



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:15 am GMT

PDB ID : 5GAD
EMDB ID : EMD-8000
Title : RNC-SRP-SR complex early state
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on : 2015-11-24
Resolution : 3.70 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 ⓘ symbol.

The types of validation reports are described at

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

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

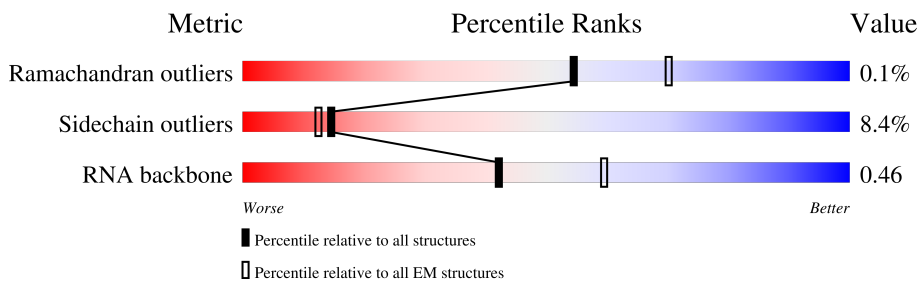
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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.



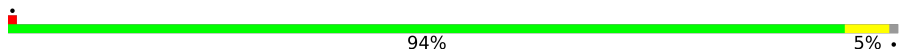
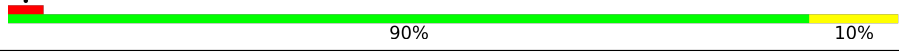

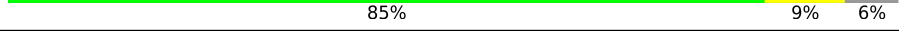
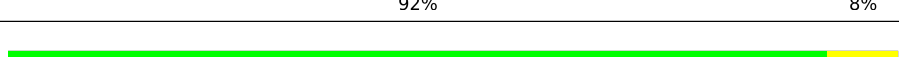
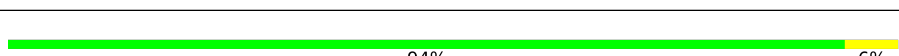
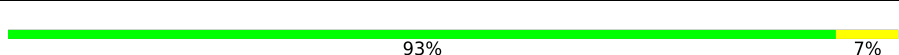
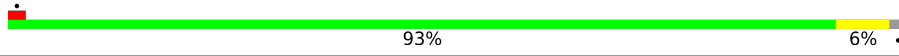
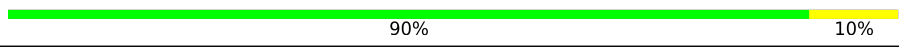
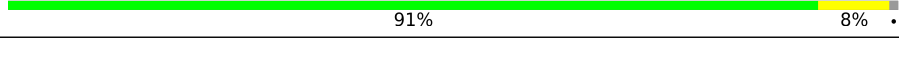
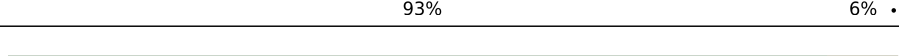
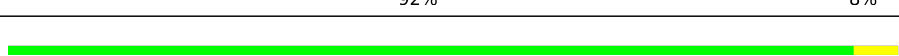

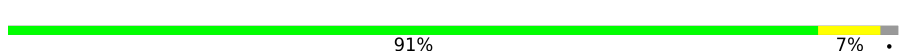
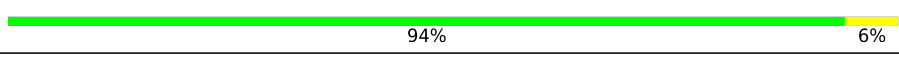

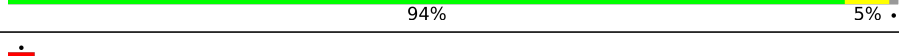

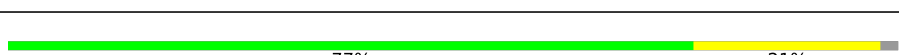
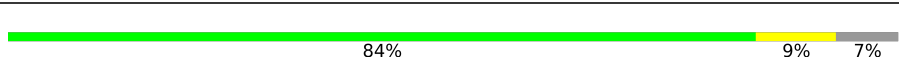

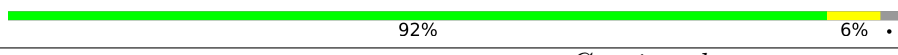



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	113	
2	2	3	
3	A	2903	
4	B	120	
5	C	273	
6	D	209	
7	E	201	
8	F	179	

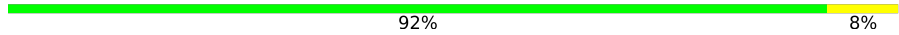
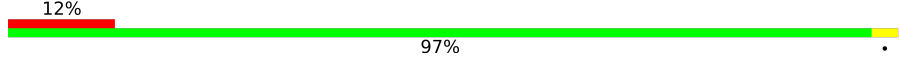

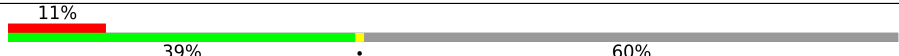
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Mol	Chain	Length	Quality of chain
9	G	177	 94% 5%
10	H	149	 90% 10%
11	I	165	 71% 5% 24%
12	J	142	 85% 9% 6%
13	K	142	 92% 8%
14	L	123	 92% 8%
15	M	144	 94% 6%
16	N	136	 93% 7%
17	O	127	 93% 6%
18	P	117	 90% 10%
19	Q	115	 91% 8%
20	R	118	 93% 6%
21	S	103	 92% 8%
22	T	110	 95% 5%
23	U	100	 87% 7% 5%
24	V	104	 91% 7%
25	W	94	 94% 6%
26	X	85	 82% 7% 11%
27	Y	78	 94% 5%
28	Z	63	 89% 10%
29	a	59	 95%
30	b	57	 77% 21%
31	c	55	 84% 9% 7%
32	d	46	 87% 13%
33	e	65	 92% 6%

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Mol	Chain	Length	Quality of chain
34	f	38	 92% 8%
35	i	450	 12% 97%
36	k	18	 11% 89% 11%
37	l	497	 11% 39% 60%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98006 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 ESRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	43	926	413	174	296	43	0	0

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	3	62	28	11	20	3	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2883	61902	27613	11397	20009	2883	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	B	120	2569	1144	468	837	120	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	271	2082	1288	423	364	7	0	0

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	209	1565	979	288	294	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	201	1552	974	283	290	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	177	1410	899	249	256	6	0	0

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	176	1323	832	243	246	2	0	0

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	149	1110	699	197	213	1	0	0

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	125	946	599	169	175	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J	134	979	619	169	185	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	K	142	1129	714	212	199	4	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	123	946	593	181	166	6	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M	144	1053	654	207	190	2	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N	136	1074	686	205	177	6	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	125	993	613	202	173	5	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	P	117	900	557	179	163	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Q	114	917	574	179	163	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	77	625	388	129	106	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Z	62	501	308	98	94	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	58	449	281	87	79	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	56	444	269	94	80	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	c	51	414	266	76	72	0	0

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	46	377	228	90	57	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	64	504	323	105	74	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	450	Total	C	N	O	S	0	0
			3337	2109	600	610	18		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	198	Total	C	N	O	S	0	0
			1492	944	266	277	5		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	1	Total	Mg	0
			1	1	
38	A	412	Total	Mg	0
			412	412	
38	B	11	Total	Mg	0
			11	11	
38	C	2	Total	Mg	0
			2	2	
38	D	1	Total	Mg	0
			1	1	
38	E	1	Total	Mg	0
			1	1	
38	P	1	Total	Mg	0
			1	1	
38	R	1	Total	Mg	0
			1	1	
38	b	1	Total	Mg	0
			1	1	

