



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:22 PM UTC

PDB ID : 7AD8 / pdb_00007ad8
EMDB ID : EMD-4970
Title : Core TFIIH-XPA-DNA complex with modelled p62 subunit
Authors : Koelmel, W.; Kuper, J.; Kisker, C.
Deposited on : 2020-09-14
Resolution : 3.50 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
Mogul : 2022.3.0, CSD as543be (2022)
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

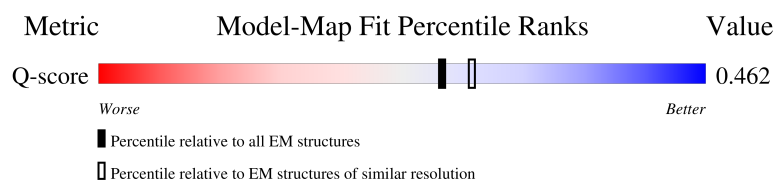
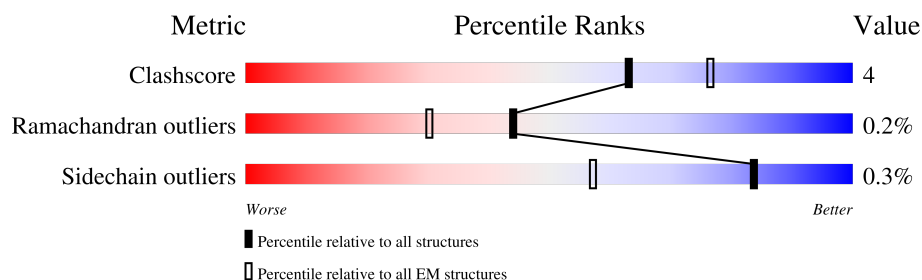
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.

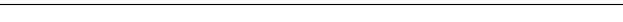
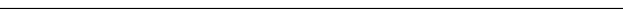
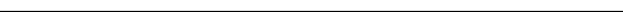


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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 $\leq 5\%$. 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	J	49	
2	K	49	
3	A	782	
4	F	71	

Continued on next page...

Mol	Chain	Length	Quality of chain
5	B	760	
6	E	308	
7	D	395	
8	C	462	
9	G	273	
10	I	548	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 21213 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 DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	19	Total	C	N	O	P	0	0
			387	184	71	113	19		

- Molecule 2 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	28	Total	C	N	O	P	0	0
			575	273	111	163	28		

- Molecule 3 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	575	Total	C	N	O	S	0	0
			4648	2977	806	837	28		

- Molecule 4 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	62	Total	C	N	O	S	0	0
			490	315	78	94	3		

- Molecule 5 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	675	Total	C	N	O	S	0	0
			5436	3490	941	976	29		

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	237	Total	C	N	O	S	0	0
			1857	1196	309	333	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	280	Total	C	N	O	S	0	0
			2182	1382	376	400	24		

- Molecule 8 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	386	Total	C	N	O	S	0	0
			3109	2016	538	543	12		

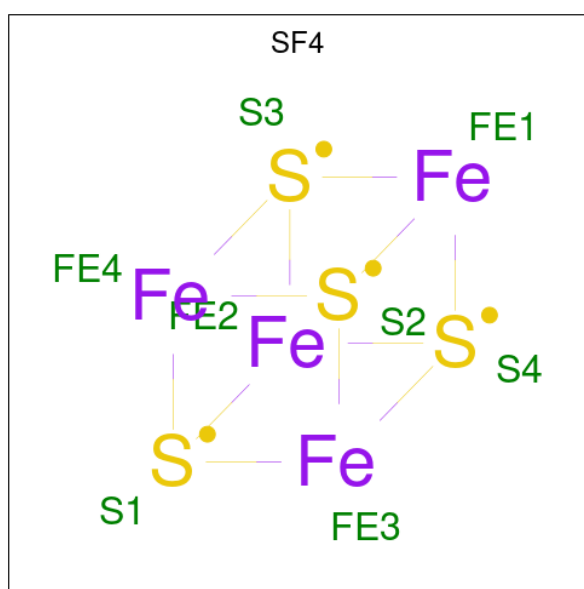
- Molecule 9 is a protein called DNA repair protein complementing XP-A cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	134	Total	C	N	O	S	0	0
			1129	710	204	206	9		

- Molecule 10 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	206	Total	C	N	O	S	0	0
			1386	860	255	265	6		

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	E	2	Total	Zn	0
			2	2	
12	D	3	Total	Zn	0
			3	3	
12	G	1	Total	Zn	0
			1	1	

PRO
SER
LYS
HIS
VAL
HIS
PRO
LEU
PHE
LYS
ARG
PHE
ARG
LYS

- Molecule 4: General transcription factor IIH subunit 5

Chain F: 

MET VAL ASN V4 L5 K6 G7 V8 L9 I10 D24 E25 K31 K32 F33 H42 A47 E48 L49 L53 M64 A65 PHE SER LEU THR GLN LYS

- Molecule 5: TFIIH basal transcription factor complex helicase XPD subunit

Chain B: 

M1 K2 L3 I17 S44 G45 T46 L52 L70 T76 G99 E100 K101 S110 S111 L115 V121 T122 R125 D131 G132 K133 Q147 H148 D149 E167 L170 P171 L177 D178 Y192 R196 V204 Y211 D219 L220 V221 S222 K223 E224

V232 A236 I239 L251 R254 T255 L256 Q267 R272 ILE LYS GLU THR ASP GLN ARG LEU ARG ASP GLU TYR ARG ARG LEU VAL GLY LEU ARG GLU THR ASP ALA HIS LEU ALA ASN PRO VAL LEU PRO ASP VAL GLN

GLU ALA VAL PRO GLY SER ILE ARG THR A326 R334 Y339 R345 V346 Q347 S353 A356 V365 I367 Q368 R369 R380 L386 D393 S408 F421 D422 D423 A429 S441 V454 S462 P463 L464 L471 T480 R487 R497 D500

T510 R511 E512 D513 V516 S528 P532 I535 S547 K565 I569 R592 I595 E606 D609 F610 V611 M657 R666 D681 K682 F684 A685 R686 K689 L693 I697 N707 M724 F728 HIS ARG GLU ASP GLN LEU

SER LEU SER LEU SER LEU GLN LEU SER LEU THR LEU ARG ILE GLU GLN ILE ALA GLN LEU

- Molecule 6: General transcription factor IIH subunit 3

Chain E: 

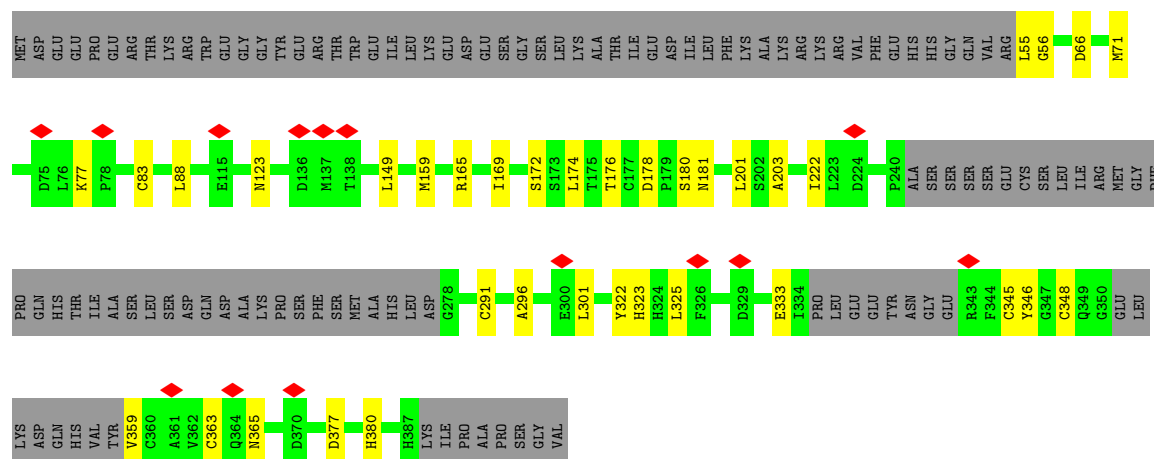
MET VAL ASP GLU GLU L5 L11 L12 Q25 K28 E29 Q31 F32 T33 L34 D39 M42 V43 L44 R53 A58 Q65 G73 LYS ASN GLY ARG LEU GLY ASP PHE GLY ASP PRO GLY ASN PRO PRO PHE ASN PRO GLY SER GLY LYS ASP

