Full wwPDB EM Validation Report (i)

Aug 19, 2026 – 10:35 pm BST

PDB ID	:	9SQV / pdb_00009sqv
EMDB ID	:	EMD-55118
Title	:	Cryo-EM structure of the ARISCdC(E33A):K63-Ub4 complex (Composite map)
Authors	:	Foglizzo, M.; Degtjarik, O.; Zeqiraj, E.
Deposited on	:	2025-09-23
Resolution	:	3.21 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 (i) 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 (i)) were used in the production of this report:

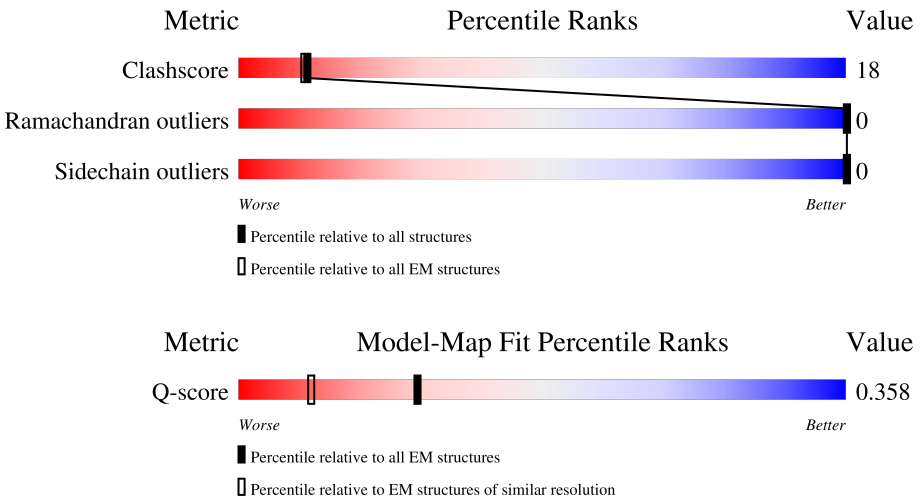
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.21 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	14613 (2.71 - 3.71)

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 <=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	G	76	32% 63% 37%
1	H	76	22% 75% 25%
2	C	302	• 59% 18% 24%
2	D	302	• 62% 14% 24%

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Mol	Chain	Length	Quality of chain
3	A	316	60% 18% 21%
3	B	316	8% 58% 17% 25%
4	E	385	5% 53% 9% 38%
4	F	385	16% 43% 18% 39%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12545 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 Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	76	602	378	105	118	1	0	0
1	H	76	601	378	105	117	1	0	0

- Molecule 2 is a protein called BRCA1-A complex subunit Abraxas 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	230	1842	1171	314	349	8	0	0
2	D	229	1835	1167	314	346	8	0	0

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-36	MET	-	initiating methionine	UNP Q6UWZ7
C	-35	TRP	-	expression tag	UNP Q6UWZ7
C	-34	SER	-	expression tag	UNP Q6UWZ7
C	-33	HIS	-	expression tag	UNP Q6UWZ7
C	-32	PRO	-	expression tag	UNP Q6UWZ7
C	-31	GLN	-	expression tag	UNP Q6UWZ7
C	-30	PHE	-	expression tag	UNP Q6UWZ7
C	-29	GLU	-	expression tag	UNP Q6UWZ7
C	-28	LYS	-	expression tag	UNP Q6UWZ7
C	-27	GLY	-	expression tag	UNP Q6UWZ7
C	-26	GLY	-	expression tag	UNP Q6UWZ7
C	-25	GLY	-	expression tag	UNP Q6UWZ7
C	-24	SER	-	expression tag	UNP Q6UWZ7
C	-23	GLY	-	expression tag	UNP Q6UWZ7
C	-22	GLY	-	expression tag	UNP Q6UWZ7
C	-21	GLY	-	expression tag	UNP Q6UWZ7
C	-20	SER	-	expression tag	UNP Q6UWZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	GLY	-	expression tag	UNP Q6UWZ7
C	-18	GLY	-	expression tag	UNP Q6UWZ7
C	-17	SER	-	expression tag	UNP Q6UWZ7
C	-16	ALA	-	expression tag	UNP Q6UWZ7
C	-15	TRP	-	expression tag	UNP Q6UWZ7
C	-14	SER	-	expression tag	UNP Q6UWZ7
C	-13	HIS	-	expression tag	UNP Q6UWZ7
C	-12	PRO	-	expression tag	UNP Q6UWZ7
C	-11	GLN	-	expression tag	UNP Q6UWZ7
C	-10	PHE	-	expression tag	UNP Q6UWZ7
C	-9	GLU	-	expression tag	UNP Q6UWZ7
C	-8	LYS	-	expression tag	UNP Q6UWZ7
C	-7	LEU	-	expression tag	UNP Q6UWZ7
C	-6	GLU	-	expression tag	UNP Q6UWZ7
C	-5	VAL	-	expression tag	UNP Q6UWZ7
C	-4	LEU	-	expression tag	UNP Q6UWZ7
C	-3	PHE	-	expression tag	UNP Q6UWZ7
C	-2	GLN	-	expression tag	UNP Q6UWZ7
C	-1	GLY	-	expression tag	UNP Q6UWZ7
C	0	THR	-	expression tag	UNP Q6UWZ7
D	-36	MET	-	initiating methionine	UNP Q6UWZ7
D	-35	TRP	-	expression tag	UNP Q6UWZ7
D	-34	SER	-	expression tag	UNP Q6UWZ7
D	-33	HIS	-	expression tag	UNP Q6UWZ7
D	-32	PRO	-	expression tag	UNP Q6UWZ7
D	-31	GLN	-	expression tag	UNP Q6UWZ7
D	-30	PHE	-	expression tag	UNP Q6UWZ7
D	-29	GLU	-	expression tag	UNP Q6UWZ7
D	-28	LYS	-	expression tag	UNP Q6UWZ7
D	-27	GLY	-	expression tag	UNP Q6UWZ7
D	-26	GLY	-	expression tag	UNP Q6UWZ7
D	-25	GLY	-	expression tag	UNP Q6UWZ7
D	-24	SER	-	expression tag	UNP Q6UWZ7
D	-23	GLY	-	expression tag	UNP Q6UWZ7
D	-22	GLY	-	expression tag	UNP Q6UWZ7
D	-21	GLY	-	expression tag	UNP Q6UWZ7
D	-20	SER	-	expression tag	UNP Q6UWZ7
D	-19	GLY	-	expression tag	UNP Q6UWZ7
D	-18	GLY	-	expression tag	UNP Q6UWZ7
D	-17	SER	-	expression tag	UNP Q6UWZ7
D	-16	ALA	-	expression tag	UNP Q6UWZ7
D	-15	TRP	-	expression tag	UNP Q6UWZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	SER	-	expression tag	UNP Q6UWZ7
D	-13	HIS	-	expression tag	UNP Q6UWZ7
D	-12	PRO	-	expression tag	UNP Q6UWZ7
D	-11	GLN	-	expression tag	UNP Q6UWZ7
D	-10	PHE	-	expression tag	UNP Q6UWZ7
D	-9	GLU	-	expression tag	UNP Q6UWZ7
D	-8	LYS	-	expression tag	UNP Q6UWZ7
D	-7	LEU	-	expression tag	UNP Q6UWZ7
D	-6	GLU	-	expression tag	UNP Q6UWZ7
D	-5	VAL	-	expression tag	UNP Q6UWZ7
D	-4	LEU	-	expression tag	UNP Q6UWZ7
D	-3	PHE	-	expression tag	UNP Q6UWZ7
D	-2	GLN	-	expression tag	UNP Q6UWZ7
D	-1	GLY	-	expression tag	UNP Q6UWZ7
D	0	THR	-	expression tag	UNP Q6UWZ7

- Molecule 3 is a protein called Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	249	2007	1259	361	374	13	1	0
3	B	237	1898	1194	338	353	13	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ALA	GLU	engineered mutation	UNP P46736
B	33	ALA	GLU	engineered mutation	UNP P46736

- Molecule 4 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	235	1856	1193	308	345	10	0	0
4	E	240	1902	1224	314	354	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP Q9NXR7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q9NXR7
E	-1	GLY	-	expression tag	UNP Q9NXR7
E	0	ALA	-	expression tag	UNP Q9NXR7

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

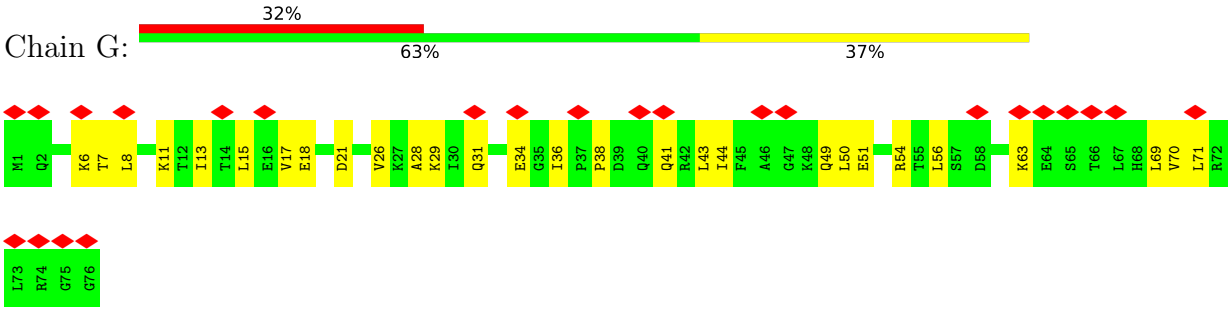
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0
			Total	Zn	
5	B	1	1	1	0

3 Residue-property plots (i)

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.

