Full wwPDB EM Validation Report

Aug 13, 2026 – 01:41 pm BST

PDB ID	:	9SMR / pdb_00009smr
EMDB ID	:	EMD-55040
Title	:	Structure of apo BRCA1-A complex in presence of K63-oligoUbATA
Authors	:	Murachelli, A.G.; Sixma, T.K.
Deposited on	:	2025-09-09
Resolution	:	3.25 Å(reported)
Based on initial model	:	9SMN

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:

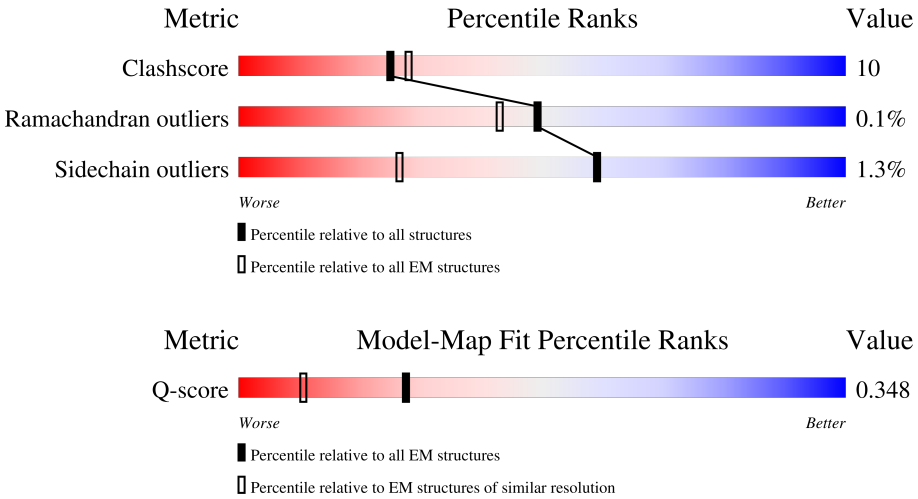
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

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	A	409	59% 16% 24%
1	F	409	52% 11% 37%
2	B	316	64% 18% 18%
2	G	316	61% 17% • 19%

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Mol	Chain	Length	Quality of chain
3	C	383	
3	H	383	
4	D	349	
4	I	349	
5	E	171	
5	J	171	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19528 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 BRCA1-A complex subunit Abraxas 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	309	Total 2480	C 1565	N 433	O 469	S 13	0	0
1	F	258	Total 2060	C 1298	N 356	O 397	S 9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	259	Total 2079	C 1301	N 369	O 395	S 14	0	0
2	G	256	Total 2057	C 1289	N 366	O 388	S 14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	381	Total 3060	C 1981	N 501	O 564	S 14	0	0
3	H	383	Total 3078	C 1993	N 504	O 567	S 14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	237	Total 1889	C 1206	N 306	O 359	S 18	0	0
4	I	237	Total 1889	C 1206	N 306	O 359	S 18	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q9NWV8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	ALA	-	expression tag	UNP Q9NWV8
D	-17	HIS	-	expression tag	UNP Q9NWV8
D	-16	HIS	-	expression tag	UNP Q9NWV8
D	-15	HIS	-	expression tag	UNP Q9NWV8
D	-14	HIS	-	expression tag	UNP Q9NWV8
D	-13	HIS	-	expression tag	UNP Q9NWV8
D	-12	HIS	-	expression tag	UNP Q9NWV8
D	-11	SER	-	expression tag	UNP Q9NWV8
D	-10	ALA	-	expression tag	UNP Q9NWV8
D	-9	ALA	-	expression tag	UNP Q9NWV8
D	-8	LEU	-	expression tag	UNP Q9NWV8
D	-7	GLU	-	expression tag	UNP Q9NWV8
D	-6	VAL	-	expression tag	UNP Q9NWV8
D	-5	LEU	-	expression tag	UNP Q9NWV8
D	-4	PHE	-	expression tag	UNP Q9NWV8
D	-3	GLN	-	expression tag	UNP Q9NWV8
D	-2	GLY	-	expression tag	UNP Q9NWV8
D	-1	PRO	-	expression tag	UNP Q9NWV8
D	0	GLY	-	expression tag	UNP Q9NWV8
I	-19	MET	-	initiating methionine	UNP Q9NWV8
I	-18	ALA	-	expression tag	UNP Q9NWV8
I	-17	HIS	-	expression tag	UNP Q9NWV8
I	-16	HIS	-	expression tag	UNP Q9NWV8
I	-15	HIS	-	expression tag	UNP Q9NWV8
I	-14	HIS	-	expression tag	UNP Q9NWV8
I	-13	HIS	-	expression tag	UNP Q9NWV8
I	-12	HIS	-	expression tag	UNP Q9NWV8
I	-11	SER	-	expression tag	UNP Q9NWV8
I	-10	ALA	-	expression tag	UNP Q9NWV8
I	-9	ALA	-	expression tag	UNP Q9NWV8
I	-8	LEU	-	expression tag	UNP Q9NWV8
I	-7	GLU	-	expression tag	UNP Q9NWV8
I	-6	VAL	-	expression tag	UNP Q9NWV8
I	-5	LEU	-	expression tag	UNP Q9NWV8
I	-4	PHE	-	expression tag	UNP Q9NWV8
I	-3	GLN	-	expression tag	UNP Q9NWV8
I	-2	GLY	-	expression tag	UNP Q9NWV8
I	-1	PRO	-	expression tag	UNP Q9NWV8
I	0	GLY	-	expression tag	UNP Q9NWV8

- Molecule 5 is a protein called BRCA1-A complex subunit RAP80.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	58	Total	C	N	O	S	0	0
			466	305	78	80	3		
5	J	58	Total	C	N	O	S	0	0
			466	305	78	80	3		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	243	MET	-	initiating methionine	UNP Q96RL1
E	244	ALA	-	expression tag	UNP Q96RL1
E	245	SER	-	expression tag	UNP Q96RL1
E	246	TRP	-	expression tag	UNP Q96RL1
E	247	SER	-	expression tag	UNP Q96RL1
E	248	HIS	-	expression tag	UNP Q96RL1
E	249	PRO	-	expression tag	UNP Q96RL1
E	250	GLN	-	expression tag	UNP Q96RL1
E	251	PHE	-	expression tag	UNP Q96RL1
E	252	GLU	-	expression tag	UNP Q96RL1
E	253	LYS	-	expression tag	UNP Q96RL1
E	254	GLY	-	expression tag	UNP Q96RL1
E	255	ALA	-	expression tag	UNP Q96RL1
E	256	LEU	-	expression tag	UNP Q96RL1
E	257	GLU	-	expression tag	UNP Q96RL1
E	258	VAL	-	expression tag	UNP Q96RL1
E	259	LEU	-	expression tag	UNP Q96RL1
E	260	PHE	-	expression tag	UNP Q96RL1
E	261	GLN	-	expression tag	UNP Q96RL1
E	262	GLY	-	expression tag	UNP Q96RL1
E	263	PRO	-	expression tag	UNP Q96RL1
E	264	GLY	-	expression tag	UNP Q96RL1
J	243	MET	-	initiating methionine	UNP Q96RL1
J	244	ALA	-	expression tag	UNP Q96RL1
J	245	SER	-	expression tag	UNP Q96RL1
J	246	TRP	-	expression tag	UNP Q96RL1
J	247	SER	-	expression tag	UNP Q96RL1
J	248	HIS	-	expression tag	UNP Q96RL1
J	249	PRO	-	expression tag	UNP Q96RL1
J	250	GLN	-	expression tag	UNP Q96RL1
J	251	PHE	-	expression tag	UNP Q96RL1
J	252	GLU	-	expression tag	UNP Q96RL1
J	253	LYS	-	expression tag	UNP Q96RL1
J	254	GLY	-	expression tag	UNP Q96RL1
J	255	ALA	-	expression tag	UNP Q96RL1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	256	LEU	-	expression tag	UNP Q96RL1
J	257	GLU	-	expression tag	UNP Q96RL1
J	258	VAL	-	expression tag	UNP Q96RL1
J	259	LEU	-	expression tag	UNP Q96RL1
J	260	PHE	-	expression tag	UNP Q96RL1
J	261	GLN	-	expression tag	UNP Q96RL1
J	262	GLY	-	expression tag	UNP Q96RL1
J	263	PRO	-	expression tag	UNP Q96RL1
J	264	GLY	-	expression tag	UNP Q96RL1

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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.

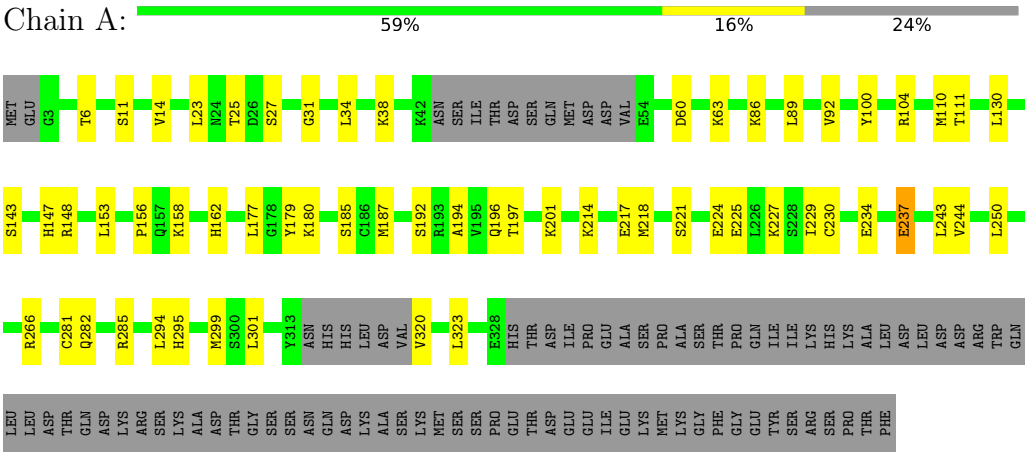
Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total O 1 1	0
7	G	1	Total O 1 1	0

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.

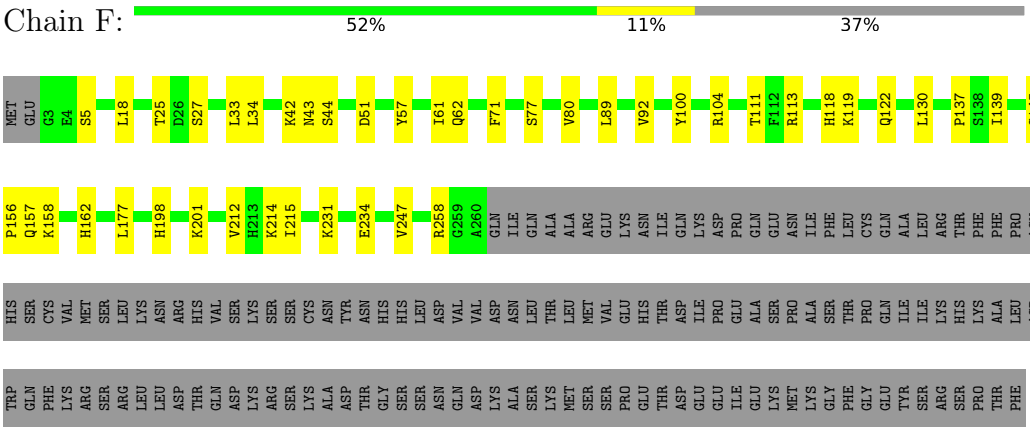
• Molecule 1: BRCA1-A complex subunit Abraxas 1

Chain A:



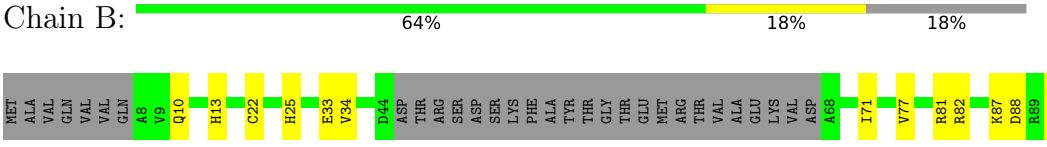
• Molecule 1: BRCA1-A complex subunit Abraxas 1

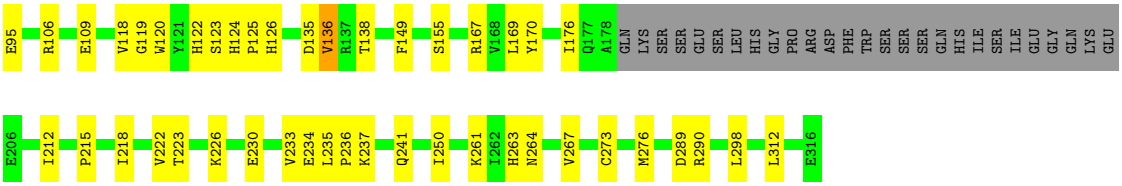
Chain F:

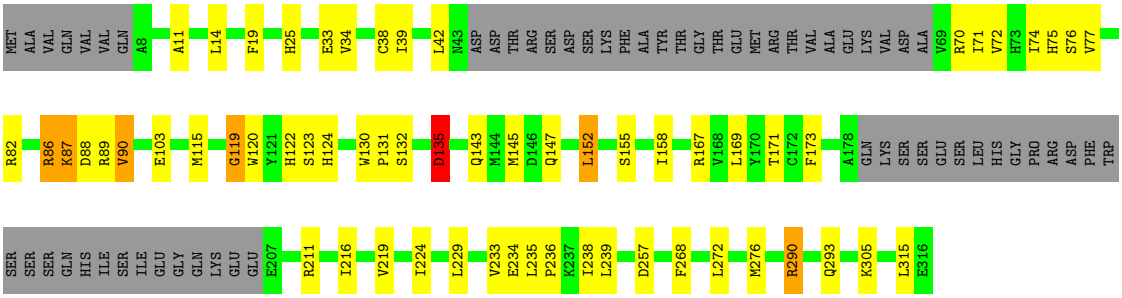


• Molecule 2: Lys-63-specific deubiquitinase BRCC36

Chain B:





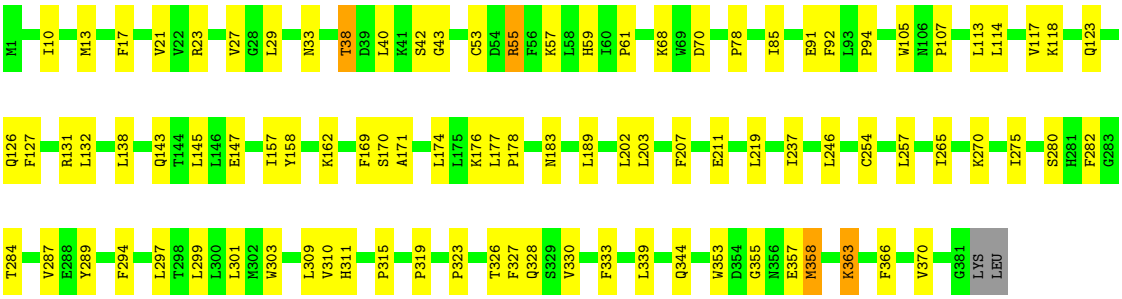


• Molecule 2: Lys-63-specific deubiquitinase BRCC36

Chain G:

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

Chain C:

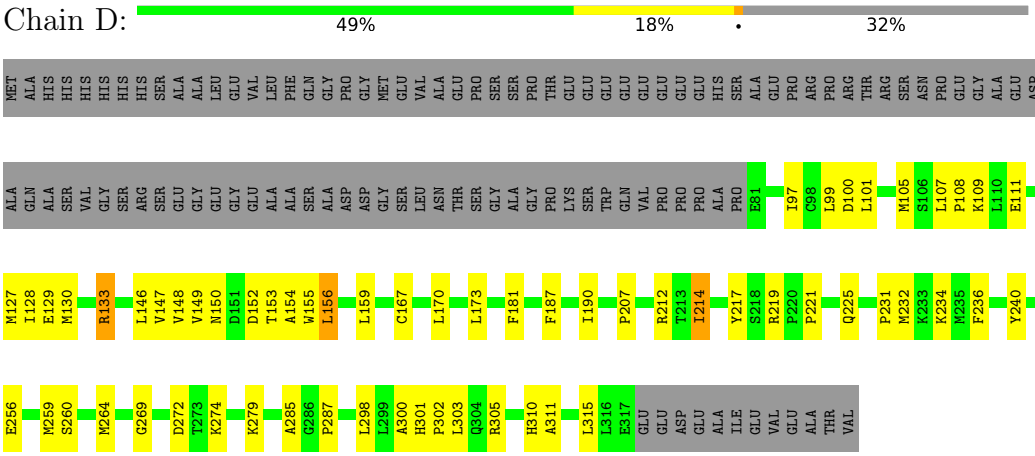


• Molecule 3: BRISC and BRCA1-A complex member 2

Chain H:

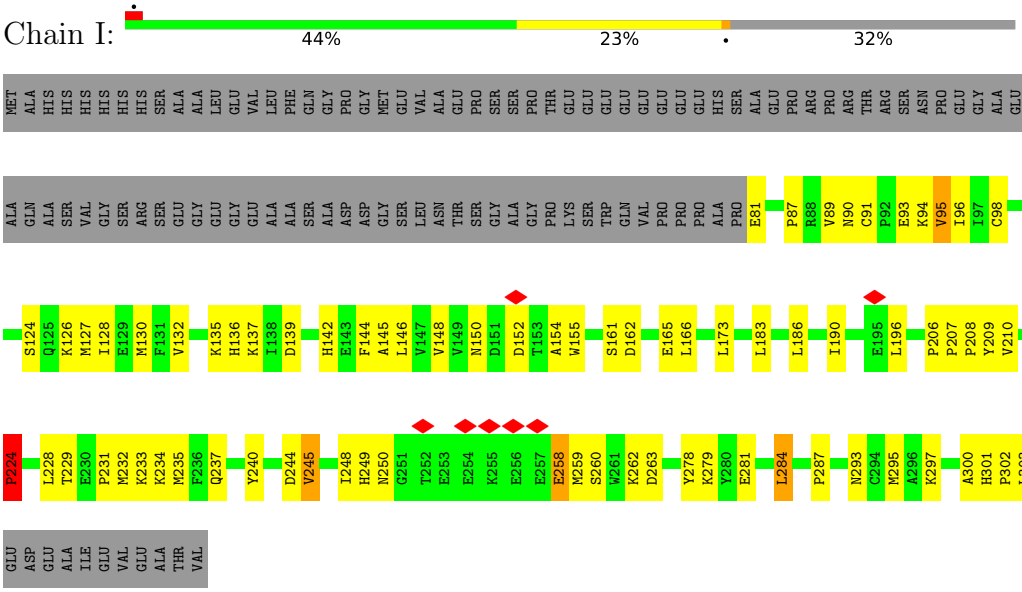
• Molecule 4: BRISC and BRCA1-A complex member 1

Chain D:



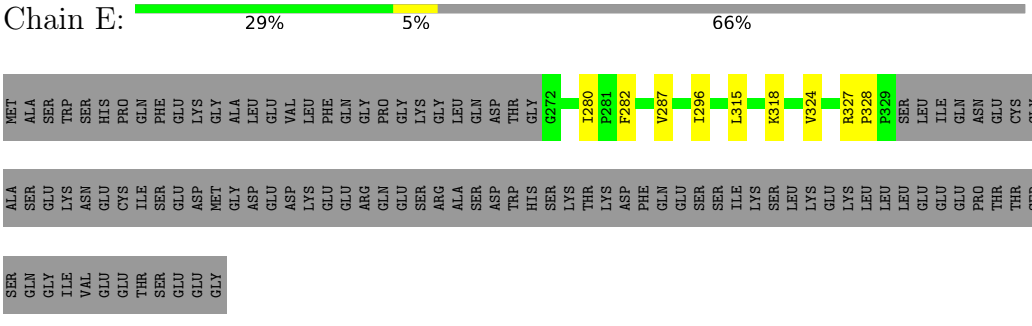
• Molecule 4: BRISC and BRCA1-A complex member 1

Chain I:



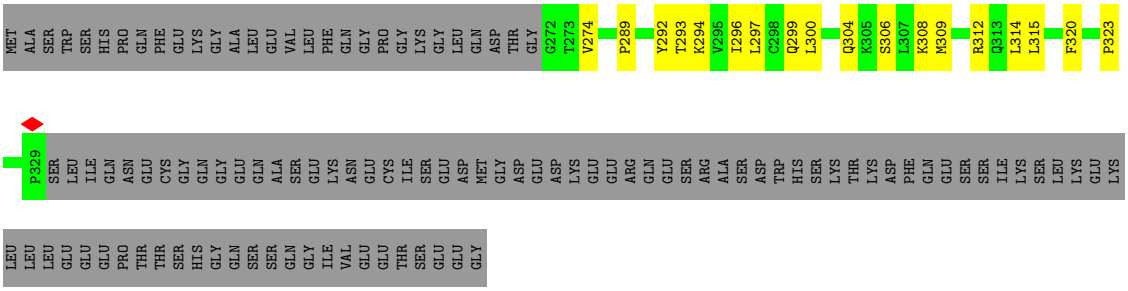
• Molecule 5: BRCA1-A complex subunit RAP80

Chain E:



• Molecule 5: BRCA1-A complex subunit RAP80

Chain J:


MET ALA SER TRP SER HIS PRO GLN PHE GLU LYS GLY ALA LEU GLU VAL LEU PHE GLN GLY PRO GLY LYS GLY LEU GLN ASP THR GLY G272 T273 V274 P289 Y292 T293 K294 V295 I296 L297 C298 Q299 L300 Q304 K305 S306 L307 K308 M309 R312 Q313 L314 L315 F320 P323
P329 SER LEU ILE GLN ASN GLU CYS GLY GLN GLY GLU GLN ALA SER GLU LYS ASN GLU CYS ILE SER GLU ASP MET GLY ASP GLU ASP LYS GLU GLU ARG GLN GLU SER ARG ALA SER ASP TRP HIS SER LYS THR LYS ASP PHE GLN GLU SER SER ILE LYS SER LEU LYS GLU LYS
LEU LEU LEU GLU GLU GLU PRO THR THR SER HIS GLY GLN SER SER GLN GLY ILE VAL GLU GLU THR SER GLU GLU GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	279338	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.421	Depositor
Minimum map value	-0.158	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	551.7936, 551.7936, 551.7936	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2773, 1.2773, 1.2773	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	0.18	0/2522	0.44	0/3386
1	F	0.24	0/2095	0.36	0/2815
2	B	0.47	2/2115 (0.1%)	0.73	8/2857 (0.3%)
2	G	0.39	0/2093	0.70	4/2827 (0.1%)
3	C	0.18	0/3151	0.47	0/4288
3	H	0.21	0/3169	0.52	2/4310 (0.0%)
4	D	0.22	0/1934	0.46	0/2623
4	I	0.25	0/1934	0.53	2/2623 (0.1%)
5	E	0.16	0/480	0.37	0/652
5	J	0.11	0/480	0.36	0/652
All	All	0.27	2/19973 (0.0%)	0.53	16/27033 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	G	0	3
3	H	0	1
4	D	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	LYS	C-N	12.92	1.50	1.33
2	B	88	ASP	C-N	6.73	1.43	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	135	ASP	CA-CB-CG	9.42	122.02	112.60
3	H	49	PRO	N-CA-C	8.15	124.86	113.53
2	B	87	LYS	O-C-N	7.45	132.03	122.87
4	I	258	GLU	CB-CA-C	-7.24	108.21	116.54
3	H	51	PRO	N-CA-CB	-7.02	95.88	103.25
2	B	88	ASP	CA-C-N	7.00	132.97	122.47
2	B	88	ASP	C-N-CA	7.00	132.97	122.47
2	B	122	HIS	N-CA-C	6.59	118.15	108.86
2	B	119	GLY	CA-C-N	-6.41	112.56	122.87
2	B	119	GLY	C-N-CA	-6.41	112.56	122.87
2	G	87	LYS	O-C-N	6.40	130.50	123.27
2	B	136	VAL	CB-CA-C	-6.03	104.14	112.04
4	I	224	PRO	N-CA-CB	-5.93	97.02	103.25
2	B	123	SER	CA-CB-OG	5.66	122.42	111.10
2	G	119	GLY	CA-C-N	-5.66	112.97	122.92
2	G	119	GLY	C-N-CA	-5.66	112.97	122.92

