WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Jun 12, 2024 – 02:24 PM EDT

PDB ID	:	8UTS
EMDB ID	:	EMD-42548
Title	:	KIF1A[1-393] APO in complex with a microtubule
Authors	:	Benoit, M.P.M.H.; Rao, L.; Asenjo, A.B.; Gennerich, A.; Sosa, H.
Deposited on	:	2023-10-31
Resolution	:	2.70 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		4.5%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
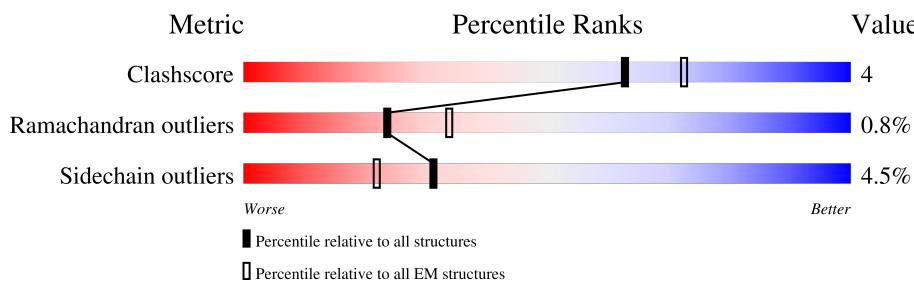
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	K	438	50% / 70% 9% · 19%
2	A	451	17% / 91% 6% ·
3	B	445	16% / 82% 13% · ·
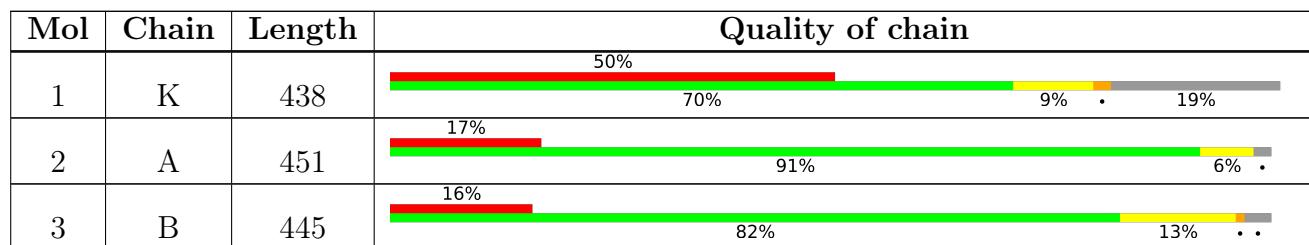
2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 9748 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 Kinesin-like protein KIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	354	2781	1720	493	552	16	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	394	GLY	-	linker	UNP Q12756
K	395	ALA	-	linker	UNP Q12756
K	396	GLY	-	linker	UNP Q12756
K	397	VAL	-	linker	UNP Q12756
K	398	LYS	-	linker	UNP Q12756
K	399	GLN	-	linker	UNP Q12756
K	400	LEU	-	linker	UNP Q12756
K	401	GLU	-	linker	UNP Q12756
K	402	ASP	-	linker	UNP Q12756
K	403	LYS	-	linker	UNP Q12756
K	404	VAL	-	linker	UNP Q12756
K	405	GLU	-	linker	UNP Q12756
K	406	GLU	-	linker	UNP Q12756
K	407	LEU	-	linker	UNP Q12756
K	408	ALA	-	linker	UNP Q12756
K	409	SER	-	linker	UNP Q12756
K	410	LYS	-	linker	UNP Q12756
K	411	ASN	-	linker	UNP Q12756
K	412	TYR	-	linker	UNP Q12756
K	413	HIS	-	linker	UNP Q12756
K	414	LEU	-	linker	UNP Q12756
K	415	GLU	-	linker	UNP Q12756
K	416	ASN	-	linker	UNP Q12756
K	417	GLU	-	linker	UNP Q12756
K	418	VAL	-	linker	UNP Q12756
K	419	ALA	-	linker	UNP Q12756
K	420	ARG	-	linker	UNP Q12756
K	421	LEU	-	linker	UNP Q12756

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	422	LYS	-	linker	UNP Q12756
K	423	LYS	-	linker	UNP Q12756
K	424	LEU	-	linker	UNP Q12756
K	425	VAL	-	linker	UNP Q12756
K	426	GLU	-	expression tag	UNP Q12756
K	427	PHE	-	expression tag	UNP Q12756
K	428	THR	-	expression tag	UNP Q12756
K	429	SER	-	expression tag	UNP Q12756
K	430	ALA	-	expression tag	UNP Q12756
K	431	TRP	-	expression tag	UNP Q12756
K	432	SER	-	expression tag	UNP Q12756
K	433	HIS	-	expression tag	UNP Q12756
K	434	PRO	-	expression tag	UNP Q12756
K	435	GLN	-	expression tag	UNP Q12756
K	436	PHE	-	expression tag	UNP Q12756
K	437	GLU	-	expression tag	UNP Q12756
K	438	LYS	-	expression tag	UNP Q12756

- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	440	3437	2175	584	656	22	0	0

- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	433	3407	2136	583	661	27	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP
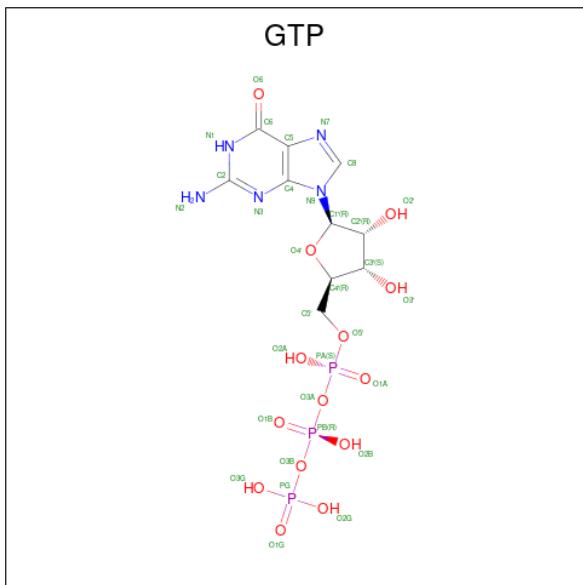
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

GDP
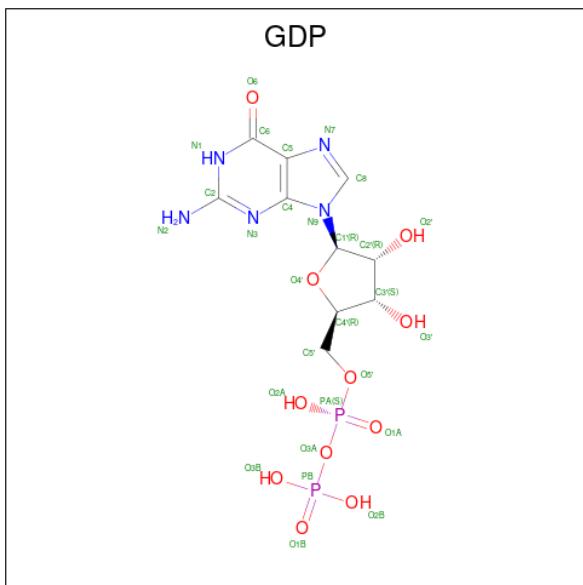
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).
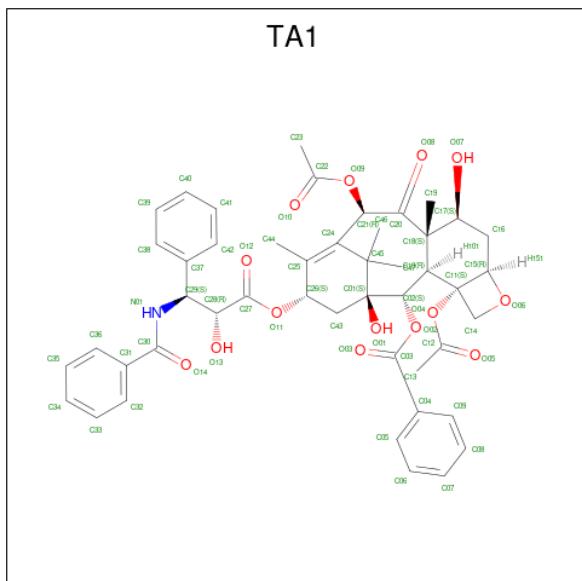
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			62	47	1	14	

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: Kinesin-like protein KIF1A
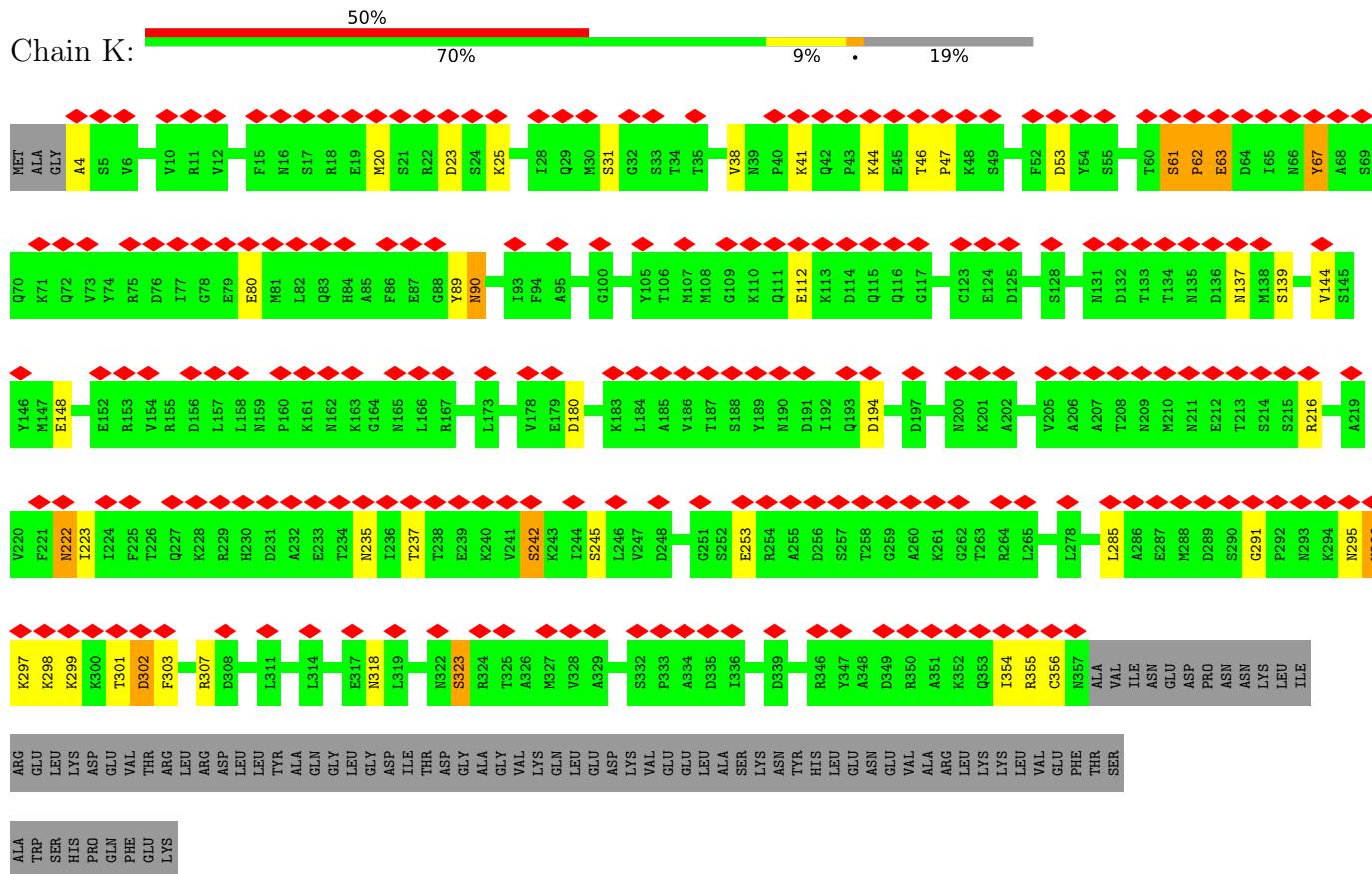
• Molecule 2: Tubulin alpha-1B chain

