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

- Molecule 17 is a protein called S10_plectin domain-containing protein.

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

- Molecule 18 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 20 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 22 is a protein called uS13.

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

- Molecule 23 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 24 is a protein called uS10.

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

- Molecule 25 is a protein called 40S ribosomal protein S21.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82
W	81	LYS	GLN	conflict	UNP G1TM82

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	36	Total	C	N	O	S	0	0
			280	171	50	58	1		

- Molecule 28 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	M	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 29 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	O	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 30 is a protein called uS15.

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

- Molecule 31 is a protein called Uncharacterized protein.

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

- Molecule 32 is a protein called uS8.

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

- Molecule 33 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	142	Total	C	N	O	S	0	0
			1106	698	220	184	4		

- Molecule 34 is a protein called eS27.

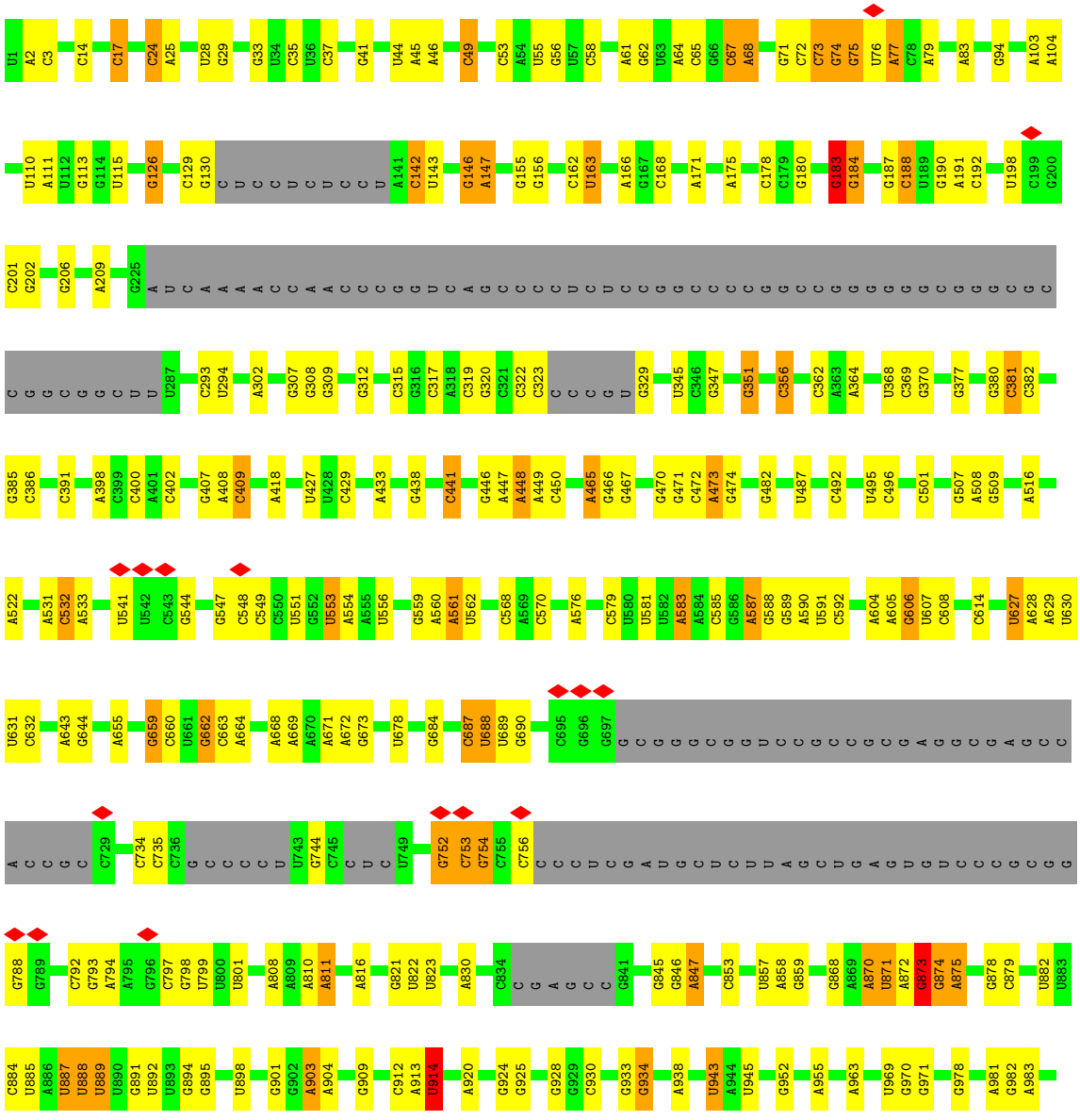
Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

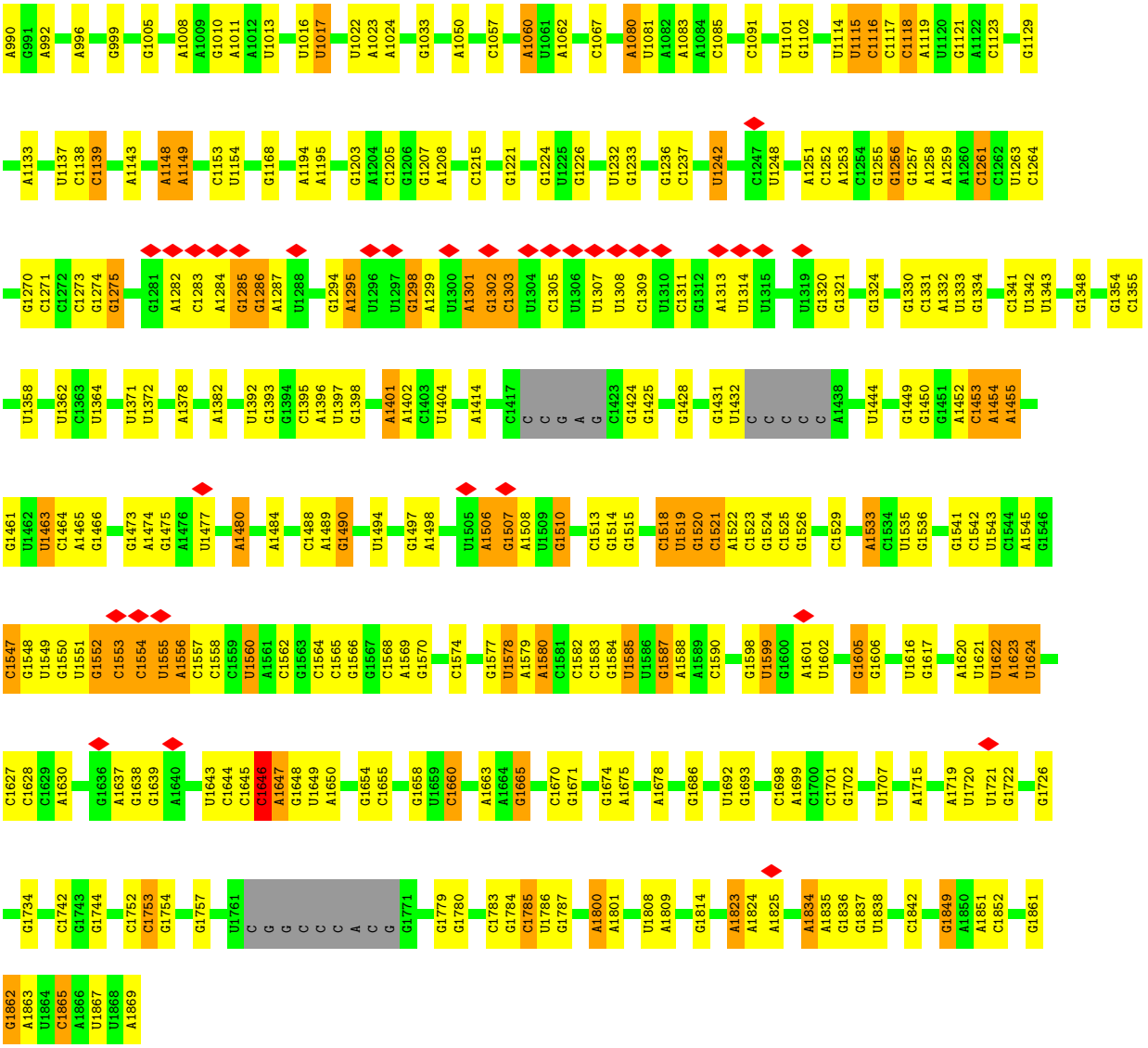
3 Residue-property plots (i)

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

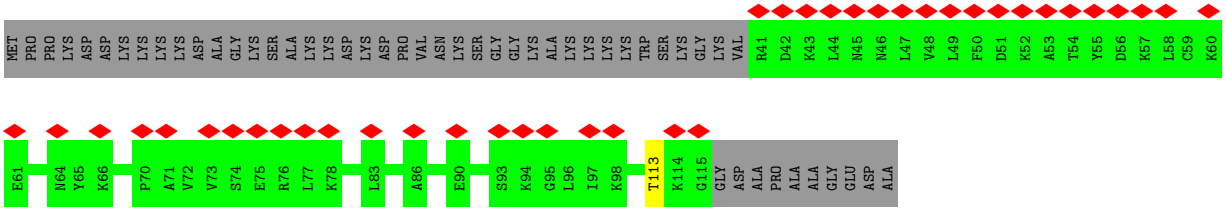
Chain A:





