



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:24 PM UTC

PDB ID : 9CL1 / pdb_00009cl1
EMDB ID : EMD-45658
Title : Particulate methane monooxygenase in 0.02% DDM
Authors : Tucci, F.J.; Rosenzweig, A.C.
Deposited on : 2024-07-10
Resolution : 2.89 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

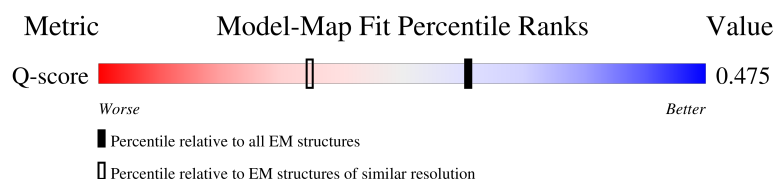
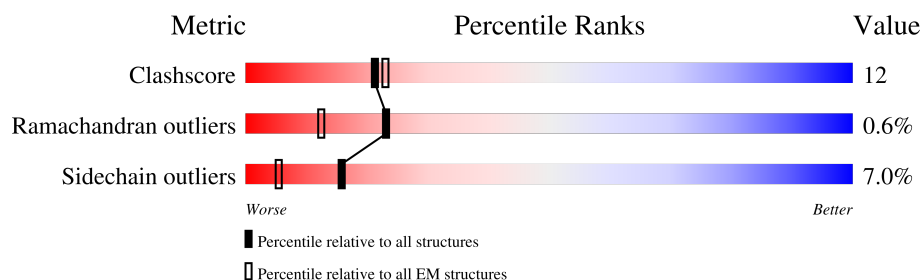
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.89 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.



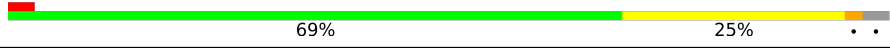
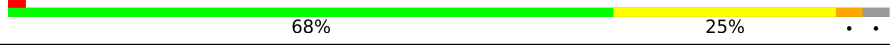
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12148 (2.39 - 3.39)

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	Aa	382	
1	Ab	382	
1	Ac	382	
2	Ca	239	

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Mol	Chain	Length	Quality of chain
2	Cb	239	 66%30%.
2	Cc	239	 67%28%.
3	Ba	237	 69%25%. .
3	Bb	237	 68%25%. .
3	Bc	237	 69%25%. .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20772 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 Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	Ab	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	Ac	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		

- Molecule 2 is a protein called Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ca	238	Total	C	N	O	S	0	0
			1958	1317	312	318	11		
2	Cb	238	Total	C	N	O	S	0	0
			1958	1317	312	318	11		
2	Cc	238	Total	C	N	O	S	0	0
			1958	1317	312	318	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ca	256	SER	THR	conflict	UNP Q607G3
Cb	256	SER	THR	conflict	UNP Q607G3
Cc	256	SER	THR	conflict	UNP Q607G3

- Molecule 3 is a protein called Methane monooxygenase, C subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ba	229	Total	C	N	O	S	0	0
			1894	1283	291	316	4		
3	Bb	229	Total	C	N	O	S	0	0
			1894	1283	291	316	4		
3	Bc	229	Total	C	N	O	S	0	0
			1894	1283	291	316	4		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ba	43	ALA	ARG	conflict	UNP Q60C16
Ba	52	THR	VAL	conflict	UNP Q60C16
Ba	55	LEU	ILE	conflict	UNP Q60C16
Ba	56	ALA	GLY	conflict	UNP Q60C16
Ba	270	ALA	-	insertion	UNP Q60C16
Ba	271	GLN	SER	conflict	UNP Q60C16
Ba	272	GLY	HIS	conflict	UNP Q60C16
Ba	273	GLY	LEU	conflict	UNP Q60C16
Ba	274	LEU	PHE	conflict	UNP Q60C16
Ba	275	GLY	GLU	conflict	UNP Q60C16
Ba	276	GLN	ARG	conflict	UNP Q60C16
Ba	277	SER	ASP	conflict	UNP Q60C16
Bb	43	ALA	ARG	conflict	UNP Q60C16
Bb	52	THR	VAL	conflict	UNP Q60C16
Bb	55	LEU	ILE	conflict	UNP Q60C16
Bb	56	ALA	GLY	conflict	UNP Q60C16
Bb	270	ALA	-	insertion	UNP Q60C16
Bb	271	GLN	SER	conflict	UNP Q60C16
Bb	272	GLY	HIS	conflict	UNP Q60C16
Bb	273	GLY	LEU	conflict	UNP Q60C16
Bb	274	LEU	PHE	conflict	UNP Q60C16
Bb	275	GLY	GLU	conflict	UNP Q60C16
Bb	276	GLN	ARG	conflict	UNP Q60C16
Bb	277	SER	ASP	conflict	UNP Q60C16
Bc	43	ALA	ARG	conflict	UNP Q60C16
Bc	52	THR	VAL	conflict	UNP Q60C16
Bc	55	LEU	ILE	conflict	UNP Q60C16
Bc	56	ALA	GLY	conflict	UNP Q60C16
Bc	270	ALA	-	insertion	UNP Q60C16
Bc	271	GLN	SER	conflict	UNP Q60C16
Bc	272	GLY	HIS	conflict	UNP Q60C16
Bc	273	GLY	LEU	conflict	UNP Q60C16
Bc	274	LEU	PHE	conflict	UNP Q60C16
Bc	275	GLY	GLU	conflict	UNP Q60C16
Bc	276	GLN	ARG	conflict	UNP Q60C16
Bc	277	SER	ASP	conflict	UNP Q60C16

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	Aa	2	Total 2	Cu 2	0
4	Ba	1	Total 1	Cu 1	0
4	Bb	1	Total 1	Cu 1	0
4	Bc	1	Total 1	Cu 1	0
4	Ab	2	Total 2	Cu 2	0
4	Ac	2	Total 2	Cu 2	0

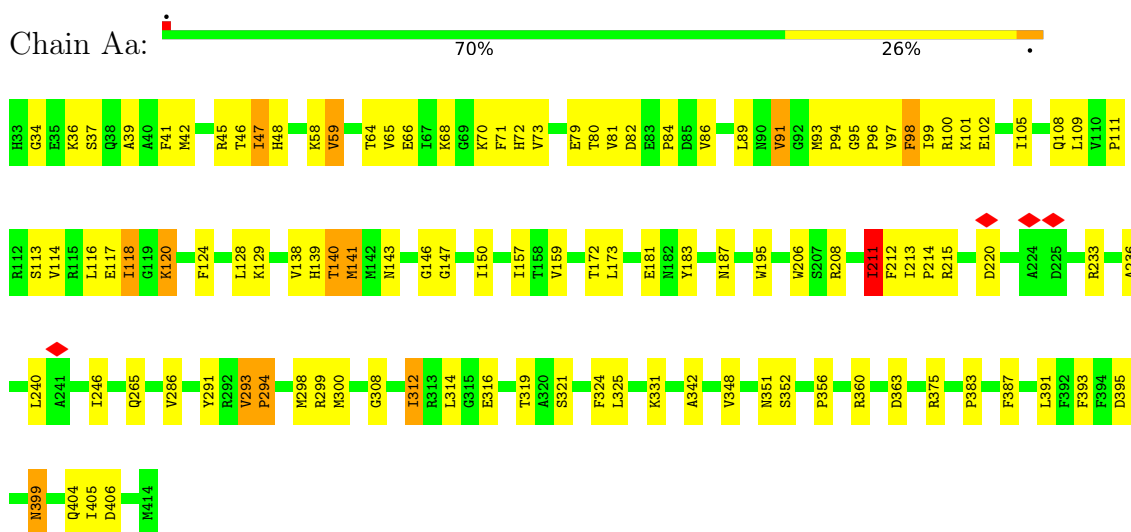
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	Aa	32	Total 32	O 32	0
5	Ca	8	Total 8	O 8	0
5	Ba	12	Total 12	O 12	0
5	Bb	12	Total 12	O 12	0
5	Bc	12	Total 12	O 12	0
5	Ab	32	Total 32	O 32	0
5	Ac	32	Total 32	O 32	0
5	Cb	8	Total 8	O 8	0
5	Cc	8	Total 8	O 8	0

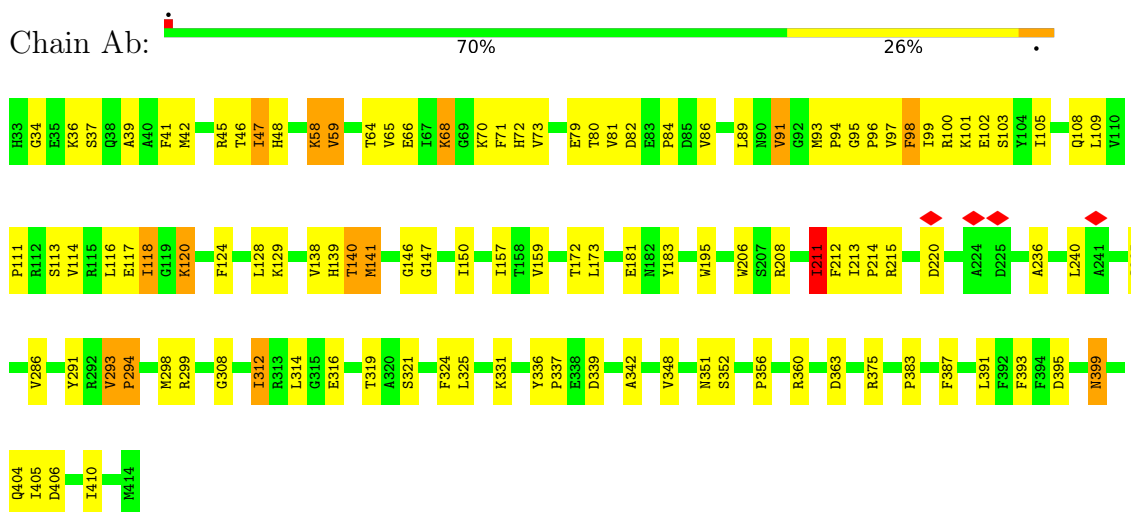
3 Residue-property plots

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.

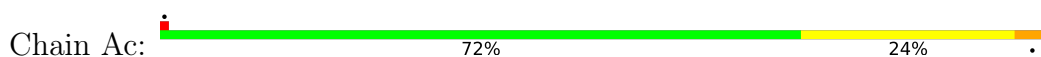
- Molecule 1: Particulate methane monooxygenase alpha subunit

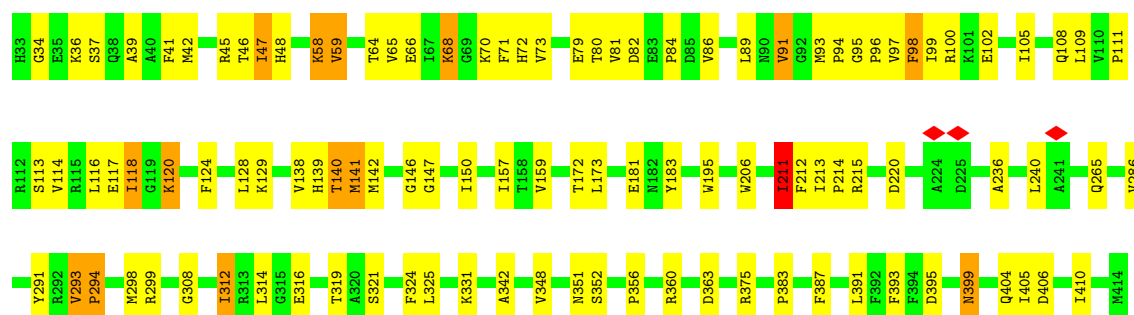


- Molecule 1: Particulate methane monooxygenase alpha subunit

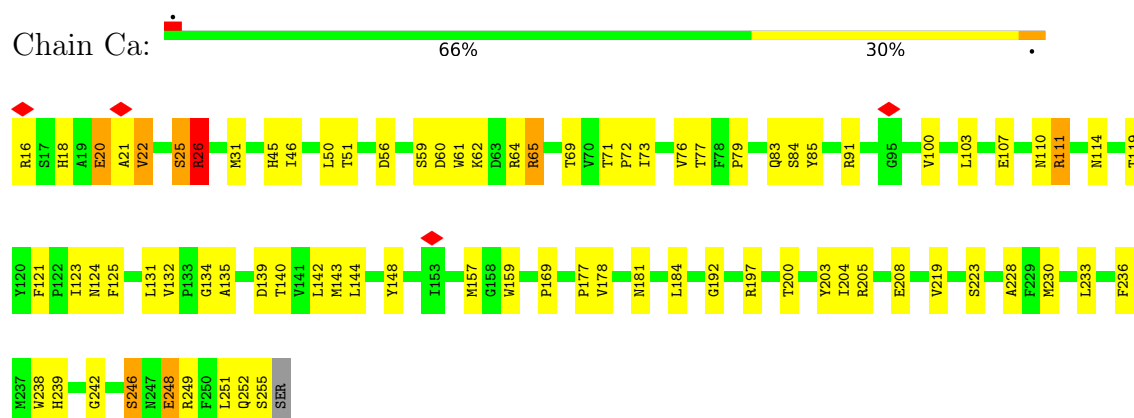


- Molecule 1: Particulate methane monooxygenase alpha subunit

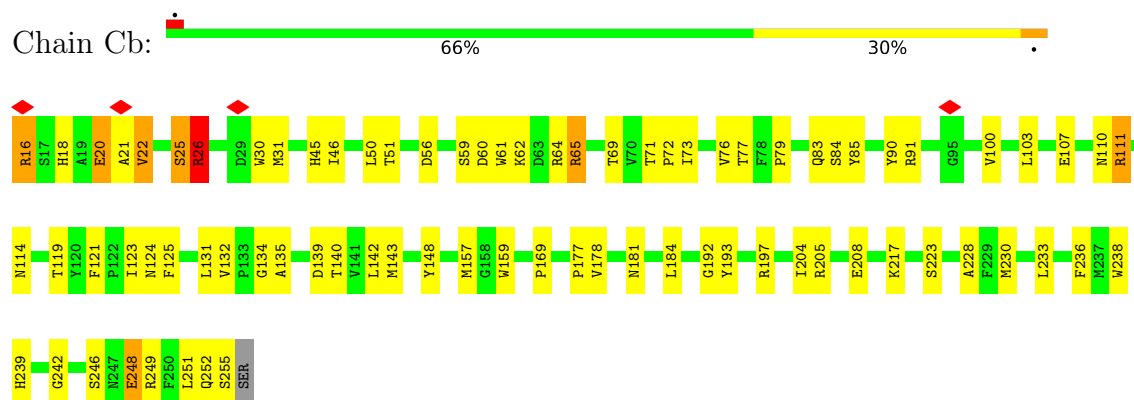




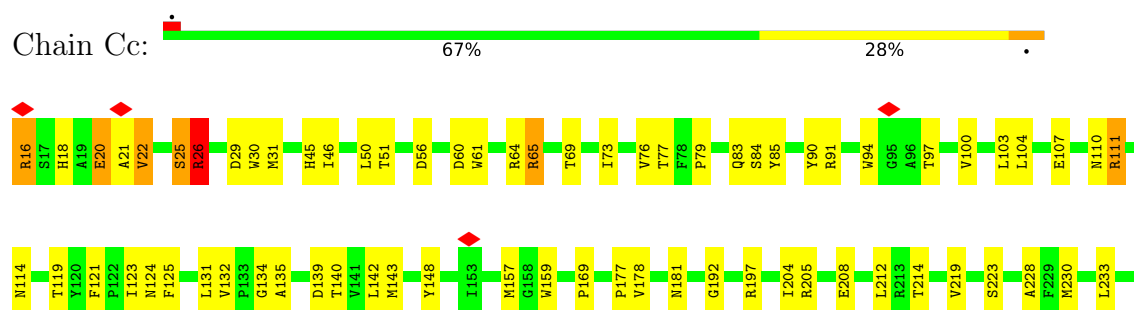
• Molecule 2: Particulate methane monooxygenase beta subunit



