



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:58 PM UTC

PDB ID : 6H3C / pdb_00006h3c
EMDB ID : EMD-0132
Title : Cryo-EM structure of the BRISC complex bound to SHMT2
Authors : Bunker, R.D.; Rabl, J.; Thoma, N.H.
Deposited on : 2018-07-18
Resolution : 3.90 Å (reported)
Based on initial models : 6GVW, 5V7I

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:

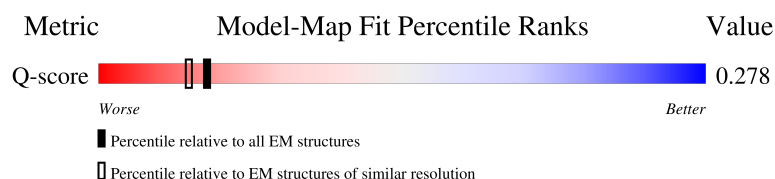
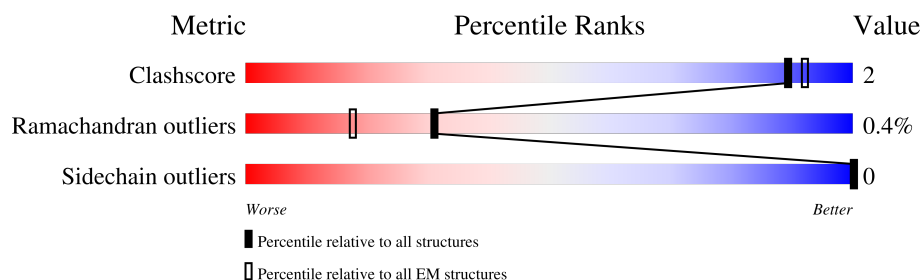
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	
1	F	434	
2	B	335	
2	G	335	

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Mol	Chain	Length	Quality of chain
3	C	402	
3	H	402	
4	D	352	
4	I	352	
5	E	507	
5	J	507	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49982 atoms, of which 24860 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 BRISC complex subunit Abraxas 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	255	Total	C	H	N	O	S	0	0
			4134	1305	2052	375	395	7		
1	F	255	Total	C	H	N	O	S	0	0
			4134	1305	2052	375	395	7		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q15018
A	-17	HIS	-	expression tag	UNP Q15018
A	-16	HIS	-	expression tag	UNP Q15018
A	-15	HIS	-	expression tag	UNP Q15018
A	-14	HIS	-	expression tag	UNP Q15018
A	-13	HIS	-	expression tag	UNP Q15018
A	-12	HIS	-	expression tag	UNP Q15018
A	-11	VAL	-	expression tag	UNP Q15018
A	-10	ASP	-	expression tag	UNP Q15018
A	-9	GLU	-	expression tag	UNP Q15018
A	-8	ASN	-	expression tag	UNP Q15018
A	-7	LEU	-	expression tag	UNP Q15018
A	-6	TYR	-	expression tag	UNP Q15018
A	-5	PHE	-	expression tag	UNP Q15018
A	-4	GLN	-	expression tag	UNP Q15018
A	-3	GLY	-	expression tag	UNP Q15018
A	-2	GLY	-	expression tag	UNP Q15018
A	-1	GLY	-	expression tag	UNP Q15018
A	0	ARG	-	expression tag	UNP Q15018
F	-18	MET	-	initiating methionine	UNP Q15018
F	-17	HIS	-	expression tag	UNP Q15018
F	-16	HIS	-	expression tag	UNP Q15018
F	-15	HIS	-	expression tag	UNP Q15018
F	-14	HIS	-	expression tag	UNP Q15018
F	-13	HIS	-	expression tag	UNP Q15018
F	-12	HIS	-	expression tag	UNP Q15018

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	VAL	-	expression tag	UNP Q15018
F	-10	ASP	-	expression tag	UNP Q15018
F	-9	GLU	-	expression tag	UNP Q15018
F	-8	ASN	-	expression tag	UNP Q15018
F	-7	LEU	-	expression tag	UNP Q15018
F	-6	TYR	-	expression tag	UNP Q15018
F	-5	PHE	-	expression tag	UNP Q15018
F	-4	GLN	-	expression tag	UNP Q15018
F	-3	GLY	-	expression tag	UNP Q15018
F	-2	GLY	-	expression tag	UNP Q15018
F	-1	GLY	-	expression tag	UNP Q15018
F	0	ARG	-	expression tag	UNP Q15018

- Molecule 2 is a protein called Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	258	Total	C	H	N	O	S	0	0
			4122	1295	2053	366	394	14		
2	G	258	Total	C	H	N	O	S	0	0
			4122	1295	2053	366	394	14		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP P46736
B	-17	HIS	-	expression tag	UNP P46736
B	-16	HIS	-	expression tag	UNP P46736
B	-15	HIS	-	expression tag	UNP P46736
B	-14	HIS	-	expression tag	UNP P46736
B	-13	HIS	-	expression tag	UNP P46736
B	-12	HIS	-	expression tag	UNP P46736
B	-11	VAL	-	expression tag	UNP P46736
B	-10	ASP	-	expression tag	UNP P46736
B	-9	GLU	-	expression tag	UNP P46736
B	-8	ASN	-	expression tag	UNP P46736
B	-7	LEU	-	expression tag	UNP P46736
B	-6	TYR	-	expression tag	UNP P46736
B	-5	PHE	-	expression tag	UNP P46736
B	-4	GLN	-	expression tag	UNP P46736
B	-3	GLY	-	expression tag	UNP P46736
B	-2	GLY	-	expression tag	UNP P46736
B	-1	GLY	-	expression tag	UNP P46736

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ARG	-	expression tag	UNP P46736
G	-18	MET	-	initiating methionine	UNP P46736
G	-17	HIS	-	expression tag	UNP P46736
G	-16	HIS	-	expression tag	UNP P46736
G	-15	HIS	-	expression tag	UNP P46736
G	-14	HIS	-	expression tag	UNP P46736
G	-13	HIS	-	expression tag	UNP P46736
G	-12	HIS	-	expression tag	UNP P46736
G	-11	VAL	-	expression tag	UNP P46736
G	-10	ASP	-	expression tag	UNP P46736
G	-9	GLU	-	expression tag	UNP P46736
G	-8	ASN	-	expression tag	UNP P46736
G	-7	LEU	-	expression tag	UNP P46736
G	-6	TYR	-	expression tag	UNP P46736
G	-5	PHE	-	expression tag	UNP P46736
G	-4	GLN	-	expression tag	UNP P46736
G	-3	GLY	-	expression tag	UNP P46736
G	-2	GLY	-	expression tag	UNP P46736
G	-1	GLY	-	expression tag	UNP P46736
G	0	ARG	-	expression tag	UNP P46736

- Molecule 3 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	383	Total	C	H	N	O	S	0	0
			6077	1993	2999	504	567	14		
3	H	383	Total	C	H	N	O	S	0	0
			6077	1993	2999	504	567	14		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	initiating methionine	UNP Q9NXR7
C	-17	HIS	-	expression tag	UNP Q9NXR7
C	-16	HIS	-	expression tag	UNP Q9NXR7
C	-15	HIS	-	expression tag	UNP Q9NXR7
C	-14	HIS	-	expression tag	UNP Q9NXR7
C	-13	HIS	-	expression tag	UNP Q9NXR7
C	-12	HIS	-	expression tag	UNP Q9NXR7
C	-11	VAL	-	expression tag	UNP Q9NXR7
C	-10	ASP	-	expression tag	UNP Q9NXR7
C	-9	GLU	-	expression tag	UNP Q9NXR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	ASN	-	expression tag	UNP Q9NXR7
C	-7	LEU	-	expression tag	UNP Q9NXR7
C	-6	TYR	-	expression tag	UNP Q9NXR7
C	-5	PHE	-	expression tag	UNP Q9NXR7
C	-4	GLN	-	expression tag	UNP Q9NXR7
C	-3	GLY	-	expression tag	UNP Q9NXR7
C	-2	GLY	-	expression tag	UNP Q9NXR7
C	-1	GLY	-	expression tag	UNP Q9NXR7
C	0	ARG	-	expression tag	UNP Q9NXR7
H	-18	MET	-	initiating methionine	UNP Q9NXR7
H	-17	HIS	-	expression tag	UNP Q9NXR7
H	-16	HIS	-	expression tag	UNP Q9NXR7
H	-15	HIS	-	expression tag	UNP Q9NXR7
H	-14	HIS	-	expression tag	UNP Q9NXR7
H	-13	HIS	-	expression tag	UNP Q9NXR7
H	-12	HIS	-	expression tag	UNP Q9NXR7
H	-11	VAL	-	expression tag	UNP Q9NXR7
H	-10	ASP	-	expression tag	UNP Q9NXR7
H	-9	GLU	-	expression tag	UNP Q9NXR7
H	-8	ASN	-	expression tag	UNP Q9NXR7
H	-7	LEU	-	expression tag	UNP Q9NXR7
H	-6	TYR	-	expression tag	UNP Q9NXR7
H	-5	PHE	-	expression tag	UNP Q9NXR7
H	-4	GLN	-	expression tag	UNP Q9NXR7
H	-3	GLY	-	expression tag	UNP Q9NXR7
H	-2	GLY	-	expression tag	UNP Q9NXR7
H	-1	GLY	-	expression tag	UNP Q9NXR7
H	0	ARG	-	expression tag	UNP Q9NXR7

- Molecule 4 is a protein called BRISC and BRCA1-A complex member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	237	Total	C	H	N	O	S	0	0
			3761	1206	1872	306	359	18		
4	I	237	Total	C	H	N	O	S	0	0
			3761	1206	1872	306	359	18		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-22	MET	-	initiating methionine	UNP Q9NWX8
D	-21	ALA	-	expression tag	UNP Q9NWX8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	SER	-	expression tag	UNP Q9NWX8
D	-19	TRP	-	expression tag	UNP Q9NWX8
D	-18	SER	-	expression tag	UNP Q9NWX8
D	-17	HIS	-	expression tag	UNP Q9NWX8
D	-16	PRO	-	expression tag	UNP Q9NWX8
D	-15	GLN	-	expression tag	UNP Q9NWX8
D	-14	PHE	-	expression tag	UNP Q9NWX8
D	-13	GLU	-	expression tag	UNP Q9NWX8
D	-12	LYS	-	expression tag	UNP Q9NWX8
D	-11	VAL	-	expression tag	UNP Q9NWX8
D	-10	ASP	-	expression tag	UNP Q9NWX8
D	-9	GLU	-	expression tag	UNP Q9NWX8
D	-8	ASN	-	expression tag	UNP Q9NWX8
D	-7	LEU	-	expression tag	UNP Q9NWX8
D	-6	TYR	-	expression tag	UNP Q9NWX8
D	-5	PHE	-	expression tag	UNP Q9NWX8
D	-4	GLN	-	expression tag	UNP Q9NWX8
D	-3	GLY	-	expression tag	UNP Q9NWX8
D	-2	GLY	-	expression tag	UNP Q9NWX8
D	-1	GLY	-	expression tag	UNP Q9NWX8
D	0	ARG	-	expression tag	UNP Q9NWX8
I	-22	MET	-	initiating methionine	UNP Q9NWX8
I	-21	ALA	-	expression tag	UNP Q9NWX8
I	-20	SER	-	expression tag	UNP Q9NWX8
I	-19	TRP	-	expression tag	UNP Q9NWX8
I	-18	SER	-	expression tag	UNP Q9NWX8
I	-17	HIS	-	expression tag	UNP Q9NWX8
I	-16	PRO	-	expression tag	UNP Q9NWX8
I	-15	GLN	-	expression tag	UNP Q9NWX8
I	-14	PHE	-	expression tag	UNP Q9NWX8
I	-13	GLU	-	expression tag	UNP Q9NWX8
I	-12	LYS	-	expression tag	UNP Q9NWX8
I	-11	VAL	-	expression tag	UNP Q9NWX8
I	-10	ASP	-	expression tag	UNP Q9NWX8
I	-9	GLU	-	expression tag	UNP Q9NWX8
I	-8	ASN	-	expression tag	UNP Q9NWX8
I	-7	LEU	-	expression tag	UNP Q9NWX8
I	-6	TYR	-	expression tag	UNP Q9NWX8
I	-5	PHE	-	expression tag	UNP Q9NWX8
I	-4	GLN	-	expression tag	UNP Q9NWX8
I	-3	GLY	-	expression tag	UNP Q9NWX8
I	-2	GLY	-	expression tag	UNP Q9NWX8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP Q9NWX8
I	0	ARG	-	expression tag	UNP Q9NWX8