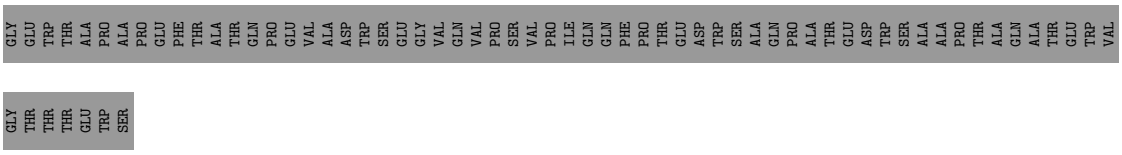
• Molecule 2: eS25

Chain a:



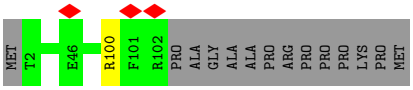
• Molecule 3: 40S ribosomal protein SA

Chain B:



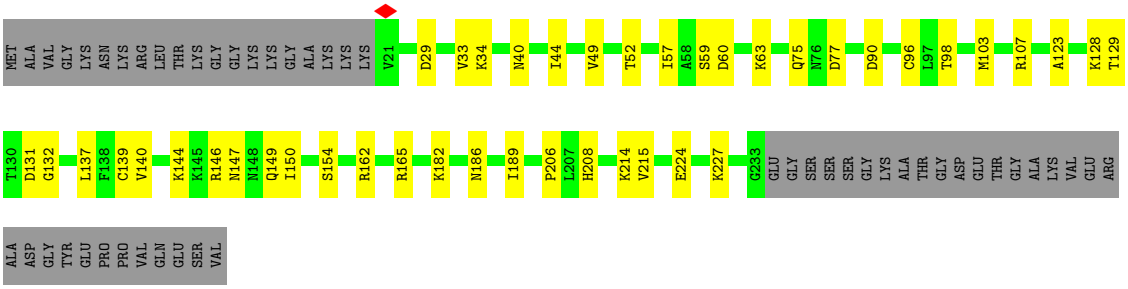
• Molecule 4: 40S ribosomal protein S26

Chain b:



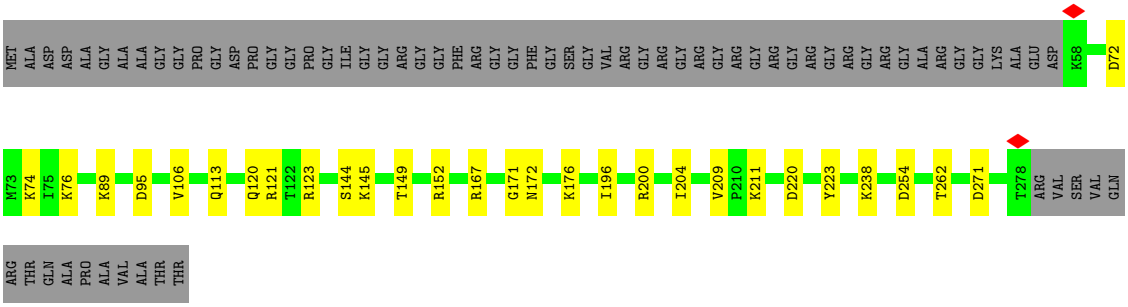
• Molecule 5: eS1

Chain C:



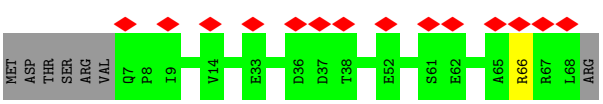
• Molecule 6: uS5

Chain D:



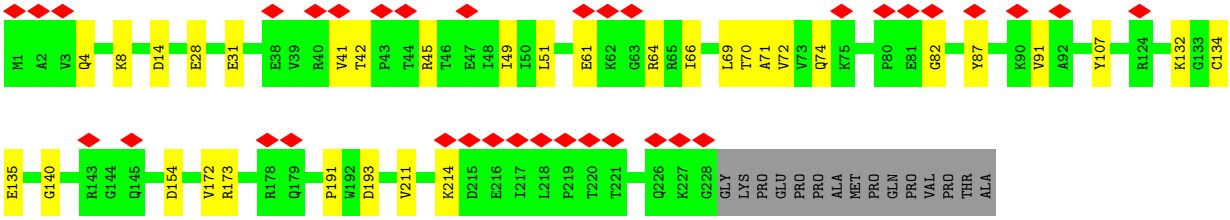
• Molecule 7: eS28

Chain d:

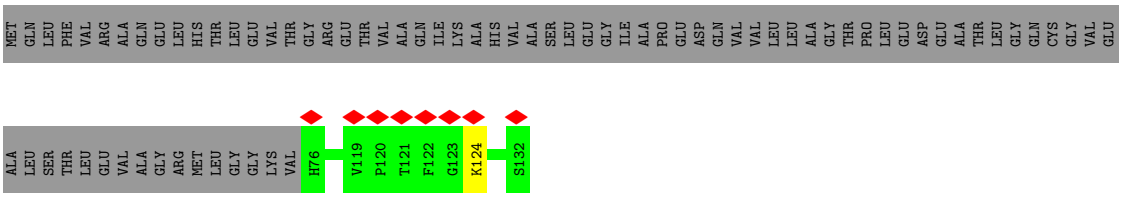


• Molecule 8: Ribosomal protein S3

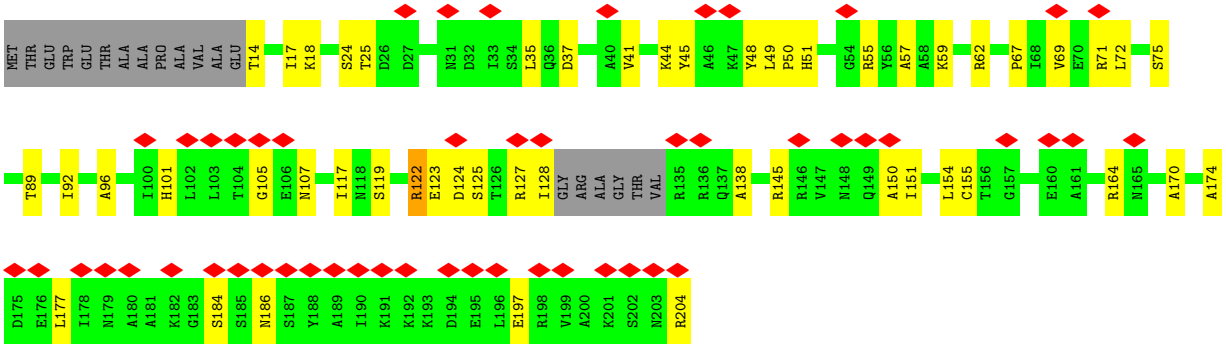
Chain E:



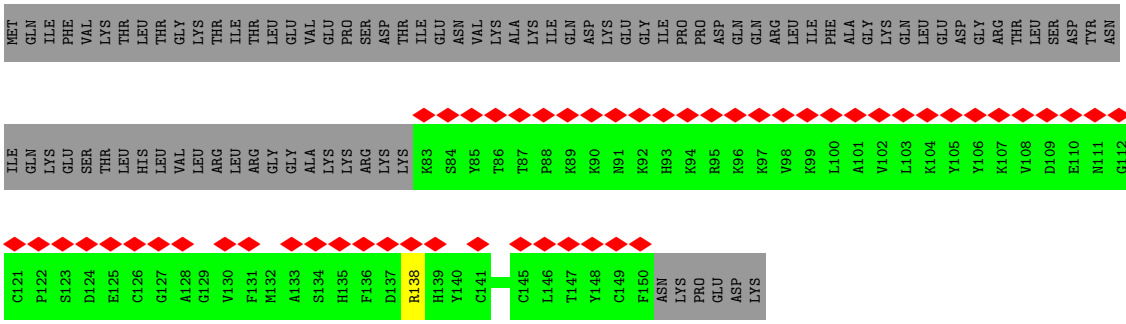
• Molecule 9: eS30



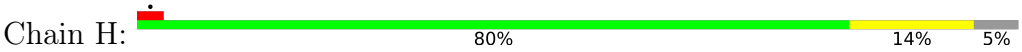
• Molecule 10: uS7

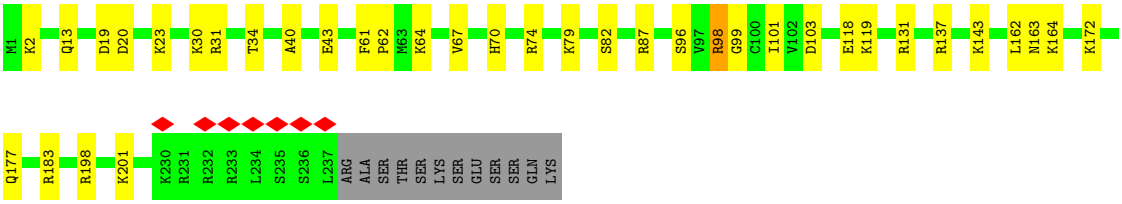


• Molecule 11: eS31



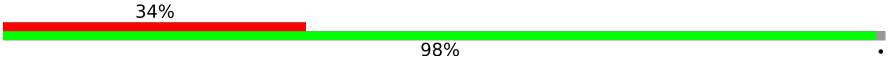
• Molecule 12: eS6

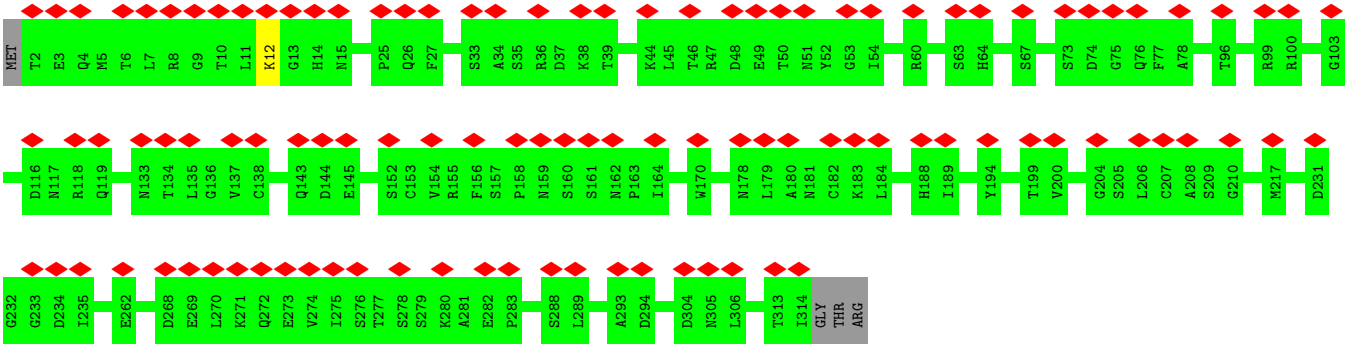




• Molecule 13: RACK1

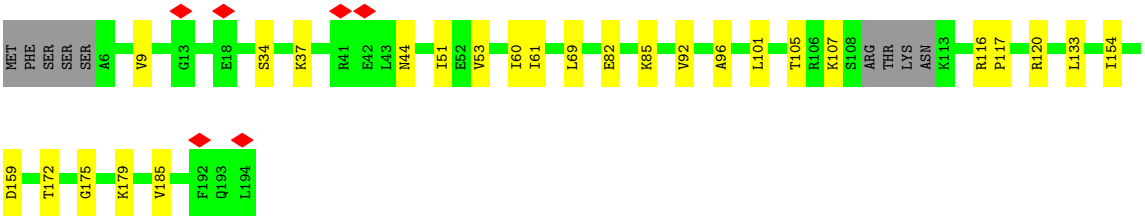
Chain h:





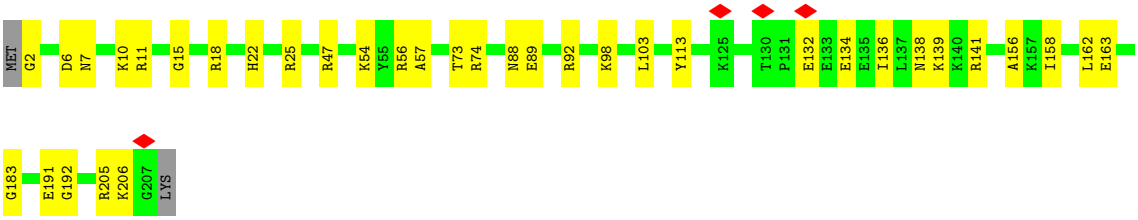
• Molecule 14: eS7

Chain I:



• Molecule 15: eS8

Chain J:

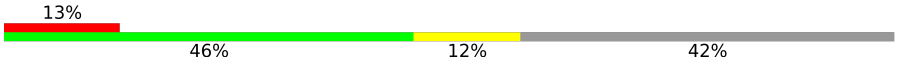


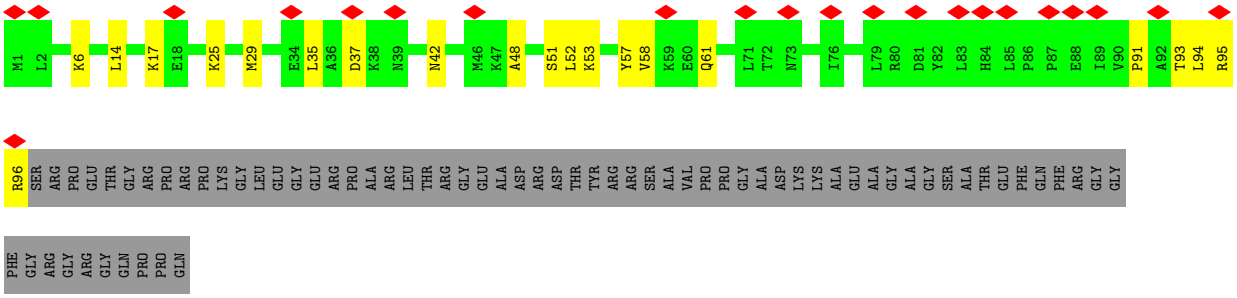
• Molecule 16: uS4

Chain K:

• Molecule 17: S10_plectin domain-containing protein

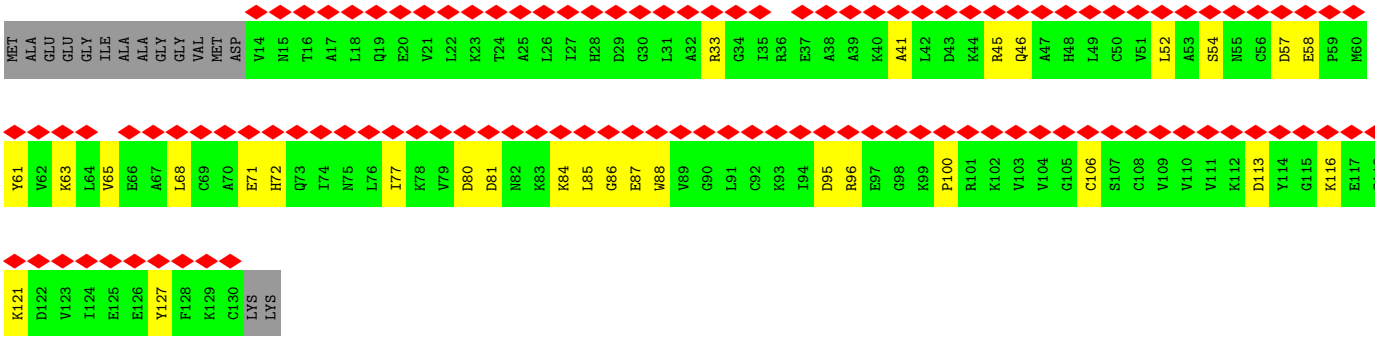
Chain L:





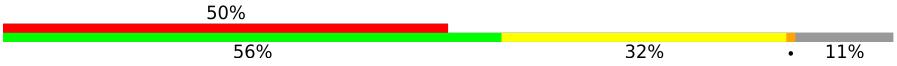
• Molecule 18: eS12

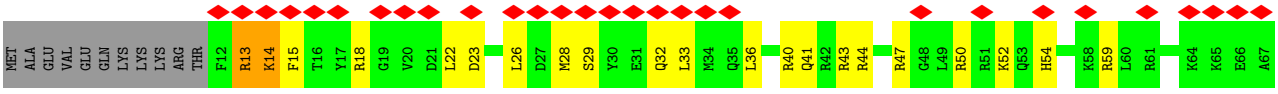
Chain N:

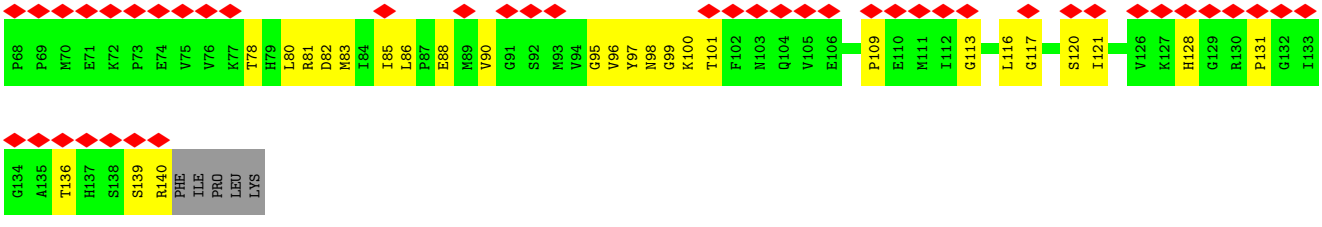


• Molecule 19: uS19

Chain Q:

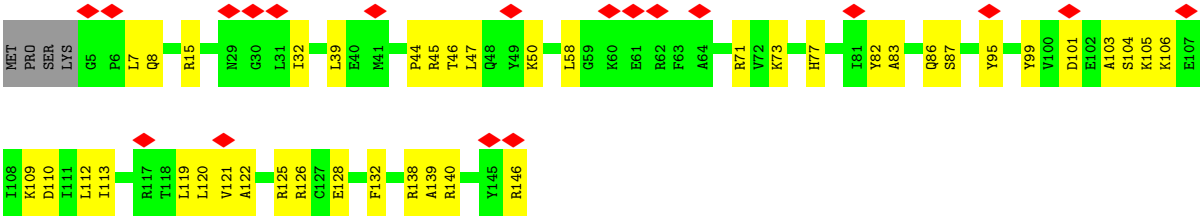




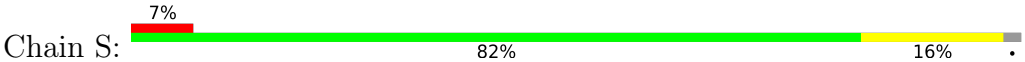


• Molecule 20: Uncharacterized protein

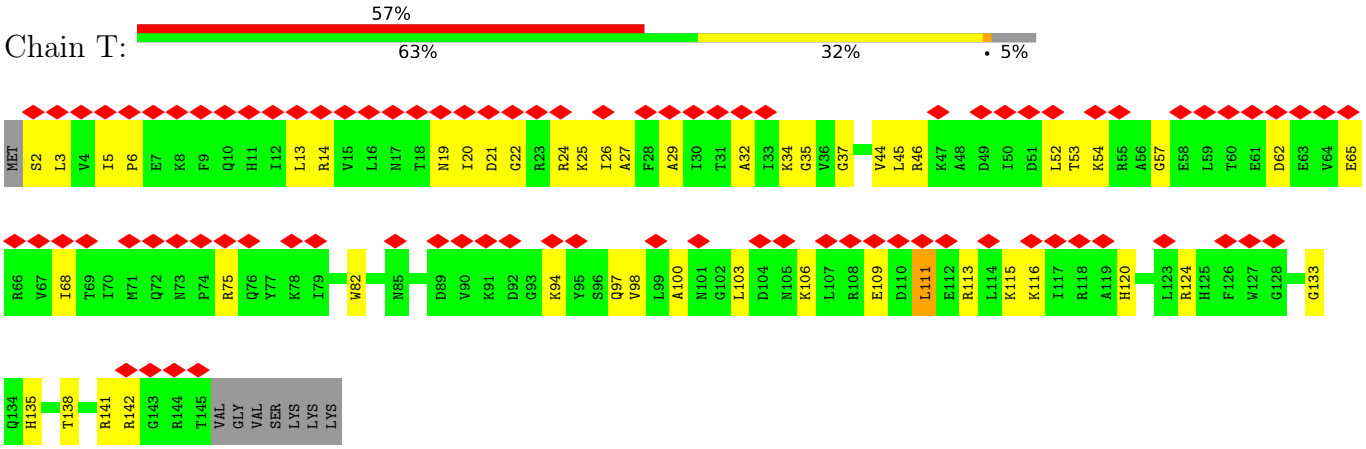
Chain R:



• Molecule 21: eS17

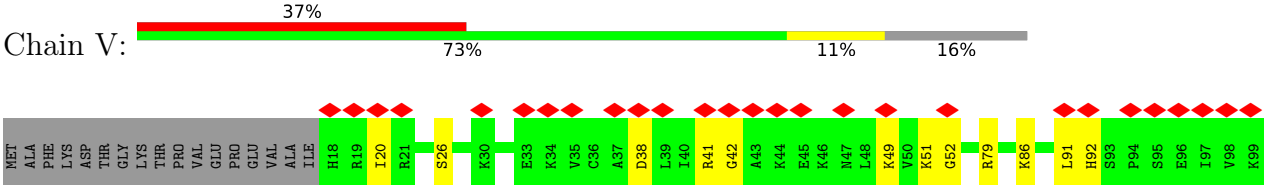


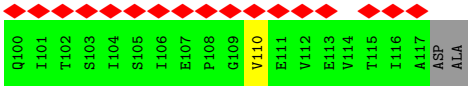
• Molecule 22: uS13



• Molecule 23: Uncharacterized protein

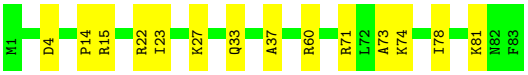
• Molecule 24: uS10





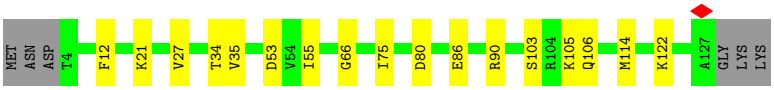
• Molecule 25: 40S ribosomal protein S21

Chain W:



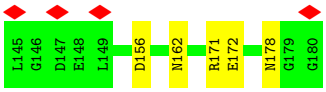
• Molecule 26: 40S ribosomal protein S24

Chain Z:



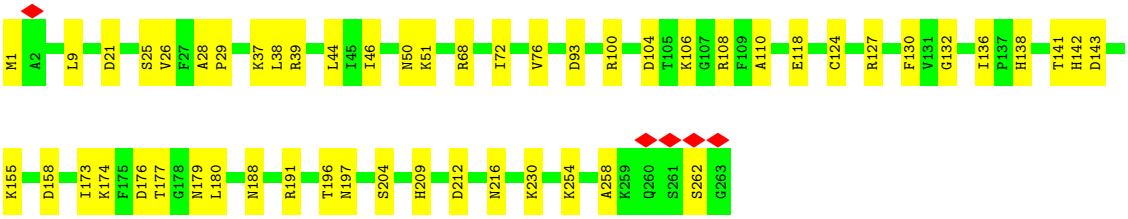
• Molecule 27: Host translation inhibitor nsp1

Chain F:



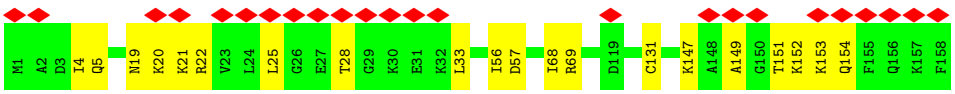
• Molecule 28: 40S ribosomal protein S4

Chain M:



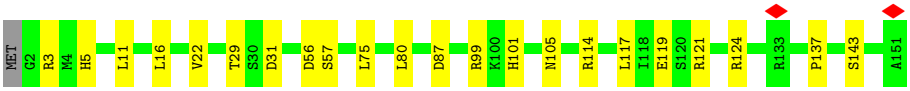
• Molecule 29: uS17

Chain O:



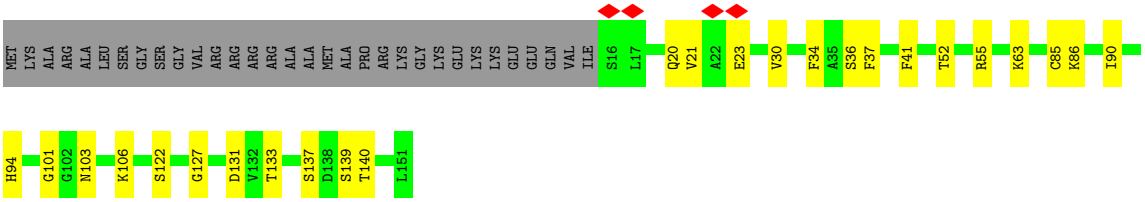
• Molecule 30: uS15

Chain P:



• Molecule 31: Uncharacterized protein

Chain X:

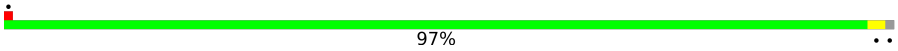


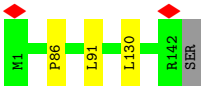
• Molecule 32: uS8

Chain Y:

• Molecule 33: Uncharacterized protein

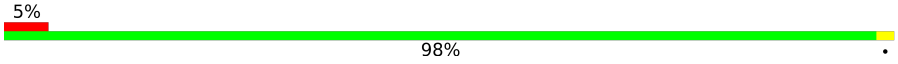
Chain c:

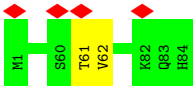




• Molecule 34: eS27

Chain e:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	353927	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.392	Depositor
Minimum map value	-2.806	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	341.75998, 341.75998, 341.75998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.83	0/40509	1.04	175/63128 (0.3%)
2	a	0.29	0/604	0.60	0/810
3	B	0.42	0/1747	0.50	0/2374
4	b	0.45	0/828	0.51	0/1109
5	C	0.40	0/1756	0.51	0/2350
6	D	0.47	0/1753	0.51	0/2369
7	d	0.27	0/490	0.49	0/656
8	E	0.33	0/1796	0.52	0/2417
9	f	0.39	0/462	0.49	0/607
10	G	0.28	0/1492	0.50	0/2005
11	g	0.28	0/567	0.54	0/753
12	H	0.36	0/1946	0.49	0/2590
13	h	0.28	0/2493	0.54	0/3394
14	I	0.36	0/1510	0.55	0/2022
15	J	0.44	0/1715	0.52	0/2287
16	K	0.44	0/1550	0.49	0/2069
17	L	0.28	0/834	0.48	0/1125
18	N	0.30	0/918	0.61	0/1233
19	Q	0.28	0/1079	0.50	0/1441
20	R	0.29	0/1146	0.52	0/1534
21	S	0.32	0/1082	0.51	0/1452
22	T	0.31	0/1208	0.59	1/1618 (0.1%)
23	U	0.27	0/1115	0.50	1/1493 (0.1%)
24	V	0.27	0/805	0.50	0/1081
25	W	0.41	0/643	0.49	0/860
26	Z	0.43	0/1028	0.51	0/1366
27	F	0.37	0/285	0.44	0/384
28	M	0.45	0/2125	0.60	0/2856
29	O	0.48	0/1319	0.63	1/1761 (0.1%)
30	P	0.42	0/1232	0.59	2/1656 (0.1%)
31	X	0.38	0/1029	0.66	0/1380
32	Y	0.49	0/1051	0.56	0/1406
33	c	0.45	0/1124	0.61	1/1500 (0.1%)
34	e	0.43	0/673	0.63	0/902

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.65	0/79914	0.85	181/115988 (0.2%)

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
3	B	0	1
5	C	0	1
8	E	0	1
28	M	0	1
29	O	0	2
30	P	0	1
31	X	0	3
33	c	0	1
34	e	0	2
All	All	0	13

There are no bond length outliers.