D327 K336 R339 S340 I341 D345 G365 G366 D367 T381 E386 L391 K394 L397 H406 V409 G410 E411 G412 M413 E414 E423 D424 M425 Y432 E433 E434 V437 D438 S439 V440 GLU GLY GLU GLY GLU GLU GLU GLY GLU GLU TYR

• Molecule 3: Tubulin beta-2B chain

Chain B:

16%

82%   13%

M1 R2 E3 G10 N14 D26 D31 Y36 H37 G38 D39 S40 D41 E45 R46 E53 A54 T55 G56 N57 K58 D67 L68 M73 D74 R77 P80 F81 I84 D88 Q94 E108 E111 D114 D118 R121 K122 E123 S124 E125

D128 G140 T143 G144 S145 T149 I152 S153 E157 E158 D161 M164 S172 P173 K174 D177 V180 N184 E194 D197 D203 L207 Y208 D209 F212 R213 T221 Y222 G223 D224 L225 N226 S230 D249 K252 N256 M267

R276 G277 S278 Q279 R282 A283 L284 L289 T290 Q291 Q292 M293 F294 K297 C303 R306 H307 G308 R309 R320 M321 S322 D327 M330 V342 E343 W344 N348 V349 K350 D355 R359 K362 M363 S364 A365 S371 T372 A373 I374 Q375 E376 R380 K392

G402 M403 D404 E405 M406 T409 N414 D417 E421 Y422 Q423 Q424 Y425 Q426 D427 A428 T429 A430 D431 F432 Q433 GLY GLU PHE GLU GLU GLU GLU GLY GLU ASP GLU ALA

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=168.09°, rise=5.61 Å, axial sym=C1	Depositor
Number of segments used	685161	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 $(e^-/\text{Å}^2)$	62.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.017	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	364.416, 364.416, 364.416	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, TA1, GDP, MG

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	K	0.30	0/2825	0.61	0/3810
2	A	0.28	0/3515	0.56	0/4772
3	B	0.31	0/3482	0.61	0/4716
All	All	0.30	0/9822	0.59	0/13298

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	K	2781	0	2757	34	0
2	A	3437	0	3349	13	0
3	B	3407	0	3280	41	0
4	A	32	0	12	2	0
5	A	1	0	0	0	0
6	B	28	0	12	1	0
7	B	62	0	51	0	0
All	All	9748	0	9461	84	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 (84) 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:B:429:THR:HG23	3:B:430:ALA:H	1.39	0.87
1:K:307:ARG:NE	3:B:417:ASP:OD2	2.22	0.72
1:K:291:GLY:O	1:K:295:ASN:N	2.24	0.70
3:B:431:ASP:O	3:B:432:GLU:HB2	1.91	0.70
1:K:4:ALA:N	1:K:323:SER:O	2.27	0.67
2:A:145:THR:OG1	4:A:501:GTP:O2G	2.07	0.67
3:B:342:VAL:HG13	3:B:344:TRP:CD1	2.30	0.66
1:K:61:SER:HB3	1:K:62:PRO:CD	2.26	0.65
3:B:373:ALA:O	3:B:375:GLN:N	2.29	0.65
2:A:15:GLN:NE2	4:A:501:GTP:O6	2.31	0.64
1:K:89:TYR:O	1:K:242:SER:OG	2.15	0.64
3:B:149:THR:HA	3:B:152:ILE:HD12	1.80	0.63
2:A:76:ASP:OD2	3:B:46:ARG:NH2	2.32	0.63
3:B:180:VAL:O	3:B:184:ASN:ND2	2.31	0.62
3:B:372:THR:OG1	3:B:426:GLN:HG3	2.01	0.60
2:A:367:ASP:N	2:A:367:ASP:OD1	2.35	0.60
1:K:303:PHE:CE1	3:B:421:GLU:HG2	2.37	0.60
1:K:61:SER:HB3	1:K:62:PRO:HD2	1.82	0.59
1:K:295:ASN:O	1:K:296:LYS:HB3	2.01	0.59
3:B:423:GLN:O	3:B:424:GLN:C	2.41	0.59
1:K:23:ASP:OD1	1:K:25:LYS:NZ	2.29	0.58
1:K:38:VAL:HG12	1:K:47:PRO:HG3	1.85	0.57
1:K:38:VAL:HG12	1:K:47:PRO:HB3	1.85	0.57
1:K:307:ARG:NH1	3:B:414:ASN:OD1	2.37	0.57
3:B:372:THR:CB	3:B:426:GLN:HG3	2.36	0.56
3:B:392:LYS:NZ	3:B:405:GLU:OE1	2.30	0.55
1:K:62:PRO:HA	1:K:67:TYR:CD1	2.42	0.54
1:K:297:LYS:O	1:K:299:LYS:HG2	2.08	0.54
2:A:1:MET:N	2:A:3:GLU:OE2	2.41	0.53
3:B:226:ASN:O	3:B:230:SER:OG	2.18	0.53
3:B:373:ALA:C	3:B:375:GLN:N	2.62	0.53
3:B:207:LEU:HB3	3:B:225:LEU:HD22	1.91	0.52
1:K:38:VAL:HG12	1:K:47:PRO:CB	2.40	0.52
3:B:67:ASP:OD1	3:B:68:LEU:N	2.43	0.52
3:B:121:ARG:NH1	3:B:158:GLU:OE2	2.44	0.51
3:B:429:THR:O	3:B:430:ALA:HB3	2.09	0.51
1:K:62:PRO:O	1:K:63:GLU:C	2.49	0.50
3:B:207:LEU:HD13	3:B:225:LEU:HB3	1.94	0.50
3:B:309:ARG:NE	3:B:428:ALA:HB2	2.27	0.50
1:K:61:SER:C	1:K:63:GLU:H	2.14	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:429:THR:HG23	3:B:430:ALA:N	2.17	0.50
3:B:145:SER:O	3:B:149:THR:HG23	2.12	0.49
3:B:372:THR:HG21	3:B:426:GLN:HG3	1.93	0.49
2:A:151:SER:HA	2:A:193:THR:HG21	1.94	0.49
2:A:223:THR:OG1	2:A:224:TYR:N	2.46	0.49
1:K:302:ASP:OD2	1:K:302:ASP:N	2.47	0.48
3:B:143:THR:N	6:B:501:GDP:O1B	2.47	0.47
3:B:252:LYS:O	3:B:256:ASN:ND2	2.47	0.47
1:K:112:GLU:N	1:K:112:GLU:OE1	2.48	0.47
3:B:371:SER:OG	3:B:372:THR:N	2.47	0.47
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.96	0.47
3:B:427:ASP:O	3:B:428:ALA:HB3	2.14	0.47
2:A:406:HIS:HA	2:A:409:VAL:HG22	1.96	0.47
1:K:38:VAL:HG12	1:K:47:PRO:CG	2.45	0.46
1:K:295:ASN:O	1:K:296:LYS:CB	2.63	0.46
3:B:373:ALA:C	3:B:375:GLN:H	2.17	0.46
1:K:297:LYS:C	1:K:299:LYS:N	2.69	0.46
2:A:76:ASP:OD1	2:A:79:ARG:NH1	2.49	0.46
3:B:431:ASP:O	3:B:432:GLU:CB	2.64	0.45
1:K:216:ARG:NH1	1:K:253:GLU:OE2	2.50	0.45
3:B:161:ASP:OD1	3:B:161:ASP:N	2.47	0.45
1:K:237:THR:OG1	1:K:237:THR:O	2.31	0.44
1:K:90:ASN:OD1	1:K:90:ASN:N	2.51	0.44
3:B:308:GLY:HA2	3:B:426:GLN:NE2	2.33	0.43
2:A:60:LYS:HG2	2:A:61:HIS:N	2.32	0.43
1:K:297:LYS:HG2	1:K:299:LYS:H	1.84	0.43
3:B:348:ASN:N	3:B:348:ASN:OD1	2.50	0.43
1:K:297:LYS:C	1:K:299:LYS:H	2.21	0.42
3:B:221:THR:OG1	3:B:222:TYR:N	2.52	0.42
1:K:144:VAL:HG12	1:K:223:ILE:HG12	2.02	0.42
1:K:222:ASN:N	1:K:222:ASN:OD1	2.52	0.42
3:B:10:GLY:O	3:B:14:ASN:ND2	2.48	0.42
1:K:62:PRO:HA	1:K:67:TYR:CE1	2.54	0.42
1:K:245:SER:OG	1:K:318:ASN:ND2	2.53	0.41
3:B:289:LEU:HD11	3:B:363:MET:HG3	2.03	0.41
1:K:23:ASP:CG	1:K:25:LYS:HZ1	2.19	0.41
3:B:406:MET:O	3:B:409:THR:OG1	2.30	0.41
2:A:273:ALA:HB2	2:A:295:CYS:SG	2.60	0.41
3:B:81:PHE:O	3:B:84:ILE:HG22	2.20	0.41
1:K:63:GLU:O	1:K:67:TYR:HB3	2.21	0.41
1:K:318:ASN:OD1	1:K:318:ASN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:263:PRO:O	2:A:266:HIS:ND1	2.47	0.41
3:B:372:THR:CG2	3:B:426:GLN:HG3	2.50	0.41
3:B:364:SER:OG	3:B:365:ALA:N	2.54	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	K	352/438 (80%)	317 (90%)	30 (8%)	5 (1%)	11	28
2	A	438/451 (97%)	422 (96%)	16 (4%)	0	100	100
3	B	431/445 (97%)	406 (94%)	20 (5%)	5 (1%)	13	32
All	All	1221/1334 (92%)	1145 (94%)	66 (5%)	10 (1%)	24	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	429	THR
3	B	432	GLU
3	B	374	ILE
3	B	428	ALA
3	B	430	ALA
1	K	46	THR
1	K	63	GLU
1	K	296	LYS
1	K	62	PRO
1	K	61	SER

