WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Nov 24, 2022 – 03:25 PM EST

|		
PDB ID	:	7SQR
EMDB ID	:	EMD-25391
Title	:	201phi2-1 Chimallin localized tetramer reconstruction
Authors	:	Laughlin, T.G.; Deep, A.; Prichard, A.M.; Seitz, C.; Gu, Y.; Enustun, E.; Suslov, S.; Khanna, K.; Birkholz, E.A.; Amaro, R.E.; Pogliano, J.; Corbett, K.D.; Villa, E.
Deposited on	:	2021-11-06
Resolution	:	3.40 Å(reported)
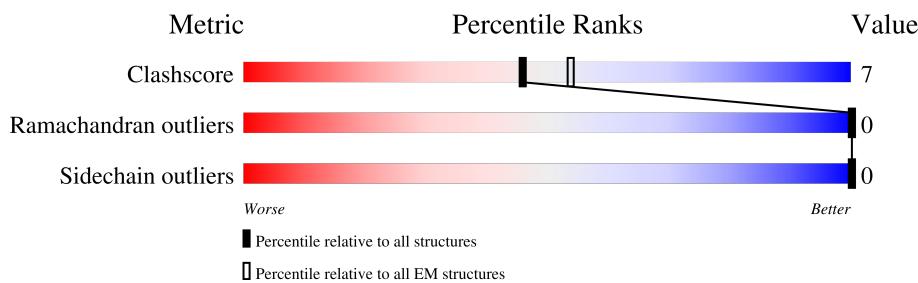
1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.40 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.
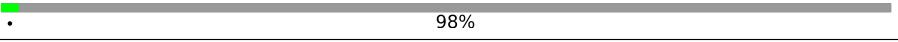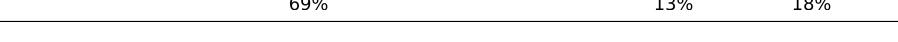

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	634	69% 13% 18%
1	B	634	97%
1	C	634	98%
1	D	634	69% 13% 18%
1	E	634	97%
1	F	634	98%
1	G	634	69% 13% 18%
1	H	634	97%

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Mol	Chain	Length	Quality of chain
1	I	634	98%
1	J	634	69% 13% 18%
1	K	634	97%
1	L	634	98%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 17272 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 Chimallin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	522	Total C N O S					0	0
			4072 2542 737 781 12						
1	B	22	Total C N O S					0	0
			163 97 33 31 2						
1	C	10	Total C N O					0	0
			83 54 12 17						
1	D	522	Total C N O S					0	0
			4072 2542 737 781 12						
1	E	22	Total C N O S					0	0
			163 97 33 31 2						
1	F	10	Total C N O					0	0
			83 54 12 17						
1	G	522	Total C N O S					0	0
			4072 2542 737 781 12						
1	H	22	Total C N O S					0	0
			163 97 33 31 2						
1	I	10	Total C N O					0	0
			83 54 12 17						
1	J	522	Total C N O S					0	0
			4072 2542 737 781 12						
1	K	22	Total C N O S					0	0
			163 97 33 31 2						
1	L	10	Total C N O					0	0
			83 54 12 17						

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B3FIW8
A	-1	ASN	-	expression tag	UNP B3FIW8
A	0	ALA	-	expression tag	UNP B3FIW8
B	-2	SER	-	expression tag	UNP B3FIW8
B	-1	ASN	-	expression tag	UNP B3FIW8
B	0	ALA	-	expression tag	UNP B3FIW8

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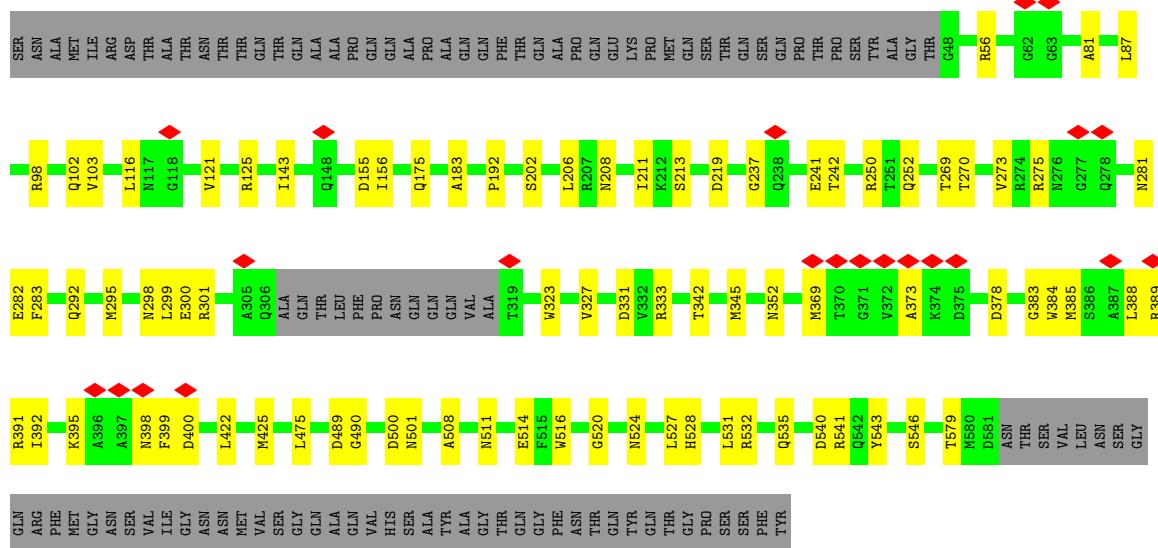
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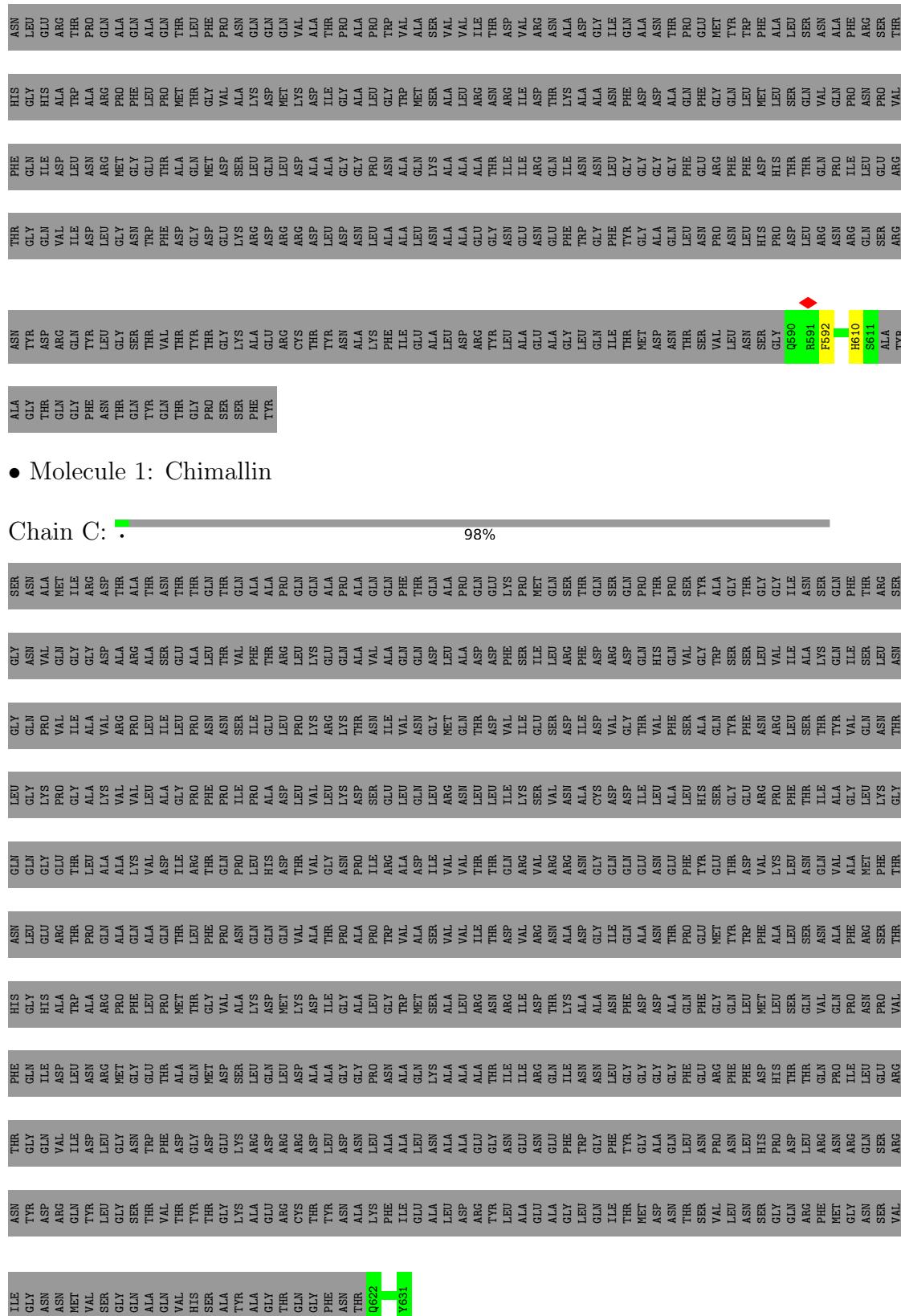
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP B3FIW8
C	-1	ASN	-	expression tag	UNP B3FIW8
C	0	ALA	-	expression tag	UNP B3FIW8
D	-2	SER	-	expression tag	UNP B3FIW8
D	-1	ASN	-	expression tag	UNP B3FIW8
D	0	ALA	-	expression tag	UNP B3FIW8
E	-2	SER	-	expression tag	UNP B3FIW8
E	-1	ASN	-	expression tag	UNP B3FIW8
E	0	ALA	-	expression tag	UNP B3FIW8
F	-2	SER	-	expression tag	UNP B3FIW8
F	-1	ASN	-	expression tag	UNP B3FIW8
F	0	ALA	-	expression tag	UNP B3FIW8
G	-2	SER	-	expression tag	UNP B3FIW8
G	-1	ASN	-	expression tag	UNP B3FIW8
G	0	ALA	-	expression tag	UNP B3FIW8
H	-2	SER	-	expression tag	UNP B3FIW8
H	-1	ASN	-	expression tag	UNP B3FIW8
H	0	ALA	-	expression tag	UNP B3FIW8
I	-2	SER	-	expression tag	UNP B3FIW8
I	-1	ASN	-	expression tag	UNP B3FIW8
I	0	ALA	-	expression tag	UNP B3FIW8
J	-2	SER	-	expression tag	UNP B3FIW8
J	-1	ASN	-	expression tag	UNP B3FIW8
J	0	ALA	-	expression tag	UNP B3FIW8
K	-2	SER	-	expression tag	UNP B3FIW8
K	-1	ASN	-	expression tag	UNP B3FIW8
K	0	ALA	-	expression tag	UNP B3FIW8
L	-2	SER	-	expression tag	UNP B3FIW8
L	-1	ASN	-	expression tag	UNP B3FIW8
L	0	ALA	-	expression tag	UNP B3FIW8

