



Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 08:12 AM EDT

PDB ID : 9B7X / pdb_00009b7x
EMDB ID : EMD-44327
Title : Fab3-7 in complex with the capsid of Adeno-associated virus type 9
Authors : Mietzsch, M.; McKenna, R.
Deposited on : 2024-03-27
Resolution : 2.76 Å(reported)

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 ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

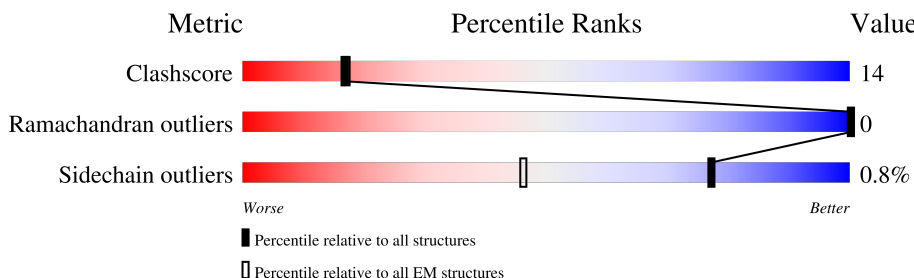
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	
1	B	736	
1	C	736	
1	D	736	
1	E	736	
1	F	736	
2	H	129	
3	L	111	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19103 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3166	2007	544	604	11		
1	B	200	Total	C	N	O	S	0	0
			1548	963	279	299	7		
1	C	506	Total	C	N	O	S	0	0
			4039	2549	703	773	14		
1	D	400	Total	C	N	O	S	0	0
			3166	2007	544	604	11		
1	E	172	Total	C	N	O	S	0	0
			1333	829	238	261	5		
1	F	506	Total	C	N	O	S	0	0
			4039	2549	703	773	14		

- Molecule 2 is a protein called Fab3-7 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	129	Total	C	N	O	S	0	0
			1005	635	167	201	2		

- Molecule 3 is a protein called Fab3-7 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			806	498	133	172	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Ca	0
			1	1	



Chain H:

78%

20%

..



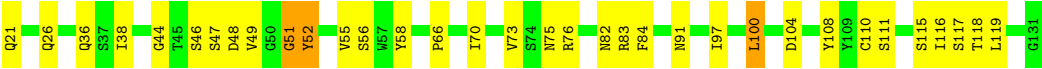
● Molecule 3: Fab3-7 light chain

Chain L:

69%

28%

.



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1008032	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	17.653	Depositor
Minimum map value	-8.986	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	185.0, 185.0, 185.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.925, 0.925, 0.925	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/3263	0.56	4/4446 (0.1%)
1	B	0.38	0/1588	0.54	0/2157
1	C	0.45	0/4160	0.65	6/5667 (0.1%)
1	D	0.38	0/3263	0.56	3/4446 (0.1%)
1	E	0.39	0/1366	0.55	0/1859
1	F	0.45	0/4160	0.62	7/5667 (0.1%)
2	H	0.52	0/1032	0.74	3/1410 (0.2%)
3	L	0.56	0/822	0.75	3/1117 (0.3%)
All	All	0.43	0/19654	0.61	26/26769 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	48	ASP	N-CA-C	10.29	122.25	111.14
2	H	131	TYR	N-CA-C	8.67	122.37	108.41
2	H	124	GLU	N-CA-C	7.70	119.67	111.28
1	A	269	SER	N-CA-C	7.12	120.82	110.28
1	A	264	THR	N-CA-C	-6.87	103.72	111.07
1	A	268	SER	N-CA-C	6.81	118.79	111.36
3	L	49	VAL	CB-CA-C	-6.70	106.02	111.71
1	F	539	GLY	N-CA-C	6.62	120.67	112.73
3	L	51	GLY	N-CA-C	6.58	120.62	112.73
1	D	268	SER	N-CA-C	6.40	123.23	113.51
1	F	364	LEU	CA-C-N	6.40	124.33	119.66
1	F	364	LEU	C-N-CA	6.40	124.33	119.66
2	H	130	LYS	N-CA-C	-5.90	99.58	109.07
1	C	492	THR	N-CA-C	-5.74	101.35	109.96
1	F	552	ASN	N-CA-C	5.69	119.42	111.74
1	C	551	ASP	N-CA-C	5.59	118.51	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	503	TRP	CA-C-N	5.54	125.20	119.05
1	D	503	TRP	C-N-CA	5.54	125.20	119.05
1	C	364	LEU	CA-C-N	5.36	123.58	119.66
1	C	364	LEU	C-N-CA	5.36	123.58	119.66
1	C	289	PHE	N-CA-C	5.34	117.18	111.36
1	A	252	TYR	N-CA-C	5.34	117.43	108.73
1	F	551	ASP	N-CA-C	5.29	117.53	108.90
1	C	281	TRP	N-CA-C	5.23	116.85	110.41
1	F	723	GLU	CA-C-N	5.23	124.85	119.05
1	F	723	GLU	C-N-CA	5.23	124.85	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3166	0	2977	96	0
1	B	1548	0	1464	49	0
1	C	4039	0	3793	159	0
1	D	3166	0	2977	83	0
1	E	1333	0	1264	44	0
1	F	4039	0	3793	138	0
2	H	1005	0	953	31	0
3	L	806	0	767	36	0
4	C	1	0	0	0	0
All	All	19103	0	17988	507	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 14.