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	K	311/383 (81%)	287 (92%)	24 (8%)	13	30
2	A	371/379 (98%)	362 (98%)	9 (2%)	49	77
3	B	374/383 (98%)	359 (96%)	15 (4%)	31	60
All	All	1056/1145 (92%)	1008 (96%)	48 (4%)	31	55

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	20	MET
1	K	31	SER
1	K	41	LYS
1	K	44	LYS
1	K	53	ASP
1	K	67	TYR
1	K	80	GLU
1	K	90	ASN
1	K	137	ASN
1	K	139	SER
1	K	148	GLU
1	K	180	ASP
1	K	194	ASP
1	K	222	ASN
1	K	235	ASN
1	K	242	SER
1	K	285	LEU
1	K	298	LYS
1	K	301	THR
1	K	302	ASP
1	K	323	SER
1	K	354	ILE
1	K	355	ARG
1	K	356	CYS
2	A	84	ARG
2	A	108	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	112	LYS
2	A	178	SER
2	A	196	GLU
2	A	345	ASP
2	A	381	THR
2	A	425	MET
2	A	432	TYR
3	B	2	ARG
3	B	31	ASP
3	B	36	TYR
3	B	73	MET
3	B	125	GLU
3	B	153	SER
3	B	164	MET
3	B	172	SER
3	B	197	ASP
3	B	209	ASP
3	B	322	SER
3	B	342	VAL
3	B	344	TRP
3	B	425	TYR
3	B	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	85	GLN
3	B	375	GLN
3	B	426	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
7	TA1	B	502	-	68,68,68	0.63	0	105,105,105	1.59	18 (17%)
6	GDP	B	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
4	GTP	A	501	5	26,34,34	1.13	2 (7%)	32,54,54	1.68	7 (21%)

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
7	TA1	B	502	-	-	7/41/127/127	0/7/7/7
6	GDP	B	501	-	-	5/12/32/32	0/3/3/3
4	GTP	A	501	5	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	C5-C6	-4.06	1.39	1.47
6	B	501	GDP	C6-N1	-2.64	1.33	1.37
4	A	501	GTP	C2-N3	2.19	1.38	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	502	TA1	O04-C11-C14	5.12	119.27	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	502	TA1	O08-C20-C21	-4.68	113.20	119.30
7	B	502	TA1	C21-C24-C25	-4.54	114.03	120.40
7	B	502	TA1	O04-C11-C10	-4.50	102.05	109.24
7	B	502	TA1	C10-C18-C20	-4.25	109.00	116.31
4	A	501	GTP	PA-O3A-PB	-4.18	118.47	132.83
6	B	501	GDP	PA-O3A-PB	-3.90	119.45	132.83
4	A	501	GTP	PB-O3B-PG	-3.81	119.74	132.83
7	B	502	TA1	C18-C20-C21	3.52	129.48	121.44
7	B	502	TA1	C11-O04-C12	3.50	128.13	119.06
4	A	501	GTP	C5-C6-N1	3.28	119.75	113.95
6	B	501	GDP	C3'-C2'-C1'	3.17	105.75	100.98
4	A	501	GTP	C8-N7-C5	3.08	108.86	102.99
4	A	501	GTP	C3'-C2'-C1'	3.07	105.60	100.98
4	A	501	GTP	C2-N1-C6	-2.97	119.63	125.10
7	B	502	TA1	C47-C45-C46	-2.90	97.71	106.26
7	B	502	TA1	C02-O02-C03	2.85	123.19	117.79
7	B	502	TA1	C45-C01-C02	2.57	114.72	111.91
6	B	501	GDP	C8-N7-C5	2.51	107.77	102.99
7	B	502	TA1	C45-C24-C21	2.50	127.18	118.78
6	B	501	GDP	C5-C6-N1	2.44	118.26	113.95
7	B	502	TA1	O09-C21-C20	2.41	114.92	108.69
7	B	502	TA1	C47-C45-C24	2.39	122.55	112.83
7	B	502	TA1	C01-C45-C24	-2.38	102.88	105.22
7	B	502	TA1	C11-C10-C02	2.29	116.14	111.66
7	B	502	TA1	C37-C29-N01	2.17	116.37	112.11
7	B	502	TA1	C16-C15-C11	2.15	122.63	119.61
7	B	502	TA1	C10-C18-C17	2.13	110.69	106.54
4	A	501	GTP	O6-C6-C5	-2.12	120.24	124.37

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	GDP	PA-O3A-PB-O3B
6	B	501	GDP	C5'-O5'-PA-O2A
7	B	502	TA1	C14-C11-O04-C12
7	B	502	TA1	O05-C12-O04-C11
7	B	502	TA1	C13-C12-O04-C11
7	B	502	TA1	O10-C22-O09-C21
7	B	502	TA1	C23-C22-O09-C21
6	B	501	GDP	C5'-O5'-PA-O3A
4	A	501	GTP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	502	TA1	C15-C11-O04-C12
6	B	501	GDP	C5'-O5'-PA-O1A
7	B	502	TA1	C28-C29-N01-C30
6	B	501	GDP	PA-O3A-PB-O1B
4	A	501	GTP	PA-O3A-PB-O2B
4	A	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GDP	1	0
4	A	501	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TA1 B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 501