• Molecule 2: Particulate methane monooxygenase beta subunit



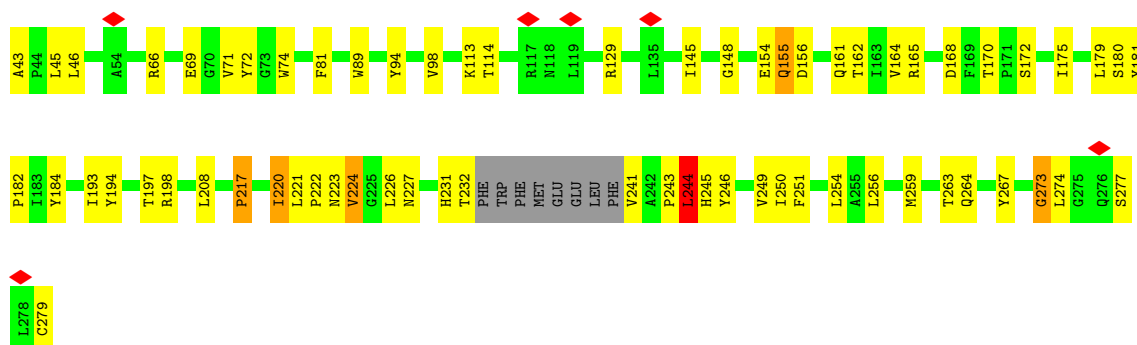
• Molecule 2: Particulate methane monooxygenase beta subunit





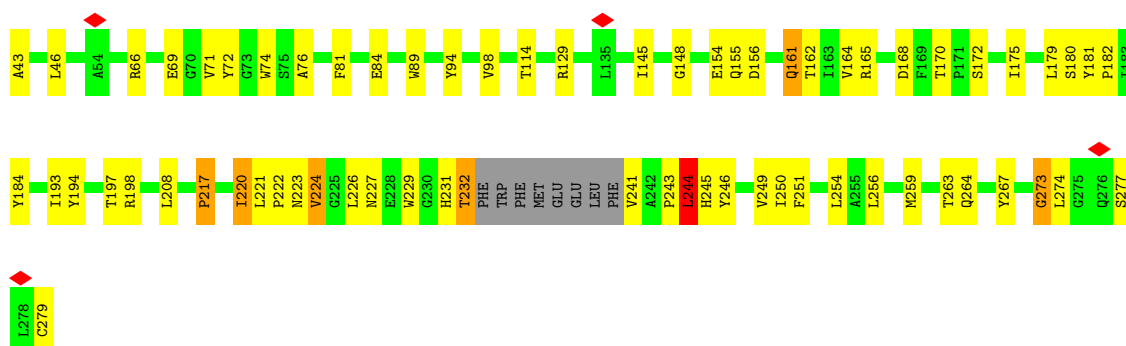
• Molecule 3: Methane monooxygenase, C subunit

Chain Ba: 69% 25%



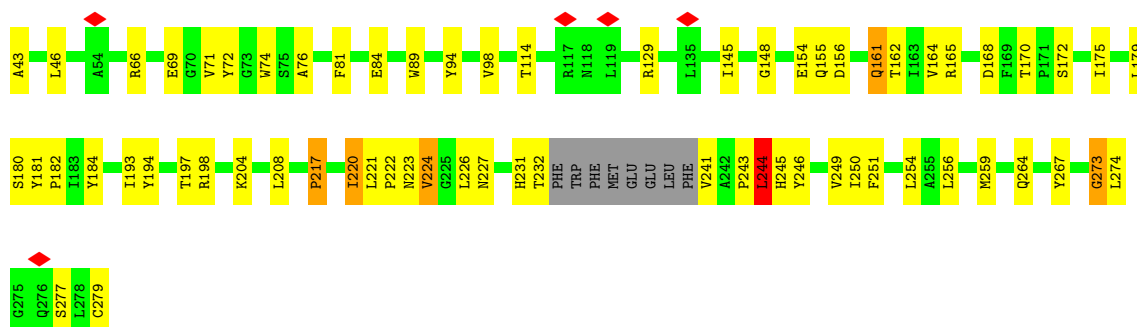
• Molecule 3: Methane monooxygenase, C subunit

Chain Bb: 68% 25%



• Molecule 3: Methane monooxygenase, C subunit

Chain Bc: 69% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109356	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 ($e^-/\text{\AA}^2$)	52.484	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.512	Depositor
Minimum map value	-3.622	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.145	Depositor
Recommended contour level	0.355	Depositor
Map size ($\text{\AA}$)	273.664, 273.664, 273.664	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.069, 1.069, 1.069	Depositor

5 Model quality

5.1 Standard geometry

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

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	Aa	0.50	0/3099	0.81	8/4215 (0.2%)
1	Ab	0.50	0/3099	0.81	8/4215 (0.2%)
1	Ac	0.50	0/3099	0.81	8/4215 (0.2%)
2	Ca	0.32	0/2034	0.55	0/2783
2	Cb	0.32	0/2034	0.55	0/2783
2	Cc	0.32	0/2034	0.55	0/2783
3	Ba	0.43	0/1968	0.66	2/2698 (0.1%)
3	Bb	0.43	0/1968	0.66	2/2698 (0.1%)
3	Bc	0.43	0/1968	0.66	2/2698 (0.1%)
All	All	0.44	0/21303	0.70	30/29088 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Aa	0	2
1	Ab	0	2
1	Ac	0	2
2	Ca	0	2
2	Cb	0	2
2	Cc	0	2
All	All	0	12

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	139	HIS	CB-CA-C	-8.58	92.36	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ab	139	HIS	CB-CA-C	-8.57	92.38	109.35
1	Ac	139	HIS	CB-CA-C	-8.56	92.40	109.35
1	Ac	71	PHE	CA-CB-CG	7.40	121.20	113.80
1	Aa	71	PHE	CA-CB-CG	7.37	121.17	113.80
1	Ab	71	PHE	CA-CB-CG	7.37	121.17	113.80
1	Ac	48	HIS	CB-CG-CD2	-7.26	121.77	131.20
1	Aa	48	HIS	CB-CG-ND1	7.23	133.54	122.70
1	Ac	48	HIS	CB-CG-ND1	7.21	133.52	122.70
1	Aa	48	HIS	CB-CG-CD2	-7.21	121.83	131.20
1	Ab	48	HIS	CB-CG-CD2	-7.19	121.85	131.20
1	Ab	48	HIS	CB-CG-ND1	7.19	133.49	122.70
1	Ab	98	PHE	CA-CB-CG	6.38	120.18	113.80
1	Aa	98	PHE	CA-CB-CG	6.36	120.16	113.80
1	Ac	98	PHE	CA-CB-CG	6.32	120.12	113.80
1	Aa	41	PHE	N-CA-C	-6.17	105.41	113.12
1	Ac	41	PHE	N-CA-C	-6.16	105.42	113.12
1	Ab	41	PHE	N-CA-C	-6.15	105.43	113.12
3	Ba	155	GLN	N-CA-C	-5.94	104.88	111.71
3	Bb	155	GLN	N-CA-C	-5.92	104.91	111.71
3	Bc	155	GLN	N-CA-C	-5.91	104.92	111.71
1	Ac	294	PRO	CA-C-N	-5.46	115.72	121.35
1	Ac	294	PRO	C-N-CA	-5.46	115.72	121.35
1	Ab	294	PRO	CA-C-N	-5.44	115.75	121.35
1	Ab	294	PRO	C-N-CA	-5.44	115.75	121.35
1	Aa	294	PRO	CA-C-N	-5.38	115.81	121.35
1	Aa	294	PRO	C-N-CA	-5.38	115.81	121.35
3	Bc	217	PRO	N-CA-CB	-5.18	97.81	103.25
3	Ba	217	PRO	N-CA-CB	-5.14	97.86	103.25
3	Bb	217	PRO	N-CA-CB	-5.13	97.86	103.25

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Aa	211	ILE	Peptide
1	Aa	293	VAL	Peptide
1	Ab	211	ILE	Peptide
1	Ab	293	VAL	Peptide
1	Ac	211	ILE	Peptide
1	Ac	293	VAL	Peptide
2	Ca	16	ARG	Sidechain
2	Ca	26	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	Cb	16	ARG	Sidechain
2	Cb	26	ARG	Sidechain
2	Cc	16	ARG	Sidechain
2	Cc	26	ARG	Sidechain

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	Aa	3017	0	2980	72	0
1	Ab	3017	0	2980	72	0
1	Ac	3017	0	2980	70	0
2	Ca	1958	0	1915	72	0
2	Cb	1958	0	1915	74	0
2	Cc	1958	0	1915	69	0
3	Ba	1894	0	1840	57	0
3	Bb	1894	0	1840	60	0
3	Bc	1894	0	1840	56	0
4	Aa	2	0	0	0	0
4	Ab	2	0	0	0	0
4	Ac	2	0	0	0	0
4	Ba	1	0	0	0	0
4	Bb	1	0	0	0	0
4	Bc	1	0	0	0	0
5	Aa	32	0	0	2	0
5	Ab	32	0	0	1	0
5	Ac	32	0	0	2	0
5	Ba	12	0	0	3	0
5	Bb	12	0	0	3	0
5	Bc	12	0	0	3	0
5	Ca	8	0	0	3	0
5	Cb	8	0	0	3	0
5	Cc	8	0	0	3	0
All	All	20772	0	20205	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 12.