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	501	C	N1-C2-O2	13.71	127.12	118.90
1	A	501	C	C2-N1-C1'	13.53	133.69	118.80
1	A	1453	C	C2-N1-C1'	12.78	132.85	118.80
1	A	1453	C	N1-C2-O2	12.09	126.16	118.90
1	A	293	C	N1-C2-O2	10.97	125.48	118.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	43	SER	Peptide
5	C	189	ILE	Peptide
8	E	41	VAL	Peptide
28	M	204	SER	Peptide
29	O	4	ILE	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	A	36229	0	18300	208	0
2	a	598	0	656	0	0
3	B	1710	0	1708	13	0
4	b	814	0	867	0	0
5	C	1729	0	1803	29	0
6	D	1716	0	1806	19	0
7	d	488	0	514	0	0
8	E	1768	0	1866	21	0
9	f	457	0	502	0	0
10	G	1471	0	1522	37	0
11	g	555	0	567	0	0
12	H	1923	0	2089	29	0
13	h	2436	0	2393	0	0
14	I	1488	0	1582	15	0
15	J	1686	0	1772	23	0
16	K	1525	0	1640	20	0
17	L	810	0	836	13	0
18	N	908	0	939	18	0
19	Q	1058	0	1104	36	0
20	R	1128	0	1195	29	0
21	S	1068	0	1121	19	0
22	T	1190	0	1249	33	0
23	U	1097	0	1132	31	0
24	V	795	0	862	9	0
25	W	636	0	637	10	0
26	Z	1011	0	1083	13	0
27	F	280	0	250	4	0
28	M	2083	0	2189	35	0
29	O	1296	0	1374	9	0
30	P	1208	0	1294	14	0
31	X	1016	0	1039	16	0
32	Y	1034	0	1080	11	0
33	c	1106	0	1179	0	0
34	e	659	0	683	0	0
All	All	74976	0	58833	594	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 6.

The worst 5 of 594 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:A:1091:C:HO2'	32:Y:2:VAL:N	1.78	0.82
1:A:925:G:H1	1:A:1017:U:H3	1.34	0.76
1:A:928:G:H1	1:A:1013:U:H3	1.38	0.72
1:A:1286:G:H21	1:A:1313:A:H62	1.44	0.65
5:C:149:GLN:HE22	5:C:154:SER:HB3	1.61	0.64

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	73/125 (58%)	66 (90%)	7 (10%)	0	100	100
3	B	215/295 (73%)	209 (97%)	6 (3%)	0	100	100
4	b	99/115 (86%)	93 (94%)	6 (6%)	0	100	100
5	C	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
6	D	219/293 (75%)	216 (99%)	3 (1%)	0	100	100
7	d	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
8	E	226/243 (93%)	212 (94%)	14 (6%)	0	100	100
9	f	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
10	G	181/204 (89%)	170 (94%)	11 (6%)	0	100	100
11	g	66/156 (42%)	56 (85%)	10 (15%)	0	100	100
12	H	235/249 (94%)	226 (96%)	9 (4%)	0	100	100
13	h	311/317 (98%)	281 (90%)	30 (10%)	0	100	100
14	I	181/194 (93%)	172 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	J	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
16	K	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
17	L	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
18	N	115/132 (87%)	101 (88%)	14 (12%)	0	100	100
19	Q	127/145 (88%)	115 (91%)	12 (9%)	0	100	100
20	R	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
21	S	130/135 (96%)	117 (90%)	13 (10%)	0	100	100
22	T	142/152 (93%)	127 (89%)	15 (11%)	0	100	100
23	U	139/145 (96%)	130 (94%)	9 (6%)	0	100	100
24	V	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
25	W	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
26	Z	122/130 (94%)	121 (99%)	1 (1%)	0	100	100
27	F	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
28	M	261/263 (99%)	237 (91%)	24 (9%)	0	100	100
29	O	156/158 (99%)	137 (88%)	18 (12%)	1 (1%)	25	50
30	P	148/151 (98%)	137 (93%)	11 (7%)	0	100	100
31	X	134/168 (80%)	108 (81%)	26 (19%)	0	100	100
32	Y	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	19	43
33	c	140/143 (98%)	128 (91%)	11 (8%)	1 (1%)	22	46
34	e	82/84 (98%)	73 (89%)	9 (11%)	0	100	100
All	All	4789/5544 (86%)	4455 (93%)	331 (7%)	3 (0%)	54	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	O	5	GLN
33	c	130	LEU
32	Y	67	GLY

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	66/103 (64%)	65 (98%)	1 (2%)	65	86
3	B	180/245 (74%)	179 (99%)	1 (1%)	86	95
4	b	88/98 (90%)	87 (99%)	1 (1%)	73	90
5	C	194/231 (84%)	194 (100%)	0	100	100
6	D	187/225 (83%)	184 (98%)	3 (2%)	62	85
7	d	55/62 (89%)	54 (98%)	1 (2%)	59	83
8	E	190/202 (94%)	190 (100%)	0	100	100
9	f	47/106 (44%)	46 (98%)	1 (2%)	53	80
10	G	158/170 (93%)	156 (99%)	2 (1%)	69	87
11	g	61/140 (44%)	60 (98%)	1 (2%)	62	85
12	H	207/218 (95%)	206 (100%)	1 (0%)	88	96
13	h	272/275 (99%)	271 (100%)	1 (0%)	91	97
14	I	165/174 (95%)	165 (100%)	0	100	100
15	J	178/180 (99%)	177 (99%)	1 (1%)	86	95
16	K	161/168 (96%)	161 (100%)	0	100	100
17	L	87/136 (64%)	86 (99%)	1 (1%)	73	90
18	N	99/108 (92%)	97 (98%)	2 (2%)	55	81
19	Q	115/130 (88%)	112 (97%)	3 (3%)	46	75
20	R	117/121 (97%)	115 (98%)	2 (2%)	60	84
21	S	119/121 (98%)	119 (100%)	0	100	100
22	T	125/132 (95%)	124 (99%)	1 (1%)	81	93
23	U	111/115 (96%)	110 (99%)	1 (1%)	78	92
24	V	92/107 (86%)	92 (100%)	0	100	100
25	W	67/67 (100%)	67 (100%)	0	100	100
26	Z	107/112 (96%)	107 (100%)	0	100	100
27	F	29/31 (94%)	29 (100%)	0	100	100
28	M	225/225 (100%)	224 (100%)	1 (0%)	91	97
29	O	142/142 (100%)	141 (99%)	1 (1%)	84	94
30	P	130/131 (99%)	130 (100%)	0	100	100
31	X	106/130 (82%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	Y	112/113 (99%)	112 (100%)	0	100 100
33	c	114/115 (99%)	114 (100%)	0	100 100
34	e	76/76 (100%)	76 (100%)	0	100 100
All	All	4182/4709 (89%)	4156 (99%)	26 (1%)	86 95

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	L	6	LYS
19	Q	13	ARG
28	M	254	LYS
18	N	63	LYS
19	Q	14	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
22	T	17	ASN
29	O	112	HIS
22	T	19	ASN
26	Z	106	GLN
30	P	5	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1685/1869 (90%)	354 (21%)	15 (0%)

5 of 354 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	C
1	A	17	C
1	A	25	A
1	A	33	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	627	U
1	A	1395	C
1	A	688	U
1	A	1646	C
1	A	874	G

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)

There are no chain breaks in this entry.

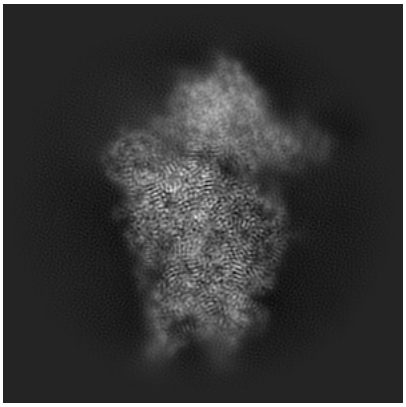
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22432. These allow visual inspection of the internal detail of the map and identification of artifacts.