- Molecule 5 is a protein called Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	440	Total	C	H	N	O	S	0	0
			6893	2172	3452	616	638	15		
5	J	440	Total	C	H	N	O	S	0	0
			6893	2172	3452	616	638	15		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-23	MET	-	initiating methionine	UNP P34897
E	-22	GLY	-	expression tag	UNP P34897
E	-21	SER	-	expression tag	UNP P34897
E	-20	SER	-	expression tag	UNP P34897
E	-19	HIS	-	expression tag	UNP P34897
E	-18	HIS	-	expression tag	UNP P34897
E	-17	HIS	-	expression tag	UNP P34897
E	-16	HIS	-	expression tag	UNP P34897
E	-15	HIS	-	expression tag	UNP P34897
E	-14	HIS	-	expression tag	UNP P34897
E	-13	SER	-	expression tag	UNP P34897
E	-12	SER	-	expression tag	UNP P34897
E	-11	GLY	-	expression tag	UNP P34897
E	-10	LEU	-	expression tag	UNP P34897
E	-9	VAL	-	expression tag	UNP P34897
E	-8	PRO	-	expression tag	UNP P34897
E	-7	ARG	-	expression tag	UNP P34897
E	-6	GLY	-	expression tag	UNP P34897
E	-5	SER	-	expression tag	UNP P34897
E	264	THR	ALA	cloning artifact	UNP P34897
J	-23	MET	-	initiating methionine	UNP P34897
J	-22	GLY	-	expression tag	UNP P34897
J	-21	SER	-	expression tag	UNP P34897
J	-20	SER	-	expression tag	UNP P34897
J	-19	HIS	-	expression tag	UNP P34897
J	-18	HIS	-	expression tag	UNP P34897
J	-17	HIS	-	expression tag	UNP P34897
J	-16	HIS	-	expression tag	UNP P34897

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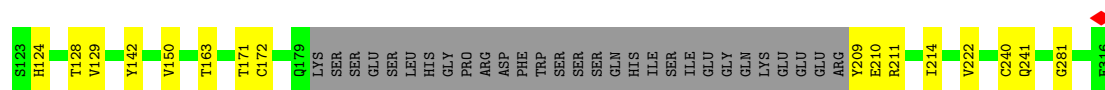
Chain	Residue	Modelled	Actual	Comment	Reference
J	-15	HIS	-	expression tag	UNP P34897
J	-14	HIS	-	expression tag	UNP P34897
J	-13	SER	-	expression tag	UNP P34897
J	-12	SER	-	expression tag	UNP P34897
J	-11	GLY	-	expression tag	UNP P34897
J	-10	LEU	-	expression tag	UNP P34897
J	-9	VAL	-	expression tag	UNP P34897
J	-8	PRO	-	expression tag	UNP P34897
J	-7	ARG	-	expression tag	UNP P34897
J	-6	GLY	-	expression tag	UNP P34897
J	-5	SER	-	expression tag	UNP P34897
J	264	THR	ALA	cloning artifact	UNP P34897

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

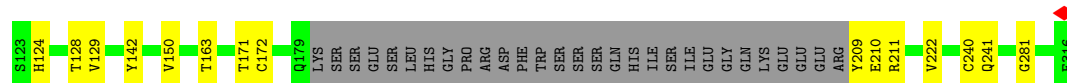
Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total Zn 1 1	0
6	G	1	Total Zn 1 1	0

- Molecule 7 is water.

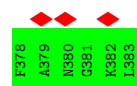
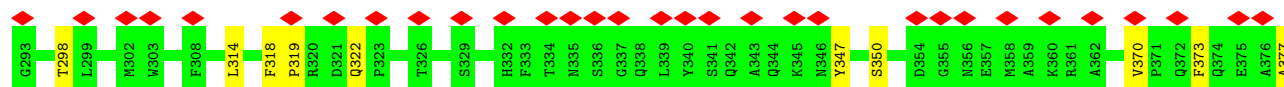
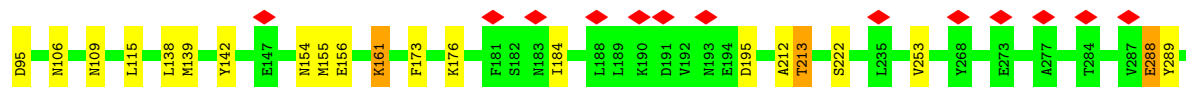
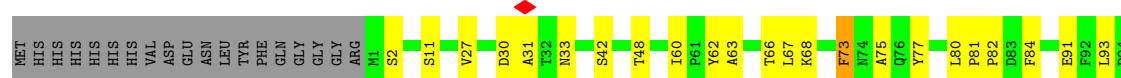
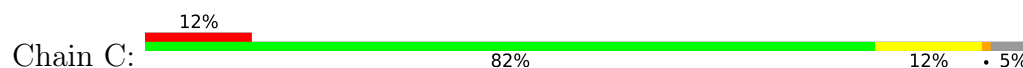
Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total H O 3 2 1	0
7	G	1	Total H O 3 2 1	0



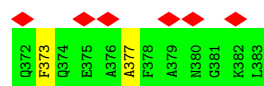
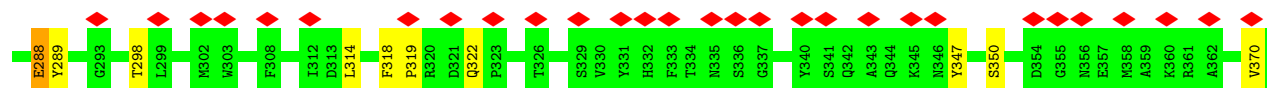
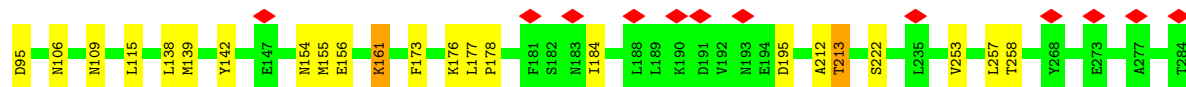
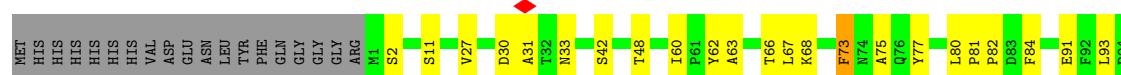
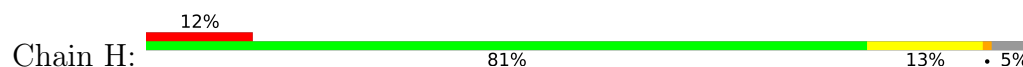
- Molecule 2: Lys-63-specific deubiquitinase BRCC36



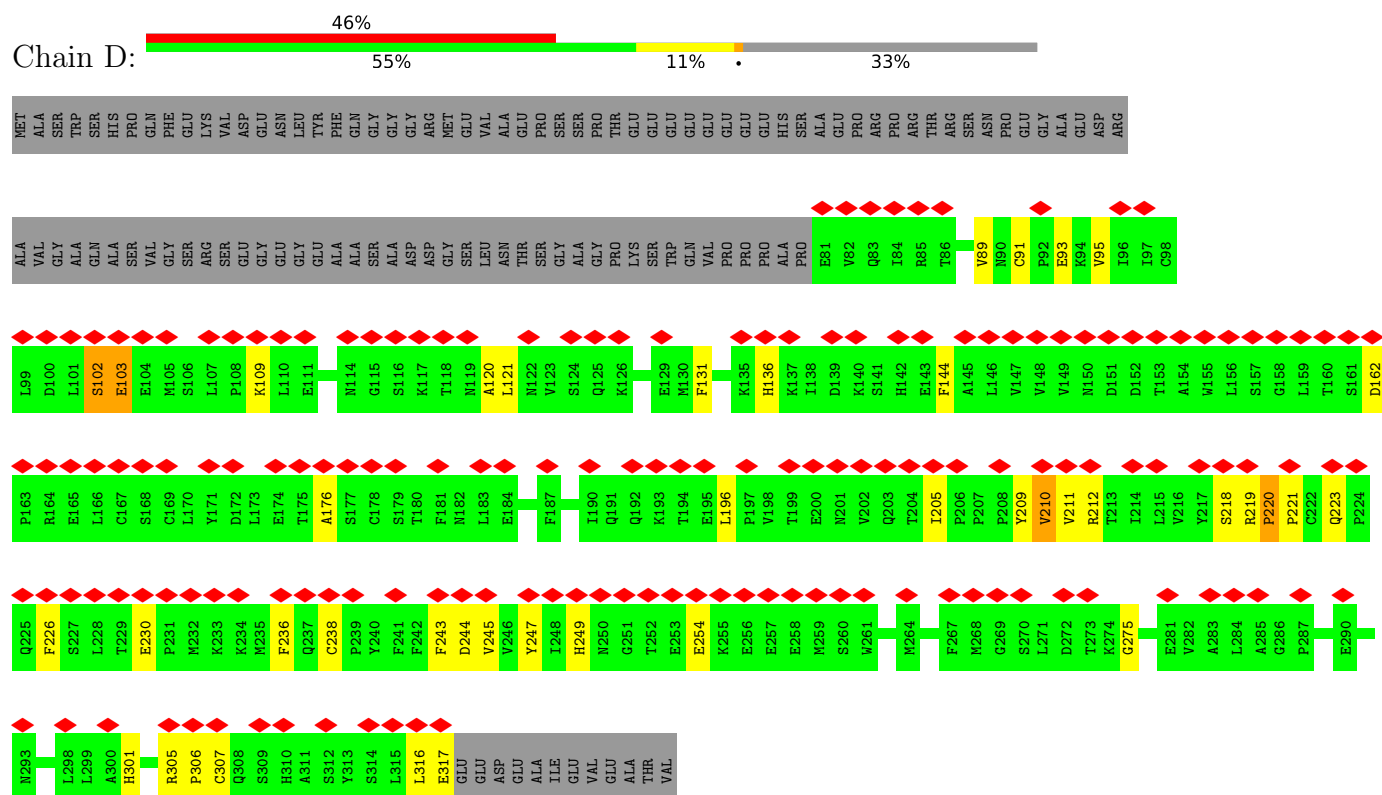
- Molecule 3: BRISC and BRCA1-A complex member 2



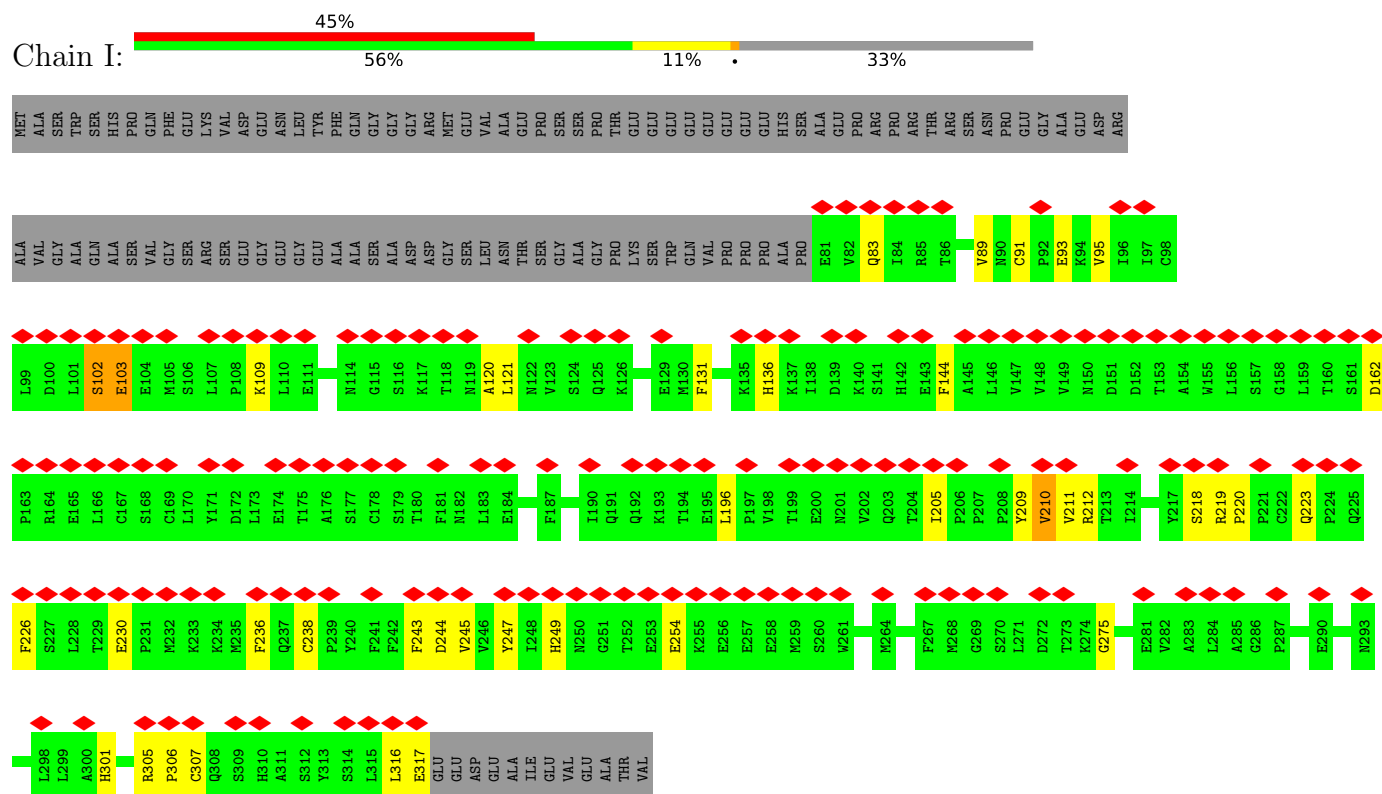
- Molecule 3: BRISC and BRCA1-A complex member 2



