



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:18 PM UTC

PDB ID : 9KB9 / pdb_00009kb9
EMDB ID : EMD-62221
Title : Cryo-EM structure of LGR4-RSPO2-ZNRF3 complex (2:2:2)
Authors : Peng, Y.; Fujimura, A.; Asami, J.; Zhang, Z.; Shimizu, T.; Ohto, U.
Deposited on : 2024-10-30
Resolution : 3.59 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:

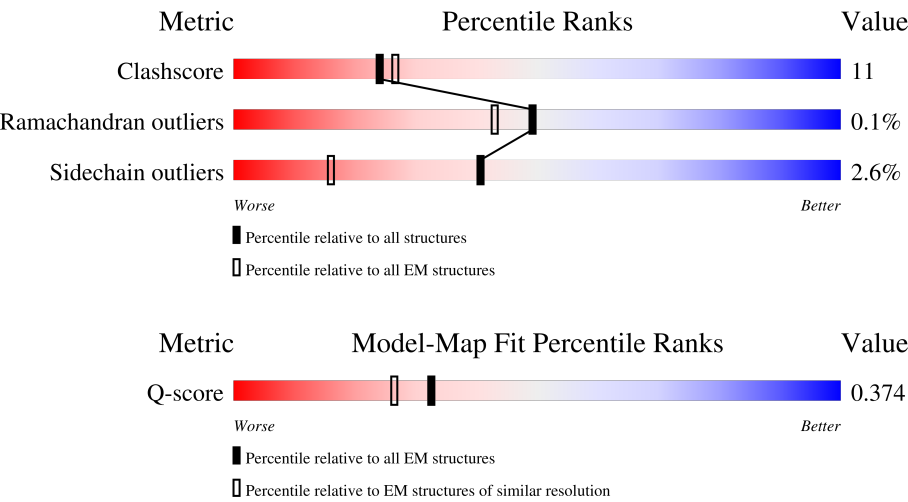
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.59 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	12565 (3.09 - 4.09)

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	845	
1	D	845	
2	C	231	
2	E	231	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	160	52%12%35%
3	F	160	49%16%35%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16352 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 Leucine-rich repeat-containing G-protein coupled receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	748	Total	C	N	O	S	0	0
			5834	3783	962	1060	29		
1	D	748	Total	C	N	O	S	0	0
			5834	3783	962	1060	29		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	823	GLU	-	expression tag	UNP Q9BXB1
A	824	ASN	-	expression tag	UNP Q9BXB1
A	825	LEU	-	expression tag	UNP Q9BXB1
A	826	TYR	-	expression tag	UNP Q9BXB1
A	827	PHE	-	expression tag	UNP Q9BXB1
A	828	GLN	-	expression tag	UNP Q9BXB1
A	829	GLY	-	expression tag	UNP Q9BXB1
A	830	ASP	-	expression tag	UNP Q9BXB1
A	831	TYR	-	expression tag	UNP Q9BXB1
A	832	LYS	-	expression tag	UNP Q9BXB1
A	833	ASP	-	expression tag	UNP Q9BXB1
A	834	ASP	-	expression tag	UNP Q9BXB1
A	835	ASP	-	expression tag	UNP Q9BXB1
A	836	ASP	-	expression tag	UNP Q9BXB1
A	837	LYS	-	expression tag	UNP Q9BXB1
A	838	HIS	-	expression tag	UNP Q9BXB1
A	839	HIS	-	expression tag	UNP Q9BXB1
A	840	HIS	-	expression tag	UNP Q9BXB1
A	841	HIS	-	expression tag	UNP Q9BXB1
A	842	HIS	-	expression tag	UNP Q9BXB1
A	843	HIS	-	expression tag	UNP Q9BXB1
A	844	HIS	-	expression tag	UNP Q9BXB1
A	845	HIS	-	expression tag	UNP Q9BXB1
D	823	GLU	-	expression tag	UNP Q9BXB1
D	824	ASN	-	expression tag	UNP Q9BXB1
D	825	LEU	-	expression tag	UNP Q9BXB1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	826	TYR	-	expression tag	UNP Q9BXB1
D	827	PHE	-	expression tag	UNP Q9BXB1
D	828	GLN	-	expression tag	UNP Q9BXB1
D	829	GLY	-	expression tag	UNP Q9BXB1
D	830	ASP	-	expression tag	UNP Q9BXB1
D	831	TYR	-	expression tag	UNP Q9BXB1
D	832	LYS	-	expression tag	UNP Q9BXB1
D	833	ASP	-	expression tag	UNP Q9BXB1
D	834	ASP	-	expression tag	UNP Q9BXB1
D	835	ASP	-	expression tag	UNP Q9BXB1
D	836	ASP	-	expression tag	UNP Q9BXB1
D	837	LYS	-	expression tag	UNP Q9BXB1
D	838	HIS	-	expression tag	UNP Q9BXB1
D	839	HIS	-	expression tag	UNP Q9BXB1
D	840	HIS	-	expression tag	UNP Q9BXB1
D	841	HIS	-	expression tag	UNP Q9BXB1
D	842	HIS	-	expression tag	UNP Q9BXB1
D	843	HIS	-	expression tag	UNP Q9BXB1
D	844	HIS	-	expression tag	UNP Q9BXB1
D	845	HIS	-	expression tag	UNP Q9BXB1

- Molecule 2 is a protein called E3 ubiquitin-protein ligase ZNRF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	190	Total 1488	C 950	N 256	O 276	S 6	0	0
2	E	190	Total 1488	C 950	N 256	O 276	S 6	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	MET	-	initiating methionine	UNP Q9ULT6
C	38	GLU	-	expression tag	UNP Q9ULT6
C	39	THR	-	expression tag	UNP Q9ULT6
C	40	GLY	-	expression tag	UNP Q9ULT6
C	41	LEU	-	expression tag	UNP Q9ULT6
C	42	ARG	-	expression tag	UNP Q9ULT6
C	43	TRP	-	expression tag	UNP Q9ULT6
C	44	LEU	-	expression tag	UNP Q9ULT6
C	45	LEU	-	expression tag	UNP Q9ULT6
C	46	LEU	-	expression tag	UNP Q9ULT6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	VAL	-	expression tag	UNP Q9ULT6
C	48	ALA	-	expression tag	UNP Q9ULT6
C	49	VAL	-	expression tag	UNP Q9ULT6
C	50	LEU	-	expression tag	UNP Q9ULT6
C	51	LYS	-	expression tag	UNP Q9ULT6
C	52	GLY	-	expression tag	UNP Q9ULT6
C	53	VAL	-	expression tag	UNP Q9ULT6
C	54	GLN	-	expression tag	UNP Q9ULT6
C	55	CYS	-	expression tag	UNP Q9ULT6
E	37	MET	-	initiating methionine	UNP Q9ULT6
E	38	GLU	-	expression tag	UNP Q9ULT6
E	39	THR	-	expression tag	UNP Q9ULT6
E	40	GLY	-	expression tag	UNP Q9ULT6
E	41	LEU	-	expression tag	UNP Q9ULT6
E	42	ARG	-	expression tag	UNP Q9ULT6
E	43	TRP	-	expression tag	UNP Q9ULT6
E	44	LEU	-	expression tag	UNP Q9ULT6
E	45	LEU	-	expression tag	UNP Q9ULT6
E	46	LEU	-	expression tag	UNP Q9ULT6
E	47	VAL	-	expression tag	UNP Q9ULT6
E	48	ALA	-	expression tag	UNP Q9ULT6
E	49	VAL	-	expression tag	UNP Q9ULT6
E	50	LEU	-	expression tag	UNP Q9ULT6
E	51	LYS	-	expression tag	UNP Q9ULT6
E	52	GLY	-	expression tag	UNP Q9ULT6
E	53	VAL	-	expression tag	UNP Q9ULT6
E	54	GLN	-	expression tag	UNP Q9ULT6
E	55	CYS	-	expression tag	UNP Q9ULT6

- Molecule 3 is a protein called R-spondin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	104	Total	C	N	O	S	0	0
			826	504	152	151	19		
3	F	104	Total	C	N	O	S	0	0
			826	504	152	151	19		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	144	GLU	-	expression tag	UNP Q6UXX9
B	145	ASN	-	expression tag	UNP Q6UXX9

Continued on next page...

Continued from previous page...

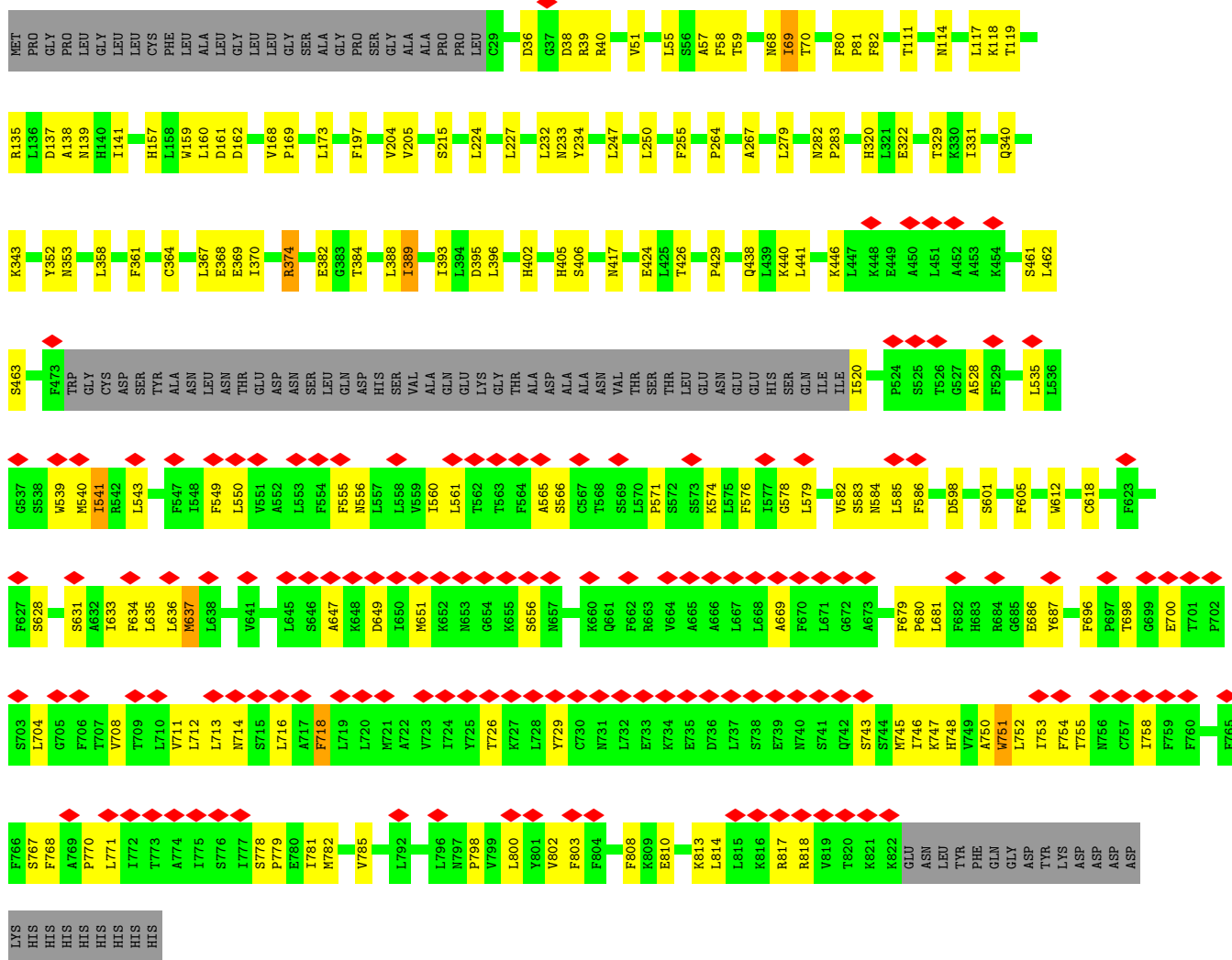
Chain	Residue	Modelled	Actual	Comment	Reference
B	146	LEU	-	expression tag	UNP Q6UXX9
B	147	TYR	-	expression tag	UNP Q6UXX9
B	148	PHE	-	expression tag	UNP Q6UXX9
B	149	GLN	-	expression tag	UNP Q6UXX9
B	150	GLY	-	expression tag	UNP Q6UXX9
B	151	HIS	-	expression tag	UNP Q6UXX9
B	152	HIS	-	expression tag	UNP Q6UXX9
B	153	HIS	-	expression tag	UNP Q6UXX9
B	154	HIS	-	expression tag	UNP Q6UXX9
B	155	HIS	-	expression tag	UNP Q6UXX9
B	156	HIS	-	expression tag	UNP Q6UXX9
B	157	HIS	-	expression tag	UNP Q6UXX9
B	158	HIS	-	expression tag	UNP Q6UXX9
B	159	HIS	-	expression tag	UNP Q6UXX9
B	160	HIS	-	expression tag	UNP Q6UXX9
F	144	GLU	-	expression tag	UNP Q6UXX9
F	145	ASN	-	expression tag	UNP Q6UXX9
F	146	LEU	-	expression tag	UNP Q6UXX9
F	147	TYR	-	expression tag	UNP Q6UXX9
F	148	PHE	-	expression tag	UNP Q6UXX9
F	149	GLN	-	expression tag	UNP Q6UXX9
F	150	GLY	-	expression tag	UNP Q6UXX9
F	151	HIS	-	expression tag	UNP Q6UXX9
F	152	HIS	-	expression tag	UNP Q6UXX9
F	153	HIS	-	expression tag	UNP Q6UXX9
F	154	HIS	-	expression tag	UNP Q6UXX9
F	155	HIS	-	expression tag	UNP Q6UXX9
F	156	HIS	-	expression tag	UNP Q6UXX9
F	157	HIS	-	expression tag	UNP Q6UXX9
F	158	HIS	-	expression tag	UNP Q6UXX9
F	159	HIS	-	expression tag	UNP Q6UXX9
F	160	HIS	-	expression tag	UNP Q6UXX9

