



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:56 PM UTC

PDB ID : 9C7Q / pdb_00009c7q
EMDB ID : EMD-45284
Title : Diheteromeric NMDA receptor GluN1/GluN2A, in complex with glycine and glutamate
Authors : Jalali-Yazdi, F.; Kim, J.; Gouaux, E.
Deposited on : 2024-06-11
Resolution : 4.05 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
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

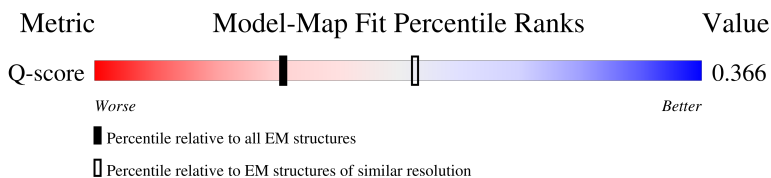
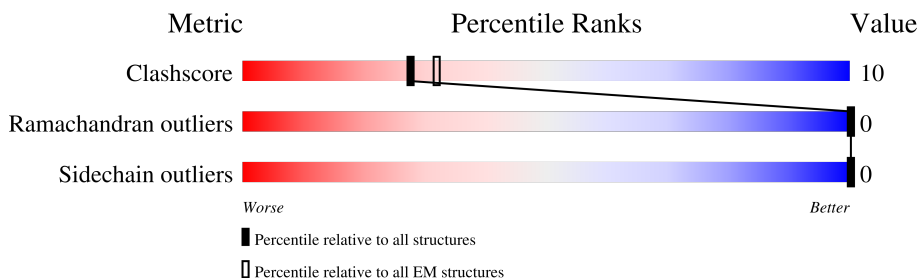
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.05 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	6569 (3.55 - 4.55)

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	1108	<div> <div>14%</div> <div>54%</div> <div>18%</div> <div>28%</div> </div>
1	C	1108	<div> <div>12%</div> <div>55%</div> <div>17%</div> <div>28%</div> </div>
2	B	1126	<div> <div>14%</div> <div>54%</div> <div>16%</div> <div>30%</div> </div>
2	D	1126	<div> <div>13%</div> <div>53%</div> <div>17%</div> <div>30%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25046 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 Glutamate receptor ionotropic, NMDA 1, Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			6295	4010	1091	1158	36		
1	C	795	Total	C	N	O	S	0	0
			6283	4003	1089	1155	36		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	848	LEU	-	linker	UNP P35439
A	849	VAL	-	linker	UNP P35439
A	850	PRO	-	linker	UNP P35439
A	851	ARG	-	linker	UNP P35439
A	852	GLY	-	linker	UNP P35439
A	853	SER	-	linker	UNP P35439
A	854	ALA	-	linker	UNP P35439
A	855	ALA	-	linker	UNP P35439
A	856	ALA	-	linker	UNP P35439
A	857	ALA	-	linker	UNP P35439
A	858	VAL	-	linker	UNP P35439
A	921	LEU	PHE	conflict	UNP P42212
A	922	THR	SER	conflict	UNP P42212
A	1063	LYS	ALA	conflict	UNP P42212
A	1088	LEU	HIS	conflict	UNP P42212
A	1096	SER	-	expression tag	UNP P42212
A	1097	GLY	-	expression tag	UNP P42212
A	1098	LEU	-	expression tag	UNP P42212
A	1099	ARG	-	expression tag	UNP P42212
A	1100	SER	-	expression tag	UNP P42212
A	1101	HIS	-	expression tag	UNP P42212
A	1102	HIS	-	expression tag	UNP P42212
A	1103	HIS	-	expression tag	UNP P42212
A	1104	HIS	-	expression tag	UNP P42212
A	1105	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1106	HIS	-	expression tag	UNP P42212
A	1107	HIS	-	expression tag	UNP P42212
A	1108	HIS	-	expression tag	UNP P42212
C	848	LEU	-	linker	UNP P35439
C	849	VAL	-	linker	UNP P35439
C	850	PRO	-	linker	UNP P35439
C	851	ARG	-	linker	UNP P35439
C	852	GLY	-	linker	UNP P35439
C	853	SER	-	linker	UNP P35439
C	854	ALA	-	linker	UNP P35439
C	855	ALA	-	linker	UNP P35439
C	856	ALA	-	linker	UNP P35439
C	857	ALA	-	linker	UNP P35439
C	858	VAL	-	linker	UNP P35439
C	921	LEU	PHE	conflict	UNP P42212
C	922	THR	SER	conflict	UNP P42212
C	1063	LYS	ALA	conflict	UNP P42212
C	1088	LEU	HIS	conflict	UNP P42212
C	1096	SER	-	expression tag	UNP P42212
C	1097	GLY	-	expression tag	UNP P42212
C	1098	LEU	-	expression tag	UNP P42212
C	1099	ARG	-	expression tag	UNP P42212
C	1100	SER	-	expression tag	UNP P42212
C	1101	HIS	-	expression tag	UNP P42212
C	1102	HIS	-	expression tag	UNP P42212
C	1103	HIS	-	expression tag	UNP P42212
C	1104	HIS	-	expression tag	UNP P42212
C	1105	HIS	-	expression tag	UNP P42212
C	1106	HIS	-	expression tag	UNP P42212
C	1107	HIS	-	expression tag	UNP P42212
C	1108	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A, Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	787	Total	C	N	O	S	0	0
			6234	4024	1017	1158	35		
2	D	787	Total	C	N	O	S	0	0
			6234	4024	1017	1158	35		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP Q00959
B	757	THR	SER	conflict	UNP Q00959
B	866	LEU	-	linker	UNP Q00959
B	867	VAL	-	linker	UNP Q00959
B	868	PRO	-	linker	UNP Q00959
B	869	ARG	-	linker	UNP Q00959
B	870	GLY	-	linker	UNP Q00959
B	871	SER	-	linker	UNP Q00959
B	872	ALA	-	linker	UNP Q00959
B	873	ALA	-	linker	UNP Q00959
B	874	ALA	-	linker	UNP Q00959
B	875	ALA	-	linker	UNP Q00959
B	876	VAL	-	linker	UNP Q00959
B	939	LEU	PHE	conflict	UNP P42212
B	940	THR	SER	conflict	UNP P42212
B	1081	LYS	ALA	conflict	UNP P42212
B	1106	LEU	HIS	conflict	UNP P42212
B	1114	SER	-	expression tag	UNP P42212
B	1115	GLY	-	expression tag	UNP P42212
B	1116	LEU	-	expression tag	UNP P42212
B	1117	ARG	-	expression tag	UNP P42212
B	1118	SER	-	expression tag	UNP P42212
B	1119	TRP	-	expression tag	UNP P42212
B	1120	SER	-	expression tag	UNP P42212
B	1121	HIS	-	expression tag	UNP P42212
B	1122	PRO	-	expression tag	UNP P42212
B	1123	GLN	-	expression tag	UNP P42212
B	1124	PHE	-	expression tag	UNP P42212
B	1125	GLU	-	expression tag	UNP P42212
B	1126	LYS	-	expression tag	UNP P42212
D	?	-	MET	deletion	UNP Q00959
D	757	THR	SER	conflict	UNP Q00959
D	866	LEU	-	linker	UNP Q00959
D	867	VAL	-	linker	UNP Q00959
D	868	PRO	-	linker	UNP Q00959
D	869	ARG	-	linker	UNP Q00959
D	870	GLY	-	linker	UNP Q00959
D	871	SER	-	linker	UNP Q00959
D	872	ALA	-	linker	UNP Q00959
D	873	ALA	-	linker	UNP Q00959
D	874	ALA	-	linker	UNP Q00959
D	875	ALA	-	linker	UNP Q00959
D	876	VAL	-	linker	UNP Q00959

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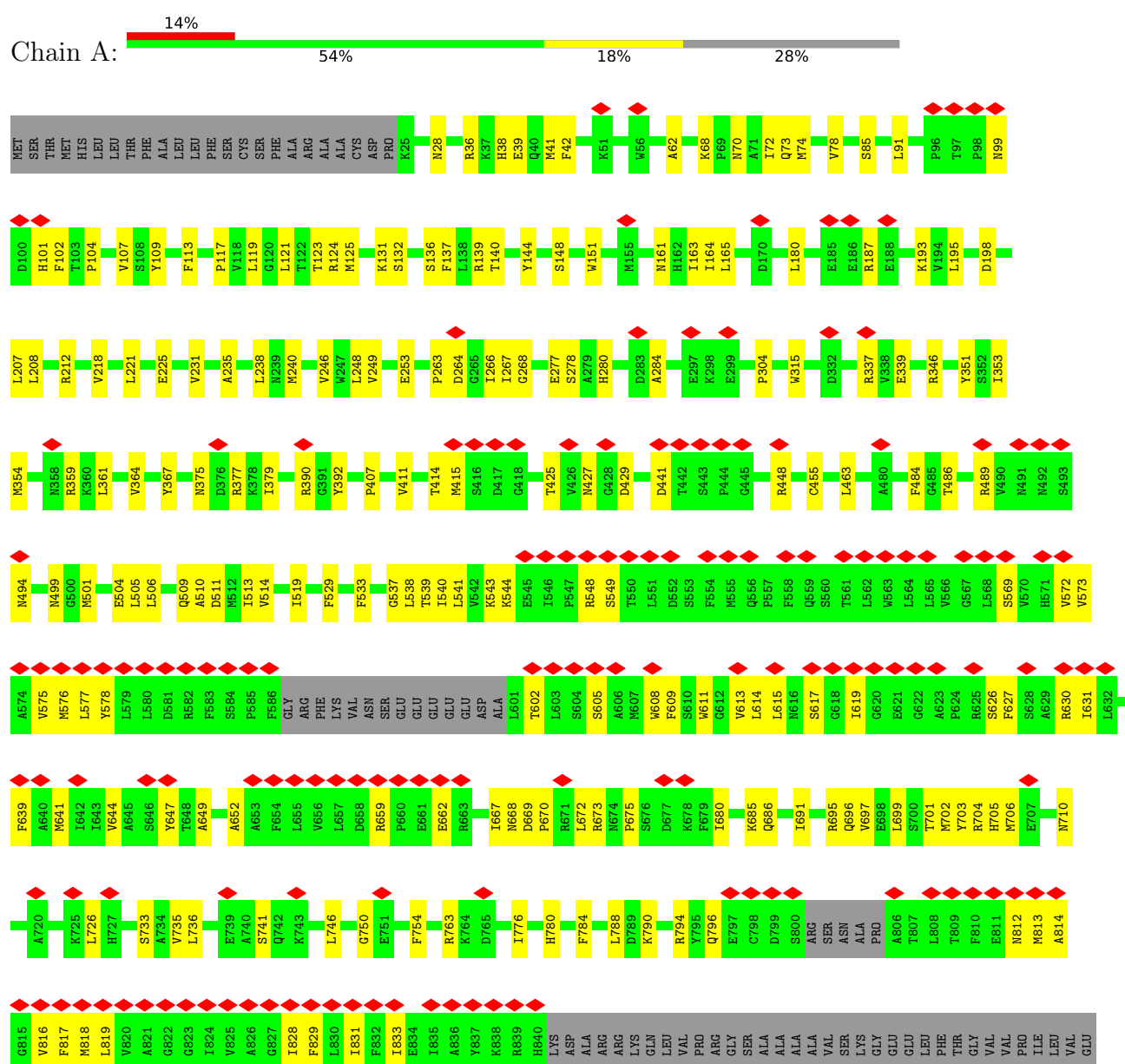
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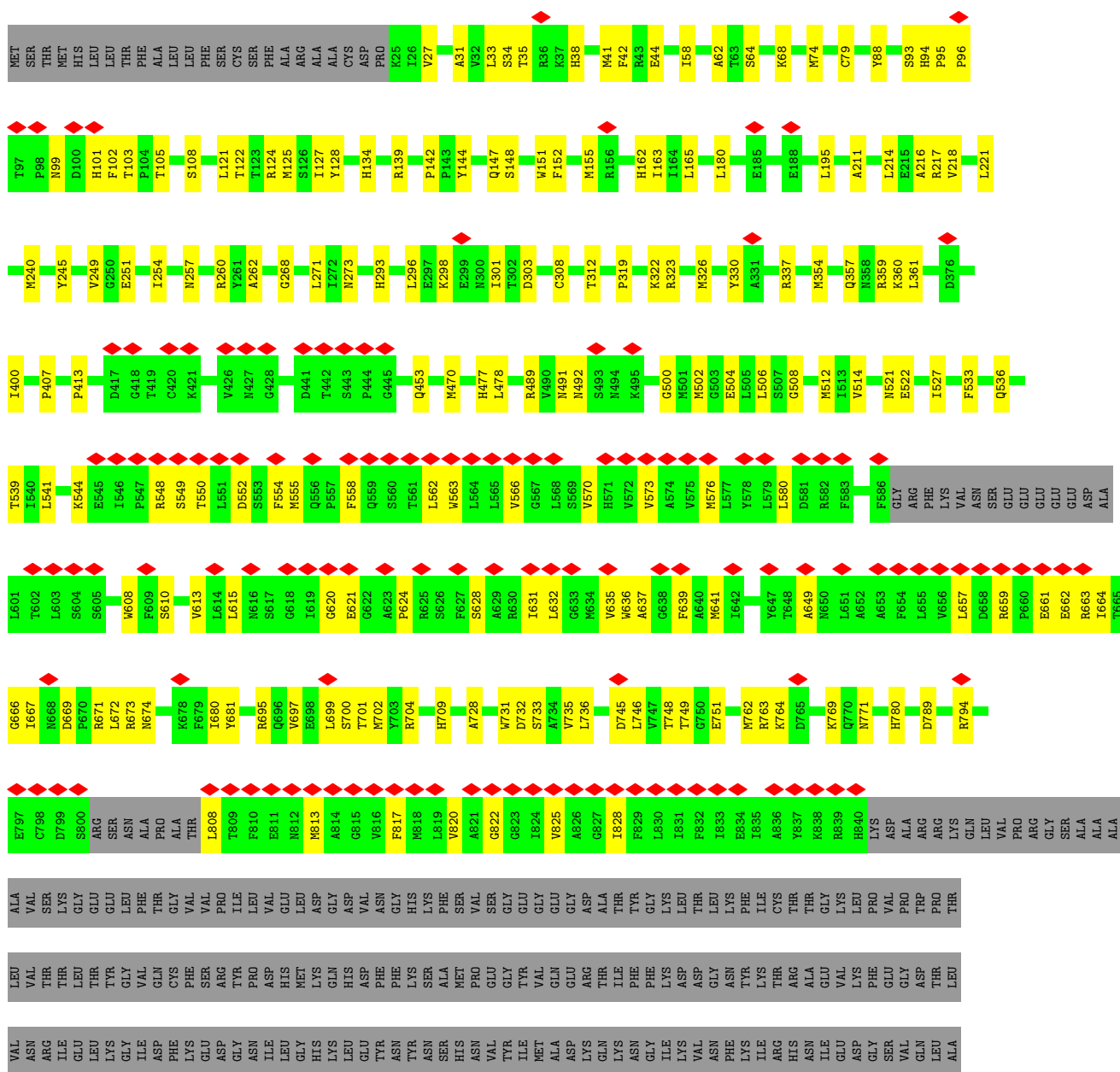
Chain	Residue	Modelled	Actual	Comment	Reference
D	939	LEU	PHE	conflict	UNP P42212
D	940	THR	SER	conflict	UNP P42212
D	1081	LYS	ALA	conflict	UNP P42212
D	1106	LEU	HIS	conflict	UNP P42212
D	1114	SER	-	expression tag	UNP P42212
D	1115	GLY	-	expression tag	UNP P42212
D	1116	LEU	-	expression tag	UNP P42212
D	1117	ARG	-	expression tag	UNP P42212
D	1118	SER	-	expression tag	UNP P42212
D	1119	TRP	-	expression tag	UNP P42212
D	1120	SER	-	expression tag	UNP P42212
D	1121	HIS	-	expression tag	UNP P42212
D	1122	PRO	-	expression tag	UNP P42212
D	1123	GLN	-	expression tag	UNP P42212
D	1124	PHE	-	expression tag	UNP P42212
D	1125	GLU	-	expression tag	UNP P42212
D	1126	LYS	-	expression tag	UNP P42212