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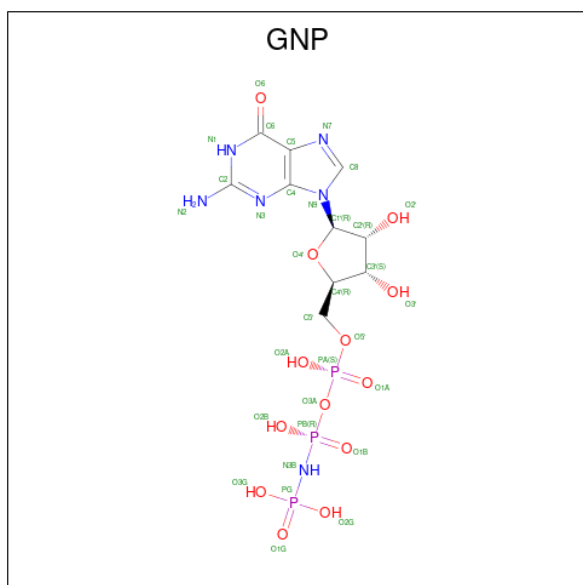
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Mol	Chain	Residues	Atoms		AltConf
38	i	1	Total	Mg	0
			1	1	
38	l	1	Total	Mg	0
			1	1	

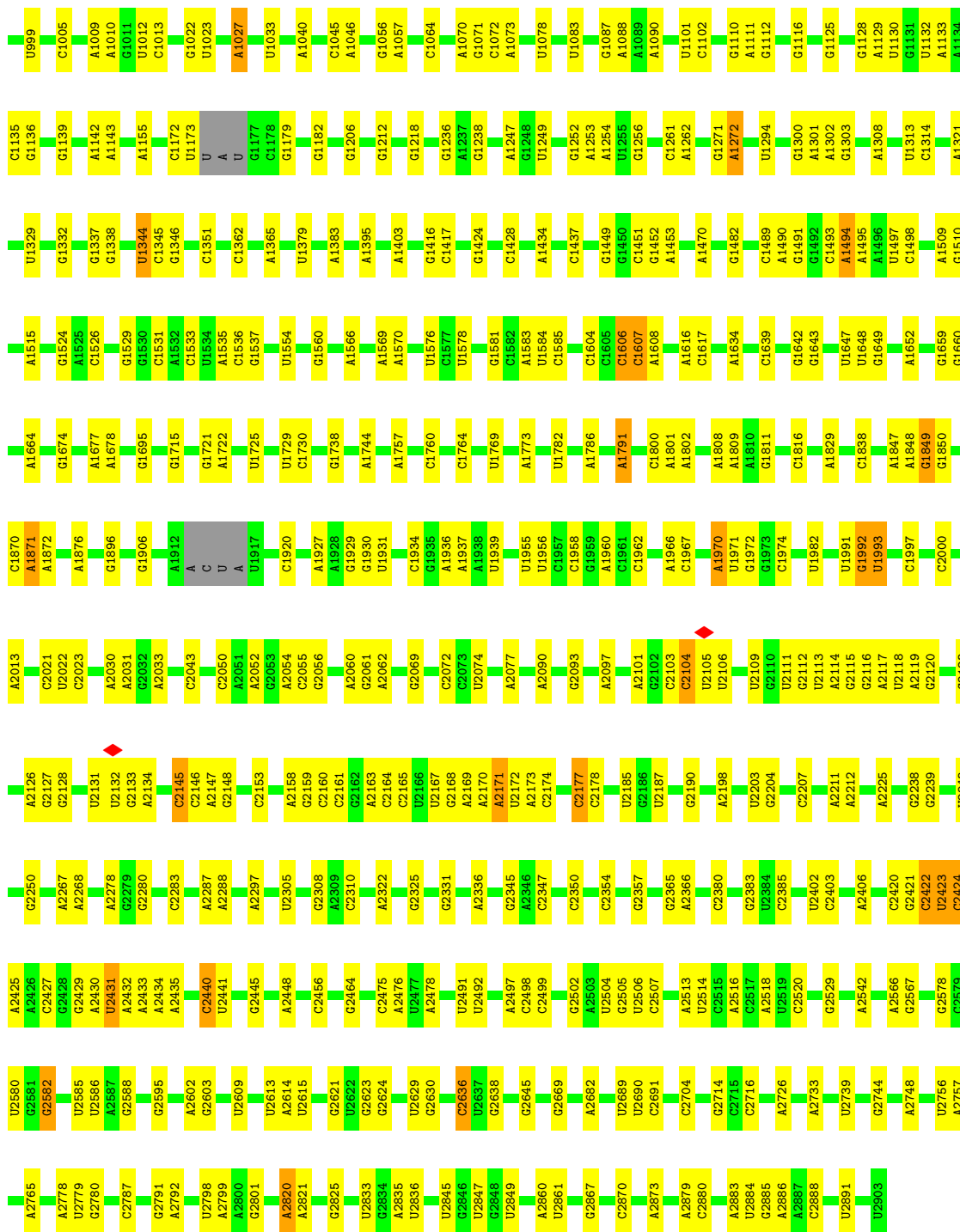
- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

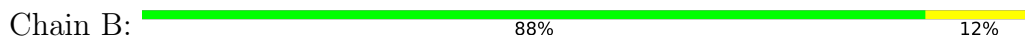
- Molecule 40 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).




Mol	Chain	Residues	Atoms					AltConf
40	i	1	Total	C	N	O	P	0
			32	10	6	13	3	
40	l	1	Total	C	N	O	P	0
			32	10	6	13	3	



• Molecule 4: 5S rRNA



• Molecule 5: 50S ribosomal protein L2

Chain C:  90% 9%



- Molecule 6: 50S ribosomal protein L3

Chain D:  95% 5%




- Molecule 7: 50S ribosomal protein L4

Chain E:  93% 7%



- Molecule 8: 50S ribosomal protein L5

Chain F:  89% 10%

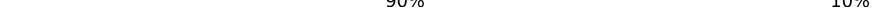


- Molecule 9: 50S ribosomal protein L6

Chain G:  94% 5%



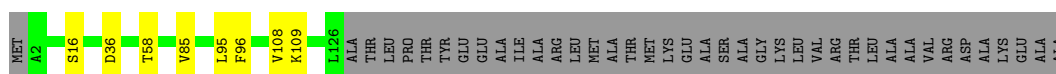
- Molecule 10: 50S ribosomal protein L9

Chain H:  90% 10%




- Molecule 11: 50S ribosomal protein L10

Chain I:  71% 5% 24%



- Molecule 12: 50S ribosomal protein L11

Chain J:  85% 9% 6%



- Molecule 13: 50S ribosomal protein L13

Chain K:  92% 8%



- Molecule 14: 50S ribosomal protein L14

Chain L:  92% 8%



- Molecule 15: 50S ribosomal protein L15

Chain M:  94% 6%



- Molecule 16: 50S ribosomal protein L16

Chain N:  93% 7%




- Molecule 17: 50S ribosomal protein L17

Chain O:  93% 6%




- Molecule 18: 50S ribosomal protein L18

Chain P:  90% 10%



- Molecule 19: 50S ribosomal protein L19

Chain Q:  91% 8%




- Molecule 20: 50S ribosomal protein L20

Chain R:  93% 6%



- Molecule 21: 50S ribosomal protein L21

Chain S:  92% 8%




- Molecule 22: 50S ribosomal protein L22

Chain T:  95% 5%




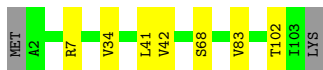
- Molecule 23: 50S ribosomal protein L23

