Full wwPDB EM Validation Report

Nov 21, 2022 – 09:42 PM EST

PDB ID	:	3J42
EMDB ID	:	EMD-5674
Title	:	Obstruction of Dengue Virus Maturation by Fab Fragments of the 2H2 Antibody
Authors	:	Wang, Z.; Pennington, J.G.; Jiang, W.; Rossmann, M.G.
Deposited on	:	2013-06-13
Resolution	:	21.00 Å(reported)
Based on initial models	:	3C6D, 4KVC

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:

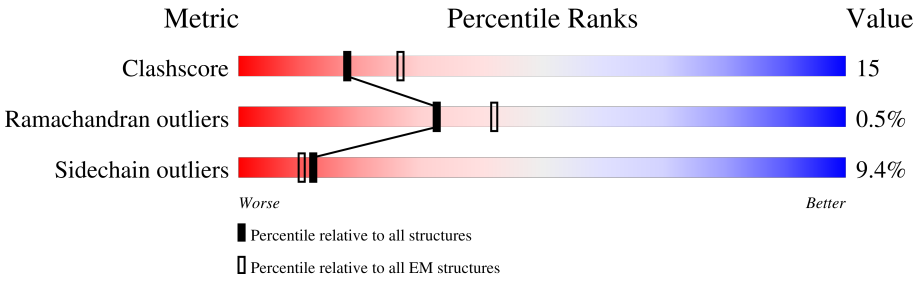
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 21.00 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	390	99%
1	B	390	99%
1	C	390	100%
2	D	81	100%
2	E	81	99%
2	F	81	99%
3	G	221	5% 76% 19%
3	I	221	6% 72% 24%

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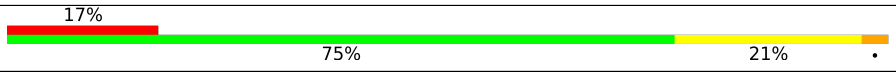
Mol	Chain	Length	Quality of chain
3	K	221	
4	H	212	
4	J	212	
4	L	212	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11226 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 Envelope protein E.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	390	Total C 390 390	0	390
1	B	390	Total C 390 390	0	390
1	C	390	Total C 390 390	0	390

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ILE	MET	CONFLICT	UNP O11875
A	?	-	GLY	DELETION	UNP O11875
A	?	-	GLY	DELETION	UNP O11875
A	?	-	GLN	DELETION	UNP O11875
A	139	VAL	ILE	CONFLICT	UNP O11875
A	162	VAL	ILE	CONFLICT	UNP O11875
A	?	-	PHE	DELETION	UNP O11875
A	?	-	ASN	DELETION	UNP O11875
A	390	ASP	ASN	CONFLICT	UNP O11875
B	6	ILE	MET	CONFLICT	UNP O11875
B	?	-	GLY	DELETION	UNP O11875
B	?	-	GLY	DELETION	UNP O11875
B	?	-	GLN	DELETION	UNP O11875
B	139	VAL	ILE	CONFLICT	UNP O11875
B	162	VAL	ILE	CONFLICT	UNP O11875
B	?	-	PHE	DELETION	UNP O11875
B	?	-	ASN	DELETION	UNP O11875
B	390	ASP	ASN	CONFLICT	UNP O11875
C	6	ILE	MET	CONFLICT	UNP O11875
C	?	-	GLY	DELETION	UNP O11875
C	?	-	GLY	DELETION	UNP O11875
C	?	-	GLN	DELETION	UNP O11875
C	139	VAL	ILE	CONFLICT	UNP O11875
C	162	VAL	ILE	CONFLICT	UNP O11875

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	DELETION	UNP O11875
C	?	-	ASN	DELETION	UNP O11875
C	390	ASP	ASN	CONFLICT	UNP O11875

- Molecule 2 is a protein called PrM.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	D	81	Total C 81 81	0	81
2	E	81	Total C 81 81	0	81
2	F	81	Total C 81 81	0	81

- Molecule 3 is a protein called Ig heavy chain V region MOPC 21, Igh protein chimera.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	G	216	Total C N O S 1633 1034 274 317 8	0	0
3	I	216	Total C N O S 1633 1034 274 317 8	0	0
3	K	216	Total C N O S 1633 1034 274 317 8	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	104	HIS	-	LINKER	UNP Q6PIP8
G	105	TYR	-	LINKER	UNP Q6PIP8
G	180	GLY	ASP	CONFLICT	UNP Q6PIP8
G	199	THR	SER	CONFLICT	UNP Q6PIP8
I	104	HIS	-	LINKER	UNP Q6PIP8
I	105	TYR	-	LINKER	UNP Q6PIP8
I	180	GLY	ASP	CONFLICT	UNP Q6PIP8
I	199	THR	SER	CONFLICT	UNP Q6PIP8
K	104	HIS	-	LINKER	UNP Q6PIP8
K	105	TYR	-	LINKER	UNP Q6PIP8
K	180	GLY	ASP	CONFLICT	UNP Q6PIP8
K	199	THR	SER	CONFLICT	UNP Q6PIP8

- Molecule 4 is a protein called Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	212	Total	C	N	O	S	0	0
			1638	1017	275	338	8		
4	J	212	Total	C	N	O	S	0	0
			1638	1017	275	338	8		
4	L	212	Total	C	N	O	S	0	0
			1638	1017	275	338	8		

There are 9 discrepancies between the modelled and reference sequences:

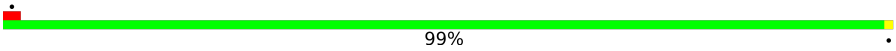
Chain	Residue	Modelled	Actual	Comment	Reference
H	1030	GLY	VAL	CONFLICT	UNP P01634
H	1091	SER	GLY	CONFLICT	UNP P01634
H	1094	THR	TYR	CONFLICT	UNP P01634
J	1030	GLY	VAL	CONFLICT	UNP P01634
J	1091	SER	GLY	CONFLICT	UNP P01634
J	1094	THR	TYR	CONFLICT	UNP P01634
L	1030	GLY	VAL	CONFLICT	UNP P01634
L	1091	SER	GLY	CONFLICT	UNP P01634
L	1094	THR	TYR	CONFLICT	UNP P01634

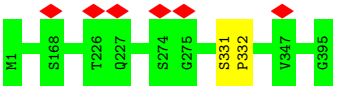
3 Residue-property plots (i)

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: Envelope protein E

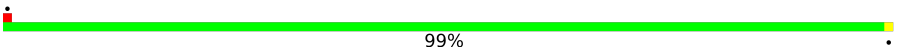
Chain A:

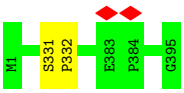




• Molecule 1: Envelope protein E

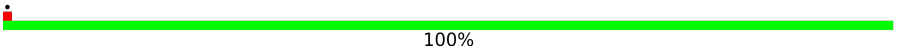
Chain B:

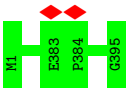




• Molecule 1: Envelope protein E

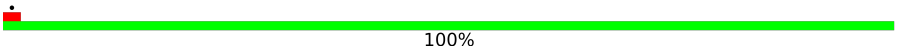
Chain C:

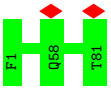




• Molecule 2: PrM

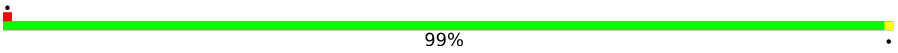
Chain D:

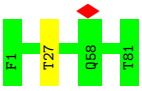




• Molecule 2: PrM

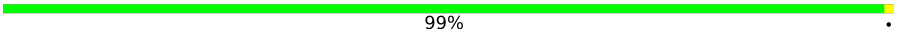
Chain E:





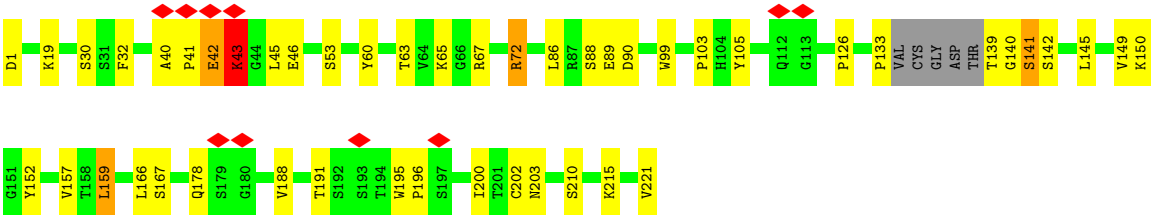
• Molecule 2: PrM

Chain F:



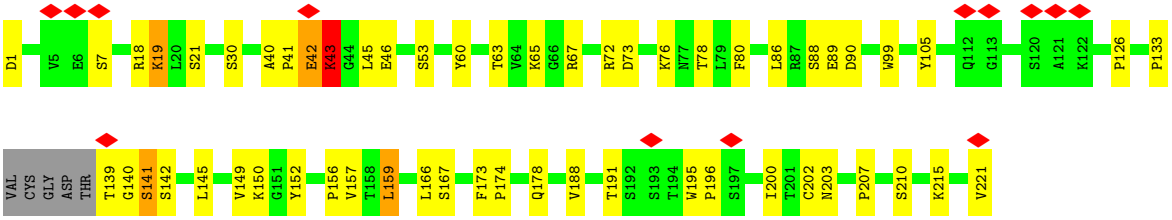
• Molecule 3: Ig heavy chain V region MOPC 21, Igh protein chimera

Chain G:



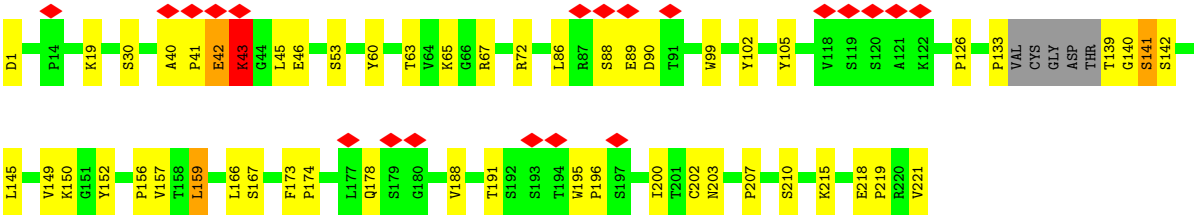
• Molecule 3: Ig heavy chain V region MOPC 21, Igh protein chimera

Chain I:



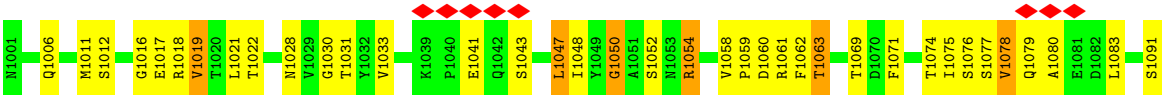
• Molecule 3: Ig heavy chain V region MOPC 21, Igh protein chimera

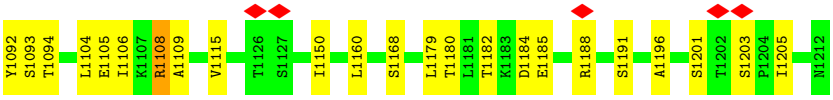
Chain K:



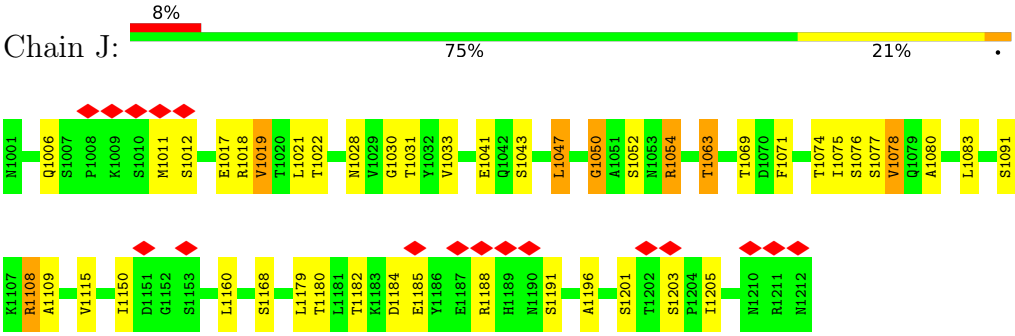
• Molecule 4: Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera

Chain H:

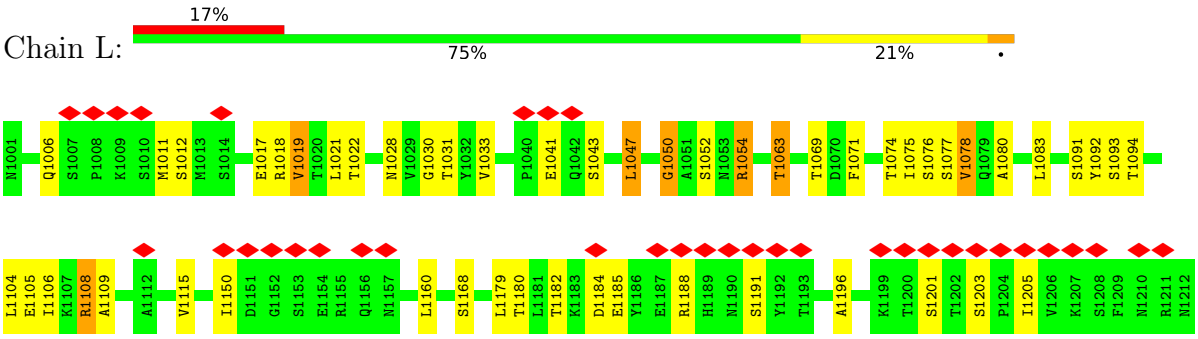




• Molecule 4: Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera



• Molecule 4: Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	378	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Film	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	51040	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	13.343	Depositor
Minimum map value	-4.581	Depositor
Average map value	0.617	Depositor
Map value standard deviation	1.820	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	892.8, 892.8, 892.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.72, 3.72, 3.72	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
3	G	0.62	1/1678 (0.1%)	0.65	0/2290
3	I	0.61	1/1678 (0.1%)	0.65	0/2290
3	K	0.61	1/1678 (0.1%)	0.65	0/2290
4	H	0.76	2/1674 (0.1%)	0.68	2/2273 (0.1%)
4	J	0.76	2/1674 (0.1%)	0.68	2/2273 (0.1%)
4	L	0.76	2/1674 (0.1%)	0.68	2/2273 (0.1%)
All	All	0.69	9/10056 (0.1%)	0.67	6/13689 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1092	TYR	CE2-CZ	-6.20	1.30	1.38
4	L	1092	TYR	CE2-CZ	-6.17	1.30	1.38
4	J	1092	TYR	CE2-CZ	-6.16	1.30	1.38
3	K	46	GLU	CD-OE2	-5.11	1.20	1.25
3	G	46	GLU	CD-OE2	-5.08	1.20	1.25
4	H	1092	TYR	CB-CG	-5.05	1.44	1.51
3	I	46	GLU	CD-OE2	-5.04	1.20	1.25
4	L	1092	TYR	CB-CG	-5.04	1.44	1.51
4	J	1092	TYR	CB-CG	-5.04	1.44	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1047	LEU	CA-CB-CG	7.42	132.35	115.30
4	J	1047	LEU	CA-CB-CG	7.38	132.28	115.30
4	L	1047	LEU	CA-CB-CG	7.38	132.28	115.30
4	H	1050	GLY	C-N-CA	-5.27	108.52	121.70
4	L	1050	GLY	C-N-CA	-5.25	108.58	121.70
4	J	1050	GLY	C-N-CA	-5.25	108.58	121.70

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	390	0	0	1	0
1	B	390	0	0	1	0
1	C	390	0	0	0	0
2	D	81	0	0	0	0
2	E	81	0	0	3	0
2	F	81	0	0	1	0
3	G	1633	0	1585	53	0
3	I	1633	0	1584	115	0
3	K	1633	0	1585	54	0
4	H	1638	0	1564	94	0
4	J	1638	0	1565	31	0
4	L	1638	0	1565	31	0
All	All	11226	0	9448	307	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 15.