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	290	ARG	Sidechain
4	D	133	ARG	Sidechain
2	G	119	GLY	Mainchain
2	G	290	ARG	Sidechain
2	G	86	ARG	Sidechain
3	H	36	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	A	2480	0	2479	52	0
1	F	2060	0	2054	39	0
2	B	2079	0	2062	36	0
2	G	2057	0	2047	53	0
3	C	3060	0	2977	62	0
3	H	3078	0	3001	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1889	0	1871	51	0
4	I	1889	0	1871	62	0
5	E	466	0	472	9	0
5	J	466	0	472	17	0
6	B	1	0	0	1	0
6	G	1	0	0	0	0
7	B	1	0	0	0	0
7	G	1	0	0	0	0
All	All	19528	0	19306	406	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (406) 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)
4:I:186:LEU:CD2	4:I:215:LEU:HD22	2.04	0.88
2:B:273:CYS:HA	2:B:276:MET:HE2	1.58	0.84
4:I:96:ILE:HG23	4:I:145:ALA:HB3	1.61	0.81
1:A:237:GLU:HG3	2:B:223:THR:HB	1.61	0.80
2:G:90:VAL:HG21	2:G:122:HIS:CD2	2.17	0.79
4:I:259:MET:HG3	4:I:263:ASP:HB2	1.67	0.77
2:G:131:PRO:HG3	2:G:173:PHE:CG	2.22	0.75
1:F:234:GLU:HG3	2:G:229:LEU:HD23	1.67	0.75
2:B:124:HIS:NE2	6:B:401:ZN:ZN	1.51	0.75
4:I:231:PRO:HA	4:I:234:LYS:HE2	1.72	0.72
4:D:259:MET:HB2	4:D:264:MET:HE2	1.69	0.72
4:I:249:HIS:HE1	4:I:281:GLU:HB2	1.54	0.71
3:C:183:ASN:HB2	3:C:265:ILE:HD13	1.73	0.71
3:C:132:LEU:HD22	3:C:157:ILE:HG21	1.72	0.71
1:F:212:VAL:HG13	2:G:268:PHE:HE2	1.56	0.71
3:H:24:ASN:HD22	3:H:114:LEU:HD21	1.57	0.70
2:G:131:PRO:HG3	2:G:173:PHE:CD1	2.28	0.69
4:I:90:ASN:HB3	4:I:304:GLN:HE22	1.57	0.69
2:G:33:GLU:HB2	2:G:82:ARG:HH12	1.58	0.69
5:J:274:VAL:HA	4:I:81:GLU:HA	1.74	0.69
1:A:281:CYS:HB3	1:A:285:ARG:HH21	1.59	0.68
4:I:186:LEU:HD22	4:I:215:LEU:HD22	1.75	0.68
3:C:282:PHE:HZ	3:C:363:LYS:HB2	1.59	0.68
4:I:124:SER:O	4:I:127:MET:HG2	1.93	0.67
4:D:231:PRO:HA	4:D:234:LYS:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:HIS:O	2:B:155:SER:HA	1.94	0.67
3:C:353:TRP:HB2	3:C:358:MET:HE2	1.77	0.67
3:H:229:LEU:HB2	3:H:260:LYS:HE3	1.75	0.67
1:F:258:ARG:HE	2:G:315:LEU:HD11	1.60	0.67
1:A:179:TYR:HD2	2:B:250:ILE:HG13	1.61	0.66
2:G:42:LEU:HD21	2:G:70:ARG:HH21	1.61	0.66
1:F:80:VAL:HG13	1:F:80:VAL:O	1.96	0.66
3:H:270:LYS:HD3	3:H:319:PRO:HG3	1.78	0.66
3:H:339:LEU:HD23	4:I:137:LYS:HE2	1.78	0.66
3:C:38:THR:HG22	3:C:57:LYS:HB3	1.78	0.65
3:H:55:ARG:HD3	3:H:72:ILE:HG23	1.78	0.65
4:I:214:ILE:HG22	4:I:244:ASP:HB2	1.78	0.65
1:A:201:LYS:HG2	1:F:214:LYS:HE3	1.78	0.65
1:F:119:LYS:HA	1:F:122:GLN:HE21	1.63	0.63
1:A:141:THR:HG22	1:A:143:SER:H	1.63	0.63
2:G:124:HIS:O	2:G:155:SER:HA	2.00	0.62
3:C:299:LEU:HB2	3:C:310:VAL:HG23	1.82	0.61
3:H:132:LEU:HD22	3:H:157:ILE:HD13	1.81	0.61
2:G:235:LEU:HB3	2:G:236:PRO:HD3	1.83	0.61
3:H:317:PHE:HB2	3:H:321:ASP:HB2	1.83	0.61
1:A:6:THR:HG22	1:A:6:THR:O	2.01	0.61
4:I:89:VAL:HG21	4:I:206:PRO:HG3	1.82	0.61
4:I:135:LYS:HG2	4:I:142:HIS:CD2	2.36	0.61
1:A:301:LEU:HA	4:D:310:HIS:HE1	1.65	0.61
3:C:123:GLN:HA	3:C:126:GLN:HG3	1.82	0.61
1:A:244:VAL:HG11	2:B:222:VAL:HG11	1.82	0.60
5:E:327:ARG:HD3	5:E:328:PRO:HD2	1.84	0.60
1:F:104:ARG:HA	1:F:137:PRO:HD2	1.82	0.60
1:F:212:VAL:HG13	2:G:268:PHE:CE2	2.37	0.60
4:I:127:MET:SD	4:I:295:MET:HG3	2.42	0.60
3:H:311:HIS:HB2	3:H:326:THR:HB	1.83	0.60
3:C:42:SER:HA	3:C:53:CYS:HA	1.84	0.59
3:C:315:PRO:HD3	3:C:323:PRO:HA	1.83	0.59
4:D:97:ILE:HG12	4:D:214:ILE:HD11	1.84	0.59
3:H:37:ILE:HG23	3:H:56:PHE:CD2	2.38	0.59
3:C:177:LEU:HD12	3:C:254:CYS:SG	2.42	0.59
1:F:104:ARG:HG2	1:F:137:PRO:HG2	1.84	0.59
1:F:111:THR:HG22	3:H:85:ILE:HG12	1.85	0.59
2:G:42:LEU:HD13	2:G:72:VAL:CG2	2.32	0.59
3:C:270:LYS:HE3	3:C:319:PRO:HG3	1.85	0.58
3:C:311:HIS:HB2	3:C:326:THR:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:42:LEU:HD13	2:G:72:VAL:HG22	1.85	0.58
3:C:132:LEU:HD11	3:C:138:LEU:HB3	1.86	0.58
2:B:25:HIS:CE1	2:B:34:VAL:HB	2.38	0.58
3:H:29:LEU:HD12	3:H:156:GLU:HG3	1.85	0.58
4:D:221:PRO:HB3	4:D:264:MET:HG3	1.86	0.58
4:I:98:CYS:SG	4:I:186:LEU:HD13	2.44	0.57
4:I:196:LEU:HD11	4:I:235:MET:HG3	1.86	0.57
1:A:218:MET:HA	1:F:198:HIS:HD2	1.68	0.57
1:F:77:SER:HB2	3:H:96:PRO:HB2	1.87	0.57
3:H:24:ASN:ND2	3:H:114:LEU:HD21	2.20	0.57
4:D:111:GLU:HB2	4:D:287:PRO:HA	1.86	0.57
4:D:99:LEU:HD21	4:D:128:ILE:HG13	1.87	0.57
3:C:23:ARG:HE	5:E:315:LEU:HG	1.69	0.57
3:H:367:LYS:HG2	4:I:316:LEU:HD22	1.85	0.57
4:I:229:THR:H	4:I:232:MET:HE2	1.70	0.57
3:H:63:ALA:HA	3:H:174:LEU:HD22	1.86	0.56
3:H:22:VAL:HB	3:H:37:ILE:HD11	1.87	0.56
4:I:146:LEU:HD12	4:I:166:LEU:HG	1.87	0.56
3:C:189:LEU:HD21	5:E:318:LYS:HD2	1.88	0.56
4:D:128:ILE:HG22	4:D:170:LEU:HD11	1.86	0.56
4:D:310:HIS:HB3	5:E:282:PHE:CZ	2.41	0.56
3:H:220:TYR:HE1	5:J:323:PRO:HB3	1.70	0.56
3:H:59:HIS:CD2	3:H:68:LYS:HD2	2.41	0.56
1:A:282:GLN:O	1:A:285:ARG:HG2	2.06	0.55
1:A:294:LEU:HD21	5:E:287:VAL:HG11	1.88	0.55
2:G:42:LEU:CD2	2:G:70:ARG:HH21	2.19	0.55
2:B:106:ARG:O	2:B:109:GLU:HG3	2.06	0.55
1:A:104:ARG:HG3	1:A:137:PRO:HG2	1.87	0.55
3:C:114:LEU:O	3:C:118:LYS:HG3	2.06	0.54
1:F:146:THR:HA	2:G:171:THR:HG22	1.89	0.54
4:D:124:SER:HA	4:D:127:MET:HE2	1.89	0.54
3:H:168:GLU:HA	3:H:210:THR:HB	1.89	0.54
4:I:293:ASN:O	4:I:297:LYS:HG3	2.07	0.54
1:F:25:THR:HG22	1:F:27:SER:H	1.71	0.54
3:H:350:SER:HB3	3:H:353:TRP:CD2	2.43	0.54
1:A:194:ALA:O	1:A:197:THR:HG22	2.08	0.54
2:G:34:VAL:HG22	2:G:123:SER:HB3	1.90	0.54
3:H:177:LEU:HD23	3:H:257:LEU:HD22	1.89	0.54
4:D:100:ASP:HB3	4:D:217:TYR:HA	1.89	0.54
3:H:132:LEU:HD11	3:H:138:LEU:HB3	1.90	0.54
3:H:330:VAL:HA	4:I:130:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:357:GLU:O	3:H:361:ARG:HG2	2.07	0.53
4:I:93:GLU:HG2	4:I:95:VAL:HG22	1.90	0.53
3:C:275:ILE:HG13	3:C:294:PHE:HB3	1.88	0.53
3:C:10:ILE:HG13	3:C:40:LEU:HD21	1.89	0.53
1:A:148:ARG:HH11	2:B:167:ARG:HH21	1.57	0.53
3:H:56:PHE:CZ	3:H:71:ILE:HD12	2.43	0.53
1:F:145:SER:HA	2:G:216:ILE:HG22	1.89	0.53
2:G:25:HIS:NE2	2:G:34:VAL:HB	2.24	0.53
3:C:282:PHE:HA	4:D:315:LEU:HD13	1.91	0.53
4:D:107:LEU:HG	4:D:109:LYS:HG2	1.92	0.53
3:H:287:VAL:HG13	4:I:300:ALA:HA	1.91	0.53
4:D:302:PRO:HA	4:D:305:ARG:HD3	1.92	0.52
2:B:230:GLU:O	2:B:234:GLU:HG2	2.09	0.52
3:C:145:LEU:HD11	3:C:246:LEU:HD23	1.91	0.52
3:C:301:LEU:HD21	4:D:315:LEU:HD12	1.92	0.52
3:C:91:GLU:HG3	3:C:127:PHE:HZ	1.75	0.52
3:H:209:ASP:HB2	3:H:214:GLN:HG2	1.91	0.52
3:C:309:LEU:HD13	3:C:328:GLN:NE2	2.24	0.52
2:G:42:LEU:HD21	2:G:70:ARG:HE	1.75	0.52
5:J:306:SER:HA	5:J:309:MET:HE3	1.92	0.52
4:I:87:PRO:HB2	4:I:89:VAL:HG23	1.91	0.52
4:I:94:LYS:HZ2	4:I:209:TYR:HB2	1.75	0.52
1:A:38:LYS:HD2	1:A:60:ASP:OD2	2.11	0.51
2:B:13:HIS:CD2	2:B:71:ILE:HG21	2.45	0.51
3:C:330:VAL:HA	4:D:130:MET:HE2	1.92	0.51
2:G:152:LEU:HA	2:G:171:THR:O	2.10	0.51
2:B:237:LYS:HG2	2:B:241:GLN:HE21	1.75	0.51
1:A:243:LEU:HD12	2:B:298:LEU:HD12	1.91	0.51
2:B:22:CYS:SG	2:B:77:VAL:HG11	2.50	0.51
3:C:70:ASP:HB2	3:C:85:ILE:HB	1.93	0.51
3:C:113:LEU:O	3:C:117:VAL:HG23	2.11	0.51
3:C:177:LEU:HD21	3:C:203:LEU:HB2	1.93	0.51
5:J:296:ILE:O	5:J:299:GLN:HG2	2.11	0.51
3:C:237:ILE:HG23	5:E:324:VAL:HG11	1.93	0.50
4:I:233:LYS:O	4:I:237:GLN:HG2	2.11	0.50
2:B:125:PRO:O	2:B:126:HIS:HB2	2.11	0.50
4:I:228:LEU:HD12	4:I:228:LEU:H	1.76	0.50
1:A:63:LYS:HG3	2:B:289:ASP:OD2	2.12	0.50
3:C:29:LEU:HD22	3:C:176:LYS:HE3	1.93	0.50
3:H:193:ASN:HA	5:J:314:LEU:HD21	1.93	0.50
3:H:328:GLN:HG3	3:H:340:TYR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:O	1:A:196:GLN:HG2	2.11	0.50
1:A:224:GLU:HA	1:A:227:LYS:HE2	1.93	0.50
2:B:167:ARG:HD3	2:B:169:LEU:HD11	1.93	0.50
3:H:40:LEU:HG	3:H:53:CYS:HB3	1.93	0.50
1:A:31:GLY:HA3	1:A:100:TYR:CZ	2.47	0.50
3:C:289:TYR:HB3	3:C:297:LEU:HD13	1.93	0.50
3:C:333:PHE:HZ	4:D:130:MET:HB2	1.76	0.50
3:H:223:PRO:HD3	5:J:320:PHE:HA	1.94	0.50
4:I:111:GLU:HB3	4:I:287:PRO:HA	1.94	0.49
3:C:59:HIS:CE1	3:C:68:LYS:HG2	2.48	0.49
2:G:238:ILE:HG13	2:G:239:LEU:N	2.28	0.49
4:I:249:HIS:CE1	4:I:281:GLU:HB2	2.42	0.49
4:I:135:LYS:HG2	4:I:142:HIS:HD2	1.76	0.49
3:H:56:PHE:HE1	3:H:73:PHE:HE2	1.59	0.49
3:H:70:ASP:HB3	3:H:85:ILE:HB	1.94	0.49
3:C:170:SER:HA	3:C:207:PHE:O	2.13	0.49
1:F:42:LYS:HE2	1:F:44:SER:HB2	1.95	0.49
2:G:11:ALA:HB3	2:G:71:ILE:HG22	1.95	0.49
3:H:127:PHE:CZ	3:H:131:ARG:HD2	2.47	0.49
5:J:294:LYS:HA	5:J:297:LEU:HD12	1.93	0.49
3:C:33:ASN:HB2	3:C:61:PRO:HB3	1.95	0.49
4:D:236:PHE:HD1	4:D:272:ASP:HB2	1.77	0.49
3:C:333:PHE:CZ	4:D:130:MET:HB2	2.48	0.49
1:A:250:LEU:O	1:A:254:ILE:HG13	2.13	0.48
1:A:140:ILE:HD11	1:A:148:ARG:CZ	2.43	0.48
3:C:174:LEU:HD11	3:C:202:LEU:HB3	1.95	0.48
3:C:284:THR:HB	4:D:311:ALA:HA	1.95	0.48
3:C:287:VAL:HG13	4:D:300:ALA:HA	1.95	0.48
3:H:73:PHE:CD1	3:H:82:PRO:HB3	2.47	0.48
3:C:43:GLY:HA3	3:C:55:ARG:NH1	2.29	0.48
1:F:118:HIS:CD2	1:F:156:PRO:HD2	2.48	0.48
4:I:278:TYR:CE2	4:I:305:ARG:HD2	2.49	0.48
3:C:327:PHE:HB2	3:C:344:GLN:HE22	1.77	0.48
3:H:14:LEU:HD11	3:H:75:ALA:HA	1.94	0.48
3:H:313:ASP:HB3	3:H:324:THR:HB	1.94	0.48
3:H:83:ASP:OD1	3:H:84:PHE:N	2.46	0.48
3:H:241:PRO:HG2	3:H:244:GLY:HA3	1.94	0.48
4:I:223:GLN:N	4:I:224:PRO:HD3	2.29	0.48
1:A:110:MET:HE1	1:A:156:PRO:HG3	1.96	0.48
2:B:235:LEU:HB3	2:B:236:PRO:HD3	1.95	0.48
1:F:34:LEU:HD21	1:F:92:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:GLN:O	3:C:147:GLU:HG3	2.14	0.48
3:H:272:ARG:CZ	5:J:300:LEU:HD13	2.44	0.48
4:D:100:ASP:HA	4:D:149:VAL:HB	1.96	0.48
3:H:7:LEU:HD22	5:J:315:LEU:HD21	1.95	0.47
4:D:129:GLU:O	4:D:133:ARG:HG3	2.14	0.47
4:D:187:PHE:HD2	4:D:232:MET:HE3	1.79	0.47
4:D:256:GLU:HG3	4:D:260:SER:HB2	1.94	0.47
2:G:233:VAL:O	2:G:236:PRO:HD2	2.14	0.47
1:F:215:ILE:HG13	2:G:272:LEU:HD23	1.96	0.47
2:G:86:ARG:CZ	2:G:89:ARG:HG2	2.44	0.47
4:I:128:ILE:O	4:I:132:VAL:HG23	2.15	0.47
4:D:146:LEU:HD22	4:D:156:LEU:HB2	1.95	0.47
2:G:33:GLU:HB2	2:G:82:ARG:NH1	2.28	0.47