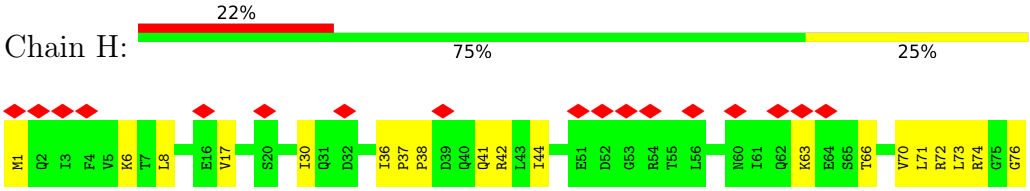
- Molecule 1: Ubiquitin

Chain G:



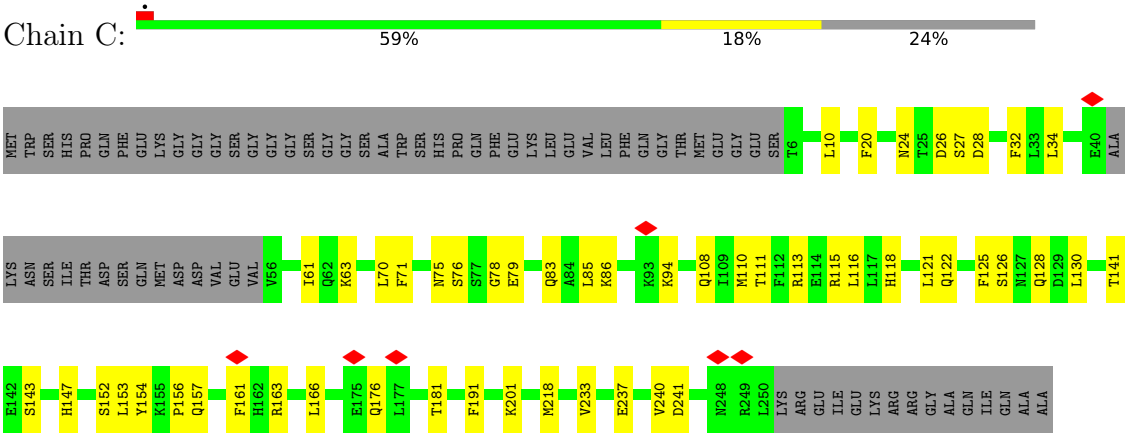
- Molecule 1: Ubiquitin

Chain H:



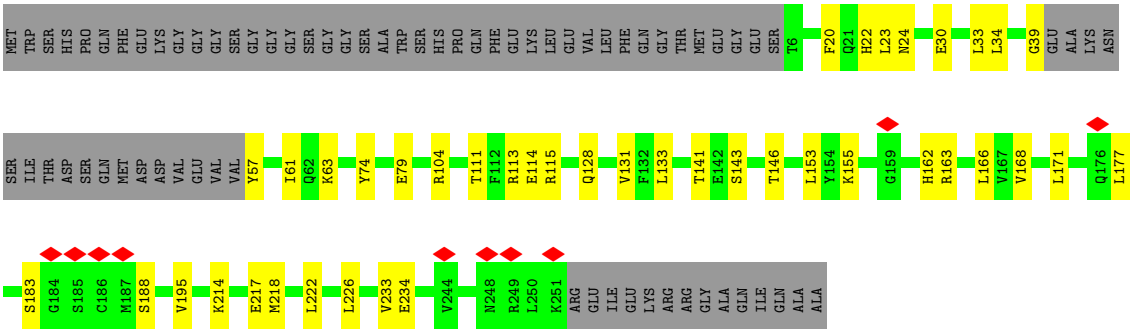
- Molecule 2: BRCA1-A complex subunit Abraxas 1

Chain C:



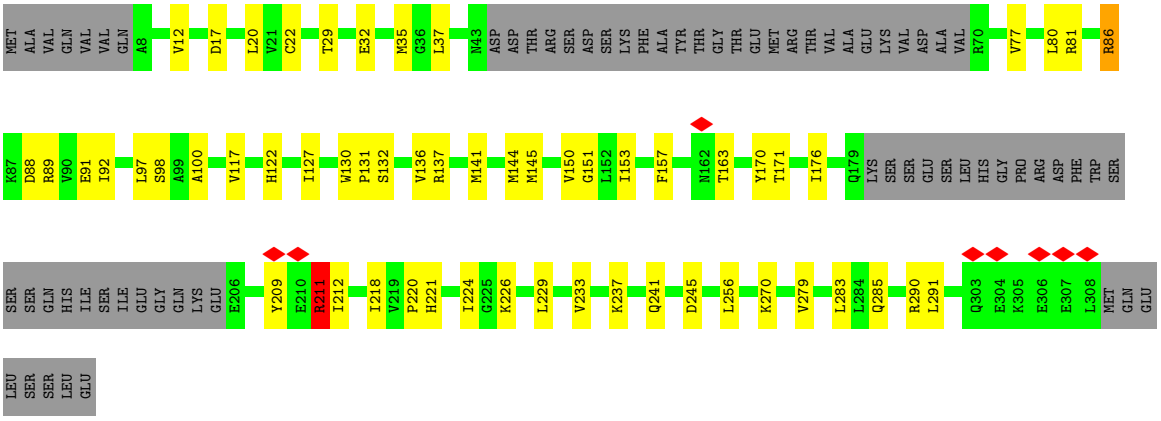
- Molecule 2: BRCA1-A complex subunit Abraxas 1

Chain D:



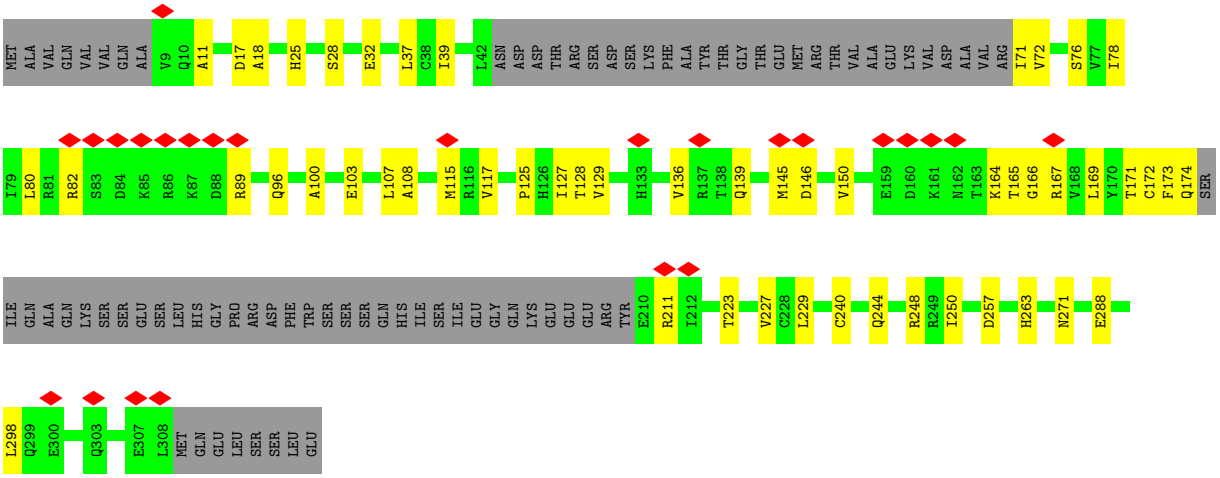
- Molecule 3: Lys-63-specific deubiquitinase BRCC36

Chain A:



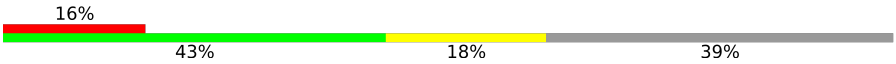
- Molecule 3: Lys-63-specific deubiquitinase BRCC36

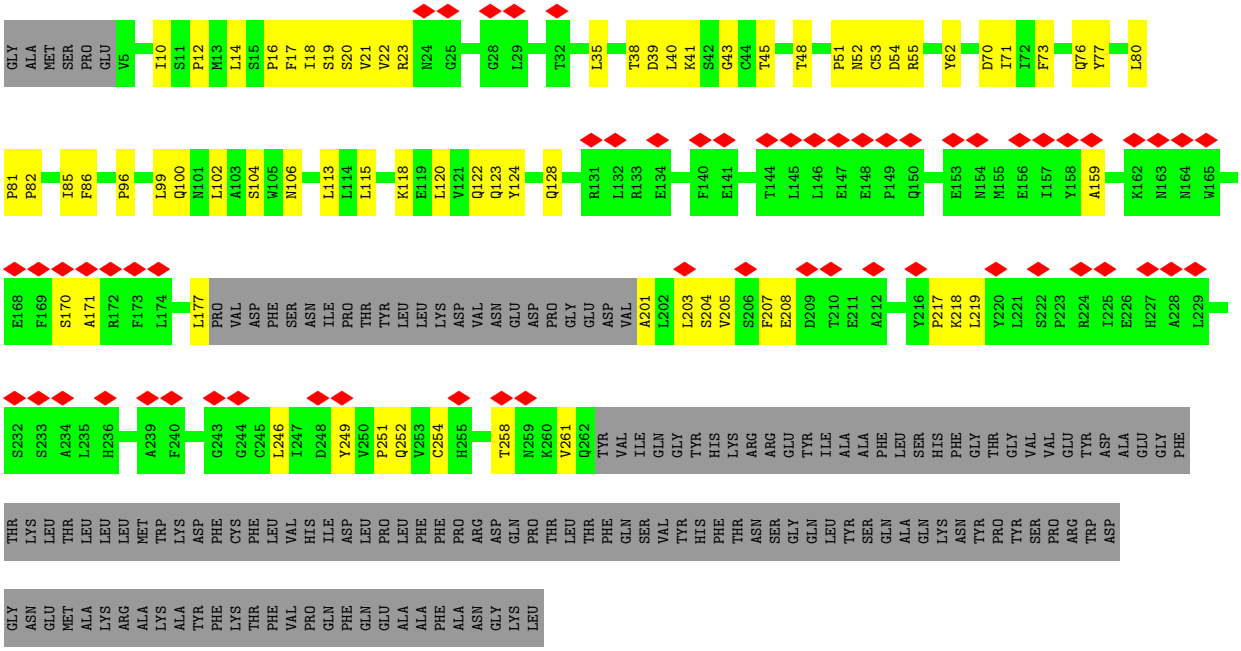
Chain B:



- Molecule 4: BRISC and BRCA1-A complex member 2

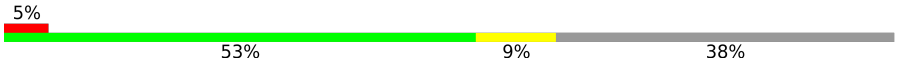
Chain F:

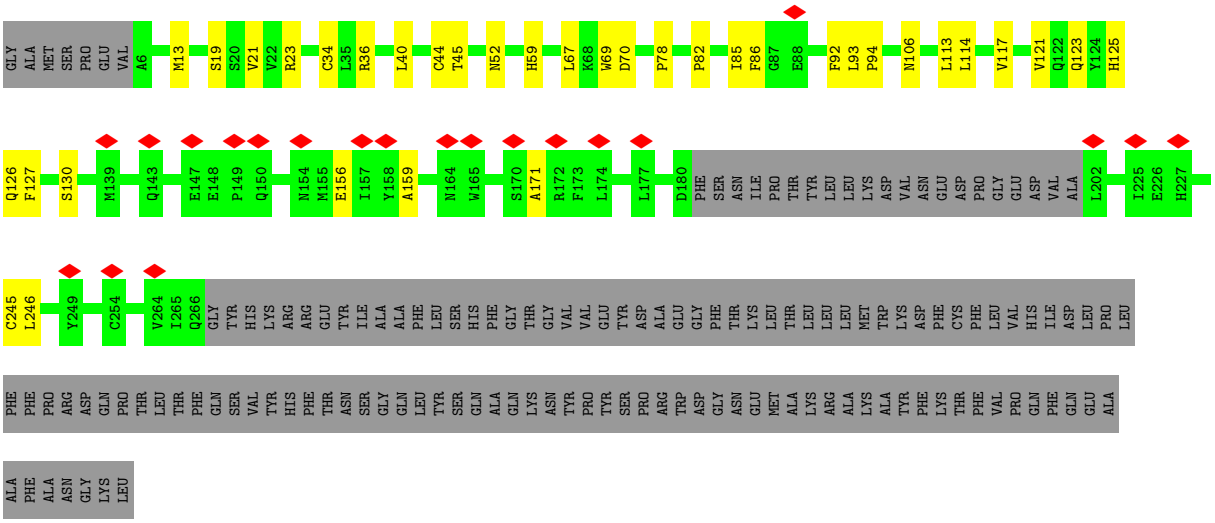




- Molecule 4: BRISC and BRCA1-A complex member 2

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54452	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 ($e^-/Å^2$)	45.8	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.266	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.0572	Depositor
Map size (Å)	296.0, 296.0, 296.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	G	0.08	0/608	0.22	0/816
1	H	0.07	0/607	0.18	0/816
2	C	0.18	0/1876	0.35	0/2523
2	D	0.10	0/1869	0.22	0/2512
3	A	0.32	0/2047	0.54	2/2767 (0.1%)
3	B	0.11	0/1933	0.26	0/2614
4	E	0.18	0/1952	0.34	0/2657
4	F	0.10	0/1904	0.29	0/2590
All	All	0.18	0/12796	0.34	2/17295 (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
3	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	211	ARG	CB-CA-C	-11.08	92.11	109.61
3	A	211	ARG	N-CA-CB	-9.20	94.38	109.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	211	ARG	Sidechain
3	A	86	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	G	602	0	628	85	0
1	H	601	0	628	40	0
2	C	1842	0	1838	49	0
2	D	1835	0	1836	50	0
3	A	2007	0	1997	86	0
3	B	1898	0	1895	77	0
4	E	1902	0	1874	30	0
4	F	1856	0	1832	55	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12545	0	12528	408	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 18.