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

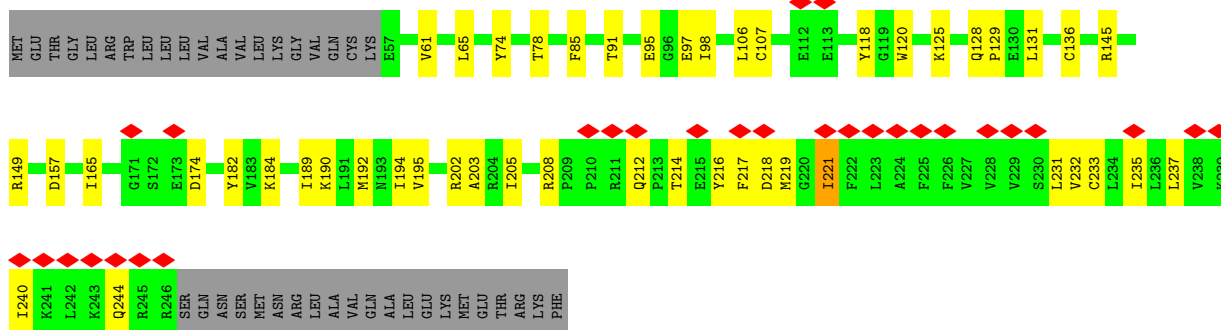


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

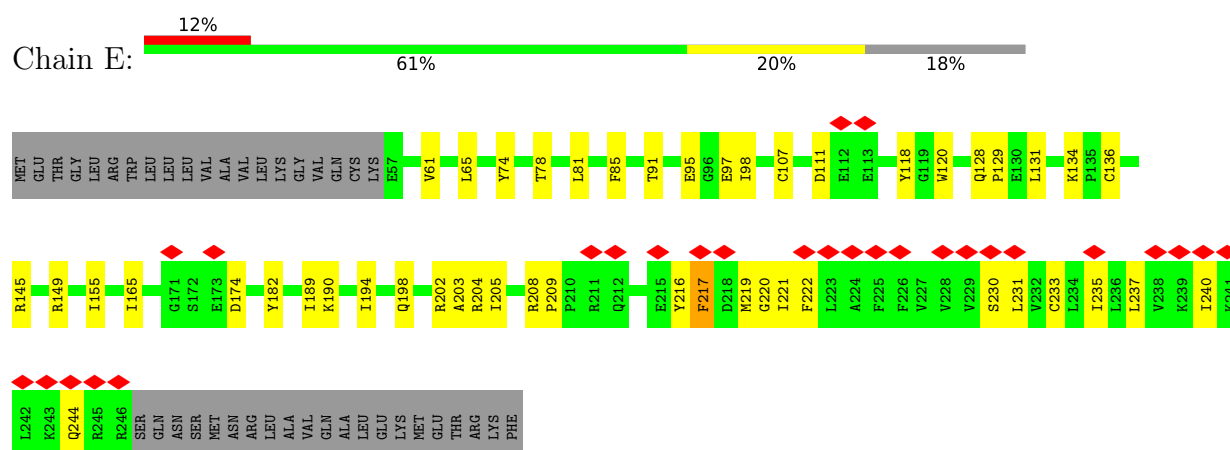
Chain D:



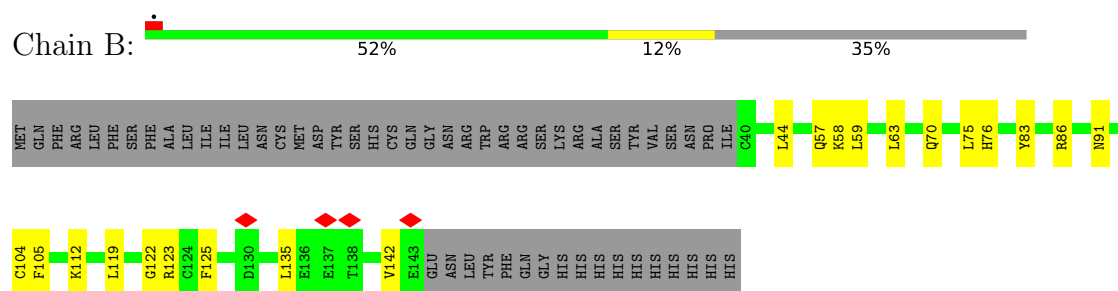
Chain C:



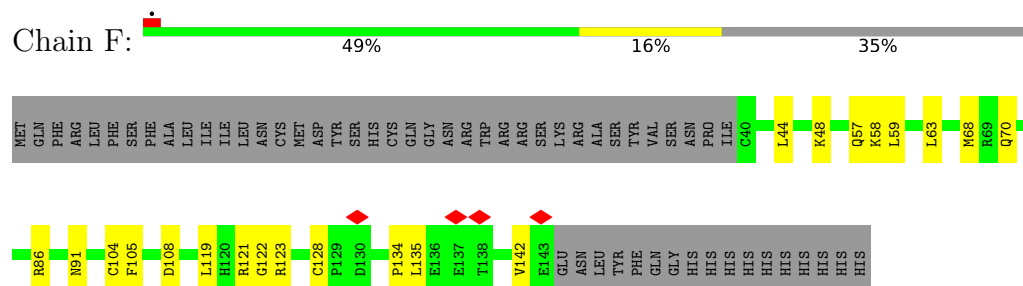
- Molecule 2: E3 ubiquitin-protein ligase ZNRF3



- Molecule 3: R-spondin-2



- Molecule 3: R-spondin-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.635	Depositor
Minimum map value	-0.328	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.137	Depositor
Map size (Å)	348.6, 348.6, 348.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.245, 1.245, 1.245	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	0.22	0/5971	0.37	0/8116
1	D	0.23	0/5971	0.39	1/8116 (0.0%)
2	C	0.24	0/1516	0.41	0/2055
2	E	0.23	0/1516	0.37	0/2055
3	B	0.25	0/844	0.35	0/1124
3	F	0.24	0/844	0.34	0/1124
All	All	0.23	0/16662	0.38	1/22590 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	541	ILE	N-CA-C	-9.90	102.27	111.67

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	5834	0	5892	143	0
1	D	5834	0	5890	131	0
2	C	1488	0	1517	41	0
2	E	1488	0	1517	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	826	0	755	15	0
3	F	826	0	755	17	0
4	A	28	0	26	0	0
4	D	28	0	26	0	0
All	All	16352	0	16378	352	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 11.