3 Residue-property plots

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

- Molecule 1: Glutamate receptor ionotropic, NMDA 1, Green fluorescent protein chimera







PRO	ASP	ASN	HIS	TYR	LEU	SER	THR	GLN	SER	LYS	LEU	SER	LYS	ASP	PRO	ASN	GLU	LYS	ARG	ASP	HIS	MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	LEU	GLY	MET	ASP	GLU	LEU	TYR	LYS	SER	GLY	LEU	ARG	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	165000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0112	Depositor
Map size (\AA)	247.79999, 247.79999, 247.79999	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.826, 0.826, 0.826	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/6436	0.34	0/8719
1	C	0.13	0/6424	0.34	0/8702
2	B	0.13	0/6387	0.33	0/8678
2	D	0.13	0/6387	0.32	0/8678
All	All	0.13	0/25634	0.33	0/34777

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6295	0	6269	154	0
1	C	6283	0	6257	121	0
2	B	6234	0	6146	119	0
2	D	6234	0	6146	145	0
All	All	25046	0	24818	481	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 10.

All (481) 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:533:PHE:HB3	1:A:776:ILE:HD11	1.55	0.86
1:A:619:ILE:CG2	2:D:628:LYS:HB3	2.14	0.78
2:D:83:ILE:HD11	2:D:112:MET:HE2	1.65	0.78
1:A:354:MET:HB3	1:A:361:LEU:HD12	1.67	0.77
1:C:674:ASN:HD21	2:D:798:ILE:HD11	1.50	0.77
1:A:608:TRP:HZ2	2:D:629:ILE:HG13	1.51	0.75
1:A:619:ILE:HG21	2:D:628:LYS:HB3	1.67	0.75
1:A:218:VAL:HG12	1:A:246:VAL:HB	1.67	0.75
1:A:608:TRP:HZ2	2:D:629:ILE:CG1	2.01	0.74
2:B:94:ARG:HE	2:B:316:ALA:HB3	1.54	0.73
1:A:608:TRP:CZ2	2:D:629:ILE:CG1	2.72	0.72
1:C:34:SER:HB2	1:C:96:PRO:HD3	1.72	0.71
1:C:508:GLY:HA2	1:C:763:ARG:HH11	1.55	0.71
1:A:28:ASN:ND2	1:A:85:SER:OG	2.24	0.71
1:A:489:ARG:HH11	1:A:494:ASN:H	1.36	0.70
2:D:612:VAL:HA	2:D:638:ALA:HB1	1.73	0.70
1:C:298:LYS:HB2	1:C:301:ILE:HD11	1.74	0.70
1:C:548:ARG:NH1	1:C:549:SER:O	2.26	0.69
1:A:608:TRP:CZ2	2:D:629:ILE:HG12	2.28	0.68
2:B:730:ASP:OD1	2:B:760:TYR:OH	2.11	0.68
1:A:499:ASN:ND2	1:A:686:GLN:OE1	2.26	0.67
2:D:39:LEU:HB3	2:D:74:MET:HE1	1.75	0.67
1:A:337:ARG:NH2	1:A:339:GLU:OE2	2.27	0.67
2:B:175:THR:HG22	2:B:176:ILE:H	1.60	0.67
2:B:58:GLU:HG3	2:B:60:ALA:H	1.60	0.67
1:A:113:PHE:HE1	2:B:106:GLN:HG2	1.59	0.66
1:A:608:TRP:CZ2	2:D:629:ILE:HG13	2.28	0.66
1:C:697:VAL:HG12	2:D:431:ARG:HG3	1.78	0.66
1:A:814:ALA:HB1	1:A:818:MET:HE2	1.78	0.66
1:C:155:MET:HE1	1:C:163:ILE:HG21	1.78	0.66
1:C:262:ALA:O	1:C:359:ARG:NH1	2.29	0.66
2:D:207:ASP:OD2	2:D:208:THR:N	2.29	0.66
1:A:78:VAL:HG21	1:A:107:VAL:HG23	1.78	0.65
1:A:541:LEU:HD11	1:A:746:LEU:HB3	1.76	0.65
1:C:124:ARG:NH1	1:C:251:GLU:OE1	2.29	0.65
1:A:195:LEU:HB3	1:A:207:LEU:HD12	1.78	0.65
1:A:685:LYS:HB2	1:A:710:ASN:HB3	1.78	0.65
1:C:93:SER:HB3	1:C:121:LEU:HD12	1.78	0.65
2:B:419:VAL:HG21	2:B:479:LEU:HD21	1.79	0.65
2:D:206:LEU:HD22	2:D:215:THR:HB	1.77	0.65
1:A:68:LYS:H	1:A:74:MET:HE1	1.62	0.65
1:A:608:TRP:HH2	2:D:629:ILE:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:HD2	1:A:266:ILE:HD11	1.79	0.64
1:A:132:SER:HB3	2:B:178:PRO:HB2	1.78	0.64
2:B:364:ILE:HG22	2:B:374:LYS:HA	1.79	0.64
1:A:407:PRO:HG3	1:A:735:VAL:HA	1.80	0.64
2:B:707:PHE:O	2:B:709:GLN:NE2	2.31	0.63
2:D:729:TYR:HB3	2:D:734:LEU:HD21	1.79	0.63
2:D:37:ALA:HB2	2:D:95:ILE:HG21	1.81	0.63
1:A:484:PHE:HA	1:A:501:MET:HE3	1.81	0.63
1:C:659:ARG:O	1:C:661:GLU:N	2.31	0.63
2:D:78:ASP:OD1	2:D:81:SER:OG	2.13	0.63
1:C:550:THR:OG1	1:C:552:ASP:OD1	2.17	0.62
1:A:165:LEU:HD22	1:A:180:LEU:HD23	1.82	0.62
2:D:233:LYS:HA	2:D:261:VAL:HG23	1.80	0.62
2:D:365:VAL:HG11	2:D:390:TRP:HH2	1.64	0.62
2:D:535:VAL:HG22	2:D:728:ILE:HG12	1.80	0.62
1:A:703:TYR:HA	1:A:706:MET:HG2	1.82	0.62
1:C:354:MET:SD	1:C:361:LEU:HB3	2.39	0.62
1:A:614:LEU:HD12	1:A:615:LEU:HG	1.82	0.62
1:A:790:LYS:HD3	1:A:794:ARG:HG3	1.81	0.62
1:A:641:MET:HG2	2:B:615:ASN:ND2	2.14	0.61
2:D:436:CYS:HB3	2:D:477:LEU:HD23	1.81	0.61
1:A:38:HIS:HA	1:A:41:MET:HE3	1.82	0.61
1:A:659:ARG:NH2	1:A:662:GLU:OE2	2.33	0.61
1:C:669:ASP:HB3	1:C:672:LEU:HD23	1.83	0.61
2:B:279:VAL:HG12	2:B:363:VAL:HG22	1.82	0.60
2:B:229:LEU:HB3	2:B:257:VAL:HG12	1.82	0.60
2:D:279:VAL:HG12	2:D:363:VAL:HG22	1.82	0.60
2:D:557:VAL:HA	2:D:560:MET:HE2	1.83	0.60
1:A:608:TRP:CH2	2:D:629:ILE:HA	2.35	0.60
2:B:552:PRO:O	1:C:808:LEU:N	2.35	0.60
1:A:543:LYS:NZ	1:A:544:LYS:O	2.34	0.60
2:B:127:ILE:HG23	2:B:291:ARG:HB3	1.82	0.60
2:B:553:PHE:HD1	1:C:813:MET:HE3	1.67	0.60
2:B:76:ARG:NH1	2:B:103:ASP:OD1	2.34	0.60
1:C:681:TYR:HB3	1:C:728:ALA:HB3	1.84	0.59
2:B:557:VAL:O	2:B:561:MET:HG2	2.02	0.59
2:B:600:THR:HB	2:B:603:LYS:HG3	1.83	0.59
1:A:102:PHE:HE1	1:A:125:MET:HG2	1.67	0.59
1:A:266:ILE:HG22	1:A:268:GLY:H	1.67	0.59
2:D:433:THR:HG22	2:D:457:LYS:HB3	1.84	0.59
1:A:113:PHE:CE1	2:B:106:GLN:HG2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:LYS:NZ	1:C:326:MET:SD	2.74	0.58
2:B:629:ILE:HG12	1:C:608:TRP:HH2	1.67	0.58
2:B:690:GLU:OE2	2:B:701:HIS:NE2	2.37	0.58
1:A:131:LYS:NZ	1:A:137:PHE:O	2.37	0.58
2:B:162:MET:HE1	2:B:228:LEU:HD11	1.85	0.58
2:B:701:HIS:O	2:B:705:THR:HG23	2.03	0.58
2:D:155:ALA:HA	2:D:158:MET:HE2	1.86	0.58
2:D:532:GLY:HA3	2:D:754:ILE:HG23	1.85	0.58
1:C:544:LYS:O	1:C:663:ARG:NH1	2.37	0.58
2:B:783:GLY:HA3	1:C:695:ARG:HH12	1.68	0.57
1:A:647:TYR:HE1	2:D:640:ILE:CD1	2.16	0.57
1:A:608:TRP:CH2	2:D:629:ILE:HG12	2.39	0.57
2:D:561:MET:HA	2:D:564:MET:HE2	1.85	0.57
2:B:680:ARG:NH2	2:B:722:GLY:O	2.37	0.57
1:C:700:SER:OG	1:C:704:ARG:NH2	2.38	0.57
1:A:575:VAL:HA	1:A:578:TYR:CE1	2.40	0.57
1:A:641:MET:HA	1:A:644:VAL:HG12	1.86	0.57
1:A:121:LEU:HD22	1:A:280:HIS:HB3	1.87	0.57
2:B:169:VAL:HA	2:B:199:ASP:HB2	1.88	0.56
1:A:264:ASP:OD1	1:A:359:ARG:NH1	2.37	0.56
1:A:484:PHE:O	1:A:501:MET:HG2	2.04	0.56
2:B:37:ALA:HB2	2:B:95:ILE:HG21	1.88	0.56
1:C:662:GLU:O	1:C:671:ARG:NH1	2.39	0.56
1:A:208:LEU:HD21	1:A:231:VAL:HG23	1.88	0.55
1:A:505:LEU:HA	1:A:510:ALA:HB3	1.88	0.55
2:B:51:LEU:HA	2:B:54:LEU:HD12	1.87	0.55
1:A:253:GLU:N	1:A:253:GLU:OE1	2.39	0.55
1:A:353:ILE:C	1:A:354:MET:HE2	2.32	0.55
2:D:599:PHE:HA	2:D:603:LYS:HD3	1.87	0.55
1:A:668:ASN:HA	1:A:673:ARG:HH21	1.71	0.55
1:A:539:THR:HG23	1:A:736:LEU:HD12	1.89	0.55
1:A:667:ILE:O	1:A:673:ARG:NH2	2.39	0.55
2:D:364:ILE:HG22	2:D:374:LYS:HA	1.87	0.55
2:D:373:GLU:OE2	2:D:386:ARG:NH1	2.39	0.55
1:A:486:THR:HB	1:A:691:ILE:HD11	1.89	0.55
2:B:693:ILE:HG22	2:B:701:HIS:HB2	1.88	0.55
1:A:212:ARG:NH2	1:A:238:LEU:O	2.39	0.55
1:C:649:ALA:HB1	2:D:650:ALA:HB2	1.89	0.55
2:D:79:PRO:O	2:D:83:ILE:HD12	2.07	0.55
2:D:229:LEU:HB3	2:D:257:VAL:HG12	1.89	0.54
2:D:134:ILE:HG21	2:D:150:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:ILE:HD11	2:D:348:LEU:HB2	1.89	0.54
1:A:573:VAL:HA	1:A:576:MET:HG2	1.88	0.54
1:A:647:TYR:HE1	2:D:640:ILE:HD13	1.72	0.54
1:A:501:MET:SD	1:A:513:ILE:HD11	2.48	0.54
2:B:537:VAL:HG12	2:B:726:ALA:HA	1.89	0.54
2:D:487:LYS:HD2	2:D:686:ASN:HA	1.90	0.54
1:C:407:PRO:HG3	1:C:735:VAL:HA	1.90	0.54
2:D:801:ASN:OD1	2:D:802:GLU:N	2.40	0.54
2:B:154:GLN:O	2:B:158:MET:HG2	2.08	0.54
2:B:553:PHE:HB2	2:B:558:TRP:NE1	2.22	0.54
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.89	0.54
2:D:693:ILE:HG22	2:D:701:HIS:HB2	1.89	0.54
2:B:661:VAL:HG22	2:B:668:LYS:HD3	1.90	0.54
2:D:780:GLN:NE2	2:D:784:ASP:OD2	2.41	0.54
2:B:298:ILE:HD11	2:B:348:LEU:HB3	1.90	0.53
1:A:630:ARG:NH1	2:B:606:TRP:CE3	2.76	0.53
1:C:558:PHE:HE2	2:D:816:MET:HE1	1.72	0.53
2:B:611:LEU:HD11	2:B:634:TRP:HD1	1.72	0.53
1:C:271:LEU:HD23	1:C:273:ASN:H	1.74	0.53
2:D:521:VAL:HG12	2:D:522:VAL:HG13	1.90	0.53
1:A:814:ALA:O	1:A:818:MET:HG2	2.08	0.53
1:A:817:PHE:CZ	2:D:560:MET:HE3	2.43	0.53
2:D:508:ALA:HB3	2:D:763:ALA:HB3	1.91	0.53
2:D:76:ARG:HD3	2:D:77:THR:H	1.74	0.53