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)
2:Cb:65:ARG:NH1	5:Cb:301:HOH:O	2.03	0.91
2:Ca:65:ARG:NH1	5:Ca:301:HOH:O	2.03	0.90
2:Cc:65:ARG:NH1	5:Cc:301:HOH:O	2.03	0.90
3:Ba:162:THR:HG21	2:Cb:119:THR:HG21	1.55	0.89
2:Ca:119:THR:HG21	3:Bb:162:THR:HG21	1.60	0.82
3:Bc:162:THR:HG21	2:Cc:119:THR:HG21	1.63	0.81
3:Ba:46:LEU:CD1	2:Cb:31:MET:HE1	2.13	0.78
3:Ba:259:MET:HE3	2:Cb:85:TYR:HB2	1.65	0.77
3:Ba:46:LEU:HD13	2:Cb:31:MET:HE1	1.67	0.76
1:Ac:109:LEU:HD22	2:Cc:181:ASN:HB2	1.67	0.76
2:Ca:31:MET:HE1	3:Bb:46:LEU:HD13	1.67	0.76
2:Ca:85:TYR:HB2	3:Bb:259:MET:HE3	1.68	0.75
1:Aa:211:ILE:HG12	1:Aa:212:PHE:H	1.53	0.73
1:Ab:211:ILE:HG12	1:Ab:212:PHE:H	1.53	0.73
2:Ca:31:MET:HE1	3:Bb:46:LEU:CD1	2.17	0.72
3:Ba:162:THR:HG21	2:Cb:119:THR:CG2	2.19	0.72
1:Ac:211:ILE:HG12	1:Ac:212:PHE:H	1.53	0.72
3:Ba:243:PRO:C	3:Ba:245:HIS:H	1.98	0.71
1:Aa:39:ALA:HB3	1:Aa:42:MET:HG2	1.73	0.71
1:Ab:39:ALA:HB3	1:Ab:42:MET:HG2	1.73	0.71
3:Bb:243:PRO:C	3:Bb:245:HIS:H	1.98	0.70
3:Bc:46:LEU:CD1	2:Cc:31:MET:HE1	2.21	0.70
1:Ac:39:ALA:HB3	1:Ac:42:MET:HG2	1.73	0.70
3:Bc:46:LEU:HD13	2:Cc:31:MET:HE1	1.72	0.70
3:Ba:154:GLU:OE2	2:Cb:111:ARG:NH1	2.25	0.69
3:Bc:243:PRO:C	3:Bc:245:HIS:H	1.98	0.69
2:Ca:56:ASP:HB3	2:Ca:111:ARG:HH22	1.59	0.68
2:Cb:169:PRO:HG2	5:Cb:302:HOH:O	1.94	0.68
2:Ca:169:PRO:HG2	5:Ca:302:HOH:O	1.94	0.68
1:Ac:181:GLU:OE1	5:Ac:601:HOH:O	2.12	0.68
2:Cc:169:PRO:HG2	5:Cc:302:HOH:O	1.94	0.68
1:Ab:213:ILE:HG23	1:Ab:214:PRO:HD3	1.76	0.68
1:Aa:181:GLU:OE1	5:Aa:601:HOH:O	2.12	0.67
2:Ca:111:ARG:NH1	3:Bb:154:GLU:OE2	2.28	0.67
2:Cb:56:ASP:HB3	2:Cb:111:ARG:HH22	1.59	0.67
2:Cc:56:ASP:HB3	2:Cc:111:ARG:HH22	1.59	0.67
1:Aa:213:ILE:HG23	1:Aa:214:PRO:HD3	1.76	0.66
1:Ab:181:GLU:OE1	5:Ab:601:HOH:O	2.12	0.66
2:Ca:119:THR:CG2	3:Bb:162:THR:HG21	2.24	0.66
3:Bc:154:GLU:OE2	2:Cc:111:ARG:NH1	2.29	0.66
1:Ab:109:LEU:HD22	2:Cb:181:ASN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bc:259:MET:HE3	2:Cc:85:TYR:HB2	1.78	0.65
1:Ab:236:ALA:HB1	2:Cb:140:THR:HG23	1.78	0.65
1:Ac:213:ILE:HG23	1:Ac:214:PRO:HD3	1.76	0.65
2:Ca:110:ASN:OD1	2:Ca:114:ASN:ND2	2.26	0.64
3:Bc:220:ILE:HG13	3:Bc:251:PHE:HB2	1.80	0.64
1:Aa:172:THR:HA	2:Ca:178:VAL:HG23	1.79	0.64
1:Aa:89:LEU:HB2	1:Aa:105:ILE:HD11	1.80	0.64
1:Aa:236:ALA:HB1	2:Ca:140:THR:HG23	1.80	0.64
2:Ca:83:GLN:NE2	2:Ca:139:ASP:OD1	2.31	0.64
1:Ab:206:TRP:HZ2	2:Cb:143:MET:HE2	1.62	0.64
3:Bc:162:THR:HG21	2:Cc:119:THR:CG2	2.27	0.63
2:Cc:83:GLN:NE2	2:Cc:139:ASP:OD1	2.31	0.63
1:Ab:89:LEU:HB2	1:Ab:105:ILE:HD11	1.80	0.63
3:Ba:223:ASN:HD21	3:Ba:226:LEU:HD23	1.63	0.63
2:Cb:83:GLN:NE2	2:Cb:139:ASP:OD1	2.31	0.63
3:Bb:220:ILE:HG13	3:Bb:251:PHE:HB2	1.80	0.63
3:Bb:223:ASN:HD21	3:Bb:226:LEU:HD23	1.63	0.63
2:Cb:110:ASN:OD1	2:Cb:114:ASN:ND2	2.26	0.63
3:Bc:223:ASN:HD21	3:Bc:226:LEU:HD23	1.63	0.63
1:Ac:89:LEU:HB2	1:Ac:105:ILE:HD11	1.80	0.63
2:Cc:110:ASN:OD1	2:Cc:114:ASN:ND2	2.26	0.63
3:Ba:220:ILE:HG13	3:Ba:251:PHE:HB2	1.80	0.62
1:Aa:183:TYR:O	2:Ca:124:ASN:ND2	2.32	0.62
1:Ab:206:TRP:CZ2	2:Cb:143:MET:HE2	2.35	0.62
3:Ba:245:HIS:HB3	2:Cb:50:LEU:CD1	2.29	0.61
1:Ab:314:LEU:HD11	1:Ab:391:LEU:HD22	1.84	0.60
1:Ac:314:LEU:HD11	1:Ac:391:LEU:HD22	1.84	0.60
1:Ab:172:THR:HA	2:Cb:178:VAL:HG23	1.84	0.60
3:Bc:164:VAL:O	5:Bc:401:HOH:O	2.17	0.60
2:Ca:50:LEU:CD1	3:Bb:245:HIS:HB3	2.32	0.60
1:Aa:316:GLU:HG3	1:Aa:325:LEU:HD13	1.84	0.59
1:Aa:314:LEU:HD11	1:Aa:391:LEU:HD22	1.84	0.59
1:Aa:109:LEU:HD22	2:Ca:181:ASN:HB2	1.84	0.59
1:Ab:316:GLU:HG3	1:Ab:325:LEU:HD13	1.84	0.59
1:Ab:352:SER:O	1:Ab:360:ARG:NH2	2.32	0.59
1:Ab:195:TRP:HB3	2:Cb:132:VAL:HB	1.84	0.59
1:Ac:236:ALA:HB1	2:Cc:140:THR:HG23	1.84	0.59
3:Ba:164:VAL:O	5:Ba:401:HOH:O	2.17	0.58
1:Ac:117:GLU:HB2	1:Ac:120:LYS:HG3	1.85	0.58
3:Bc:243:PRO:C	3:Bc:245:HIS:N	2.61	0.58
1:Ac:183:TYR:O	2:Cc:124:ASN:ND2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:316:GLU:HG3	1:Ac:325:LEU:HD13	1.84	0.58
1:Ac:195:TRP:HB3	2:Cc:132:VAL:HB	1.85	0.58
1:Ac:352:SER:O	1:Ac:360:ARG:NH2	2.32	0.58
1:Aa:352:SER:O	1:Aa:360:ARG:NH2	2.32	0.58
1:Ab:211:ILE:O	1:Ab:214:PRO:HD2	2.04	0.58
1:Aa:211:ILE:O	1:Aa:214:PRO:HD2	2.04	0.58
2:Ca:69:THR:OG1	2:Ca:223:SER:OG	2.22	0.58
3:Bb:243:PRO:C	3:Bb:245:HIS:N	2.61	0.58
1:Aa:117:GLU:HB2	1:Aa:120:LYS:HG3	1.85	0.57
1:Aa:348:VAL:HB	1:Aa:351:ASN:HB2	1.86	0.57
3:Bb:164:VAL:O	5:Bb:401:HOH:O	2.17	0.57
1:Ab:117:GLU:HB2	1:Ab:120:LYS:HG3	1.85	0.57
2:Cc:69:THR:OG1	2:Cc:223:SER:OG	2.22	0.57
1:Aa:265:GLN:HA	1:Ab:383:PRO:O	2.04	0.57
1:Ac:395:ASP:OD1	1:Ac:399:ASN:N	2.38	0.57
1:Ac:211:ILE:HG23	2:Cc:29:ASP:CG	2.30	0.57
1:Ab:265:GLN:HA	1:Ac:383:PRO:O	2.05	0.57
1:Aa:383:PRO:O	1:Ac:265:GLN:HA	2.04	0.57
1:Aa:395:ASP:OD1	1:Aa:399:ASN:N	2.38	0.57
2:Cb:46:ILE:O	2:Cb:50:LEU:HB2	2.05	0.57
2:Ca:46:ILE:O	2:Ca:50:LEU:HB2	2.05	0.56
3:Ba:243:PRO:C	3:Ba:245:HIS:N	2.61	0.56
1:Ab:395:ASP:OD1	1:Ab:399:ASN:N	2.38	0.56
1:Ac:211:ILE:O	1:Ac:214:PRO:HD2	2.04	0.56
2:Cb:69:THR:OG1	2:Cb:223:SER:OG	2.22	0.56
2:Cc:46:ILE:O	2:Cc:50:LEU:HB2	2.05	0.56
1:Aa:138:VAL:HG21	1:Aa:157:ILE:HD12	1.88	0.56
1:Ab:183:TYR:O	2:Cb:124:ASN:ND2	2.38	0.56
1:Ac:72:HIS:CE1	1:Ac:404:GLN:HE21	2.24	0.56
3:Bb:164:VAL:C	5:Bb:401:HOH:O	2.49	0.56
3:Bc:164:VAL:C	5:Bc:401:HOH:O	2.49	0.55
2:Ca:85:TYR:OH	3:Bb:263:THR:OG1	2.24	0.55
1:Ac:348:VAL:HB	1:Ac:351:ASN:HB2	1.86	0.55
1:Ab:72:HIS:CE1	1:Ab:404:GLN:HE21	2.24	0.55
1:Ab:138:VAL:HG21	1:Ab:157:ILE:HD12	1.88	0.55
1:Ab:348:VAL:HB	1:Ab:351:ASN:HB2	1.86	0.55
1:Ab:331:LYS:NZ	1:Ab:331:LYS:HB3	2.22	0.55
1:Aa:72:HIS:CE1	1:Aa:404:GLN:HE21	2.24	0.55
3:Ba:71:VAL:HG12	3:Ba:72:TYR:CD1	2.42	0.55
3:Bb:256:LEU:HG	3:Bb:259:MET:SD	2.47	0.55
1:Ac:138:VAL:HG21	1:Ac:157:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ba:164:VAL:C	5:Ba:401:HOH:O	2.49	0.55
1:Aa:331:LYS:NZ	1:Aa:331:LYS:HB3	2.22	0.55
3:Ba:256:LEU:HG	3:Ba:259:MET:SD	2.47	0.55
3:Bc:256:LEU:HG	3:Bc:259:MET:SD	2.47	0.55
1:Ac:240:LEU:HB2	2:Cc:140:THR:HG21	1.89	0.55
2:Cb:100:VAL:HG21	2:Cb:135:ALA:HB2	1.89	0.55
3:Bb:71:VAL:HG12	3:Bb:72:TYR:CD1	2.42	0.55
1:Ac:331:LYS:NZ	1:Ac:331:LYS:HB3	2.22	0.54
2:Cc:60:ASP:HB3	2:Cc:205:ARG:HD2	1.89	0.54
1:Ab:312:ILE:HG12	1:Ab:393:PHE:HB3	1.89	0.54
2:Cb:60:ASP:HB3	2:Cb:205:ARG:HD2	1.89	0.54
2:Ca:60:ASP:HB3	2:Ca:205:ARG:HD2	1.89	0.54
1:Aa:312:ILE:HG12	1:Aa:393:PHE:HB3	1.89	0.54
2:Ca:83:GLN:HG2	2:Ca:142:LEU:HD22	1.90	0.54
3:Bc:71:VAL:HG12	3:Bc:72:TYR:CD1	2.42	0.54
1:Aa:195:TRP:HB3	2:Ca:132:VAL:HB	1.90	0.54
2:Ca:100:VAL:HG21	2:Ca:135:ALA:HB2	1.89	0.54
2:Cb:60:ASP:OD2	2:Cb:192:GLY:HA3	2.08	0.54
2:Cb:83:GLN:HG2	2:Cb:142:LEU:HD22	1.90	0.54
2:Cc:83:GLN:HG2	2:Cc:142:LEU:HD22	1.90	0.54
2:Cc:100:VAL:HG21	2:Cc:135:ALA:HB2	1.89	0.54
1:Ac:206:TRP:HZ2	2:Cc:143:MET:HE2	1.72	0.54
1:Aa:124:PHE:CE2	1:Aa:140:THR:HG21	2.43	0.53
3:Bc:208:LEU:HD13	2:Cc:251:LEU:HD11	1.90	0.53
3:Ba:46:LEU:HD11	2:Cb:31:MET:HE1	1.88	0.53
1:Aa:206:TRP:HZ2	2:Ca:143:MET:HE2	1.73	0.53
1:Ac:312:ILE:HG12	1:Ac:393:PHE:HB3	1.89	0.53
1:Ac:124:PHE:CE2	1:Ac:140:THR:HG21	2.43	0.53
1:Ab:124:PHE:CE2	1:Ab:140:THR:HG21	2.43	0.53
2:Cc:60:ASP:OD2	2:Cc:192:GLY:HA3	2.08	0.53
2:Ca:60:ASP:OD2	2:Ca:192:GLY:HA3	2.08	0.52
3:Bc:94:TYR:O	3:Bc:98:VAL:HG23	2.09	0.52
3:Ba:251:PHE:HA	3:Ba:254:LEU:HD23	1.92	0.52
3:Bb:94:TYR:O	3:Bb:98:VAL:HG23	2.09	0.52
3:Bb:251:PHE:HA	3:Bb:254:LEU:HD23	1.92	0.52
2:Cc:134:GLY:HA3	2:Cc:159:TRP:CD1	2.45	0.52
2:Ca:50:LEU:HB3	3:Bb:249:VAL:HG22	1.91	0.52
3:Ba:71:VAL:HG12	3:Ba:72:TYR:HD1	1.75	0.52
1:Aa:213:ILE:CG2	1:Aa:214:PRO:HD3	2.40	0.52
3:Ba:94:TYR:O	3:Ba:98:VAL:HG23	2.09	0.52
1:Aa:206:TRP:CZ2	2:Ca:143:MET:HE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ba:267:TYR:OH	1:Ab:220:ASP:OD2	2.23	0.52
3:Ba:181:TYR:HA	3:Ba:184:TYR:CE2	2.45	0.52
3:Bc:181:TYR:HA	3:Bc:184:TYR:CE2	2.45	0.51
3:Bc:251:PHE:HA	3:Bc:254:LEU:HD23	1.92	0.51
1:Ac:299:ARG:NH2	1:Ac:363:ASP:OD2	2.43	0.51
1:Ac:286:VAL:HG21	1:Ac:405:ILE:HG23	1.92	0.51
3:Bb:181:TYR:HA	3:Bb:184:TYR:CE2	2.45	0.51
3:Ba:74:TRP:HZ3	1:Ab:94:PRO:HB2	1.76	0.51
3:Bc:221:LEU:HB3	3:Bc:222:PRO:HD3	1.93	0.51
1:Ab:299:ARG:NH2	1:Ab:363:ASP:OD2	2.43	0.51
1:Ac:213:ILE:CG2	1:Ac:214:PRO:HD3	2.40	0.51
2:Cb:134:GLY:HA3	2:Cb:159:TRP:CD1	2.45	0.51
3:Bb:221:LEU:HB3	3:Bb:222:PRO:HD3	1.93	0.51
1:Ab:286:VAL:HG21	1:Ab:405:ILE:HG23	1.92	0.51
2:Ca:134:GLY:HA3	2:Ca:159:TRP:CD1	2.45	0.51
3:Ba:249:VAL:HG22	2:Cb:50:LEU:HB3	1.93	0.51
1:Ab:91:VAL:HG21	1:Ab:128:LEU:HD21	1.93	0.51
1:Ac:91:VAL:HG21	1:Ac:128:LEU:HD21	1.93	0.51
1:Ac:172:THR:HA	2:Cc:178:VAL:HG23	1.93	0.51
2:Ca:85:TYR:CB	3:Bb:259:MET:HE3	2.40	0.51
3:Ba:221:LEU:HB3	3:Ba:222:PRO:HD3	1.93	0.51
3:Bb:71:VAL:HG12	3:Bb:72:TYR:HD1	1.75	0.51
1:Aa:286:VAL:HG21	1:Aa:405:ILE:HG23	1.92	0.51
3:Ba:246:TYR:O	3:Ba:250:ILE:HG12	2.11	0.50
1:Ab:213:ILE:CG2	1:Ab:214:PRO:HD3	2.40	0.50
1:Aa:299:ARG:NH2	1:Aa:363:ASP:OD2	2.43	0.50
3:Ba:170:THR:HG22	5:Ba:403:HOH:O	2.11	0.50
1:Aa:91:VAL:HG21	1:Aa:128:LEU:HD21	1.93	0.50
3:Bc:71:VAL:HG12	3:Bc:72:TYR:HD1	1.75	0.50
3:Ba:259:MET:HE3	2:Cb:85:TYR:CB	2.39	0.50
3:Bb:246:TYR:O	3:Bb:250:ILE:HG12	2.11	0.50
3:Ba:264:GLN:CG	2:Cb:248:GLU:HG2	2.41	0.50
3:Bb:170:THR:HG22	5:Bb:403:HOH:O	2.11	0.50
1:Ac:81:VAL:HG13	1:Ac:147:GLY:HA3	1.94	0.50
1:Aa:99:ILE:HG13	1:Aa:129:LYS:HB3	1.94	0.50
3:Bc:74:TRP:HZ3	1:Ac:94:PRO:HB2	1.77	0.50
3:Bc:170:THR:HG22	5:Bc:403:HOH:O	2.11	0.50
3:Ba:175:ILE:O	3:Ba:179:LEU:HB3	2.12	0.49
3:Bc:175:ILE:O	3:Bc:179:LEU:HB3	2.12	0.49
1:Ab:81:VAL:HG13	1:Ab:147:GLY:HA3	1.94	0.49
3:Bb:175:ILE:O	3:Bb:179:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bc:246:TYR:O	3:Bc:250:ILE:HG12	2.11	0.49
3:Bc:249:VAL:HG22	2:Cc:50:LEU:HB3	1.94	0.49
3:Bb:231:HIS:CE1	3:Bb:244:LEU:HD11	2.48	0.49
3:Ba:231:HIS:CE1	3:Ba:244:LEU:HD11	2.48	0.49
1:Ab:99:ILE:HG13	1:Ab:129:LYS:HB3	1.94	0.49
1:Ac:173:LEU:HD12	2:Cc:177:PRO:HB2	1.94	0.49
1:Aa:81:VAL:HG13	1:Aa:147:GLY:HA3	1.94	0.48
3:Bc:194:TYR:CE2	3:Bc:198:ARG:HD2	2.48	0.48
3:Ba:264:GLN:HG3	2:Cb:248:GLU:HG2	1.95	0.48
1:Ac:319:THR:O	1:Ac:321:SER:N	2.46	0.48
2:Ca:110:ASN:HD22	3:Bb:154:GLU:CD	2.21	0.48
1:Ab:84:PRO:HD2	1:Ab:118:ILE:HD11	1.95	0.48
1:Ab:319:THR:O	1:Ab:321:SER:N	2.46	0.48
3:Ba:194:TYR:CE2	3:Ba:198:ARG:HD2	2.48	0.48
3:Bc:204:LYS:O	2:Cc:252:GLN:NE2	2.46	0.48
3:Bc:245:HIS:HB3	2:Cc:50:LEU:CD1	2.42	0.48
1:Aa:220:ASP:OD2	3:Bb:267:TYR:OH	2.22	0.48
3:Bc:231:HIS:CE1	3:Bc:244:LEU:HD11	2.48	0.48
1:Ac:99:ILE:HG13	1:Ac:129:LYS:HB3	1.94	0.48
2:Cb:125:PHE:HZ	2:Cb:197:ARG:HH11	1.61	0.48
1:Aa:84:PRO:HD2	1:Aa:118:ILE:HD11	1.95	0.48
3:Bc:264:GLN:HG3	2:Cc:248:GLU:HG2	1.95	0.48
1:Ac:206:TRP:CZ2	2:Cc:143:MET:HE2	2.48	0.48
2:Cc:125:PHE:HZ	2:Cc:197:ARG:HH11	1.61	0.48
1:Aa:94:PRO:HB2	3:Bb:74:TRP:HZ3	1.78	0.48
2:Cb:20:GLU:H	2:Cb:20:GLU:HG3	1.56	0.48
1:Aa:319:THR:O	1:Aa:321:SER:N	2.46	0.48
2:Ca:103:LEU:O	2:Ca:107:GLU:HG3	2.14	0.48
2:Cc:103:LEU:O	2:Cc:107:GLU:HG3	2.14	0.48
1:Ac:84:PRO:HD2	1:Ac:118:ILE:HD11	1.95	0.47
3:Ba:114:THR:O	3:Ba:114:THR:HG22	2.14	0.47
3:Ba:241:VAL:HG22	2:Cb:51:THR:O	2.14	0.47
3:Bb:193:ILE:O	3:Bb:197:THR:HG23	2.14	0.47
1:Ac:141:MET:HE2	1:Ac:141:MET:HB2	1.62	0.47
2:Cb:79:PRO:O	2:Cb:83:GLN:HB2	2.14	0.47
2:Ca:248:GLU:HG2	3:Bb:264:GLN:CG	2.45	0.47
2:Cb:103:LEU:O	2:Cb:107:GLU:HG3	2.14	0.47
3:Bb:194:TYR:CE2	3:Bb:198:ARG:HD2	2.48	0.47
3:Bc:193:ILE:O	3:Bc:197:THR:HG23	2.14	0.47
1:Aa:211:ILE:HG12	1:Aa:212:PHE:CD1	2.50	0.47
3:Bc:114:THR:HG22	3:Bc:114:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ca:31:MET:HE1	3:Bb:46:LEU:HD11	1.95	0.47