All (307) 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)
3:I:42:GLU:HA	3:I:43:LYS:CG	1.43	1.48
3:G:42:GLU:HA	3:G:43:LYS:CG	1.43	1.47
3:K:42:GLU:CA	3:K:43:LYS:HG2	1.46	1.46
3:G:42:GLU:CA	3:G:43:LYS:HG2	1.46	1.46
3:K:42:GLU:HA	3:K:43:LYS:CG	1.43	1.45
3:I:42:GLU:CA	3:I:43:LYS:HG2	1.46	1.44
4:H:1076:SER:O	3:I:19:LYS:HE3	1.19	1.34
4:H:1060:ASP:OD1	3:I:73:ASP:CB	1.74	1.32
4:H:1060:ASP:C	3:I:80:PHE:HZ	1.38	1.26
4:H:1060:ASP:O	3:I:80:PHE:HZ	1.11	1.23
4:H:1060:ASP:O	3:I:80:PHE:CZ	1.90	1.23
4:H:1058:VAL:CG1	3:I:76:LYS:HE3	1.69	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1058:VAL:CG1	3:I:76:LYS:CE	2.27	1.11
4:H:1060:ASP:OD1	3:I:73:ASP:HB3	0.92	1.09
3:K:139:THR:N	3:K:140:GLY:HA3	1.61	1.09
3:G:139:THR:N	3:G:140:GLY:HA3	1.61	1.08
3:I:139:THR:N	3:I:140:GLY:HA3	1.61	1.06
4:H:1060:ASP:C	3:I:80:PHE:CZ	2.28	1.02
4:H:1077:SER:OG	3:I:19:LYS:O	1.80	0.99
3:I:42:GLU:HA	3:I:43:LYS:CB	1.93	0.99
4:H:1058:VAL:HG11	3:I:76:LYS:CE	1.92	0.98
3:G:42:GLU:HA	3:G:43:LYS:CB	1.93	0.98
4:H:1058:VAL:HG12	3:I:76:LYS:HE3	1.44	0.98
4:H:1076:SER:O	3:I:19:LYS:CE	2.12	0.98
4:H:1061:ARG:HA	3:I:80:PHE:CE1	1.97	0.97
3:K:42:GLU:HA	3:K:43:LYS:CB	1.93	0.97
4:H:1058:VAL:HG12	3:I:76:LYS:CE	1.92	0.95
4:H:1061:ARG:HG2	3:I:21:SER:OG	1.67	0.94
3:K:139:THR:N	3:K:140:GLY:CA	2.29	0.94
3:I:139:THR:N	3:I:140:GLY:CA	2.29	0.94
4:H:1076:SER:C	3:I:19:LYS:HG2	1.88	0.94
4:H:1054:ARG:NE	3:I:73:ASP:OD2	2.02	0.92
3:G:139:THR:N	3:G:140:GLY:CA	2.29	0.91
4:H:1054:ARG:HA	3:I:76:LYS:HZ1	1.32	0.91
4:L:1083:LEU:HD21	4:L:1106:ILE:HG13	1.55	0.89
4:H:1076:SER:C	3:I:19:LYS:HE3	1.93	0.89
4:J:1083:LEU:HD21	4:J:1106:ILE:HG13	1.55	0.88
3:K:42:GLU:HA	3:K:43:LYS:HG2	0.88	0.88
4:H:1079:GLN:NE2	3:I:7:SER:OG	2.06	0.87
3:G:42:GLU:HA	3:G:43:LYS:HG2	0.88	0.87
3:I:42:GLU:HA	3:I:43:LYS:HG2	0.88	0.87
4:H:1054:ARG:HA	3:I:76:LYS:NZ	1.87	0.86
4:H:1083:LEU:HD21	4:H:1106:ILE:HG13	1.55	0.86
4:L:1054:ARG:HH21	4:L:1063:THR:HA	1.41	0.85
4:H:1054:ARG:HH21	4:H:1063:THR:HA	1.41	0.84
3:I:140:GLY:O	3:I:141:SER:HB3	1.76	0.84
3:K:41:PRO:O	3:K:43:LYS:HE2	1.79	0.83
3:K:140:GLY:O	3:K:141:SER:HB3	1.76	0.83
3:G:140:GLY:O	3:G:141:SER:HB3	1.76	0.83
3:I:41:PRO:O	3:I:43:LYS:HE2	1.79	0.83
3:G:41:PRO:O	3:G:43:LYS:HE2	1.79	0.82
3:G:42:GLU:C	3:G:43:LYS:HG2	2.00	0.82
4:H:1058:VAL:CG1	3:I:76:LYS:HE2	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:42:GLU:C	3:K:43:LYS:HG2	2.00	0.82
4:J:1054:ARG:HH21	4:J:1063:THR:HA	1.42	0.82
3:K:42:GLU:CB	3:K:43:LYS:HE2	2.10	0.82
3:I:42:GLU:C	3:I:43:LYS:HG2	2.00	0.81
3:G:42:GLU:CB	3:G:43:LYS:HE2	2.10	0.81
3:I:42:GLU:CB	3:I:43:LYS:HE2	2.10	0.80
4:H:1016:GLY:HA3	3:I:18:ARG:CZ	2.11	0.80
3:K:41:PRO:O	3:K:43:LYS:CE	2.30	0.79
3:G:41:PRO:O	3:G:43:LYS:CE	2.30	0.79
3:I:41:PRO:O	3:I:43:LYS:CE	2.30	0.79
4:H:1077:SER:N	3:I:19:LYS:HG2	1.99	0.78
3:I:140:GLY:O	3:I:141:SER:CB	2.30	0.77
3:G:67:ARG:NH2	3:G:90:ASP:OD2	2.17	0.77
3:K:67:ARG:NH2	3:K:90:ASP:OD2	2.17	0.77
2:E:27:THR:CA	3:G:103:PRO:CD	2.63	0.77
3:I:42:GLU:HB2	3:I:43:LYS:HE2	1.67	0.76
3:I:67:ARG:NH2	3:I:90:ASP:OD2	2.17	0.76
3:G:42:GLU:HB2	3:G:43:LYS:HE2	1.67	0.76
4:H:1033:VAL:O	4:H:1050:GLY:O	2.04	0.75
4:H:1058:VAL:CB	3:I:76:LYS:HE3	2.16	0.75
3:I:42:GLU:CB	3:I:43:LYS:HG2	2.17	0.75
4:J:1033:VAL:O	4:J:1050:GLY:O	2.04	0.75
3:K:42:GLU:HB2	3:K:43:LYS:HE2	1.67	0.75
4:L:1033:VAL:O	4:L:1050:GLY:O	2.04	0.75
4:H:1060:ASP:CG	3:I:73:ASP:HB3	2.04	0.75
3:G:42:GLU:CB	3:G:43:LYS:HG2	2.17	0.74
3:K:42:GLU:CB	3:K:43:LYS:HG2	2.17	0.73
2:E:27:THR:CA	3:G:103:PRO:HD2	2.18	0.73
4:H:1077:SER:CB	3:I:19:LYS:O	2.38	0.71
3:I:42:GLU:CA	3:I:43:LYS:HE2	2.21	0.71
3:G:42:GLU:CA	3:G:43:LYS:HE2	2.21	0.71
4:H:1061:ARG:HA	3:I:80:PHE:CZ	2.26	0.71
3:G:42:GLU:CA	3:G:43:LYS:CG	2.29	0.70
4:H:1061:ARG:HA	3:I:80:PHE:HE1	1.55	0.70
3:K:42:GLU:CA	3:K:43:LYS:HE2	2.21	0.70
4:J:1115:VAL:HG21	4:J:1205:ILE:HD13	1.74	0.69
3:G:133:PRO:HD3	3:G:145:LEU:HD23	1.75	0.69
4:H:1115:VAL:HG21	4:H:1205:ILE:HD13	1.75	0.69
3:K:133:PRO:HD3	3:K:145:LEU:HD23	1.75	0.68
3:I:133:PRO:HD3	3:I:145:LEU:HD23	1.75	0.68
4:L:1115:VAL:HG21	4:L:1205:ILE:HD13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:140:GLY:O	3:G:141:SER:CB	2.30	0.68
3:K:140:GLY:O	3:K:141:SER:CB	2.30	0.67
4:H:1058:VAL:HG11	3:I:76:LYS:HE2	1.69	0.67
4:H:1054:ARG:CD	3:I:73:ASP:OD2	2.43	0.67
3:G:42:GLU:HG2	3:G:43:LYS:HG2	1.76	0.67
3:I:42:GLU:HG2	3:I:43:LYS:HG2	1.76	0.67
4:L:1080:ALA:HA	4:L:1106:ILE:HD11	1.77	0.67
4:J:1196:ALA:HB3	4:J:1205:ILE:HD11	1.77	0.66
3:I:42:GLU:CA	3:I:43:LYS:CB	2.70	0.66
3:K:42:GLU:HG2	3:K:43:LYS:HG2	1.76	0.66
3:G:42:GLU:HA	3:G:43:LYS:CD	2.25	0.66
4:H:1196:ALA:HB3	4:H:1205:ILE:HD11	1.77	0.66
4:H:1060:ASP:CG	3:I:80:PHE:CE2	2.69	0.66
3:K:42:GLU:HA	3:K:43:LYS:CD	2.24	0.66
4:L:1196:ALA:HB3	4:L:1205:ILE:HD11	1.77	0.66
4:J:1080:ALA:HA	4:J:1106:ILE:HD11	1.77	0.66
4:H:1080:ALA:HA	4:H:1106:ILE:HD11	1.77	0.65
4:L:1052:SER:O	4:L:1054:ARG:NH1	2.29	0.65
4:H:1054:ARG:CA	3:I:76:LYS:NZ	2.59	0.65
3:I:41:PRO:O	3:I:43:LYS:NZ	2.30	0.65
4:J:1052:SER:O	4:J:1054:ARG:NH1	2.29	0.65
3:K:140:GLY:O	3:K:142:SER:N	2.30	0.65
3:K:41:PRO:O	3:K:43:LYS:NZ	2.30	0.64
3:I:140:GLY:O	3:I:142:SER:N	2.30	0.64
3:G:42:GLU:CA	3:G:43:LYS:CB	2.70	0.64
4:H:1052:SER:O	4:H:1054:ARG:NH1	2.29	0.64
4:H:1054:ARG:CZ	3:I:73:ASP:OD2	2.46	0.64
3:G:41:PRO:O	3:G:43:LYS:NZ	2.30	0.64
4:H:1061:ARG:CA	3:I:80:PHE:CE1	2.79	0.63
4:H:1060:ASP:N	3:I:78:THR:OG1	2.26	0.63
4:H:1060:ASP:OD1	3:I:73:ASP:HB2	1.92	0.63
3:K:42:GLU:CA	3:K:43:LYS:CB	2.70	0.63
3:G:140:GLY:O	3:G:142:SER:N	2.30	0.62
3:I:42:GLU:HA	3:I:43:LYS:CD	2.25	0.62
3:G:42:GLU:CG	3:G:43:LYS:HG2	2.30	0.61
4:H:1054:ARG:CA	3:I:76:LYS:HZ1	2.09	0.61
3:K:42:GLU:CG	3:K:43:LYS:HG2	2.30	0.61
4:L:1182:THR:OG1	4:L:1184:ASP:OD1	2.12	0.61
3:I:42:GLU:CG	3:I:43:LYS:HG2	2.30	0.60
3:K:42:GLU:CA	3:K:43:LYS:CG	2.29	0.59
4:H:1060:ASP:O	3:I:80:PHE:CE2	2.53	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1061:ARG:N	3:I:80:PHE:CZ	2.71	0.59
4:H:1076:SER:C	3:I:19:LYS:CE	2.58	0.58
3:K:42:GLU:HA	3:K:43:LYS:HE2	1.85	0.58
4:H:1182:THR:OG1	4:H:1184:ASP:OD1	2.12	0.58
4:J:1019:VAL:HG11	4:J:1104:LEU:HD11	1.86	0.57
4:H:1058:VAL:HB	3:I:76:LYS:HE3	1.84	0.57
3:G:42:GLU:HG2	3:G:43:LYS:CG	2.35	0.57
3:G:42:GLU:HA	3:G:43:LYS:HE2	1.85	0.56
4:J:1182:THR:OG1	4:J:1184:ASP:OD1	2.13	0.56
4:H:1058:VAL:HG12	3:I:76:LYS:HE2	1.72	0.56
4:H:1019:VAL:HG11	4:H:1104:LEU:HD11	1.86	0.56
4:H:1077:SER:HB3	3:I:19:LYS:HB3	1.88	0.56
4:L:1019:VAL:HG11	4:L:1104:LEU:HD11	1.86	0.56
3:K:42:GLU:HG2	3:K:43:LYS:CG	2.35	0.55
4:H:1076:SER:O	3:I:19:LYS:HG2	2.06	0.55
3:I:42:GLU:CA	3:I:43:LYS:CG	2.29	0.55
3:I:42:GLU:HG2	3:I:43:LYS:CG	2.35	0.55
4:H:1061:ARG:CA	3:I:80:PHE:CZ	2.89	0.55
4:H:1061:ARG:N	3:I:80:PHE:HZ	1.99	0.55
4:H:1062:PHE:HB2	3:I:76:LYS:HE2	1.89	0.54
3:I:40:ALA:HB1	3:I:41:PRO:HD2	1.90	0.54
3:K:40:ALA:HB1	3:K:41:PRO:HD2	1.90	0.54
4:H:1006:GLN:HG2	4:H:1021:LEU:HD21	1.91	0.53
4:L:1006:GLN:HG2	4:L:1021:LEU:HD21	1.90	0.53
3:G:166:LEU:HD11	3:G:200:ILE:HD12	1.91	0.53
4:H:1048:ILE:CD1	3:I:76:LYS:HZ3	2.22	0.52
