



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:43 AM UTC

PDB ID : 9BD8 / pdb_00009bd8
EMDB ID : EMD-44446
Title : ApoB 100 beta barrel bound to LDLR beta propeller
Authors : Dearborn, A.D.; Reimund, M.; Graziano, G.; Lei, H.; Kumar, A.; Neufeld, E.B.; Remaley, A.T.; Marcotrigiano, J.
Deposited on : 2024-04-11
Resolution : 4.80 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

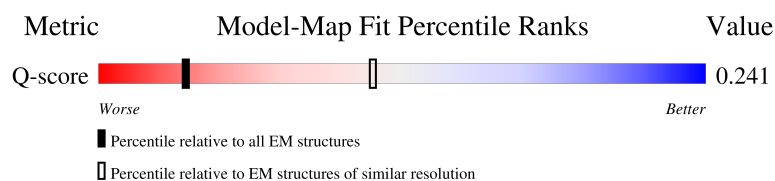
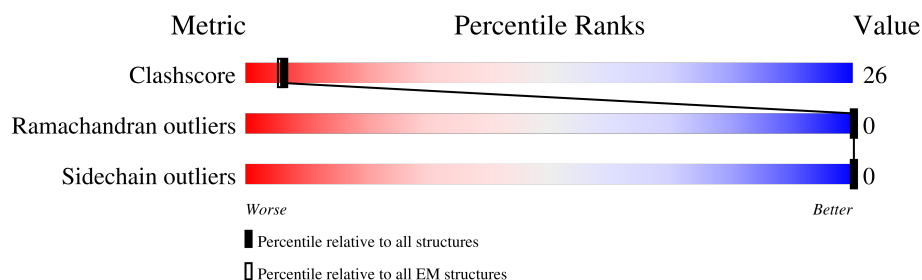
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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	4563	 6% 15% 16% 63% 90%
2	B	860	 15% 16% 69%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5369 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.

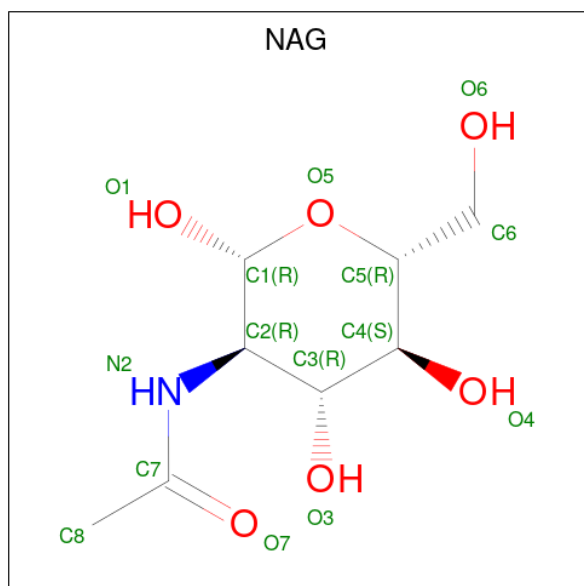
- Molecule 1 is a protein called Apolipoprotein B-100.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	462	Total	C	N	O	S	0	0
			3423	2163	565	680	15		

- Molecule 2 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	264	Total	C	N	O	S	0	0
			1932	1235	314	378	5		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	

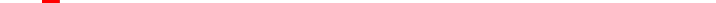






LYS PHE ILE ALA GLU SER LYS ARG LEU ILE LEU LEU SER GLN ASN HIS THR PHE LEU ILE TYR THR ILE GLU LEU LYS LYS LEU GLN SER THR THR VAL MET ASN PRO TYR MET LYS LEU ALA PRO GLY GLU LEU THR ILE ILE LEU

- Molecule 2: Low-density lipoprotein receptor

Chain B:  15% 16% 69%

ASP CYS ARG ASP TRP SER ASP GLU PRO LYS LEU CYS GLY THR ASN CYS LEU ASP ASN CYS GLY TYR VAL HIS CYS ASN ASP LYS LEU CYS ASP ASP PHE GLN LEU VAL ALA ARG CYS ASP ASP ASP ASP ASP ASP

PRO	ASP	THR	CYS	SER	GLN	LEU	CYS	VAL	ASN	LEU	GLU	GLY	TYR	LYS	CYS	GLN	CYS	GLU	GLY	PHE	GLN	LEU	ASP	PRO	HIS	THR	LYS	ALA	CYS	LYS	ALA	VAL	GLY	SER	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1416	1427	1428
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

E435	E436	A437	A438	I441	Y442	W443	S444	D445	L446	S447	M450	I451	C452	S453	T454	R458	ALA	HIS	GLY	VAL	SER	SER	Y465	D466	T467	V468	I469	S470	T471	D472	I473	D477	G478	L479	A480	V481	D482	W483	L484	H485	S486	N487	L488	Y489	W490	T491	D492	S493	V494	L495	G496	T497	V498
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

V500	A501	D502	T503	K504	R508	K509	T510	R513	E514	N515	G516	S517	K518	P519	R520	A521	I522	V523	V527	F530	M531	V532	W533	T534	D535	W536	G537	T538	P539	K541	L542	K543	K544	G545	G546	L547	V550	D551	S554	L555	V556	N559	W562	P563	N564	D569	L570
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

L654	F655	H656	N657	L658	T659	Q660	P661	G662	N665	H666	C667	GLU	ARG	THR	THR	LEU	SER	ASN	GLY	GLY	CYS	GLN	TTR	LEU	CYS	PRO	PRO	ALA	ALA	GLN	ILE	ASN	ASN	PRO	PRO	HIS	SER	SER	PRO	LYS	PHI	THR	CYS	ALA	CYS	PRO	ASP	GLY	MET	LEU	LEU	ALA	ALA	ARG	ASP	MET	ARG	SER	CYS	THR	LEU	THR	GLU
------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	GLU	ALA	ALA	ALA	VAL	ALA	THR	GLN	ARG	SER	THR	VAL	VAL	ARG	LEU	LYS	VAL	SER	SER	THR	ALA	ALA	VAL	VAL	ARG	THR	GLN	HIS	THR	THR	THR	THR	THR	ARG	PRO	PRO	VAL	VAL	ASP	THR	THR	SER	ARG	LEU	LEU	GLY	GLY	ALA	ALA	THR	THR	PRO	GLY	GLY	LEU	THR	THR	THR	VAL	GLU	VAL	VAL	IIE	MET	MET	SER	HIS	GLN	ALA	LEU	LEU	GLY	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	ALA	GLY	GLY	GLY	ASN	GLU	LYS	LYS	PRO	SER	SER	VAL	ALA	LEU	VAL	VAL	PRO	PHE	LEU	LEU	VAL	VAL	LEU	LEU	GLY	VAL	PHE	LEU	LEU	TRP	LYS	ASN	ASN	TRP	TRP	ASN	SER	ASN	ILE	ASN	PHE	ASP	ASN	PRO	VAL	VAL	THR	GLN	GLY	THR	THR	THR	GLU	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU VAL HIS ILE CYS HIS ASN GLN ASP GLY TYR SER TYR PRO SER ARG GLN MET VAL SER LEU GLU ASP ASP VAL ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	522863	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 ($e^-/\text{\AA}^2$)	51.38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.76, 557.76, 557.76	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6600001, 1.6600001, 1.6600001	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/3483	0.33	0/4744
2	B	0.14	0/1978	0.39	0/2723
All	All	0.13	0/5461	0.35	0/7467

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

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	3423	0	3243	157	0
2	B	1932	0	1728	110	0
3	A	14	0	13	0	0
All	All	5369	0	4984	264	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 26.

