



## Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 08:33 PM EST

PDB ID : 6NUW  
EMDB ID : EMD-0523  
Title : Yeast Ctf19 complex  
Authors : Hinshaw, S.M.; Harrison, S.C.  
Deposited on : 2019-02-03  
Resolution : 4.25 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

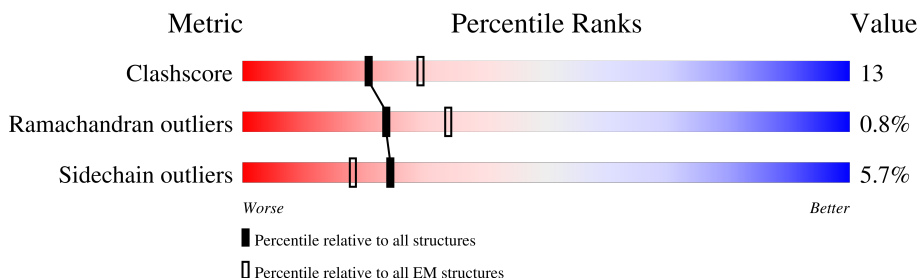
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.25 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)
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	248	<div> <div>6%</div> <div>62%</div> <div>35%</div> <div>..</div> </div>
2	C	371	<div> <div>34%</div> <div>16%</div> <div>48%</div> <div>.</div> </div>
3	D	369	<div> <div>29%</div> <div>19%</div> <div>5%</div> <div>47%</div> <div>.</div> </div>
4	E	461	<div> <div>6%</div> <div>54%</div> <div>23%</div> <div>20%</div> <div>.</div> </div>
5	F	406	<div> <div>14%</div> <div>39%</div> <div>7%</div> <div>53%</div> </div>
6	G	241	<div> <div>17%</div> <div>65%</div> <div>7%</div> <div>27%</div> <div>.</div> </div>
7	I	330	<div> <div>11%</div> <div>41%</div> <div>10%</div> <div>49%</div> </div>
8	H	773	<div> <div>33%</div> <div>6%</div> <div>61%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	Y	773	<div><div></div><div>19%81%</div></div>
9	J	153	<div><div></div><div>24%75%20%</div></div>
10	X	126	<div><div></div><div>95%5%</div></div>
11	M	75	<div><div></div><div>95%5%</div></div>
12	U	23	<div><div></div><div>87%100%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16292 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 Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	244	Total	C	N	O	S	0	0
			1962	1256	324	370	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P38265
B	-1	ASN	-	expression tag	UNP P38265
B	0	ALA	-	expression tag	UNP P38265

- Molecule 2 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	194	Total	C	N	O	S	0	0
			1601	1039	261	297	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q06675
C	-1	ASN	-	expression tag	UNP Q06675
C	0	ALA	-	expression tag	UNP Q06675

- Molecule 3 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	196	Total	C	N	O	S	0	0
			1578	1011	277	280	10		

- Molecule 4 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	369	Total	C	N	O	S	0	0
			2851	1848	492	500	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	expression tag	UNP P38907
E	-1	ASN	-	expression tag	UNP P38907
E	0	ALA	-	expression tag	UNP P38907

- Molecule 5 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	190	Total	C	N	O	S	0	0
			1360	835	247	273	5		

- Molecule 6 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	176	Total	C	N	O	S	0	0
			1114	678	212	222	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	SER	-	expression tag	UNP Q12493
G	-1	ASN	-	expression tag	UNP Q12493
G	0	ALA	-	expression tag	UNP Q12493

- Molecule 7 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	168	Total	C	N	O	S	0	0
			1295	807	231	253	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	325	HIS	-	expression tag	UNP P38313
I	326	HIS	-	expression tag	UNP P38313
I	327	HIS	-	expression tag	UNP P38313
I	328	HIS	-	expression tag	UNP P38313

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	329	HIS	-	expression tag	UNP P38313
I	330	HIS	-	expression tag	UNP P38313

- Molecule 8 is a protein called Inner kinetochore subunit CTF3, Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	302	Total	C	N	O	S	0	0
			1668	1026	319	322	1		
8	Y	150	Total	C	N	O		0	0
			746	446	150	150			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	SER	-	expression tag	UNP Q12748
H	-1	ASN	-	expression tag	UNP Q12748
H	0	ALA	-	expression tag	UNP Q12748
Y	-2	SER	-	expression tag	UNP Q12748
Y	-1	ASN	-	expression tag	UNP Q12748
Y	0	ALA	-	expression tag	UNP Q12748

- Molecule 9 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	147	Total	C	N	O	0	0
			997	618	184	195		

- Molecule 10 is a protein called Inner kinetochore subunit Mcm22.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	126	Total	C	N	O	0	0
			630	378	126	126		

- Molecule 11 is a protein called Inner kinetochore subunit Mcm16.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	75	Total	C	N	O	0	0
			375	225	75	75		

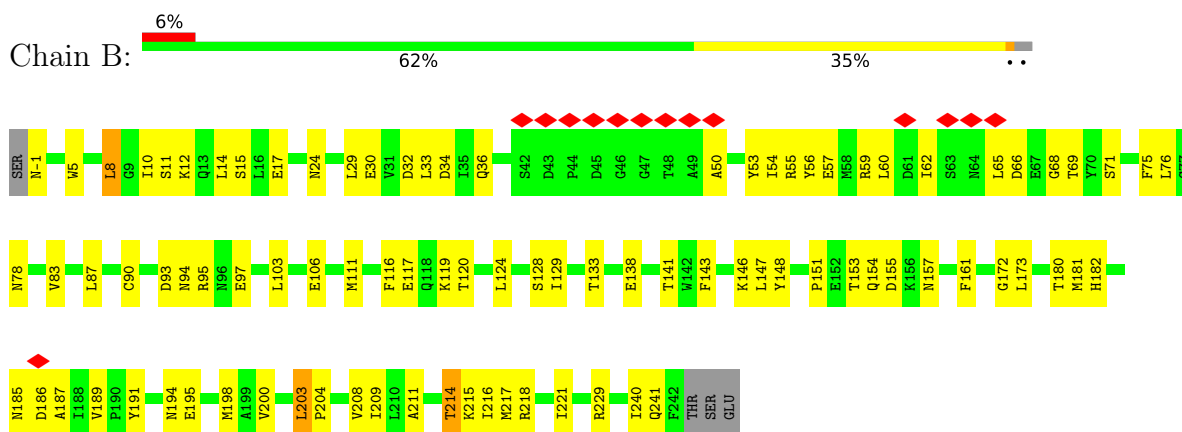
- Molecule 12 is a protein called Unknown (unassigned).

Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	23	Total	C	N	O	0	0
			115	69	23	23		

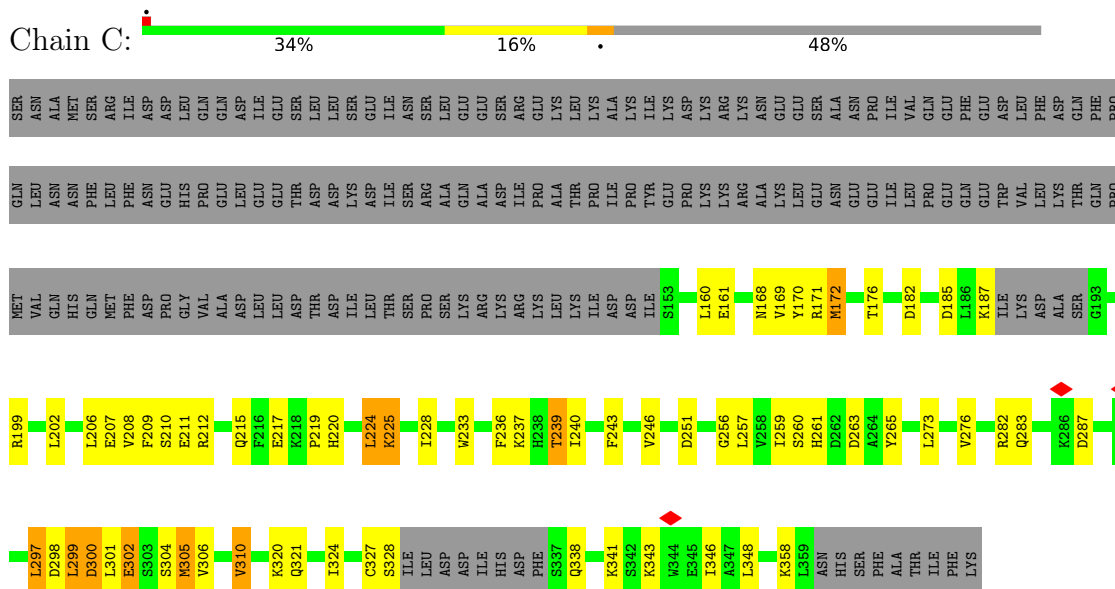
### 3 Residue-property plots

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.

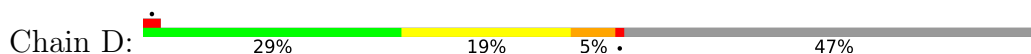
#### • Molecule 1: Inner kinetochore subunit IML3



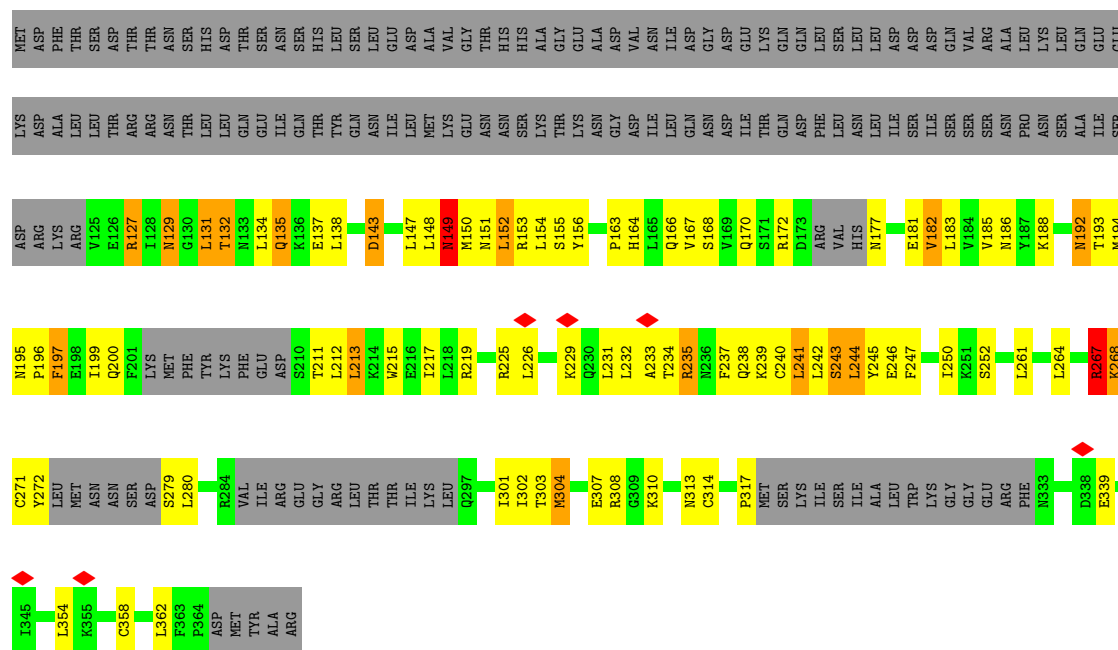
#### • Molecule 2: Inner kinetochore subunit MCM21