3:K:99:TRP:CZ2	3:K:105:TYR:HB3	2.45	0.52
2:E:27:THR:CA	3:G:103:PRO:CG	2.88	0.52
3:K:166:LEU:HD11	3:K:200:ILE:HD12	1.91	0.52
4:J:1006:GLN:HG2	4:J:1021:LEU:HD21	1.91	0.52
3:G:40:ALA:HB1	3:G:41:PRO:HD2	1.90	0.52
3:G:99:TRP:CZ2	3:G:105:TYR:HB3	2.45	0.52
4:H:1108:ARG:HD3	4:H:1109:ALA:O	2.10	0.51
3:I:42:GLU:HA	3:I:43:LYS:HE2	1.85	0.51
4:L:1108:ARG:HD3	4:L:1109:ALA:O	2.10	0.51
3:I:166:LEU:HD11	3:I:200:ILE:HD12	1.91	0.51
3:K:42:GLU:C	3:K:43:LYS:CG	2.71	0.51
4:H:1062:PHE:O	3:I:76:LYS:HD2	2.10	0.51
3:I:99:TRP:CZ2	3:I:105:TYR:HB3	2.45	0.51
4:H:1077:SER:HB3	3:I:19:LYS:O	2.10	0.51
4:J:1108:ARG:HD3	4:J:1109:ALA:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:210:SER:O	3:I:210:SER:OG	2.29	0.51
4:H:1019:VAL:HG23	4:H:1075:ILE:HB	1.93	0.51
4:J:1019:VAL:HG23	4:J:1075:ILE:HB	1.93	0.51
3:I:221:VAL:O	3:I:221:VAL:CG1	2.59	0.51
3:G:210:SER:O	3:G:210:SER:OG	2.29	0.50
4:L:1019:VAL:HG23	4:L:1075:ILE:HB	1.93	0.50
3:G:126:PRO:HB3	3:G:152:TYR:HB3	1.94	0.50
3:G:221:VAL:CG1	3:G:221:VAL:O	2.59	0.50
3:I:42:GLU:OE2	3:I:42:GLU:O	2.30	0.50
4:J:1201:SER:OG	4:J:1203:SER:O	2.24	0.50
3:K:221:VAL:O	3:K:221:VAL:CG1	2.59	0.50
4:L:1017:GLU:O	4:L:1078:VAL:HG12	2.12	0.50
4:J:1017:GLU:O	4:J:1078:VAL:HG12	2.12	0.49
3:K:210:SER:O	3:K:210:SER:OG	2.29	0.49
4:H:1017:GLU:O	4:H:1078:VAL:HG12	2.12	0.49
3:I:42:GLU:C	3:I:43:LYS:CG	2.71	0.49
4:L:1083:LEU:HD22	4:L:1105:GLU:HA	1.94	0.49
3:G:42:GLU:OE2	3:G:42:GLU:O	2.30	0.49
3:I:126:PRO:HB3	3:I:152:TYR:HB3	1.94	0.49
3:K:126:PRO:HB3	3:K:152:TYR:HB3	1.94	0.49
3:I:42:GLU:HA	3:I:43:LYS:CE	2.43	0.49
3:K:195:TRP:CD1	3:K:196:PRO:HA	2.48	0.49
3:G:42:GLU:C	3:G:43:LYS:CG	2.71	0.49
3:K:42:GLU:HA	3:K:43:LYS:CE	2.43	0.49
3:G:195:TRP:CD1	3:G:196:PRO:HA	2.48	0.48
4:H:1184:ASP:OD1	4:H:1185:GLU:N	2.47	0.48
4:J:1184:ASP:OD1	4:J:1185:GLU:N	2.46	0.48
3:K:42:GLU:OE2	3:K:42:GLU:O	2.30	0.48
4:H:1083:LEU:HD22	4:H:1105:GLU:HA	1.94	0.48
3:I:195:TRP:CD1	3:I:196:PRO:HA	2.48	0.48
4:J:1083:LEU:HD22	4:J:1105:GLU:HA	1.94	0.48
4:L:1184:ASP:OD1	4:L:1185:GLU:N	2.47	0.48
3:K:63:THR:O	3:K:67:ARG:NH1	2.47	0.48
4:H:1059:PRO:O	3:I:76:LYS:HD3	2.14	0.48
3:G:42:GLU:HA	3:G:43:LYS:CE	2.43	0.48
2:F:26:LYS:CA	3:K:102:TYR:O	2.62	0.47
4:H:1188:ARG:HD3	4:H:1188:ARG:HA	1.68	0.47
4:L:1188:ARG:HA	4:L:1188:ARG:HD3	1.68	0.47
3:G:60:TYR:HB2	3:G:65:LYS:HG3	1.96	0.47
3:K:60:TYR:HB2	3:K:65:LYS:HG3	1.96	0.47
3:I:99:TRP:HH2	4:J:1091:SER:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:42:GLU:CB	3:K:43:LYS:CE	2.90	0.47
3:I:63:THR:O	3:I:67:ARG:NH1	2.47	0.47
4:J:1196:ALA:HB3	4:J:1205:ILE:CD1	2.44	0.47
3:K:99:TRP:HH2	4:L:1091:SER:HB2	1.79	0.47
3:I:60:TYR:HB2	3:I:65:LYS:HG3	1.96	0.47
4:H:1196:ALA:HB3	4:H:1205:ILE:CD1	2.44	0.46
3:G:99:TRP:HH2	4:H:1091:SER:HB2	1.79	0.46
4:H:1006:GLN:HE21	4:H:1021:LEU:HD21	1.81	0.46
4:H:1061:ARG:CA	3:I:80:PHE:HE1	2.23	0.46
4:J:1006:GLN:HE21	4:J:1021:LEU:HD21	1.81	0.46
4:H:1201:SER:OG	4:H:1203:SER:O	2.24	0.46
3:K:149:VAL:HG21	3:K:159:LEU:HD21	1.97	0.46
4:H:1060:ASP:HA	3:I:76:LYS:HB2	1.98	0.46
4:L:1076:SER:HA	4:L:1077:SER:HA	1.71	0.46
4:H:1060:ASP:OD2	3:I:80:PHE:CE2	2.69	0.46
3:I:149:VAL:HG21	3:I:159:LEU:HD21	1.97	0.46
3:G:166:LEU:HD13	3:G:188:VAL:HG21	1.97	0.46
3:I:166:LEU:HD13	3:I:188:VAL:HG21	1.97	0.46
4:J:1076:SER:HA	4:J:1077:SER:HA	1.71	0.46
3:G:63:THR:O	3:G:67:ARG:NH1	2.47	0.45
3:G:149:VAL:HG21	3:G:159:LEU:HD21	1.97	0.45
3:K:166:LEU:HD13	3:K:188:VAL:HG21	1.97	0.45
4:L:1006:GLN:HE21	4:L:1021:LEU:HD21	1.81	0.45
4:H:1054:ARG:HD3	3:I:73:ASP:OD2	2.16	0.45
4:H:1060:ASP:OD1	3:I:80:PHE:CE2	2.70	0.45
3:K:42:GLU:HA	3:K:43:LYS:HB3	1.94	0.45
3:I:139:THR:HG23	3:I:139:THR:O	2.16	0.45
3:K:139:THR:O	3:K:139:THR:HG23	2.15	0.45
3:I:221:VAL:O	3:I:221:VAL:HG13	2.17	0.45
3:G:42:GLU:CB	3:G:43:LYS:CE	2.90	0.44
3:G:139:THR:HG23	3:G:139:THR:O	2.16	0.44
4:L:1196:ALA:HB3	4:L:1205:ILE:CD1	2.44	0.44
3:G:30:SER:O	3:G:53:SER:HB2	2.17	0.44
4:H:1019:VAL:HG11	4:H:1104:LEU:CD1	2.47	0.44
3:K:40:ALA:O	3:K:43:LYS:HA	2.18	0.44
4:J:1188:ARG:HA	4:J:1188:ARG:HD3	1.68	0.44
3:I:40:ALA:O	3:I:43:LYS:HA	2.18	0.44
3:G:150:LYS:HZ1	4:H:1180:THR:HG23	1.83	0.44
4:H:1019:VAL:O	4:H:1074:THR:HA	2.18	0.44
3:K:30:SER:O	3:K:53:SER:HB2	2.17	0.43
4:H:1063:THR:HG23	4:H:1074:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:221:VAL:O	3:K:221:VAL:HG13	2.17	0.43
4:H:1061:ARG:CG	3:I:21:SER:OG	2.53	0.43
4:J:1063:THR:HG23	4:J:1074:THR:OG1	2.19	0.43
4:L:1063:THR:HG23	4:L:1074:THR:OG1	2.19	0.43
4:L:1201:SER:OG	4:L:1203:SER:O	2.24	0.43
3:I:173:PHE:HA	3:I:174:PRO:HD3	1.92	0.43
4:L:1019:VAL:HG11	4:L:1104:LEU:CD1	2.47	0.43
3:I:30:SER:O	3:I:53:SER:HB2	2.17	0.43
4:H:1058:VAL:HG11	3:I:76:LYS:HE3	1.63	0.43
4:J:1019:VAL:HG11	4:J:1104:LEU:CD1	2.47	0.43
3:G:40:ALA:O	3:G:43:LYS:HA	2.18	0.43
3:G:221:VAL:O	3:G:221:VAL:HG13	2.17	0.43
4:H:1060:ASP:CG	3:I:80:PHE:CZ	2.92	0.42
4:H:1071:PHE:CD1	4:H:1071:PHE:N	2.87	0.42
3:I:150:LYS:HZ1	4:J:1180:THR:HG23	1.84	0.42
3:K:218:GLU:HA	3:K:219:PRO:HD3	1.89	0.42
3:I:178:GLN:HB3	4:J:1160:LEU:HD21	2.01	0.42
4:L:1071:PHE:CD1	4:L:1071:PHE:N	2.87	0.42
4:H:1054:ARG:HA	3:I:76:LYS:HZ2	1.77	0.42
4:J:1019:VAL:O	4:J:1074:THR:HA	2.18	0.42
4:L:1019:VAL:O	4:L:1074:THR:HA	2.18	0.42
3:K:150:LYS:HZ1	4:L:1180:THR:HG23	1.85	0.42
3:K:178:GLN:HB3	4:L:1160:LEU:HD21	2.01	0.42
4:J:1071:PHE:CD1	4:J:1071:PHE:N	2.87	0.42
3:G:40:ALA:HB1	3:G:41:PRO:CD	2.50	0.42
4:L:1012:SER:HA	4:L:1105:GLU:HG2	2.02	0.42
3:G:178:GLN:HB3	4:H:1160:LEU:HD21	2.01	0.42
4:H:1012:SER:HA	4:H:1105:GLU:HG2	2.02	0.42
3:K:40:ALA:HB1	3:K:41:PRO:CD	2.50	0.42
4:H:1060:ASP:OD1	3:I:80:PHE:HE2	2.02	0.42
3:I:40:ALA:HB1	3:I:41:PRO:CD	2.50	0.42
4:H:1150:ILE:HD11	4:H:1179:LEU:HD21	2.03	0.41
4:L:1150:ILE:HD11	4:L:1179:LEU:HD21	2.03	0.41
4:H:1076:SER:HA	4:H:1077:SER:HA	1.71	0.41
3:G:32:PHE:O	3:G:72:ARG:NH2	2.45	0.41
4:J:1012:SER:HA	4:J:1105:GLU:HG2	2.02	0.41
4:J:1115:VAL:HG21	4:J:1205:ILE:CD1	2.48	0.41
4:H:1016:GLY:O	3:I:18:ARG:HG3	2.20	0.41
4:L:1019:VAL:CG2	4:L:1075:ILE:HB	2.51	0.41
3:I:42:GLU:CB	3:I:43:LYS:CE	2.90	0.41
3:I:156:PRO:O	3:I:207:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:1019:VAL:CG2	4:J:1075:ILE:HB	2.51	0.41
4:J:1150:ILE:HD11	4:J:1179:LEU:HD21	2.03	0.41
1:A:331:SER:CA	1:A:332:PRO:CA	2.99	0.41
3:K:173:PHE:HA	3:K:174:PRO:HD3	1.92	0.41
1:B:331:SER:CA	1:B:332:PRO:CA	2.99	0.40
4:L:1033:VAL:HG11	4:L:1071:PHE:CD2	2.57	0.40
4:H:1019:VAL:CG2	4:H:1075:ILE:HB	2.51	0.40
3:K:156:PRO:O	3:K:207:PRO:HD2	2.21	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	
3	G	212/221 (96%)	205 (97%)	6 (3%)	1 (0%)	29	69
3	I	212/221 (96%)	205 (97%)	6 (3%)	1 (0%)	29	69
3	K	212/221 (96%)	205 (97%)	6 (3%)	1 (0%)	29	69
4	H	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	29	69
4	J	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	29	69
4	L	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	29	69
All	All	1266/1299 (98%)	1227 (97%)	33 (3%)	6 (0%)	32	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	43	LYS
3	I	43	LYS
3	K	43	LYS
4	H	1030	GLY

