



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:10 PM UTC

PDB ID : 9CL5 / pdb_00009cl5
EMDB ID : EMD-45662
Title : particulate methane monooxygenase in native membranes
Authors : Tucci, F.J.; Rosenzweig, A.C.
Deposited on : 2024-07-10
Resolution : 2.48 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

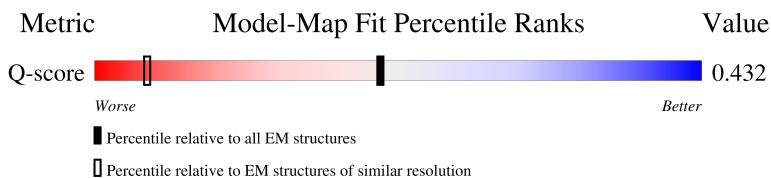
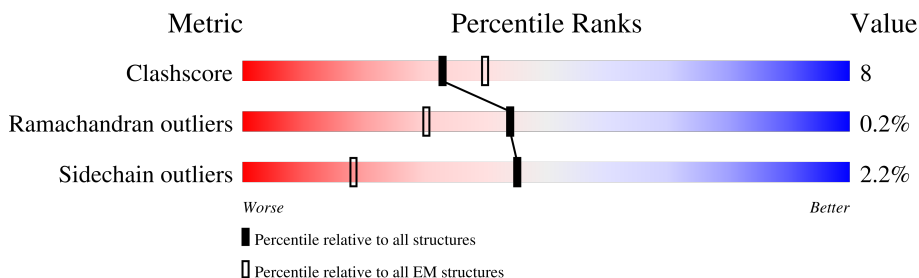
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.48 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.



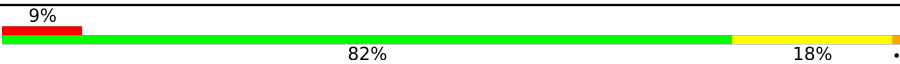
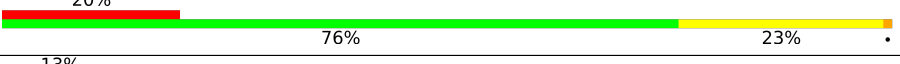
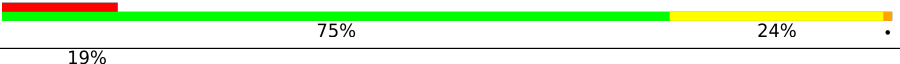
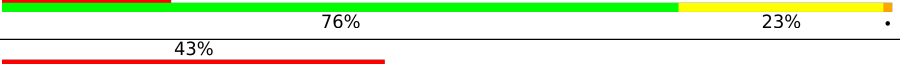
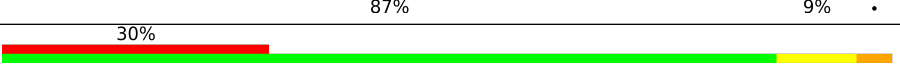
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6178 (1.98 - 2.98)

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	Ba	244	7% 76% 24%
1	Bb	244	11% 76% 24%
1	Bc	244	6% 75% 24%
2	Aa	388	7% 80% 19% .

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Mol	Chain	Length	Quality of chain
2	Ab	388	
2	Ac	388	
3	Ca	241	
3	Cb	241	
3	Cc	241	
4	Da	23	
4	Db	23	
4	Dc	23	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22272 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 Methane monooxygenase/ammonia monooxygenase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ba	244	Total	C	N	O	S	0	0
			1974	1336	311	316	11		
1	Bb	244	Total	C	N	O	S	0	0
			1974	1336	311	316	11		
1	Bc	244	Total	C	N	O	S	0	0
			1974	1336	311	316	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ba	151	VAL	ILE	conflict	UNP A0A5R8QJU8
Bb	151	VAL	ILE	conflict	UNP A0A5R8QJU8
Bc	151	VAL	ILE	conflict	UNP A0A5R8QJU8

- Molecule 2 is a protein called Methane monooxygenase/ammonia monooxygenase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aa	388	Total	C	N	O	S	0	0
			3026	1946	521	555	4		
2	Ab	388	Total	C	N	O	S	0	0
			3026	1946	521	555	4		
2	Ac	388	Total	C	N	O	S	0	0
			3026	1946	521	555	4		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	49	GLN	ALA	conflict	UNP A0A431PQN7
Aa	60	GLU	ASP	conflict	UNP A0A431PQN7
Aa	200	PHE	LEU	conflict	UNP A0A431PQN7
Aa	204	VAL	ILE	conflict	UNP A0A431PQN7

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	210	THR	ALA	conflict	UNP A0A431PQN7
Aa	214	ARG	LYS	conflict	UNP A0A431PQN7
Aa	219	LYS	ARG	conflict	UNP A0A431PQN7
Aa	220	ALA	PRO	conflict	UNP A0A431PQN7
Aa	277	VAL	ALA	conflict	UNP A0A431PQN7
Aa	283	ASN	GLN	conflict	UNP A0A431PQN7
Aa	309	ASN	GLY	conflict	UNP A0A431PQN7
Aa	314	LEU	VAL	conflict	UNP A0A431PQN7
Aa	330	ASP	SER	conflict	UNP A0A431PQN7
Aa	334	THR	SER	conflict	UNP A0A431PQN7
Aa	350	VAL	ASN	conflict	UNP A0A431PQN7
Aa	352	ALA	ASP	conflict	UNP A0A431PQN7
Aa	354	PRO	-	insertion	UNP A0A431PQN7
Aa	360	ALA	SER	conflict	UNP A0A431PQN7
Aa	396	SER	THR	conflict	UNP A0A431PQN7
Aa	402	TYR	PHE	conflict	UNP A0A431PQN7
Aa	404	SER	ALA	conflict	UNP A0A431PQN7
Ab	49	GLN	ALA	conflict	UNP A0A431PQN7
Ab	60	GLU	ASP	conflict	UNP A0A431PQN7
Ab	200	PHE	LEU	conflict	UNP A0A431PQN7
Ab	204	VAL	ILE	conflict	UNP A0A431PQN7
Ab	210	THR	ALA	conflict	UNP A0A431PQN7
Ab	214	ARG	LYS	conflict	UNP A0A431PQN7
Ab	219	LYS	ARG	conflict	UNP A0A431PQN7
Ab	220	ALA	PRO	conflict	UNP A0A431PQN7
Ab	277	VAL	ALA	conflict	UNP A0A431PQN7
Ab	283	ASN	GLN	conflict	UNP A0A431PQN7
Ab	309	ASN	GLY	conflict	UNP A0A431PQN7
Ab	314	LEU	VAL	conflict	UNP A0A431PQN7
Ab	330	ASP	SER	conflict	UNP A0A431PQN7
Ab	334	THR	SER	conflict	UNP A0A431PQN7
Ab	350	VAL	ASN	conflict	UNP A0A431PQN7
Ab	352	ALA	ASP	conflict	UNP A0A431PQN7
Ab	354	PRO	-	insertion	UNP A0A431PQN7
Ab	360	ALA	SER	conflict	UNP A0A431PQN7
Ab	396	SER	THR	conflict	UNP A0A431PQN7
Ab	402	TYR	PHE	conflict	UNP A0A431PQN7
Ab	404	SER	ALA	conflict	UNP A0A431PQN7
Ac	49	GLN	ALA	conflict	UNP A0A431PQN7
Ac	60	GLU	ASP	conflict	UNP A0A431PQN7
Ac	200	PHE	LEU	conflict	UNP A0A431PQN7
Ac	204	VAL	ILE	conflict	UNP A0A431PQN7

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Chain	Residue	Modelled	Actual	Comment	Reference
Ac	210	THR	ALA	conflict	UNP A0A431PQN7
Ac	214	ARG	LYS	conflict	UNP A0A431PQN7
Ac	219	LYS	ARG	conflict	UNP A0A431PQN7
Ac	220	ALA	PRO	conflict	UNP A0A431PQN7
Ac	277	VAL	ALA	conflict	UNP A0A431PQN7
Ac	283	ASN	GLN	conflict	UNP A0A431PQN7
Ac	309	ASN	GLY	conflict	UNP A0A431PQN7
Ac	314	LEU	VAL	conflict	UNP A0A431PQN7
Ac	330	ASP	SER	conflict	UNP A0A431PQN7
Ac	334	THR	SER	conflict	UNP A0A431PQN7
Ac	350	VAL	ASN	conflict	UNP A0A431PQN7
Ac	352	ALA	ASP	conflict	UNP A0A431PQN7
Ac	354	PRO	-	insertion	UNP A0A431PQN7
Ac	360	ALA	SER	conflict	UNP A0A431PQN7
Ac	396	SER	THR	conflict	UNP A0A431PQN7
Ac	402	TYR	PHE	conflict	UNP A0A431PQN7
Ac	404	SER	ALA	conflict	UNP A0A431PQN7

- Molecule 3 is a protein called Particulate methane monooxygenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ca	241	Total	C	N	O	S	0	0
			1982	1337	311	325	9		
3	Cb	241	Total	C	N	O	S	0	0
			1982	1337	311	325	9		
3	Cc	241	Total	C	N	O	S	0	0
			1982	1337	311	325	9		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ca	29	VAL	ALA	conflict	UNP W6D653
Ca	30	LEU	VAL	conflict	UNP W6D653
Ca	96	THR	ALA	conflict	UNP W6D653
Ca	240	MET	GLY	conflict	UNP W6D653
Ca	246	VAL	ILE	conflict	UNP W6D653
Ca	252	LYS	ALA	conflict	UNP W6D653
Cb	29	VAL	ALA	conflict	UNP W6D653
Cb	30	LEU	VAL	conflict	UNP W6D653
Cb	96	THR	ALA	conflict	UNP W6D653
Cb	240	MET	GLY	conflict	UNP W6D653
Cb	246	VAL	ILE	conflict	UNP W6D653

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Chain	Residue	Modelled	Actual	Comment	Reference
Cb	252	LYS	ALA	conflict	UNP W6D653
Cc	29	VAL	ALA	conflict	UNP W6D653
Cc	30	LEU	VAL	conflict	UNP W6D653
Cc	96	THR	ALA	conflict	UNP W6D653
Cc	240	MET	GLY	conflict	UNP W6D653
Cc	246	VAL	ILE	conflict	UNP W6D653
Cc	252	LYS	ALA	conflict	UNP W6D653

- Molecule 4 is a protein called particulate methane monooxygenase supernumerary helix.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Da	23	Total	C	N	O	S	0	0
			167	112	27	25	3		
4	Db	23	Total	C	N	O	S	0	0
			167	112	27	25	3		
4	Dc	23	Total	C	N	O	S	0	0
			167	112	27	25	3		

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	Aa	1	Total	Cu	0
			1	1	
5	Ca	1	Total	Cu	0
			1	1	
5	Ab	1	Total	Cu	0
			1	1	
5	Ac	1	Total	Cu	0
			1	1	
5	Cb	1	Total	Cu	0
			1	1	
5	Cc	1	Total	Cu	0
			1	1	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	Ba	55	Total	O	0
			55	55	
6	Aa	167	Total	O	0
			167	167	

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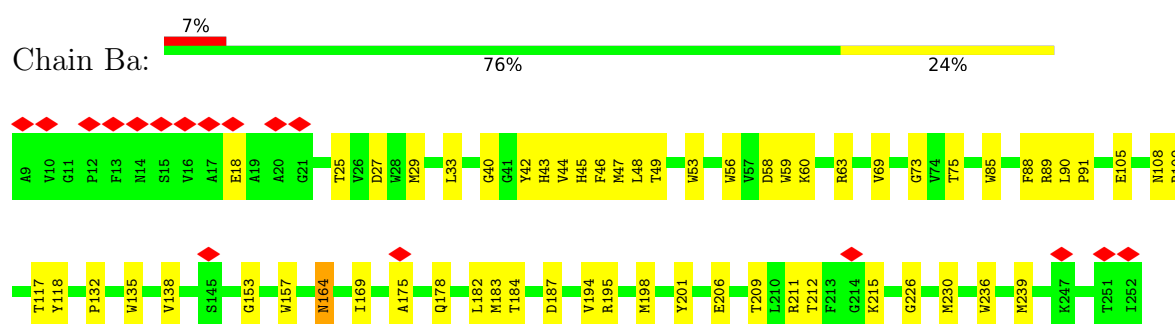
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Mol	Chain	Residues	Atoms		AltConf
6	Ca	49	Total 49	O 49	0
6	Da	3	Total 3	O 3	0
6	Bb	54	Total 54	O 54	0
6	Bc	54	Total 54	O 54	0
6	Ab	166	Total 166	O 166	0
6	Ac	167	Total 167	O 167	0
6	Cb	49	Total 49	O 49	0
6	Cc	49	Total 49	O 49	0
6	Db	3	Total 3	O 3	0
6	Dc	3	Total 3	O 3	0

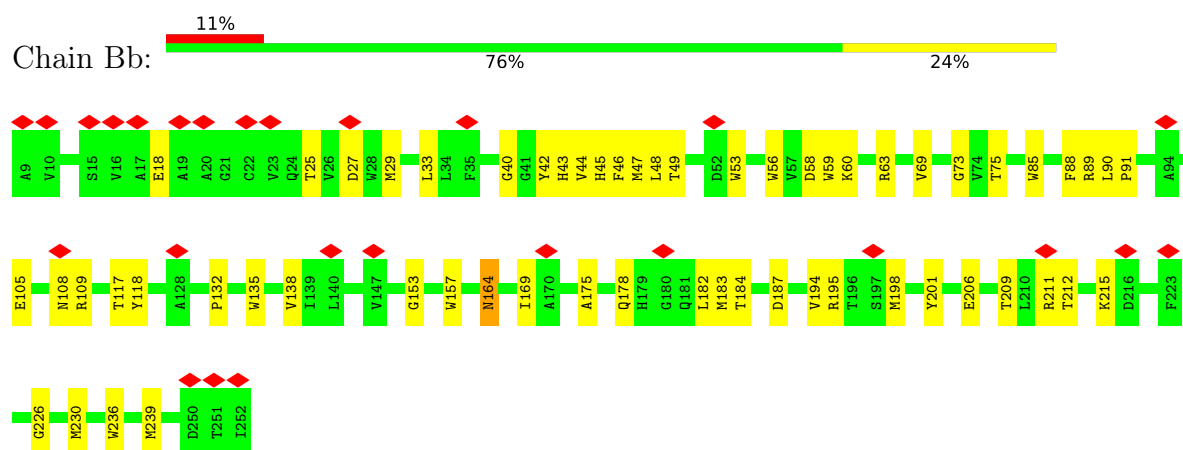
3 Residue-property plots

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.