All (352) 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:A:555:PHE:HB3	1:A:798:PRO:HB2	1.63	0.78
1:D:579:LEU:HD13	1:D:635:LEU:HD22	1.74	0.70
1:D:555:PHE:HB3	1:D:798:PRO:HB2	1.74	0.69
1:D:680:PRO:HB2	1:D:687:TYR:CE1	2.29	0.67
1:D:204:VAL:HG12	1:D:205:VAL:HG23	1.77	0.67
1:A:556:ASN:ND2	1:A:584:ASN:HB3	2.11	0.66
1:A:204:VAL:HG12	1:A:205:VAL:HG23	1.78	0.66
1:D:755:THR:HA	1:D:758:ILE:HB	1.77	0.65
1:D:39:ARG:HB3	1:D:59:THR:HA	1.78	0.65
1:A:579:LEU:HD13	1:A:635:LEU:HD22	1.77	0.65
1:A:39:ARG:HB3	1:A:59:THR:HA	1.79	0.64
2:C:219:MET:HE2	2:E:220:GLY:HA3	1.77	0.64
1:D:633:ILE:HA	1:D:636:LEU:HD12	1.80	0.64
1:D:556:ASN:HD21	1:D:585:LEU:HB2	1.63	0.64
1:D:758:ILE:HG21	2:E:230:SER:HB3	1.81	0.63
3:B:135:LEU:HD13	3:B:142:VAL:HG11	1.81	0.63
1:D:751:TRP:O	1:D:755:THR:HG23	1.99	0.62
1:A:749:VAL:HA	1:A:752:LEU:HD12	1.81	0.62
2:C:216:TYR:CE2	1:D:781:ILE:HG22	2.34	0.62
1:A:711:VAL:HA	1:A:714:ASN:ND2	2.15	0.62
1:A:389:ILE:HG13	1:A:390:SER:H	1.63	0.62
1:D:778:SER:O	1:D:781:ILE:HG12	1.99	0.62
1:A:696:PHE:HB3	1:A:698:THR:HG23	1.81	0.62
1:D:369:GLU:HG3	1:D:393:ILE:HB	1.80	0.62
1:A:759:PHE:HB3	1:A:793:PRO:HG3	1.82	0.62
2:C:217:PHE:CE1	1:D:541:ILE:HG12	2.35	0.61
1:A:748:HIS:CE1	1:A:752:LEU:HD11	2.35	0.61
1:A:700:GLU:HB2	1:A:704:LEU:HD23	1.82	0.61
3:F:135:LEU:HD13	3:F:142:VAL:HG11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:HIS:HA	1:A:751:TRP:CE3	2.36	0.60
1:A:538:SER:H	1:A:541:ILE:HD13	1.65	0.60
2:C:221:ILE:HG21	1:D:541:ILE:HG13	1.84	0.60
1:A:173:LEU:HD12	1:A:200:LEU:HD11	1.84	0.60
1:A:556:ASN:HD21	1:A:584:ASN:HB3	1.66	0.60
1:D:535:LEU:HD13	1:D:598:ASP:HA	1.84	0.59
2:E:240:ILE:HG22	2:E:244:GLN:HE21	1.67	0.59
1:A:369:GLU:HG3	1:A:393:ILE:HB	1.83	0.59
1:A:583:SER:HA	1:A:586:PHE:CD1	2.37	0.59
2:C:240:ILE:HG22	2:C:244:GLN:HE21	1.68	0.59
2:E:219:MET:HA	2:E:222:PHE:HB2	1.85	0.58
1:D:578:GLY:O	1:D:582:VAL:HG23	2.03	0.58
1:A:778:SER:O	1:A:781:ILE:HG12	2.04	0.58
1:D:782:MET:HA	1:D:785:VAL:HG22	1.86	0.58
1:A:777:ILE:HB	1:A:781:ILE:HD11	1.85	0.58
1:A:255:PHE:HE1	1:A:279:LEU:HB3	1.69	0.57
1:A:680:PRO:HB3	1:A:686:GLU:HB2	1.87	0.57
1:D:584:ASN:ND2	1:D:798:PRO:HD3	2.20	0.57
1:D:748:HIS:HA	1:D:751:TRP:CE3	2.39	0.57
1:A:712:LEU:HD11	1:A:764:ALA:HB1	1.85	0.57
1:D:197:PHE:HB2	1:D:224:LEU:HD11	1.87	0.57
1:D:227:LEU:HD23	1:D:247:LEU:HD13	1.87	0.57
2:E:237:LEU:HA	2:E:240:ILE:HD12	1.86	0.57
1:A:578:GLY:O	1:A:582:VAL:HG23	2.03	0.57
1:A:365:HIS:HB3	1:A:389:ILE:HD11	1.87	0.57
1:A:745:MET:HA	1:A:748:HIS:HB3	1.86	0.57
1:D:745:MET:HA	1:D:748:HIS:HB3	1.87	0.57
1:D:700:GLU:HB2	1:D:704:LEU:HD23	1.86	0.57
1:D:393:ILE:HD12	1:D:417:ASN:HB2	1.87	0.56
1:A:552:ALA:O	1:A:556:ASN:HB2	2.04	0.56
1:D:556:ASN:O	1:D:560:ILE:HG12	2.06	0.56
1:A:810:GLU:HA	1:A:813:LYS:HD2	1.87	0.55
1:D:169:PRO:O	1:D:173:LEU:HD23	2.06	0.55
2:C:235:ILE:HD11	1:D:803:PHE:CG	2.41	0.55
1:A:546:TRP:O	1:A:550:LEU:HD22	2.06	0.55
1:D:583:SER:HA	1:D:586:PHE:CD1	2.41	0.55
1:D:601:SER:HB2	1:D:605:PHE:HA	1.88	0.55
3:F:59:LEU:HD13	3:F:74:CYS:HB3	1.89	0.55
1:A:402:HIS:HB3	1:A:424:GLU:HB2	1.88	0.55
2:C:219:MET:CE	2:E:220:GLY:HA3	2.37	0.55
1:D:711:VAL:HA	1:D:714:ASN:ND2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ASP:HB2	3:F:86:ARG:HH21	1.73	0.54
1:A:601:SER:HB2	1:A:605:PHE:HA	1.89	0.54
1:A:38:ASP:HB3	1:A:40:ARG:HG3	1.90	0.54
2:C:107:CYS:HB3	2:C:136:CYS:SG	2.48	0.54
1:D:810:GLU:HA	1:D:813:LYS:HD2	1.90	0.54
1:A:64:ILE:HG21	1:A:69:ILE:HD11	1.90	0.54
2:C:120:TRP:HZ2	2:C:149:ARG:HB2	1.73	0.54
1:A:186:LEU:HD12	3:B:86:ARG:HB3	1.89	0.53
2:C:237:LEU:HA	2:C:240:ILE:HD12	1.89	0.53
1:A:535:LEU:HD13	1:A:598:ASP:HA	1.90	0.53
1:A:694:LEU:HD12	1:A:695:PRO:HD2	1.91	0.53
1:D:329:THR:HG23	1:D:331:ILE:HG12	1.90	0.53
1:D:402:HIS:HB3	1:D:424:GLU:HB2	1.91	0.53
1:D:612:TRP:CZ2	1:D:618:CYS:HA	2.44	0.53
1:A:541:ILE:HD12	1:A:541:ILE:H	1.73	0.53
1:A:749:VAL:O	1:A:753:ILE:HG22	2.08	0.53
1:D:38:ASP:HB3	1:D:40:ARG:HG3	1.91	0.52
1:A:169:PRO:HG2	1:A:173:LEU:HD23	1.91	0.52
1:A:718:PHE:CZ	1:A:753:ILE:HD13	2.45	0.52
1:D:364:CYS:HB3	1:D:367:LEU:HB2	1.92	0.52
1:D:680:PRO:HB3	1:D:686:GLU:HB2	1.92	0.52
1:A:781:ILE:HA	2:E:216:TYR:CE2	2.44	0.52
1:A:781:ILE:HG13	1:A:782:MET:N	2.25	0.52
1:D:750:ALA:O	1:D:753:ILE:HG22	2.10	0.52
1:D:168:VAL:HG21	1:D:197:PHE:HE1	1.75	0.52
1:A:540:MET:HA	1:A:543:LEU:HD12	1.91	0.52
1:D:539:TRP:CD1	1:D:539:TRP:H	2.28	0.52
1:A:556:ASN:O	1:A:560:ILE:HG12	2.09	0.51
1:A:576:PHE:HD1	1:A:579:LEU:HD11	1.75	0.51
2:E:231:LEU:O	2:E:235:ILE:HG22	2.10	0.51
1:A:138:ALA:HB2	3:B:86:ARG:NH2	2.24	0.51
1:D:752:LEU:HD23	1:D:800:LEU:HD23	1.91	0.51
1:A:612:TRP:CZ2	1:A:618:CYS:HA	2.45	0.51
1:A:752:LEU:HD23	1:A:800:LEU:HD23	1.92	0.50
1:D:264:PRO:HG2	1:D:267:ALA:HB2	1.93	0.50
2:E:65:LEU:HD21	2:E:198:GLN:HG3	1.92	0.50
1:A:329:THR:HG23	1:A:331:ILE:HG12	1.93	0.50
1:D:367:LEU:HD23	1:D:368:GLU:N	2.27	0.50
1:D:528:ALA:HB3	1:D:779:PRO:HB2	1.93	0.50
2:C:65:LEU:HD21	2:C:194:ILE:HD11	1.94	0.50
1:A:135:ARG:HG2	1:A:159:TRP:CE3	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:HB2	1:A:224:LEU:HD11	1.94	0.50
1:A:547:PHE:O	1:A:551:VAL:HG13	2.12	0.50
1:A:629:SER:O	1:A:633:ILE:HG13	2.12	0.50
1:A:264:PRO:HG2	1:A:267:ALA:HB2	1.94	0.49
2:C:74:TYR:HD2	2:E:118:TYR:HD1	1.60	0.49
2:C:216:TYR:CZ	1:D:781:ILE:HG22	2.48	0.49
1:A:227:LEU:HD23	1:A:247:LEU:HD13	1.94	0.49
1:A:751:TRP:HB2	1:A:800:LEU:HD21	1.95	0.49
1:D:438:GLN:HG2	1:D:461:SER:HB3	1.93	0.49
1:D:634:PHE:HB3	1:D:669:ALA:HB1	1.95	0.49
1:D:649:ASP:HB2	1:D:656:SER:HB3	1.95	0.49
2:E:240:ILE:O	2:E:244:GLN:HG3	2.12	0.49
1:D:57:ALA:HB1	1:D:81:PRO:HD2	1.95	0.49
1:D:718:PHE:CE2	1:D:753:ILE:HD11	2.47	0.49
1:A:711:VAL:HA	1:A:714:ASN:HD21	1.77	0.49
3:B:57:GLN:HG2	3:B:58:LYS:H	1.78	0.49
1:A:159:TRP:CZ2	3:B:105:PHE:HD1	2.31	0.48
2:C:221:ILE:HD13	1:D:540:MET:HB3	1.94	0.48
2:C:190:LYS:O	2:C:194:ILE:HG22	2.13	0.48
2:E:120:TRP:HZ2	2:E:149:ARG:HB3	1.78	0.48
1:D:539:TRP:O	1:D:540:MET:HB2	2.13	0.48
1:A:118:LYS:HG2	1:A:119:THR:HG23	1.95	0.48
1:A:247:LEU:HD12	1:A:250:LEU:HD22	1.94	0.48
1:A:781:ILE:HG13	1:A:782:MET:H	1.79	0.48
1:D:161:ASP:OD2	3:F:86:ARG:HG3	2.13	0.48
1:D:340:GLN:HA	1:D:343:LYS:NZ	2.29	0.48
1:A:367:LEU:HD23	1:A:368:GLU:N	2.28	0.48
1:D:743:SER:HA	1:D:746:ILE:HB	1.95	0.48
1:D:118:LYS:O	1:D:141:ILE:HA	2.13	0.48
1:D:586:PHE:HB2	1:D:628:SER:OG	2.14	0.48
1:D:814:LEU:HB3	1:D:817:ARG:HH21	1.79	0.48
1:A:114:ASN:HD22	3:B:76:HIS:CD2	2.32	0.48
1:A:181:ALA:HB1	3:B:105:PHE:CE2	2.49	0.48
1:D:679:PHE:HB3	1:D:680:PRO:HD3	1.96	0.48
1:D:138:ALA:HB2	3:F:86:ARG:NH2	2.28	0.47
2:C:232:VAL:HA	2:C:235:ILE:HG22	1.95	0.47
1:D:718:PHE:HE2	1:D:753:ILE:HD11	1.79	0.47
1:A:782:MET:HA	1:A:785:VAL:HG22	1.95	0.47
1:D:138:ALA:HA	1:D:162:ASP:HB3	1.97	0.47
2:E:189:ILE:HG13	2:E:190:LYS:N	2.30	0.47
1:D:135:ARG:HG2	1:D:159:TRP:CE3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:O	1:A:141:ILE:HA	2.14	0.47
2:C:208:ARG:NH2	1:D:520:ILE:HG21	2.30	0.47
1:D:647:ALA:O	1:D:651:MET:HG2	2.15	0.47
1:D:751:TRP:HD1	2:E:237:LEU:HD12	1.79	0.47
2:E:98:ILE:HD11	2:E:203:ALA:HB2	1.97	0.47
3:F:57:GLN:HG2	3:F:58:LYS:H	1.80	0.47
1:A:57:ALA:HB1	1:A:81:PRO:HD2	1.95	0.47
1:A:55:LEU:HB2	1:A:80:PHE:HE2	1.80	0.47
1:D:114:ASN:HD22	3:F:76:HIS:CD2	2.33	0.47
1:D:708:VAL:HA	1:D:711:VAL:HG22	1.97	0.47
2:E:190:LYS:O	2:E:194:ILE:HG22	2.15	0.47
3:B:122:GLY:C	3:B:123:ARG:HD2	2.39	0.46
1:D:224:LEU:HB3	1:D:227:LEU:HB2	1.97	0.46
1:A:368:GLU:HB3	1:A:369:GLU:OE1	2.16	0.46
1:D:561:LEU:O	1:D:565:ALA:HB3	2.14	0.46
2:C:216:TYR:HE2	1:D:781:ILE:HA	1.80	0.46
1:D:55:LEU:HB2	1:D:80:PHE:HE2	1.80	0.46
1:A:361:PHE:HB3	1:A:388:LEU:HD21	1.98	0.46
1:D:118:LYS:HG2	1:D:119:THR:HG23	1.97	0.46
2:C:240:ILE:O	2:C:244:GLN:HG3	2.16	0.46
3:B:63:LEU:HD13	3:B:70:GLN:HE21	1.80	0.46
1:A:571:PRO:HG2	1:A:574:LYS:HG3	1.98	0.46
1:D:68:ASN:O	1:D:69:ILE:C	2.59	0.46
1:D:576:PHE:HD1	1:D:579:LEU:HD11	1.81	0.46
1:A:694:LEU:HD12	1:A:695:PRO:CD	2.46	0.46
1:A:814:LEU:HB3	1:A:817:ARG:HH21	1.81	0.46
1:D:549:PHE:CD2	1:D:550:LEU:HD22	2.51	0.46
1:D:696:PHE:HB3	1:D:698:THR:HG23	1.98	0.45