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Chimallin

Chain A:

• Molecule 1: Chimallin

Chain B:

• Molecule 1: Chimallin

Chain C: 98%

• Molecule 1: Chimallin

Chain D: 69%   13%   18%

• Molecule 1: Chimallin

Chain E: 97%

• Molecule 1: Chimallin

Chain F:

98%

Q622 Y631

• Molecule 1: Chimallin

Chain G:

69% 13% 18%

G48 R56 G62 G63 A81 L87

R98 Q102 V103 L116 N117 G118 V121 R125 I143 Q148 D155 I156 Q175 A183 P192 S202 L206 R207 N208 I211 K212 S213 D219 G237 Q238 E241 T242 R250 T251 Q252 T269 T270 V273 R274 R275 N276 G277 Q278 N281

E282 F283 Q292 M295 N298 L299 E300 R301 A305 Q306 T319 V327 D331 V332 R333 T342 M345 N352 R355 M369 T370 G371 V372 A373 K374 D375 D378 L382 G383 W384 A387 L388 R389 N390

R391 I392 K395 A396 A397 N398 F399 D400 L422 M425 L475 Q480 V481 I482 D489 G490 D500 N501 A508 N511 E514 F515 W516 G520 N524 L527 H528 L531 R532 Q535 D540 R541 Q542 Y543 S546 T579 M580 D581

• Molecule 1: Chimallin

Chain H: 97%

SER ASN ALA MET ILE ARG ASP ASP THR ALA THR ASN THR THR GLN THR GLN ALA ALA PRO GLN GLN ALA PRO ALA GLN GLN PHE THR GLN ALA PRO GLN GLU LYS PRO MET GLN SER THR GLN SER GLN PRO THR PRO SER TYR ALA GLY THR GLY ILE GLY ILE ASN SER GLN PHE THR ARG SER

GLY ASN VAL GLN GLY GLY ASP ALA ARG ALA ALA SER GLU ALA LEU THR VAL PHE THR ARG LEU LYS GLU GLN ALA VAL GLN GLN ASP LEU ALA ASP ASP PHE SER ILE LEU ARG PHE ASP ARG GLN HIS GLN VAL GLY TRP SER SER LEU VAL ILE ALA LYS GLN ILE SER LEU ASN

GLY GLN PRO VAL ILE ALA VAL ARG PRO LEU ILE LEU PRO ASN SER ILE GLU LEU PRO LYS ARG LYS THR ASN ILE VAL ASN GLY MET GLN THR ASP ILE GLU SER ASP ILE ASP VAL GLY THR VAL PHE SER ALA GLN LEU TYR PHE ASN ARG LEU SER THR TYR VAL GLN ASN THR

LEU GLY LYS PRO GLY ALA LYS VAL VAL LEU ALA GLY PRO PHE PRO ILE PRO ALA ASP LEU VAL LEU LYS ASP SER GLU LEU GLN LEU ARG ASN LEU ILE LYS SER VAL ALA CYS ASP ILE LEU ALA LEU HIS SER GLY GLU ARG PRO PHE ILE ALA GLY LEU LYS GLY

GLN GLN GLY GLU THR LEU ALA ALA LYS VAL ASP ILE ARG THR GLN PRO LEU HIS ASP THR VAL GLY ASN PRO ILE ARG ALA ASP ILE VAL VAL THR THR GLN ARG VAL ARG ASN GLY GLN GLU GLU ASN GLU PHE TYR GLU THR ASP VAL LYS LEU ASN GLN VAL ALA MET PHE THR

ASN LEU GLU ARG THR PRO GLN ALA GLN ALA GLN THR LEU PHE PRO ASN GLN GLN GLN VAL ALA THR PRO ALA PRO TRP VAL ALA SER VAL VAL ILE THR ASP VAL ARG ASN ALA ASP GLY ILE LEU ALA ASN THR PRO GLU MET TYR TRP ALA LEU LEU SER ASN ALA PHE ARG SER THR

HIS GLY HIS ALA TRP ALA ARG PRO PHE LEU PRO MET THR GLY VAL ALA LYS ASP MET LYS ASP ILE GLY ALA LEU GLY TRP MET SER ALA LEU ARG ASN ILE ASP LYS ALA ALA ASN PHE ASP ALA GLN PHE GLY GLN LEU MET LEU SER GLN VAL GLN PRO ASN PRO VAL

PHE GLN ILE LEU ASN MET GLY THR ALA MET ASP GLY LYS ARG ASP SER LEU GLN LEU ASP ALA ALA GLY GLY PRO ASN ALA GLN LYS ALA ALA THR ILE LEU ARG GLN ILE LEU ASN LEU GLY GLY GLY PHE ASP ARG PHE ASP HIS THR GLN GLN PRO ILE LEU GLU ARG

THR GLY GLN VAL ILE ASP LEU GLY ASN TRP PHE ASP GLY ASP GLU LYS ARG ASP ARG ASP ASP LEU ASP ASN LEU ALA LEU ASN ALA GLU GLY GLU ASN GLU PHE TRP GLY PHE TYR GLY ALA GLN LEU ASN PRO ASN LEU HIS PRO ASP LEU ARG ASN ARG GLN SER ARG

ASN TYR ASP ARG GLN TYR LEU GLY SER THR VAL THR TYR THR GLY LYS ALA GLU ALA ARG CYS THR SER THR TYR ASN ALA LYS GLU ILE GLU GLN ALA LEU ASP ARG TYR LEU ALA GLU GLY LEU GLN ILE GLN THR MET ASP ASN THR SER VAL LEU ASN SER GLY **Q590 R591 F592** **H610 S611** ALA TYR

ALA GLY THR GLN GLY PHE ASN THR GLN TYR GLN GLY PRO SER SER PHE TYR

• Molecule 1: Chimallin

Chain I: 98%

SER ASN ALA MET ILE ARG ASP ASP THR ALA THR ASN THR THR GLN THR GLN ALA ALA PRO GLN GLN ALA PRO ALA GLN GLN PHE THR GLN ALA PRO GLN GLU LYS PRO MET GLN SER THR GLN SER GLN PRO THR PRO SER TYR ALA GLY THR GLY ILE GLY ILE ASN SER GLN PHE THR ARG SER

GLY ASN VAL GLN GLY GLY ASP ALA ARG ALA ALA SER GLU ALA LEU THR VAL PHE THR ARG LEU LYS GLU GLN ALA VAL GLN GLN ASP LEU ALA ASP ASP PHE SER ILE LEU ARG PHE ASP ARG GLN HIS GLN VAL GLY TRP SER SER LEU VAL ILE ALA LYS GLN ILE SER LEU ASN

GLY GLN PRO VAL ILE ALA VAL ARG PRO LEU ILE LEU PRO ASN SER ILE GLU LEU PRO LYS ARG LYS THR ASN ILE VAL ASN GLY MET GLN THR ASP ILE GLU SER ASP ILE ASP VAL GLY THR VAL PHE SER ALA GLN LEU TYR PHE ASN ARG LEU SER THR TYR VAL GLN ASN THR

LEU GLY LYS PRO GLY ALA LYS VAL VAL LEU ALA GLY PRO PHE PRO ILE PRO ALA ASP LEU VAL LEU LYS ASP SER GLU LEU GLN LEU ARG ASN LEU ILE LYS SER VAL ALA CYS ASP ILE LEU ALA LEU HIS SER GLY GLU ARG PRO PHE ILE ALA GLY LEU LYS GLY

GLN GLN GLY GLU THR LEU ALA ALA LYS VAL ASP ILE ARG THR GLN PRO LEU HIS ASP THR VAL GLY ASN PRO ILE ARG ALA ASP ILE VAL VAL THR THR GLN ARG VAL ARG ASN GLY GLN GLU GLU ASN GLU PHE TYR GLU THR ASP VAL LYS LEU ASN GLN VAL ALA MET PHE THR

ASN LEU GLU ARG THR PRO GLN ALA GLN ALA GLN THR LEU PHE PRO ASN GLN GLN GLN VAL ALA THR PRO ALA PRO TRP VAL ALA SER VAL VAL ILE THR ASP VAL ARG ASN ALA ASP GLY ILE LEU ALA ASN THR PRO GLU MET TYR TRP ALA LEU LEU SER ASN ALA PHE ARG SER THR

• Molecule 1: Chimallin

Chain J:

69%   13%   18%

• Molecule 1: Chimallin

Chain K:

97%

- Molecule 1: Chimallin

Chain L: 98%

Q590 R591 F592 H610 S611

Q622 Y631

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	664363	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction performed during 3D reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	42.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	200.19205, 200.19205, 200.19205	wwPDB
Map dimensions	148, 148, 148	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.352649, 1.352649, 1.352649	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.25	0/4147	0.53	0/5627
1	B	0.25	0/164	0.64	0/218
1	C	0.25	0/86	0.34	0/116
1	D	0.25	0/4147	0.53	0/5627
1	E	0.26	0/164	0.64	0/218
1	F	0.26	0/86	0.34	0/116
1	G	0.25	0/4147	0.53	0/5627
1	H	0.26	0/164	0.64	0/218
1	I	0.26	0/86	0.34	0/116
1	J	0.25	0/4147	0.53	0/5627
1	K	0.25	0/164	0.64	0/218
1	L	0.25	0/86	0.34	0/116
All	All	0.25	0/17588	0.53	0/23844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4072	0	3995	60	0
1	B	163	0	155	2	0
1	C	83	0	69	0	0
1	D	4072	0	3995	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	163	0	155	2	0
1	F	83	0	69	0	0
1	G	4072	0	3995	60	0
1	H	163	0	155	2	0
1	I	83	0	69	0	0
1	J	4072	0	3995	60	0
1	K	163	0	155	2	0
1	L	83	0	69	0	0
All	All	17272	0	16876	225	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 7.