All (507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:SER:CB	3:L:75:ASN:HD21	1.61	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:SER:HB2	3:L:75:ASN:HD21	1.17	1.05
1:C:726:PRO:O	2:H:124:GLU:HG2	1.55	1.05
3:L:55:VAL:HG12	3:L:73:VAL:HG22	1.35	1.03
1:A:255:HIS:ND1	1:A:653:PRO:HB3	1.76	1.00
1:F:495:GLN:HE22	1:F:533:ARG:HE	1.02	0.97
1:F:706:TYR:CD1	2:H:50:ASN:HB2	1.99	0.97
1:A:495:GLN:HE22	1:A:533:ARG:HE	0.95	0.93
1:C:708:SER:CB	3:L:75:ASN:ND2	2.32	0.91
1:A:255:HIS:CE1	1:A:653:PRO:HB3	2.06	0.90
1:B:590:GLN:HA	1:C:497:ASN:HD22	1.36	0.89
1:D:358:SER:O	1:F:442:GLN:NE2	2.05	0.88
1:C:287:ASN:O	1:C:618:ILE:HG13	1.75	0.87
1:C:562:ASN:HB3	2:H:126:ILE:HG13	1.57	0.86
3:L:55:VAL:CG1	3:L:73:VAL:HG22	2.05	0.86
1:C:495:GLN:HE22	1:C:533:ARG:HE	1.24	0.86
1:A:495:GLN:HE22	1:A:533:ARG:NE	1.73	0.86
1:C:562:ASN:HB3	2:H:126:ILE:CG1	2.07	0.85
1:A:495:GLN:NE2	1:A:533:ARG:HE	1.75	0.83
1:C:712:GLU:OE2	1:C:725:ARG:NH2	2.12	0.82
1:F:495:GLN:HE22	1:F:533:ARG:NE	1.78	0.81
1:F:706:TYR:CE1	2:H:50:ASN:HB2	2.14	0.81
1:E:429:SER:O	1:F:382:LEU:HG	1.81	0.80
1:C:563:GLU:OE2	1:C:613:TYR:OH	1.98	0.80
1:D:566:ILE:HD12	1:D:570:ASN:HD22	1.47	0.80
1:A:566:ILE:HD12	1:A:570:ASN:HD22	1.47	0.80
1:F:495:GLN:NE2	1:F:533:ARG:HE	1.78	0.80
1:C:495:GLN:NE2	1:C:533:ARG:HE	1.78	0.79
1:F:706:TYR:HE2	2:H:119:ARG:HG3	1.48	0.79
1:F:706:TYR:CE2	2:H:119:ARG:HG3	2.19	0.78
1:B:590:GLN:HA	1:C:497:ASN:ND2	1.99	0.77
1:A:250:PRO:HG3	1:A:373:MET:HE3	1.68	0.76
1:E:566:ILE:HD12	1:E:570:ASN:HD22	1.49	0.76
1:A:497:ASN:HD22	1:C:589:ALA:C	1.94	0.76
3:L:47:SER:HB2	3:L:115:SER:OG	1.85	0.76
2:H:117:GLN:HE22	2:H:131:TYR:HA	1.51	0.76
1:A:485:ARG:NH2	1:A:576:SER:OG	2.20	0.75
1:B:566:ILE:HD12	1:B:570:ASN:HD22	1.49	0.75
1:C:281:TRP:CE2	1:C:650:LYS:HD2	2.22	0.75
1:C:562:ASN:HB3	2:H:126:ILE:CD1	2.16	0.74
1:A:511:LEU:HD21	1:C:568:THR:O	1.88	0.74
1:A:358:SER:O	1:C:442:GLN:NE2	2.21	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:THR:HG23	1:C:502:ALA:HB2	1.69	0.74
1:D:485:ARG:NH2	1:D:576:SER:OG	2.20	0.73
3:L:55:VAL:HG12	3:L:73:VAL:CG2	2.15	0.73
1:B:585:GLN:OE1	1:C:501:PHE:CZ	2.42	0.73
1:E:447:LEU:HD23	1:F:537:LEU:CD1	2.19	0.72
1:C:707:LYS:NZ	1:F:529:GLU:OE2	2.23	0.72
1:A:253:ASN:C	1:A:253:ASN:HD22	1.98	0.71
1:C:562:ASN:HD22	1:C:562:ASN:H	1.36	0.71
1:A:382:LEU:HG	1:C:429:SER:O	1.91	0.71
1:B:496:ASN:HD22	1:B:496:ASN:H	1.39	0.71
1:F:706:TYR:HD1	2:H:50:ASN:HB2	1.56	0.70
1:D:255:HIS:CG	1:D:653:PRO:HB3	2.27	0.69
1:C:562:ASN:HB3	2:H:126:ILE:HD11	1.74	0.69
1:F:712:GLU:OE1	1:F:725:ARG:NH2	2.25	0.69
1:C:708:SER:HB3	3:L:75:ASN:ND2	2.06	0.69
1:C:708:SER:HB3	3:L:75:ASN:HD21	1.55	0.69
1:A:501:PHE:CZ	1:C:585:GLN:OE1	2.45	0.69
1:D:353:PRO:HB3	1:F:430:GLN:HE22	1.58	0.69
1:C:726:PRO:O	2:H:124:GLU:CG	2.38	0.68
1:A:247:TRP:CD1	1:A:679:VAL:HG23	2.29	0.68
1:C:562:ASN:CB	2:H:126:ILE:HD11	2.24	0.68
1:A:255:HIS:CE1	1:A:653:PRO:CB	2.78	0.67
1:C:287:ASN:O	1:C:618:ILE:CG1	2.42	0.67
1:A:581:ALA:O	1:B:485:ARG:HD2	1.95	0.67
1:D:247:TRP:CD1	1:D:679:VAL:HG23	2.29	0.67
1:D:503:TRP:HZ3	1:D:517:LEU:HB2	1.58	0.67
1:D:353:PRO:HB3	1:F:430:GLN:NE2	2.11	0.66
1:C:495:GLN:HE22	1:C:533:ARG:NE	1.93	0.66
1:A:254:ASN:N	1:A:254:ASN:HD22	1.92	0.66
1:A:265:SER:OG	1:A:274:TYR:OH	2.11	0.66
3:L:21:GLN:HE22	3:L:118:THR:HB	1.60	0.66
1:E:581:ALA:O	1:F:485:ARG:HD2	1.96	0.65
2:H:48:ILE:HG23	2:H:53:TRP:HE1	1.60	0.65
1:C:490:SER:HB2	1:C:534:PHE:CE1	2.32	0.65
1:F:566:ILE:HD12	1:F:570:ASN:HD22	1.60	0.64
1:C:503:TRP:N	1:C:504:PRO:CD	2.60	0.64
1:E:506:ALA:HB2	1:E:537:LEU:HD22	1.78	0.64
1:F:364:LEU:HD12	1:F:364:LEU:N	2.12	0.64
1:A:503:TRP:HB3	1:A:504:PRO:HD3	1.80	0.64
3:L:83:ARG:NH1	3:L:104:ASP:OD2	2.25	0.64
1:A:497:ASN:ND2	1:C:589:ALA:C	2.56	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:THR:HG22	1:D:647:ILE:HG12	1.80	0.64
1:C:262:ASN:HD22	1:C:273:ALA:HA	1.64	0.63
3:L:21:GLN:N	3:L:21:GLN:OE1	2.30	0.63
1:E:500:GLU:OE1	1:E:500:GLU:HA	1.98	0.63
1:A:346:THR:HG22	1:A:647:ILE:HG12	1.80	0.63
1:C:532:ASP:O	2:H:126:ILE:HG23	1.97	0.63
1:C:708:SER:HB2	3:L:75:ASN:ND2	2.00	0.63
1:F:466:ALA:HB1	1:F:474:GLN:HG2	1.81	0.63
1:A:387:GLN:OE1	1:F:707:LYS:HE2	1.99	0.62
1:C:466:ALA:HB1	1:C:474:GLN:HG2	1.81	0.62
1:B:490:SER:HB3	1:B:496:ASN:HD21	1.65	0.62
1:F:262:ASN:HD22	1:F:273:ALA:HA	1.64	0.62
1:D:255:HIS:CD2	1:D:653:PRO:HB3	2.35	0.62
1:B:599:GLN:OE1	1:C:598:ASN:ND2	2.32	0.62
1:D:503:TRP:HB3	1:D:504:PRO:HD3	1.82	0.62
1:D:503:TRP:N	1:D:504:PRO:CD	2.63	0.61
1:D:581:ALA:O	1:E:485:ARG:HD2	2.01	0.61
1:F:565:GLU:OE1	1:F:565:GLU:N	2.26	0.60
1:C:250:PRO:HG3	1:C:373:MET:HE3	1.84	0.60
1:C:285:ASP:O	1:C:363:CYS:HA	2.00	0.60
1:F:247:TRP:CD1	1:F:679:VAL:HG23	2.37	0.60
1:D:599:GLN:OE1	1:E:598:ASN:ND2	2.32	0.60
1:B:496:ASN:HD22	1:B:496:ASN:N	1.99	0.60
1:C:503:TRP:H	1:C:504:PRO:CD	2.15	0.60
1:F:230:CYS:SG	1:F:244:THR:N	2.74	0.59
1:F:323:LYS:NZ	1:F:336:ASN:OD1	2.32	0.59
1:D:290:HIS:HD2	1:D:615:GLN:HA	1.68	0.59
1:A:548:THR:HG23	1:A:557:LYS:HB3	1.85	0.59
1:A:290:HIS:HD2	1:A:615:GLN:HA	1.68	0.59
1:D:548:THR:HG23	1:D:557:LYS:HB3	1.85	0.59
1:A:353:PRO:HB3	1:C:430:GLN:HE22	1.67	0.59
1:F:250:PRO:HG3	1:F:373:MET:HE3	1.84	0.59
1:A:253:ASN:O	1:A:253:ASN:ND2	2.35	0.59
1:C:230:CYS:SG	1:C:244:THR:N	2.74	0.59
1:A:255:HIS:CE1	1:A:653:PRO:CA	2.86	0.59
1:C:247:TRP:CD1	1:C:679:VAL:HG23	2.37	0.59
1:A:255:HIS:ND1	1:A:653:PRO:CB	2.62	0.59
1:C:313:LEU:HB3	1:C:415:TYR:HB3	1.85	0.58
1:C:425:SER:CB	1:C:729:THR:HG22	2.34	0.58
1:F:313:LEU:HB3	1:F:415:TYR:HB3	1.85	0.58
1:E:485:ARG:HH21	1:E:576:SER:N	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ARG:HH21	1:B:576:SER:N	2.02	0.58
1:F:364:LEU:H	1:F:364:LEU:CD1	2.16	0.58
1:C:296:ARG:NE	1:F:698:GLU:HG2	2.19	0.58
1:C:490:SER:OG	1:C:495:GLN:HG3	2.04	0.57
1:A:485:ARG:HD2	1:C:581:ALA:O	2.04	0.57
1:D:250:PRO:HG3	1:D:373:MET:HE3	1.86	0.57
1:F:712:GLU:CD	1:F:725:ARG:NH2	2.62	0.57
1:C:696:ASN:ND2	1:F:711:VAL:CG1	2.67	0.57
1:D:367:PHE:CE2	1:D:369:ALA:HB3	2.39	0.57
1:C:259:GLN:NE2	1:C:275:PHE:HE1	2.03	0.57
1:A:658:PRO:HG2	1:F:250:PRO:HB3	1.86	0.57
1:E:447:LEU:HD23	1:F:537:LEU:HD13	1.86	0.57
1:A:367:PHE:CE2	1:A:369:ALA:HB3	2.39	0.57
1:A:502:ALA:HB2	1:C:450:THR:HG23	1.86	0.57
1:F:364:LEU:HD12	1:F:364:LEU:H	1.69	0.56
1:F:545:LYS:HG3	1:F:557:LYS:O	2.04	0.56
1:B:429:SER:O	1:C:382:LEU:HG	2.06	0.56
1:C:355:VAL:H	1:C:646:GLN:NE2	2.04	0.56
1:A:503:TRP:N	1:A:504:PRO:CD	2.68	0.56
1:F:259:GLN:NE2	1:F:275:PHE:HE1	2.03	0.56
2:H:131:TYR:N	2:H:131:TYR:CD2	2.73	0.56
1:C:323:LYS:NZ	1:C:336:ASN:OD1	2.32	0.56
1:A:255:HIS:CE1	1:A:653:PRO:HA	2.41	0.56
1:E:430:GLN:HE22	1:F:353:PRO:HB3	1.71	0.56
1:D:503:TRP:H	1:D:504:PRO:CD	2.19	0.56
1:C:696:ASN:HD22	1:F:711:VAL:CG1	2.19	0.55
3:L:111:SER:OG	3:L:119:LEU:HD11	2.06	0.55
1:A:501:PHE:CE1	1:C:585:GLN:OE1	2.58	0.55
1:F:355:VAL:H	1:F:646:GLN:NE2	2.04	0.55
1:E:447:LEU:HD23	1:F:537:LEU:HD11	1.87	0.55
1:E:503:TRP:HB3	1:E:504:PRO:HD3	1.87	0.55
1:C:418:GLU:OE2	1:C:641:LYS:N	2.40	0.55
1:F:707:LYS:HG3	1:F:707:LYS:O	2.05	0.55
1:C:355:VAL:H	1:C:646:GLN:HE22	1.55	0.55
1:D:269:SER:HB3	1:D:272:ASN:HB2	1.88	0.55
1:F:418:GLU:OE2	1:F:641:LYS:N	2.40	0.55
1:C:435:LEU:HD21	1:C:736:LEU:HB3	1.89	0.55
1:C:250:PRO:HB3	1:D:658:PRO:HG2	1.89	0.54
1:E:450:THR:OG1	1:F:500:GLU:HA	2.07	0.54
1:F:425:SER:CB	1:F:729:THR:HG22	2.37	0.54
1:A:325:VAL:HG22	1:A:334:ILE:HG12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:ALA:HB1	1:D:517:LEU:CD1	2.36	0.54
1:F:415:TYR:OH	1:F:642:HIS:O	2.24	0.54
3:L:55:VAL:HG13	3:L:73:VAL:HA	1.89	0.54
1:C:431:SER:HA	1:C:568:THR:HB	1.89	0.54
1:F:690:GLU:HG3	1:F:732:LEU:HD13	1.90	0.54
3:L:21:GLN:NE2	3:L:116:ILE:HD11	2.22	0.54
1:C:375:PRO:HA	1:D:662:PHE:CD1	2.42	0.54
1:F:545:LYS:CG	1:F:557:LYS:O	2.56	0.54
1:F:529:GLU:OE1	1:F:567:LYS:HE3	2.07	0.54
1:C:426:TYR:CD1	1:C:426:TYR:C	2.86	0.54
1:F:435:LEU:HD21	1:F:736:LEU:HB3	1.88	0.54
1:E:430:GLN:NE2	1:F:353:PRO:HB3	2.22	0.54
1:D:380:LEU:HD13	1:F:434:ARG:HD2	1.90	0.54
1:C:326:THR:O	1:C:333:THR:N	2.35	0.53
1:A:353:PRO:HB3	1:C:430:GLN:NE2	2.22	0.53
1:A:497:ASN:HB2	1:C:586:SER:O	2.07	0.53
1:A:503:TRP:H	1:A:504:PRO:CD	2.21	0.53
1:D:624:HIS:O	1:F:428:HIS:HE1	1.92	0.53
