wwPDB EM Validation Summary Report

Dec 15, 2024 – 05:31 AM EST

PDB ID	:	1Z7Z
EMDB ID	:	EMD-1114
Title	:	Cryo-em structure of human coxsackievirus A21 complexed with five domain icam-1kilifi
Authors	:	Xiao, C.; Bator-Kelly, C.M.; Rieder, E.; Chipman, P.R.; Craig, A.; Kuhn, R.J.; Wimmer, E.; Rossmann, M.G.
Deposited on	:	2005-03-28
Resolution	:	8.00 Å(reported)
Based on initial models	:	1Z7S, 1IAM

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:

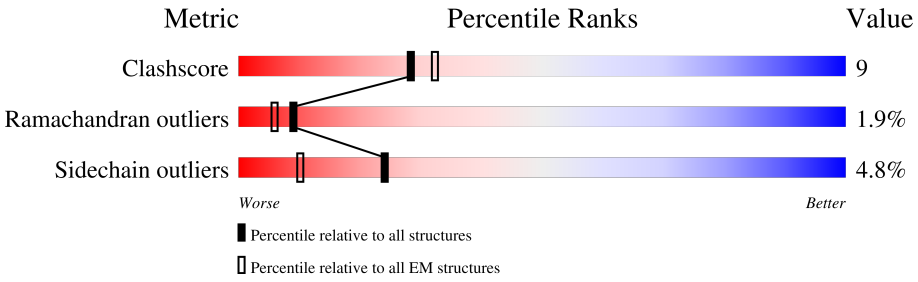
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	286	67% 6% 25%
2	2	272	87% 8%
3	3	234	74% 8% 18%
4	4	12	92% 8%
5	5	6	50% 17% 17% 17%
6	I	450	60% 74% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	I	457	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	214	Total	C	N	O	S	0	0
			1723	1102	295	317	9		

- Molecule 2 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	263	Total	C	N	O	S	0	0
			2042	1297	345	389	11		

- Molecule 3 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	192	Total	C	N	O	S	0	0
			1493	955	246	274	18		

- Molecule 4 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	12	Total	C	N	O	0	0
			94	62	13	19		

- Molecule 5 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	5	Total	C	N	O	0	0
			38	24	8	6		

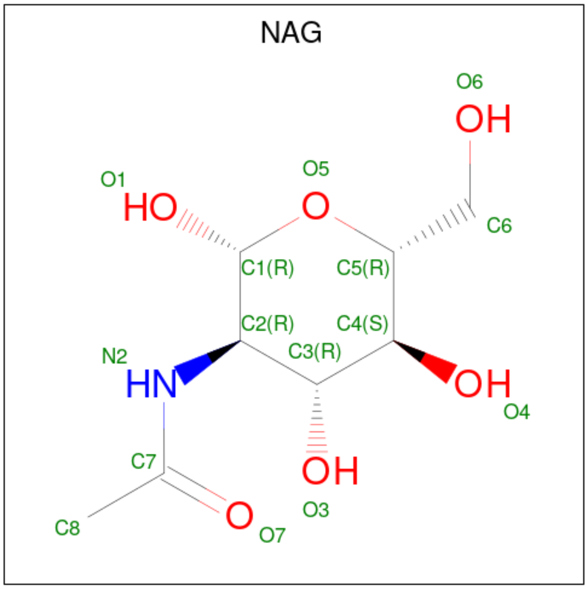
- Molecule 6 is a protein called Intercellular adhesion molecule-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	434	Total	C	N	O	S	0	0
			3322	2073	577	655	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	29	MET	LYS	engineered mutation	UNP P05362

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



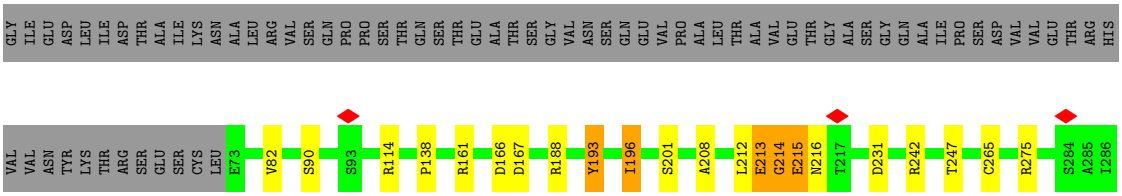
Mol	Chain	Residues	Atoms	AltConf
7	I	1	Total C N O 14 8 1 5	0
7	I	1	Total C N O 14 8 1 5	0
7	I	1	Total C N O 14 8 1 5	0
7	I	1	Total C N O 14 8 1 5	0
7	I	1	Total C N O 14 8 1 5	0
7	I	1	Total C N O 14 8 1 5	0
7	I	1	Total C N O 14 8 1 5	0
7	I	1	Total C N O 14 8 1 5	0

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.

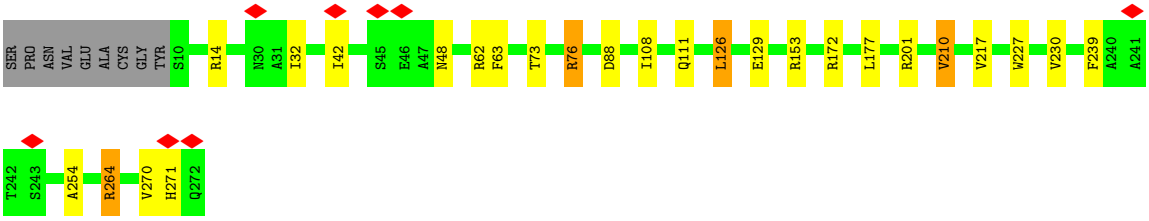
• Molecule 1: human coxsackievirus A21

Chain 1:



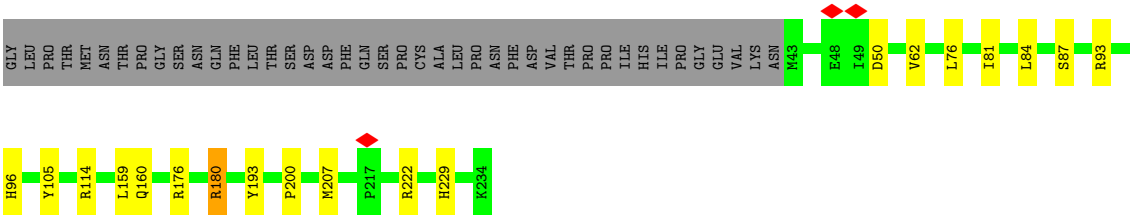
• Molecule 2: human coxsackievirus A21

Chain 2:



• Molecule 3: human coxsackievirus A21

Chain 3:

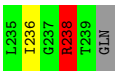


• Molecule 4: human coxsackievirus A21

Chain 4:

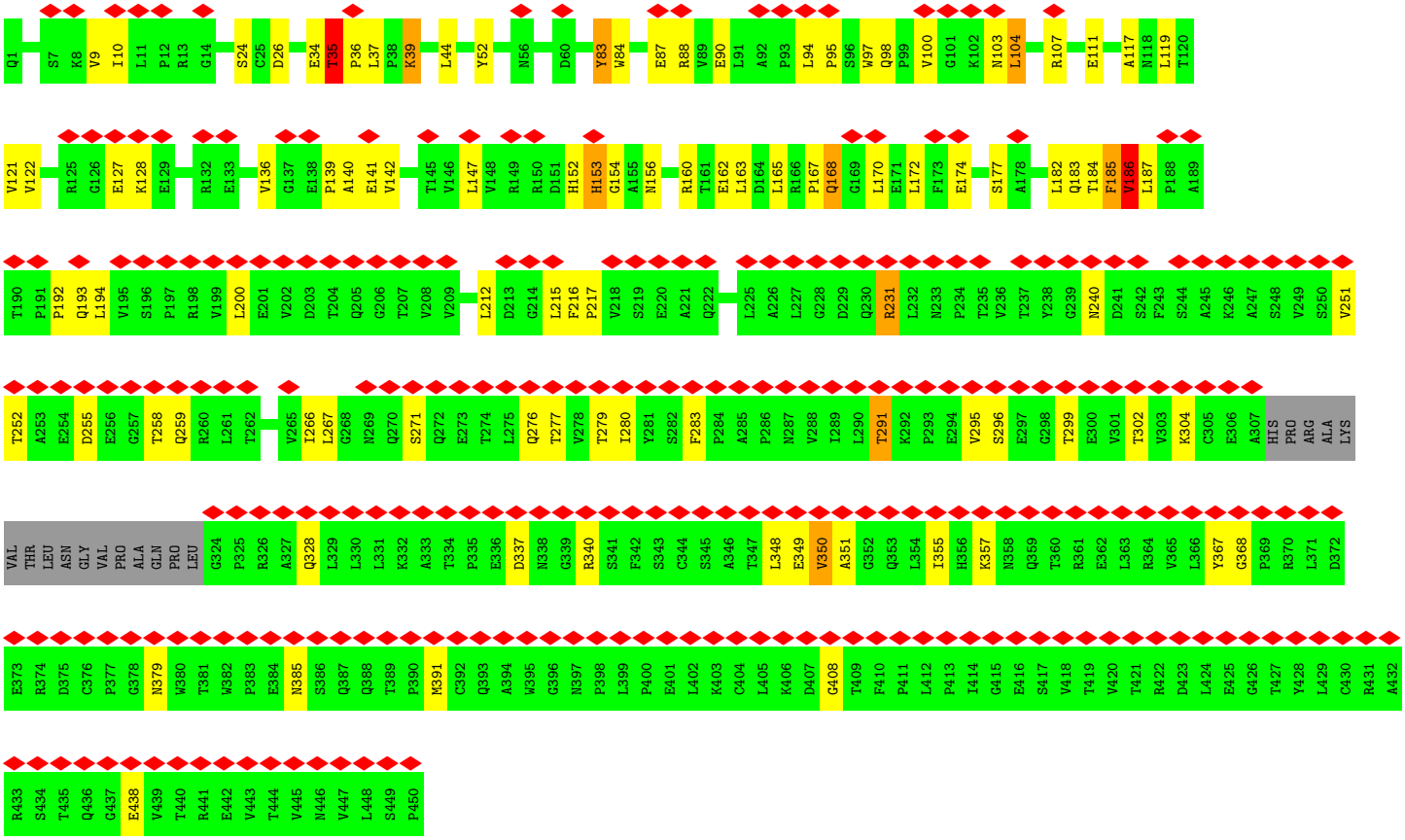
• Molecule 5: human coxsackievirus A21

Chain 5:



• Molecule 6: Intercellular adhesion molecule-1

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4704	Depositor
Resolution determination method	Not provided	
CTF correction method	REVERSED CTF WITH WEINER FACTOR FOR EACH PARTICLE	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	26	Depositor
Minimum defocus (nm)	700.00	Depositor
Maximum defocus (nm)	3000.00	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	512.800	Depositor
Minimum map value	-396.970	Depositor
Average map value	-1.831	Depositor
Map value standard deviation	51.307	Depositor
Recommended contour level	101	Depositor
Map size (Å)	742, 742, 742	wwPDB
Map dimensions	371, 371, 371	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2, 2, 2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.77	0/1777	1.06	3/2419 (0.1%)
2	2	0.71	0/2098	1.03	6/2870 (0.2%)
3	3	0.71	0/1531	1.06	4/2078 (0.2%)
4	4	0.70	0/95	1.02	0/128
5	5	0.74	0/37	1.95	1/48 (2.1%)
6	I	0.50	0/3388	0.83	3/4629 (0.1%)
All	All	0.65	0/8926	0.98	17/12172 (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
1	1	0	1
2	2	0	1
3	3	0	3
5	5	0	1
All	All	0	6

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	76	ARG	NE-CZ-NH2	-8.53	116.04	120.30
6	I	186	VAL	CA-C-N	-7.40	100.92	117.20
5	5	238	ARG	NE-CZ-NH1	7.15	123.88	120.30
2	2	264	ARG	NE-CZ-NH1	7.04	123.82	120.30
3	3	114	ARG	NE-CZ-NH1	6.64	123.62	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	193	TYR	Sidechain
2	2	172	ARG	Sidechain
3	3	105	TYR	Sidechain
3	3	87	SER	Peptide
3	3	93	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1723	0	1648	17	0
2	2	2042	0	1966	12	0
3	3	1493	0	1490	3	0
4	4	94	0	100	0	0
5	5	38	0	44	0	0
6	I	3322	0	3303	124	0
7	I	112	0	104	17	0
All	All	8824	0	8655	149	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 9.

