



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 08:17 AM EST

PDB ID : 7KPX  
EMDB ID : EMD-22991  
Title : Structure of the yeast CKM  
Authors : Li, Y.C.; Chao, T.C.; Kim, H.J.; Cholko, T.; Chen, S.F.; Nakanishi, K.; Chang, C.E.; Murakami, K.; Garcia, B.A.; Boyer, T.G.; Tsai, K.L.  
Deposited on : 2020-11-12  
Resolution : 4.40 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>.

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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



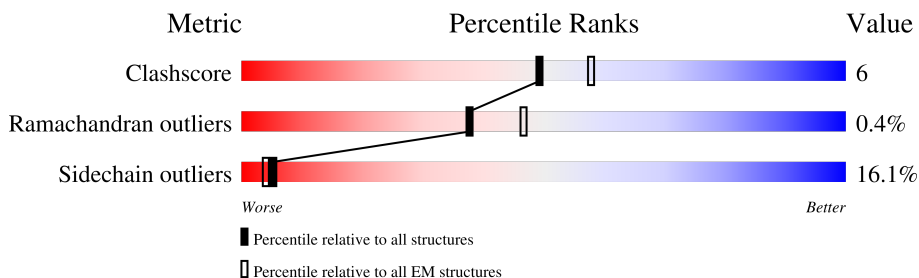
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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  $\geq 3$ , 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	A	555	<div> <div>12%</div> <div>47%</div> <div>15%</div> <div>•</div> <div>36%</div> </div>
2	B	352	<div> <div>8%</div> <div>63%</div> <div>18%</div> <div>•</div> <div>18%</div> </div>
3	C	1427	<div> <div>40%</div> <div>81%</div> <div>12%</div> <div>•</div> <div>5%</div> </div>
4	D	1420	<div> <div>5%</div> <div>47%</div> <div>13%</div> <div>•</div> <div>38%</div> </div>



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20762 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 Meiotic mRNA stability protein kinase SSN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	357	Total	C	N	O	S	0	0
			2952	1919	512	507	14		

- Molecule 2 is a protein called RNA polymerase II holoenzyme cyclin-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	290	Total	C	N	O	S	0	0
			2436	1591	404	429	12		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	324	SER	-	expression tag	UNP P47821
B	325	MET	-	expression tag	UNP P47821
B	326	GLU	-	expression tag	UNP P47821
B	327	LYS	-	expression tag	UNP P47821
B	328	ARG	-	expression tag	UNP P47821
B	329	ARG	-	expression tag	UNP P47821
B	330	TRP	-	expression tag	UNP P47821
B	331	LYS	-	expression tag	UNP P47821
B	332	LYS	-	expression tag	UNP P47821
B	333	ASN	-	expression tag	UNP P47821
B	334	PHE	-	expression tag	UNP P47821
B	335	ILE	-	expression tag	UNP P47821
B	336	ALA	-	expression tag	UNP P47821
B	337	VAL	-	expression tag	UNP P47821
B	338	SER	-	expression tag	UNP P47821
B	339	ALA	-	expression tag	UNP P47821
B	340	ALA	-	expression tag	UNP P47821
B	341	ASN	-	expression tag	UNP P47821
B	342	ARG	-	expression tag	UNP P47821
B	343	PHE	-	expression tag	UNP P47821
B	344	LYS	-	expression tag	UNP P47821

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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	LYS	-	expression tag	UNP P47821
B	346	ILE	-	expression tag	UNP P47821
B	347	SER	-	expression tag	UNP P47821
B	348	SER	-	expression tag	UNP P47821
B	349	SER	-	expression tag	UNP P47821
B	350	GLY	-	expression tag	UNP P47821
B	351	ALA	-	expression tag	UNP P47821
B	352	LEU	-	expression tag	UNP P47821

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1352	Total	C	N	O	S	0	0
			8362	5201	1544	1600	17		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 13.

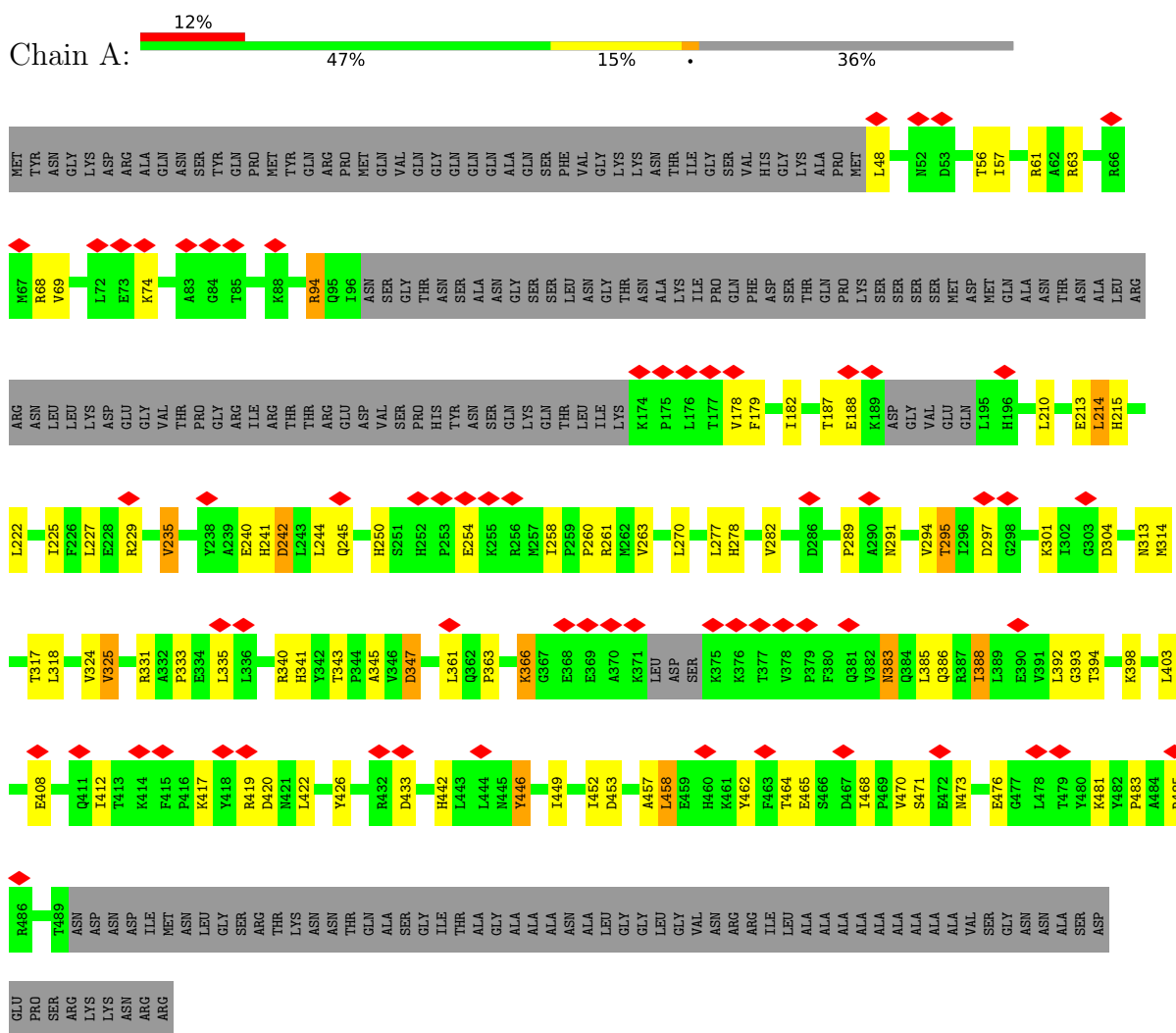
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	876	Total	C	N	O	S	0	0
			7012	4530	1176	1272	34		



### 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.

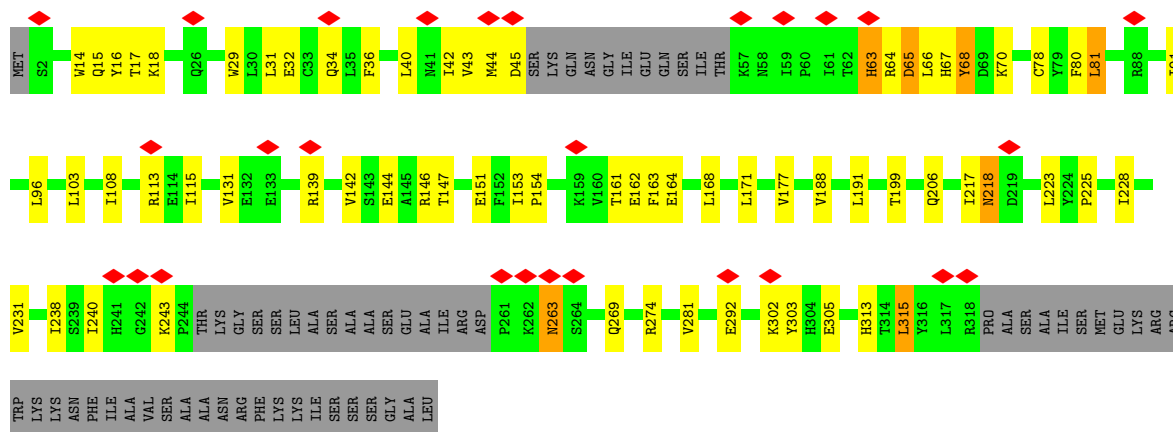
- Molecule 1: Meiotic mRNA stability protein kinase SSN3