All (408) 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:G:15:LEU:CD1	1:G:29:LYS:CE	1.85	1.53
1:G:51:GLU:CD	1:G:54:ARG:NH1	1.75	1.42
3:B:107:LEU:CB	3:B:115:MET:HE1	1.47	1.41
1:G:15:LEU:CD1	1:G:29:LYS:CG	1.98	1.41
3:B:107:LEU:CB	3:B:115:MET:CE	2.00	1.40
1:G:15:LEU:HD11	1:G:29:LYS:CG	1.51	1.39
3:B:107:LEU:HB2	3:B:115:MET:CE	1.53	1.37
1:G:15:LEU:HD11	1:G:29:LYS:CD	1.55	1.36
1:G:51:GLU:OE1	1:G:54:ARG:CZ	1.73	1.36
3:B:107:LEU:CB	3:B:115:MET:SD	2.16	1.32
1:G:51:GLU:OE1	1:G:54:ARG:NH1	1.61	1.32
4:F:62:TYR:CE2	4:F:124:TYR:HE2	1.49	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:107:LEU:CD1	3:B:115:MET:HE1	1.60	1.30
3:B:107:LEU:HB2	3:B:115:MET:SD	1.72	1.29
1:G:15:LEU:CD2	1:G:29:LYS:HG2	1.63	1.28
1:G:15:LEU:CD1	1:G:29:LYS:HG2	1.58	1.27
1:G:21:ASP:OD1	1:G:56:LEU:HD12	1.32	1.26
1:G:15:LEU:HD11	1:G:29:LYS:CE	1.53	1.26
1:G:15:LEU:CD2	1:G:29:LYS:CG	2.15	1.24
3:B:78:ILE:HG13	3:B:103:GLU:OE2	1.40	1.20
1:G:15:LEU:CG	1:G:29:LYS:HG2	1.71	1.19
1:G:15:LEU:CD1	1:G:29:LYS:HE2	1.65	1.16
1:G:15:LEU:HD21	1:G:29:LYS:CG	1.72	1.16
2:D:104:ARG:HH11	4:E:44:CYS:C	1.52	1.16
3:B:107:LEU:CG	3:B:115:MET:HE1	1.75	1.15
1:G:15:LEU:CD1	1:G:29:LYS:HE3	1.64	1.15
3:A:224:ILE:HD12	3:A:290:ARG:NH2	1.63	1.12
3:A:224:ILE:HD12	3:A:290:ARG:CZ	1.79	1.11
3:B:129:VAL:HG21	3:B:169:LEU:HD11	1.16	1.11
1:G:15:LEU:HD13	1:G:29:LYS:HE3	1.34	1.10
4:F:62:TYR:CE2	4:F:124:TYR:CE2	2.39	1.09
1:G:15:LEU:HD21	1:G:29:LYS:HG2	1.27	1.09
1:G:63:LYS:NZ	1:H:76:GLY:C	2.12	1.06
3:B:107:LEU:CD1	3:B:115:MET:CE	2.33	1.06
3:B:107:LEU:HB3	3:B:115:MET:HE1	1.38	1.06
3:B:78:ILE:HG13	3:B:103:GLU:CD	1.80	1.05
3:B:107:LEU:HB3	3:B:115:MET:SD	1.95	1.05
3:B:139:GLN:HE22	3:B:174:GLN:HA	1.19	1.05
1:G:63:LYS:HZ1	1:H:76:GLY:C	1.63	1.05
3:B:107:LEU:HB3	3:B:115:MET:CE	1.85	1.04
2:C:118:HIS:CE1	2:C:130:LEU:HD22	1.93	1.03
2:D:104:ARG:NH1	4:E:44:CYS:C	2.16	1.03
1:G:26:VAL:CG2	1:G:56:LEU:HD11	1.89	1.03
1:G:15:LEU:HD21	1:G:29:LYS:CB	1.88	1.03
2:C:20:PHE:O	2:C:24:ASN:ND2	1.93	1.02
3:B:107:LEU:C	3:B:115:MET:SD	2.44	1.00
1:G:15:LEU:HD12	1:G:29:LYS:HE2	1.39	0.99
3:A:130:TRP:CE3	3:A:211:ARG:NH1	2.30	0.99
3:A:131:PRO:HD2	3:A:211:ARG:CD	1.93	0.99
2:D:104:ARG:NH1	4:E:45:THR:N	2.09	0.99
4:F:62:TYR:CD2	4:F:124:TYR:HE2	1.80	0.98
1:G:51:GLU:OE2	1:G:54:ARG:NH1	1.95	0.98
2:D:153:LEU:HD11	2:D:166:LEU:CD1	1.94	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:HD11	2:D:166:LEU:HD13	1.46	0.97
3:B:78:ILE:CG1	3:B:103:GLU:OE2	2.13	0.96
2:D:104:ARG:HH12	4:E:45:THR:CA	1.77	0.96
3:B:129:VAL:CG2	3:B:169:LEU:HD11	1.95	0.96
3:B:139:GLN:NE2	3:B:174:GLN:HA	1.80	0.96
1:G:63:LYS:HZ3	1:H:76:GLY:HA2	1.31	0.95
1:G:26:VAL:HG21	1:G:56:LEU:HD11	1.46	0.95
3:A:131:PRO:CD	3:A:211:ARG:HD3	1.96	0.95
3:A:130:TRP:HE3	3:A:211:ARG:HH11	1.15	0.95
1:G:15:LEU:HD12	1:G:29:LYS:CE	1.87	0.94
1:G:26:VAL:HG21	1:G:56:LEU:HD21	1.49	0.94
3:A:131:PRO:CG	3:A:211:ARG:HD3	1.96	0.94
1:H:73:LEU:HG	3:A:35:MET:HE1	1.50	0.94
1:G:21:ASP:OD1	1:G:56:LEU:CD1	2.14	0.93
2:D:104:ARG:HH12	4:E:45:THR:N	1.67	0.92
2:C:118:HIS:CE1	2:C:130:LEU:CD2	2.52	0.92
1:G:15:LEU:HD11	1:G:29:LYS:HG2	1.20	0.91
1:H:73:LEU:CD2	3:A:35:MET:HE2	2.00	0.91
3:A:131:PRO:HD2	3:A:211:ARG:HD3	1.48	0.91
1:G:63:LYS:HZ3	1:H:76:GLY:CA	1.84	0.91
3:B:107:LEU:HD13	3:B:115:MET:HE1	1.52	0.91
1:H:6:LYS:HD2	1:H:66:THR:CG2	2.01	0.90
1:G:15:LEU:HD13	1:G:29:LYS:CG	1.99	0.90
4:E:106:ASN:OD1	4:E:106:ASN:O	1.90	0.90
4:F:17:PHE:HB3	4:F:113:LEU:HD22	1.53	0.90
3:B:107:LEU:HD12	3:B:115:MET:CE	2.01	0.90
1:G:15:LEU:HD13	1:G:29:LYS:CE	1.95	0.89
1:H:6:LYS:HD2	1:H:66:THR:HG21	1.53	0.88
1:G:15:LEU:HD21	1:G:29:LYS:HB3	1.56	0.88
3:A:131:PRO:HG2	3:A:211:ARG:CD	2.04	0.88
1:G:15:LEU:CD1	1:G:29:LYS:HG3	2.01	0.87
1:G:15:LEU:CD1	1:G:29:LYS:CD	2.29	0.86
2:D:104:ARG:NH1	4:E:45:THR:HA	1.89	0.86
1:G:63:LYS:HD3	3:A:127:ILE:HG21	1.58	0.86
2:D:104:ARG:NH1	4:E:45:THR:CA	2.38	0.85
3:B:39:ILE:CD1	3:B:107:LEU:HD12	2.06	0.85
1:G:51:GLU:CD	1:G:54:ARG:HH12	1.76	0.84
1:H:70:VAL:HG12	1:H:71:LEU:N	1.93	0.83
1:G:15:LEU:HD13	1:G:29:LYS:HG3	1.60	0.83
2:D:34:LEU:HD12	2:D:63:LYS:HD3	1.61	0.82
3:A:131:PRO:CG	3:A:211:ARG:CD	2.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:86:ARG:HG3	3:A:88:ASP:H	1.44	0.81
4:F:17:PHE:O	4:F:113:LEU:HD23	1.79	0.81
3:A:141:MET:HA	3:A:144:MET:HE2	1.62	0.81
4:F:62:TYR:CZ	4:F:124:TYR:CE2	2.68	0.80
1:H:70:VAL:HG12	1:H:71:LEU:H	1.46	0.80
3:A:131:PRO:CD	3:A:211:ARG:CD	2.58	0.80
1:G:26:VAL:HG21	1:G:56:LEU:CD1	2.12	0.80
3:B:145:MET:O	3:B:146:ASP:OD1	2.00	0.79
2:D:234:GLU:OE2	3:A:226:LYS:HD3	1.82	0.79
2:D:153:LEU:CD1	2:D:166:LEU:HD13	2.11	0.79
1:G:51:GLU:OE1	1:G:54:ARG:NE	2.16	0.78
1:G:63:LYS:NZ	1:H:76:GLY:CA	2.44	0.78
4:F:62:TYR:CD2	4:F:124:TYR:CE2	2.65	0.78
3:A:130:TRP:HE3	3:A:211:ARG:NH1	1.72	0.78
3:A:86:ARG:HD2	3:A:88:ASP:OD1	1.84	0.78
1:G:26:VAL:HG21	1:G:56:LEU:CD2	2.14	0.78
3:B:78:ILE:CD1	3:B:103:GLU:OE2	2.31	0.78
4:F:70:ASP:HB2	4:F:85:ILE:HB	1.65	0.78
4:E:70:ASP:HB2	4:E:85:ILE:HB	1.66	0.77
1:G:15:LEU:CD2	1:G:29:LYS:HG3	2.12	0.77
1:G:21:ASP:CG	1:G:56:LEU:HD12	2.09	0.77
1:H:30:ILE:HG13	1:H:41:GLN:HE22	1.51	0.76
2:C:118:HIS:CD2	2:C:156:PRO:HG2	2.19	0.76
1:G:11:LYS:NZ	1:G:13:ILE:HG22	1.99	0.76
1:G:51:GLU:CD	1:G:54:ARG:HH11	1.93	0.76
2:C:118:HIS:HE1	2:C:130:LEU:CD2	2.00	0.75
1:H:73:LEU:HG	3:A:35:MET:CE	2.16	0.75
3:A:86:ARG:HD2	3:A:89:ARG:HG3	1.70	0.74
3:A:86:ARG:CD	3:A:88:ASP:OD1	2.36	0.74
1:G:15:LEU:HD11	1:G:29:LYS:HE2	1.35	0.74
1:G:15:LEU:HD22	1:G:29:LYS:CG	2.17	0.73
1:H:42:ARG:HH21	1:H:72:ARG:HH21	1.35	0.72
1:H:73:LEU:HD23	3:A:35:MET:HE2	1.69	0.72
3:A:131:PRO:HG2	3:A:211:ARG:HD2	1.71	0.72
3:B:108:ALA:N	3:B:115:MET:SD	2.63	0.72
4:F:115:LEU:HA	4:F:118:LYS:HB2	1.72	0.72
2:C:34:LEU:HD12	2:C:94:LYS:HB2	1.72	0.71
2:D:104:ARG:HH12	4:E:45:THR:HA	1.47	0.71
2:C:118:HIS:HE1	2:C:130:LEU:HD23	1.56	0.70
3:B:107:LEU:HB2	3:B:115:MET:HE2	1.71	0.70
3:B:39:ILE:CD1	3:B:107:LEU:CD1	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:LEU:HD22	1:G:29:LYS:HG3	1.74	0.69
3:B:139:GLN:OE1	3:B:173:PHE:CE2	2.44	0.69
1:G:26:VAL:HG22	1:G:56:LEU:HD11	1.72	0.69
1:H:70:VAL:CG1	1:H:71:LEU:H	2.04	0.69
2:C:76:SER:O	2:C:113:ARG:NH1	2.25	0.69
2:C:78:GLY:HA3	2:C:116:LEU:HD23	1.72	0.69
1:G:15:LEU:CG	1:G:29:LYS:CG	2.49	0.69
1:G:26:VAL:HG21	1:G:56:LEU:CG	2.23	0.69
3:B:107:LEU:CA	3:B:115:MET:SD	2.80	0.69
3:A:224:ILE:CD1	3:A:290:ARG:NH2	2.51	0.68
3:B:107:LEU:HD12	3:B:115:MET:HE2	1.75	0.68
3:A:224:ILE:CD1	3:A:290:ARG:CZ	2.66	0.68
3:B:39:ILE:HD11	3:B:76:SER:OG	1.93	0.67
1:G:15:LEU:CD2	1:G:29:LYS:HB3	2.24	0.67
3:A:176:ILE:HG12	3:A:212:ILE:HG21	1.77	0.67
1:H:1:MET:HB3	1:H:63:LYS:HG2	1.77	0.66
1:H:70:VAL:CG1	1:H:71:LEU:N	2.58	0.66
3:B:39:ILE:HD12	3:B:115:MET:CE	2.26	0.66
4:F:251:PRO:HA	4:F:254:CYS:HB2	1.78	0.65
1:H:42:ARG:NH2	1:H:72:ARG:HH21	1.95	0.65
2:D:153:LEU:HD11	2:D:166:LEU:HD12	1.80	0.64
3:A:131:PRO:CB	3:A:211:ARG:HD3	2.27	0.64
2:C:201:LYS:NZ	2:D:217:GLU:OE1	2.29	0.64
2:D:133:LEU:HD13	2:D:153:LEU:HD23	1.80	0.64
1:H:73:LEU:CD2	3:A:35:MET:CE	2.76	0.63
4:F:10:ILE:HA	4:F:53:CYS:HB2	1.80	0.63
1:H:37:PRO:HD3	3:A:144:MET:SD	2.39	0.63
2:D:226:LEU:HD23	3:A:233:VAL:HB	1.82	0.62
3:B:139:GLN:OE1	3:B:211:ARG:NH1	2.33	0.62
2:C:122:GLN:HE22	2:C:157:GLN:HE21	1.47	0.61
3:B:82:ARG:NH2	3:B:89:ARG:O	2.32	0.61
4:E:19:SER:O	4:E:23:ARG:N	2.33	0.61
2:D:163:ARG:NH1	3:A:163:THR:O	2.32	0.61
1:G:51:GLU:CD	1:G:54:ARG:CZ	2.46	0.61
1:G:21:ASP:CG	1:G:56:LEU:CD1	2.71	0.61
3:A:137:ARG:HG2	3:A:141:MET:HE2	1.81	0.61
4:E:34:CYS:O	4:E:36:ARG:HG2	2.01	0.60
2:D:23:LEU:HD13	3:A:218:ILE:HG21	1.82	0.60
1:H:6:LYS:CD	1:H:66:THR:CG2	2.78	0.60
4:F:100:GLN:O	4:F:104:SER:OG	2.19	0.60
3:A:224:ILE:HD12	3:A:290:ARG:NE	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:LEU:HB2	2:D:63:LYS:HB3	1.84	0.60
2:D:234:GLU:OE2	3:A:226:LYS:HB2	2.02	0.60
3:B:39:ILE:HD12	3:B:115:MET:HE2	1.82	0.59
1:H:30:ILE:HD11	1:H:41:GLN:OE1	2.03	0.59
2:D:234:GLU:OE2	3:A:226:LYS:CD	2.49	0.59
1:H:73:LEU:HD21	3:A:35:MET:HE2	1.84	0.59
3:B:107:LEU:HD13	3:B:115:MET:CE	2.21	0.59
1:H:44:ILE:HD12	3:A:98:SER:HB3	1.85	0.58
4:F:19:SER:O	4:F:23:ARG:N	2.36	0.58
1:G:13:ILE:HD13	1:G:34:GLU:OE2	2.02	0.58
4:F:77:TYR:HB3	4:F:80:LEU:HG	1.85	0.58
3:A:12:VAL:HG21	3:A:150:VAL:HG11	1.86	0.58
4:F:62:TYR:CZ	4:F:124:TYR:CD2	2.91	0.58
2:D:153:LEU:CG	2:D:166:LEU:HD13	2.34	0.58
2:D:39:GLY:HA2	2:D:57:TYR:HA	1.86	0.57
2:C:176:GLN:O	3:B:271:ASN:ND2	2.38	0.57
1:H:6:LYS:HD2	1:H:66:THR:HG23	1.84	0.57
1:G:15:LEU:CD2	1:G:29:LYS:CB	2.64	0.56
1:H:73:LEU:CG	3:A:35:MET:CE	2.84	0.56
3:A:212:ILE:HG13	3:A:212:ILE:O	2.04	0.56
4:F:17:PHE:O	4:F:113:LEU:CD2	2.52	0.56
2:C:26:ASP:OD2	4:F:45:THR:HG22	2.05	0.56
2:C:122:GLN:NE2	2:C:157:GLN:HE21	2.04	0.56
2:C:118:HIS:ND1	2:C:130:LEU:HD22	2.20	0.56
2:D:24:ASN:HA	3:A:220:PRO:HB3	1.87	0.56
4:F:48:THR:HB	4:F:52:ASN:HD22	1.71	0.56
1:G:11:LYS:HZ1	1:G:13:ILE:HG22	1.67	0.56
2:C:113:ARG:NH2	4:F:82:PRO:O	2.37	0.56
3:B:78:ILE:HG13	3:B:103:GLU:OE1	2.04	0.56
2:C:241:ASP:HB2	3:B:223:THR:HG21	1.88	0.56
4:F:14:LEU:HD13	4:F:17:PHE:HD2	1.70	0.56
1:G:44:ILE:HG12	1:G:49:GLN:HG2	1.88	0.56
3:A:136:VAL:HG21	3:A:209:TYR:HA	1.88	0.56
1:H:6:LYS:CD	1:H:66:THR:HG23	2.35	0.55
3:A:211:ARG:HH21	3:A:211:ARG:HB2	1.72	0.55
2:C:75:ASN:HB3	2:C:79:GLU:HG3	1.87	0.55
2:C:122:GLN:OE1	2:C:157:GLN:NE2	2.39	0.55
3:B:39:ILE:HD12	3:B:107:LEU:HD12	1.87	0.55
3:A:17:ASP:OD2	3:A:221:HIS:ND1	2.27	0.55
2:C:111:THR:O	2:C:115:ARG:HG3	2.07	0.55