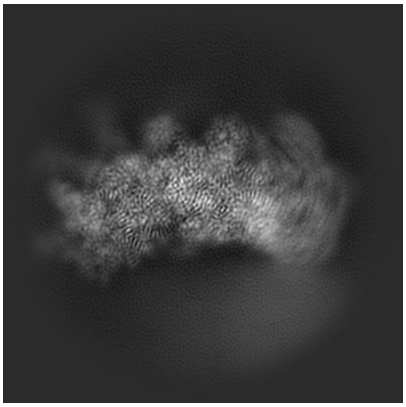
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

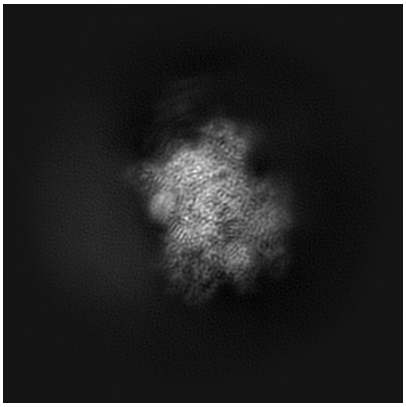
6.1.1 Primary map



X



Y

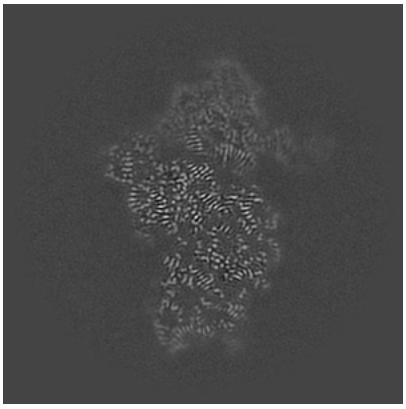


Z

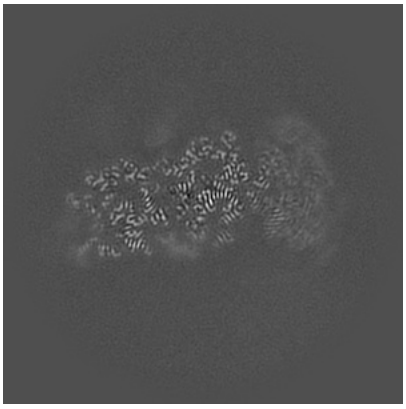
The images above show the map projected in three orthogonal directions.

6.2 Central slices

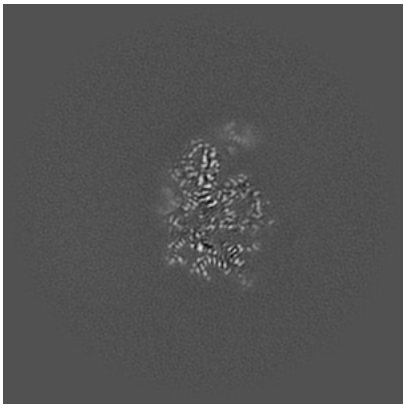
6.2.1 Primary map



X Index: 160



Y Index: 160

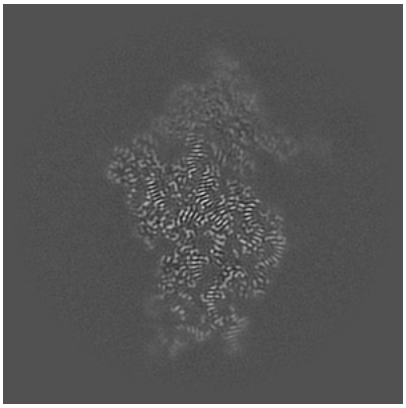


Z Index: 160

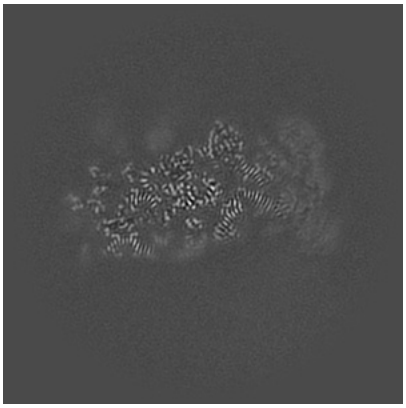
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

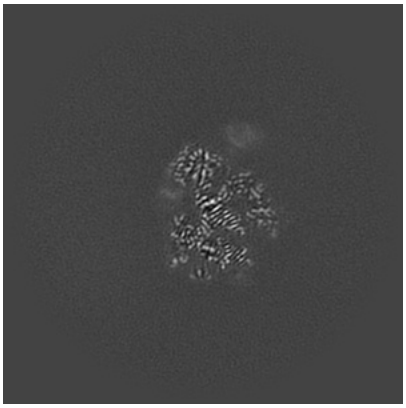
6.3.1 Primary map



X Index: 165



Y Index: 154

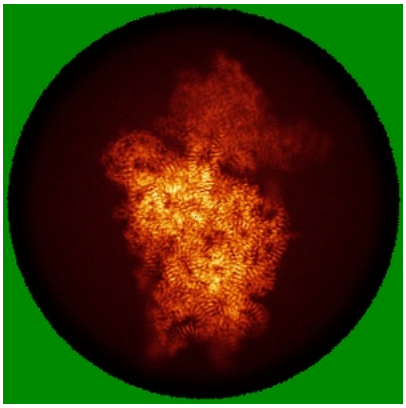


Z Index: 165

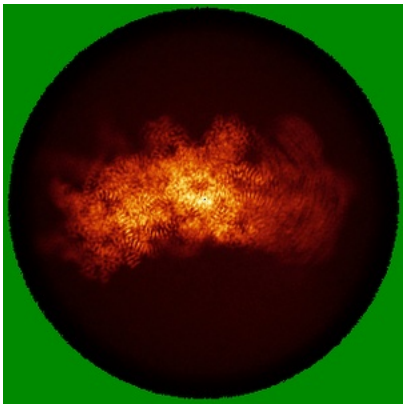
The images above show the largest variance slices of the map in three orthogonal directions.

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

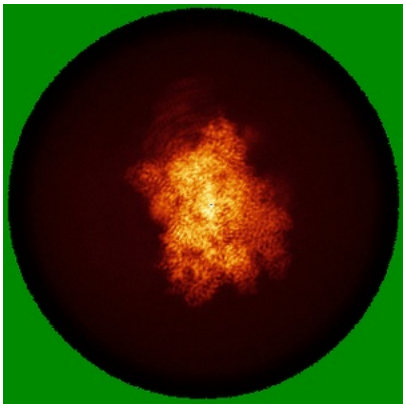
6.4.1 Primary map



X



Y



Z

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 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

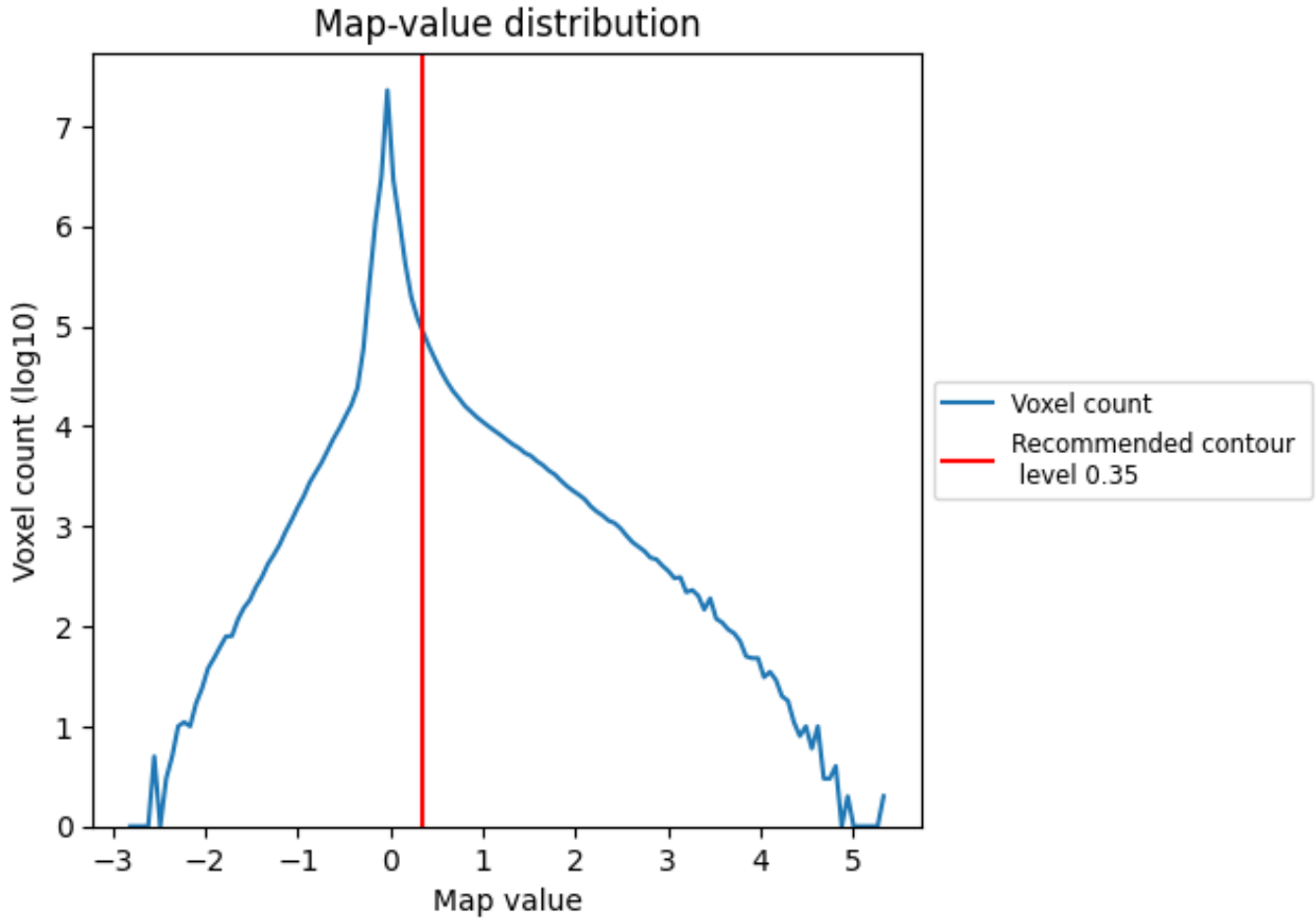
6.6 Mask visualisation (i)