3:Bc:223:ASN:O	3:Bc:224:VAL:C	2.58	0.47
1:Ac:324:PHE:HA	1:Ac:342:ALA:HB3	1.97	0.47
2:Cc:79:PRO:O	2:Cc:83:GLN:HB2	2.15	0.47
2:Ca:79:PRO:O	2:Ca:83:GLN:HB2	2.15	0.47
3:Ba:245:HIS:HB3	2:Cb:50:LEU:HD12	1.96	0.47
3:Bc:264:GLN:CG	2:Cc:248:GLU:HG2	2.44	0.47
1:Ac:211:ILE:HG12	1:Ac:212:PHE:CD1	2.50	0.47
2:Cb:100:VAL:HG13	2:Cb:131:LEU:HB2	1.97	0.47
2:Ca:100:VAL:HG13	2:Ca:131:LEU:HB2	1.97	0.47
2:Ca:125:PHE:HZ	2:Ca:197:ARG:HH11	1.61	0.47
3:Ba:148:GLY:HA2	3:Ba:180:SER:HB2	1.97	0.47
1:Ab:211:ILE:HG12	1:Ab:212:PHE:CD1	2.50	0.47
1:Ab:215:ARG:NH1	2:Cb:91:ARG:O	2.47	0.47
2:Cb:45:HIS:CE1	2:Cb:107:GLU:HG2	2.50	0.47
3:Bc:181:TYR:HB2	3:Bc:182:PRO:HD3	1.97	0.47
2:Cb:84:SER:HA	2:Cb:148:TYR:HE2	1.80	0.47
2:Ca:45:HIS:CE1	2:Ca:107:GLU:HG2	2.50	0.46
3:Ba:223:ASN:O	3:Ba:224:VAL:C	2.58	0.46
2:Ca:20:GLU:H	2:Ca:20:GLU:HG3	1.56	0.46
3:Ba:193:ILE:O	3:Ba:197:THR:HG23	2.14	0.46
3:Bb:148:GLY:HA2	3:Bb:180:SER:HB2	1.97	0.46
1:Ab:324:PHE:HA	1:Ab:342:ALA:HB3	1.96	0.46
2:Ca:61:TRP:HH2	2:Ca:204:ILE:HG22	1.81	0.46
1:Ab:141:MET:HE2	1:Ab:141:MET:HB2	1.62	0.46
2:Cc:45:HIS:CE1	2:Cc:107:GLU:HG2	2.50	0.46
2:Ca:233:LEU:HD21	3:Ba:251:PHE:HZ	1.79	0.46
3:Bc:243:PRO:O	3:Bc:245:HIS:N	2.48	0.46
2:Ca:242:GLY:O	2:Ca:246:SER:OG	2.32	0.46
3:Bb:114:THR:HG22	3:Bb:114:THR:O	2.14	0.46
3:Bb:223:ASN:O	3:Bb:224:VAL:C	2.58	0.46
2:Cc:100:VAL:HG13	2:Cc:131:LEU:HB2	1.97	0.46
1:Aa:147:GLY:O	2:Cc:212:LEU:HB2	2.16	0.46
2:Ca:84:SER:HA	2:Ca:148:TYR:HE2	1.80	0.46
3:Bb:181:TYR:HB2	3:Bb:182:PRO:HD3	1.97	0.46
3:Bc:148:GLY:HA2	3:Bc:180:SER:HB2	1.97	0.46
1:Ab:211:ILE:HG12	1:Ab:212:PHE:N	2.27	0.46
2:Cc:84:SER:HA	2:Cc:148:TYR:HE2	1.80	0.46
1:Aa:211:ILE:HG12	1:Aa:212:PHE:N	2.26	0.46
3:Ba:243:PRO:O	3:Ba:245:HIS:N	2.48	0.46
1:Ab:173:LEU:HD12	2:Cb:177:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:68:LYS:HE2	1:Ac:68:LYS:HB2	1.34	0.46
1:Ab:399:ASN:N	1:Ab:399:ASN:OD1	2.49	0.45
2:Cc:56:ASP:HB3	2:Cc:111:ARG:NH2	2.29	0.45
1:Ab:96:PRO:HG2	2:Cb:121:PHE:CD1	2.51	0.45
2:Cc:61:TRP:HH2	2:Cc:204:ILE:HG22	1.81	0.45
1:Aa:324:PHE:HA	1:Aa:342:ALA:HB3	1.97	0.45
3:Bb:243:PRO:O	3:Bb:245:HIS:N	2.48	0.45
2:Cb:242:GLY:O	2:Cb:246:SER:OG	2.32	0.45
3:Bc:43:ALA:O	3:Bc:129:ARG:NH2	2.49	0.45
3:Bc:154:GLU:CD	2:Cc:110:ASN:HD22	2.24	0.45
3:Bc:241:VAL:HG22	2:Cc:51:THR:O	2.17	0.45
3:Bc:251:PHE:HZ	2:Cb:233:LEU:HD21	1.81	0.45
2:Cb:56:ASP:HB3	2:Cb:111:ARG:NH2	2.29	0.45
2:Cb:61:TRP:HH2	2:Cb:204:ILE:HG22	1.81	0.45
3:Ba:181:TYR:HB2	3:Ba:182:PRO:HD3	1.97	0.45
1:Ab:94:PRO:HG2	1:Ab:97:VAL:HG11	1.99	0.45
3:Ba:155:GLN:HB2	2:Cb:114:ASN:ND2	2.31	0.45
2:Ca:51:THR:O	3:Bb:241:VAL:HG22	2.17	0.45
1:Ac:82:ASP:HB2	1:Ac:146:GLY:HA3	1.99	0.45
1:Ab:68:LYS:HB2	1:Ab:68:LYS:HE2	1.34	0.45
2:Ca:25:SER:O	2:Ca:26:ARG:C	2.60	0.45
1:Ac:291:TYR:CE2	1:Ac:293:VAL:HG22	2.52	0.45
2:Ca:110:ASN:ND2	3:Bb:154:GLU:HB3	2.32	0.44
3:Bb:229:TRP:CD1	2:Cc:223:SER:HA	2.51	0.44
2:Ca:73:ILE:HG12	2:Ca:230:MET:HB3	1.99	0.44
3:Bc:161:GLN:H	3:Bc:161:GLN:HG2	1.67	0.44
2:Cb:208:GLU:HB3	5:Cb:303:HOH:O	2.18	0.44
1:Aa:399:ASN:N	1:Aa:399:ASN:OD1	2.49	0.44
2:Ca:56:ASP:HB3	2:Ca:111:ARG:NH2	2.29	0.44
3:Ba:43:ALA:O	3:Ba:129:ARG:NH2	2.49	0.44
1:Ab:291:TYR:CE2	1:Ab:293:VAL:HG22	2.52	0.44
1:Ac:94:PRO:HG2	1:Ac:97:VAL:HG11	1.99	0.44
1:Ab:73:VAL:HG11	1:Ab:84:PRO:HG3	2.00	0.44
1:Ab:240:LEU:HB2	2:Cb:140:THR:HG21	2.00	0.44
1:Ac:399:ASN:N	1:Ac:399:ASN:OD1	2.49	0.44
5:Ac:616:HOH:O	2:Cc:104:LEU:HD13	2.17	0.44
1:Aa:291:TYR:CE2	1:Aa:293:VAL:HG22	2.52	0.44
1:Ab:211:ILE:CG1	1:Ab:212:PHE:H	2.28	0.44
1:Ac:58:LYS:HE2	1:Ac:58:LYS:HB2	1.28	0.44
1:Aa:94:PRO:HG2	1:Aa:97:VAL:HG11	1.99	0.44
1:Aa:173:LEU:HD12	2:Ca:177:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:211:ILE:HG12	1:Ac:212:PHE:N	2.26	0.44
1:Aa:47:ILE:HG13	1:Aa:150:ILE:HG21	2.00	0.44
2:Ca:248:GLU:HG2	3:Bb:264:GLN:HG3	1.99	0.44
1:Ab:208:ARG:HD2	1:Ab:208:ARG:HA	1.73	0.44
1:Ac:206:TRP:HB2	2:Cc:94:TRP:CZ3	2.53	0.44
1:Ac:410:ILE:HD13	2:Cb:184:LEU:HB2	2.00	0.44
2:Cc:73:ILE:HG12	2:Cc:230:MET:HB3	1.99	0.44
1:Aa:73:VAL:HG11	1:Aa:84:PRO:HG3	1.99	0.44
3:Ba:69:GLU:HG3	3:Ba:89:TRP:HH2	1.82	0.44
1:Ab:82:ASP:HB2	1:Ab:146:GLY:HA3	1.99	0.44
2:Cc:208:GLU:HB3	5:Cc:303:HOH:O	2.18	0.44
1:Aa:82:ASP:HB2	1:Aa:146:GLY:HA3	1.99	0.43
3:Ba:154:GLU:CD	2:Cb:110:ASN:HD22	2.26	0.43
2:Cc:157:MET:HA	2:Cc:228:ALA:HB1	2.00	0.43
2:Cc:25:SER:O	2:Cc:26:ARG:C	2.60	0.43
1:Aa:96:PRO:HG2	2:Ca:121:PHE:CD1	2.54	0.43
1:Aa:101:LYS:HD2	1:Aa:101:LYS:HA	1.71	0.43
2:Ca:50:LEU:HD12	3:Bb:245:HIS:HB3	1.99	0.43
3:Bb:43:ALA:O	3:Bb:129:ARG:NH2	2.49	0.43
3:Bb:69:GLU:HG3	3:Bb:89:TRP:HH2	1.82	0.43
3:Bc:69:GLU:HG3	3:Bc:89:TRP:HH2	1.82	0.43
1:Ac:93:MET:HE2	1:Ac:93:MET:HB3	1.60	0.43
1:Ac:215:ARG:NH1	2:Cc:91:ARG:O	2.50	0.43
3:Bc:208:LEU:HB2	2:Cc:251:LEU:HG	1.99	0.43
1:Ab:195:TRP:O	2:Cb:132:VAL:HG11	2.17	0.43
1:Ac:73:VAL:HG11	1:Ac:84:PRO:HG3	2.00	0.43
2:Cb:25:SER:O	2:Cb:26:ARG:C	2.60	0.43
1:Aa:363:ASP:OD1	1:Aa:363:ASP:C	2.62	0.43
1:Ac:363:ASP:OD1	1:Ac:363:ASP:C	2.62	0.43
2:Ca:208:GLU:HB3	5:Ca:303:HOH:O	2.18	0.43
3:Bc:267:TYR:OH	1:Ac:220:ASP:OD2	2.24	0.43
1:Ac:96:PRO:HG2	2:Cc:121:PHE:CD1	2.54	0.43
2:Cb:73:ILE:HG12	2:Cb:230:MET:HB3	1.99	0.43
3:Ba:81:PHE:CE2	1:Ab:375:ARG:HD2	2.54	0.43
3:Ba:154:GLU:HB3	2:Cb:110:ASN:ND2	2.33	0.43
3:Bc:246:TYR:HA	3:Bc:249:VAL:HG23	2.00	0.43
1:Ab:363:ASP:C	1:Ab:363:ASP:OD1	2.62	0.43
2:Cb:157:MET:HA	2:Cb:228:ALA:HB1	2.00	0.43
1:Aa:143:ASN:HB3	2:Ca:203:TYR:OH	2.18	0.43
1:Aa:240:LEU:HB2	2:Ca:140:THR:HG21	2.00	0.43
1:Aa:59:VAL:HG23	1:Aa:159:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:95:GLY:O	1:Aa:97:VAL:N	2.52	0.43
1:Aa:187:ASN:ND2	5:Aa:605:HOH:O	2.41	0.43
2:Ca:157:MET:HA	2:Ca:228:ALA:HB1	2.00	0.43
3:Ba:263:THR:OG1	2:Cb:85:TYR:OH	2.28	0.43
3:Bb:156:ASP:HB2	3:Bb:172:SER:HB2	2.00	0.43
3:Bb:223:ASN:O	3:Bb:226:LEU:N	2.52	0.43
3:Bb:246:TYR:HA	3:Bb:249:VAL:HG23	2.00	0.43
3:Ba:156:ASP:HB2	3:Ba:172:SER:HB2	2.00	0.42
3:Bc:46:LEU:HD11	2:Cc:31:MET:HE1	2.01	0.42
1:Ab:47:ILE:HG13	1:Ab:150:ILE:HG21	2.00	0.42
1:Ac:47:ILE:HG13	1:Ac:150:ILE:HG21	2.00	0.42
2:Cb:83:GLN:HG2	2:Cb:142:LEU:CD2	2.49	0.42
2:Ca:77:THR:HB	2:Ca:238:TRP:CE2	2.54	0.42
3:Ba:246:TYR:HA	3:Ba:249:VAL:HG23	2.00	0.42
2:Cb:85:TYR:OH	2:Cb:90:TYR:OH	2.30	0.42
1:Aa:37:SER:OG	3:Bb:165:ARG:NH1	2.52	0.42
2:Ca:83:GLN:HG2	2:Ca:142:LEU:CD2	2.49	0.42
2:Ca:184:LEU:HB2	1:Ab:410:ILE:HD13	2.00	0.42
3:Ba:165:ARG:NH1	1:Ab:37:SER:OG	2.52	0.42
1:Aa:109:LEU:C	1:Aa:111:PRO:HD3	2.44	0.42
3:Bc:223:ASN:O	3:Bc:226:LEU:N	2.52	0.42
2:Cb:26:ARG:HD2	2:Cb:26:ARG:HA	1.28	0.42
2:Cc:83:GLN:HG2	2:Cc:142:LEU:CD2	2.49	0.42
2:Cc:242:GLY:O	2:Cc:246:SER:OG	2.32	0.42
1:Aa:93:MET:HE1	1:Aa:98:PHE:HB2	2.01	0.42
3:Bc:154:GLU:OE1	2:Cc:45:HIS:NE2	2.53	0.42
1:Ab:58:LYS:HE2	1:Ab:58:LYS:HB2	1.28	0.42
1:Ab:93:MET:HE1	1:Ab:98:PHE:HB2	2.01	0.42
1:Ac:298:MET:HE1	1:Ac:387:PHE:CD2	2.55	0.42
3:Bb:161:GLN:H	3:Bb:161:GLN:HG2	1.67	0.42
3:Bc:156:ASP:HB2	3:Bc:172:SER:HB2	2.00	0.42
1:Ab:84:PRO:HB2	1:Ab:116:LEU:HB2	2.02	0.42
1:Ac:142:MET:HE2	1:Ac:142:MET:HB2	1.89	0.42
1:Ac:215:ARG:HD3	2:Cc:90:TYR:O	2.18	0.42
2:Cb:77:THR:HB	2:Cb:238:TRP:CE2	2.54	0.42
1:Aa:93:MET:HE2	1:Aa:93:MET:HB3	1.60	0.42
3:Bc:165:ARG:NH1	1:Ac:37:SER:OG	2.53	0.42
1:Ac:59:VAL:HG23	1:Ac:159:VAL:HG22	2.00	0.42
1:Ac:93:MET:HE1	1:Ac:98:PHE:HB2	2.01	0.42
1:Ac:109:LEU:C	1:Ac:111:PRO:HD3	2.44	0.42
2:Cc:77:THR:HB	2:Cc:238:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ab:59:VAL:HG23	1:Ab:159:VAL:HG22	2.00	0.42
1:Ab:298:MET:HE1	1:Ab:387:PHE:CD2	2.55	0.42
3:Ba:273:GLY:O	3:Ba:274:LEU:C	2.63	0.42
1:Ab:109:LEU:C	1:Ab:111:PRO:HD3	2.44	0.42
2:Cc:21:ALA:O	2:Cc:22:VAL:C	2.63	0.42
2:Ca:21:ALA:O	2:Ca:22:VAL:C	2.63	0.41
1:Ac:95:GLY:O	1:Ac:97:VAL:N	2.52	0.41
3:Bb:232:THR:HG23	2:Cc:214:THR:HA	2.01	0.41
3:Bc:76:ALA:HB1	3:Bc:84:GLU:HB3	2.02	0.41
3:Bc:81:PHE:CE2	1:Ac:375:ARG:HD2	2.55	0.41
1:Aa:64:THR:HA	1:Aa:128:LEU:O	2.21	0.41
1:Aa:300:MET:HE3	1:Aa:300:MET:HB2	1.93	0.41
1:Ac:64:THR:HA	1:Ac:128:LEU:O	2.21	0.41
1:Ac:84:PRO:HB2	1:Ac:116:LEU:HB2	2.02	0.41
1:Ac:308:GLY:O	1:Ac:356:PRO:HB3	2.20	0.41
1:Aa:45:ARG:NH2	1:Aa:406:ASP:OD1	2.54	0.41
1:Aa:215:ARG:NH1	2:Ca:91:ARG:O	2.53	0.41
1:Aa:298:MET:HE1	1:Aa:387:PHE:CD2	2.55	0.41
1:Aa:308:GLY:O	1:Aa:356:PRO:HB3	2.20	0.41
3:Bb:66:ARG:C	3:Bb:66:ARG:HD3	2.45	0.41
3:Bb:273:GLY:O	3:Bb:274:LEU:C	2.63	0.41
1:Ab:101:LYS:HD2	1:Ab:101:LYS:HA	1.72	0.41
1:Ab:308:GLY:O	1:Ab:356:PRO:HB3	2.20	0.41
2:Cc:20:GLU:H	2:Cc:20:GLU:HG3	1.56	0.41
1:Ab:96:PRO:CG	2:Cb:121:PHE:CE1	3.04	0.41
1:Ac:45:ARG:NH2	1:Ac:406:ASP:OD1	2.54	0.41
2:Cb:45:HIS:HE1	2:Cb:107:GLU:HG2	1.85	0.41
2:Ca:59:SER:HA	2:Ca:62:LYS:HG3	2.03	0.41
2:Ca:64:ARG:HH21	2:Ca:208:GLU:CD	2.29	0.41
3:Bb:256:LEU:HD12	3:Bb:256:LEU:HA	1.91	0.41
1:Ab:45:ARG:NH2	1:Ab:406:ASP:OD1	2.54	0.41
1:Ab:103:SER:N	2:Cb:193:TYR:OH	2.53	0.41
2:Cb:59:SER:HA	2:Cb:62:LYS:HG3	2.03	0.41
3:Ba:66:ARG:HD3	3:Ba:66:ARG:C	2.45	0.41
3:Ba:208:LEU:HD13	2:Cb:251:LEU:HD11	2.01	0.41
1:Ab:64:THR:HA	1:Ab:128:LEU:O	2.21	0.41
2:Ca:26:ARG:HA	2:Ca:26:ARG:HD2	1.27	0.41
2:Ca:197:ARG:HE	2:Ca:200:THR:HG1	1.67	0.41
2:Ca:208:GLU:OE1	2:Ca:219:VAL:HG21	2.21	0.41
2:Ca:251:LEU:HD11	3:Bb:208:LEU:HD13	2.03	0.41
3:Bb:76:ALA:HB1	3:Bb:84:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bb:251:PHE:HZ	2:Cc:233:LEU:HD21	1.85	0.41
3:Bc:66:ARG:HD3	3:Bc:66:ARG:C	2.45	0.41
3:Bc:273:GLY:O	3:Bc:274:LEU:C	2.63	0.41
1:Ab:95:GLY:O	1:Ab:97:VAL:N	2.52	0.41
2:Cb:64:ARG:HH21	2:Cb:208:GLU:CD	2.29	0.41
2:Cb:71:THR:HB	2:Cb:72:PRO:HD3	2.03	0.41
2:Cc:208:GLU:OE1	2:Cc:219:VAL:HG21	2.21	0.41
1:Aa:84:PRO:HB2	1:Aa:116:LEU:HB2	2.02	0.41
1:Aa:208:ARG:HA	1:Aa:208:ARG:HD2	1.73	0.41
3:Ba:45:LEU:HD23	3:Ba:45:LEU:HA	1.93	0.41
2:Cb:21:ALA:O	2:Cb:22:VAL:C	2.63	0.41
1:Aa:141:MET:HE2	1:Aa:141:MET:HB2	1.62	0.41
3:Ba:223:ASN:O	3:Ba:226:LEU:N	2.52	0.41
1:Aa:233:ARG:HH21	2:Ca:144:LEU:HA	1.86	0.40
2:Ca:110:ASN:ND2	3:Bb:154:GLU:CG	2.83	0.40
3:Ba:154:GLU:OE1	2:Cb:45:HIS:NE2	2.54	0.40
2:Cc:64:ARG:HH21	2:Cc:208:GLU:CD	2.29	0.40
2:Cc:97:THR:OG1	2:Cc:139:ASP:OD2	2.24	0.40
2:Ca:71:THR:HB	2:Ca:72:PRO:HD3	2.03	0.40
1:Ab:336:TYR:CG	1:Ab:337:PRO:HD2	2.57	0.40
2:Cb:236:PHE:O	2:Cb:239:HIS:HB3	2.21	0.40
2:Ca:45:HIS:HE1	2:Ca:107:GLU:HG2	1.85	0.40
3:Bc:256:LEU:HD12	3:Bc:256:LEU:HA	1.91	0.40
2:Cb:217:LYS:HE2	2:Cb:217:LYS:HB2	1.92	0.40
1:Aa:96:PRO:CG	2:Ca:121:PHE:CE1	3.04	0.40
1:Aa:375:ARG:HD2	3:Bb:81:PHE:CE2	2.55	0.40
2:Cb:30:TRP:HA	2:Cb:30:TRP:CE3	2.57	0.40
1:Aa:246:ILE:HD13	1:Aa:246:ILE:HA	1.94	0.40
2:Ca:236:PHE:O	2:Ca:239:HIS:HB3	2.21	0.40
2:Cc:30:TRP:HA	2:Cc:30:TRP:CE3	2.57	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	Aa	380/382 (100%)	358 (94%)	20 (5%)	2 (0%)	24	54
1	Ab	380/382 (100%)	358 (94%)	20 (5%)	2 (0%)	24	54
1	Ac	380/382 (100%)	358 (94%)	20 (5%)	2 (0%)	24	54
2	Ca	236/239 (99%)	220 (93%)	16 (7%)	0	100	100
2	Cb	236/239 (99%)	221 (94%)	15 (6%)	0	100	100
2	Cc	236/239 (99%)	220 (93%)	16 (7%)	0	100	100
3	Ba	225/237 (95%)	214 (95%)	8 (4%)	3 (1%)	9	32
3	Bb	225/237 (95%)	214 (95%)	8 (4%)	3 (1%)	9	32
3	Bc	225/237 (95%)	214 (95%)	8 (4%)	3 (1%)	9	32
All	All	2523/2574 (98%)	2377 (94%)	131 (5%)	15 (1%)	23	51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Ba	244	LEU
3	Bb	244	LEU
3	Bc	244	LEU
3	Ba	273	GLY
3	Bb	273	GLY
3	Bc	273	GLY
3	Ba	224	VAL
3	Bb	224	VAL
3	Bc	224	VAL
1	Aa	34	GLY
1	Ab	34	GLY
1	Ac	34	GLY
1	Aa	294	PRO
1	Ab	294	PRO
1	Ac	294	PRO