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Mol	Chain	Res	Type
4	J	1030	GLY
4	L	1030	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
3	G	183/187 (98%)	166 (91%)	17 (9%)	9 28
3	I	183/187 (98%)	166 (91%)	17 (9%)	9 28
3	K	183/187 (98%)	166 (91%)	17 (9%)	9 28
4	H	188/188 (100%)	170 (90%)	18 (10%)	8 27
4	J	188/188 (100%)	170 (90%)	18 (10%)	8 27
4	L	188/188 (100%)	170 (90%)	18 (10%)	8 27
All	All	1113/1125 (99%)	1008 (91%)	105 (9%)	12 28

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	1	ASP
3	G	19	LYS
3	G	42	GLU
3	G	43	LYS
3	G	45	LEU
3	G	72	ARG
3	G	86	LEU
3	G	88	SER
3	G	89	GLU
3	G	141	SER
3	G	157	VAL
3	G	159	LEU
3	G	167	SER
3	G	191	THR
3	G	202	CYS
3	G	203	ASN

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Mol	Chain	Res	Type
3	G	215	LYS
4	H	1011	MET
4	H	1018	ARG
4	H	1019	VAL
4	H	1022	THR
4	H	1028	ASN
4	H	1031	THR
4	H	1041	GLU
4	H	1043	SER
4	H	1047	LEU
4	H	1054	ARG
4	H	1063	THR
4	H	1069	THR
4	H	1078	VAL
4	H	1093	SER
4	H	1094	THR
4	H	1108	ARG
4	H	1168	SER
4	H	1191	SER
3	I	1	ASP
3	I	19	LYS
3	I	42	GLU
3	I	43	LYS
3	I	45	LEU
3	I	72	ARG
3	I	86	LEU
3	I	88	SER
3	I	89	GLU
3	I	141	SER
3	I	157	VAL
3	I	159	LEU
3	I	167	SER
3	I	191	THR
3	I	202	CYS
3	I	203	ASN
3	I	215	LYS
4	J	1011	MET
4	J	1018	ARG
4	J	1019	VAL
4	J	1022	THR
4	J	1028	ASN
4	J	1031	THR

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Mol	Chain	Res	Type
4	J	1041	GLU
4	J	1043	SER
4	J	1047	LEU
4	J	1054	ARG
4	J	1063	THR
4	J	1069	THR
4	J	1078	VAL
4	J	1093	SER
4	J	1094	THR
4	J	1108	ARG
4	J	1168	SER
4	J	1191	SER
3	K	1	ASP
3	K	19	LYS
3	K	42	GLU
3	K	43	LYS
3	K	45	LEU
3	K	72	ARG
3	K	86	LEU
3	K	88	SER
3	K	89	GLU
3	K	141	SER
3	K	157	VAL
3	K	159	LEU
3	K	167	SER
3	K	191	THR
3	K	202	CYS
3	K	203	ASN
3	K	215	LYS
4	L	1011	MET
4	L	1018	ARG
4	L	1019	VAL
4	L	1022	THR
4	L	1028	ASN
4	L	1031	THR
4	L	1041	GLU
4	L	1043	SER
4	L	1047	LEU
4	L	1054	ARG
4	L	1063	THR
4	L	1069	THR
4	L	1078	VAL

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Mol	Chain	Res	Type
4	L	1093	SER
4	L	1094	THR
4	L	1108	ARG
4	L	1168	SER
4	L	1191	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	H	1079	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.

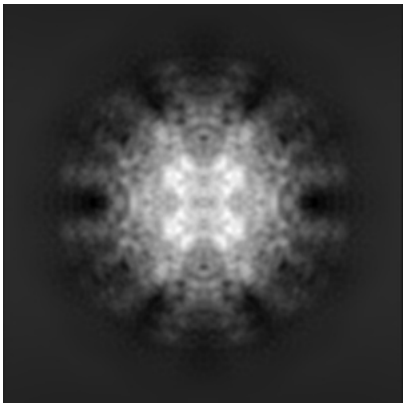
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5674. These allow visual inspection of the internal detail of the map and identification of artifacts.