1:A:528:ALA:HB3	1:A:779:PRO:HG2	1.98	0.45
2:E:128:GLN:OE1	2:E:129:PRO:HD2	2.16	0.45
1:A:155:LEU:HD23	1:A:176:LEU:HD11	1.98	0.45
1:A:586:PHE:HB2	1:A:628:SER:OG	2.16	0.45
1:A:781:ILE:HA	2:E:216:TYR:HE2	1.81	0.45
1:D:540:MET:HA	1:D:543:LEU:HD12	1.99	0.45
1:A:224:LEU:HB3	1:A:227:LEU:HB2	1.98	0.45
1:A:561:LEU:O	1:A:565:ALA:HB3	2.15	0.45
1:D:631:SER:O	1:D:635:LEU:HG	2.16	0.45
1:A:549:PHE:CE2	1:A:550:LEU:HD13	2.51	0.45
1:A:633:ILE:HG22	1:A:637:MET:CE	2.46	0.45
1:D:367:LEU:HD21	1:D:370:ILE:HG13	1.98	0.45
1:D:137:ASP:HB3	1:D:161:ASP:OD1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:748:HIS:HA	1:D:751:TRP:CZ3	2.51	0.45
1:A:138:ALA:HB2	3:B:86:ARG:HH22	1.82	0.45
1:A:647:ALA:O	1:A:651:MET:HG2	2.16	0.45
1:A:742:GLN:HA	1:A:745:MET:HE1	1.99	0.45
1:A:748:HIS:O	1:A:752:LEU:HG	2.16	0.45
1:D:571:PRO:HG2	1:D:574:LYS:HG3	1.98	0.45
1:D:767:SER:O	1:D:770:PRO:HD2	2.17	0.45
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.70	0.45
1:A:282:ASN:OD1	1:A:283:PRO:HD2	2.16	0.45
1:A:382:GLU:HB2	1:A:405:HIS:CG	2.52	0.45
2:C:189:ILE:HG13	2:C:190:LYS:N	2.30	0.45
3:F:63:LEU:HD13	3:F:70:GLN:HE21	1.82	0.45
3:F:122:GLY:C	3:F:123:ARG:HD2	2.42	0.45
1:A:585:LEU:HD22	1:A:585:LEU:HA	1.70	0.44
1:A:634:PHE:HA	1:A:637:MET:HG2	1.99	0.44
2:C:118:TYR:HD1	2:E:74:TYR:HD2	1.66	0.44
1:A:788:ILE:O	1:A:792:LEU:HB2	2.16	0.44
2:C:235:ILE:HD11	1:D:803:PHE:HB3	2.00	0.44
3:F:83:TYR:HB3	3:F:104:CYS:SG	2.57	0.44
1:A:111:THR:HA	1:A:135:ARG:HB2	2.00	0.44
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.87	0.44
1:D:633:ILE:O	1:D:636:LEU:HB2	2.17	0.44
2:E:134:LYS:NZ	2:E:136:CYS:HA	2.32	0.44
1:A:781:ILE:HG13	1:A:782:MET:SD	2.57	0.44
1:D:711:VAL:HA	1:D:714:ASN:HD21	1.80	0.44
2:E:81:LEU:HD21	2:E:190:LYS:HG2	1.99	0.44
1:A:704:LEU:HD13	1:A:704:LEU:HA	1.89	0.44
1:A:540:MET:HB2	2:E:221:ILE:CD1	2.48	0.44
2:C:145:ARG:O	2:C:149:ARG:HG2	2.17	0.44
1:A:713:LEU:O	1:A:716:LEU:HG	2.18	0.44
3:B:123:ARG:HD2	3:B:123:ARG:N	2.33	0.44
1:D:556:ASN:ND2	1:D:585:LEU:HB2	2.29	0.44
1:D:637:MET:HE3	1:D:637:MET:HB3	1.67	0.43
2:C:74:TYR:CD2	2:E:118:TYR:HD1	2.36	0.43
1:D:282:ASN:OD1	1:D:283:PRO:HD2	2.18	0.43
1:D:802:VAL:HG22	1:D:808:PHE:CE1	2.53	0.43
2:E:95:GLU:OE2	2:E:202:ARG:HD3	2.18	0.43
1:A:167:GLU:OE1	1:A:167:GLU:N	2.52	0.43
1:D:331:ILE:HD11	1:D:353:ASN:ND2	2.34	0.43
1:D:382:GLU:HB2	1:D:405:HIS:CG	2.53	0.43
1:D:584:ASN:HD21	1:D:798:PRO:HD3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:PHE:HA	1:A:579:LEU:HG	2.00	0.43
1:A:331:ILE:HD11	1:A:353:ASN:ND2	2.33	0.43
1:D:111:THR:HA	1:D:135:ARG:HB2	2.01	0.43
1:D:440:LYS:C	1:D:441:LEU:HD22	2.43	0.43
3:B:59:LEU:HD12	3:B:59:LEU:HA	1.78	0.43
1:D:389:ILE:HD12	1:D:389:ILE:H	1.83	0.43
1:A:726:THR:HA	1:A:729:TYR:CD2	2.53	0.43
1:D:233:ASN:HB3	1:D:234:TYR:HD1	1.84	0.43
1:A:189:ILE:HG13	1:A:211:ASN:HD21	1.84	0.43
1:A:686:GLU:HB3	1:A:704:LEU:HD21	1.99	0.43
2:E:95:GLU:HG3	2:E:204:ARG:HG3	2.00	0.43
1:A:718:PHE:HD1	1:A:721:MET:SD	2.42	0.43
1:A:72:LEU:HB2	1:A:96:ILE:HD13	2.01	0.43
1:A:340:GLN:HA	1:A:343:LYS:NZ	2.34	0.43
2:C:61:VAL:HG22	2:C:205:ILE:HG12	2.00	0.43
1:D:440:LYS:HZ2	1:D:440:LYS:HG3	1.65	0.43
1:A:250:LEU:HD21	1:A:253:LEU:HB2	2.01	0.42
3:B:83:TYR:HB3	3:B:104:CYS:SG	2.59	0.42
2:E:208:ARG:HD3	2:E:209:PRO:HD2	2.01	0.42
1:D:320:HIS:HE1	1:D:322:GLU:OE2	2.01	0.42
2:E:145:ARG:CZ	2:E:149:ARG:HH21	2.32	0.42
3:F:123:ARG:HD2	3:F:123:ARG:N	2.34	0.42
1:A:426:THR:HG22	1:A:446:LYS:HB3	2.01	0.42
1:D:39:ARG:CZ	1:D:58:PHE:HB3	2.49	0.42
1:D:395:ASP:O	1:D:396:LEU:HD23	2.20	0.42
1:D:754:PHE:O	1:D:758:ILE:HG12	2.20	0.42
2:E:111:ASP:OD2	2:E:149:ARG:HG3	2.19	0.42
2:C:174:ASP:OD2	2:C:174:ASP:N	2.51	0.42
1:D:117:LEU:HB2	1:D:139:ASN:OD1	2.19	0.42
1:D:779:PRO:HA	1:D:782:MET:HE1	2.00	0.42
2:E:174:ASP:OD1	2:E:174:ASP:N	2.52	0.42
3:F:108:ASP:OD1	3:F:108:ASP:C	2.62	0.42
1:A:797:ASN:N	1:A:798:PRO:HD2	2.35	0.42
1:A:807:LYS:HB2	1:A:807:LYS:HE2	1.88	0.42
2:C:98:ILE:HD11	2:C:203:ALA:HB2	2.01	0.42
1:D:255:PHE:HE1	1:D:279:LEU:HB3	1.85	0.42
1:D:686:GLU:HB3	1:D:704:LEU:HD21	2.01	0.42
1:A:406:SER:HA	1:A:429:PRO:HB3	2.02	0.42
1:A:584:ASN:OD1	1:A:794:ALA:HB1	2.19	0.42
2:E:155:ILE:HD11	2:E:205:ILE:HD11	2.02	0.42
3:F:121:ARG:HA	3:F:121:ARG:HD2	1.95	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:HB3	1:A:234:TYR:HD1	1.84	0.42
1:A:540:MET:HB2	2:E:221:ILE:HD12	2.01	0.42
2:C:165:ILE:HG12	2:C:182:TYR:CE2	2.54	0.42
2:C:216:TYR:CE1	2:E:219:MET:HG3	2.55	0.42
1:D:160:LEU:HD23	1:D:160:LEU:HA	1.78	0.42
2:E:85:PHE:HB3	2:E:91:THR:HG22	2.01	0.42
2:E:165:ILE:HG12	2:E:182:TYR:CE2	2.55	0.42
1:A:389:ILE:CG1	1:A:390:SER:H	2.29	0.42
2:C:218:ASP:O	2:C:221:ILE:HG13	2.20	0.42
1:D:159:TRP:CZ2	3:F:105:PHE:HD2	2.38	0.42
1:A:212:LYS:HE2	1:A:212:LYS:HB3	1.82	0.42
1:A:540:MET:HE2	2:E:221:ILE:HD11	2.01	0.42
2:C:125:LYS:HA	2:C:157:ASP:HB3	2.02	0.42
2:C:219:MET:SD	2:E:216:TYR:CE1	3.13	0.42
3:B:123:ARG:HB2	3:B:125:PHE:CE2	2.55	0.42
1:D:704:LEU:HD13	1:D:704:LEU:HA	1.90	0.42
1:D:768:PHE:CD1	1:D:771:LEU:HD12	2.55	0.42
2:E:131:LEU:HD12	2:E:131:LEU:HA	1.94	0.42
2:C:128:GLN:OE1	2:C:129:PRO:HD2	2.20	0.41
1:D:713:LEU:O	1:D:716:LEU:HG	2.19	0.41
1:D:726:THR:HA	1:D:729:TYR:CD2	2.55	0.41
3:F:128:CYS:HB2	3:F:134:PRO:HD3	2.01	0.41
1:A:39:ARG:CZ	1:A:58:PHE:HB3	2.50	0.41
1:A:352:TYR:CE2	1:A:374:ARG:HD3	2.55	0.41
1:A:586:PHE:HB2	1:A:628:SER:CB	2.50	0.41
1:A:767:SER:O	1:A:770:PRO:HD2	2.21	0.41
1:D:358:LEU:HD23	1:D:358:LEU:HA	1.84	0.41
2:E:217:PHE:O	2:E:221:ILE:HG23	2.20	0.41
1:A:395:ASP:O	1:A:396:LEU:HD23	2.20	0.41
1:A:802:VAL:HG22	1:A:808:PHE:CZ	2.56	0.41
3:B:112:LYS:HE2	3:B:112:LYS:HB2	1.94	0.41
1:D:58:PHE:HA	1:D:82:PHE:HD2	1.85	0.41
1:D:232:LEU:HD23	1:D:232:LEU:HA	1.87	0.41
1:A:40:ARG:HA	1:A:61:ALA:HB3	2.03	0.41
1:A:90:GLY:HA2	1:A:114:ASN:O	2.21	0.41
1:A:175:ASN:C	1:A:176:LEU:HD22	2.45	0.41
1:A:255:PHE:CE1	1:A:279:LEU:HB3	2.53	0.41
1:A:751:TRP:HD1	2:C:237:LEU:HD12	1.85	0.41
1:A:803:PHE:CD1	2:E:235:ILE:HD11	2.56	0.41
1:A:73:PRO:HG2	1:A:76:ALA:HB2	2.03	0.41
1:A:539:TRP:NE1	1:A:540:MET:HG3	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:235:ILE:HD11	1:D:803:PHE:CB	2.50	0.41
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.92	0.41
1:A:108:LYS:HB3	1:A:108:LYS:HE3	1.81	0.41
1:A:564:PHE:CZ	1:A:578:GLY:HA3	2.56	0.41
2:E:107:CYS:SG	2:E:136:CYS:HB2	2.61	0.41
3:F:68:MET:HE2	3:F:68:MET:HB3	1.78	0.41
1:A:58:PHE:HA	1:A:82:PHE:HD2	1.85	0.41
1:A:800:LEU:O	1:A:804:PHE:HB2	2.21	0.41
2:C:106:LEU:O	2:C:145:ARG:HG2	2.20	0.41
2:C:131:LEU:HD12	2:C:131:LEU:HA	1.85	0.41
1:D:352:TYR:CE2	1:D:374:ARG:HD3	2.56	0.41
1:D:406:SER:HA	1:D:429:PRO:HB3	2.02	0.41
1:D:681:LEU:N	1:D:687:TYR:HE1	2.19	0.41
2:E:97:GLU:HA	2:E:202:ARG:HA	2.03	0.41
3:F:48:LYS:HA	3:F:48:LYS:HD3	1.89	0.41
1:D:462:LEU:HD12	1:D:463:SER:H	1.87	0.40
1:D:582:VAL:O	1:D:585:LEU:HB3	2.20	0.40
1:A:138:ALA:HA	1:A:162:ASP:HB2	2.02	0.40
1:A:314:ASN:O	1:A:315:LEU:HD23	2.20	0.40
1:A:759:PHE:O	1:A:762:PRO:HD2	2.21	0.40
2:C:97:GLU:H	2:C:97:GLU:CD	2.28	0.40
2:C:212:GLN:HE22	2:C:214:THR:HB	1.86	0.40
1:D:361:PHE:HB2	1:D:384:THR:O	2.20	0.40
1:D:426:THR:HG22	1:D:446:LYS:HB3	2.02	0.40
1:D:582:VAL:HG12	1:D:586:PHE:CZ	2.57	0.40
1:A:361:PHE:HB2	1:A:384:THR:O	2.21	0.40
1:A:438:GLN:HE22	1:A:440:LYS:NZ	2.19	0.40
1:A:696:PHE:CZ	1:A:786:THR:HG21	2.56	0.40
2:E:61:VAL:HB	2:E:81:LEU:HB2	2.03	0.40
1:A:439:LEU:O	1:A:462:LEU:HA	2.22	0.40
1:A:571:PRO:HD2	1:A:574:LYS:HD2	2.03	0.40
2:C:85:PHE:HB3	2:C:91:THR:HG22	2.04	0.40
2:C:95:GLU:OE2	2:C:202:ARG:HD3	2.22	0.40
1:D:36:ASP:OD2	1:D:40:ARG:HB2	2.22	0.40
1:D:224:LEU:HD22	1:D:227:LEU:HD22	2.03	0.40
1:D:566:SER:HA	1:D:818:ARG:NE	2.35	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	744/845 (88%)	701 (94%)	42 (6%)	1 (0%)	48	79
1	D	744/845 (88%)	695 (93%)	48 (6%)	1 (0%)	48	79
2	C	188/231 (81%)	178 (95%)	10 (5%)	0	100	100
2	E	188/231 (81%)	180 (96%)	8 (4%)	0	100	100
3	B	102/160 (64%)	97 (95%)	5 (5%)	0	100	100
3	F	102/160 (64%)	96 (94%)	6 (6%)	0	100	100
All	All	2068/2472 (84%)	1947 (94%)	119 (6%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ILE
1	D	69	ILE