The worst 5 of 149 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)
6:I:103:ASN:HD21	7:I:451:NAG:C1	0.93	1.58
6:I:279:THR:CG2	6:I:350:VAL:HG23	1.23	1.55
6:I:279:THR:CG2	6:I:350:VAL:CG2	2.02	1.38
6:I:279:THR:HG21	6:I:350:VAL:CG2	1.52	1.37
6:I:279:THR:CB	6:I:350:VAL:HG23	1.55	1.34

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
1	1	212/286 (74%)	185 (87%)	19 (9%)	8 (4%)	2 19
2	2	261/272 (96%)	242 (93%)	17 (6%)	2 (1%)	16 55
3	3	190/234 (81%)	176 (93%)	13 (7%)	1 (0%)	25 64
4	4	10/12 (83%)	10 (100%)	0	0	100 100
5	5	3/6 (50%)	1 (33%)	0	2 (67%)	0 0
6	I	430/450 (96%)	407 (95%)	15 (4%)	8 (2%)	6 32
All	All	1106/1260 (88%)	1021 (92%)	64 (6%)	21 (2%)	9 32

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	213	GLU
1	1	214	GLY
5	5	238	ARG
6	I	35	THR
6	I	36	PRO

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
1	1	188/249 (76%)	182 (97%)	6 (3%)	34 53
2	2	223/230 (97%)	212 (95%)	11 (5%)	21 42
3	3	170/208 (82%)	163 (96%)	7 (4%)	26 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	4	12/12 (100%)	11 (92%)	1 (8%)	9 27
5	5	4/5 (80%)	4 (100%)	0	100 100
6	I	382/395 (97%)	360 (94%)	22 (6%)	17 38
All	All	979/1099 (89%)	932 (95%)	47 (5%)	24 43

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I	39	LYS
6	I	163	LEU
6	I	87	GLU
6	I	122	VAL
6	I	168	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
6	I	168	GLN
6	I	359	GLN
6	I	436	GLN
6	I	388	GLN
6	I	397	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	I	454	6	14,14,15	0.60	0	17,19,21	0.78	1 (5%)
7	NAG	I	453	6	14,14,15	0.74	0	17,19,21	0.86	0
7	NAG	I	456	6	14,14,15	0.78	0	17,19,21	1.29	4 (23%)
7	NAG	I	452	-	14,14,15	0.69	0	17,19,21	1.24	2 (11%)
7	NAG	I	458	6	14,14,15	0.64	0	17,19,21	0.69	0
7	NAG	I	451	6	14,14,15	3.74	2 (14%)	17,19,21	2.12	4 (23%)
7	NAG	I	457	6	14,14,15	0.74	1 (7%)	17,19,21	0.75	0
7	NAG	I	455	-	14,14,15	0.72	0	17,19,21	1.11	1 (5%)

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
7	NAG	I	454	6	-	1/6/23/26	0/1/1/1
7	NAG	I	453	6	-	0/6/23/26	0/1/1/1
7	NAG	I	456	6	-	2/6/23/26	0/1/1/1
7	NAG	I	452	-	-	0/6/23/26	0/1/1/1
7	NAG	I	458	6	-	4/6/23/26	0/1/1/1
7	NAG	I	451	6	-	0/6/23/26	0/1/1/1
7	NAG	I	457	6	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	I	455	-	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	451	NAG	C1-C2	12.68	1.69	1.52
7	I	451	NAG	C3-C2	4.76	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	457	NAG	C1-C2	2.17	1.55	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	451	NAG	C1-O5-C5	6.07	120.33	112.19
7	I	451	NAG	C1-C2-N2	3.47	115.91	110.43
7	I	455	NAG	C2-N2-C7	-3.29	118.49	122.90
7	I	451	NAG	O5-C5-C6	-2.73	102.36	107.66
7	I	452	NAG	C6-C5-C4	2.69	119.64	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	I	457	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	456	NAG	C8-C7-N2-C2
7	I	456	NAG	O7-C7-N2-C2
7	I	457	NAG	C8-C7-N2-C2
7	I	457	NAG	O7-C7-N2-C2
7	I	458	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	454	NAG	1	0
7	I	456	NAG	1	0
7	I	452	NAG	4	0
7	I	451	NAG	4	0
7	I	457	NAG	6	0
7	I	455	NAG	2	0

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.

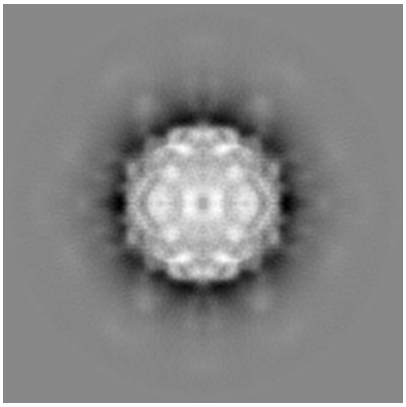
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1114. These allow visual inspection of the internal detail of the map and identification of artifacts.