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	Aa	323/323 (100%)	298 (92%)	25 (8%)	12	35
1	Ab	323/323 (100%)	297 (92%)	26 (8%)	11	34
1	Ac	323/323 (100%)	298 (92%)	25 (8%)	12	35
2	Ca	204/205 (100%)	190 (93%)	14 (7%)	14	41
2	Cb	204/205 (100%)	190 (93%)	14 (7%)	14	41
2	Cc	204/205 (100%)	189 (93%)	15 (7%)	13	38
3	Ba	192/200 (96%)	181 (94%)	11 (6%)	18	49
3	Bb	192/200 (96%)	182 (95%)	10 (5%)	21	52
3	Bc	192/200 (96%)	182 (95%)	10 (5%)	21	52
All	All	2157/2184 (99%)	2007 (93%)	150 (7%)	16	40

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	36	LYS
1	Aa	46	THR
1	Aa	47	ILE
1	Aa	58	LYS
1	Aa	59	VAL
1	Aa	65	VAL
1	Aa	66	GLU
1	Aa	68	LYS
1	Aa	70	LYS
1	Aa	79	GLU
1	Aa	80	THR
1	Aa	86	VAL
1	Aa	91	VAL
1	Aa	100	ARG
1	Aa	102	GLU
1	Aa	108	GLN
1	Aa	113	SER
1	Aa	114	VAL
1	Aa	118	ILE
1	Aa	120	LYS
1	Aa	140	THR
1	Aa	141	MET
1	Aa	211	ILE
1	Aa	312	ILE

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Mol	Chain	Res	Type
1	Aa	399	ASN
2	Ca	18	HIS
2	Ca	20	GLU
2	Ca	22	VAL
2	Ca	25	SER
2	Ca	26	ARG
2	Ca	65	ARG
2	Ca	76	VAL
2	Ca	111	ARG
2	Ca	123	ILE
2	Ca	246	SER
2	Ca	248	GLU
2	Ca	249	ARG
2	Ca	252	GLN
2	Ca	255	SER
3	Ba	113	LYS
3	Ba	145	ILE
3	Ba	161	GLN
3	Ba	168	ASP
3	Ba	217	PRO
3	Ba	220	ILE
3	Ba	227	ASN
3	Ba	232	THR
3	Ba	244	LEU
3	Ba	277	SER
3	Ba	279	CYS
3	Bb	145	ILE
3	Bb	161	GLN
3	Bb	168	ASP
3	Bb	217	PRO
3	Bb	220	ILE
3	Bb	227	ASN
3	Bb	232	THR
3	Bb	244	LEU
3	Bb	277	SER
3	Bb	279	CYS
3	Bc	145	ILE
3	Bc	161	GLN
3	Bc	168	ASP
3	Bc	217	PRO
3	Bc	220	ILE
3	Bc	227	ASN