Bond lengths

Bond angles

Torsions

Rings
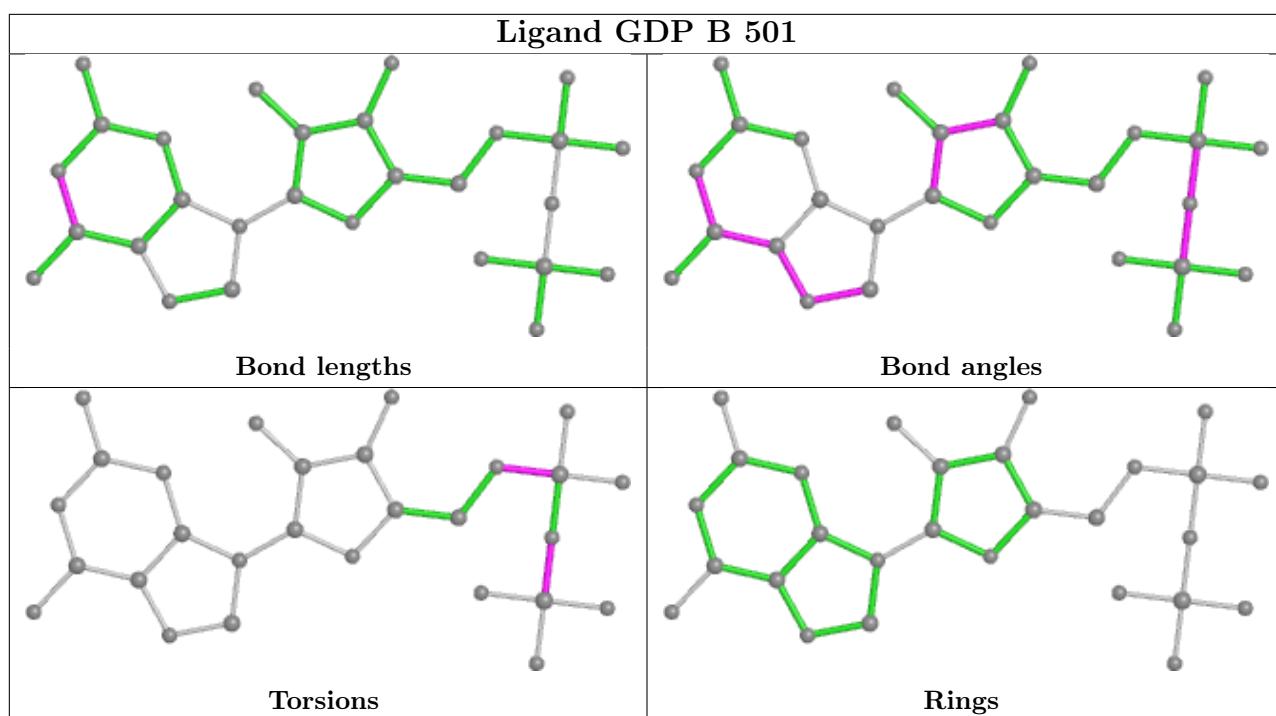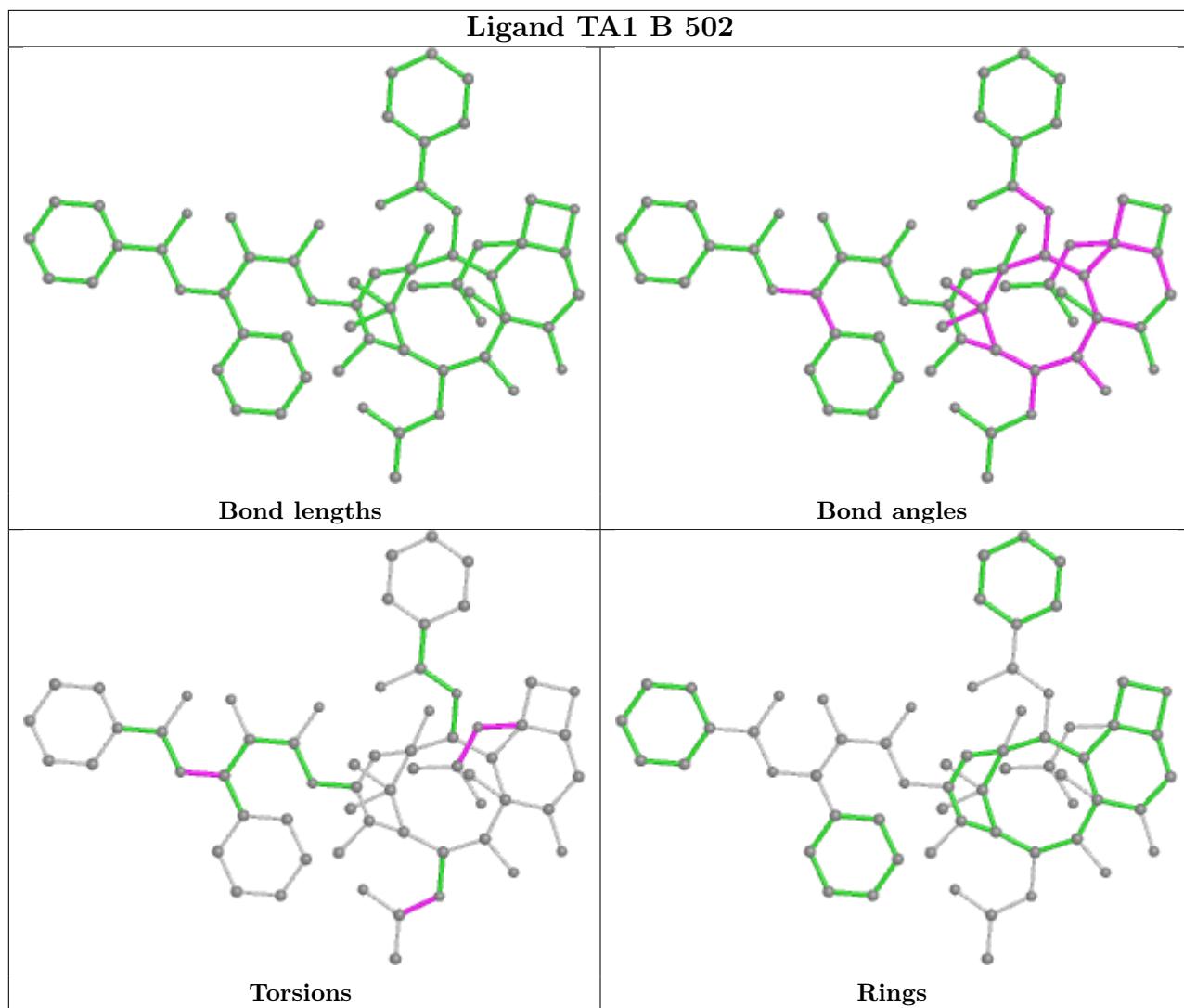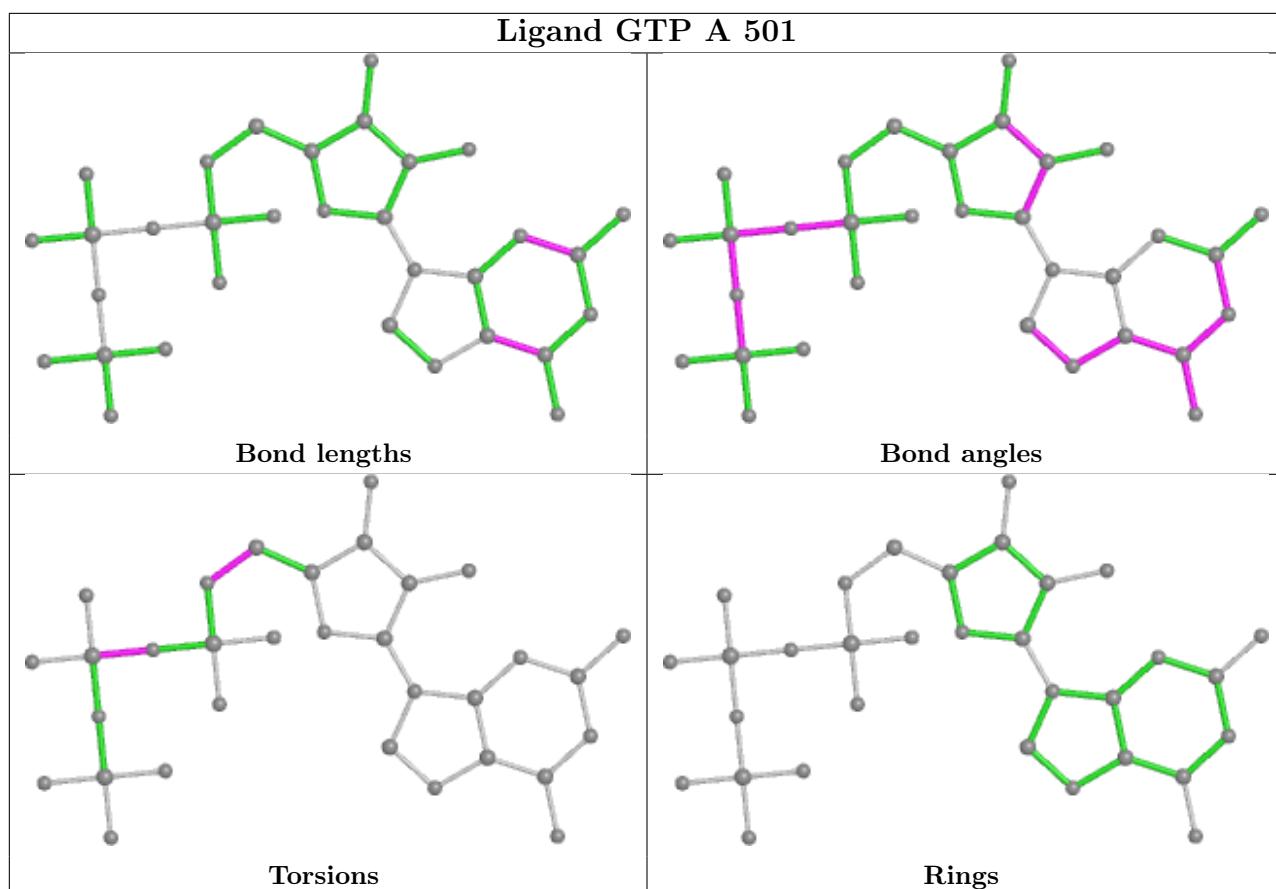
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-42548. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ
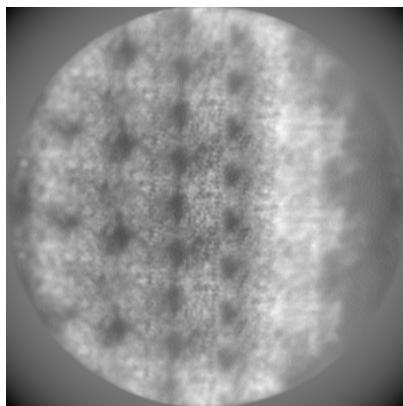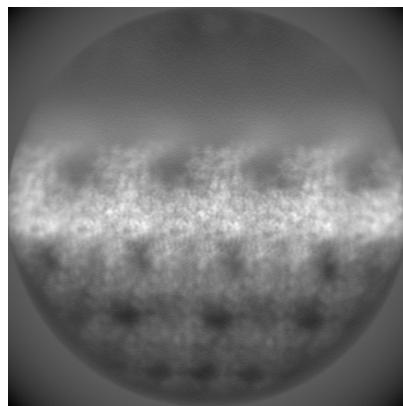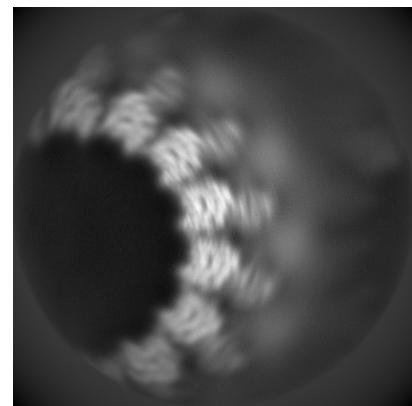
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

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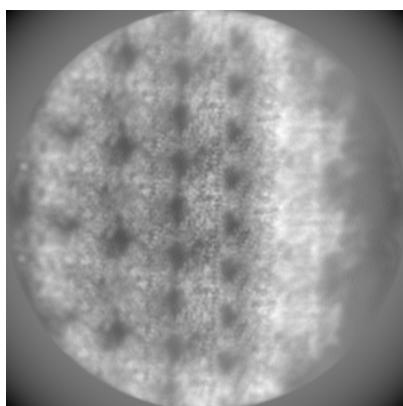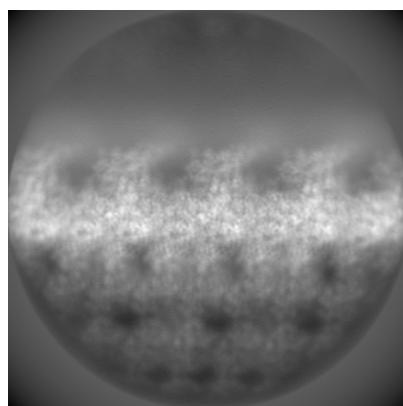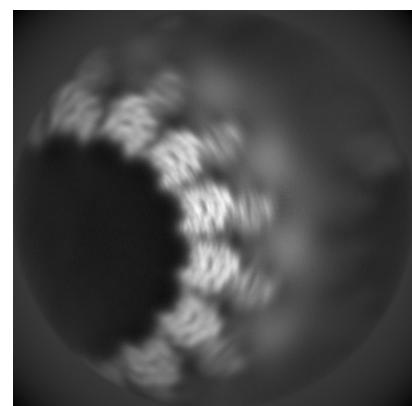
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
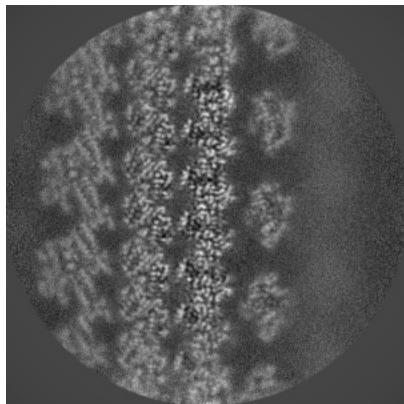
6.2.1   Primary map
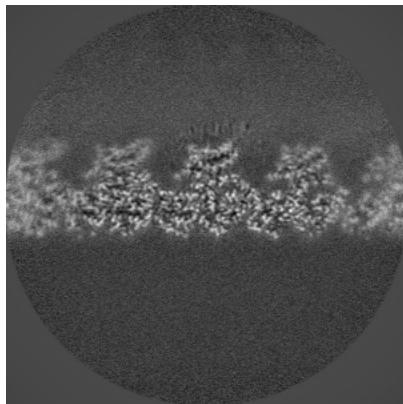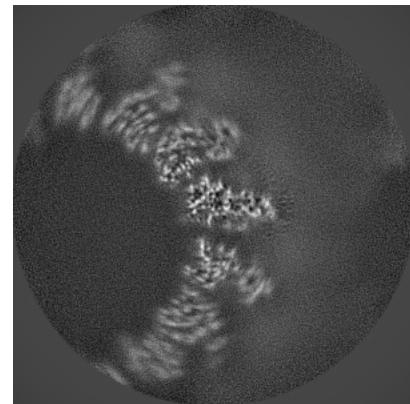
X Index: 208	Y Index: 208	Z Index: 208