1:A:425:THR:OG1	1:A:427:ASN:OD1	2.21	0.53
2:D:39:LEU:HD23	2:D:72:LEU:HB3	1.91	0.53
2:D:560:MET:HA	2:D:563:VAL:HG12	1.89	0.53
2:B:365:VAL:HG11	2:B:390:TRP:HH2	1.74	0.53
1:C:148:SER:HA	1:C:151:TRP:CE3	2.44	0.52
2:B:214:LYS:O	2:B:215:THR:OG1	2.22	0.52
1:C:354:MET:HE2	1:C:354:MET:HA	1.90	0.52
1:C:562:LEU:O	1:C:566:VAL:N	2.37	0.52
1:A:619:ILE:CG2	2:D:628:LYS:CB	2.87	0.52
2:B:486:GLY:HA2	2:B:494:ASN:O	2.09	0.52
2:B:570:ALA:O	2:B:574:PHE:HD2	1.92	0.52
1:C:573:VAL:O	1:C:576:MET:HG3	2.09	0.52
2:D:94:ARG:NH2	2:D:316:ALA:O	2.43	0.52
1:C:697:VAL:HB	2:D:432:ASN:HD22	1.75	0.52
1:C:789:ASP:OD2	1:C:794:ARG:NH2	2.43	0.52
1:A:68:LYS:N	1:A:74:MET:HE1	2.25	0.52
1:A:390:ARG:NH1	1:A:392:TYR:O	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:TRP:HB3	2:B:226:VAL:HG21	1.91	0.52
2:B:496:MET:HE2	2:B:508:ALA:HB1	1.91	0.52
1:C:554:PHE:CE2	1:C:555:MET:HE2	2.45	0.51
1:C:641:MET:HB2	2:D:615:ASN:HD21	1.76	0.51
1:A:615:LEU:CD1	2:D:632:SER:HB2	2.41	0.51
1:A:533:PHE:HA	1:A:780:HIS:NE2	2.25	0.51
1:A:641:MET:SD	2:B:615:ASN:HB2	2.51	0.51
1:C:563:TRP:O	1:C:566:VAL:HG12	2.11	0.51
1:A:148:SER:HA	1:A:151:TRP:CE3	2.46	0.51
1:A:697:VAL:HG12	2:B:431:ARG:HD2	1.93	0.51
2:B:464:LEU:HD22	2:B:509:VAL:HG11	1.93	0.51
1:C:152:PHE:HA	1:C:155:MET:HG2	1.92	0.51
1:C:163:ILE:HG22	1:C:218:VAL:HB	1.91	0.51
2:D:42:HIS:HB2	2:D:75:ASN:HA	1.92	0.51
2:D:304:SER:O	2:D:308:GLU:HG2	2.10	0.51
1:A:511:ASP:OD1	1:A:763:ARG:NH2	2.42	0.50
2:D:286:TYR:CE2	2:D:291:ARG:HG2	2.46	0.50
2:D:536:MET:SD	2:D:746:LEU:HB3	2.50	0.50
1:A:140:THR:O	1:A:346:ARG:NH2	2.40	0.50
1:C:808:LEU:HB2	1:C:813:MET:HE1	1.92	0.50
2:D:226:VAL:HG22	2:D:254:PHE:HB2	1.93	0.50
2:B:576:PHE:HE1	2:B:623:LYS:H	1.59	0.50
1:A:573:VAL:O	1:A:577:LEU:HD23	2.11	0.50
2:B:228:LEU:HD23	2:B:256:ILE:HB	1.93	0.50
1:A:125:MET:O	1:A:139:ARG:NH1	2.40	0.50
1:A:441:ASP:O	1:A:448:ARG:NH1	2.44	0.50
1:A:161:ASN:HA	1:A:187:ARG:HH22	1.77	0.50
1:C:624:PRO:HD2	2:D:606:TRP:HH2	1.77	0.50
1:A:699:LEU:O	1:A:702:MET:HB2	2.11	0.49
2:D:339:VAL:O	2:D:349:SER:OG	2.21	0.49
2:B:532:GLY:O	2:B:731:ALA:N	2.45	0.49
2:D:680:ARG:NH2	2:D:722:GLY:O	2.44	0.49
1:A:680:ILE:HG12	1:A:726:LEU:HD23	1.93	0.49
1:A:814:ALA:HA	1:A:817:PHE:HD2	1.77	0.49
2:D:782:VAL:HG22	2:D:787:MET:HE1	1.94	0.49
1:A:41:MET:SD	1:A:278:SER:OG	2.65	0.49
1:A:427:ASN:ND2	1:A:429:ASP:OD2	2.45	0.49
1:C:254:ILE:HD13	1:C:268:GLY:HA3	1.93	0.49
2:D:127:ILE:HG23	2:D:291:ARG:HB3	1.95	0.49
1:A:375:ASN:HD21	1:A:377:ARG:HG2	1.77	0.49
2:D:326:LYS:HG2	2:D:328:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:MET:HG3	1:C:127:ILE:HG22	1.94	0.49
1:A:649:ALA:HB1	2:B:650:ALA:HB2	1.95	0.49
2:D:540:SER:HB2	2:D:660:GLN:NE2	2.28	0.49
1:A:109:TYR:HB3	2:B:112:MET:HE2	1.95	0.49
1:C:94:HIS:HD2	1:C:122:THR:HG23	1.78	0.48
1:C:620:GLY:O	1:C:621:GLU:HG3	2.13	0.48
1:A:38:HIS:NE2	1:A:277:GLU:OE1	2.46	0.48
2:B:137:ASP:N	2:B:137:ASP:OD1	2.43	0.48
1:C:470:MET:HE2	1:C:771:ASN:HB3	1.95	0.48
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.94	0.48
1:C:95:PRO:HD3	1:C:103:THR:HG21	1.93	0.48
1:C:257:ASN:O	1:C:260:ARG:HG2	2.12	0.48
1:C:354:MET:HG3	1:C:361:LEU:HD22	1.95	0.48
2:D:169:VAL:HA	2:D:199:ASP:HB3	1.95	0.48
2:D:464:LEU:HB2	2:D:509:VAL:HG21	1.95	0.48
2:D:307:LEU:HD21	2:D:313:ILE:HG12	1.94	0.48
2:B:86:VAL:HG11	2:B:116:ILE:HG21	1.96	0.48
1:C:211:ALA:HA	1:C:214:LEU:HD12	1.96	0.48
1:C:144:TYR:O	1:C:147:GLN:HB2	2.13	0.48
2:B:90:MET:HG3	2:B:122:ILE:HD11	1.96	0.48
1:A:104:PRO:HG3	1:A:123:THR:HG21	1.96	0.48
2:B:433:THR:HG22	2:B:457:LYS:HD3	1.95	0.48
2:B:789:GLU:HA	2:B:792:THR:HG22	1.95	0.48
2:D:413:GLU:HG3	2:D:415:PRO:HD2	1.95	0.47
1:A:117:PRO:HA	1:A:136:SER:HB2	1.96	0.47
2:B:377:LYS:NZ	2:B:379:GLU:OE1	2.42	0.47
1:C:822:GLY:HA2	1:C:825:VAL:HG12	1.96	0.47
2:B:282:ASP:OD1	2:B:282:ASP:N	2.47	0.47
2:D:306:MET:HE3	2:D:332:HIS:ND1	2.30	0.47
2:B:676:SER:OG	2:B:677:PRO:HD3	2.14	0.47
1:C:502:MET:HE1	1:C:527:ILE:HD13	1.95	0.47
1:C:522:GLU:OE2	1:C:522:GLU:N	2.46	0.47
2:B:460:CYS:HB3	2:B:509:VAL:HG22	1.96	0.47
1:C:533:PHE:HA	1:C:780:HIS:NE2	2.29	0.47
2:D:47:THR:O	2:D:51:LEU:HG	2.14	0.47
2:D:294:ASP:O	2:D:298:ILE:HG12	2.15	0.47
2:D:676:SER:OG	2:D:677:PRO:HD3	2.15	0.47
2:B:76:ARG:HH12	2:B:104:THR:HB	1.79	0.47
1:C:558:PHE:HB2	1:C:563:TRP:CH2	2.50	0.47
2:B:649:LEU:O	2:B:653:ILE:HG12	2.15	0.47
1:C:413:PRO:HA	1:C:453:GLN:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HD12	1:A:514:VAL:HG21	1.96	0.46
1:A:695:ARG:HH12	2:D:783:GLY:HA3	1.80	0.46
2:D:419:VAL:HG21	2:D:479:LEU:HD21	1.97	0.46
1:A:741:SER:HB3	1:A:796:GLN:HB3	1.98	0.46
2:B:130:GLY:H	2:B:133:MET:HE1	1.81	0.46
2:D:75:ASN:OD1	2:D:76:ARG:N	2.48	0.46
1:A:99:ASN:HD22	1:A:101:HIS:CE1	2.33	0.46
1:A:619:ILE:HD11	2:D:631:VAL:HG12	1.97	0.46
1:C:68:LYS:N	1:C:74:MET:HE3	2.30	0.46
1:C:701:THR:HA	1:C:704:ARG:NH1	2.31	0.46
2:D:133:MET:O	2:D:146:GLN:NE2	2.40	0.46
1:A:164:ILE:HG13	1:A:193:LYS:HB3	1.98	0.46
1:C:330:TYR:O	1:C:337:ARG:NH2	2.48	0.46
2:B:341:VAL:HG22	2:B:349:SER:HA	1.98	0.46
2:B:442:ILE:HG22	2:B:443:ASN:HD22	1.81	0.46
1:A:538:LEU:HG	1:A:754:PHE:HD2	1.81	0.46
2:D:497:ILE:HD11	2:D:512:LEU:HD21	1.97	0.46
1:A:235:ALA:HB1	1:A:240:MET:HB3	1.98	0.46
2:B:829:LEU:HA	2:B:832:ILE:HG12	1.98	0.46
1:C:570:VAL:HG23	1:C:610:SER:HB2	1.97	0.46
1:C:667:ILE:O	1:C:673:ARG:NH2	2.42	0.46
1:C:664:ILE:O	1:C:749:THR:OG1	2.25	0.46
1:C:762:MET:HE1	1:C:769:LYS:HA	1.98	0.46
2:D:40:LEU:O	2:D:73:LEU:HA	2.16	0.46
2:B:772:ARG:HH12	1:C:764:LYS:HZ2	1.62	0.46
1:C:357:GLN:O	1:C:360:LYS:N	2.44	0.46
1:C:632:LEU:HA	1:C:635:VAL:HG12	1.98	0.46
1:A:626:SER:O	1:A:630:ARG:HG2	2.16	0.45
1:A:652:ALA:HA	2:D:647:ALA:HB1	1.97	0.45
2:B:635:ALA:HB3	1:C:615:LEU:HD13	1.98	0.45
2:D:157:VAL:HG13	2:D:279:VAL:HG11	1.97	0.45
2:B:611:LEU:HD11	2:B:634:TRP:CD1	2.51	0.45
2:B:661:VAL:HG11	2:B:669:PHE:CE2	2.51	0.45
2:D:204:ILE:HD12	2:D:218:GLN:HB3	1.98	0.45
2:D:288:LEU:HA	2:D:291:ARG:HD2	1.98	0.45
2:D:415:PRO:HB3	2:D:736:TYR:CG	2.52	0.45
1:C:58:ILE:HG21	1:C:296:LEU:HD13	1.98	0.45
1:C:312:THR:HG21	2:D:76:ARG:HG2	1.98	0.45
2:D:35:ASN:HB2	2:D:95:ILE:HA	1.98	0.45
2:D:682:GLY:HA2	2:D:704:MET:HG3	1.99	0.45
2:B:600:THR:HG22	2:B:602:GLY:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:675:TYR:HB3	2:B:677:PRO:HD2	1.98	0.45
2:D:437:ARG:HG3	2:D:478:TYR:HB2	1.97	0.45
2:D:507:MET:HE2	2:D:764:LEU:HD21	1.99	0.45
1:C:195:LEU:HD11	1:C:211:ALA:HB2	1.99	0.45
2:D:713:GLU:O	2:D:717:VAL:HG22	2.17	0.45
1:C:142:PRO:HD2	1:C:271:LEU:HD11	1.99	0.45
1:A:602:THR:N	1:A:605:SER:OG	2.37	0.45
1:A:675:PRO:HB3	1:A:705:HIS:ND1	2.32	0.45
1:A:695:ARG:NH1	2:D:783:GLY:HA3	2.31	0.45
2:B:191:VAL:HG13	2:B:198:TRP:HB2	1.99	0.45
2:B:538:SER:HA	2:B:746:LEU:HD23	1.98	0.45
1:A:669:ASP:HB3	1:A:672:LEU:HB3	1.99	0.44
2:B:639:VAL:HA	2:B:642:LEU:HG	1.99	0.44
2:B:791:GLU:O	2:B:795:LEU:N	2.48	0.44
2:D:272:PHE:O	2:D:370:ARG:NH1	2.45	0.44
2:D:421:ASP:OD1	2:D:454:LYS:NZ	2.50	0.44
2:D:572:ALA:HB2	2:D:630:MET:HE1	1.98	0.44
1:A:510:ALA:O	1:A:763:ARG:NH2	2.44	0.44
2:B:89:LEU:HB3	2:B:95:ILE:HD13	1.99	0.44
2:B:246:LEU:HD12	2:D:220:LYS:HB3	1.98	0.44
1:C:102:PHE:HB3	1:C:105:THR:OG1	2.18	0.44
1:C:477:HIS:ND1	1:C:478:LEU:O	2.50	0.44
2:D:100:PHE:HE1	2:D:102:ASP:HB2	1.83	0.44
2:D:298:ILE:HD11	2:D:348:LEU:HD13	1.99	0.44
2:B:172:LEU:HD11	2:B:183:PHE:HE2	1.81	0.44
2:B:306:MET:HE2	2:B:313:ILE:HG22	1.98	0.44
2:D:259:SER:HB2	2:D:280:SER:HA	1.99	0.44
2:D:422:ILE:HD12	2:D:422:ILE:H	1.83	0.44
1:A:42:PHE:CE2	1:A:62:ALA:HB1	2.52	0.44
1:A:611:TRP:HA	1:A:614:LEU:HG	2.00	0.44
1:C:500:GLY:O	1:C:504:GLU:HG2	2.17	0.44
2:D:210:PHE:O	2:D:215:THR:OG1	2.35	0.44
1:A:39:GLU:HA	1:A:42:PHE:HB3	2.00	0.44
1:A:72:ILE:HD13	2:B:115:PHE:CE2	2.53	0.44
1:A:248:LEU:HD23	1:A:267:ILE:HB	1.98	0.44