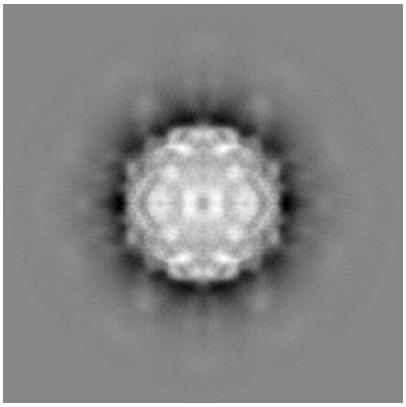
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

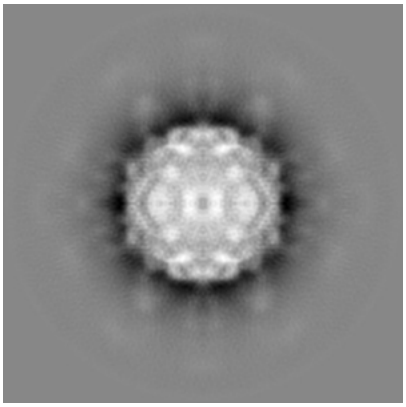
6.1.1 Primary map



X



Y

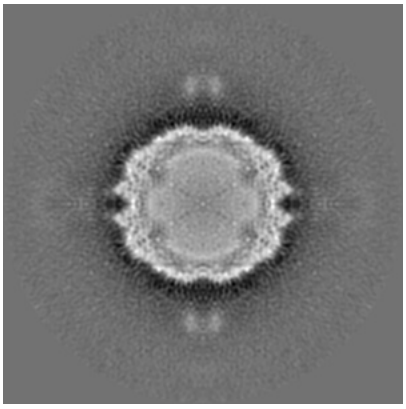


Z

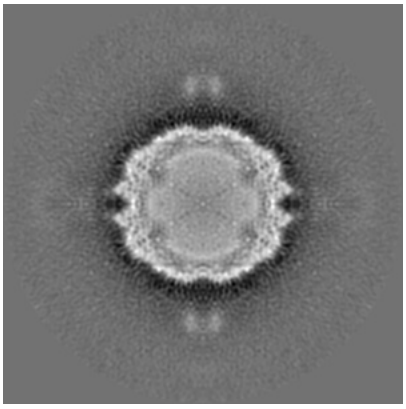
The images above show the map projected in three orthogonal directions.

6.2 Central slices

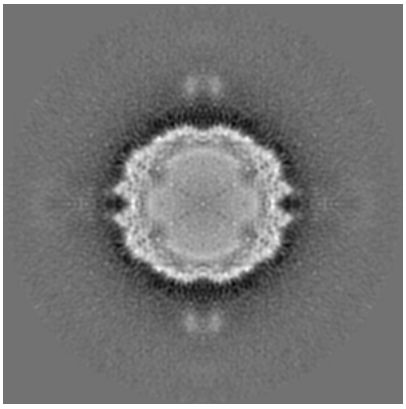
6.2.1 Primary map



X Index: 185



Y Index: 185

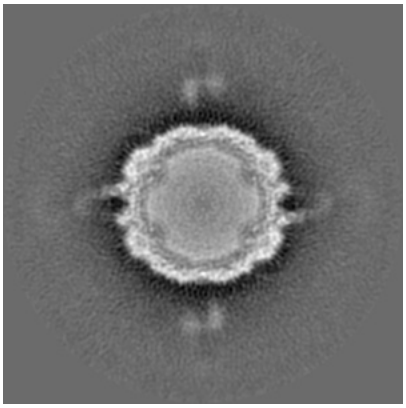


Z Index: 185

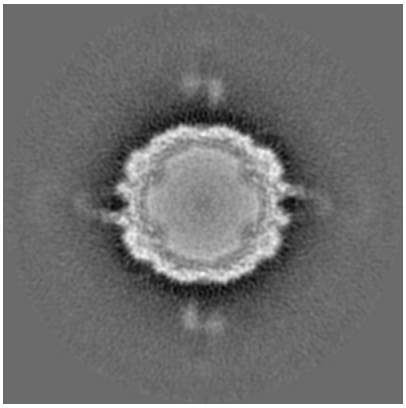
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

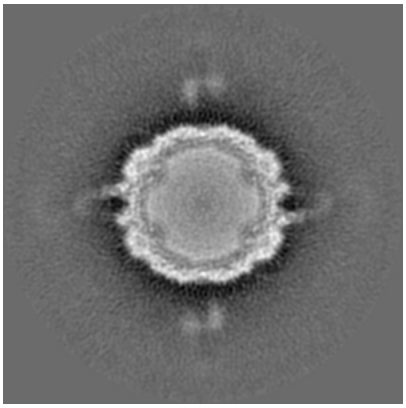
6.3.1 Primary map



X Index: 188



Y Index: 182

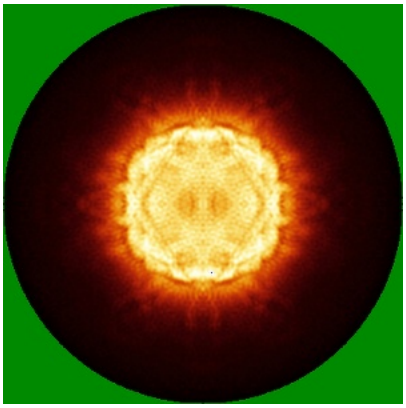


Z Index: 188

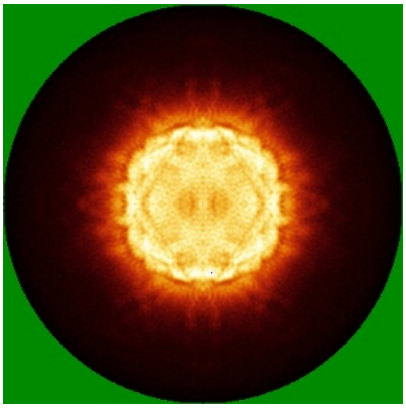
The images above show the largest variance slices of the map in three orthogonal directions.