All (264) 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:B:468:VAL:HG12	2:B:469:ILE:HG12	1.60	0.81
2:B:540:ALA:HB1	2:B:562:TRP:H	1.47	0.80
1:A:294:ILE:HG22	1:A:296:SER:H	1.53	0.74
2:B:480:ALA:HB3	2:B:489:TYR:HB2	1.70	0.74
1:A:238:LEU:HB2	1:A:269:PRO:HD3	1.69	0.73
2:B:470:SER:O	2:B:508:ARG:NH1	2.21	0.73
2:B:570:LEU:HD13	2:B:658:LEU:HD23	1.71	0.72
2:B:404:THR:HG21	2:B:432:LEU:HD21	1.70	0.72
2:B:536:TRP:HA	2:B:540:ALA:HA	1.74	0.69
1:A:158:ARG:NH1	1:A:307:GLY:O	2.26	0.69
2:B:477:ASP:HB2	2:B:491:THR:HG23	1.74	0.69
1:A:977:THR:HG22	1:A:1003:LEU:HA	1.75	0.69
1:A:82:LEU:HD11	1:A:90:PHE:HB3	1.76	0.67
1:A:45:ARG:HB3	1:A:255:HIS:HA	1.77	0.67
1:A:158:ARG:HG3	1:A:182:VAL:HG12	1.78	0.66
1:A:942:LEU:HB3	1:A:953:ILE:HD12	1.76	0.66
1:A:980:ALA:HB3	1:A:1000:ARG:HB2	1.78	0.66
1:A:60:SER:HG	1:A:74:THR:HG1	1.44	0.65
1:A:60:SER:HA	1:A:282:VAL:HG12	1.78	0.65
1:A:906:PHE:O	1:A:937:SER:N	2.30	0.65
1:A:163:ALA:O	1:A:247:TYR:OH	2.15	0.64
1:A:828:HIS:HD2	1:A:855:ALA:HB1	1.61	0.64
1:A:287:LYS:NZ	1:A:288:LEU:O	2.31	0.64
2:B:574:ARG:HH11	2:B:588:ILE:HA	1.63	0.64
1:A:221:GLY:O	1:A:356:ARG:NH1	2.31	0.63
2:B:484:ILE:O	2:B:665:ASN:ND2	2.31	0.63
1:A:54:TYR:HA	1:A:288:LEU:HA	1.81	0.63
2:B:452:CYS:HA	2:B:468:VAL:HB	1.79	0.63
2:B:630:SER:HB3	2:B:640:ASN:HB2	1.81	0.63
1:A:243:GLN:HE22	1:A:245:CYS:HB2	1.64	0.62
1:A:884:VAL:HG22	1:A:902:ASN:HD22	1.63	0.62
1:A:325:VAL:HG22	1:A:354:GLU:HB3	1.81	0.62
1:A:265:HIS:HB2	1:A:280:ALA:HB3	1.81	0.62
2:B:499:SER:HA	2:B:510:THR:HA	1.82	0.62
1:A:288:LEU:HD21	1:A:291:THR:HG23	1.81	0.62
1:A:189:HIS:ND1	1:A:206:GLU:O	2.33	0.62
2:B:622:ASP:HB3	2:B:625:ASN:HB2	1.82	0.62
1:A:60:SER:OG	1:A:74:THR:OG1	2.18	0.61
2:B:488:ILE:N	2:B:501:ALA:O	2.23	0.61
1:A:156:ILE:O	1:A:160:ILE:HG12	2.00	0.61
1:A:331:GLU:OE1	1:A:331:GLU:N	2.31	0.61
1:A:207:ARG:NE	1:A:243:GLN:OE1	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:GLY:N	1:A:878:SER:O	2.34	0.61
1:A:960:ARG:HA	1:A:982:SER:HA	1.81	0.60
1:A:50:ARG:NH1	1:A:291:THR:O	2.34	0.60
1:A:902:ASN:OD1	1:A:943:HIS:ND1	2.34	0.60
2:B:521:ALA:H	2:B:534:THR:HB	1.66	0.60
1:A:831:PHE:HD2	1:A:854:ILE:HG12	1.67	0.60
2:B:563:PRO:HA	2:B:579:ASP:HA	1.84	0.60
1:A:158:ARG:NH1	1:A:309:ALA:O	2.35	0.59
1:A:192:VAL:HG11	1:A:195:ARG:HB2	1.85	0.59
2:B:403:PHE:HB2	2:B:652:MET:HE1	1.85	0.59
2:B:518:LYS:NZ	2:B:519:PRO:O	2.32	0.58
1:A:144:TYR:HB3	1:A:302:GLY:HA3	1.85	0.58
1:A:55:ASN:N	1:A:287:LYS:O	2.35	0.58
1:A:143:LEU:HB2	1:A:306:MET:HB2	1.84	0.58
1:A:380:GLN:OE1	1:A:380:GLN:N	2.37	0.57
1:A:155:ASN:HD21	1:A:311:GLU:HG2	1.69	0.57
1:A:208:ASP:O	1:A:211:GLN:NE2	2.37	0.57
1:A:209:LEU:HB2	1:A:241:SER:HB2	1.86	0.57
1:A:133:LEU:HD12	1:A:141:VAL:HG21	1.87	0.57
1:A:840:THR:HB	1:A:844:LEU:H	1.69	0.57
2:B:564:ASN:HB3	2:B:609:PHE:HA	1.86	0.57
1:A:48:HIS:CE1	2:B:648:SER:HA	2.40	0.56
2:B:519:PRO:HA	2:B:535:ASP:HA	1.88	0.56
2:B:620:TRP:NE1	2:B:629:PHE:HB3	2.20	0.56
2:B:623:ILE:HG13	2:B:624:ILE:HG23	1.87	0.56
2:B:401:LEU:HD12	2:B:652:MET:HG3	1.87	0.56
2:B:617:LYS:N	2:B:633:ARG:HB2	2.21	0.56
1:A:206:GLU:OE2	1:A:242:SER:OG	2.24	0.55
2:B:404:THR:HG22	2:B:409:VAL:HG22	1.87	0.55
1:A:195:ARG:HG3	1:A:197:GLY:H	1.70	0.55
2:B:402:PHE:HD2	2:B:653:VAL:HG23	1.72	0.55
2:B:577:TRP:NE1	2:B:586:SER:OG	2.40	0.55
1:A:183:TYR:HD2	1:A:207:ARG:HH12	1.53	0.55
2:B:579:ASP:HB2	2:B:582:LEU:HB2	1.90	0.54
2:B:586:SER:HB3	2:B:597:THR:HG22	1.89	0.54
1:A:937:SER:OG	1:A:1001:LEU:O	2.14	0.54
1:A:209:LEU:HD12	1:A:241:SER:HB3	1.90	0.54
2:B:654:LEU:HG	2:B:655:PHE:H	1.73	0.54
1:A:356:ARG:NH1	1:A:385:CYS:O	2.41	0.53
2:B:432:LEU:HA	2:B:479:LEU:HD22	1.89	0.53
2:B:444:SER:HB3	2:B:479:LEU:HD11	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:THR:HG23	1:A:183:TYR:H	1.74	0.53
1:A:65:PRO:HD3	1:A:279:VAL:HB	1.90	0.53
1:A:963:TRP:N	1:A:979:GLY:O	2.42	0.53
2:B:398:ILE:O	2:B:656:HIS:ND1	2.41	0.53
2:B:578:VAL:HG22	2:B:611:LEU:HD22	1.91	0.53
1:A:213:ASP:N	1:A:213:ASP:OD1	2.41	0.53
1:A:263:GLU:HB3	1:A:282:VAL:HG22	1.91	0.52
1:A:377:ILE:O	1:A:380:GLN:NE2	2.33	0.52
1:A:830:ILE:HD13	1:A:853:VAL:HG13	1.91	0.52
1:A:241:SER:HB3	1:A:265:HIS:CD2	2.44	0.52
1:A:209:LEU:HD11	1:A:263:GLU:HG3	1.92	0.52
1:A:905:PHE:CD2	1:A:938:GLY:HA2	2.44	0.52
1:A:212:CYS:HB2	1:A:215:PHE:CD2	2.45	0.52
1:A:828:HIS:CD2	1:A:855:ALA:HB1	2.45	0.51
1:A:128:ARG:HH22	1:A:150:PRO:HG3	1.75	0.51
1:A:188:THR:HG22	1:A:207:ARG:HG2	1.93	0.51
1:A:40:PRO:HB2	1:A:43:ALA:HB2	1.93	0.51
2:B:628:ILE:O	2:B:641:LEU:HA	2.11	0.51
1:A:155:ASN:O	1:A:158:ARG:HG2	2.10	0.51
1:A:979:GLY:HA2	1:A:1001:LEU:HA	1.92	0.51
2:B:400:TYR:HE1	2:B:413:THR:HG22	1.75	0.51
2:B:398:ILE:HG22	2:B:655:PHE:HE2	1.76	0.51
2:B:543:LYS:HA	2:B:554:SER:HA	1.93	0.51
1:A:76:ILE:HD13	1:A:99:LEU:HB3	1.92	0.51
2:B:400:TYR:H	2:B:655:PHE:HB3	1.76	0.50
1:A:103:TYR:CZ	1:A:112:LEU:HB3	2.45	0.50
1:A:183:TYR:OH	1:A:841:GLY:N	2.43	0.50
1:A:263:GLU:HB3	1:A:282:VAL:CG2	2.41	0.50
1:A:53:THR:O	1:A:289:GLU:N	2.34	0.50
2:B:435:GLU:HG3	2:B:438:SER:HB2	1.92	0.50
2:B:655:PHE:CG	2:B:656:HIS:N	2.80	0.50
2:B:401:LEU:HB3	2:B:652:MET:SD	2.51	0.50
2:B:436:VAL:HG22	2:B:657:ASN:HA	1.94	0.50
2:B:618:VAL:HG13	2:B:620:TRP:HZ3	1.76	0.50
1:A:186:CYS:SG	1:A:207:ARG:NH1	2.84	0.50
1:A:276:TYR:CZ	1:A:996:THR:HG22	2.47	0.50
2:B:450:MET:HB2	2:B:469:ILE:O	2.12	0.50
2:B:538:THR:OG1	2:B:539:PRO:HD3	2.12	0.50
1:A:271:SER:HB2	1:A:276:TYR:HB3	1.93	0.50
1:A:50:ARG:HD2	1:A:291:THR:HB	1.93	0.49
1:A:49:LEU:N	1:A:84:VAL:O	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLN:O	1:A:393:HIS:ND1	2.41	0.49
1:A:172:GLU:OE1	1:A:174:LYS:N	2.46	0.49
2:B:405:ASN:ND2	2:B:408:GLU:HB3	2.28	0.49
1:A:290:ASP:OD1	1:A:291:THR:N	2.45	0.49
2:B:483:TRP:HB3	2:B:660:GLN:NE2	2.27	0.49
1:A:243:GLN:NE2	1:A:261:CYS:HB3	2.27	0.49
2:B:408:GLU:OE1	2:B:409:VAL:N	2.45	0.49
1:A:323:GLU:O	1:A:326:LEU:HG	2.12	0.49
2:B:492:ASP:OD1	2:B:493:SER:N	2.46	0.49
1:A:905:PHE:HD2	1:A:938:GLY:HA2	1.77	0.48
1:A:240:SER:HB3	1:A:268:LEU:HD21	1.95	0.48
2:B:482:ASP:OD1	2:B:485:HIS:N	2.46	0.48
1:A:223:SER:HB2	1:A:384:GLN:O	2.13	0.48
2:B:487:ASN:HA	2:B:502:ASP:HA	1.95	0.48