- Molecule 4: BRISC and BRCA1-A complex member 1

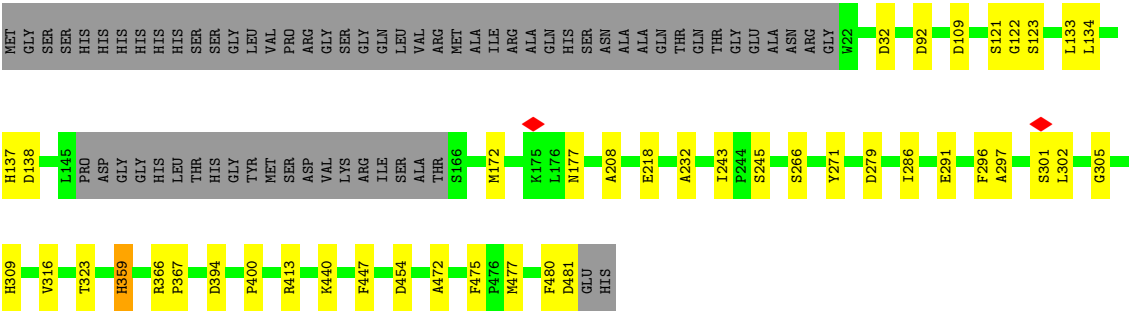


- Molecule 4: BRISC and BRCA1-A complex member 1



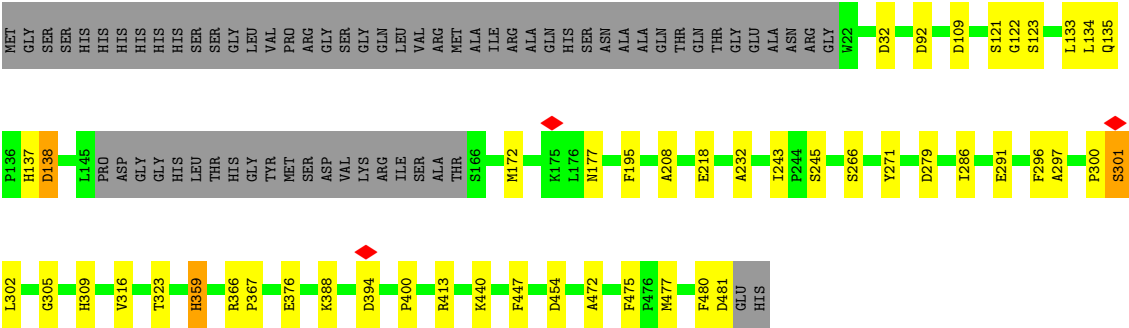
- Molecule 5: Serine hydroxymethyltransferase, mitochondrial

Chain E: 78% 8% 13%



• Molecule 5: Serine hydroxymethyltransferase, mitochondrial

Chain J: 77% 9% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	35595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF was determined using GCTF. CTF was corrected within RELION.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	58140	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00816	Depositor
Map size ($\text{\AA}$)	301.0, 301.0, 301.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	1/2120 (0.0%)	1.24	7/2856 (0.2%)
1	F	1.16	1/2120 (0.0%)	1.24	7/2856 (0.2%)
2	B	1.15	1/2105 (0.0%)	1.24	18/2845 (0.6%)
2	G	1.15	1/2105 (0.0%)	1.24	16/2845 (0.6%)
3	C	1.05	1/3169 (0.0%)	1.42	48/4310 (1.1%)
3	H	1.05	1/3169 (0.0%)	1.42	48/4310 (1.1%)
4	D	1.03	1/1934 (0.1%)	1.57	43/2623 (1.6%)
4	I	1.03	1/1934 (0.1%)	1.57	45/2623 (1.7%)
5	E	1.11	3/3508 (0.1%)	1.30	39/4744 (0.8%)
5	J	1.11	3/3508 (0.1%)	1.30	40/4744 (0.8%)
All	All	1.10	14/25672 (0.1%)	1.35	311/34756 (0.9%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	359	HIS	CB-CG	-8.20	1.38	1.50
5	J	359	HIS	CB-CG	-8.20	1.38	1.50
2	G	122	HIS	CB-CG	-7.33	1.39	1.50
2	B	122	HIS	CB-CG	-7.26	1.40	1.50
4	I	220	PRO	CA-C	6.59	1.55	1.51
4	D	220	PRO	CA-C	6.50	1.55	1.51
3	C	370	VAL	CA-CB	-6.29	1.50	1.54
1	A	141	HIS	CB-CG	-6.08	1.41	1.50
1	F	141	HIS	CB-CG	-6.08	1.41	1.50
3	H	370	VAL	CA-CB	-6.06	1.51	1.54
5	J	309	HIS	CB-CG	-5.19	1.42	1.50
5	E	309	HIS	CB-CG	-5.18	1.42	1.50
5	J	447	PHE	CG-CD2	-5.07	1.28	1.38
5	E	447	PHE	CG-CD2	-5.06	1.28	1.38