2:B:831:LEU:HD23	2:B:831:LEU:HA	1.88	0.44
1:C:541:LEU:HD11	1:C:746:LEU:HB3	1.99	0.44
1:C:680:ILE:HD11	1:C:709:HIS:CG	2.53	0.44
2:D:737:LYS:HA	2:D:737:LYS:HD3	1.83	0.44
2:B:59:GLN:O	2:B:61:THR:HG23	2.18	0.44
2:B:334:LEU:HB3	2:B:338:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG13	1:C:88:TYR:CD1	2.53	0.44
1:C:303:ASP:OD1	1:C:303:ASP:N	2.50	0.44
1:A:615:LEU:CD2	2:D:636:PHE:HB2	2.48	0.44
1:A:784:PHE:CZ	1:A:788:LEU:HD21	2.53	0.44
1:A:829:PHE:O	1:A:833:ILE:HG12	2.17	0.44
2:B:683:THR:OG1	2:B:728:ILE:O	2.29	0.44
1:C:41:MET:O	1:C:44:GLU:HG3	2.18	0.44
1:C:165:LEU:HD11	1:C:180:LEU:HD23	1.98	0.44
2:D:708:ASN:OD1	2:D:709:GLN:N	2.51	0.44
1:C:817:PHE:HA	1:C:820:VAL:HG12	2.00	0.44
2:D:778:LEU:O	2:D:782:VAL:HG23	2.18	0.44
1:A:828:ILE:O	1:A:831:ILE:HG22	2.18	0.43
1:C:35:THR:O	1:C:38:HIS:HB2	2.18	0.43
1:C:319:PRO:C	1:C:323:ARG:HE	2.25	0.43
1:C:613:VAL:HG11	1:C:636:TRP:CD1	2.53	0.43
2:D:282:ASP:OD1	2:D:282:ASP:N	2.51	0.43
1:A:548:ARG:HE	1:A:549:SER:H	1.66	0.43
2:B:286:TYR:CE2	2:B:291:ARG:HG3	2.53	0.43
2:B:514:ILE:HD11	2:B:761:GLY:HA3	2.01	0.43
1:A:163:ILE:HA	1:A:218:VAL:HG23	2.00	0.43
1:A:639:PHE:CD1	2:B:823:LEU:HD22	2.53	0.43
1:A:669:ASP:O	1:A:673:ARG:N	2.43	0.43
2:B:408:ILE:HG23	2:B:507:MET:HG3	2.00	0.43
1:A:121:LEU:HD21	1:A:284:ALA:HB2	2.00	0.43
1:A:813:MET:O	1:A:813:MET:HG2	2.19	0.43
1:C:162:HIS:HB3	1:C:216:ALA:HB2	1.99	0.43
1:A:608:TRP:CH2	2:D:629:ILE:CG1	3.01	0.43
2:D:729:TYR:HB3	2:D:734:LEU:CD2	2.49	0.43
2:D:787:MET:HA	2:D:790:LEU:HB2	2.01	0.43
2:B:410:THR:HA	2:B:496:MET:HE3	1.99	0.43
1:C:35:THR:OG1	1:C:38:HIS:ND1	2.49	0.43
1:C:99:ASN:HB2	1:C:101:HIS:CD2	2.53	0.43
2:B:611:LEU:HD13	2:B:635:ALA:HB2	2.00	0.43
1:C:42:PHE:CE2	1:C:62:ALA:HB1	2.53	0.43
1:A:198:ASP:OD1	1:A:198:ASP:N	2.51	0.43
1:A:304:PRO:HG3	1:A:315:TRP:CZ2	2.53	0.43
1:A:609:PHE:O	1:A:613:VAL:HG22	2.19	0.43
1:A:790:LYS:HD3	1:A:790:LYS:HA	1.79	0.43
2:B:772:ARG:O	2:B:776:LEU:HD23	2.18	0.43
1:C:217:ARG:HD2	1:C:245:TYR:CZ	2.53	0.43
1:C:639:PHE:HZ	2:D:822:MET:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:THR:OG1	1:A:415:MET:N	2.51	0.43
1:A:816:VAL:HA	1:A:819:LEU:HG	2.00	0.43
2:B:204:ILE:HD13	2:B:222:ILE:HD11	2.00	0.43
2:B:274:SER:HB2	2:B:394:LYS:O	2.19	0.43
2:B:422:ILE:HD12	2:B:422:ILE:H	1.84	0.43
1:C:825:VAL:O	1:C:828:ILE:HG22	2.18	0.43
2:D:235:GLU:O	2:D:239:ILE:HG12	2.19	0.43
2:D:561:MET:HA	2:D:564:MET:HG2	2.01	0.43
1:A:519:ILE:HD12	1:A:529:PHE:CD2	2.54	0.43
2:B:782:VAL:HG22	2:B:787:MET:HG3	2.00	0.43
1:A:696:GLN:OE1	1:A:699:LEU:N	2.44	0.42
2:B:780:GLN:HB2	1:C:521:ASN:ND2	2.34	0.42
1:C:628:SER:HA	1:C:631:ILE:HG12	2.01	0.42
2:D:94:ARG:HH12	2:D:318:ALA:HA	1.84	0.42
1:A:351:TYR:HB2	1:A:367:TYR:HB3	2.01	0.42
1:A:641:MET:HE3	1:A:641:MET:HB3	1.91	0.42
2:D:63:LEU:HB2	2:D:64:PRO:HD3	2.01	0.42
2:D:507:MET:HE1	2:D:774:ILE:HD11	2.01	0.42
1:A:70:ASN:HD21	1:A:73:GLN:HG3	1.84	0.42
1:C:31:ALA:O	1:C:64:SER:HA	2.20	0.42
1:C:514:VAL:O	1:C:514:VAL:HG23	2.19	0.42
2:D:76:ARG:HA	2:D:76:ARG:NE	2.35	0.42
2:B:667:LYS:HA	2:B:667:LYS:HD3	1.71	0.42
2:B:740:ARG:NH1	2:B:794:TRP:O	2.52	0.42
2:B:816:MET:HA	2:B:816:MET:HE2	2.00	0.42
1:C:632:LEU:HD11	2:D:830:SER:HB3	2.01	0.42
1:C:699:LEU:O	1:C:702:MET:HG2	2.19	0.42
2:D:208:THR:OG1	2:D:209:SER:N	2.49	0.42
1:A:364:VAL:HG11	1:A:379:ILE:HD13	2.02	0.42
1:A:540:ILE:HD13	1:A:750:GLY:HA3	2.00	0.42
2:B:601:ILE:O	2:B:605:ILE:HG13	2.20	0.42
1:C:506:LEU:HD23	1:C:506:LEU:HA	1.87	0.42
1:A:249:VAL:HB	1:A:253:GLU:HB2	2.01	0.42
1:A:504:GLU:OE1	1:A:509:GLN:HB3	2.20	0.42
1:A:816:VAL:O	1:A:819:LEU:HG	2.18	0.42
2:B:158:MET:HE1	2:B:257:VAL:C	2.45	0.42
2:B:162:MET:HE3	2:B:162:MET:HB2	1.97	0.42
2:B:523:ASP:OD2	2:B:771:LYS:HD2	2.19	0.42
2:B:682:GLY:HA2	2:B:704:MET:HG2	2.02	0.42
2:D:493:TRP:NE1	2:D:521:VAL:HG21	2.35	0.42
2:D:573:VAL:HG21	2:D:601:ILE:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:OE2	1:A:225:GLU:N	2.50	0.42
1:A:617:SER:HB3	2:D:635:ALA:CB	2.50	0.42
1:C:58:ILE:HD11	1:C:293:HIS:CD2	2.54	0.42
1:C:108:SER:OG	1:C:134:HIS:ND1	2.42	0.42
1:C:240:MET:HE2	1:C:240:MET:HA	2.01	0.42
1:C:666:GLY:HA3	1:C:751:GLU:HG3	2.01	0.42
2:D:230:TYR:HD1	2:D:258:PRO:HG3	1.85	0.42
1:A:569:SER:HA	1:A:572:VAL:HG12	2.01	0.42
1:A:812:ASN:HD22	1:A:812:ASN:C	2.27	0.42
1:C:41:MET:HA	1:C:44:GLU:HG3	2.02	0.42
1:C:762:MET:CE	1:C:769:LYS:HA	2.50	0.42
2:D:104:THR:HG23	2:D:106:GLN:H	1.85	0.42
1:A:36:ARG:HA	1:A:39:GLU:CD	2.45	0.42
2:B:608:LEU:HD12	2:B:634:TRP:NE1	2.35	0.42
1:C:128:TYR:HB2	1:C:139:ARG:NH2	2.35	0.42
2:B:533:ILE:HG13	2:B:692:ASN:HD22	1.84	0.41
1:C:536:GLN:HB2	1:C:733:SER:HB3	2.02	0.41
1:A:615:LEU:HD22	2:D:636:PHE:HB2	2.03	0.41
1:A:701:THR:O	1:A:704:ARG:HB2	2.20	0.41
2:D:37:ALA:HB1	2:D:89:LEU:HD23	2.02	0.41
1:A:91:LEU:HD11	1:A:119:LEU:HD12	2.02	0.41
1:A:411:VAL:HG12	1:A:455:CYS:SG	2.59	0.41
1:A:619:ILE:HG23	2:D:628:LYS:HG2	2.01	0.41
1:C:613:VAL:HG13	1:C:637:ALA:HA	2.03	0.41
2:D:59:GLN:OE1	2:D:59:GLN:N	2.54	0.41
2:D:408:ILE:HG12	2:D:507:MET:HG2	2.03	0.41
2:D:615:ASN:HB2	2:D:617:VAL:HG13	2.02	0.41
2:B:165:TYR:CZ	2:B:385:LEU:HD13	2.56	0.41
2:D:568:VAL:HG12	2:D:608:LEU:HD21	2.02	0.41
1:A:670:PRO:HB2	2:B:798:ILE:HG12	2.02	0.41
2:B:788:GLU:HA	2:B:791:GLU:HG3	2.03	0.41
1:C:125:MET:HB3	1:C:128:TYR:HE2	1.86	0.41
2:D:493:TRP:HE1	2:D:521:VAL:HG21	1.85	0.41
1:A:608:TRP:HE1	2:D:625:THR:HG23	1.84	0.41
2:B:407:SER:OG	2:B:505:ALA:HA	2.21	0.41
1:C:748:THR:OG1	1:C:749:THR:N	2.53	0.41
2:D:630:MET:SD	2:D:631:VAL:HG23	2.61	0.41
2:B:426:THR:HG22	2:B:428:THR:HG22	2.03	0.41
1:C:400:ILE:HD13	1:C:512:MET:HB3	2.02	0.41
1:C:558:PHE:CE2	2:D:816:MET:HE1	2.54	0.41
1:C:657:LEU:HB2	1:C:659:ARG:HE	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:ASP:OD1	1:C:745:ASP:N	2.52	0.41
1:A:240:MET:HE2	1:A:240:MET:HA	2.02	0.41
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.89	0.41
1:A:537:GLY:O	1:A:733:SER:N	2.54	0.41
2:B:143:THR:HG22	2:B:335:HIS:CE1	2.56	0.41
2:B:764:LEU:HD11	2:B:774:ILE:HD12	2.03	0.41
1:C:489:ARG:HB2	2:D:195:PHE:CE2	2.56	0.41
2:D:48:GLU:HG2	2:D:71:ALA:HB3	2.03	0.41
2:D:531:THR:HG21	2:D:760:TYR:CE2	2.56	0.41
1:A:124:ARG:HB2	1:A:144:TYR:CZ	2.56	0.41
1:C:31:ALA:HB1	1:C:33:LEU:HD23	2.02	0.41
2:D:34:LEU:HB2	2:D:65:LEU:HD12	2.02	0.41
2:D:576:PHE:HE1	2:D:623:LYS:H	1.69	0.41
1:A:602:THR:H	1:A:605:SER:HG	1.60	0.40
2:B:788:GLU:O	2:B:791:GLU:HG3	2.20	0.40
2:D:659:ASP:OD1	2:D:659:ASP:N	2.53	0.40
1:A:627:PHE:O	1:A:631:ILE:HG12	2.21	0.40
2:B:415:PRO:HB3	2:B:736:TYR:CG	2.56	0.40
2:B:661:VAL:HG11	2:B:669:PHE:HE2	1.86	0.40
2:B:739:GLY:HA3	2:B:797:GLY:HA3	2.04	0.40
1:C:539:THR:HG23	1:C:736:LEU:HD12	2.04	0.40
1:C:576:MET:O	1:C:580:LEU:HG	2.20	0.40
1:A:615:LEU:HD13	2:D:632:SER:HB2	2.04	0.40
2:B:244:ARG:HD2	2:B:396:PHE:CE1	2.57	0.40
1:C:79:CYS:HB3	1:C:308:CYS:HB3	2.03	0.40
1:C:491:ASN:OD1	1:C:492:ASN:N	2.55	0.40
2:B:497:ILE:HD11	2:B:512:LEU:HD21	2.03	0.40
1:C:731:TRP:CG	1:C:732:ASP:H	2.39	0.40
2:D:557:VAL:HG12	2:D:561:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	791/1108 (71%)	772 (98%)	19 (2%)	0	100	100
1	C	789/1108 (71%)	765 (97%)	24 (3%)	0	100	100
2	B	781/1126 (69%)	748 (96%)	33 (4%)	0	100	100
2	D	781/1126 (69%)	747 (96%)	34 (4%)	0	100	100
All	All	3142/4468 (70%)	3032 (96%)	110 (4%)	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	686/956 (72%)	686 (100%)	0	100	100
1	C	685/956 (72%)	685 (100%)	0	100	100
2	B	689/977 (70%)	689 (100%)	0	100	100
2	D	689/977 (70%)	689 (100%)	0	100	100
All	All	2749/3866 (71%)	2749 (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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	47	ASN
1	A	59	GLN
1	A	99	ASN
1	A	616	ASN
1	A	709	HIS
2	B	381	GLN
2	B	387	HIS
2	B	670	GLN
2	B	765	GLN