1:C:415:TYR:OH	1:C:642:HIS:O	2.24	0.53
1:D:325:VAL:HG22	1:D:334:ILE:HG12	1.89	0.53
1:F:355:VAL:H	1:F:646:GLN:HE22	1.55	0.53
1:A:340:SER:HA	1:F:321:GLN:HE22	1.72	0.53
1:D:485:ARG:HD2	1:F:581:ALA:O	2.09	0.53
1:C:371:VAL:HG12	1:D:667:LEU:HD12	1.90	0.53
1:C:690:GLU:HG3	1:C:732:LEU:HD13	1.90	0.53
1:D:261:SER:H	1:D:264:THR:HB	1.74	0.53
1:D:265:SER:OG	1:D:274:TYR:OH	2.25	0.53
2:H:128:ASP:N	2:H:128:ASP:OD1	2.35	0.53
1:F:536:PRO:HB2	1:F:539:GLY:HA3	1.89	0.53
1:F:548:THR:HG22	1:F:553:VAL:HG11	1.91	0.53
1:A:503:TRP:H	1:A:504:PRO:HD2	1.74	0.52
1:F:364:LEU:N	1:F:364:LEU:CD1	2.73	0.52
1:F:425:SER:HB3	1:F:729:THR:HG22	1.91	0.52
1:C:354:TYR:CE2	1:C:356:LEU:HB2	2.45	0.52
1:D:361:GLU:HG3	1:D:362:GLY:H	1.74	0.52
1:B:581:ALA:O	1:C:485:ARG:HD2	2.09	0.52
1:A:343:GLN:HG2	1:A:404:MET:HG2	1.92	0.52
1:C:321:GLN:HE22	1:D:340:SER:HA	1.75	0.52
1:C:490:SER:HB2	1:C:534:PHE:HE1	1.74	0.52
1:F:326:THR:O	1:F:333:THR:N	2.35	0.52
1:F:262:ASN:OD1	1:F:263:SER:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:SER:HB2	1:A:534:PHE:CE1	2.46	0.51
1:C:262:ASN:OD1	1:C:263:SER:N	2.43	0.51
1:C:425:SER:HB2	1:C:729:THR:HG22	1.92	0.51
1:F:354:TYR:CE2	1:F:356:LEU:HB2	2.45	0.51
1:F:712:GLU:OE2	1:F:725:ARG:NH2	2.40	0.51
1:B:568:THR:O	1:C:511:LEU:HD21	2.10	0.51
1:D:490:SER:HB2	1:D:534:PHE:CE1	2.46	0.51
1:A:361:GLU:HG3	1:A:362:GLY:H	1.74	0.51
1:B:506:ALA:HB1	1:B:517:LEU:CD1	2.41	0.51
1:D:343:GLN:HG2	1:D:404:MET:HG2	1.92	0.51
1:D:498:ASN:HB2	1:F:459:GLN:NE2	2.25	0.51
1:E:439:LEU:HD21	1:F:278:SER:HB3	1.92	0.51
1:F:447:LEU:HD12	1:F:462:LYS:O	2.10	0.51
3:L:36:GLN:O	3:L:100:LEU:HD12	2.11	0.51
1:D:254:ASN:N	1:D:254:ASN:HD22	2.10	0.50
1:D:490:SER:HB3	1:D:496:ASN:OD1	2.11	0.50
1:E:506:ALA:HB1	1:E:517:LEU:CD1	2.41	0.50
1:B:590:GLN:CA	1:C:497:ASN:HD22	2.18	0.50
2:H:66:TRP:HZ3	3:L:118:THR:HG23	1.76	0.50
1:F:725:ARG:HB2	1:F:726:PRO:HD2	1.93	0.50
1:A:599:GLN:OE1	1:B:598:ASN:ND2	2.42	0.50
1:C:696:ASN:ND2	1:F:711:VAL:HG11	2.27	0.50
1:D:307:GLY:HA2	1:D:423:HIS:O	2.12	0.50
1:B:572:VAL:HG12	1:B:574:THR:H	1.77	0.50
2:H:53:TRP:HB3	2:H:97:PHE:CZ	2.46	0.50
1:A:271:ASP:OD1	1:A:515:ASN:HB2	2.12	0.50
1:C:708:SER:CA	3:L:75:ASN:ND2	2.75	0.50
1:F:566:ILE:HD12	1:F:570:ASN:ND2	2.26	0.50
1:C:447:LEU:HD12	1:C:462:LYS:O	2.11	0.49
1:F:262:ASN:ND2	1:F:273:ALA:HA	2.27	0.49
1:A:254:ASN:N	1:A:254:ASN:ND2	2.60	0.49
1:A:426:TYR:CD1	1:A:426:TYR:C	2.90	0.49
1:B:463:PHE:CE2	1:C:555:ALA:HA	2.48	0.49
3:L:70:ILE:HD13	3:L:76:ARG:HB3	1.95	0.49
1:A:608:GLN:HE22	1:B:625:THR:HA	1.78	0.49
1:B:585:GLN:OE1	1:C:501:PHE:CE2	2.66	0.49
1:C:262:ASN:ND2	1:C:273:ALA:HA	2.27	0.49
1:D:424:SER:HB2	1:D:426:TYR:CE2	2.47	0.49
1:D:563:GLU:O	1:D:566:ILE:HG12	2.13	0.49
1:C:249:LEU:HB2	1:C:374:ILE:HD12	1.95	0.48
1:F:283:TYR:HB3	1:F:648:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:ALA:HB1	1:E:517:LEU:HD11	1.94	0.48
1:F:367:PHE:CE2	1:F:369:ALA:HB3	2.48	0.48
1:E:589:ALA:C	1:F:497:ASN:ND2	2.72	0.48
1:A:380:LEU:HD21	1:C:438:PRO:HB3	1.95	0.48
1:C:500:GLU:O	1:C:500:GLU:HG3	2.13	0.48
1:C:284:PHE:CE1	1:C:679:VAL:HG21	2.49	0.48
1:C:425:SER:HB3	1:C:729:THR:HG22	1.94	0.48
1:C:700:GLN:HB2	1:F:702:THR:HB	1.95	0.48
1:D:503:TRP:CZ3	1:D:517:LEU:HB2	2.45	0.48
1:E:437:ASN:HB2	1:F:355:VAL:HB	1.95	0.48
1:F:655:PRO:HA	1:F:670:PHE:HA	1.96	0.48
1:C:485:ARG:HG2	1:C:486:GLN:N	2.28	0.48
1:D:290:HIS:CD2	1:D:615:GLN:HA	2.48	0.48
1:F:229:HIS:O	1:F:244:THR:OG1	2.31	0.48
1:D:355:VAL:HB	1:F:437:ASN:HB2	1.95	0.48
1:F:485:ARG:HG2	1:F:486:GLN:N	2.28	0.47
1:A:389:VAL:HA	1:F:707:LYS:HA	1.97	0.47
1:A:563:GLU:O	1:A:566:ILE:HG12	2.13	0.47
1:F:249:LEU:HB2	1:F:374:ILE:HD12	1.95	0.47
2:H:43:VAL:HG22	2:H:46:GLY:O	2.14	0.47
1:A:290:HIS:CD2	1:A:615:GLN:HA	2.48	0.47
1:A:357:GLY:O	1:C:477:ASN:ND2	2.48	0.47
1:B:590:GLN:CA	1:C:497:ASN:ND2	2.73	0.47
1:C:373:MET:HE2	1:D:662:PHE:HA	1.96	0.47
1:C:427:ALA:O	1:C:733:THR:HA	2.14	0.47
1:A:255:HIS:CG	1:A:653:PRO:HB3	2.46	0.47
1:A:283:TYR:HB3	1:A:648:LEU:HD13	1.96	0.47
1:C:424:SER:HB2	1:C:426:TYR:CE2	2.50	0.47
1:C:708:SER:HA	3:L:75:ASN:ND2	2.30	0.47
1:D:322:VAL:HG11	1:D:340:SER:HB2	1.96	0.47
1:E:572:VAL:HG12	1:E:574:THR:H	1.77	0.47
1:D:501:PHE:CZ	1:F:585:GLN:OE1	2.68	0.47
1:A:485:ARG:HG2	1:A:486:GLN:N	2.28	0.47
1:C:295:PRO:HB2	1:F:697:PRO:HD3	1.96	0.47
1:D:322:VAL:CG1	1:D:673:GLN:HE21	2.28	0.47
1:E:427:ALA:CB	1:F:391:ARG:HD3	2.44	0.47
1:E:506:ALA:HB2	1:E:537:LEU:CD2	2.45	0.47
1:E:603:PRO:HB3	1:F:630:HIS:HB3	1.97	0.47
2:H:66:TRP:CZ3	3:L:118:THR:HG23	2.50	0.47
1:A:358:SER:HB2	1:A:360:HIS:CD2	2.50	0.47
1:B:496:ASN:N	1:B:496:ASN:ND2	2.60	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:THR:OG1	1:D:377:TYR:O	2.21	0.47
1:D:503:TRP:H	1:D:504:PRO:HD2	1.79	0.47
1:F:285:ASP:O	1:F:364:LEU:CD1	2.62	0.47
1:C:655:PRO:HA	1:C:670:PHE:HA	1.96	0.47
1:E:449:LYS:HA	1:F:500:GLU:OE2	2.14	0.47
1:A:322:VAL:HG11	1:A:340:SER:HB2	1.96	0.47
1:D:485:ARG:HG2	1:D:486:GLN:N	2.28	0.47
1:E:532:ASP:OD1	1:E:532:ASP:N	2.46	0.47
2:H:24:GLN:HG3	2:H:138:GLN:HE22	1.80	0.47
1:D:384:ASP:CG	3:L:82:ASN:HD21	2.23	0.46
1:D:309:ARG:NH1	1:D:420:VAL:O	2.47	0.46
3:L:21:GLN:HE22	3:L:118:THR:CB	2.27	0.46
1:E:563:GLU:O	1:E:566:ILE:HG12	2.15	0.46
1:A:497:ASN:HA	1:C:587:ALA:HA	1.97	0.46
1:B:485:ARG:HH21	1:B:576:SER:H	1.63	0.46
1:C:503:TRP:HB3	1:C:504:PRO:HD3	1.98	0.46
1:B:437:ASN:HB2	1:C:355:VAL:HB	1.98	0.46
1:D:283:TYR:HB3	1:D:648:LEU:HD13	1.96	0.46
1:D:503:TRP:N	1:D:504:PRO:HD2	2.31	0.46
1:E:527:HIS:ND1	1:E:531:GLU:O	2.49	0.46
1:E:485:ARG:NH2	1:E:576:SER:OG	2.48	0.46
1:A:309:ARG:NH1	1:A:420:VAL:O	2.47	0.46
2:H:131:TYR:H	2:H:131:TYR:HD2	1.61	0.46
1:D:358:SER:HB2	1:D:360:HIS:CD2	2.50	0.46
1:A:322:VAL:CG1	1:A:673:GLN:HE21	2.28	0.46
1:B:563:GLU:O	1:B:566:ILE:HG12	2.16	0.46
1:C:525:ALA:HB2	1:C:567:LYS:HA	1.98	0.46
1:F:346:THR:HG22	1:F:647:ILE:HG12	1.98	0.46
1:A:313:LEU:HB2	1:A:417:PHE:HE2	1.81	0.45
1:C:340:SER:OG	1:C:673:GLN:NE2	2.50	0.45
1:C:346:THR:HG22	1:C:647:ILE:HG12	1.98	0.45
1:E:471:MET:O	1:E:476:ARG:NH2	2.49	0.45
1:B:471:MET:O	1:B:476:ARG:NH2	2.49	0.45
1:B:485:ARG:NH2	1:B:576:SER:OG	2.49	0.45
1:F:545:LYS:NZ	1:F:556:ASP:O	2.43	0.45
2:H:25:GLU:HB2	2:H:140:THR:HG23	1.99	0.45
1:C:562:ASN:HD22	1:C:562:ASN:N	2.03	0.45
3:L:56:SER:HA	3:L:70:ILE:O	2.17	0.45
1:E:477:ASN:ND2	1:F:357:GLY:O	2.50	0.45
3:L:46:SER:O	3:L:51:GLY:N	2.49	0.45
1:B:426:TYR:CD1	1:B:426:TYR:C	2.95	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:PRO:HD3	1:B:635:MET:HG2	1.99	0.45
1:F:281:TRP:CE2	1:F:650:LYS:HD2	2.51	0.45
1:B:527:HIS:ND1	1:B:531:GLU:O	2.49	0.45
1:C:712:GLU:CD	1:C:725:ARG:HH21	2.25	0.45
1:D:313:LEU:HB2	1:D:417:PHE:CE2	2.52	0.45
1:D:313:LEU:HB2	1:D:417:PHE:HE2	1.81	0.45
1:F:284:PHE:CE1	1:F:679:VAL:HG21	2.52	0.45
1:A:503:TRP:N	1:A:504:PRO:HD2	2.30	0.45
1:A:608:GLN:NE2	1:B:625:THR:HA	2.31	0.45
1:E:485:ARG:HH21	1:E:576:SER:H	1.63	0.45
1:C:364:LEU:N	1:C:364:LEU:CD1	2.80	0.45
1:E:589:ALA:C	1:F:497:ASN:HD22	2.26	0.45
1:C:284:PHE:CZ	1:C:679:VAL:HG21	2.52	0.44
1:D:624:HIS:O	1:F:428:HIS:CE1	2.71	0.44
1:F:340:SER:OG	1:F:673:GLN:NE2	2.50	0.44
1:A:313:LEU:HB2	1:A:417:PHE:CE2	2.52	0.44
1:A:418:GLU:HG2	1:A:640:MET:HE3	2.00	0.44
1:B:490:SER:HB3	1:B:496:ASN:ND2	2.30	0.44
1:F:249:LEU:HD12	1:F:250:PRO:HD2	1.99	0.44
1:C:615:GLN:HE22	1:C:726:PRO:HA	1.81	0.44
1:D:418:GLU:HG2	1:D:640:MET:HE3	2.00	0.44
1:E:503:TRP:N	1:E:504:PRO:CD	2.81	0.44
1:B:428:HIS:NE2	1:B:608:GLN:NE2	2.65	0.44
1:C:249:LEU:HD12	1:C:250:PRO:HD2	1.99	0.44
1:D:320:ILE:O	1:D:407:THR:OG1	2.33	0.44
3:L:38:ILE:HD12	3:L:100:LEU:HG	1.99	0.44
1:B:427:ALA:CB	1:C:391:ARG:HD3	2.48	0.44
1:C:503:TRP:H	1:C:504:PRO:HD3	1.83	0.44
1:D:255:HIS:CE1	1:D:653:PRO:HB3	2.52	0.44
1:D:542:ILE:HG22	1:F:445:TYR:HB2	1.99	0.44
1:A:399:TYR:OH	1:F:297:ASP:OD2	2.35	0.43
1:C:562:ASN:O	1:C:562:ASN:ND2	2.51	0.43
1:C:695:TRP:HE1	1:F:721:TYR:HE1	1.66	0.43
3:L:44:GLY:O	3:L:91:ASN:HB3	2.18	0.43
1:C:433:ASP:OD1	1:C:433:ASP:N	2.50	0.43
1:F:288:ARG:HH21	1:F:615:GLN:HB3	1.82	0.43
1:C:529:GLU:OE1	1:C:529:GLU:HA	2.18	0.43
1:D:418:GLU:OE2	1:D:641:LYS:N	2.50	0.43
1:D:506:ALA:HB1	1:D:517:LEU:HD13	2.01	0.43
1:F:424:SER:HB2	1:F:426:TYR:CE2	2.54	0.43