GLY LYS TYR L103 V112 E113 K116 D117 T120 LYS SER ASP ILE LYS GLN H128 R146 V151 LYS ASP ASN GLN M157 M175 L227 L241 R252 L261 C268 S269 N277 F278 C285 GLU THR PHE LYS ILE SER LEU PRO PRO VAL

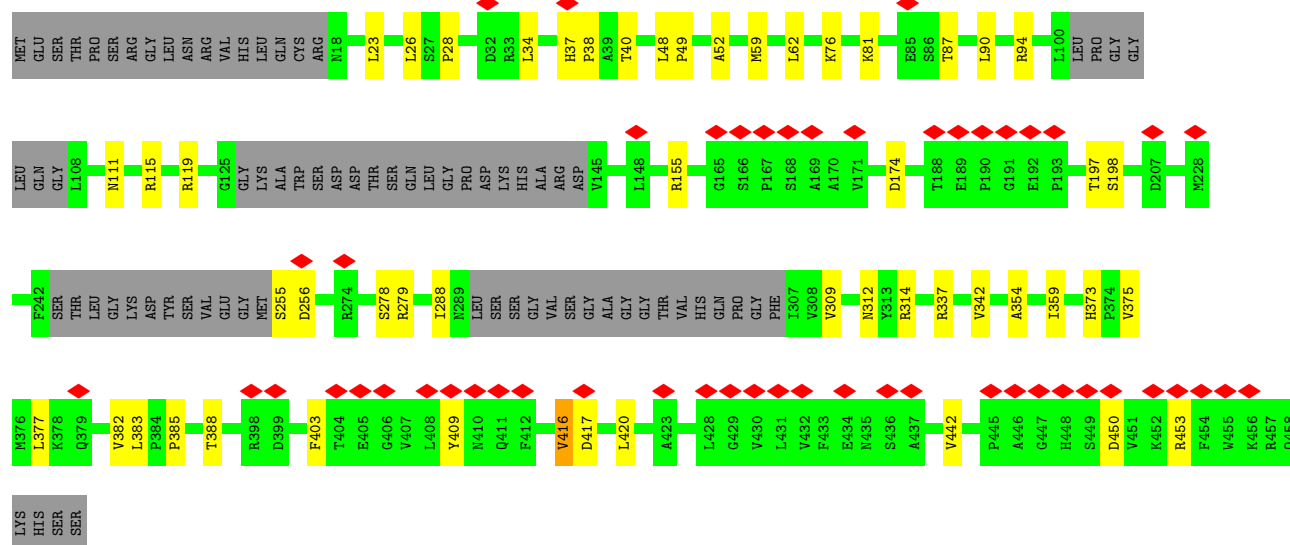
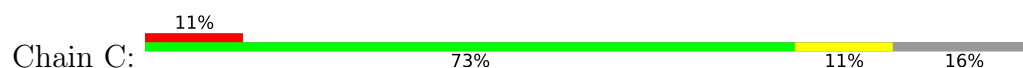
LEU LYS ALA LYS LYS LYS LYS LYS VAL SER ALA

- Molecule 7: General transcription factor IIH subunit 2

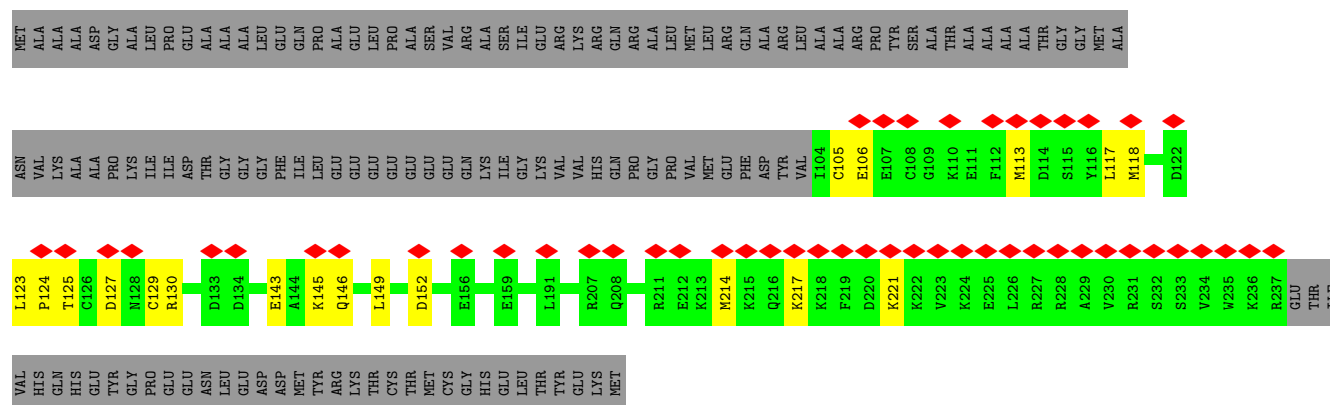
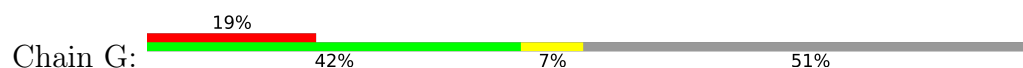
Chain D: 



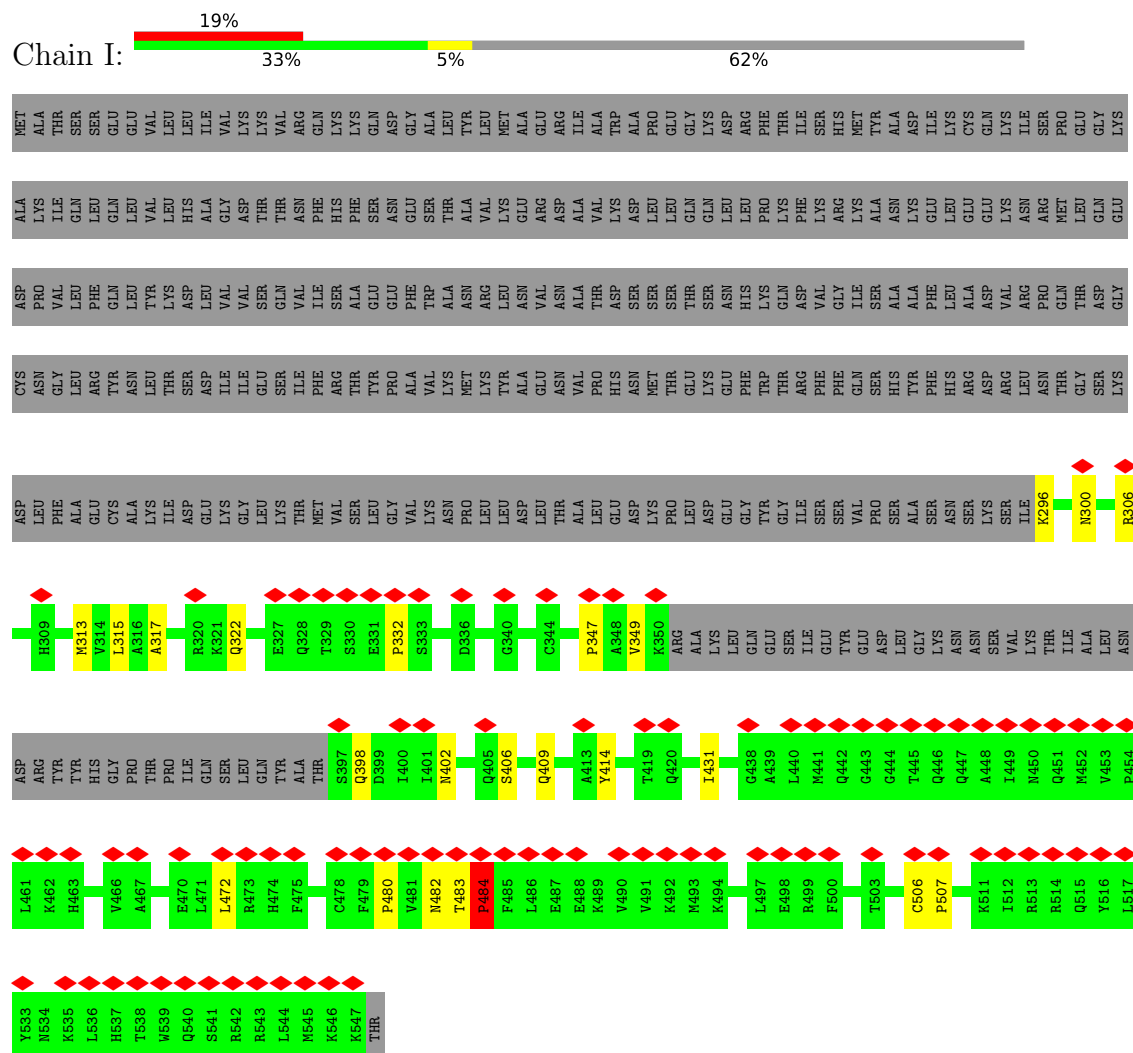
• Molecule 8: General transcription factor IIH subunit 4



