Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:41 PM UTC

PDB ID	:	7JMN / pdb_00007jmn
EMDB ID	:	EMD-22397
Title	:	Tail module of Mediator complex
Authors	:	Zhang, H.Q.; Chen, D.C.
Deposited on	:	2020-08-02
Resolution	:	3.58 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

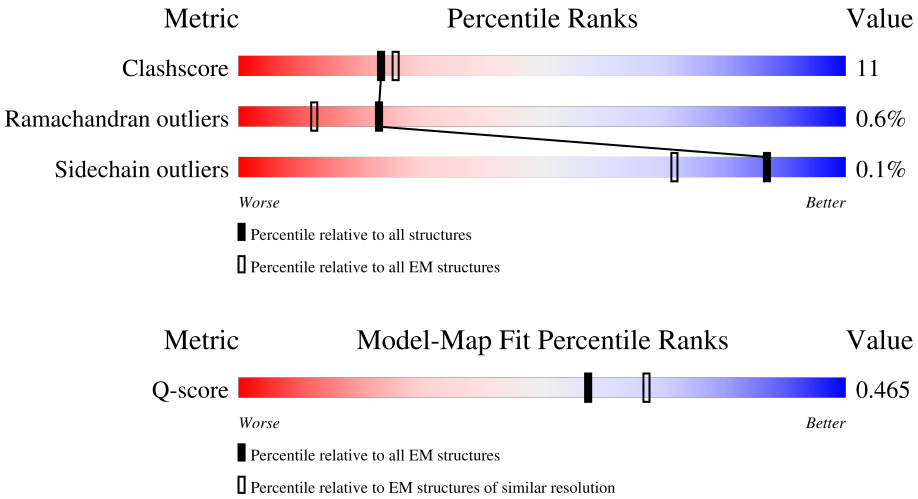
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12629 (3.08 - 4.08)

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	E	1099	42% 11% 47%
2	N	1168	14% · 83%
3	P	1130	52% 20% 28%
4	O	1625	8% · 90%

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Mol	Chain	Length	Quality of chain
5	X	52	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13633 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 Mediator of RNA polymerase II transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	584	Total	C	N	O	S	0	0
			4467	2851	745	846	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	228	ILE	LEU	conflict	UNP G0SGD2

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	198	Total	C	N	O	S	0	0
			1439	905	272	260	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	822	ASP	GLN	conflict	UNP G0SCL5
N	908	GLN	GLU	conflict	UNP G0SCL5

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	810	Total	C	N	O	S	0	0
			6178	3911	1074	1167	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	180	PRO	LEU	conflict	UNP G0SEV7
P	327	TRP	GLY	conflict	UNP G0SEV7

- Molecule 4 is a protein called MED15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	164	Total	C	N	O	S	0	0
			1290	788	248	245	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	117	LYS	ALA	conflict	UNP G0SHL5
O	308	GLU	GLN	conflict	UNP G0SHL5

- Molecule 5 is a protein called Unknown peptide.

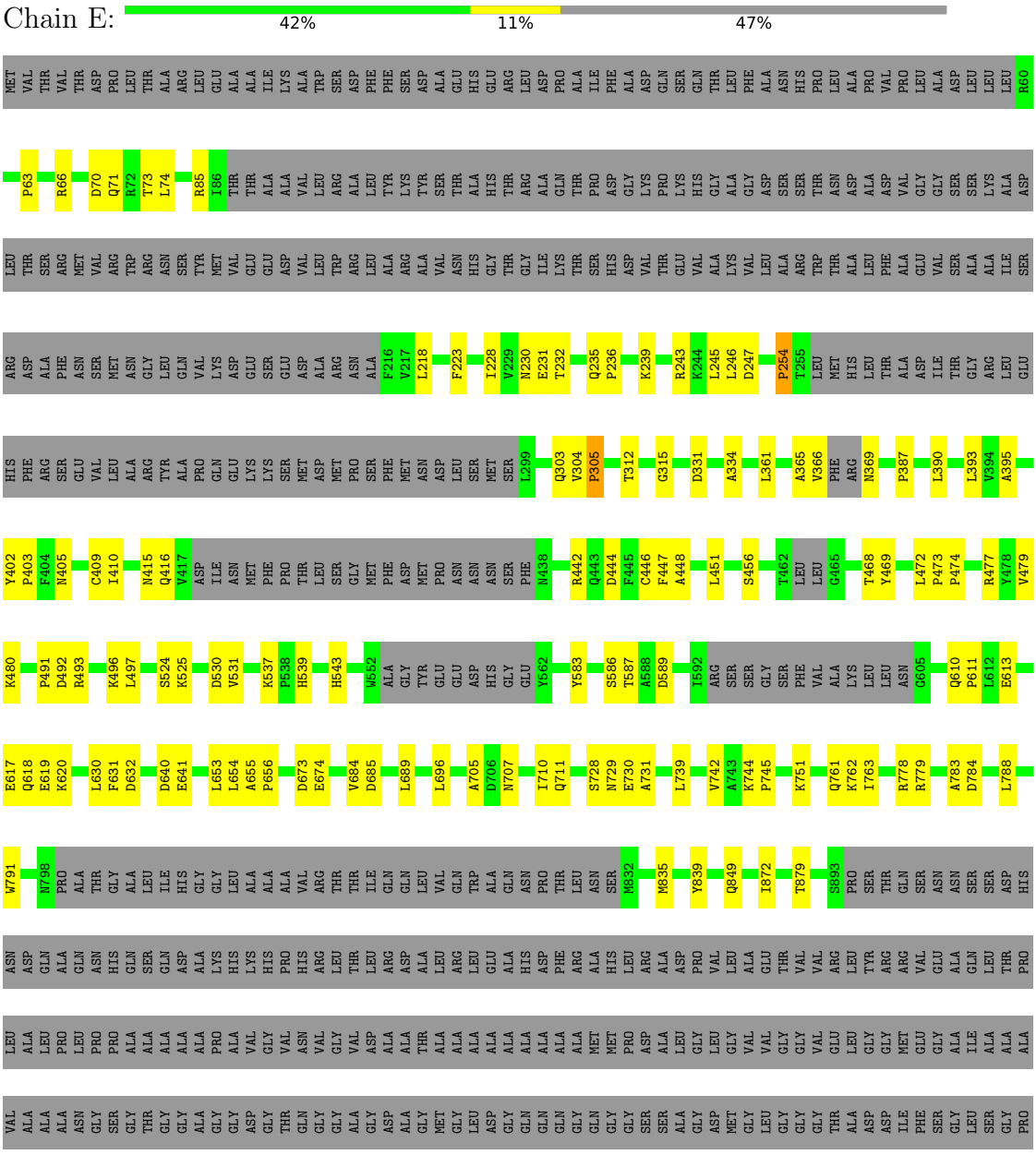
Mol	Chain	Residues	Atoms				AltConf	Trace
5	X	52	Total	C	N	O	0	0
			259	155	52	52		

3 Residue-property plots (i)

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

- Molecule 1: Mediator of RNA polymerase II transcription subunit 5

Chain E:

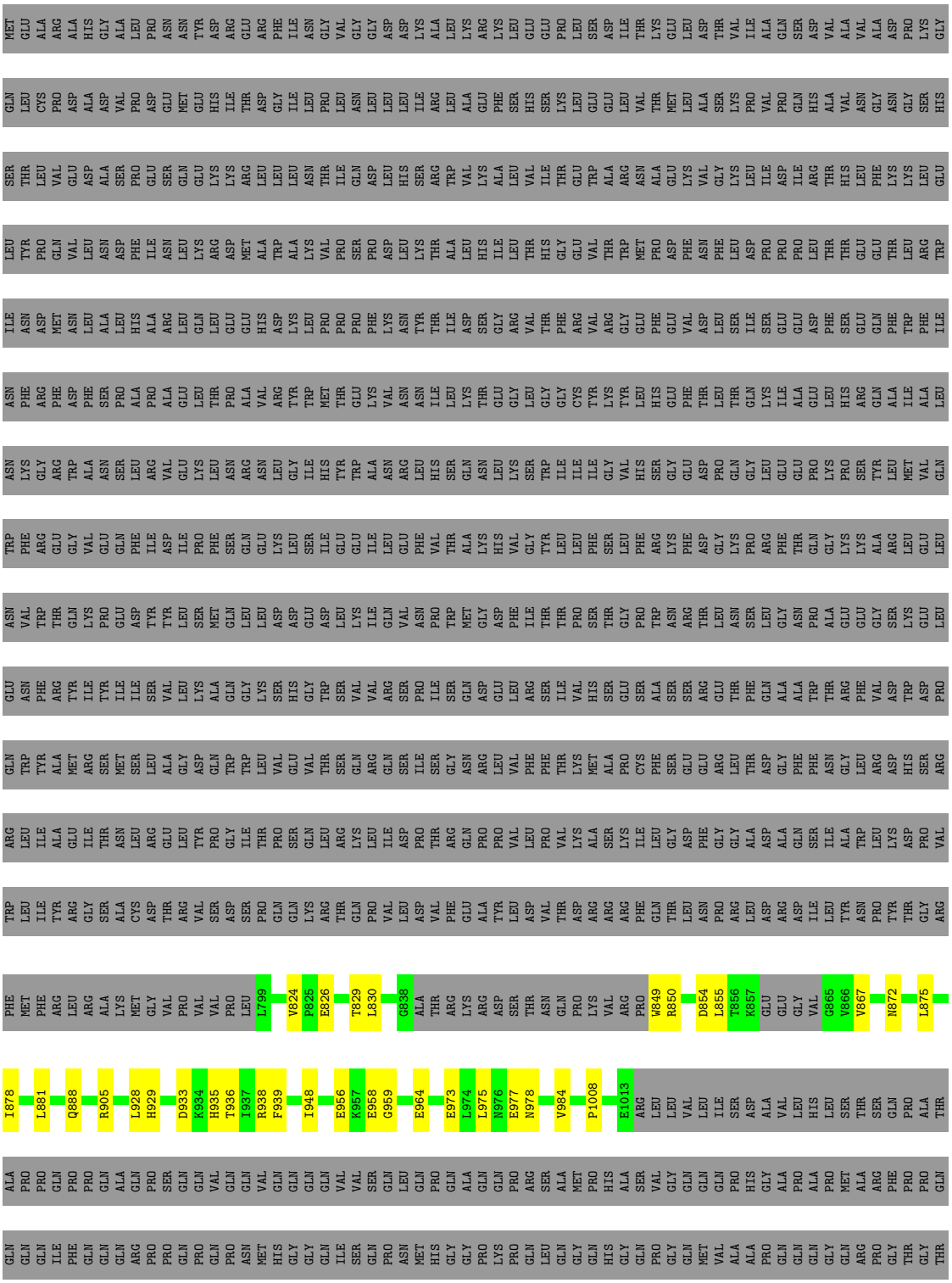




• Molecule 2: Mediator of RNA polymerase II transcription subunit 14

Chain N:



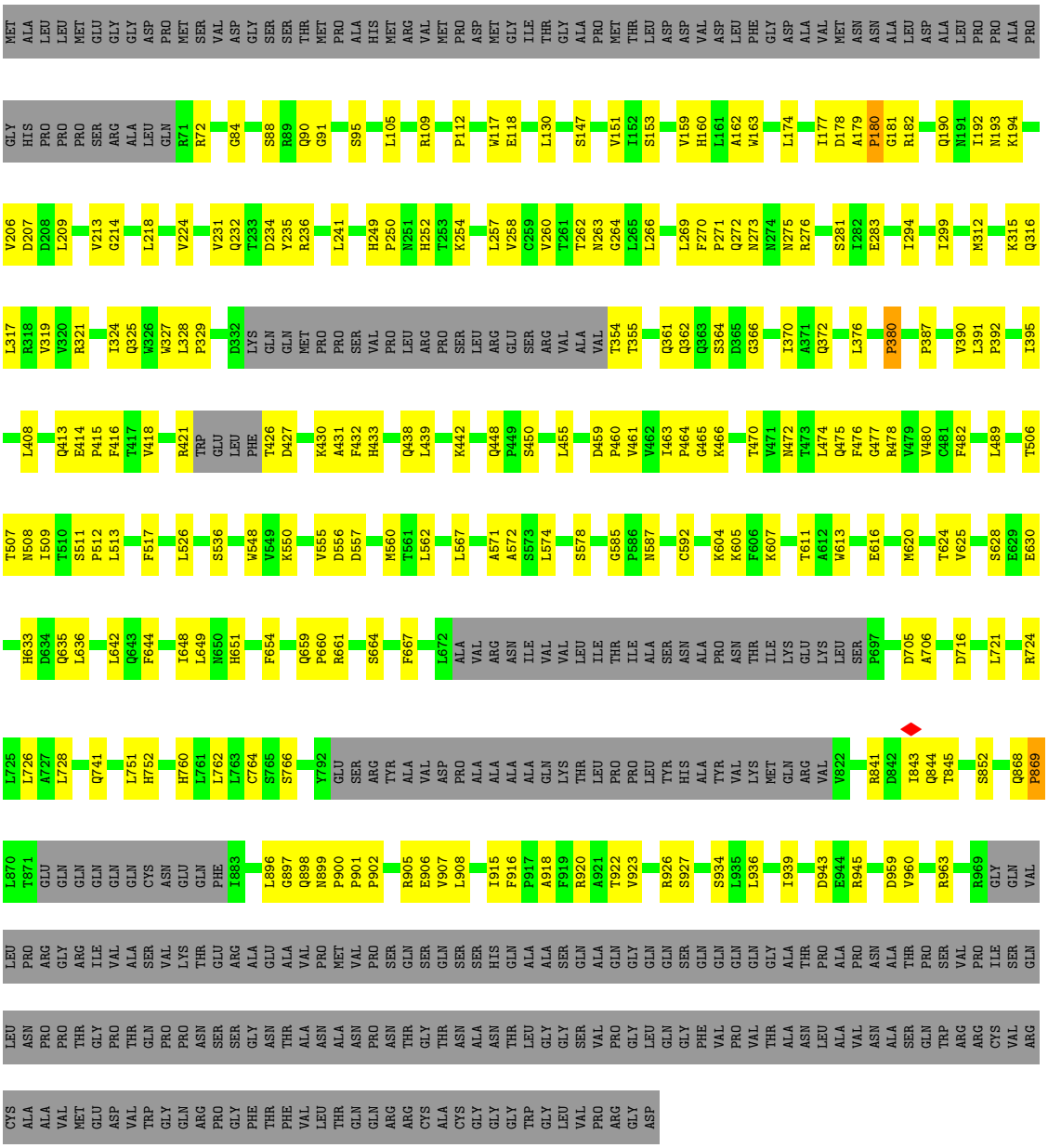




• Molecule 3: Mediator of RNA polymerase II transcription subunit 16

Chain P:

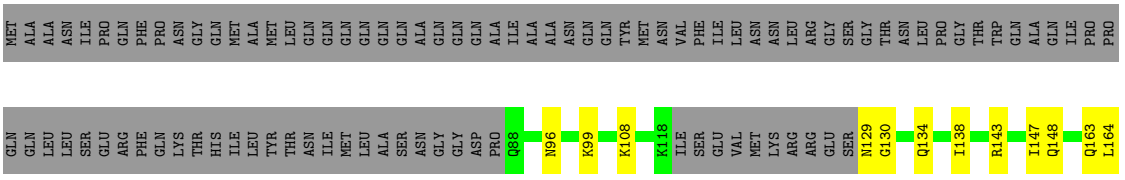


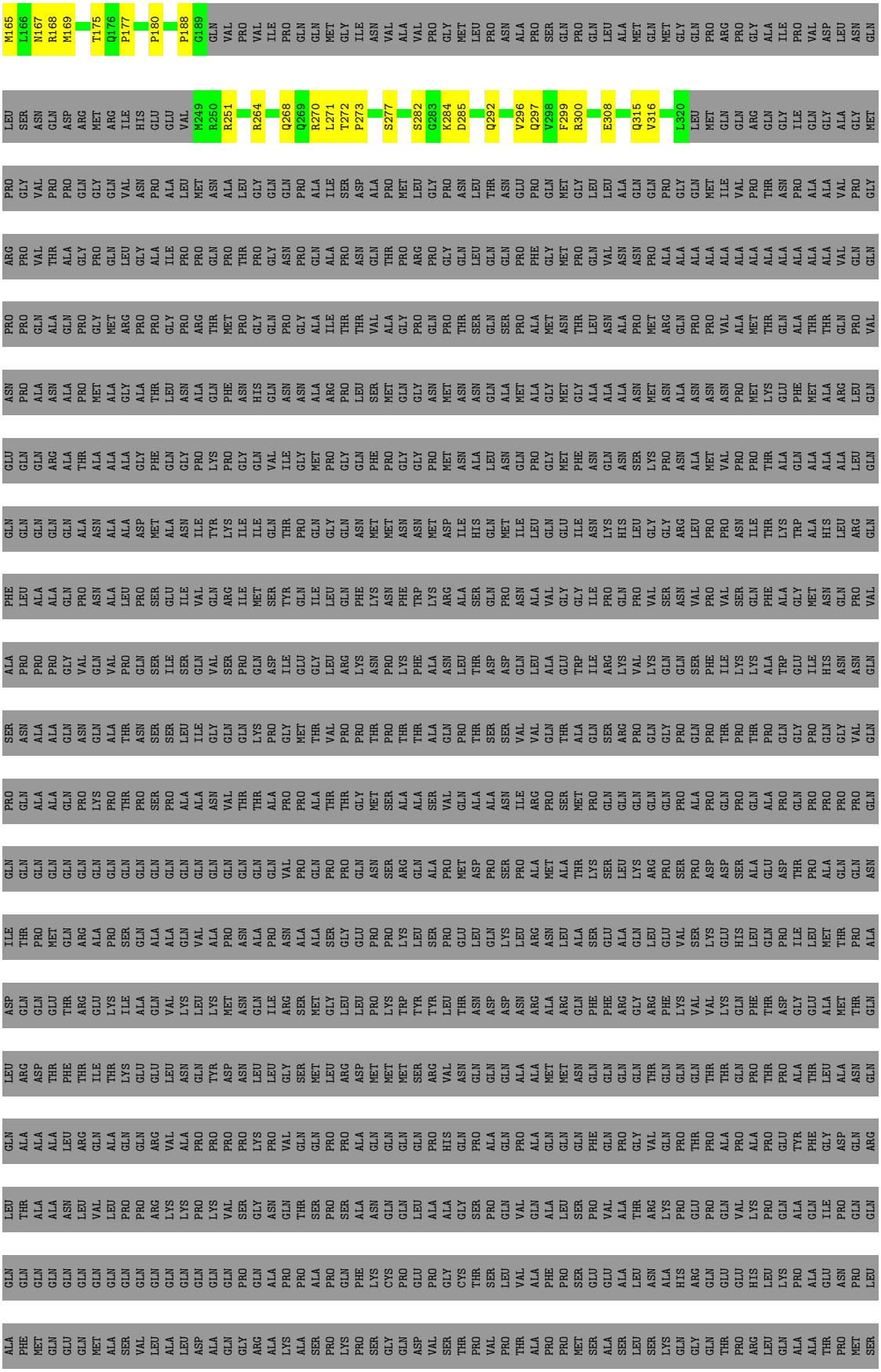


• Molecule 4: MED15

Chain O:






M165 L166 N167 R168 M169 T175 Q176 P177 P180 P188 G189
M249 R250 R251 R264 Q268 Q269 R270 L271 T272 P273 S277 S282 G283 K284 D285 Q292 V296 Q297 V298 F299 R300 E308 Q315 V316 L320

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

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

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

LYS GLY PHE GLY PHE LEU ASP GLY THR LEU GLY GLU GLY GLN GLN GLU SER GLY GLN GLY GLN GLY GLY GLN GLY GLN PRO GLU VAL MET VAL ILE GLU

- Molecule 5: Unknown peptide

Chain X: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.610	Depositor
Minimum map value	-1.096	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	526.07996, 526.07996, 526.07996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	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	E	0.17	0/4548	0.43	2/6191 (0.0%)
2	N	0.20	0/1464	0.52	2/1988 (0.1%)
3	P	0.19	0/6315	0.52	4/8611 (0.0%)
4	O	0.17	0/1300	0.44	1/1749 (0.1%)
All	All	0.18	0/13627	0.49	9/18539 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	254	PRO	N-CA-CB	7.96	111.61	103.25
3	P	380	PRO	N-CA-CB	7.55	111.18	103.25
3	P	869	PRO	N-CA-CB	7.46	111.08	103.25
1	E	305	PRO	N-CA-CB	7.45	111.07	103.25
4	O	188	PRO	N-CA-CB	6.25	110.55	102.86
2	N	1008	PRO	N-CA-CB	6.06	110.23	103.44
2	N	984	VAL	N-CA-C	-5.48	107.14	112.29
3	P	555	VAL	CA-C-N	5.23	131.53	121.54
3	P	555	VAL	C-N-CA	5.23	131.53	121.54

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	E	4467	0	4409	87	0
2	N	1439	0	1304	22	0
3	P	6178	0	6027	170	0
4	O	1290	0	1289	27	0
5	X	259	0	64	0	0
All	All	13633	0	13093	295	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 11.