All (225) 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:A:540:ASP:OD2	1:A:541:ARG:N	2.28	0.67
1:A:527:LEU:HD22	1:A:532:ARG:HG2	1.77	0.67
1:D:540:ASP:OD2	1:D:541:ARG:N	2.28	0.67
1:J:527:LEU:HD22	1:J:532:ARG:HG2	1.77	0.67
1:A:281:ASN:ND2	1:J:102:GLN:OE1	2.26	0.66
1:G:540:ASP:OD2	1:G:541:ARG:N	2.28	0.66
1:G:527:LEU:HD22	1:G:532:ARG:HG2	1.77	0.65
1:D:527:LEU:HD22	1:D:532:ARG:HG2	1.77	0.65
1:J:540:ASP:OD2	1:J:541:ARG:N	2.28	0.65
1:G:102:GLN:OE1	1:J:281:ASN:ND2	2.26	0.65
1:A:102:GLN:OE1	1:D:281:ASN:ND2	2.26	0.64
1:J:192:PRO:HD3	1:J:425:MET:HG3	1.81	0.63
1:A:192:PRO:HD3	1:A:425:MET:HG3	1.81	0.63
1:D:192:PRO:HD3	1:D:425:MET:HG3	1.81	0.62
1:G:192:PRO:HD3	1:G:425:MET:HG3	1.81	0.62
1:D:102:GLN:OE1	1:G:281:ASN:ND2	2.26	0.61
1:D:514:GLU:OE2	1:D:543:TYR:OH	2.18	0.61
1:G:378:ASP:OD2	1:G:391:ARG:NH2	2.33	0.61
1:A:378:ASP:OD2	1:A:391:ARG:NH2	2.33	0.61
1:G:514:GLU:OE2	1:G:543:TYR:OH	2.18	0.61
1:D:378:ASP:OD2	1:D:391:ARG:NH2	2.33	0.61
1:A:508:ALA:HB1	1:A:511:ASN:OD1	2.01	0.61
1:J:378:ASP:OD2	1:J:391:ARG:NH2	2.33	0.61
1:J:508:ALA:HB1	1:J:511:ASN:OD1	2.01	0.61
1:D:508:ALA:HB1	1:D:511:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:508:ALA:HB1	1:G:511:ASN:OD1	2.01	0.60
1:D:175:GLN:NE2	1:D:183:ALA:O	2.35	0.60
1:J:514:GLU:OE2	1:J:543:TYR:OH	2.18	0.60
1:G:175:GLN:NE2	1:G:183:ALA:O	2.35	0.60
1:J:175:GLN:NE2	1:J:183:ALA:O	2.35	0.59
1:A:175:GLN:NE2	1:A:183:ALA:O	2.35	0.59
1:A:514:GLU:OE2	1:A:543:TYR:OH	2.18	0.59
1:D:579:THR:HG22	1:E:610:HIS:HB3	1.86	0.58
1:A:579:THR:HG22	1:B:610:HIS:HB3	1.86	0.58
1:J:579:THR:HG22	1:K:610:HIS:HB3	1.86	0.58
1:G:579:THR:HG22	1:H:610:HIS:HB3	1.86	0.57
1:A:373:ALA:HB2	1:A:395:LYS:HE3	1.86	0.56
1:G:384:TRP:O	1:G:389:ARG:NH2	2.38	0.56
1:J:373:ALA:HB2	1:J:395:LYS:HE3	1.87	0.56
1:D:273:VAL:HG22	1:D:275:ARG:HG2	1.87	0.56
1:D:373:ALA:HB2	1:D:395:LYS:HE3	1.87	0.56
1:G:273:VAL:HG22	1:G:275:ARG:HG2	1.87	0.56
1:D:384:TRP:O	1:D:389:ARG:NH2	2.38	0.56
1:J:384:TRP:O	1:J:389:ARG:NH2	2.38	0.56
1:A:384:TRP:O	1:A:389:ARG:NH2	2.38	0.55
1:G:373:ALA:HB2	1:G:395:LYS:HE3	1.87	0.55
1:A:273:VAL:HG22	1:A:275:ARG:HG2	1.87	0.55
1:J:273:VAL:HG22	1:J:275:ARG:HG2	1.87	0.55
1:D:56:ARG:NE	1:G:219:ASP:OD1	2.40	0.55
1:A:56:ARG:NE	1:D:219:ASP:OD1	2.40	0.55
1:G:56:ARG:NE	1:J:219:ASP:OD1	2.40	0.54
1:A:219:ASP:OD1	1:J:56:ARG:NE	2.40	0.53
1:G:342:THR:H	1:G:345:MET:HE3	1.74	0.53
1:J:369:MET:O	1:J:395:LYS:NZ	2.35	0.53
1:D:342:THR:H	1:D:345:MET:HE3	1.74	0.53
1:J:342:THR:H	1:J:345:MET:HE3	1.74	0.52
1:A:342:THR:H	1:A:345:MET:HE3	1.74	0.52
1:D:102:GLN:HB3	1:G:281:ASN:ND2	2.26	0.51
1:A:102:GLN:HB3	1:D:281:ASN:ND2	2.26	0.51
1:G:143:ILE:HD13	1:G:531:LEU:HD11	1.93	0.50
1:A:281:ASN:ND2	1:J:102:GLN:HB3	2.26	0.50
1:D:143:ILE:HD13	1:D:531:LEU:HD11	1.93	0.50
1:G:102:GLN:HB3	1:J:281:ASN:ND2	2.26	0.50
1:G:298:ASN:ND2	1:G:300:GLU:OE2	2.45	0.50
1:J:143:ILE:HD13	1:J:531:LEU:HD11	1.93	0.50
1:J:298:ASN:ND2	1:J:300:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:TRP:NE1	1:B:592:PHE:O	2.39	0.50
1:D:301:ARG:HH11	1:D:516:TRP:HH2	1.60	0.50
1:A:143:ILE:HD13	1:A:531:LEU:HD11	1.93	0.49
1:A:298:ASN:ND2	1:A:300:GLU:OE2	2.45	0.49
1:G:301:ARG:HH11	1:G:516:TRP:HH2	1.60	0.49
1:A:301:ARG:HH11	1:A:516:TRP:HH2	1.60	0.49
1:J:301:ARG:HH11	1:J:516:TRP:HH2	1.60	0.49
1:J:155:ASP:OD1	1:J:156:ILE:N	2.46	0.49
1:A:116:LEU:HD12	1:A:121:VAL:HG21	1.95	0.49
1:D:298:ASN:ND2	1:D:300:GLU:OE2	2.45	0.49
1:G:116:LEU:HD12	1:G:121:VAL:HG21	1.95	0.49
1:J:116:LEU:HD12	1:J:121:VAL:HG21	1.95	0.48
1:D:116:LEU:HD12	1:D:121:VAL:HG21	1.95	0.48
1:D:155:ASP:OD1	1:D:156:ILE:N	2.46	0.48
1:G:155:ASP:OD1	1:G:156:ILE:N	2.46	0.48
1:G:500:ASP:OD1	1:G:500:ASP:N	2.47	0.48
1:D:500:ASP:OD1	1:D:500:ASP:N	2.47	0.48
1:J:398:ASN:OD1	1:J:399:PHE:N	2.47	0.48
1:A:155:ASP:OD1	1:A:156:ILE:N	2.46	0.47
1:D:398:ASN:OD1	1:D:399:PHE:N	2.47	0.47
1:G:269:THR:HG22	1:G:292:GLN:HG3	1.96	0.47
1:G:398:ASN:OD1	1:G:399:PHE:N	2.47	0.47
1:A:192:PRO:CD	1:A:425:MET:HG3	2.45	0.47
1:D:527:LEU:HD21	1:D:531:LEU:HB2	1.97	0.47
1:A:398:ASN:OD1	1:A:399:PHE:N	2.47	0.47
1:J:269:THR:HG22	1:J:292:GLN:HG3	1.96	0.47
1:A:269:THR:HG22	1:A:292:GLN:HG3	1.96	0.47
1:J:527:LEU:HD21	1:J:531:LEU:HB2	1.97	0.47
1:A:500:ASP:N	1:A:500:ASP:OD1	2.47	0.46
1:D:527:LEU:HD23	1:D:528:HIS:O	2.15	0.46
1:G:527:LEU:HD21	1:G:531:LEU:HB2	1.97	0.46
1:A:383:GLY:HA3	1:A:392:ILE:HD12	1.98	0.46
1:D:192:PRO:CD	1:D:425:MET:HG3	2.45	0.46
1:D:269:THR:HG22	1:D:292:GLN:HG3	1.96	0.46
1:J:383:GLY:HA3	1:J:392:ILE:HD12	1.98	0.46
1:J:500:ASP:OD1	1:J:500:ASP:N	2.47	0.46
1:J:527:LEU:HD23	1:J:528:HIS:O	2.15	0.46
1:A:527:LEU:HD21	1:A:531:LEU:HB2	1.97	0.46
1:J:192:PRO:CD	1:J:425:MET:HG3	2.44	0.46
1:J:282:GLU:HG3	1:J:283:PHE:HD1	1.81	0.46
1:J:301:ARG:NH1	1:J:516:TRP:HH2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ARG:NH1	1:D:516:TRP:HH2	2.13	0.46
1:G:301:ARG:NH1	1:G:516:TRP:HH2	2.13	0.46
1:D:489:ASP:OD1	1:D:490:GLY:N	2.47	0.46
1:D:383:GLY:HA3	1:D:392:ILE:HD12	1.98	0.46
1:D:531:LEU:O	1:D:535:GLN:HG2	2.16	0.46
1:G:516:TRP:NE1	1:H:592:PHE:O	2.39	0.46
1:J:541:ARG:NH2	1:J:546:SER:HA	2.31	0.46
1:D:282:GLU:HG3	1:D:283:PHE:HD1	1.81	0.45
1:G:541:ARG:NH2	1:G:546:SER:HA	2.31	0.45
1:D:331:ASP:OD2	1:D:333:ARG:NH2	2.45	0.45
1:G:282:GLU:HG3	1:G:283:PHE:HD1	1.81	0.45
1:G:383:GLY:HA3	1:G:392:ILE:HD12	1.98	0.45
1:G:531:LEU:O	1:G:535:GLN:HG2	2.16	0.45
1:D:541:ARG:NH2	1:D:546:SER:HA	2.31	0.45
1:J:531:LEU:O	1:J:535:GLN:HG2	2.16	0.45
1:A:282:GLU:HG3	1:A:283:PHE:HD1	1.81	0.45
1:A:527:LEU:HD23	1:A:528:HIS:O	2.15	0.45
1:A:531:LEU:O	1:A:535:GLN:HG2	2.16	0.45