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Mol	Chain	Res	Type
3	Bc	232	THR
3	Bc	244	LEU
3	Bc	277	SER
3	Bc	279	CYS
1	Ab	36	LYS
1	Ab	46	THR
1	Ab	47	ILE
1	Ab	58	LYS
1	Ab	59	VAL
1	Ab	65	VAL
1	Ab	66	GLU
1	Ab	68	LYS
1	Ab	70	LYS
1	Ab	79	GLU
1	Ab	80	THR
1	Ab	86	VAL
1	Ab	91	VAL
1	Ab	100	ARG
1	Ab	102	GLU
1	Ab	108	GLN
1	Ab	113	SER
1	Ab	114	VAL
1	Ab	118	ILE
1	Ab	120	LYS
1	Ab	140	THR
1	Ab	141	MET
1	Ab	211	ILE
1	Ab	312	ILE
1	Ab	339	ASP
1	Ab	399	ASN
1	Ac	36	LYS
1	Ac	46	THR
1	Ac	47	ILE
1	Ac	58	LYS
1	Ac	59	VAL
1	Ac	65	VAL
1	Ac	66	GLU
1	Ac	68	LYS
1	Ac	70	LYS
1	Ac	79	GLU
1	Ac	80	THR
1	Ac	86	VAL

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Mol	Chain	Res	Type
1	Ac	91	VAL
1	Ac	100	ARG
1	Ac	102	GLU
1	Ac	108	GLN
1	Ac	113	SER
1	Ac	114	VAL
1	Ac	118	ILE
1	Ac	120	LYS
1	Ac	140	THR
1	Ac	141	MET
1	Ac	211	ILE
1	Ac	312	ILE
1	Ac	399	ASN
2	Cb	16	ARG
2	Cb	18	HIS
2	Cb	20	GLU
2	Cb	22	VAL
2	Cb	25	SER
2	Cb	26	ARG
2	Cb	65	ARG
2	Cb	76	VAL
2	Cb	111	ARG
2	Cb	123	ILE
2	Cb	248	GLU
2	Cb	249	ARG
2	Cb	252	GLN
2	Cb	255	SER
2	Cc	16	ARG
2	Cc	18	HIS
2	Cc	20	GLU
2	Cc	22	VAL
2	Cc	25	SER
2	Cc	26	ARG
2	Cc	65	ARG
2	Cc	76	VAL
2	Cc	111	ARG
2	Cc	123	ILE
2	Cc	246	SER
2	Cc	248	GLU
2	Cc	249	ARG
2	Cc	252	GLN
2	Cc	255	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	404	GLN
2	Ca	83	GLN
3	Ba	223	ASN
3	Ba	231	HIS
3	Bb	223	ASN
3	Bc	223	ASN
1	Ab	404	GLN
1	Ac	404	GLN
2	Cb	83	GLN
2	Cc	83	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

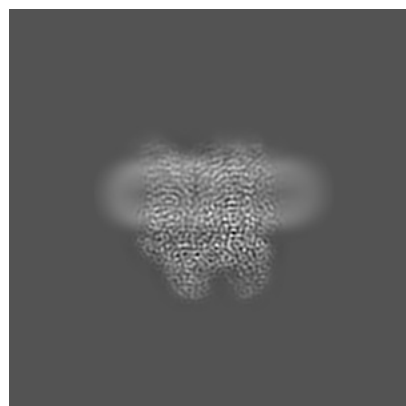
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45658. These allow visual inspection of the internal detail of the map and identification of artifacts.

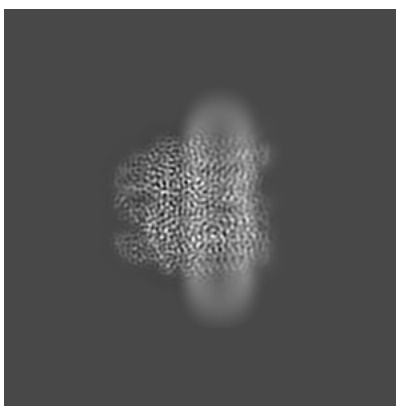
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

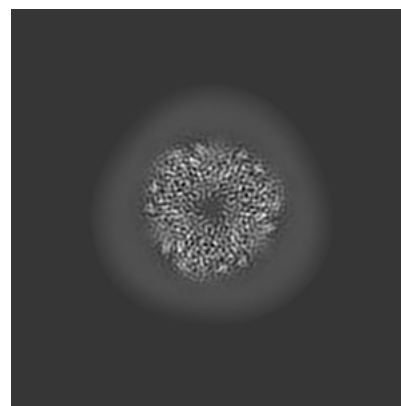
6.1.1 Primary map



X

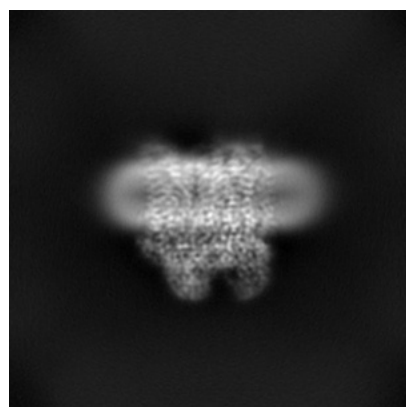


Y

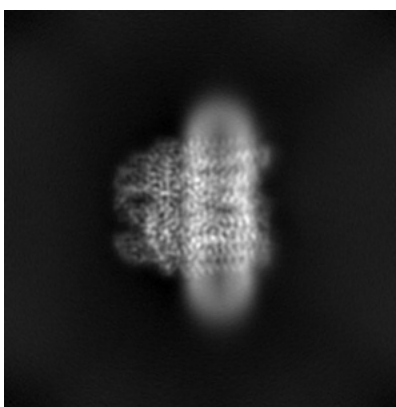


Z

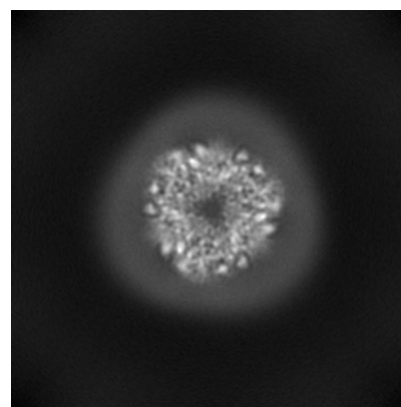
6.1.2 Raw map



X



Y



Z

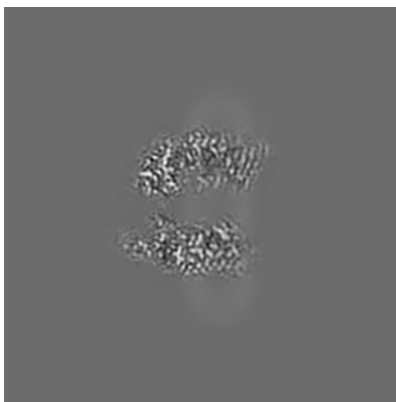
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

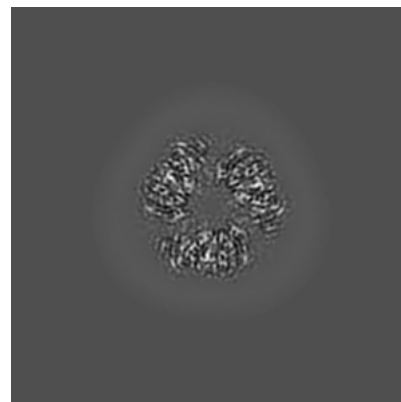
6.2.1 Primary map



X Index: 128

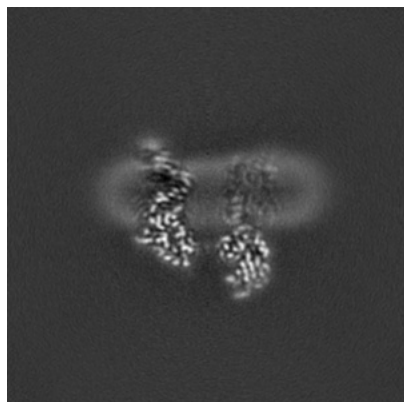


Y Index: 128

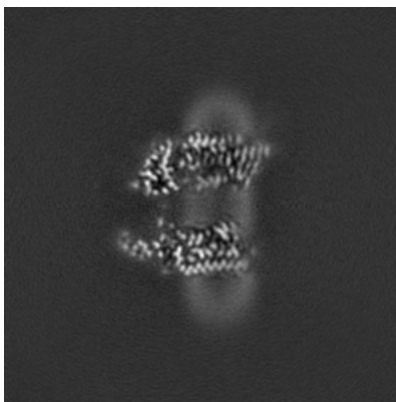


Z Index: 128

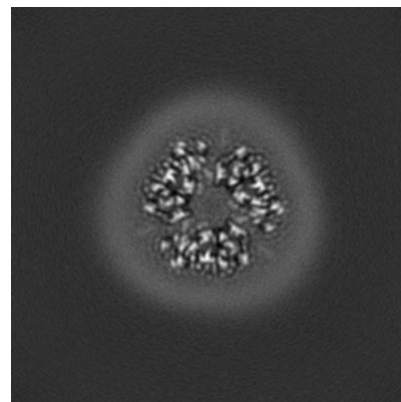
6.2.2 Raw map



X Index: 128



Y Index: 128

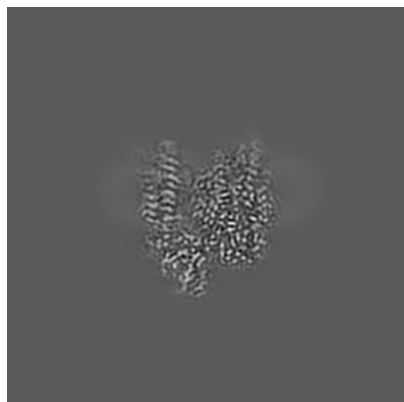


Z Index: 128

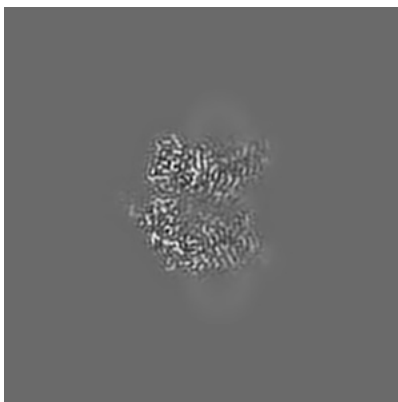
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 107

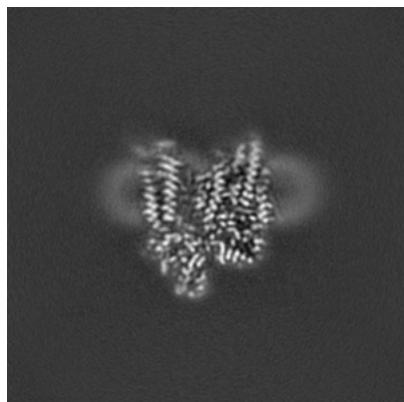


Y Index: 141

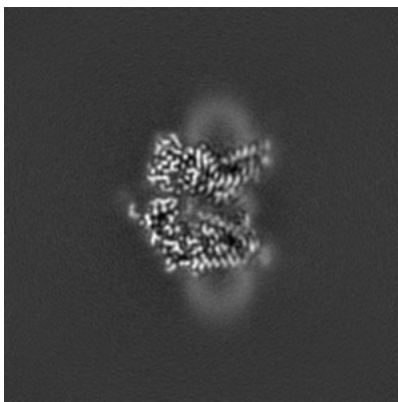


Z Index: 104

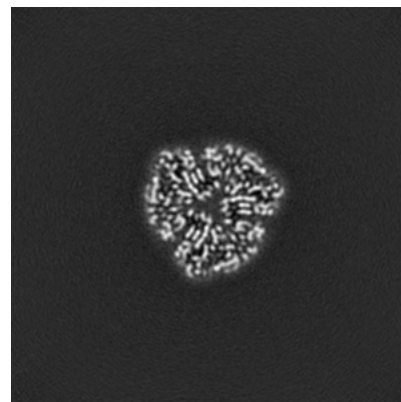
6.3.2 Raw map



X Index: 108



Y Index: 141

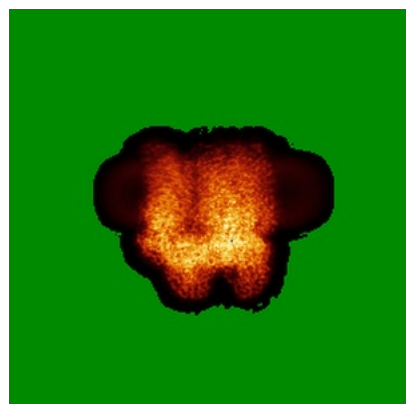


Z Index: 104

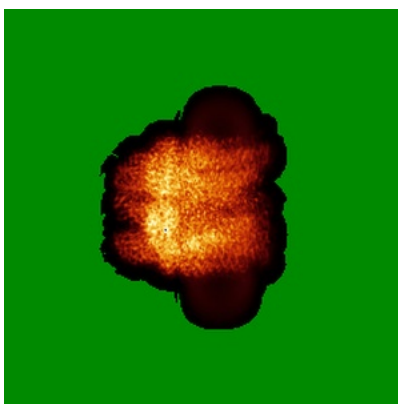
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

