Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 01:13 PM EST

PDB ID	:	3J30
EMDB ID	:	EMD-5580
Title	:	Electron Cryo-microscopy of Chikungunya VLP in complex with neutralizing antibody Fab CHK152
Authors	:	Sun, S.; Xiang, Y.; Rossmann, M.G.
Deposited on	:	2013-01-28
Resolution	:	16.00 Å(reported)
Based on initial model	:	4GQ8

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

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

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

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

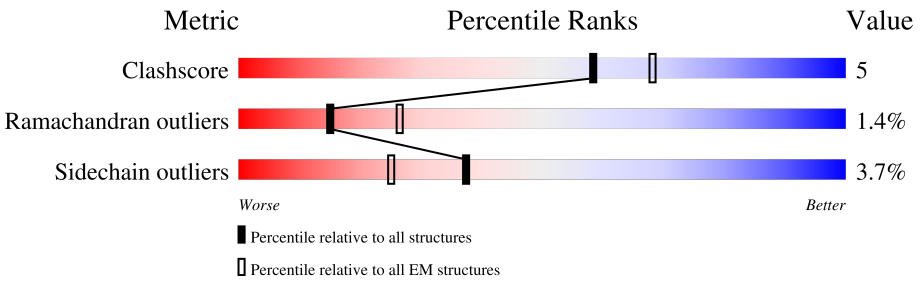
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 16.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	217	• 85% 13% •
1	C	217	7% 86% 12% •
1	E	217	14% 87% 11% •
1	G	217	6% 86% 12% •
2	B	217	6% 84% 14% •
2	D	217	17% 83% 16% •
2	F	217	18% 83% 15% •
2	H	217	12% 84% 14% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13228 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 CHK152 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	217	1676	1041	285	344	6	0	0
1	C	217	1676	1041	285	344	6	0	0
1	E	217	1676	1041	285	344	6	0	0
1	G	217	1676	1041	285	344	6	0	0

- Molecule 2 is a protein called CHK152 heavy chain.

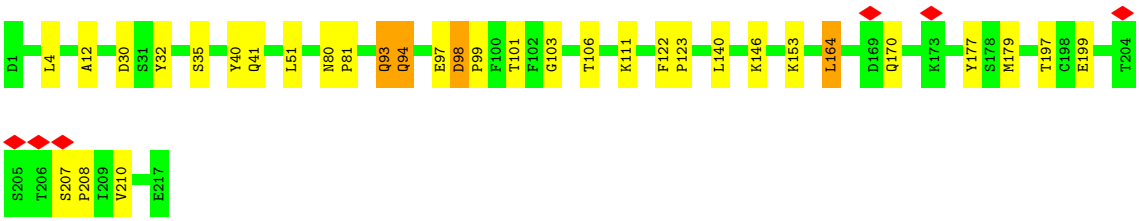
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	217	1631	1035	263	326	7	0	0
2	D	217	1631	1035	263	326	7	0	0
2	F	217	1631	1035	263	326	7	0	0
2	H	217	1631	1035	263	326	7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

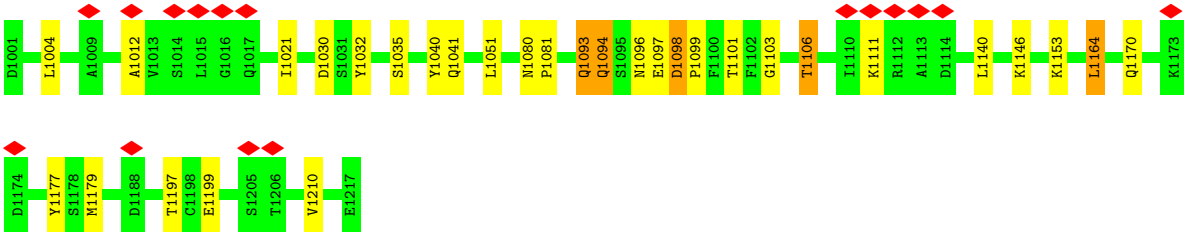
• Molecule 1: CHK152 light chain

Chain A:



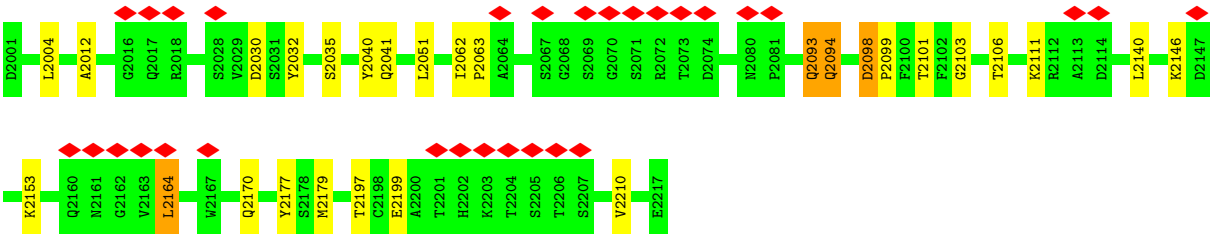
• Molecule 1: CHK152 light chain

Chain C:



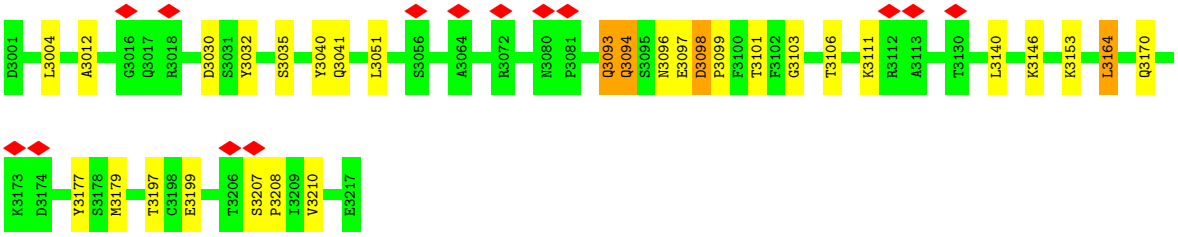
• Molecule 1: CHK152 light chain

Chain E:



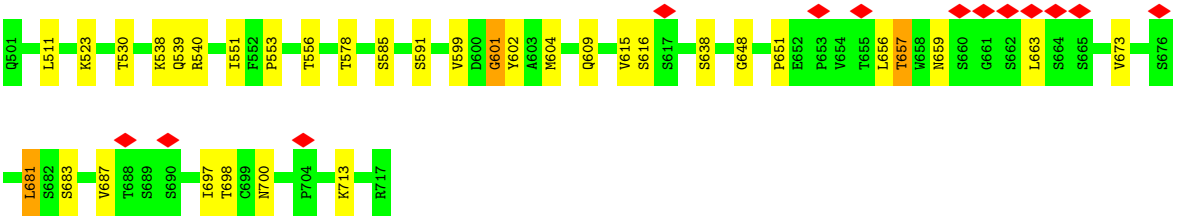
• Molecule 1: CHK152 light chain

Chain G:



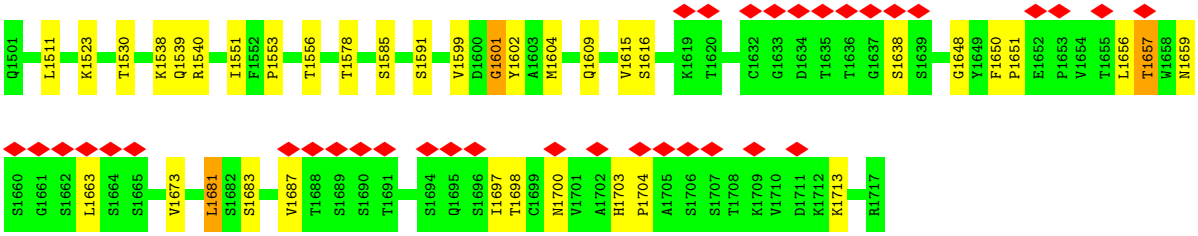
- Molecule 2: CHK152 heavy chain

Chain B:



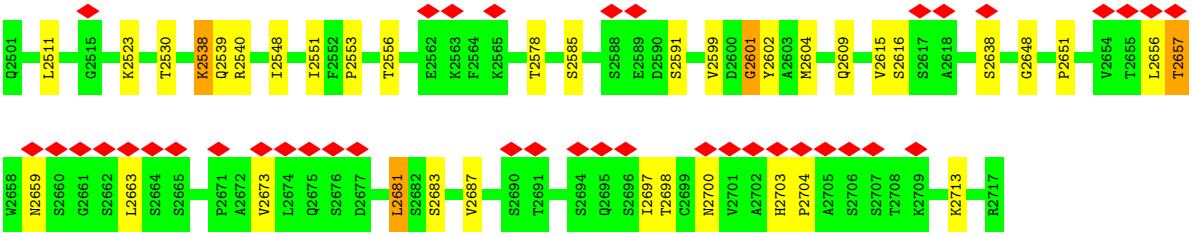
- Molecule 2: CHK152 heavy chain

Chain D:



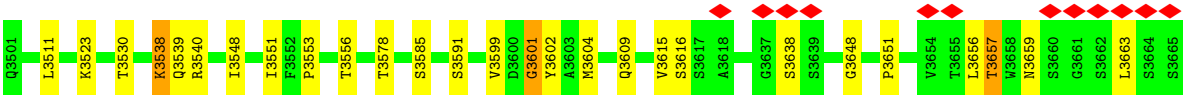
- Molecule 2: CHK152 heavy chain

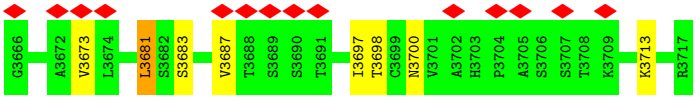
Chain F:



- Molecule 2: CHK152 heavy chain

Chain H:




G3666
A3672
V3673
L3674
L3681
S3682
S3683
V3687
T3688
S3689
S3690
T3691
I3697
T3698
C3699
N3700
V3701
A3702
H3703
P3704
A3705
S3706
S3707
T3708
K3709
K3713
R3717

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	2106	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	35600	Depositor
Image detector	Not provided	
Maximum map value	6.737	Depositor
Minimum map value	-3.880	Depositor
Average map value	0.179	Depositor
Map value standard deviation	1.188	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	888.0, 888.0, 888.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.22, 2.22, 2.22	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.31	0/1713	0.45	0/2327
1	C	0.31	0/1713	0.45	0/2327
1	E	0.31	0/1713	0.45	0/2327
1	G	0.31	0/1713	0.45	0/2327
2	B	0.31	0/1674	0.48	0/2287
2	D	0.31	0/1674	0.48	0/2287
2	F	0.31	0/1674	0.48	0/2287
2	H	0.31	0/1674	0.48	0/2287
All	All	0.31	0/13548	0.46	0/18456

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1676	0	1605	17	0
1	C	1676	0	1602	17	0
1	E	1676	0	1602	13	0
1	G	1676	0	1602	15	0
2	B	1631	0	1591	16	0
2	D	1631	0	1591	18	0
2	F	1631	0	1591	18	0
2	H	1631	0	1591	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13228	0	12775	127	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 5.