• Molecule 9: DNA repair protein complementing XP-A cells



Chain I:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227776	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 ($e^-/\text{\AA}^2$)	41	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	0.150	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	J	0.27	0/433	0.45	0/665
2	K	0.31	0/646	0.47	0/994
3	A	0.26	0/4748	0.54	1/6416 (0.0%)
4	F	0.19	0/495	0.45	0/668
5	B	0.27	1/5556 (0.0%)	0.54	2/7522 (0.0%)
6	E	0.21	0/1890	0.43	0/2561
7	D	0.20	0/2228	0.46	0/3017
8	C	0.22	0/3178	0.53	1/4307 (0.0%)
9	G	0.17	0/1149	0.51	0/1531
10	I	0.23	0/1404	0.81	5/1914 (0.3%)
All	All	0.24	1/21727 (0.0%)	0.54	9/29595 (0.0%)

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
3	A	0	1
5	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	122	THR	C-N	6.74	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	332	PRO	N-CA-CB	10.55	110.69	101.83
5	B	76	THR	CA-C-N	10.29	126.72	120.24
5	B	76	THR	C-N-CA	10.29	126.72	120.24
10	I	484	PRO	N-CA-CB	7.95	111.60	103.25
3	A	152	ILE	N-CA-C	-7.07	105.89	112.96
10	I	480	PRO	N-CA-CB	7.03	110.63	103.25
10	I	347	PRO	N-CA-CB	6.99	110.58	102.33
10	I	507	PRO	N-CA-CB	6.74	110.99	103.44
8	C	416	VAL	N-CA-C	-5.66	108.33	113.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	81	ASP	Peptide
5	B	462	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	J	387	0	214	4	0
2	K	575	0	314	8	0
3	A	4648	0	4704	45	0
4	F	490	0	499	8	0
5	B	5436	0	5483	41	0
6	E	1857	0	1895	12	0
7	D	2182	0	2173	22	0
8	C	3109	0	3155	32	0
9	G	1129	0	1147	12	0
10	I	1386	0	1156	11	0
11	B	8	0	0	0	0
12	D	3	0	0	0	0
12	E	2	0	0	0	0
12	G	1	0	0	0	0
All	All	21213	0	20740	176	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 4.