3:L:84:PHE:CD1	3:L:97:ILE:HG12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TRP:HB3	1:A:372:PHE:CZ	2.53	0.43
1:C:696:ASN:OD1	1:C:696:ASN:N	2.49	0.43
1:E:478:TYR:CE2	1:F:623:PRO:HD3	2.54	0.43
1:A:493:VAL:HG12	1:C:461:LEU:HD13	2.00	0.43
1:C:541:LEU:O	1:C:561:THR:HG22	2.18	0.43
1:D:247:TRP:HB3	1:D:372:PHE:CZ	2.53	0.43
2:H:37:LEU:HD11	2:H:142:VAL:HG11	2.01	0.43
1:A:259:GLN:OE1	1:F:710:ASN:OD1	2.37	0.43
1:C:283:TYR:O	1:C:375:PRO:HD2	2.19	0.43
1:C:434:ARG:HA	1:C:434:ARG:HD3	1.84	0.43
1:F:322:VAL:HG11	1:F:673:GLN:HE21	1.84	0.43
1:F:285:ASP:O	1:F:363:CYS:HA	2.18	0.43
1:A:355:VAL:H	1:A:646:GLN:NE2	2.16	0.42
1:D:621:LYS:HB2	1:D:643:PRO:HG3	2.01	0.42
1:D:355:VAL:H	1:D:646:GLN:NE2	2.16	0.42
1:A:323:LYS:NZ	1:A:336:ASN:OD1	2.30	0.42
3:L:47:SER:O	3:L:52:TYR:HE2	2.02	0.42
1:A:428:HIS:CE1	1:B:624:HIS:O	2.73	0.42
1:D:628:ASN:HB3	1:F:606:VAL:HG12	2.02	0.42
1:E:449:LYS:HE3	1:F:552:ASN:HD21	1.85	0.42
1:F:354:TYR:CZ	1:F:356:LEU:HB2	2.55	0.42
1:A:382:LEU:HG	1:C:429:SER:C	2.43	0.42
1:B:424:SER:OG	1:C:626:ASP:OD1	2.37	0.42
1:C:379:TYR:OH	1:C:395:TYR:N	2.51	0.42
1:C:495:GLN:H	1:C:495:GLN:HG2	1.62	0.42
1:C:563:GLU:OE1	1:C:610:ARG:HG3	2.19	0.42
2:H:54:ASN:OD1	2:H:69:TYR:HB3	2.20	0.42
1:A:313:LEU:HD13	1:A:314:ASN:N	2.35	0.42
1:A:344:VAL:HA	1:A:648:LEU:O	2.19	0.42
1:A:607:TRP:HE1	1:A:630:HIS:CD2	2.38	0.42
1:A:621:LYS:HB2	1:A:643:PRO:HG3	2.01	0.42
1:C:322:VAL:HG11	1:C:673:GLN:HE21	1.84	0.42
1:F:425:SER:HB2	1:F:729:THR:HG22	2.00	0.42
1:F:621:LYS:HB2	1:F:643:PRO:HG3	2.01	0.42
1:A:423:HIS:NE2	1:A:612:VAL:HG22	2.34	0.42
1:C:283:TYR:CE1	1:C:375:PRO:CG	3.03	0.42
1:C:343:GLN:HG2	1:C:404:MET:HG2	2.02	0.42
1:D:288:ARG:HD3	1:D:363:CYS:SG	2.60	0.42
1:D:323:LYS:NZ	1:D:336:ASN:OD1	2.30	0.42
1:E:427:ALA:HB1	1:F:391:ARG:HD3	2.02	0.42
1:E:506:ALA:CB	1:E:537:LEU:HD22	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:LYS:HE2	1:F:412:GLN:OE1	2.20	0.42
1:F:434:ARG:HD3	1:F:434:ARG:HA	1.84	0.42
1:F:519:ASN:HA	1:F:520:PRO:HA	1.94	0.42
1:A:355:VAL:H	1:A:646:GLN:HE22	1.68	0.42
1:A:418:GLU:OE2	1:A:641:LYS:N	2.50	0.42
1:A:478:TYR:CE2	1:B:623:PRO:HD3	2.55	0.42
1:B:428:HIS:HE1	1:C:624:HIS:O	2.03	0.42
1:C:364:LEU:N	1:C:364:LEU:HD12	2.34	0.42
1:C:460:THR:O	1:C:461:LEU:HD12	2.20	0.42
1:C:537:LEU:HB3	1:C:538:SER:H	1.57	0.42
1:B:461:LEU:HD13	1:C:493:VAL:HG12	2.02	0.41
1:C:314:ASN:HB3	1:C:682:GLU:HB3	2.01	0.41
1:C:612:VAL:O	1:C:729:THR:OG1	2.37	0.41
1:D:313:LEU:HD13	1:D:314:ASN:N	2.35	0.41
1:D:344:VAL:HA	1:D:648:LEU:O	2.19	0.41
1:F:615:GLN:HE22	1:F:726:PRO:HA	1.85	0.41
1:A:529:GLU:OE1	1:A:567:LYS:HE3	2.20	0.41
1:D:355:VAL:H	1:D:646:GLN:HE22	1.68	0.41
1:F:316:LYS:HB2	1:F:680:SER:OG	2.20	0.41
1:F:460:THR:O	1:F:461:LEU:HD12	2.20	0.41
1:A:585:GLN:OE1	1:B:501:PHE:CZ	2.73	0.41
1:B:430:GLN:NE2	1:C:353:PRO:HB3	2.36	0.41
1:C:540:SER:HB3	1:C:561:THR:O	2.20	0.41
1:D:351:GLN:O	1:F:735:ASN:ND2	2.53	0.41
2:H:70:VAL:HB	2:H:88:VAL:HG12	2.01	0.41
1:C:316:LYS:HE2	1:C:412:GLN:OE1	2.20	0.41
1:C:352:LEU:HD21	1:C:400:PHE:CE2	2.56	0.41
1:D:520:PRO:HD3	1:D:635:MET:HG2	2.03	0.41
1:E:434:ARG:HD2	1:F:380:LEU:HD13	2.02	0.41
1:F:352:LEU:HD21	1:F:400:PHE:CE2	2.56	0.41
3:L:58:TYR:O	3:L:108:TYR:HA	2.20	0.41
1:A:343:GLN:HE21	1:A:404:MET:HE3	1.85	0.41
1:C:621:LYS:HB2	1:C:643:PRO:HG3	2.01	0.41
1:F:275:PHE:HB3	1:F:383:ASN:HB3	2.03	0.41
1:C:354:TYR:CZ	1:C:356:LEU:HB2	2.55	0.41
1:F:314:ASN:HB3	1:F:682:GLU:HB3	2.01	0.41
1:A:288:ARG:HD3	1:A:363:CYS:SG	2.60	0.41
1:A:520:PRO:HD3	1:A:635:MET:HG2	2.03	0.41
1:B:466:ALA:HB1	1:B:474:GLN:HG2	2.03	0.41
1:B:484:TYR:O	1:B:524:MET:HE1	2.21	0.41
1:C:323:LYS:HB3	1:C:334:ILE:HG23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ALA:HB1	1:E:474:GLN:HG2	2.03	0.41
2:H:136:TRP:CE3	3:L:66:PRO:HD2	2.56	0.41
1:C:308:PHE:HA	1:C:686:GLU:O	2.21	0.41
1:D:607:TRP:HE1	1:D:630:HIS:CD2	2.38	0.41
1:F:696:ASN:OD1	1:F:696:ASN:N	2.49	0.41
1:F:715:VAL:HA	1:F:720:VAL:O	2.21	0.41
1:B:586:SER:O	1:C:497:ASN:HB2	2.21	0.41
1:E:460:THR:O	1:E:461:LEU:HD12	2.21	0.41
1:F:323:LYS:HB3	1:F:334:ILE:HG23	2.03	0.41
1:F:612:VAL:O	1:F:729:THR:OG1	2.37	0.41
2:H:66:TRP:CZ2	2:H:68:GLY:HA2	2.55	0.41
1:C:244:THR:HA	1:C:679:VAL:O	2.21	0.41
1:C:519:ASN:HA	1:C:520:PRO:HA	1.94	0.41
1:F:308:PHE:HA	1:F:686:GLU:O	2.21	0.41
2:H:128:ASP:OD2	3:L:117:SER:OG	2.37	0.41
3:L:26:GLN:HE21	3:L:110:CYS:HB2	1.85	0.41
3:L:75:ASN:HD22	3:L:75:ASN:HA	1.65	0.41
1:A:428:HIS:HE1	1:B:624:HIS:O	2.04	0.40
1:B:433:ASP:OD1	1:B:433:ASP:N	2.48	0.40
1:B:460:THR:O	1:B:461:LEU:HD12	2.21	0.40
1:C:238:ARG:HD2	1:C:684:GLU:OE2	2.21	0.40
1:C:275:PHE:HB3	1:C:383:ASN:HB3	2.03	0.40
1:C:306:TRP:CZ3	1:C:734:ARG:NH1	2.89	0.40
1:D:495:GLN:HE22	1:D:533:ARG:NE	2.19	0.40
1:D:529:GLU:OE1	1:D:567:LYS:HE3	2.20	0.40
1:E:589:ALA:O	1:F:497:ASN:ND2	2.52	0.40
1:F:244:THR:HA	1:F:679:VAL:O	2.21	0.40
1:A:279:THR:OG1	1:A:377:TYR:O	2.21	0.40
1:C:367:PHE:HE1	1:D:396:CYS:HB2	1.86	0.40
1:C:484:TYR:O	1:C:524:MET:HE1	2.21	0.40
1:D:254:ASN:N	1:D:254:ASN:ND2	2.69	0.40
1:D:650:LYS:HE3	1:D:650:LYS:HB2	1.92	0.40
1:F:427:ALA:O	1:F:733:THR:HA	2.21	0.40
1:A:628:ASN:HB3	1:C:606:VAL:HG12	2.04	0.40
1:D:343:GLN:HE21	1:D:404:MET:HE3	1.85	0.40
1:E:433:ASP:OD1	1:E:433:ASP:N	2.48	0.40
1:F:548:THR:CG2	1:F:553:VAL:HG11	2.51	0.40
1:A:367:PHE:HE2	1:A:369:ALA:HB3	1.86	0.40
1:A:406:ARG:N	1:A:409:ASN:OD1	2.47	0.40
1:C:316:LYS:HB2	1:C:680:SER:OG	2.20	0.40
1:C:650:LYS:HE3	1:C:650:LYS:HB2	1.92	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:ILE:CG2	1:F:445:TYR:HB2	2.52	0.40
1:E:484:TYR:O	1:E:524:MET:HE1	2.21	0.40
1:F:317:LEU:HD13	1:F:679:VAL:HG22	2.04	0.40
1:F:343:GLN:HG2	1:F:404:MET:HG2	2.02	0.40
1:F:426:TYR:CD1	1:F:426:TYR:C	2.99	0.40
1:F:484:TYR:O	1:F:524:MET:HE1	2.21	0.40
1:A:269:SER:HB3	1:A:272:ASN:HD22	1.86	0.40
1:A:341:THR:HG22	1:A:406:ARG:HG3	2.04	0.40
1:B:420:VAL:HG11	1:B:640:MET:HG2	2.03	0.40
1:C:559:MET:SD	1:C:726:PRO:HD3	2.62	0.40
1:C:699:ILE:HG12	1:F:703:SER:O	2.21	0.40
1:F:712:GLU:CD	1:F:725:ARG:HH22	2.19	0.40
2:H:109:THR:HG23	2:H:143:THR:HA	2.03	0.40
3:L:84:PHE:HD1	3:L:97:ILE:HG12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	394/736 (54%)	383 (97%)	11 (3%)	0	100	100
1	B	194/736 (26%)	189 (97%)	5 (3%)	0	100	100
1	C	502/736 (68%)	488 (97%)	14 (3%)	0	100	100
1	D	394/736 (54%)	381 (97%)	13 (3%)	0	100	100
1	E	168/736 (23%)	164 (98%)	4 (2%)	0	100	100
1	F	502/736 (68%)	491 (98%)	11 (2%)	0	100	100
2	H	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
3	L	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
All	All	2390/4656 (51%)	2327 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	347/615 (56%)	345 (99%)	2 (1%)	84	90
1	B	168/615 (27%)	167 (99%)	1 (1%)	84	90
1	C	443/615 (72%)	438 (99%)	5 (1%)	70	83
1	D	347/615 (56%)	346 (100%)	1 (0%)	91	95
1	E	145/615 (24%)	145 (100%)	0	100	100
1	F	443/615 (72%)	441 (100%)	2 (0%)	86	92
2	H	113/113 (100%)	109 (96%)	4 (4%)	31	52
3	L	91/91 (100%)	89 (98%)	2 (2%)	47	68
All	All	2097/3894 (54%)	2080 (99%)	17 (1%)	77	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	254	ASN
1	B	496	ASN
1	C	429	SER
1	C	491	THR
1	C	495	GLN
1	C	537	LEU
1	C	562	ASN
1	D	254	ASN
1	F	717	THR
1	F	725	ARG
2	H	48	ILE
2	H	124	GLU
2	H	127	THR
2	H	131	TYR
3	L	52	TYR
3	L	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	A	259	GLN
1	A	262	ASN
1	A	272	ASN
1	A	343	GLN
1	A	546	GLN
1	A	584	HIS
1	A	608	GLN
1	A	624	HIS
1	A	642	HIS
1	A	646	GLN
1	A	651	ASN
1	A	678	GLN
1	B	452	ASN
1	B	496	ASN
1	B	585	GLN
1	B	608	GLN
1	B	624	HIS
1	B	642	HIS
1	C	305	ASN
1	C	321	GLN
1	C	495	GLN
1	C	515	ASN
1	C	552	ASN
1	C	562	ASN
1	C	608	GLN
1	C	624	HIS
1	C	642	HIS
1	C	646	GLN
1	C	673	GLN
1	C	691	ASN
1	C	700	GLN
1	D	253	ASN
1	D	254	ASN
1	D	255	HIS
1	D	343	GLN
1	D	546	GLN
1	D	624	HIS
1	D	642	HIS
1	D	646	GLN
1	D	651	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	688	GLN
1	E	430	GLN
1	E	452	ASN
1	E	585	GLN
1	E	608	GLN
1	F	305	ASN
1	F	321	GLN
1	F	428	HIS
1	F	495	GLN
1	F	515	ASN
1	F	585	GLN
1	F	608	GLN
1	F	624	HIS
1	F	642	HIS
1	F	646	GLN
1	F	673	GLN
1	F	700	GLN
1	F	704	ASN
1	F	709	ASN
2	H	71	HIS
2	H	117	GLN
3	L	21	GLN
3	L	61	HIS
3	L	75	ASN
3	L	82	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