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	658/737 (89%)	641 (97%)	17 (3%)	40	62
1	D	658/737 (89%)	645 (98%)	13 (2%)	48	66
2	C	163/199 (82%)	156 (96%)	7 (4%)	26	52
2	E	163/199 (82%)	160 (98%)	3 (2%)	51	68
3	B	92/144 (64%)	88 (96%)	4 (4%)	26	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	92/144 (64%)	88 (96%)	4 (4%)	26	52
All	All	1826/2160 (84%)	1778 (97%)	48 (3%)	41	62

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	70	THR
1	A	155	LEU
1	A	179	LEU
1	A	215	SER
1	A	255	PHE
1	A	374	ARG
1	A	388	LEU
1	A	389	ILE
1	A	412	LEU
1	A	415	ILE
1	A	522	CYS
1	A	585	LEU
1	A	593	ILE
1	A	594	LEU
1	A	690	SER
1	A	753	ILE
2	C	78	THR
2	C	184	LYS
2	C	192	MET
2	C	195	VAL
2	C	221	ILE
2	C	231	LEU
2	C	233	CYS
3	B	44	LEU
3	B	75	LEU
3	B	91	ASN
3	B	119	LEU
1	D	51	VAL
1	D	70	THR
1	D	157	HIS
1	D	215	SER
1	D	250	LEU
1	D	374	ARG
1	D	388	LEU
1	D	389	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	637	MET
1	D	712	LEU
1	D	718	PHE
1	D	747	LYS
1	D	751	TRP
2	E	78	THR
2	E	217	PHE
2	E	233	CYS
3	F	44	LEU
3	F	75	LEU
3	F	91	ASN
3	F	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	114	ASN
1	A	116	GLN
1	A	336	ASN
2	C	108	ASN
2	C	193	ASN
2	C	244	GLN
3	B	70	GLN
1	D	79	ASN
1	D	114	ASN
1	D	154	GLN
1	D	180	GLN
1	D	336	ASN
2	E	244	GLN
3	F	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1002	1	14,14,15	0.74	0	17,19,21	0.87	1 (5%)
4	NAG	A	1001	1	14,14,15	0.73	0	17,19,21	0.81	0
4	NAG	A	1002	1	14,14,15	0.73	0	17,19,21	0.80	0
4	NAG	D	1001	1	14,14,15	0.77	0	17,19,21	1.14	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1002	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1001	NAG	C2-N2-C7	2.66	126.47	122.90
4	D	1002	NAG	C2-N2-C7	2.02	125.61	122.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	C8-C7-N2-C2
4	A	1002	NAG	O7-C7-N2-C2
4	D	1002	NAG	C8-C7-N2-C2
4	D	1002	NAG	O7-C7-N2-C2
4	D	1001	NAG	C1-C2-N2-C7
4	D	1001	NAG	C3-C2-N2-C7
4	D	1002	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.

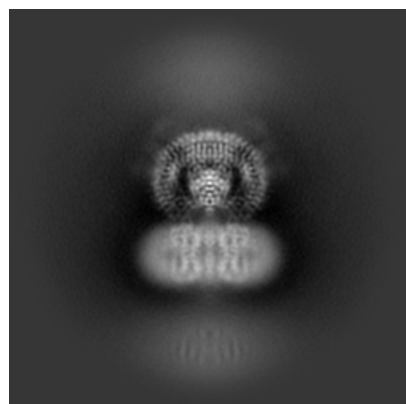
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62221. These allow visual inspection of the internal detail of the map and identification of artifacts.

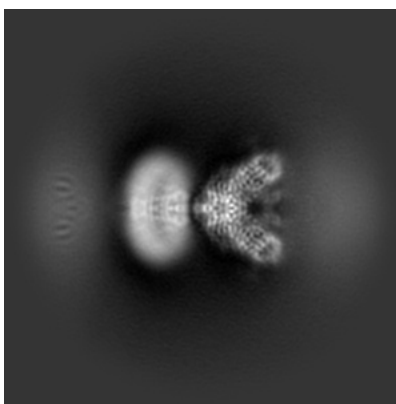
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

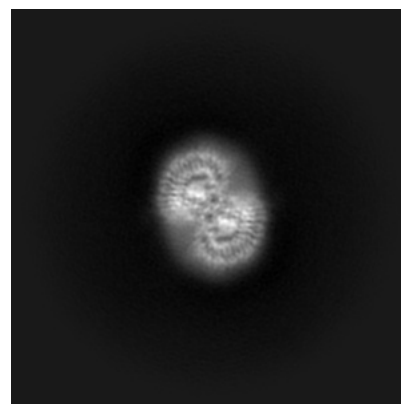
6.1.1 Primary map



X

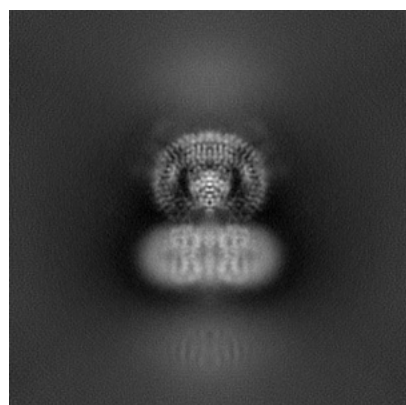


Y

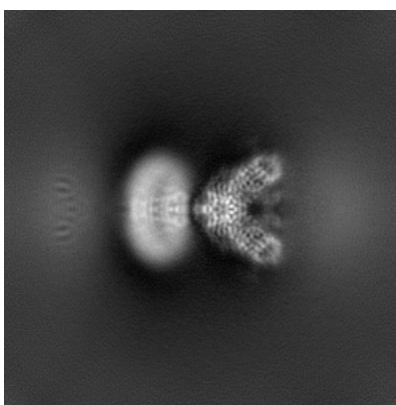


Z

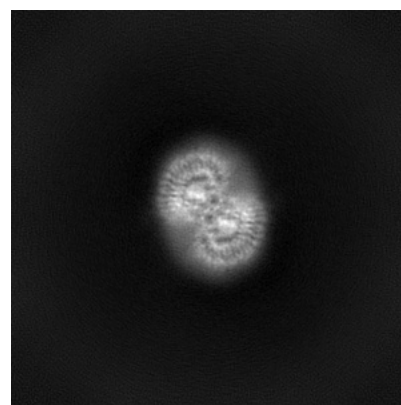
6.1.2 Raw map



X



Y

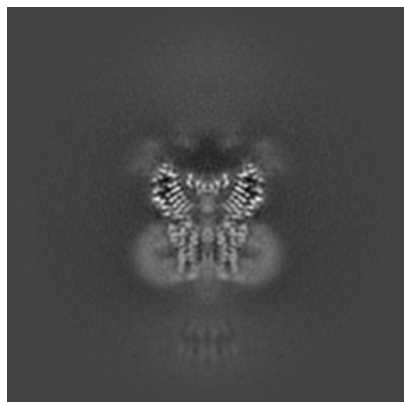


Z

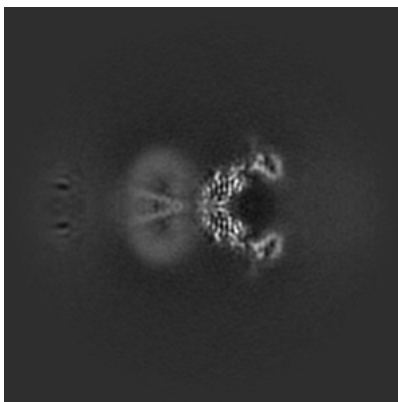
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