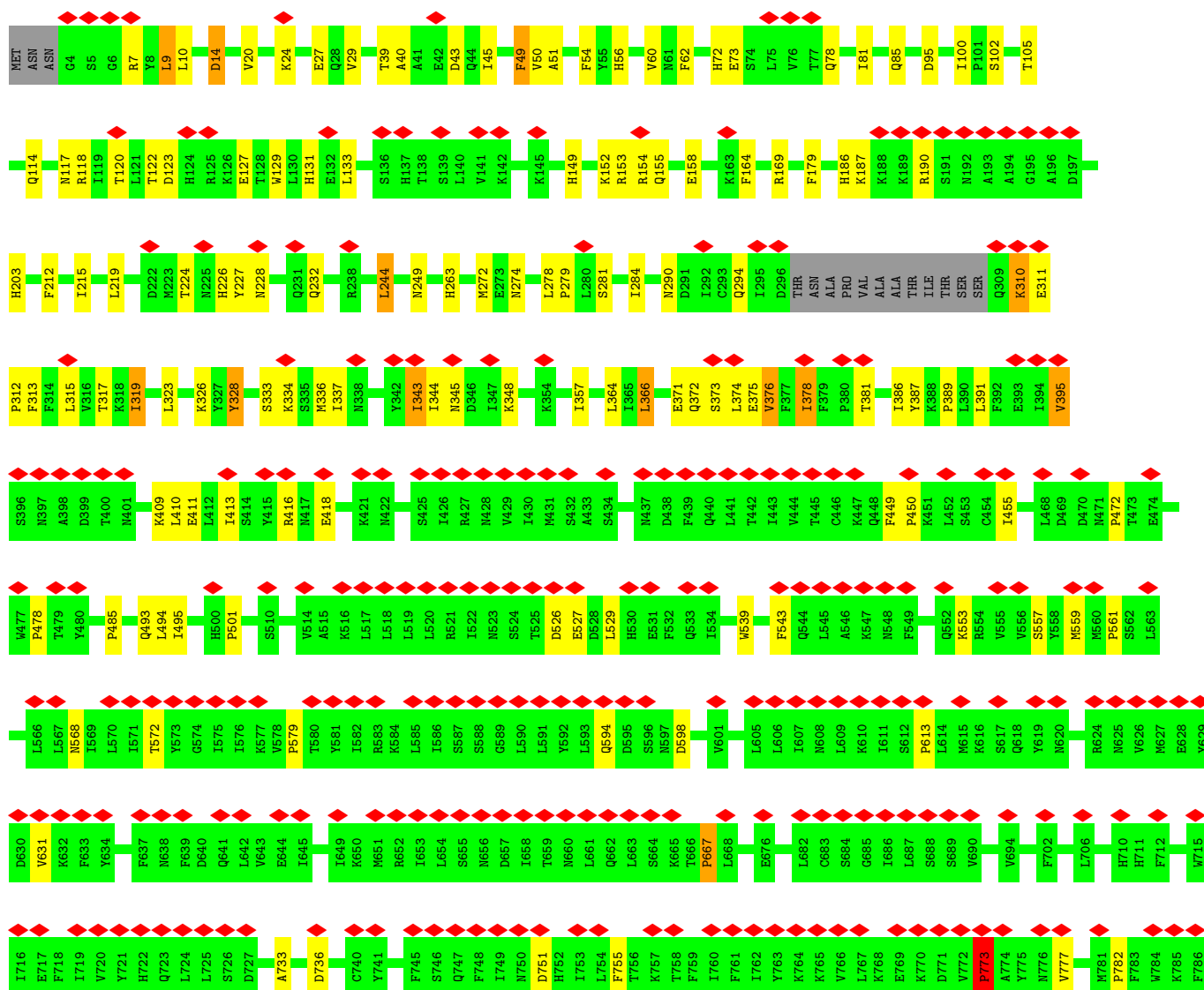
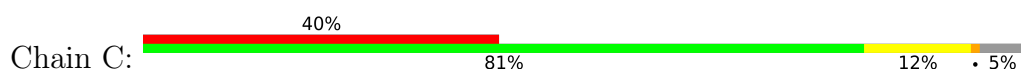
- Molecule 2: RNA polymerase II holoenzyme cyclin-like subunit







• Molecule 3: Mediator of RNA polymerase II transcription subunit 12













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138178	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 ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.28	0/3030	0.53	0/4098
2	B	0.30	0/2505	0.49	0/3407
3	C	0.39	0/8467	0.59	24/11647 (0.2%)
4	D	0.30	0/7183	0.55	0/9753
All	All	0.33	0/21185	0.56	24/28905 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	613	PRO	N-CA-CB	6.34	110.91	103.30
3	C	1316	PRO	N-CA-CB	6.26	110.81	103.30
3	C	485	PRO	N-CA-CB	6.19	110.72	103.30
3	C	494	LEU	N-CA-C	6.15	127.60	111.00
3	C	1106	PRO	N-CA-CB	6.01	110.51	103.30
3	C	478	PRO	N-CA-CB	5.96	110.45	103.30
3	C	1000	PRO	N-CA-CB	5.96	110.45	103.30
3	C	450	PRO	N-CA-CB	5.90	110.38	103.30
3	C	667	PRO	N-CA-CB	5.86	110.33	103.30
3	C	1255	PRO	N-CA-CB	5.86	110.33	103.30
3	C	1297	PRO	N-CA-CB	5.85	110.32	103.30
3	C	936	PRO	N-CA-CB	5.82	110.28	103.30
3	C	773	PRO	N-CA-CB	5.79	110.25	103.30
3	C	1315	PRO	N-CA-CB	5.79	110.25	103.30
3	C	1308	PRO	N-CA-CB	5.77	110.23	103.30
3	C	792	PRO	N-CA-CB	5.73	110.18	103.30
3	C	501	PRO	N-CA-CB	5.71	110.15	103.30
3	C	847	PRO	N-CA-CB	5.67	110.10	103.30
3	C	1252	PRO	N-CA-CB	5.58	109.99	103.30
3	C	472	PRO	N-CA-CB	5.43	109.82	103.30
3	C	495	ILE	N-CA-C	5.15	124.91	111.00
3	C	579	PRO	N-CA-CB	5.14	109.47	103.30
3	C	782	PRO	N-CA-CB	5.11	109.44	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	561	PRO	N-CA-CB	5.10	109.42	103.30

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	2952	0	2987	39	0
2	B	2436	0	2430	27	0
3	C	8362	0	5809	96	0
4	D	7012	0	7104	90	0
All	All	20762	0	18330	240	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 6.