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Mol	Chain	Res	Type
2	B	810	GLN
1	C	742	GLN
2	D	42	HIS
2	D	44	HIS
2	D	68	ASN
2	D	323	GLN
2	D	356	GLN
2	D	621	ASN
2	D	686	ASN
2	D	696	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

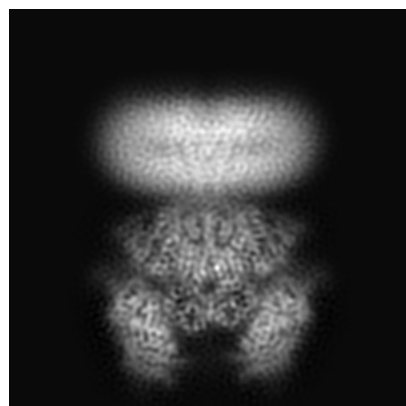
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45284. These allow visual inspection of the internal detail of the map and identification of artifacts.

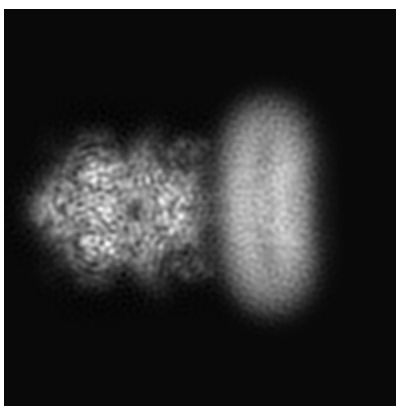
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

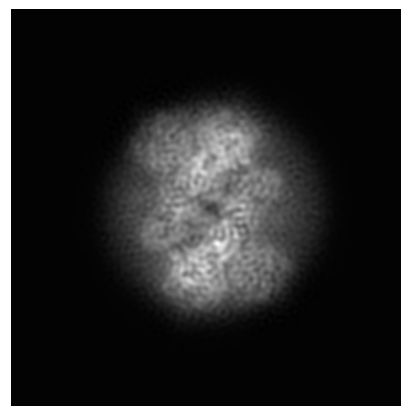
6.1.1 Primary map



X

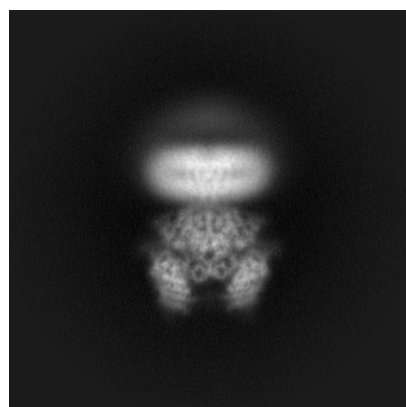


Y

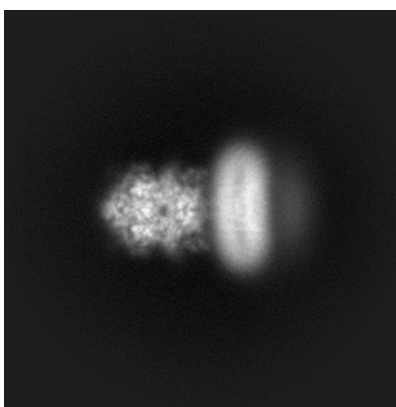


Z

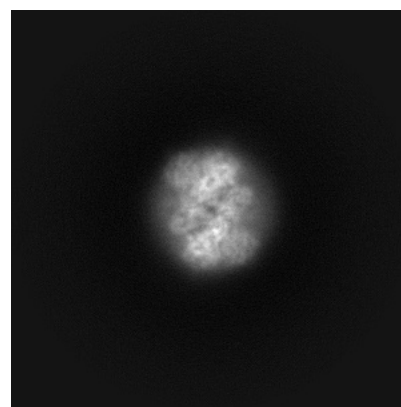
6.1.2 Raw map



X



Y

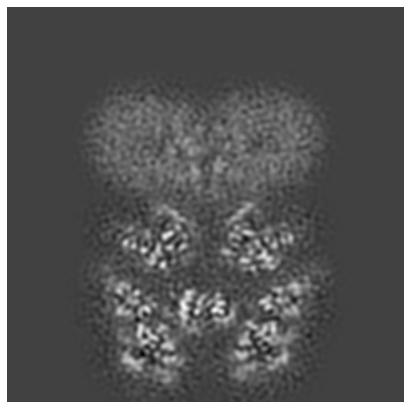


Z

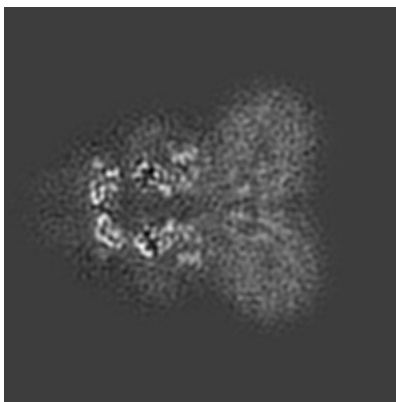
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