6.2.2   Raw map
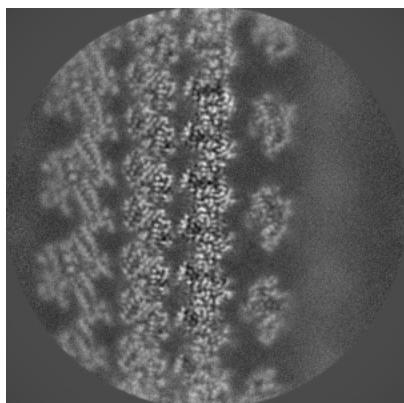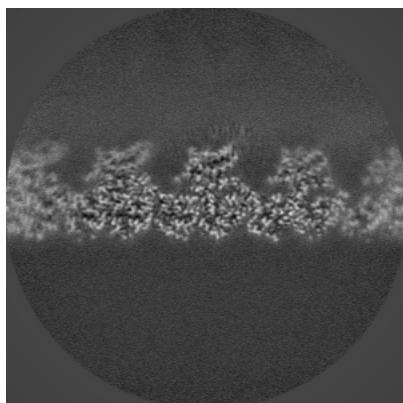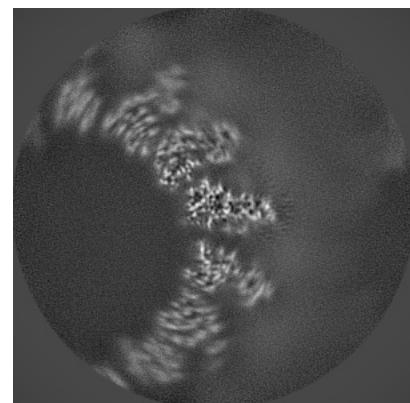
X Index: 208	Y Index: 208	Z Index: 208

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

6.3 Largest variance slices (i)

6.3.1 Primary map
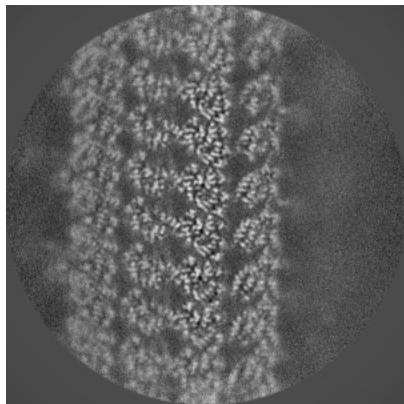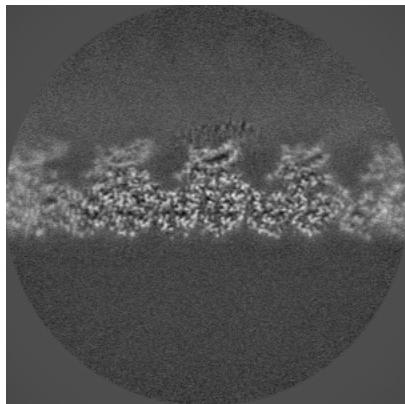
| X Index: 189 | Y Index: 210 | Z Index: 225 |
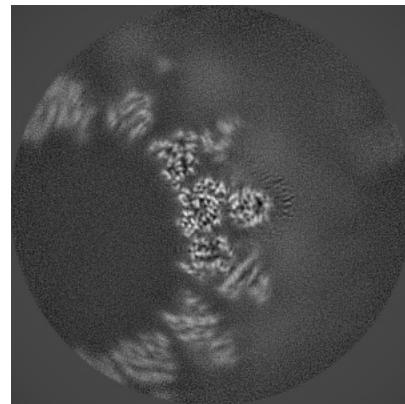
6.3.2 Raw map
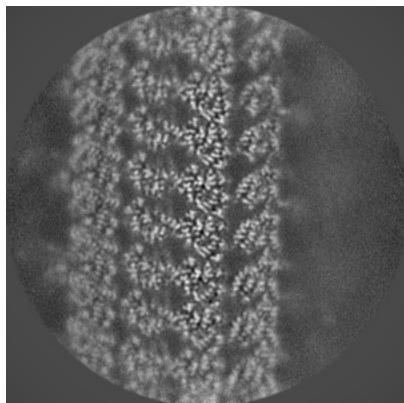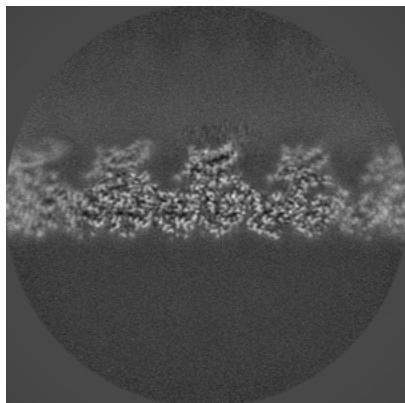
| X Index: 189 | Y Index: 209 | Z Index: 225 |
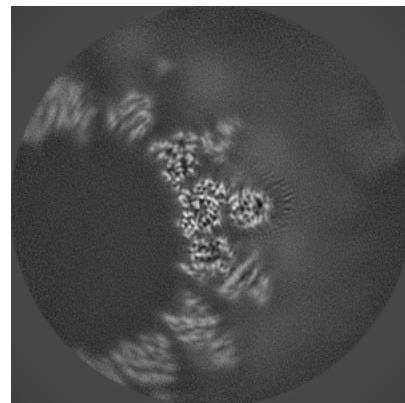
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
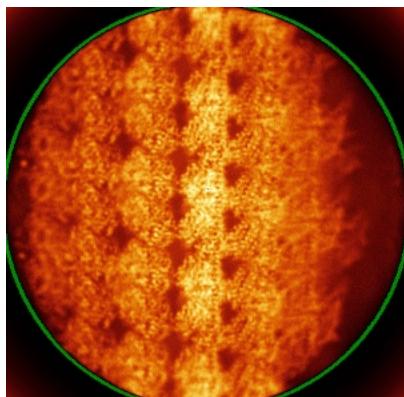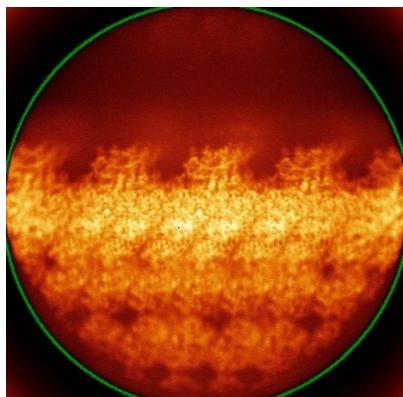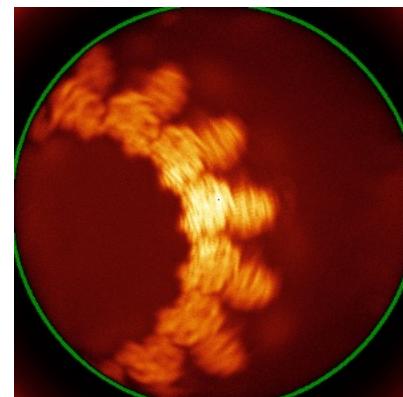
X
Y
Z