1:A:322:ALA:O	1:A:325:VAL:HB	2.13	0.48
2:B:626:GLU:HG2	2:B:646:LEU:N	2.29	0.48
1:A:363:VAL:HG11	1:A:389:GLN:HB2	1.96	0.48
1:A:906:PHE:N	1:A:937:SER:HB3	2.28	0.48
2:B:402:PHE:HD1	2:B:411:LYS:HA	1.79	0.48
1:A:378:THR:HG22	1:A:382:LEU:HD23	1.95	0.48
1:A:310:PHE:CD2	1:A:839:PRO:HB3	2.48	0.47
1:A:295:ASN:ND2	2:B:563:PRO:O	2.47	0.47
2:B:534:THR:HA	2:B:542:ILE:HD12	1.95	0.47
1:A:837:GLU:OE2	1:A:846:LEU:N	2.40	0.47
2:B:403:PHE:CZ	2:B:646:LEU:HB3	2.49	0.47
2:B:643:ALA:HB3	2:B:646:LEU:HD11	1.95	0.47
2:B:405:ASN:HD21	2:B:408:GLU:HB3	1.80	0.47
2:B:522:ILE:HD12	2:B:532:TYR:O	2.14	0.47
1:A:75:ARG:O	1:A:99:LEU:HA	2.15	0.47
2:B:523:VAL:O	2:B:531:MET:HB2	2.15	0.47
1:A:132:LYS:NZ	1:A:133:LEU:O	2.48	0.47
1:A:267:PHE:CZ	1:A:269:PRO:HG2	2.50	0.47
2:B:472:ASP:HB3	2:B:473:ILE:H	1.58	0.47
1:A:225:LEU:HD11	1:A:383:VAL:HG22	1.97	0.46
1:A:39:CYS:HA	1:A:137:GLU:HA	1.97	0.46
1:A:225:LEU:O	1:A:829:TYR:OH	2.24	0.46
2:B:483:TRP:CG	2:B:660:GLN:HB3	2.50	0.46
1:A:205:THR:HG23	1:A:245:CYS:HB3	1.97	0.46
1:A:52:TYR:HB3	1:A:54:TYR:CE1	2.50	0.46
2:B:588:ILE:HG23	2:B:593:GLY:H	1.80	0.46
1:A:191:THR:N	1:A:204:SER:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:VAL:HA	1:A:901:MET:O	2.16	0.46
1:A:906:PHE:H	1:A:937:SER:HB3	1.81	0.46
1:A:53:THR:HG23	1:A:81:GLU:HG3	1.97	0.46
1:A:228:ILE:HB	1:A:832:MET:HA	1.98	0.46
2:B:492:ASP:HB3	2:B:494:VAL:HG12	1.98	0.46
1:A:173:ALA:O	1:A:192:VAL:N	2.37	0.45
1:A:937:SER:HA	1:A:1001:LEU:HG	1.98	0.45
1:A:39:CYS:SG	1:A:87:LEU:HB3	2.56	0.45
1:A:235:LEU:HA	1:A:238:LEU:HG	1.98	0.45
1:A:255:HIS:CD2	1:A:257:ALA:H	2.34	0.45
2:B:473:ILE:HB	2:B:492:ASP:OD2	2.15	0.45
2:B:530:PHE:HA	2:B:545:GLY:O	2.16	0.45
2:B:577:TRP:NE1	2:B:586:SER:HG	2.14	0.45
2:B:442:TYR:CD1	2:B:453:SER:HB3	2.52	0.45
2:B:656:HIS:HB3	2:B:658:LEU:HD13	1.99	0.44
1:A:153:ILE:HG22	1:A:157:LYS:HD2	1.99	0.44
1:A:260:ILE:HG12	1:A:285:THR:HG23	1.98	0.44
2:B:445:ASP:OD1	2:B:446:LEU:N	2.51	0.44
1:A:887:MET:SD	1:A:899:VAL:HG12	2.58	0.44
1:A:962:SER:HA	1:A:980:ALA:HA	1.98	0.44
1:A:45:ARG:HH11	1:A:166:VAL:HG13	1.83	0.44
1:A:174:LYS:HA	1:A:191:THR:HA	1.99	0.44
2:B:496:GLY:N	2:B:517:SER:O	2.51	0.44
1:A:243:GLN:NE2	1:A:244:SER:O	2.51	0.44
2:B:453:SER:O	2:B:466:ASP:HA	2.18	0.44
2:B:656:HIS:O	2:B:658:LEU:HD12	2.17	0.43
1:A:56:TYR:CE2	1:A:58:ALA:HB2	2.53	0.43
2:B:416:ARG:C	2:B:642:LEU:HD11	2.43	0.43
2:B:607:HIS:HB3	2:B:609:PHE:HE1	1.82	0.43
2:B:441:ILE:O	2:B:453:SER:HA	2.18	0.43
1:A:45:ARG:NH1	1:A:166:VAL:HG13	2.33	0.43
2:B:495:LEU:HB2	2:B:515:ASN:HA	1.99	0.43
1:A:831:PHE:CE2	1:A:854:ILE:HG23	2.53	0.43
1:A:170:THR:O	1:A:195:ARG:NH2	2.37	0.43
1:A:329:LEU:HD13	1:A:351:LEU:HG	2.01	0.43
2:B:632:ASN:OD1	2:B:633:ARG:N	2.51	0.43
1:A:45:ARG:HD2	1:A:166:VAL:HG11	2.00	0.43
1:A:189:HIS:O	1:A:205:THR:HA	2.19	0.43
1:A:233:ARG:O	1:A:237:THR:HG23	2.19	0.43
1:A:270:PHE:HB2	1:A:995:LEU:HD22	2.00	0.42
2:B:559:ASN:O	2:B:582:LEU:HD11	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HD13	1:A:832:MET:HB2	2.02	0.42
1:A:268:LEU:HD22	1:A:274:ASN:HB2	2.01	0.42
2:B:407:HIS:H	2:B:427:ARG:HA	1.84	0.42
2:B:545:GLY:HA2	2:B:551:ASP:O	2.19	0.42
1:A:58:ALA:HB3	1:A:76:ILE:CG2	2.49	0.42
1:A:325:VAL:O	1:A:328:THR:OG1	2.32	0.42
1:A:356:ARG:HA	1:A:387:GLN:HG3	2.02	0.42
2:B:428:ASN:HD22	2:B:447:SER:HB3	1.84	0.42
2:B:607:HIS:HB3	2:B:609:PHE:CE1	2.55	0.42
1:A:48:HIS:NE2	2:B:648:SER:HA	2.35	0.42
1:A:74:THR:HG23	1:A:897:SER:HB3	2.01	0.42
1:A:185:ASN:N	1:A:213:ASP:OD1	2.52	0.42
1:A:48:HIS:CD2	1:A:48:HIS:H	2.36	0.42
2:B:404:THR:OG1	2:B:650:GLU:HB2	2.19	0.42
2:B:583:HIS:CE1	2:B:606:ALA:HA	2.54	0.42
1:A:52:TYR:HE2	1:A:255:HIS:HB2	1.84	0.42
1:A:62:SER:HB3	1:A:887:MET:SD	2.60	0.42
1:A:334:LYS:HB2	1:A:334:LYS:HE2	1.87	0.42
1:A:903:THR:HA	1:A:940:ASN:HA	2.01	0.42
2:B:495:LEU:HD13	2:B:516:GLY:H	1.84	0.42
1:A:63:GLY:C	1:A:279:VAL:HG12	2.44	0.41
1:A:212:CYS:HB2	1:A:215:PHE:HD2	1.85	0.41
2:B:483:TRP:NE1	2:B:662:ARG:O	2.51	0.41
2:B:555:LEU:HD12	2:B:556:VAL:N	2.35	0.41
2:B:582:LEU:O	2:B:584:SER:N	2.53	0.41
1:A:50:ARG:HG2	1:A:253:ARG:HH12	1.85	0.41
1:A:181:THR:HG23	1:A:183:TYR:N	2.33	0.41
1:A:359:SER:OG	1:A:362:ALA:N	2.46	0.41
2:B:480:ALA:HB2	2:B:522:ILE:HG23	2.01	0.41
1:A:73:ALA:H	1:A:102:VAL:HG12	1.86	0.41
2:B:450:MET:SD	2:B:450:MET:N	2.93	0.41
2:B:578:VAL:HG12	2:B:585:ILE:HG13	2.01	0.41
2:B:616:ASP:HA	2:B:633:ARG:HB3	2.03	0.41
2:B:622:ASP:OD1	2:B:623:ILE:N	2.54	0.41
1:A:58:ALA:HA	1:A:283:THR:O	2.21	0.41
1:A:349:ASN:C	1:A:349:ASN:HD22	2.29	0.41
1:A:836:PHE:CE2	1:A:848:ILE:HB	2.56	0.41
2:B:491:THR:HA	2:B:497:THR:O	2.20	0.41
2:B:569:ASP:N	2:B:569:ASP:OD1	2.54	0.41
1:A:53:THR:HG21	1:A:79:LYS:HE3	2.03	0.41
2:B:531:MET:HE1	2:B:547:LEU:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:ALA:HB1	2:B:646:LEU:HD21	2.03	0.41
1:A:50:ARG:HH11	1:A:291:THR:HB	1.86	0.41
1:A:146:GLU:OE1	1:A:148:ASP:N	2.47	0.41
2:B:518:LYS:HG3	2:B:536:TRP:NE1	2.36	0.41
1:A:980:ALA:N	1:A:1000:ARG:O	2.50	0.40
2:B:520:ARG:HA	2:B:520:ARG:HD2	1.84	0.40
2:B:522:ILE:HD13	2:B:533:TRP:HB3	2.03	0.40
1:A:243:GLN:NE2	1:A:245:CYS:HB2	2.34	0.40
1:A:831:PHE:CD2	1:A:854:ILE:HG12	2.53	0.40
1:A:76:ILE:HD12	1:A:98:THR:C	2.46	0.40
2:B:551:ASP:OD1	2:B:551:ASP:N	2.44	0.40
2:B:621:THR:HG23	2:B:627:ALA:O	2.22	0.40
1:A:360:ASP:O	1:A:364:THR:OG1	2.31	0.40
2:B:480:ALA:O	2:B:489:TYR:N	2.38	0.40
2:B:534:THR:HA	2:B:542:ILE:HG23	2.03	0.40
1:A:158:ARG:HA	1:A:161:ILE:HG12	2.02	0.40
2:B:496:GLY:O	2:B:513:ARG:HA	2.21	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	446/4563 (10%)	425 (95%)	21 (5%)	0	100	100
2	B	260/860 (30%)	225 (86%)	35 (14%)	0	100	100
All	All	706/5423 (13%)	650 (92%)	56 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	366/4080 (9%)	366 (100%)	0	100	100
2	B	193/755 (26%)	193 (100%)	0	100	100
All	All	559/4835 (12%)	559 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	246	GLN
1	A	340	GLN
1	A	900	GLN
1	A	902	ASN
2	B	425	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	4601	1	14,14,15	0.70	0	17,19,21	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	4601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