2:G:131:PRO:HG2	2:G:211:ARG:HD2	1.95	0.47
4:I:150:ASN:C	4:I:152:ASP:H	2.23	0.47
1:A:214:LYS:HD3	1:F:201:LYS:HB3	1.95	0.47
1:A:258:ARG:O	1:A:262:ILE:HG13	2.15	0.47
3:C:219:LEU:HD21	3:C:257:LEU:HD21	1.97	0.47
5:J:306:SER:O	5:J:309:MET:HG2	2.15	0.47
1:A:214:LYS:O	1:A:217:GLU:HG2	2.15	0.47
3:C:91:GLU:HG3	3:C:127:PHE:CZ	2.50	0.47
4:I:139:ASP:HB3	4:I:142:HIS:CD2	2.49	0.47
3:H:260:LYS:HE2	3:H:264:VAL:HG21	1.95	0.47
3:C:339:LEU:HD23	4:D:130:MET:HE1	1.96	0.46
5:J:289:PRO:O	5:J:293:THR:HG23	2.16	0.46
4:I:93:GLU:H	4:I:142:HIS:CE1	2.32	0.46
4:D:214:ILE:HG22	4:D:244:ASP:HB2	1.97	0.46
3:H:246:LEU:O	3:H:250:VAL:HG23	2.16	0.46
4:D:101:LEU:HB3	4:D:150:ASN:HD21	1.81	0.46
3:H:92:PHE:O	3:H:94:PRO:HD3	2.15	0.46
3:H:137:ARG:O	3:H:141:GLU:HG2	2.15	0.46
4:I:248:ILE:HG22	4:I:284:LEU:HG	1.96	0.46
1:A:25:THR:HG22	1:A:27:SER:H	1.80	0.46
3:H:91:GLU:HG3	3:H:127:PHE:CZ	2.49	0.46
3:H:303:TRP:HB3	3:H:306:PHE:HB3	1.96	0.46
3:H:24:ASN:HD21	3:H:114:LEU:HD11	1.81	0.46
3:H:35:LEU:HD23	3:H:61:PRO:HD2	1.96	0.46
3:H:281:HIS:O	3:H:282:PHE:HD1	1.98	0.46
4:I:136:HIS:HE1	4:I:161:SER:HB3	1.80	0.46
4:I:301:HIS:CD2	4:I:303:LEU:HB2	2.51	0.46
3:H:36:ARG:HB2	3:H:59:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:212:ARG:HD3	4:D:302:PRO:HG3	1.98	0.46
1:F:130:LEU:N	1:F:157:GLN:HE22	2.14	0.46
3:H:54:ASP:O	3:H:73:PHE:HD2	1.99	0.46
4:I:121:LEU:HD11	4:I:173:LEU:HD23	1.98	0.46
4:I:124:SER:O	4:I:128:ILE:HG12	2.16	0.45
4:I:207:PRO:HB3	4:I:240:TYR:CZ	2.51	0.45
4:I:260:SER:H	4:I:262:LYS:HE2	1.80	0.45
4:D:150:ASN:C	4:D:152:ASP:H	2.24	0.45
1:F:5:SER:HA	1:F:57:TYR:HB2	1.97	0.45
4:I:119:ASN:HD21	4:I:121:LEU:HB3	1.81	0.45
3:H:299:LEU:HB2	3:H:310:VAL:CG1	2.46	0.45
3:C:17:PHE:O	3:C:21:VAL:HG23	2.16	0.45
4:D:148:VAL:HG22	4:D:154:ALA:O	2.17	0.45
3:H:376:ALA:HA	3:H:379:ALA:HB3	1.97	0.45
4:I:279:LYS:HB2	4:I:279:LYS:HE3	1.72	0.45
3:C:303:TRP:HA	3:C:303:TRP:CE3	2.51	0.45
4:I:132:VAL:HG21	4:I:166:LEU:HD22	1.98	0.45
4:D:107:LEU:HD12	4:D:108:PRO:HD2	1.98	0.45
3:C:246:LEU:HD12	3:C:246:LEU:HA	1.80	0.45
3:H:54:ASP:OD1	3:H:55:ARG:HG3	2.17	0.45
3:H:210:THR:HG23	3:H:211:GLU:HG3	1.99	0.45
2:B:81:ARG:HH12	2:B:241:GLN:HB3	1.81	0.45
2:G:143:GLN:HG3	2:G:147:GLN:HA	1.99	0.45
4:I:186:LEU:HD23	4:I:215:LEU:HD22	1.97	0.45
1:F:43:ASN:HB2	1:F:51:ASP:HB3	1.98	0.45
1:F:71:PHE:HZ	1:F:113:ARG:HH11	1.65	0.45
3:H:146:LEU:HA	3:H:152:GLY:HA3	1.99	0.45
4:D:269:GLY:HA3	4:D:279:LYS:HD3	1.98	0.44
5:J:292:TYR:O	5:J:296:ILE:HG12	2.17	0.44
1:A:89:LEU:HD22	1:A:92:VAL:HG21	1.99	0.44
1:A:221:SER:O	1:A:225:GLU:HG2	2.17	0.44
2:G:219:VAL:HG22	3:H:47:LEU:HD21	1.98	0.44
3:H:7:LEU:HD12	3:H:10:ILE:HD11	1.99	0.44
5:J:296:ILE:O	5:J:300:LEU:HG	2.17	0.44
1:A:254:ILE:HG12	2:B:312:LEU:HD13	1.99	0.44
2:G:87:LYS:O	2:G:88:ASP:C	2.60	0.44
3:H:111:GLU:OE1	3:H:114:LEU:HD23	2.17	0.44
4:D:101:LEU:HB3	4:D:150:ASN:ND2	2.32	0.44
2:G:234:GLU:O	2:G:238:ILE:HG23	2.17	0.44
3:H:271:ARG:HD2	3:H:294:PHE:HB2	1.99	0.44
4:I:295:MET:HE3	4:I:295:MET:HB3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HE3	1:A:86:LYS:HB2	1.81	0.44
1:A:262:ILE:HG22	1:A:266:ARG:HE	1.83	0.44
2:B:93:SER:HB2	2:B:95:GLU:HG2	2.00	0.44
3:H:7:LEU:O	3:H:10:ILE:HG12	2.18	0.44
3:H:118:LYS:O	3:H:121:VAL:HG12	2.18	0.44
2:B:120:TRP:H	2:B:120:TRP:CD1	2.35	0.44
4:D:147:VAL:HG22	4:D:155:TRP:CD1	2.53	0.44
1:F:148:ARG:HD2	2:G:167:ARG:HH11	1.83	0.44
1:A:201:LYS:HE2	1:A:201:LYS:HB3	1.78	0.44
1:A:230:CYS:O	1:A:234:GLU:HG2	2.18	0.44
1:F:139:ILE:HG23	1:F:147:HIS:CD2	2.53	0.44
4:I:250:ASN:HA	4:I:284:LEU:HB2	2.00	0.44
4:D:109:LYS:HB3	4:D:285:ALA:HA	2.00	0.43
1:A:6:THR:O	1:A:6:THR:CG2	2.66	0.43
3:C:27:VAL:HG11	3:C:117:VAL:HG12	2.00	0.43
3:H:32:THR:HG23	5:J:320:PHE:HB2	2.00	0.43
1:F:33:LEU:HD11	1:F:100:TYR:HB3	2.00	0.43
2:G:272:LEU:O	2:G:276:MET:HG3	2.18	0.43
2:B:264:ASN:HA	2:B:267:VAL:HG22	2.00	0.43
1:F:62:GLN:HE21	1:F:62:GLN:HB2	1.66	0.43
1:A:177:LEU:HD12	1:F:177:LEU:HD22	2.00	0.43
1:A:180:LYS:HG3	2:B:263:HIS:CE1	2.54	0.43
5:E:280:ILE:HD12	5:E:280:ILE:H	1.83	0.43
1:A:158:LYS:HE2	1:A:158:LYS:HB3	1.83	0.43
4:I:302:PRO:HA	4:I:305:ARG:HD3	2.01	0.43
2:B:33:GLU:HB2	2:B:82:ARG:NH1	2.34	0.43
2:B:81:ARG:HH22	2:B:241:GLN:CD	2.26	0.43
2:B:90:VAL:HG21	2:B:120:TRP:CZ3	2.54	0.43
3:C:366:PHE:O	3:C:370:VAL:HG23	2.19	0.43
4:D:149:VAL:HG22	4:D:153:THR:HG22	2.01	0.43
3:H:248:ASP:O	3:H:251:PRO:HD2	2.19	0.43
4:I:155:TRP:HZ2	4:I:190:ILE:HG23	1.82	0.43
2:B:118:VAL:O	2:B:149:PHE:HA	2.18	0.43
4:D:129:GLU:HG3	4:D:167:CYS:SG	2.58	0.43
4:D:246:VAL:HG21	4:D:298:LEU:HD11	2.00	0.43
2:G:229:LEU:HG	2:G:229:LEU:O	2.19	0.43
2:B:10:GLN:O	2:B:215:PRO:HD2	2.19	0.43
3:C:158:TYR:O	3:C:171:ALA:HA	2.19	0.43
2:G:120:TRP:H	2:G:120:TRP:CD1	2.37	0.43
3:H:192:VAL:HG22	3:H:193:ASN:H	1.84	0.43
1:A:299:MET:SD	5:E:280:ILE:HG12	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:162:ASP:HB3	4:I:165:GLU:HG3	2.00	0.43
2:G:145:MET:HE2	2:G:145:MET:HB3	1.88	0.42
1:F:247:VAL:N	2:G:305:LYS:HZ1	2.17	0.42
2:G:42:LEU:HD21	2:G:70:ARG:NH2	2.32	0.42
2:G:132:SER:O	2:G:135:ASP:HB2	2.19	0.42
2:G:158:ILE:O	2:G:167:ARG:HG2	2.18	0.42
4:I:91:CYS:SG	4:I:210:VAL:HG23	2.59	0.42
1:A:224:GLU:HA	1:A:227:LYS:CE	2.49	0.42
3:C:127:PHE:CZ	3:C:131:ARG:HD3	2.55	0.42
3:C:355:GLY:C	3:C:357:GLU:H	2.25	0.42
3:H:132:LEU:HD21	3:H:142:TYR:HB2	2.01	0.42
3:C:162:LYS:HD3	3:C:169:PHE:CD1	2.54	0.42
4:I:126:LYS:HD3	4:I:126:LYS:HA	1.91	0.42
3:H:149:PRO:O	3:H:153:GLU:HG2	2.19	0.42
3:C:177:LEU:HA	3:C:178:PRO:HD3	1.84	0.42
4:I:208:PRO:HB2	4:I:209:TYR:CD1	2.55	0.42
1:A:111:THR:HG22	3:C:85:ILE:HG12	2.01	0.42
4:D:301:HIS:CE1	4:D:303:LEU:HB2	2.55	0.42
3:C:13:MET:SD	3:C:78:PRO:HG3	2.59	0.42
3:H:56:PHE:CE1	3:H:73:PHE:HE2	2.38	0.42
4:D:274:LYS:HB2	4:D:274:LYS:HE3	1.83	0.42
2:G:152:LEU:HD12	2:G:152:LEU:H	1.85	0.42
3:H:308:PHE:HA	3:H:328:GLN:O	2.19	0.42
1:F:148:ARG:HG3	2:G:169:LEU:HG	2.01	0.41
2:G:75:HIS:HB2	2:G:115:MET:HE3	2.02	0.41
1:A:234:GLU:CD	2:B:226:LYS:HD3	2.45	0.41
2:B:233:VAL:O	2:B:236:PRO:HD2	2.20	0.41
3:H:188:LEU:HD12	3:H:292:GLU:HB3	2.01	0.41
5:J:304:GLN:O	5:J:308:LYS:HG3	2.21	0.41
4:I:135:LYS:HB3	4:I:144:PHE:HZ	1.85	0.41
1:A:147:HIS:HB2	2:B:170:TYR:CZ	2.56	0.41
1:F:89:LEU:HB3	1:F:92:VAL:HG11	2.02	0.41
3:H:54:ASP:HB3	3:H:75:ALA:HB2	2.02	0.41
2:B:135:ASP:O	2:B:138:THR:N	2.54	0.41
1:F:158:LYS:HD2	1:F:162:HIS:HE1	1.85	0.41
2:G:90:VAL:CG1	2:G:120:TRP:HZ3	2.33	0.41
3:H:306:PHE:CE2	3:H:308:PHE:HB3	2.55	0.41
4:I:183:LEU:HD12	4:I:183:LEU:H	1.85	0.41
1:A:158:LYS:HB2	1:A:162:HIS:ND1	2.35	0.41
1:F:231:LYS:HA	1:F:234:GLU:HB2	2.02	0.41
2:G:38:CYS:HB3	2:G:74:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:26:LYS:HA	3:H:35:LEU:HD21	2.01	0.41
3:H:198:GLU:HB3	5:J:312:ARG:NH1	2.35	0.41
4:I:245:VAL:O	4:I:279:LYS:HA	2.21	0.41
3:H:353:TRP:CZ3	3:H:361:ARG:HG3	2.55	0.41
3:H:356:ASN:OD1	3:H:357:GLU:N	2.54	0.41
3:H:357:GLU:HA	3:H:360:LYS:HG2	2.03	0.41
4:I:136:HIS:CE1	4:I:161:SER:HB3	2.56	0.41
4:D:128:ILE:HD13	4:D:128:ILE:HA	1.83	0.41
4:D:181:PHE:CG	4:D:219:ARG:HG3	2.54	0.41
1:F:139:ILE:HG23	1:F:147:HIS:HD2	1.86	0.41
2:G:39:ILE:HD11	2:G:76:SER:HB2	2.02	0.41
3:H:17:PHE:O	3:H:21:VAL:HG23	2.21	0.41
4:I:148:VAL:HG23	4:I:154:ALA:HB3	2.02	0.41
4:I:207:PRO:HA	4:I:208:PRO:HD3	1.97	0.41
1:A:34:LEU:HB2	1:A:63:LYS:HB3	2.03	0.41
1:A:11:SER:HB2	1:A:14:VAL:HG23	2.03	0.41
3:C:299:LEU:HB2	3:C:310:VAL:CG2	2.49	0.41
4:D:234:LYS:HB2	4:D:234:LYS:HE3	1.84	0.41
2:G:122:HIS:HE1	2:G:135:ASP:OD1	2.04	0.41
2:G:130:TRP:O	2:G:131:PRO:C	2.63	0.41
2:G:235:LEU:O	2:G:238:ILE:HG12	2.20	0.41
3:H:13:MET:SD	3:H:78:PRO:HG2	2.60	0.41
3:H:303:TRP:CG	3:H:304:LYS:N	2.89	0.41
3:C:40:LEU:HG	3:C:53:CYS:HB3	2.03	0.41
3:C:92:PHE:CZ	3:C:94:PRO:HG3	2.56	0.41
3:C:105:TRP:HE1	3:C:107:PRO:HB3	1.86	0.41
4:D:155:TRP:CH2	4:D:159:LEU:HG	2.56	0.41
4:D:187:PHE:HA	4:D:190:ILE:HD12	2.03	0.41
2:G:42:LEU:HD13	2:G:72:VAL:HG23	2.02	0.41
3:H:48:THR:HA	3:H:49:PRO:HD2	1.94	0.41
1:A:23:LEU:HD13	2:B:218:ILE:HG21	2.04	0.40
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.95	0.40
1:A:320:VAL:HG23	1:A:323:LEU:HD12	2.03	0.40
2:G:14:LEU:HD23	2:G:19:PHE:HB2	2.03	0.40
3:H:24:ASN:OD1	3:H:25:GLY:N	2.54	0.40
1:A:229:ILE:HD12	1:A:229:ILE:HA	1.94	0.40
3:C:280:SER:HB2	5:E:296:ILE:HD12	2.03	0.40
1:A:185:SER:HB3	1:A:187:MET:HE1	2.04	0.40
2:B:261:LYS:HE3	2:B:261:LYS:HB2	1.92	0.40
3:C:57:LYS:HG3	3:C:70:ASP:OD1	2.21	0.40
4:D:121:LEU:HD11	4:D:173:LEU:HD23	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:207:PRO:HB3	4:D:240:TYR:CE2	2.57	0.40
1:F:33:LEU:HD22	1:F:61:ILE:HG21	2.03	0.40
2:G:131:PRO:HB3	2:G:173:PHE:CZ	2.56	0.40
4:I:222:CYS:SG	4:I:223:GLN:N	2.93	0.40
4:D:105:MET:C	4:D:107:LEU:H	2.29	0.40
4:D:187:PHE:CZ	4:D:236:PHE:HZ	2.39	0.40
1:F:130:LEU:H	1:F:157:GLN:HE22	1.69	0.40
5:J:314:LEU:HD12	5:J:314:LEU:HA	1.85	0.40
1:A:234:GLU:OE2	2:B:226:LYS:HA	2.22	0.40
1:F:80:VAL:O	1:F:80:VAL:CG1	2.66	0.40
1:F:118:HIS:CE1	1:F:130:LEU:HB3	2.57	0.40
2:G:290:ARG:HD2	2:G:293:GLN:CD	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/409 (74%)	282 (93%)	21 (7%)	0	100	100
1	F	256/409 (63%)	245 (96%)	11 (4%)	0	100	100
2	B	253/316 (80%)	244 (96%)	9 (4%)	0	100	100
2	G	250/316 (79%)	240 (96%)	10 (4%)	0	100	100
3	C	379/383 (99%)	352 (93%)	27 (7%)	0	100	100
3	H	381/383 (100%)	358 (94%)	22 (6%)	1 (0%)	36	66
4	D	235/349 (67%)	218 (93%)	17 (7%)	0	100	100
4	I	235/349 (67%)	213 (91%)	21 (9%)	1 (0%)	30	59
5	E	56/171 (33%)	55 (98%)	1 (2%)	0	100	100
5	J	56/171 (33%)	55 (98%)	1 (2%)	0	100	100
All	All	2404/3256 (74%)	2262 (94%)	140 (6%)	2 (0%)	49	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	51	PRO
4	I	224	PRO