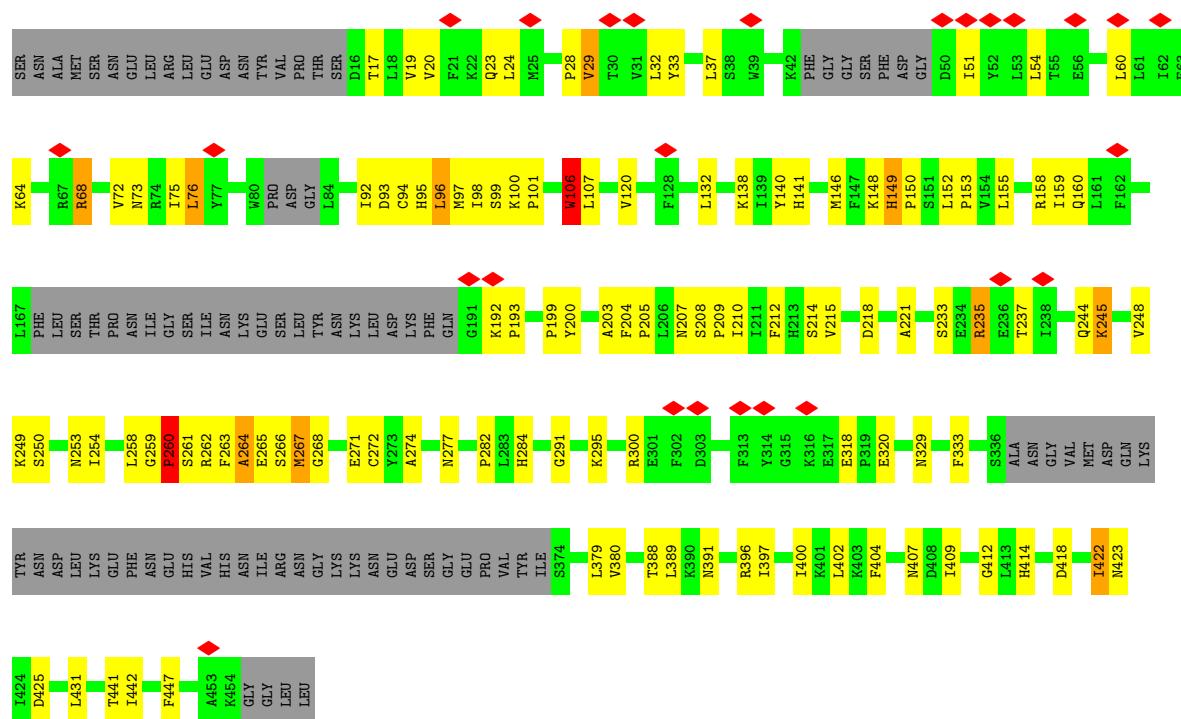
#### • Molecule 3: Inner kinetochore subunit CTF19



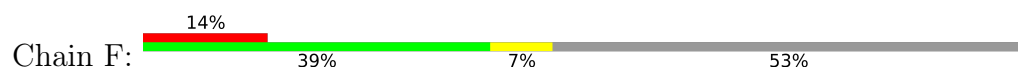




• Molecule 4: Inner kinetochore subunit CHL4

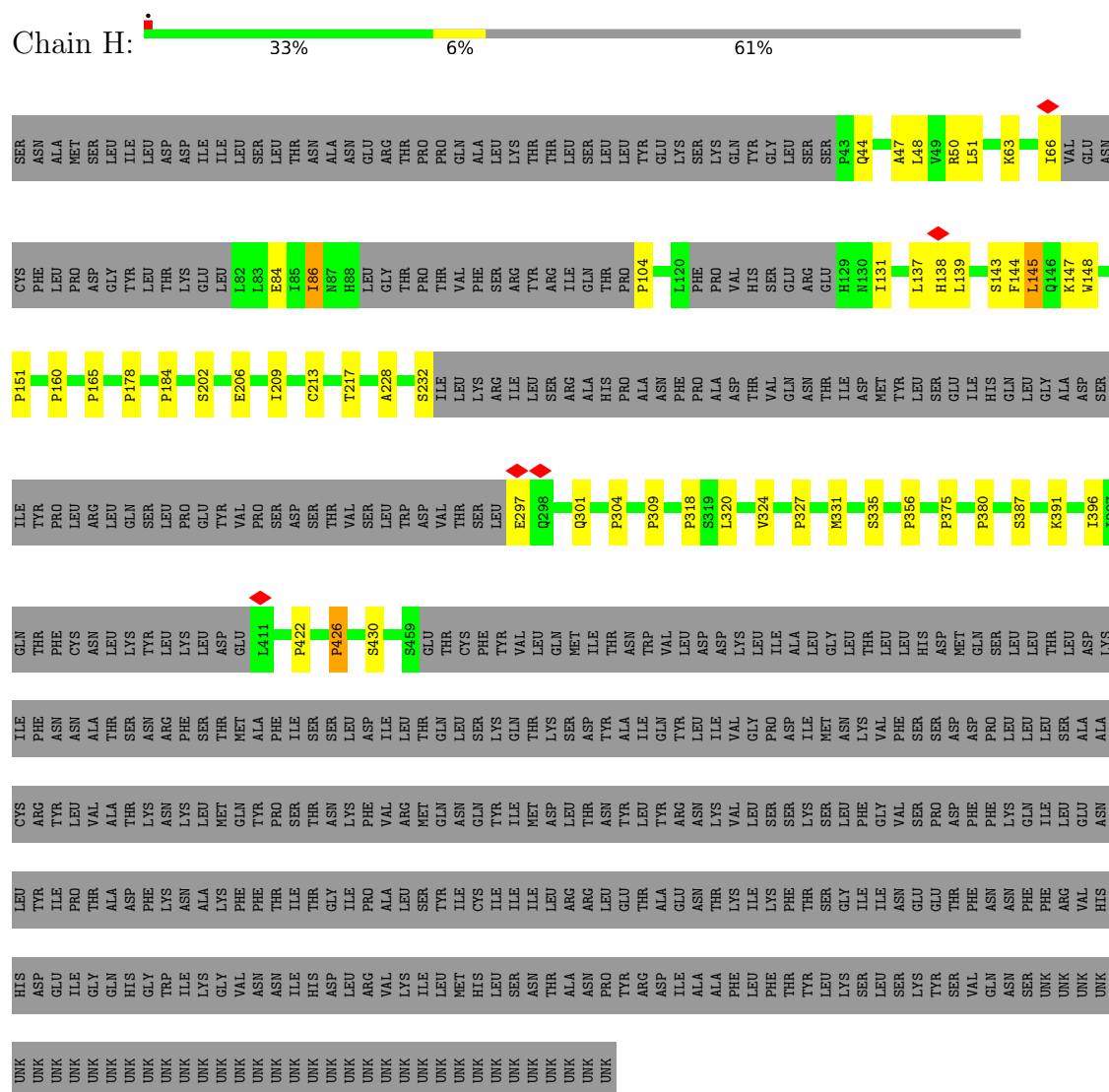


• Molecule 5: Inner kinetochore subunit OKP1

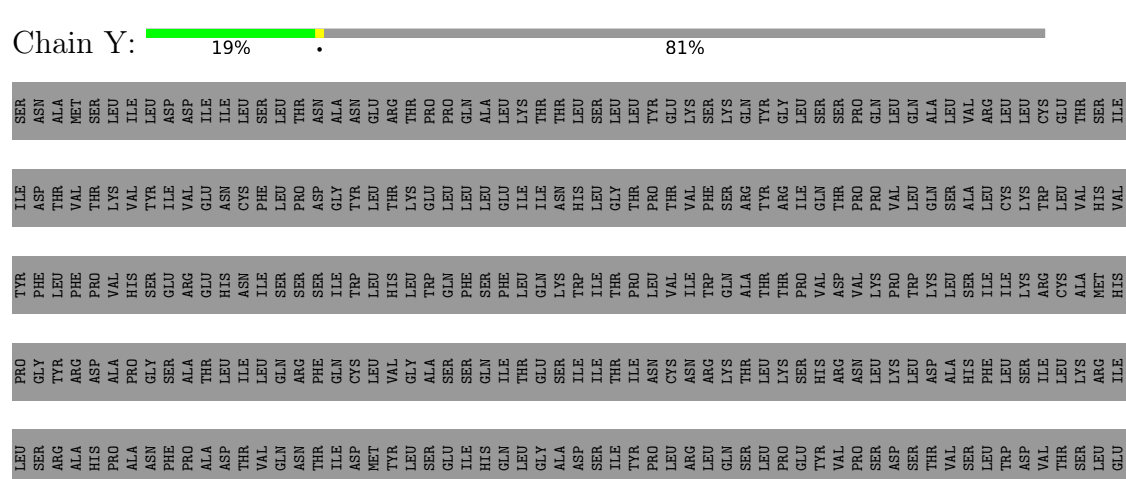




● Molecule 8: Inner kinetochore subunit CTF3, Inner kinetochore subunit CTF3



● Molecule 8: Inner kinetochore subunit CTF3, Inner kinetochore subunit CTF3





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	119469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47	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	0.175	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	373.92, 373.92, 373.92	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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	B	0.76	1/2002 (0.0%)	0.83	2/2713 (0.1%)
2	C	0.79	0/1630	0.87	1/2190 (0.0%)
3	D	0.52	0/1598	0.77	1/2146 (0.0%)
4	E	0.74	1/2912 (0.0%)	0.88	6/3943 (0.2%)
5	F	0.36	0/1367	0.65	2/1845 (0.1%)
6	G	0.36	0/1115	0.62	2/1513 (0.1%)
7	I	0.37	0/1303	0.76	1/1754 (0.1%)
8	H	0.46	0/1674	0.74	16/2316 (0.7%)
8	Y	0.37	0/556	0.51	2/768 (0.3%)
9	J	0.36	0/1006	0.65	3/1371 (0.2%)
All	All	0.59	2/15163 (0.0%)	0.77	36/20559 (0.2%)

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	C	0	1
3	D	0	6
4	E	0	8
6	G	0	1
8	H	0	2
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	106	TRP	CB-CG	-7.07	1.37	1.50
1	B	5	TRP	CB-CG	-5.75	1.39	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	260	PRO	CA-N-CD	-8.54	99.54	111.50
9	J	129	PRO	N-CA-CB	7.12	111.85	103.30
9	J	46	LEU	CA-CB-CG	6.74	130.81	115.30
8	H	184	PRO	N-CA-CB	6.51	111.11	103.30
5	F	340	ILE	CG1-CB-CG2	-6.17	97.82	111.40
8	H	422	PRO	N-CA-CB	6.04	110.55	103.30
8	H	104	PRO	N-CA-CB	6.03	110.54	103.30
8	H	151	PRO	N-CA-CB	6.02	110.53	103.30
4	E	193	PRO	N-CA-CB	6.00	110.50	103.30
3	D	317	PRO	N-CA-CB	5.88	110.36	103.30
8	H	86	ILE	CG1-CB-CG2	-5.88	98.47	111.40
6	G	62	LEU	CA-CB-CG	5.83	128.71	115.30
8	H	178	PRO	N-CA-CB	5.83	110.30	103.30
2	C	297	LEU	CA-CB-CG	5.81	128.66	115.30
5	F	224	PRO	N-CA-CB	5.80	110.26	103.30
8	H	165	PRO	N-CA-CB	5.78	110.24	103.30
8	H	318	PRO	N-CA-CB	5.75	110.20	103.30
8	H	375	PRO	N-CA-CB	5.70	110.14	103.30
6	G	35	PRO	N-CA-CB	5.68	110.11	103.30
9	J	137	PRO	N-CA-CB	5.53	109.94	103.30
8	H	380	PRO	N-CA-CB	5.48	109.88	103.30
8	Y	318	PRO	N-CA-CB	5.47	109.86	103.30
8	H	304	PRO	N-CA-CB	5.46	109.85	103.30
4	E	76	LEU	CA-CB-CG	5.44	127.82	115.30
4	E	402	LEU	CB-CG-CD2	-5.42	101.78	111.00
8	H	160	PRO	N-CA-CB	5.42	109.80	103.30
8	H	309	PRO	N-CA-CB	5.41	109.80	103.30
8	Y	356	PRO	N-CA-CB	5.40	109.78	103.30
8	H	356	PRO	N-CA-CB	5.29	109.64	103.30
1	B	90	CYS	C-N-CA	5.28	133.39	122.30
7	I	191	ASP	CB-CG-OD2	5.22	123.00	118.30
8	H	327	PRO	N-CA-CB	5.13	109.45	103.30
4	E	259	GLY	C-N-CD	5.07	139.05	128.40
1	B	173	LEU	CA-CB-CG	-5.05	103.69	115.30
4	E	106	TRP	CA-CB-CG	-5.04	104.13	113.70
8	H	426	PRO	N-CA-CB	5.03	109.34	103.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	310	VAL	Peptide
3	D	147	LEU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
3	D	149	ASN	Peptide
3	D	167	VAL	Peptide
3	D	197	PHE	Peptide
3	D	213	LEU	Peptide
3	D	304	MET	Peptide
4	E	140	TYR	Peptide
4	E	149	HIS	Peptide
4	E	152	LEU	Peptide
4	E	153	PRO	Peptide
4	E	235	ARG	Peptide
4	E	29	VAL	Peptide
4	E	422	ILE	Peptide
4	E	423	ASN	Peptide
6	G	90	LYS	Peptide
8	H	138	HIS	Peptide
8	H	143	SER	Peptide