All (240) 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:C:373:SER:HB2	3:C:1318:GLN:CB	1.77	1.15
3:C:102:SER:CB	3:C:1413:ASN:HD21	1.60	1.13
3:C:373:SER:CB	3:C:1318:GLN:CB	2.29	1.10
3:C:102:SER:HB2	3:C:1413:ASN:HD21	1.05	1.09
3:C:311:GLU:CG	3:C:312:PRO:HD3	1.88	1.03
3:C:311:GLU:HG3	3:C:312:PRO:CD	1.88	1.02
3:C:311:GLU:HG3	3:C:312:PRO:HD3	0.99	0.98
3:C:373:SER:O	3:C:1318:GLN:CA	2.13	0.96
3:C:100:ILE:CG2	3:C:1408:ASN:HD21	1.80	0.95
3:C:373:SER:C	3:C:1318:GLN:CB	2.35	0.94
3:C:373:SER:O	3:C:1318:GLN:CB	2.16	0.93
3:C:102:SER:HB2	3:C:1413:ASN:ND2	1.84	0.92
3:C:1413:ASN:HD22	4:D:1284:TYR:HE2	1.15	0.92
3:C:373:SER:O	3:C:1318:GLN:HA	1.71	0.91
3:C:334:LYS:HD3	3:C:345:ASN:HD22	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:373:SER:O	3:C:1317:PHE:O	1.89	0.89
3:C:310:LYS:H	3:C:310:LYS:CE	1.88	0.86
3:C:102:SER:CB	3:C:1413:ASN:ND2	2.41	0.81
3:C:310:LYS:H	3:C:310:LYS:HE2	1.47	0.79
3:C:334:LYS:HD3	3:C:345:ASN:ND2	1.99	0.77
2:B:65:ASP:OD1	2:B:65:ASP:N	2.19	0.73
3:C:100:ILE:CG2	3:C:1408:ASN:ND2	2.51	0.73
4:D:198:HIS:HE1	4:D:262:LEU:HD11	1.54	0.72
3:C:100:ILE:HG23	3:C:1408:ASN:HD21	1.55	0.71
4:D:198:HIS:CE1	4:D:262:LEU:HD11	2.27	0.69
3:C:102:SER:HB3	3:C:1413:ASN:HD21	1.52	0.69
3:C:373:SER:OG	3:C:1318:GLN:CB	2.40	0.69
3:C:311:GLU:OE2	3:C:312:PRO:HG3	1.93	0.69
4:D:198:HIS:CE1	4:D:262:LEU:CD1	2.76	0.69
2:B:66:LEU:O	2:B:67:HIS:ND1	2.27	0.68
4:D:198:HIS:HE1	4:D:262:LEU:CD1	2.08	0.67
4:D:262:LEU:HD13	4:D:262:LEU:N	2.09	0.67
2:B:63:HIS:CE1	2:B:66:LEU:HB2	2.29	0.67
4:D:1024:LYS:O	4:D:1027:PRO:HD2	1.94	0.66
1:A:363:PRO:HG2	1:A:366:LYS:HB3	1.76	0.65
2:B:66:LEU:O	2:B:67:HIS:CG	2.49	0.65
3:C:1413:ASN:ND2	4:D:1284:TYR:HE2	1.90	0.65
3:C:311:GLU:CG	3:C:312:PRO:CD	2.64	0.63
4:D:262:LEU:HD13	4:D:262:LEU:H	1.63	0.62
3:C:526:ASP:O	3:C:529:LEU:N	2.33	0.62
4:D:290:ASP:HB2	4:D:295:HIS:HB2	1.82	0.61
3:C:14:ASP:OD1	3:C:14:ASP:N	2.33	0.61
3:C:310:LYS:H	3:C:310:LYS:HE3	1.65	0.61
3:C:343:ILE:HG13	3:C:343:ILE:O	1.99	0.60
3:C:1143:ILE:HA	3:C:1150:VAL:CB	2.31	0.60
3:C:315:LEU:O	3:C:319:ILE:HB	2.02	0.60
3:C:100:ILE:HG21	3:C:1408:ASN:OD1	2.02	0.60
1:A:245:GLN:NE2	1:A:483:PRO:O	2.35	0.59
2:B:78:CYS:HA	2:B:81:LEU:HD23	1.84	0.59
4:D:156:ASN:OD1	4:D:156:ASN:N	2.34	0.59
4:D:262:LEU:C	4:D:262:LEU:HD22	2.22	0.59
3:C:773:PRO:O	3:C:777:VAL:N	2.28	0.59
3:C:1136:GLN:O	3:C:1140:MET:N	2.28	0.59
4:D:1255:PHE:HB2	4:D:1332:TRP:HE1	1.67	0.58
4:D:96:ASP:N	4:D:96:ASP:OD1	2.37	0.58
3:C:373:SER:CA	3:C:1318:GLN:CB	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1005:LEU:HD21	4:D:1049:ILE:HG23	1.86	0.57
3:C:374:LEU:O	3:C:1317:PHE:CB	2.53	0.57
4:D:1037:ASN:N	4:D:1037:ASN:OD1	2.35	0.57
4:D:1062:PRO:O	4:D:1063:ASN:ND2	2.38	0.57
3:C:45:ILE:O	3:C:49:PHE:HB2	2.03	0.57
3:C:493:GLN:CB	3:C:559:MET:CB	2.82	0.57
3:C:539:TRP:CB	3:C:598:ASP:CB	2.82	0.57
3:C:455:ILE:N	3:C:1129:LEU:CB	2.67	0.57
1:A:343:THR:HG23	1:A:345:ALA:H	1.70	0.57
4:D:1342:CYS:HG	4:D:1347:SER:HG	1.51	0.56
4:D:948:ASN:N	4:D:948:ASN:OD1	2.38	0.56
4:D:262:LEU:HD22	4:D:262:LEU:O	2.06	0.55
4:D:14:LEU:HB3	4:D:898:ARG:HH21	1.72	0.55
3:C:102:SER:HB3	3:C:1413:ASN:ND2	2.17	0.55
4:D:1287:GLU:OE2	4:D:1289:ARG:NH2	2.40	0.54
4:D:1344:HIS:ND1	4:D:1345:SER:O	2.40	0.54
3:C:279:PRO:HG3	3:C:357:ILE:HD11	1.89	0.54
2:B:146:ARG:HD3	2:B:153:ILE:HG23	1.89	0.54
3:C:133:LEU:O	3:C:169:ARG:NH1	2.41	0.54
1:A:297:ASP:OD1	1:A:473:ASN:ND2	2.41	0.54
4:D:27:ASN:N	4:D:27:ASN:OD1	2.40	0.54
4:D:1029:ILE:O	4:D:1066:LEU:HA	2.08	0.53
1:A:383:ASN:OD1	1:A:383:ASN:N	2.40	0.53
4:D:146:LEU:HD21	4:D:170:LEU:HD12	1.89	0.53
3:C:1199:ASN:O	3:C:1241:GLN:CB	2.56	0.53
3:C:1095:PHE:CB	3:C:1141:GLN:CB	2.87	0.53
3:C:310:LYS:HE2	3:C:310:LYS:N	2.20	0.53
4:D:18:TYR:HA	4:D:898:ARG:HA	1.90	0.53
2:B:63:HIS:ND1	2:B:66:LEU:HB2	2.24	0.53
3:C:1420:ARG:NH1	4:D:915:TYR:OH	2.42	0.53
4:D:215:THR:O	4:D:218:LEU:HB3	2.09	0.53
3:C:1011:MET:O	3:C:1014:LEU:CB	2.58	0.52
4:D:837:THR:OG1	4:D:1396:ARG:NH1	2.42	0.52
4:D:1042:GLU:OE1	4:D:1046:LYS:NZ	2.42	0.52
3:C:1393:TYR:OH	3:C:1397:MET:SD	2.68	0.52
4:D:1074:ASP:N	4:D:1074:ASP:OD1	2.43	0.52
1:A:56:THR:OG1	1:A:57:ILE:N	2.37	0.52
3:C:333:SER:OG	3:C:334:LYS:N	2.43	0.52
1:A:222:LEU:HD21	1:A:225:ILE:HD11	1.92	0.51
3:C:409:LYS:HG3	3:C:413:ILE:HD13	1.91	0.51
3:C:373:SER:O	3:C:1317:PHE:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1159:SER:OG	4:D:1161:ASP:OD1	2.29	0.51
4:D:1326:CYS:SG	4:D:1327:ASP:N	2.83	0.51
3:C:123:ASP:O	3:C:127:GLU:HB3	2.11	0.51
4:D:854:ALA:O	4:D:858:VAL:HB	2.11	0.51
4:D:198:HIS:CE1	4:D:262:LEU:HD13	2.46	0.50
4:D:928:LYS:NZ	4:D:930:ASP:OD2	2.43	0.50
1:A:244:LEU:HG	1:A:289:PRO:HB2	1.94	0.50
4:D:1034:PRO:HA	4:D:1071:ILE:O	2.12	0.50
2:B:206:GLN:NE2	3:C:62:PHE:O	2.44	0.50
3:C:1413:ASN:ND2	4:D:1284:TYR:CE2	2.74	0.50
4:D:1106:HIS:ND1	4:D:1175:GLN:OE1	2.45	0.49
1:A:61:ARG:NH2	2:B:162:GLU:OE1	2.45	0.49
4:D:192:PRO:HD3	4:D:274:LEU:HD12	1.94	0.49
4:D:1026:VAL:N	4:D:1027:PRO:CD	2.75	0.49
3:C:1376:CYS:SG	3:C:1377:THR:N	2.85	0.49
4:D:1375:ASP:OD1	4:D:1375:ASP:N	2.44	0.49
3:C:375:GLU:O	3:C:409:LYS:NZ	2.46	0.49
4:D:1279:ASP:OD1	4:D:1279:ASP:N	2.45	0.49
1:A:347:ASP:N	1:A:347:ASP:OD1	2.44	0.49
2:B:217:ILE:O	2:B:218:ASN:ND2	2.27	0.49
3:C:272:MET:O	3:C:326:LYS:NZ	2.44	0.48
1:A:68:ARG:NH1	1:A:227:LEU:O	2.45	0.48
4:D:1029:ILE:HG12	4:D:1066:LEU:HB3	1.94	0.48
1:A:242:ASP:OD1	1:A:245:GLN:N	2.46	0.48
1:A:74:LYS:HG3	1:A:94:ARG:HH22	1.78	0.48
4:D:115:ARG:NH1	4:D:225:SER:OG	2.40	0.47
4:D:921:HIS:O	4:D:922:HIS:ND1	2.47	0.47
4:D:301:LEU:HA	4:D:304:ILE:HG22	1.95	0.47
3:C:526:ASP:O	3:C:527:GLU:C	2.53	0.47
4:D:1220:LEU:HD21	4:D:1382:ILE:HG23	1.96	0.47
4:D:1377:HIS:CE1	4:D:1378:ILE:HG13	2.50	0.47
2:B:225:PRO:HD2	2:B:228:ILE:HD12	1.97	0.47
2:B:263:ASN:N	2:B:263:ASN:OD1	2.47	0.47
4:D:1176:GLY:HA3	4:D:1205:LEU:HD11	1.96	0.47
1:A:449:ILE:HD12	3:C:43:ASP:HB2	1.97	0.47
2:B:17:THR:OG1	2:B:18:LYS:N	2.48	0.47
2:B:144:GLU:HA	2:B:147:THR:HG22	1.97	0.47
3:C:117:ASN:OD1	3:C:117:ASN:N	2.47	0.46
4:D:1258:GLU:HG3	4:D:1329:ASP:HB3	1.97	0.46
4:D:14:LEU:HD22	4:D:898:ARG:HD2	1.98	0.46
4:D:132:PHE:HB3	4:D:135:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:859:THR:O	4:D:859:THR:OG1	2.34	0.46
3:C:311:GLU:N	3:C:312:PRO:CD	2.78	0.46
4:D:262:LEU:CD2	4:D:263:LEU:O	2.63	0.46
4:D:131:GLN:HG2	4:D:133:GLY:H	1.81	0.46
4:D:262:LEU:CD1	4:D:262:LEU:N	2.76	0.46
1:A:182:ILE:HG12	1:A:235:VAL:HG12	1.98	0.45
3:C:1354:VAL:HG23	4:D:878:LYS:HE2	1.98	0.45
2:B:243:LYS:HG3	3:C:81:ILE:HG21	1.98	0.45
4:D:1078:ASN:HB3	4:D:1081:VAL:HG23	1.98	0.45
4:D:936:LYS:HD2	4:D:936:LYS:HA	1.84	0.45
4:D:942:PRO:HA	4:D:943:PRO:HD3	1.86	0.45
1:A:260:PRO:HA	1:A:263:VAL:HG12	1.97	0.45
1:A:325:VAL:HG21	1:A:335:LEU:HD22	1.98	0.45
3:C:1409:ASP:OD1	3:C:1409:ASP:N	2.43	0.45
1:A:291:ASN:OD1	1:A:291:ASN:N	2.49	0.45
1:A:442:HIS:HB3	1:A:452:ILE:HG21	1.99	0.45
2:B:68:TYR:HB3	2:B:113:ARG:HH22	1.82	0.45
4:D:15:SER:OG	4:D:16:SER:N	2.50	0.45
4:D:158:ASP:OD1	4:D:158:ASP:N	2.49	0.45
2:B:15:GLN:NE2	2:B:223:LEU:O	2.49	0.45
3:C:311:GLU:CD	3:C:312:PRO:N	2.70	0.45
3:C:313:PHE:O	3:C:313:PHE:CD1	2.70	0.45
3:C:376:VAL:HG12	3:C:378:ILE:HG22	1.99	0.45
3:C:553:LYS:O	3:C:557:SER:N	2.47	0.44
4:D:1224:LEU:O	4:D:1312:ARG:NH1	2.50	0.44
1:A:313:ASN:OD1	1:A:313:ASN:N	2.50	0.44
2:B:31:LEU:O	2:B:34:GLN:NE2	2.50	0.44
3:C:39:THR:OG1	3:C:40:ALA:N	2.49	0.44
2:B:161:THR:HA	2:B:164:GLU:HB3	2.00	0.44
3:C:568:ASN:HA	3:C:572:THR:CB	2.48	0.44
4:D:134:ASN:OD1	4:D:134:ASN:N	2.50	0.44
4:D:262:LEU:C	4:D:262:LEU:CD2	2.86	0.44
1:A:240:GLU:HB2	1:A:295:THR:HA	2.00	0.44
3:C:1013:LEU:O	3:C:1016:ASP:N	2.50	0.44
1:A:333:PRO:HG2	1:A:446:TYR:HB3	2.00	0.43
3:C:418:GLU:H	3:C:418:GLU:HG2	1.67	0.43
4:D:1252:LYS:HD3	4:D:1307:ALA:HB1	1.99	0.43
2:B:238:ILE:HD13	2:B:238:ILE:HA	1.90	0.43
3:C:100:ILE:HG22	3:C:1408:ASN:HD21	1.75	0.43
4:D:971:GLN:O	4:D:975:ASN:HB2	2.18	0.43
4:D:252:THR:HG21	4:D:1160:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:835:THR:HG23	4:D:836:PRO:HD3	2.01	0.43
3:C:244:LEU:HD21	3:C:284:ILE:HD11	2.00	0.43
4:D:1169:LEU:O	4:D:1177:SER:HA	2.19	0.43
1:A:471:SER:OG	1:A:473:ASN:O	2.36	0.43
2:B:40:LEU:HD13	2:B:315:LEU:HD23	2.00	0.43
4:D:907:LYS:HB3	4:D:1299:VAL:HB	2.00	0.43
3:C:751:ASP:O	3:C:755:PHE:N	2.48	0.43
1:A:393:GLY:O	1:A:446:TYR:OH	2.31	0.43
1:A:452:ILE:HG12	1:A:457:ALA:HB2	2.01	0.43
2:B:32:GLU:OE1	2:B:64:ARG:HD2	2.19	0.43
1:A:250:HIS:HB3	1:A:361:LEU:HD21	2.00	0.42
3:C:328:TYR:HD1	3:C:328:TYR:HA	1.78	0.42
1:A:242:ASP:OD2	1:A:485:ARG:NH2	2.53	0.42
1:A:317:THR:OG1	1:A:318:LEU:N	2.52	0.42
1:A:341:HIS:CD2	3:C:54:PHE:HB3	2.54	0.42
3:C:154:ARG:O	3:C:158:GLU:HB2	2.19	0.42
3:C:733:ALA:O	3:C:736:ASP:N	2.53	0.42
2:B:240:ILE:HD11	3:C:78:GLN:HB3	2.01	0.42
4:D:14:LEU:HB2	4:D:1256:ILE:HG23	2.01	0.42
1:A:426:TYR:HE2	1:A:433:ASP:HA	1.84	0.42
3:C:409:LYS:HD2	3:C:409:LYS:HA	1.84	0.42
4:D:871:LYS:HE2	4:D:871:LYS:HB2	1.75	0.42
2:B:153:ILE:HD12	2:B:154:PRO:HD2	2.02	0.42
3:C:543:PHE:HA	3:C:594:GLN:CB	2.50	0.42
4:D:1157:SER:HB2	4:D:1220:LEU:HB2	2.02	0.42
4:D:1257:ASP:OD2	4:D:1266:LYS:NZ	2.53	0.42
1:A:340:ARG:HG3	3:C:51:ALA:HA	2.01	0.41
4:D:984:LEU:O	4:D:993:GLY:N	2.49	0.41
1:A:394:THR:HG21	1:A:417:LYS:HG3	2.02	0.41
2:B:115:ILE:HD13	2:B:115:ILE:HA	1.88	0.41
3:C:809:TYR:O	3:C:812:GLU:CB	2.68	0.41
1:A:458:LEU:HD12	1:A:458:LEU:HA	1.87	0.41
2:B:108:ILE:HD13	2:B:108:ILE:HA	1.88	0.41
3:C:114:GLN:NE2	3:C:1390:ASN:OD1	2.43	0.41
3:C:152:LYS:HG3	3:C:155:GLN:HB2	2.03	0.41
3:C:449:PHE:CB	3:C:1084:ALA:HB2	2.50	0.41
3:C:1013:LEU:O	3:C:1014:LEU:C	2.58	0.41
4:D:840:VAL:HG11	4:D:850:LEU:HD21	2.01	0.41
1:A:385:LEU:HD12	1:A:385:LEU:HA	1.92	0.41
4:D:1192:ASP:OD1	4:D:1192:ASP:N	2.54	0.41
1:A:74:LYS:O	1:A:94:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:HD2	2:B:70:LYS:HA	1.74	0.41
3:C:372:GLN:HG2	3:C:375:GLU:H	1.86	0.41
4:D:32:ILE:N	4:D:88:ASP:OD2	2.51	0.41
3:C:9:LEU:HD22	3:C:9:LEU:HA	1.82	0.41
4:D:867:LEU:H	4:D:867:LEU:HG	1.58	0.41
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.94	0.41
1:A:291:ASN:HD22	1:A:304:ASP:HB3	1.86	0.41
1:A:385:LEU:HA	1:A:388:ILE:HG22	2.02	0.41
3:C:366:LEU:HD21	3:C:395:VAL:HG11	2.02	0.41
3:C:386:ILE:HG13	3:C:389:PRO:HD2	2.03	0.41
4:D:821:LEU:HD13	4:D:821:LEU:HA	1.93	0.41
4:D:935:ILE:HG12	4:D:940:PHE:HB2	2.02	0.41
4:D:984:LEU:HD12	4:D:984:LEU:HA	1.91	0.41
4:D:851:ASP:N	4:D:851:ASP:OD1	2.54	0.41
4:D:1121:GLN:H	4:D:1121:GLN:HG2	1.66	0.41
4:D:1309:SER:O	4:D:1309:SER:OG	2.33	0.40
4:D:21:GLU:HB3	4:D:159:LEU:HB3	2.03	0.40
1:A:214:LEU:HD12	1:A:214:LEU:HA	1.96	0.40
4:D:123:LEU:HD23	4:D:123:LEU:HA	1.88	0.40
3:C:105:THR:OG1	3:C:105:THR:O	2.40	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	349/555 (63%)	308 (88%)	41 (12%)	0	100	100
2	B	284/352 (81%)	259 (91%)	25 (9%)	0	100	100
3	C	1344/1427 (94%)	1267 (94%)	67 (5%)	10 (1%)	22	62
4	D	870/1420 (61%)	782 (90%)	88 (10%)	0	100	100
All	All	2847/3754 (76%)	2616 (92%)	221 (8%)	10 (0%)	38	72