Chain U:  87% 7% 5%



- Molecule 24: 50S ribosomal protein L24

Chain V:  91% 7%

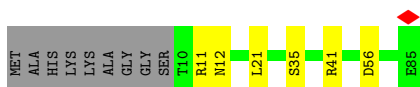
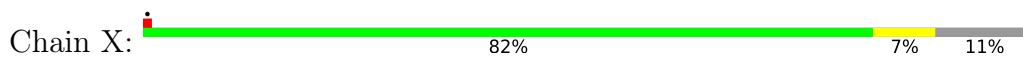


- Molecule 25: 50S ribosomal protein L25

Chain W:  94% 6%



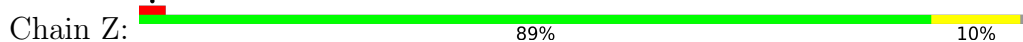
- Molecule 26: 50S ribosomal protein L27



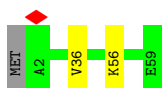
- Molecule 27: 50S ribosomal protein L28



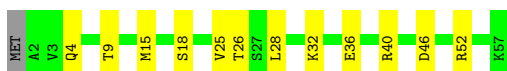
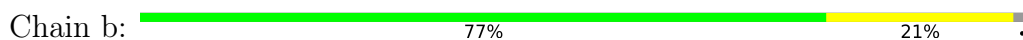
- Molecule 28: 50S ribosomal protein L29



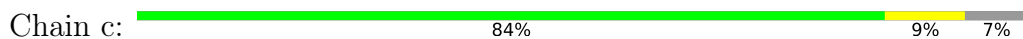
- Molecule 29: 50S ribosomal protein L30



- Molecule 30: 50S ribosomal protein L32



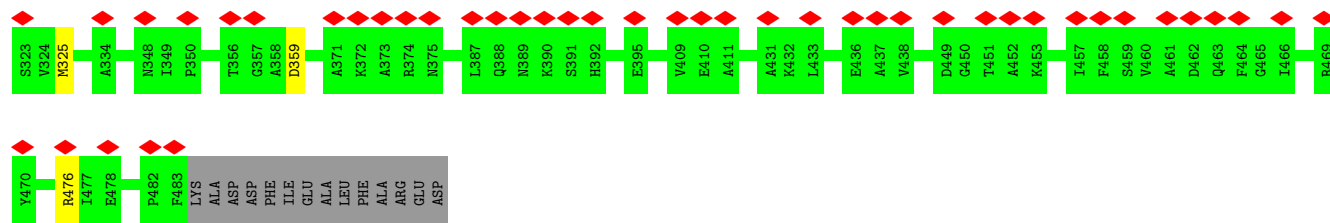
- Molecule 31: 50S ribosomal protein L33



- Molecule 32: 50S ribosomal protein L34



- Molecule 33: 50S ribosomal protein L35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	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	0.234	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	443.2, 443.2, 443.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.385, 1.385, 1.385	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GNP

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	1	0.30	0/1037	0.99	2/1616 (0.1%)
2	2	0.56	0/68	1.26	1/103 (1.0%)
3	A	0.68	13/69329 (0.0%)	1.17	188/108152 (0.2%)
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.48	0/2121	0.65	0/2852
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1434	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.59	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.64	3/763 (0.4%)	0.73	1/1021 (0.1%)
24	V	0.38	0/787	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.33	0/500	0.47	0/661
29	a	0.38	0/453	0.56	0/605
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.31	0/2942	0.51	0/3950
36	k	0.32	0/137	0.58	0/186
37	l	0.37	0/1511	1.08	3/2040 (0.1%)
All	All	0.61	16/105341 (0.0%)	1.04	199/157282 (0.1%)

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
5	C	0	1
9	G	0	1
12	J	0	1
35	i	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.88	1.33	1.37
23	U	89	GLU	N-CA	6.84	1.60	1.46
3	A	1254	A	N9-C4	-6.35	1.34	1.37
3	A	2114	A	N9-C4	6.24	1.41	1.37
3	A	1321	A	N9-C4	6.01	1.41	1.37

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	l	476	ARG	NE-CZ-NH2	-25.15	107.72	120.30
37	l	476	ARG	NE-CZ-NH1	-25.05	107.78	120.30
37	l	476	ARG	NH1-CZ-NH2	22.82	144.50	119.40
3	A	2423	U	C6-N1-C2	-12.22	113.67	121.00
3	A	1838	C	C6-N1-C2	9.47	124.09	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	i	240	LEU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
9	G	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	22	59
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	19	56
12	J	132/142 (93%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	U	93/100 (93%)	89 (96%)	3 (3%)	1 (1%)	14	50
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	56/63 (89%)	54 (96%)	2 (4%)	0	100	100
29	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
30	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	i	378/450 (84%)	361 (96%)	17 (4%)	0	100	100
36	k	16/18 (89%)	11 (69%)	5 (31%)	0	100	100
37	l	196/497 (39%)	189 (96%)	7 (4%)	0	100	100
All	All	4018/4539 (88%)	3876 (96%)	139 (4%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

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	
5	C	216/218 (99%)	192 (89%)	24 (11%)	6	28
6	D	164/164 (100%)	154 (94%)	10 (6%)	18	50
7	E	165/165 (100%)	152 (92%)	13 (8%)	12	42
8	F	148/150 (99%)	130 (88%)	18 (12%)	5	24
9	G	137/138 (99%)	129 (94%)	8 (6%)	20	52
10	H	114/114 (100%)	100 (88%)	14 (12%)	4	24
11	I	95/123 (77%)	89 (94%)	6 (6%)	18	49
12	J	104/110 (94%)	93 (89%)	11 (11%)	6	30
13	K	116/116 (100%)	105 (90%)	11 (10%)	8	34
14	L	104/104 (100%)	94 (90%)	10 (10%)	8	34
15	M	103/103 (100%)	94 (91%)	9 (9%)	10	38
16	N	109/109 (100%)	100 (92%)	9 (8%)	11	40
17	O	102/103 (99%)	95 (93%)	7 (7%)	15	46
18	P	87/87 (100%)	75 (86%)	12 (14%)	3	21
19	Q	99/100 (99%)	90 (91%)	9 (9%)	9	36
20	R	89/90 (99%)	82 (92%)	7 (8%)	12	42
21	S	84/84 (100%)	76 (90%)	8 (10%)	8	34
22	T	93/93 (100%)	88 (95%)	5 (5%)	22	54
23	U	82/84 (98%)	76 (93%)	6 (7%)	14	44
24	V	83/85 (98%)	76 (92%)	7 (8%)	11	40
25	W	78/78 (100%)	72 (92%)	6 (8%)	13	43
26	X	57/63 (90%)	51 (90%)	6 (10%)	7	30
27	Y	67/68 (98%)	63 (94%)	4 (6%)	19	50
28	Z	54/55 (98%)	48 (89%)	6 (11%)	6	28
29	a	48/49 (98%)	46 (96%)	2 (4%)	30	59
30	b	47/48 (98%)	35 (74%)	12 (26%)	0	4
31	c	45/49 (92%)	40 (89%)	5 (11%)	6	28
32	d	38/38 (100%)	32 (84%)	6 (16%)	2	16
33	e	51/52 (98%)	47 (92%)	4 (8%)	12	42
34	f	34/34 (100%)	31 (91%)	3 (9%)	10	38
35	i	311/313 (99%)	298 (96%)	13 (4%)	30	59
36	k	17/17 (100%)	15 (88%)	2 (12%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	l	156/405 (38%)	153 (98%)	3 (2%)	57 76
All	All	3297/3609 (91%)	3021 (92%)	276 (8%)	14 40