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	A	281/373 (75%)	278 (99%)	3 (1%)	65	75
1	F	233/373 (62%)	232 (100%)	1 (0%)	84	84
2	B	235/286 (82%)	232 (99%)	3 (1%)	61	73
2	G	233/286 (82%)	226 (97%)	7 (3%)	36	59
3	C	335/337 (99%)	330 (98%)	5 (2%)	57	71
3	H	337/337 (100%)	335 (99%)	2 (1%)	78	81
4	D	219/305 (72%)	216 (99%)	3 (1%)	59	72
4	I	219/305 (72%)	215 (98%)	4 (2%)	51	69
5	E	52/150 (35%)	52 (100%)	0	100	100
5	J	52/150 (35%)	52 (100%)	0	100	100
All	All	2196/2902 (76%)	2168 (99%)	28 (1%)	59	73

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	A	237	GLU
1	A	295	HIS
2	B	136	VAL
2	B	176	ILE
2	B	212	ILE
3	C	38	THR
3	C	55	ARG
3	C	211	GLU
3	C	358	MET

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Mol	Chain	Res	Type
3	C	363	LYS
4	D	156	LEU
4	D	214	ILE
4	D	225	GLN
1	F	18	LEU
2	G	77	VAL
2	G	90	VAL
2	G	103	GLU
2	G	135	ASP
2	G	152	LEU
2	G	224	ILE
2	G	257	ASP
3	H	51	PRO
3	H	91	GLU
4	I	95	VAL
4	I	245	VAL
4	I	258	GLU
4	I	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	62	GLN
1	A	120	ASN
1	A	176	GLN
1	A	196	GLN
1	A	198	HIS
1	A	223	GLN
2	B	143	GLN
2	B	147	GLN
2	B	217	HIS
2	B	241	GLN
2	B	285	GLN
3	C	123	GLN
3	C	128	GLN
3	C	150	GLN
3	C	154	ASN
3	C	193	ASN
3	C	311	HIS
3	C	342	GLN
3	C	344	GLN

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Mol	Chain	Res	Type
4	D	83	GLN
4	D	250	ASN
1	F	62	GLN
1	F	105	HIS
1	F	118	HIS
1	F	151	HIS
1	F	157	GLN
1	F	198	HIS
2	G	13	HIS
2	G	43	ASN
2	G	143	GLN
3	H	74	ASN
3	H	164	ASN
3	H	255	HIS
3	H	311	HIS
3	H	344	GLN
5	J	275	ASN
4	I	125	GLN
4	I	136	HIS
4	I	249	HIS
4	I	301	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

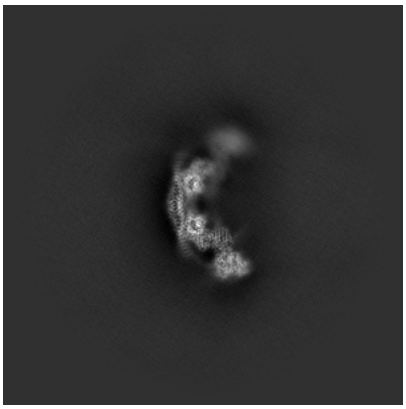
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55040. These allow visual inspection of the internal detail of the map and identification of artifacts.