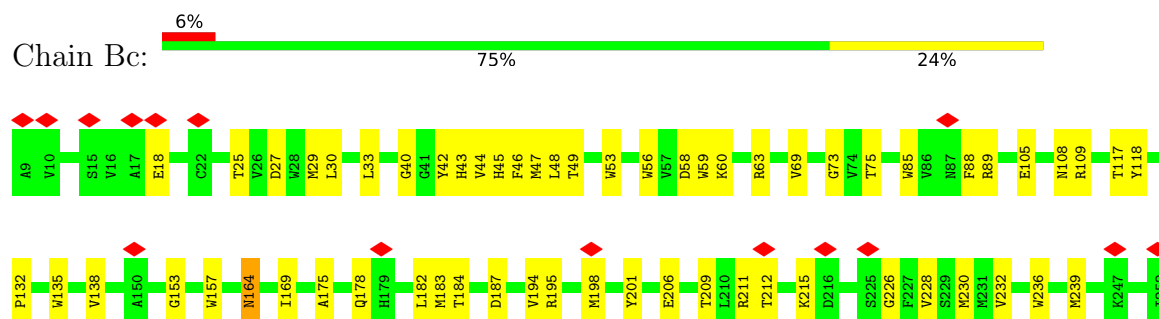
- Molecule 1: Methane monooxygenase/ammonia monooxygenase subunit A



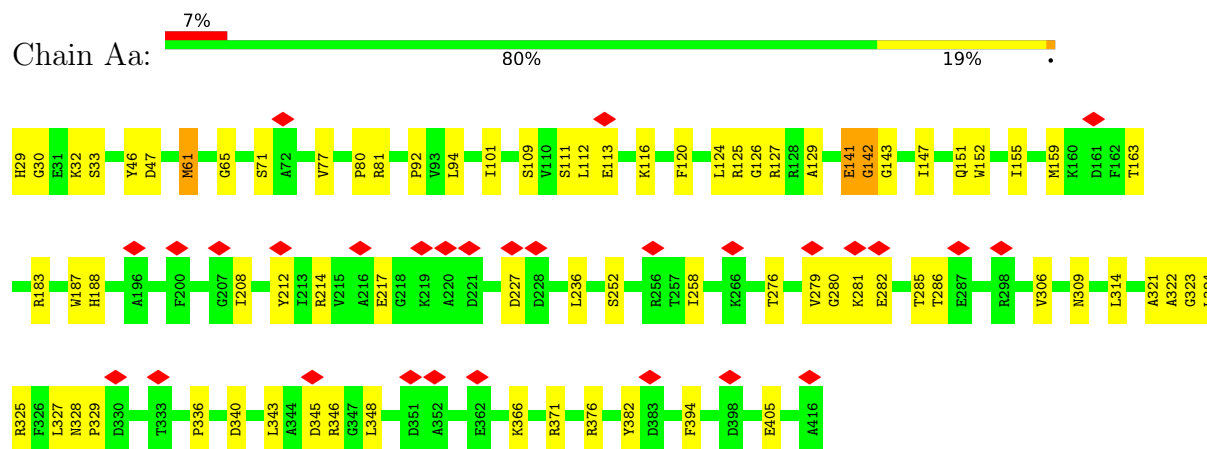
- Molecule 1: Methane monooxygenase/ammonia monooxygenase subunit A



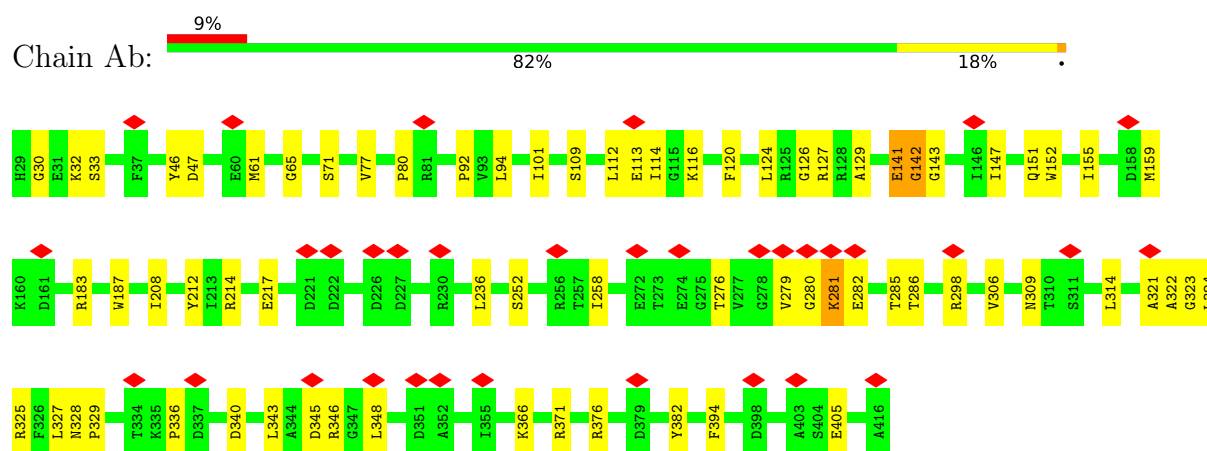
- Molecule 1: Methane monooxygenase/ammonia monooxygenase subunit A



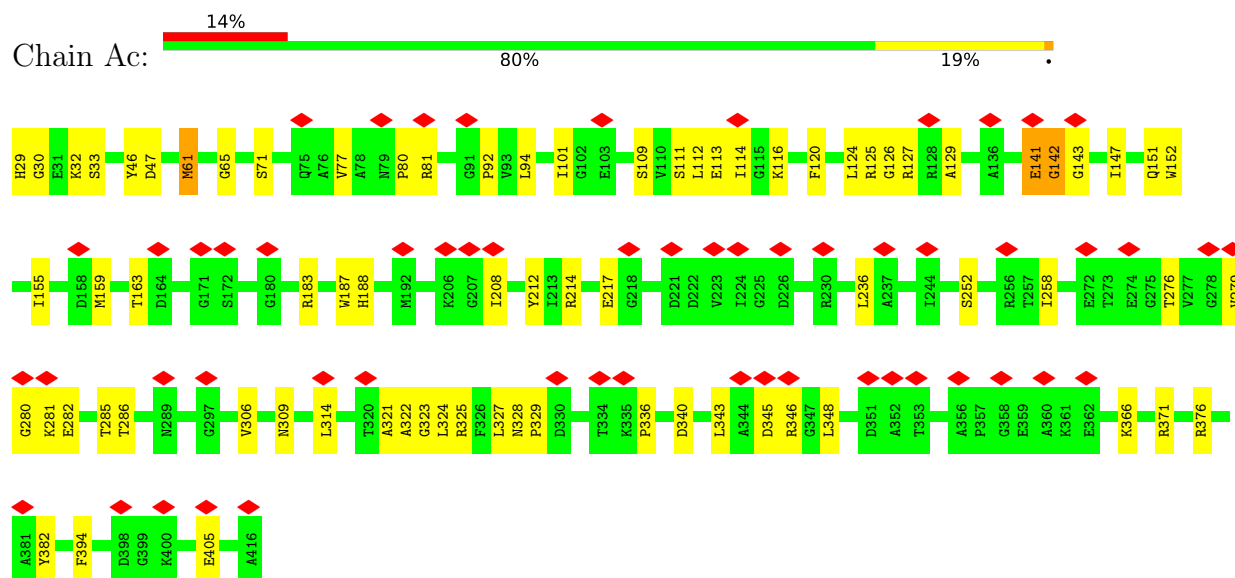
- Molecule 2: Methane monooxygenase/ammonia monooxygenase subunit B



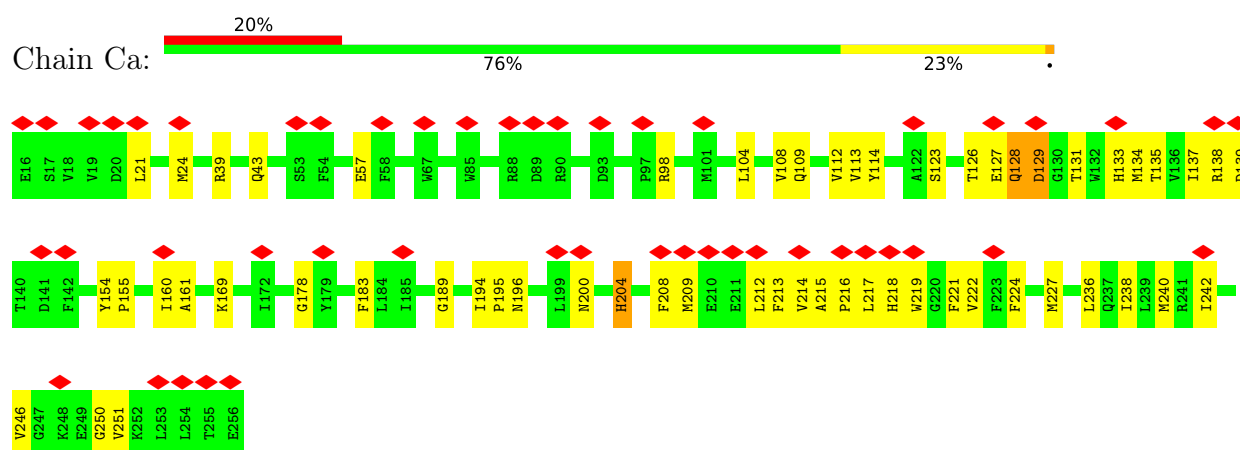
- Molecule 2: Methane monooxygenase/ammonia monooxygenase subunit B



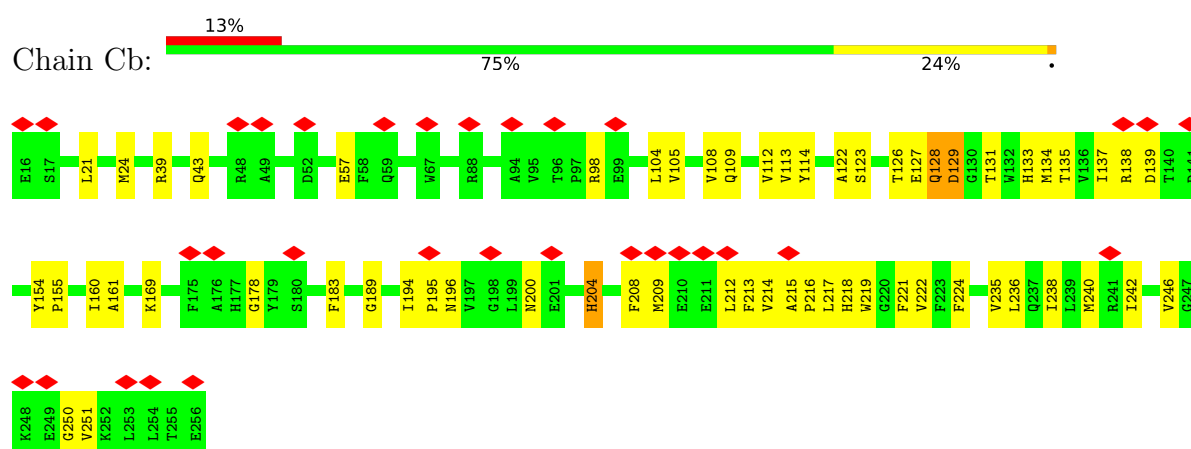
- Molecule 2: Methane monooxygenase/ammonia monooxygenase subunit B



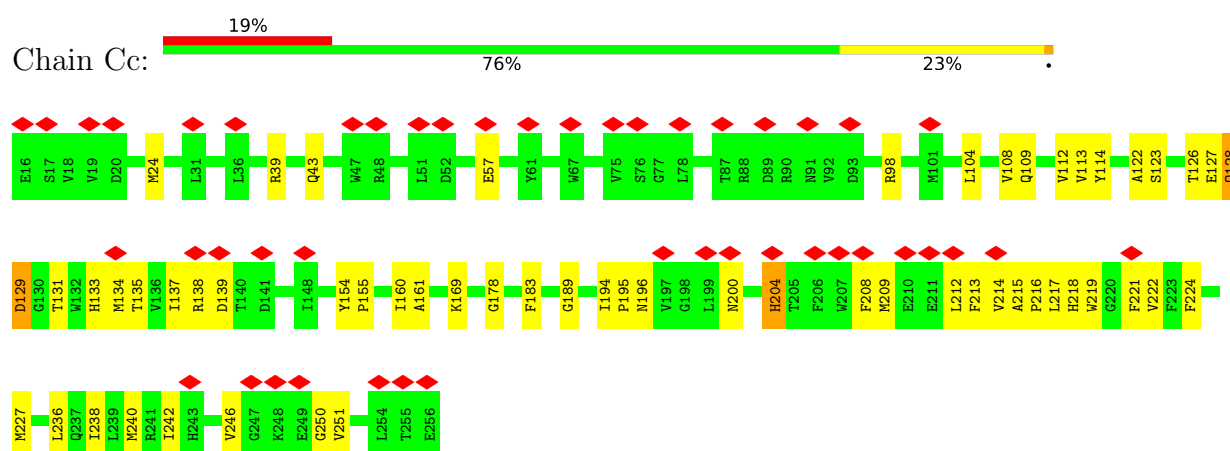
- Molecule 3: Particulate methane monooxygenase subunit C