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	GLU	N-CA-C	9.04	124.14	113.20
2	G	210	GLU	N-CA-C	9.02	124.12	113.20
3	H	42	SER	N-CA-C	8.87	121.91	111.71
3	C	42	SER	N-CA-C	8.86	121.90	111.71
4	I	249	HIS	CA-CB-CG	8.85	122.65	113.80
4	D	249	HIS	CA-CB-CG	8.83	122.63	113.80
5	E	279	ASP	CA-C-N	8.74	128.39	119.82
5	E	279	ASP	C-N-CA	8.74	128.39	119.82
5	J	279	ASP	CA-C-N	8.72	128.37	119.82
5	J	279	ASP	C-N-CA	8.72	128.37	119.82
3	H	80	LEU	CA-C-N	8.60	125.85	119.66
3	H	80	LEU	C-N-CA	8.60	125.85	119.66
3	C	80	LEU	CA-C-N	8.56	125.83	119.66
3	C	80	LEU	C-N-CA	8.56	125.83	119.66
2	G	211	ARG	N-CA-C	8.37	122.57	110.10
2	B	211	ARG	N-CA-C	8.36	122.55	110.10
4	D	220	PRO	CA-C-N	8.22	128.71	119.92
4	D	220	PRO	C-N-CA	8.22	128.71	119.92
4	I	220	PRO	CA-C-N	8.21	128.71	119.92
4	I	220	PRO	C-N-CA	8.21	128.71	119.92
2	B	163	THR	N-CA-C	-8.14	104.23	114.56
5	E	305	GLY	CA-C-N	8.05	128.00	120.03
5	E	305	GLY	C-N-CA	8.05	128.00	120.03
4	D	196	LEU	CA-C-N	8.04	128.19	120.31
4	D	196	LEU	C-N-CA	8.04	128.19	120.31
4	I	196	LEU	CA-C-N	8.04	128.19	120.31
4	I	196	LEU	C-N-CA	8.04	128.19	120.31
4	I	243	PHE	CA-CB-CG	8.03	121.83	113.80
5	J	305	GLY	CA-C-N	8.02	127.97	120.03
5	J	305	GLY	C-N-CA	8.02	127.97	120.03
4	D	243	PHE	CA-CB-CG	7.99	121.79	113.80
2	G	163	THR	N-CA-C	-7.79	104.26	114.31
2	B	150	VAL	CA-C-N	-7.72	116.85	122.18
2	B	150	VAL	C-N-CA	-7.72	116.85	122.18
5	J	172	MET	CA-C-N	7.71	127.66	120.03
5	J	172	MET	C-N-CA	7.71	127.66	120.03
2	G	150	VAL	CA-C-N	-7.71	116.86	122.18
2	G	150	VAL	C-N-CA	-7.71	116.86	122.18
5	E	172	MET	CA-C-N	7.69	127.64	120.03
5	E	172	MET	C-N-CA	7.69	127.64	120.03
5	E	286	ILE	CA-C-N	7.68	127.63	120.03
5	E	286	ILE	C-N-CA	7.68	127.63	120.03
5	J	286	ILE	CA-C-N	7.67	127.63	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	286	ILE	C-N-CA	7.67	127.63	120.03
4	D	162	ASP	CA-C-N	7.64	127.36	119.56
4	D	162	ASP	C-N-CA	7.64	127.36	119.56
4	I	162	ASP	CA-C-N	7.64	127.35	119.56
4	I	162	ASP	C-N-CA	7.64	127.35	119.56
4	I	205	ILE	CA-C-N	7.59	125.13	119.66
4	I	205	ILE	C-N-CA	7.59	125.13	119.66
4	D	205	ILE	CA-C-N	7.58	125.12	119.66
4	D	205	ILE	C-N-CA	7.58	125.12	119.66
5	J	177	ASN	CA-C-N	7.41	127.11	119.56
5	J	177	ASN	C-N-CA	7.41	127.11	119.56
5	E	177	ASN	CA-C-N	7.40	127.11	119.56
5	E	177	ASN	C-N-CA	7.40	127.11	119.56
4	I	95	VAL	N-CA-C	7.38	118.53	107.75
4	D	95	VAL	N-CA-C	7.38	118.52	107.75
1	A	43	SER	N-CA-C	-7.35	101.07	110.19
1	F	212	VAL	N-CA-C	-7.33	94.10	109.34
4	D	305	ARG	CA-C-N	7.32	127.75	119.92
4	D	305	ARG	C-N-CA	7.32	127.75	119.92
1	F	43	SER	N-CA-C	-7.32	101.12	110.19
1	A	212	VAL	N-CA-C	-7.30	94.17	109.34
4	D	91	CYS	CA-C-N	7.27	127.19	119.85
4	D	91	CYS	C-N-CA	7.27	127.19	119.85
4	I	305	ARG	CA-C-N	7.25	127.67	119.92
4	I	305	ARG	C-N-CA	7.25	127.67	119.92
4	I	91	CYS	CA-C-N	7.24	127.16	119.85
4	I	91	CYS	C-N-CA	7.24	127.16	119.85
5	E	245	SER	CA-C-N	7.17	126.88	119.56
5	E	245	SER	C-N-CA	7.17	126.88	119.56
5	J	245	SER	CA-C-N	7.14	126.85	119.56
5	J	245	SER	C-N-CA	7.14	126.85	119.56
5	E	296	PHE	CA-CB-CG	-7.13	106.67	113.80
5	J	296	PHE	CA-CB-CG	-7.12	106.69	113.80
3	H	81	PRO	CA-C-N	7.04	127.44	119.83
3	H	81	PRO	C-N-CA	7.04	127.44	119.83
3	C	81	PRO	CA-C-N	7.04	127.43	119.83
3	C	81	PRO	C-N-CA	7.04	127.43	119.83
4	D	244	ASP	CA-CB-CG	7.03	119.63	112.60
4	I	244	ASP	CA-CB-CG	6.99	119.59	112.60
5	J	123	SER	N-CA-C	-6.94	100.21	110.20
5	E	123	SER	N-CA-C	-6.92	100.23	110.20
5	J	109	ASP	CA-C-N	6.84	127.41	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	109	ASP	C-N-CA	6.84	127.41	119.47
4	D	238	CYS	CA-C-N	6.83	126.97	119.87
4	D	238	CYS	C-N-CA	6.83	126.97	119.87
5	E	477	MET	CA-C-N	6.83	127.28	120.52
5	E	477	MET	C-N-CA	6.83	127.28	120.52
5	E	109	ASP	CA-C-N	6.83	127.39	119.47
5	E	109	ASP	C-N-CA	6.83	127.39	119.47
5	J	477	MET	CA-C-N	6.82	127.28	120.52
5	J	477	MET	C-N-CA	6.82	127.28	120.52
4	I	238	CYS	CA-C-N	6.78	126.92	119.87
4	I	238	CYS	C-N-CA	6.78	126.92	119.87
2	B	124	HIS	CA-C-N	6.65	126.90	119.32
2	B	124	HIS	C-N-CA	6.65	126.90	119.32
2	G	124	HIS	CA-C-N	6.62	126.86	119.32
2	G	124	HIS	C-N-CA	6.62	126.86	119.32
3	H	48	THR	CA-C-N	6.58	126.76	120.31
3	H	48	THR	C-N-CA	6.58	126.76	120.31
5	J	323	THR	CA-C-N	6.57	126.26	119.56
5	J	323	THR	C-N-CA	6.57	126.26	119.56
5	E	302	LEU	N-CA-C	-6.55	105.30	113.55
5	E	323	THR	CA-C-N	6.55	126.24	119.56
5	E	323	THR	C-N-CA	6.55	126.24	119.56
3	C	48	THR	CA-C-N	6.54	126.72	120.31
3	C	48	THR	C-N-CA	6.54	126.72	120.31
5	J	302	LEU	N-CA-C	-6.53	105.32	113.55
5	E	92	ASP	CA-CB-CG	6.53	119.13	112.60
5	J	92	ASP	CA-CB-CG	6.51	119.11	112.60
3	C	195	ASP	CA-C-N	6.47	126.16	119.56
3	C	195	ASP	C-N-CA	6.47	126.16	119.56
3	H	11	SER	CA-C-N	6.46	126.96	119.47
3	H	11	SER	C-N-CA	6.46	126.96	119.47
3	H	195	ASP	CA-C-N	6.45	126.14	119.56
3	H	195	ASP	C-N-CA	6.45	126.14	119.56
3	C	11	SER	CA-C-N	6.44	126.94	119.47
3	C	11	SER	C-N-CA	6.44	126.94	119.47
4	I	219	ARG	CA-C-N	6.44	124.36	119.66
4	I	219	ARG	C-N-CA	6.44	124.36	119.66
2	G	222	VAL	N-CA-C	6.38	117.38	111.45
4	D	219	ARG	CA-C-N	6.36	124.30	119.66
4	D	219	ARG	C-N-CA	6.36	124.30	119.66
4	I	226	PHE	N-CA-C	6.35	119.75	109.40
2	B	222	VAL	N-CA-C	6.34	117.35	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	93	LEU	CA-C-N	6.33	126.28	119.76
3	H	93	LEU	C-N-CA	6.33	126.28	119.76
3	C	93	LEU	CA-C-N	6.33	126.28	119.76
3	C	93	LEU	C-N-CA	6.33	126.28	119.76
4	D	226	PHE	N-CA-C	6.32	119.71	109.40
5	J	245	SER	N-CA-C	6.24	117.51	109.65
2	B	281	GLY	CA-C-N	6.23	126.42	119.32
2	B	281	GLY	C-N-CA	6.23	126.42	119.32
5	E	245	SER	N-CA-C	6.22	117.49	109.65
2	G	281	GLY	CA-C-N	6.20	126.39	119.32
2	G	281	GLY	C-N-CA	6.20	126.39	119.32
3	C	322	GLN	CA-C-N	6.18	126.15	120.03
3	C	322	GLN	C-N-CA	6.18	126.15	120.03
3	C	109	ASN	CA-C-N	6.14	126.60	119.47
3	C	109	ASN	C-N-CA	6.14	126.60	119.47
3	H	322	GLN	CA-C-N	6.13	126.10	120.03
3	H	322	GLN	C-N-CA	6.13	126.10	120.03
1	A	122	VAL	CA-C-N	6.13	126.03	119.28
1	A	122	VAL	C-N-CA	6.13	126.03	119.28
1	F	122	VAL	CA-C-N	6.13	126.02	119.28
1	F	122	VAL	C-N-CA	6.13	126.02	119.28
4	I	301	HIS	CA-C-N	6.13	126.58	119.47
4	I	301	HIS	C-N-CA	6.13	126.58	119.47
1	F	174	LYS	N-CA-C	6.13	118.88	110.24
3	H	109	ASN	CA-C-N	6.12	126.57	119.47
3	H	109	ASN	C-N-CA	6.12	126.57	119.47
5	E	122	GLY	N-CA-C	-6.12	107.25	115.21
4	D	131	PHE	CA-CB-CG	6.11	119.91	113.80
4	D	301	HIS	CA-C-N	6.10	126.55	119.47
4	D	301	HIS	C-N-CA	6.10	126.55	119.47
4	D	103	GLU	N-CA-C	6.09	121.41	111.37
5	J	122	GLY	N-CA-C	-6.08	107.30	115.21
1	A	174	LYS	N-CA-C	6.08	118.81	110.24
5	E	359	HIS	CA-CB-CG	-6.07	107.73	113.80
4	I	131	PHE	CA-CB-CG	6.07	119.87	113.80
2	B	93	SER	CA-C-N	6.06	126.50	119.47
2	B	93	SER	C-N-CA	6.06	126.50	119.47
2	G	93	SER	CA-C-N	6.05	126.49	119.47
2	G	93	SER	C-N-CA	6.05	126.49	119.47
4	I	103	GLU	N-CA-C	6.05	121.36	111.37
5	J	359	HIS	CA-CB-CG	-6.05	107.75	113.80
4	D	245	VAL	N-CA-C	6.04	116.99	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	245	VAL	N-CA-C	6.02	116.97	108.17
4	I	236	PHE	N-CA-C	-6.00	104.82	111.36
4	D	236	PHE	N-CA-C	-5.99	104.83	111.36
5	J	475	PHE	CA-C-N	5.94	125.91	120.03
5	J	475	PHE	C-N-CA	5.94	125.91	120.03
5	E	475	PHE	CA-C-N	5.88	125.85	120.03
5	E	475	PHE	C-N-CA	5.88	125.85	120.03
3	C	253	VAL	N-CA-C	-5.85	104.81	110.72
3	C	156	GLU	CA-C-N	-5.82	115.97	123.19
3	C	156	GLU	C-N-CA	-5.82	115.97	123.19
3	H	156	GLU	CA-C-N	-5.82	115.97	123.19
3	H	156	GLU	C-N-CA	-5.82	115.97	123.19
3	H	253	VAL	N-CA-C	-5.82	104.84	110.72
3	H	115	LEU	N-CA-C	-5.81	104.38	112.45
3	C	115	LEU	N-CA-C	-5.80	104.39	112.45
4	I	93	GLU	N-CA-C	5.79	118.64	109.50
4	D	144	PHE	N-CA-C	5.76	118.61	109.50
4	D	93	GLU	N-CA-C	5.76	118.60	109.50
4	I	144	PHE	N-CA-C	5.74	118.57	109.50
3	H	106	ASN	CA-C-N	5.67	125.35	119.56
3	H	106	ASN	C-N-CA	5.67	125.35	119.56
3	C	314	LEU	CA-C-N	5.65	125.60	119.78
3	C	314	LEU	C-N-CA	5.65	125.60	119.78
4	I	102	SER	N-CA-C	5.64	122.81	110.80
3	H	184	ILE	CA-C-N	5.63	125.58	119.78
3	H	184	ILE	C-N-CA	5.63	125.58	119.78
4	D	102	SER	N-CA-C	5.62	122.77	110.80
3	H	314	LEU	CA-C-N	5.62	125.57	119.78
3	H	314	LEU	C-N-CA	5.62	125.57	119.78
3	C	106	ASN	CA-C-N	5.61	125.28	119.56
3	C	106	ASN	C-N-CA	5.61	125.28	119.56
4	I	89	VAL	N-CA-C	5.60	116.55	108.48
4	D	89	VAL	N-CA-C	5.60	116.54	108.48
1	F	206	ILE	N-CA-C	-5.59	105.27	110.53
5	E	208	ALA	N-CA-C	5.59	117.37	111.28
3	C	184	ILE	CA-C-N	5.58	125.53	119.78
3	C	184	ILE	C-N-CA	5.58	125.53	119.78
1	A	206	ILE	N-CA-C	-5.58	105.29	110.53
2	B	45	ASP	CA-CB-CG	5.57	118.17	112.60
5	J	208	ALA	N-CA-C	5.57	117.35	111.28
2	G	45	ASP	CA-CB-CG	5.56	118.16	112.60
3	H	350	SER	N-CA-C	-5.56	103.22	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	289	TYR	CA-C-N	5.54	130.24	121.99
3	H	289	TYR	C-N-CA	5.54	130.24	121.99
3	C	289	TYR	CA-C-N	5.53	130.23	121.99
3	C	289	TYR	C-N-CA	5.53	130.23	121.99
1	A	198	ASP	N-CA-C	5.52	118.36	111.24
1	F	198	ASP	N-CA-C	5.51	118.35	111.24
5	J	316	VAL	CB-CA-C	-5.50	104.93	111.97
5	E	316	VAL	CB-CA-C	-5.49	104.94	111.97
3	C	350	SER	N-CA-C	-5.46	103.30	108.22
3	H	347	TYR	N-CA-C	5.46	114.42	108.14
2	B	209	TYR	CA-C-N	5.46	132.85	121.94
2	B	209	TYR	C-N-CA	5.46	132.85	121.94
2	G	209	TYR	CA-C-N	5.45	132.84	121.94
2	G	209	TYR	C-N-CA	5.45	132.84	121.94
2	B	29	THR	N-CA-C	5.45	117.46	109.24
2	G	29	THR	N-CA-C	5.44	117.45	109.24
4	D	223	GLN	CA-C-N	5.43	126.63	119.84
4	D	223	GLN	C-N-CA	5.43	126.63	119.84
3	C	347	TYR	N-CA-C	5.43	114.38	108.14
4	I	223	GLN	CA-C-N	5.42	126.61	119.84
4	I	223	GLN	C-N-CA	5.42	126.61	119.84
5	E	32	ASP	CA-C-N	5.42	125.08	119.56
5	E	32	ASP	C-N-CA	5.42	125.08	119.56
3	H	106	ASN	N-CA-C	-5.41	103.23	109.93
5	J	32	ASP	CA-C-N	5.40	125.07	119.56
5	J	32	ASP	C-N-CA	5.40	125.07	119.56
5	E	297	ALA	N-CA-C	-5.38	106.76	113.38
5	J	297	ALA	N-CA-C	-5.38	106.76	113.38
3	C	106	ASN	N-CA-C	-5.38	103.27	109.93
4	D	247	TYR	N-CA-C	5.35	117.80	108.76
5	E	232	ALA	CA-C-N	-5.35	114.09	122.65
5	E	232	ALA	C-N-CA	-5.35	114.09	122.65
3	C	2	SER	CA-C-N	5.34	125.01	119.56
3	C	2	SER	C-N-CA	5.34	125.01	119.56
3	H	95	ASP	CA-C-N	5.33	125.00	119.56
3	H	95	ASP	C-N-CA	5.33	125.00	119.56
5	E	133	LEU	N-CA-C	5.33	119.91	113.41
3	C	347	TYR	CA-C-N	5.32	126.50	119.84
3	C	347	TYR	C-N-CA	5.32	126.50	119.84
4	I	247	TYR	N-CA-C	5.32	117.76	108.76
5	J	232	ALA	CA-C-N	-5.32	114.14	122.65
5	J	232	ALA	C-N-CA	-5.32	114.14	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	133	LEU	N-CA-C	5.32	119.90	113.41
3	H	347	TYR	CA-C-N	5.31	126.48	119.84
3	H	347	TYR	C-N-CA	5.31	126.48	119.84
4	D	230	GLU	CA-C-N	5.31	124.97	119.56
4	D	230	GLU	C-N-CA	5.31	124.97	119.56
3	C	84	PHE	CA-CB-CG	-5.30	108.50	113.80
3	H	84	PHE	CA-CB-CG	-5.30	108.50	113.80
3	H	2	SER	CA-C-N	5.29	124.95	119.56
3	H	2	SER	C-N-CA	5.29	124.95	119.56
3	C	95	ASP	CA-C-N	5.28	124.95	119.56
3	C	95	ASP	C-N-CA	5.28	124.95	119.56
4	I	230	GLU	CA-C-N	5.26	124.92	119.56
4	I	230	GLU	C-N-CA	5.26	124.92	119.56
4	I	249	HIS	CB-CA-C	-5.23	103.58	112.00
4	D	249	HIS	CB-CA-C	-5.22	103.59	112.00
3	H	288	GLU	CB-CG-CD	5.18	121.42	112.60
3	C	288	GLU	CB-CG-CD	5.18	121.40	112.60
3	H	73	PHE	CA-CB-CG	5.16	118.96	113.80
4	D	209	TYR	CA-C-N	5.16	131.26	121.97
4	D	209	TYR	C-N-CA	5.16	131.26	121.97
4	I	209	TYR	CA-C-N	5.15	131.24	121.97
4	I	209	TYR	C-N-CA	5.15	131.24	121.97
3	H	77	TYR	CA-C-N	5.13	124.79	119.56
3	H	77	TYR	C-N-CA	5.13	124.79	119.56
3	C	77	TYR	CA-C-N	5.13	124.79	119.56
3	C	77	TYR	C-N-CA	5.13	124.79	119.56
4	D	218	SER	N-CA-C	-5.12	99.90	110.80
4	I	218	SER	N-CA-C	-5.12	99.90	110.80
3	C	73	PHE	CA-CB-CG	5.11	118.91	113.80
4	D	136	HIS	N-CA-C	-5.10	106.65	112.92
3	C	222	SER	CA-C-N	5.10	126.21	119.84
3	C	222	SER	C-N-CA	5.10	126.21	119.84
4	D	275	GLY	CA-C-O	-5.08	118.72	122.23
3	H	173	PHE	CA-CB-CG	5.08	118.88	113.80
4	I	136	HIS	N-CA-C	-5.07	106.68	112.92
3	H	222	SER	CA-C-N	5.06	126.17	119.84
3	H	222	SER	C-N-CA	5.06	126.17	119.84
5	J	138	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	214	ILE	CA-C-N	5.05	125.05	119.90
2	B	214	ILE	C-N-CA	5.05	125.05	119.90
4	I	275	GLY	CA-C-O	-5.05	118.75	122.23
4	D	212	ARG	NE-CZ-NH2	-5.05	114.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	243	ILE	CA-C-N	5.05	125.05	119.90
5	E	243	ILE	C-N-CA	5.05	125.05	119.90
5	J	243	ILE	CA-C-N	5.04	125.04	119.90
5	J	243	ILE	C-N-CA	5.04	125.04	119.90
5	E	138	ASP	CA-CB-CG	5.04	117.64	112.60
3	C	173	PHE	CA-CB-CG	5.04	118.84	113.80
4	I	212	ARG	NE-CZ-NH2	-5.04	114.67	119.20
3	C	73	PHE	N-CA-C	5.03	121.52	110.80
3	C	161	LYS	N-CA-C	-5.03	102.34	110.14
5	J	195	PHE	CA-CB-CG	-5.03	108.77	113.80
5	J	134	LEU	N-CA-C	5.03	117.93	110.14
3	H	161	LYS	N-CA-C	-5.02	102.36	110.14
3	H	73	PHE	N-CA-C	5.02	121.49	110.80
4	I	83	GLN	CA-C-N	-5.01	116.22	122.48
4	I	83	GLN	C-N-CA	-5.01	116.22	122.48
5	E	134	LEU	N-CA-C	5.01	117.90	110.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2082	2052	2054	7	0
1	F	2082	2052	2054	7	0
2	B	2069	2053	2051	5	0
2	G	2069	2053	2051	5	0
3	C	3078	2999	3001	15	0
3	H	3078	2999	3001	17	0
4	D	1889	1872	1871	9	0
4	I	1889	1872	1871	6	0
5	E	3441	3452	3451	9	0
5	J	3441	3452	3451	12	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
7	B	1	2	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1	2	0	0	0
All	All	25122	24860	24856	90	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 2.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:SER:O	1:F:44:GLN:C	2.43	0.60
4:D:316:LEU:O	4:D:317:GLU:C	2.47	0.58
1:A:43:SER:O	1:A:44:GLN:C	2.43	0.58
4:I:316:LEU:O	4:I:317:GLU:C	2.47	0.57
1:F:211:GLN:C	1:F:212:VAL:O	2.45	0.56
5:J:359:HIS:ND1	5:J:359:HIS:N	2.53	0.55
5:J:480:PHE:O	5:J:481:ASP:C	2.51	0.55
4:D:210:VAL:HG12	4:D:211:VAL:H	1.73	0.54
5:E:480:PHE:O	5:E:481:ASP:C	2.51	0.54
4:I:109:LYS:NZ	4:I:254:GLU:OE2	2.42	0.53
4:D:102:SER:OG	4:D:176:ALA:O	2.22	0.53
4:I:210:VAL:HG12	4:I:211:VAL:H	1.73	0.53
4:D:109:LYS:NZ	4:D:254:GLU:OE2	2.42	0.52
1:F:212:VAL:O	1:F:213:TYR:HB3	2.09	0.52
1:A:212:VAL:O	1:A:213:TYR:HB3	2.09	0.51
1:A:211:GLN:C	1:A:212:VAL:O	2.45	0.51
4:I:306:PRO:O	4:I:307:CYS:C	2.54	0.50
3:H:60:ILE:N	3:H:66:THR:O	2.45	0.50
3:C:60:ILE:N	3:C:66:THR:O	2.45	0.50
4:D:306:PRO:O	4:D:307:CYS:C	2.54	0.49
4:I:102:SER:OG	4:I:103:GLU:N	2.44	0.49
1:F:198:ASP:N	1:F:198:ASP:OD1	2.45	0.49
1:A:198:ASP:OD1	1:A:198:ASP:N	2.45	0.48
3:C:288:GLU:HG2	3:C:298:THR:HB	1.95	0.48
3:H:68:LYS:NZ	5:J:218:GLU:OE2	2.47	0.48
3:H:288:GLU:HG2	3:H:298:THR:HB	1.96	0.48
4:D:102:SER:OG	4:D:103:GLU:N	2.44	0.47
3:C:68:LYS:NZ	5:E:218:GLU:OE2	2.47	0.47
3:C:27:VAL:H	3:C:33:ASN:HD21	1.62	0.46
1:A:48:THR:OG1	1:A:49:GLU:N	2.49	0.46
3:C:62:TYR:O	3:C:63:ALA:C	2.57	0.46
3:C:138:LEU:O	3:C:139:MET:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:ILE:N	2:B:142:TYR:OH	2.45	0.46
5:J:271:TYR:CE1	5:J:291:GLU:HB3	2.51	0.46
5:J:366:ARG:N	5:J:367:PRO:CD	2.79	0.46
3:H:62:TYR:O	3:H:63:ALA:C	2.57	0.45
3:H:27:VAL:H	3:H:33:ASN:HD21	1.62	0.45
5:E:359:HIS:ND1	5:E:359:HIS:N	2.53	0.45
5:E:271:TYR:CE1	5:E:291:GLU:HB3	2.51	0.45
2:G:171:THR:OG1	2:G:172:CYS:N	2.48	0.45
5:E:366:ARG:N	5:E:367:PRO:CD	2.79	0.45
1:A:172:GLU:O	1:A:173:TYR:C	2.60	0.45
3:H:66:THR:O	3:H:67:LEU:C	2.60	0.45
2:B:171:THR:OG1	2:B:172:CYS:N	2.48	0.45
2:B:128:THR:OG1	2:B:129:VAL:N	2.49	0.45
3:H:73:PHE:HB3	3:H:82:PRO:HA	1.99	0.45
3:C:66:THR:O	3:C:67:LEU:C	2.59	0.44
3:H:138:LEU:O	3:H:139:MET:C	2.58	0.44
5:E:121:SER:N	5:E:266:SER:HA	2.32	0.44
1:F:48:THR:OG1	1:F:49:GLU:N	2.49	0.44
4:D:102:SER:OG	4:D:176:ALA:N	2.45	0.44
2:G:128:THR:OG1	2:G:129:VAL:N	2.49	0.44
1:A:42:ASP:C	1:A:43:SER:O	2.58	0.44
2:B:45:ASP:O	2:B:46:THR:C	2.60	0.44
5:J:121:SER:N	5:J:266:SER:HA	2.33	0.44
3:C:73:PHE:HB3	3:C:82:PRO:HA	1.98	0.43
2:G:45:ASP:O	2:G:46:THR:C	2.60	0.43
2:G:92:ILE:N	2:G:142:TYR:OH	2.45	0.43
5:J:376:GLU:OE1	5:J:388:LYS:NZ	2.44	0.43
1:F:42:ASP:C	1:F:43:SER:O	2.58	0.43
3:C:318:PHE:N	3:C:319:PRO:CD	2.81	0.43
3:H:318:PHE:N	3:H:319:PRO:CD	2.81	0.43
3:C:91:GLU:OE1	3:C:161:LYS:NZ	2.51	0.43
1:F:172:GLU:O	1:F:173:TYR:C	2.60	0.42
3:H:257:LEU:O	3:H:258:THR:C	2.63	0.42
5:E:440:LYS:NZ	5:E:454:ASP:OD2	2.53	0.42
5:J:413:ARG:NH2	5:J:472:ALA:O	2.53	0.42
2:G:240:CYS:SG	2:G:241:GLN:N	2.92	0.42
3:C:30:ASP:OD1	3:C:31:ALA:N	2.53	0.42
2:B:240:CYS:SG	2:B:241:GLN:N	2.92	0.41
5:E:413:ARG:NH2	5:E:472:ALA:O	2.53	0.41
3:C:212:ALA:O	3:C:213:THR:CB	2.68	0.41
4:D:220:PRO:HA	4:D:221:PRO:HD3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:440:LYS:NZ	5:J:454:ASP:OD2	2.53	0.41
3:H:30:ASP:OD1	3:H:31:ALA:N	2.53	0.41
3:C:373:PHE:CD1	3:C:377:ALA:HB3	2.56	0.41
3:H:91:GLU:OE1	3:H:161:LYS:NZ	2.51	0.41
3:H:212:ALA:O	3:H:213:THR:CB	2.68	0.41
4:I:120:ALA:O	4:I:121:LEU:C	2.62	0.41
5:J:300:PRO:O	5:J:301:SER:HB2	2.21	0.41
3:H:177:LEU:HA	3:H:178:PRO:HD3	1.90	0.41
5:J:135:GLN:O	5:J:138:ASP:HB2	2.21	0.41
3:C:154:ASN:HB3	3:C:176:LYS:H	1.86	0.40
3:H:373:PHE:CD1	3:H:377:ALA:HB3	2.56	0.40
3:C:138:LEU:O	3:C:142:TYR:HB3	2.20	0.40
4:D:120:ALA:O	4:D:121:LEU:C	2.62	0.40
3:H:138:LEU:O	3:H:142:TYR:HB3	2.20	0.40
3:H:154:ASN:HB3	3:H:176:LYS:H	1.86	0.40
5:E:394:ASP:OD2	5:E:400:PRO:HA	2.22	0.40
5:J:394:ASP:OD2	5:J:400:PRO:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/434 (58%)	238 (94%)	14 (6%)	1 (0%)	30	64
1	F	253/434 (58%)	237 (94%)	15 (6%)	1 (0%)	30	64
2	B	252/335 (75%)	248 (98%)	4 (2%)	0	100	100
2	G	252/335 (75%)	248 (98%)	4 (2%)	0	100	100
3	C	381/402 (95%)	352 (92%)	26 (7%)	3 (1%)	16	50
3	H	381/402 (95%)	353 (93%)	25 (7%)	3 (1%)	16	50
4	D	235/352 (67%)	212 (90%)	22 (9%)	1 (0%)	30	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	235/352 (67%)	212 (90%)	22 (9%)	1 (0%)	30	64
5	E	436/507 (86%)	417 (96%)	17 (4%)	2 (0%)	24	59
5	J	436/507 (86%)	417 (96%)	17 (4%)	2 (0%)	24	59
All	All	3114/4060 (77%)	2934 (94%)	166 (5%)	14 (0%)	31	64