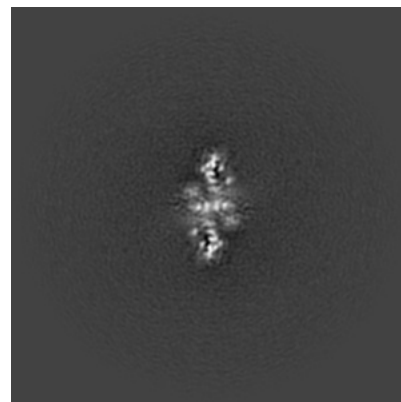
6.2.1 Primary map



X Index: 140

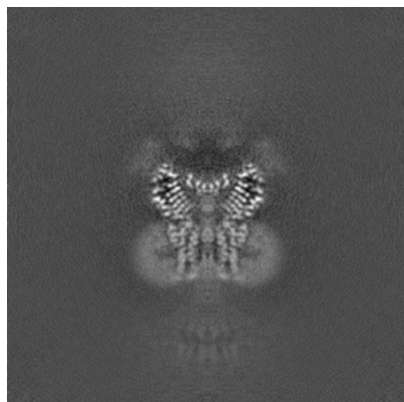


Y Index: 140

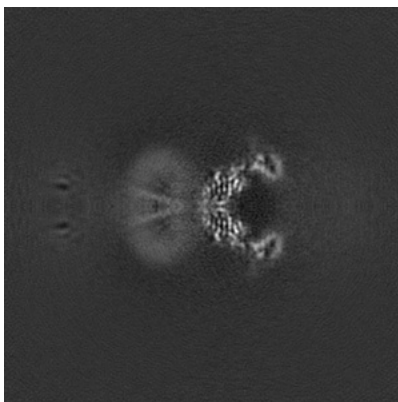


Z Index: 140

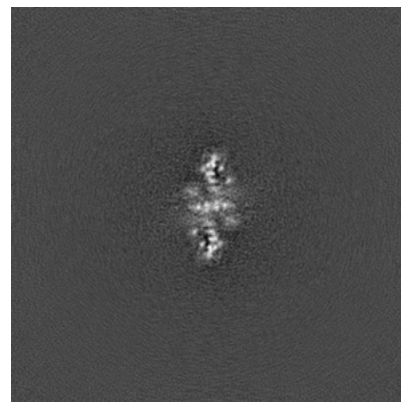
6.2.2 Raw map



X Index: 140



Y Index: 140

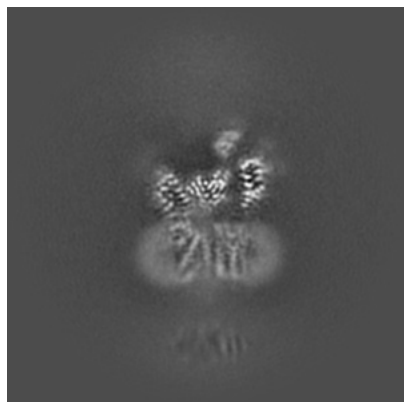


Z Index: 140

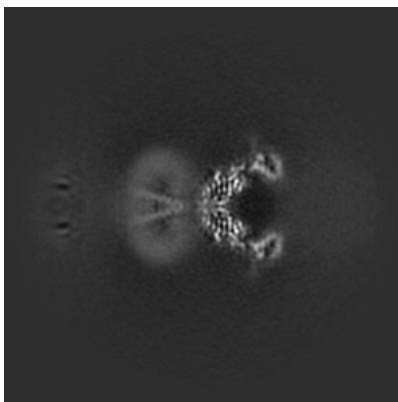
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

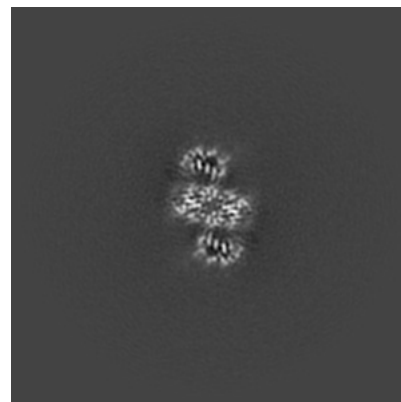
6.3.1 Primary map



X Index: 134

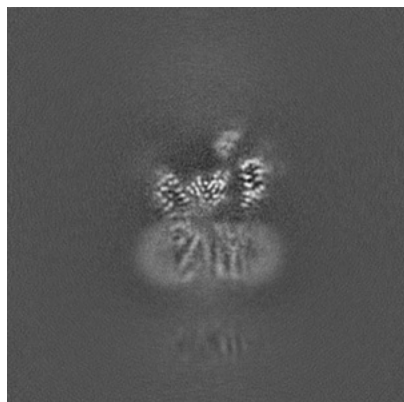


Y Index: 140

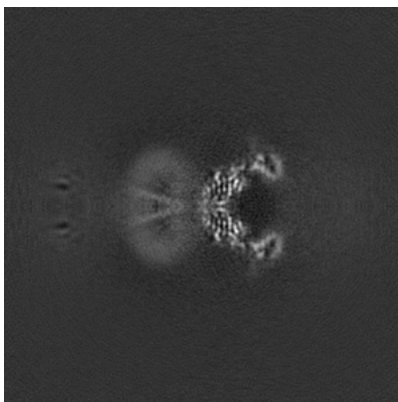


Z Index: 158

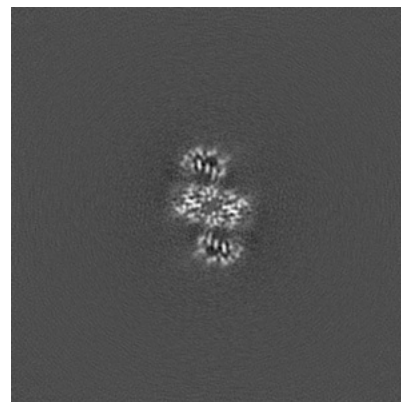
6.3.2 Raw map



X Index: 134



Y Index: 140

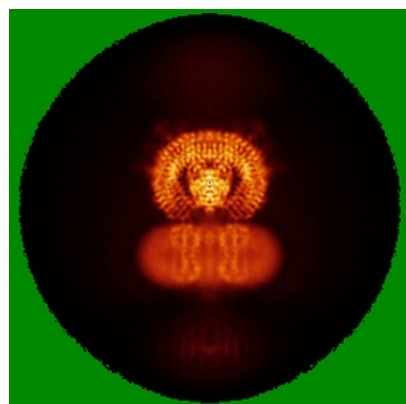


Z Index: 158

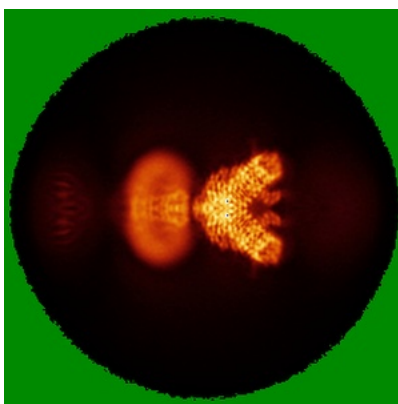
The images above show the largest variance slices of the map in three orthogonal directions.

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

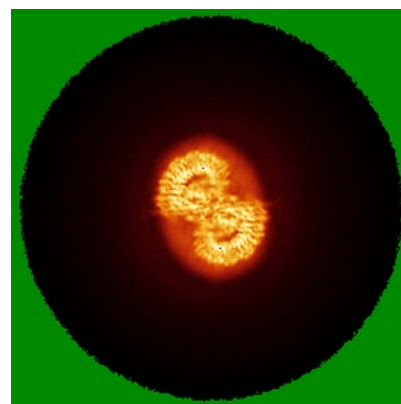
6.4.1 Primary map



X

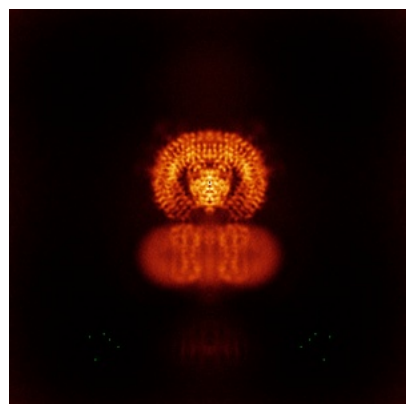


Y

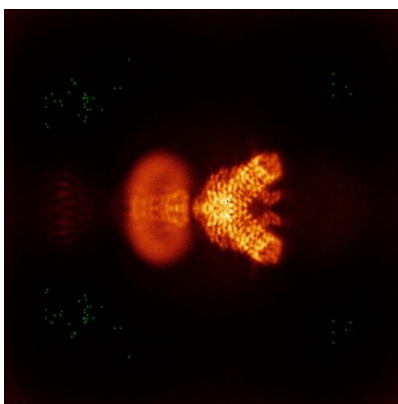


Z

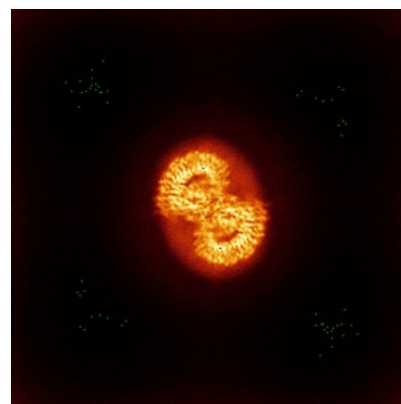
6.4.2 Raw map



X



Y

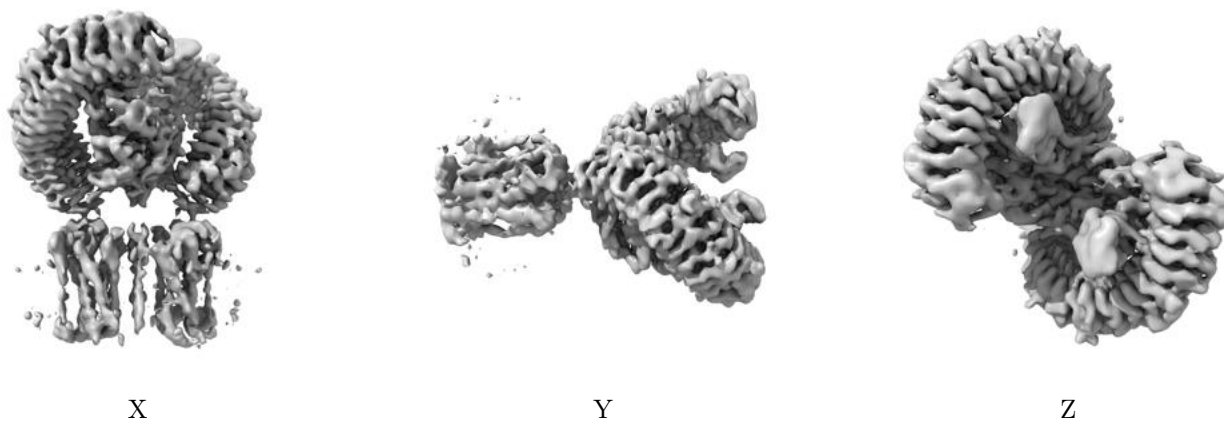


Z

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.

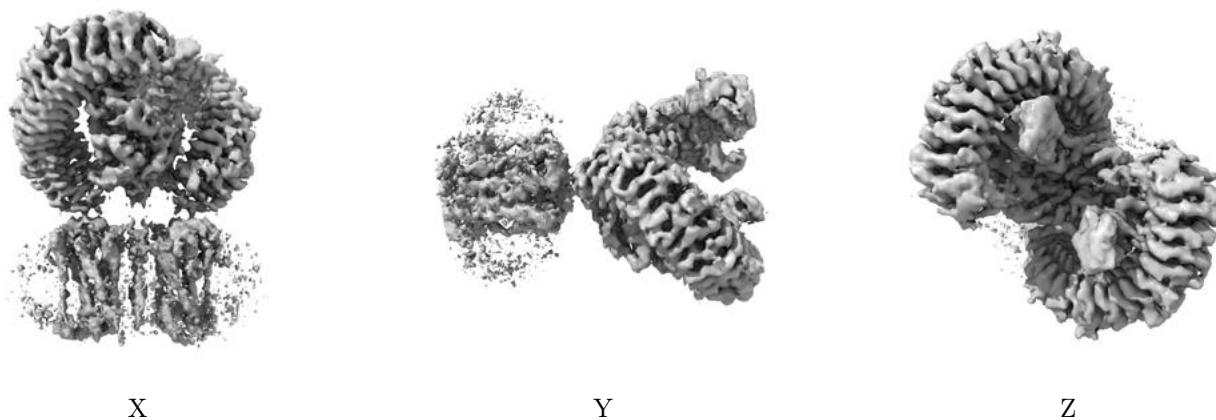
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.137. 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.