2:C:233:VAL:HG12	3:B:229:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:VAL:HG12	3:A:151:GLY:N	2.22	0.54
4:F:120:LEU:HA	4:F:123:GLN:HG2	1.89	0.54
3:B:129:VAL:HG11	3:B:169:LEU:CD1	2.37	0.54
3:B:136:VAL:HG13	3:B:211:ARG:HE	1.71	0.54
2:D:115:ARG:NH2	4:E:93:LEU:HD13	2.23	0.54
2:C:118:HIS:CE1	2:C:130:LEU:HD23	2.33	0.54
3:A:29:THR:HG21	3:A:32:GLU:HB2	1.89	0.54
2:D:141:THR:OG1	2:D:143:SER:O	2.26	0.54
3:B:25:HIS:O	3:B:28:SER:OG	2.24	0.54
4:F:205:VAL:HA	4:F:217:PRO:HA	1.89	0.53
4:F:204:SER:O	4:F:218:LYS:N	2.30	0.53
2:D:20:PHE:HB2	3:A:20:LEU:HD13	1.89	0.53
3:B:37:LEU:CD1	3:B:80:LEU:HD11	2.38	0.53
3:B:96:GLN:O	3:B:100:ALA:N	2.40	0.53
4:F:21:VAL:HG12	4:F:35:LEU:HD23	1.90	0.53
2:C:122:GLN:HE22	2:C:157:GLN:NE2	2.06	0.53
2:C:153:LEU:HD22	2:C:166:LEU:HD13	1.89	0.53
2:C:218:MET:HE2	2:D:195:VAL:HG22	1.89	0.53
4:E:13:MET:SD	4:E:78:PRO:HG3	2.48	0.53
2:D:128:GLN:N	2:D:128:GLN:OE1	2.42	0.53
1:G:11:LYS:HZ2	1:G:13:ILE:HG22	1.73	0.53
4:E:123:GLN:OE1	4:E:126:GLN:OE1	2.25	0.53
3:B:80:LEU:HD21	3:B:96:GLN:NE2	2.24	0.53
1:G:15:LEU:HD12	1:G:29:LYS:HE3	1.65	0.53
3:B:257:ASP:OD1	3:B:257:ASP:N	2.36	0.52
4:F:177:LEU:N	4:F:201:ALA:O	2.43	0.52
4:E:159:ALA:HA	4:E:171:ALA:HA	1.91	0.52
1:G:18:GLU:O	1:G:21:ASP:OD1	2.28	0.52
1:H:74:ARG:HD2	3:A:91:GLU:HG3	1.91	0.52
2:C:181:THR:HG22	3:B:250:ILE:HD11	1.90	0.52
2:C:83:GLN:HA	2:C:86:LYS:HE3	1.91	0.52
1:G:7:THR:HA	1:G:69:LEU:HB3	1.92	0.52
2:C:152:SER:HB3	3:B:165:THR:HG22	1.90	0.52
1:G:18:GLU:O	1:G:21:ASP:CG	2.53	0.52
1:G:51:GLU:OE1	1:G:54:ARG:CD	2.56	0.52
2:D:113:ARG:NH2	4:E:82:PRO:O	2.43	0.52
3:B:108:ALA:HB2	3:B:115:MET:HB2	1.92	0.52
2:D:133:LEU:HD13	2:D:153:LEU:CD2	2.40	0.51
1:G:63:LYS:CE	1:H:76:GLY:O	2.58	0.51
3:B:39:ILE:HD13	3:B:107:LEU:HD12	1.89	0.51
3:B:240:CYS:SG	3:B:244:GLN:NE2	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:233:VAL:HA	3:A:283:LEU:HD21	1.93	0.51
4:F:62:TYR:CE1	4:F:124:TYR:CD2	2.99	0.51
3:A:176:ILE:HG12	3:A:212:ILE:CG2	2.40	0.51
3:B:37:LEU:HG	3:B:80:LEU:HD11	1.92	0.51
2:C:27:SER:OG	2:C:28:ASP:N	2.43	0.51
2:C:28:ASP:HB2	2:C:70:LEU:HD11	1.93	0.51
4:F:62:TYR:CE1	4:F:124:TYR:HD2	2.29	0.50
4:F:128:GLN:NE2	4:F:159:ALA:O	2.44	0.50
1:H:70:VAL:HG11	3:A:97:LEU:HD13	1.94	0.50
3:A:131:PRO:HB2	3:A:211:ARG:HD3	1.93	0.50
3:B:128:THR:HG22	3:B:129:VAL:H	1.75	0.50
4:F:249:TYR:HA	4:F:252:GLN:HB3	1.92	0.50
1:G:6:LYS:O	1:G:69:LEU:N	2.34	0.50
2:D:30:GLU:OE1	2:D:74:TYR:OH	2.25	0.50
4:F:12:PRO:HD3	4:F:51:PRO:HG2	1.92	0.50
1:H:30:ILE:HD11	1:H:41:GLN:CD	2.37	0.49
3:A:81:ARG:HH22	3:A:245:ASP:CG	2.21	0.49
4:E:44:CYS:SG	4:E:52:ASN:ND2	2.85	0.49
3:B:244:GLN:OE1	3:B:248:ARG:NH2	2.46	0.48
2:C:108:GLN:O	2:C:154:TYR:OH	2.29	0.48
3:A:80:LEU:HB2	3:A:92:ILE:HD13	1.95	0.48
3:A:37:LEU:HD13	3:A:117:VAL:HG11	1.95	0.48
2:D:177:LEU:HD22	3:A:270:LYS:HD3	1.94	0.48
2:C:32:PHE:HE1	2:C:121:LEU:HD21	1.79	0.48
3:A:270:LYS:HG3	3:B:263:HIS:CD2	2.48	0.48
2:D:168:VAL:HB	3:A:157:PHE:HE1	1.78	0.48
1:H:36:ILE:HG13	3:A:144:MET:O	2.14	0.48
4:F:86:PHE:HE1	4:F:120:LEU:HD13	1.79	0.48
3:B:139:GLN:CD	3:B:211:ARG:HH12	2.22	0.47
4:F:21:VAL:HG23	4:F:113:LEU:HD23	1.96	0.47
3:A:176:ILE:CG1	3:A:212:ILE:HG21	2.44	0.47
4:E:117:VAL:O	4:E:121:VAL:HG13	2.15	0.47
1:G:63:LYS:CE	1:H:76:GLY:C	2.87	0.47
3:B:125:PRO:O	3:B:127:ILE:HG13	2.15	0.47
4:F:258:THR:HA	4:F:261:VAL:HG22	1.97	0.47
4:E:127:PHE:O	4:E:130:SER:OG	2.30	0.47
3:B:39:ILE:HD11	3:B:107:LEU:CD1	2.42	0.46
3:B:17:ASP:OD1	3:B:18:ALA:N	2.48	0.46
4:E:113:LEU:O	4:E:117:VAL:HG23	2.16	0.46
4:F:22:VAL:HG12	4:F:22:VAL:O	2.16	0.46
4:F:122:GLN:HB2	4:F:123:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:59:HIS:HA	4:E:67:LEU:O	2.16	0.46
1:G:8:LEU:HD23	1:G:70:VAL:HA	1.98	0.46
2:C:141:THR:HG22	2:C:143:SER:H	1.79	0.46
2:C:10:LEU:HD12	2:C:61:ILE:HB	1.97	0.46
1:G:7:THR:HG23	1:G:69:LEU:HD23	1.97	0.46
2:C:161:PHE:HE1	2:C:163:ARG:HH21	1.63	0.46
4:F:76:GLN:C	4:F:77:TYR:HD1	2.24	0.46
2:D:183:SER:HB3	3:A:256:LEU:HD22	1.98	0.46
3:A:131:PRO:HD2	3:A:211:ARG:NE	2.28	0.46
4:F:171:ALA:O	4:F:207:PHE:N	2.32	0.45
1:H:70:VAL:HG11	3:A:97:LEU:CD1	2.46	0.45
4:E:21:VAL:HA	4:E:114:LEU:HG	1.98	0.45
2:C:237:GLU:HA	2:C:240:VAL:HG12	1.98	0.45
4:F:106:ASN:OD1	4:F:106:ASN:N	2.49	0.45
3:B:37:LEU:HG	3:B:80:LEU:CD1	2.47	0.45
3:A:285:GLN:O	3:A:285:GLN:NE2	2.46	0.45
4:F:35:LEU:HD22	4:F:35:LEU:H	1.81	0.45
3:A:291:LEU:HA	3:A:291:LEU:HD12	1.69	0.45
1:G:26:VAL:CG2	1:G:56:LEU:HD21	2.35	0.44
3:B:171:THR:OG1	3:B:172:CYS:N	2.50	0.44
4:E:123:GLN:O	4:E:127:PHE:N	2.49	0.44
1:G:51:GLU:OE1	1:G:54:ARG:HD2	2.17	0.44
2:C:116:LEU:HD21	4:F:96:PRO:HG3	1.99	0.44
4:F:246:LEU:HA	4:F:249:TYR:HB2	1.98	0.44
2:C:122:GLN:CD	2:C:157:GLN:HE21	2.26	0.44
1:G:38:PRO:O	1:G:41:GLN:HG2	2.18	0.44
4:F:43:GLY:HA3	4:F:55:ARG:HH21	1.83	0.44
1:H:8:LEU:HD11	3:A:100:ALA:HB3	2.00	0.44
2:C:125:PHE:O	2:C:126:SER:C	2.61	0.44
3:A:86:ARG:HD3	3:A:88:ASP:OD1	2.16	0.44
3:B:250:ILE:HD13	3:B:250:ILE:HA	1.89	0.44
4:F:99:LEU:HD22	4:F:102:LEU:HD23	2.00	0.44
2:C:71:PHE:CE2	4:F:81:PRO:HD2	2.52	0.44
2:D:131:VAL:HG12	2:D:155:LYS:CG	2.48	0.44
2:D:146:THR:HG23	3:A:171:THR:HG22	2.00	0.44
1:G:36:ILE:HD13	1:G:71:LEU:HD21	2.00	0.43
1:H:37:PRO:CD	3:A:144:MET:SD	3.06	0.43
1:H:1:MET:HE3	1:H:17:VAL:HG23	1.99	0.43
2:D:155:LYS:HB2	2:D:162:HIS:HD2	1.83	0.43
3:A:141:MET:CA	3:A:144:MET:HE2	2.40	0.43
3:B:107:LEU:HD22	3:B:227:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:170:SER:HA	4:F:208:GLU:HA	2.00	0.43
2:D:131:VAL:HG12	2:D:155:LYS:HG2	1.99	0.43
3:A:145:MET:HE3	3:A:145:MET:HB2	1.82	0.43
4:E:21:VAL:HG11	4:E:113:LEU:HD23	2.00	0.43
1:G:17:VAL:HB	1:G:21:ASP:OD2	2.18	0.43
3:A:132:SER:O	3:A:136:VAL:HG22	2.19	0.43
4:E:69:TRP:CD1	4:E:86:PHE:HA	2.54	0.43
1:G:11:LYS:HZ2	1:G:13:ILE:CG2	2.32	0.43
1:G:26:VAL:CG2	1:G:56:LEU:CD1	2.75	0.43
2:C:122:GLN:HE21	2:C:128:GLN:HA	1.83	0.43
2:D:33:LEU:HD13	2:D:61:ILE:HD13	2.00	0.43
3:B:37:LEU:HD11	3:B:80:LEU:HD11	2.00	0.43
1:G:43:LEU:HD13	1:G:43:LEU:HA	1.91	0.43
3:A:22:CYS:SG	3:A:77:VAL:HG11	2.59	0.43
1:G:21:ASP:OD2	1:G:56:LEU:HD11	2.19	0.43
2:C:110:MET:HE2	2:C:115:ARG:HG2	2.01	0.42
4:E:92:PHE:CZ	4:E:94:PRO:HG3	2.53	0.42
4:F:10:ILE:HG21	4:F:18:ILE:HG21	2.00	0.42
3:A:150:VAL:CG1	3:A:151:GLY:N	2.82	0.42
2:D:111:THR:OG1	2:D:114:GLU:HG3	2.18	0.42
3:A:86:ARG:CG	3:A:89:ARG:H	2.32	0.42
3:A:224:ILE:HD12	3:A:290:ARG:HH21	1.69	0.42
3:B:298:LEU:HD23	3:B:298:LEU:HA	1.81	0.42
1:G:21:ASP:OD2	1:G:56:LEU:CD1	2.67	0.42
4:F:38:THR:HG22	4:F:39:ASP:CG	2.45	0.42
4:F:41:LYS:HB2	4:F:55:ARG:HG3	2.00	0.42
4:F:203:LEU:HA	4:F:219:LEU:HA	2.02	0.42
2:C:32:PHE:CE1	2:C:121:LEU:HD21	2.55	0.42
2:C:63:LYS:HD3	2:C:94:LYS:HZ3	1.85	0.42
2:D:22:HIS:HE2	2:D:104:ARG:HG3	1.84	0.42
3:B:164:LYS:HE2	3:B:164:LYS:HB3	1.79	0.42
1:G:50:LEU:HD23	1:G:50:LEU:HA	1.85	0.42
3:B:11:ALA:HB3	3:B:71:ILE:HG22	2.01	0.42
3:A:35:MET:HB3	3:A:122:HIS:HB2	2.01	0.42
3:A:81:ARG:NH2	3:A:245:ASP:OD2	2.45	0.42
4:E:125:HIS:NE2	4:E:156:GLU:HA	2.35	0.41
2:D:233:VAL:HG12	3:A:229:LEU:HD11	2.01	0.41
2:C:154:TYR:OH	2:C:163:ARG:NH1	2.53	0.41
3:A:153:ILE:O	3:A:170:TYR:HA	2.20	0.41
3:B:139:GLN:CD	3:B:211:ARG:NH1	2.78	0.41
1:G:28:ALA:HA	1:G:31:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:SER:OG	3:B:288:GLU:OE2	2.38	0.41
3:A:86:ARG:HG3	3:A:88:ASP:N	2.25	0.41
4:F:54:ASP:O	4:F:73:PHE:HB2	2.20	0.41
4:E:40:LEU:HD23	4:E:40:LEU:HA	1.77	0.41
1:G:63:LYS:NZ	1:H:76:GLY:O	2.50	0.41
2:C:147:HIS:O	3:B:169:LEU:HB2	2.20	0.41
2:C:201:LYS:HE3	2:D:214:LYS:HG2	2.02	0.41
3:B:32:GLU:O	3:B:125:PRO:HG3	2.21	0.41
1:G:11:LYS:NZ	1:G:13:ILE:CG2	2.77	0.41
1:H:37:PRO:HA	1:H:38:PRO:HD3	1.95	0.41
2:D:79:GLU:H	2:D:79:GLU:HG2	1.68	0.41
2:D:218:MET:HE3	2:D:218:MET:HB2	1.90	0.41
3:A:229:LEU:O	3:A:233:VAL:HG13	2.21	0.41
3:B:39:ILE:HG22	3:B:117:VAL:HG22	2.03	0.41
3:B:166:GLY:C	3:B:167:ARG:HG3	2.45	0.41
4:F:18:ILE:HD12	4:F:19:SER:N	2.35	0.41
4:F:38:THR:HG22	4:F:39:ASP:OD1	2.20	0.41
4:E:245:CYS:O	4:E:246:LEU:C	2.64	0.41
3:A:237:LYS:O	3:A:241:GLN:HG3	2.21	0.41
3:B:37:LEU:CG	3:B:80:LEU:HD11	2.51	0.40
3:B:72:VAL:HG21	3:B:150:VAL:HG21	2.03	0.40
4:F:71:ILE:HD13	4:F:71:ILE:HA	1.88	0.40
2:C:85:LEU:HD12	2:C:85:LEU:HA	1.80	0.40
2:C:191:PHE:HA	2:D:222:LEU:HD21	2.03	0.40
2:D:171:LEU:HD22	3:A:279:VAL:HG21	2.03	0.40
4:F:10:ILE:HD11	4:F:40:LEU:HD22	2.03	0.40
4:F:16:PRO:O	4:F:20:SER:OG	2.21	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	G	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
1	H	74/76 (97%)	74 (100%)	0	0	100	100
2	C	226/302 (75%)	214 (95%)	12 (5%)	0	100	100
2	D	225/302 (74%)	216 (96%)	9 (4%)	0	100	100
3	A	244/316 (77%)	235 (96%)	9 (4%)	0	100	100
3	B	231/316 (73%)	224 (97%)	7 (3%)	0	100	100
4	E	236/385 (61%)	221 (94%)	15 (6%)	0	100	100
4	F	231/385 (60%)	219 (95%)	12 (5%)	0	100	100
All	All	1541/2158 (71%)	1475 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	G	68/68 (100%)	68 (100%)	0	100	100
1	H	68/68 (100%)	68 (100%)	0	100	100
2	C	209/265 (79%)	209 (100%)	0	100	100
2	D	208/265 (78%)	208 (100%)	0	100	100
3	A	226/285 (79%)	226 (100%)	0	100	100
3	B	215/285 (75%)	215 (100%)	0	100	100
4	E	213/337 (63%)	213 (100%)	0	100	100
4	F	207/337 (61%)	207 (100%)	0	100	100
All	All	1414/1910 (74%)	1414 (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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	68	HIS
1	H	41	GLN
2	C	118	HIS
2	C	122	GLN
2	C	157	GLN
2	C	176	GLN
2	D	162	HIS
3	A	174	GLN
3	B	293	GLN
4	F	76	GLN
4	F	255	HIS
4	E	106	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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)