All (127) 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)
2:F:2656:LEU:HD13	2:F:2683:SER:HB2	1.80	0.64
2:D:1656:LEU:HD13	2:D:1683:SER:HB2	1.80	0.64
2:H:3656:LEU:HD13	2:H:3683:SER:HB2	1.80	0.64
2:B:656:LEU:HD13	2:B:683:SER:HB2	1.80	0.63
1:G:3040:TYR:HE1	1:G:3093:GLN:HG2	1.64	0.63
1:C:1040:TYR:HE1	1:C:1093:GLN:HG2	1.64	0.63
1:A:40:TYR:HE1	1:A:93:GLN:HG2	1.64	0.62
1:E:2098:ASP:HB3	1:E:2099:PRO:HD3	1.81	0.62
1:E:2030:ASP:HA	1:E:2035:SER:HA	1.81	0.62
1:C:1030:ASP:HA	1:C:1035:SER:HA	1.81	0.62
1:E:2040:TYR:HE1	1:E:2093:GLN:HG2	1.64	0.61
1:G:3030:ASP:HA	1:G:3035:SER:HA	1.81	0.61
1:G:3098:ASP:HB3	1:G:3099:PRO:HD3	1.81	0.61
1:A:98:ASP:HB3	1:A:99:PRO:HD3	1.81	0.61
1:A:30:ASP:HA	1:A:35:SER:HA	1.81	0.60
1:C:1098:ASP:HB3	1:C:1099:PRO:HD3	1.81	0.60
2:B:615:VAL:HA	2:B:616:SER:HB2	1.84	0.60
2:H:3615:VAL:HA	2:H:3616:SER:HB2	1.84	0.59
2:F:2615:VAL:HA	2:F:2616:SER:HB2	1.84	0.58
2:D:1615:VAL:HA	2:D:1616:SER:HB2	1.84	0.57
2:F:2591:SER:HB3	2:F:2615:VAL:H	1.76	0.51
2:B:698:THR:HG22	2:B:713:LYS:HG2	1.92	0.51
2:D:1591:SER:HB3	2:D:1615:VAL:H	1.76	0.51
2:F:2698:THR:HG22	2:F:2713:LYS:HG2	1.92	0.51
2:H:3591:SER:HB3	2:H:3615:VAL:H	1.76	0.51
2:H:3698:THR:HG22	2:H:3713:LYS:HG2	1.92	0.50
1:A:12:ALA:HB1	1:A:111:LYS:HG3	1.94	0.50
2:B:615:VAL:CA	2:B:616:SER:HB2	2.42	0.50
2:D:1698:THR:HG22	2:D:1713:LYS:HG2	1.92	0.50
2:B:591:SER:HB3	2:B:615:VAL:H	1.76	0.50
2:H:3615:VAL:CA	2:H:3616:SER:HB2	2.42	0.50
1:G:3012:ALA:HB1	1:G:3111:LYS:HG3	1.94	0.49
1:E:2012:ALA:HB1	1:E:2111:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1615:VAL:CA	2:D:1616:SER:HB2	2.42	0.49
1:C:1012:ALA:HB1	1:C:1111:LYS:HG3	1.94	0.49
1:C:1094:GLN:NE2	1:C:1101:THR:OG1	2.46	0.48
2:F:2615:VAL:CA	2:F:2616:SER:HB2	2.42	0.48
2:H:3530:THR:HA	2:H:3553:PRO:HB2	1.96	0.48
1:A:41:GLN:HB2	1:A:51:LEU:HD11	1.96	0.48
2:F:2530:THR:HA	2:F:2553:PRO:HB2	1.96	0.48
1:E:2041:GLN:HB2	1:E:2051:LEU:HD11	1.96	0.48
2:B:530:THR:HA	2:B:553:PRO:HB2	1.96	0.48
2:D:1530:THR:HA	2:D:1553:PRO:HB2	1.96	0.48
1:E:2094:GLN:NE2	1:E:2101:THR:OG1	2.46	0.47
1:A:4:LEU:HB2	1:A:103:GLY:HA2	1.97	0.47
1:G:3004:LEU:HB2	1:G:3103:GLY:HA2	1.97	0.47
1:G:3041:GLN:HB2	1:G:3051:LEU:HD11	1.96	0.47
1:E:2004:LEU:HB2	1:E:2103:GLY:HA2	1.97	0.47
1:C:1041:GLN:HB2	1:C:1051:LEU:HD11	1.96	0.47
1:G:3094:GLN:NE2	1:G:3101:THR:OG1	2.46	0.47
2:B:601:GLY:HA2	2:B:602:TYR:HA	1.57	0.46
1:C:1004:LEU:HB2	1:C:1103:GLY:HA2	1.97	0.46
2:D:1601:GLY:HA2	2:D:1602:TYR:HA	1.57	0.46
2:D:1656:LEU:HD11	2:D:1681:LEU:HD21	1.98	0.46
2:B:656:LEU:HD11	2:B:681:LEU:HD21	1.98	0.46
2:H:3656:LEU:HD11	2:H:3681:LEU:HD21	1.98	0.46
2:F:2656:LEU:HD11	2:F:2681:LEU:HD21	1.98	0.46
1:G:3140:LEU:HD12	1:G:3179:MET:HB3	1.98	0.45
1:E:2140:LEU:HD12	1:E:2179:MET:HB3	1.98	0.45
1:A:164:LEU:HD11	2:B:673:VAL:HB	1.98	0.45
1:C:1140:LEU:HD12	1:C:1179:MET:HB3	1.98	0.45
1:C:1164:LEU:HD11	2:D:1673:VAL:HB	1.98	0.45
2:D:1657:THR:HB	2:D:1700:ASN:HB2	1.99	0.45
2:F:2659:ASN:HD21	2:F:2697:ILE:HA	1.82	0.45
1:A:94:GLN:NE2	1:A:101:THR:OG1	2.46	0.45
1:A:140:LEU:HD12	1:A:179:MET:HB3	1.98	0.45
2:H:3659:ASN:HD21	2:H:3697:ILE:HA	1.82	0.45
1:E:2164:LEU:HD11	2:F:2673:VAL:HB	1.98	0.44
1:G:3164:LEU:HD11	2:H:3673:VAL:HB	1.98	0.44
2:B:657:THR:HB	2:B:700:ASN:HB2	1.99	0.44
2:D:1659:ASN:HD21	2:D:1697:ILE:HA	1.82	0.44
1:C:1153:LYS:HB2	1:C:1197:THR:OG1	2.18	0.44
2:F:2657:THR:HB	2:F:2700:ASN:HB2	1.99	0.44
2:H:3601:GLY:HA2	2:H:3602:TYR:HA	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HB2	1:A:197:THR:OG1	2.18	0.44
2:B:659:ASN:HD21	2:B:697:ILE:HA	1.82	0.44
1:E:2199:GLU:HG3	1:E:2210:VAL:HG22	2.00	0.44
2:B:659:ASN:HD22	2:B:663:LEU:HD12	1.83	0.44
1:A:80:ASN:HA	1:A:81:PRO:HA	1.83	0.44
1:C:1199:GLU:HG3	1:C:1210:VAL:HG22	2.00	0.44
2:D:1703:HIS:HA	2:D:1704:PRO:HD3	1.84	0.44
1:A:199:GLU:HG3	1:A:210:VAL:HG22	2.00	0.43
1:E:2153:LYS:HB2	1:E:2197:THR:OG1	2.18	0.43
1:G:3170:GLN:HG3	1:G:3177:TYR:CZ	2.54	0.43
1:G:3199:GLU:HG3	1:G:3210:VAL:HG22	2.00	0.43
2:H:3657:THR:HB	2:H:3700:ASN:HB2	1.99	0.43
2:F:2511:LEU:HG	2:F:2651:PRO:HG3	2.00	0.43
1:A:207:SER:HA	1:A:208:PRO:HD3	1.88	0.43
2:D:1511:LEU:HG	2:D:1651:PRO:HG3	2.00	0.43
2:F:2601:GLY:HA2	2:F:2602:TYR:HA	1.57	0.43
2:H:3523:LYS:HG2	2:H:3578:THR:HG22	2.01	0.43
1:C:1170:GLN:HG3	1:C:1177:TYR:CZ	2.54	0.43
2:F:2599:VAL:HG22	2:F:2604:MET:HA	2.01	0.43
2:H:3659:ASN:HD22	2:H:3663:LEU:HD12	1.83	0.43
2:F:2659:ASN:HD22	2:F:2663:LEU:HD12	1.83	0.42
1:A:122:PHE:HA	1:A:123:PRO:HD3	1.90	0.42
2:B:511:LEU:HG	2:B:651:PRO:HG3	2.00	0.42
2:D:1523:LYS:HG2	2:D:1578:THR:HG22	2.01	0.42
2:D:1659:ASN:HD22	2:D:1663:LEU:HD12	1.83	0.42
1:E:2170:GLN:HG3	1:E:2177:TYR:CZ	2.54	0.42
1:G:3153:LYS:HB2	1:G:3197:THR:OG1	2.18	0.42
1:G:3097:GLU:HA	1:G:3098:ASP:HA	1.87	0.42
2:B:599:VAL:HG22	2:B:604:MET:HA	2.01	0.42
2:D:1599:VAL:HG22	2:D:1604:MET:HA	2.01	0.42
2:F:2523:LYS:HG2	2:F:2578:THR:HG22	2.01	0.42
2:H:3511:LEU:HG	2:H:3651:PRO:HG3	2.00	0.42
2:B:523:LYS:HG2	2:B:578:THR:HG22	2.01	0.42
1:A:97:GLU:HA	1:A:98:ASP:HA	1.87	0.41
2:B:599:VAL:HG22	2:B:604:MET:HG2	2.03	0.41
1:C:1098:ASP:HB3	1:C:1099:PRO:CD	2.50	0.41
2:H:3599:VAL:HG22	2:H:3604:MET:HA	2.01	0.41
1:A:170:GLN:HG3	1:A:177:TYR:CZ	2.54	0.41
2:D:1599:VAL:HG22	2:D:1604:MET:HG2	2.03	0.41
2:F:2599:VAL:HG22	2:F:2604:MET:HG2	2.02	0.41
1:G:3207:SER:HA	1:G:3208:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2062:ILE:HA	1:E:2063:PRO:HD3	1.94	0.41
1:C:1021:ILE:HG23	1:C:1106:THR:HG21	2.03	0.41
2:D:1650:PHE:HA	2:D:1651:PRO:HA	1.87	0.41
2:F:2538:LYS:HB2	2:F:2548:ILE:HD11	2.03	0.41
1:C:1096:ASN:HB3	1:C:1097:GLU:H	1.71	0.40
2:H:3599:VAL:HG22	2:H:3604:MET:HG2	2.02	0.40
1:C:1097:GLU:HA	1:C:1098:ASP:HA	1.87	0.40
2:H:3538:LYS:HB2	2:H:3548:ILE:HD11	2.03	0.40
1:G:3096:ASN:HB3	1:G:3097:GLU:H	1.71	0.40
2:F:2703:HIS:HA	2:F:2704:PRO:HD3	1.84	0.40
1:A:98:ASP:HB3	1:A:99:PRO:CD	2.50	0.40
1:C:1080:ASN:HA	1:C:1081:PRO:HA	1.83	0.40