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

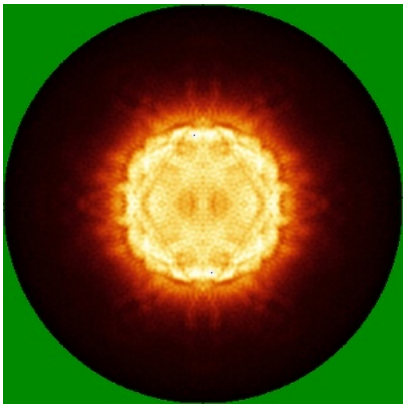
6.4.1 Primary map



X



Y

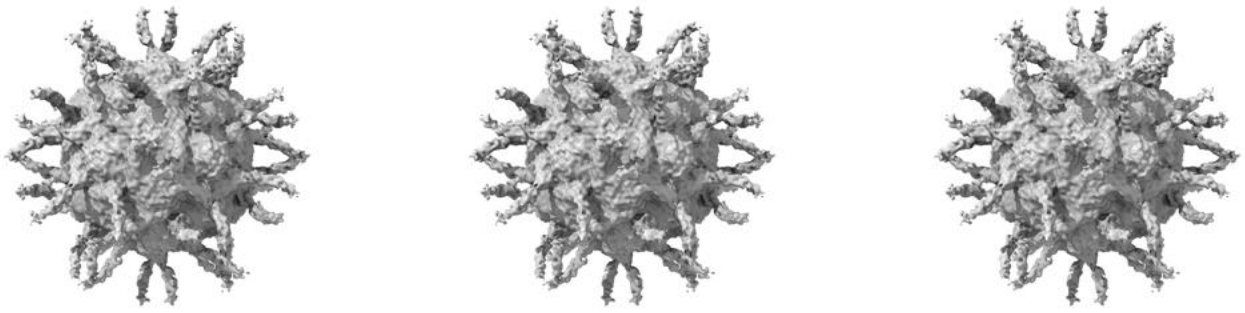


Z

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

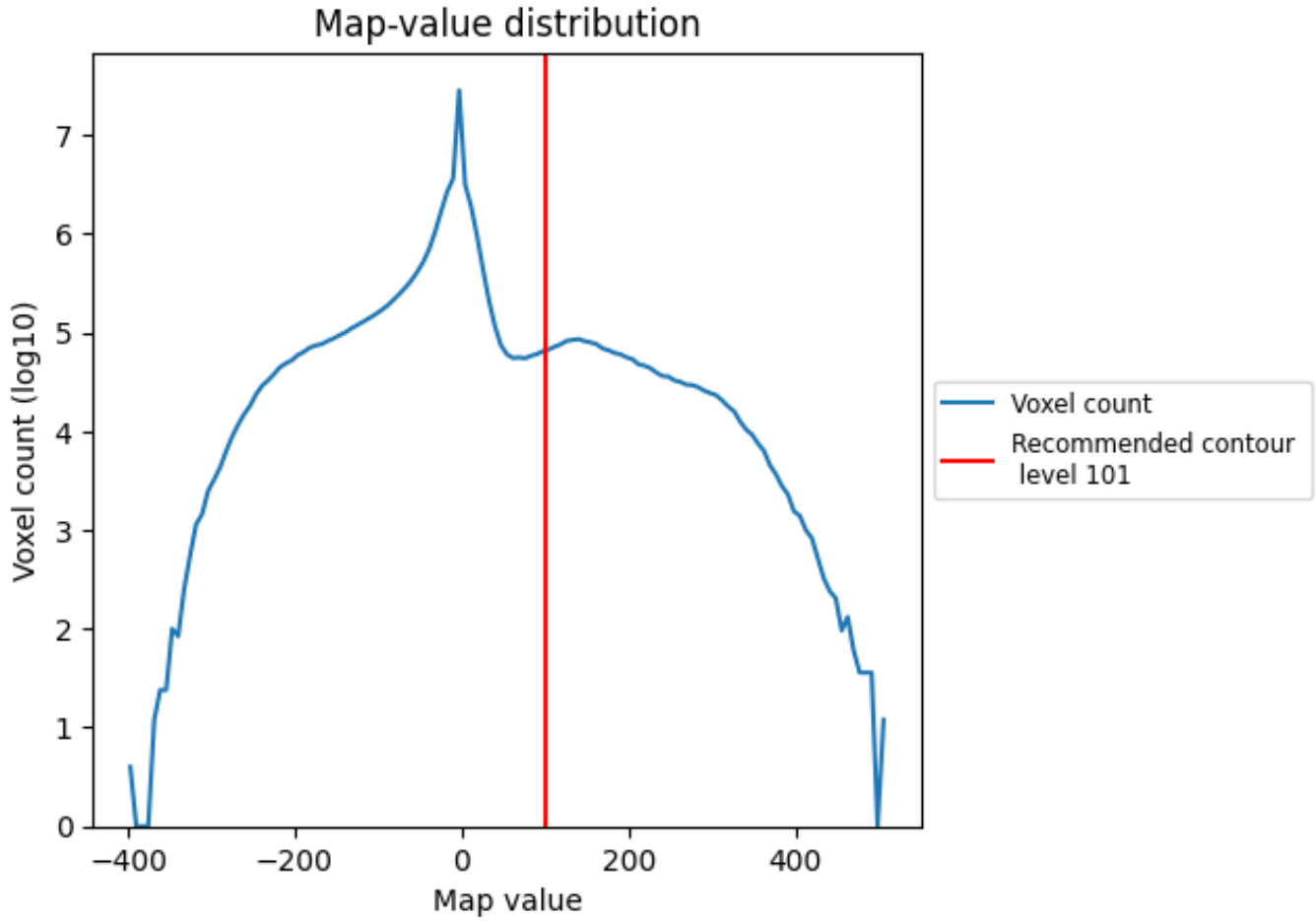
6.6 Mask visualisation (i)