6.4.2 Raw map

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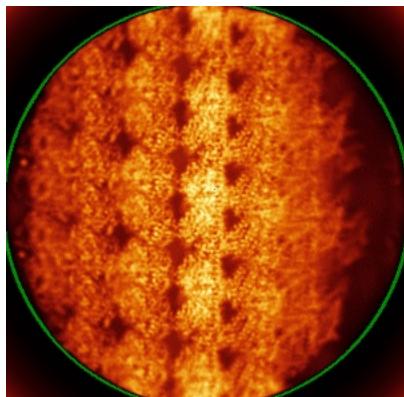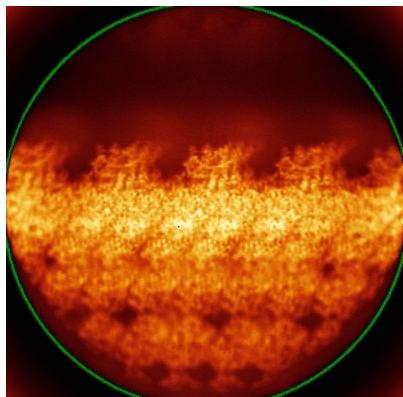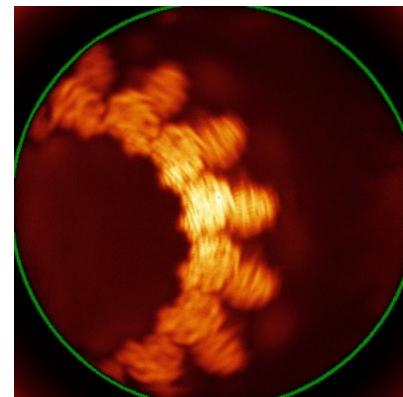
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
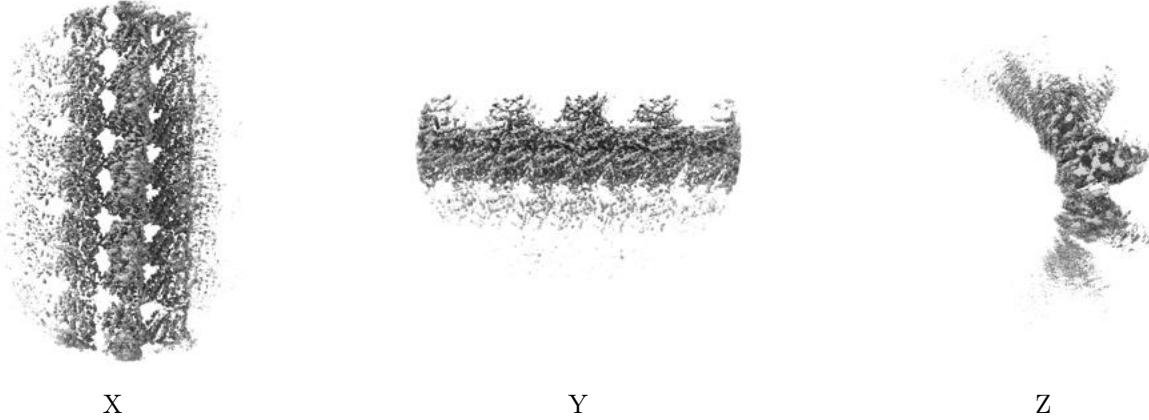
The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X   Y   Z
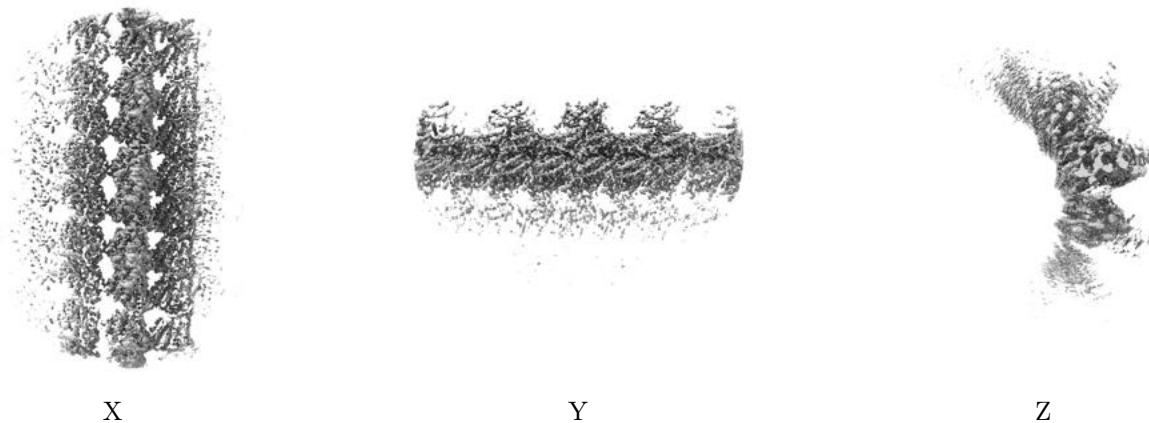
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 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_42548_msk_1.map (i)
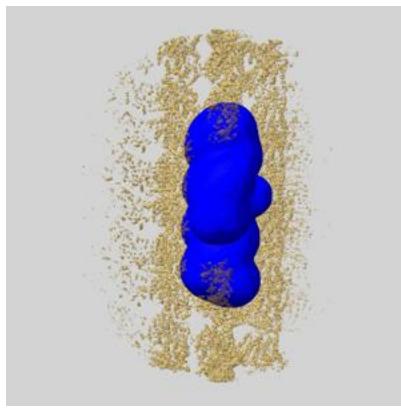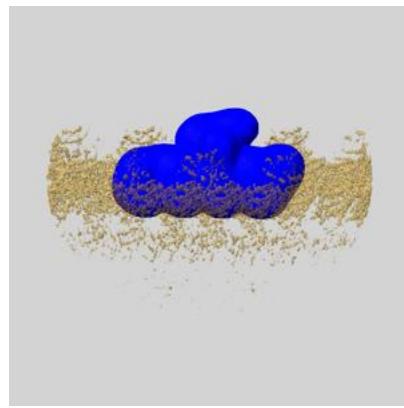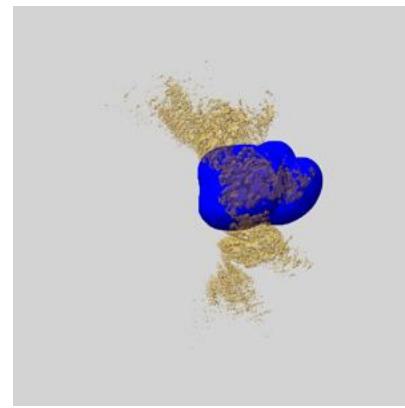
X   Y   Z

6.6.2 emd_42548_msk_2.map (i)
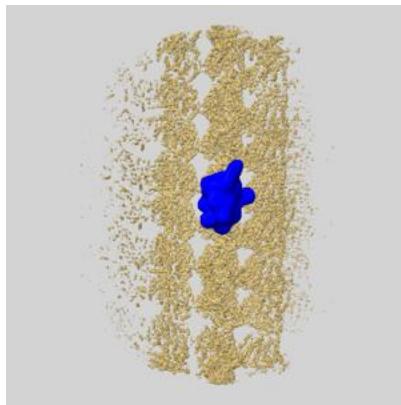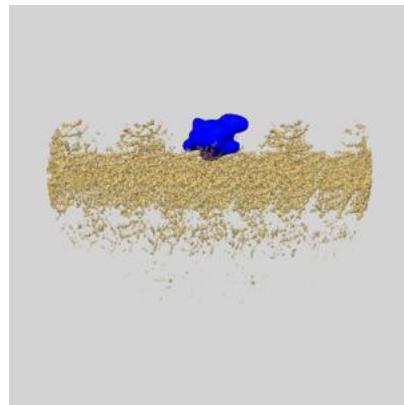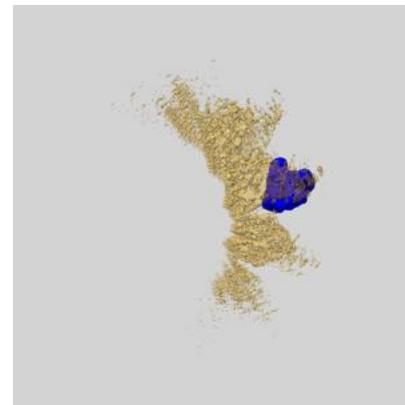
X   Y   Z

6.6.3 emd_42548_msk_3.map ⓘ

| X | Y | Z |
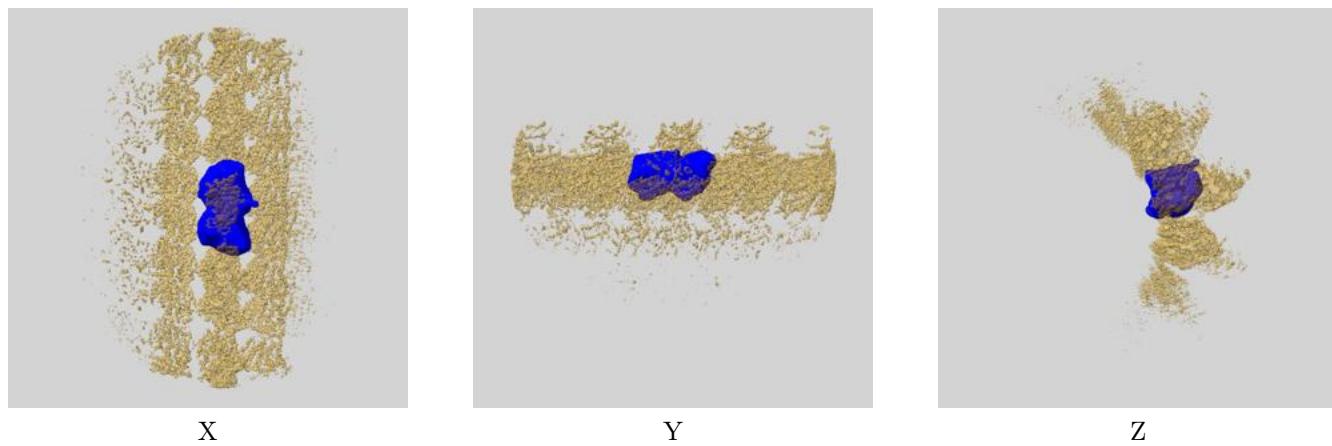
6.6.4 emd_42548_msk_4.map ⓘ