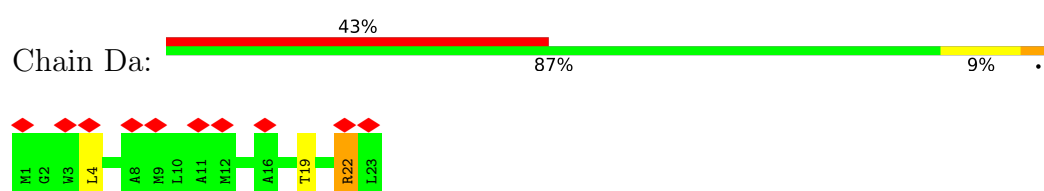
• Molecule 3: Particulate methane monooxygenase subunit C



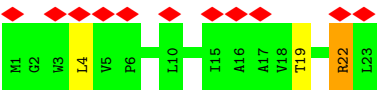
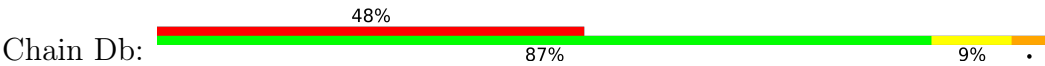
• Molecule 3: Particulate methane monooxygenase subunit C



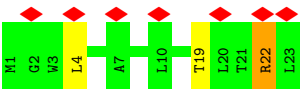
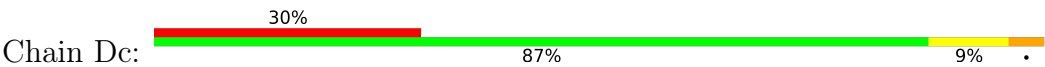
• Molecule 4: particulate methane monooxygenase supernumerary helix



- Molecule 4: particulate methane monooxygenase supernumerary helix



- Molecule 4: particulate methane monooxygenase supernumerary helix



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160646	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.921	Depositor
Minimum map value	-0.508	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.179	Depositor
Map size ($\text{\AA}$)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83000004, 0.83000004, 0.83000004	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	Ba	0.14	0/2052	0.31	0/2814
1	Bb	0.14	0/2052	0.31	0/2814
1	Bc	0.15	0/2052	0.31	0/2814
2	Aa	0.22	0/3103	0.39	0/4227
2	Ab	0.22	0/3103	0.39	0/4227
2	Ac	0.22	0/3103	0.39	0/4227
3	Ca	0.24	0/2052	0.51	3/2801 (0.1%)
3	Cb	0.24	0/2052	0.51	3/2801 (0.1%)
3	Cc	0.24	0/2052	0.51	3/2801 (0.1%)
4	Da	0.90	0/169	1.12	0/231
4	Db	0.90	0/169	1.12	0/231
4	Dc	0.91	0/169	1.13	0/231
All	All	0.25	0/22128	0.44	9/30219 (0.0%)

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
2	Aa	0	2
2	Ab	0	2
2	Ac	0	2
4	Da	0	1
4	Db	0	1
4	Dc	0	1
All	All	0	9

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Ca	129	ASP	CA-CB-CG	10.05	122.65	112.60
3	Cb	129	ASP	CA-CB-CG	10.03	122.63	112.60
3	Cc	129	ASP	CA-CB-CG	10.02	122.62	112.60
3	Ca	128	GLN	N-CA-C	-5.67	105.46	112.38
3	Cc	128	GLN	N-CA-C	-5.66	105.47	112.38
3	Cb	128	GLN	N-CA-C	-5.65	105.49	112.38
3	Cc	204	HIS	CA-CB-CG	5.61	119.41	113.80
3	Cb	204	HIS	CA-CB-CG	5.58	119.38	113.80
3	Ca	204	HIS	CA-CB-CG	5.57	119.37	113.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Aa	141	GLU	Peptide
2	Aa	46	TYR	Peptide
2	Ab	141	GLU	Peptide
2	Ab	46	TYR	Peptide
2	Ac	141	GLU	Peptide
2	Ac	46	TYR	Peptide
4	Da	22	ARG	Sidechain
4	Db	22	ARG	Sidechain
4	Dc	22	ARG	Sidechain

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	Ba	1974	0	1932	50	0
1	Bb	1974	0	1932	47	0
1	Bc	1974	0	1932	51	0
2	Aa	3026	0	3015	51	0
2	Ab	3026	0	3015	47	0
2	Ac	3026	0	3015	50	0
3	Ca	1982	0	1960	49	0
3	Cb	1982	0	1960	52	0
3	Cc	1982	0	1960	51	0
4	Da	167	0	192	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Db	167	0	192	0	0
4	Dc	167	0	192	0	0
5	Aa	1	0	0	0	0
5	Ab	1	0	0	0	0
5	Ac	1	0	0	0	0
5	Ca	1	0	0	0	0
5	Cb	1	0	0	0	0
5	Cc	1	0	0	0	0
6	Aa	167	0	0	5	0
6	Ab	166	0	0	5	0
6	Ac	167	0	0	5	0
6	Ba	55	0	0	3	0
6	Bb	54	0	0	3	0
6	Bc	54	0	0	3	0
6	Ca	49	0	0	2	0
6	Cb	49	0	0	2	0
6	Cc	49	0	0	2	0
6	Da	3	0	0	0	0
6	Db	3	0	0	0	0
6	Dc	3	0	0	0	0
All	All	22272	0	21297	359	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 8.