All (295) 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:E:228:ILE:HG21	1:E:246:LEU:HD22	1.54	0.89
1:E:409:CYS:SG	1:E:442:ARG:NH2	2.55	0.80
3:P:118:GLU:HA	3:P:548:TRP:HH2	1.51	0.76
1:E:231:GLU:HB3	1:E:239:LYS:HZ3	1.52	0.75
3:P:325:GLN:HE22	3:P:327:TRP:HB3	1.50	0.74
3:P:506:THR:HG22	3:P:507:THR:H	1.52	0.73
2:N:849:TRP:HB2	2:N:872:ASN:HD22	1.52	0.72
4:O:177:PRO:HA	4:O:308:GLU:HG2	1.71	0.72
3:P:648:ILE:HD13	3:P:945:ARG:HB2	1.70	0.72
3:P:415:PRO:HB3	3:P:433:HIS:HB2	1.72	0.72
3:P:387:PRO:HB2	3:P:416:PHE:HB3	1.71	0.72
3:P:607:LYS:NZ	3:P:635:GLN:O	2.23	0.71
3:P:624:THR:HG22	3:P:625:VAL:H	1.54	0.70
2:N:878:ILE:HG12	4:O:180:PRO:HG2	1.73	0.70
3:P:413:GLN:NE2	3:P:438:GLN:OE1	2.19	0.69
2:N:850:ARG:O	2:N:872:ASN:ND2	2.26	0.69
1:E:66:ARG:HE	3:P:206:VAL:HG21	1.59	0.68
3:P:659:GLN:NE2	3:P:764:CYS:SG	2.67	0.68
3:P:324:ILE:HG23	3:P:364:SER:HB2	1.73	0.67
2:N:958:GLU:HG2	2:N:959:GLY:H	1.59	0.67
3:P:273:ASN:O	3:P:275:ASN:ND2	2.27	0.67
4:O:315:GLN:HG2	4:O:316:VAL:H	1.60	0.67
3:P:843:ILE:HD12	3:P:927:SER:HA	1.75	0.67
3:P:273:ASN:HB2	3:P:281:SER:HB3	1.77	0.66
3:P:315:LYS:HD2	3:P:321:ARG:HE	1.61	0.65
1:E:619:GLU:HG3	1:E:620:LYS:HG3	1.78	0.65
3:P:232:GLN:HE22	3:P:241:LEU:HD22	1.63	0.64
4:O:264:ARG:O	4:O:268:GLN:NE2	2.31	0.64
3:P:118:GLU:OE2	3:P:550:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:625:VAL:HG12	3:P:766:SER:HB2	1.80	0.63
1:E:761:GLN:HG3	1:E:762:LYS:H	1.64	0.63
3:P:899:ASN:OD1	3:P:900:PRO:HD3	1.98	0.63
3:P:159:VAL:HB	3:P:178:ASP:HB3	1.81	0.62
2:N:928:LEU:HB2	2:N:936:THR:HG23	1.82	0.62
1:E:366:VAL:O	1:E:369:ASN:ND2	2.33	0.61
3:P:901:PRO:HB2	3:P:902:PRO:HD3	1.83	0.61
3:P:661:ARG:HH21	3:P:963:ARG:HH11	1.49	0.61
2:N:824:VAL:HG22	2:N:826:GLU:H	1.65	0.61
2:N:881:LEU:HD11	4:O:108:LYS:HD2	1.81	0.61
1:E:530:ASP:OD1	1:E:583:TYR:OH	2.15	0.60
3:P:90:GLN:OE1	3:P:91:GLY:N	2.36	0.59
4:O:167:ASN:HD22	4:O:168:ARG:HD3	1.67	0.59
1:E:387:PRO:HA	1:E:390:LEU:HB3	1.85	0.59
3:P:651:HIS:CG	3:P:751:LEU:HB3	2.37	0.59
1:E:707:ASN:HD21	1:E:710:ILE:HD12	1.68	0.58
4:O:164:LEU:O	4:O:168:ARG:NH2	2.35	0.58
3:P:117:TRP:CD1	3:P:592:CYS:HB3	2.38	0.58
3:P:234:ASP:OD2	3:P:236:ARG:NH2	2.36	0.58
3:P:959:ASP:OD1	3:P:960:VAL:N	2.35	0.58
1:E:696:LEU:HD11	1:E:742:VAL:HG21	1.86	0.58
3:P:180:PRO:HB3	3:P:207:ASP:H	1.67	0.58
3:P:414:GLU:OE1	3:P:415:PRO:HD3	2.04	0.57
3:P:915:ILE:HG22	3:P:918:ALA:H	1.69	0.57
3:P:179:ALA:O	3:P:181:GLY:N	2.38	0.56
1:E:447:PHE:HA	1:E:451:LEU:HD13	1.87	0.56
1:E:228:ILE:HG13	1:E:246:LEU:HB2	1.86	0.56
1:E:402:TYR:O	1:E:405:ASN:N	2.31	0.56
1:E:783:ALA:HB3	3:P:294:ILE:HD11	1.86	0.56
3:P:130:LEU:HD22	3:P:153:SER:HB3	1.88	0.56
3:P:354:THR:OG1	3:P:355:THR:N	2.39	0.56
3:P:506:THR:HG22	3:P:507:THR:HG23	1.87	0.56
3:P:257:LEU:HG	3:P:258:VAL:H	1.71	0.56
4:O:96:ASN:O	4:O:99:LYS:HG2	2.06	0.56
2:N:958:GLU:OE1	2:N:958:GLU:N	2.33	0.55
3:P:232:GLN:NE2	3:P:241:LEU:HD22	2.21	0.55
1:E:849:GLN:HE22	3:P:316:GLN:HE21	1.54	0.55
3:P:260:VAL:HA	3:P:270:PHE:HB2	1.87	0.55
3:P:536:SER:HG	3:P:548:TRP:CD1	2.24	0.55
3:P:442:LYS:NZ	3:P:450:SER:OG	2.24	0.55
1:E:235:GLN:OE1	1:E:235:GLN:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:418:VAL:HG12	3:P:432:PHE:HB2	1.89	0.54
2:N:973:GLU:HB2	2:N:975:LEU:HD22	1.87	0.54
3:P:317:LEU:HB2	3:P:319:VAL:HG22	1.90	0.54
3:P:130:LEU:HD23	3:P:151:VAL:HG23	1.89	0.54
1:E:243:ARG:NH1	1:E:247:ASP:OD1	2.40	0.54
3:P:459:ASP:OD1	3:P:459:ASP:N	2.40	0.54
4:O:169:MET:HE2	4:O:175:THR:HG22	1.88	0.54
3:P:328:LEU:N	3:P:329:PRO:HD3	2.22	0.54
1:E:705:ALA:HA	3:P:366:GLY:HA2	1.91	0.53
3:P:177:ILE:HG12	3:P:179:ALA:H	1.73	0.53
3:P:180:PRO:O	3:P:209:LEU:HB2	2.08	0.53
1:E:613:GLU:N	1:E:613:GLU:OE1	2.41	0.53
3:P:179:ALA:HB1	3:P:180:PRO:HD2	1.91	0.53
1:E:497:LEU:HD21	1:E:531:VAL:HG12	1.90	0.53
2:N:977:GLU:O	2:N:978:ASN:ND2	2.42	0.53
1:E:243:ARG:HD2	1:E:303:GLN:HA	1.91	0.53
3:P:262:THR:OG1	3:P:263:ASN:N	2.41	0.53
4:O:272:THR:OG1	4:O:273:PRO:HD3	2.08	0.53
4:O:134:GLN:O	4:O:138:ILE:HG13	2.08	0.53
1:E:784:ASP:OD1	1:E:784:ASP:N	2.38	0.53
3:P:922:THR:O	3:P:926:ARG:NH1	2.42	0.53
4:O:268:GLN:OE1	4:O:282:SER:OG	2.24	0.53
1:E:474:PRO:HB3	1:E:480:LYS:HE2	1.90	0.52
2:N:867:VAL:HG11	2:N:888:GLN:HB3	1.91	0.52
3:P:630:GLU:HB2	3:P:633:HIS:HB3	1.91	0.52
3:P:943:ASP:OD1	3:P:943:ASP:N	2.42	0.52
1:E:71:GLN:OE1	1:E:71:GLN:N	2.43	0.52
2:N:933:ASP:O	2:N:935:HIS:ND1	2.42	0.52
3:P:651:HIS:HB2	3:P:751:LEU:HD22	1.89	0.52
1:E:492:ASP:C	1:E:493:ARG:HD3	2.34	0.52
3:P:426:THR:OG1	3:P:427:ASP:N	2.35	0.52
1:E:685:ASP:HB2	1:E:731:ALA:HB2	1.90	0.51
3:P:387:PRO:HG3	3:P:418:VAL:HB	1.91	0.51
1:E:70:ASP:OD2	1:E:791:TRP:HB2	2.11	0.51
3:P:604:LYS:O	3:P:605:LYS:HD2	2.10	0.51
3:P:896:LEU:HD13	3:P:907:VAL:HG11	1.93	0.51
1:E:66:ARG:NE	3:P:206:VAL:HG21	2.25	0.51
3:P:439:LEU:HD23	3:P:455:LEU:HD11	1.93	0.51
1:E:63:PRO:HB3	1:E:66:ARG:HH11	1.76	0.50
1:E:315:GLY:HA2	1:E:879:THR:HG21	1.93	0.50
1:E:684:VAL:HA	1:E:689:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:907:VAL:O	3:P:908:LEU:HG	2.11	0.50
3:P:95:SER:HB3	3:P:105:LEU:HD13	1.92	0.50
3:P:489:LEU:H	3:P:489:LEU:HD23	1.76	0.50
3:P:536:SER:HG	3:P:548:TRP:HD1	1.57	0.50
3:P:906:GLU:N	3:P:906:GLU:OE1	2.44	0.50
3:P:249:HIS:HB2	3:P:250:PRO:HD3	1.94	0.50
3:P:269:LEU:HD12	3:P:283:GLU:HG3	1.94	0.50
1:E:705:ALA:O	1:E:711:GLN:NE2	2.45	0.50
1:E:610:GLN:HG2	1:E:611:PRO:HD3	1.93	0.50
1:E:617:GLU:HG3	1:E:618:GLN:H	1.77	0.50
1:E:85:ARG:HH12	1:E:410:ILE:HG23	1.76	0.50
3:P:263:ASN:N	3:P:263:ASN:OD1	2.43	0.50
3:P:463:ILE:O	3:P:482:PHE:HB3	2.12	0.50
4:O:315:GLN:HG2	4:O:316:VAL:N	2.27	0.50
1:E:230:ASN:HB2	3:P:72:ARG:HH21	1.77	0.49
3:P:312:MET:HG2	3:P:395:ILE:HD11	1.94	0.49
3:P:192:ILE:O	3:P:194:LYS:N	2.45	0.49
3:P:624:THR:HG22	3:P:625:VAL:N	2.25	0.49
3:P:705:ASP:OD1	3:P:706:ALA:N	2.45	0.49
3:P:231:VAL:HG22	3:P:509:ILE:HG22	1.93	0.49
1:E:218:LEU:HB2	1:E:223:PHE:CZ	2.48	0.49
3:P:512:PRO:HA	3:P:517:PHE:HB2	1.94	0.49
3:P:649:LEU:HD22	3:P:654:PHE:HB3	1.93	0.49
3:P:218:LEU:O	3:P:257:LEU:HD11	2.13	0.49
4:O:129:ASN:OD1	4:O:130:GLY:N	2.40	0.49
2:N:854:ASP:OD1	2:N:855:LEU:N	2.45	0.48
3:P:177:ILE:HG22	3:P:182:ARG:O	2.12	0.48
3:P:254:LYS:HA	3:P:254:LYS:HD3	1.67	0.48
3:P:760:HIS:CE1	3:P:900:PRO:HG2	2.48	0.48
1:E:312:THR:HG21	1:E:872:ILE:HG23	1.96	0.48
2:N:964:GLU:OE2	3:P:934:SER:OG	2.31	0.48
3:P:433:HIS:CE1	3:P:460:PRO:HD2	2.49	0.48
3:P:476:PHE:CG	3:P:477:GLY:N	2.82	0.48
3:P:316:GLN:O	3:P:316:GLN:HG2	2.13	0.48
3:P:370:ILE:HG22	3:P:372:GLN:H	1.79	0.47
1:E:390:LEU:HA	1:E:393:LEU:O	2.14	0.47
1:E:761:GLN:C	1:E:763:ILE:H	2.22	0.47
2:N:829:THR:O	2:N:830:LEU:HD22	2.14	0.47
3:P:190:GLN:C	3:P:192:ILE:H	2.22	0.47
3:P:272:GLN:O	3:P:273:ASN:ND2	2.48	0.47
3:P:511:SER:HA	3:P:572:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:557:ASP:HB3	3:P:560:MET:HB2	1.96	0.47
3:P:726:LEU:C	3:P:728:LEU:H	2.22	0.47
1:E:232:THR:N	1:E:239:LYS:HE2	2.28	0.47
1:E:655:ALA:HB3	1:E:656:PRO:HD3	1.96	0.47
3:P:177:ILE:HG23	3:P:179:ALA:HB3	1.96	0.47