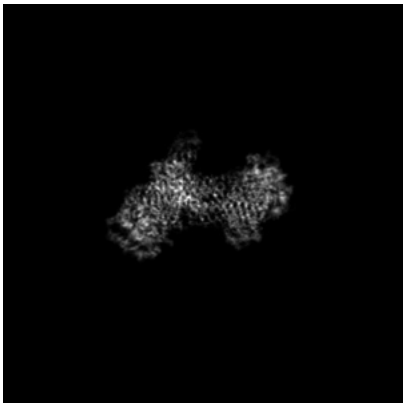
This section contains visualisations of the EMDB entry EMD-55118. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

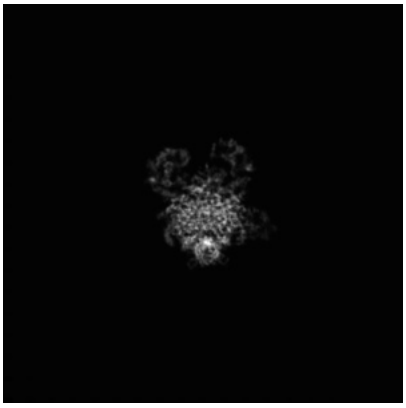
6.1 Orthogonal projections (i)

6.1.1 Primary 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: 200

Y Index: 200

Z Index: 200

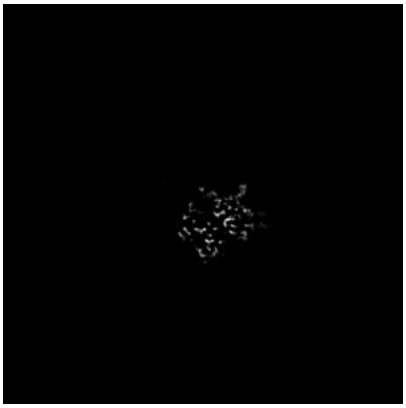
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 205

Y Index: 189

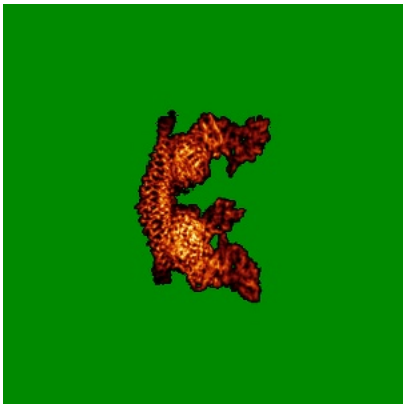


Z Index: 171

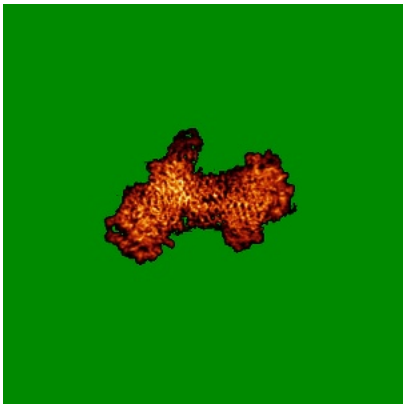
The images above show the largest variance slices of the map in three orthogonal directions.