## 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	B	1962	0	1968	54	0
2	C	1601	0	1618	88	0
3	D	1578	0	1614	125	0
4	E	2851	0	2789	94	0
5	F	1360	0	1181	14	0
6	G	1114	0	867	13	0
7	I	1295	0	1241	20	0
8	H	1668	0	945	18	0
8	Y	746	0	274	2	0
9	J	997	0	792	20	0
10	X	630	0	133	3	0
11	M	375	0	80	3	0
12	U	115	0	25	0	0
All	All	16292	0	13527	399	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 13.



All (399) 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)
3:D:234:THR:HA	3:D:235:ARG:CZ	1.41	1.47
3:D:134:LEU:CD2	3:D:150:MET:HE2	1.46	1.45
2:C:297:LEU:CD1	2:C:299:LEU:HD21	1.51	1.40
3:D:234:THR:HA	3:D:235:ARG:NH2	1.30	1.39
3:D:134:LEU:CD2	3:D:150:MET:CE	2.01	1.39
2:C:297:LEU:CD1	2:C:299:LEU:CD2	2.00	1.39
3:D:234:THR:C	3:D:235:ARG:NH1	1.90	1.25
2:C:302:GLU:OE2	4:E:207:ASN:CG	1.76	1.24
2:C:297:LEU:HD13	2:C:299:LEU:CD2	1.62	1.22
3:D:234:THR:CA	3:D:235:ARG:CZ	2.17	1.22
2:C:297:LEU:HD11	2:C:299:LEU:CD2	1.68	1.16
2:C:298:ASP:C	2:C:299:LEU:HD23	1.65	1.16
3:D:234:THR:CA	3:D:235:ARG:NH1	2.10	1.15
3:D:134:LEU:HD21	3:D:150:MET:CE	1.70	1.12
2:C:209:PHE:N	3:D:238:GLN:HE22	1.47	1.11
3:D:134:LEU:HD22	3:D:150:MET:HE3	1.30	1.09
2:C:300:ASP:OD2	2:C:305:MET:N	1.85	1.07
2:C:302:GLU:OE2	4:E:207:ASN:CB	2.04	1.03
3:D:233:ALA:C	3:D:235:ARG:HH12	1.60	1.03
2:C:297:LEU:CD1	2:C:299:LEU:HD22	1.88	1.02
2:C:297:LEU:HD11	2:C:299:LEU:HD22	1.37	1.02
3:D:234:THR:CA	3:D:235:ARG:NH2	2.23	1.01
3:D:233:ALA:O	3:D:235:ARG:NH1	1.92	1.01
2:C:302:GLU:OE2	4:E:207:ASN:ND2	1.93	1.00
2:C:219:PRO:O	4:E:262:ARG:NH2	1.96	0.99
3:D:132:THR:HG22	3:D:150:MET:HG3	1.45	0.98
2:C:300:ASP:OD1	2:C:305:MET:O	1.84	0.95
3:D:134:LEU:CD2	3:D:150:MET:HE3	1.85	0.94
2:C:209:PHE:H	3:D:238:GLN:HE22	1.13	0.90
2:C:209:PHE:N	3:D:238:GLN:NE2	2.21	0.89
3:D:239:LYS:HG3	3:D:310:LYS:NZ	1.89	0.87
2:C:302:GLU:CD	4:E:207:ASN:ND2	2.28	0.87
3:D:241:LEU:O	3:D:241:LEU:HD12	1.76	0.85
2:C:302:GLU:OE1	2:C:302:GLU:N	2.11	0.84
3:D:134:LEU:HD21	3:D:150:MET:HE2	0.86	0.83
3:D:234:THR:HA	3:D:235:ARG:HH22	1.45	0.82
2:C:302:GLU:OE2	4:E:207:ASN:HB3	1.79	0.82
3:D:215:TRP:CH2	3:D:232:LEU:HD22	2.14	0.82
2:C:209:PHE:H	3:D:238:GLN:NE2	1.76	0.80
2:C:297:LEU:HD13	2:C:299:LEU:HD23	1.64	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:LEU:HD11	3:D:131:LEU:CD2	2.13	0.78
3:D:135:GLN:HA	3:D:135:GLN:NE2	1.97	0.78
2:C:297:LEU:HD13	2:C:299:LEU:HD21	1.36	0.78
3:D:233:ALA:O	3:D:235:ARG:CZ	2.32	0.78
2:C:160:LEU:HD11	3:D:131:LEU:HD21	1.66	0.77
2:C:239:THR:OG1	4:E:262:ARG:CG	2.31	0.77
3:D:239:LYS:HD2	3:D:310:LYS:HZ2	1.49	0.77
2:C:298:ASP:C	2:C:299:LEU:CD2	2.51	0.76
2:C:239:THR:OG1	4:E:262:ARG:HG3	1.84	0.76
3:D:234:THR:C	3:D:235:ARG:CZ	2.47	0.76
2:C:297:LEU:HD11	2:C:299:LEU:HD21	1.37	0.75
3:D:239:LYS:CG	3:D:310:LYS:NZ	2.49	0.75
2:C:302:GLU:OE1	4:E:207:ASN:ND2	2.20	0.74
3:D:215:TRP:HH2	3:D:232:LEU:HD22	1.50	0.74
2:C:299:LEU:HD23	2:C:299:LEU:N	2.02	0.72
3:D:233:ALA:O	3:D:235:ARG:NH2	2.23	0.71
4:E:267:MET:SD	4:E:267:MET:N	2.63	0.71
2:C:220:HIS:HA	4:E:262:ARG:NH2	2.04	0.71
2:C:299:LEU:HB3	2:C:306:VAL:HG12	1.72	0.70
3:D:239:LYS:HG3	3:D:310:LYS:HZ1	1.56	0.69
2:C:208:VAL:C	3:D:238:GLN:HE22	1.94	0.69
3:D:150:MET:SD	3:D:150:MET:N	2.62	0.69
3:D:234:THR:O	3:D:235:ARG:NH1	2.26	0.69
3:D:234:THR:N	3:D:235:ARG:HH12	1.89	0.69
1:B:34:ASP:HB3	1:B:57:GLU:HB2	1.74	0.69
2:C:298:ASP:CA	2:C:299:LEU:HD23	2.23	0.69
2:C:301:LEU:HD13	2:C:301:LEU:C	2.14	0.68
3:D:168:SER:OG	3:D:170:GLN:NE2	2.27	0.68
3:D:215:TRP:HZ2	3:D:235:ARG:HA	1.57	0.67
3:D:170:GLN:HE22	3:D:181:GLU:HG2	1.59	0.67
4:E:32:LEU:HD22	4:E:100:LYS:NZ	2.10	0.67
3:D:131:LEU:HD12	3:D:131:LEU:O	1.95	0.67
5:F:327:ASN:O	5:F:331:GLU:HB2	1.95	0.67
3:D:239:LYS:CD	3:D:310:LYS:HZ2	2.07	0.67
2:C:239:THR:OG1	4:E:262:ARG:HG2	1.97	0.65
3:D:231:LEU:HD21	3:D:304:MET:HG2	1.78	0.65
3:D:239:LYS:HG3	3:D:310:LYS:CE	2.27	0.65
2:C:237:LYS:HG2	4:E:265:GLU:HB3	1.77	0.65
3:D:182:VAL:HG12	3:D:196:PRO:HD3	1.78	0.65
3:D:239:LYS:CD	3:D:310:LYS:NZ	2.59	0.65
2:C:263:ASP:OD1	2:C:263:ASP:N	2.29	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:243:SER:O	3:D:247:PHE:CB	2.45	0.65
8:H:48:LEU:HD13	8:H:51:LEU:HD12	1.79	0.64
4:E:19:VAL:O	4:E:23:GLN:NE2	2.30	0.64
3:D:134:LEU:HD22	3:D:150:MET:CE	1.88	0.64
3:D:272:TYR:C	3:D:279:SER:HA	2.17	0.64
1:B:68:GLY:O	1:B:95:ARG:NH2	2.31	0.63
2:C:243:PHE:CE1	2:C:301:LEU:HD11	2.33	0.63
1:B:143:PHE:HB3	1:B:211:ALA:HB3	1.80	0.63
3:D:134:LEU:HD23	3:D:150:MET:CE	2.20	0.63
3:D:234:THR:C	3:D:235:ARG:HH11	1.97	0.63
9:J:76:LEU:HG	9:J:77:GLU:HG3	1.81	0.63
4:E:263:PHE:HA	4:E:266:SER:OG	1.99	0.62
3:D:239:LYS:HD2	3:D:310:LYS:NZ	2.14	0.62
4:E:93:ASP:HA	4:E:96:LEU:HB2	1.82	0.62
3:D:239:LYS:CG	3:D:310:LYS:HZ2	2.12	0.62
3:D:271:CYS:SG	3:D:272:TYR:N	2.73	0.61
7:I:246:LEU:O	7:I:250:VAL:HB	2.00	0.61
3:D:127:ARG:HH21	3:D:127:ARG:HG3	1.65	0.61
7:I:290:LEU:O	7:I:294:HIS:ND1	2.30	0.61
8:H:63:LYS:NZ	8:H:84:GLU:OE1	2.33	0.61
1:B:172:GLY:HA2	4:E:396:ARG:HE	1.65	0.60
2:C:182:ASP:N	2:C:182:ASP:OD1	2.32	0.60
4:E:333:PHE:HD2	4:E:414:HIS:HB3	1.66	0.60
3:D:243:SER:O	3:D:247:PHE:N	2.30	0.60
4:E:263:PHE:CD2	4:E:266:SER:OG	2.54	0.60
4:E:263:PHE:CE2	4:E:274:ALA:HB1	2.36	0.60
2:C:302:GLU:CD	4:E:207:ASN:HD22	2.05	0.60
6:G:51:LYS:HB3	9:J:22:PHE:HE1	1.65	0.60
4:E:106:TRP:H	4:E:248:VAL:HG11	1.67	0.60
1:B:24:ASN:ND2	1:B:30:GLU:OE1	2.35	0.60
3:D:127:ARG:HH21	3:D:127:ARG:CG	2.15	0.60
3:D:234:THR:CA	3:D:235:ARG:HH12	2.00	0.59
2:C:300:ASP:OD1	2:C:300:ASP:N	2.35	0.59
4:E:329:ASN:ND2	4:E:418:ASP:OD1	2.35	0.59
2:C:300:ASP:CG	2:C:305:MET:H	1.98	0.59
3:D:194:MET:HG2	3:D:217:ILE:HD13	1.85	0.59
4:E:218:ASP:H	4:E:221:ALA:HB3	1.68	0.59
2:C:224:LEU:HD13	2:C:233:TRP:HB3	1.85	0.58
2:C:187:LYS:NZ	4:E:300:ARG:O	2.34	0.58
6:G:40:ARG:NH2	9:J:31:SER:OG	2.36	0.58
1:B:56:TYR:HB2	1:B:75:PHE:HB2	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:TYR:HB3	1:B:76:LEU:HD21	1.84	0.58
7:I:260:THR:O	7:I:264:LEU:HB2	2.04	0.58
3:D:339:GLU:OE2	7:I:255:ARG:NH2	2.37	0.58
1:B:154:GLN:O	1:B:157:ASN:ND2	2.37	0.57
4:E:262:ARG:HG2	4:E:262:ARG:O	2.04	0.57
2:C:185:ASP:OD1	2:C:185:ASP:N	2.37	0.57
9:J:40:GLN:HA	9:J:43:TYR:HD2	1.69	0.57
3:D:166:GLN:O	3:D:183:LEU:N	2.33	0.57
3:D:177:ASN:N	3:D:199:ILE:O	2.38	0.57
5:F:246:ASN:O	5:F:250:GLN:NE2	2.38	0.57