All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1105	GLU
3	C	1106	PRO
3	C	1255	PRO
3	C	1316	PRO
3	C	667	PRO
3	C	773	PRO
3	C	965	ILE
3	C	1315	PRO
3	C	631	VAL
3	C	1319	VAL

### 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	317/474 (67%)	265 (84%)	52 (16%)	2	14
2	B	274/323 (85%)	235 (86%)	39 (14%)	3	19
3	C	460/1357 (34%)	383 (83%)	77 (17%)	2	14
4	D	793/1300 (61%)	665 (84%)	128 (16%)	2	15
All	All	1844/3454 (53%)	1548 (84%)	296 (16%)	5	15

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	63	ARG
1	A	69	VAL
1	A	94	ARG
1	A	178	VAL
1	A	179	PHE
1	A	187	THR
1	A	188	GLU
1	A	210	LEU
1	A	213	GLU

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	215	HIS
1	A	229	ARG
1	A	235	VAL
1	A	241	HIS
1	A	242	ASP
1	A	254	GLU
1	A	258	ILE
1	A	261	ARG
1	A	270	LEU
1	A	278	HIS
1	A	282	VAL
1	A	294	VAL
1	A	295	THR
1	A	301	LYS
1	A	314	MET
1	A	324	VAL
1	A	325	VAL
1	A	331	ARG
1	A	347	ASP
1	A	366	LYS
1	A	383	ASN
1	A	386	GLN
1	A	388	ILE
1	A	392	LEU
1	A	398	LYS
1	A	403	LEU
1	A	408	GLU
1	A	412	ILE
1	A	419	ARG
1	A	420	ASP
1	A	422	LEU
1	A	446	TYR
1	A	453	ASP
1	A	458	LEU
1	A	462	TYR
1	A	464	THR
1	A	465	GLU
1	A	468	ILE
1	A	470	VAL
1	A	476	GLU
1	A	481	LYS

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Mol	Chain	Res	Type
2	B	14	TRP
2	B	16	TYR
2	B	29	TRP
2	B	36	PHE
2	B	42	ILE
2	B	43	VAL
2	B	44	MET
2	B	45	ASP
2	B	63	HIS
2	B	65	ASP
2	B	68	TYR
2	B	80	PHE
2	B	81	LEU
2	B	91	ILE
2	B	96	LEU
2	B	103	LEU
2	B	131	VAL
2	B	139	ARG
2	B	142	VAL
2	B	151	GLU
2	B	163	PHE
2	B	168	LEU
2	B	171	LEU
2	B	177	VAL
2	B	188	VAL
2	B	191	LEU
2	B	199	THR
2	B	218	ASN
2	B	231	VAL
2	B	263	ASN
2	B	269	GLN
2	B	274	ARG
2	B	281	VAL
2	B	292	GLU
2	B	302	LYS
2	B	303	TYR
2	B	305	GLU
2	B	313	HIS
2	B	315	LEU
3	C	7	ARG
3	C	9	LEU
3	C	10	LEU

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Mol	Chain	Res	Type
3	C	14	ASP
3	C	20	VAL
3	C	24	LYS
3	C	27	GLU
3	C	29	VAL
3	C	49	PHE
3	C	50	VAL
3	C	56	HIS
3	C	60	VAL
3	C	72	HIS
3	C	73	GLU
3	C	85	GLN
3	C	95	ASP
3	C	118	ARG
3	C	120	THR
3	C	122	THR
3	C	129	TRP
3	C	131	HIS
3	C	149	HIS
3	C	153	ARG
3	C	164	PHE
3	C	179	PHE
3	C	186	HIS
3	C	187	LYS
3	C	190	ARG
3	C	203	HIS
3	C	212	PHE
3	C	215	ILE
3	C	219	LEU
3	C	224	THR
3	C	226	HIS
3	C	227	TYR
3	C	228	ASN
3	C	232	GLN
3	C	244	LEU
3	C	249	ASN
3	C	263	HIS
3	C	274	ASN
3	C	278	LEU
3	C	281	SER
3	C	290	ASN
3	C	294	GLN

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Mol	Chain	Res	Type
3	C	310	LYS
3	C	317	THR
3	C	319	ILE
3	C	323	LEU
3	C	328	TYR
3	C	336	MET
3	C	337	ILE
3	C	343	ILE
3	C	344	ILE
3	C	348	LYS
3	C	364	LEU
3	C	366	LEU
3	C	371	GLU
3	C	376	VAL
3	C	378	ILE
3	C	381	THR
3	C	387	TYR
3	C	391	LEU
3	C	395	VAL
3	C	410	LEU
3	C	411	GLU
3	C	416	ARG
3	C	1353	ILE
3	C	1367	TYR
3	C	1375	VAL
3	C	1392	LYS
3	C	1396	ASP
3	C	1397	MET
3	C	1412	VAL
3	C	1421	PHE
3	C	1423	ARG
3	C	1427	HIS
4	D	7	THR
4	D	13	VAL
4	D	20	VAL
4	D	22	LYS
4	D	25	LYS
4	D	26	ILE
4	D	27	ASN
4	D	32	ILE
4	D	34	LYS
4	D	36	GLN