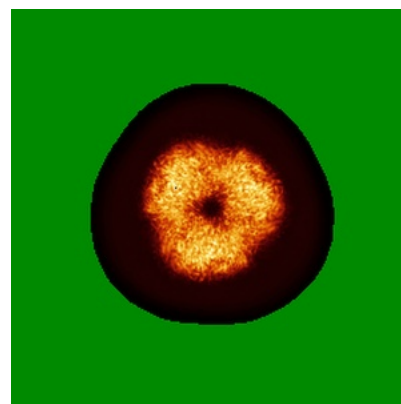
6.4.1 Primary map



X

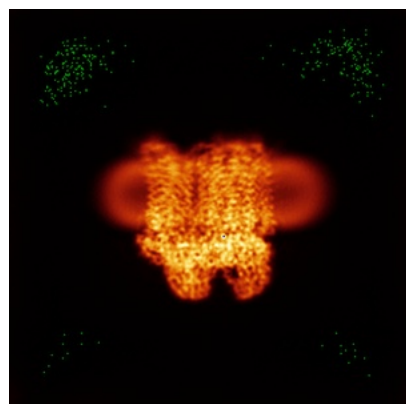


Y

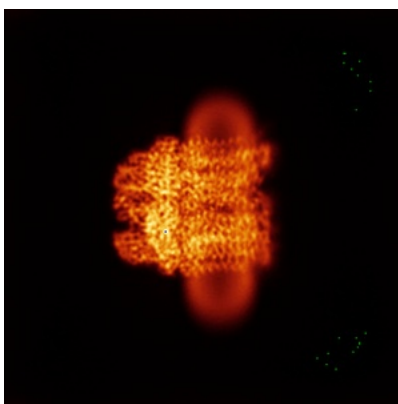


Z

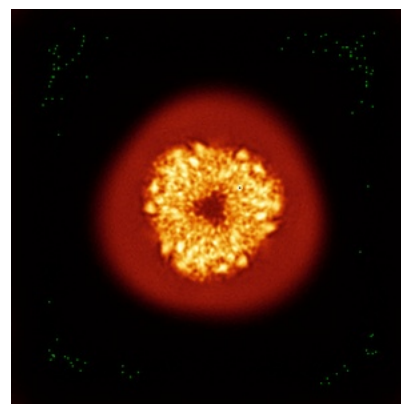
6.4.2 Raw map



X



Y

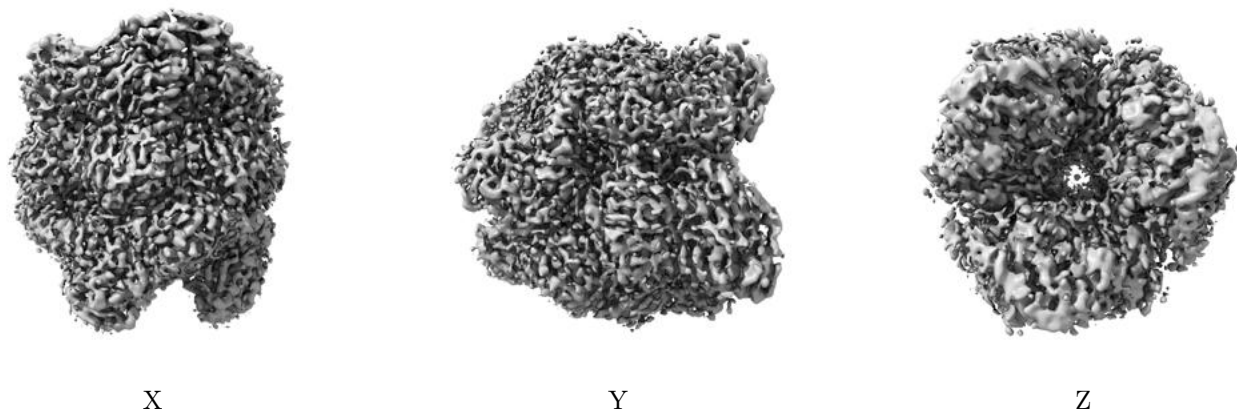


Z

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.

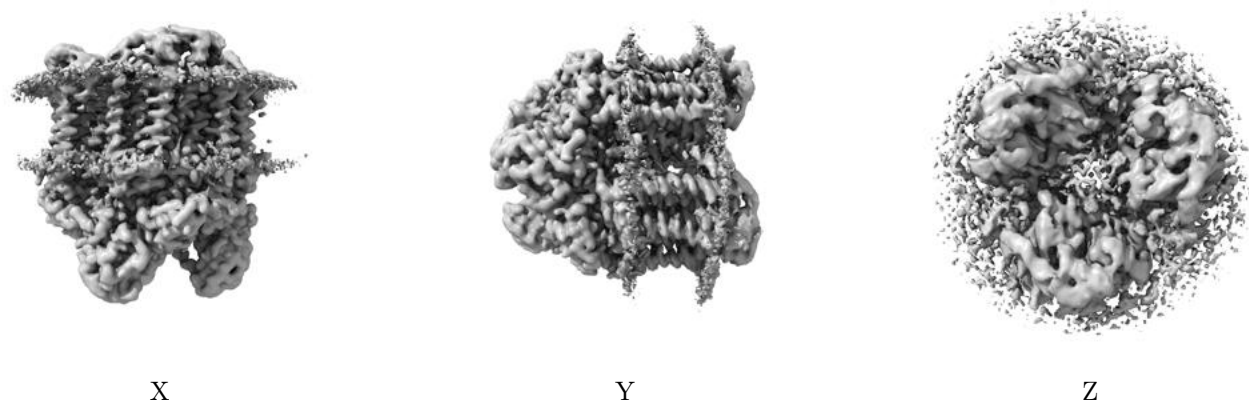
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.355. 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.

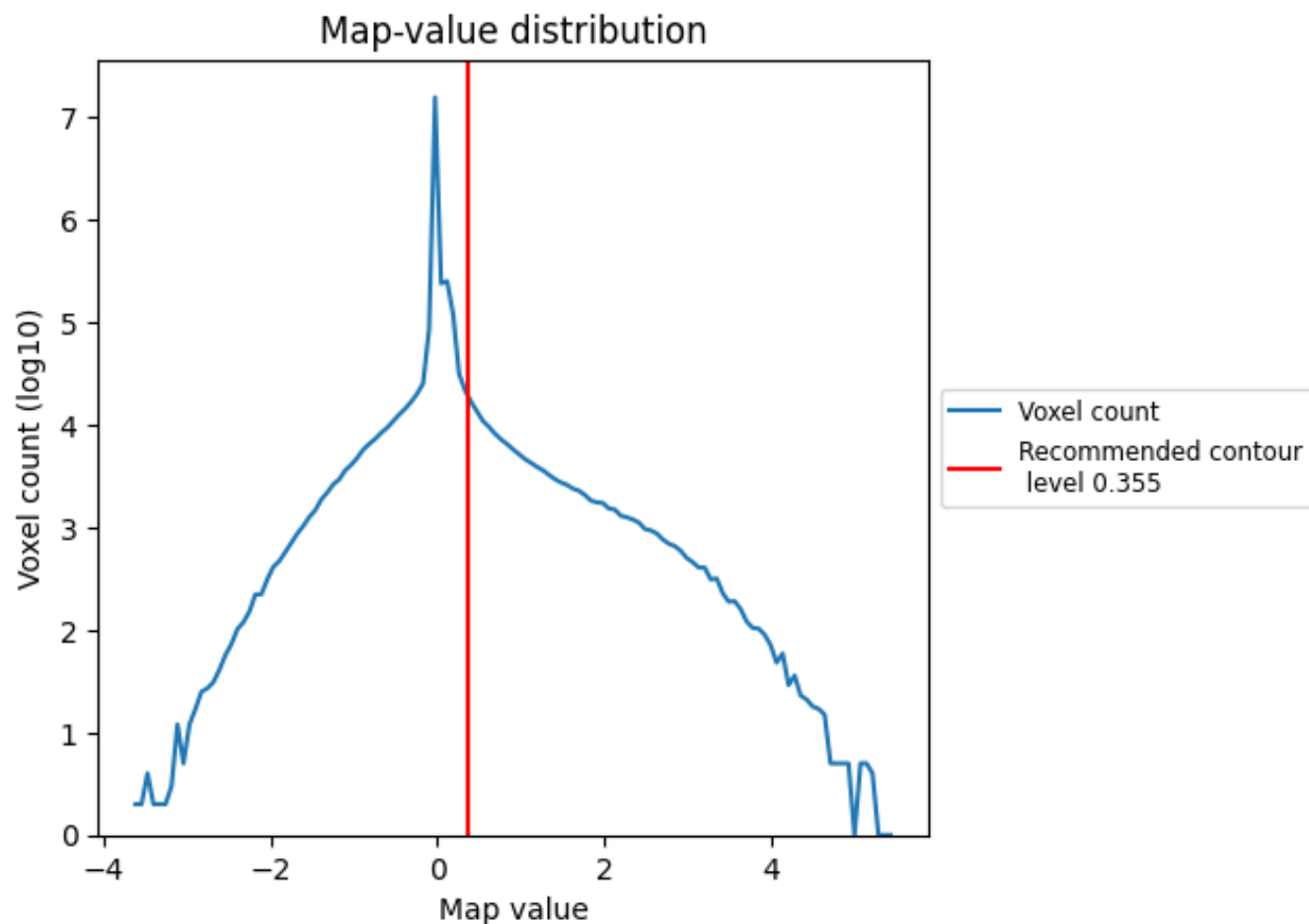
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

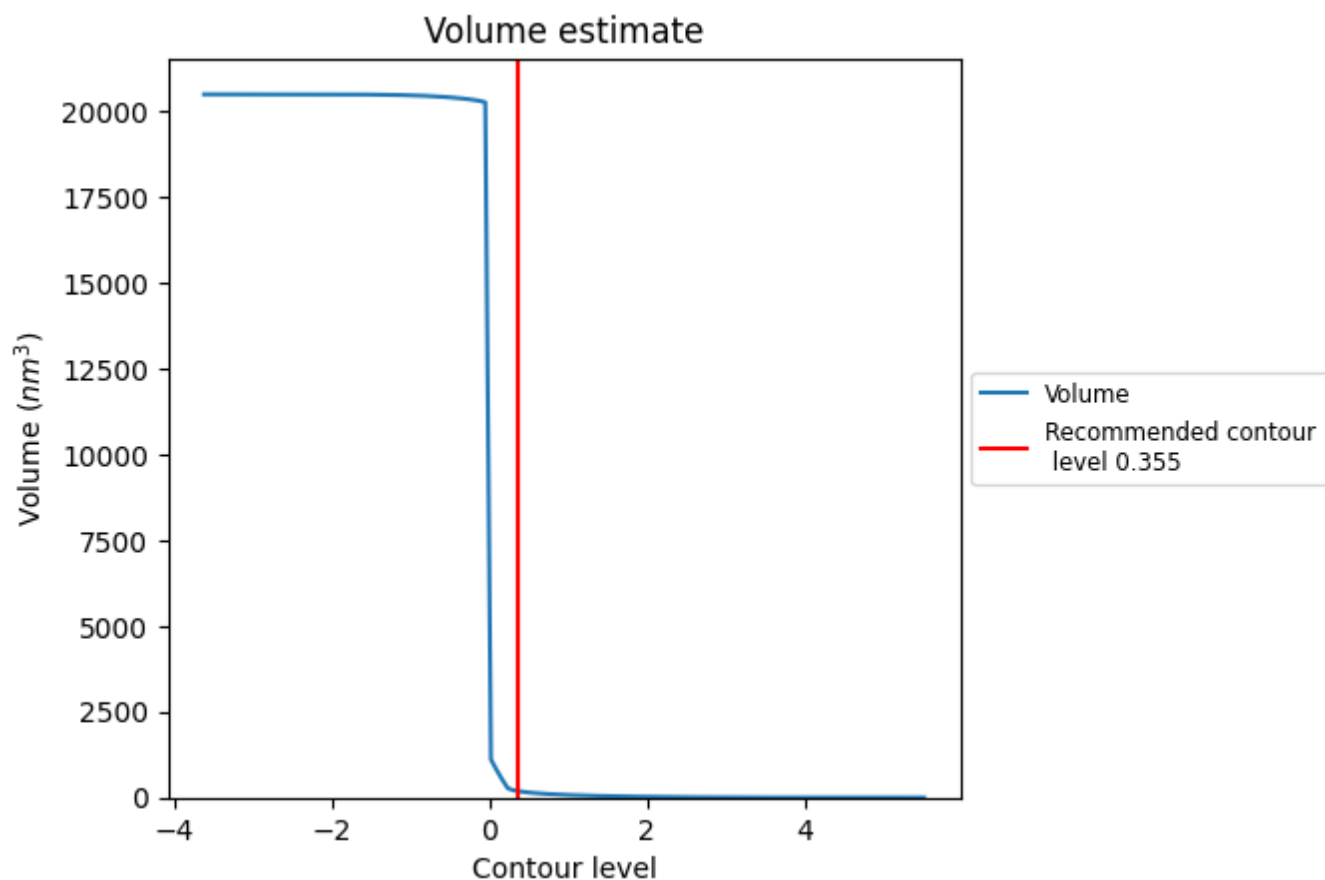
This section contains the results of statistical analysis of the map.

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.

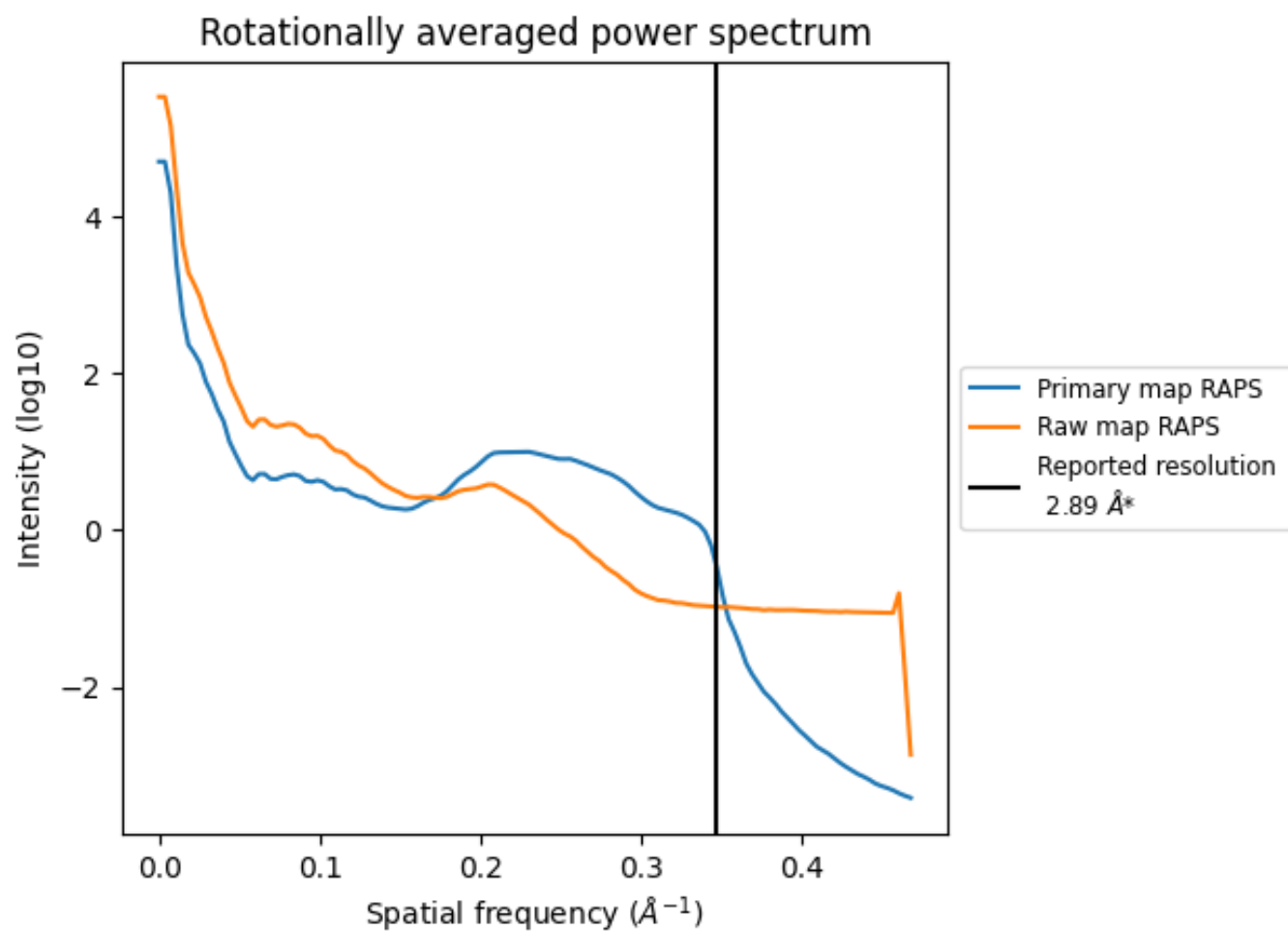
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