1:B:181:MET:SD	1:B:181:MET:N	2.78	0.57
3:D:241:LEU:HD12	3:D:241:LEU:C	2.23	0.57
6:G:90:LYS:HB3	6:G:93:LEU:HD21	1.86	0.57
6:G:119:LYS:NZ	9:J:86:SER:O	2.38	0.57
3:D:134:LEU:HD23	3:D:150:MET:HE2	1.72	0.57
4:E:97:MET:O	4:E:100:LYS:HB2	2.04	0.57
4:E:263:PHE:O	4:E:264:ALA:C	2.43	0.57
4:E:272:CYS:SG	4:E:277:ASN:ND2	2.78	0.56
1:B:-1:ASN:HB3	1:B:215:LYS:HZ2	1.70	0.56
2:C:208:VAL:HA	3:D:238:GLN:HE22	1.71	0.56
3:D:186:ASN:HD22	3:D:192:ASN:HB3	1.71	0.56
3:D:215:TRP:CZ3	3:D:232:LEU:HD22	2.40	0.56
3:D:243:SER:O	3:D:247:PHE:HB2	2.06	0.56
1:B:182:HIS:O	1:B:186:ASP:HB2	2.05	0.56
1:B:203:LEU:HD13	1:B:204:PRO:HD2	1.88	0.56
2:C:301:LEU:HD22	2:C:301:LEU:O	2.05	0.56
3:D:239:LYS:HG3	3:D:310:LYS:HE3	1.88	0.56
1:B:97:GLU:OE1	1:B:97:GLU:N	2.39	0.56
1:B:60:LEU:HD13	1:B:71:SER:HB3	1.89	0.55
1:B:133:THR:H	1:B:138:GLU:HG2	1.71	0.55
3:D:226:LEU:HD23	3:D:229:LYS:HD2	1.88	0.55
4:E:209:PRO:HG2	4:E:210:ILE:HG12	1.89	0.55
2:C:208:VAL:CA	3:D:238:GLN:HE22	2.19	0.55
4:E:99:SER:O	4:E:148:LYS:NZ	2.40	0.55
1:B:83:VAL:O	1:B:241:GLN:NE2	2.39	0.55
1:B:128:SER:O	1:B:229:ARG:NH1	2.40	0.55
4:E:120:VAL:HG12	4:E:208:SER:H	1.71	0.55
8:Y:1677:UNK:O	8:Y:1681:UNK:N	2.39	0.55
1:B:36:GLN:NE2	1:B:57:GLU:OE2	2.39	0.55
2:C:168:ASN:OD1	2:C:171:ARG:NH2	2.40	0.55
3:D:134:LEU:O	3:D:138:LEU:HB2	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:N	1:B:185:ASN:OD1	2.38	0.54
2:C:301:LEU:HD12	2:C:302:GLU:HG3	1.89	0.54
3:D:267:ARG:NH1	7:I:270:ASP:OD1	2.40	0.54
4:E:263:PHE:CE2	4:E:274:ALA:CB	2.91	0.54
2:C:260:SER:OG	2:C:261:HIS:N	2.41	0.54
8:H:147:LYS:HD2	8:H:148:TRP:HB2	1.89	0.54
3:D:134:LEU:HD23	3:D:134:LEU:N	2.23	0.54
7:I:268:GLU:O	7:I:272:LYS:N	2.40	0.54
1:B:208:VAL:HG13	1:B:216:ILE:HB	1.90	0.54
4:E:263:PHE:CZ	4:E:274:ALA:HB1	2.43	0.54
5:F:273:ARG:NH1	5:F:276:CYS:SG	2.81	0.54
1:B:157:ASN:O	4:E:407:ASN:N	2.36	0.53
7:I:178:PHE:HA	7:I:181:ILE:HD12	1.89	0.53
2:C:239:THR:HG1	4:E:262:ARG:CG	2.20	0.53
1:B:195:GLU:OE2	4:E:391:ASN:ND2	2.41	0.53
4:E:28:PRO:HG2	4:E:32:LEU:HD21	1.91	0.53
6:G:47:ILE:HA	6:G:50:ARG:HD2	1.89	0.53
8:H:50:ARG:HH22	11:M:71:UNK:HA	1.74	0.53
2:C:324:ILE:HD13	2:C:346:ILE:HG13	1.90	0.53
3:D:301:ILE:HD13	3:D:303:THR:HG23	1.91	0.53
4:E:409:ILE:O	4:E:412:GLY:N	2.42	0.53
1:B:32:ASP:HB3	1:B:59:ARG:HB3	1.92	0.52
9:J:50:ASP:N	9:J:50:ASP:OD1	2.41	0.52
1:B:187:ALA:O	1:B:191:TYR:N	2.39	0.52
4:E:37:LEU:HD11	4:E:75:ILE:HD13	1.91	0.52
3:D:235:ARG:CZ	3:D:235:ARG:N	2.73	0.52
4:E:94:CYS:SG	4:E:95:HIS:N	2.82	0.52
4:E:318:GLU:HG2	4:E:320:GLU:H	1.75	0.52
1:B:153:THR:OG1	1:B:154:GLN:N	2.44	0.51
4:E:235:ARG:HB2	4:E:237:THR:HG23	1.91	0.51
4:E:233:SER:O	4:E:237:THR:OG1	2.27	0.51
3:D:195:ASN:OD1	3:D:195:ASN:N	2.42	0.51
3:D:267:ARG:HH12	7:I:274:MET:HG3	1.76	0.51
4:E:68:ARG:H	4:E:68:ARG:HD3	1.75	0.51
2:C:300:ASP:OD2	2:C:304:SER:N	2.41	0.51
2:C:208:VAL:HA	3:D:238:GLN:NE2	2.26	0.51
5:F:350:LYS:HA	5:F:353:VAL:HB	1.93	0.51
3:D:211:THR:HG21	4:E:282:PRO:HB2	1.93	0.51
3:D:127:ARG:HD2	3:D:127:ARG:N	2.26	0.51
7:I:201:GLU:O	7:I:205:GLN:NE2	2.44	0.51
10:X:105:UNK:O	10:X:109:UNK:CB	2.59	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:307:GLU:HB3	3:D:308:ARG:HH11	1.75	0.51
8:Y:1201:UNK:O	8:Y:1206:UNK:N	2.44	0.51
2:C:220:HIS:HA	4:E:262:ARG:HH21	1.75	0.50
3:D:164:HIS:HB2	3:D:185:VAL:HB	1.92	0.50
3:D:235:ARG:N	3:D:235:ARG:CD	2.73	0.50
2:C:343:LYS:HE2	2:C:358:LYS:HB2	1.92	0.50
8:H:213:CYS:O	8:H:217:THR:CB	2.59	0.50
4:E:20:VAL:HG22	4:E:24:LEU:HD13	1.94	0.50
3:D:127:ARG:N	3:D:127:ARG:CD	2.74	0.50
4:E:51:ILE:HA	4:E:54:LEU:HB2	1.93	0.49
4:E:100:LYS:CB	4:E:101:PRO:CD	2.90	0.49
4:E:263:PHE:O	4:E:265:GLU:N	2.46	0.49
3:D:127:ARG:CG	3:D:127:ARG:NH2	2.74	0.49
5:F:279:LEU:HA	5:F:282:ASN:HD22	1.76	0.49
11:M:73:UNK:O	11:M:77:UNK:N	2.44	0.49
2:C:207:GLU:HG3	2:C:219:PRO:HB3	1.93	0.49
3:D:215:TRP:CZ2	3:D:235:ARG:HA	2.45	0.49
8:H:331:MET:O	8:H:335:SER:CB	2.60	0.49
1:B:161:PHE:HB2	4:E:404:PHE:CD1	2.48	0.49
1:B:214:THR:OG1	1:B:215:LYS:N	2.44	0.49
3:D:233:ALA:C	3:D:235:ARG:HH22	2.15	0.49
8:H:144:PHE:O	8:H:148:TRP:N	2.44	0.49
10:X:125:UNK:O	10:X:129:UNK:CB	2.61	0.49
1:B:11:SER:OG	1:B:12:LYS:N	2.46	0.49
2:C:208:VAL:HG23	2:C:276:VAL:HG23	1.93	0.49
2:C:210:SER:HG	2:C:215:GLN:H	1.60	0.49
4:E:32:LEU:HD22	4:E:100:LYS:HZ2	1.76	0.49
4:E:72:VAL:O	4:E:76:LEU:HB2	2.12	0.49
1:B:83:VAL:N	1:B:241:GLN:OE1	2.39	0.48
4:E:268:GLY:N	4:E:271:GLU:OE2	2.37	0.48
1:B:33:LEU:HD11	1:B:56:TYR:HB3	1.95	0.48
1:B:209:ILE:HG13	1:B:215:LYS:HG3	1.94	0.48
8:H:63:LYS:HA	8:H:66:ILE:HG22	1.95	0.48
6:G:108:THR:O	6:G:112:ARG:HB2	2.12	0.48
8:H:387:SER:O	8:H:391:LYS:CB	2.61	0.48
2:C:161:GLU:HB2	4:E:284:HIS:CE1	2.48	0.48
3:D:188:LYS:HE2	3:D:252:SER:HB2	1.96	0.48
1:B:8:LEU:HD11	1:B:111:MET:HB3	1.95	0.48
3:D:197:PHE:HB3	3:D:215:TRP:HA	1.96	0.48
6:G:93:LEU:HA	6:G:96:GLU:HB3	1.96	0.48
3:D:149:ASN:HA	3:D:153:ARG:HG3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:LEU:HB3	3:D:354:LEU:HD22	1.95	0.48
8:H:44:GLN:HA	8:H:47:ALA:HB3	1.94	0.48
1:B:117:GLU:OE1	1:B:119:LYS:N	2.45	0.48
4:E:235:ARG:NH1	6:G:104:GLU:OE1	2.45	0.48
2:C:265:TYR:OH	3:D:242:LEU:HD11	2.14	0.48
2:C:327:CYS:O	6:G:100:ARG:NH2	2.46	0.47
2:C:199:ARG:HH11	2:C:228:ILE:HD11	1.79	0.47
2:C:225:LYS:HD2	2:C:236:PHE:HB2	1.96	0.47
3:D:195:ASN:OD1	3:D:219:ARG:N	2.47	0.47
4:E:388:THR:HB	4:E:441:THR:HA	1.95	0.47
2:C:338:GLN:HA	2:C:341:LYS:HG2	1.96	0.47
8:H:426:PRO:O	8:H:430:SER:CB	2.61	0.47
4:E:205:PRO:HB2	4:E:260:PRO:HG3	1.96	0.47
5:F:332:LEU:HD11	5:F:334:LEU:HD23	1.97	0.47
9:J:5:GLN:HA	9:J:8:HIS:CD2	2.48	0.47
9:J:7:LEU:HD13	9:J:62:LYS:HE2	1.96	0.47
3:D:131:LEU:HB2	4:E:291:GLY:O	2.14	0.47
4:E:277:ASN:N	4:E:277:ASN:OD1	2.44	0.47
7:I:242:GLU:O	7:I:246:LEU:HB2	2.15	0.47
3:D:135:GLN:NE2	3:D:135:GLN:CA	2.73	0.47
5:F:252:LEU:HA	5:F:255:ASN:HD22	1.79	0.47
1:B:146:LYS:O	1:B:148:TYR:N	2.44	0.47
4:E:17:THR:HA	4:E:20:VAL:HG12	1.97	0.47
4:E:425:ASP:OD1	4:E:425:ASP:N	2.45	0.47
1:B:29:LEU:HD21	1:B:62:ILE:HG21	1.96	0.46
2:C:212:ARG:HH22	2:C:282:ARG:HG2	1.80	0.46
7:I:195:ILE:HD13	7:I:195:ILE:HA	1.84	0.46
7:I:196:ASN:O	7:I:200:ASN:ND2	2.48	0.46
8:H:137:LEU:HD12	8:H:137:LEU:HA	1.76	0.46
2:C:301:LEU:CD1	2:C:302:GLU:HG3	2.46	0.46
3:D:151:ASN:O	3:D:155:SER:N	2.33	0.46