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Mol	Chain	Res	Type
4	D	38	ASP
4	D	45	GLU
4	D	46	PHE
4	D	59	LEU
4	D	74	VAL
4	D	80	ILE
4	D	85	VAL
4	D	121	LEU
4	D	130	ILE
4	D	134	ASN
4	D	149	LEU
4	D	153	LEU
4	D	155	VAL
4	D	156	ASN
4	D	158	ASP
4	D	171	VAL
4	D	176	GLU
4	D	179	GLU
4	D	197	MET
4	D	198	HIS
4	D	215	THR
4	D	218	LEU
4	D	219	LEU
4	D	228	ILE
4	D	230	LEU
4	D	232	ASN
4	D	242	VAL
4	D	252	THR
4	D	255	ILE
4	D	258	TYR
4	D	262	LEU
4	D	268	LEU
4	D	273	HIS
4	D	274	LEU
4	D	284	GLU
4	D	305	ASP
4	D	307	PHE
4	D	310	LEU
4	D	826	LEU
4	D	835	THR
4	D	840	VAL
4	D	843	SER

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Mol	Chain	Res	Type
4	D	857	VAL
4	D	858	VAL
4	D	859	THR
4	D	863	ILE
4	D	867	LEU
4	D	871	LYS
4	D	877	VAL
4	D	879	ASP
4	D	884	LEU
4	D	885	ILE
4	D	886	THR
4	D	906	SER
4	D	912	LYS
4	D	916	VAL
4	D	917	PHE
4	D	918	VAL
4	D	927	VAL
4	D	935	ILE
4	D	948	ASN
4	D	952	LEU
4	D	959	LYS
4	D	963	LEU
4	D	975	ASN
4	D	982	GLU
4	D	989	GLU
4	D	994	LEU
4	D	998	LYS
4	D	1002	LYS
4	D	1023	ILE
4	D	1025	ASN
4	D	1029	ILE
4	D	1037	ASN
4	D	1041	THR
4	D	1063	ASN
4	D	1066	LEU
4	D	1070	VAL
4	D	1071	ILE
4	D	1074	ASP
4	D	1082	THR
4	D	1083	VAL
4	D	1100	LYS
4	D	1102	VAL

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Mol	Chain	Res	Type
4	D	1106	HIS
4	D	1119	THR
4	D	1120	MET
4	D	1145	ILE
4	D	1159	SER
4	D	1162	LYS
4	D	1181	THR
4	D	1187	SER
4	D	1199	TRP
4	D	1205	LEU
4	D	1213	ILE
4	D	1215	LEU
4	D	1224	LEU
4	D	1229	LEU
4	D	1238	ARG
4	D	1242	LEU
4	D	1249	ASP
4	D	1256	ILE
4	D	1259	ASP
4	D	1263	PRO
4	D	1272	THR
4	D	1279	ASP
4	D	1283	LEU
4	D	1291	ILE
4	D	1310	GLN
4	D	1313	CYS
4	D	1324	LYS
4	D	1327	ASP
4	D	1329	ASP
4	D	1332	TRP
4	D	1359	ARG
4	D	1364	LEU
4	D	1370	LEU
4	D	1377	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	63	HIS
3	C	345	ASN
3	C	1413	ASN
4	D	177	ASN

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Mol	Chain	Res	Type
4	D	198	HIS

### 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](#)

There are no chain breaks in this entry.



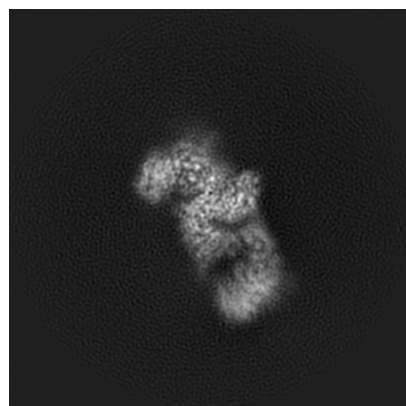
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22991. These allow visual inspection of the internal detail of the map and identification of artifacts.

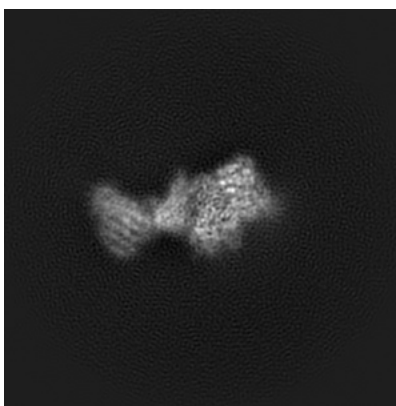
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