| X | Y | Z |
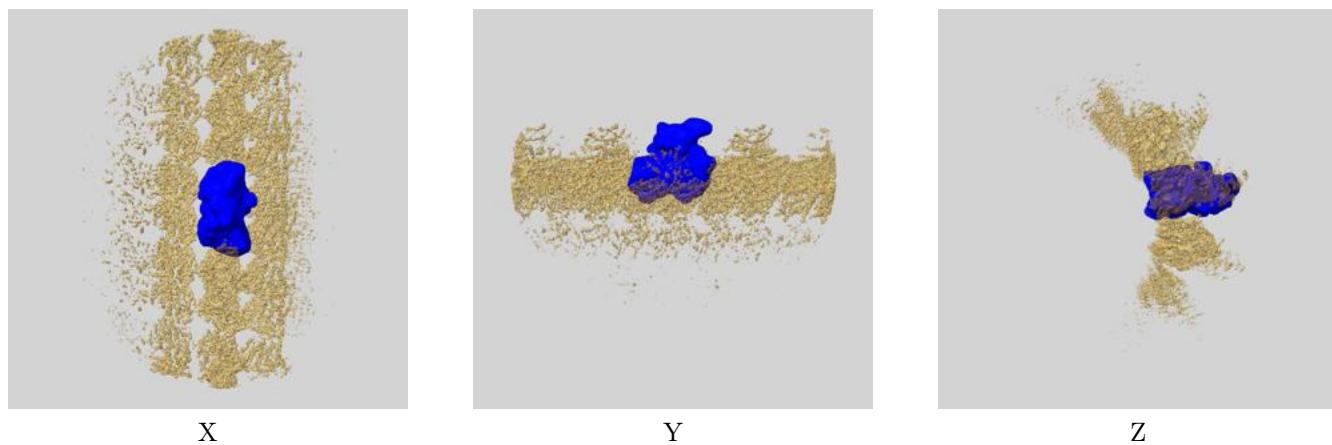
7 Map analysis ⓘ

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

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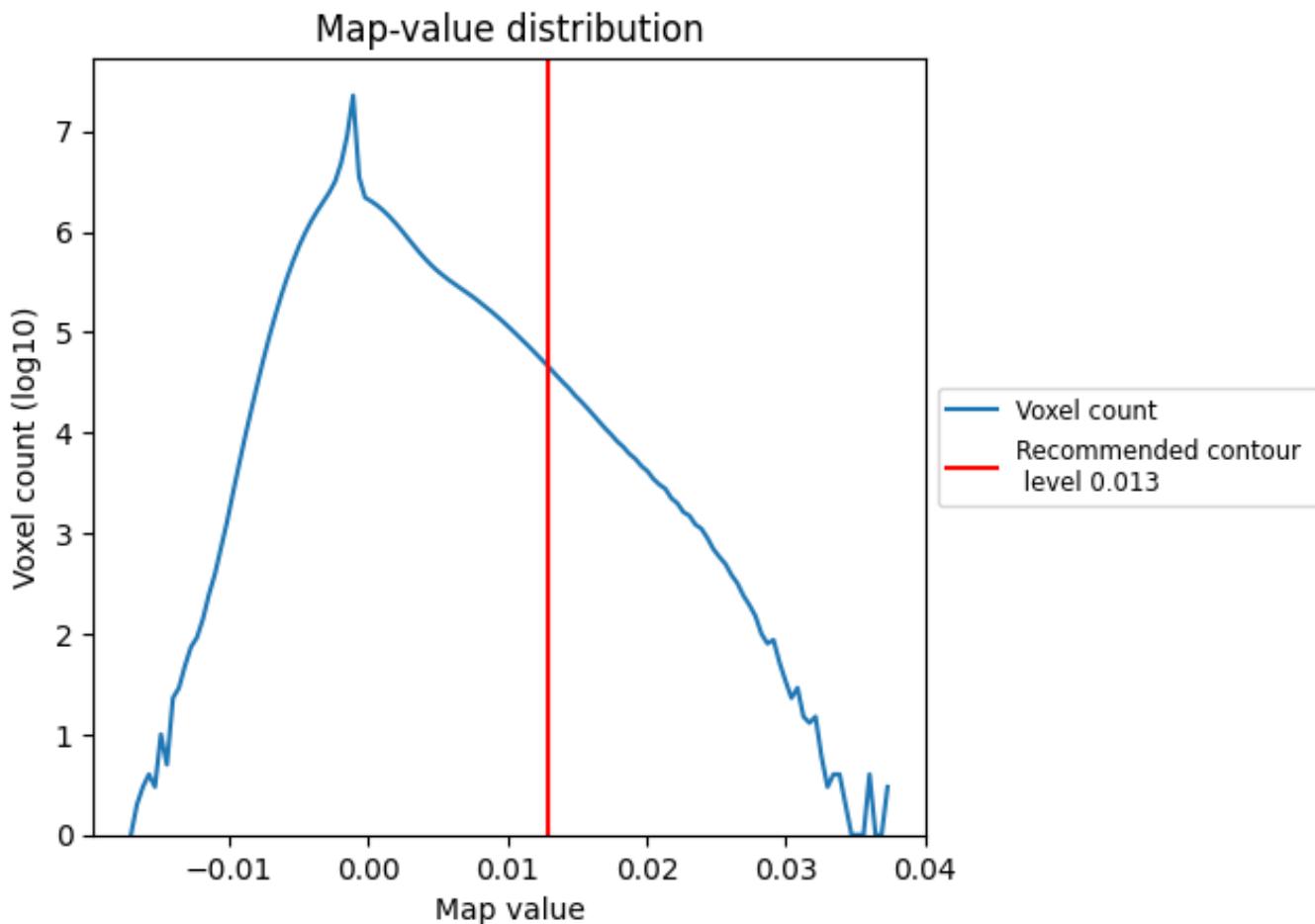
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate　(i)
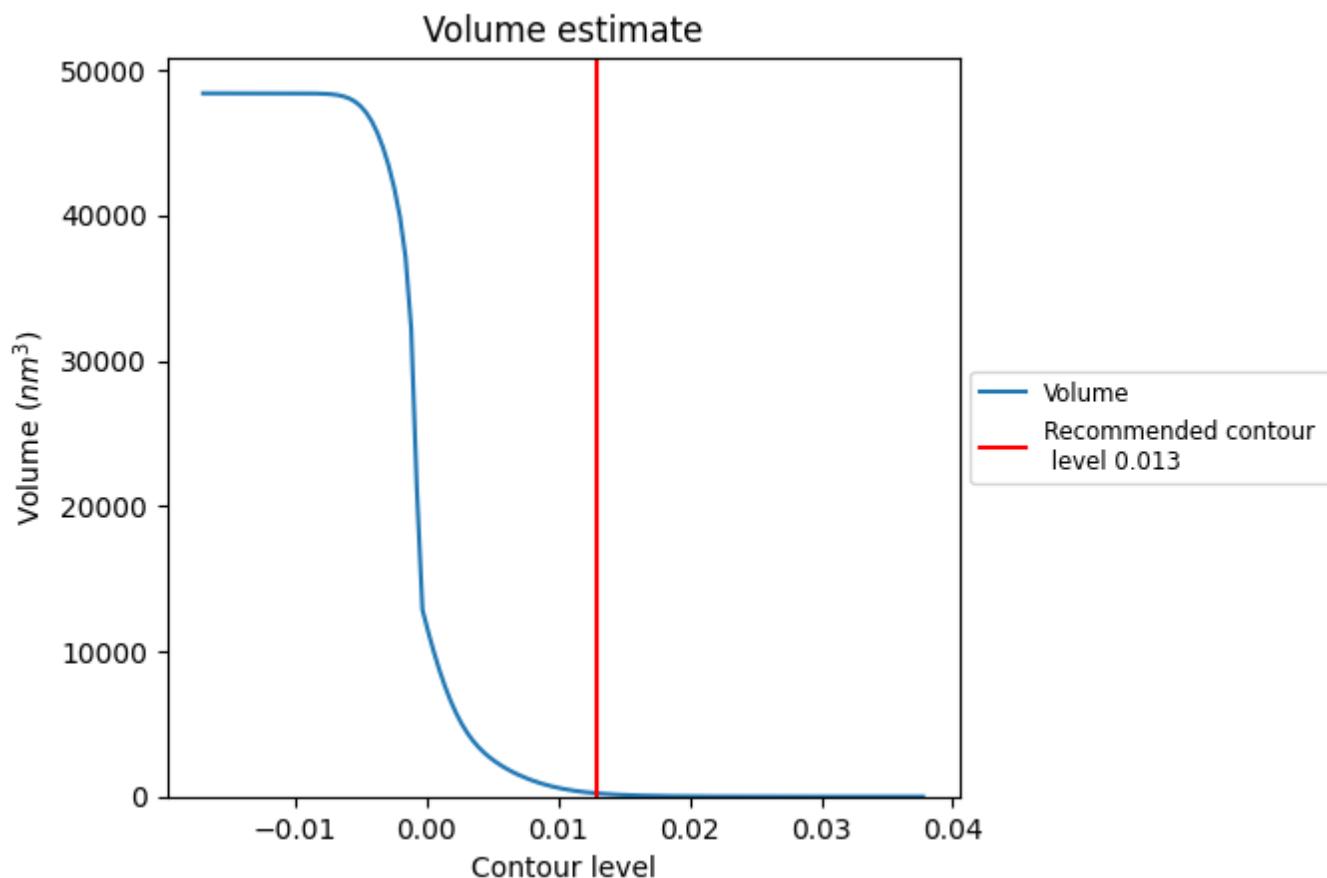
The volume at the recommended contour level is 219 nm^3; this corresponds to an approximate mass of 198 kDa.