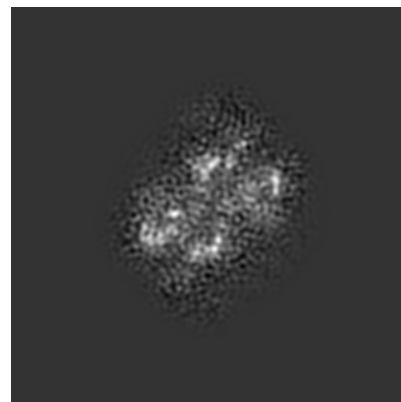
6.2.1 Primary map



X Index: 150

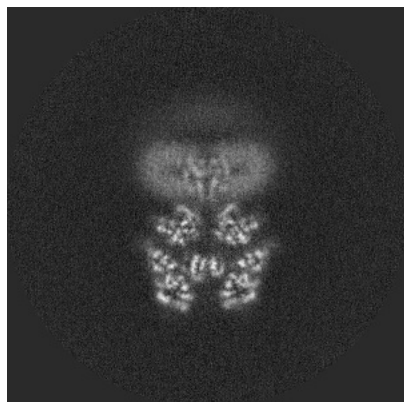


Y Index: 150

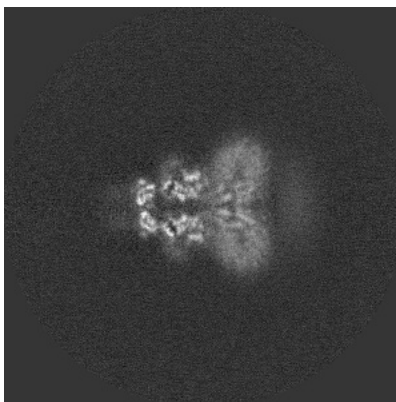


Z Index: 150

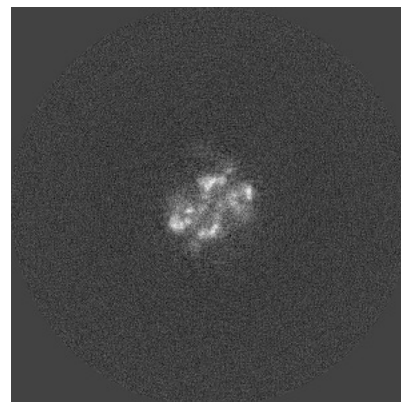
6.2.2 Raw map



X Index: 256



Y Index: 256

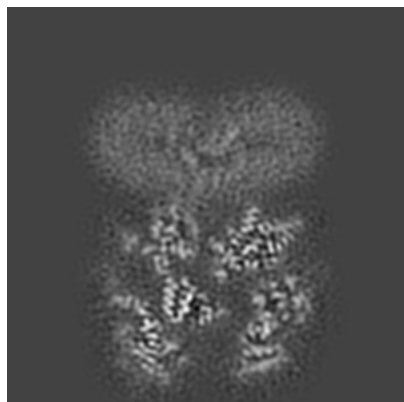


Z Index: 256

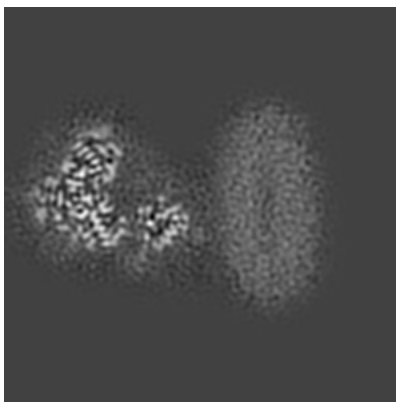
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

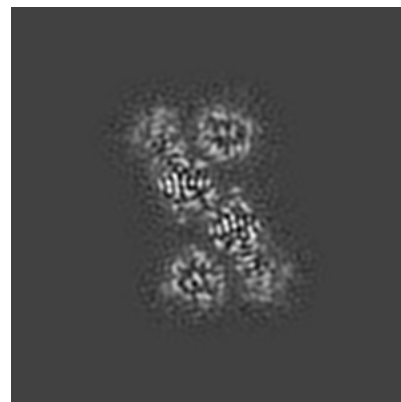
6.3.1 Primary map



X Index: 156

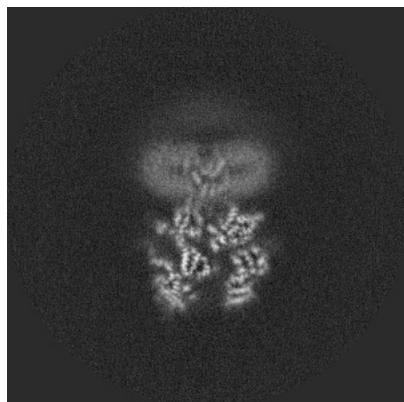


Y Index: 105

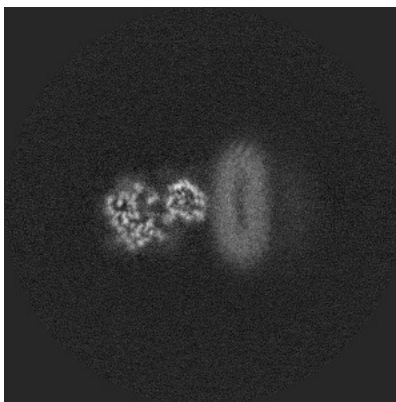


Z Index: 78

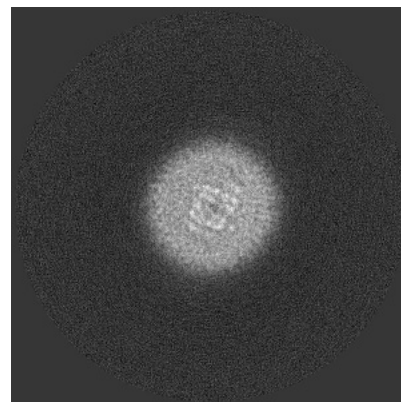
6.3.2 Raw map



X Index: 263



Y Index: 291

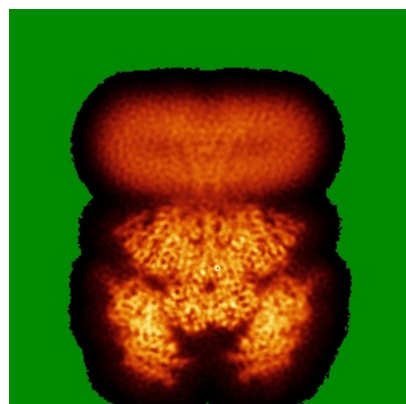


Z Index: 314

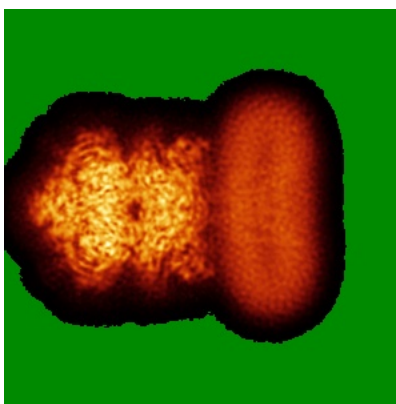
The images above show the largest variance slices of the map in three orthogonal directions.

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

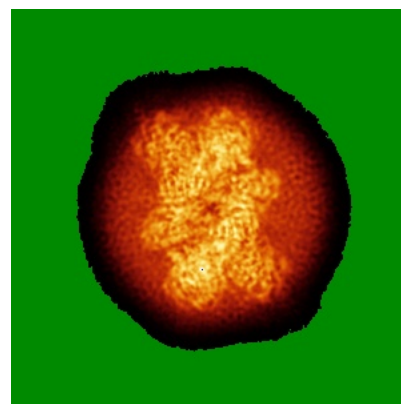
6.4.1 Primary map



X

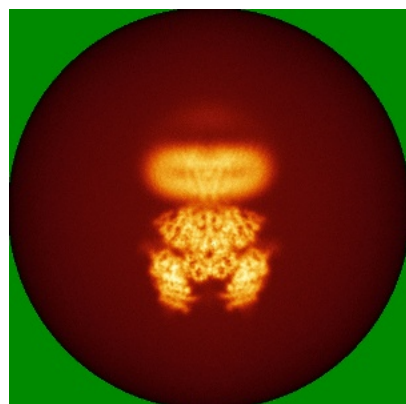


Y

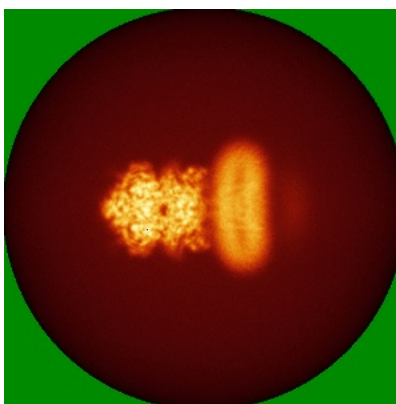


Z

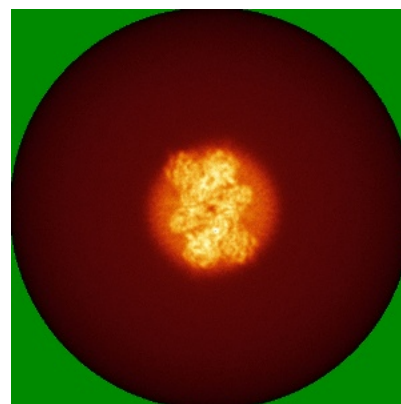
6.4.2 Raw map



X



Y

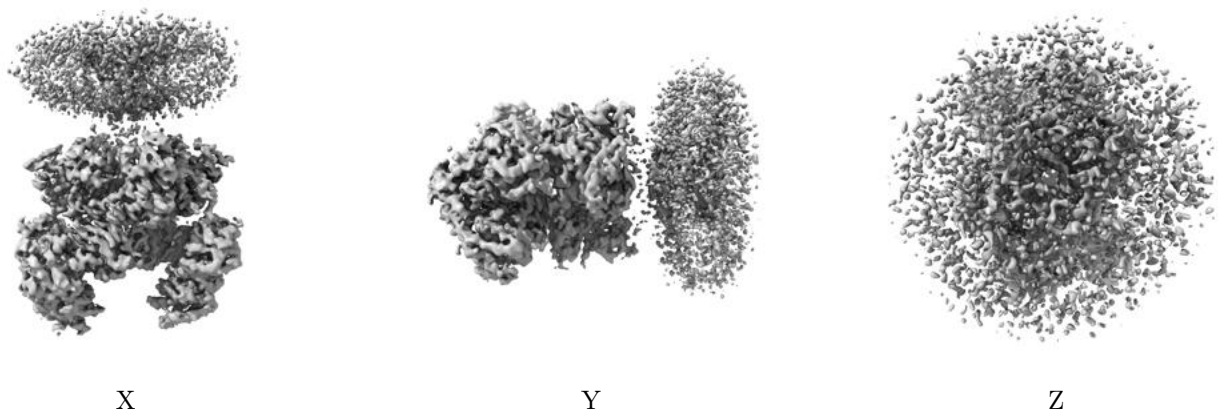


Z

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 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