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	75	ALA
3	C	213	THR
3	H	75	ALA
3	H	213	THR
4	D	210	VAL
4	I	210	VAL
5	E	137	HIS
5	E	301	SER
5	J	137	HIS
5	J	301	SER
1	A	202	VAL
1	F	202	VAL
3	C	155	MET
3	H	155	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/386 (60%)	232 (100%)	0	100	100
1	F	232/386 (60%)	232 (100%)	0	100	100
2	B	235/302 (78%)	235 (100%)	0	100	100
2	G	235/302 (78%)	235 (100%)	0	100	100
3	C	337/353 (96%)	337 (100%)	0	100	100
3	H	337/353 (96%)	337 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	219/309 (71%)	219 (100%)	0	100	100
4	I	219/309 (71%)	219 (100%)	0	100	100
5	E	364/416 (88%)	364 (100%)	0	100	100
5	J	364/416 (88%)	364 (100%)	0	100	100
All	All	2774/3532 (78%)	2774 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	34	GLN
1	A	102	GLN
1	A	151	ASN
1	A	156	GLN
1	A	217	GLN
3	C	33	ASN
3	C	101	ASN
3	C	255	HIS
1	F	24	HIS
1	F	34	GLN
1	F	102	GLN
1	F	151	ASN
1	F	156	GLN
3	H	33	ASN
3	H	255	HIS
5	E	118	GLN
5	E	187	GLN
5	E	332	GLN
5	J	118	GLN
5	J	187	GLN
5	J	332	GLN
5	J	459	GLN

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 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.

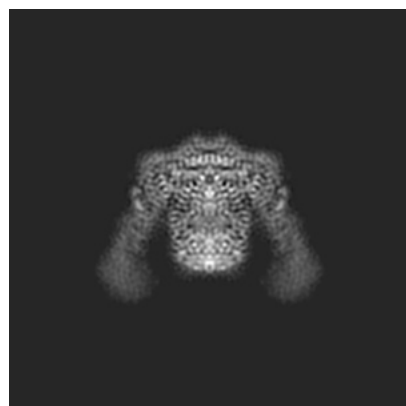
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0132. These allow visual inspection of the internal detail of the map and identification of artifacts.