1:G:527:LEU:HD23	1:G:528:HIS:O	2.15	0.45
1:G:295:MET:HE3	1:G:327:VAL:HG11	1.98	0.45
1:A:125:ARG:NH1	1:A:213:SER:OG	2.50	0.45
1:A:270:THR:OG1	1:A:352:ASN:ND2	2.49	0.45
1:A:301:ARG:NH1	1:A:516:TRP:HH2	2.13	0.45
1:G:192:PRO:CD	1:G:425:MET:HG3	2.45	0.45
1:J:516:TRP:NE1	1:K:592:PHE:O	2.39	0.45
1:A:541:ARG:NH2	1:A:546:SER:HA	2.31	0.45
1:A:400:ASP:OD1	1:A:400:ASP:N	2.50	0.45
1:A:489:ASP:OD1	1:A:490:GLY:N	2.47	0.45
1:D:87:LEU:HD11	1:D:211:ILE:HD13	1.99	0.45
1:A:87:LEU:HD11	1:A:211:ILE:HD13	1.99	0.45
1:D:400:ASP:OD1	1:D:400:ASP:N	2.50	0.45
1:G:489:ASP:OD1	1:G:490:GLY:N	2.47	0.44
1:D:516:TRP:NE1	1:E:592:PHE:O	2.39	0.44
1:G:250:ARG:NH2	1:G:252:GLN:O	2.48	0.44
1:J:270:THR:OG1	1:J:352:ASN:ND2	2.49	0.44
1:J:299:LEU:O	1:J:501:ASN:ND2	2.49	0.44
1:G:400:ASP:OD1	1:G:400:ASP:N	2.50	0.44
1:D:295:MET:HE3	1:D:327:VAL:HG11	1.99	0.44
1:D:369:MET:O	1:D:395:LYS:NZ	2.35	0.44
1:J:250:ARG:NH2	1:J:252:GLN:O	2.48	0.44
1:A:202:SER:O	1:A:206:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:295:MET:HE3	1:J:327:VAL:HG11	1.98	0.43
1:A:295:MET:HE3	1:A:327:VAL:HG11	1.98	0.43
1:A:299:LEU:O	1:A:501:ASN:ND2	2.49	0.43
1:D:242:THR:O	1:D:273:VAL:HG12	2.19	0.43
1:J:202:SER:O	1:J:206:LEU:HD23	2.18	0.43
1:J:520:GLY:O	1:J:524:ASN:HB2	2.18	0.43
1:A:520:GLY:O	1:A:524:ASN:HB2	2.18	0.43
1:D:202:SER:O	1:D:206:LEU:HD23	2.18	0.43
1:D:352:ASN:OD1	1:D:355:ARG:NH2	2.47	0.43
1:G:299:LEU:O	1:G:501:ASN:ND2	2.49	0.43
1:G:87:LEU:HD11	1:G:211:ILE:HD13	1.99	0.43
1:J:87:LEU:HD11	1:J:211:ILE:HD13	1.99	0.43
1:A:283:PHE:CD2	1:J:156:ILE:HD13	2.54	0.43
1:D:520:GLY:O	1:D:524:ASN:HB2	2.18	0.43
1:G:242:THR:O	1:G:273:VAL:HG12	2.19	0.43
1:A:242:THR:O	1:A:273:VAL:HG12	2.19	0.42
1:G:520:GLY:O	1:G:524:ASN:HB2	2.18	0.42
1:J:331:ASP:OD2	1:J:333:ARG:NH2	2.45	0.42
1:D:250:ARG:NH2	1:D:252:GLN:O	2.48	0.42
1:G:156:ILE:HD13	1:J:283:PHE:CD2	2.54	0.42
1:J:242:THR:O	1:J:273:VAL:HG12	2.19	0.42
1:G:202:SER:O	1:G:206:LEU:HD23	2.18	0.42
1:A:250:ARG:NH2	1:A:252:GLN:O	2.48	0.42
1:G:125:ARG:NH1	1:G:213:SER:OG	2.50	0.42
1:G:270:THR:OG1	1:G:352:ASN:ND2	2.49	0.42
1:J:400:ASP:N	1:J:400:ASP:OD1	2.50	0.42
1:A:156:ILE:HD13	1:D:283:PHE:CD2	2.54	0.42
1:A:331:ASP:OD2	1:A:333:ARG:NH2	2.45	0.42
1:D:156:ILE:HD13	1:G:283:PHE:CD2	2.54	0.42
1:J:125:ARG:NH1	1:J:213:SER:OG	2.50	0.42
1:D:270:THR:OG1	1:D:352:ASN:ND2	2.49	0.42
1:J:98:ARG:HA	1:J:103:VAL:HG22	2.02	0.42
1:J:208:ASN:HA	1:J:211:ILE:HG22	2.02	0.42
1:A:541:ARG:O	1:A:541:ARG:HD3	2.20	0.42
1:G:98:ARG:HA	1:G:103:VAL:HG22	2.02	0.42
1:G:208:ASN:HA	1:G:211:ILE:HG22	2.02	0.42
1:D:541:ARG:O	1:D:541:ARG:HD3	2.20	0.42
1:J:237:GLY:HA3	1:J:241:GLU:OE2	2.20	0.42
1:J:422:LEU:HD11	1:J:475:LEU:HD21	2.02	0.42
1:A:369:MET:O	1:A:395:LYS:NZ	2.35	0.41
1:D:299:LEU:O	1:D:501:ASN:ND2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:ASP:OD2	1:G:333:ARG:NH2	2.45	0.41
1:G:422:LEU:HD11	1:G:475:LEU:HD21	2.02	0.41
1:J:352:ASN:OD1	1:J:355:ARG:NH2	2.47	0.41
1:D:237:GLY:HA3	1:D:241:GLU:OE2	2.20	0.41
1:D:527:LEU:HD21	1:D:531:LEU:CB	2.51	0.41
1:J:382:LEU:HD12	1:J:382:LEU:HA	1.92	0.41
1:J:388:LEU:H	1:J:388:LEU:HD23	1.85	0.41
1:J:541:ARG:HD3	1:J:541:ARG:O	2.20	0.41
1:A:527:LEU:HD21	1:A:531:LEU:CB	2.51	0.41
1:D:388:LEU:HD23	1:D:388:LEU:H	1.85	0.41
1:A:388:LEU:HD23	1:A:388:LEU:H	1.85	0.41
1:G:382:LEU:HD12	1:G:382:LEU:HA	1.92	0.41
1:G:388:LEU:H	1:G:388:LEU:HD23	1.85	0.41
1:A:422:LEU:HD11	1:A:475:LEU:HD21	2.02	0.41
1:D:208:ASN:HA	1:D:211:ILE:HG22	2.02	0.41
1:D:254:LEU:HD23	1:D:254:LEU:HA	1.95	0.41
1:J:480:GLN:NE2	1:J:482:ILE:HD11	2.36	0.41
1:A:208:ASN:HA	1:A:211:ILE:HG22	2.02	0.41
1:A:237:GLY:HA3	1:A:241:GLU:OE2	2.20	0.41
1:D:98:ARG:HA	1:D:103:VAL:HG22	2.02	0.41
1:D:422:LEU:HD11	1:D:475:LEU:HD21	2.02	0.41
1:D:480:GLN:NE2	1:D:482:ILE:HD11	2.36	0.41
1:G:237:GLY:HA3	1:G:241:GLU:OE2	2.20	0.41
1:G:527:LEU:HD21	1:G:531:LEU:CB	2.50	0.41
1:G:541:ARG:O	1:G:541:ARG:HD3	2.20	0.41
1:J:527:LEU:HD21	1:J:531:LEU:CB	2.51	0.41
1:A:81:ALA:HB1	1:A:87:LEU:HD13	2.03	0.41
1:D:125:ARG:NH1	1:D:213:SER:OG	2.50	0.41
1:A:323:TRP:HZ2	1:A:385:MET:SD	2.45	0.40
1:A:385:MET:H	1:A:385:MET:HG2	1.74	0.40
1:G:480:GLN:NE2	1:G:482:ILE:HD11	2.36	0.40
1:J:323:TRP:HZ2	1:J:385:MET:SD	2.45	0.40
1:A:98:ARG:HA	1:A:103:VAL:HG22	2.02	0.40
1:G:81:ALA:HB1	1:G:87:LEU:HD13	2.03	0.40
1:D:385:MET:H	1:D:385:MET:HG2	1.74	0.40
1:G:352:ASN:OD1	1:G:355:ARG:NH2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/634 (82%)	501 (97%)	17 (3%)	0	100	100
1	B	20/634 (3%)	20 (100%)	0	0	100	100
1	C	8/634 (1%)	8 (100%)	0	0	100	100
1	D	518/634 (82%)	501 (97%)	17 (3%)	0	100	100
1	E	20/634 (3%)	20 (100%)	0	0	100	100
1	F	8/634 (1%)	8 (100%)	0	0	100	100
1	G	518/634 (82%)	501 (97%)	17 (3%)	0	100	100
1	H	20/634 (3%)	20 (100%)	0	0	100	100
1	I	8/634 (1%)	8 (100%)	0	0	100	100
1	J	518/634 (82%)	501 (97%)	17 (3%)	0	100	100
1	K	20/634 (3%)	20 (100%)	0	0	100	100
1	L	8/634 (1%)	8 (100%)	0	0	100	100
All	All	2184/7608 (29%)	2116 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/522 (83%)	431 (100%)	0	100	100
1	B	18/522 (3%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	9/522 (2%)	9 (100%)	0	100	100
1	D	431/522 (83%)	431 (100%)	0	100	100
1	E	18/522 (3%)	18 (100%)	0	100	100
1	F	9/522 (2%)	9 (100%)	0	100	100
1	G	431/522 (83%)	431 (100%)	0	100	100
1	H	18/522 (3%)	18 (100%)	0	100	100
1	I	9/522 (2%)	9 (100%)	0	100	100
1	J	431/522 (83%)	431 (100%)	0	100	100
1	K	18/522 (3%)	18 (100%)	0	100	100
1	L	9/522 (2%)	9 (100%)	0	100	100
All	All	1832/6264 (29%)	1832 (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. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