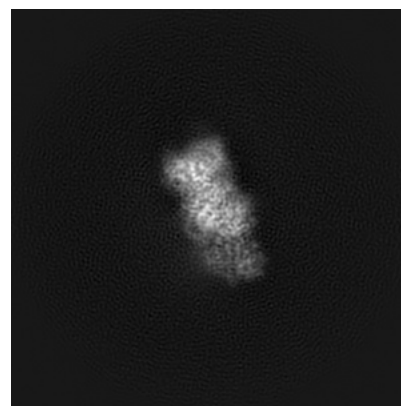
#### 6.1.1 Primary map



X

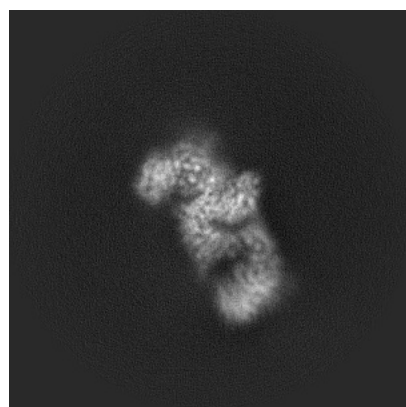


Y

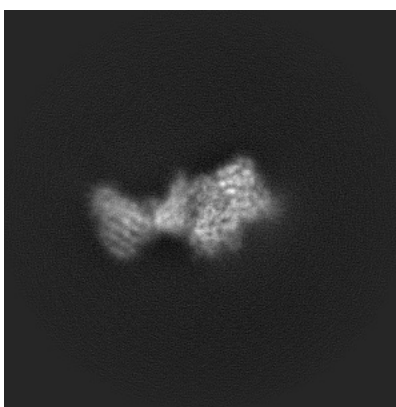


Z

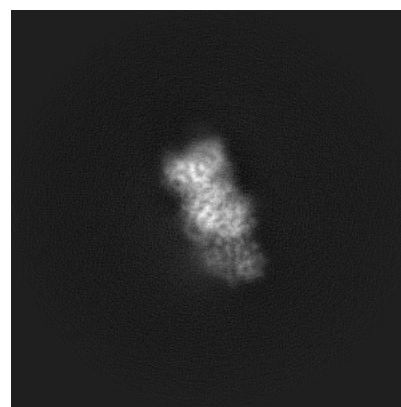
#### 6.1.2 Raw map



X



Y



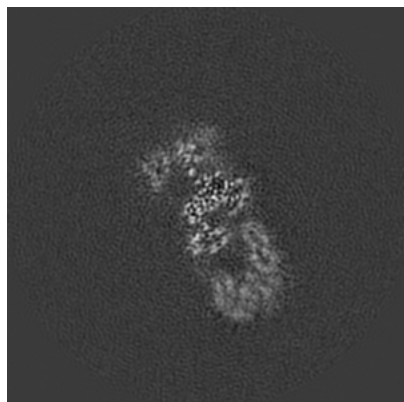
Z

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

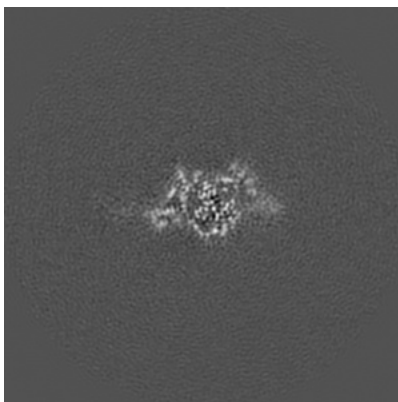


## 6.2 Central slices [i](#)

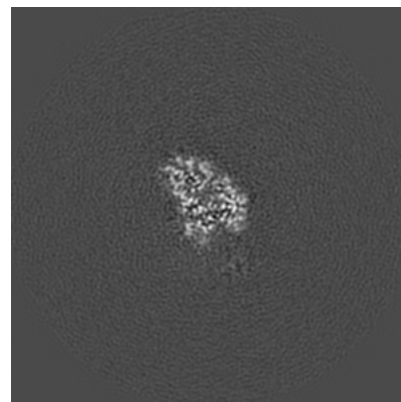
### 6.2.1 Primary map



X Index: 192

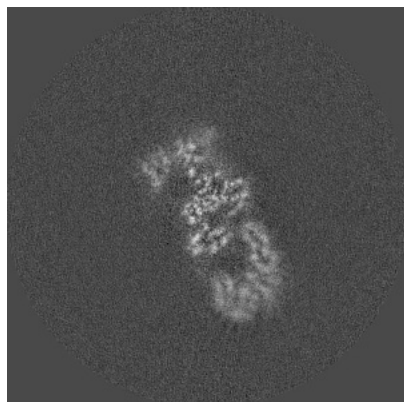


Y Index: 192

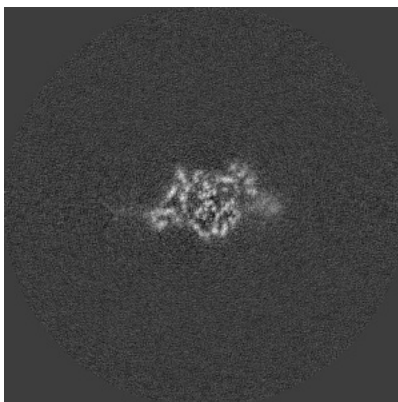


Z Index: 192

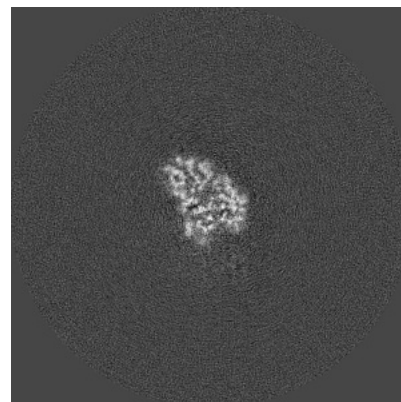
### 6.2.2 Raw map



X Index: 192



Y Index: 192



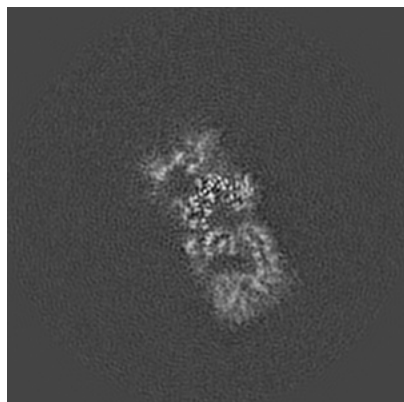
Z Index: 192

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

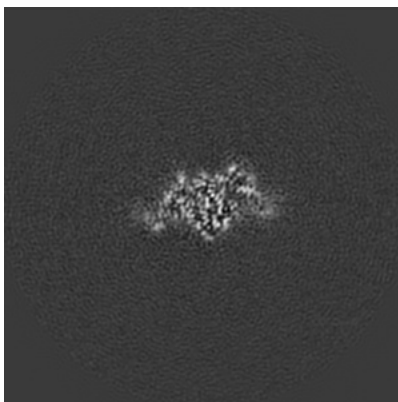


## 6.3 Largest variance slices [i](#)

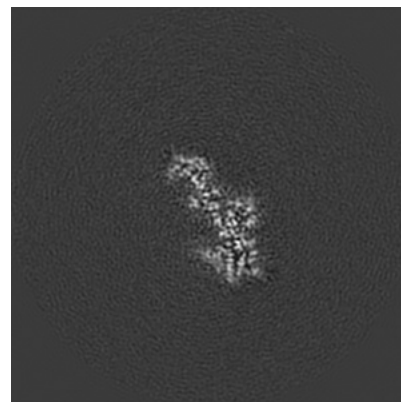
### 6.3.1 Primary map



X Index: 188

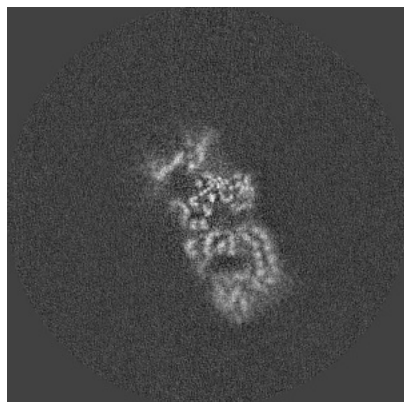


Y Index: 189

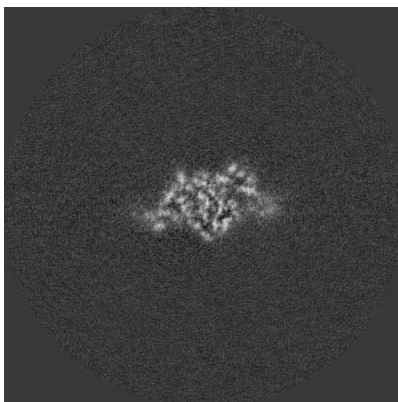


Z Index: 219

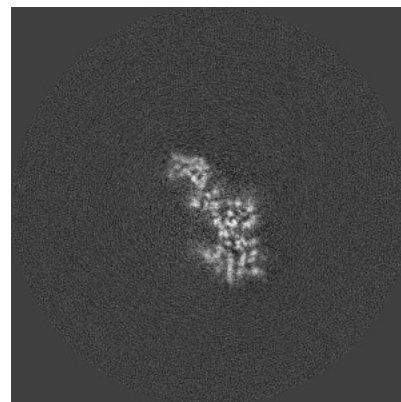
### 6.3.2 Raw map



X Index: 187



Y Index: 190



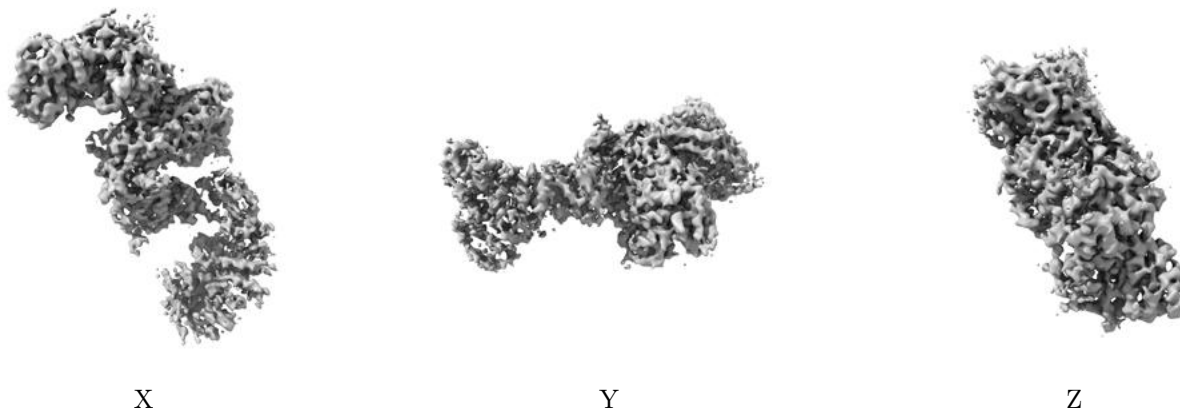
Z Index: 220

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



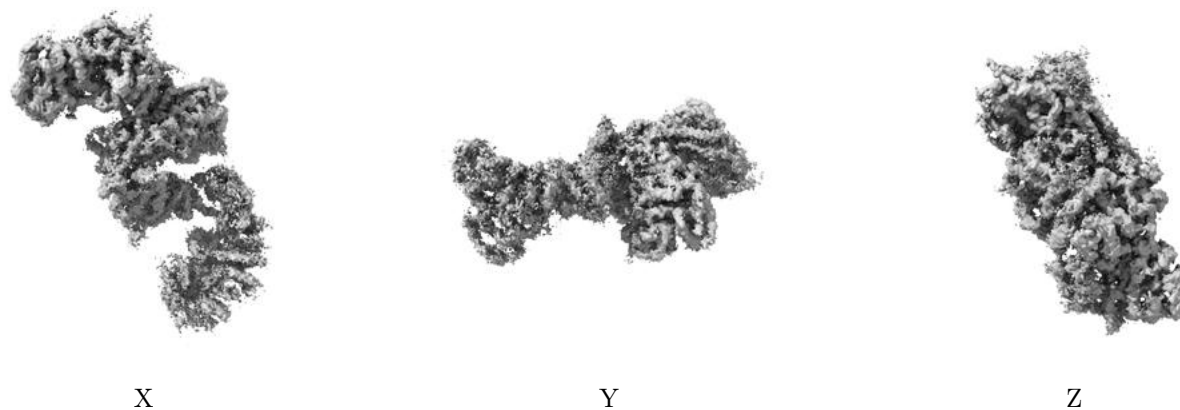
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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.

### 6.4.2 Raw map



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 [i](#)

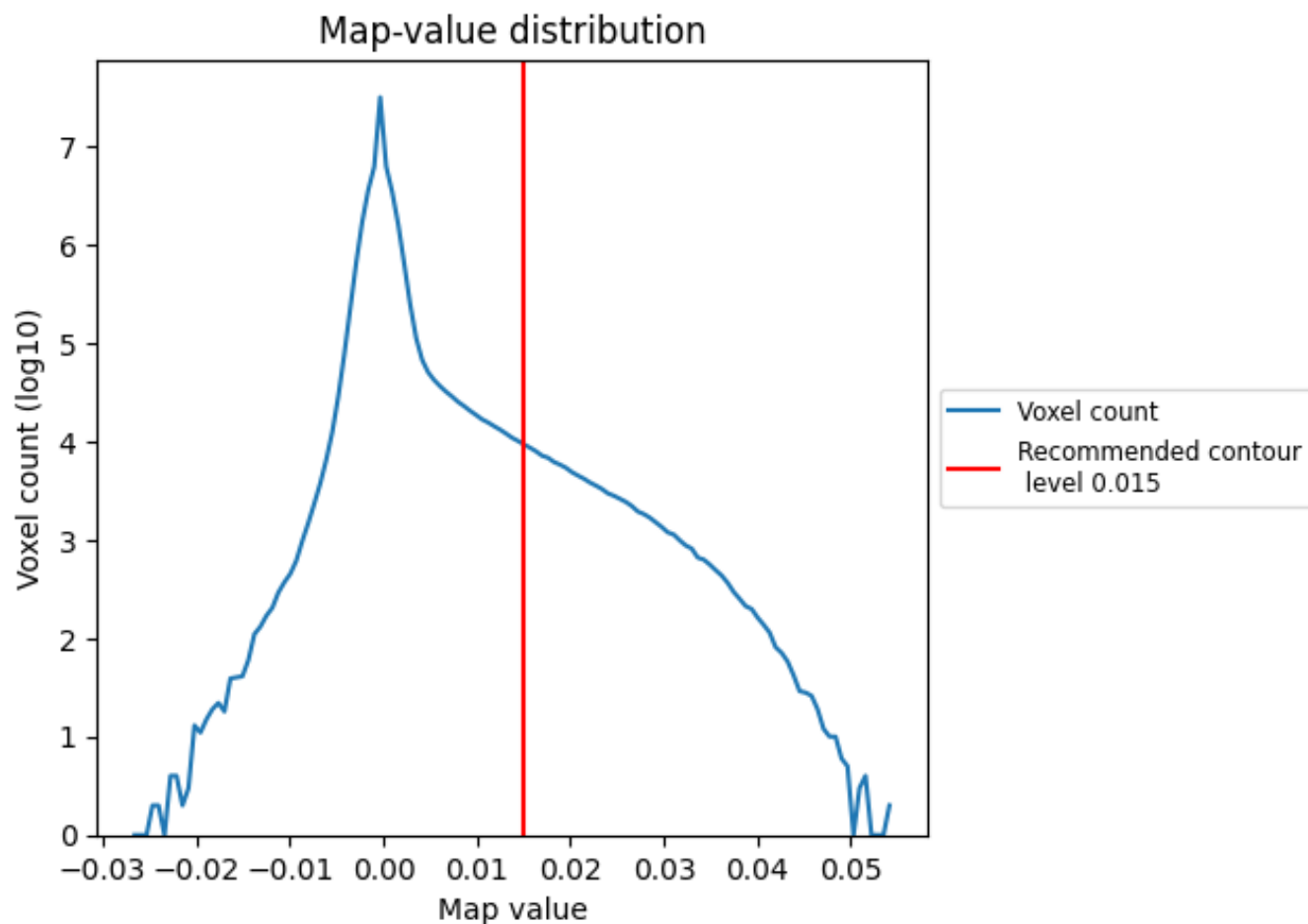
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