All (359) 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:Ac:282:GLU:HA	2:Ac:309:ASN:O	1.66	0.96
2:Aa:282:GLU:HA	2:Aa:309:ASN:O	1.66	0.94
2:Ab:282:GLU:HA	2:Ab:309:ASN:O	1.66	0.94
2:Aa:141:GLU:O	2:Aa:143:GLY:N	2.08	0.86
2:Ac:141:GLU:O	2:Ac:143:GLY:N	2.08	0.86
2:Ab:141:GLU:O	2:Ab:143:GLY:N	2.08	0.86
2:Aa:279:VAL:HG12	2:Aa:280:GLY:H	1.45	0.81
2:Ac:279:VAL:HG12	2:Ac:280:GLY:H	1.45	0.79
2:Ab:279:VAL:HG12	2:Ab:280:GLY:H	1.46	0.78
3:Cb:129:ASP:OD2	6:Cb:401:HOH:O	2.04	0.74
3:Cc:129:ASP:OD2	6:Cc:401:HOH:O	2.04	0.74
3:Ca:129:ASP:OD2	6:Ca:401:HOH:O	2.04	0.74
6:Ba:343:HOH:O	3:Cc:137:ILE:CD1	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ca:137:ILE:CD1	6:Bb:343:HOH:O	2.39	0.70
3:Cc:126:THR:O	3:Cc:129:ASP:HB3	1.92	0.70
6:Bc:343:HOH:O	3:Cb:137:ILE:CD1	2.38	0.70
3:Cb:126:THR:O	3:Cb:129:ASP:HB3	1.92	0.70
3:Ca:126:THR:O	3:Ca:129:ASP:HB3	1.92	0.69
2:Ab:113:GLU:HB2	2:Ab:116:LYS:HD2	1.77	0.67
2:Aa:113:GLU:HB2	2:Aa:116:LYS:HD2	1.77	0.67
2:Ac:113:GLU:HB2	2:Ac:116:LYS:HD2	1.77	0.66
6:Ba:343:HOH:O	3:Cc:137:ILE:HD11	1.95	0.66
1:Bb:209:THR:OG1	1:Bb:212:THR:OG1	2.14	0.65
3:Ca:137:ILE:HD11	6:Bb:343:HOH:O	1.97	0.64
3:Cb:138:ARG:HH12	3:Cb:204:HIS:CD2	2.16	0.64
1:Ba:105:GLU:O	1:Ba:109:ARG:HG2	1.98	0.64
3:Ca:138:ARG:HH12	3:Ca:204:HIS:CD2	2.16	0.64
6:Bc:343:HOH:O	3:Cb:137:ILE:HD11	1.96	0.64
3:Cc:138:ARG:HH12	3:Cc:204:HIS:CD2	2.16	0.63
1:Bb:105:GLU:O	1:Bb:109:ARG:HG2	1.98	0.63
1:Bc:105:GLU:O	1:Bc:109:ARG:HG2	1.98	0.63
1:Ba:209:THR:OG1	1:Ba:212:THR:OG1	2.14	0.63
1:Bc:209:THR:OG1	1:Bc:212:THR:OG1	2.14	0.62
1:Bc:48:LEU:HD13	3:Cb:221:PHE:HB3	1.81	0.62
1:Ba:85:TRP:O	1:Ba:89:ARG:NH1	2.33	0.61
1:Ba:42:TYR:OH	1:Ba:73:GLY:O	2.16	0.61
2:Aa:286:THR:HG22	2:Aa:306:VAL:HG22	1.83	0.61
2:Ac:286:THR:HG22	2:Ac:306:VAL:HG22	1.83	0.61
1:Bc:85:TRP:O	1:Bc:89:ARG:NH1	2.33	0.61
2:Ab:286:THR:HG22	2:Ab:306:VAL:HG22	1.83	0.61
1:Ba:48:LEU:HD13	3:Cc:221:PHE:HB3	1.83	0.61
1:Ba:60:LYS:HD3	1:Ba:169:ILE:HD11	1.83	0.60
1:Bb:85:TRP:O	1:Bb:89:ARG:NH1	2.33	0.60
1:Bc:60:LYS:HD3	1:Bc:169:ILE:HD11	1.83	0.60
2:Ab:321:ALA:HB3	2:Ab:324:LEU:HB2	1.83	0.60
2:Ac:321:ALA:HB3	2:Ac:324:LEU:HB2	1.83	0.60
1:Ba:201:TYR:HB3	2:Ab:109:SER:OG	2.02	0.59
3:Ca:221:PHE:HB3	1:Bb:48:LEU:HD13	1.83	0.59
1:Bb:60:LYS:HD3	1:Bb:169:ILE:HD11	1.83	0.59
3:Ca:169:LYS:NZ	3:Ca:178:GLY:O	2.36	0.59
1:Bc:25:THR:O	1:Bc:29:MET:HG3	2.03	0.59
3:Cb:169:LYS:NZ	3:Cb:178:GLY:O	2.36	0.59
2:Aa:321:ALA:HB3	2:Aa:324:LEU:HB2	1.83	0.59
6:Aa:604:HOH:O	1:Bc:194:VAL:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:25:THR:O	1:Ba:29:MET:HG3	2.03	0.58
1:Bc:43:HIS:ND1	3:Cb:123:SER:OG	2.29	0.58
1:Ba:45:HIS:O	1:Ba:49:THR:OG1	2.16	0.58
1:Bb:42:TYR:OH	1:Bb:73:GLY:O	2.16	0.58
1:Bb:25:THR:O	1:Bb:29:MET:HG3	2.03	0.58
2:Ab:340:ASP:O	2:Ab:371:ARG:NH1	2.37	0.58
3:Cc:169:LYS:NZ	3:Cc:178:GLY:O	2.36	0.58
1:Bb:201:TYR:HB3	2:Ac:109:SER:OG	2.03	0.58
1:Bc:42:TYR:OH	1:Bc:73:GLY:O	2.16	0.57
1:Ba:194:VAL:HG12	6:Ab:604:HOH:O	2.04	0.57
3:Cc:200:ASN:HB2	3:Cc:221:PHE:HE2	1.70	0.57
2:Aa:109:SER:OG	1:Bc:201:TYR:HB3	2.04	0.57
2:Ac:214:ARG:NH1	6:Ac:614:HOH:O	2.36	0.57
3:Ca:200:ASN:HB2	3:Ca:221:PHE:HE2	1.70	0.57
2:Aa:340:ASP:O	2:Aa:371:ARG:NH1	2.37	0.57
1:Bb:194:VAL:HG12	6:Ac:604:HOH:O	2.04	0.56
2:Ab:281:LYS:HG2	2:Ab:282:GLU:HG2	1.88	0.56
3:Cb:200:ASN:HB2	3:Cb:221:PHE:HE2	1.70	0.56
1:Bb:63:ARG:NH2	6:Bb:308:HOH:O	2.39	0.56
2:Ac:340:ASP:O	2:Ac:371:ARG:NH1	2.37	0.56
2:Ab:30:GLY:HA2	3:Cc:139:ASP:HB3	1.88	0.55
1:Bb:178:GLN:HG3	1:Bb:183:MET:HE3	1.88	0.55
1:Ba:63:ARG:NH2	6:Ba:308:HOH:O	2.39	0.55
2:Ac:281:LYS:HG2	2:Ac:282:GLU:HG2	1.88	0.55
3:Ca:139:ASP:HB3	2:Ac:30:GLY:HA2	1.88	0.55
1:Bc:63:ARG:NH2	6:Bc:308:HOH:O	2.39	0.55
3:Cb:246:VAL:HG12	3:Cb:250:GLY:HA3	1.89	0.55
2:Aa:94:LEU:HB3	2:Aa:124:LEU:HB3	1.89	0.54
2:Aa:183:ARG:NH1	6:Aa:619:HOH:O	2.40	0.54
3:Cc:246:VAL:HG12	3:Cc:250:GLY:HA3	1.90	0.54
1:Ba:43:HIS:ND1	3:Cc:123:SER:OG	2.27	0.54
3:Ca:39:ARG:HH12	3:Ca:43:GLN:HB2	1.72	0.54
2:Ab:47:ASP:O	2:Ab:65:GLY:HA2	2.08	0.54
2:Ac:94:LEU:HB3	2:Ac:124:LEU:HB3	1.89	0.54
2:Aa:281:LYS:HG2	2:Aa:282:GLU:HG2	1.88	0.54
3:Cb:39:ARG:HH12	3:Cb:43:GLN:HB2	1.72	0.54
2:Ac:183:ARG:NH1	6:Ac:619:HOH:O	2.40	0.54
2:Ab:183:ARG:NH1	6:Ab:619:HOH:O	2.40	0.54
3:Cc:39:ARG:HH12	3:Cc:43:GLN:HB2	1.72	0.54
2:Aa:30:GLY:HA2	3:Cb:139:ASP:HB3	1.89	0.54
2:Ab:94:LEU:HB3	2:Ab:124:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:178:GLN:HG3	1:Bc:183:MET:HE3	1.88	0.53
1:Ba:178:GLN:HG3	1:Ba:183:MET:HE3	1.88	0.53
2:Aa:47:ASP:O	2:Aa:65:GLY:HA2	2.08	0.53
3:Ca:246:VAL:HG12	3:Ca:250:GLY:HA3	1.90	0.53
2:Ab:142:GLY:O	3:Cc:209:MET:HG3	2.08	0.53
2:Ac:47:ASP:O	2:Ac:65:GLY:HA2	2.07	0.53
3:Ca:108:VAL:CG1	1:Bb:29:MET:HE3	2.39	0.53
1:Bc:29:MET:HE3	3:Cb:108:VAL:HG12	1.91	0.53
3:Cb:24:MET:HB2	3:Cb:109:GLN:HB3	1.91	0.53
1:Bc:29:MET:HE3	3:Cb:108:VAL:CG1	2.39	0.52
1:Ba:56:TRP:CZ2	3:Cc:134:MET:HG2	2.44	0.52
2:Aa:214:ARG:NH1	6:Aa:615:HOH:O	2.36	0.52
3:Ca:24:MET:HB2	3:Ca:109:GLN:HB3	1.91	0.52
2:Ab:214:ARG:NH1	6:Ab:614:HOH:O	2.36	0.52
1:Ba:56:TRP:HZ2	3:Cc:134:MET:HG2	1.74	0.52
3:Cc:208:PHE:CE2	3:Cc:216:PRO:HD2	2.44	0.52
3:Ca:108:VAL:HG12	1:Bb:29:MET:HE3	1.91	0.52
3:Ca:134:MET:HG2	1:Bb:56:TRP:HZ2	1.75	0.52
3:Cc:24:MET:HB2	3:Cc:109:GLN:HB3	1.91	0.52
1:Bc:56:TRP:HZ2	3:Cb:134:MET:HG2	1.75	0.52
3:Ca:134:MET:HG2	1:Bb:56:TRP:CZ2	2.45	0.52
3:Ca:208:PHE:CE2	3:Ca:216:PRO:HD2	2.44	0.52
3:Cb:208:PHE:CE2	3:Cb:216:PRO:HD2	2.44	0.52
2:Aa:142:GLY:O	3:Cb:209:MET:HG3	2.10	0.52
1:Bc:56:TRP:CZ2	3:Cb:134:MET:HG2	2.45	0.52
3:Ca:242:ILE:O	3:Ca:246:VAL:HG23	2.11	0.51
1:Bb:184:THR:HG22	2:Ac:258:ILE:HG13	1.92	0.51
1:Bc:45:HIS:O	1:Bc:49:THR:OG1	2.16	0.51
2:Ac:321:ALA:C	2:Ac:323:GLY:H	2.18	0.51
1:Ba:184:THR:HG22	2:Ab:258:ILE:HG13	1.92	0.51
3:Ca:137:ILE:HG21	2:Ac:147:ILE:HD11	1.93	0.51
3:Cb:242:ILE:O	3:Cb:246:VAL:HG23	2.10	0.51
1:Ba:29:MET:HE3	3:Cc:108:VAL:HG12	1.93	0.51
1:Ba:135:TRP:HE1	1:Ba:153:GLY:HA2	1.76	0.51
2:Aa:321:ALA:C	2:Aa:323:GLY:H	2.18	0.51
2:Ab:314:LEU:HB3	2:Ab:394:PHE:HB3	1.93	0.51
1:Ba:184:THR:OG1	1:Ba:187:ASP:OD2	2.28	0.51
1:Bc:135:TRP:HE1	1:Bc:153:GLY:HA2	1.76	0.51
1:Ba:29:MET:HE3	3:Cc:108:VAL:CG1	2.41	0.50
1:Bb:45:HIS:O	1:Bb:49:THR:OG1	2.16	0.50
3:Cc:242:ILE:O	3:Cc:246:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:47:MET:O	3:Cc:213:PHE:HD2	1.94	0.50
2:Aa:94:LEU:HD23	2:Aa:126:GLY:HA2	1.92	0.50
3:Ca:43:GLN:NE2	6:Ca:408:HOH:O	2.44	0.50
2:Ac:94:LEU:HD23	2:Ac:126:GLY:HA2	1.92	0.50
2:Ab:321:ALA:C	2:Ab:323:GLY:H	2.18	0.50
3:Ca:123:SER:OG	1:Bb:43:HIS:ND1	2.30	0.50
1:Bc:184:THR:OG1	1:Bc:187:ASP:OD2	2.28	0.50
1:Bb:138:VAL:HG11	2:Ac:236:LEU:HB2	1.94	0.50
3:Cb:43:GLN:NE2	6:Cb:408:HOH:O	2.44	0.50
2:Aa:147:ILE:HD11	3:Cb:137:ILE:HG21	1.93	0.50
3:Ca:209:MET:HG3	2:Ac:142:GLY:O	2.11	0.50
2:Aa:187:TRP:NE1	1:Bc:164:ASN:O	2.44	0.50
2:Ab:94:LEU:HD23	2:Ab:126:GLY:HA2	1.92	0.50
6:Aa:604:HOH:O	1:Bc:194:VAL:CG1	2.59	0.50
1:Bb:135:TRP:HE1	1:Bb:153:GLY:HA2	1.76	0.50
2:Ab:147:ILE:HD11	3:Cc:137:ILE:HG21	1.92	0.50
1:Ba:138:VAL:HG11	2:Ab:236:LEU:HB2	1.94	0.49
2:Aa:314:LEU:HB3	2:Aa:394:PHE:HB3	1.93	0.49
2:Ab:71:SER:OG	2:Ab:405:GLU:OE2	2.28	0.49
1:Bb:194:VAL:CG1	6:Ac:604:HOH:O	2.60	0.49
2:Ac:314:LEU:HB3	2:Ac:394:PHE:HB3	1.93	0.49
1:Bb:184:THR:OG1	1:Bb:187:ASP:OD2	2.28	0.49
2:Ac:325:ARG:HH12	2:Ac:336:PRO:HG2	1.78	0.49
3:Cc:43:GLN:NE2	6:Cc:408:HOH:O	2.44	0.49
2:Aa:325:ARG:HH12	2:Aa:336:PRO:HG2	1.78	0.49
1:Bc:47:MET:O	3:Cb:213:PHE:HD2	1.96	0.49
2:Ab:325:ARG:HH12	2:Ab:336:PRO:HG2	1.78	0.49
2:Ab:32:LYS:O	2:Ab:376:ARG:NH1	2.41	0.49
2:Aa:258:ILE:HG13	1:Bc:184:THR:HG22	1.93	0.49
3:Cb:218:HIS:O	3:Cb:221:PHE:HB2	2.13	0.48
3:Cc:218:HIS:O	3:Cc:221:PHE:HB2	2.13	0.48
2:Ac:71:SER:OG	2:Ac:405:GLU:OE2	2.28	0.48
2:Ac:279:VAL:HG12	2:Ac:280:GLY:N	2.23	0.48
2:Aa:81:ARG:O	2:Aa:111:SER:OG	2.25	0.48
2:Ab:279:VAL:HG12	2:Ab:280:GLY:N	2.23	0.48
1:Ba:164:ASN:O	2:Ab:187:TRP:NE1	2.43	0.48
2:Ab:212:TYR:OH	3:Cc:240:MET:HG2	2.13	0.48
2:Ac:32:LYS:O	2:Ac:376:ARG:NH1	2.41	0.48
2:Aa:212:TYR:OH	3:Cb:240:MET:HG2	2.13	0.48
2:Aa:236:LEU:HB2	1:Bc:138:VAL:HG11	1.95	0.48
3:Ca:240:MET:HG2	2:Ac:212:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ca:213:PHE:HD2	1:Bb:47:MET:O	1.96	0.48
3:Ca:218:HIS:O	3:Ca:221:PHE:HB2	2.13	0.48
3:Ca:128:GLN:HA	3:Ca:131:THR:HG22	1.97	0.47
2:Ac:81:ARG:O	2:Ac:111:SER:OG	2.25	0.47
3:Cb:212:LEU:HG	3:Cb:215:ALA:HB2	1.96	0.47
1:Bb:164:ASN:O	2:Ac:187:TRP:NE1	2.44	0.47
2:Aa:32:LYS:O	2:Aa:376:ARG:NH1	2.41	0.47
2:Aa:366:LYS:HE3	2:Aa:366:LYS:HB3	1.79	0.47
1:Bb:56:TRP:HB2	1:Bb:59:TRP:CD1	2.50	0.47
1:Ba:33:LEU:HB3	3:Cc:112:VAL:HG22	1.96	0.47
1:Bc:56:TRP:HB2	1:Bc:59:TRP:CD1	2.50	0.47
3:Cc:212:LEU:HG	3:Cc:215:ALA:HB2	1.96	0.47
2:Aa:329:PRO:HG3	2:Aa:346:ARG:HA	1.97	0.47