3:P:408:LEU:HD13	3:P:439:LEU:HD13	1.97	0.47
3:P:726:LEU:HG	3:P:920:ARG:HH12	1.80	0.47
3:P:852:SER:HB2	3:P:923:VAL:HG21	1.95	0.47
4:O:147:ILE:HG22	4:O:148:GLN:H	1.80	0.47
4:O:164:LEU:HD12	4:O:165:MET:HG3	1.96	0.47
1:E:492:ASP:O	1:E:493:ARG:HD3	2.15	0.47
1:E:70:ASP:HA	1:E:73:THR:HG22	1.96	0.47
3:P:327:TRP:HE3	3:P:329:PRO:HD2	1.79	0.47
3:P:466:LYS:HD3	3:P:526:LEU:O	2.15	0.47
1:E:402:TYR:N	1:E:403:PRO:HD2	2.30	0.46
1:E:415:ASN:OD1	1:E:416:GLN:N	2.37	0.46
1:E:751:LYS:HE3	1:E:751:LYS:HB2	1.74	0.46
3:P:271:PRO:HA	3:P:283:GLU:HA	1.97	0.46
3:P:475:GLN:NE2	3:P:476:PHE:O	2.48	0.46
3:P:162:ALA:HB3	3:P:174:LEU:HD21	1.96	0.46
3:P:844:GLN:O	3:P:845:THR:OG1	2.27	0.46
3:P:414:GLU:HB3	3:P:415:PRO:CD	2.45	0.46
3:P:661:ARG:HE	3:P:963:ARG:NH1	2.14	0.46
3:P:433:HIS:ND1	3:P:464:PRO:HG3	2.30	0.46
3:P:480:VAL:HG22	3:P:482:PHE:H	1.79	0.46
4:O:277:SER:O	4:O:277:SER:OG	2.31	0.46
4:O:165:MET:HA	4:O:168:ARG:HH21	1.79	0.46
1:E:468:THR:OG1	1:E:469:TYR:N	2.48	0.46
1:E:543:HIS:HE1	1:E:589:ASP:HA	1.80	0.46
2:N:875:LEU:HD11	2:N:905:ARG:HA	1.97	0.46
3:P:448:GLN:OE1	3:P:448:GLN:N	2.43	0.45
1:E:496:LYS:HE2	1:E:496:LYS:HB3	1.83	0.45
1:E:402:TYR:OH	1:E:456:SER:OG	2.12	0.45
3:P:361:GLN:CD	3:P:362:GLN:H	2.24	0.45
4:O:143:ARG:O	4:O:147:ILE:HG12	2.16	0.45
3:P:294:ILE:HG22	3:P:316:GLN:HE22	1.82	0.45
3:P:562:LEU:HB3	3:P:567:LEU:HD13	1.98	0.45
3:P:636:LEU:HD23	3:P:636:LEU:HA	1.79	0.45
3:P:716:ASP:HB3	3:P:939:ILE:HD11	1.98	0.45
3:P:179:ALA:C	3:P:181:GLY:H	2.25	0.44
3:P:578:SER:HB3	3:P:613:TRP:HH2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:284:LYS:HG2	4:O:285:ASP:H	1.82	0.44
1:E:537:LYS:HE3	1:E:537:LYS:HB3	1.84	0.44
3:P:147:SER:O	3:P:147:SER:OG	2.32	0.44
3:P:299:ILE:HG21	3:P:392:PRO:HA	2.00	0.44
3:P:841:ARG:NH2	3:P:845:THR:HG22	2.33	0.44
4:O:163:GLN:OE1	4:O:163:GLN:N	2.39	0.44
3:P:648:ILE:HD11	3:P:651:HIS:CE1	2.53	0.44
1:E:472:LEU:C	1:E:474:PRO:HD3	2.43	0.44
1:E:525:LYS:HB2	1:E:525:LYS:HE3	1.72	0.44
1:E:630:LEU:O	1:E:631:PHE:HB3	2.17	0.44
3:P:898:GLN:O	3:P:901:PRO:HD2	2.18	0.44
3:P:84:GLY:HA3	3:P:160:HIS:CE1	2.53	0.44
1:E:444:ASP:O	1:E:448:ALA:HB3	2.18	0.43
3:P:721:LEU:HA	3:P:721:LEU:HD23	1.79	0.43
3:P:214:GLY:O	3:P:262:THR:HG22	2.17	0.43
4:O:292:GLN:O	4:O:296:VAL:HG12	2.18	0.43
3:P:179:ALA:C	3:P:181:GLY:N	2.76	0.43
3:P:270:PHE:O	3:P:270:PHE:CG	2.72	0.43
3:P:418:VAL:HG12	3:P:432:PHE:CB	2.48	0.43
3:P:741:GLN:HA	3:P:905:ARG:HD2	1.99	0.43
1:E:245:LEU:HD23	1:E:245:LEU:HA	1.84	0.43
1:E:493:ARG:O	1:E:493:ARG:HG2	2.17	0.43
3:P:585:GLY:O	3:P:587:ASN:N	2.47	0.43
3:P:916:PHE:O	3:P:920:ARG:HB3	2.18	0.43
3:P:414:GLU:HB3	3:P:415:PRO:HD3	2.00	0.43
3:P:664:SER:HA	3:P:667:PHE:CD1	2.53	0.43
1:E:630:LEU:C	1:E:632:ASP:H	2.27	0.43
3:P:905:ARG:HG2	3:P:906:GLU:H	1.84	0.43
4:O:251:ARG:HH21	4:O:299:PHE:HB3	1.83	0.43
2:N:928:LEU:HD12	4:O:300:ARG:HD3	2.01	0.43
2:N:938:ARG:NH1	4:O:297:GLN:HE22	2.17	0.43
3:P:430:LYS:HG3	3:P:431:ALA:H	1.84	0.43
3:P:508:ASN:OD1	3:P:508:ASN:N	2.52	0.43
3:P:659:GLN:HB2	3:P:660:PRO:HD3	2.01	0.43
3:P:936:LEU:HD23	3:P:936:LEU:H	1.82	0.43
4:O:285:ASP:OD1	4:O:285:ASP:C	2.62	0.43
1:E:640:ASP:OD1	1:E:641:GLU:N	2.39	0.43
3:P:574:LEU:HD21	3:P:613:TRP:CD2	2.53	0.43
3:P:578:SER:HB3	3:P:613:TRP:CH2	2.54	0.43
1:E:393:LEU:HD11	1:E:395:ALA:HB3	2.01	0.43
1:E:539:HIS:HB2	1:E:543:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:421:ARG:O	3:P:421:ARG:NH2	2.45	0.43
3:P:472:ASN:C	3:P:474:LEU:H	2.27	0.43
3:P:724:ARG:HE	3:P:752:HIS:HE1	1.66	0.43
3:P:109:ARG:HH21	3:P:112:PRO:HD2	1.84	0.42
1:E:446:CYS:C	1:E:448:ALA:H	2.27	0.42
1:E:530:ASP:OD2	1:E:779:ARG:NH1	2.52	0.42
3:P:461:VAL:HG12	3:P:461:VAL:O	2.19	0.42
3:P:390:VAL:HG13	3:P:391:LEU:HD23	2.01	0.42
2:N:958:GLU:HG2	2:N:959:GLY:N	2.32	0.42
3:P:511:SER:OG	3:P:512:PRO:HD3	2.19	0.42
1:E:761:GLN:O	1:E:763:ILE:N	2.53	0.42
3:P:213:VAL:HG23	3:P:262:THR:HG23	2.01	0.42
3:P:478:ARG:HD3	3:P:478:ARG:HA	1.65	0.42
1:E:492:ASP:CG	1:E:493:ARG:H	2.26	0.42
1:E:524:SER:OG	1:E:525:LYS:N	2.53	0.42
1:E:778:ARG:HA	1:E:778:ARG:HD3	1.87	0.42
3:P:235:TYR:HD1	3:P:235:TYR:HA	1.68	0.42
1:E:728:SER:O	1:E:731:ALA:N	2.53	0.42
2:N:956:GLU:HG3	2:N:958:GLU:OE1	2.19	0.42
1:E:586:SER:OG	1:E:587:THR:N	2.53	0.41
3:P:252:HIS:O	3:P:252:HIS:CG	2.73	0.41
3:P:620:MET:HE1	3:P:628:SER:HA	2.01	0.41
4:O:270:ARG:C	4:O:271:LEU:HD22	2.45	0.41
1:E:331:ASP:OD1	1:E:334:ALA:HB3	2.19	0.41
1:E:744:LYS:HB3	1:E:745:PRO:HD3	2.02	0.41
3:P:651:HIS:CE1	3:P:751:LEU:HD13	2.55	0.41
3:P:724:ARG:HE	3:P:752:HIS:CE1	2.38	0.41
1:E:835:MET:HE2	1:E:835:MET:HB3	1.86	0.41
3:P:642:LEU:HD23	3:P:642:LEU:H	1.86	0.41
3:P:264:GLY:C	3:P:266:LEU:H	2.29	0.41
3:P:391:LEU:HD21	3:P:465:GLY:O	2.21	0.41
1:E:729:ASN:OD1	1:E:730:GLU:N	2.53	0.41
1:E:788:LEU:HD23	1:E:788:LEU:HA	1.81	0.41
2:N:929:HIS:ND1	2:N:935:HIS:HD2	2.19	0.41
3:P:376:LEU:HD12	3:P:376:LEU:HA	1.91	0.41
3:P:611:THR:HA	3:P:616:GLU:HG2	2.01	0.41
3:P:235:TYR:OH	3:P:571:ALA:HB3	2.21	0.41
3:P:276:ARG:HH21	3:P:354:THR:N	2.19	0.41
3:P:512:PRO:HB2	3:P:513:LEU:HG	2.03	0.41
1:E:74:LEU:HD21	1:E:839:TYR:HD1	1.85	0.41
1:E:365:ALA:HA	1:E:369:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:653:LEU:C	1:E:654:LEU:HD12	2.46	0.41
1:E:739:LEU:HD23	1:E:739:LEU:HA	1.92	0.41
3:P:88:SER:OG	3:P:163:TRP:NE1	2.54	0.41
3:P:193:ASN:OD1	3:P:193:ASN:N	2.53	0.41
1:E:231:GLU:HB3	1:E:239:LYS:NZ	2.29	0.41
3:P:470:THR:HG22	3:P:476:PHE:HD1	1.86	0.41
2:N:939:PHE:HB2	2:N:948:ILE:HG22	2.04	0.40
3:P:262:THR:HG1	3:P:263:ASN:H	1.69	0.40
3:P:762:LEU:HD11	3:P:897:GLY:HA3	2.03	0.40
3:P:271:PRO:HB3	3:P:283:GLU:HB3	2.03	0.40
3:P:536:SER:OG	3:P:548:TRP:HD1	2.04	0.40
3:P:843:ILE:HD12	3:P:927:SER:CA	2.49	0.40
1:E:477:ARG:NH1	1:E:479:VAL:HG21	2.37	0.40
1:E:707:ASN:ND2	1:E:710:ILE:HD12	2.32	0.40
3:P:325:GLN:NE2	3:P:327:TRP:HB3	2.29	0.40
1:E:235:GLN:HG3	1:E:239:LYS:HB2	2.04	0.40
1:E:361:LEU:HB3	1:E:835:MET:HE1	2.04	0.40
1:E:472:LEU:N	1:E:473:PRO:HD3	2.37	0.40
1:E:673:ASP:OD1	1:E:674:GLU:N	2.55	0.40
3:P:556:ASP:OD1	3:P:556:ASP:C	2.65	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	E	566/1099 (52%)	474 (84%)	87 (15%)	5 (1%)	14 46
2	N	192/1168 (16%)	148 (77%)	44 (23%)	0	100 100
3	P	798/1130 (71%)	618 (77%)	175 (22%)	5 (1%)	21 54
4	O	158/1625 (10%)	134 (85%)	24 (15%)	0	100 100
All	All	1714/5022 (34%)	1374 (80%)	330 (19%)	10 (1%)	23 54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	254	PRO
1	E	304	VAL
1	E	305	PRO
3	P	380	PRO
3	P	180	PRO
3	P	224	VAL
3	P	868	GLN
3	P	869	PRO
1	E	236	PRO
1	E	491	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	481/889 (54%)	481 (100%)	0	100	100
2	N	129/1026 (13%)	129 (100%)	0	100	100
3	P	662/947 (70%)	661 (100%)	1 (0%)	87	85
4	O	135/1327 (10%)	135 (100%)	0	100	100
All	All	1407/4189 (34%)	1406 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	644	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	226	ASN
1	E	369	ASN
1	E	416	GLN
1	E	450	GLN