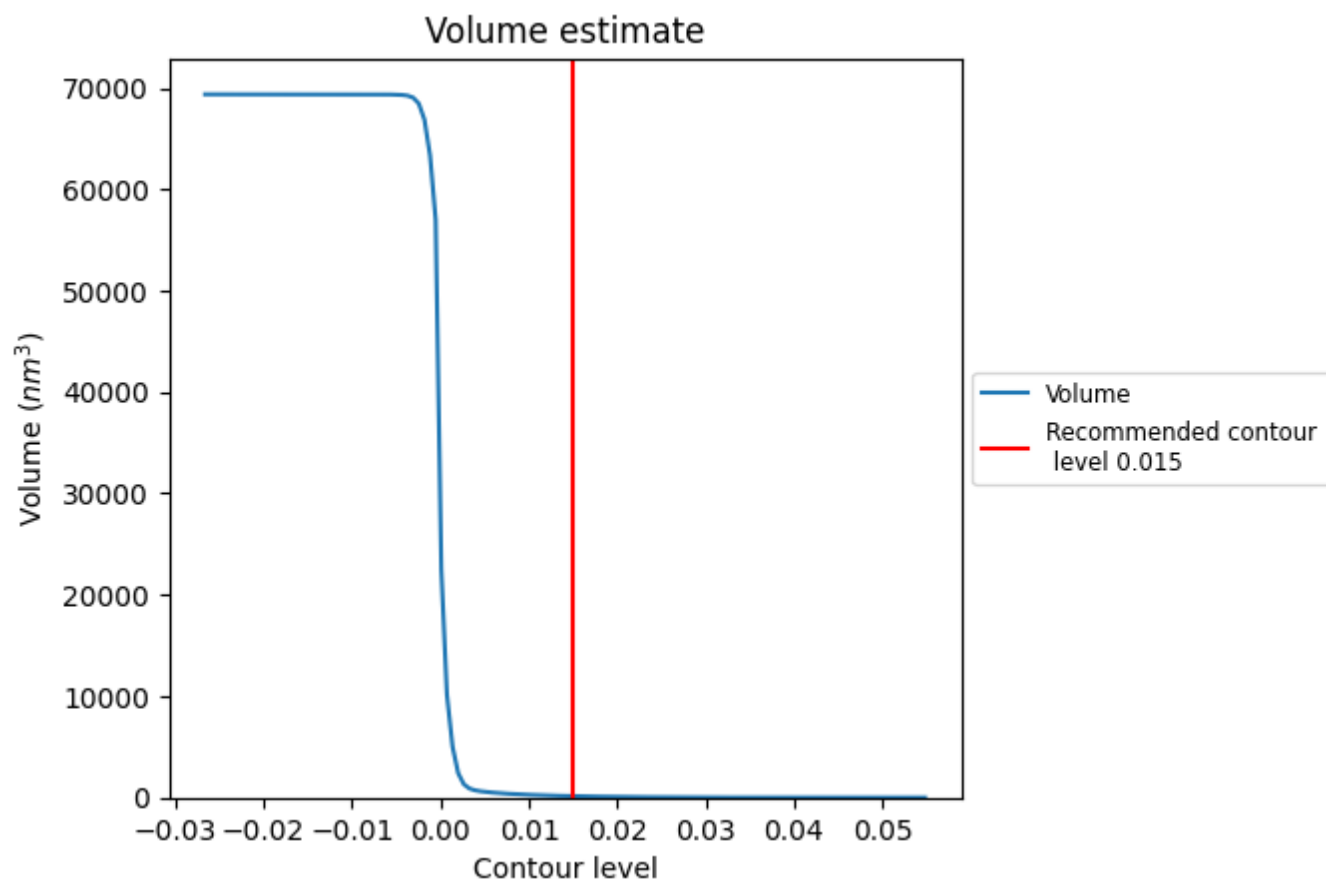
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

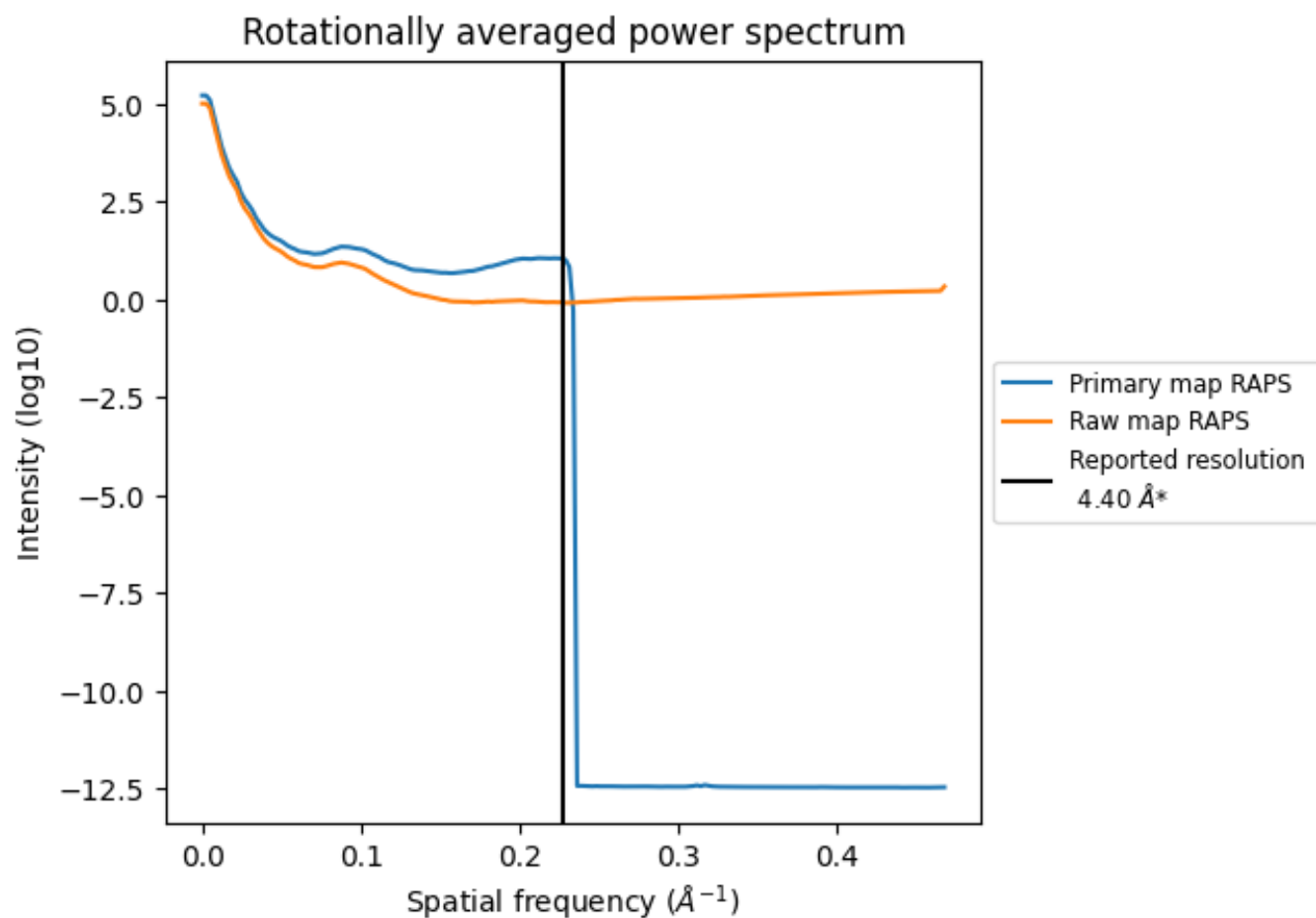


The volume at the recommended contour level is 139 nm<sup>3</sup>; this corresponds to an approximate mass of 126 kDa.

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 ⓘ



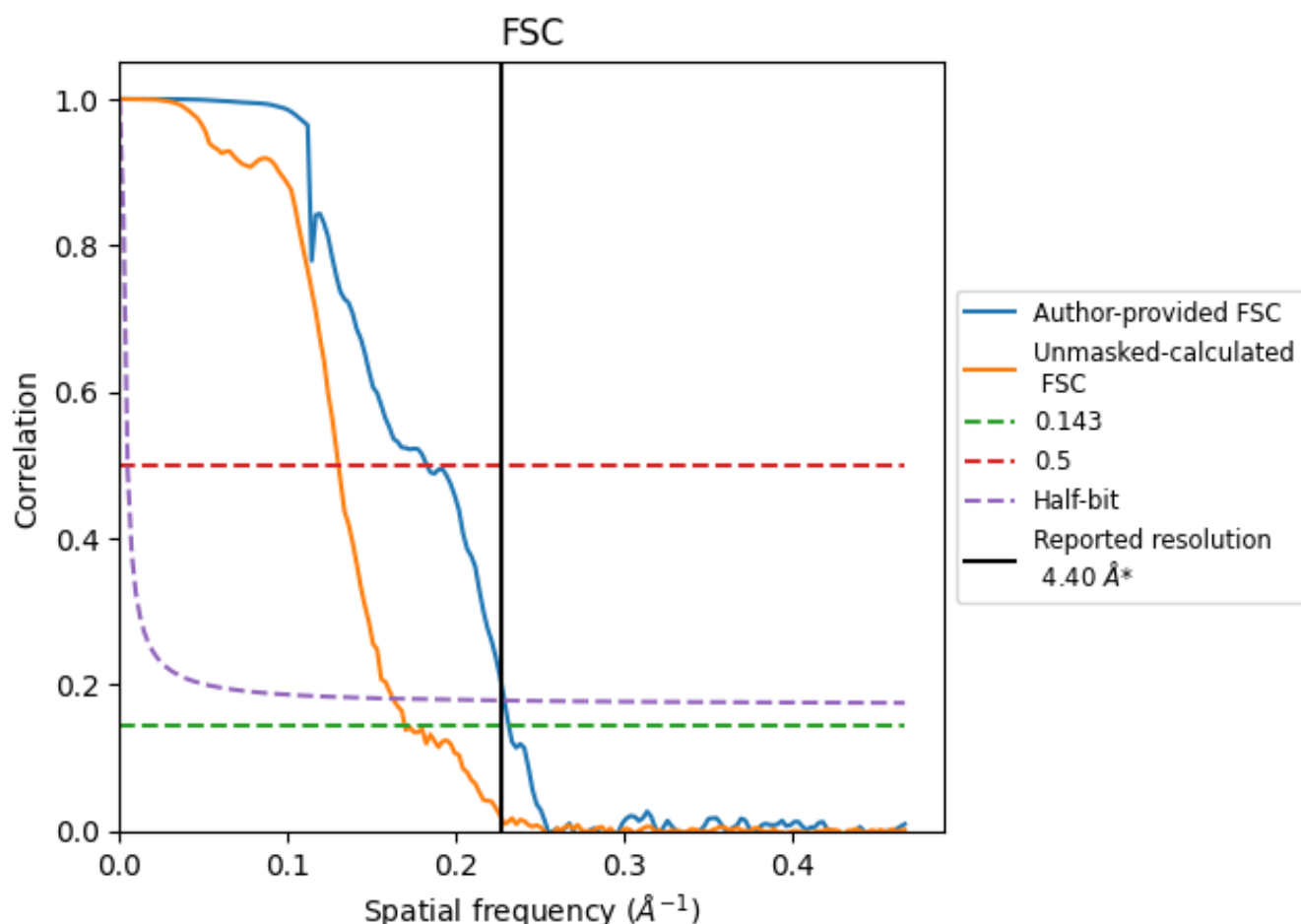
\*Reported resolution corresponds to spatial frequency of 0.227  $\text{\AA}^{-1}$