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

7 Map analysis

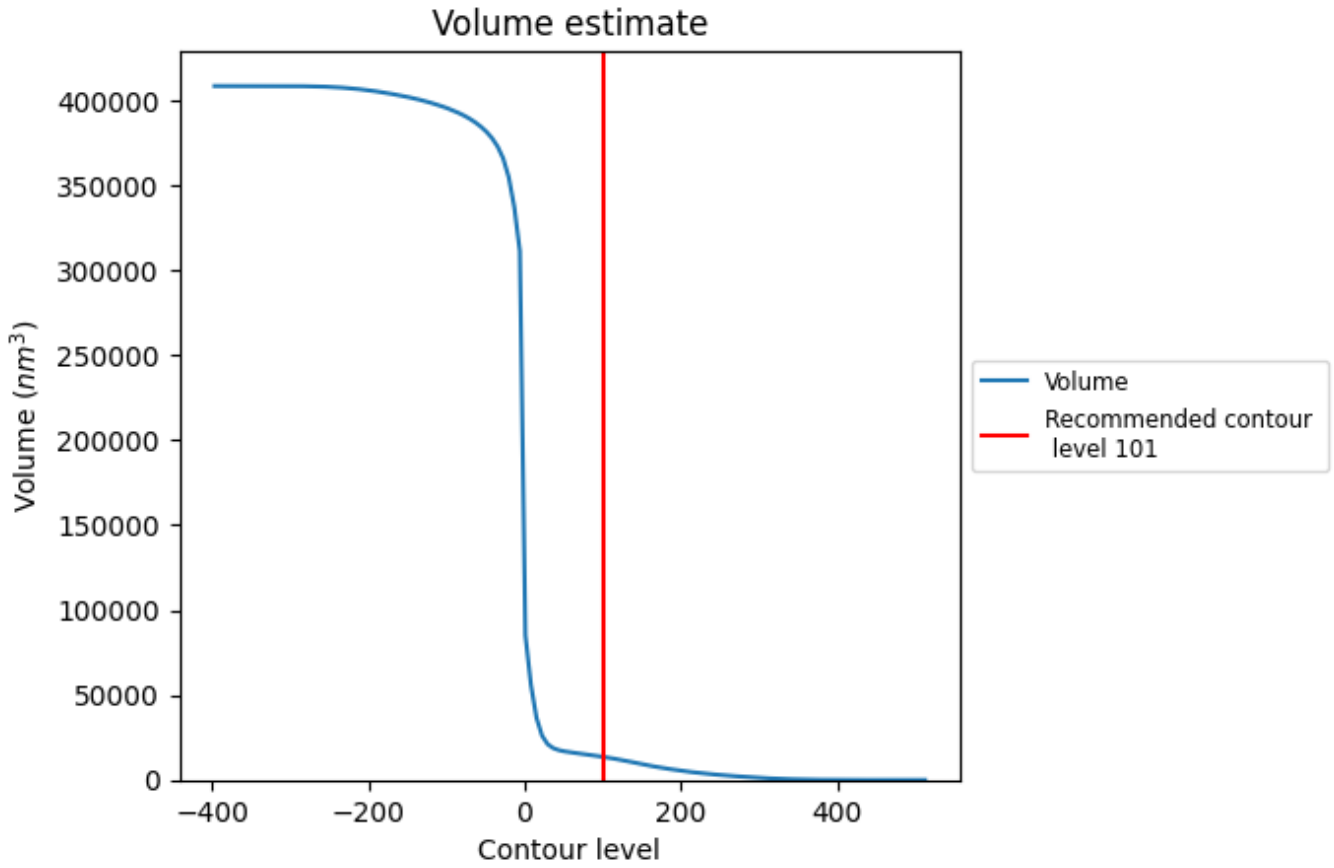
This section contains the results of statistical analysis of the map.

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.

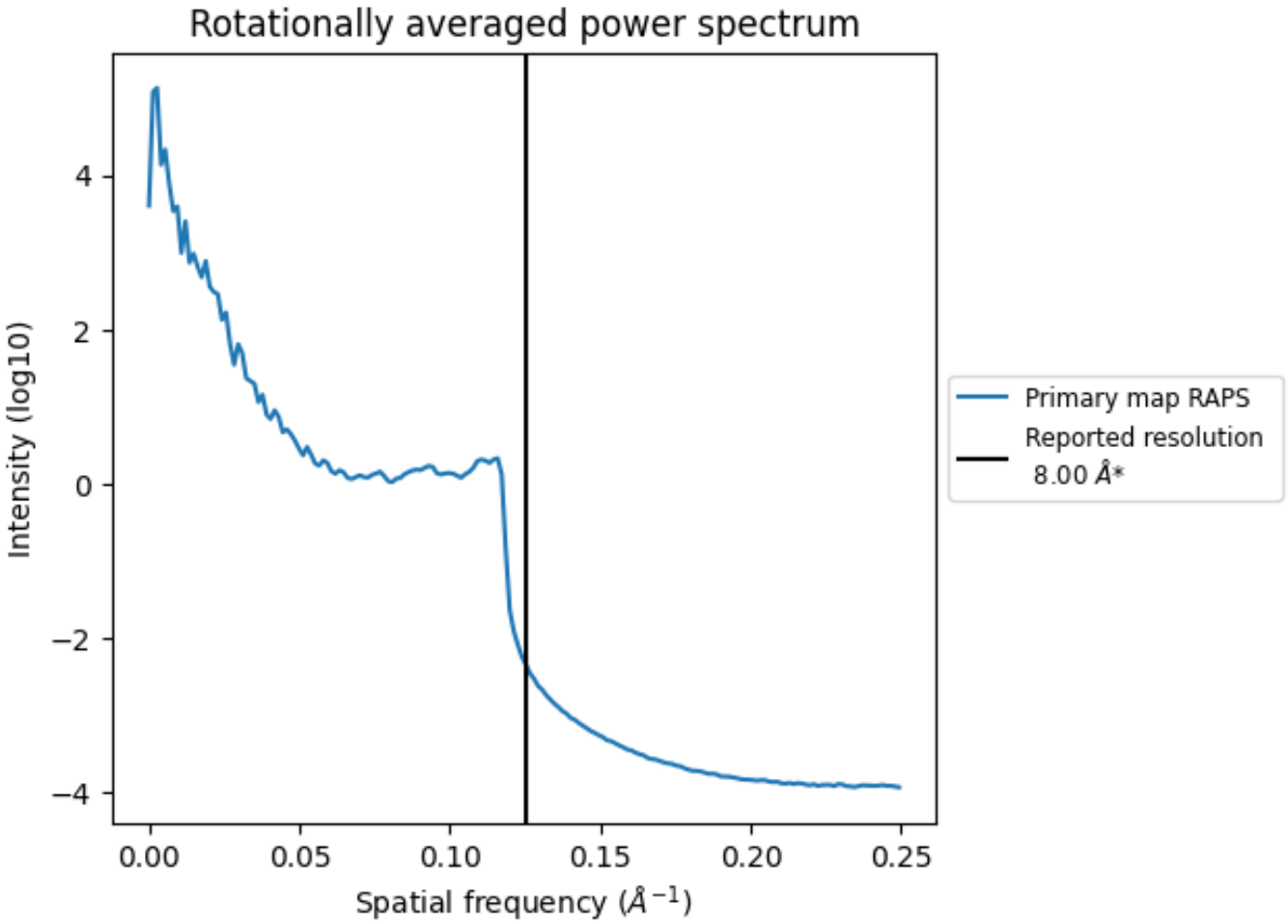
7.2 Volume estimate (i)