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Mol	Chain	Res	Type
1	E	485	GLN
1	E	505	ASN
1	E	543	HIS
1	E	708	GLN
1	E	711	GLN
1	E	843	GLN
1	E	888	ASN
2	N	872	ASN
2	N	879	ASN
2	N	944	HIS
2	N	955	HIS
3	P	190	GLN
3	P	232	GLN
3	P	273	ASN
3	P	274	ASN
3	P	275	ASN
3	P	316	GLN
3	P	325	GLN
3	P	475	GLN
3	P	587	ASN
3	P	589	HIS
3	P	633	HIS
3	P	651	HIS
3	P	659	GLN
3	P	755	ASN
3	P	861	HIS
4	O	135	ASN
4	O	146	GLN
4	O	167	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (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.

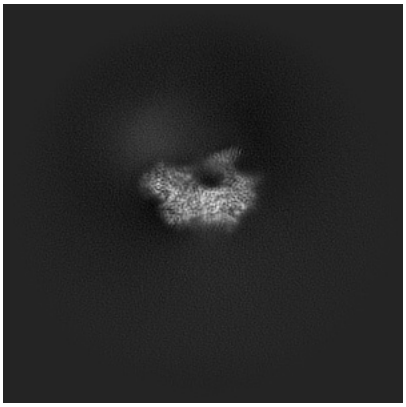
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22397. These allow visual inspection of the internal detail of the map and identification of artifacts.

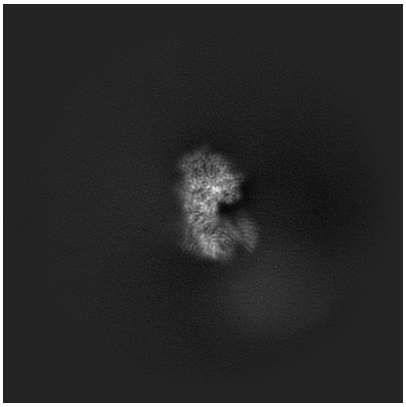
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

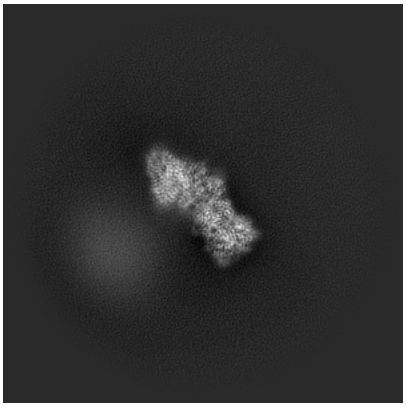
6.1.1 Primary map



X



Y

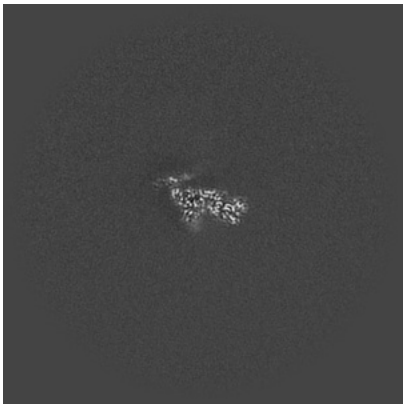


Z

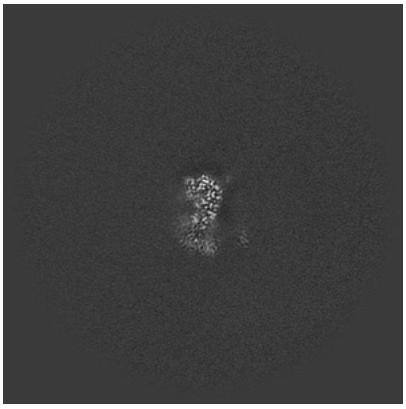
The images above show the map projected in three orthogonal directions.