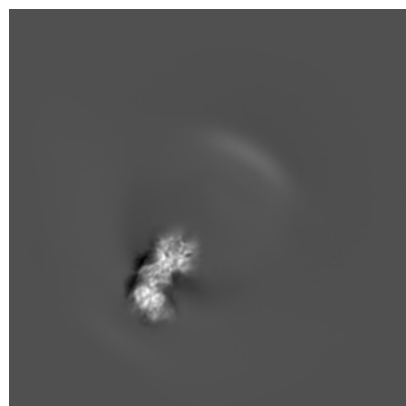
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44446. 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

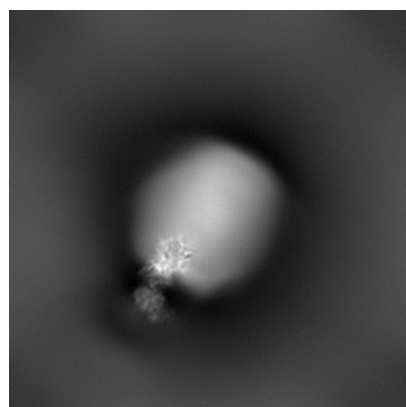


Y

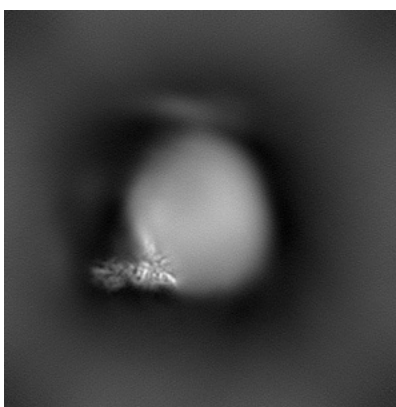


Z

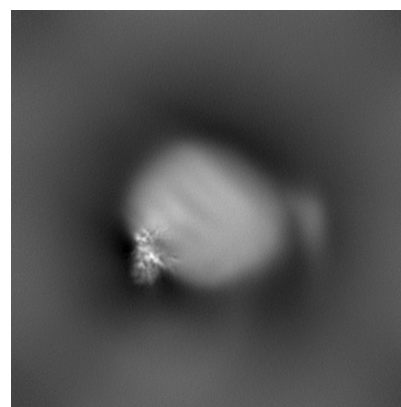
6.1.2 Raw map



X



Y

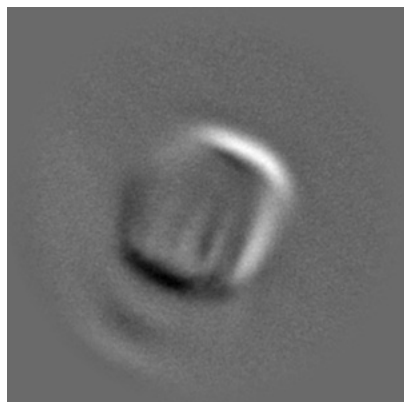


Z

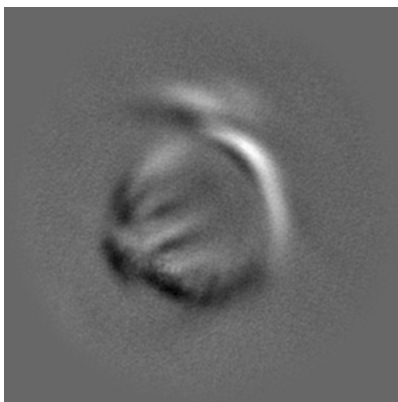
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