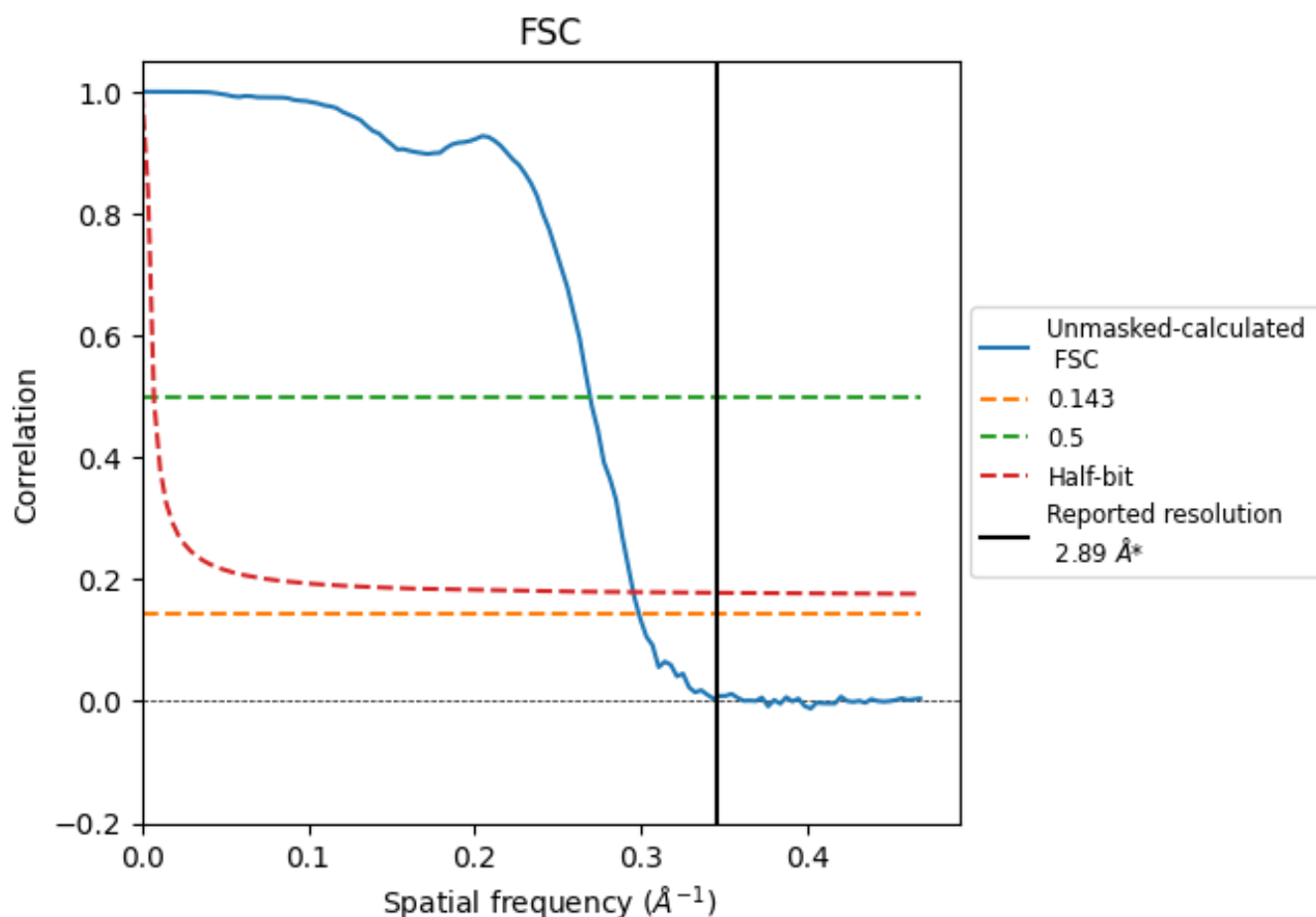


*Reported resolution corresponds to spatial frequency of $0.346 \text{ \AA}^{-1}$

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 0.346 Å⁻¹

8.2 Resolution estimates [i](#)

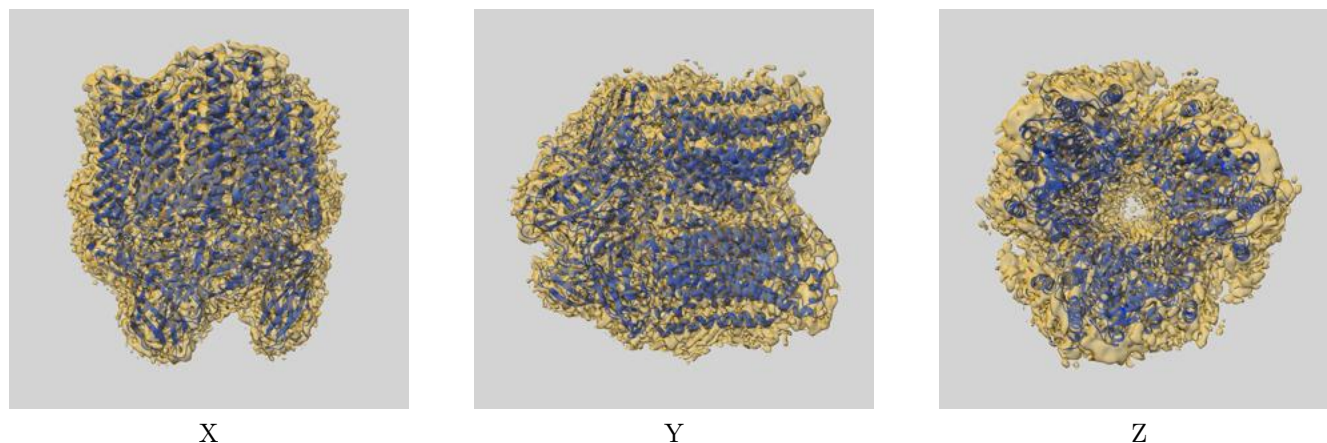
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.35	3.71	3.39

*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 3.35 differs from the reported value 2.89 by more than 10 %

9 Map-model fit [i](#)

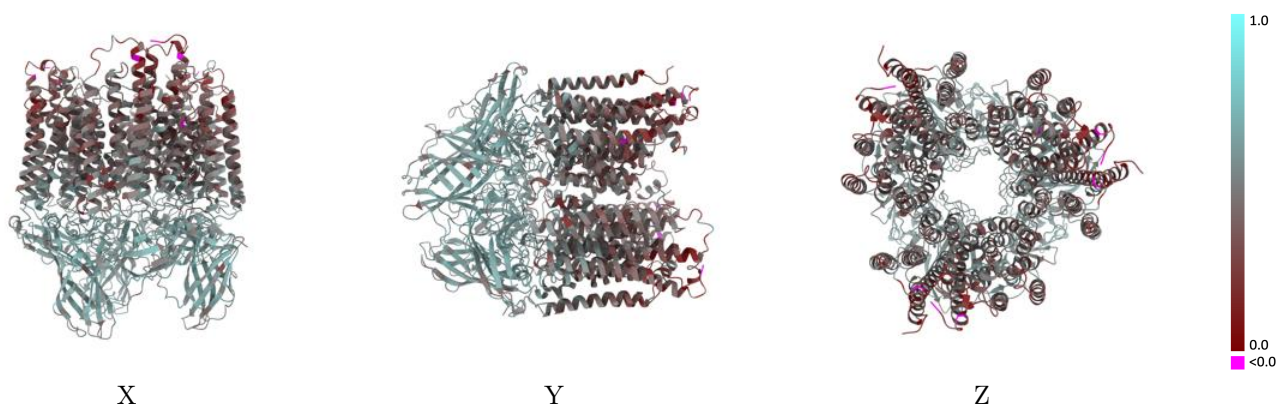
This section contains information regarding the fit between EMDB map EMD-45658 and PDB model 9CL1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



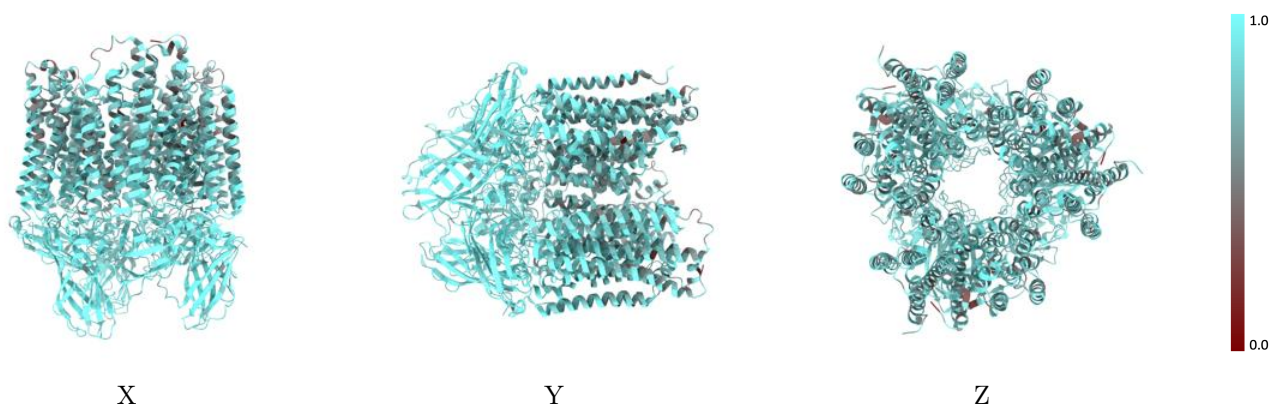
The images above show the 3D surface view of the map at the recommended contour level 0.355 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



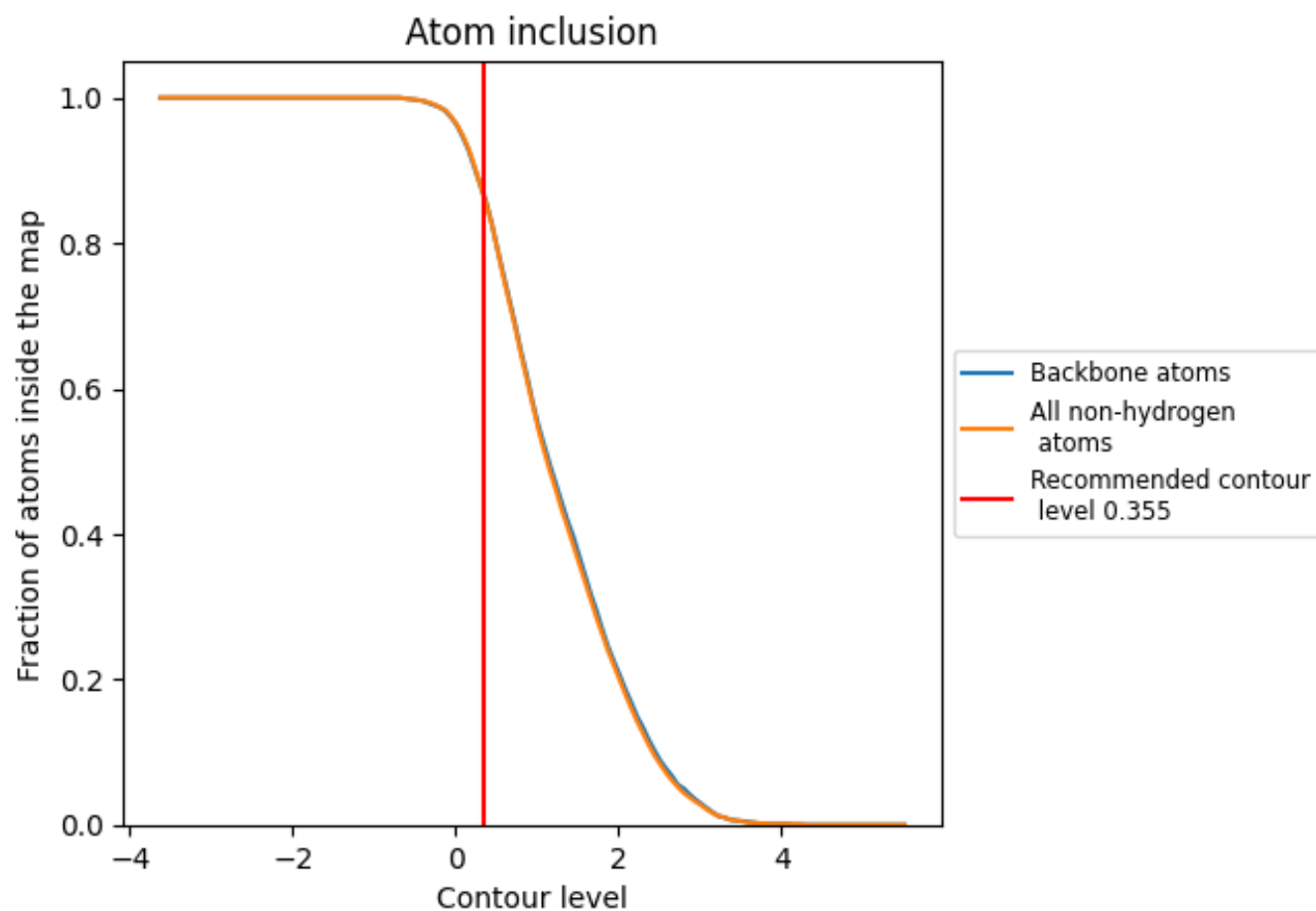
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.355).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.355) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.4750
Aa	0.9150	0.5380
Ab	0.9140	0.5390
Ac	0.9150	0.5370
Ba	0.7950	0.3950
Bb	0.8060	0.3990
Bc	0.7970	0.3970
Ca	0.8540	0.4530
Cb	0.8510	0.4490
Cc	0.8590	0.4560

1.0

0.0

<0.0