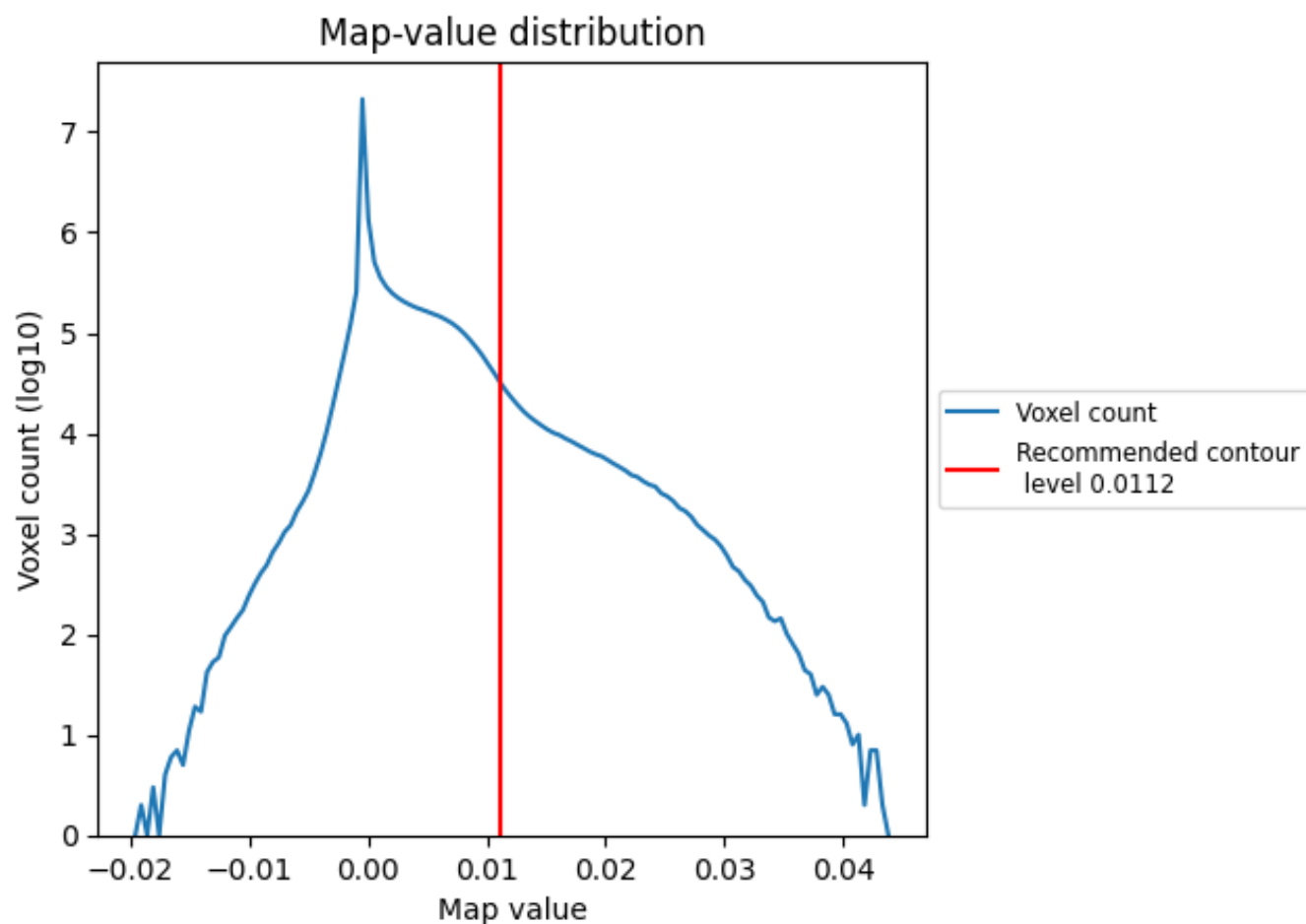
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

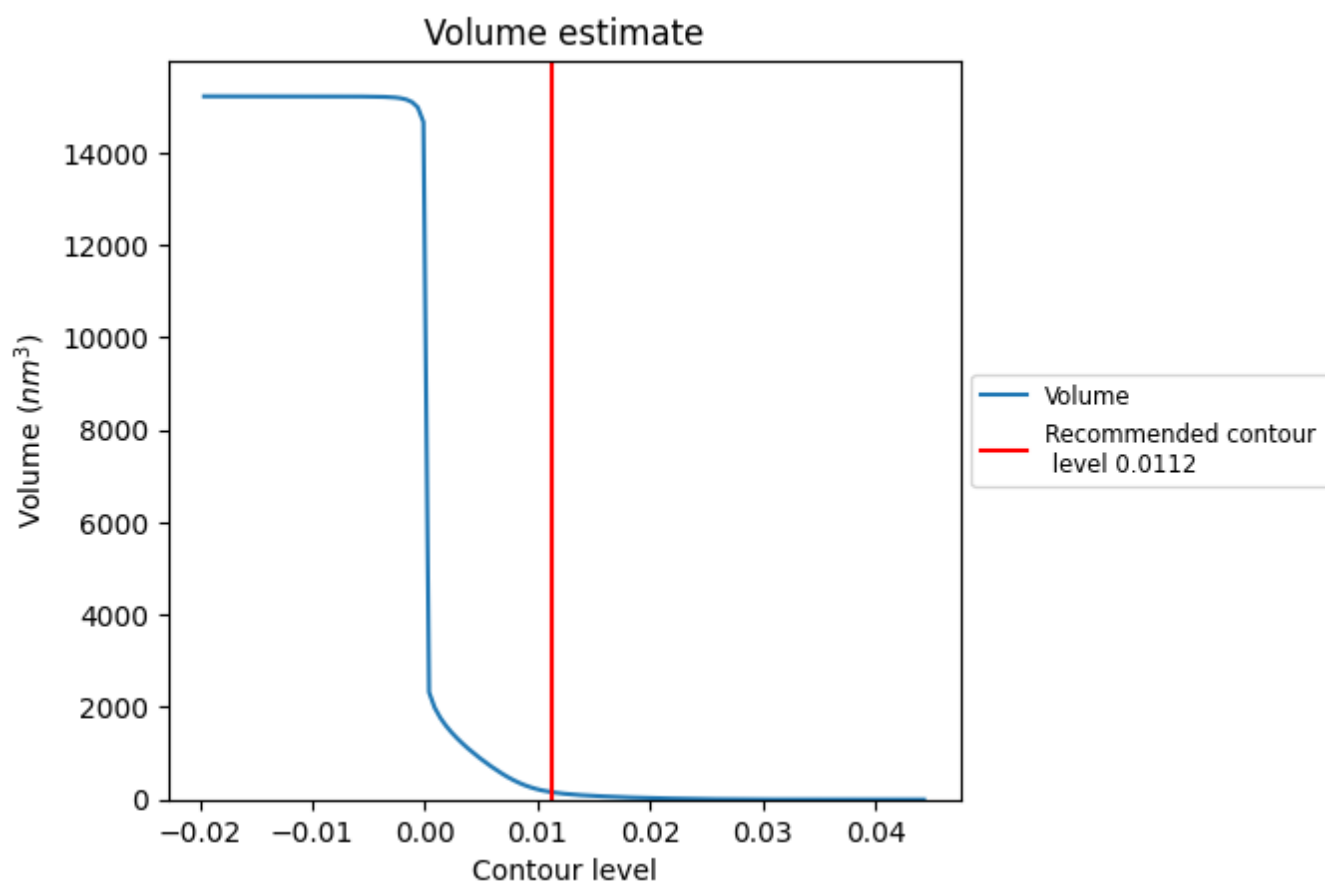
This section contains the results of statistical analysis of the map.

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.

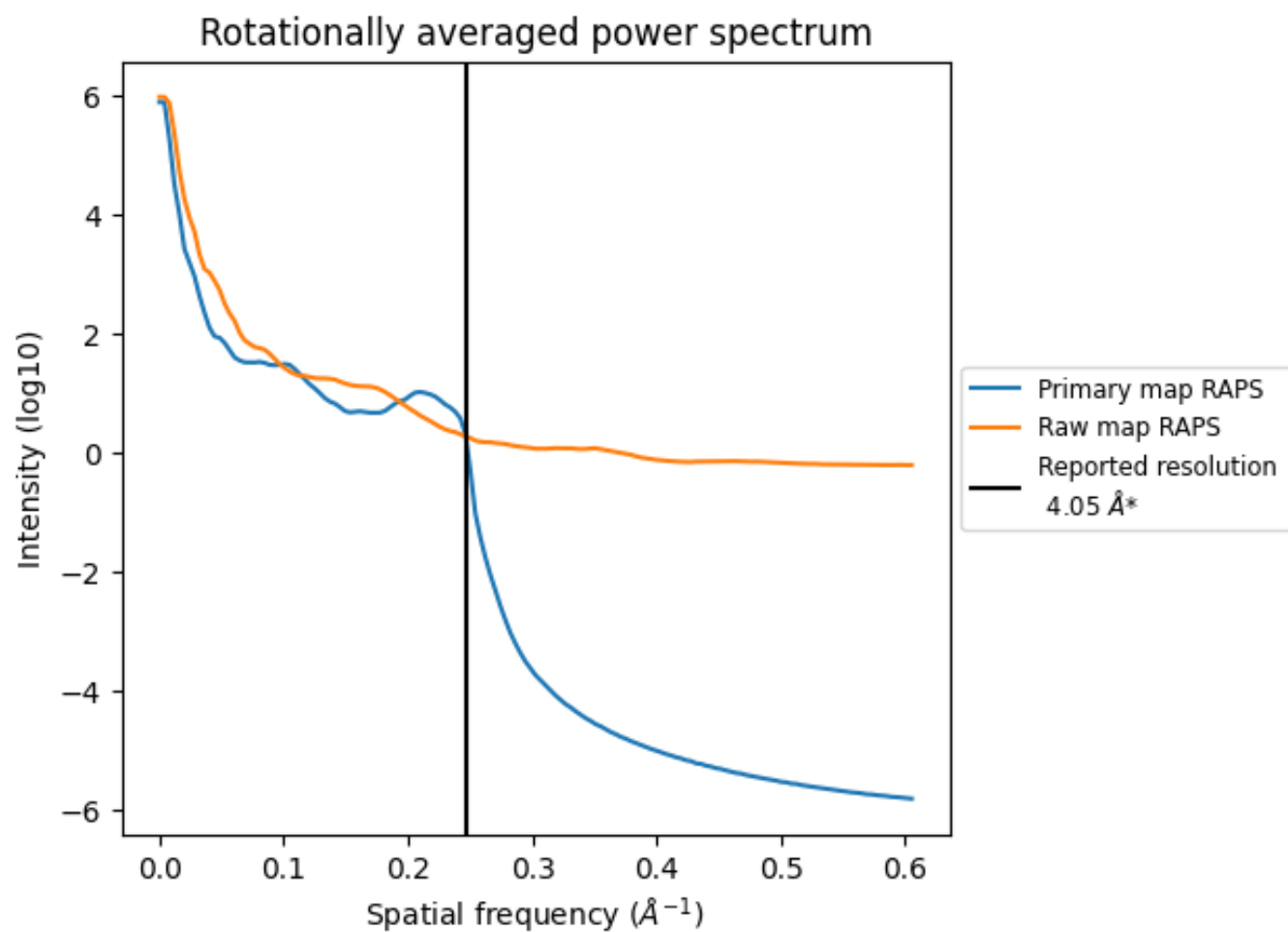
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; this corresponds to an approximate mass of 147 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 ⓘ