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	b	18	SER
30	b	46	ASP
35	i	19	ARG
12	J	55	ILE
12	J	21	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
23	U	59	ASN
32	d	29	GLN
24	V	53	ASN
28	Z	39	GLN
35	i	72	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	18 (42%)	1 (2%)
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	521 (18%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3139 (96%)	553 (18%)	20 (0%)

5 of 553 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	34	U
1	1	37	U
1	1	39	A
1	1	41	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	2158	A
3	A	2430	A
3	A	2756	U
3	A	2602	A
3	A	827	U

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](#)

Of 436 ligands modelled in this entry, 434 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	GNP	i	1400	38	29,34,34	2.06	8 (27%)	33,54,54	2.50	14 (42%)
40	GNP	l	1400	38	29,34,34	1.86	9 (31%)	33,54,54	2.33	10 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	GNP	i	1400	38	-	3/14/38/38	0/3/3/3
40	GNP	l	1400	38	-	3/14/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	i	1400	GNP	C4-N3	6.00	1.45	1.35
40	l	1400	GNP	C4-N3	5.32	1.44	1.35
40	i	1400	GNP	O4'-C1'	3.59	1.46	1.41
40	l	1400	GNP	C5-C6	3.35	1.47	1.41
40	l	1400	GNP	PB-O1B	3.21	1.51	1.46

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	i	1400	GNP	C4-C5-C6	-6.59	114.51	120.80
40	l	1400	GNP	C4-C5-C6	-6.17	114.91	120.80
40	i	1400	GNP	C2-N1-C6	5.12	124.06	115.93
40	l	1400	GNP	C2-N1-C6	4.88	123.69	115.93
40	i	1400	GNP	N3-C2-N1	-4.41	121.34	127.22

There are no chirality outliers.

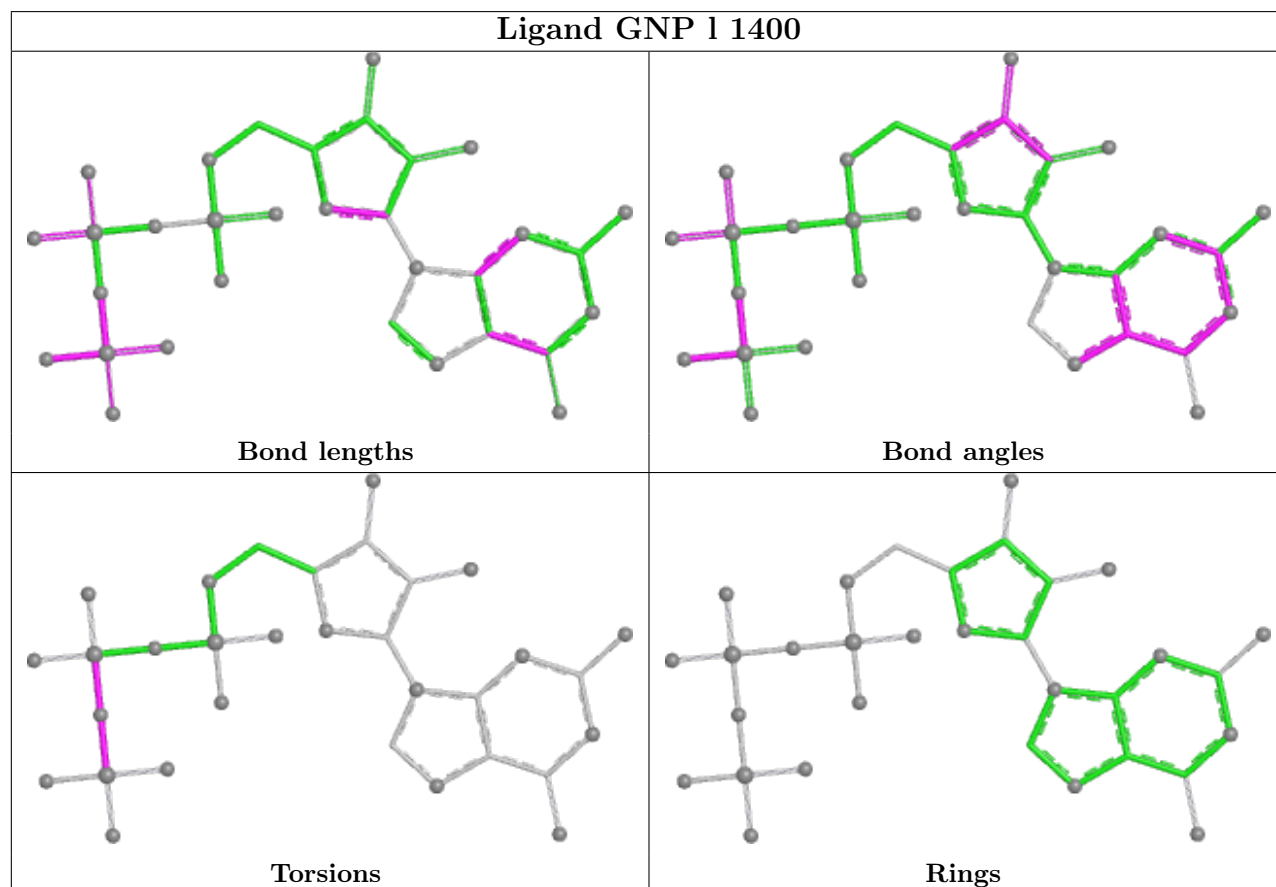
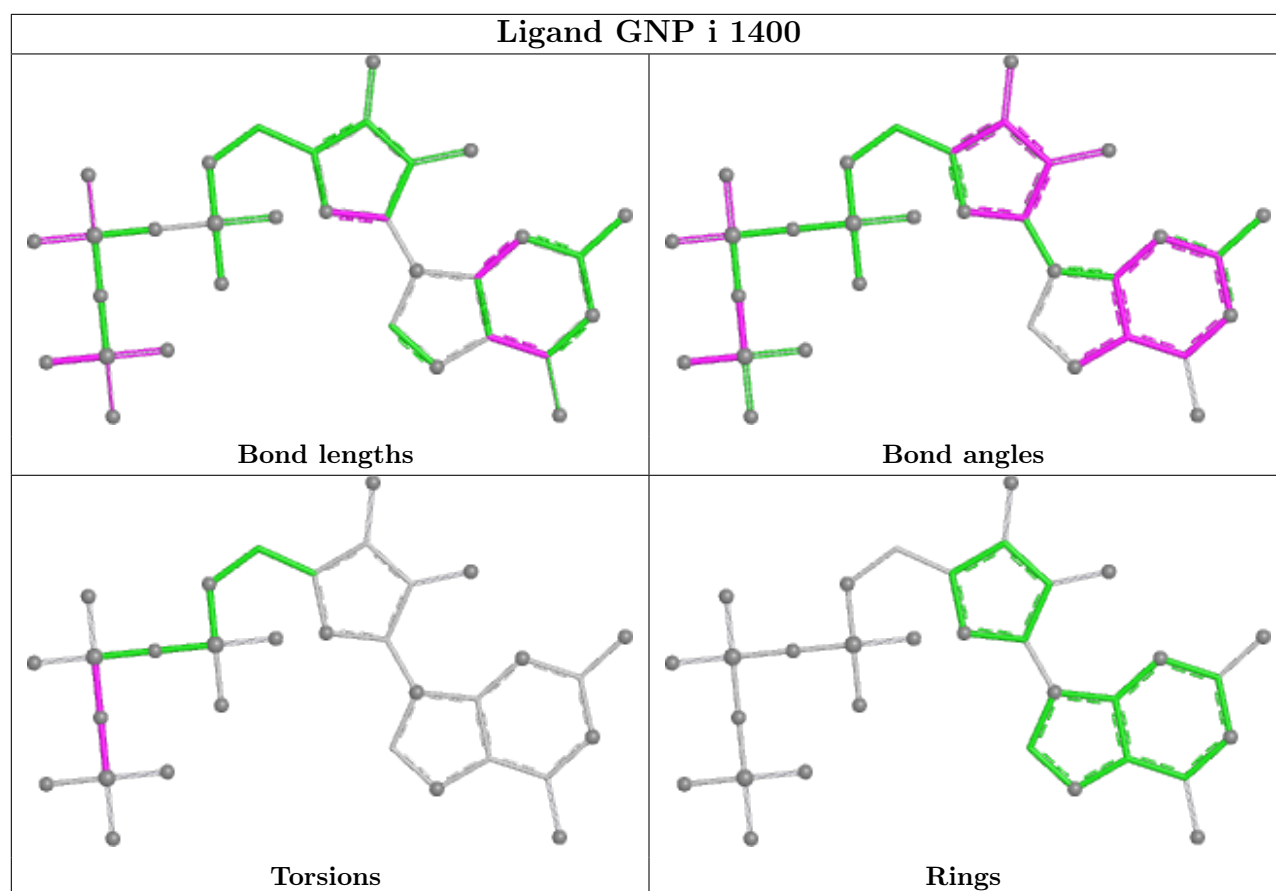
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	i	1400	GNP	PB-N3B-PG-O1G
40	i	1400	GNP	PG-N3B-PB-O1B
40	i	1400	GNP	PG-N3B-PB-O3A
40	l	1400	GNP	PB-N3B-PG-O1G
40	l	1400	GNP	PG-N3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	Z	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	15:ASN	C	16:THR	N	3.07
1	Z	40:SER	C	41:HIS	N	2.90