6.2 Central slices

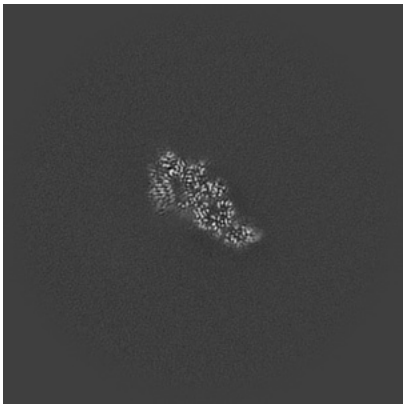
6.2.1 Primary map



X Index: 240



Y Index: 240

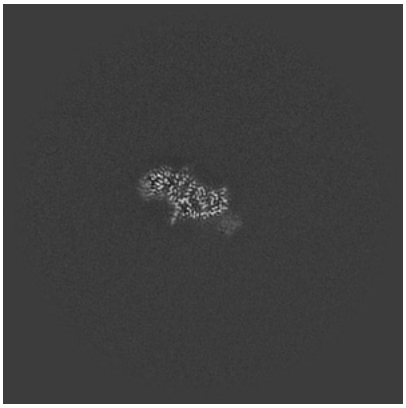


Z Index: 240

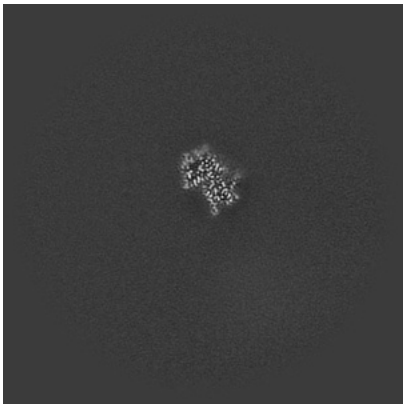
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

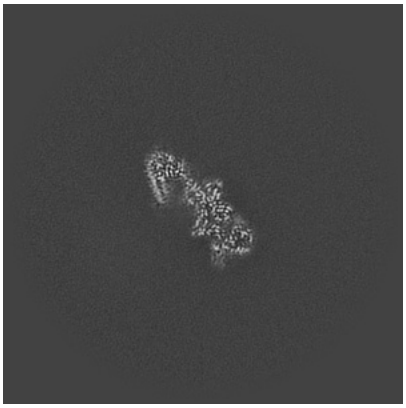
6.3.1 Primary map



X Index: 259



Y Index: 203

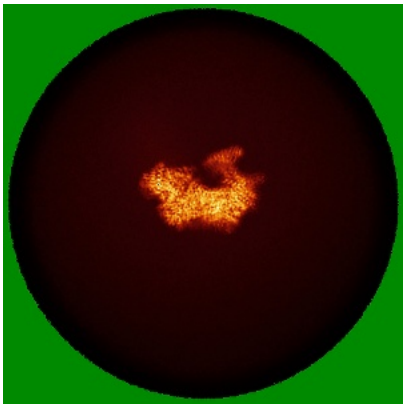


Z Index: 253

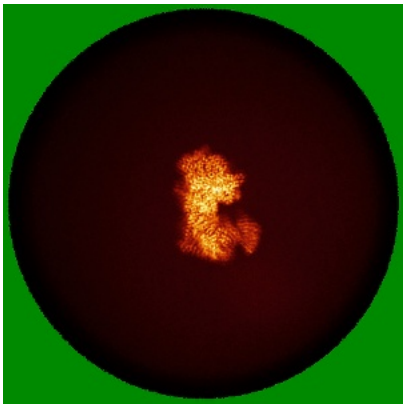
The images above show the largest variance slices of the map in three orthogonal directions.

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

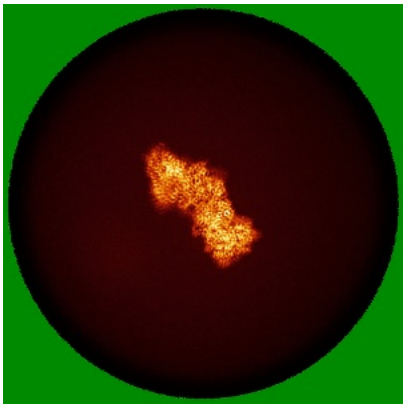
6.4.1 Primary map



X



Y

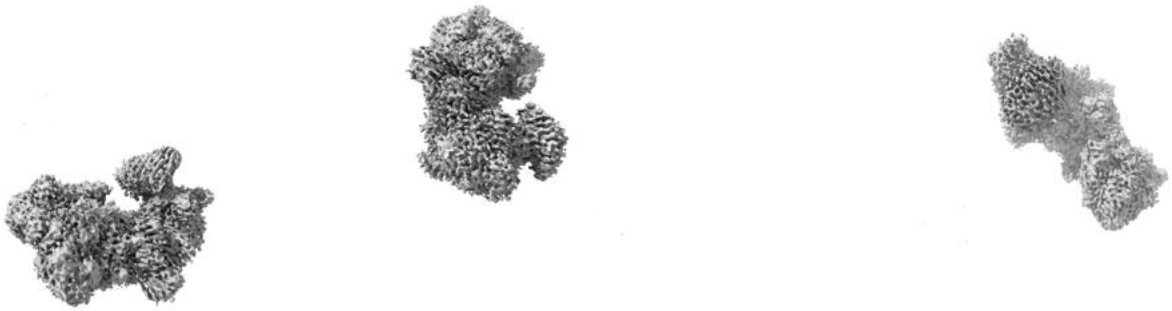


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

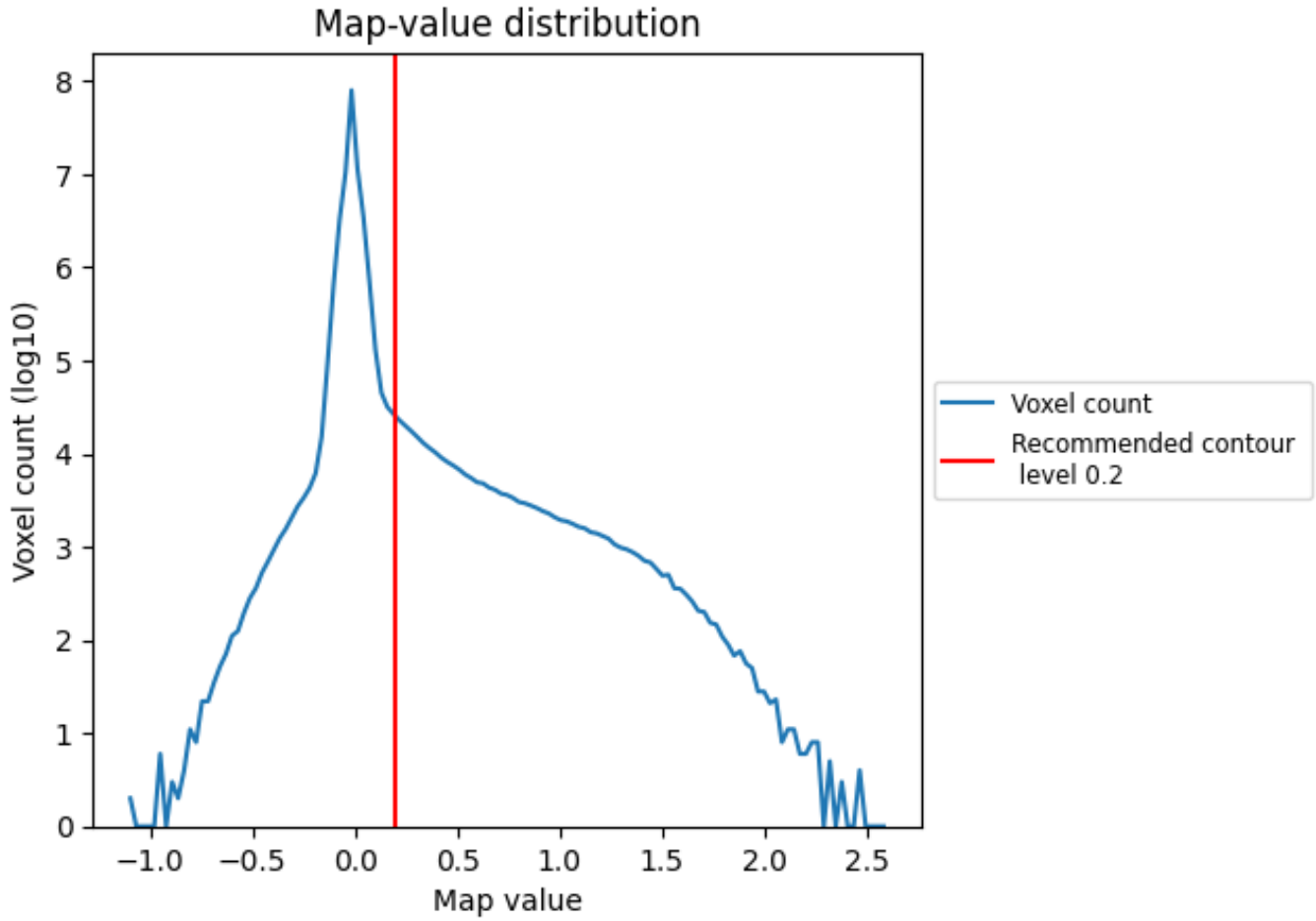
6.6 Mask visualisation (i)