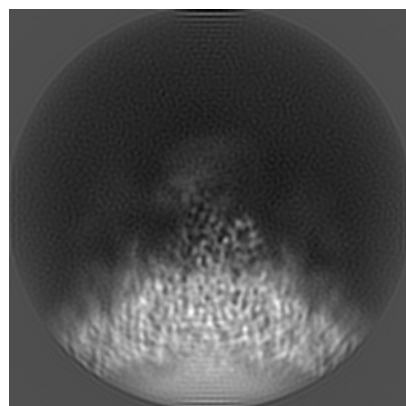
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44327. These allow visual inspection of the internal detail of the map and identification of artifacts.

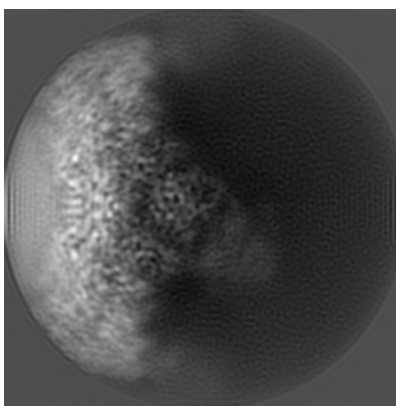
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

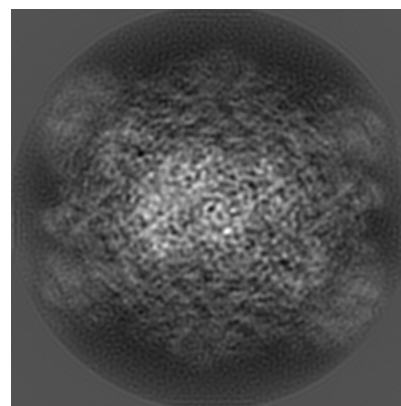
6.1.1 Primary map



X

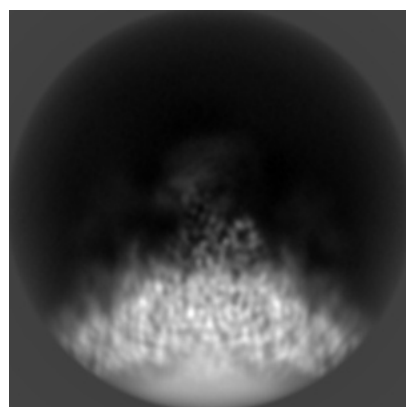


Y

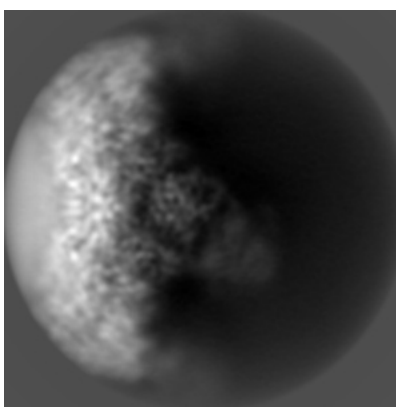


Z

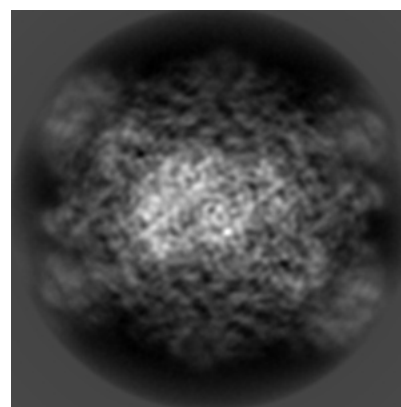
6.1.2 Raw map



X



Y

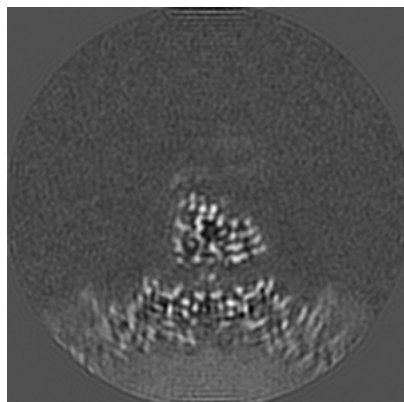


Z

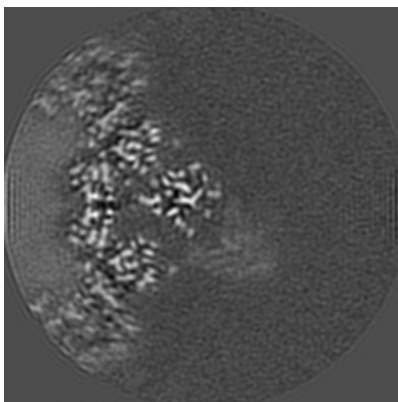
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

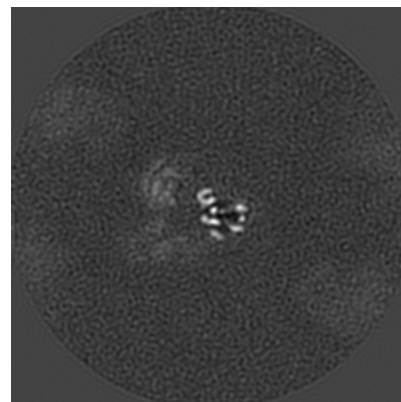
6.2.1 Primary map



X Index: 100

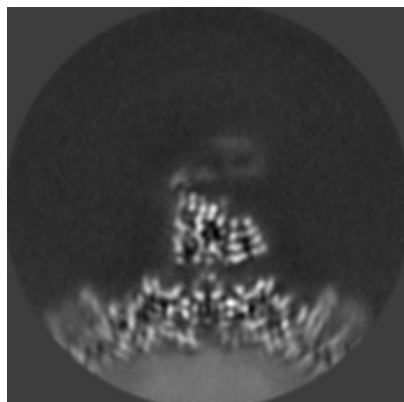


Y Index: 100

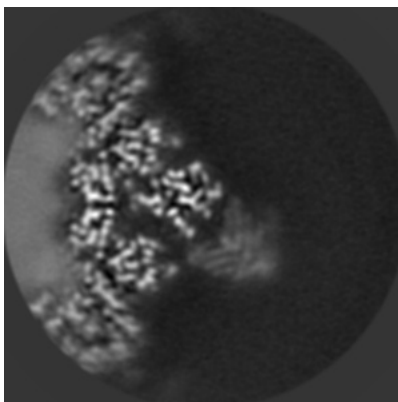


Z Index: 100

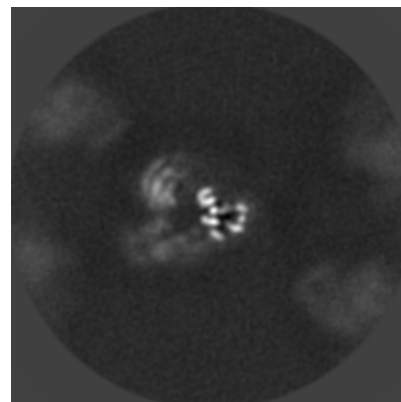
6.2.2 Raw map



X Index: 100



Y Index: 100

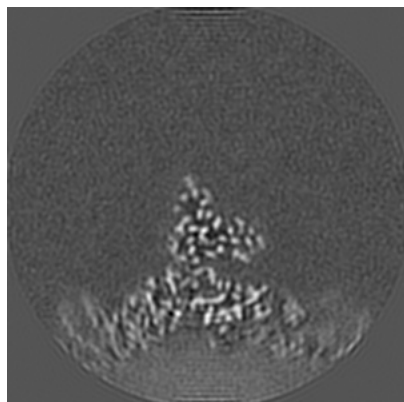


Z Index: 100

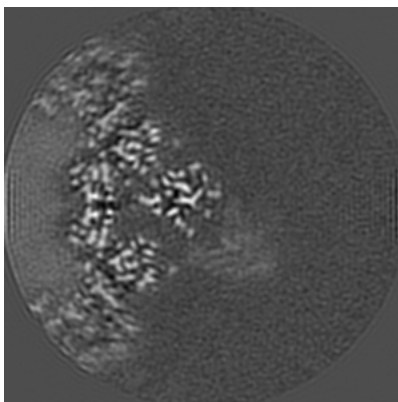
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