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

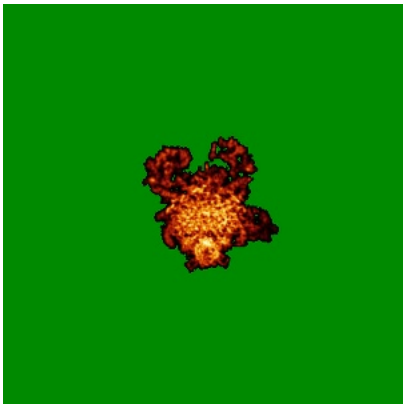
6.4.1 Primary map



X



Y

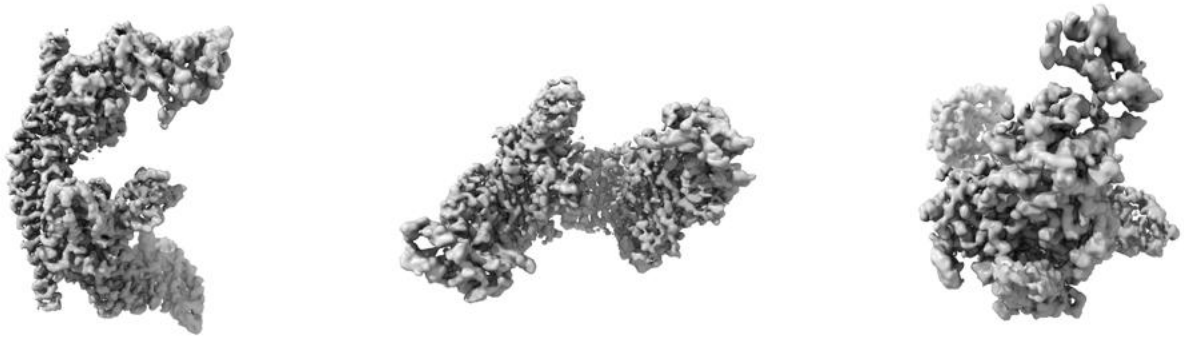


Z

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 0.0572. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

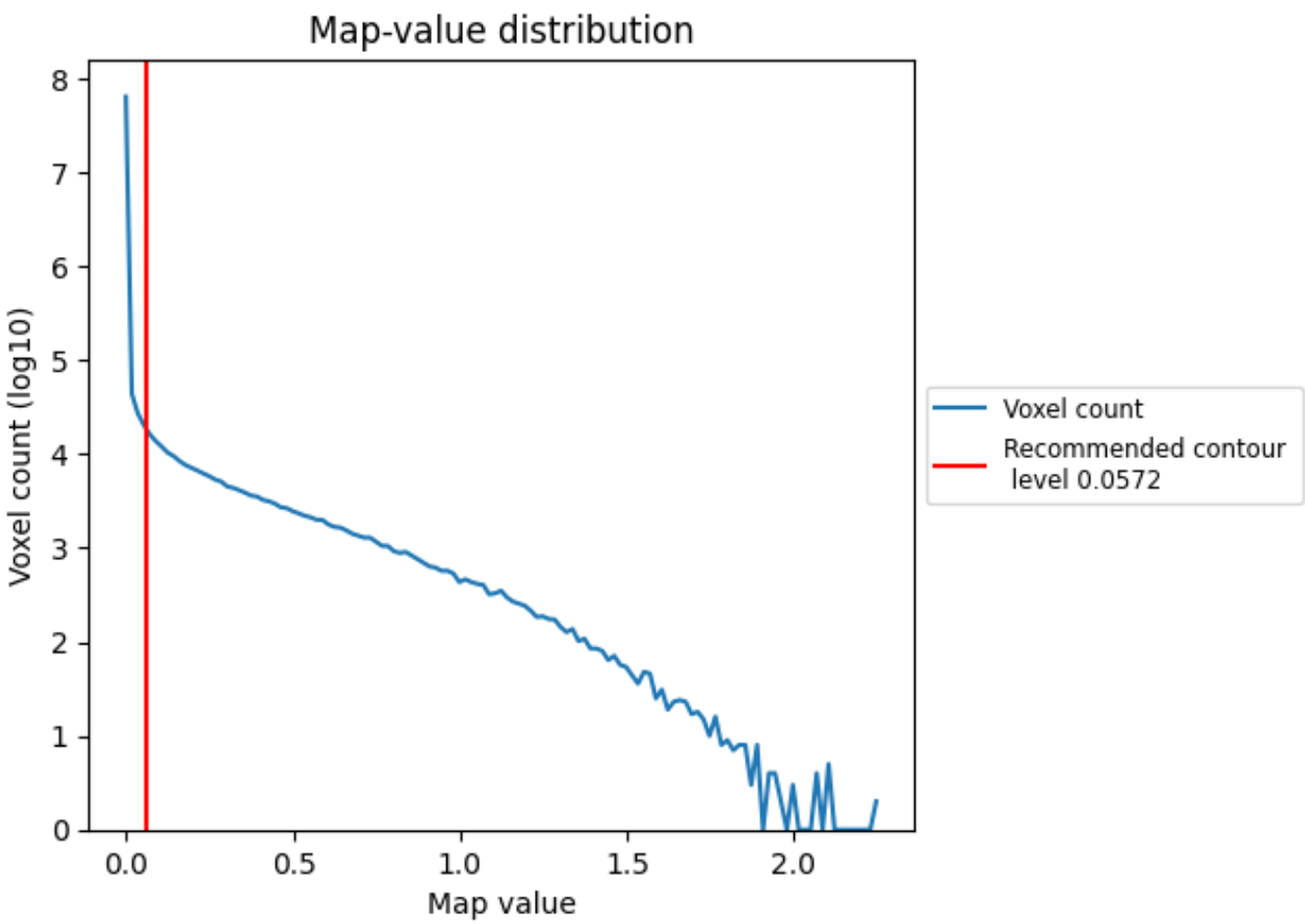
6.6 Mask visualisation (i)

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

7 Map analysis (i)

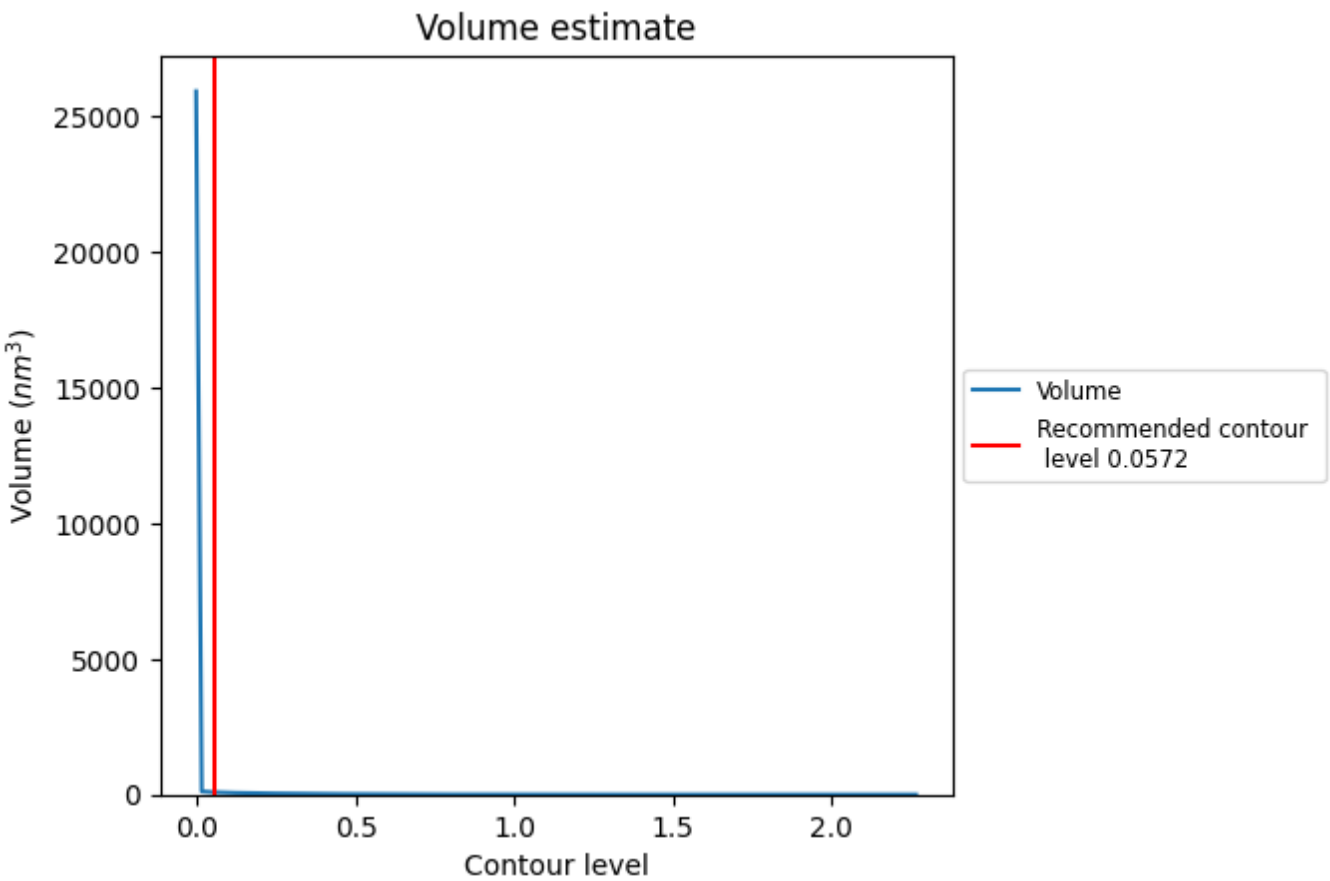
This section contains the results of statistical analysis of the map.

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.

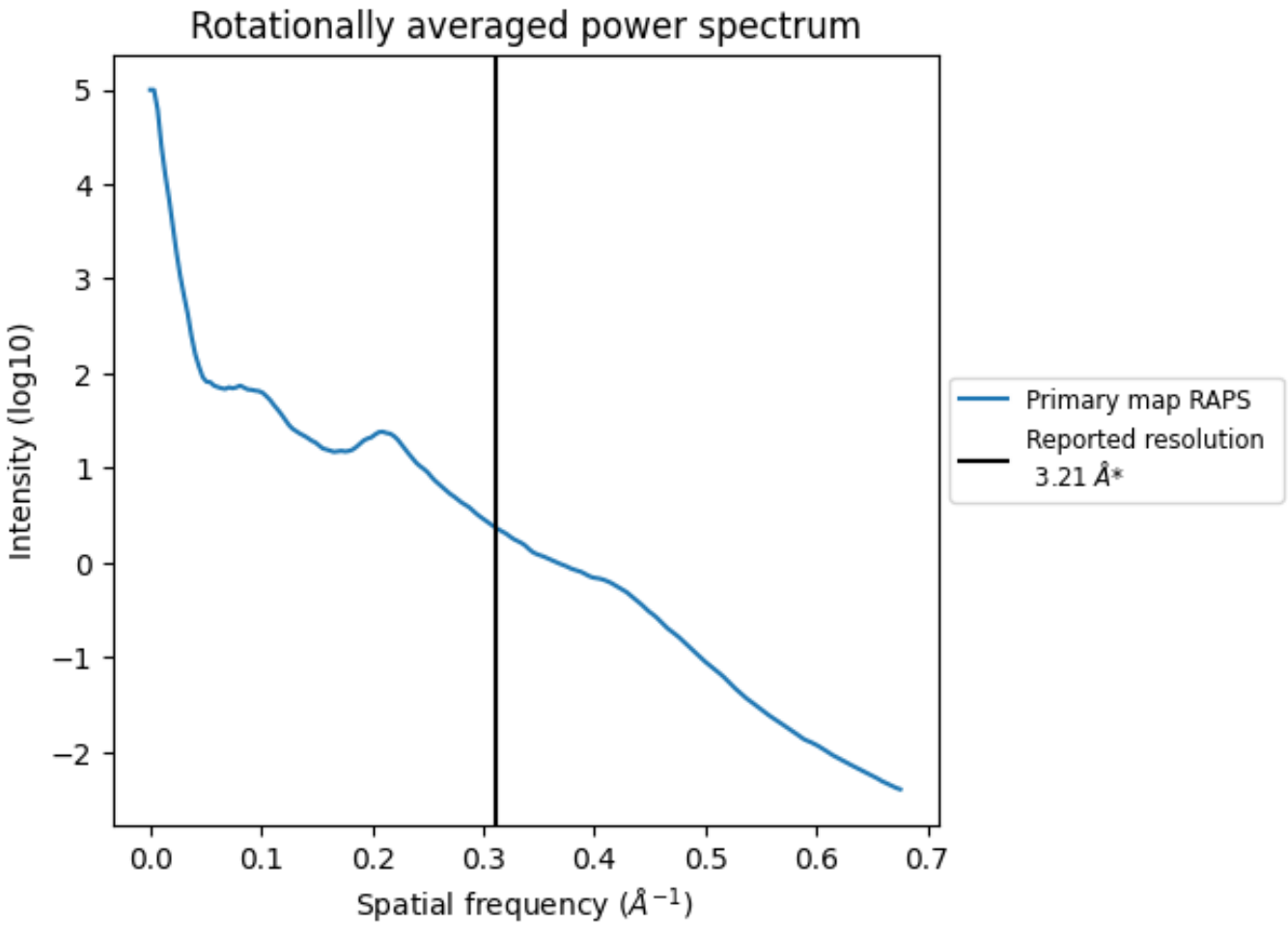
7.2 Volume estimate (i)