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

7 Map analysis

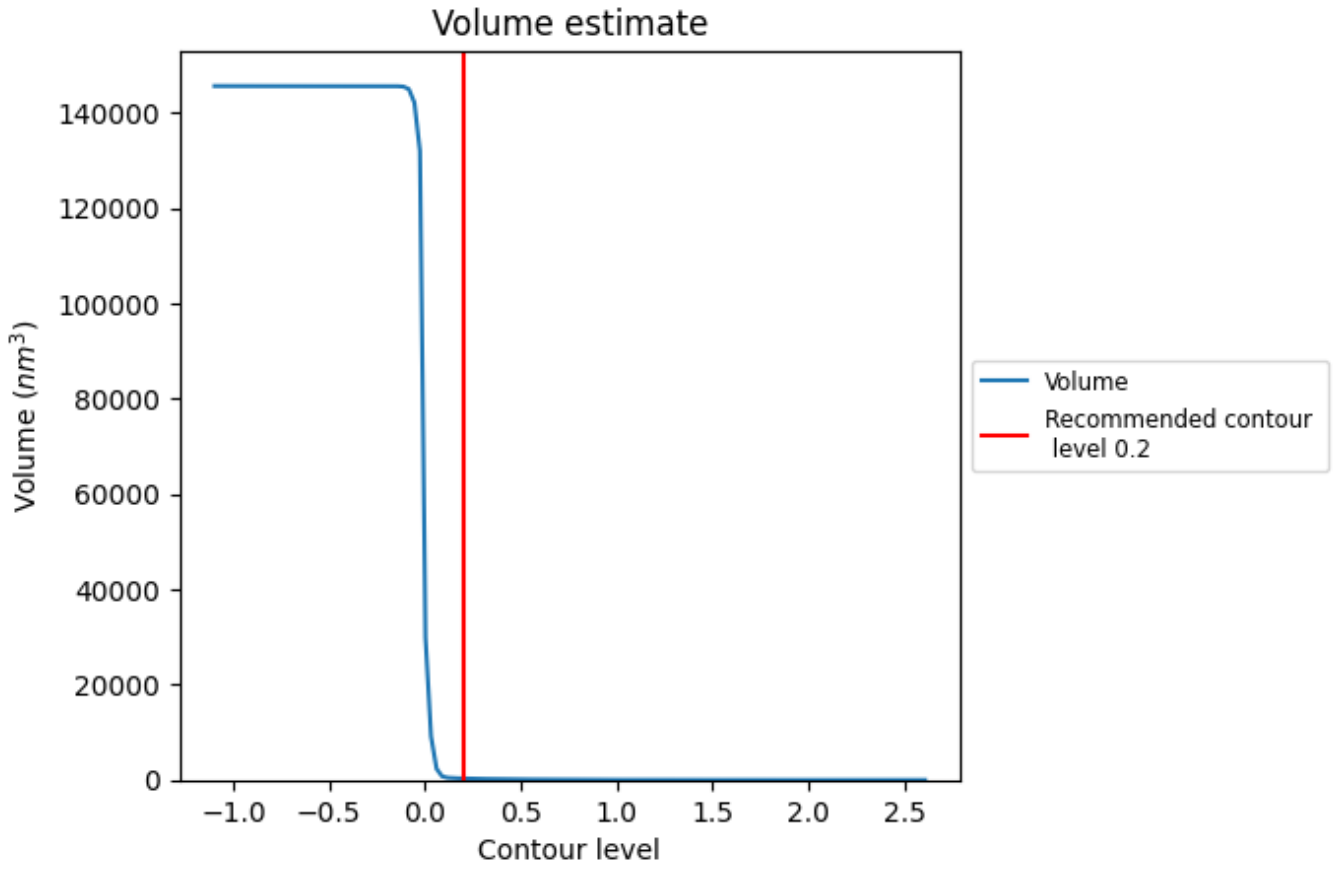
This section contains the results of statistical analysis of the map.

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.

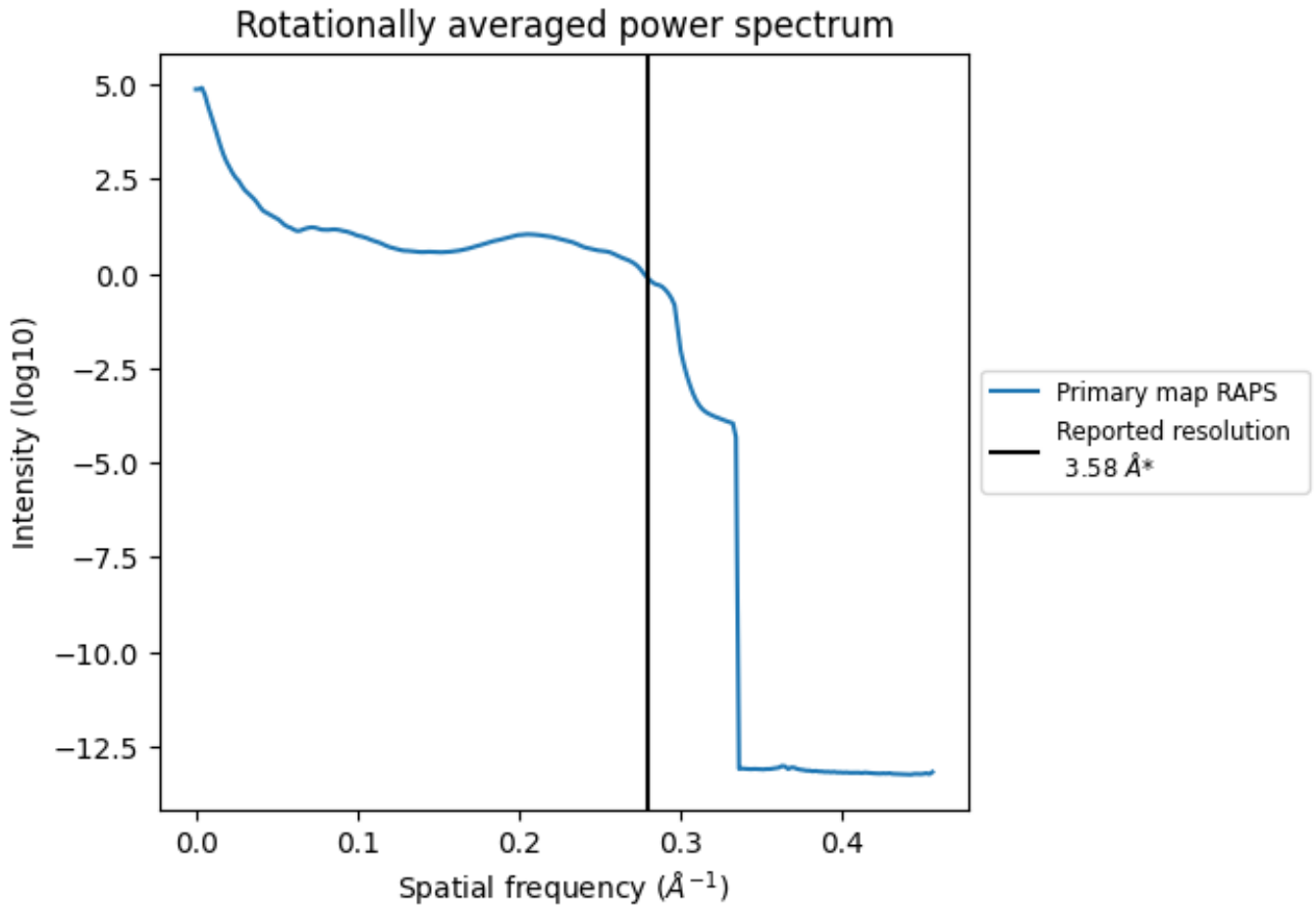
7.2 Volume estimate



The volume at the recommended contour level is 317 nm^3; this corresponds to an approximate mass of 286 kDa.