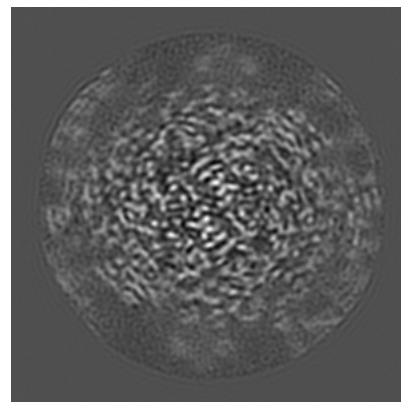
6.3.1 Primary map



X Index: 105

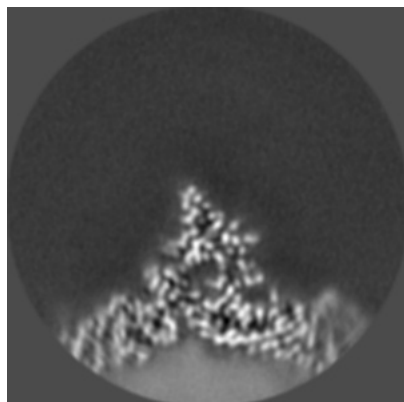


Y Index: 100

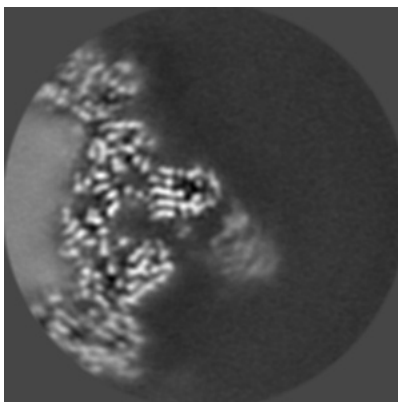


Z Index: 47

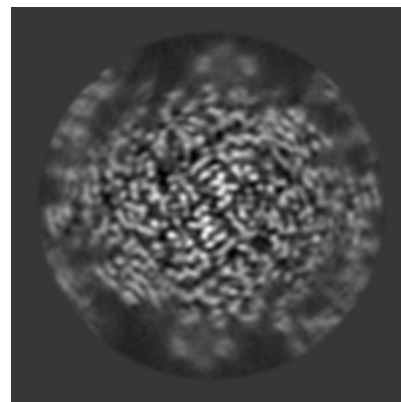
6.3.2 Raw map



X Index: 113



Y Index: 96

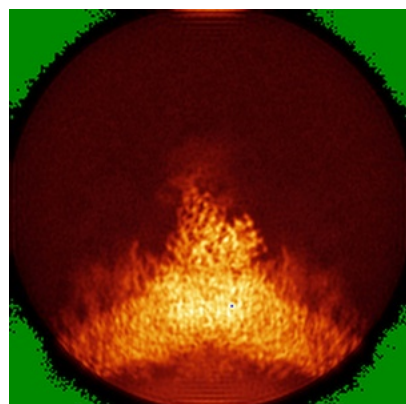


Z Index: 47

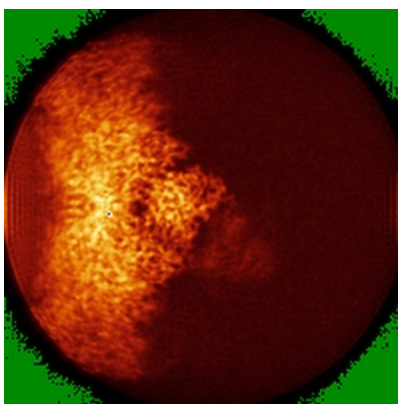
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

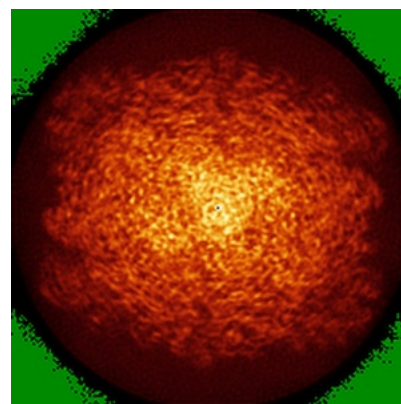
6.4.1 Primary map



X

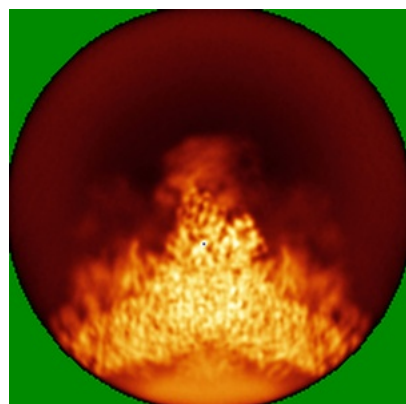


Y

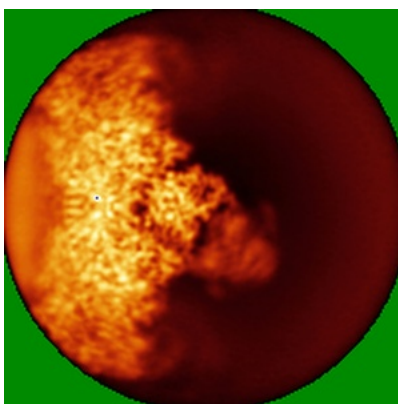


Z

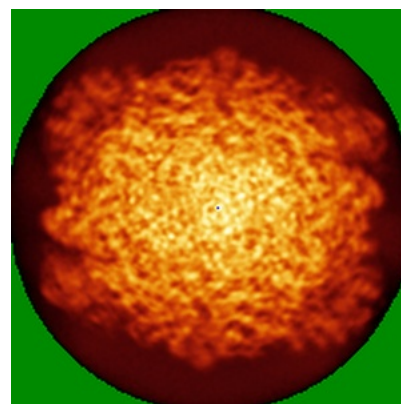
6.4.2 Raw map



X



Y

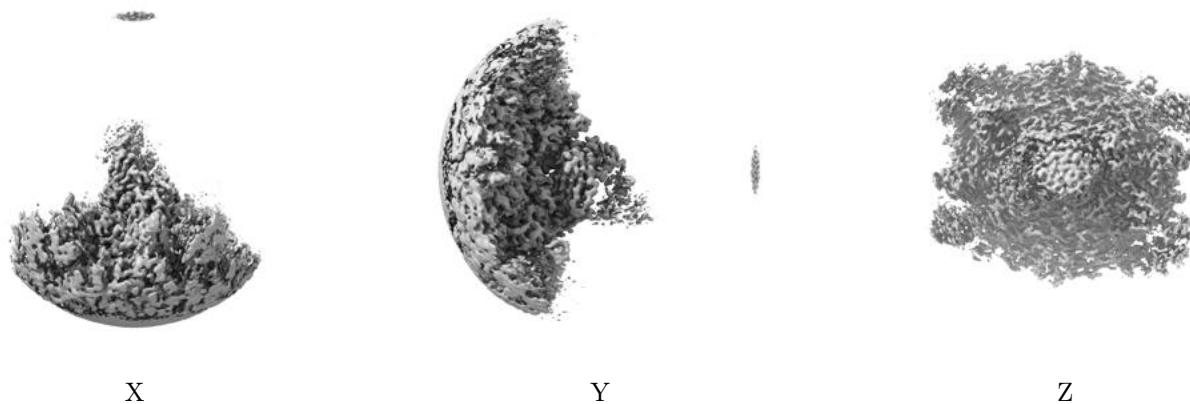


Z

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.

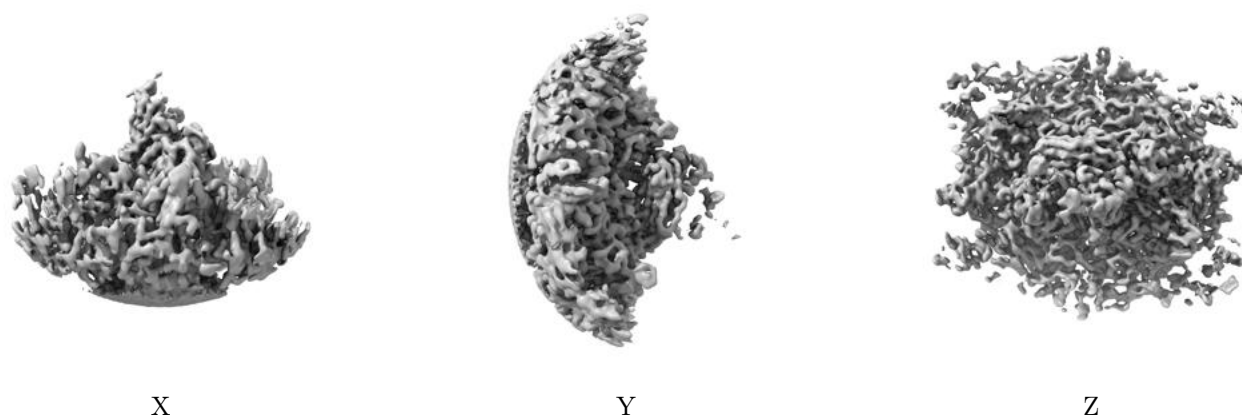
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

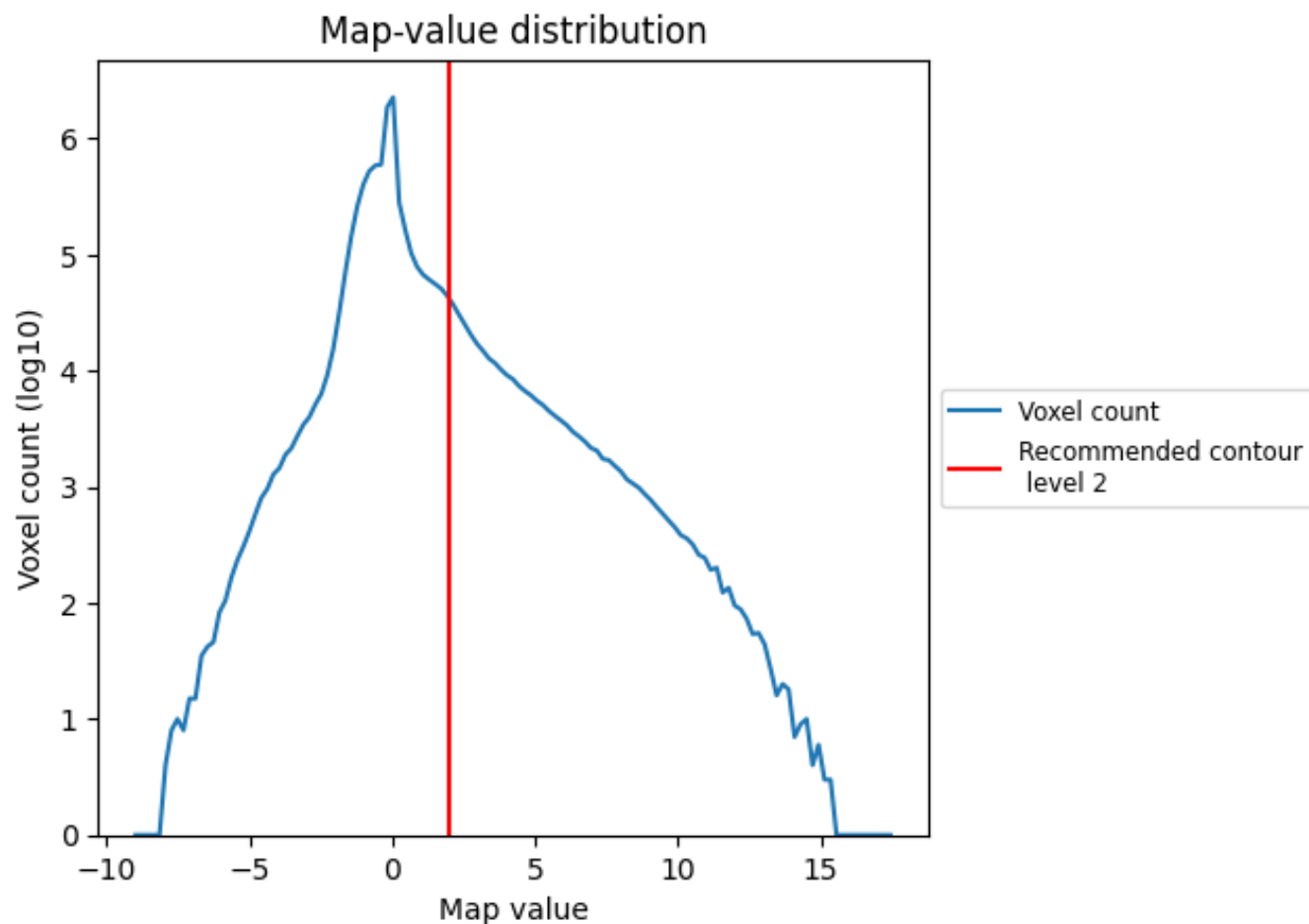
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