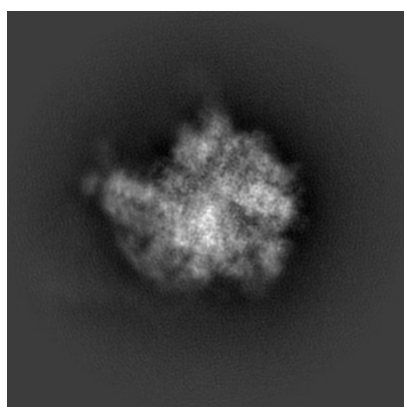
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8000. These allow visual inspection of the internal detail of the map and identification of artifacts.

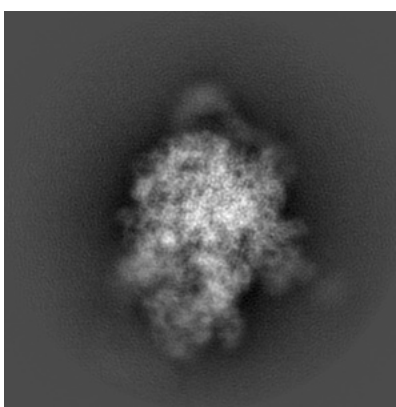
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

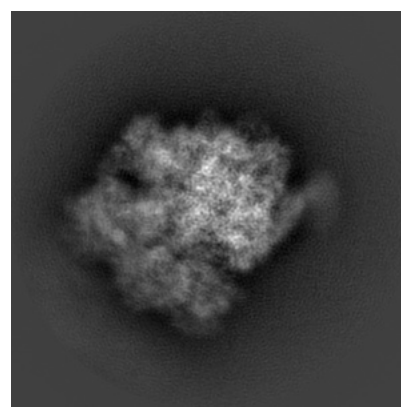
6.1.1 Primary map



X



Y

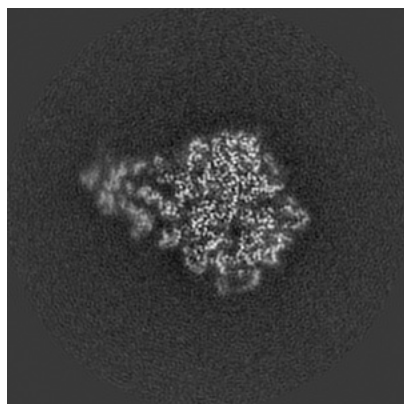


Z

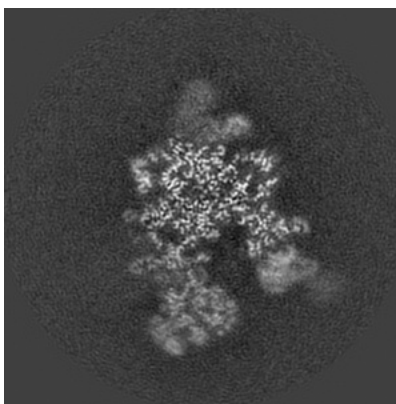
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

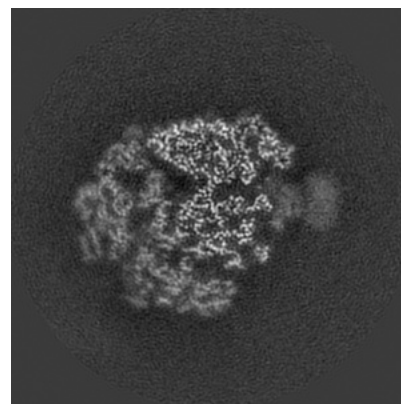
6.2.1 Primary map



X Index: 160



Y Index: 160

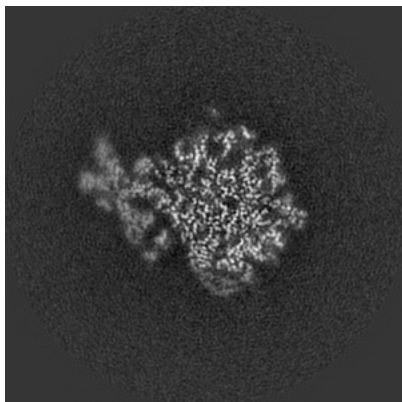


Z Index: 160

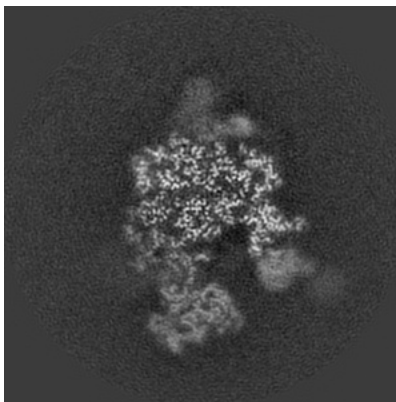
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