The volume at the recommended contour level is 13565 nm^3; this corresponds to an approximate mass of 12254 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 0.125 Å^{-1}

8 Fourier-Shell correlation

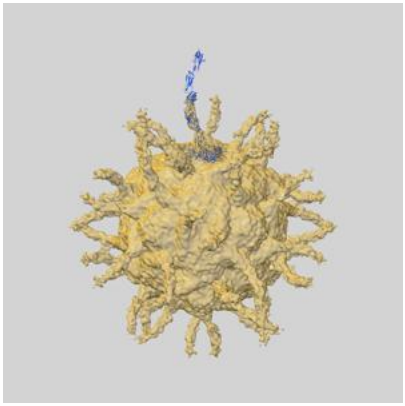
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

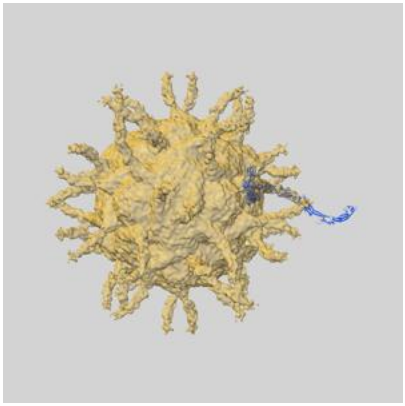
This section contains information regarding the fit between EMDB map EMD-1114 and PDB model 1Z7Z. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

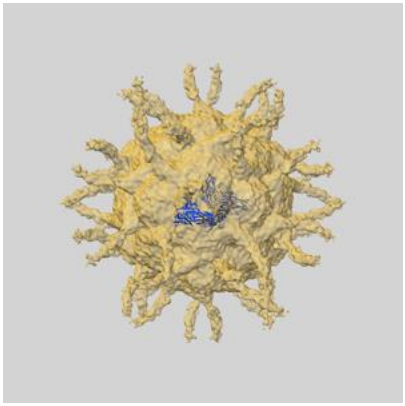
9.1.1 Map-model overlay



X

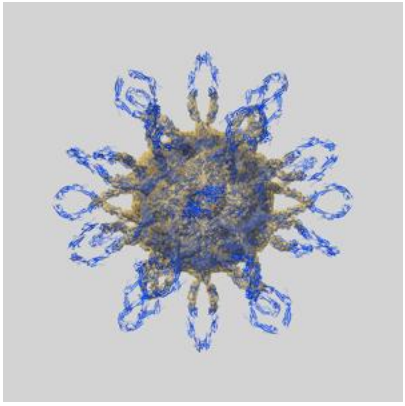


Y

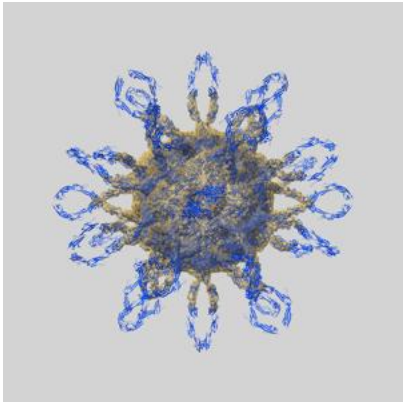


Z

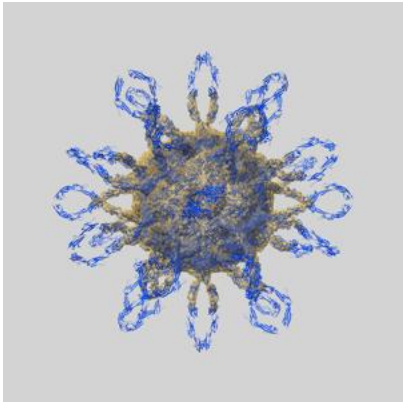
9.1.2 Map-model assembly overlay



X



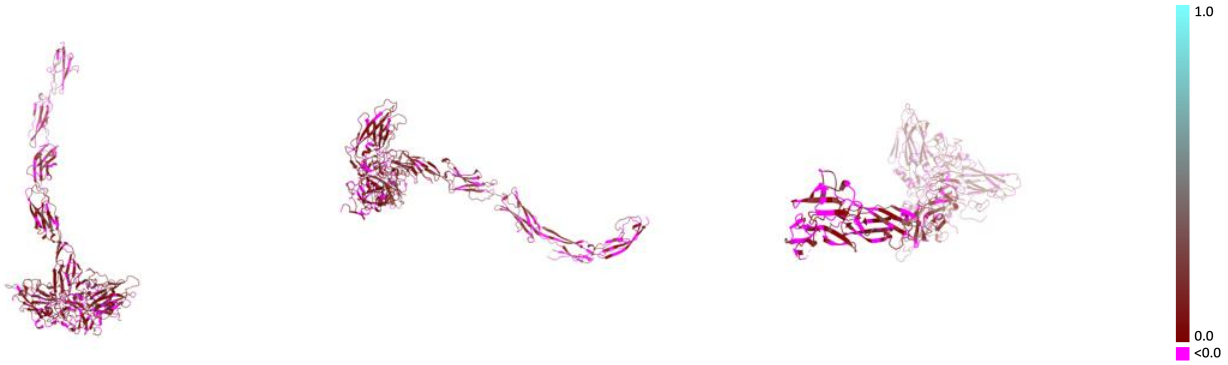
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 101.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