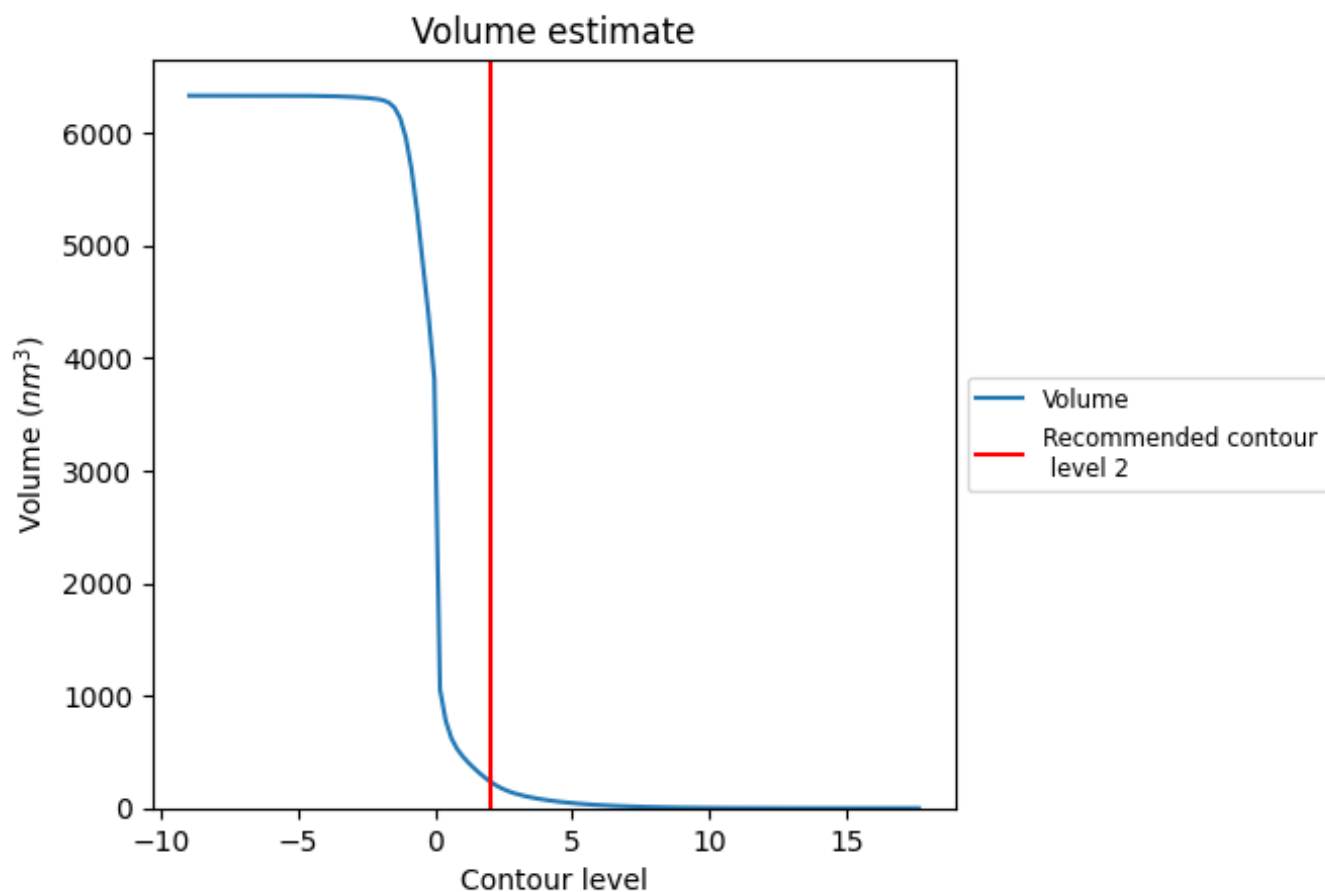
This section contains the results of statistical analysis of the map.

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.

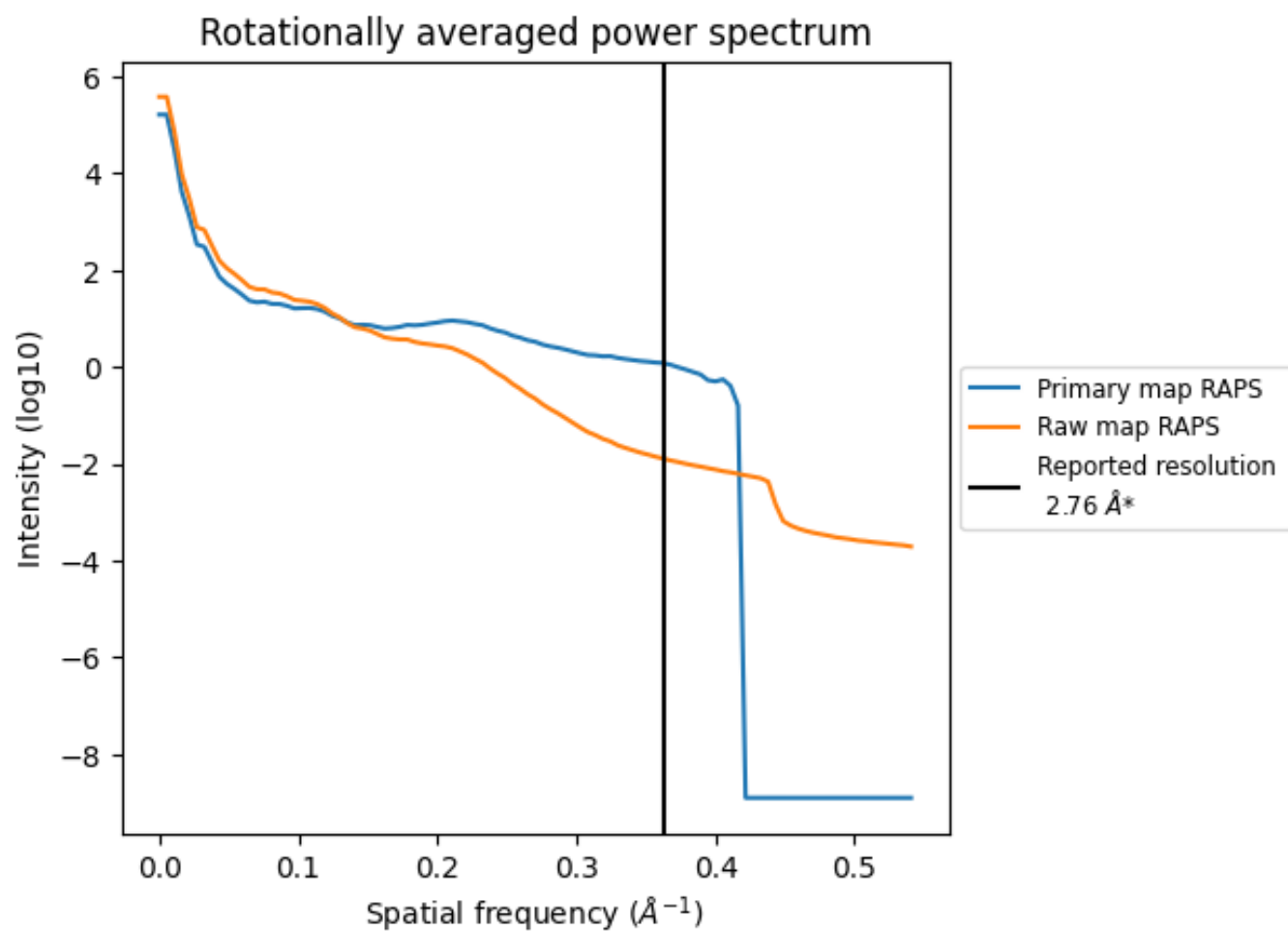
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 237 nm³; this corresponds to an approximate mass of 214 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 ⓘ

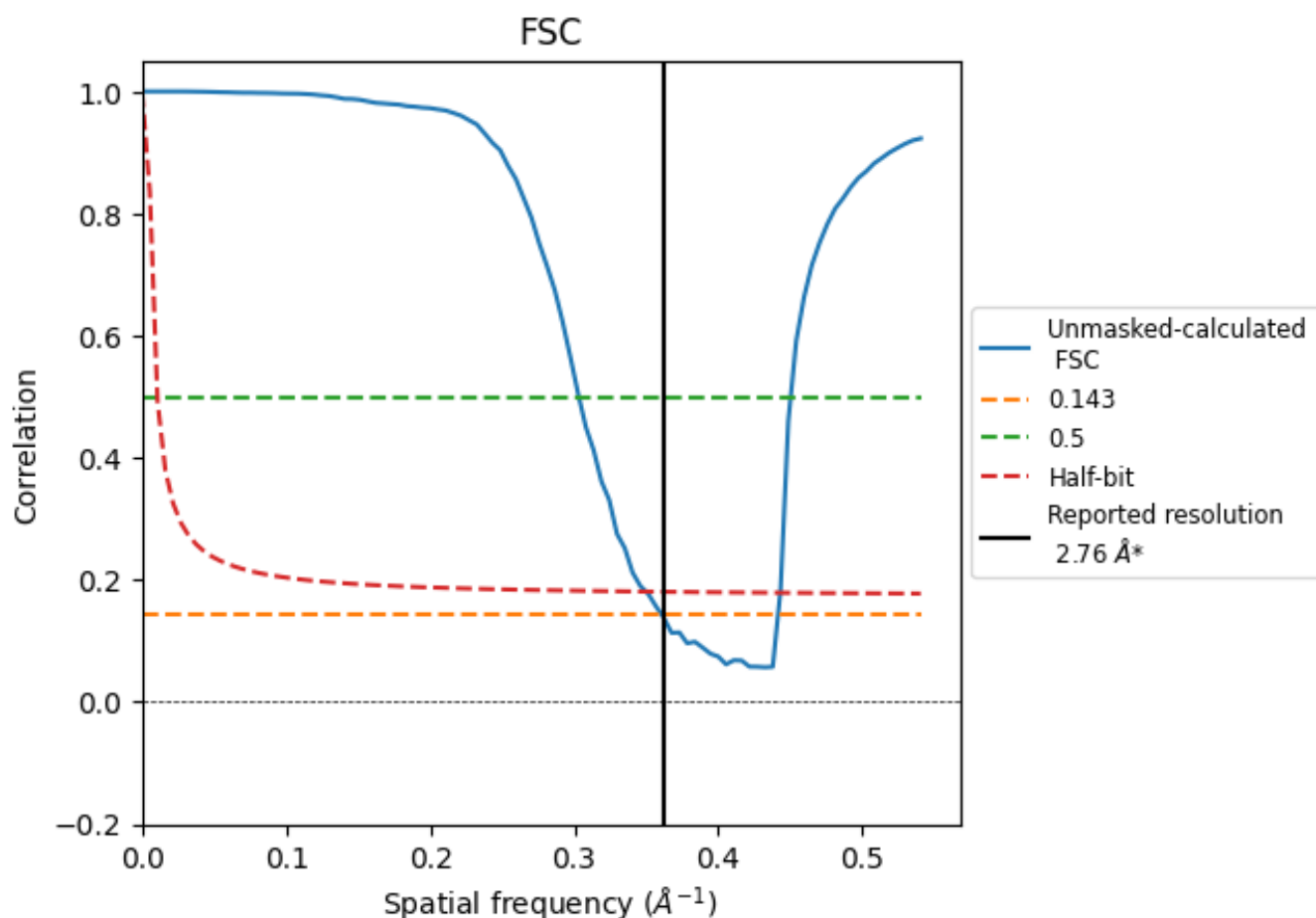


*Reported resolution corresponds to spatial frequency of 0.362 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.362 \AA^{-1}