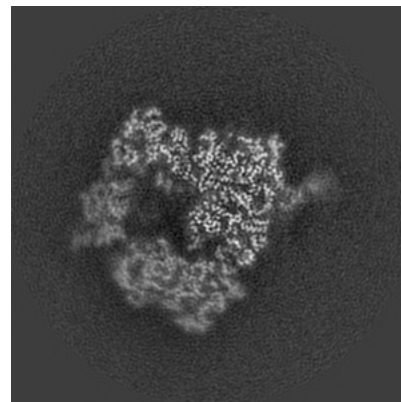
6.3.1 Primary map



X Index: 154



Y Index: 157

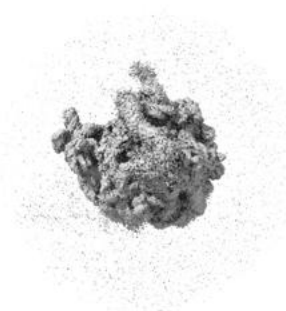


Z Index: 175

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

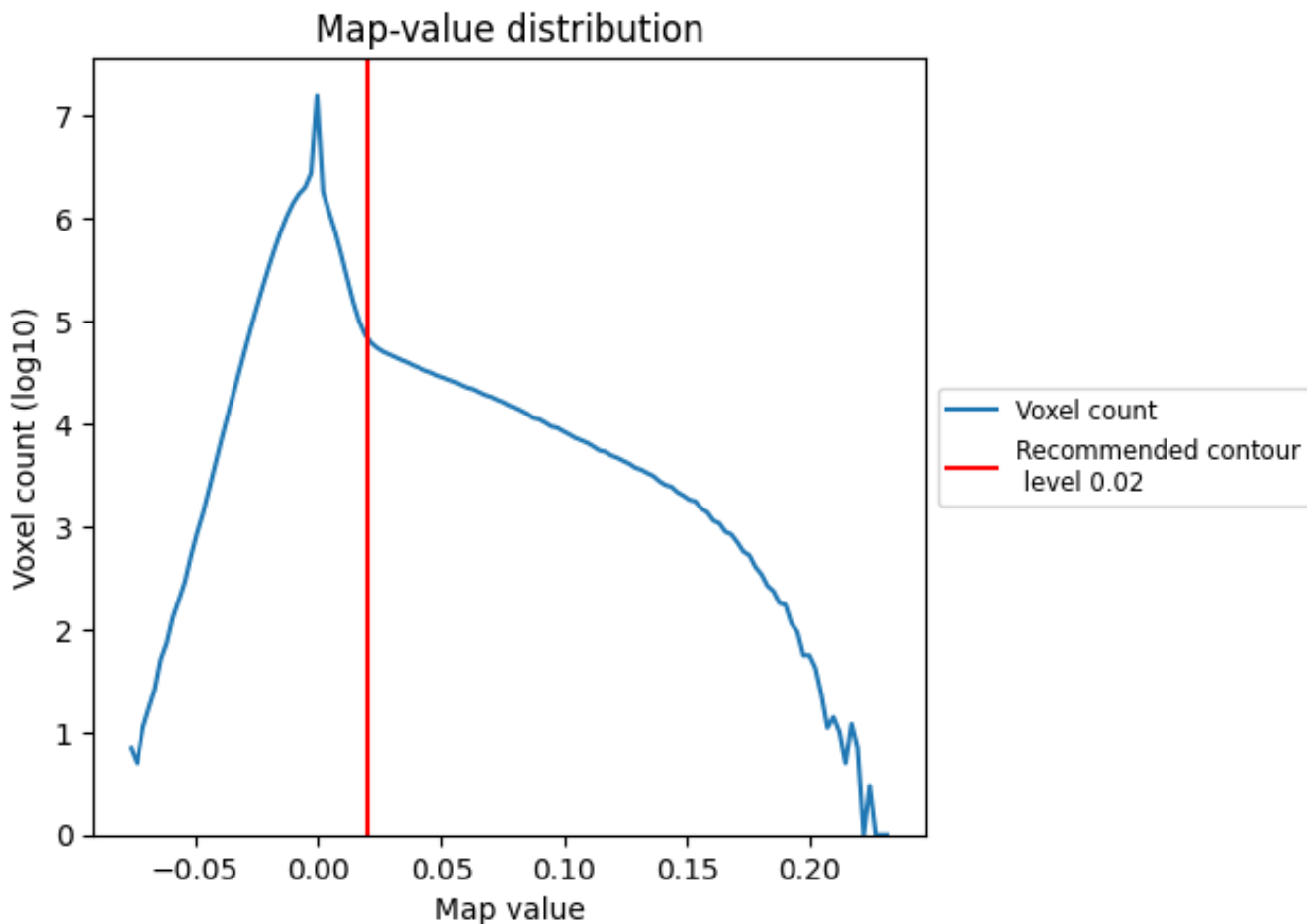
6.5 Mask visualisation

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

7 Map analysis [i](#)

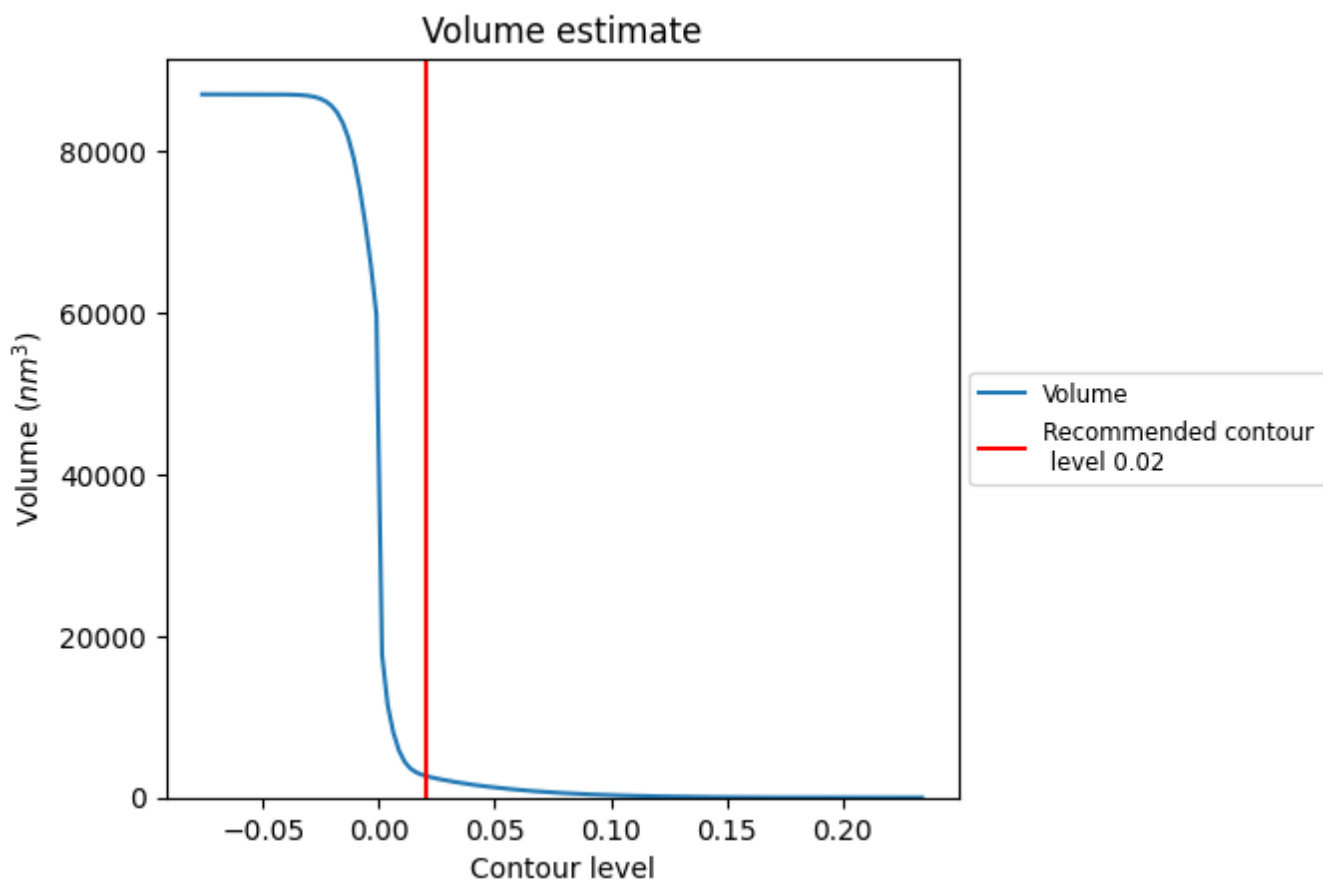
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