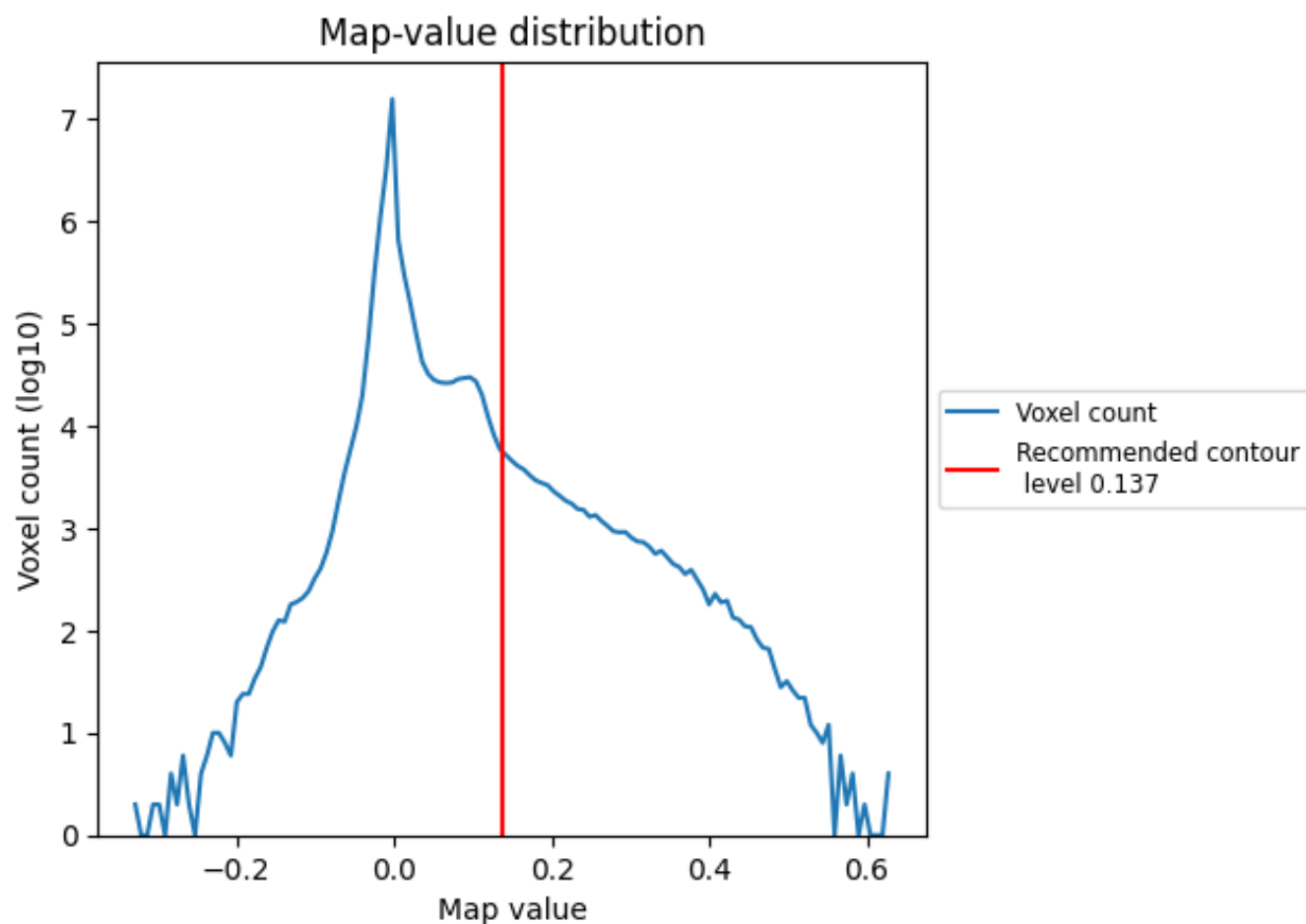
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

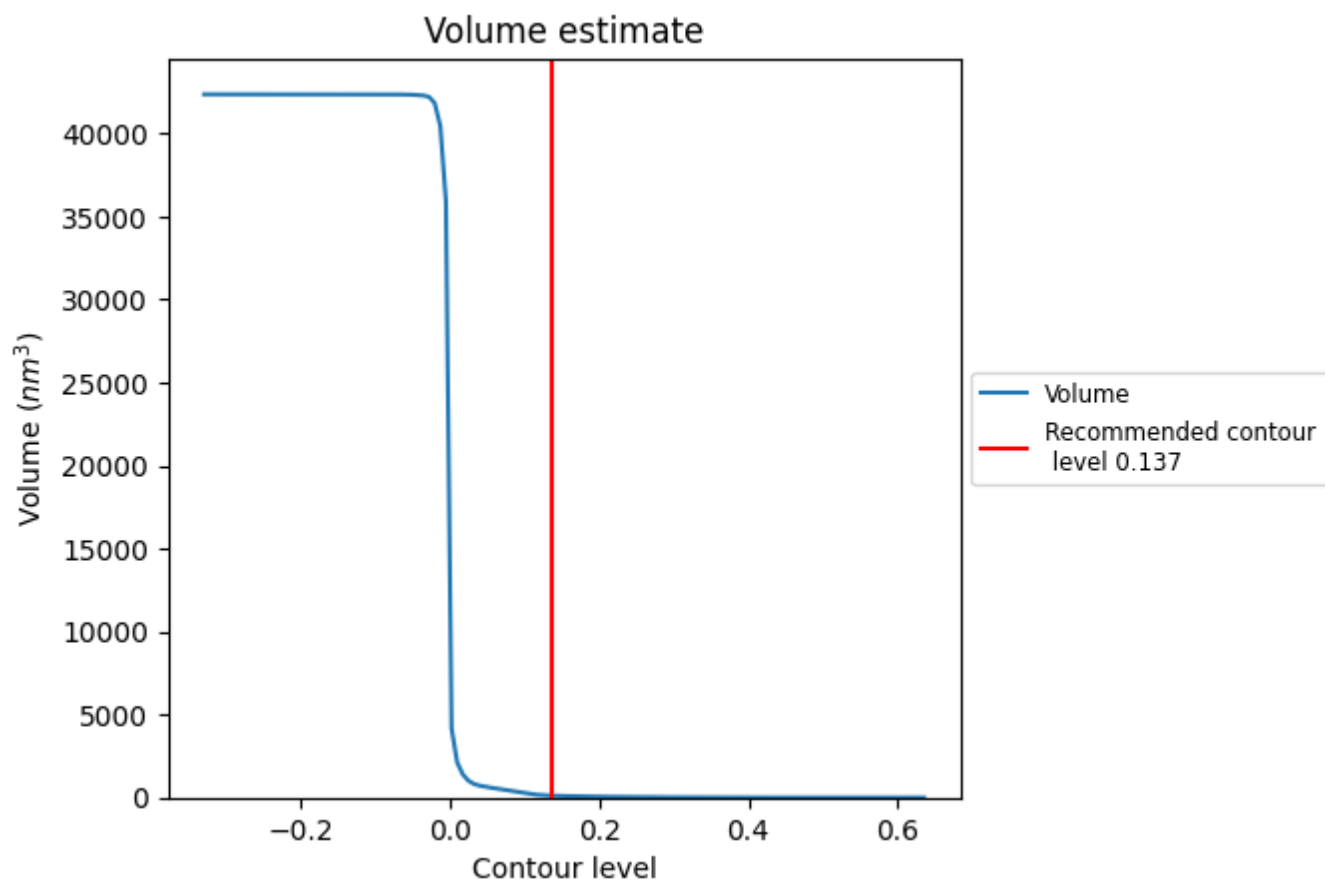
This section contains the results of statistical analysis of the map.

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.

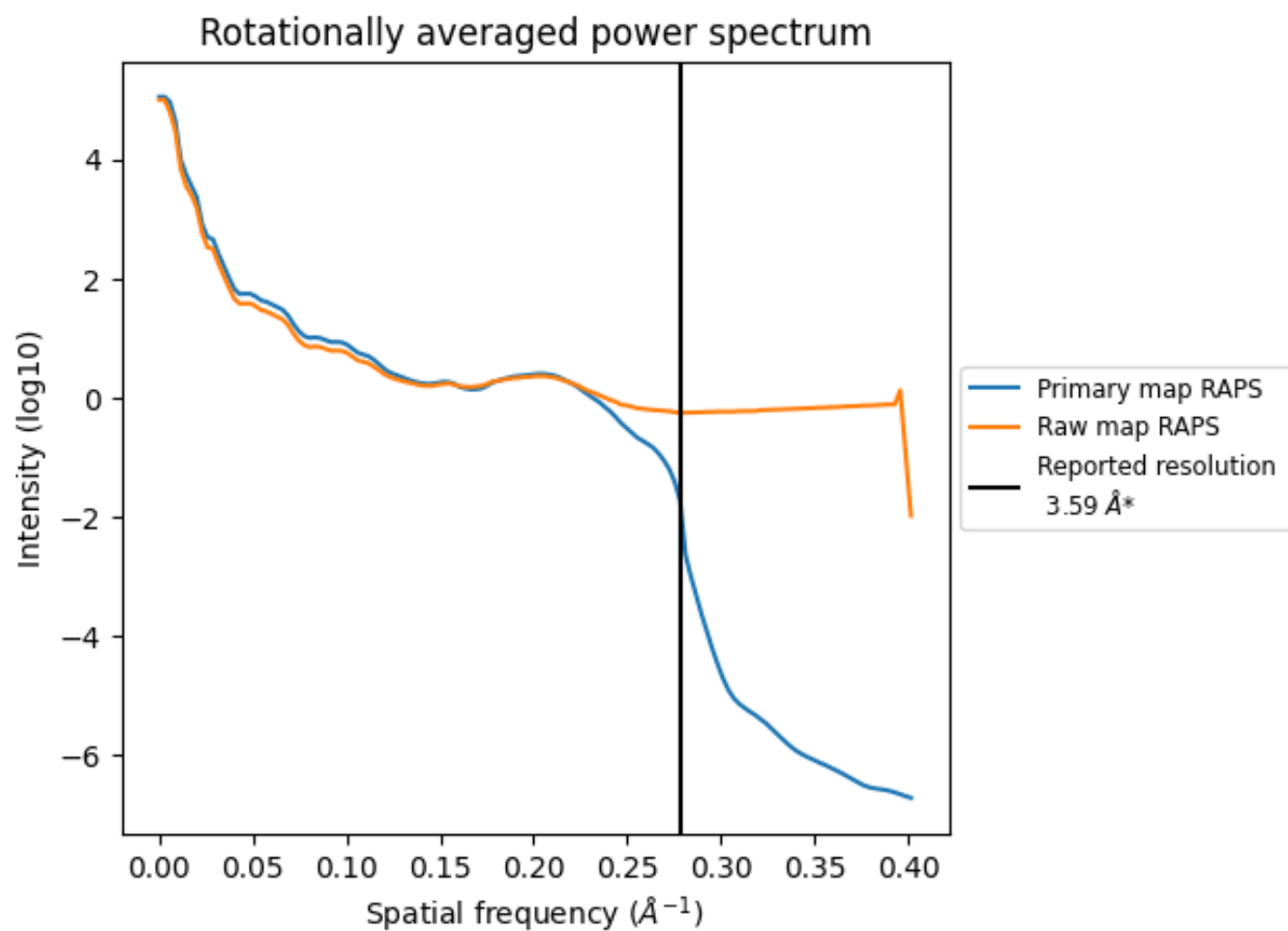
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm³; this corresponds to an approximate mass of 105 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 ⓘ