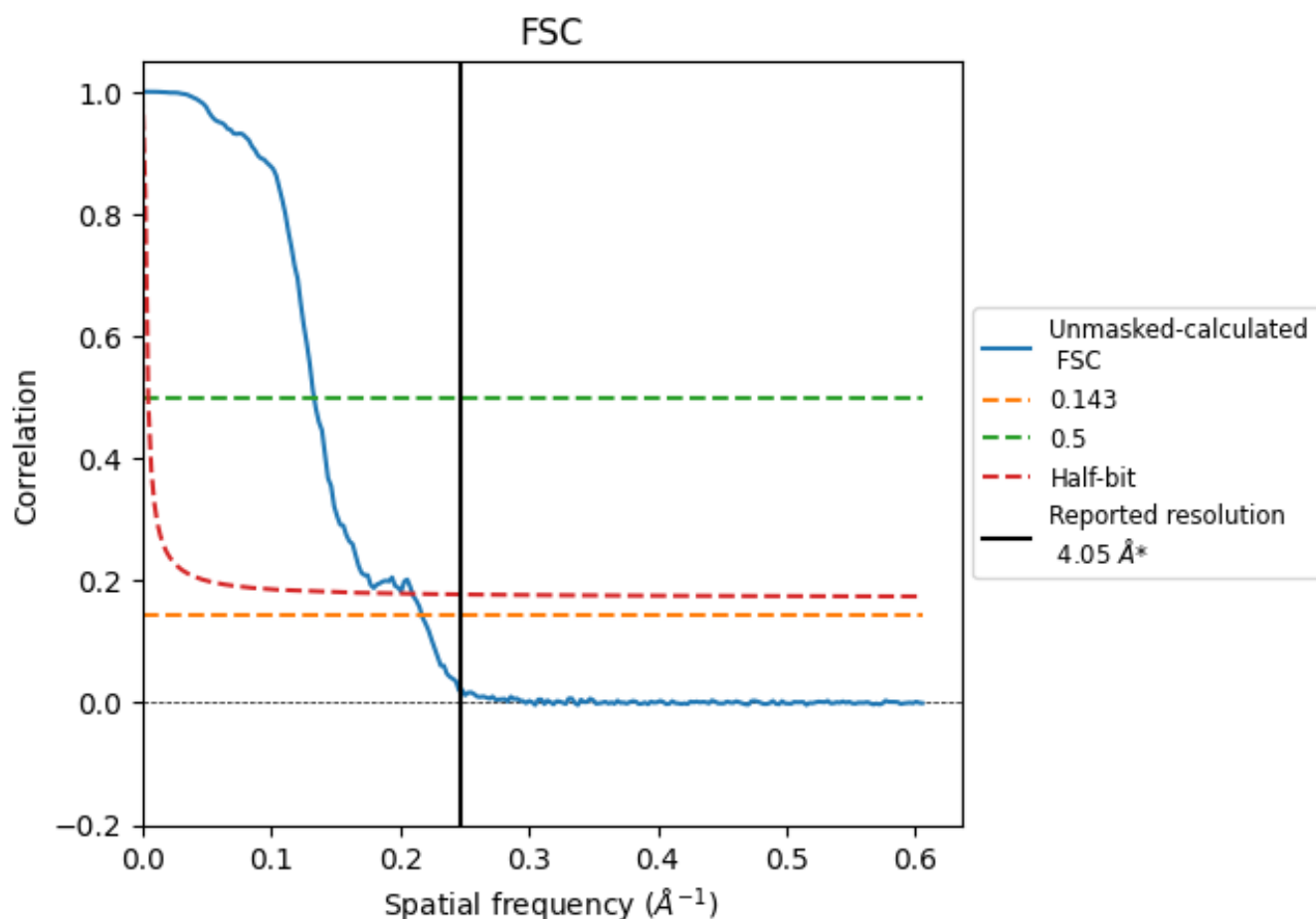


*Reported resolution corresponds to spatial frequency of 0.247 \AA^{-1}

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 0.247 \AA^{-1}

8.2 Resolution estimates [i](#)

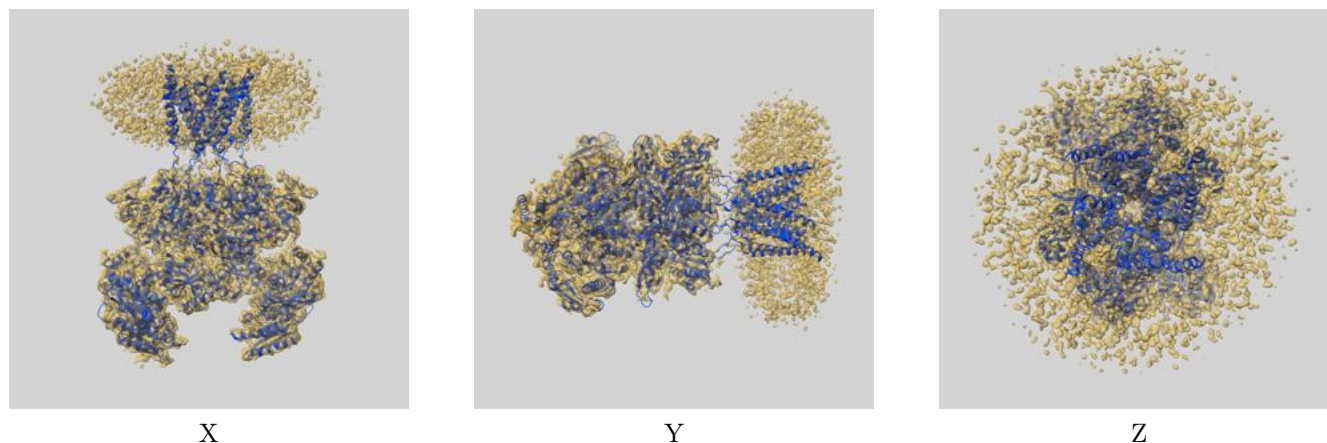
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.61	7.50	4.77

*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 4.61 differs from the reported value 4.05 by more than 10 %

9 Map-model fit [i](#)

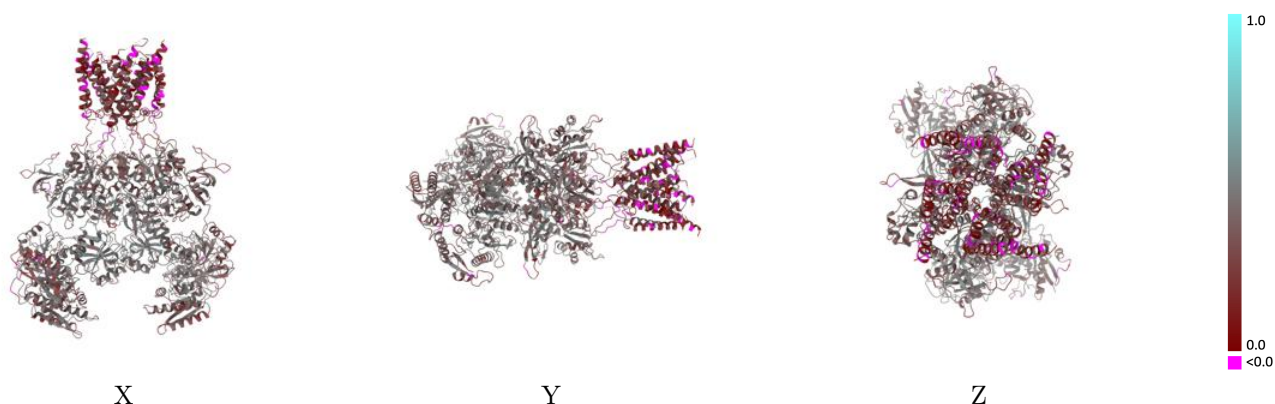
This section contains information regarding the fit between EMDB map EMD-45284 and PDB model 9C7Q. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



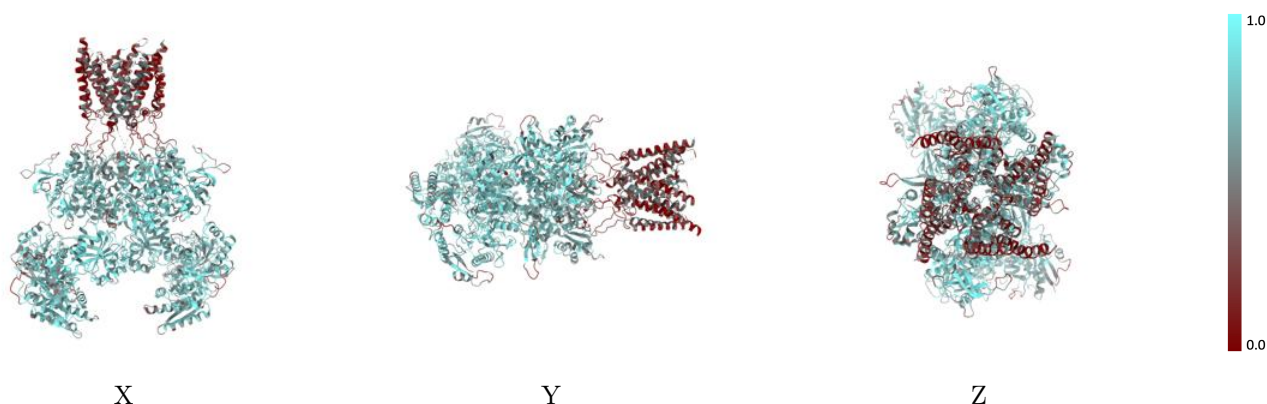
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



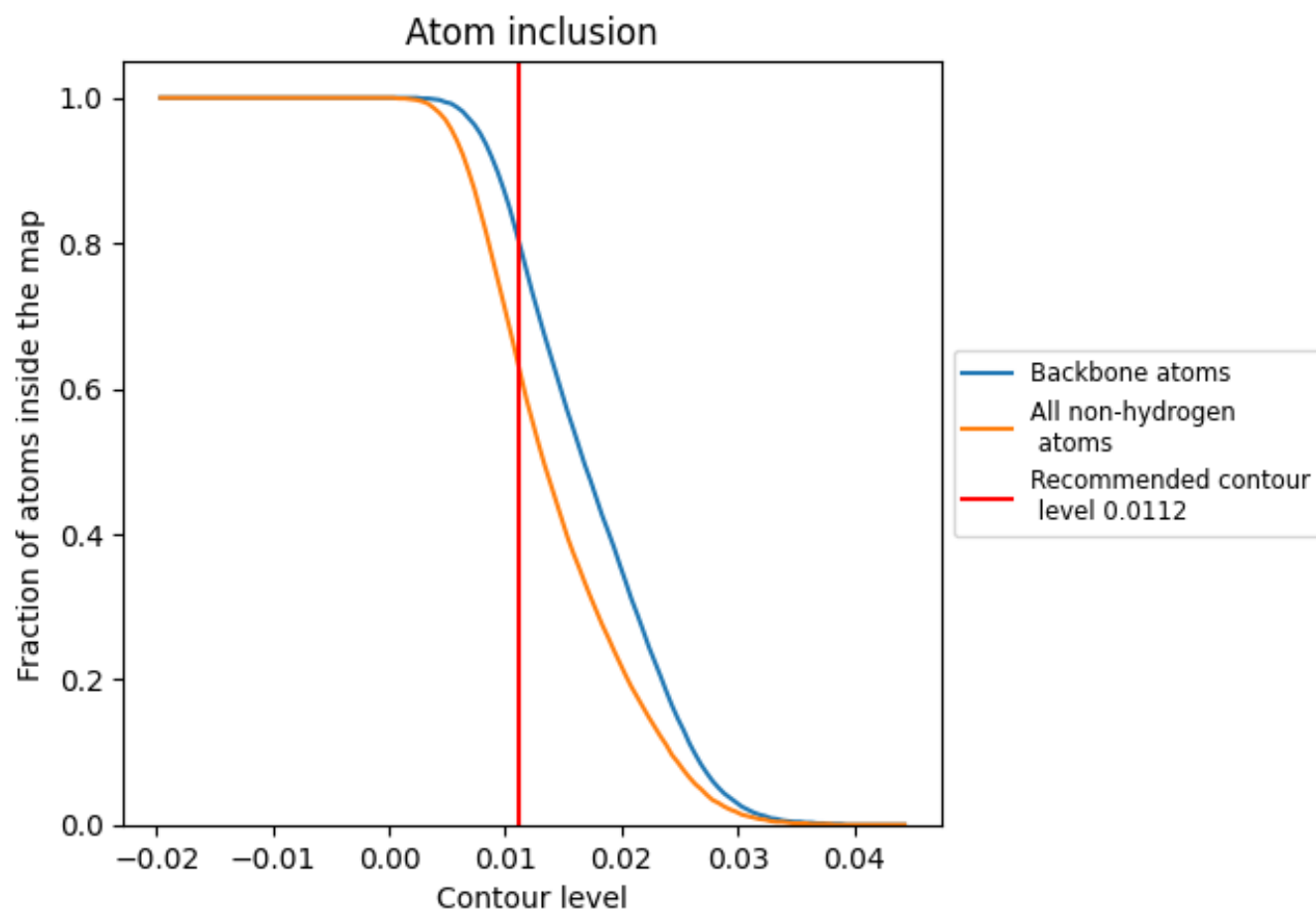
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0112).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 63% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6280	<div></div> 0.3660
A	<div></div> 0.6170	<div></div> 0.3420
B	<div></div> 0.6160	<div></div> 0.3690
C	<div></div> 0.6490	<div></div> 0.3760
D	<div></div> 0.6290	<div></div> 0.3770