3:D:314:CYS:HB3	5:F:335:MET:HB2	1.97	0.46
4:E:73:ASN:HA	4:E:76:LEU:HB3	1.96	0.46
9:J:123:GLU:O	9:J:127:ARG:CB	2.63	0.46
2:C:211:GLU:OE1	2:C:283:GLN:NE2	2.48	0.46
2:C:301:LEU:HD13	2:C:301:LEU:O	2.16	0.46
4:E:214:SER:OG	4:E:215:VAL:N	2.49	0.46
2:C:160:LEU:CD2	3:D:131:LEU:HD11	2.45	0.46
2:C:169:VAL:HA	2:C:172:MET:SD	2.56	0.46
3:D:225:ARG:HH22	7:I:306:LEU:HB3	1.81	0.46
4:E:379:LEU:HG	4:E:380:VAL:HG23	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASP:H	1:B:69:THR:HG1	1.63	0.46
4:E:442:ILE:HG22	4:E:447:PHE:HD1	1.81	0.46
3:D:143:ASP:OD1	3:D:143:ASP:N	2.46	0.45
8:H:297:GLU:O	8:H:301:GLN:CB	2.64	0.45
1:B:68:GLY:HA2	1:B:93:ASP:HB2	1.97	0.45
3:D:244:LEU:HD23	3:D:244:LEU:N	2.31	0.45
7:I:260:THR:HA	7:I:263:LEU:HD23	1.97	0.45
1:B:50:ALA:O	1:B:78:ASN:ND2	2.49	0.45
1:B:198:MET:HA	4:E:422:ILE:HG22	1.98	0.45
8:H:228:ALA:O	8:H:232:SER:N	2.44	0.45
1:B:200:VAL:HA	1:B:203:LEU:HB2	1.99	0.45
3:D:301:ILE:H	3:D:301:ILE:HG13	1.54	0.45
4:E:155:LEU:HA	4:E:203:ALA:HA	1.97	0.45
1:B:129:ILE:O	1:B:141:THR:OG1	2.32	0.45
2:C:160:LEU:HD21	3:D:131:LEU:HD11	1.98	0.45
3:D:200:GLN:HG3	3:D:213:LEU:HD13	1.99	0.45
4:E:244:GLN:HB3	4:E:245:LYS:H	1.66	0.45
5:F:365:LYS:HD2	5:F:368:LYS:HD2	1.97	0.45
2:C:240:ILE:HD11	2:C:246:VAL:HG13	1.98	0.45
3:D:186:ASN:HB2	3:D:192:ASN:HB3	1.99	0.45
1:B:155:ASP:HB2	1:B:157:ASN:HD21	1.81	0.45
3:D:163:PRO:HD2	3:D:245:TYR:HE1	1.82	0.45
4:E:158:ARG:NH1	4:E:200:TYR:HB3	2.32	0.45
1:B:65:LEU:HB2	1:B:69:THR:HG21	1.99	0.45
3:D:193:THR:OG1	3:D:194:MET:N	2.40	0.45
4:E:249:LYS:HG3	4:E:250:SER:H	1.82	0.45
5:F:340:ILE:HG22	5:F:341:LYS:H	1.80	0.45
10:X:119:UNK:O	10:X:123:UNK:CB	2.65	0.45
1:B:93:ASP:OD1	1:B:94:ASN:N	2.51	0.44
2:C:160:LEU:HD11	3:D:131:LEU:HD22	1.95	0.44
4:E:146:MET:HB2	4:E:155:LEU:HG	1.98	0.44
7:I:259:LEU:HD13	7:I:263:LEU:HD22	1.99	0.44
8:H:202:SER:O	8:H:206:GLU:CB	2.65	0.44
2:C:251:ASP:O	2:C:256:GLY:N	2.50	0.44
4:E:208:SER:OG	4:E:210:ILE:O	2.32	0.44
3:D:358:CYS:O	3:D:362:LEU:N	2.49	0.44
4:E:29:VAL:HA	4:E:33:TYR:CD2	2.53	0.44
8:H:320:LEU:O	8:H:324:VAL:N	2.51	0.44
1:B:180:THR:OG1	1:B:181:MET:N	2.50	0.44
3:D:129:ASN:OD1	3:D:129:ASN:N	2.50	0.44
5:F:269:LEU:HA	7:I:227:ILE:HD13	2.00	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:23:GLN:HA	9:J:42:TRP:HZ3	1.82	0.44
3:D:215:TRP:HH2	3:D:232:LEU:CD2	2.25	0.44
4:E:64:LYS:HD2	4:E:64:LYS:HA	1.81	0.44
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.80	0.43
4:E:29:VAL:HA	4:E:33:TYR:HD2	1.82	0.43
2:C:257:LEU:HG	2:C:259:ILE:HD11	2.00	0.43
4:E:141:HIS:NE2	4:E:159:ILE:O	2.52	0.43
9:J:62:LYS:HA	9:J:65:PHE:CE2	2.53	0.43
2:C:212:ARG:HB3	2:C:283:GLN:HE21	1.84	0.43
4:E:60:LEU:O	4:E:64:LYS:N	2.41	0.43
4:E:253:ASN:OD1	4:E:253:ASN:N	2.52	0.43
4:E:389:LEU:HB3	4:E:400:ILE:HG13	2.00	0.43
1:B:10:ILE:HD11	1:B:87:LEU:HB2	2.00	0.43
9:J:7:LEU:HD23	9:J:7:LEU:HA	1.87	0.43
1:B:-1:ASN:OD1	1:B:-1:ASN:N	2.52	0.43
1:B:15:SER:OG	1:B:17:GLU:OE1	2.29	0.43
2:C:273:LEU:HA	2:C:276:VAL:HG12	2.01	0.43
2:C:328:SER:HA	6:G:100:ARG:HH12	1.83	0.43
5:F:280:LYS:HD3	5:F:283:ASN:HD22	1.83	0.43
3:D:234:THR:CA	3:D:235:ARG:HH22	2.14	0.43
5:F:353:VAL:HG13	5:F:357:LEU:HB3	2.01	0.43
9:J:7:LEU:HB3	9:J:62:LYS:NZ	2.34	0.43
1:B:240:ILE:H	1:B:240:ILE:HG13	1.56	0.42
4:E:92:ILE:HD12	4:E:92:ILE:HA	1.78	0.42
6:G:56:ARG:HD3	6:G:56:ARG:HA	1.88	0.42
7:I:224:ARG:HA	7:I:227:ILE:HG22	2.01	0.42
9:J:49:ARG:HA	9:J:54:THR:HG21	2.01	0.42
9:J:53:VAL:O	9:J:56:GLU:HG2	2.19	0.42
2:C:199:ARG:HD2	2:C:228:ILE:HD11	2.02	0.42
2:C:320:LYS:HG3	2:C:321:GLN:H	1.83	0.42
4:E:159:ILE:HG12	4:E:199:PRO:HB3	2.00	0.42
8:H:145:LEU:HD22	8:H:145:LEU:HA	1.85	0.42
3:D:134:LEU:HD23	3:D:134:LEU:H	1.84	0.42
1:B:151:PRO:HB3	1:B:204:PRO:HG2	2.01	0.42
3:D:313:ASN:N	5:F:333:ASN:O	2.53	0.42
1:B:55:ARG:HB3	1:B:76:LEU:HD23	2.02	0.42
2:C:212:ARG:NH2	2:C:282:ARG:HG2	2.35	0.42
3:D:302:ILE:HA	3:D:313:ASN:ND2	2.35	0.42
7:I:306:LEU:HA	7:I:309:ILE:HG12	2.00	0.42
1:B:116:PHE:HB2	1:B:120:THR:HG21	2.01	0.42
4:E:132:LEU:HD13	4:E:132:LEU:HA	1.90	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:THR:CG2	3:D:150:MET:HG3	2.33	0.41
7:I:292:ILE:HA	7:I:295:PHE:CD1	2.55	0.41
1:B:217:MET:HG2	1:B:218:ARG:H	1.85	0.41
3:D:134:LEU:HA	3:D:137:GLU:OE2	2.21	0.41
4:E:98:ILE:HA	4:E:101:PRO:HD2	2.02	0.41
4:E:205:PRO:HG2	4:E:208:SER:HB3	2.01	0.41
3:D:246:GLU:O	3:D:250:ILE:HG12	2.20	0.41
4:E:37:LEU:HD13	4:E:37:LEU:HA	1.81	0.41
4:E:138:LYS:HA	4:E:138:LYS:HD2	1.88	0.41
9:J:74:ARG:NH2	9:J:78:SER:OG	2.42	0.41
4:E:397:ILE:HD12	4:E:397:ILE:HA	1.94	0.41
7:I:305:LEU:HD11	9:J:139:LEU:HA	2.02	0.41
4:E:32:LEU:HD22	4:E:100:LYS:HZ1	1.85	0.41
6:G:106:GLN:O	6:G:109:SER:OG	2.29	0.41
2:C:298:ASP:O	2:C:299:LEU:CD2	2.67	0.41
3:D:264:LEU:O	3:D:268:LYS:HG2	2.21	0.41
6:G:112:ARG:NH2	9:J:97:ILE:HA	2.36	0.41
3:D:152:LEU:HD22	3:D:152:LEU:HA	1.85	0.41
4:E:107:LEU:HD23	4:E:215:VAL:HB	2.03	0.41
4:E:158:ARG:HH22	4:E:160:GLN:HB2	1.86	0.41
3:D:243:SER:O	3:D:247:PHE:HB3	2.21	0.40
3:D:302:ILE:HA	3:D:313:ASN:HD22	1.86	0.40
4:E:254:ILE:HD12	4:E:254:ILE:HA	1.88	0.40
8:H:50:ARG:NH1	11:M:70:UNK:O	2.36	0.40
2:C:210:SER:HB3	2:C:217:GLU:OE2	2.20	0.40
3:D:244:LEU:N	3:D:244:LEU:CD2	2.83	0.40
9:J:70:SER:HA	9:J:73:LEU:HG	2.03	0.40
3:D:151:ASN:O	3:D:154:LEU:N	2.54	0.40
9:J:16:LEU:HD13	9:J:16:LEU:HA	1.95	0.40
2:C:212:ARG:NE	2:C:287:ASP:OD2	2.54	0.40
2:C:224:LEU:H	2:C:224:LEU:HG	1.42	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	B	242/248 (98%)	203 (84%)	38 (16%)	1 (0%)	34	72
2	C	188/371 (51%)	160 (85%)	28 (15%)	0	100	100
3	D	184/369 (50%)	139 (76%)	43 (23%)	2 (1%)	14	52
4	E	359/461 (78%)	275 (77%)	78 (22%)	6 (2%)	9	44
5	F	184/406 (45%)	167 (91%)	16 (9%)	1 (0%)	29	68
6	G	168/241 (70%)	151 (90%)	16 (10%)	1 (1%)	25	65
7	I	162/330 (49%)	150 (93%)	12 (7%)	0	100	100
8	H	290/773 (38%)	242 (83%)	45 (16%)	3 (1%)	15	54
8	Y	103/773 (13%)	91 (88%)	12 (12%)	0	100	100
9	J	143/153 (94%)	121 (85%)	20 (14%)	2 (1%)	11	47
All	All	2023/4125 (49%)	1699 (84%)	308 (15%)	16 (1%)	24	60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	129	PRO
4	E	295	LYS
8	H	209	ILE
4	E	264	ALA
6	G	35	PRO
3	D	280	LEU
4	E	192	LYS
9	J	128	SER
1	B	147	LEU
3	D	267	ARG
4	E	260	PRO
8	H	396	ILE
4	E	150	PRO
5	F	223	PHE
8	H	131	ILE
4	E	149	HIS