There are no ligands in this entry.

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.
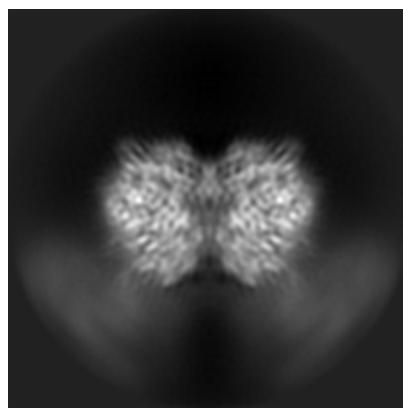
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-25391. These allow visual inspection of the internal detail of the map and identification of artifacts.
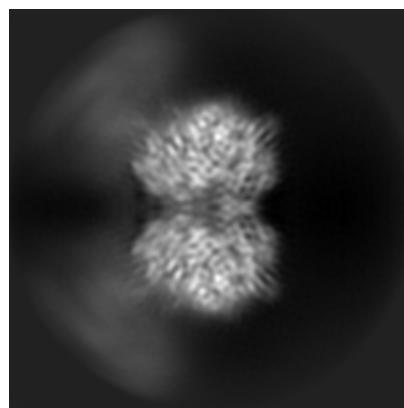
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
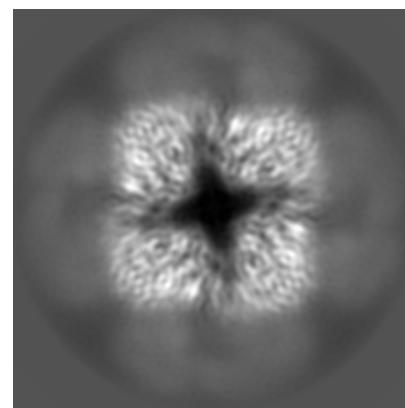
6.1.1 Primary map

X
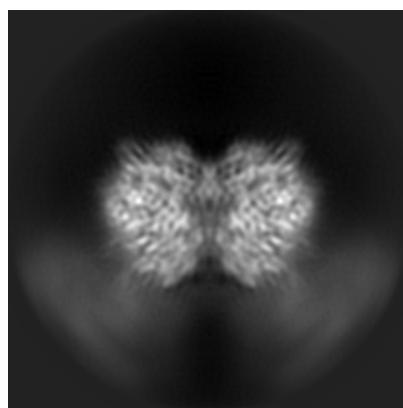
Y
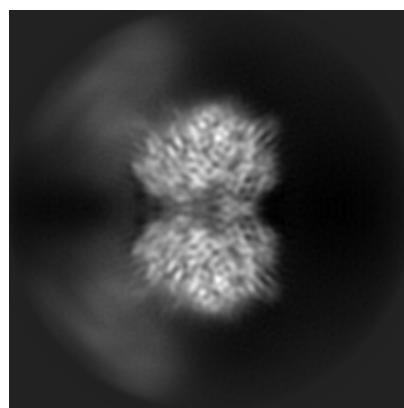
Z
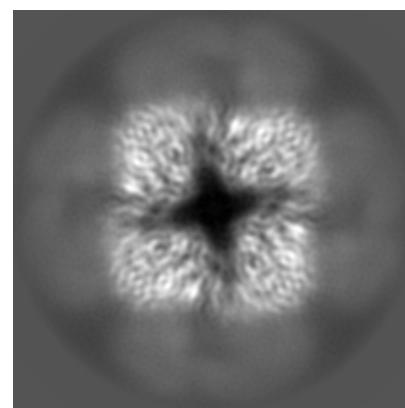
6.1.2 Raw map

X

Y

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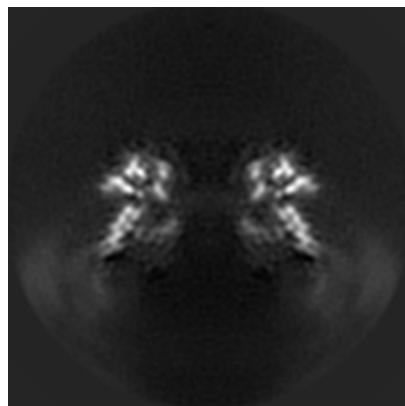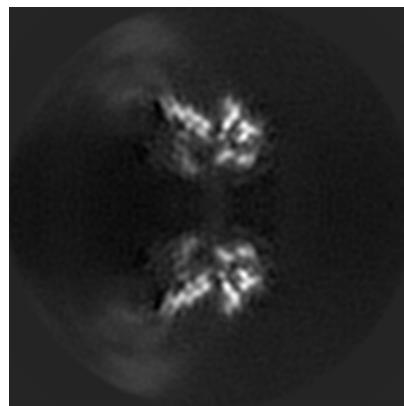
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
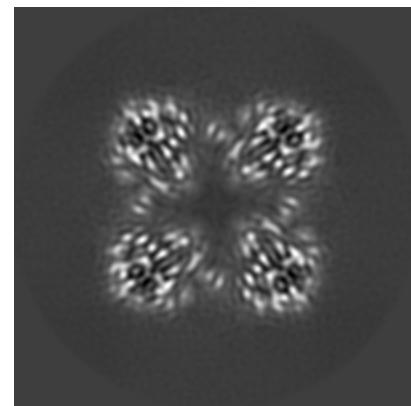
6.2.1 Primary map
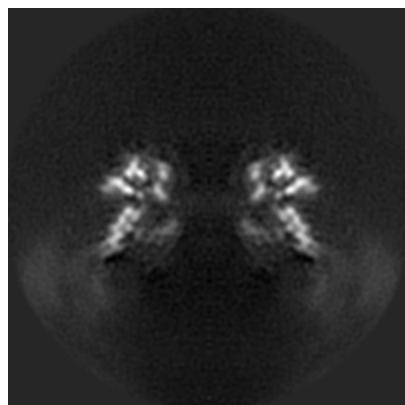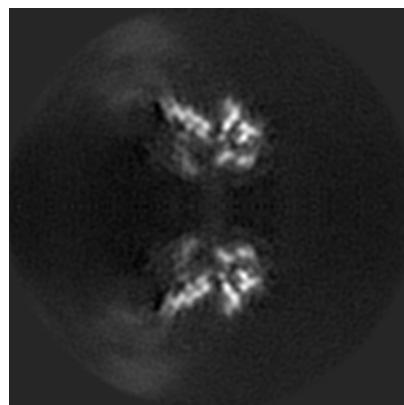
| X Index: 74 | Y Index: 74 | Z Index: 74 |
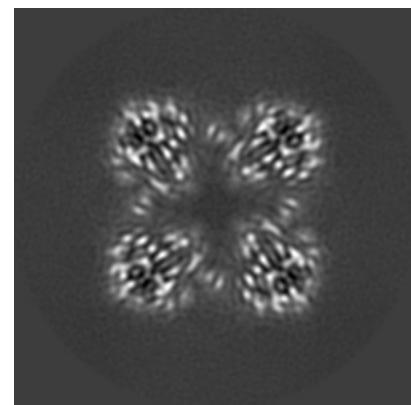
6.2.2 Raw map
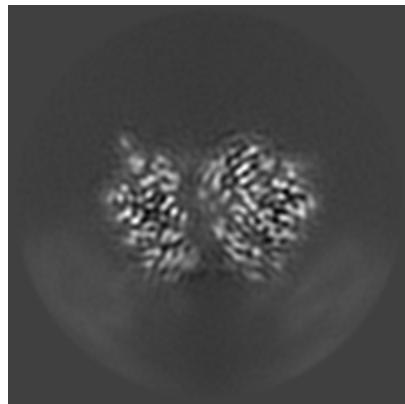
| X Index: 74 | Y Index: 74 | Z Index: 74 |
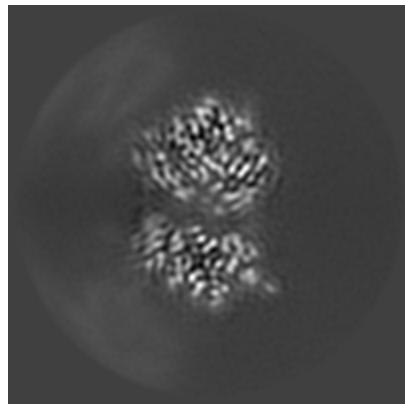
The images above show central slices of the map in three orthogonal directions.