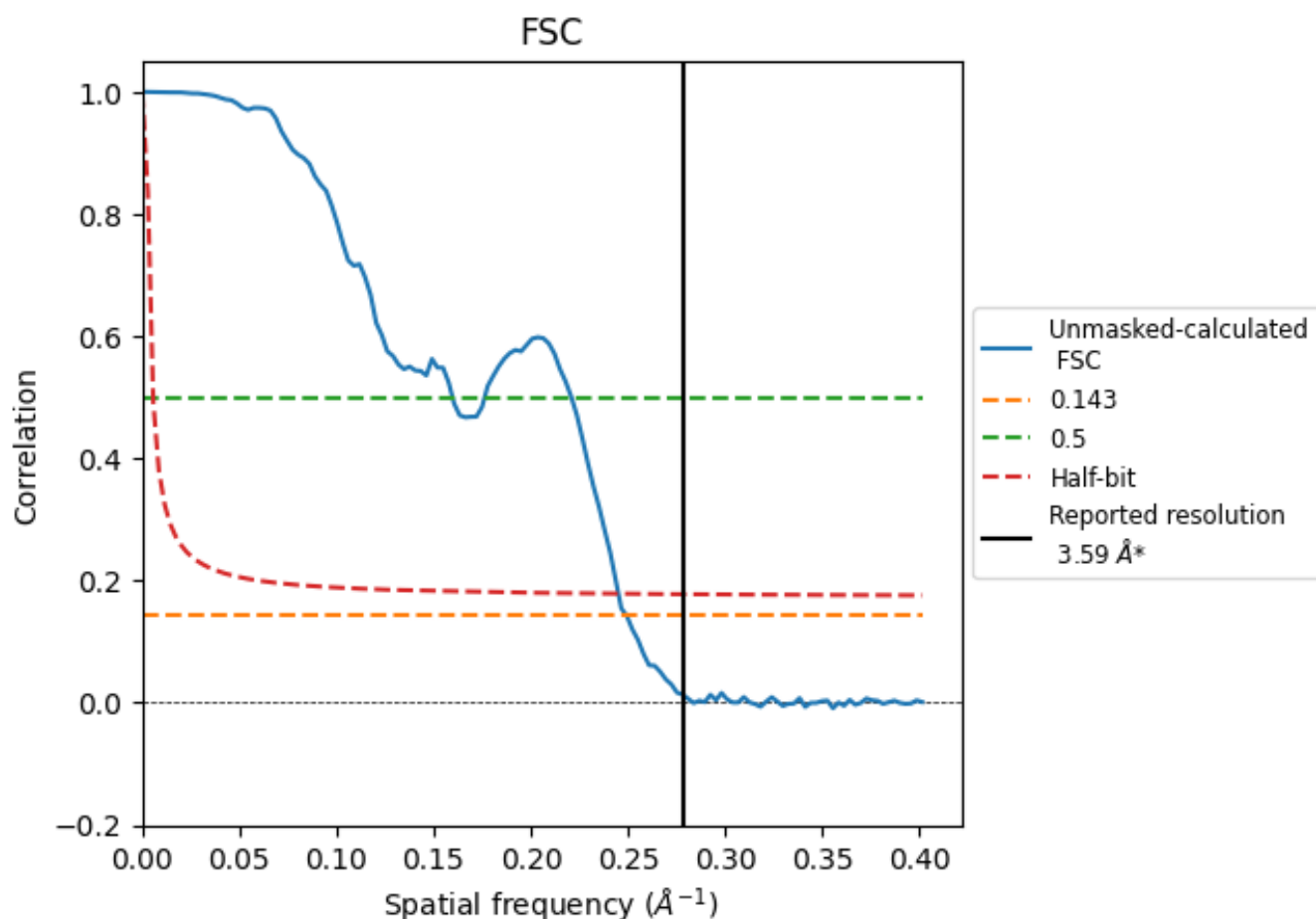


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 $0.279 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

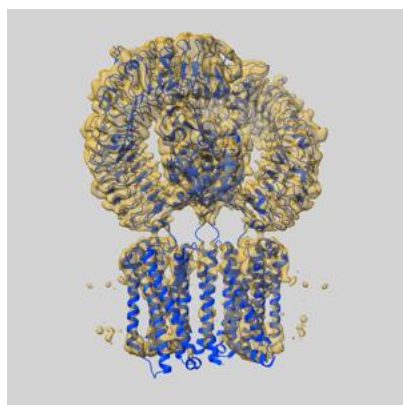
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	6.26	4.08

*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 4.01 differs from the reported value 3.59 by more than 10 %

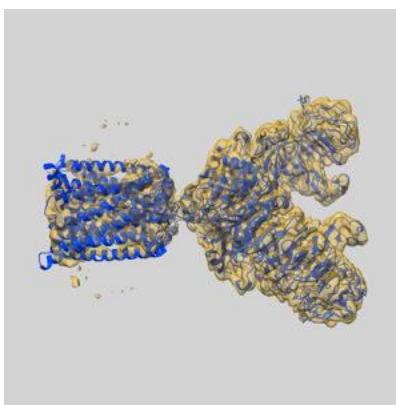
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62221 and PDB model 9KB9. Per-residue inclusion information can be found in section [3](#) on page [9](#).

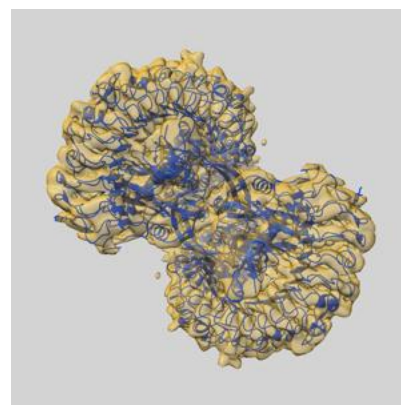
9.1 Map-model overlay [i](#)



X



Y



Z

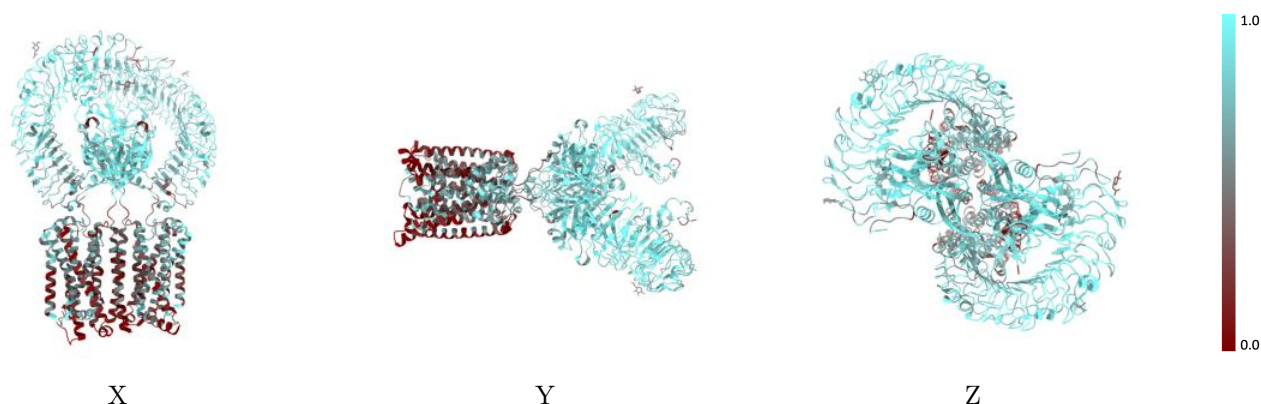
The images above show the 3D surface view of the map at the recommended contour level 0.137 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



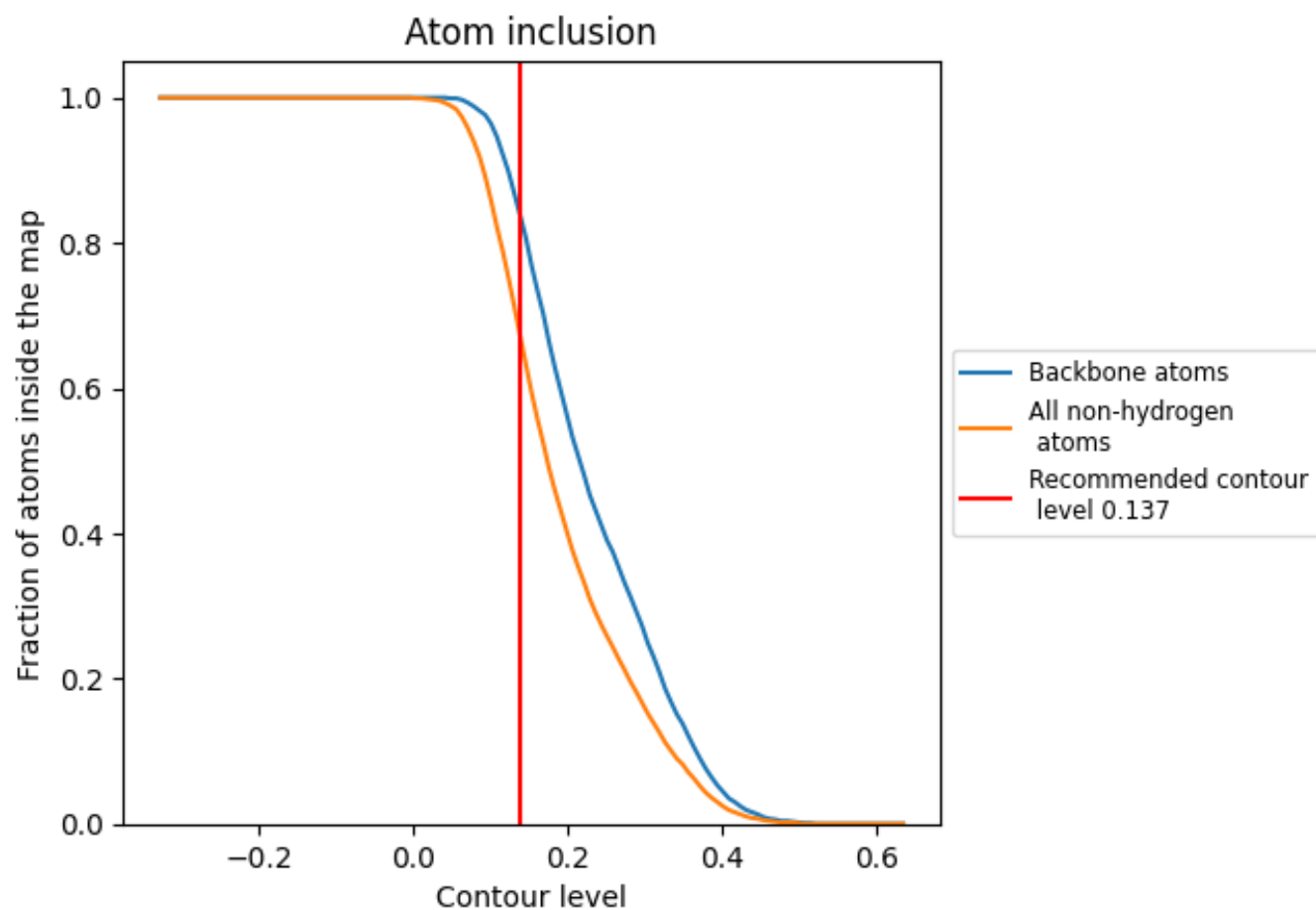
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.137).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 68% 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 (0.137) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.3740
A	0.6490	0.3600
B	0.8400	0.4370
C	0.7140	0.3960
D	0.6490	0.3580
E	0.7200	0.3950
F	0.8440	0.4370

1.0

0.0

<0.0