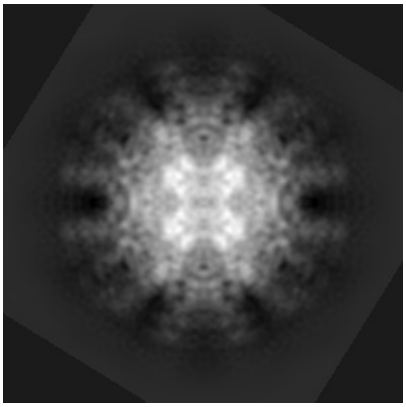
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

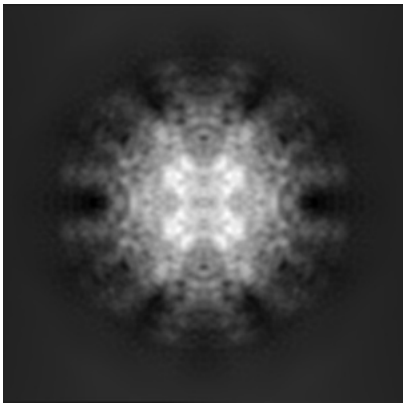
6.1.1 Primary map



X



Y

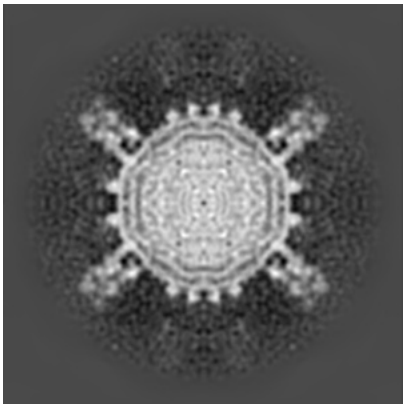


Z

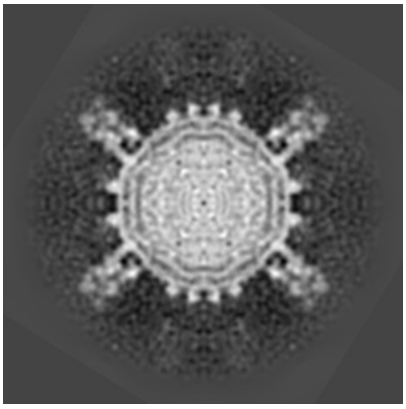
The images above show the map projected in three orthogonal directions.

6.2 Central slices

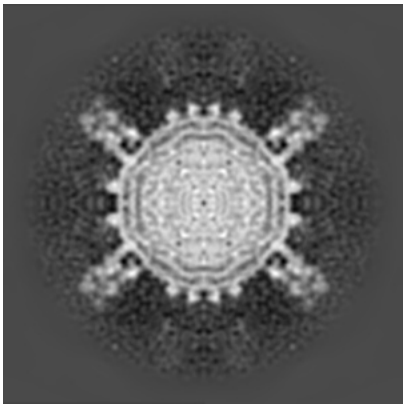
6.2.1 Primary map



X Index: 120



Y Index: 120

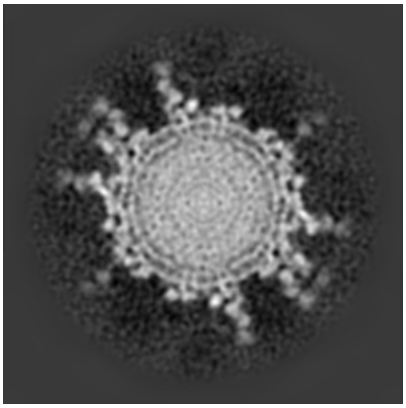


Z Index: 120

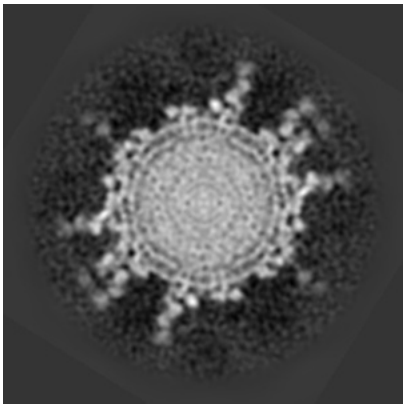
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

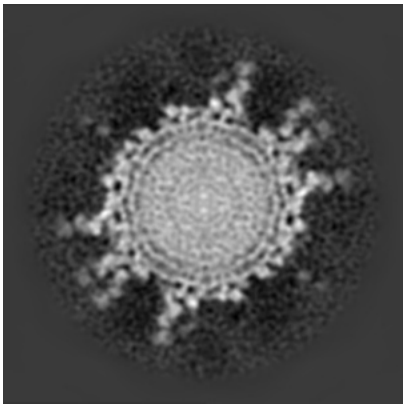
6.3.1 Primary map



X Index: 114



Y Index: 126

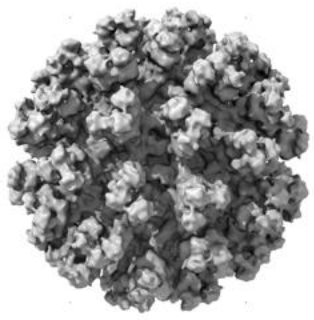


Z Index: 127

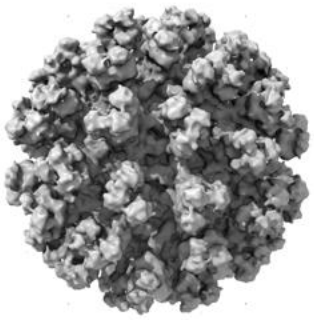
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

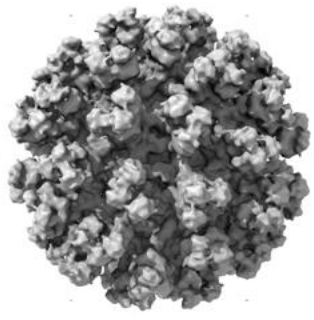
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

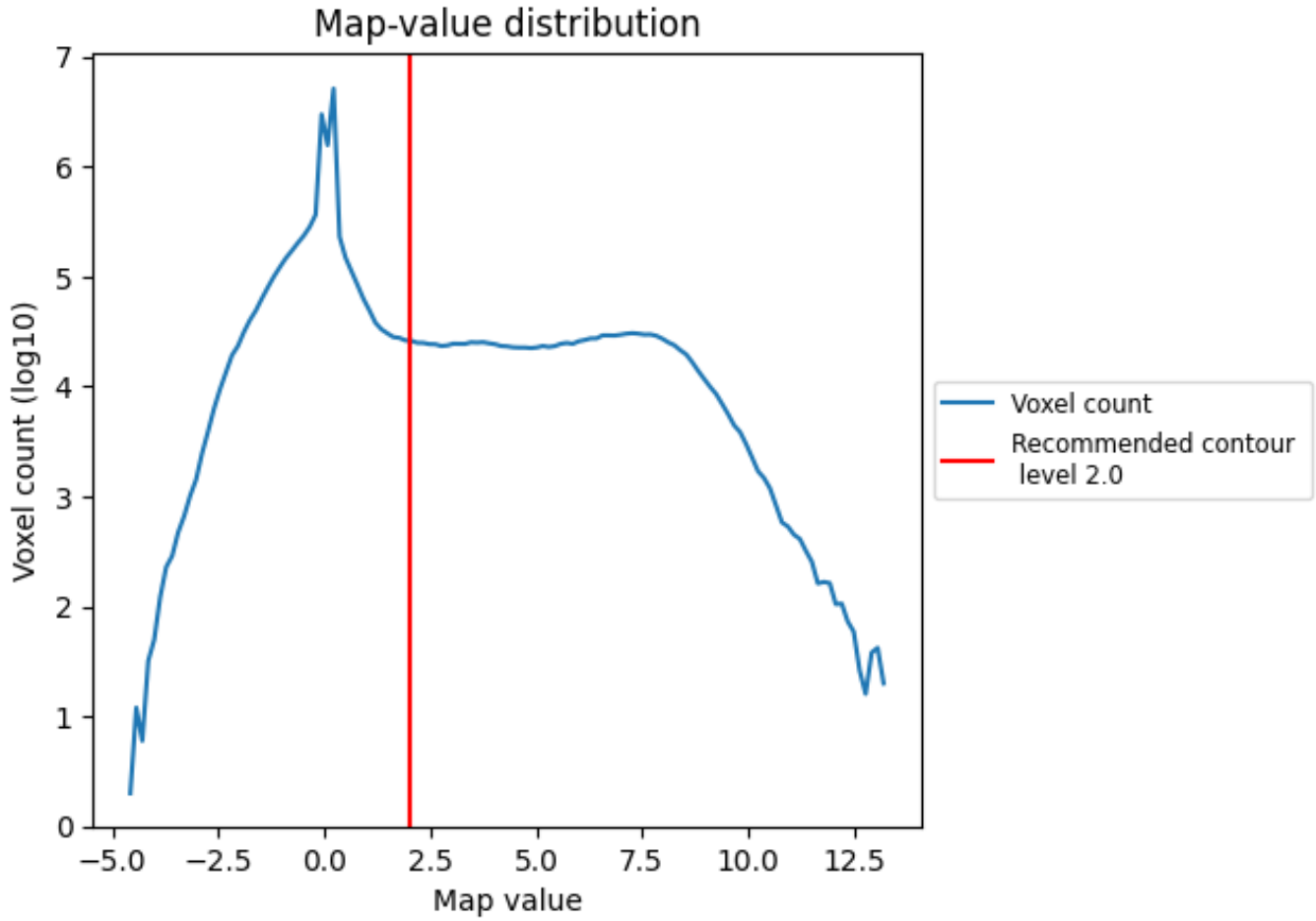
6.5 Mask visualisation (i)