8.2 Resolution estimates [i](#)

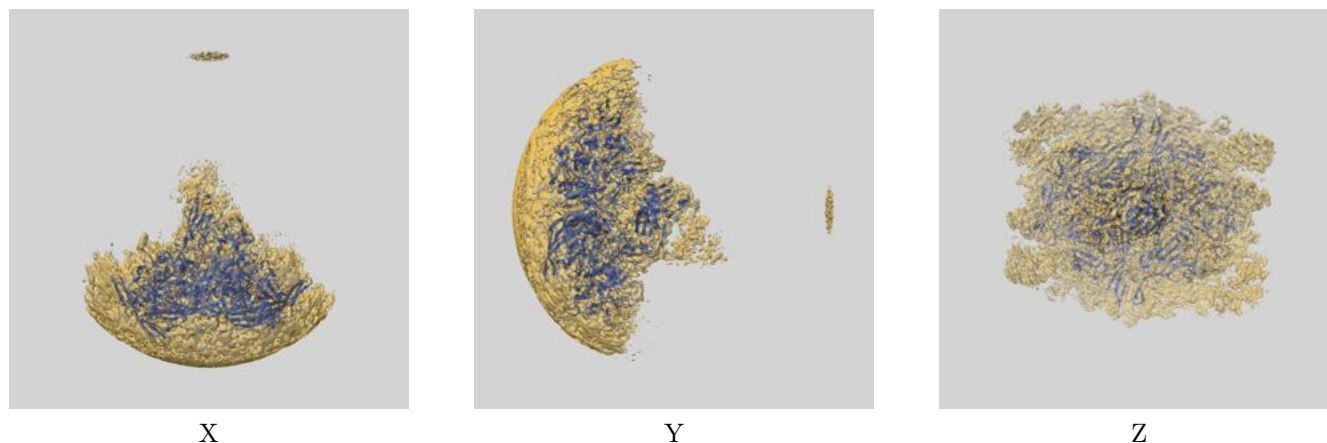
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.77	3.30	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

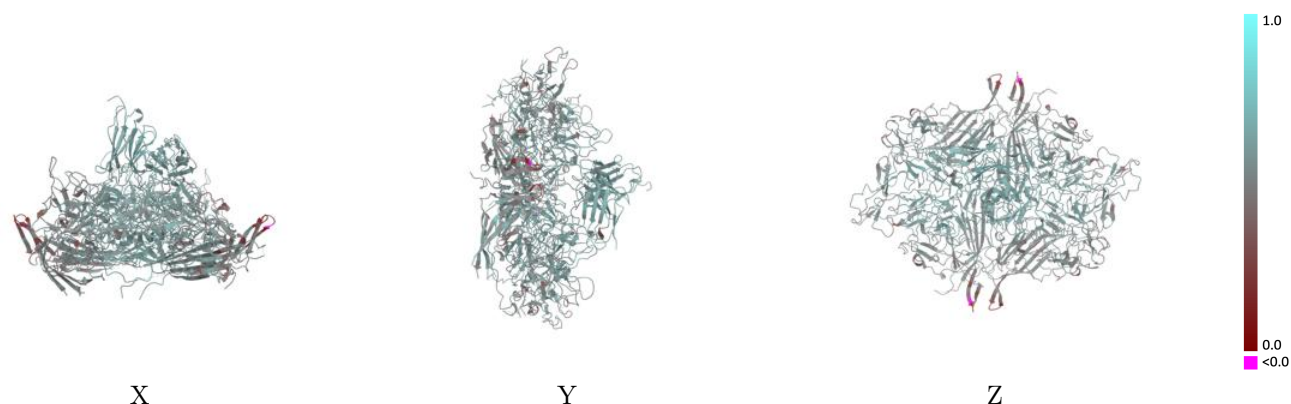
This section contains information regarding the fit between EMDB map EMD-44327 and PDB model 9B7X. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



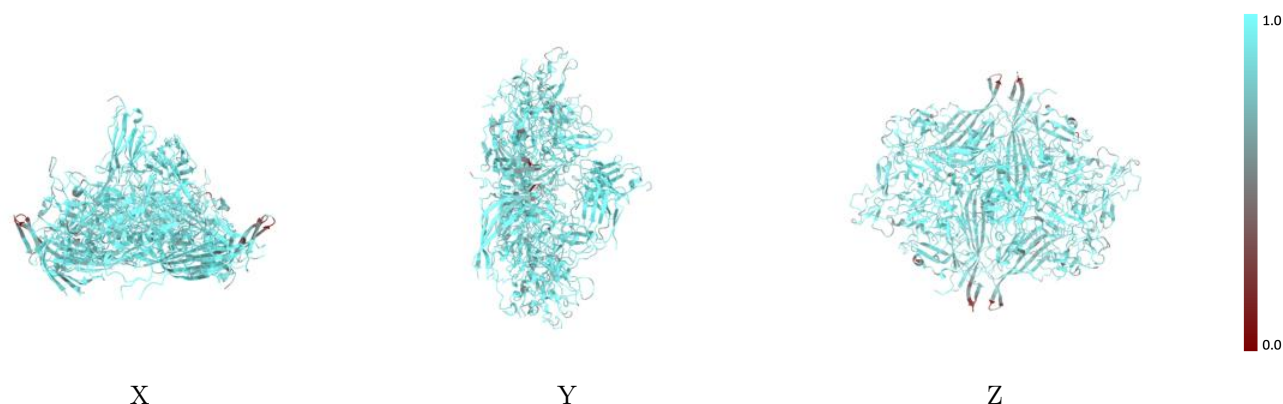
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



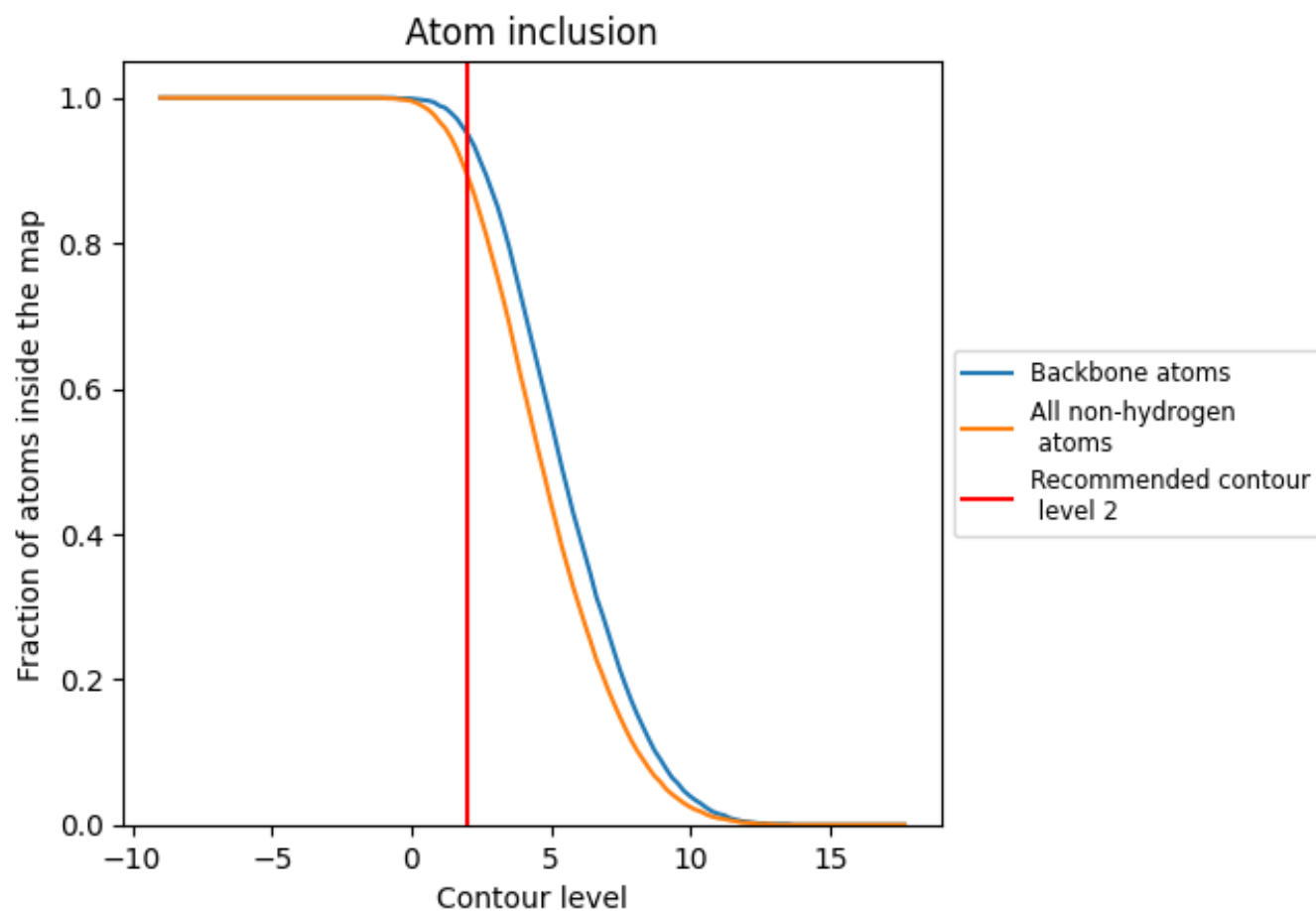
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8930	<div><div></div></div> 0.5490
A	<div><div></div></div> 0.8650	<div><div></div></div> 0.5150
B	<div><div></div></div> 0.8820	<div><div></div></div> 0.5540
C	<div><div></div></div> 0.8990	<div><div></div></div> 0.5500
D	<div><div></div></div> 0.8860	<div><div></div></div> 0.5380
E	<div><div></div></div> 0.8840	<div><div></div></div> 0.5500
F	<div><div></div></div> 0.9040	<div><div></div></div> 0.5580
H	<div><div></div></div> 0.9370	<div><div></div></div> 0.6070
L	<div><div></div></div> 0.9240	<div><div></div></div> 0.6030

1.0

0.0

<0.0