The volume at the recommended contour level is 85 nm^3; this corresponds to an approximate mass of 77 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

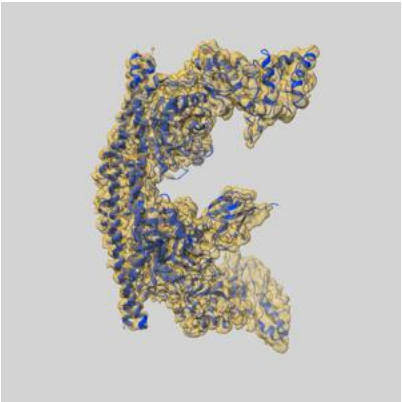
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

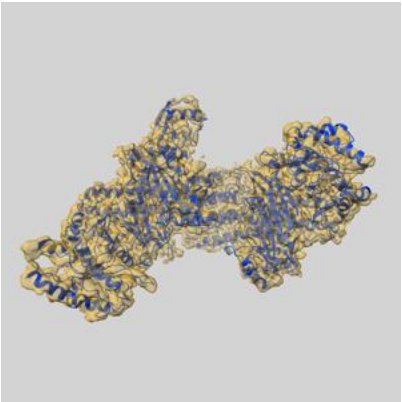
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55118 and PDB model 9SQV. Per-residue inclusion information can be found in section 3 on page 8.

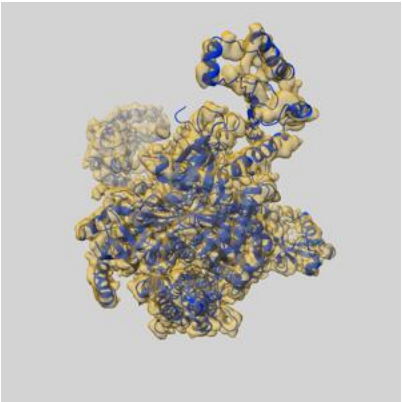
9.1 Map-model overlay (i)



X



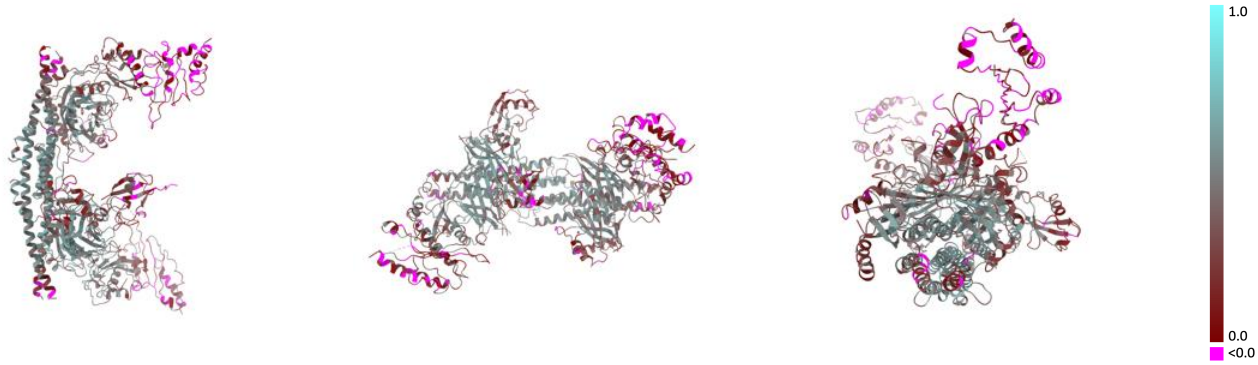
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0572 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.

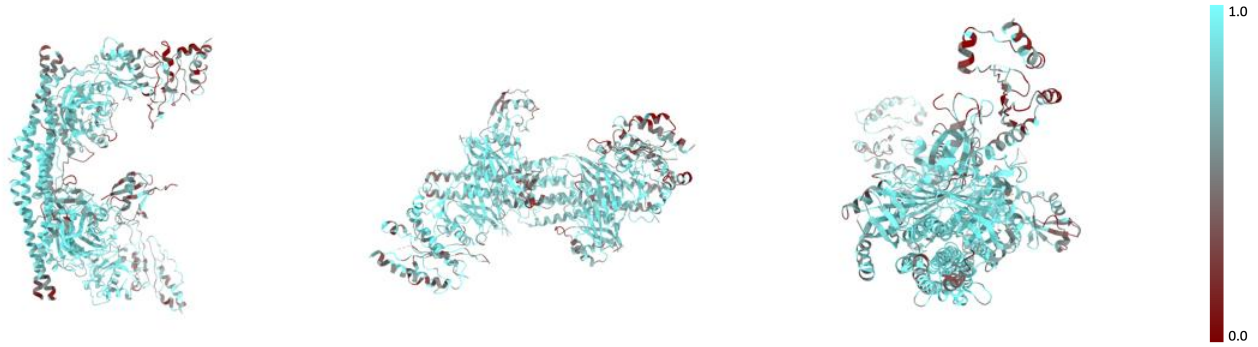
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

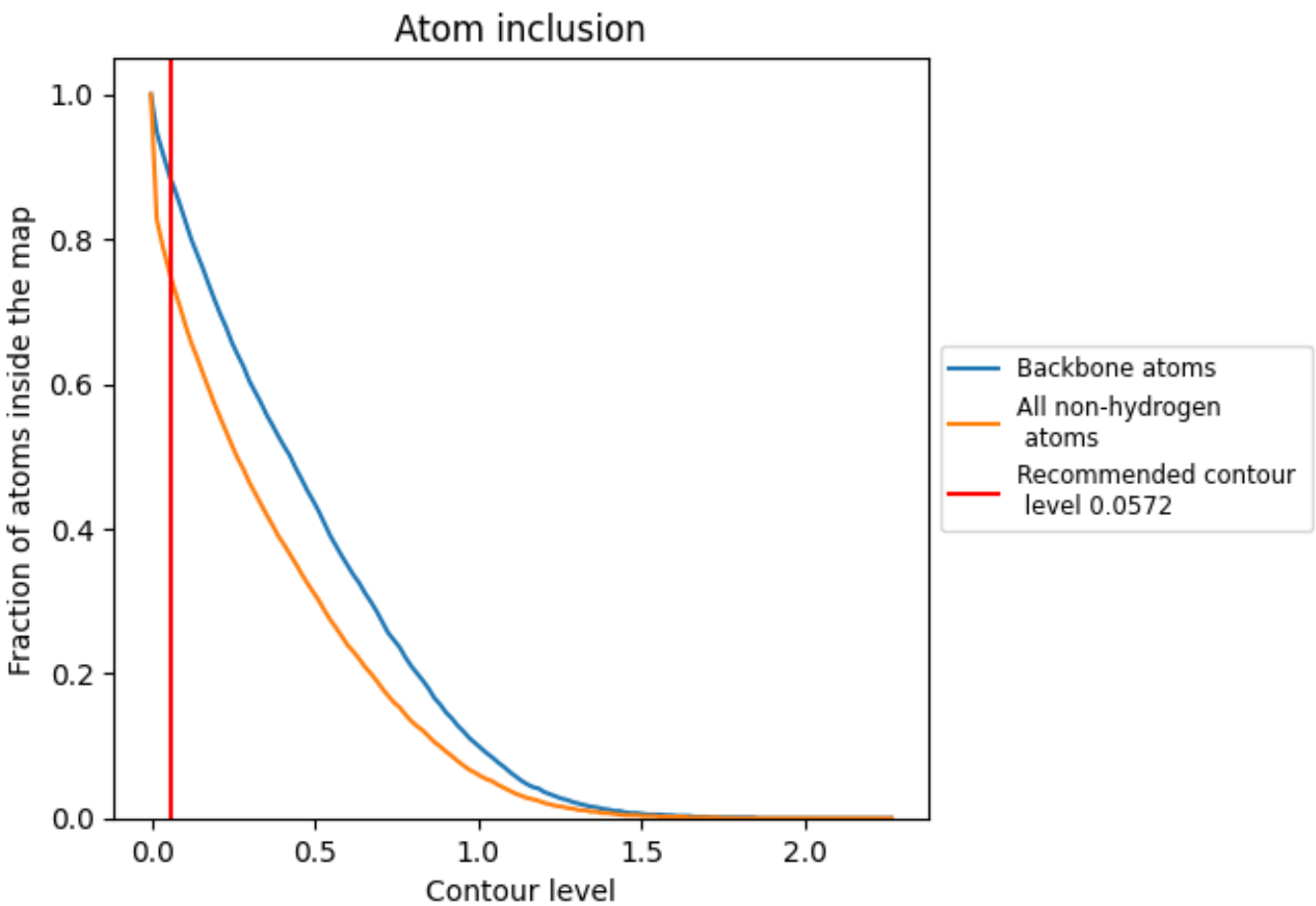
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0572).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0572) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.3580
A	0.8680	0.4860
B	0.7500	0.3780
C	0.8180	0.4340
D	0.8460	0.4820
E	0.7380	0.2790
F	0.5960	0.1640
G	0.5240	0.1850
H	0.5930	0.2850