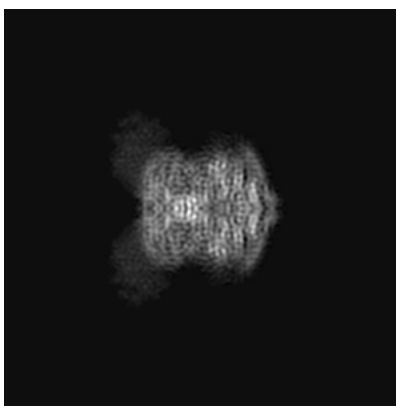
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

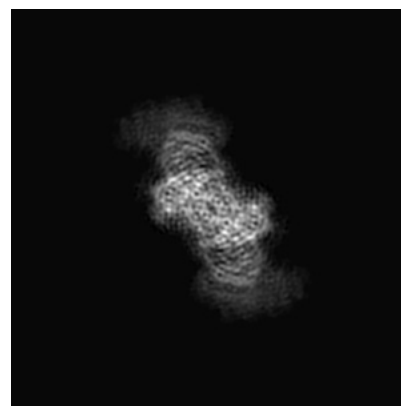
6.1.1 Primary map



X

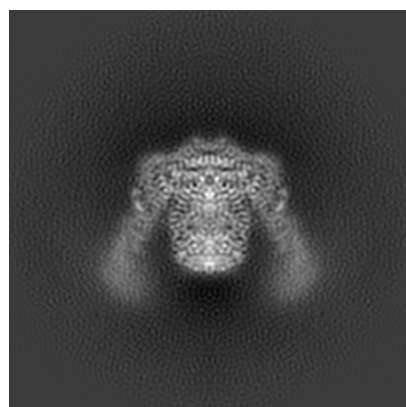


Y

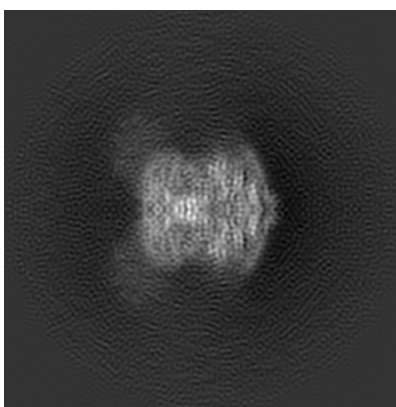


Z

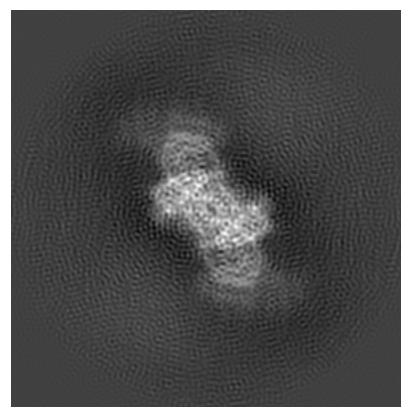
6.1.2 Raw map



X



Y

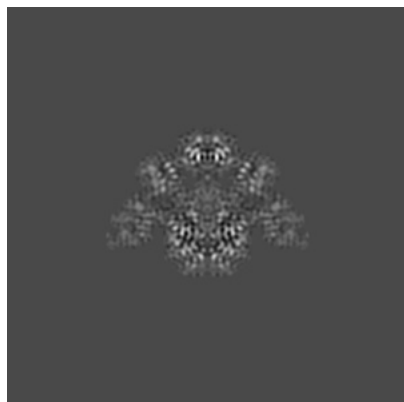


Z

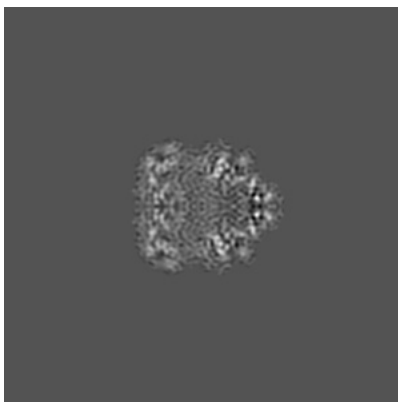
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

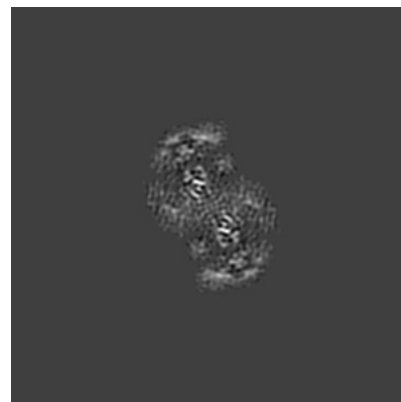
6.2.1 Primary map



X Index: 175

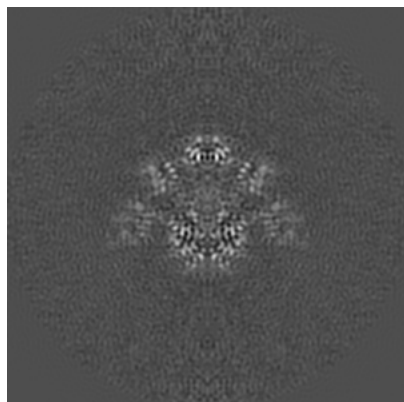


Y Index: 175

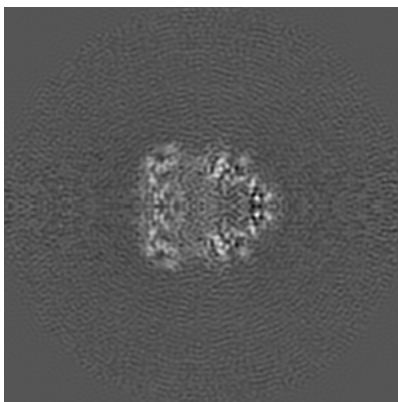


Z Index: 175

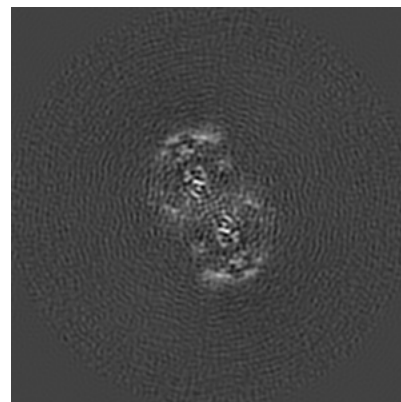
6.2.2 Raw map



X Index: 175



Y Index: 175

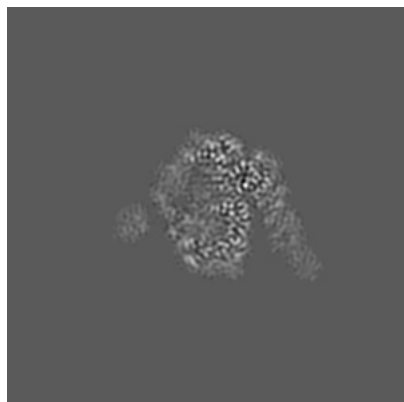


Z Index: 175

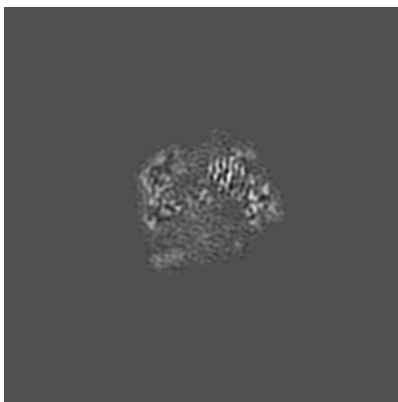
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

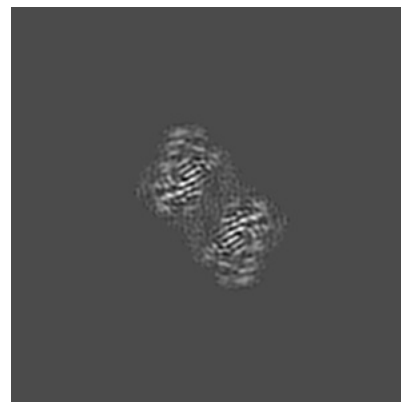
6.3.1 Primary map



X Index: 164

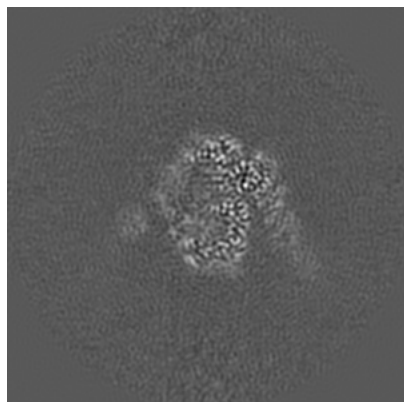


Y Index: 166

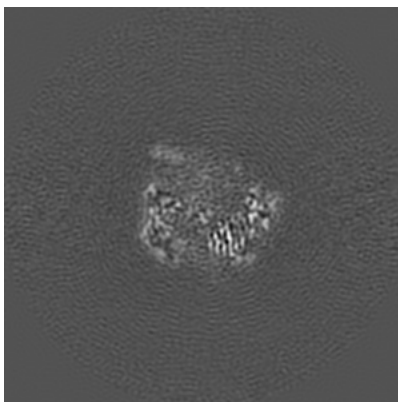


Z Index: 192

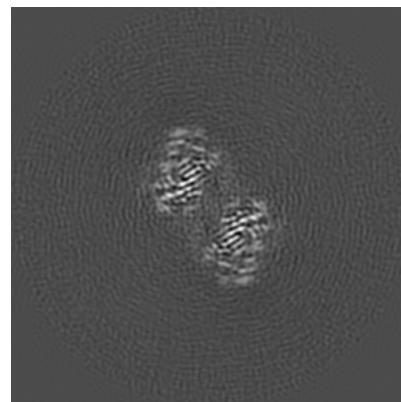
6.3.2 Raw map



X Index: 164



Y Index: 184

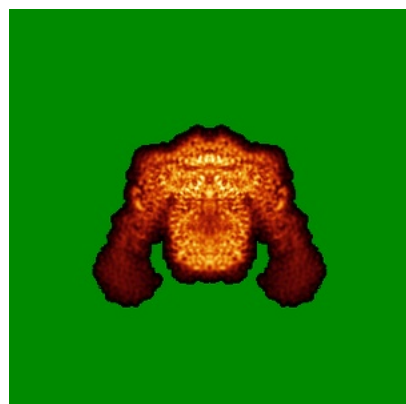


Z Index: 192

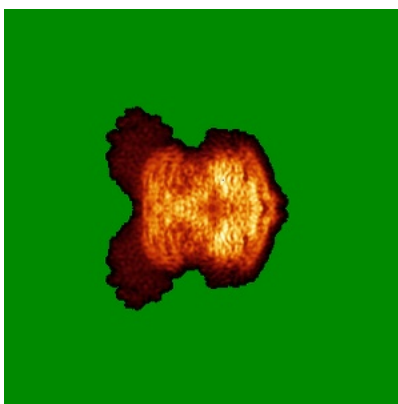
The images above show the largest variance slices of the map in three orthogonal directions.

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

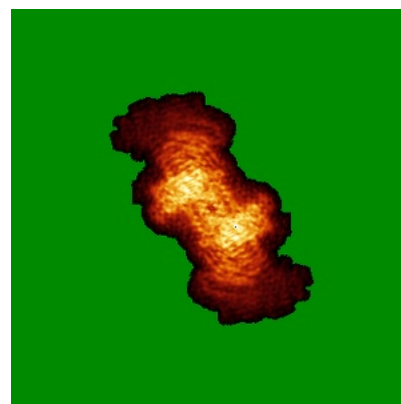
6.4.1 Primary map



X

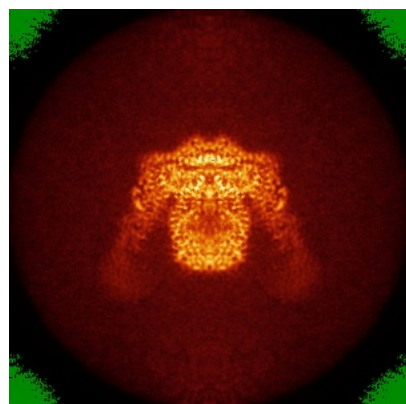


Y

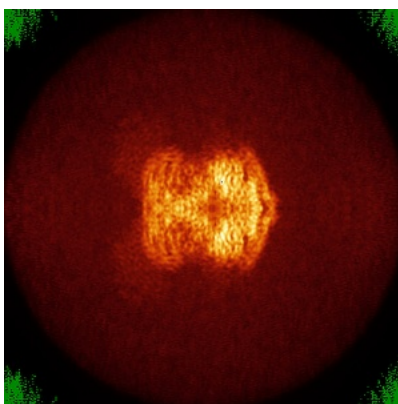


Z

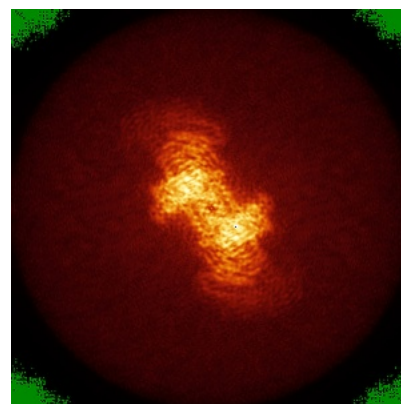
6.4.2 Raw map



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](#)

This section was not generated.