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	A	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	29	69
1	C	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	29	69
1	E	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	29	69
1	G	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	29	69
2	B	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	6	34
2	D	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	6	34
2	F	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	6	34
2	H	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	6	34
All	All	1720/1736 (99%)	1572 (91%)	124 (7%)	24 (1%)	15	46

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	601	GLY
2	D	1601	GLY
2	F	2601	GLY
2	H	3601	GLY
2	B	556	THR
2	B	585	SER
2	B	638	SER
2	D	1556	THR
2	D	1585	SER
2	D	1638	SER
2	F	2556	THR
2	F	2585	SER
2	F	2638	SER
2	H	3556	THR
2	H	3585	SER
2	H	3638	SER
1	A	98	ASP
1	C	1098	ASP
1	E	2098	ASP
1	G	3098	ASP
2	B	648	GLY
2	D	1648	GLY
2	F	2648	GLY
2	H	3648	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	
1	A	191/191 (100%)	185 (97%)	6 (3%)	40	62
1	C	191/191 (100%)	185 (97%)	6 (3%)	40	62
1	E	191/191 (100%)	185 (97%)	6 (3%)	40	62
1	G	191/191 (100%)	185 (97%)	6 (3%)	40	62
2	B	187/187 (100%)	179 (96%)	8 (4%)	29	53
2	D	187/187 (100%)	179 (96%)	8 (4%)	29	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	187/187 (100%)	179 (96%)	8 (4%)	29	53
2	H	187/187 (100%)	179 (96%)	8 (4%)	29	53
All	All	1512/1512 (100%)	1456 (96%)	56 (4%)	37	58

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	93	GLN
1	A	94	GLN
1	A	106	THR
1	A	146	LYS
1	A	164	LEU
2	B	538	LYS
2	B	539	GLN
2	B	540	ARG
2	B	551	ILE
2	B	609	GLN
2	B	657	THR
2	B	681	LEU
2	B	687	VAL
1	C	1032	TYR
1	C	1093	GLN
1	C	1094	GLN
1	C	1106	THR
1	C	1146	LYS
1	C	1164	LEU
2	D	1538	LYS
2	D	1539	GLN
2	D	1540	ARG
2	D	1551	ILE
2	D	1609	GLN
2	D	1657	THR
2	D	1681	LEU
2	D	1687	VAL
1	E	2032	TYR
1	E	2093	GLN
1	E	2094	GLN
1	E	2106	THR
1	E	2146	LYS
1	E	2164	LEU

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Mol	Chain	Res	Type
2	F	2538	LYS
2	F	2539	GLN
2	F	2540	ARG
2	F	2551	ILE
2	F	2609	GLN
2	F	2657	THR
2	F	2681	LEU
2	F	2687	VAL
1	G	3032	TYR
1	G	3093	GLN
1	G	3094	GLN
1	G	3106	THR
1	G	3146	LYS
1	G	3164	LEU
2	H	3538	LYS
2	H	3539	GLN
2	H	3540	ARG
2	H	3551	ILE
2	H	3609	GLN
2	H	3657	THR
2	H	3681	LEU
2	H	3687	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	96	ASN
2	B	539	GLN
1	C	1042	GLN
1	C	1094	GLN
1	C	1096	ASN
2	D	1539	GLN
1	E	2042	GLN
1	E	2096	ASN
2	F	2539	GLN
1	G	3042	GLN
1	G	3094	GLN
1	G	3096	ASN
2	H	3539	GLN

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 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.

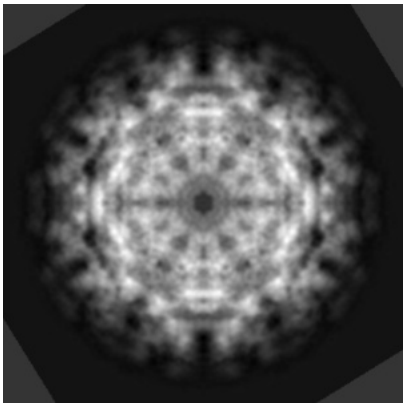
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5580. These allow visual inspection of the internal detail of the map and identification of artifacts.

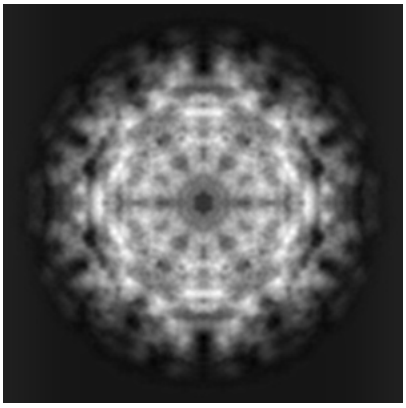
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