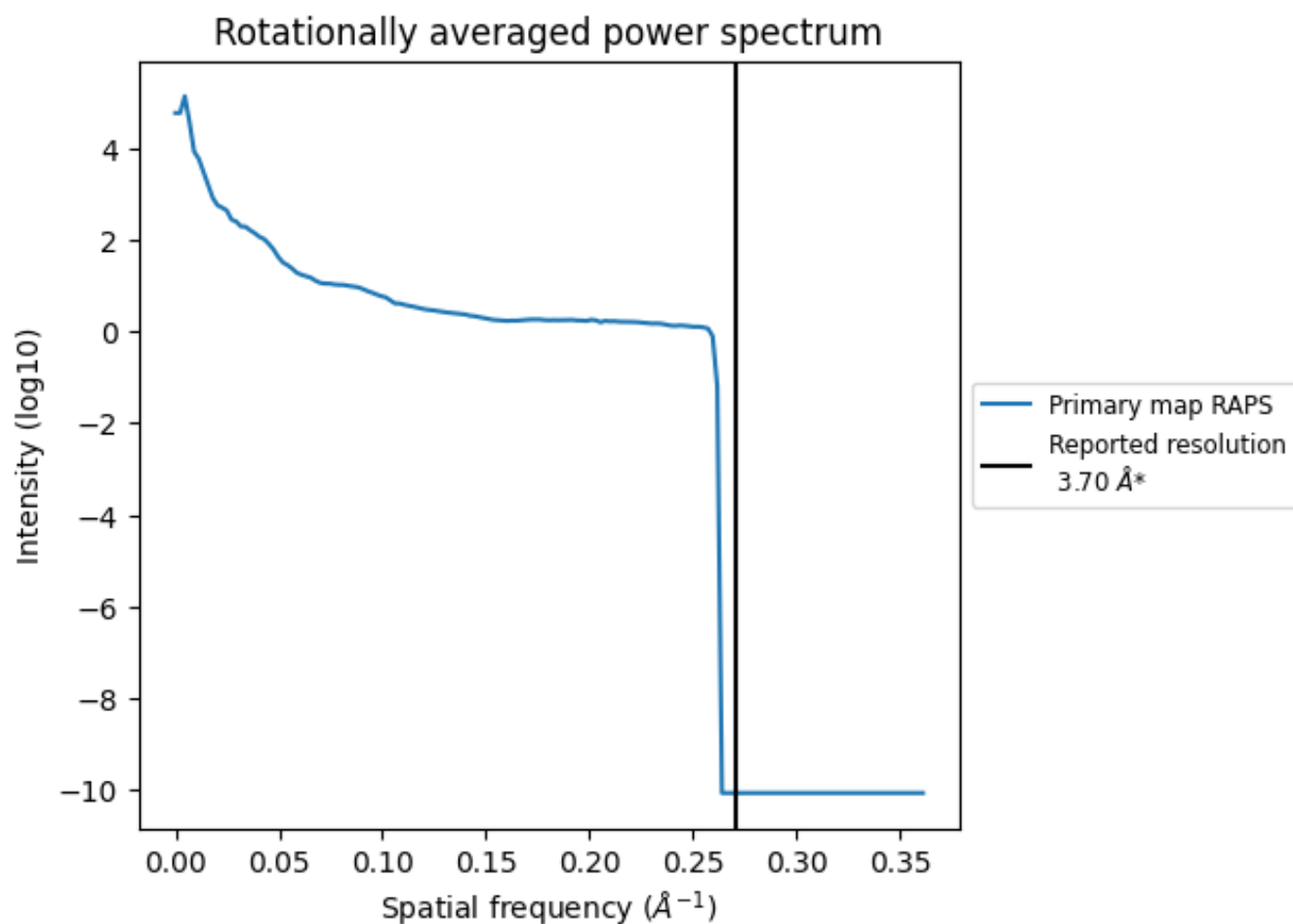
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2699 nm^3 ; this corresponds to an approximate mass of 2438 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 0.270 Å⁻¹

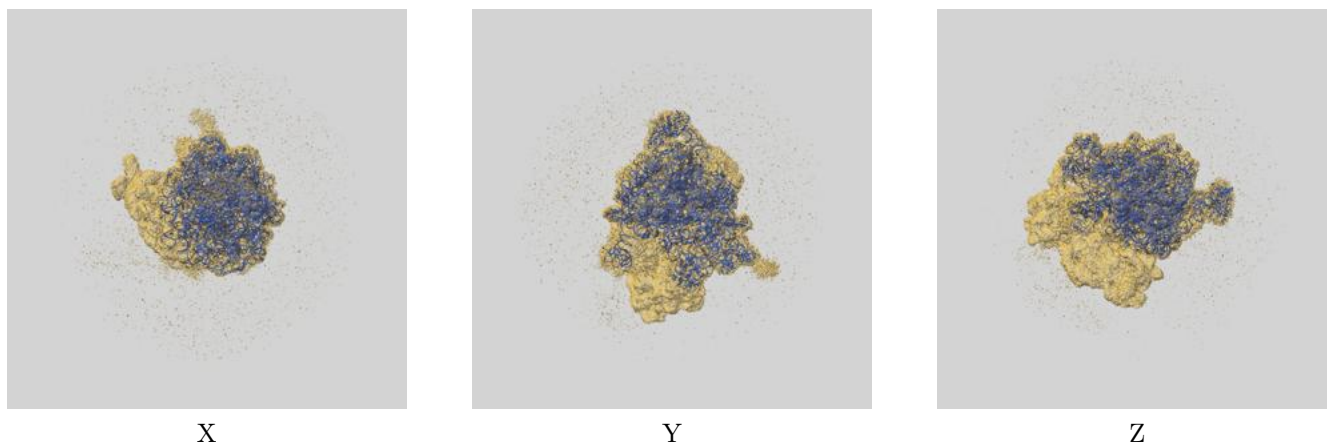
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

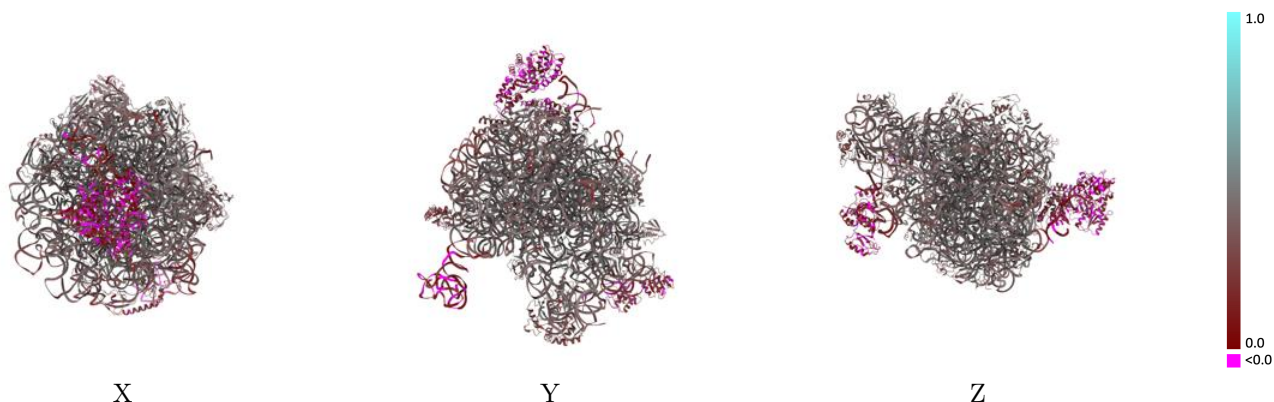
This section contains information regarding the fit between EMDB map EMD-8000 and PDB model 5GAD. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