6.3　Largest variance slices ⓘ
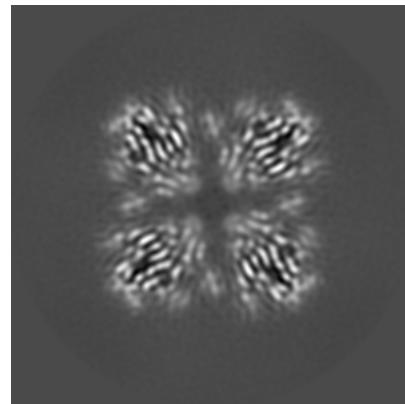
6.3.1　Primary map
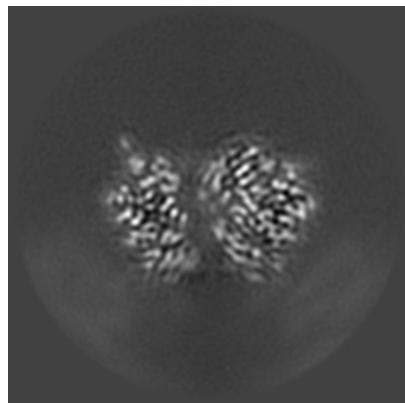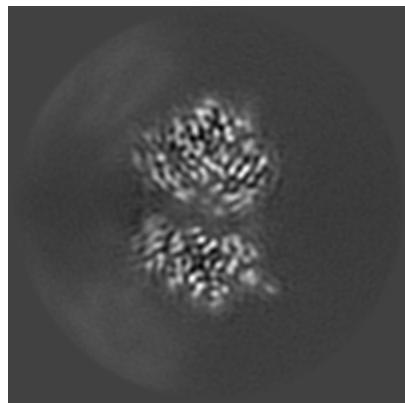
| X Index: 50 | Y Index: 98 | Z Index: 71 |
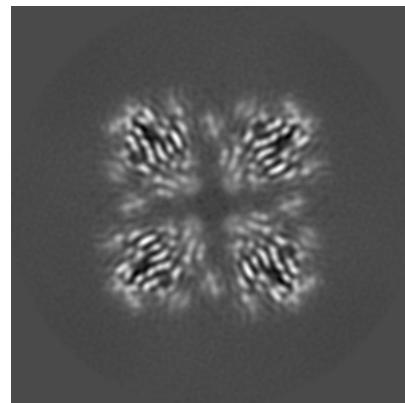
6.3.2　Raw map
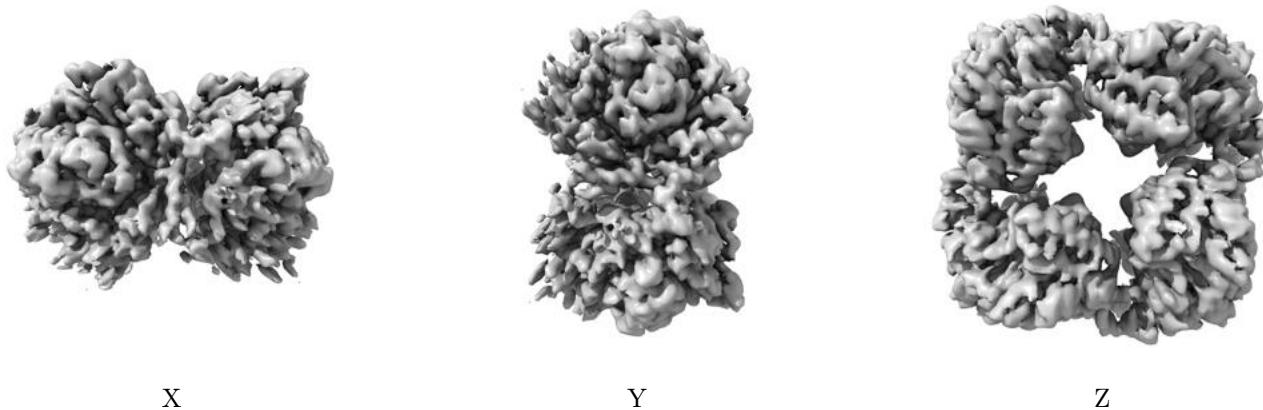
| X Index: 50 | Y Index: 98 | Z Index: 71 |

The images above show the largest variance slices of the map in three orthogonal directions.
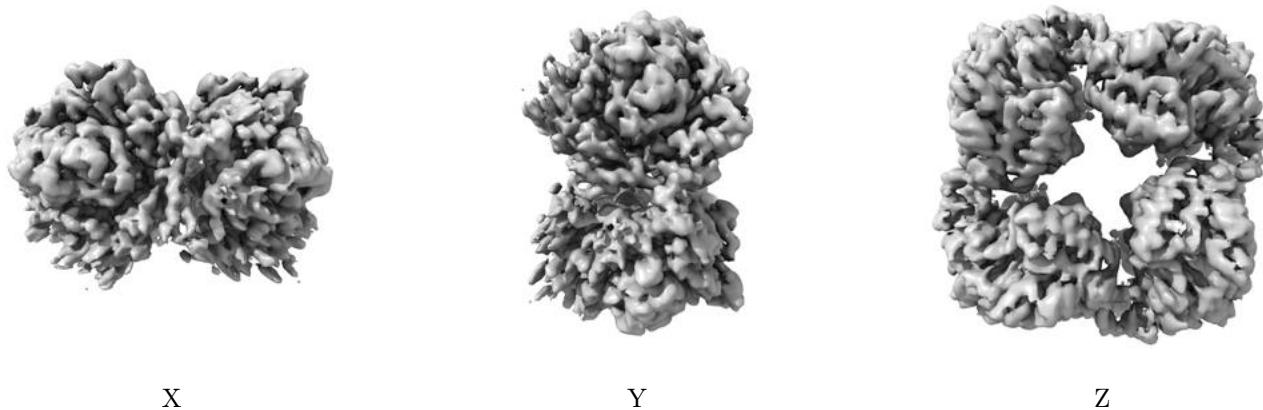
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.
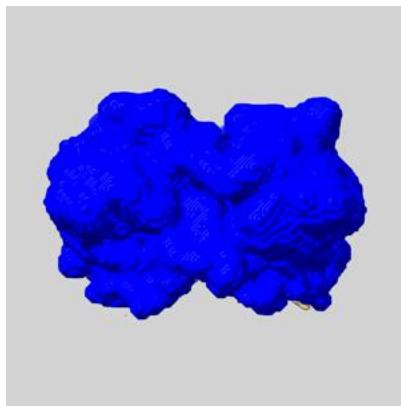
6.5　Mask visualisation ⓘ

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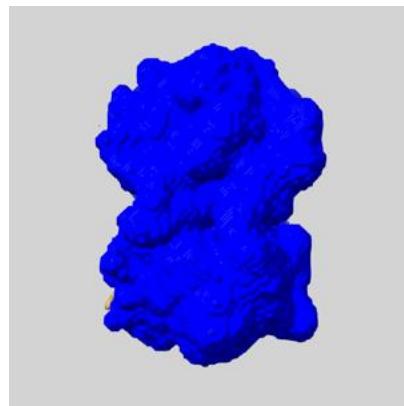
A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure
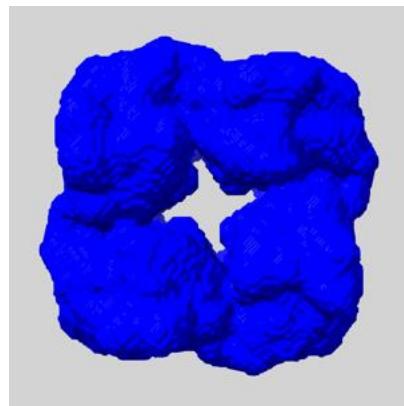
6.5.1　emd_25391_msk_1.map ⓘ

X　　　　　　　　　　　Y　　　　　　　　　　　Z
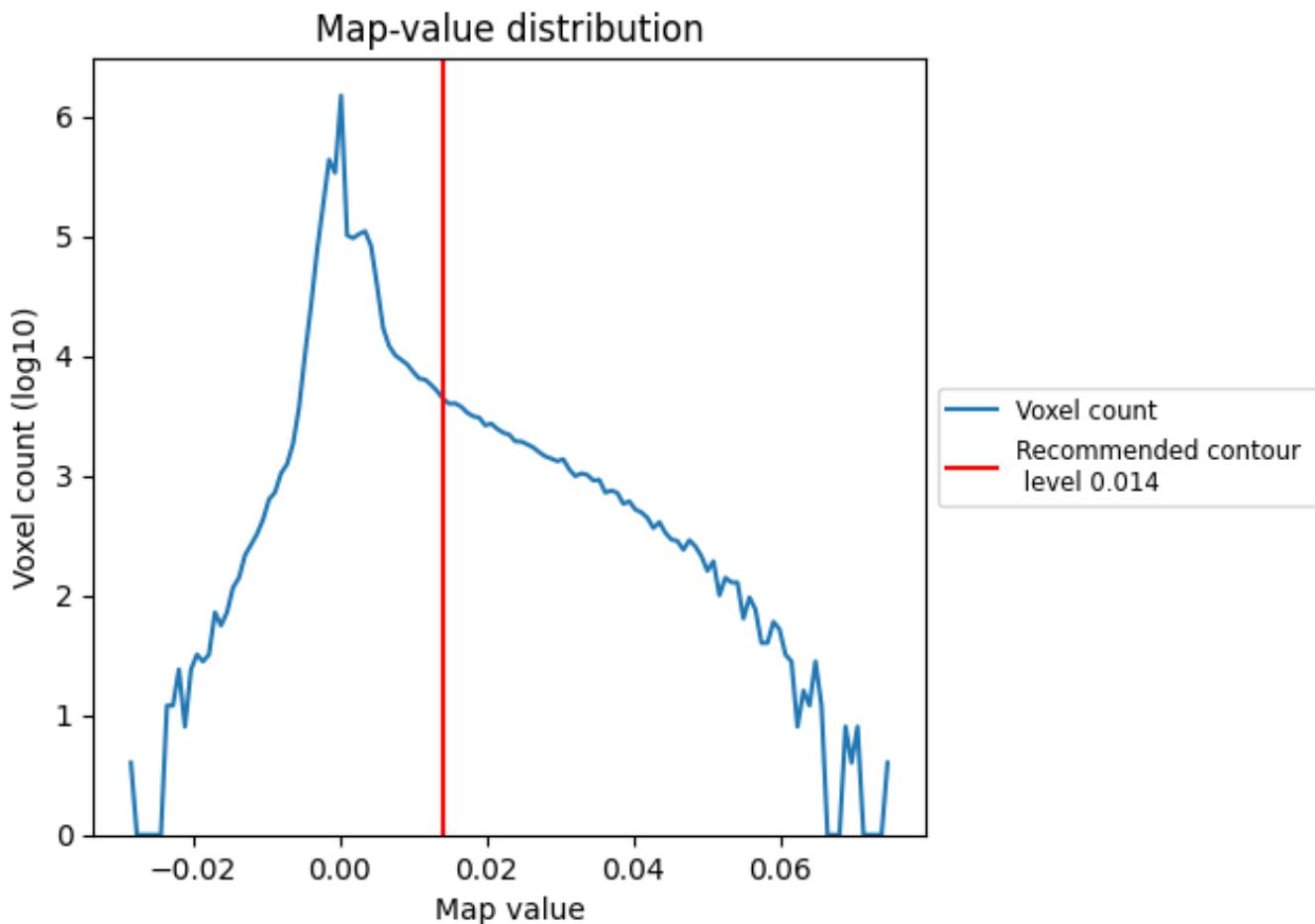
7   Map analysis ⓘ
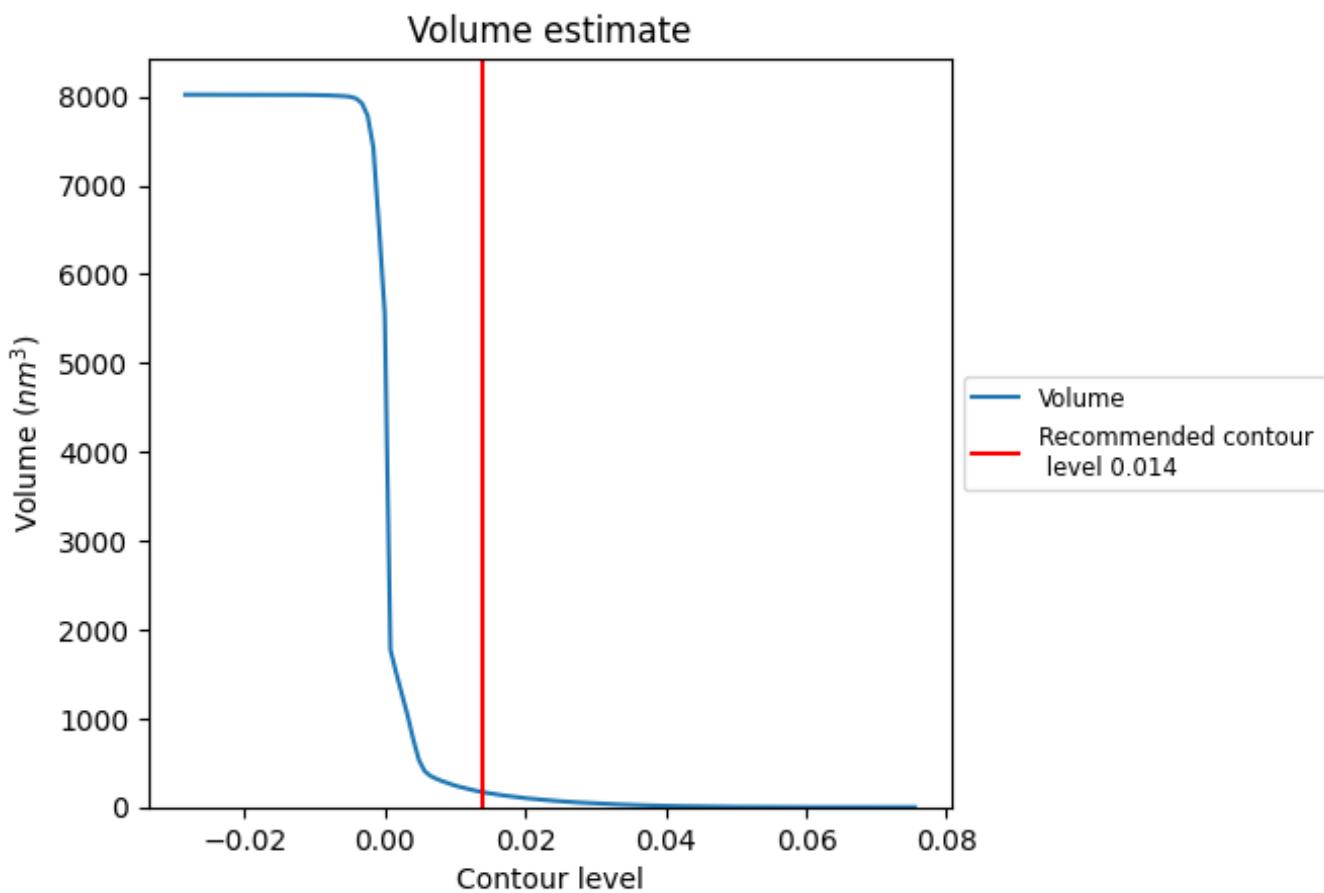
This section contains the results of statistical analysis of the map.