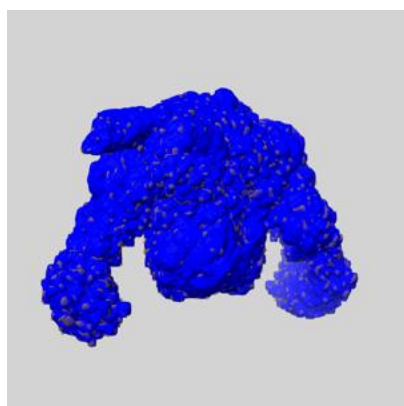
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

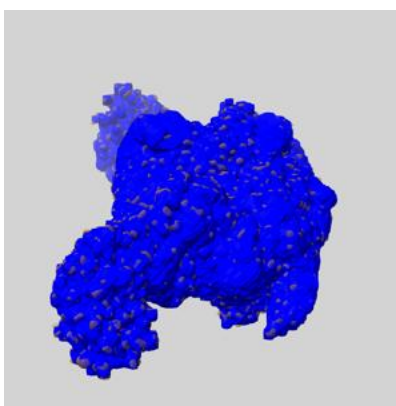
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

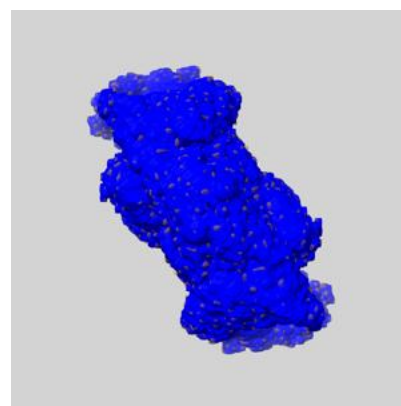
6.6.1 emd_0132_msk_1.map [i](#)



X



Y

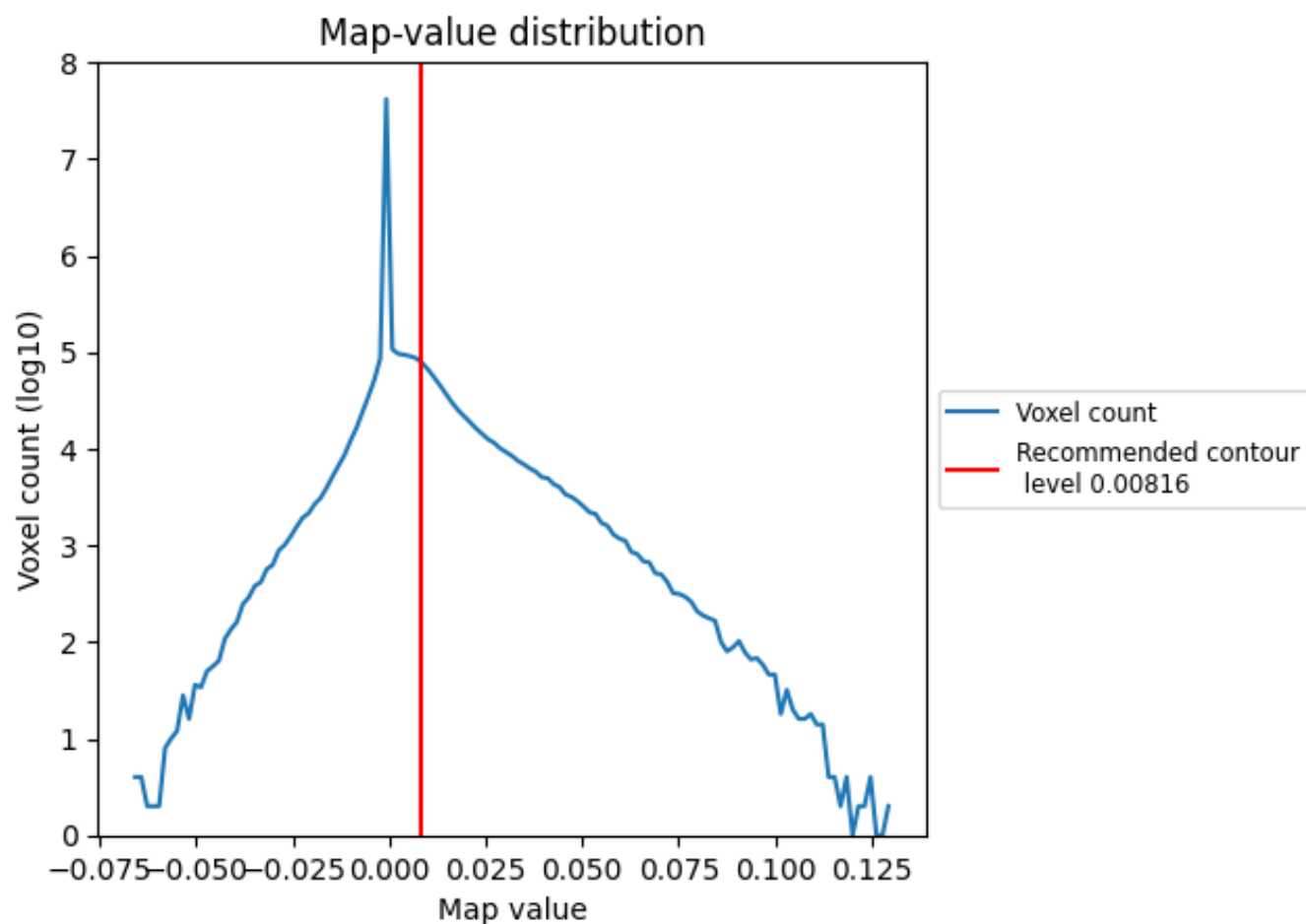


Z

7 Map analysis [i](#)

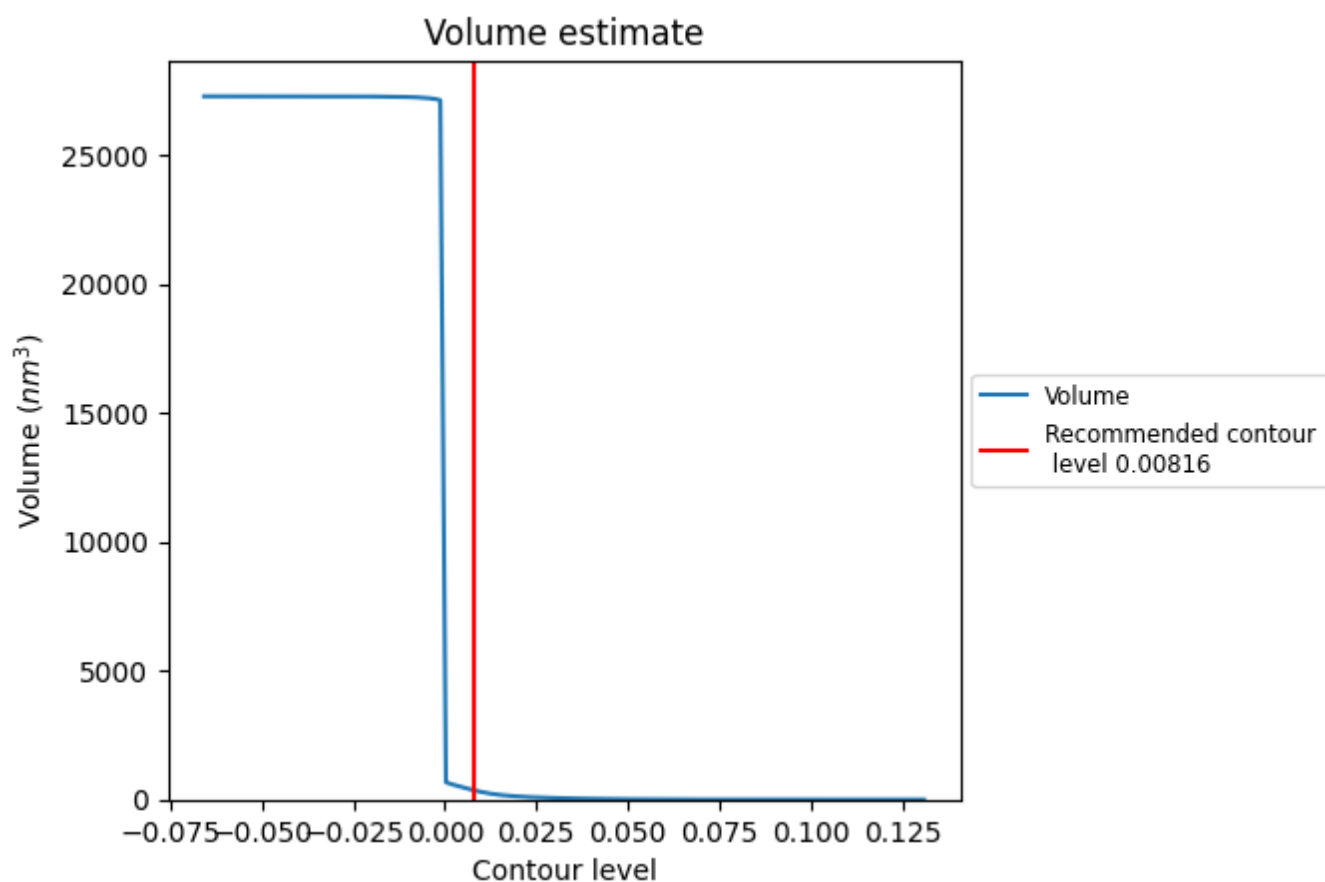
This section contains the results of statistical analysis of the map.

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.

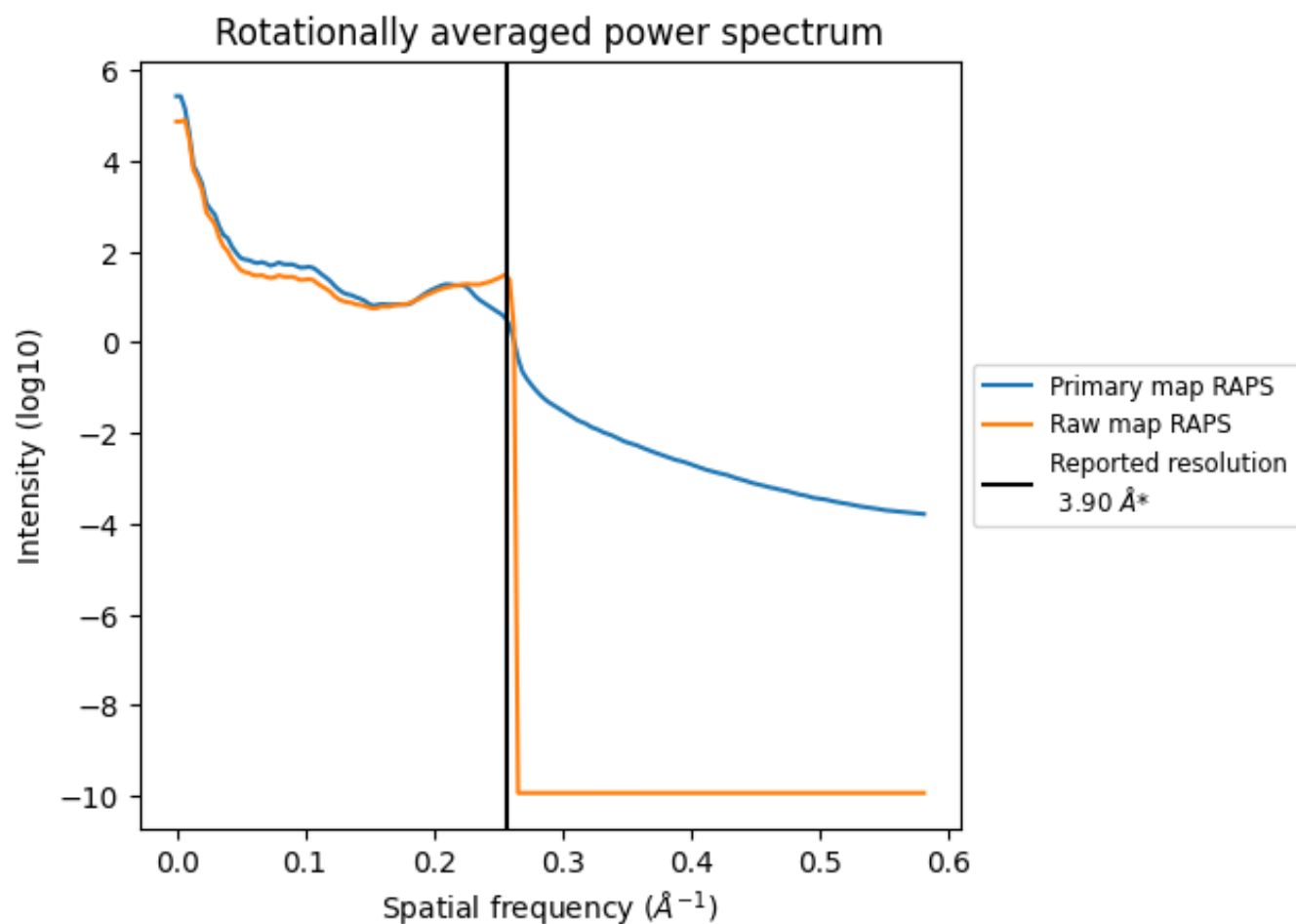
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 354 nm³; this corresponds to an approximate mass of 320 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 ⓘ