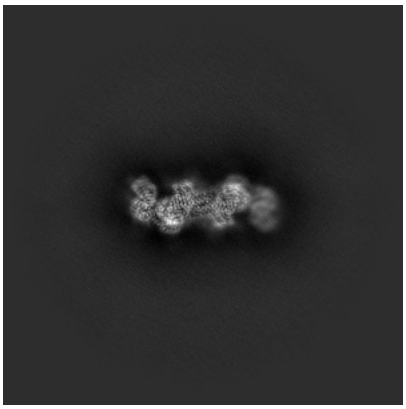
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

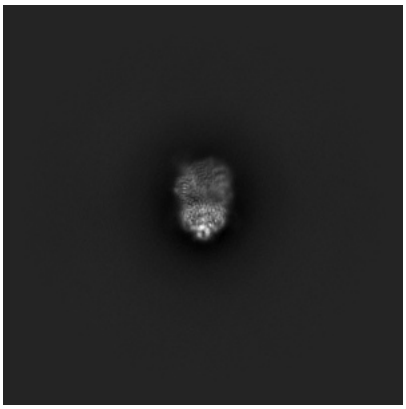
6.1.1 Primary map



X

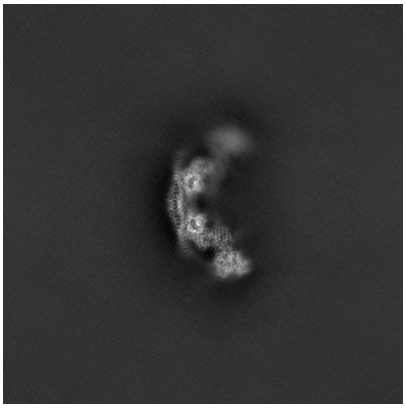


Y

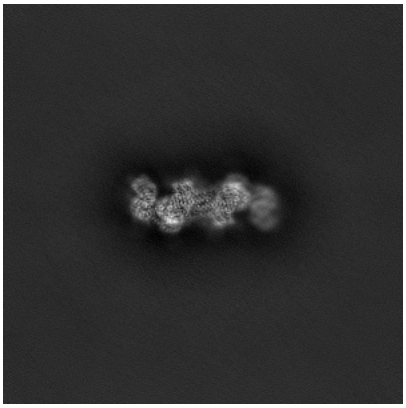


Z

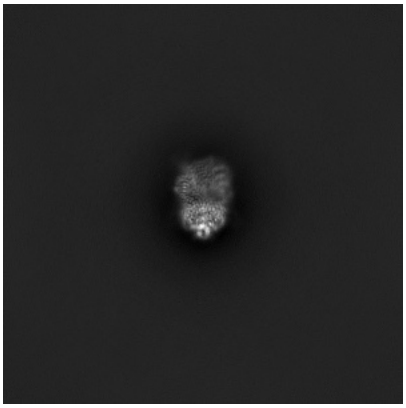
6.1.2 Raw map



X



Y

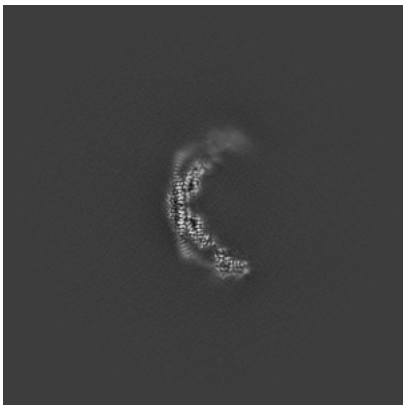


Z

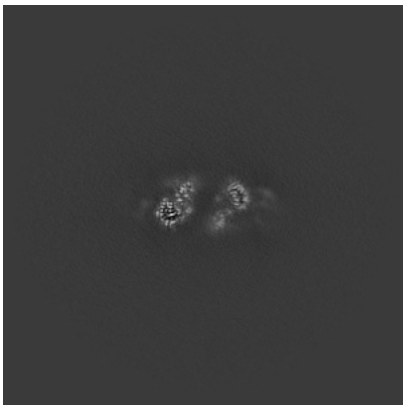
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

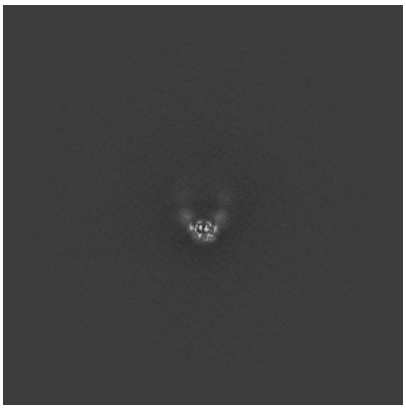
6.2.1 Primary map



X Index: 216

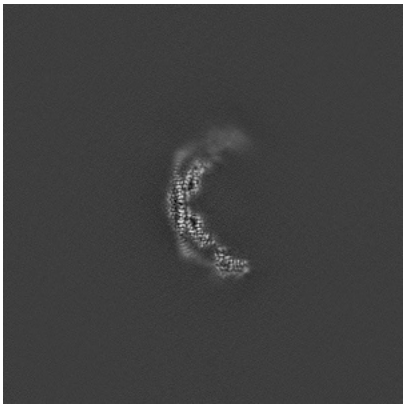


Y Index: 216

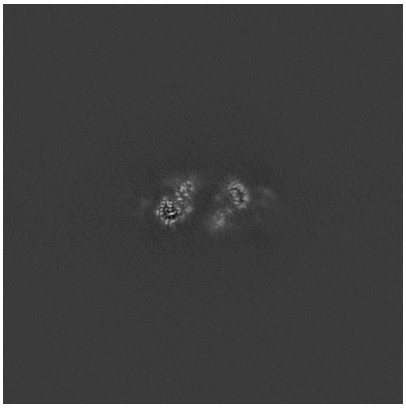


Z Index: 216

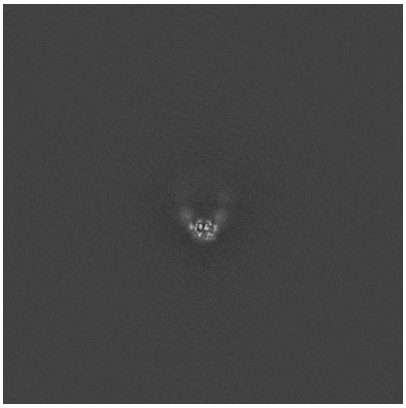
6.2.2 Raw map



X Index: 216



Y Index: 216

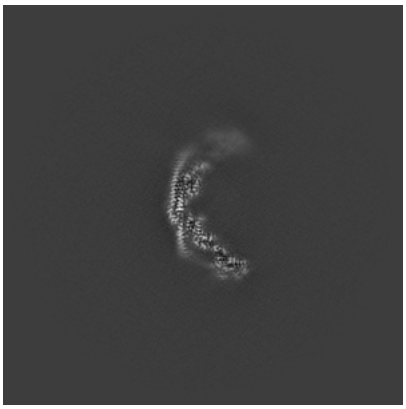


Z Index: 216

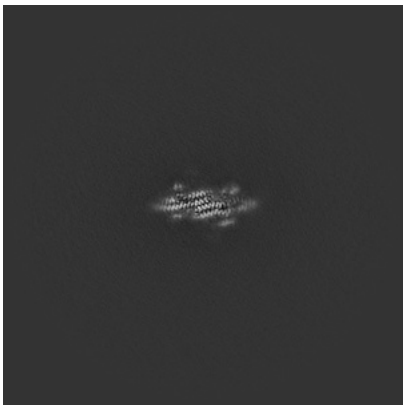
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

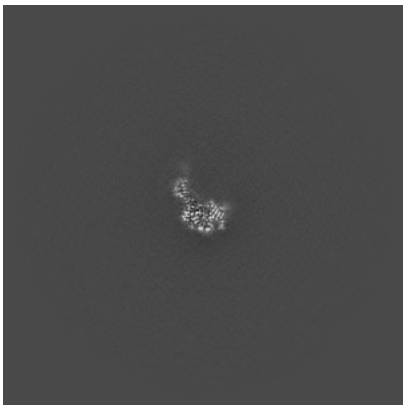
6.3.1 Primary map



X Index: 213

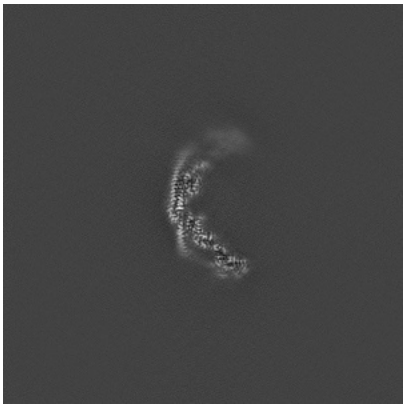


Y Index: 191

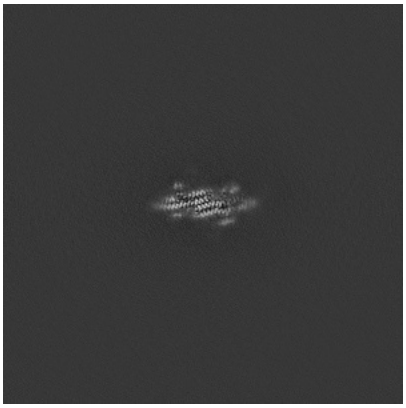


Z Index: 187

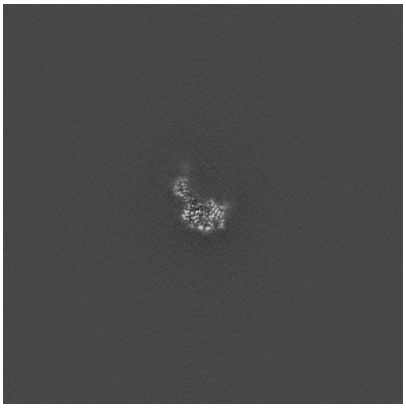
6.3.2 Raw map



X Index: 213



Y Index: 191

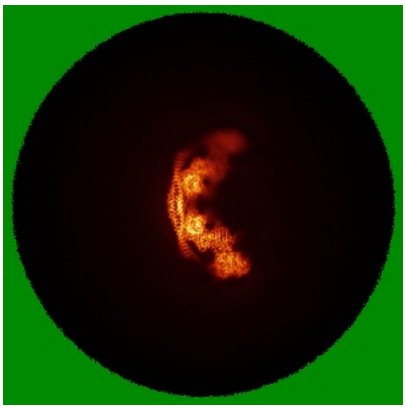


Z Index: 187

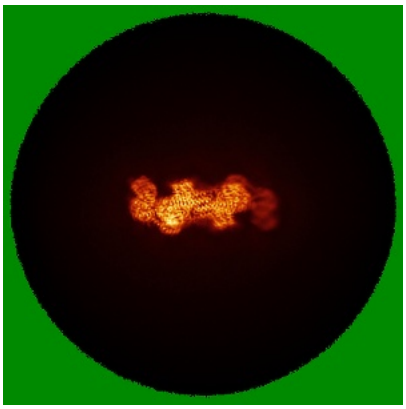
The images above show the largest variance slices of the map in three orthogonal directions.

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

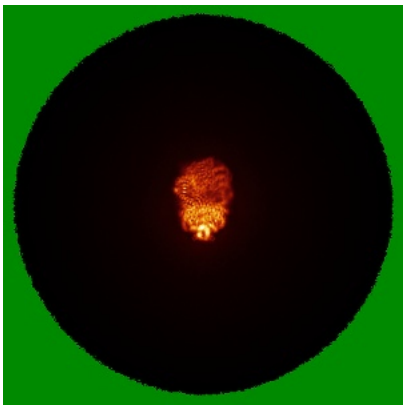
6.4.1 Primary map



X

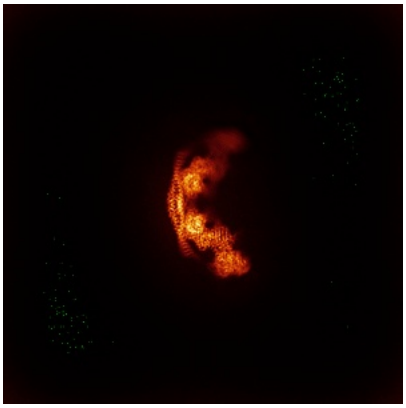


Y

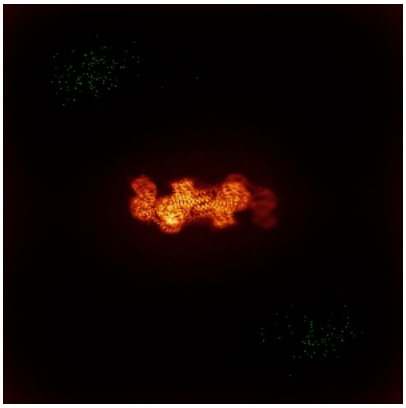


Z

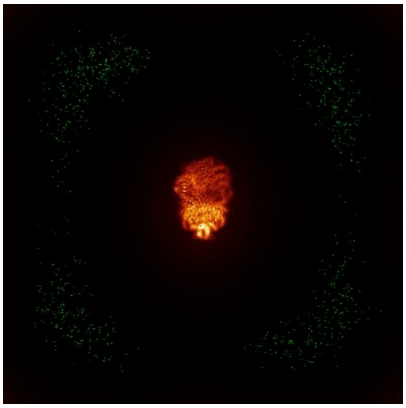
6.4.2 Raw map



X



Y

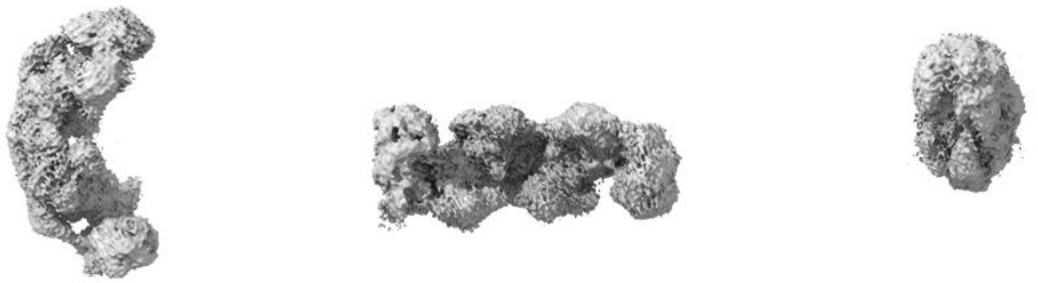


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

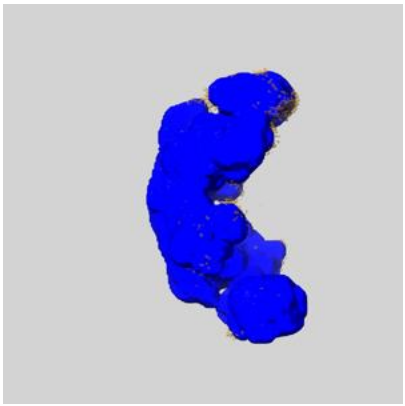
6.6 Mask visualisation (i)