### 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	B	219/223 (98%)	209 (95%)	10 (5%)	27	54
2	C	183/349 (52%)	169 (92%)	14 (8%)	13	39
3	D	176/344 (51%)	154 (88%)	22 (12%)	4	22
4	E	291/418 (70%)	281 (97%)	10 (3%)	37	61
5	F	120/378 (32%)	114 (95%)	6 (5%)	24	51
6	G	72/221 (33%)	68 (94%)	4 (6%)	21	49
7	I	133/314 (42%)	128 (96%)	5 (4%)	33	58
8	H	47/685 (7%)	44 (94%)	3 (6%)	17	44
9	J	73/143 (51%)	72 (99%)	1 (1%)	67	80
All	All	1314/3075 (43%)	1239 (94%)	75 (6%)	24	48

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LEU
1	B	54	ILE
1	B	103	LEU
1	B	106	GLU
1	B	124	LEU
1	B	189	VAL
1	B	194	ASN
1	B	203	LEU
1	B	214	THR
1	B	221	ILE
2	C	170	TYR
2	C	172	MET
2	C	176	THR
2	C	202	LEU
2	C	206	LEU
2	C	224	LEU
2	C	225	LYS
2	C	239	THR
2	C	299	LEU
2	C	300	ASP
2	C	302	GLU
2	C	305	MET
2	C	310	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	348	LEU
3	D	127	ARG
3	D	129	ASN
3	D	131	LEU
3	D	132	THR
3	D	135	GLN
3	D	143	ASP
3	D	148	LEU
3	D	149	ASN
3	D	152	LEU
3	D	156	TYR
3	D	172	ARG
3	D	182	VAL
3	D	192	ASN
3	D	212	LEU
3	D	235	ARG
3	D	237	PHE
3	D	240	CYS
3	D	241	LEU
3	D	243	SER
3	D	244	LEU
3	D	267	ARG
3	D	268	LYS
4	E	68	ARG
4	E	96	LEU
4	E	106	TRP
4	E	204	PHE
4	E	212	PHE
4	E	245	LYS
4	E	258	LEU
4	E	261	SER
4	E	267	MET
4	E	431	LEU
5	F	262	LEU
5	F	286	ARG
5	F	290	LYS
5	F	333	ASN
5	F	356	LEU
5	F	371	LYS
6	G	49	LYS
6	G	69	ASN
6	G	98	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	G	112	ARG
7	I	176	ARG
7	I	187	ARG
7	I	240	GLN
7	I	263	LEU
7	I	303	ASN
8	H	86	ILE
8	H	139	LEU
8	H	145	LEU
9	J	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	ASN
1	B	194	ASN
3	D	149	ASN
3	D	151	ASN
3	D	170	GLN
3	D	186	ASN
3	D	192	ASN
3	D	238	GLN
3	D	313	ASN
4	E	23	GLN
4	E	133	GLN
4	E	149	HIS
4	E	207	ASN
4	E	284	HIS
4	E	391	ASN
4	E	423	ASN
5	F	250	GLN
5	F	255	ASN
5	F	278	ASN
5	F	282	ASN
5	F	283	ASN
5	F	333	ASN
5	F	382	HIS
7	I	200	ASN
7	I	205	GLN
7	I	228	GLN
7	I	303	ASN
9	J	5	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	X	2
8	Y	1
11	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	1213:UNK	C	1667:UNK	N	26.06
1	X	129:UNK	C	136:UNK	N	14.95
1	M	128:UNK	C	149:UNK	N	10.69
1	X	168:UNK	C	175:UNK	N	9.72

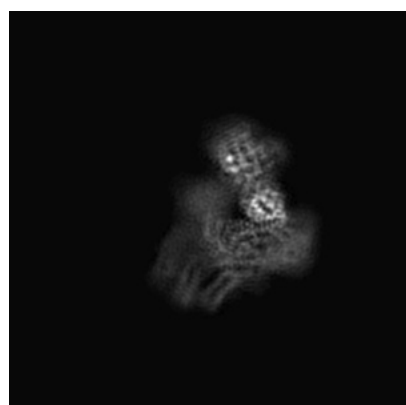
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0523. These allow visual inspection of the internal detail of the map and identification of artifacts.

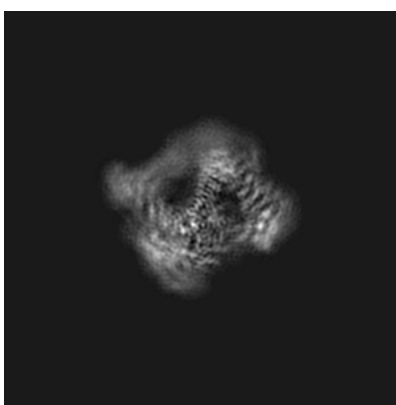
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

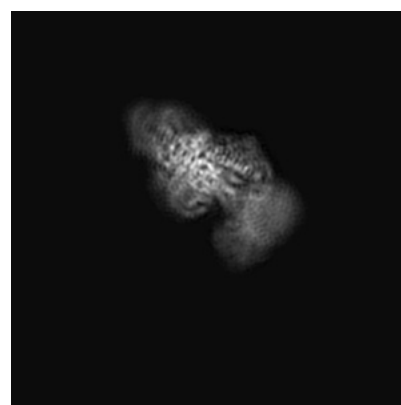
#### 6.1.1 Primary map



X



Y

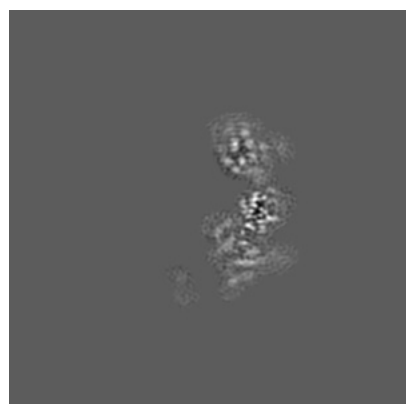


Z

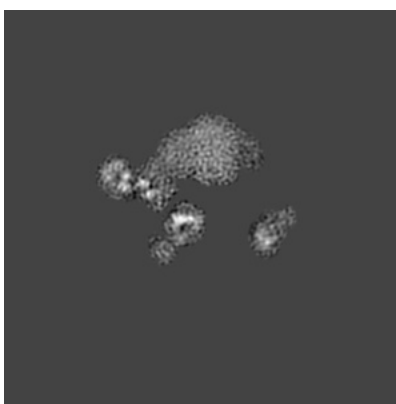
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

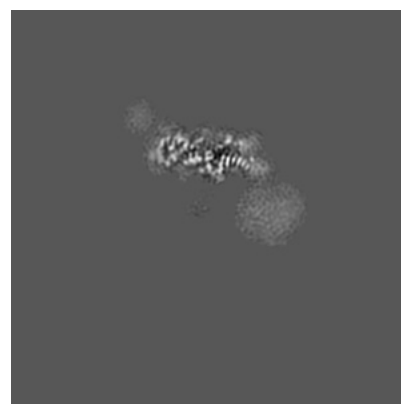
#### 6.2.1 Primary map



X Index: 152



Y Index: 152



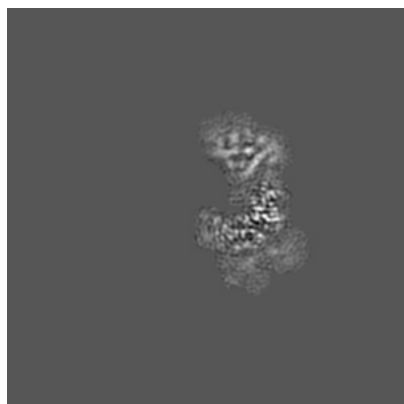
Z Index: 152



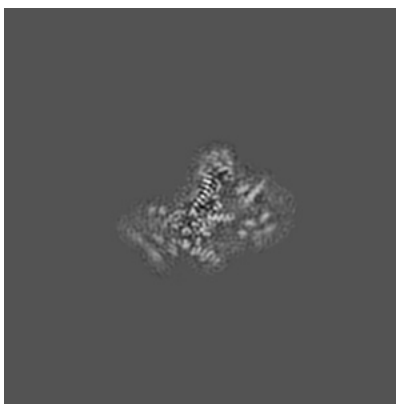
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

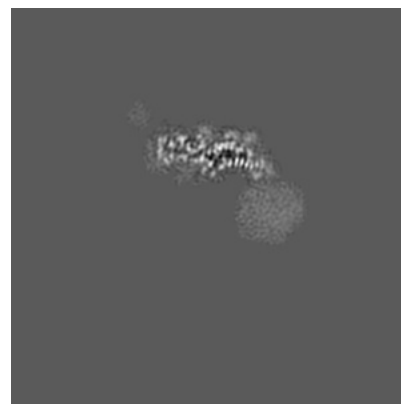
### 6.3.1 Primary map



X Index: 140



Y Index: 188



Z Index: 156

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

## 6.4 Orthogonal surface views [i](#)

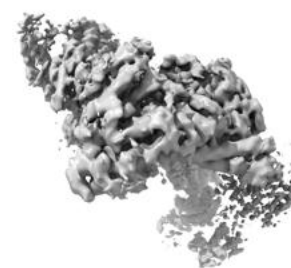
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