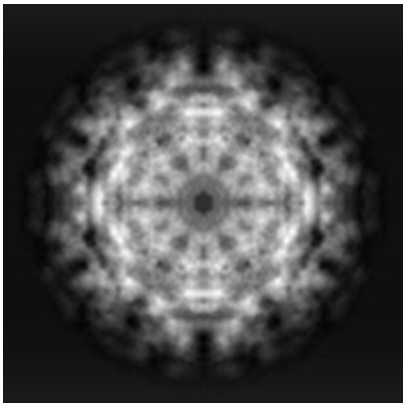
6.1.1 Primary map



X



Y

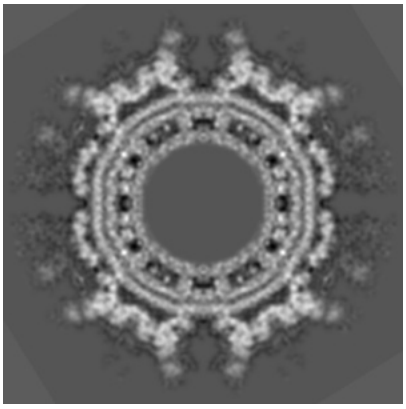


Z

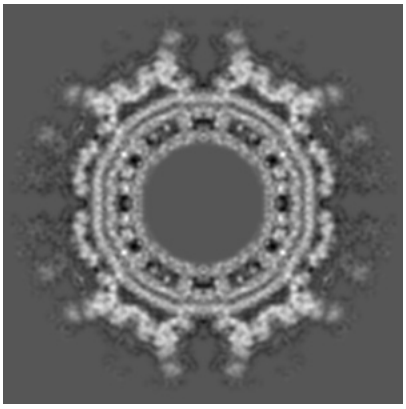
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

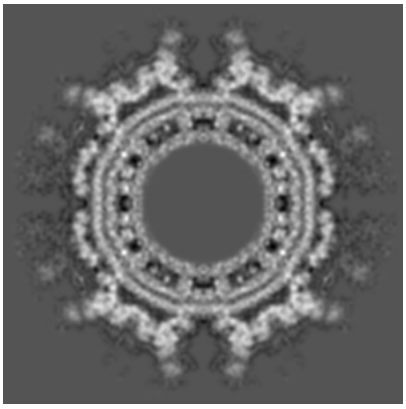
6.2.1 Primary map



X Index: 200



Y Index: 200

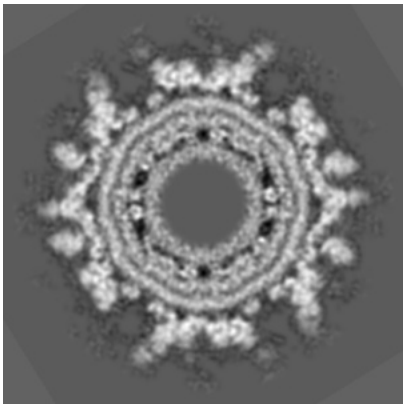


Z Index: 200

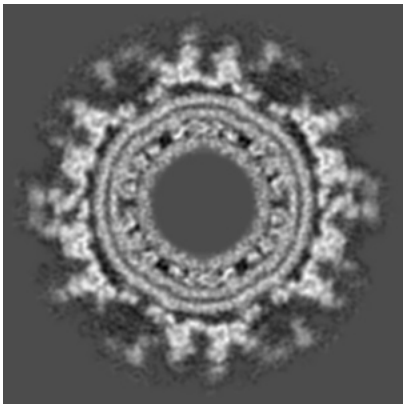
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

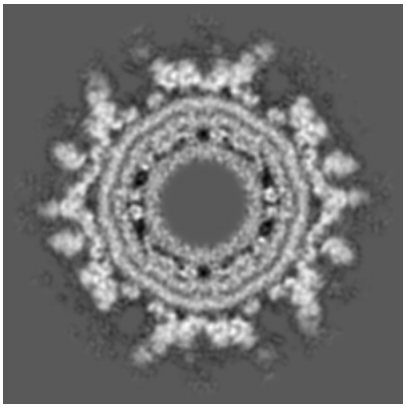
6.3.1 Primary map



X Index: 157



Y Index: 231

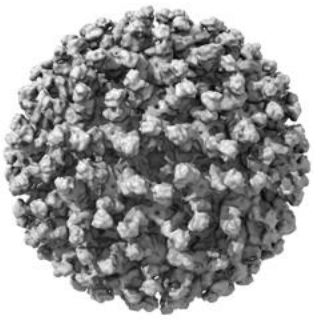


Z Index: 157

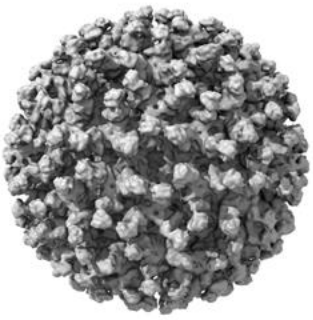
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

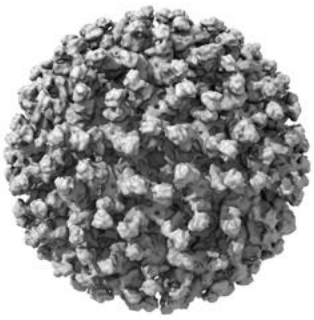
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

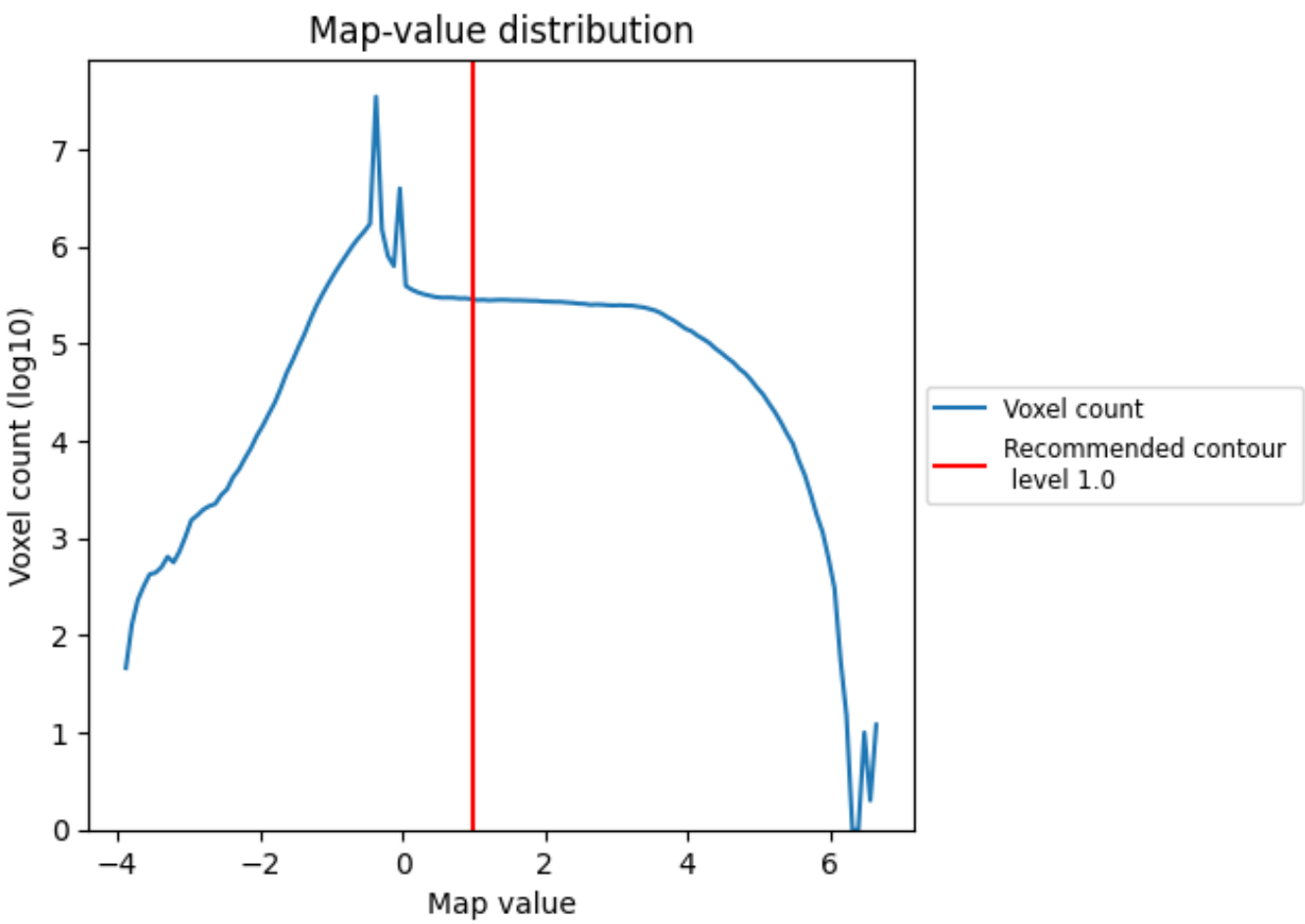
6.5 Mask visualisation (i)