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

7 Map analysis

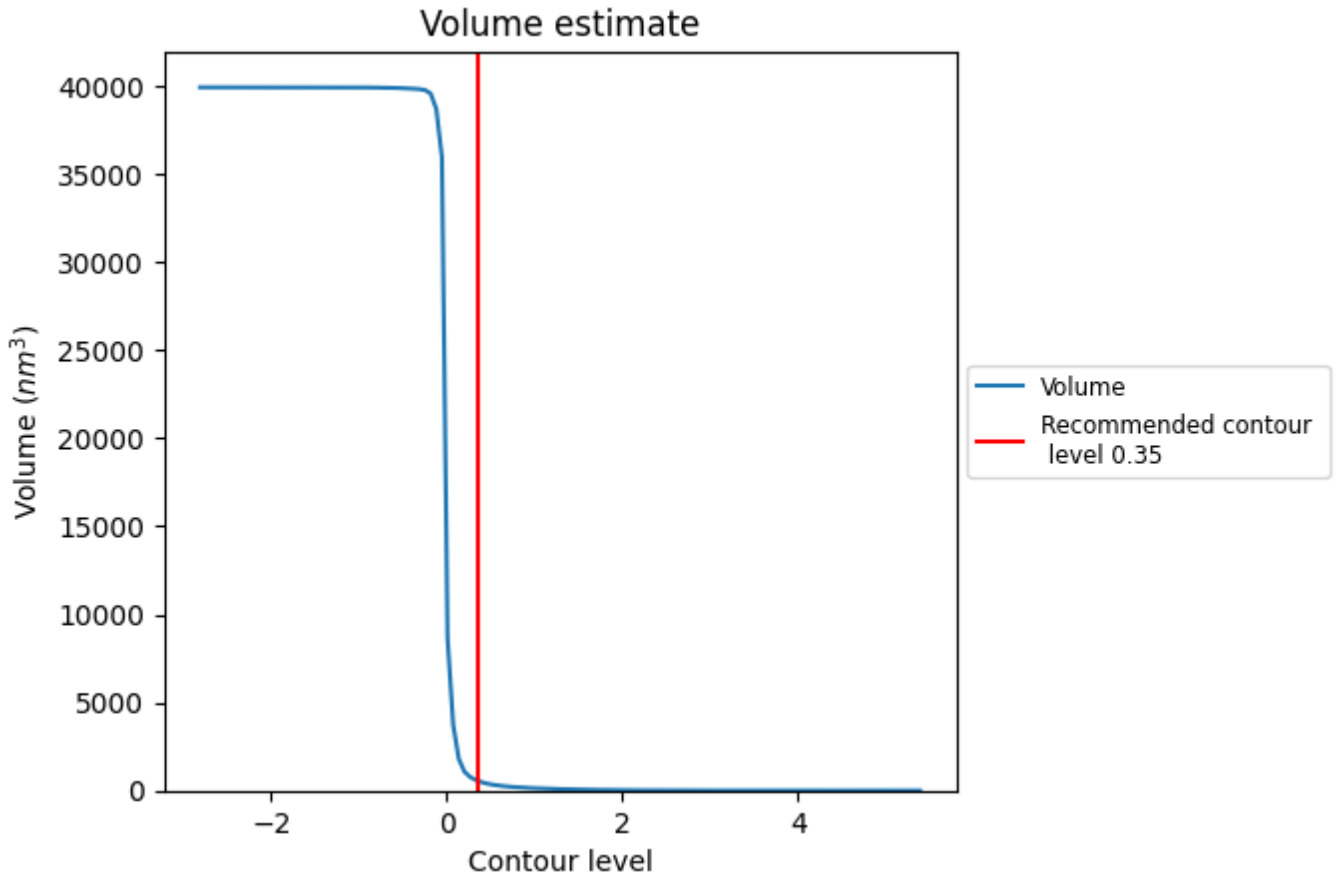
This section contains the results of statistical analysis of the map.

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.

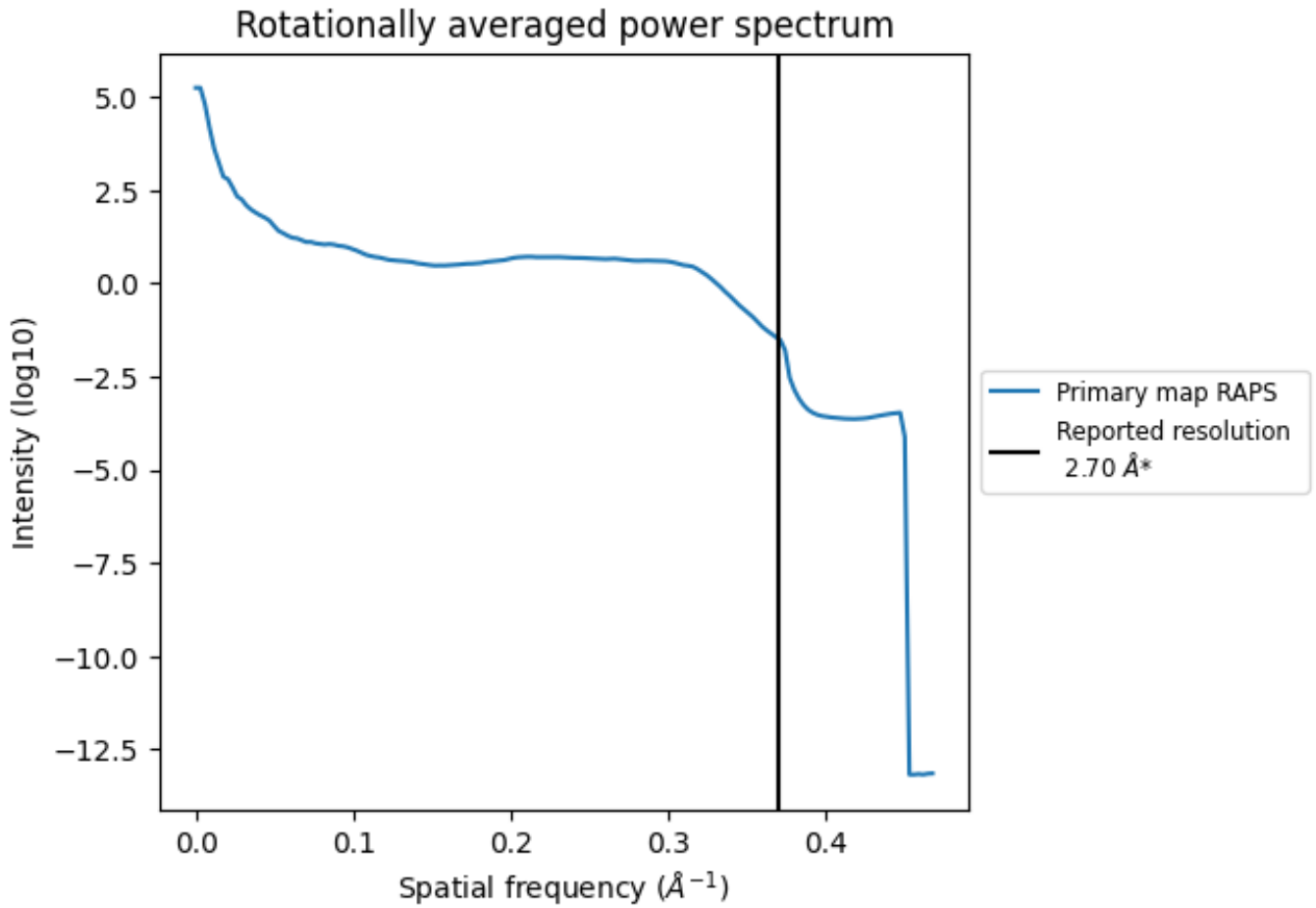
7.2 Volume estimate (i)



The volume at the recommended contour level is 567 nm^3; this corresponds to an approximate mass of 512 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 0.370 $Å^{-1}$

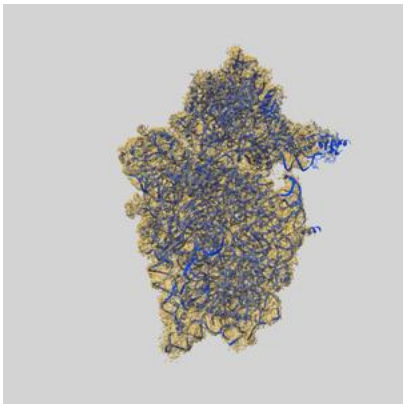
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

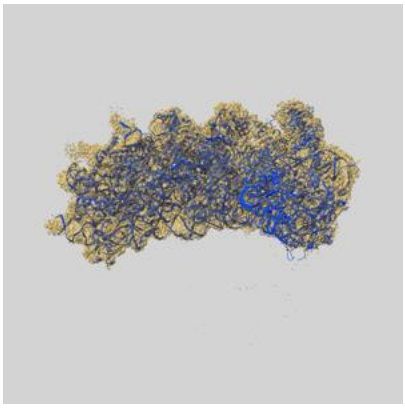
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22432 and PDB model 7JQB. Per-residue inclusion information can be found in section 3 on page 11.