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.
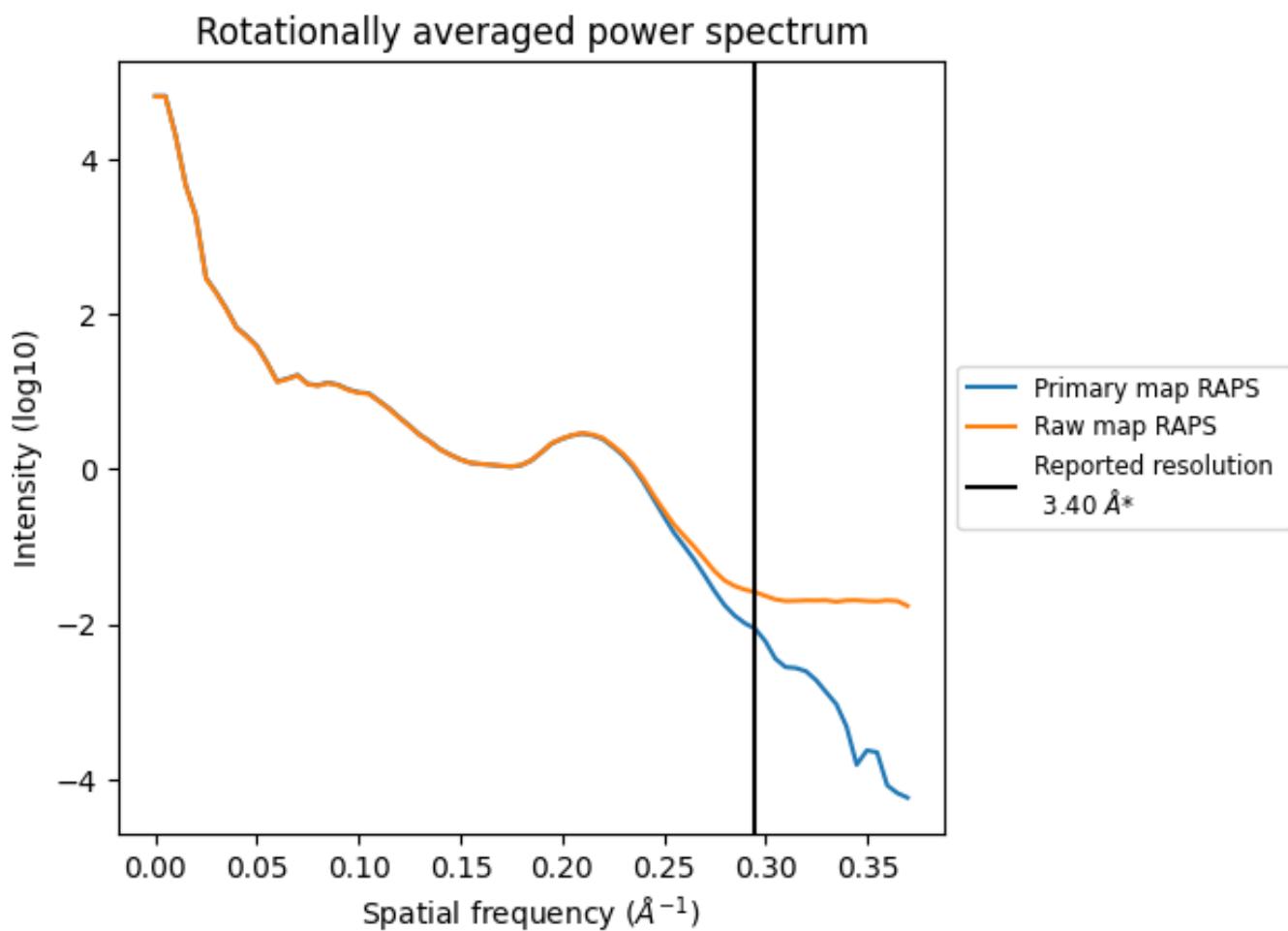
7.2 Volume estimate ⓘ