2:Ab:116:LYS:NZ	6:Ab:611:HOH:O	2.35	0.47
2:Ab:217:GLU:OE1	3:Cc:251:VAL:HG11	2.15	0.47
1:Ba:18:GLU:OE2	3:Cc:98:ARG:NH2	2.48	0.46
2:Aa:71:SER:OG	2:Aa:405:GLU:OE2	2.28	0.46
1:Ba:56:TRP:HB2	1:Ba:59:TRP:CD1	2.50	0.46
2:Ac:116:LYS:NZ	6:Ac:612:HOH:O	2.35	0.46
2:Ac:328:ASN:HB2	2:Ac:348:LEU:HD22	1.98	0.46
3:Cc:128:GLN:HA	3:Cc:131:THR:HG22	1.97	0.46
2:Aa:151:GLN:HG3	2:Aa:152:TRP:N	2.31	0.46
2:Ab:328:ASN:HB2	2:Ab:348:LEU:HD22	1.97	0.46
3:Cc:131:THR:O	3:Cc:135:THR:HG23	2.16	0.46
1:Ba:53:TRP:CZ3	3:Cc:214:VAL:HG11	2.51	0.46
1:Ba:194:VAL:CG1	6:Ab:604:HOH:O	2.60	0.46
2:Aa:328:ASN:HB2	2:Aa:348:LEU:HD22	1.98	0.46
3:Ca:131:THR:O	3:Ca:135:THR:HG23	2.16	0.46
2:Aa:279:VAL:HG12	2:Aa:280:GLY:N	2.22	0.46
2:Aa:327:LEU:HD11	2:Aa:343:LEU:HD11	1.98	0.46
2:Ab:151:GLN:HG3	2:Ab:152:TRP:N	2.31	0.46
2:Ac:329:PRO:HG3	2:Ac:346:ARG:HA	1.97	0.46
3:Cb:39:ARG:NH1	3:Cb:43:GLN:HB2	2.31	0.46
3:Cb:128:GLN:HA	3:Cb:131:THR:HG22	1.97	0.46
3:Ca:212:LEU:HG	3:Ca:215:ALA:HB2	1.96	0.46
2:Ab:327:LEU:HD12	2:Ab:345:ASP:HA	1.98	0.46
2:Ab:329:PRO:HG3	2:Ab:346:ARG:HA	1.97	0.46
2:Ac:151:GLN:HG3	2:Ac:152:TRP:N	2.31	0.46
3:Ca:39:ARG:NH1	3:Ca:43:GLN:HB2	2.31	0.45
1:Bc:33:LEU:HB3	3:Cb:112:VAL:HG22	1.98	0.45
1:Bc:195:ARG:HB2	1:Bc:198:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:327:LEU:HD11	2:Ab:343:LEU:HD11	1.98	0.45
2:Ac:80:PRO:HB2	2:Ac:112:LEU:HB2	1.98	0.45
3:Ca:133:HIS:CE1	3:Ca:138:ARG:HD2	2.52	0.45
1:Bc:53:TRP:CZ3	3:Cb:214:VAL:HG11	2.52	0.45
3:Cc:39:ARG:NH1	3:Cc:43:GLN:HB2	2.31	0.45
1:Ba:175:ALA:HB1	1:Ba:182:LEU:HD11	1.99	0.45
3:Ca:112:VAL:HG22	1:Bb:33:LEU:HB3	1.99	0.45
3:Cb:131:THR:O	3:Cb:135:THR:HG23	2.16	0.45
3:Cc:133:HIS:CE1	3:Cc:138:ARG:HD2	2.52	0.45
2:Aa:327:LEU:HD12	2:Aa:345:ASP:HA	1.98	0.45
1:Bc:175:ALA:HB1	1:Bc:182:LEU:HD11	1.99	0.45
1:Ba:195:ARG:HB2	1:Ba:198:MET:HB2	1.98	0.45
1:Bb:226:GLY:O	1:Bb:230:MET:HG3	2.17	0.45
1:Bc:215:LYS:HA	2:Ac:382:TYR:CZ	2.52	0.45
3:Cb:216:PRO:HA	3:Cb:219:TRP:HD1	1.82	0.45
1:Ba:226:GLY:O	1:Ba:230:MET:HG3	2.17	0.44
2:Aa:77:VAL:HG13	2:Aa:143:GLY:HA3	1.99	0.44
3:Ca:209:MET:O	1:Bc:211:ARG:NE	2.49	0.44
1:Ba:215:LYS:HA	2:Aa:382:TYR:CZ	2.53	0.44
1:Bb:175:ALA:HB1	1:Bb:182:LEU:HD11	1.99	0.44
1:Bb:195:ARG:HB2	1:Bb:198:MET:HB2	1.98	0.44
3:Cb:133:HIS:CE1	3:Cb:138:ARG:HD2	2.52	0.44
2:Ac:77:VAL:HG13	2:Ac:143:GLY:HA3	1.99	0.44
3:Ca:104:LEU:HD22	3:Ca:238:ILE:HG23	1.99	0.44
1:Bb:215:LYS:HA	2:Ab:382:TYR:CZ	2.52	0.44
3:Ca:216:PRO:HA	3:Ca:219:TRP:HD1	1.82	0.44
2:Ac:327:LEU:HD11	2:Ac:343:LEU:HD11	1.98	0.44
3:Cc:216:PRO:HA	3:Cc:219:TRP:HD1	1.82	0.44
2:Aa:80:PRO:HB2	2:Aa:112:LEU:HB2	1.99	0.44
2:Aa:227:ASP:OD1	2:Aa:227:ASP:N	2.48	0.44
2:Ab:80:PRO:HB2	2:Ab:112:LEU:HB2	1.99	0.44
2:Ab:279:VAL:CG1	2:Ab:280:GLY:H	2.24	0.44
1:Ba:27:ASP:OD1	2:Ab:208:ILE:HB	2.18	0.44
1:Ba:236:TRP:HA	1:Ba:239:MET:HB2	2.00	0.44
2:Aa:116:LYS:NZ	6:Aa:613:HOH:O	2.35	0.44
1:Bb:27:ASP:OD1	2:Ac:208:ILE:HB	2.18	0.44
3:Cb:104:LEU:HD22	3:Cb:238:ILE:HG23	1.99	0.44
2:Aa:346:ARG:HE	2:Aa:346:ARG:HB3	1.62	0.43
1:Bb:135:TRP:NE1	1:Bb:153:GLY:HA2	2.32	0.43
2:Ab:101:ILE:HD12	2:Ab:120:PHE:HB3	2.00	0.43
2:Ac:327:LEU:HD12	2:Ac:345:ASP:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bb:236:TRP:HA	1:Bb:239:MET:HB2	2.00	0.43
2:Ac:101:ILE:HD12	2:Ac:120:PHE:HB3	2.00	0.43
1:Ba:135:TRP:NE1	1:Ba:153:GLY:HA2	2.32	0.43
2:Aa:212:TYR:HB2	1:Bc:88:PHE:CE2	2.53	0.43
3:Ca:114:TYR:CE1	3:Ca:161:ALA:HB2	2.53	0.43
1:Bc:18:GLU:OE2	3:Cb:98:ARG:NH2	2.50	0.43
2:Ab:77:VAL:HG13	2:Ab:143:GLY:HA3	1.99	0.43
3:Ca:113:VAL:HG12	3:Ca:160:ILE:HD13	2.01	0.43
3:Ca:214:VAL:HG11	1:Bb:53:TRP:CZ3	2.53	0.43
1:Bc:135:TRP:NE1	1:Bc:153:GLY:HA2	2.32	0.43
1:Bc:226:GLY:O	1:Bc:230:MET:HG3	2.17	0.43
1:Bc:236:TRP:HA	1:Bc:239:MET:HB2	2.00	0.43
3:Ca:98:ARG:NH2	1:Bb:18:GLU:OE2	2.51	0.43
1:Ba:211:ARG:NE	3:Cb:209:MET:O	2.52	0.43
1:Bb:239:MET:HE2	1:Bb:239:MET:HB3	1.89	0.43
3:Cc:104:LEU:HD22	3:Cc:238:ILE:HG23	1.99	0.43
3:Cc:114:TYR:CE1	3:Cc:161:ALA:HB2	2.53	0.43
3:Ca:135:THR:HG21	1:Bb:117:THR:HB	2.00	0.43
3:Cb:113:VAL:HG12	3:Cb:160:ILE:HD13	2.01	0.43
3:Cb:114:TYR:CE1	3:Cb:161:ALA:HB2	2.53	0.43
2:Aa:208:ILE:HB	1:Bc:27:ASP:OD1	2.19	0.43
3:Cc:113:VAL:HG12	3:Cc:160:ILE:HD13	2.01	0.43
1:Ba:88:PHE:CE2	2:Ab:212:TYR:HB2	2.54	0.43
1:Bb:118:TYR:CD1	2:Ac:159:MET:HE1	2.54	0.43
2:Ac:279:VAL:CG1	2:Ac:280:GLY:H	2.24	0.42
2:Aa:101:ILE:HD12	2:Aa:120:PHE:HB3	2.00	0.42
3:Ca:154:TYR:HB2	3:Ca:155:PRO:HD3	2.01	0.42
1:Bc:49:THR:HG23	3:Cb:222:VAL:HG21	2.01	0.42
3:Cc:154:TYR:HB2	3:Cc:155:PRO:HD3	2.01	0.42
1:Ba:118:TYR:CD1	2:Ab:159:MET:HE1	2.55	0.42
1:Bb:88:PHE:CE2	2:Ac:212:TYR:HB2	2.55	0.42
3:Cb:154:TYR:HB2	3:Cb:155:PRO:HD3	2.01	0.42
1:Ba:49:THR:HG23	3:Cc:222:VAL:HG21	2.02	0.42
2:Aa:92:PRO:O	2:Aa:127:ARG:HD3	2.20	0.42
3:Ca:127:GLU:HB3	1:Bb:108:ASN:CG	2.44	0.42
1:Ba:40:GLY:O	1:Ba:44:VAL:HG23	2.20	0.42
1:Bb:211:ARG:NE	3:Cc:209:MET:O	2.52	0.42
1:Bc:48:LEU:HD13	3:Cb:221:PHE:CB	2.48	0.42
1:Bc:53:TRP:HZ3	3:Cb:214:VAL:HG11	1.84	0.42
1:Bc:117:THR:HB	3:Cb:135:THR:HG21	2.01	0.42
2:Ab:92:PRO:O	2:Ab:127:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Aa:217:GLU:OE1	3:Cb:251:VAL:HG11	2.20	0.42
1:Bc:40:GLY:O	1:Bc:44:VAL:HG23	2.20	0.42
2:Aa:129:ALA:HA	2:Aa:155:ILE:O	2.20	0.42
1:Bb:46:PHE:HZ	1:Bb:69:VAL:HG13	1.85	0.42
1:Bc:75:THR:HB	1:Bc:236:TRP:CE2	2.55	0.42
1:Bc:108:ASN:CG	3:Cb:127:GLU:HB3	2.44	0.42
1:Ba:53:TRP:HZ3	3:Cc:214:VAL:HG11	1.83	0.42
3:Ca:189:GLY:O	3:Ca:224:PHE:HB3	2.20	0.42
1:Bc:46:PHE:HZ	1:Bc:69:VAL:HG13	1.85	0.42
2:Ab:129:ALA:HA	2:Ab:155:ILE:O	2.20	0.42
2:Ab:298:ARG:HE	2:Ab:298:ARG:HB3	1.72	0.42
3:Cb:189:GLY:O	3:Cb:224:PHE:HB3	2.20	0.41
3:Cb:194:ILE:HB	3:Cb:195:PRO:HD3	2.02	0.41
1:Bb:132:PRO:HB3	1:Bb:157:TRP:HA	2.02	0.41
3:Ca:251:VAL:HG11	2:Ac:217:GLU:OE1	2.20	0.41
3:Cc:189:GLY:O	3:Cc:224:PHE:HB3	2.20	0.41
1:Ba:90:LEU:HA	1:Ba:91:PRO:HD3	1.93	0.41
1:Ba:117:THR:HB	3:Cc:135:THR:HG21	2.01	0.41
1:Bb:75:THR:HB	1:Bb:236:TRP:CE2	2.55	0.41
1:Ba:48:LEU:HD13	3:Cc:221:PHE:CB	2.49	0.41
1:Ba:75:THR:HB	1:Ba:236:TRP:CE2	2.55	0.41
2:Ab:71:SER:HA	2:Ab:114:ILE:HG22	2.02	0.41
3:Ca:236:LEU:O	3:Ca:240:MET:HG3	2.21	0.41
1:Bc:132:PRO:HB3	1:Bc:157:TRP:HA	2.02	0.41
2:Ac:29:HIS:N	2:Ac:29:HIS:ND1	2.69	0.41
2:Ac:71:SER:HA	2:Ac:114:ILE:HG22	2.02	0.41
1:Ba:43:HIS:NE2	3:Cc:127:GLU:OE1	2.53	0.41
1:Ba:44:VAL:CG2	3:Cc:122:ALA:HB1	2.50	0.41
2:Aa:61:MET:HE3	2:Aa:124:LEU:HD12	2.03	0.41
2:Aa:279:VAL:CG1	2:Aa:280:GLY:H	2.24	0.41
3:Ca:21:LEU:HD23	3:Ca:109:GLN:NE2	2.36	0.41
1:Bb:40:GLY:O	1:Bb:44:VAL:HG23	2.20	0.41
2:Ac:125:ARG:NH1	2:Ac:163:THR:O	2.54	0.41
2:Ac:129:ALA:HA	2:Ac:155:ILE:O	2.20	0.41
1:Ba:132:PRO:HB3	1:Ba:157:TRP:HA	2.02	0.41
1:Bc:239:MET:HE2	1:Bc:239:MET:HB3	1.89	0.41
3:Cb:236:LEU:O	3:Cb:240:MET:HG3	2.21	0.41
3:Cc:194:ILE:HB	3:Cc:195:PRO:HD3	2.02	0.41
1:Ba:46:PHE:HZ	1:Ba:69:VAL:HG13	1.85	0.41
2:Aa:159:MET:HE1	1:Bc:118:TYR:CD1	2.56	0.41
2:Ac:61:MET:HE3	2:Ac:124:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bb:90:LEU:HA	1:Bb:91:PRO:HD3	1.93	0.40
3:Ca:209:MET:HE2	3:Ca:209:MET:HA	2.04	0.40
1:Bc:228:VAL:O	1:Bc:232:VAL:HG23	2.21	0.40
2:Ab:366:LYS:HE3	2:Ab:366:LYS:HB3	1.79	0.40
2:Ac:92:PRO:O	2:Ac:127:ARG:HD3	2.20	0.40
3:Cb:105:VAL:O	3:Cb:109:GLN:HG3	2.22	0.40
3:Cc:189:GLY:HA3	3:Cc:227:MET:HG3	2.03	0.40
3:Cc:236:LEU:O	3:Cc:240:MET:HG3	2.21	0.40
1:Ba:108:ASN:CG	3:Cc:127:GLU:HB3	2.46	0.40
3:Ca:189:GLY:HA3	3:Ca:227:MET:HG3	2.03	0.40
3:Ca:222:VAL:HG21	1:Bb:49:THR:HG23	2.03	0.40
2:Ac:366:LYS:HE3	2:Ac:366:LYS:HB3	1.79	0.40
3:Cb:21:LEU:HD23	3:Cb:109:GLN:NE2	2.36	0.40
2:Aa:29:HIS:ND1	2:Aa:29:HIS:N	2.69	0.40
2:Aa:125:ARG:NH1	2:Aa:163:THR:O	2.54	0.40
3:Ca:194:ILE:HB	3:Ca:195:PRO:HD3	2.02	0.40
1:Bc:30:LEU:HD22	3:Cb:235:VAL:HG13	2.04	0.40
1:Bc:44:VAL:CG2	3:Cb:122:ALA:HB1	2.52	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	Ba	242/244 (99%)	233 (96%)	9 (4%)	0	100	100
1	Bb	242/244 (99%)	233 (96%)	9 (4%)	0	100	100
1	Bc	242/244 (99%)	233 (96%)	9 (4%)	0	100	100
2	Aa	386/388 (100%)	370 (96%)	14 (4%)	2 (0%)	24	40
2	Ab	386/388 (100%)	370 (96%)	14 (4%)	2 (0%)	24	40
2	Ac	386/388 (100%)	370 (96%)	14 (4%)	2 (0%)	24	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ca	239/241 (99%)	236 (99%)	3 (1%)	0	100	100
3	Cb	239/241 (99%)	236 (99%)	3 (1%)	0	100	100
3	Cc	239/241 (99%)	236 (99%)	3 (1%)	0	100	100
4	Da	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
4	Db	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
4	Dc	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
All	All	2664/2688 (99%)	2577 (97%)	81 (3%)	6 (0%)	44	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Aa	142	GLY
2	Ab	142	GLY
2	Ac	142	GLY
2	Aa	322	ALA
2	Ab	322	ALA
2	Ac	322	ALA