All (176) 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:J:27:DC:H42	2:K:23:DG:H1	1.36	0.73
5:B:353:SER:HB2	5:B:356:ALA:HB3	1.77	0.66
3:A:415:HIS:HE2	3:A:417:THR:HG1	1.45	0.65
7:D:345:CYS:SG	7:D:346:TYR:N	2.70	0.64
6:E:44:LEU:HD22	6:E:227:LEU:HB3	1.80	0.63
5:B:657:MET:HE3	5:B:689:LYS:HB3	1.82	0.61
3:A:443:VAL:HG12	3:A:480:LEU:HD11	1.82	0.61
5:B:192:TYR:OH	5:B:196:ARG:NH2	2.35	0.60
4:F:9:LEU:HD21	4:F:42:HIS:HD2	1.67	0.59
1:J:30:DG:H1	2:K:20:DC:H42	1.50	0.59
3:A:623:LEU:HB3	3:A:659:PHE:HB2	1.84	0.59
3:A:671:ALA:HB2	4:F:64:ASN:HA	1.85	0.58
8:C:373:HIS:HD2	8:C:375:VAL:H	1.52	0.58
6:E:252:ARG:HD3	6:E:261:LEU:HB3	1.86	0.58
10:I:398:GLN:O	10:I:402:ASN:ND2	2.37	0.58
7:D:333:GLU:OE2	7:D:359:VAL:N	2.37	0.57
9:G:105:CYS:SG	9:G:106:GLU:N	2.77	0.57
6:E:12:VAL:HG22	6:E:58:ALA:HB3	1.87	0.57
6:E:25:GLN:HA	6:E:28:LYS:HB2	1.87	0.57
5:B:423:ASP:N	5:B:423:ASP:OD1	2.38	0.56
3:A:278:GLU:OE2	3:A:452:ARG:NH1	2.39	0.56
3:A:108:CYS:SG	8:C:312:ASN:ND2	2.79	0.55
5:B:497:ARG:NH2	5:B:707:ASN:O	2.39	0.55
3:A:629:HIS:O	3:A:676:ARG:NH2	2.39	0.55
7:D:363:CYS:SG	7:D:365:ASN:ND2	2.79	0.55
4:F:4:VAL:HA	8:C:409:TYR:HA	1.87	0.55
3:A:540:LYS:HG2	3:A:662:LEU:HD23	1.89	0.55
8:C:62:LEU:HD11	10:I:431:ILE:HD11	1.89	0.54
3:A:272:VAL:HG21	3:A:280:LEU:HD22	1.89	0.54
8:C:59:MET:HA	8:C:62:LEU:HD13	1.89	0.54
3:A:693:LEU:HD12	3:A:696:MET:HE2	1.90	0.54
5:B:369:ARG:NH2	5:B:408:SER:O	2.41	0.54
9:G:214:MET:HA	9:G:217:LYS:HG2	1.88	0.53
3:A:551:HIS:HB3	3:A:556:ASP:HB2	1.91	0.53
7:D:322:TYR:O	7:D:323:HIS:ND1	2.41	0.53
3:A:588:GLU:HA	3:A:591:GLN:HG2	1.90	0.53
10:I:406:SER:O	10:I:409:GLN:NE2	2.42	0.52
2:K:32:DA:OP1	5:B:686:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:217:LYS:O	9:G:221:LYS:NZ	2.40	0.52
10:I:472:LEU:HD11	10:I:532:ALA:HB2	1.90	0.52
8:C:87:THR:HA	8:C:90:LEU:HB3	1.89	0.52
9:G:143:GLU:OE2	9:G:146:GLN:NE2	2.43	0.52
5:B:569:ILE:H	10:I:315:LEU:HD13	1.74	0.52
7:D:172:SER:HA	7:D:201:LEU:HB2	1.92	0.52
10:I:296:LYS:O	10:I:300:ASN:ND2	2.42	0.52
9:G:118:MET:HE3	9:G:124:PRO:HA	1.92	0.51
3:A:558:ILE:HB	3:A:604:THR:HG22	1.92	0.51
5:B:365:VAL:HG12	5:B:367:ILE:HG12	1.93	0.51
6:E:53:ARG:NH2	8:C:288:ILE:O	2.44	0.51
5:B:339:TYR:HB2	5:B:365:VAL:HG21	1.91	0.51
5:B:606:GLU:O	5:B:666:ARG:NH2	2.43	0.51
2:K:24:DC:H2''	2:K:25:DT:H5''	1.93	0.51
5:B:219:ASP:OD2	5:B:219:ASP:N	2.44	0.51
3:A:115:GLU:OE1	8:C:314:ARG:NH1	2.45	0.50
3:A:392:PHE:HB3	3:A:408:SER:HB2	1.93	0.50
8:C:23:LEU:HA	8:C:26:LEU:HD12	1.94	0.50
3:A:514:MET:HE1	3:A:534:TYR:HA	1.93	0.50
1:J:34:DT:H2'	1:J:35:DC:H6	1.76	0.49
3:A:556:ASP:OD1	3:A:621:ASN:ND2	2.44	0.49
5:B:52:LEU:HD21	5:B:232:VAL:HG21	1.94	0.49
3:A:137:THR:OG1	3:A:153:MET:SD	2.70	0.49
8:C:94:ARG:O	8:C:111:ASN:ND2	2.46	0.49
8:C:278:SER:OG	8:C:279:ARG:N	2.45	0.49
3:A:535:THR:HG21	3:A:564:ASN:HD22	1.78	0.49
5:B:393:ASP:OD1	5:B:393:ASP:N	2.46	0.49
5:B:110:SER:OG	5:B:111:SER:N	2.46	0.49
6:E:112:VAL:HG13	10:I:414:TYR:HD2	1.77	0.49
3:A:520:ARG:NH1	4:F:25:GLU:OE1	2.46	0.48
9:G:145:LYS:NZ	9:G:152:ASP:OD1	2.39	0.48
3:A:502:ILE:HG23	3:A:644:LEU:HB2	1.95	0.48
5:B:441:SER:HB3	5:B:471:LEU:HA	1.95	0.48
5:B:510:THR:HG22	5:B:516:VAL:HG21	1.95	0.48
3:A:408:SER:OG	3:A:409:THR:N	2.47	0.48
3:A:599:ASN:HD21	3:A:601:LYS:HB3	1.79	0.48
7:D:174:LEU:HD11	7:D:203:ALA:HB3	1.96	0.48
3:A:168:LEU:HB2	3:A:291:LEU:HD22	1.95	0.48
9:G:117:LEU:HD23	9:G:123:LEU:HB3	1.94	0.48
6:E:33:THR:OG1	6:E:34:LEU:N	2.47	0.47
3:A:467:THR:OG1	3:A:468:ALA:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:612:ASP:OD2	3:A:635:GLN:NE2	2.47	0.47
3:A:514:MET:HG2	3:A:519:TYR:HD1	1.79	0.47
8:C:417:ASP:HA	8:C:420:LEU:HB2	1.96	0.47
7:D:66:ASP:HB3	7:D:71:MET:HE2	1.97	0.47
8:C:354:ALA:HB1	8:C:359:ILE:HD12	1.96	0.47
8:C:377:LEU:HD23	8:C:382:VAL:HG11	1.97	0.47
5:B:500:ASP:N	5:B:500:ASP:OD1	2.48	0.46
5:B:528:SER:HB2	5:B:565:LYS:HD2	1.97	0.46
8:C:48:LEU:HB3	8:C:52:ALA:HB3	1.97	0.46
3:A:197:CYS:HB3	3:A:276:MET:HE2	1.97	0.46
8:C:28:PRO:HB3	8:C:94:ARG:HD3	1.96	0.46
3:A:340:LEU:HD23	3:A:491:ALA:HB2	1.97	0.46
7:D:180:SER:OG	7:D:181:ASN:N	2.49	0.46
9:G:113:MET:SD	9:G:113:MET:N	2.88	0.46
3:A:103:ILE:HD12	3:A:136:ILE:HD12	1.97	0.46
3:A:375:LYS:HD2	3:A:391:ARG:HD3	1.96	0.46
5:B:464:LEU:HD11	5:B:480:THR:HB	1.98	0.46
5:B:267:GLN:HB2	5:B:334:ARG:HH12	1.81	0.46
7:D:159:MET:O	7:D:165:ARG:NH2	2.49	0.45
7:D:149:LEU:HD21	7:D:169:ILE:HD11	1.98	0.45
7:D:176:THR:O	7:D:176:THR:OG1	2.31	0.45
5:B:487:ARG:HB3	5:B:724:MET:HE1	1.98	0.45
4:F:31:LYS:HD3	4:F:32:LYS:HG3	1.99	0.45
3:A:589:ARG:HE	3:A:589:ARG:HB2	1.59	0.45
8:C:197:THR:OG1	8:C:198:SER:N	2.50	0.45
3:A:336:GLY:HA3	3:A:488:LEU:HG	1.98	0.44
7:D:123:ASN:HD21	7:D:301:LEU:HD13	1.81	0.44
5:B:513:ASP:OD2	5:B:513:ASP:N	2.48	0.44
7:D:178:ASP:OD1	7:D:178:ASP:N	2.50	0.44
7:D:377:ASP:O	7:D:380:HIS:NE2	2.50	0.44
5:B:115:LEU:HD21	5:B:177:LEU:HD22	2.00	0.43
4:F:10:ILE:HG12	8:C:403:PHE:HD1	1.84	0.43
4:F:48:GLU:HG2	4:F:49:LEU:HG	2.01	0.43
7:D:88:LEU:HD23	7:D:88:LEU:HA	1.87	0.43
8:C:155:ARG:HD3	8:C:155:ARG:HA	1.83	0.43
5:B:251:LEU:HD23	5:B:256:LEU:HD21	2.01	0.43
6:E:241:LEU:O	8:C:76:LYS:NZ	2.45	0.43
8:C:385:PRO:HA	8:C:388:THR:HG22	2.01	0.43
3:A:613:THR:OG1	3:A:614:SER:N	2.51	0.43
8:C:255:SER:OG	8:C:256:ASP:N	2.51	0.43
7:D:172:SER:HB2	7:D:201:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:146:ARG:HD3	7:D:348:CYS:HB2	2.01	0.43
5:B:170:LEU:HA	5:B:171:PRO:HD3	1.93	0.43
3:A:643:VAL:HG21	3:A:659:PHE:HB3	2.00	0.42
5:B:592:ARG:HA	5:B:592:ARG:HD2	1.83	0.42
8:C:416:VAL:O	8:C:420:LEU:N	2.52	0.42
8:C:450:ASP:HA	8:C:453:ARG:HG3	2.01	0.42
2:K:24:DC:H5'	3:A:412:MET:SD	2.59	0.42
10:I:482:ASN:O	10:I:484:PRO:N	2.52	0.42
5:B:682:LYS:HB3	5:B:682:LYS:HE3	1.87	0.42
5:B:693:LEU:HD13	5:B:697:ILE:HG13	2.01	0.42
3:A:505:VAL:HB	3:A:685:TYR:HE2	1.83	0.42
5:B:3:LEU:HD11	5:B:17:ILE:HD13	2.01	0.42
7:D:201:LEU:HG	7:D:222:ILE:HD12	2.01	0.42
8:C:450:ASP:OD1	8:C:450:ASP:N	2.39	0.42
3:A:362:LEU:HD23	3:A:438:MET:HG2	2.01	0.42
3:A:596:PHE:HD2	3:A:618:PRO:HG2	1.84	0.42
9:G:129:CYS:SG	9:G:130:ARG:N	2.92	0.42
3:A:506:GLN:HB3	3:A:658:PHE:HB3	2.02	0.42
6:E:252:ARG:HB2	6:E:261:LEU:HD12	2.01	0.42
2:K:21:DG:H2'	2:K:22:DA:C8	2.55	0.42
2:K:41:DA:OP1	5:B:211:TYR:OH	2.32	0.42
8:C:174:ASP:N	8:C:174:ASP:OD1	2.50	0.42
10:I:313:MET:O	10:I:317:ALA:N	2.53	0.42
8:C:34:LEU:HG	8:C:40:THR:HG21	2.02	0.41
5:B:236:ALA:HB1	5:B:239:ILE:HB	2.03	0.41
5:B:681:ASP:HB3	5:B:684:PHE:HD2	1.85	0.41
7:D:77:LYS:HB3	7:D:83:CYS:HB2	2.01	0.41
1:J:22:DG:H1	2:K:28:DC:H42	1.68	0.41
5:B:532:PRO:HG3	7:D:203:ALA:HB1	2.01	0.41
8:C:337:ARG:HG3	8:C:342:VAL:HG22	2.01	0.41
5:B:535:ILE:HB	5:B:595:ILE:HG12	2.02	0.41
8:C:309:VAL:HG11	8:C:383:LEU:HD13	2.01	0.41
10:I:527:GLU:O	10:I:531:THR:OG1	2.36	0.41
5:B:547:SER:O	5:B:547:SER:OG	2.34	0.41
7:D:55:LEU:HB3	7:D:56:GLY:H	1.65	0.41
7:D:291:CYS:HB3	7:D:296:ALA:H	1.85	0.41
5:B:121:VAL:HG23	5:B:133:LYS:HB3	2.03	0.41
4:F:33:PHE:HZ	4:F:53:LEU:HB2	1.85	0.41
5:B:44:SER:OG	5:B:46:THR:O	2.34	0.41
3:A:306:ILE:H	3:A:306:ILE:HG12	1.65	0.41
3:A:469:THR:O	3:A:469:THR:OG1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:81:LYS:HA	8:C:81:LYS:HD2	1.88	0.41
3:A:628:SER:HB2	3:A:676:ARG:HH22	1.85	0.40
5:B:223:LYS:HA	5:B:223:LYS:HD2	1.93	0.40
6:E:268:CYS:SG	6:E:269:SER:N	2.94	0.40
8:C:37:HIS:CG	8:C:38:PRO:HD3	2.56	0.40
9:G:117:LEU:HD22	9:G:125:THR:HB	2.03	0.40
5:B:211:TYR:HD2	5:B:221:VAL:HG21	1.87	0.40
6:E:39:ASP:HA	6:E:42:MET:HB2	2.04	0.40
9:G:149:LEU:HD13	9:G:149:LEU:HA	1.91	0.40
3:A:353:ALA:HB1	3:A:437:LEU:HD11	2.02	0.40
5:B:70:LEU:HD23	5:B:204:VAL:HG13	2.03	0.40
9:G:127:ASP:OD1	9:G:127:ASP:N	2.45	0.40
3:A:140:LEU:HD23	3:A:140:LEU:HA	1.95	0.40
8:C:115:ARG:HH22	8:C:119:ARG:HH21	1.68	0.40
10:I:306:ARG:HA	10:I:306:ARG:HD2	1.82	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	
3	A	569/782 (73%)	508 (89%)	61 (11%)	0	100	100
4	F	60/71 (84%)	58 (97%)	2 (3%)	0	100	100
5	B	671/760 (88%)	623 (93%)	48 (7%)	0	100	100
6	E	229/308 (74%)	217 (95%)	12 (5%)	0	100	100
7	D	272/395 (69%)	255 (94%)	17 (6%)	0	100	100
8	C	376/462 (81%)	343 (91%)	32 (8%)	1 (0%)	36	67
9	G	132/273 (48%)	123 (93%)	9 (7%)	0	100	100
10	I	202/548 (37%)	182 (90%)	15 (7%)	5 (2%)	4	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2511/3599 (70%)	2309 (92%)	196 (8%)	6 (0%)	44	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	I	483	THR
10	I	484	PRO
10	I	322	GLN
8	C	49	PRO
10	I	349	VAL
10	I	506	CYS