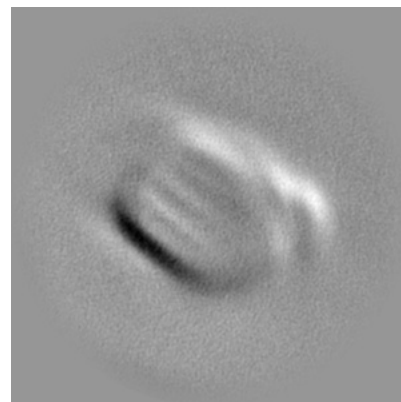
6.2.1 Primary map



X Index: 168

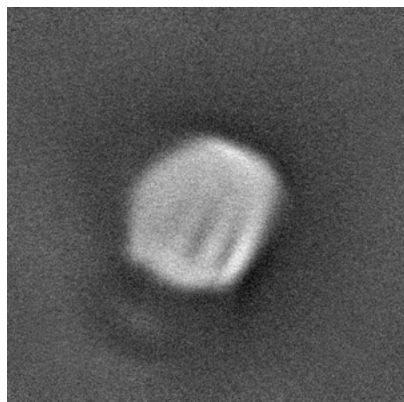


Y Index: 168

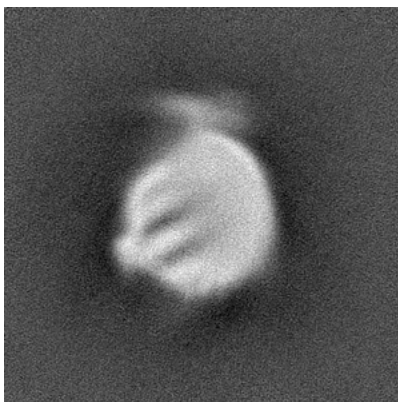


Z Index: 168

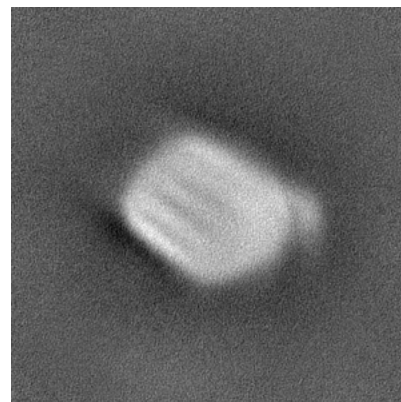
6.2.2 Raw map



X Index: 168



Y Index: 168

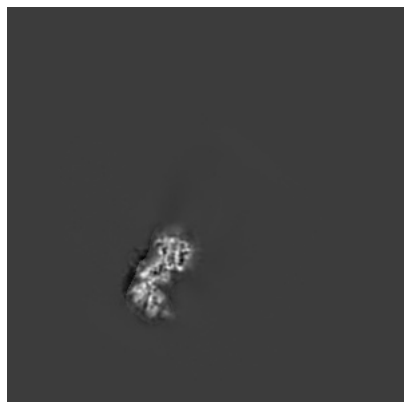


Z Index: 168

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

6.3 Largest variance slices [i](#)

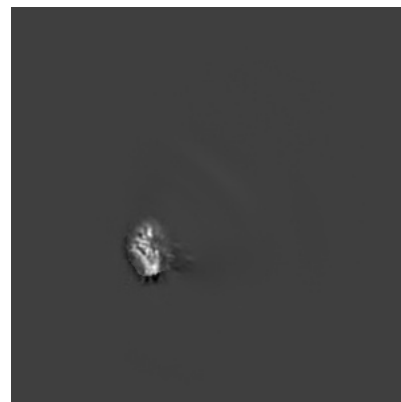
6.3.1 Primary map



X Index: 111

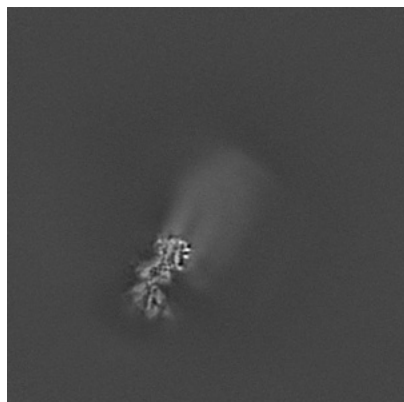


Y Index: 122

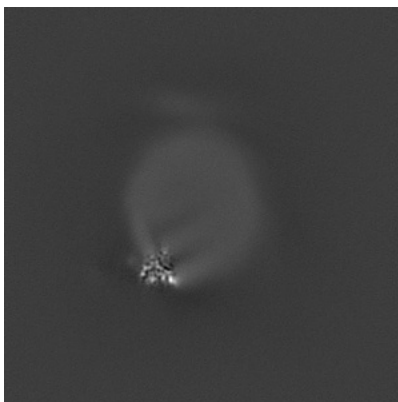


Z Index: 118

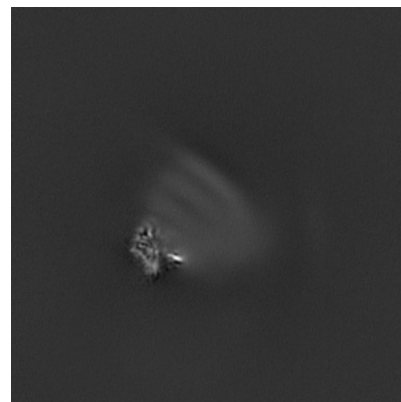
6.3.2 Raw map



X Index: 112



Y Index: 144

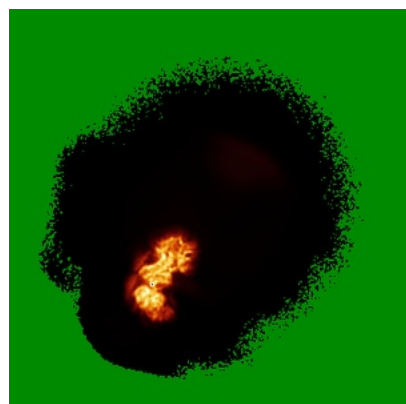


Z Index: 119

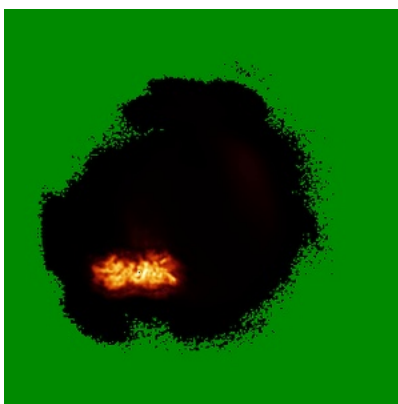
The images above show the largest variance slices of the map in three orthogonal directions.