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	Ba	202/202 (100%)	199 (98%)	3 (2%)	57	78
1	Bb	202/202 (100%)	199 (98%)	3 (2%)	57	78
1	Bc	202/202 (100%)	199 (98%)	3 (2%)	57	78
2	Aa	319/319 (100%)	313 (98%)	6 (2%)	50	73
2	Ab	319/319 (100%)	313 (98%)	6 (2%)	50	73
2	Ac	319/319 (100%)	313 (98%)	6 (2%)	50	73
3	Ca	205/205 (100%)	201 (98%)	4 (2%)	48	72
3	Cb	205/205 (100%)	201 (98%)	4 (2%)	48	72
3	Cc	205/205 (100%)	201 (98%)	4 (2%)	48	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Da	17/17 (100%)	14 (82%)	3 (18%)	2	3
4	Db	17/17 (100%)	14 (82%)	3 (18%)	2	3
4	Dc	17/17 (100%)	14 (82%)	3 (18%)	2	3
All	All	2229/2229 (100%)	2181 (98%)	48 (2%)	45	70

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

Mol	Chain	Res	Type
1	Ba	58	ASP
1	Ba	164	ASN
1	Ba	206	GLU
2	Aa	33	SER
2	Aa	61	MET
2	Aa	188	HIS
2	Aa	252	SER
2	Aa	276	THR
2	Aa	285	THR
3	Ca	57	GLU
3	Ca	183	PHE
3	Ca	196	ASN
3	Ca	217	LEU
4	Da	4	LEU
4	Da	19	THR
4	Da	22	ARG
1	Bb	58	ASP
1	Bb	164	ASN
1	Bb	206	GLU
1	Bc	58	ASP
1	Bc	164	ASN
1	Bc	206	GLU
2	Ab	33	SER
2	Ab	61	MET
2	Ab	252	SER
2	Ab	276	THR
2	Ab	281	LYS
2	Ab	285	THR
2	Ac	33	SER
2	Ac	61	MET
2	Ac	188	HIS
2	Ac	252	SER
2	Ac	276	THR

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Mol	Chain	Res	Type
2	Ac	285	THR
3	Cb	57	GLU
3	Cb	183	PHE
3	Cb	196	ASN
3	Cb	217	LEU
3	Cc	57	GLU
3	Cc	183	PHE
3	Cc	196	ASN
3	Cc	217	LEU
4	Db	4	LEU
4	Db	19	THR
4	Db	22	ARG
4	Dc	4	LEU
4	Dc	19	THR
4	Dc	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ba	87	ASN
1	Ba	108	ASN
1	Ba	179	HIS
2	Aa	44	ASN
2	Aa	104	GLN
2	Aa	123	ASN
2	Aa	139	ASN
2	Aa	151	GLN
2	Aa	188	HIS
2	Aa	308	ASN
3	Ca	59	GLN
1	Bb	87	ASN
1	Bb	108	ASN
1	Bb	179	HIS
1	Bc	87	ASN
1	Bc	108	ASN
1	Bc	179	HIS
2	Ab	44	ASN
2	Ab	79	ASN
2	Ab	123	ASN
2	Ab	139	ASN
2	Ab	151	GLN
2	Ab	188	HIS

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Mol	Chain	Res	Type
2	Ab	308	ASN
2	Ac	44	ASN
2	Ac	104	GLN
2	Ac	123	ASN
2	Ac	139	ASN
2	Ac	151	GLN
2	Ac	188	HIS
2	Ac	308	ASN
3	Cb	59	GLN
3	Cc	59	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 6 ligands modelled in this entry, 6 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 ⓘ

There are no chain breaks in this entry.

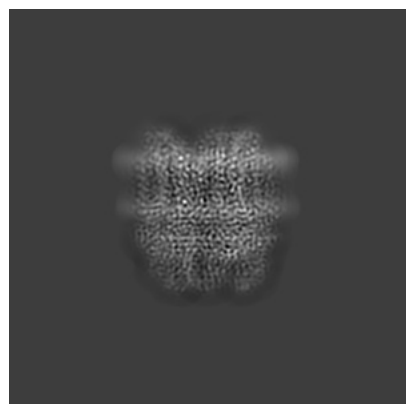
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45662. These allow visual inspection of the internal detail of the map and identification of artifacts.

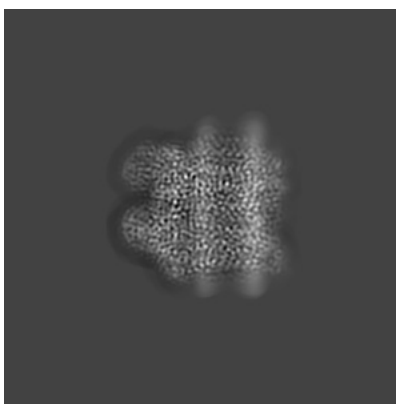
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

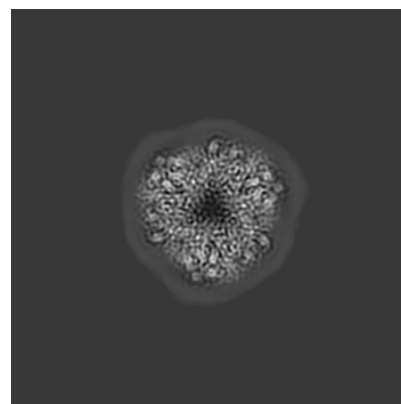
6.1.1 Primary map



X

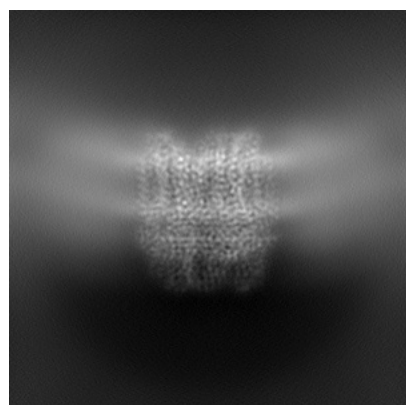


Y

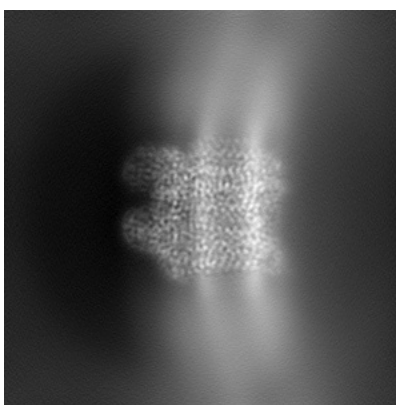


Z

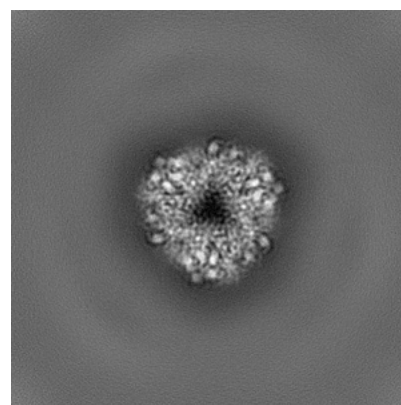
6.1.2 Raw map



X



Y



Z

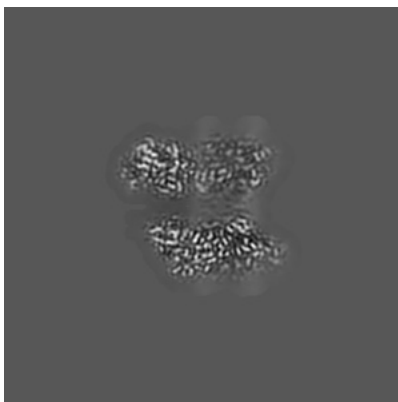
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

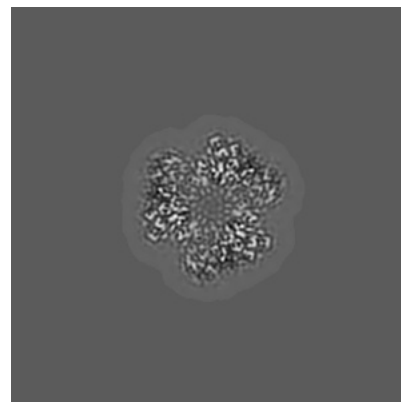
6.2.1 Primary map



X Index: 160

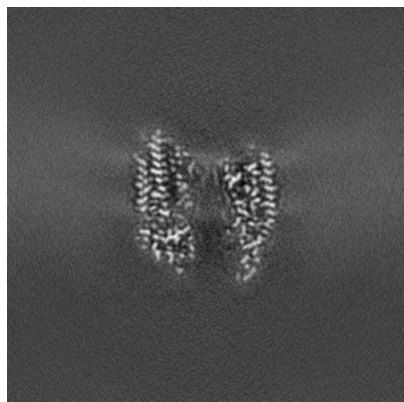


Y Index: 160

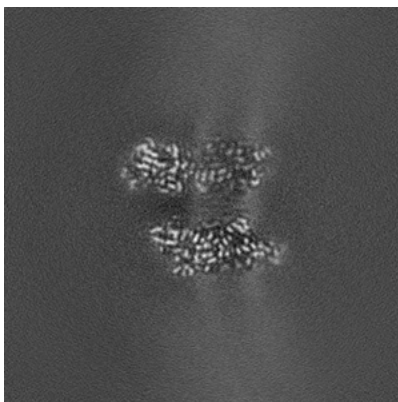


Z Index: 160

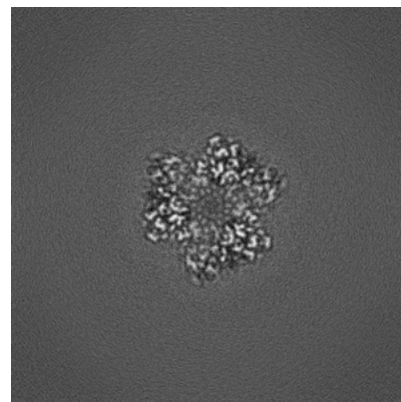
6.2.2 Raw map



X Index: 160



Y Index: 160

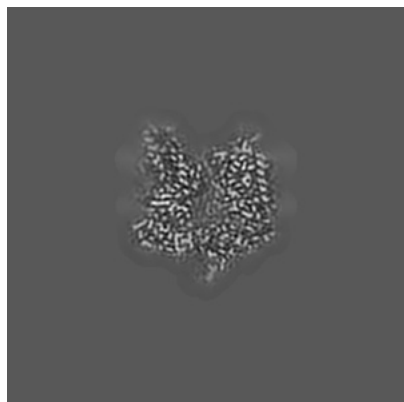


Z Index: 160

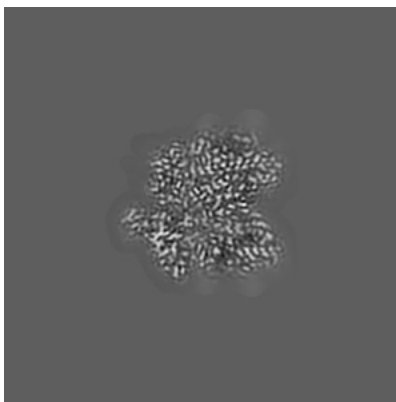
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 175

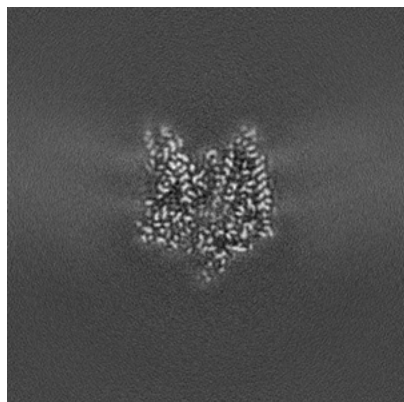


Y Index: 181

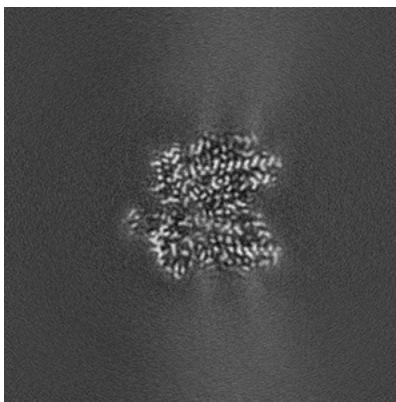


Z Index: 137

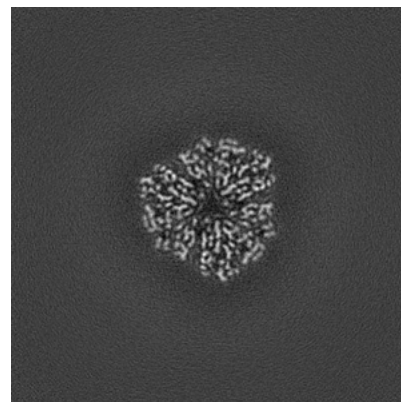
6.3.2 Raw map



X Index: 178



Y Index: 180

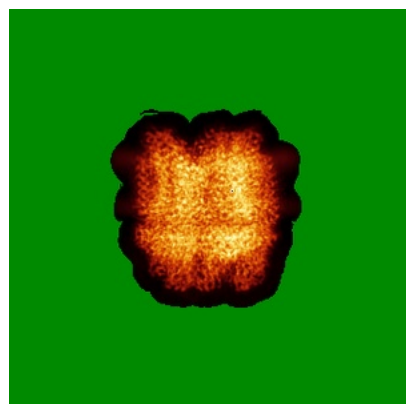


Z Index: 137

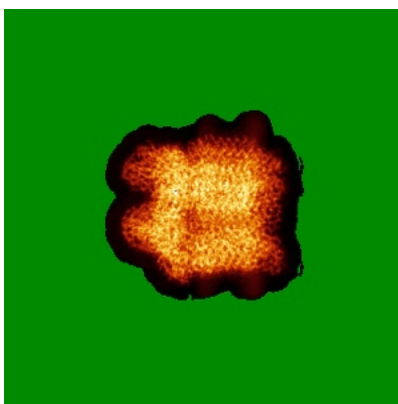
The images above show the largest variance slices of the map in three orthogonal directions.