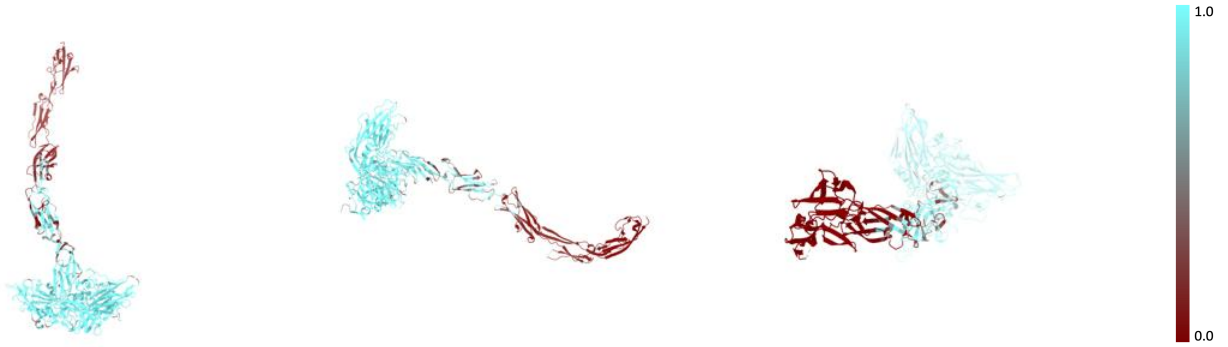
9.2 Q-score mapped to coordinate model (i)



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.

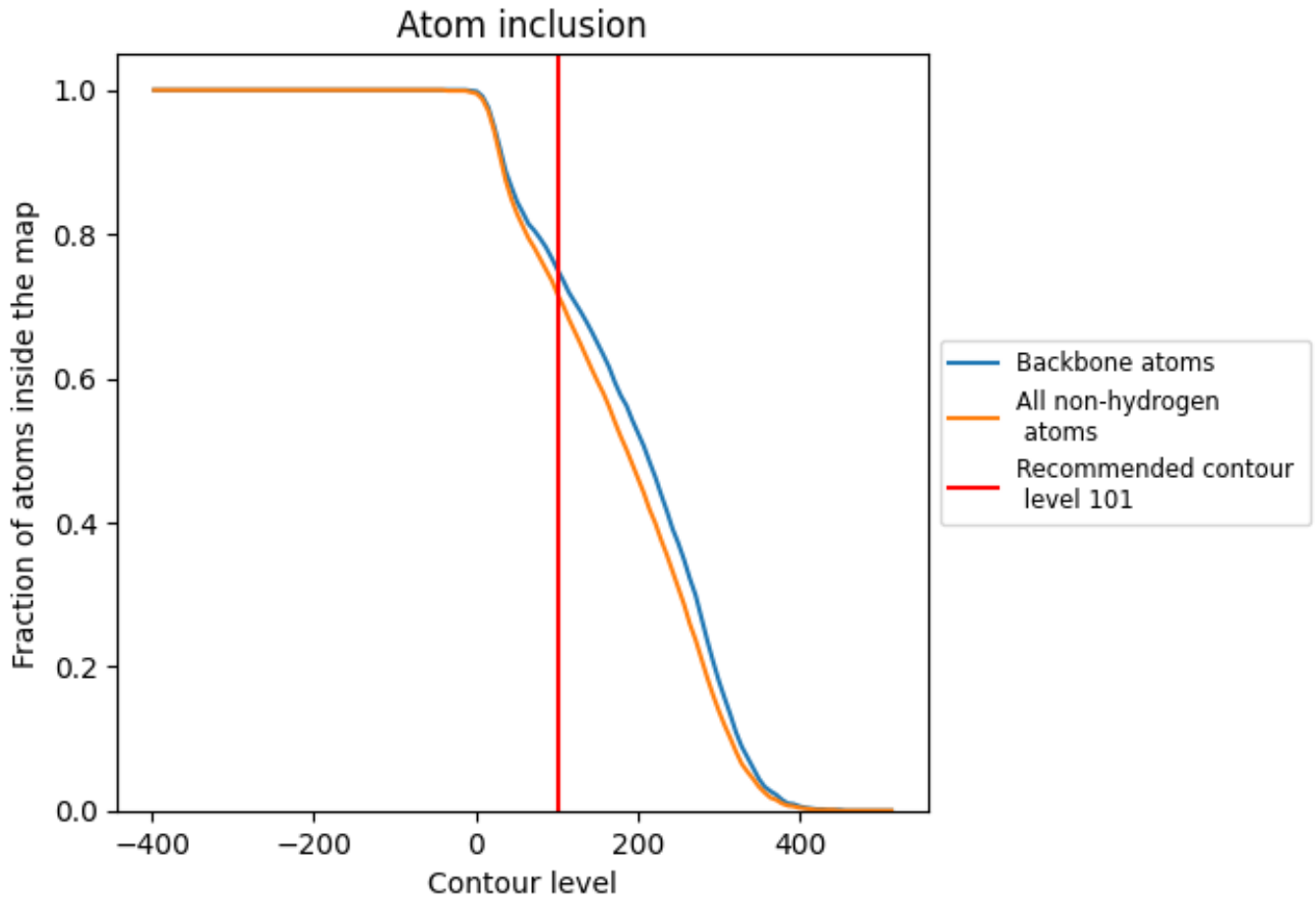
9.3 Atom inclusion mapped to coordinate model (i)



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 (101).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7160	0.0780
1	0.9760	0.0800
2	0.9510	0.0870
3	0.9670	0.0900
4	0.9680	0.1050
5	0.8890	0.1230
I	0.3290	0.0660