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.32	5.47	4.37
Unmasked-calculated*	5.89	7.68	6.15

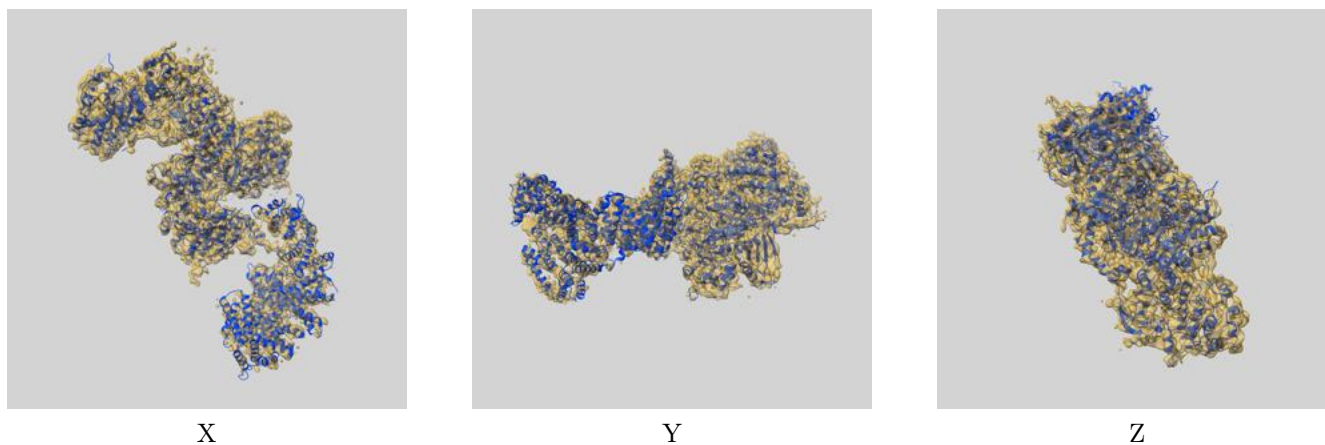
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.89 differs from the reported value 4.4 by more than 10 %



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

This section contains information regarding the fit between EMDB map EMD-22991 and PDB model 7KPX. Per-residue inclusion information can be found in section [3](#) on page [5](#).

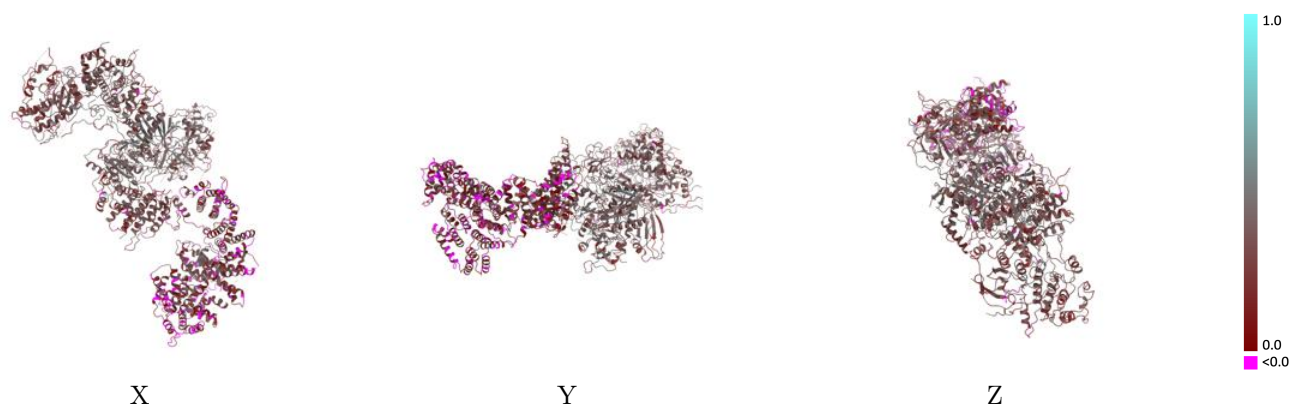
### 9.1 Map-model overlay [i](#)



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.

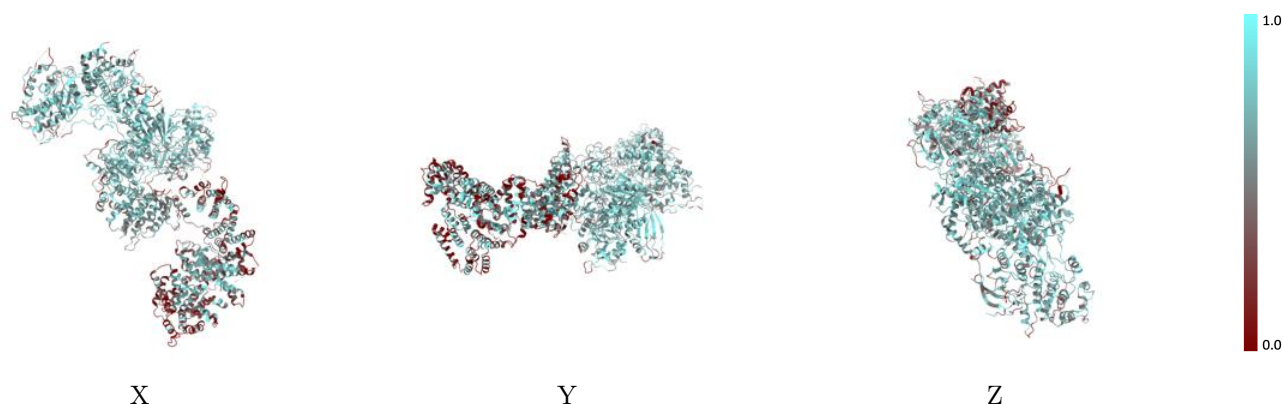


## 9.2 Q-score mapped to coordinate model [i](#)



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.

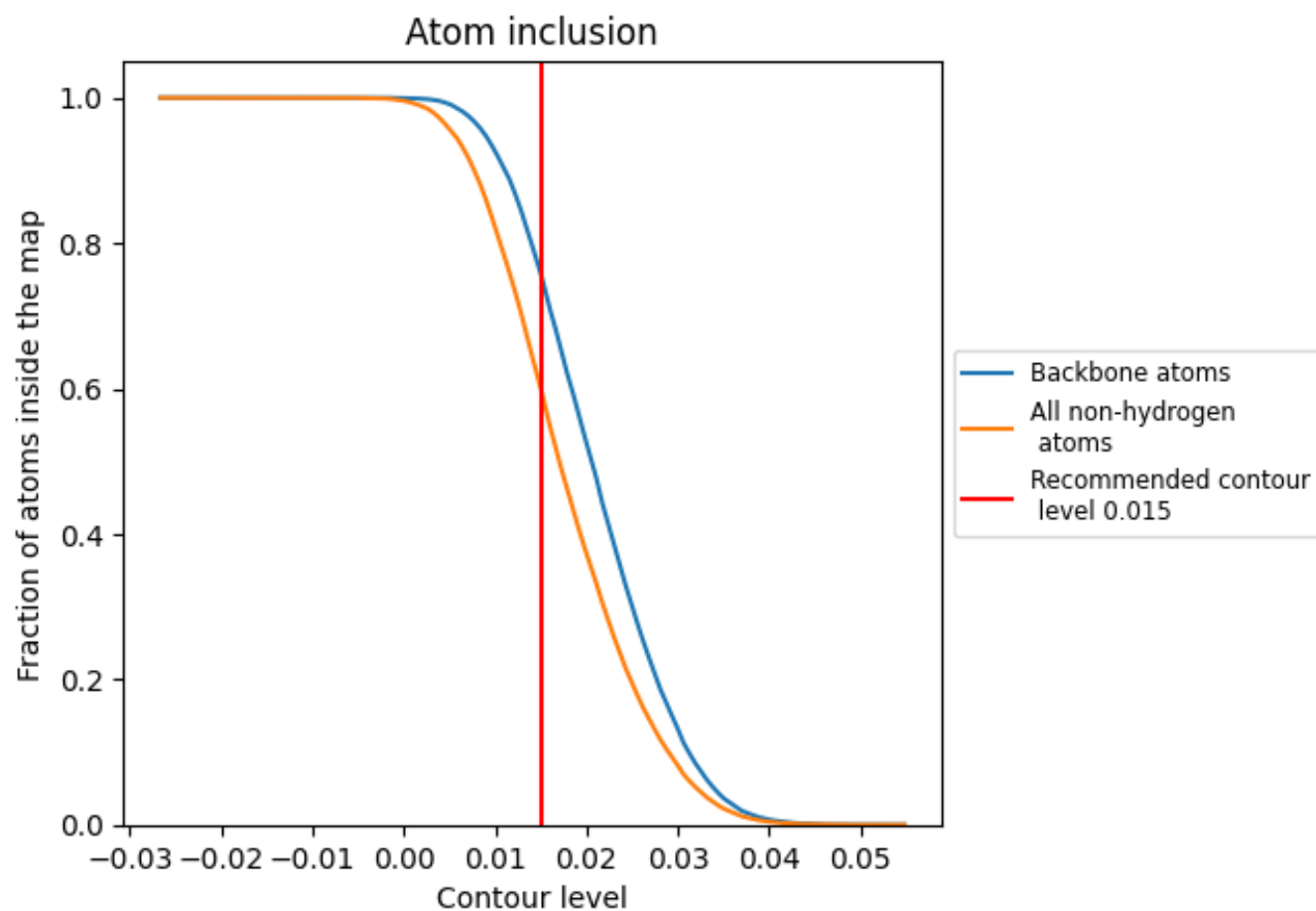
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.015).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 60% 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	<div></div> 0.5995	<div></div> 0.2960
A	<div></div> 0.6119	<div></div> 0.2970
B	<div></div> 0.6637	<div></div> 0.3280
C	<div></div> 0.5123	<div></div> 0.2290
D	<div></div> 0.6768	<div></div> 0.3630