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

7.3 Rotationally averaged power spectrum (i)

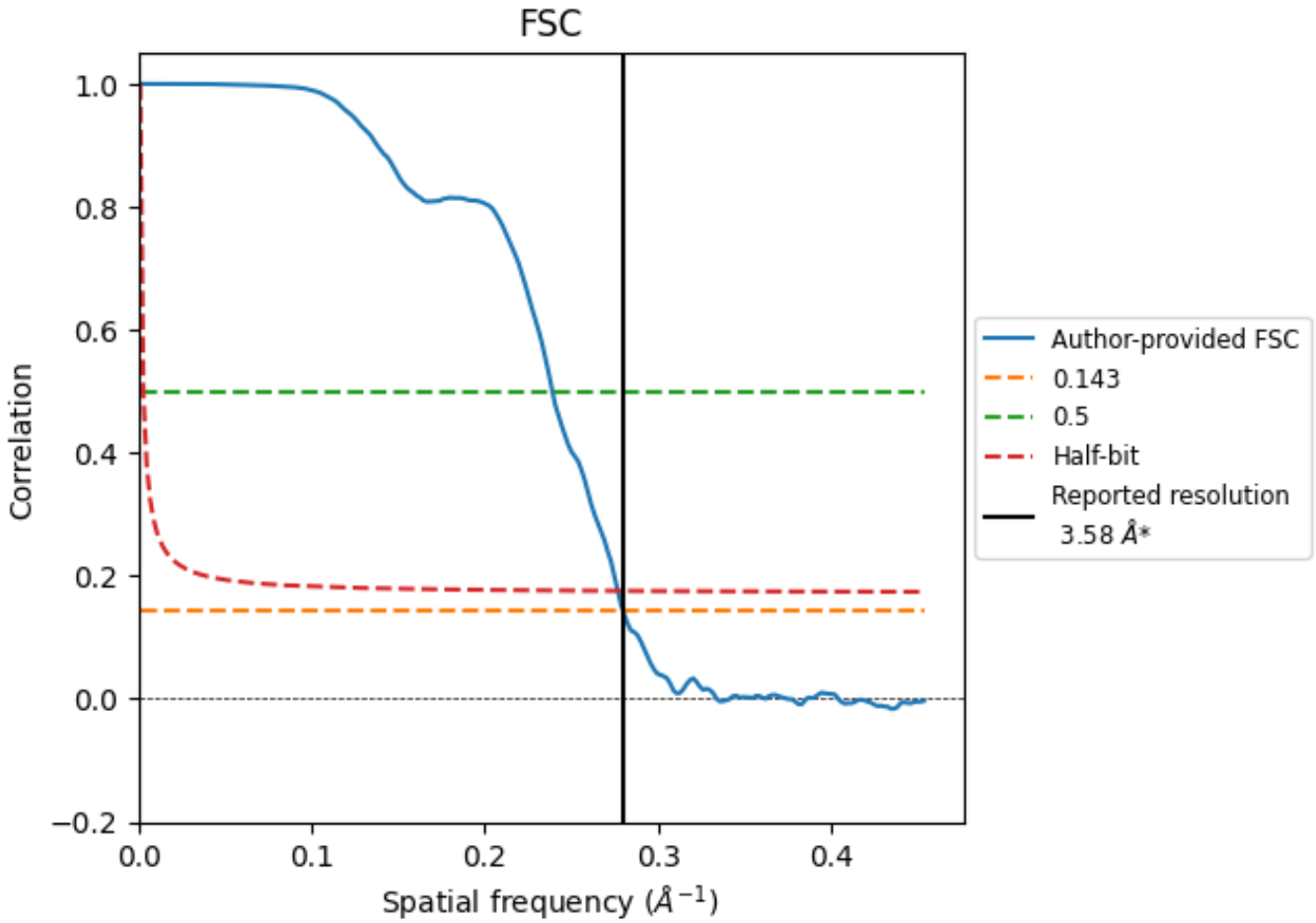


*Reported resolution corresponds to spatial frequency of 0.279 $Å^{-1}$

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 0.279 Å^{-1}

8.2 Resolution estimates (i)

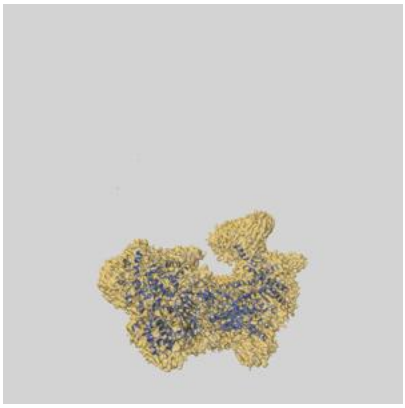
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.58	4.19	3.62
Unmasked-calculated*	-	-	-

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

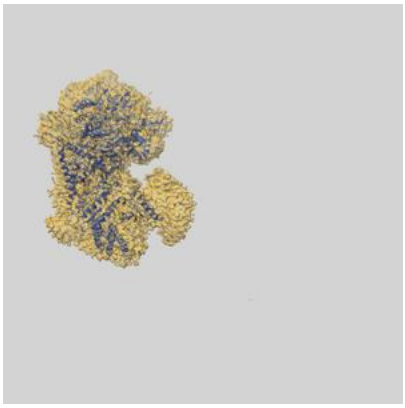
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22397 and PDB model 7JMN. Per-residue inclusion information can be found in section 3 on page 6.

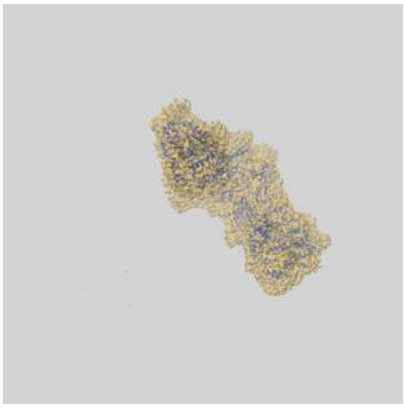
9.1 Map-model overlay



X



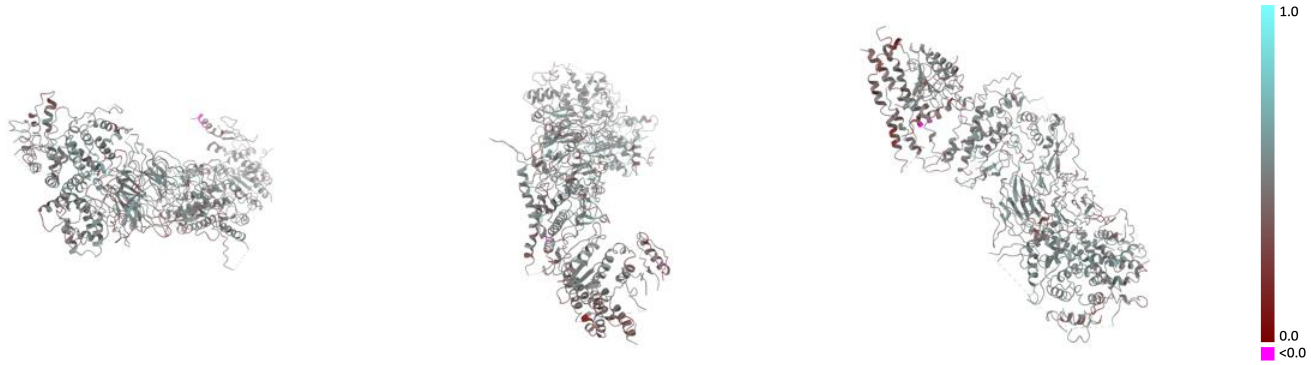
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

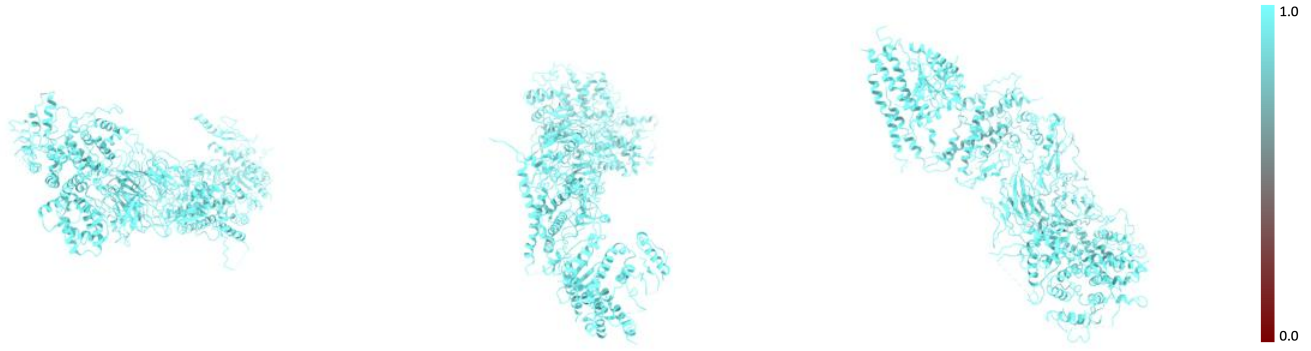
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

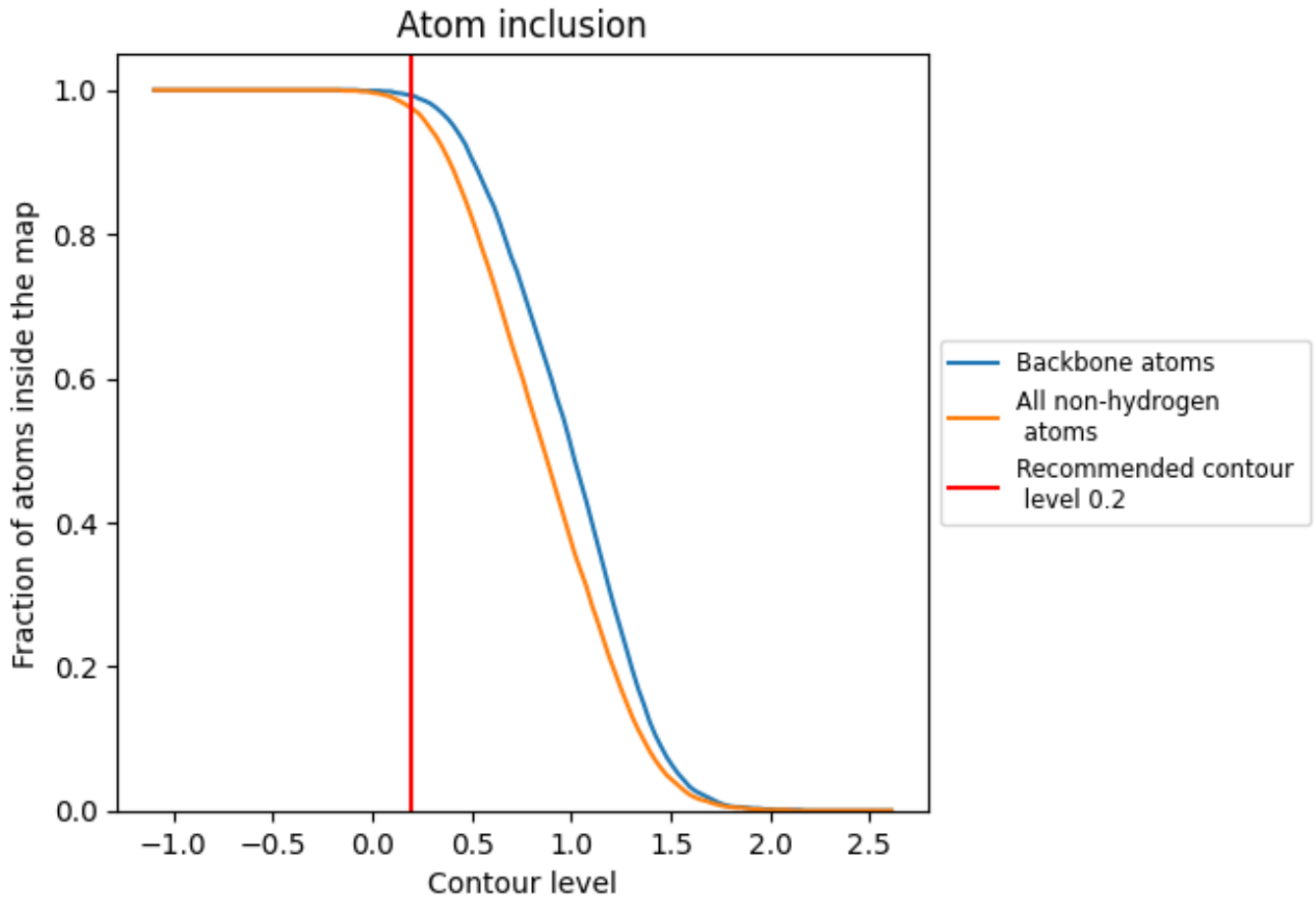
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.2) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9740	0.4650
E	0.9820	0.4830
N	0.9820	0.4530
O	0.9770	0.4230
P	0.9660	0.4640
X	0.9920	0.4970