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

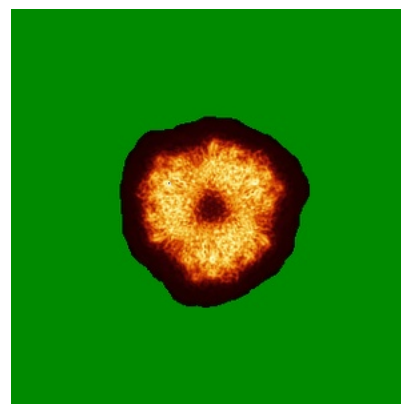
6.4.1 Primary map



X

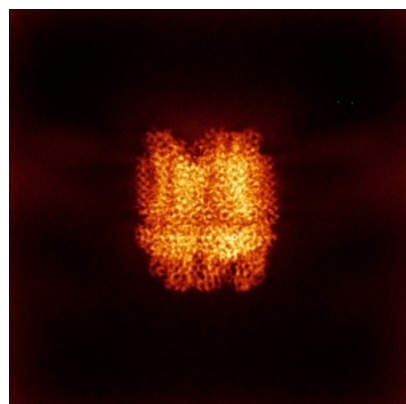


Y

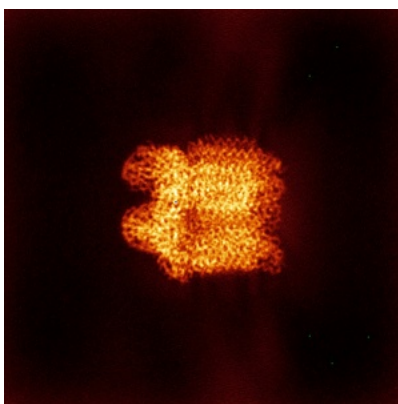


Z

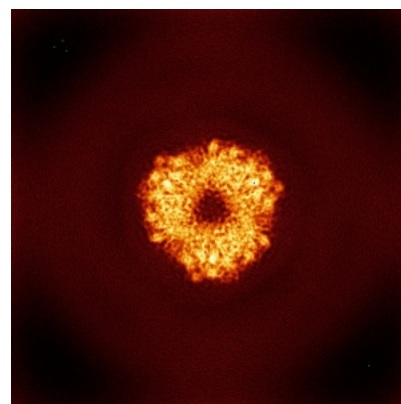
6.4.2 Raw map



X



Y

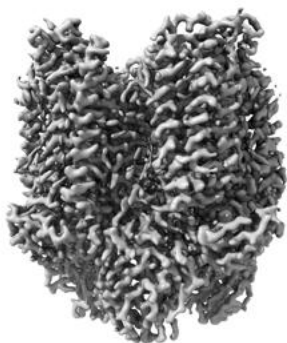


Z

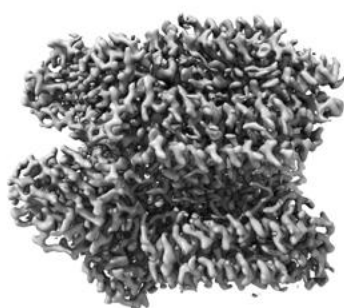
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

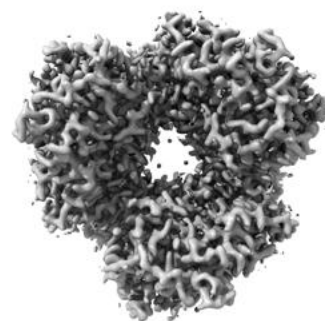
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.179. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

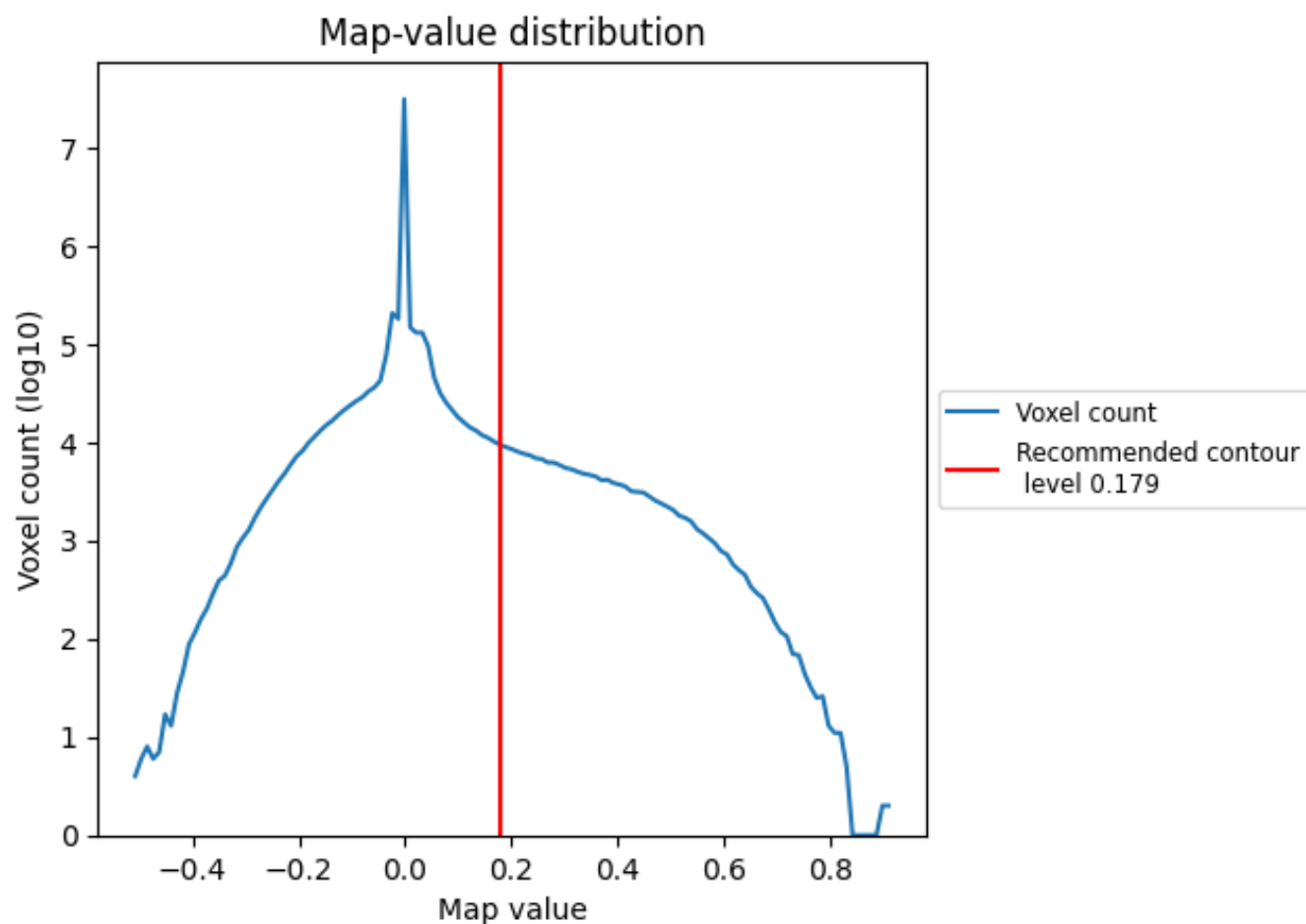
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

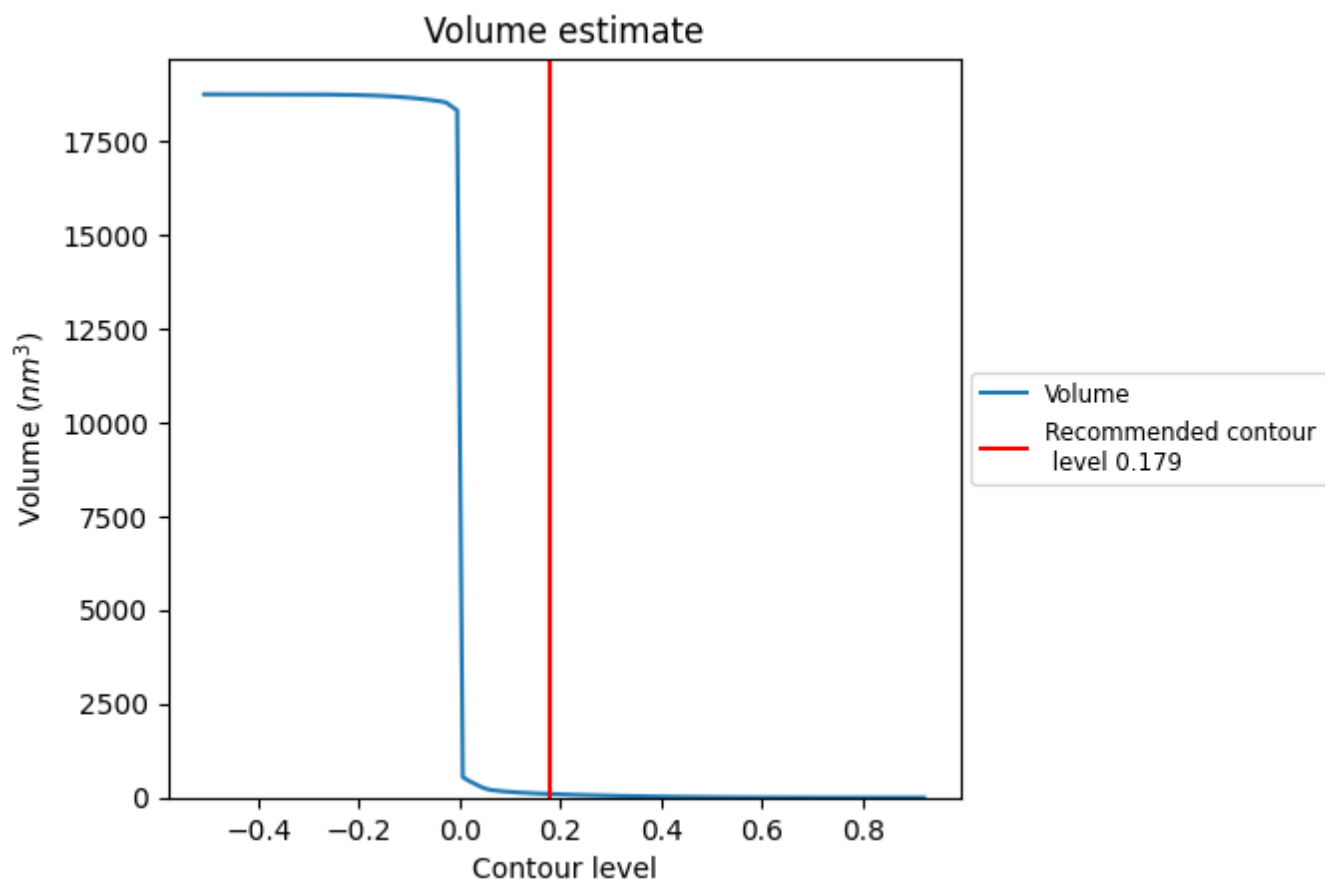
This section contains the results of statistical analysis of the map.

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.

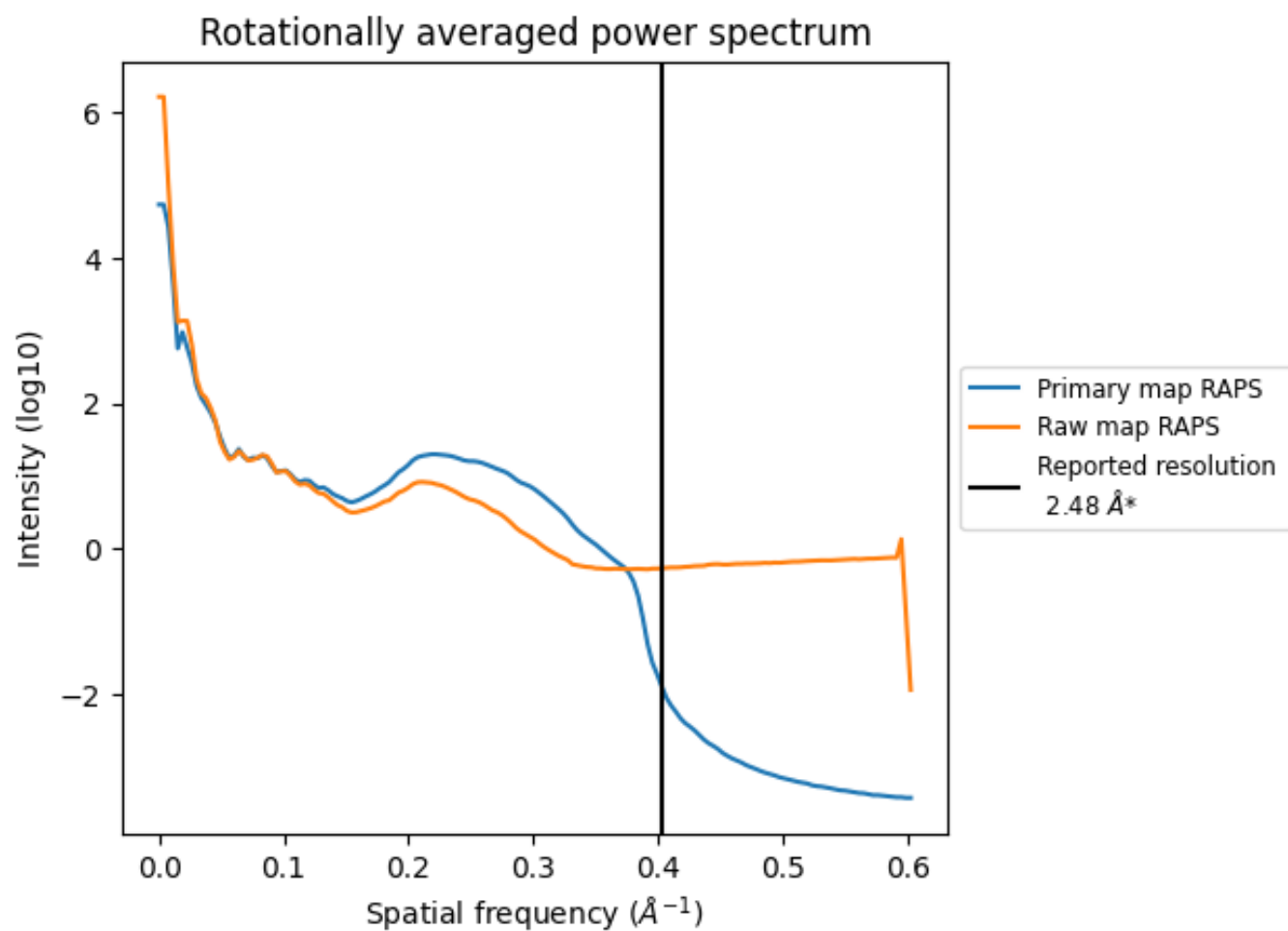
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm^3 ; this corresponds to an approximate mass of 86 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 ⓘ