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	
3	A	511/688 (74%)	509 (100%)	2 (0%)	84	81
4	F	55/64 (86%)	55 (100%)	0	100	100
5	B	589/664 (89%)	587 (100%)	2 (0%)	86	83
6	E	211/272 (78%)	210 (100%)	1 (0%)	81	80
7	D	251/352 (71%)	250 (100%)	1 (0%)	84	81
8	C	334/399 (84%)	333 (100%)	1 (0%)	86	83
9	G	126/233 (54%)	126 (100%)	0	100	100
10	I	109/484 (22%)	109 (100%)	0	100	100
All	All	2186/3156 (69%)	2179 (100%)	7 (0%)	84	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	129	VAL
3	A	510	VAL
5	B	454	VAL
5	B	611	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	11	LEU
7	D	325	LEU
8	C	442	VAL

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

Mol	Chain	Res	Type
3	A	281	GLN
3	A	492	ASN
3	A	498	ASN
3	A	537	ASN
3	A	564	ASN
3	A	598	HIS
3	A	599	ASN
4	F	27	ASN
4	F	42	HIS
4	F	51	ASN
4	F	64	ASN
5	B	92	ASN
5	B	114	ASN
5	B	135	HIS
5	B	147	GLN
5	B	203	ASN
5	B	241	ASN
5	B	250	ASN
5	B	555	GLN
5	B	659	HIS
5	B	700	HIS
5	B	726	GLN
6	E	46	ASN
6	E	108	ASN
6	E	128	HIS
6	E	204	GLN
6	E	235	GLN
7	D	60	HIS
7	D	74	GLN
7	D	147	ASN
7	D	227	HIS
8	C	116	GLN
8	C	117	ASN
8	C	224	GLN
8	C	312	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	C	345	GLN
8	C	373	HIS
8	C	390	GLN
9	G	169	ASN
10	I	300	ASN
10	I	402	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	SF4	B	1000	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	B	1000	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

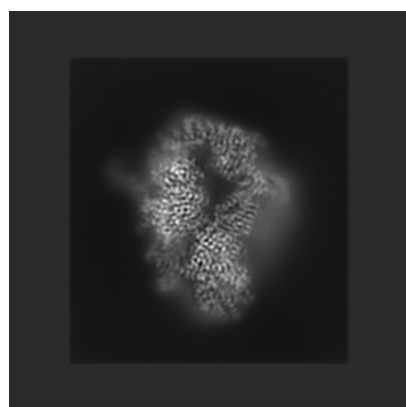
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4970. These allow visual inspection of the internal detail of the map and identification of artifacts.

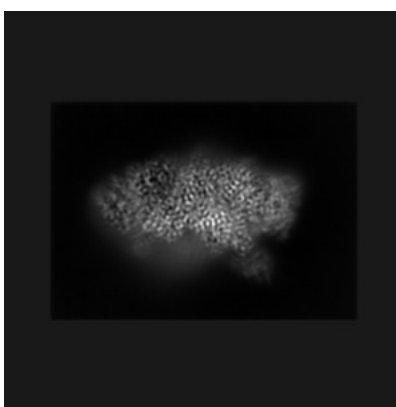
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

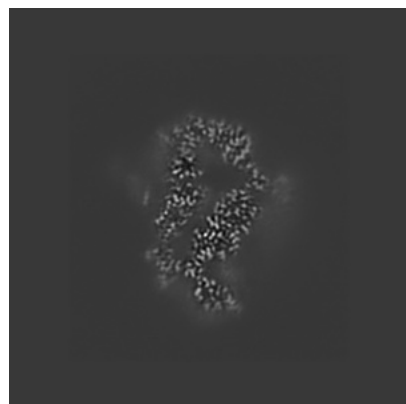


Z

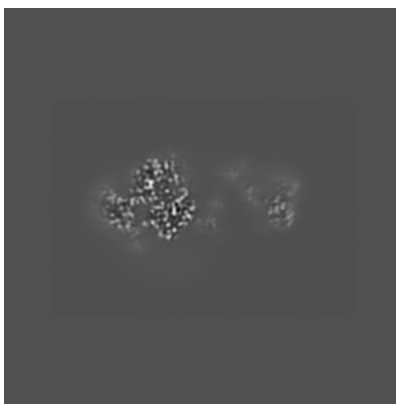
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

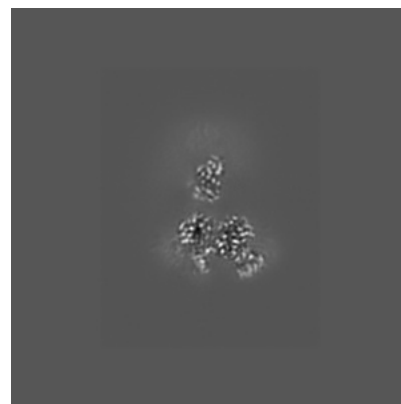
6.2.1 Primary map



X Index: 160



Y Index: 160

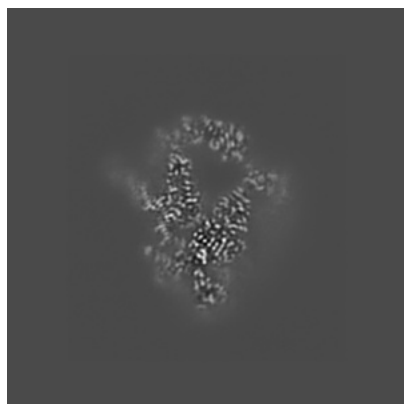


Z Index: 160

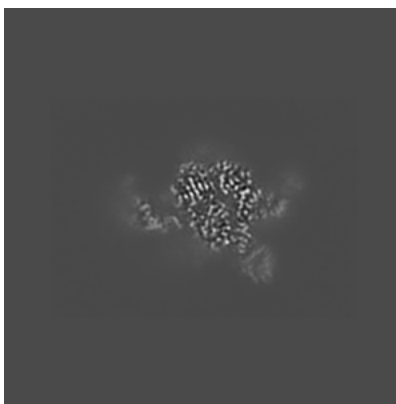
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

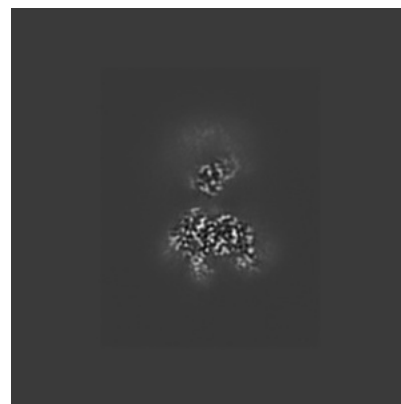
6.3.1 Primary map



X Index: 153



Y Index: 134

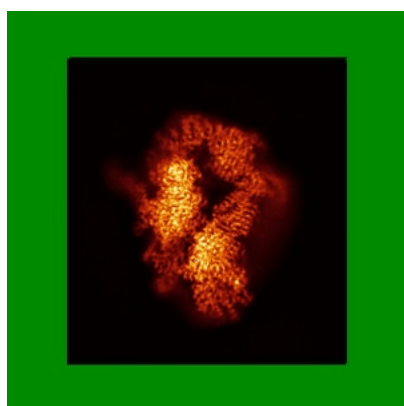


Z Index: 166

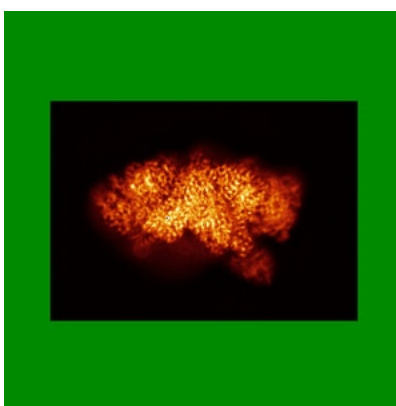
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