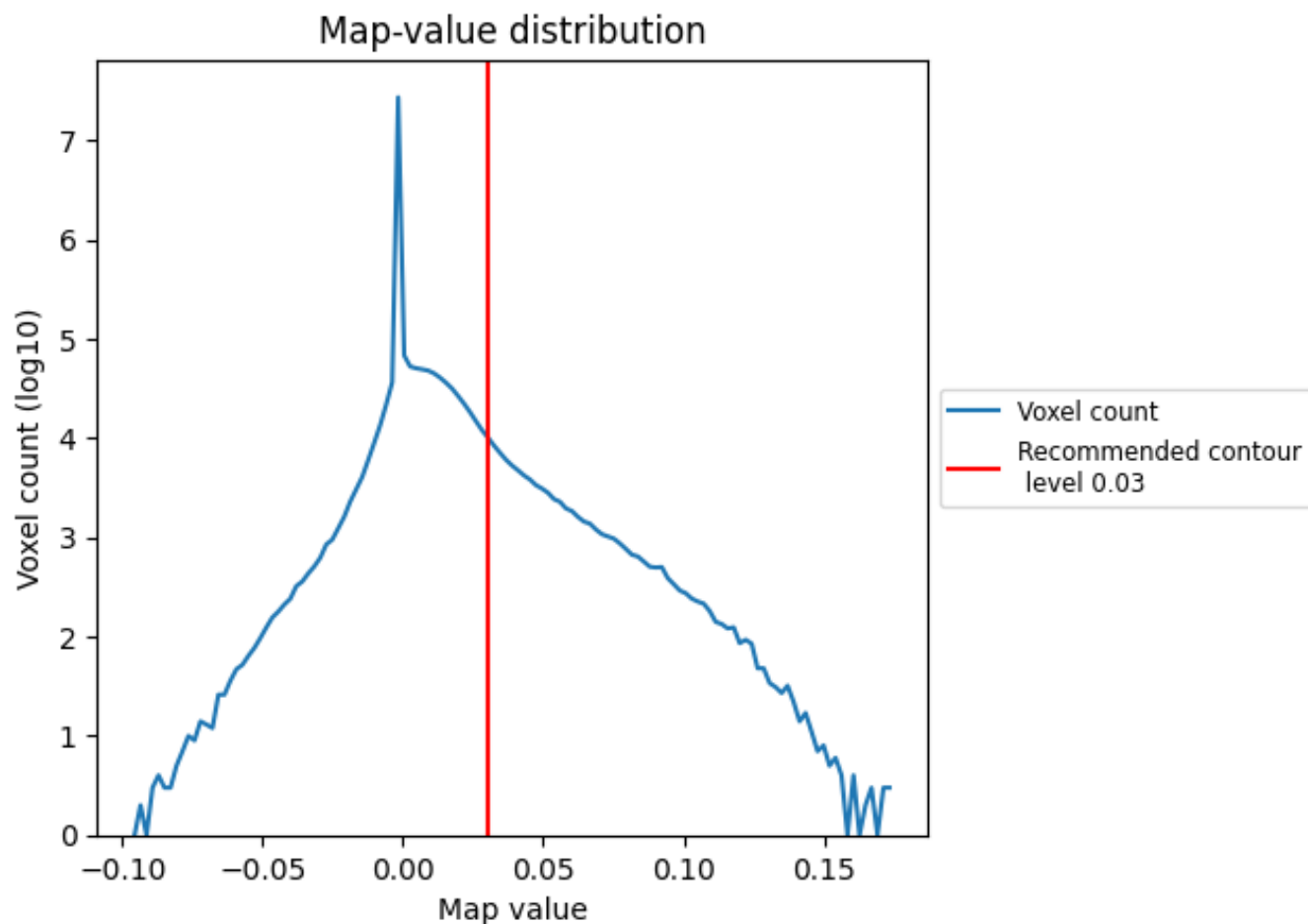
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

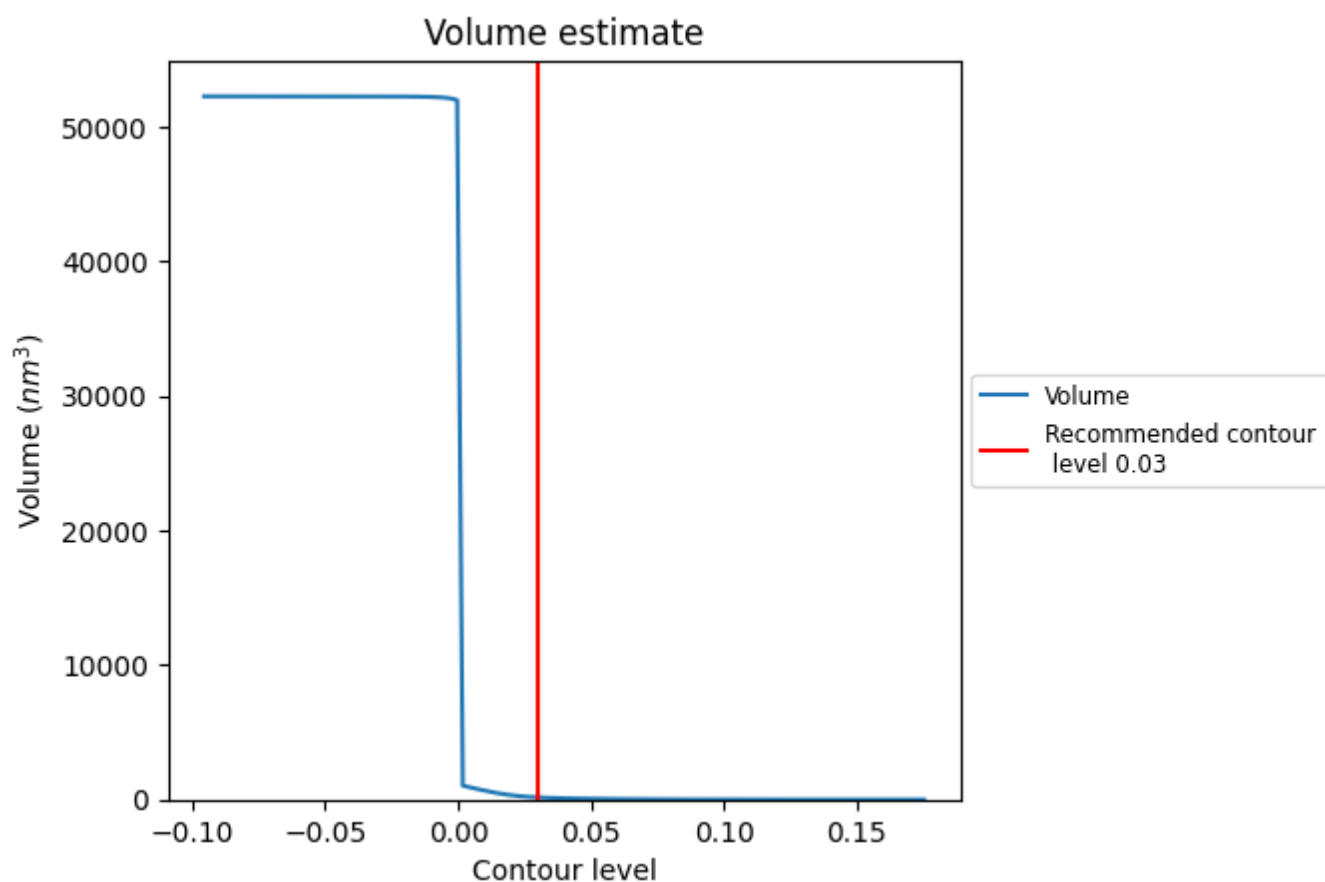
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

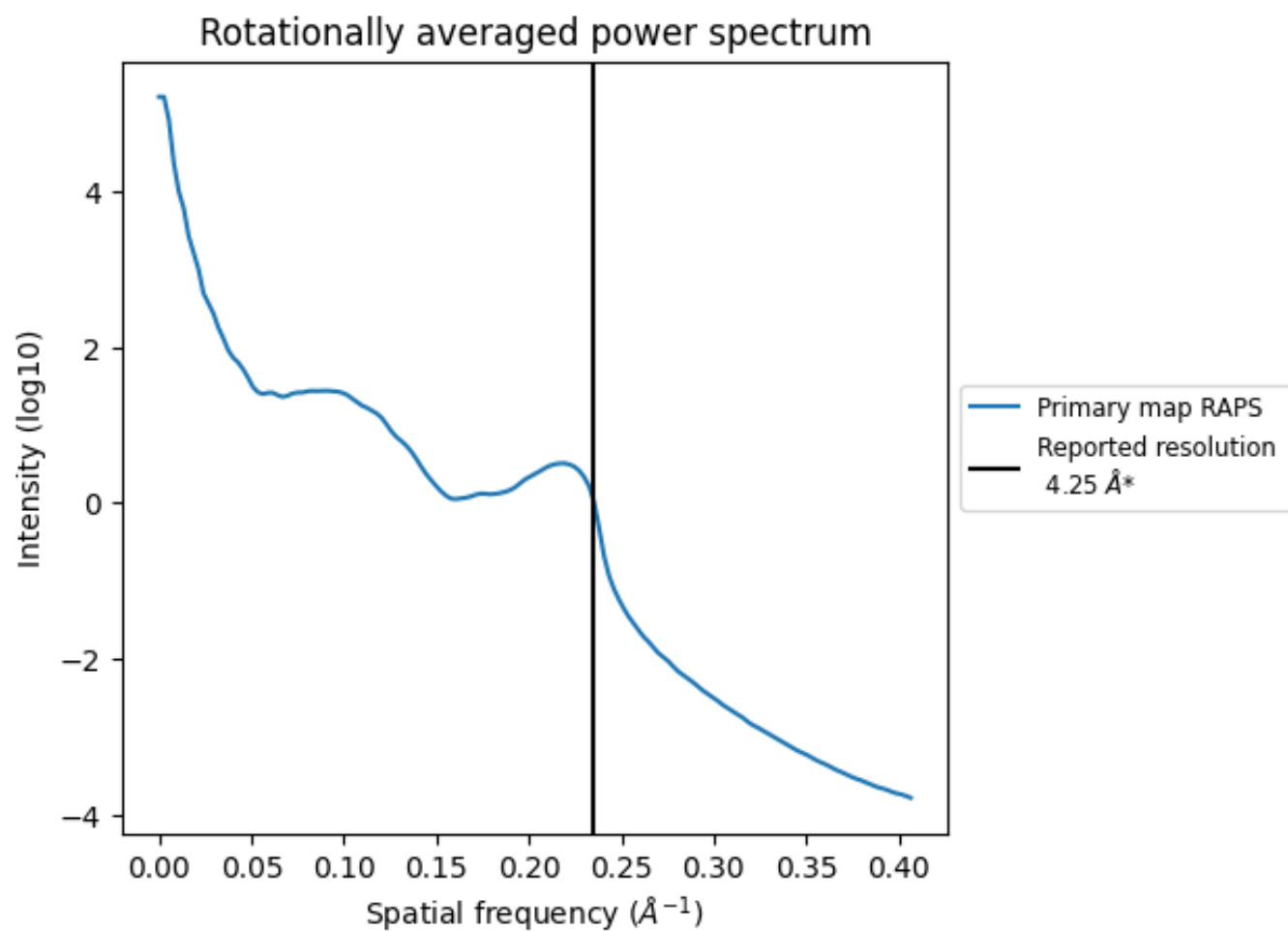
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm<sup>3</sup>; this corresponds to an approximate mass of 146 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 ⓘ