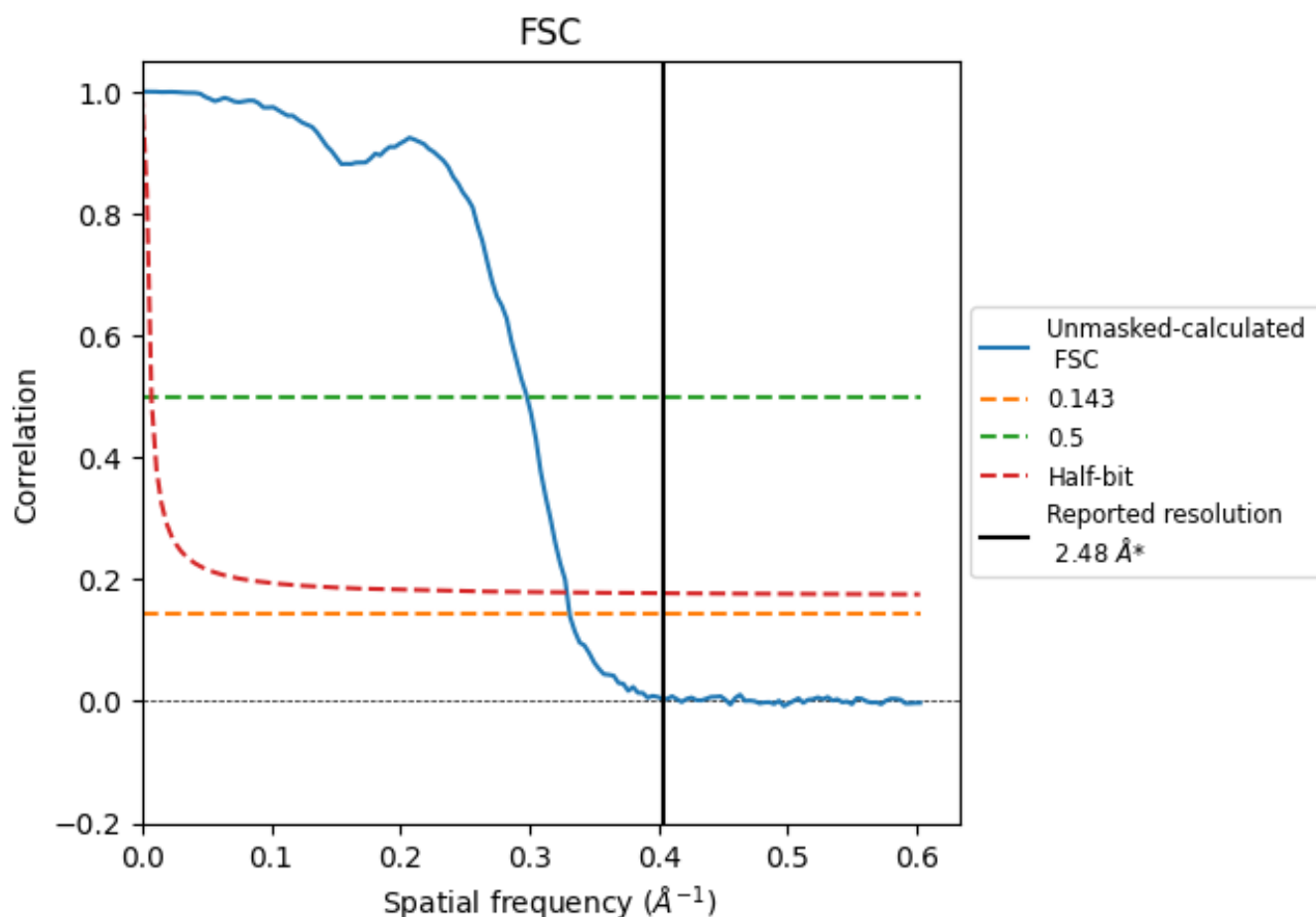


*Reported resolution corresponds to spatial frequency of $0.403 \text{ \AA}^{-1}$

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 0.403 Å⁻¹

8.2 Resolution estimates [i](#)

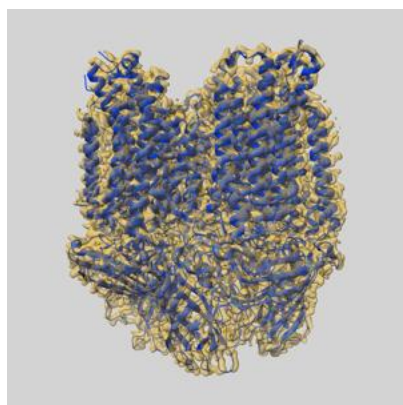
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.02	3.36	3.04

*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 3.02 differs from the reported value 2.48 by more than 10 %

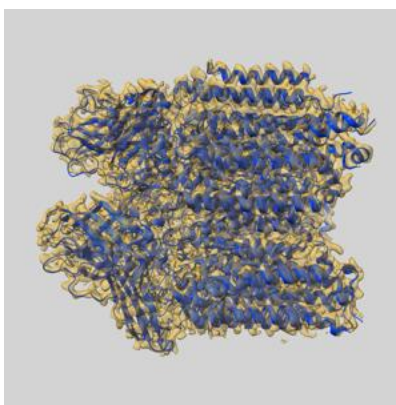
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45662 and PDB model 9CL5. Per-residue inclusion information can be found in section [3](#) on page [9](#).

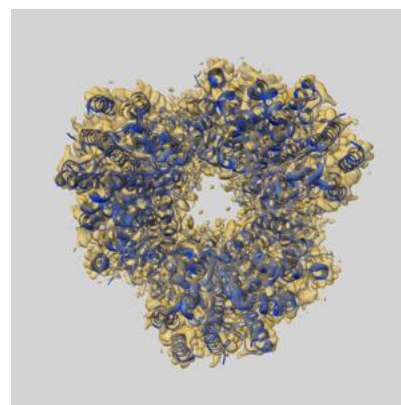
9.1 Map-model overlay [i](#)



X



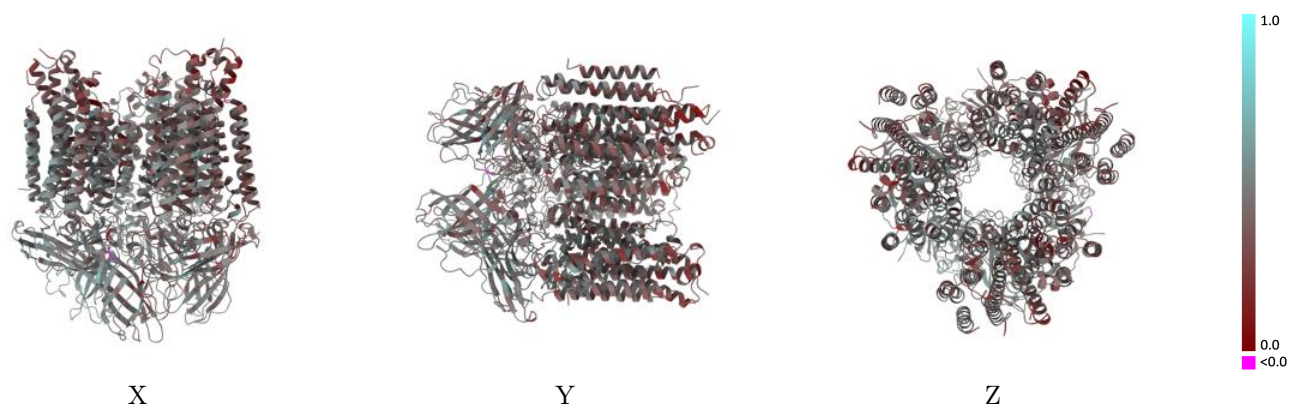
Y



Z

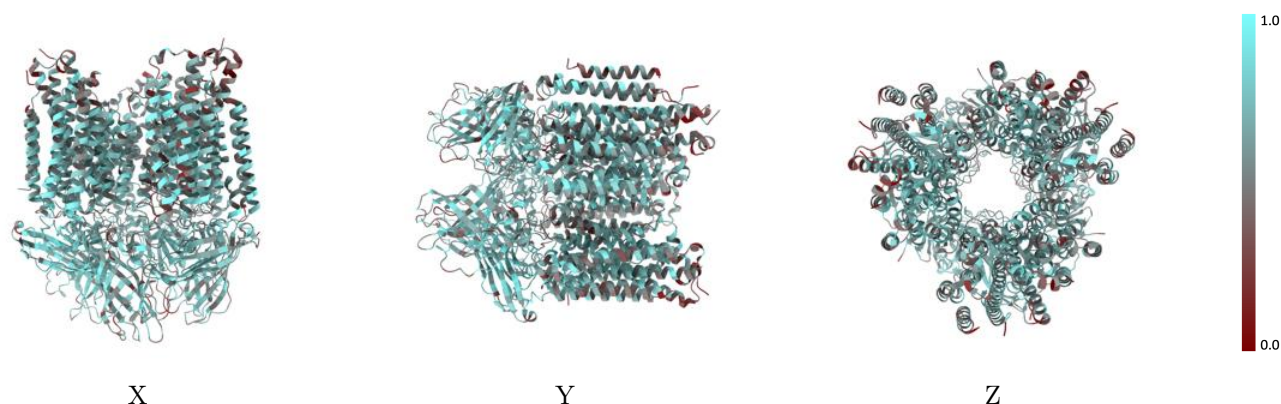
The images above show the 3D surface view of the map at the recommended contour level 0.179 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



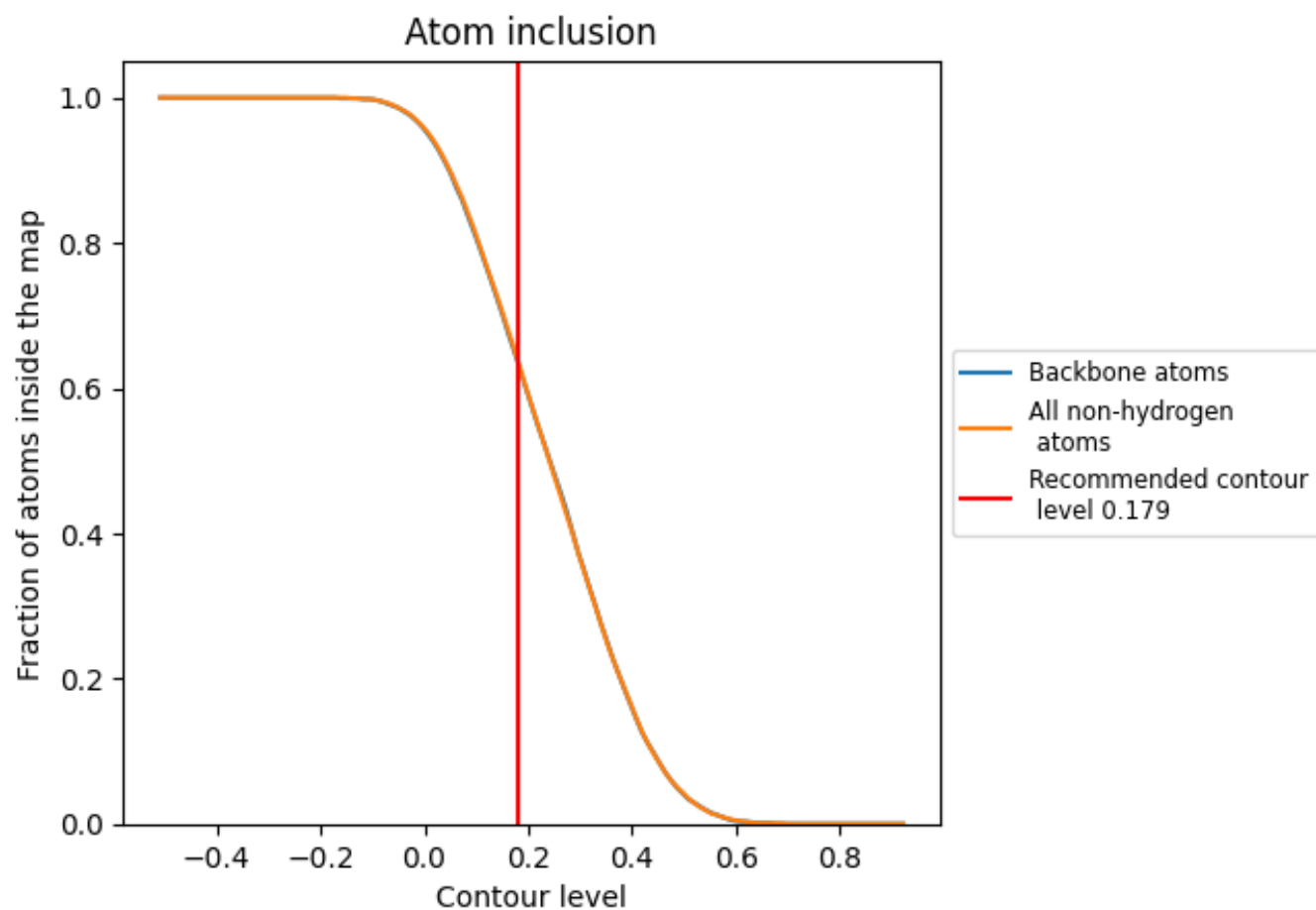
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.179).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (0.179) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.4320
Aa	 0.6980	 0.4840
Ab	 0.6730	 0.4560
Ac	 0.6330	 0.4190
Ba	 0.7160	 0.4580
Bb	 0.6600	 0.4090
Bc	 0.6810	 0.4230
Ca	 0.5710	 0.3990
Cb	 0.6080	 0.4230
Cc	 0.5730	 0.3870
Da	 0.4330	 0.3930
Db	 0.4210	 0.3800
Dc	 0.4880	 0.4640