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

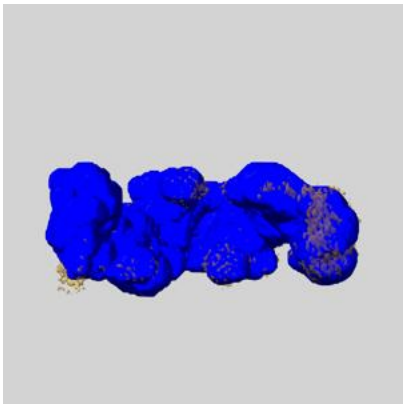
A mask typically either:

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

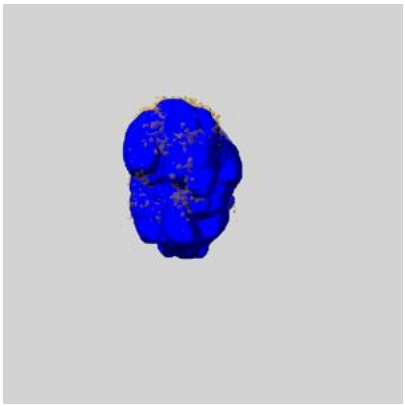
6.6.1 emd_55040_msk_1.map (i)



X



Y

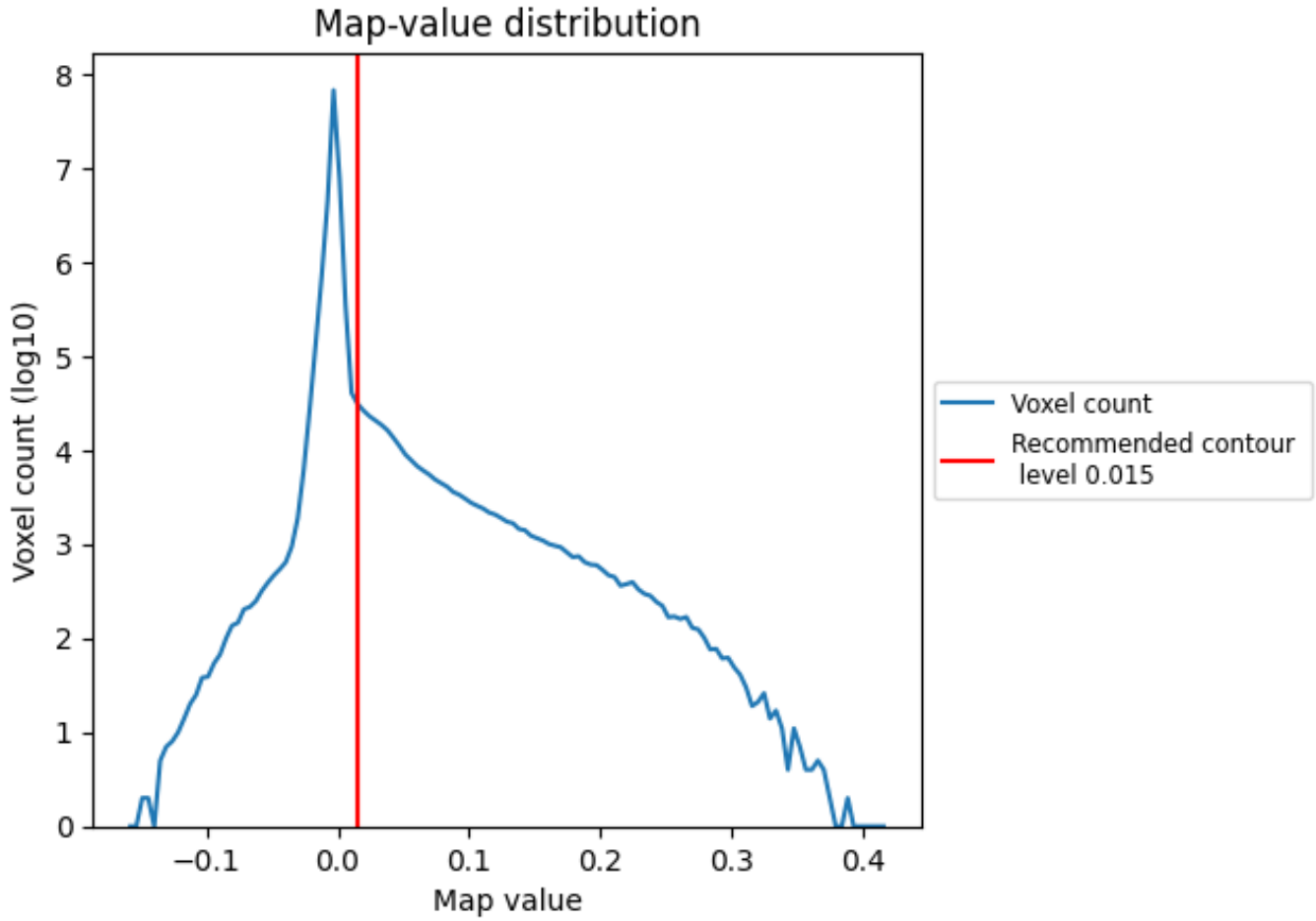


Z

7 Map analysis

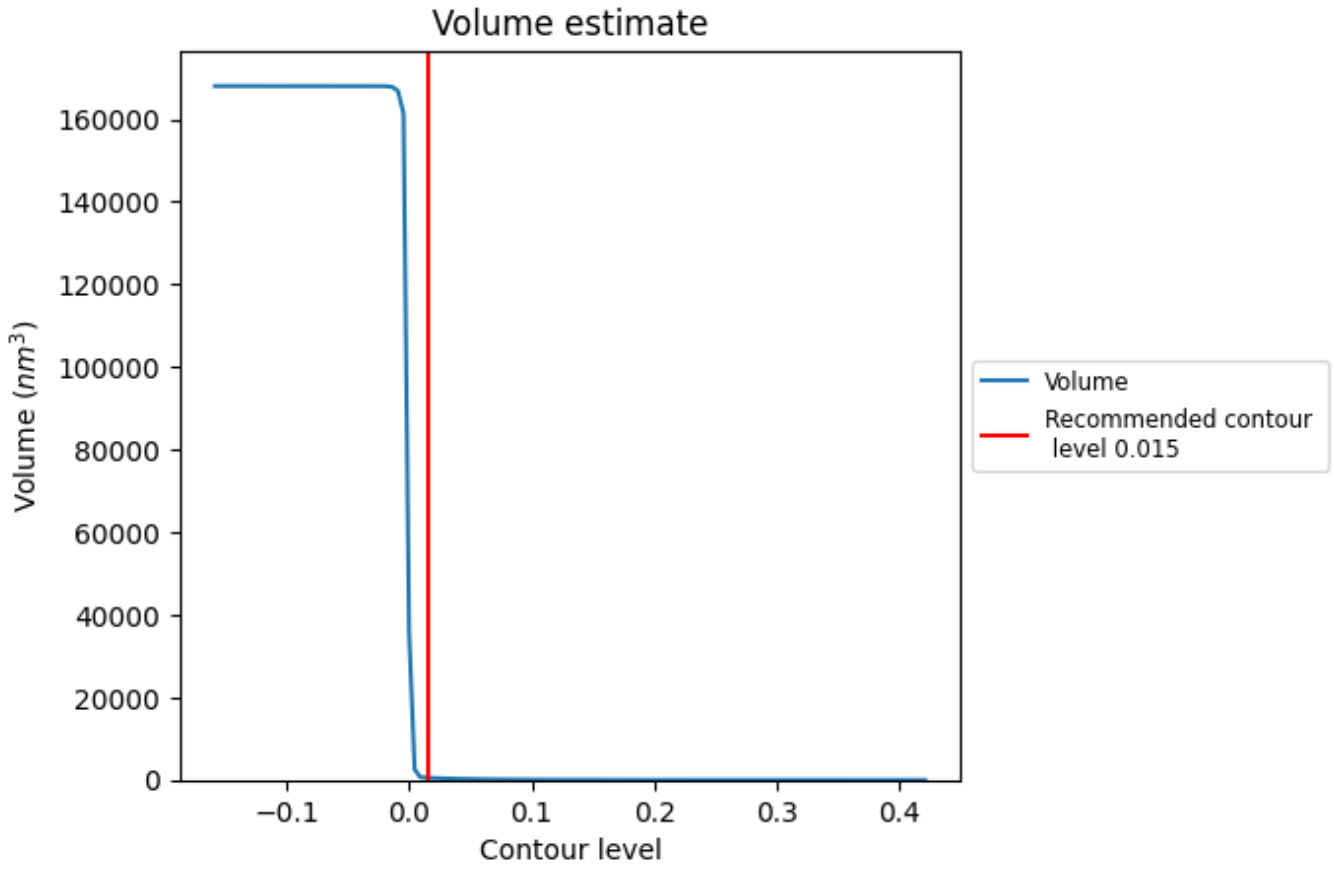
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

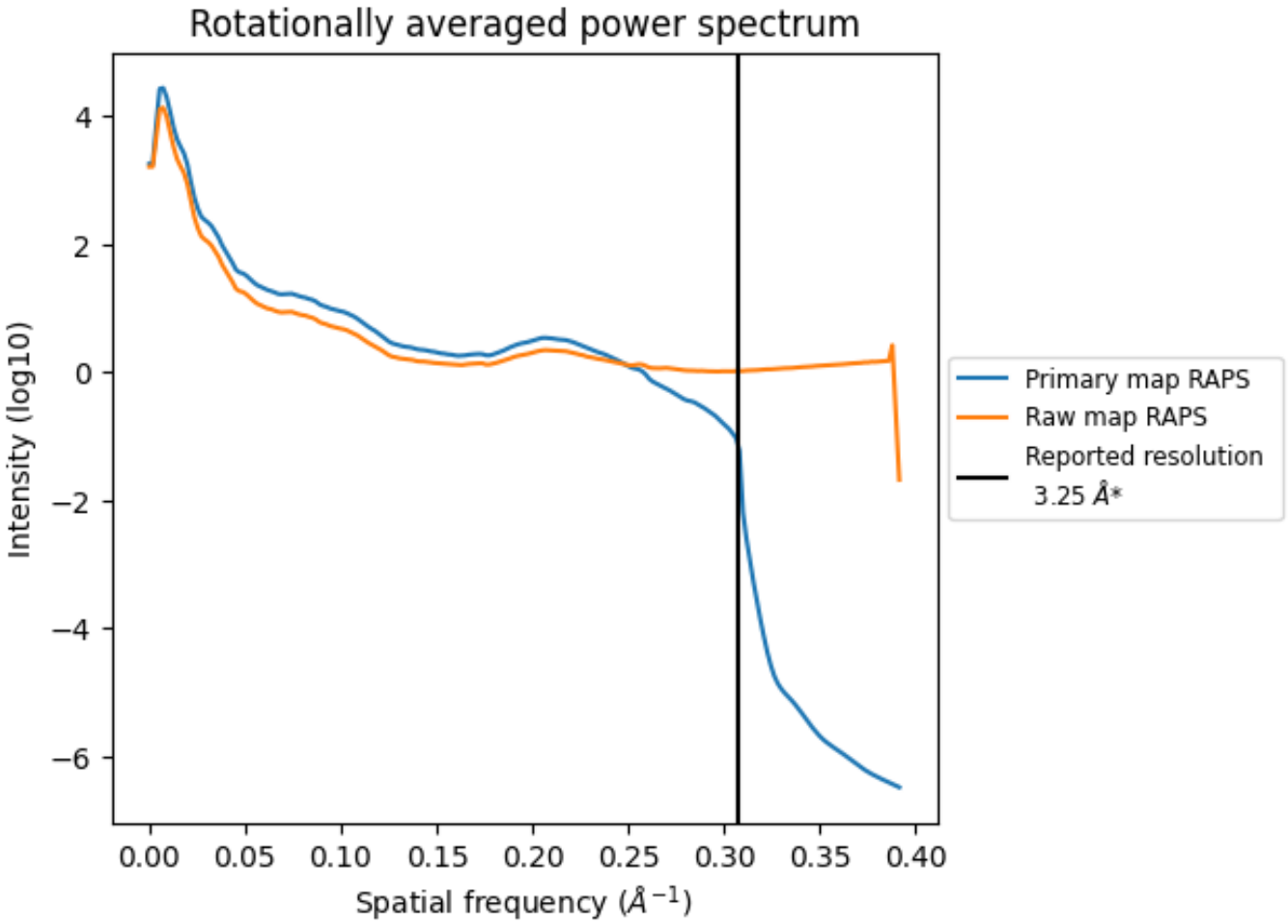
7.2 Volume estimate



The volume at the recommended contour level is 533 nm^3; this corresponds to an approximate mass of 481 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)