The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 152 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ
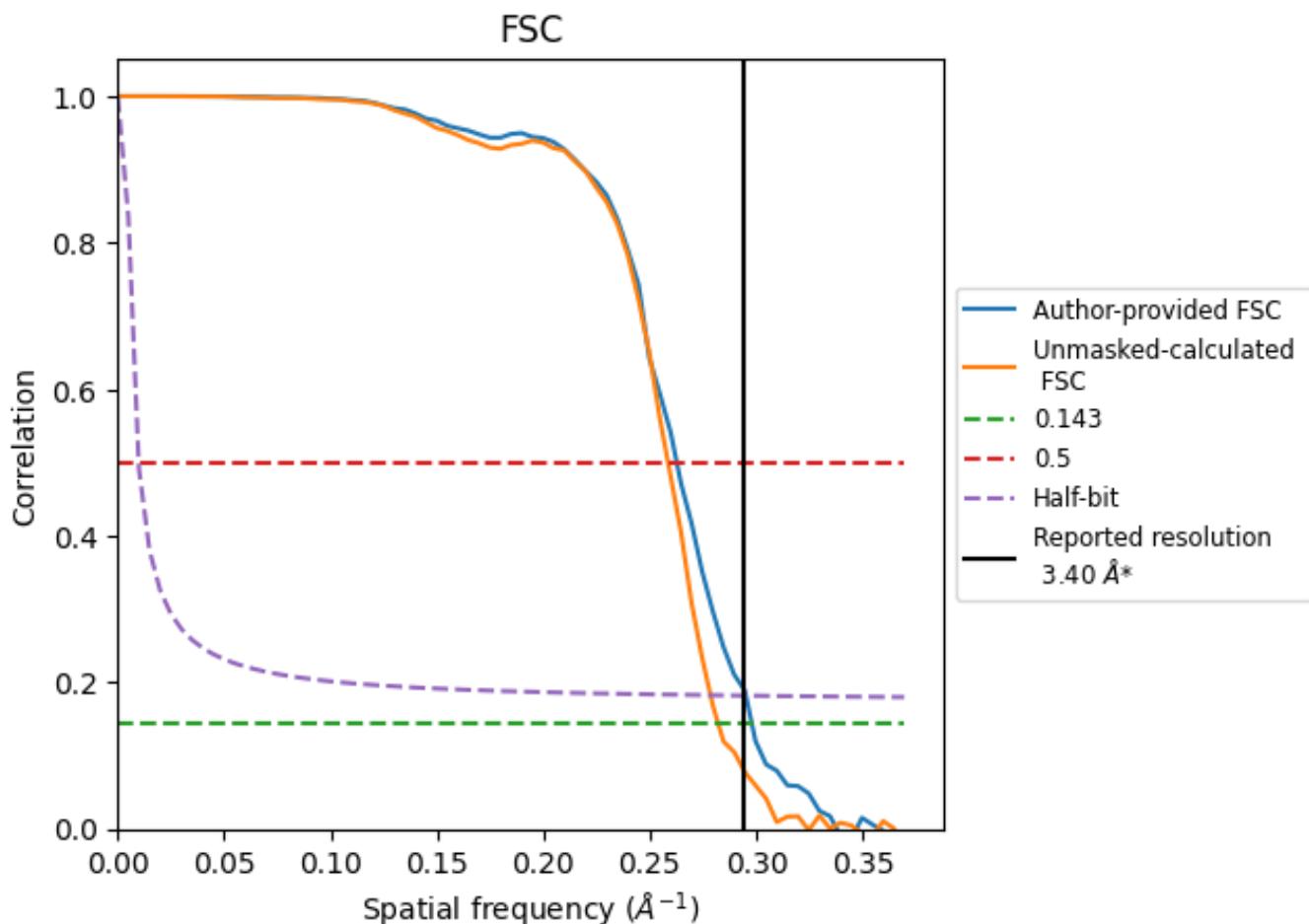
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2　Resolution estimates　ⓘ
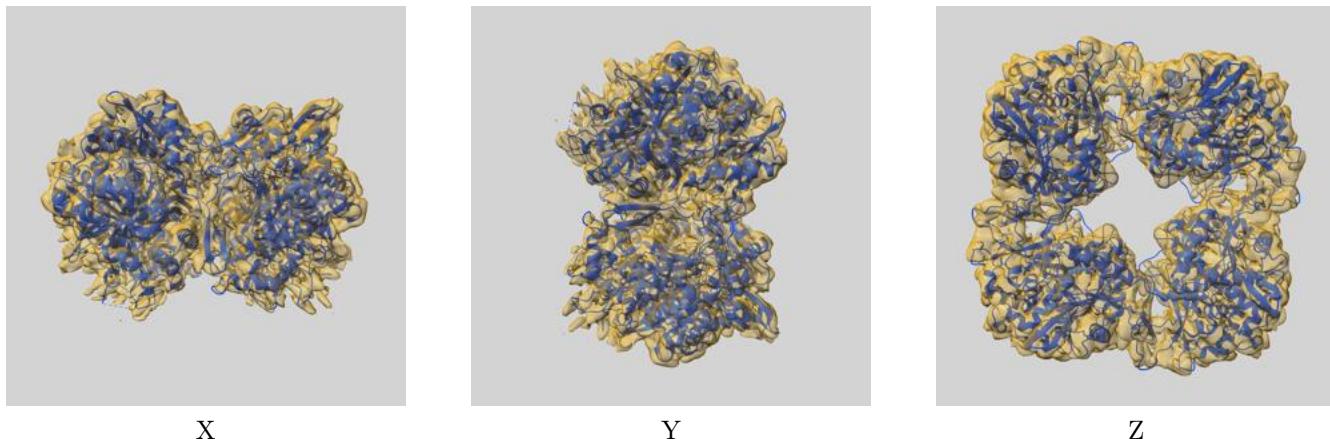
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.81	3.39
Unmasked-calculated*	3.54	3.87	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ
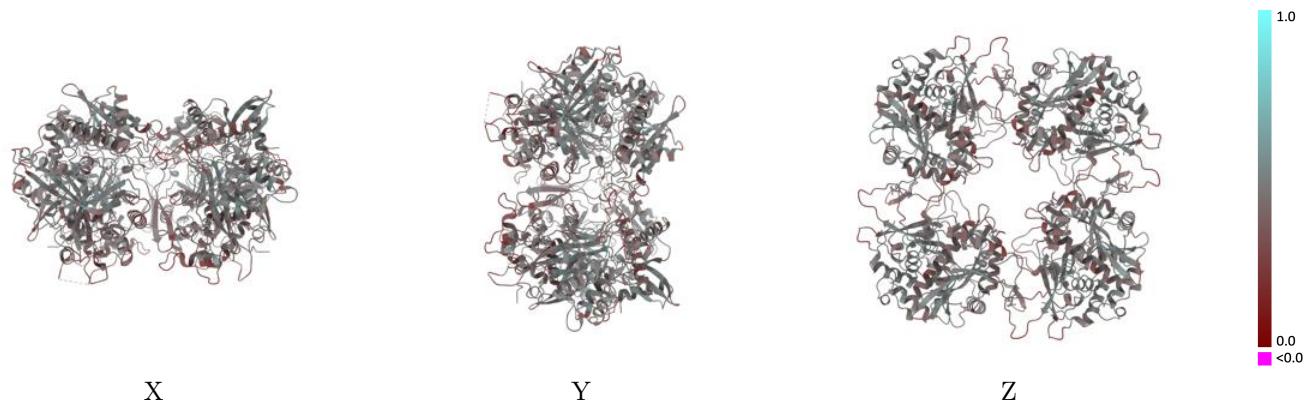
This section contains information regarding the fit between EMDB map EMD-25391 and PDB model 7SQR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

| X | Y | Z |
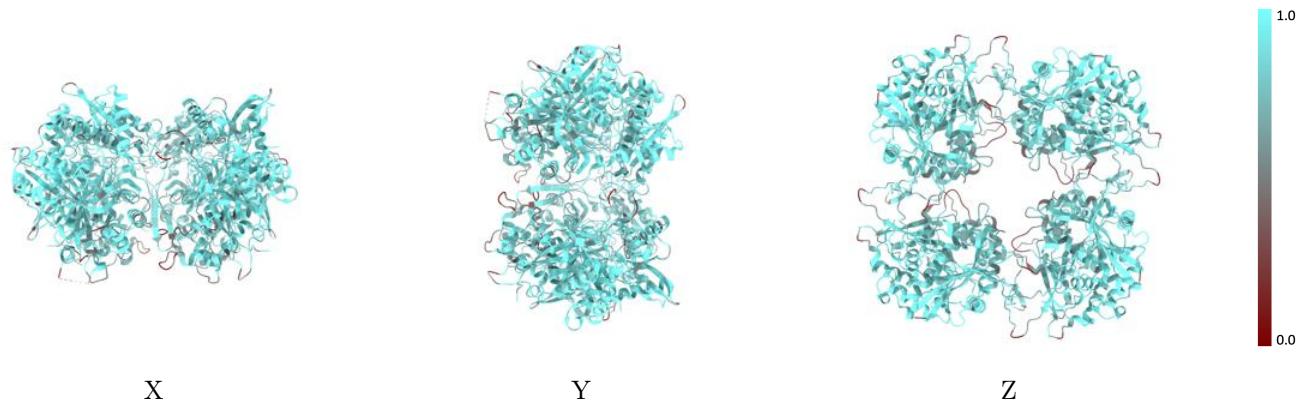
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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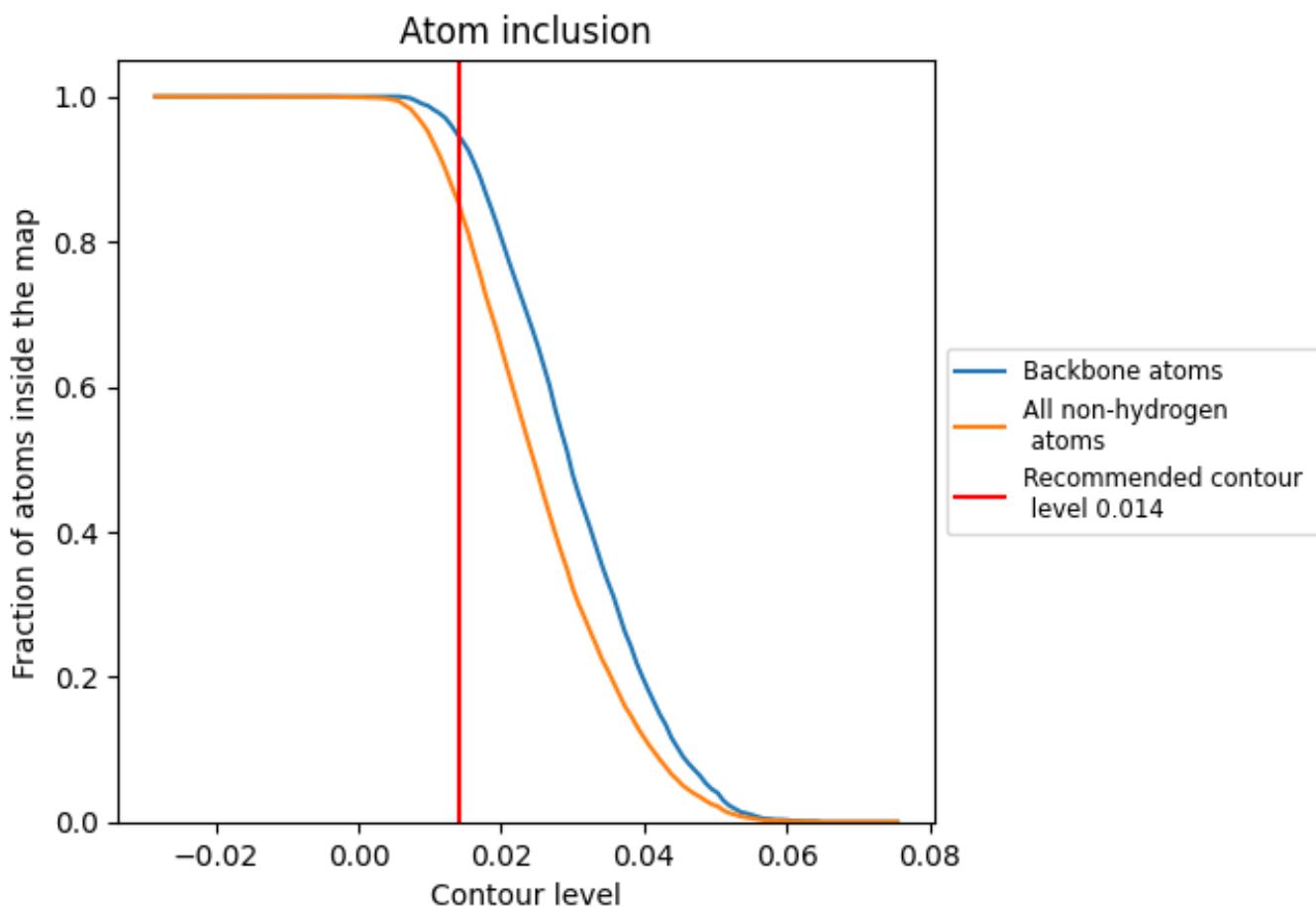
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.014).

9.4 Atom inclusion ⓘ

At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8540	0.4330
A	0.8550	0.4340
B	0.8012	0.4260
C	0.9136	0.4470
D	0.8550	0.4330
E	0.8012	0.4210
F	0.9136	0.4480
G	0.8548	0.4330
H	0.8012	0.4230
I	0.9136	0.4410
J	0.8550	0.4330
K	0.8012	0.4310
L	0.9136	0.4340

1.0

0.0
<0.0