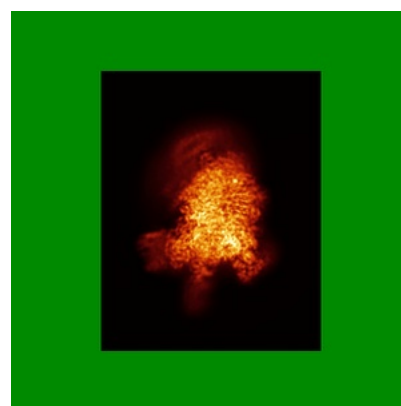
6.4.1 Primary map



X



Y

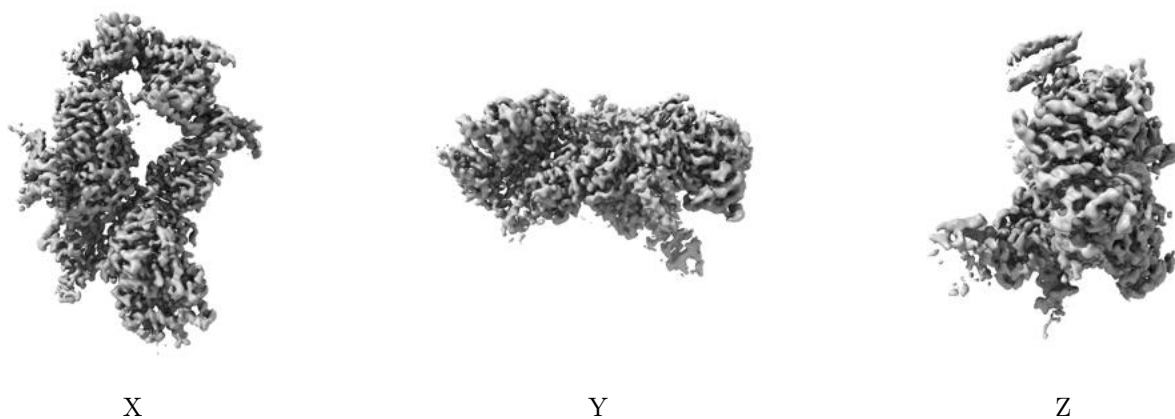


Z

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



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.

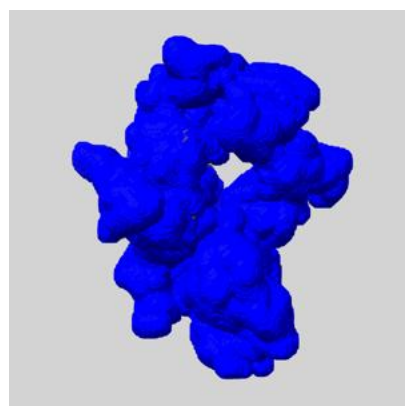
6.6 Mask visualisation [i](#)

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

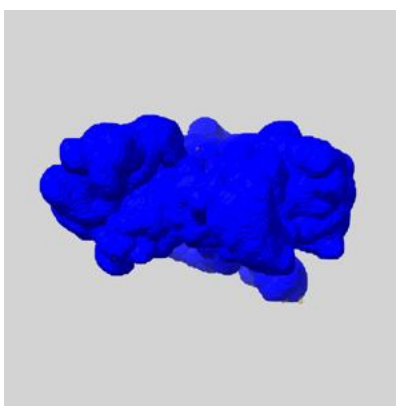
A mask typically either:

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

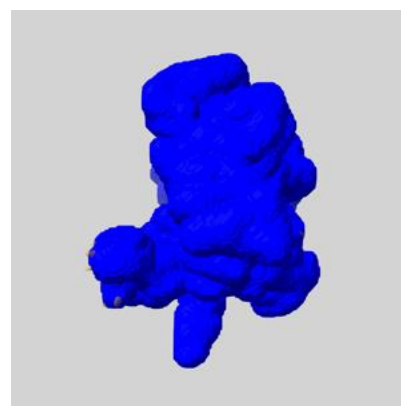
6.6.1 emd_4970_msk_1.map [i](#)