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

7 Map analysis (i)

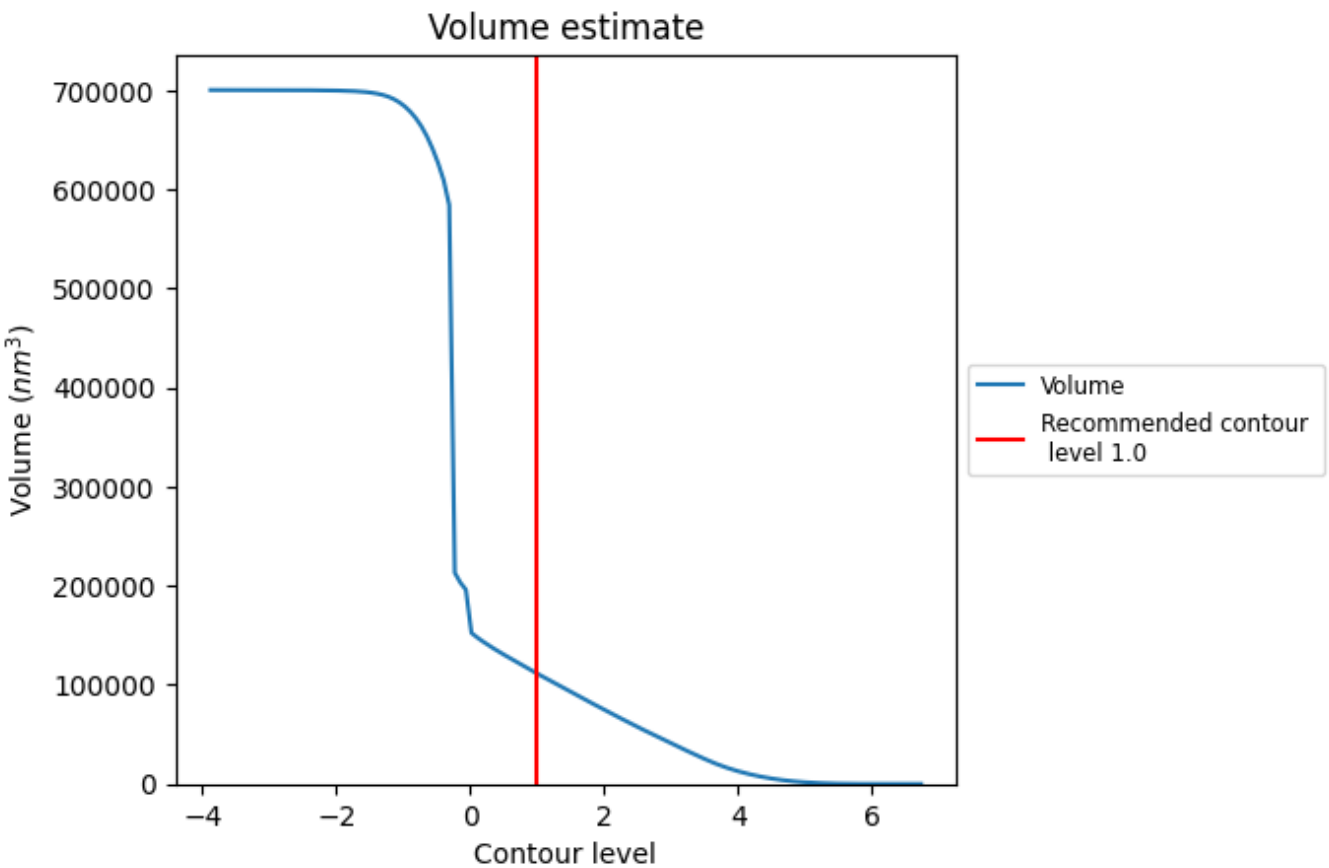
This section contains the results of statistical analysis of the map.

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.