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

7 Map analysis

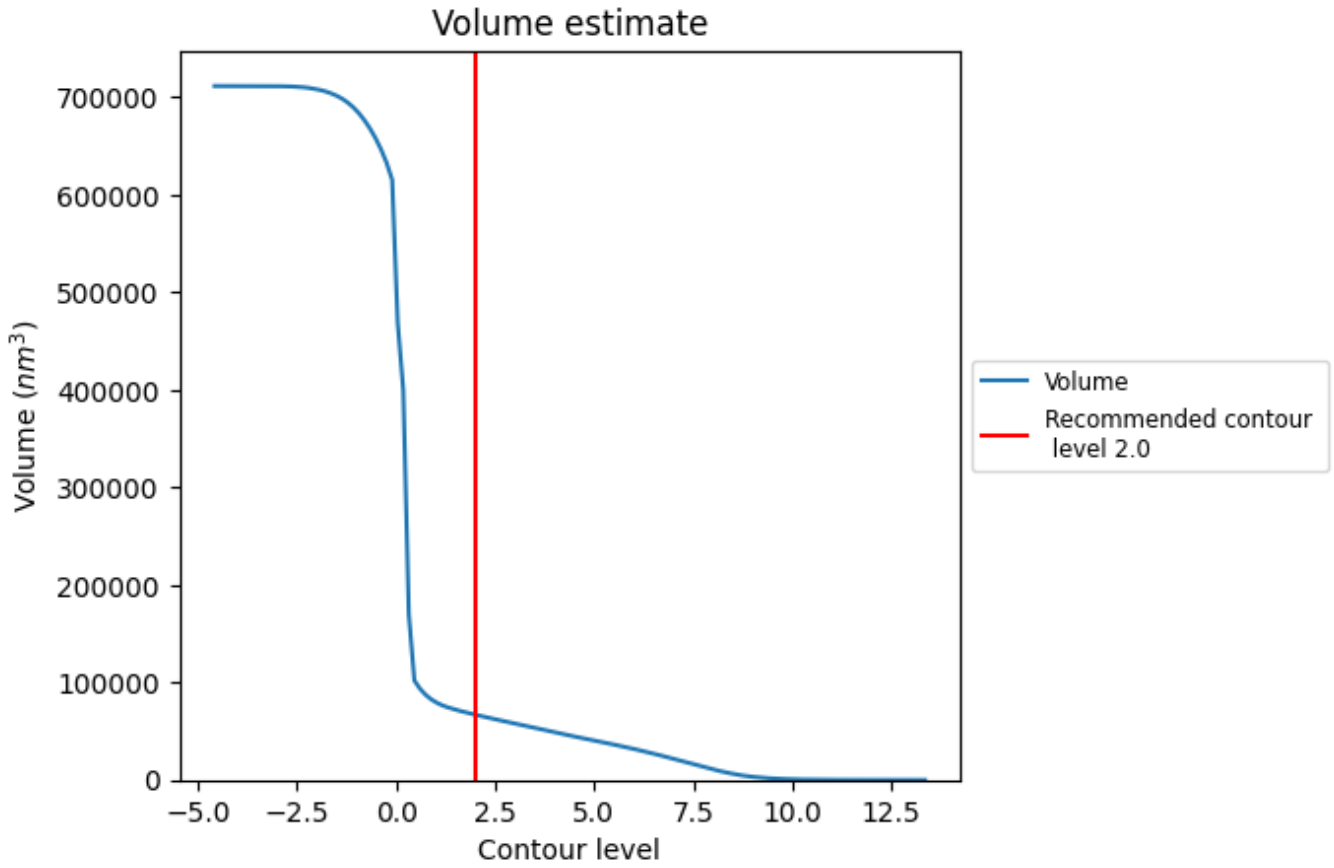
This section contains the results of statistical analysis of the map.

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.

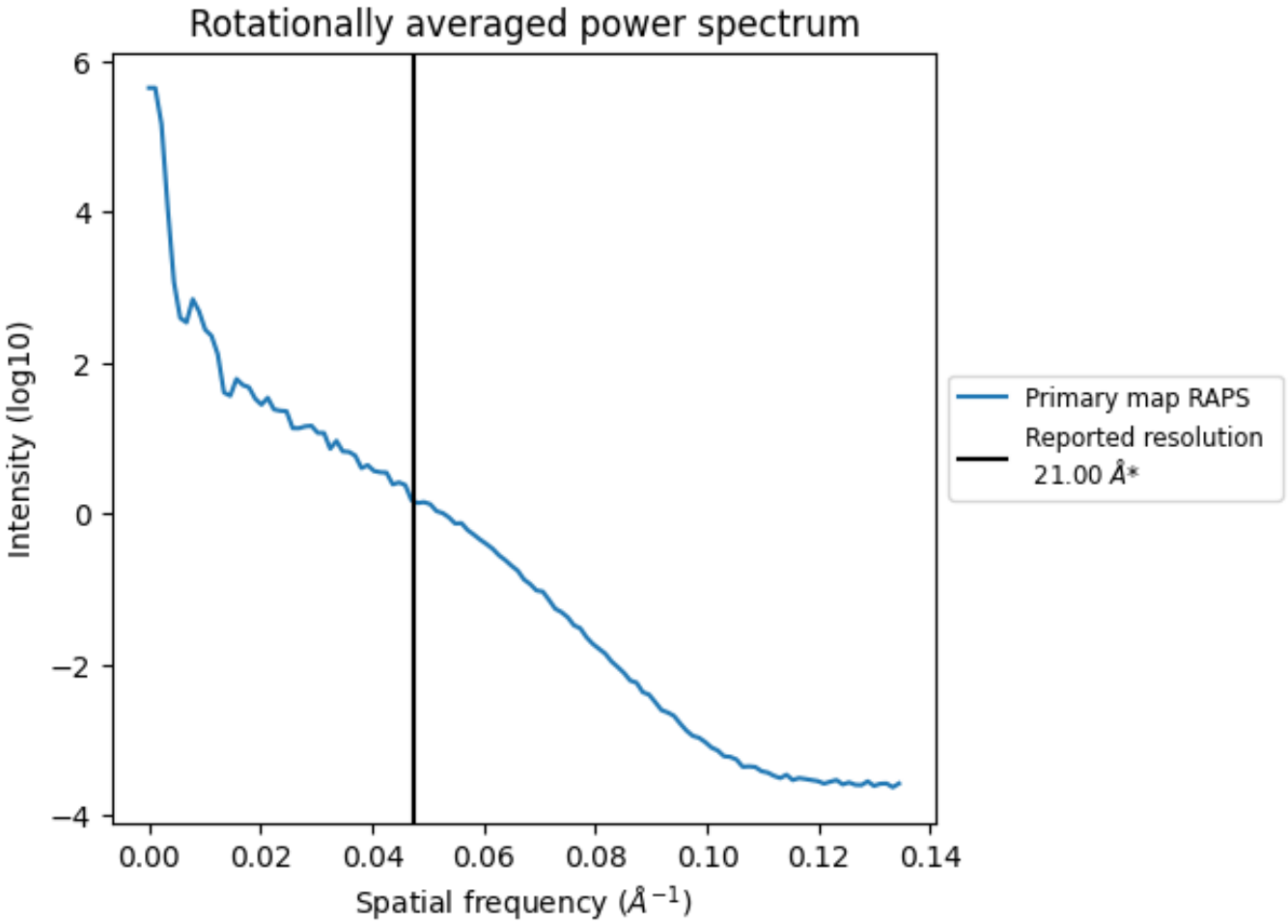
7.2 Volume estimate



The volume at the recommended contour level is 66878 nm^3; this corresponds to an approximate mass of 60412 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 0.048 Å^{-1}

8 Fourier-Shell correlation (i)

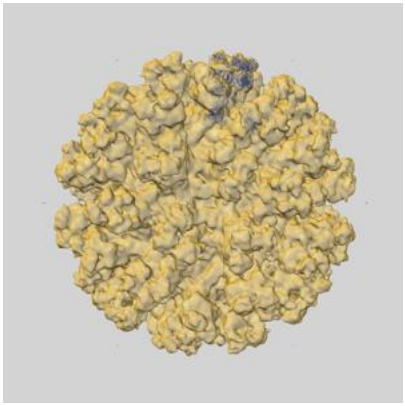
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

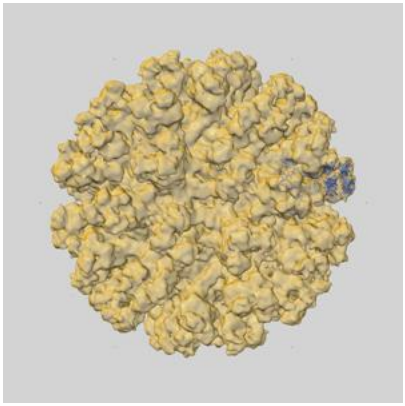
This section contains information regarding the fit between EMDB map EMD-5674 and PDB model 3J42. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