X



Y

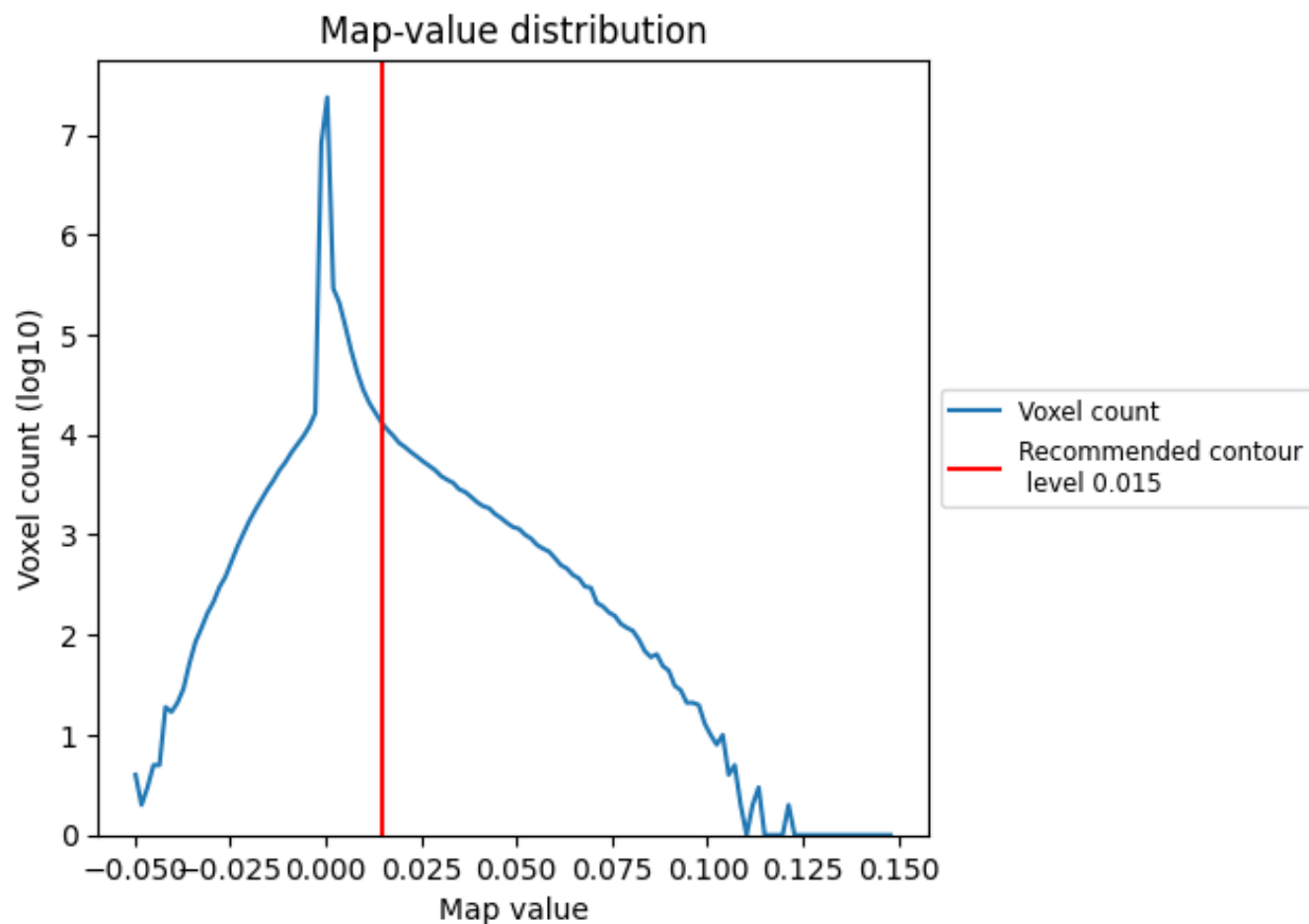


Z

7 Map analysis [i](#)

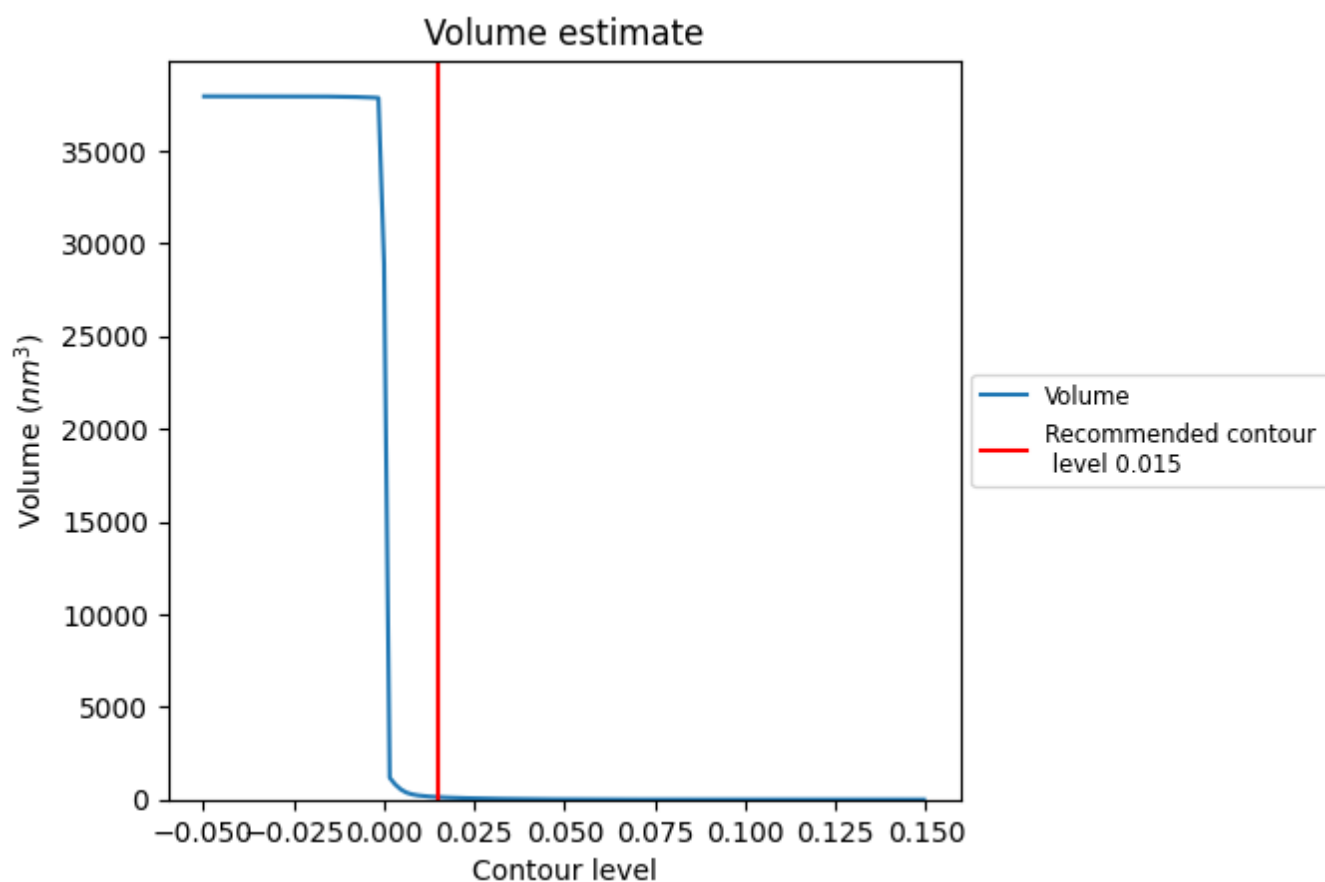
This section contains the results of statistical analysis of the map.

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.

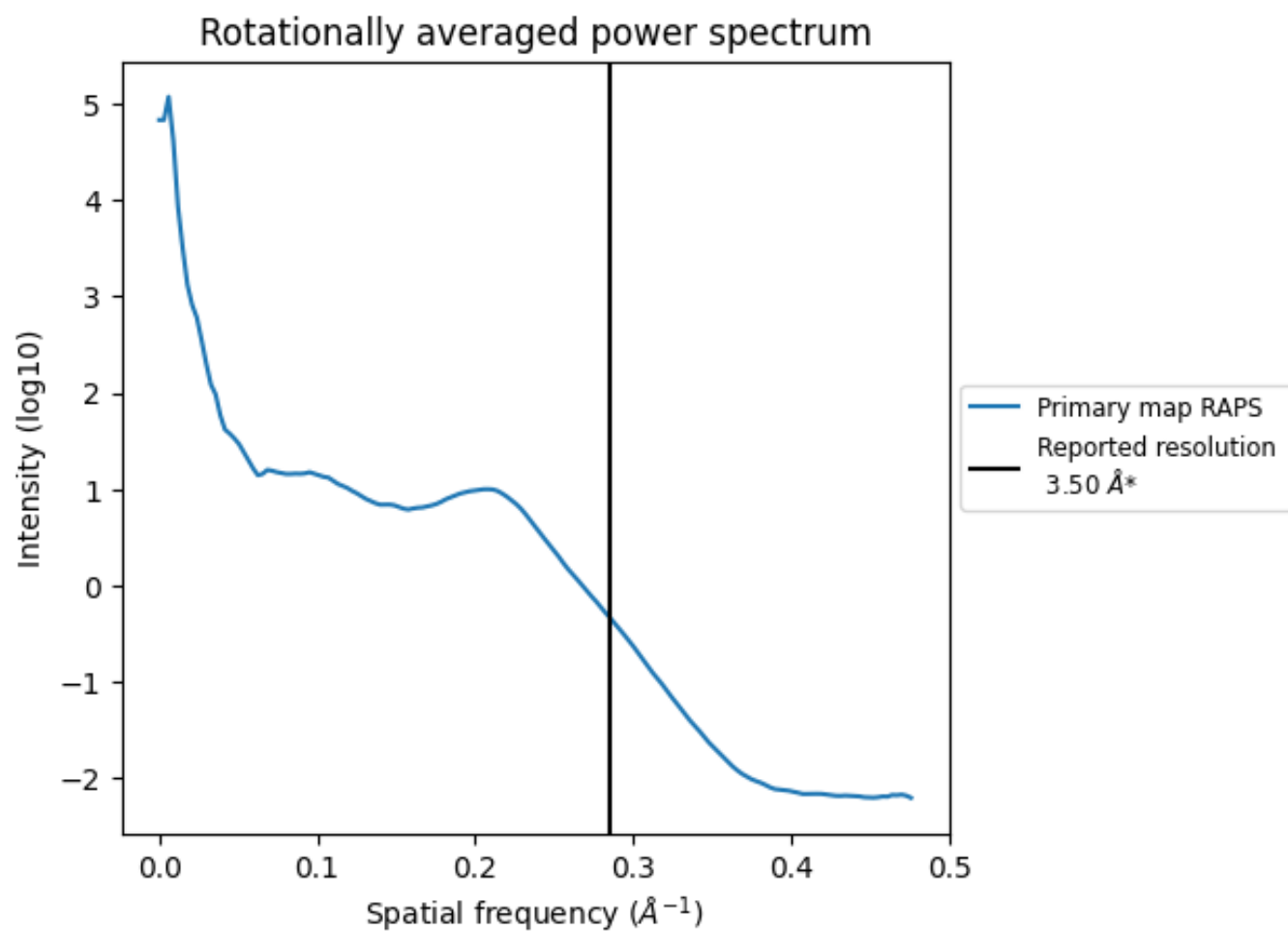
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm^3 ; this corresponds to an approximate mass of 119 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 0.286 Å⁻¹

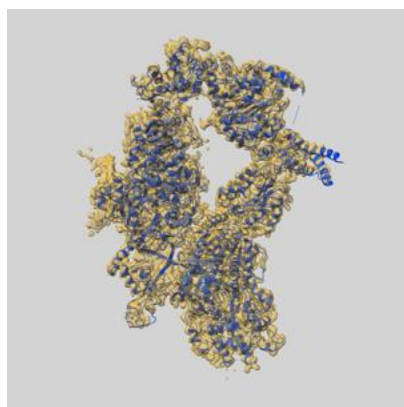
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