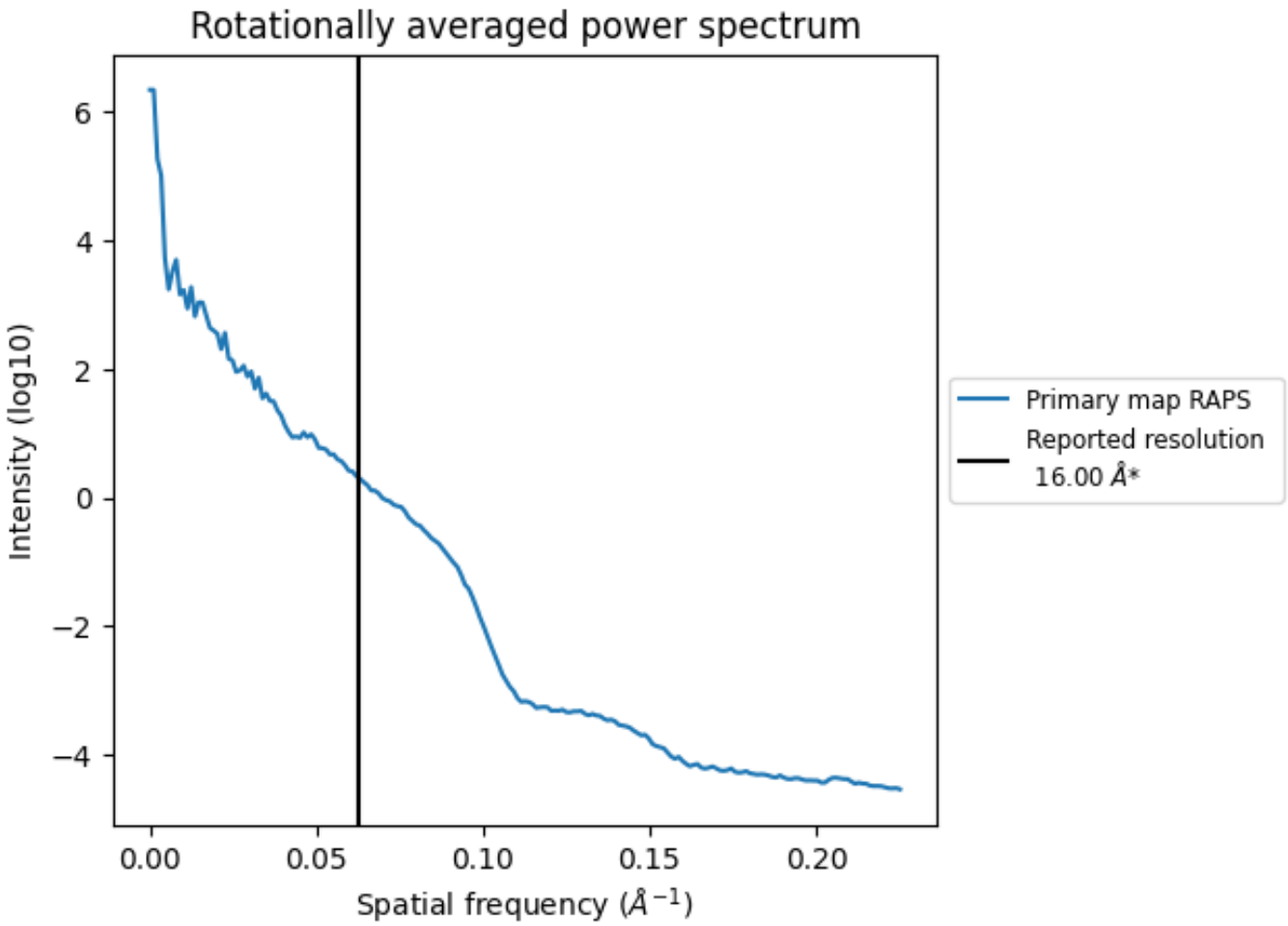
7.2 Volume estimate (i)



The volume at the recommended contour level is 111413 nm^3; this corresponds to an approximate mass of 100642 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 0.062 Å^{-1}

8 Fourier-Shell correlation (i)

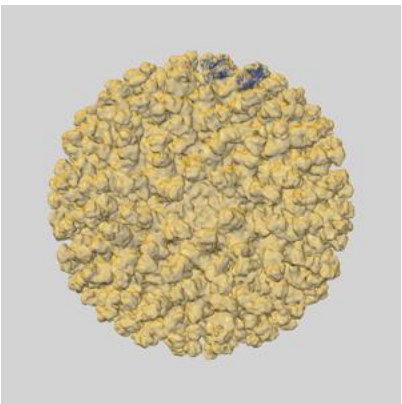
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

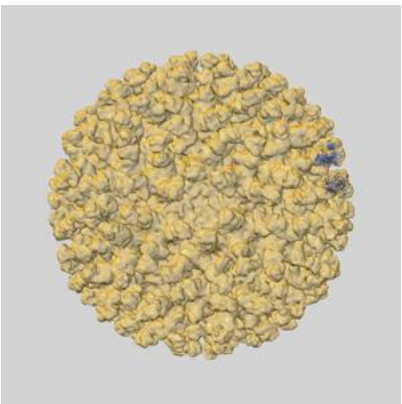
This section contains information regarding the fit between EMDB map EMD-5580 and PDB model 3J30. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

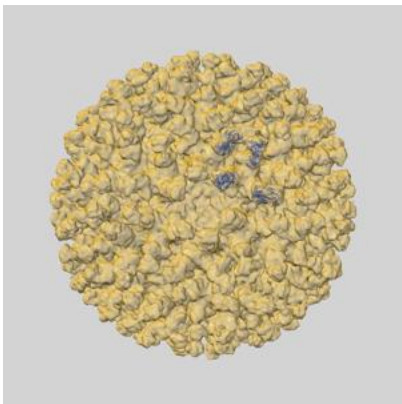
9.1.1 Map-model overlay (i)



X

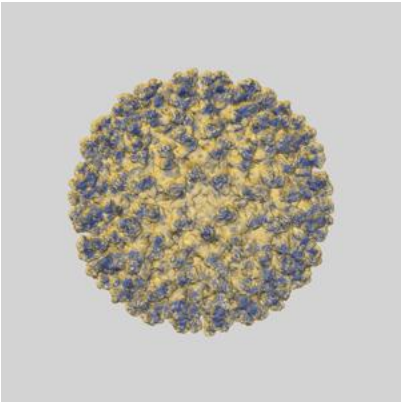


Y

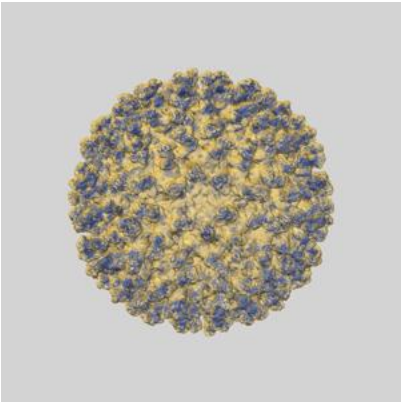


Z

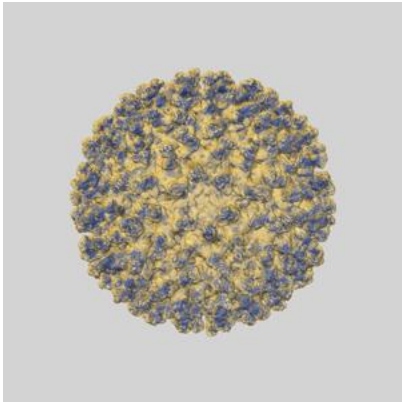
9.1.2 Map-model assembly overlay (i)