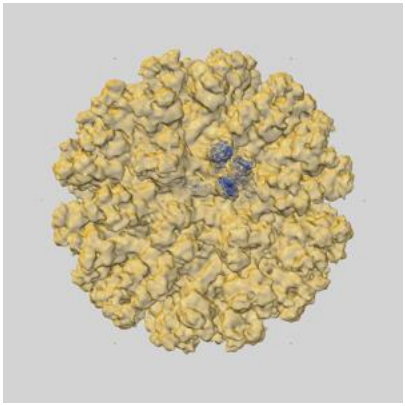
9.1.1 Map-model overlay



X

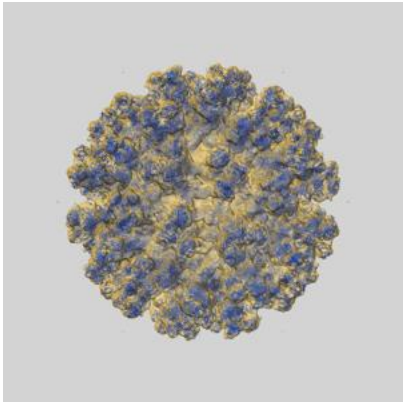


Y

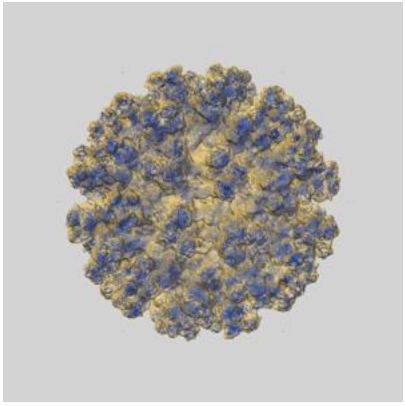


Z

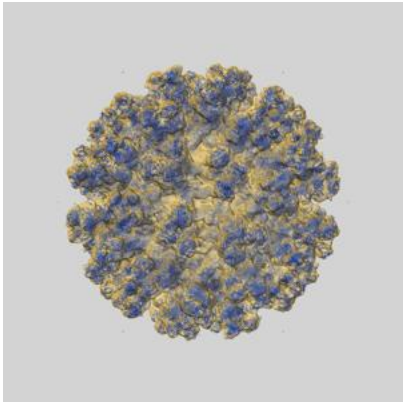
9.1.2 Map-model assembly overlay



X



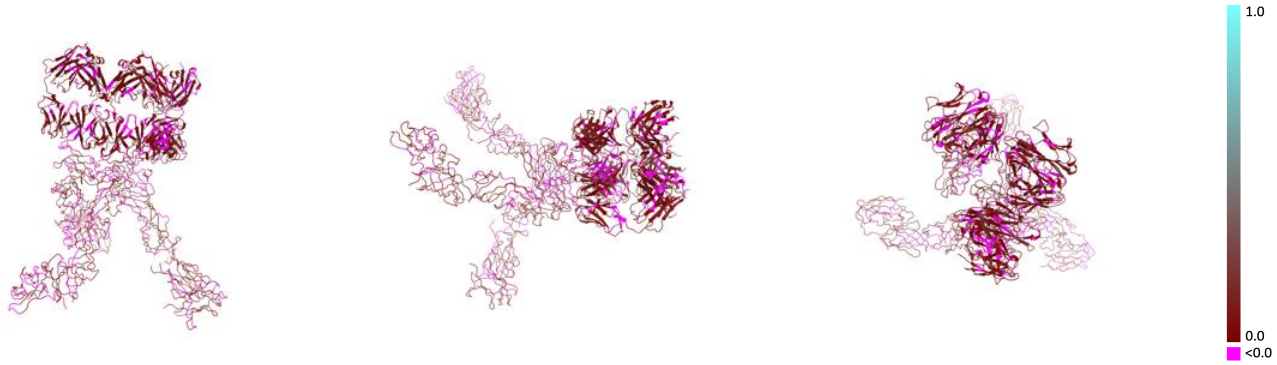
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

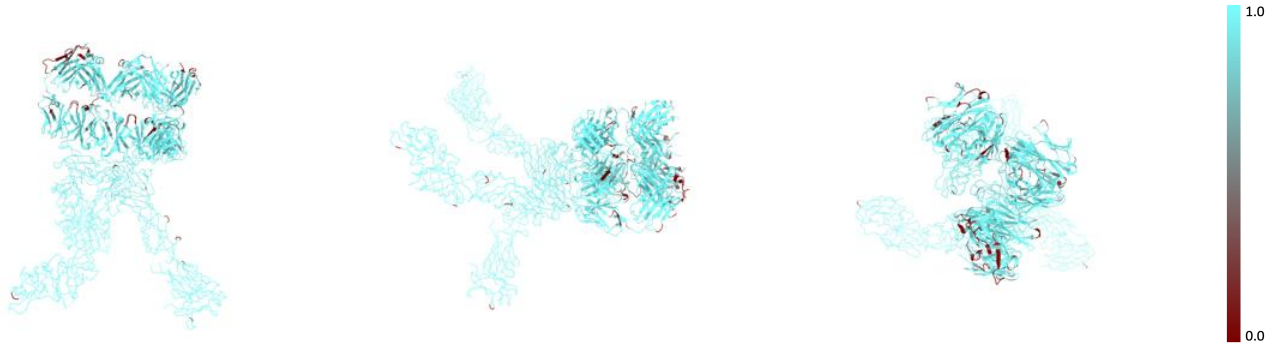
9.2 Q-score mapped to coordinate model (i)



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.

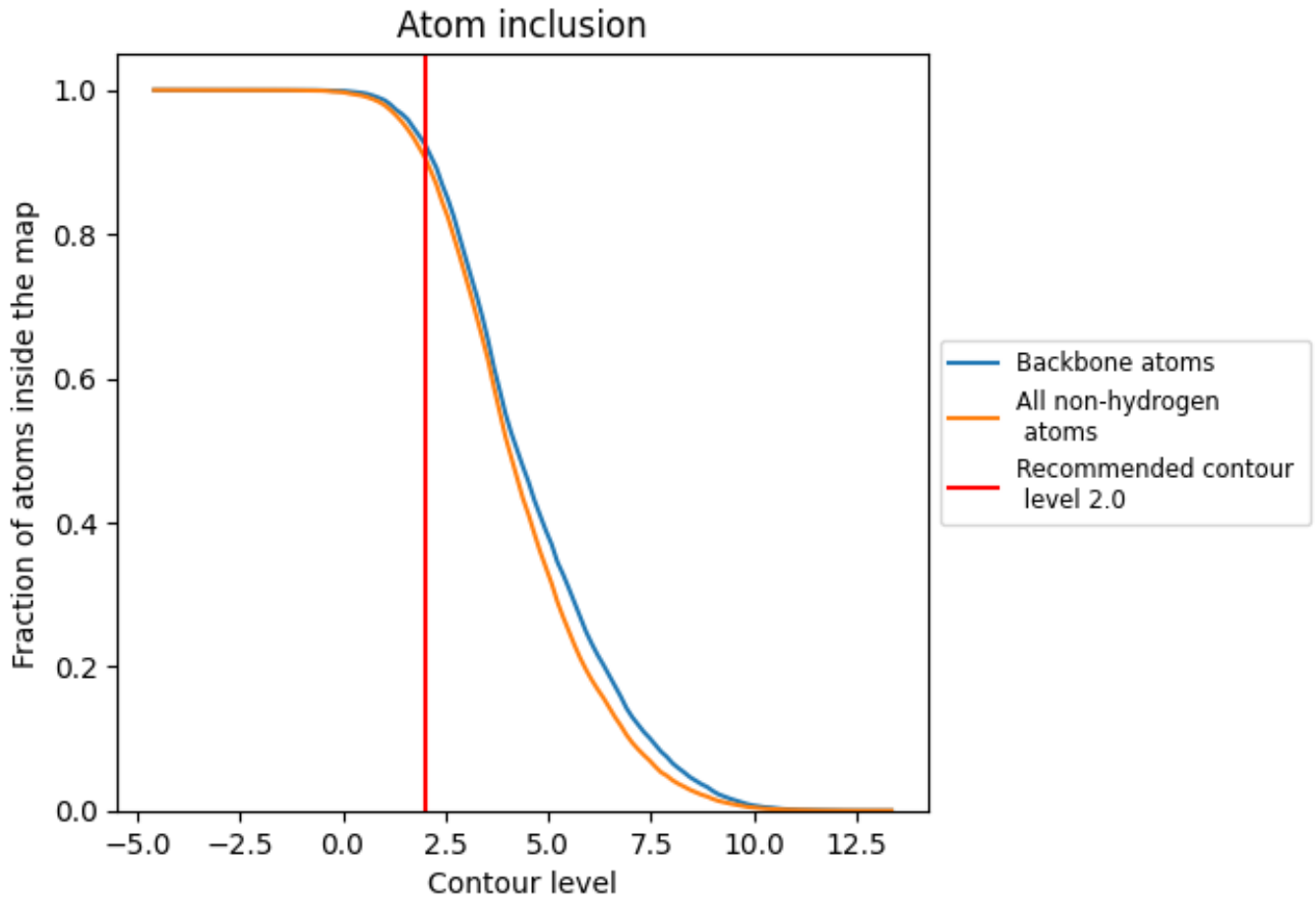
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9064	0.0620
A	0.9846	0.0710
B	0.9949	0.0500
C	0.9949	0.0570
D	0.9753	0.0270
E	0.9877	0.0510
F	1.0000	0.0290
G	0.9245	0.0580
H	0.9292	0.0610
I	0.9189	0.0520
J	0.9031	0.0610
K	0.8977	0.0700
L	0.7907	0.0720