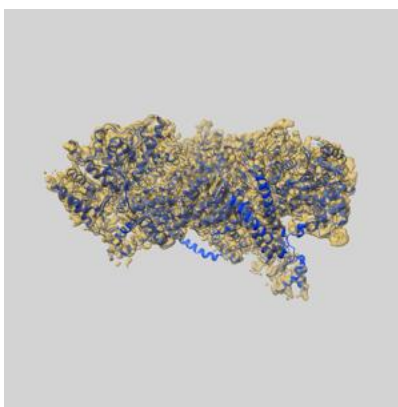
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4970 and PDB model 7AD8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

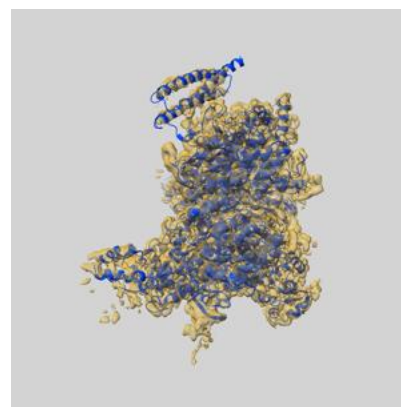
9.1 Map-model overlay [i](#)



X



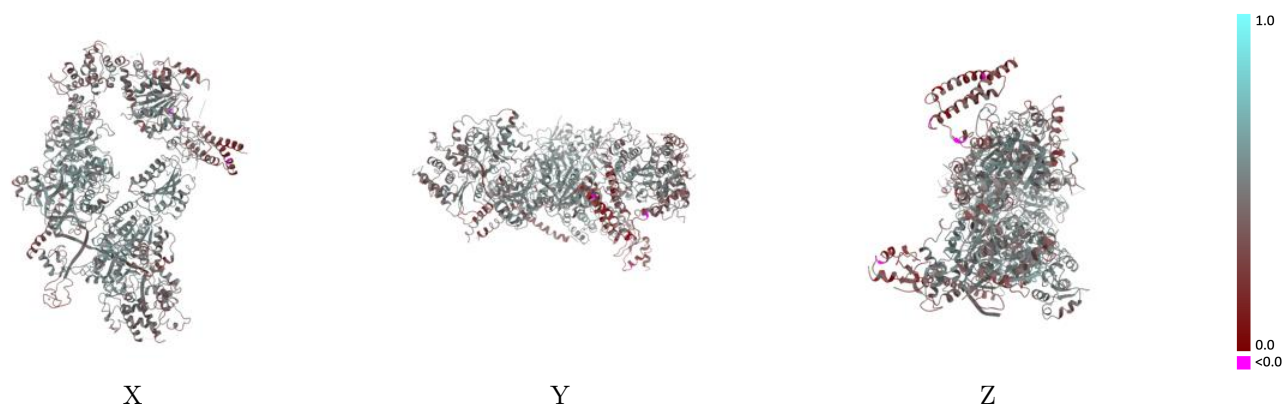
Y



Z

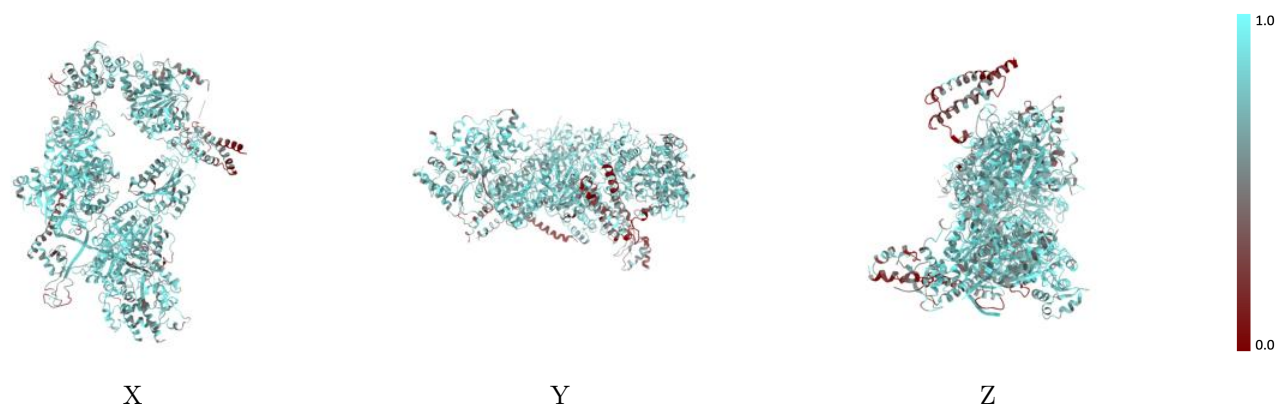
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



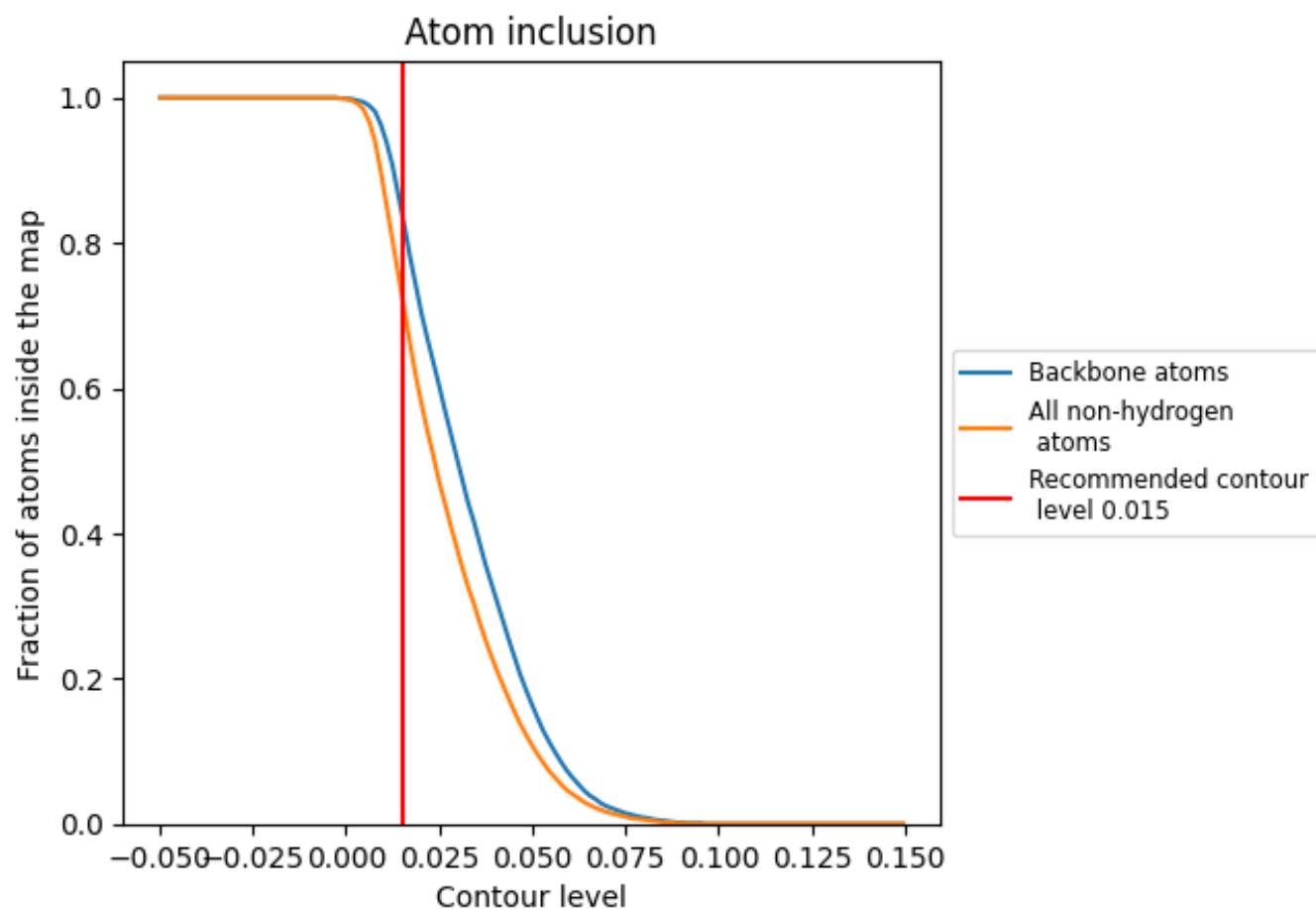
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.4620
A	0.8120	0.5130
B	0.7880	0.4910
C	0.6710	0.4220
D	0.7360	0.4810
E	0.7430	0.4800
F	0.6780	0.4310
G	0.4690	0.3580
I	0.4310	0.2970
J	0.8990	0.4740
K	0.8120	0.4700

1.0

0.0

<0.0