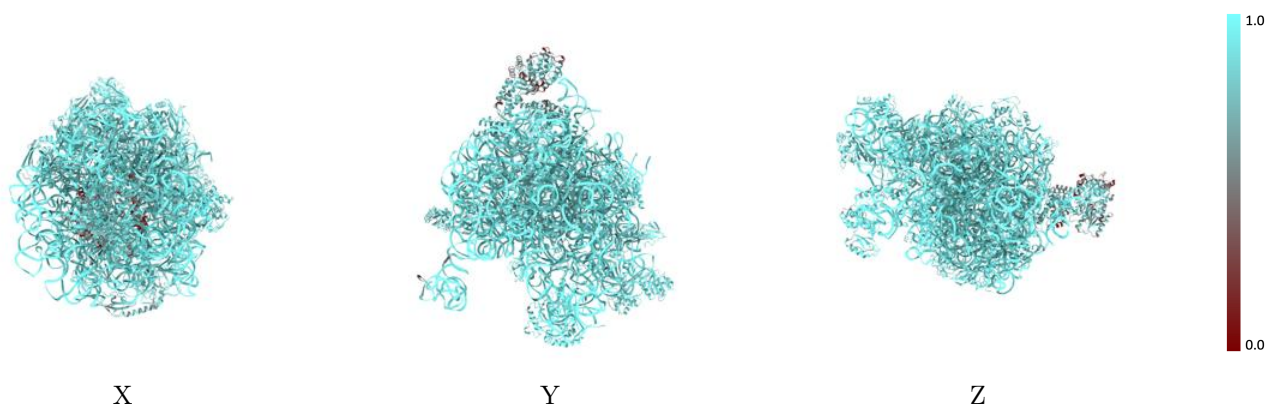
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



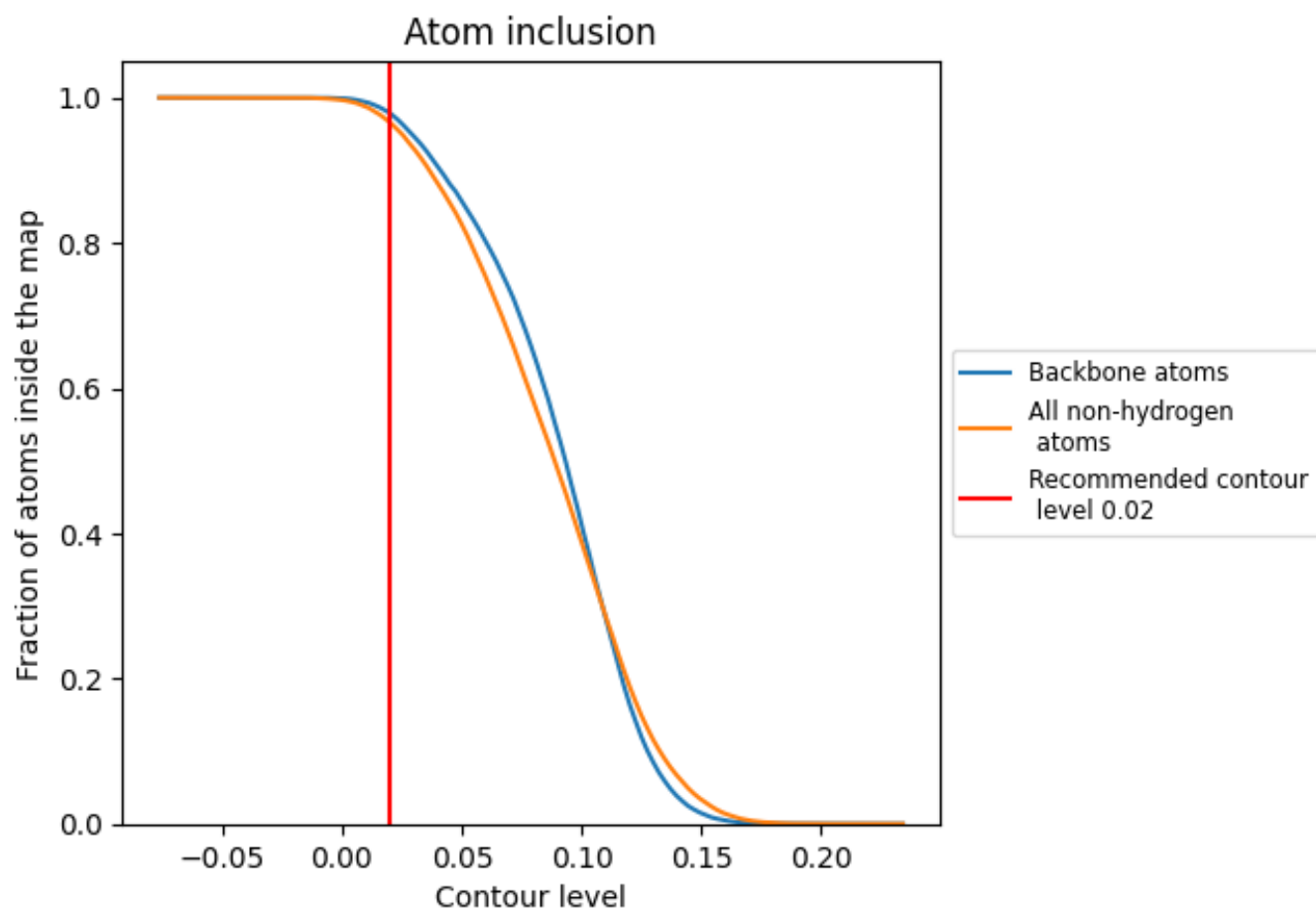
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9659	 0.3710
1	 0.9892	 0.1330
2	 0.9841	 0.4410
A	 0.9953	 0.3960
B	 0.9996	 0.3890
C	 0.9490	 0.4340
D	 0.9519	 0.4300
E	 0.9329	 0.3940
F	 0.9563	 0.3290
G	 0.9453	 0.3680
H	 0.8110	 0.2610
I	 0.9244	 0.1510
J	 0.9112	 0.0770
K	 0.9664	 0.4150
L	 0.9034	 0.4160
M	 0.9512	 0.4030
N	 0.9501	 0.4270
O	 0.9497	 0.4190
P	 0.9633	 0.3720
Q	 0.9313	 0.4000
R	 0.9769	 0.4220
S	 0.9435	 0.4150
T	 0.9139	 0.4170
U	 0.9216	 0.3880
V	 0.9322	 0.3900
W	 0.9390	 0.3980
X	 0.9521	 0.4230
Y	 0.9484	 0.4100
Z	 0.9018	 0.3350
a	 0.9474	 0.4160
b	 0.9487	 0.4200
c	 0.9286	 0.3880
d	 0.9437	 0.4280
e	 0.9389	 0.4390
f	 0.9727	 0.4150



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Chain	Atom inclusion	Q-score
i	 0.7649	 0.0780
k	 0.7737	 0.1020
l	 0.6492	 0.0230