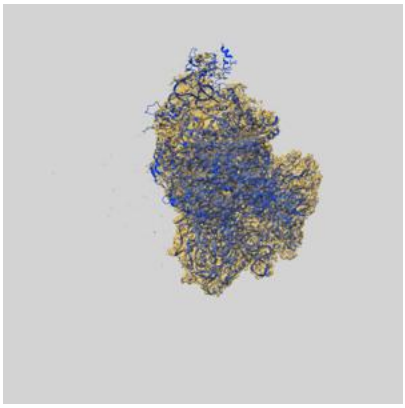
9.1 Map-model overlay



X



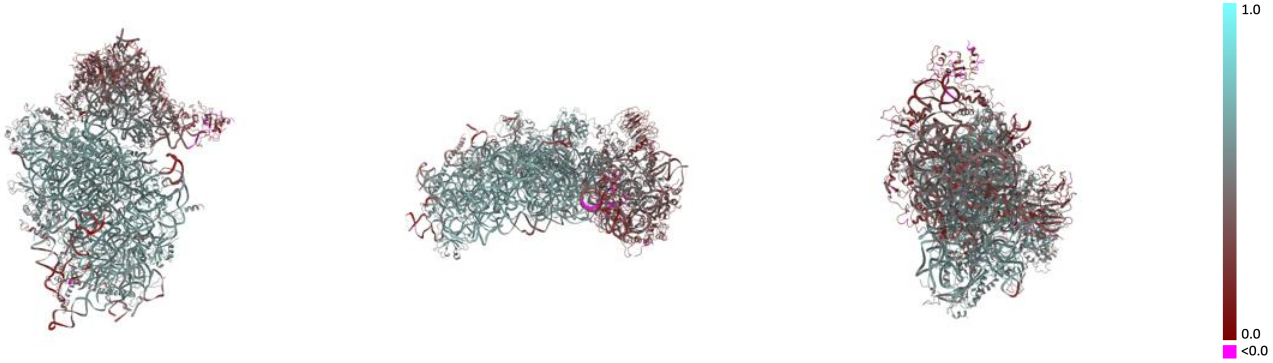
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

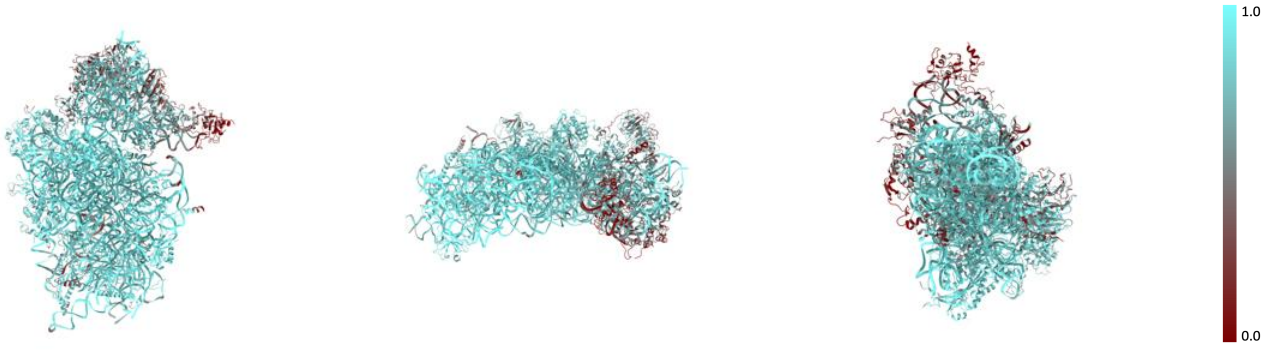
9.2 Q-score mapped to coordinate model



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.

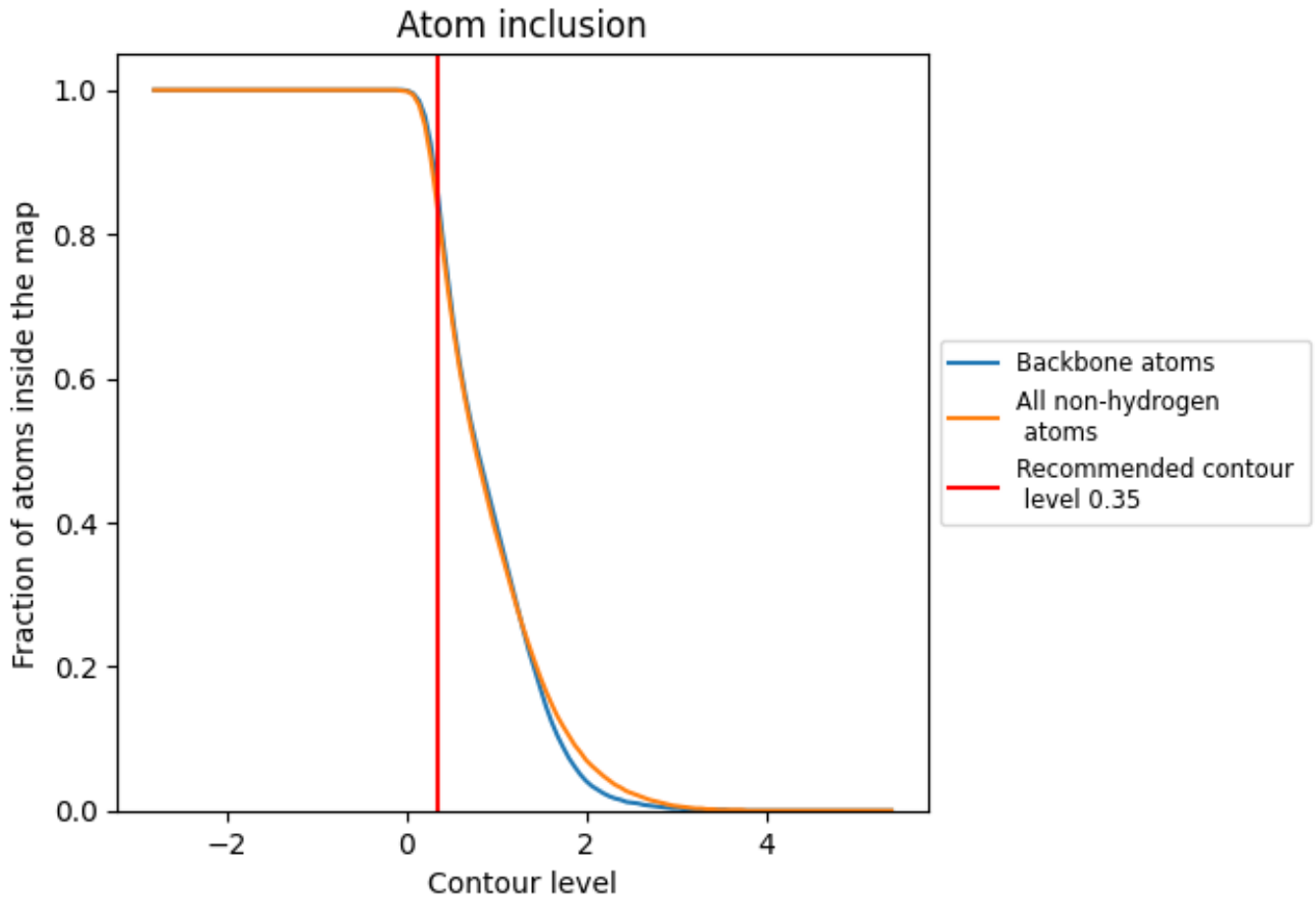
9.3 Atom inclusion mapped to coordinate model



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.4980
A	0.9220	0.5290
B	0.9140	0.5770
C	0.9110	0.5630
D	0.9200	0.5920
E	0.6710	0.4240
F	0.8320	0.5460
G	0.5910	0.3590
H	0.8750	0.5270
I	0.8250	0.5130
J	0.8890	0.5500
K	0.9040	0.5820
L	0.6110	0.3500
M	0.9050	0.5650
N	0.0430	0.1560
O	0.7970	0.5210
P	0.8980	0.5590
Q	0.3630	0.2950
R	0.6890	0.3670
S	0.7600	0.4560
T	0.4040	0.3280
U	0.6510	0.3590
V	0.4780	0.3560
W	0.9240	0.5800
X	0.8580	0.5090
Y	0.9470	0.6010
Z	0.9310	0.5800
a	0.3670	0.2860
b	0.8960	0.5660
c	0.9180	0.5810
d	0.6090	0.3920
e	0.8500	0.5320
f	0.8160	0.5310
g	0.1020	0.1760
h	0.5390	0.2980