X



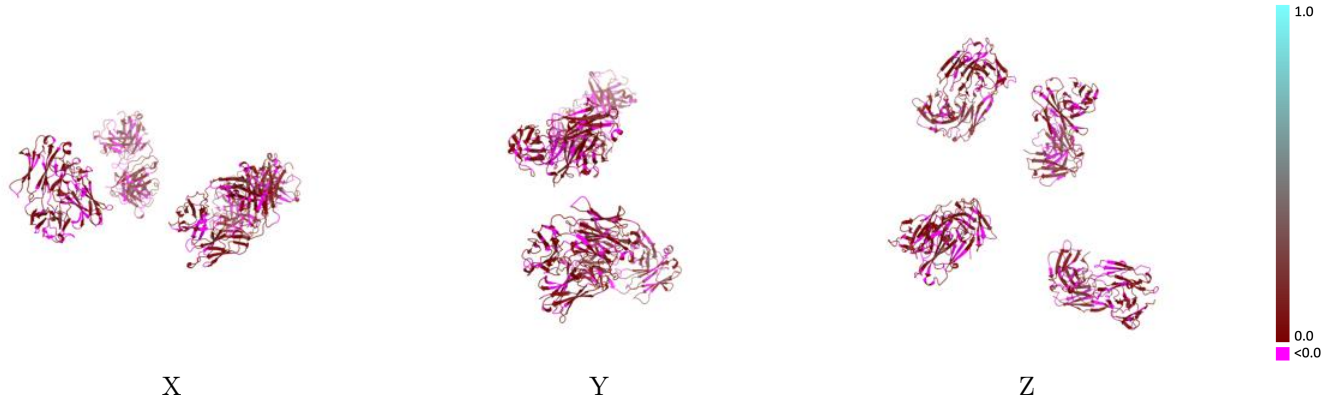
Y



Z

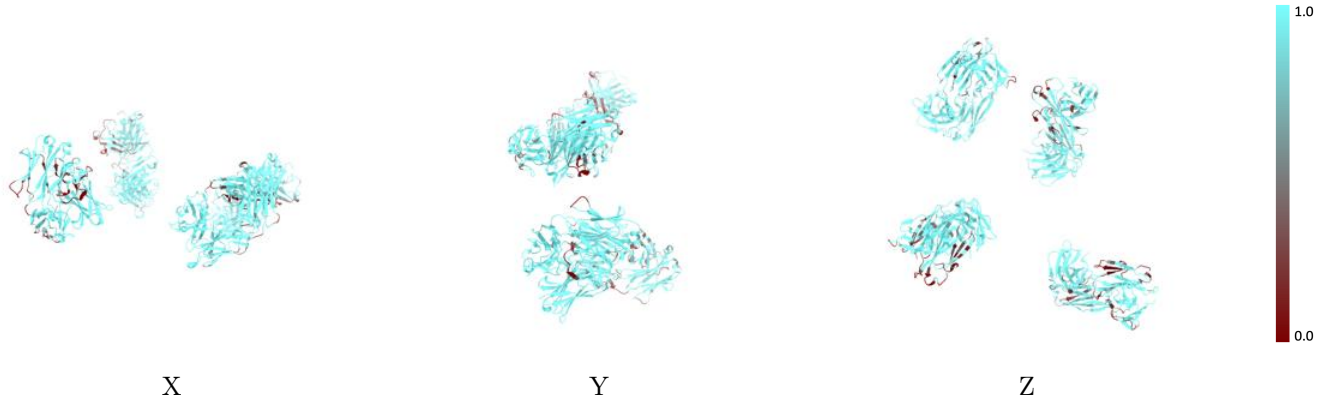
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



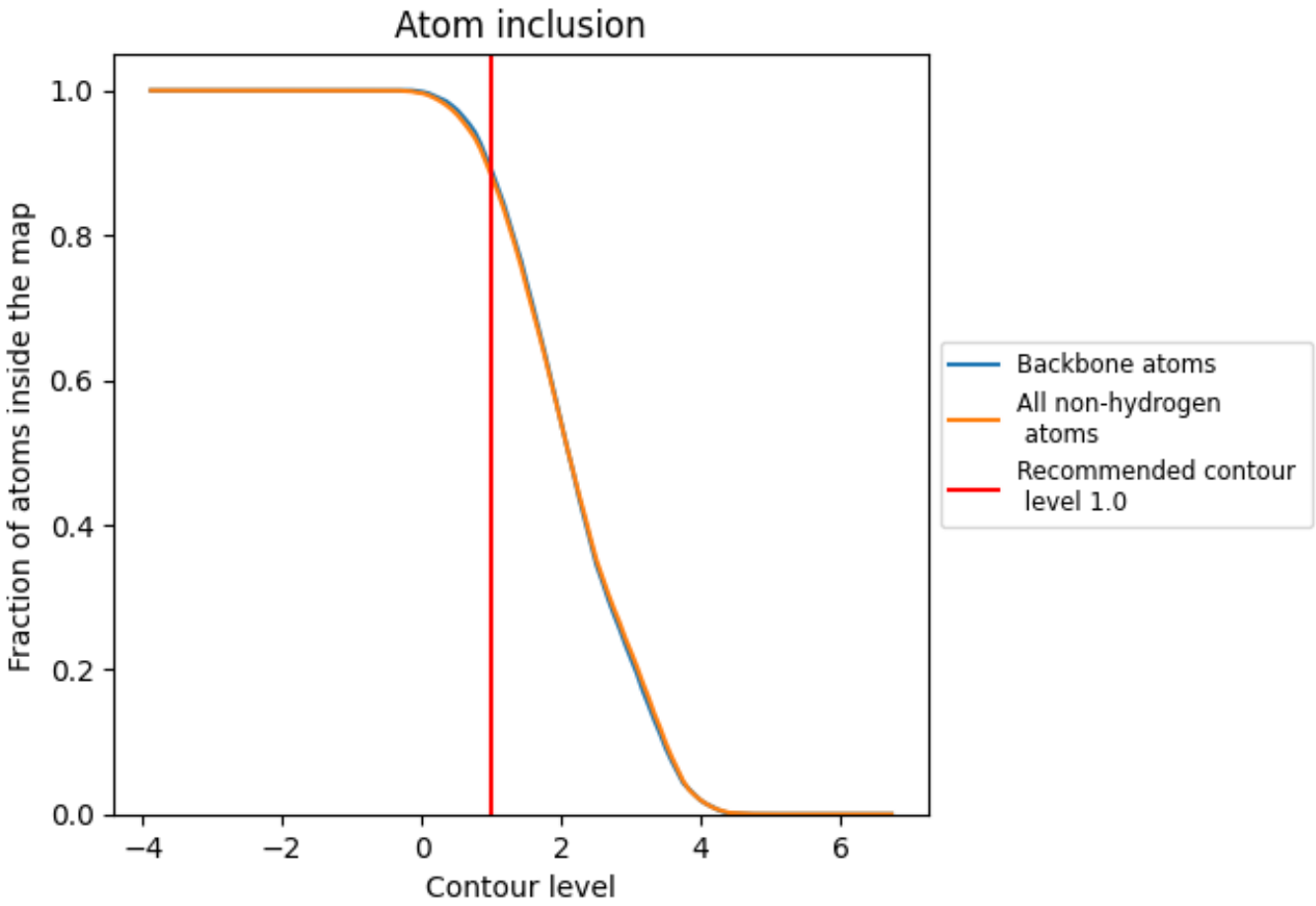
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8827	0.0500
A	0.9550	0.0620
B	0.9198	0.0610
C	0.8955	0.0580
D	0.8434	0.0500
E	0.8426	0.0450
F	0.8117	0.0210
G	0.9216	0.0510
H	0.8701	0.0500