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

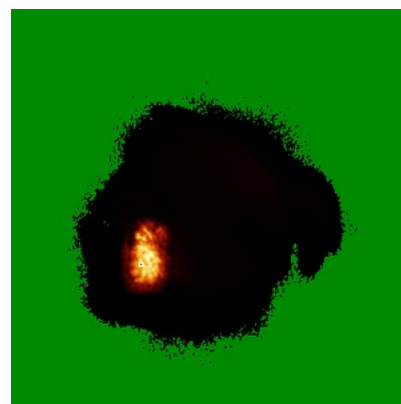
6.4.1 Primary map



X

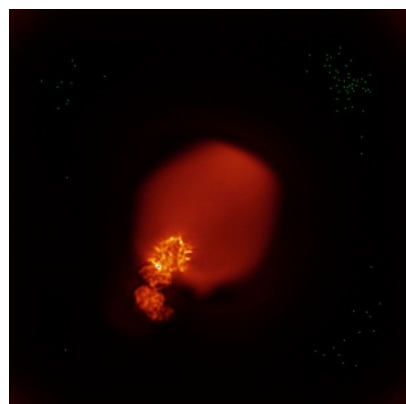


Y

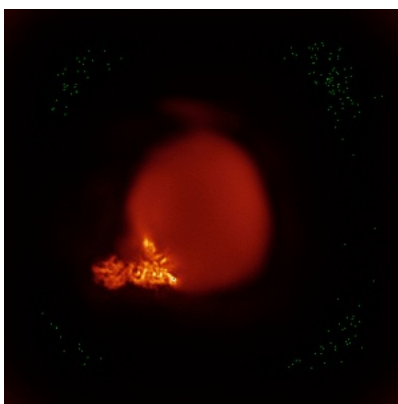


Z

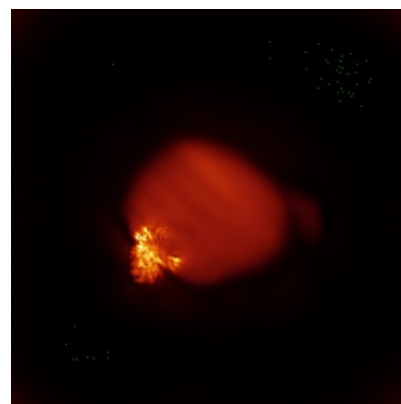
6.4.2 Raw map



X



Y

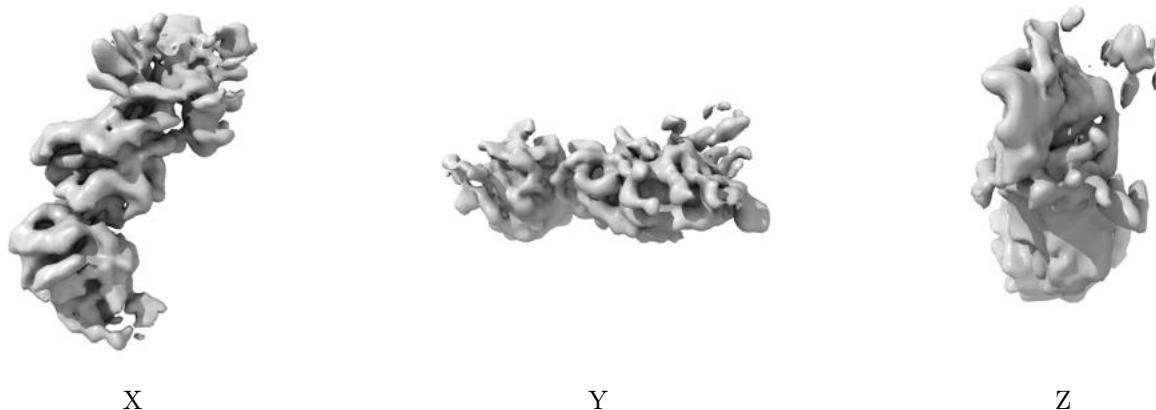


Z

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

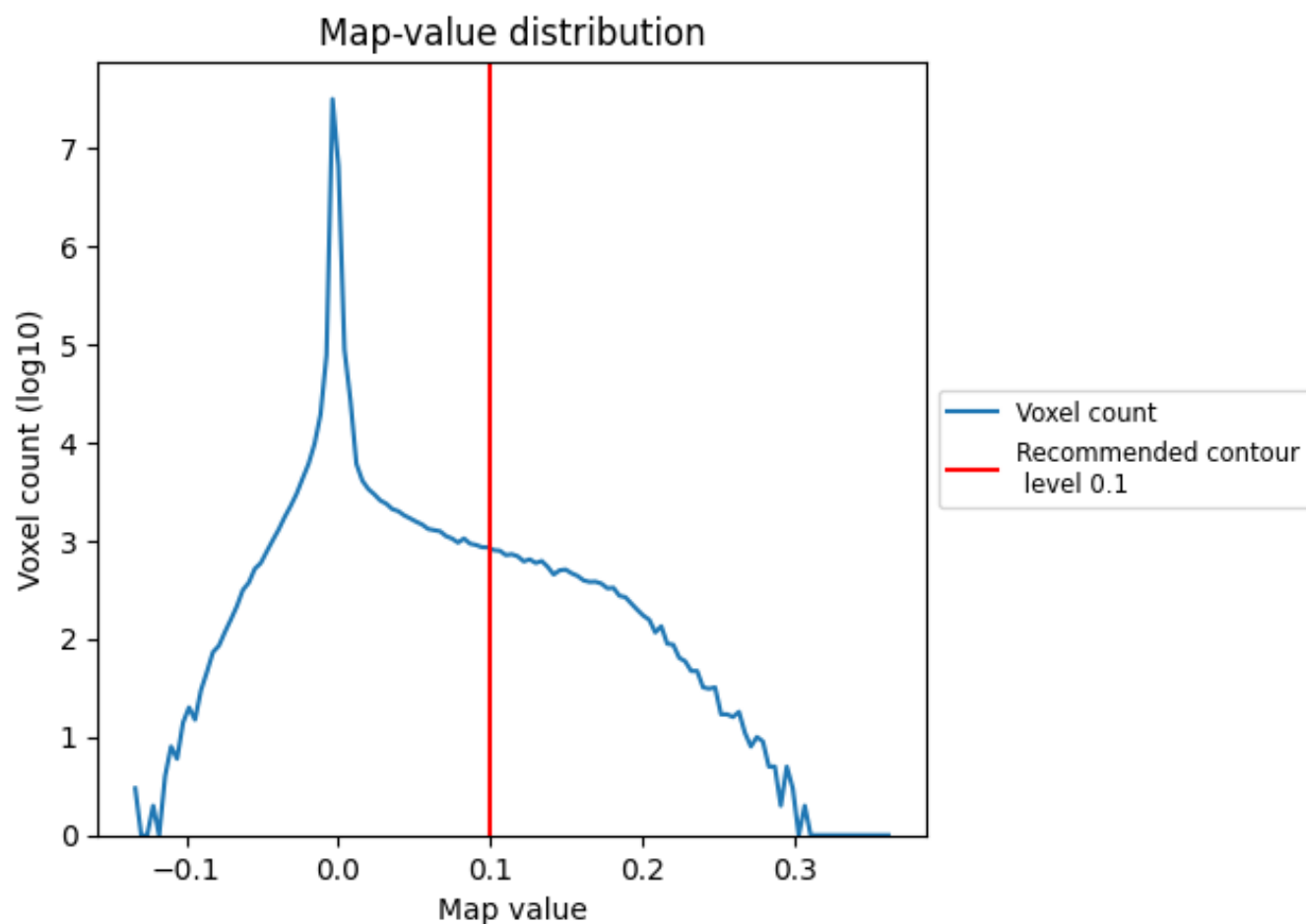
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

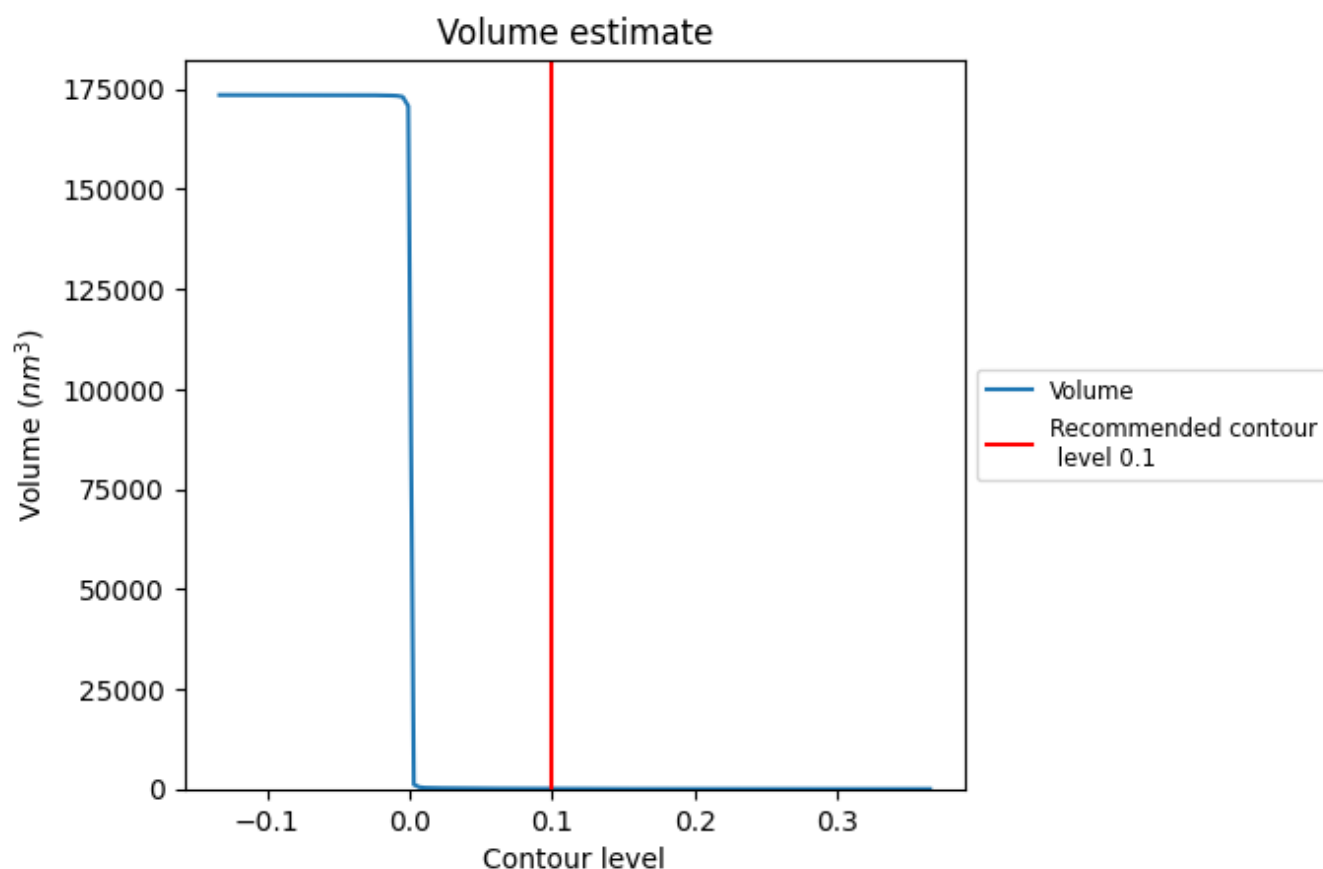
This section contains the results of statistical analysis of the map.