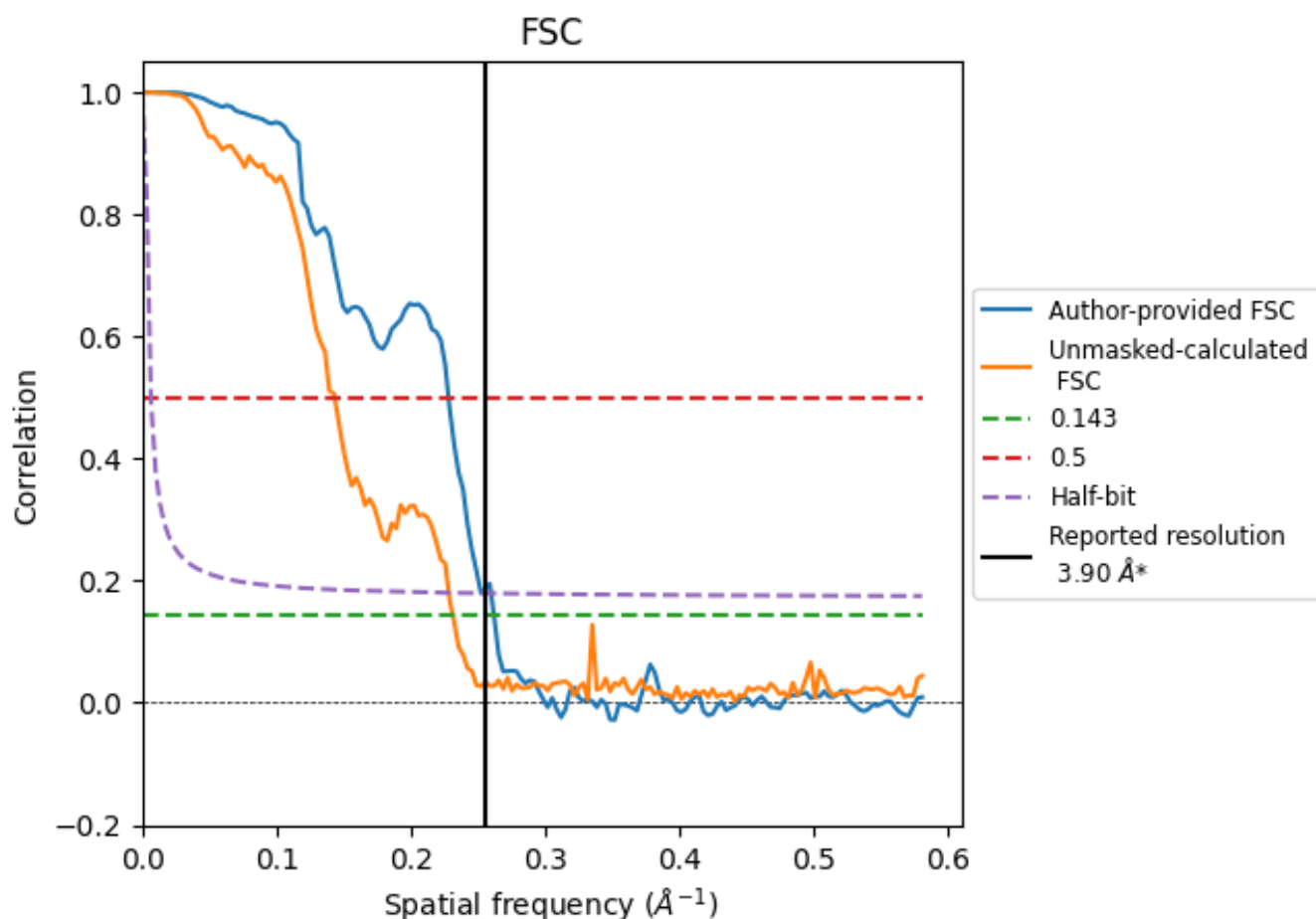


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

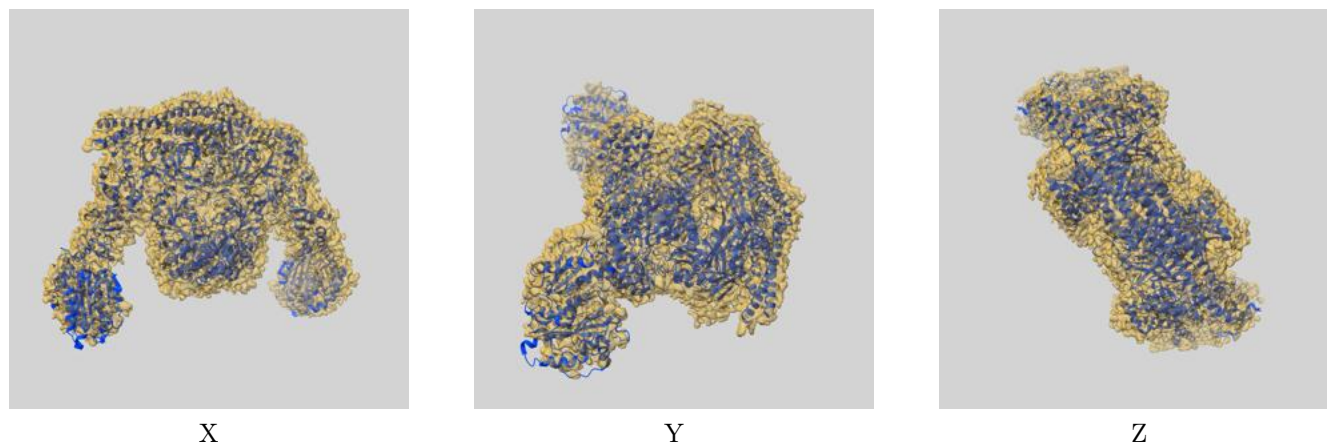
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.81	4.38	3.84
Unmasked-calculated*	4.32	6.97	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

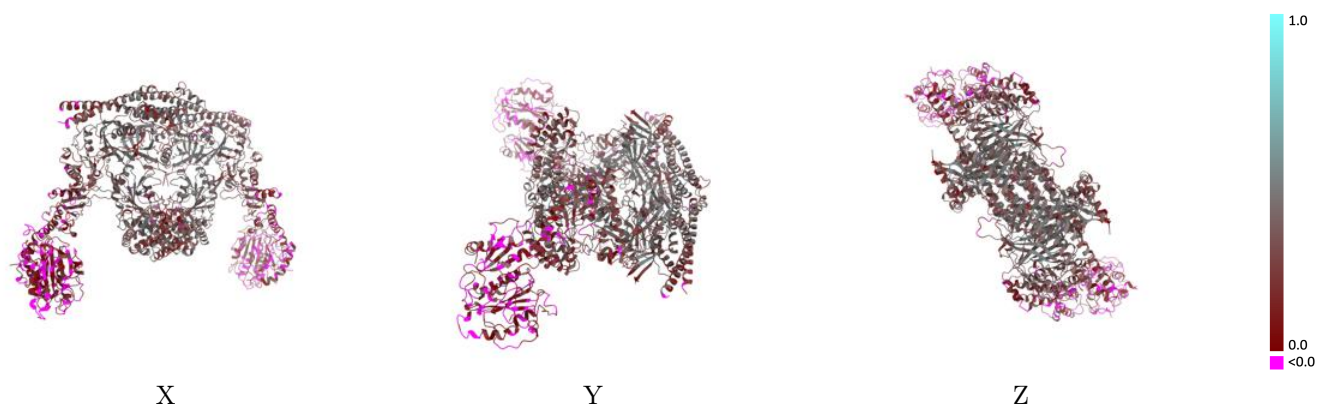
This section contains information regarding the fit between EMDB map EMD-0132 and PDB model 6H3C. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



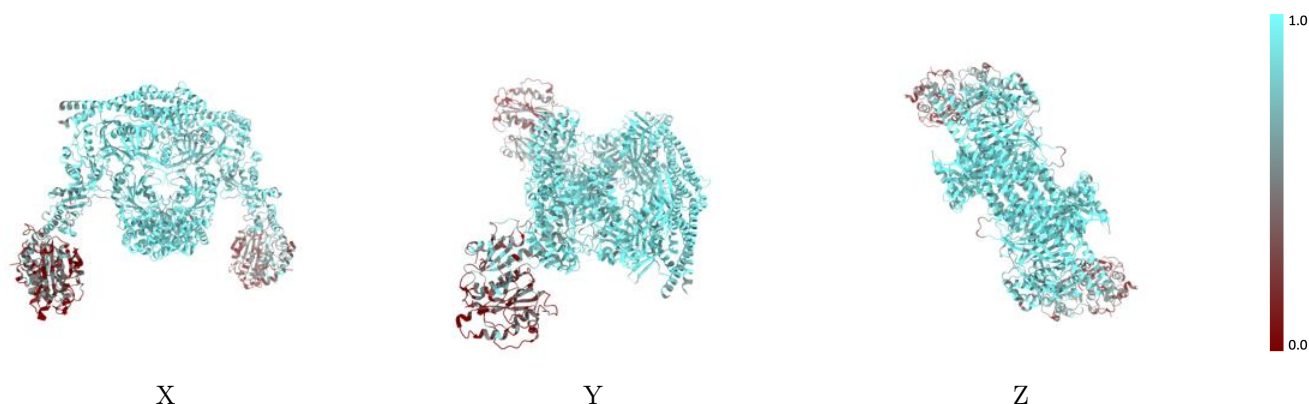
The images above show the 3D surface view of the map at the recommended contour level 0.00816 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



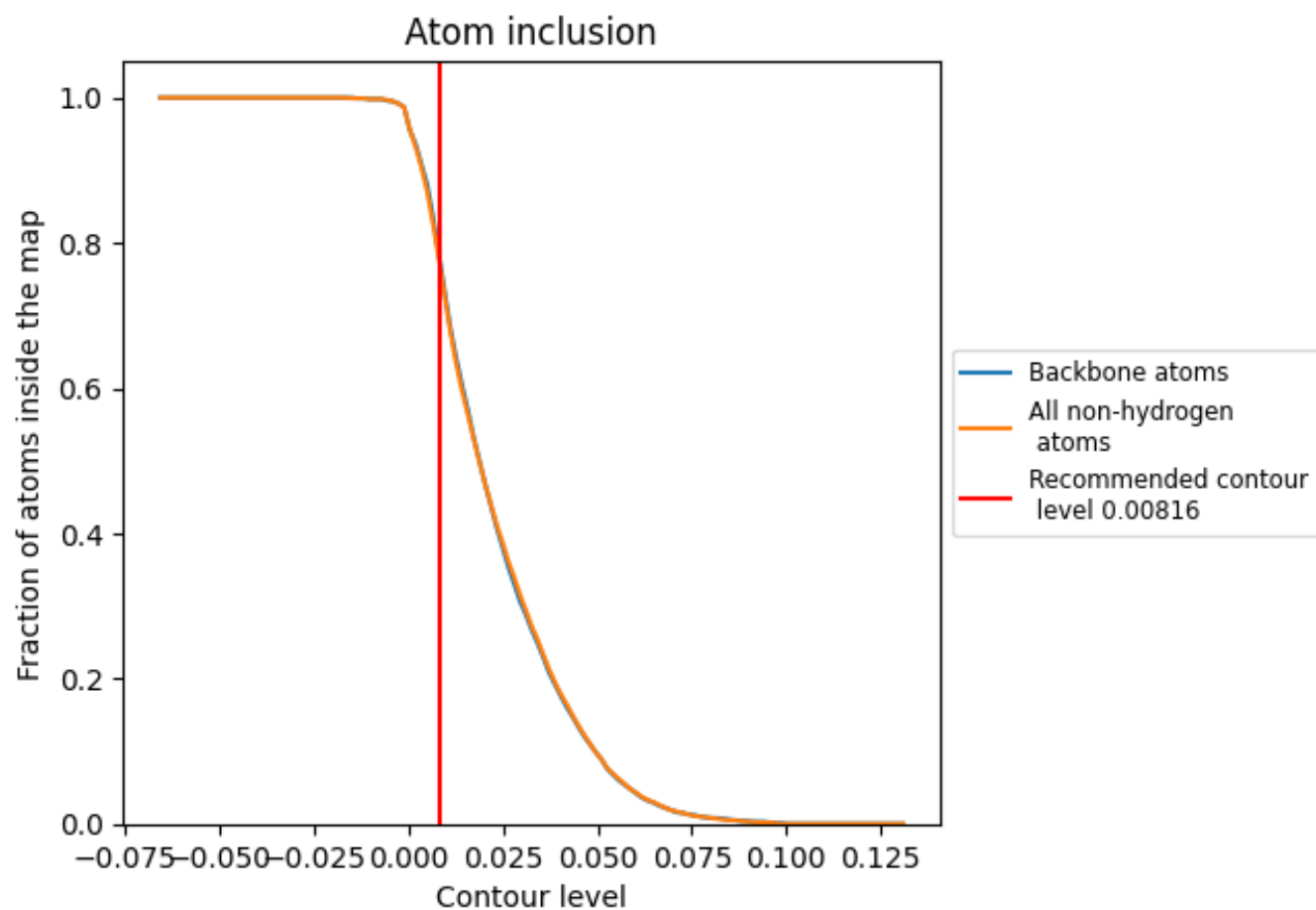
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00816).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.00816) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.2780
A	 0.9020	 0.3630
B	 0.9150	 0.3780
C	 0.7380	 0.2010
D	 0.2800	 0.0640
E	 0.9130	 0.3540
F	 0.9030	 0.3640
G	 0.9150	 0.3770
H	 0.7390	 0.2020
I	 0.2820	 0.0630
J	 0.9120	 0.3510