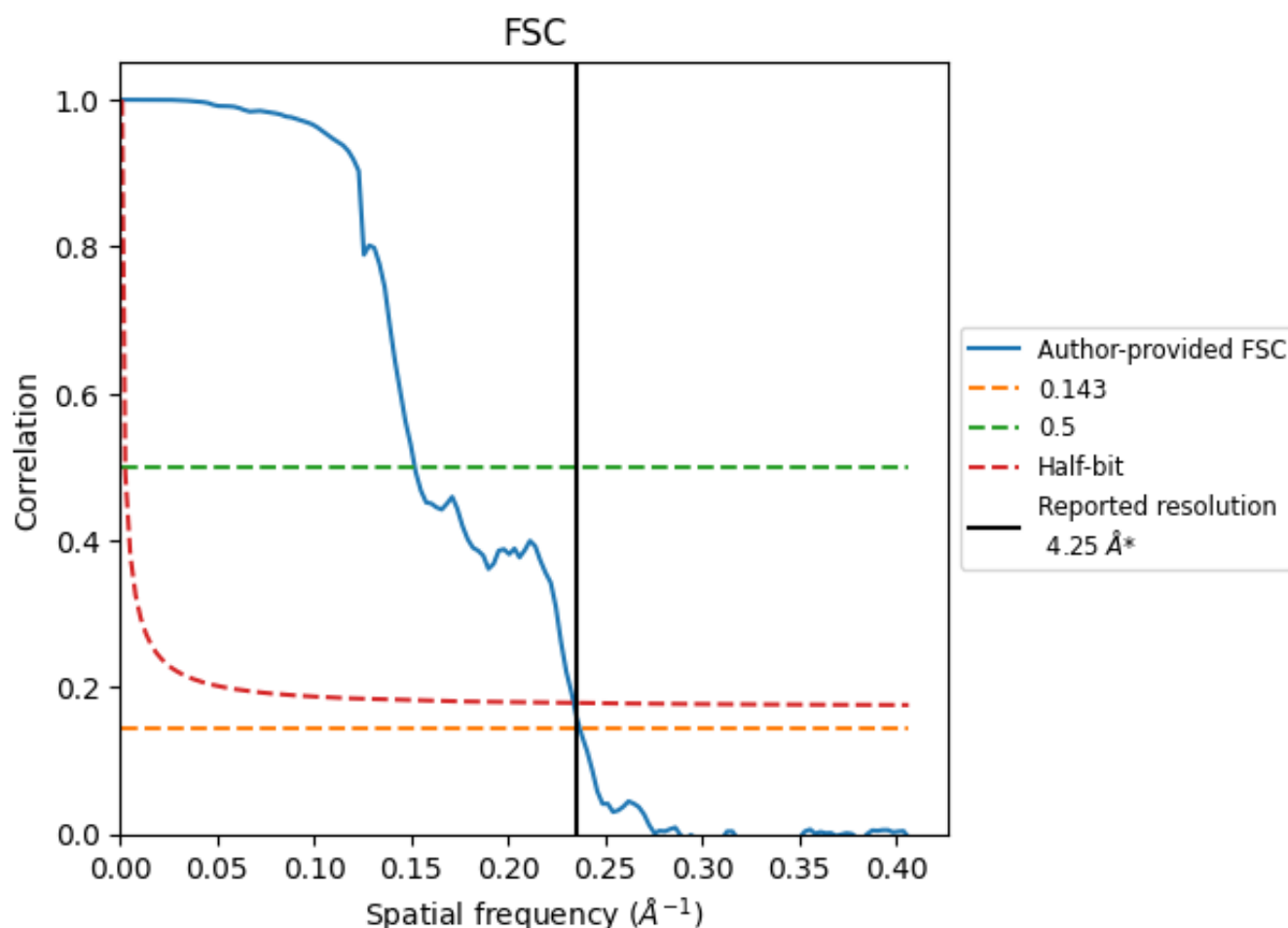


\*Reported resolution corresponds to spatial frequency of 0.235 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.235  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

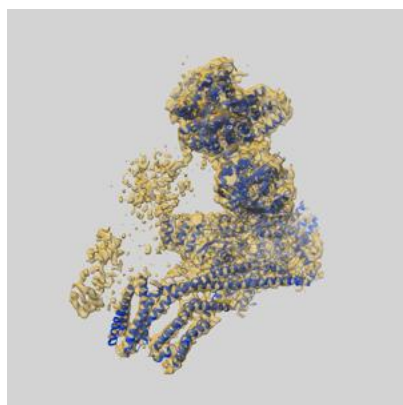
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.22	6.58	4.28
Unmasked-calculated*	-	-	-

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

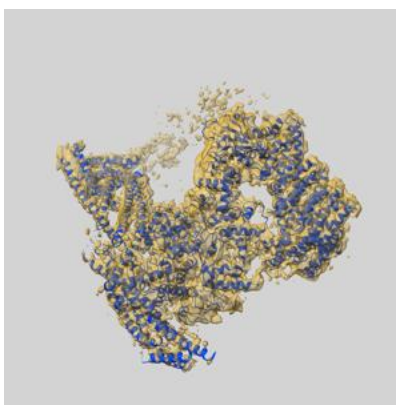
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0523 and PDB model 6NUW. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

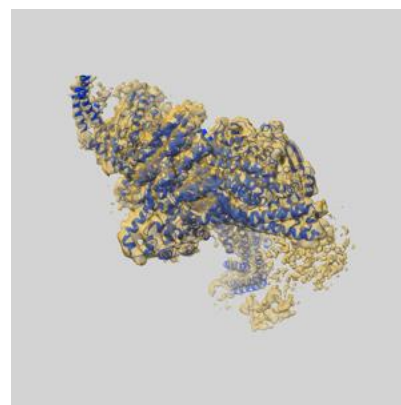
### 9.1 Map-model overlay [i](#)



X



Y

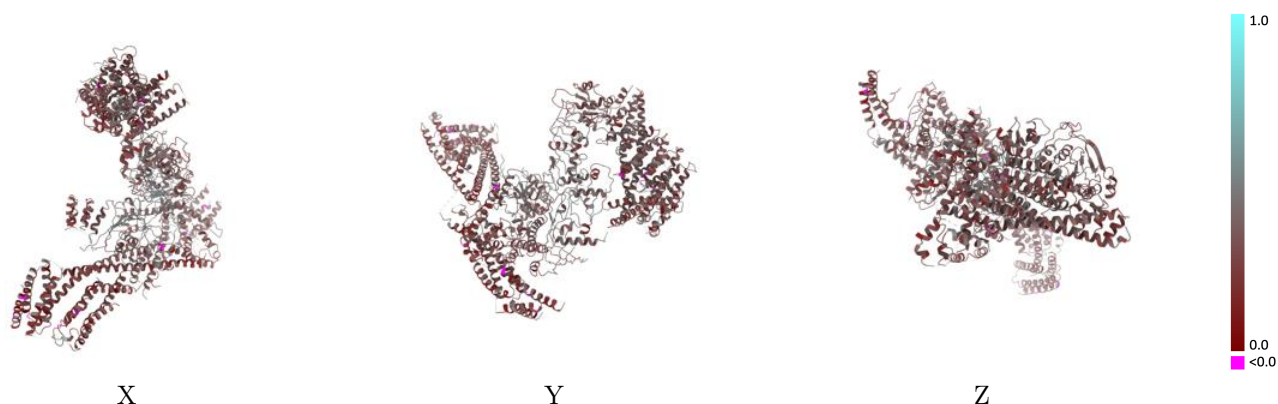


Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

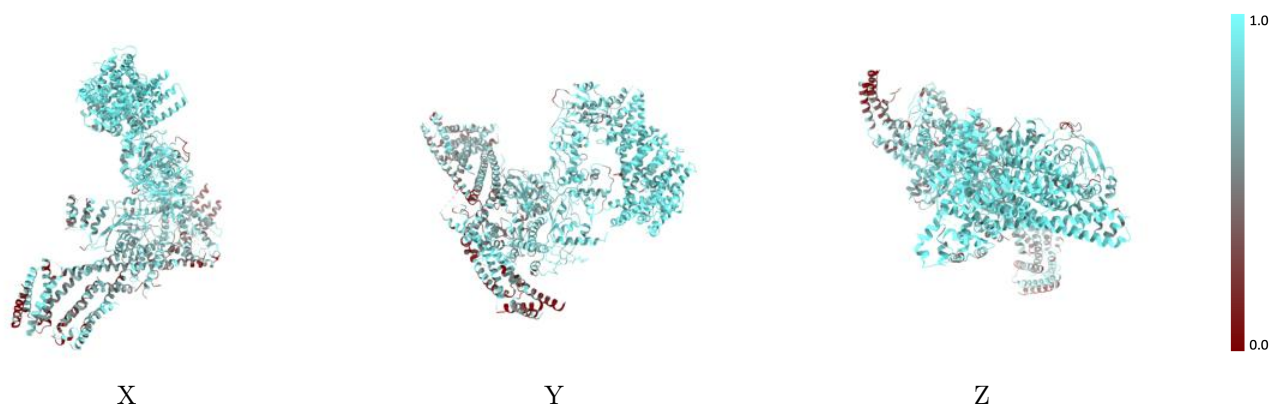


## 9.2 Q-score mapped to coordinate model [i](#)



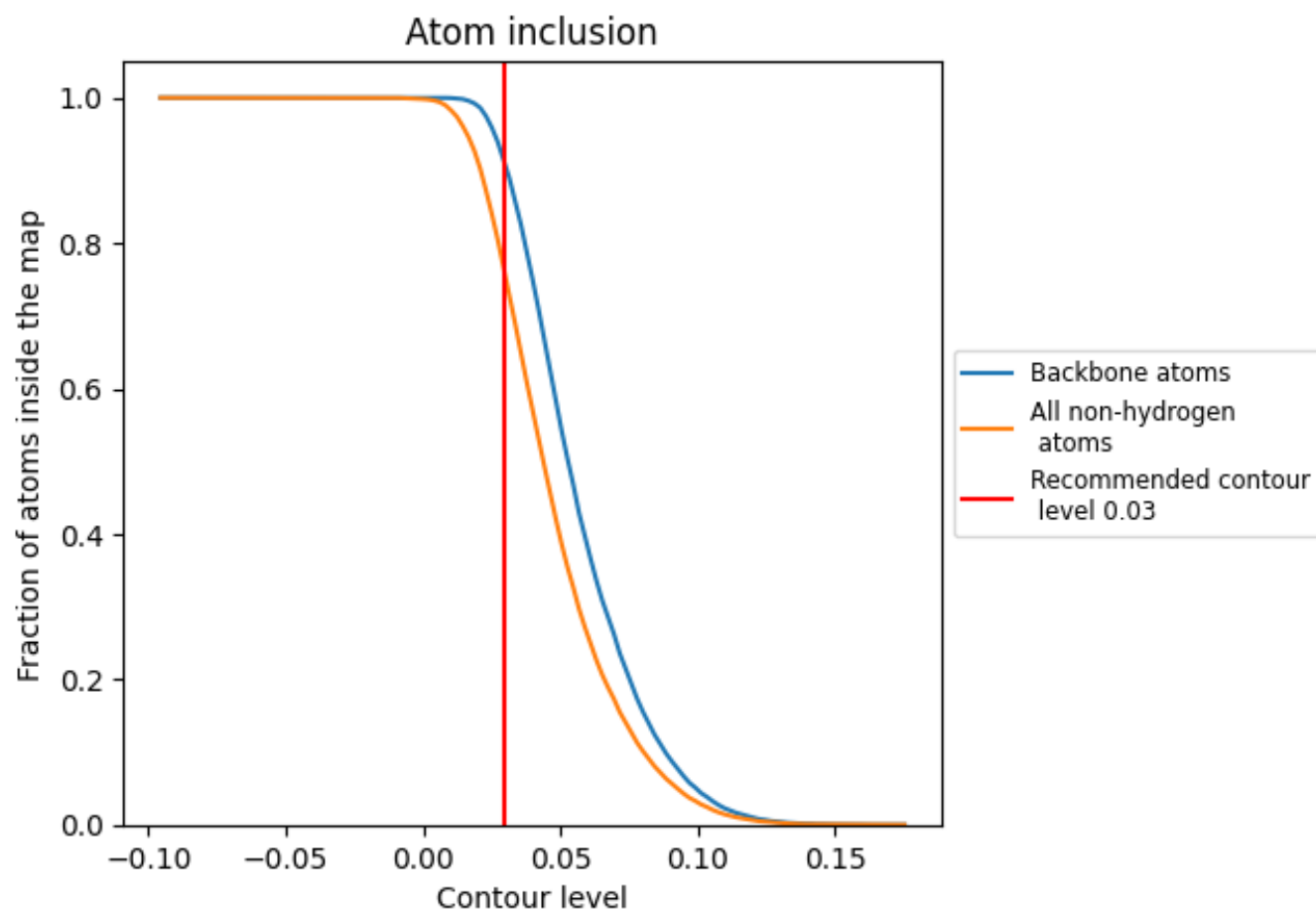
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 76% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7555	 0.3420
B	 0.8130	 0.3820
C	 0.7933	 0.3810
D	 0.7956	 0.3560
E	 0.7694	 0.3960
F	 0.5649	 0.2940
G	 0.6330	 0.3020
H	 0.9001	 0.3400
I	 0.5743	 0.2670
J	 0.5927	 0.2740
M	 0.9573	 0.3370
U	 0.1391	 0.2250
X	 0.9429	 0.3200
Y	 0.9517	 0.3310