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.

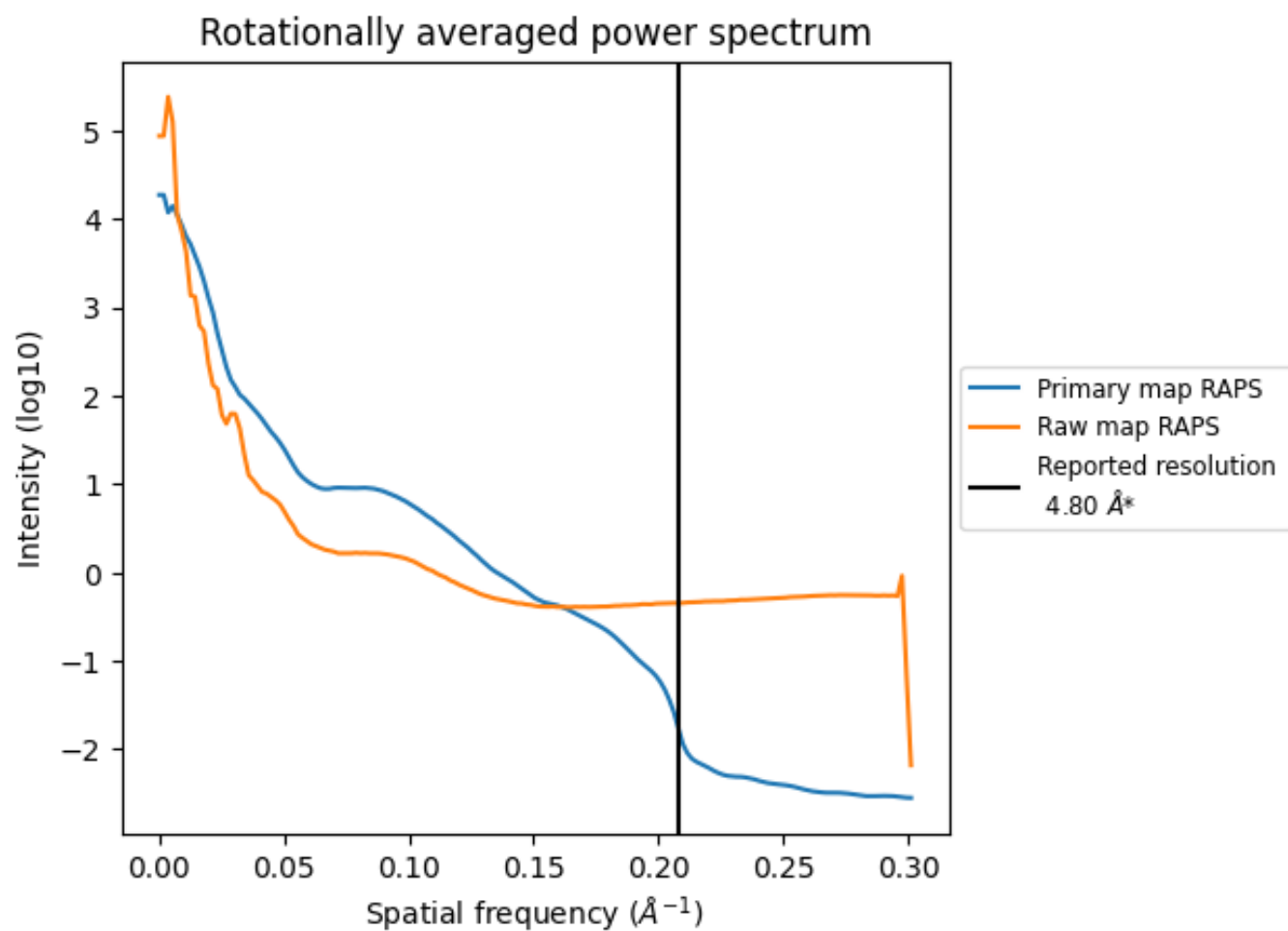
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm^3 ; this corresponds to an approximate mass of 57 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 ⓘ

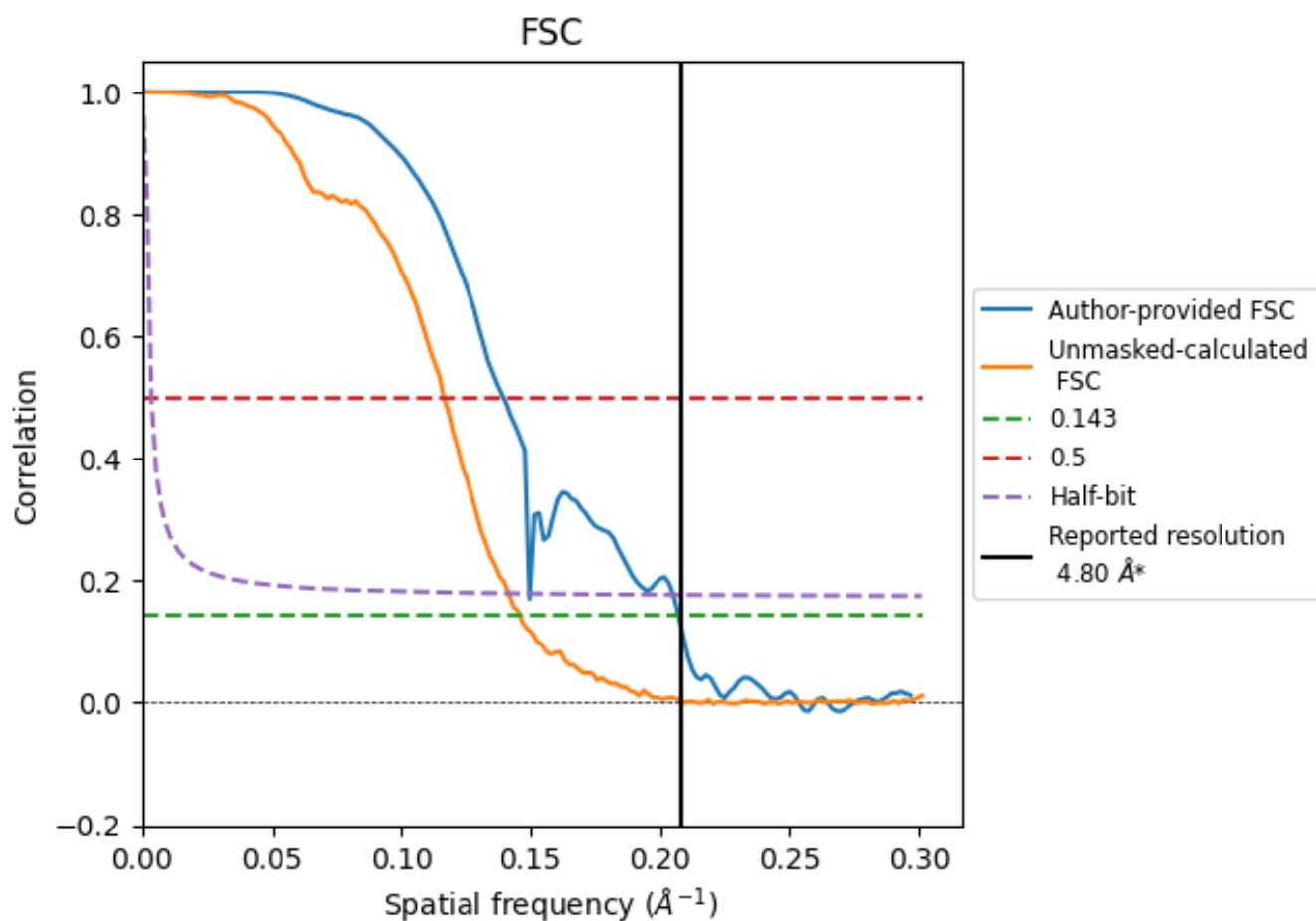


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

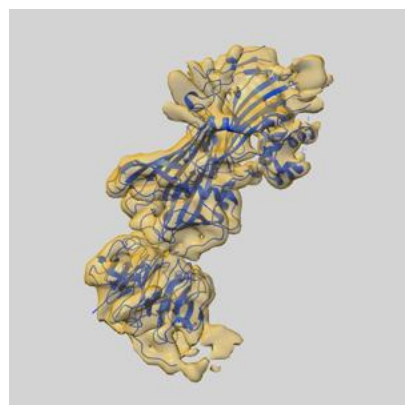
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.83	7.16	6.68
Unmasked-calculated*	6.85	8.58	7.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.85 differs from the reported value 4.8 by more than 10 %