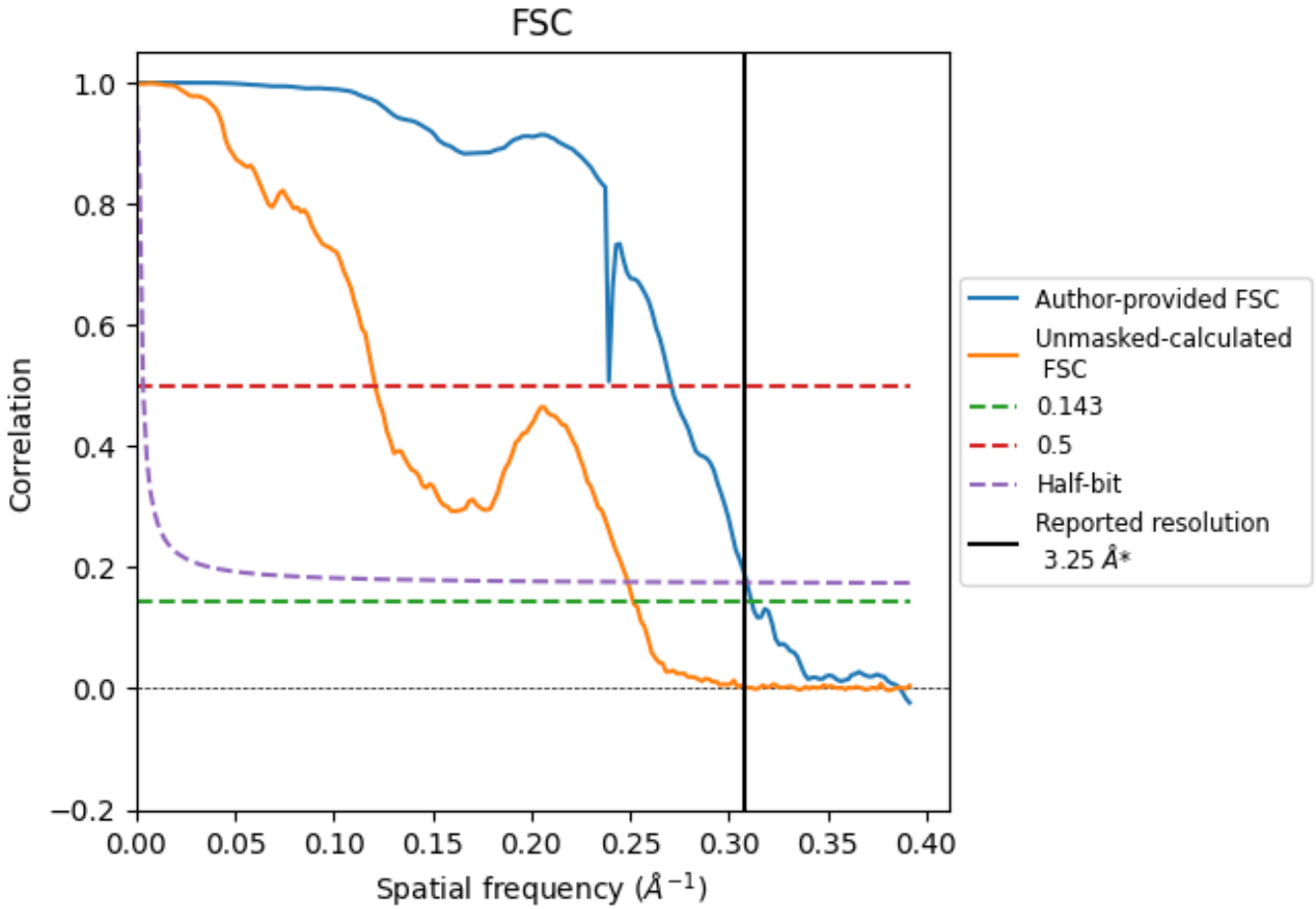


*Reported resolution corresponds to spatial frequency of 0.308 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.308 Å^{-1}

8.2 Resolution estimates (i)

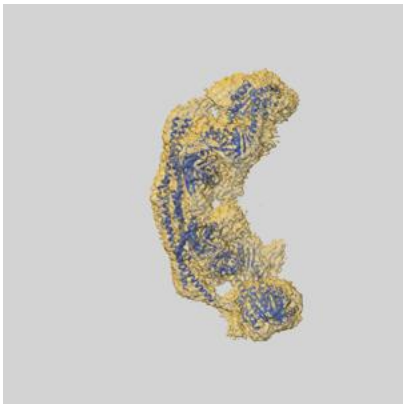
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.21	3.69	3.24
Unmasked-calculated*	3.97	8.26	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 3.25 by more than 10 %

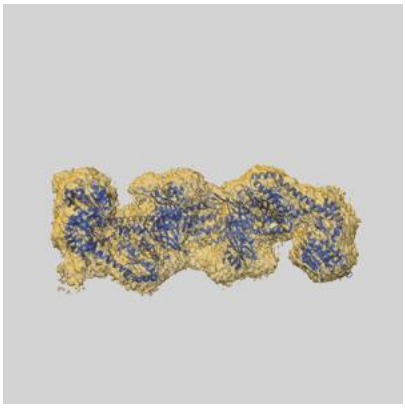
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55040 and PDB model 9SMR. Per-residue inclusion information can be found in section 3 on page 8.

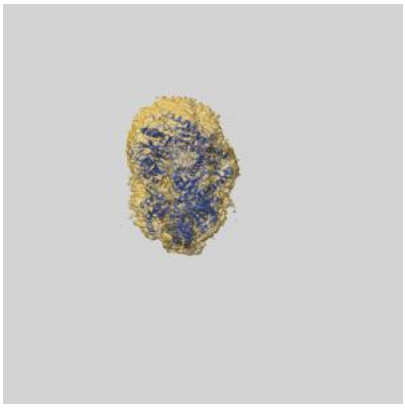
9.1 Map-model overlay



X



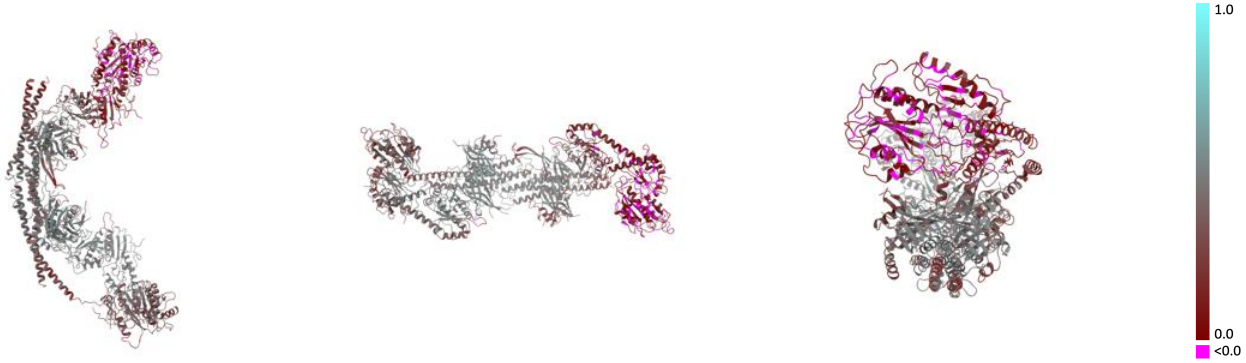
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

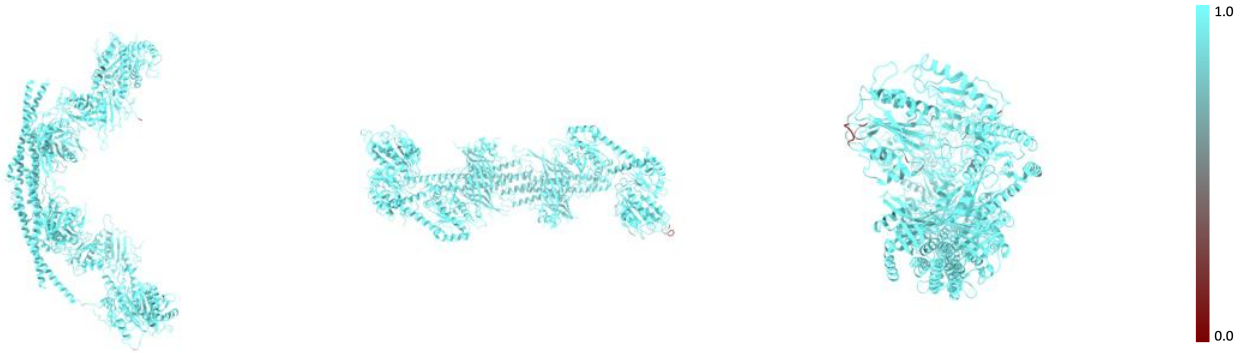
9.2 Q-score mapped to coordinate model (i)



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.

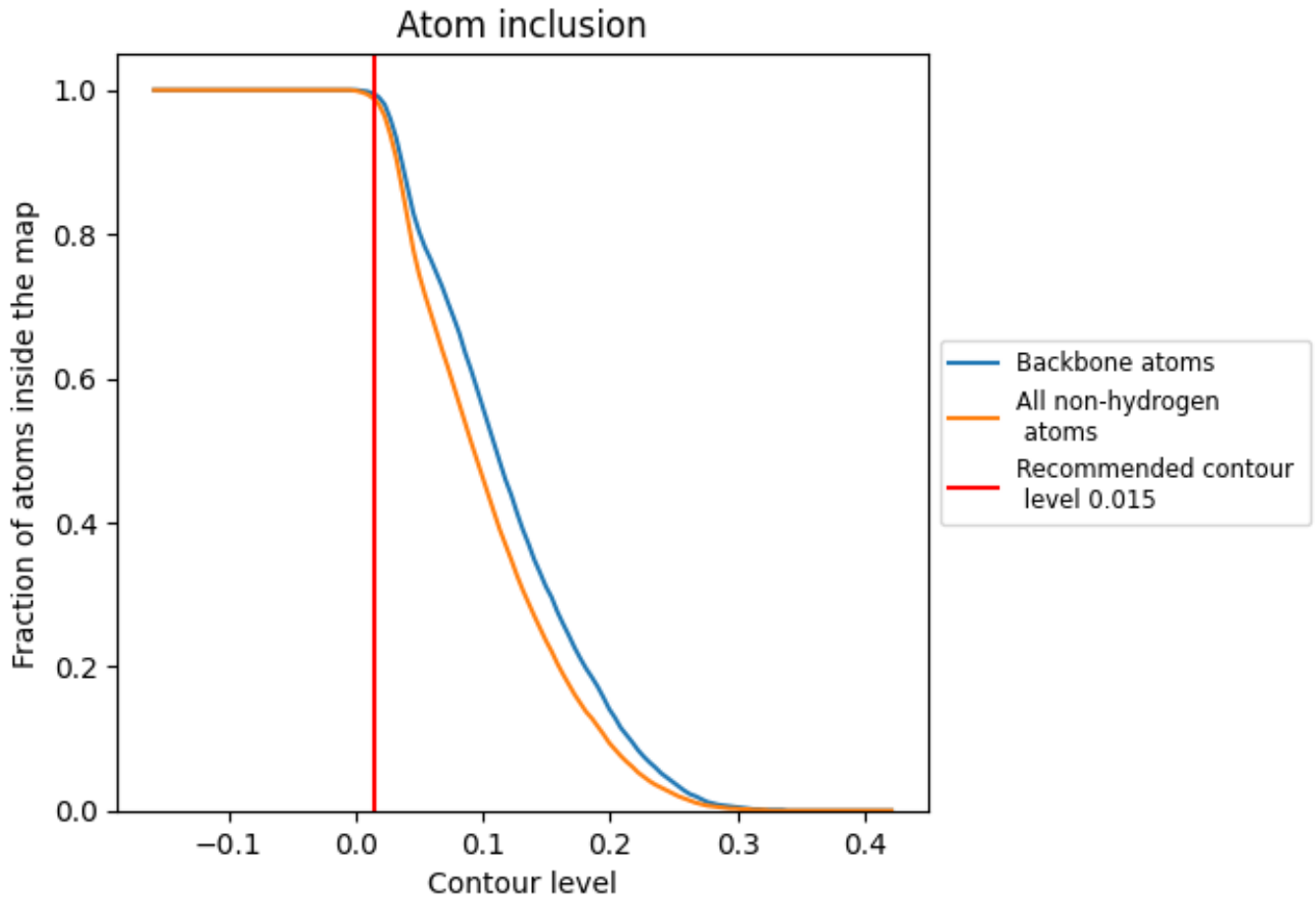
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9870	0.3480
A	0.9930	0.4330
B	0.9960	0.4470
C	0.9940	0.4390
D	0.9870	0.3720
E	0.9930	0.4470
F	0.9970	0.4140
G	0.9970	0.4040
H	0.9910	0.2040
I	0.9380	0.0890
J	0.9590	0.1320