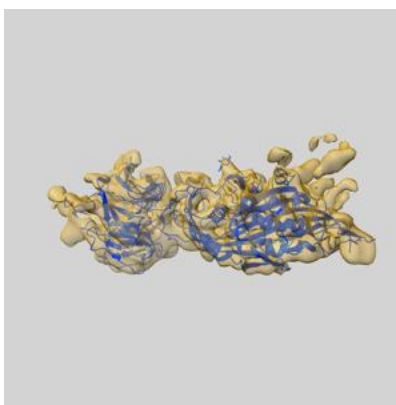
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44446 and PDB model 9BD8. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

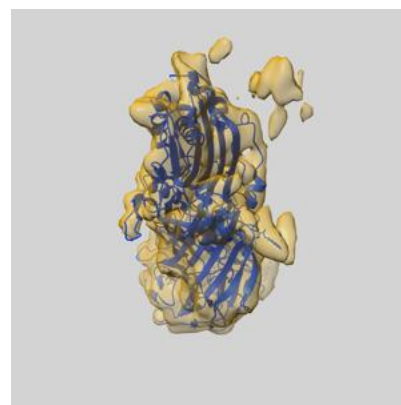
9.1 Map-model overlay [i](#)



X



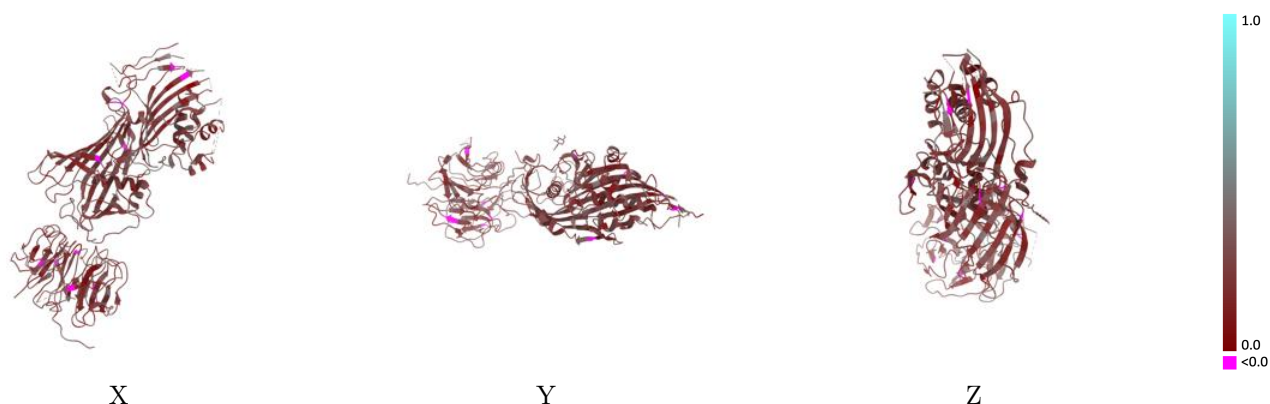
Y



Z

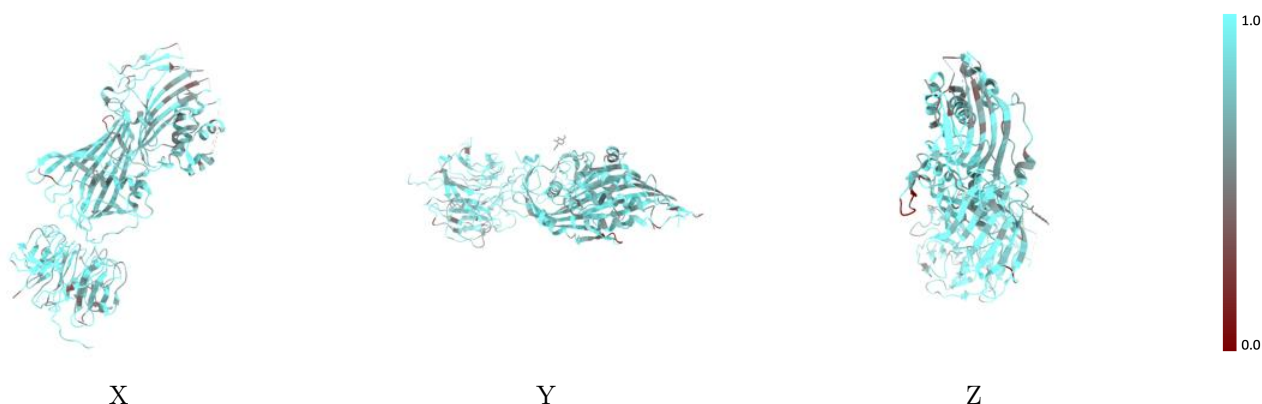
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



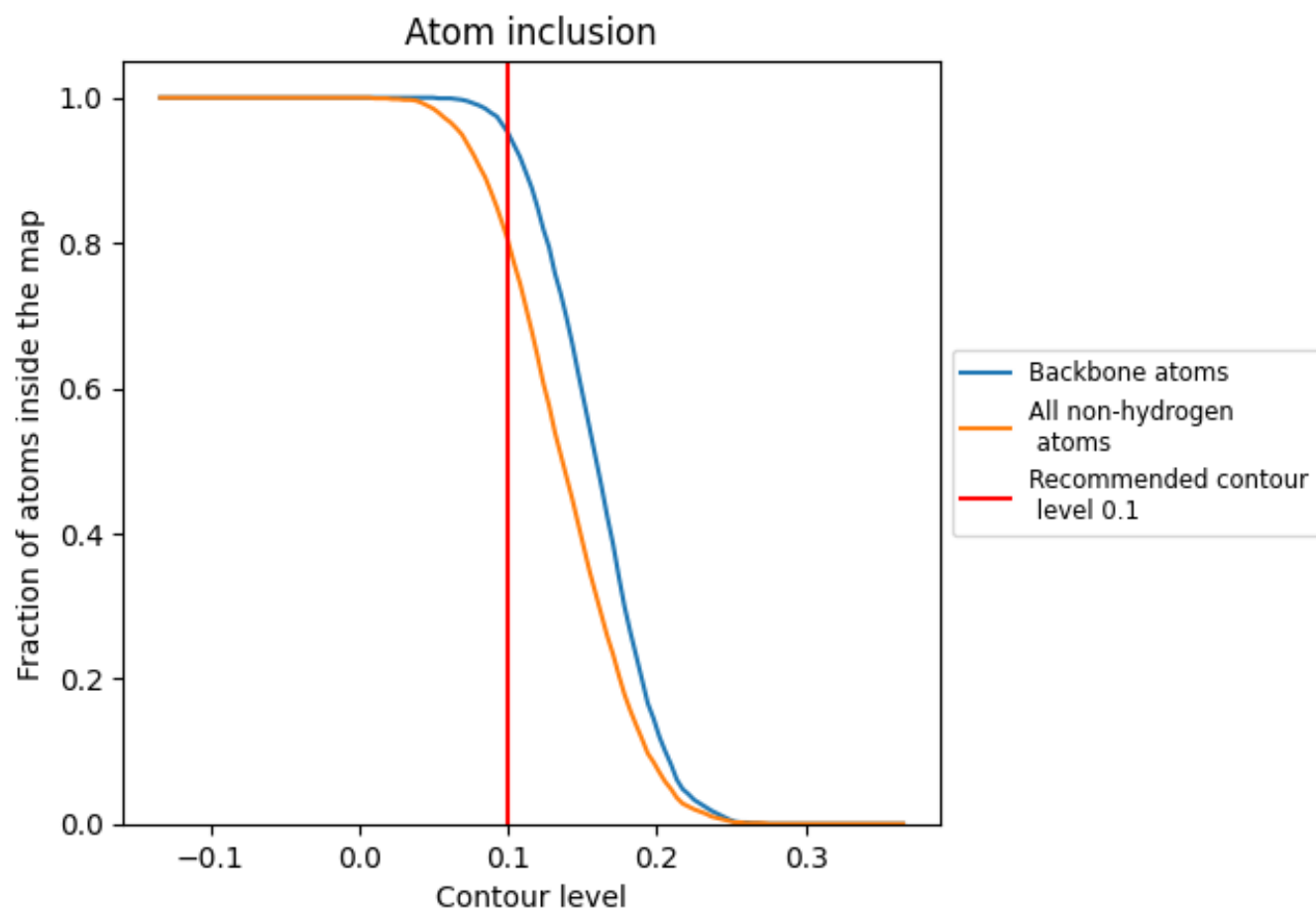
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.2410
A	0.8000	0.2480
B	0.8100	0.2270