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)
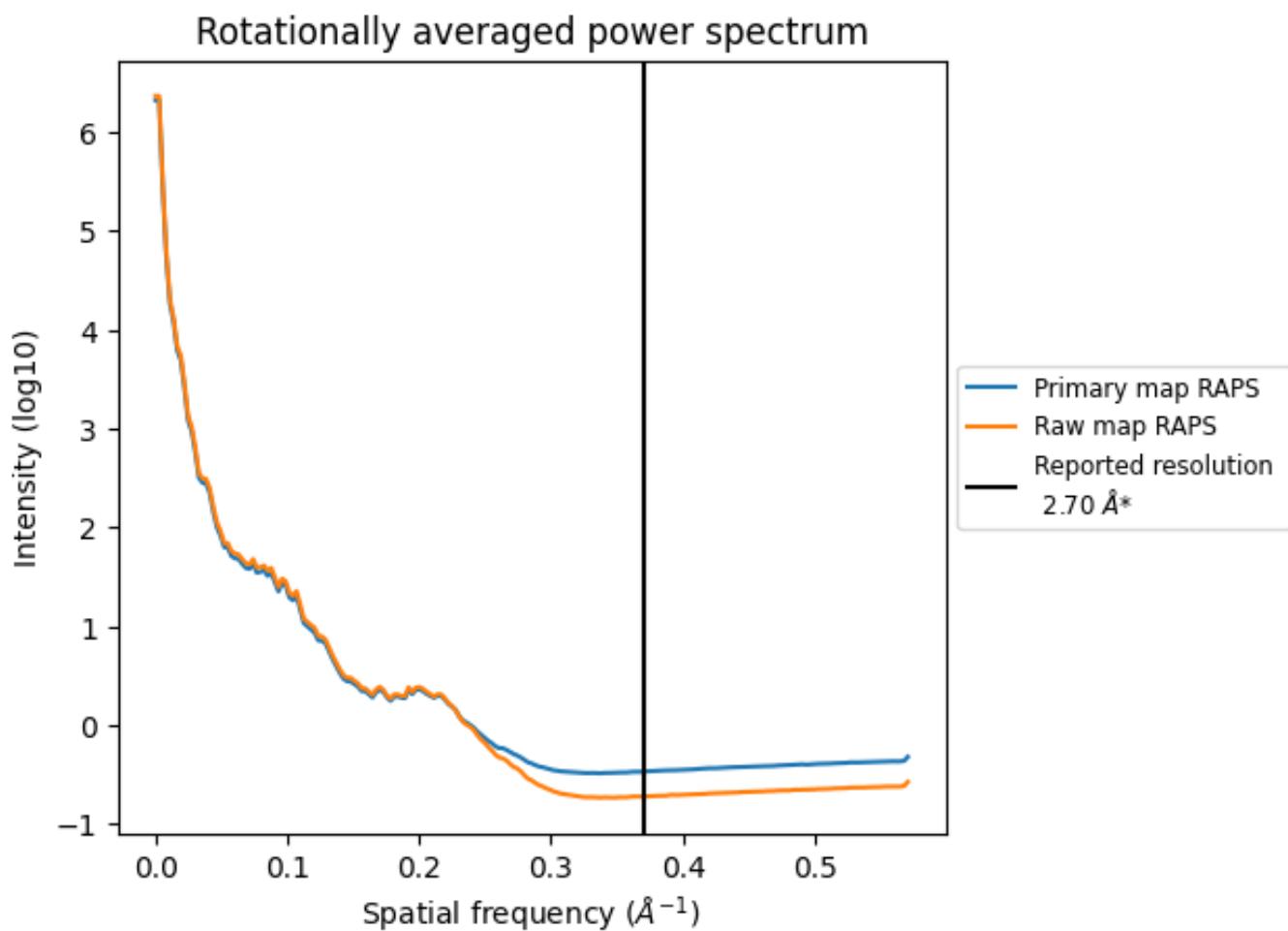
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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)
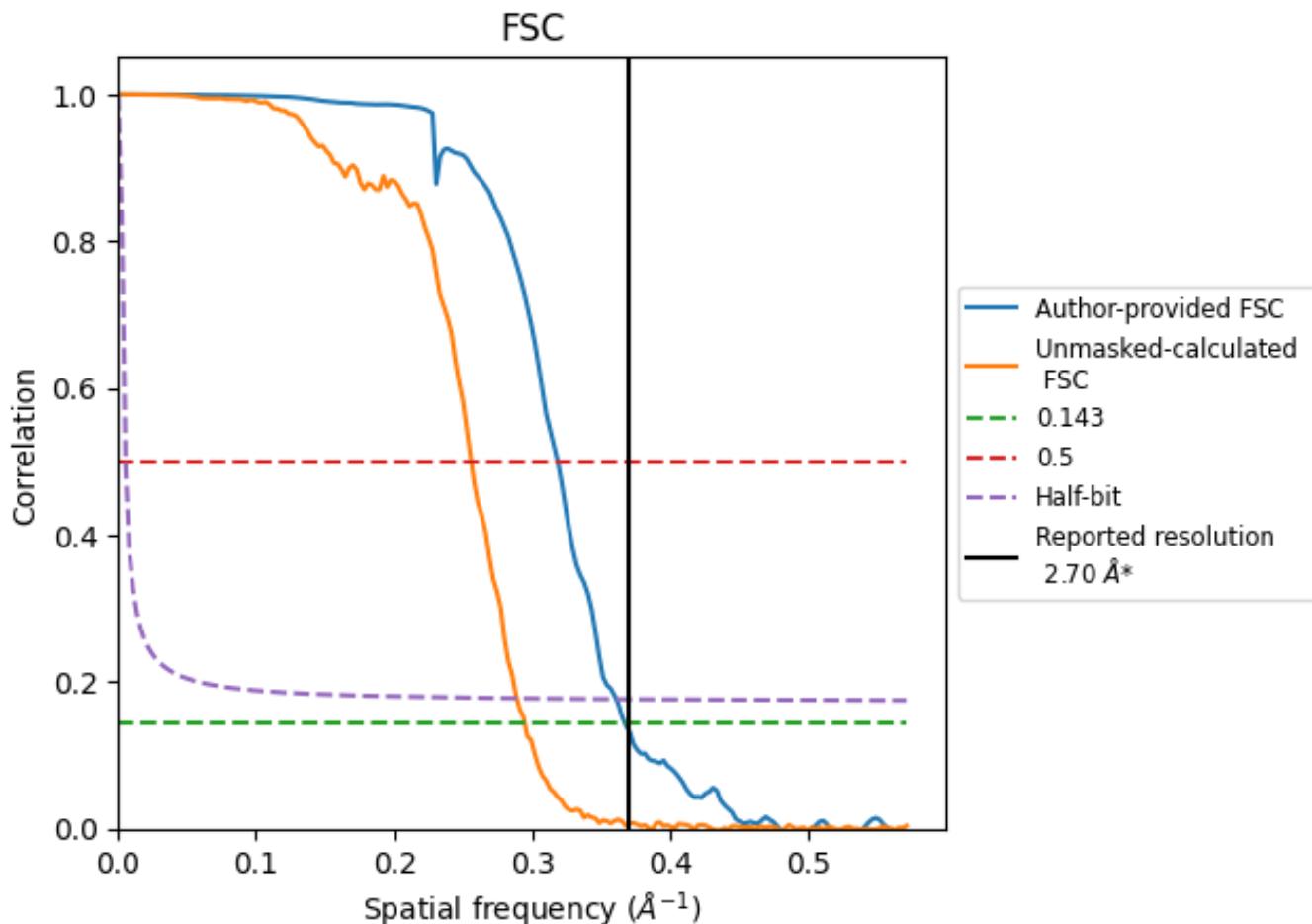
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.14	2.77
Unmasked-calculated*	3.40	3.91	3.46

*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 3.40 differs from the reported value 2.7 by more than 10 %

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-42548 and PDB model 8UTS. Per-residue inclusion information can be found in section 3 on page 7.

9.1　Map-model overlay ⓘ

| X | Y | Z |
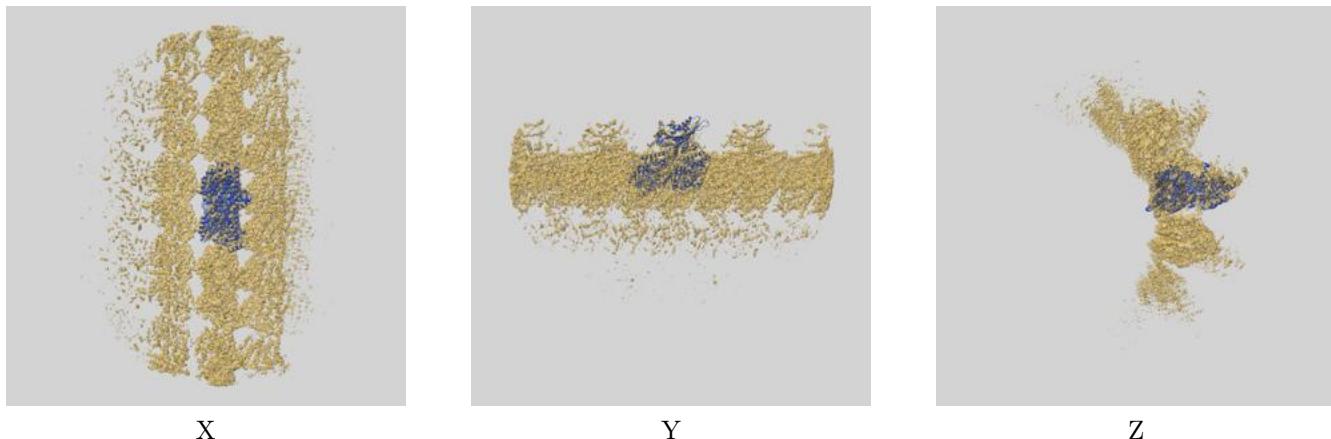
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

9.2 Q-score mapped to coordinate model ⓘ
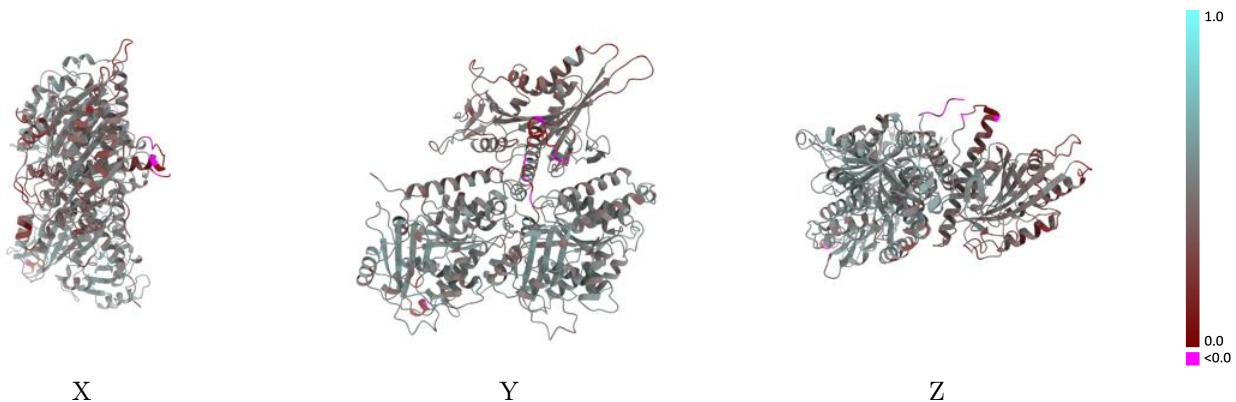
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
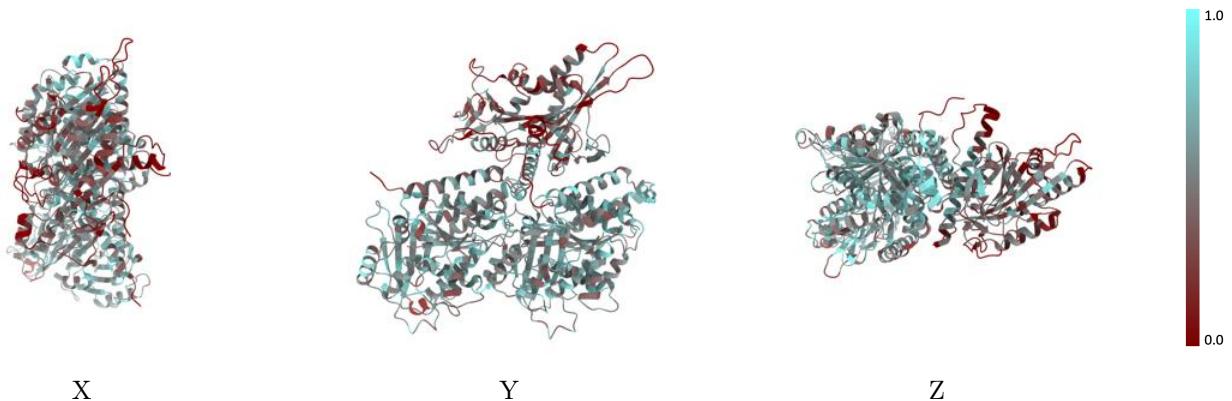
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4   Atom inclusion   ⓘ
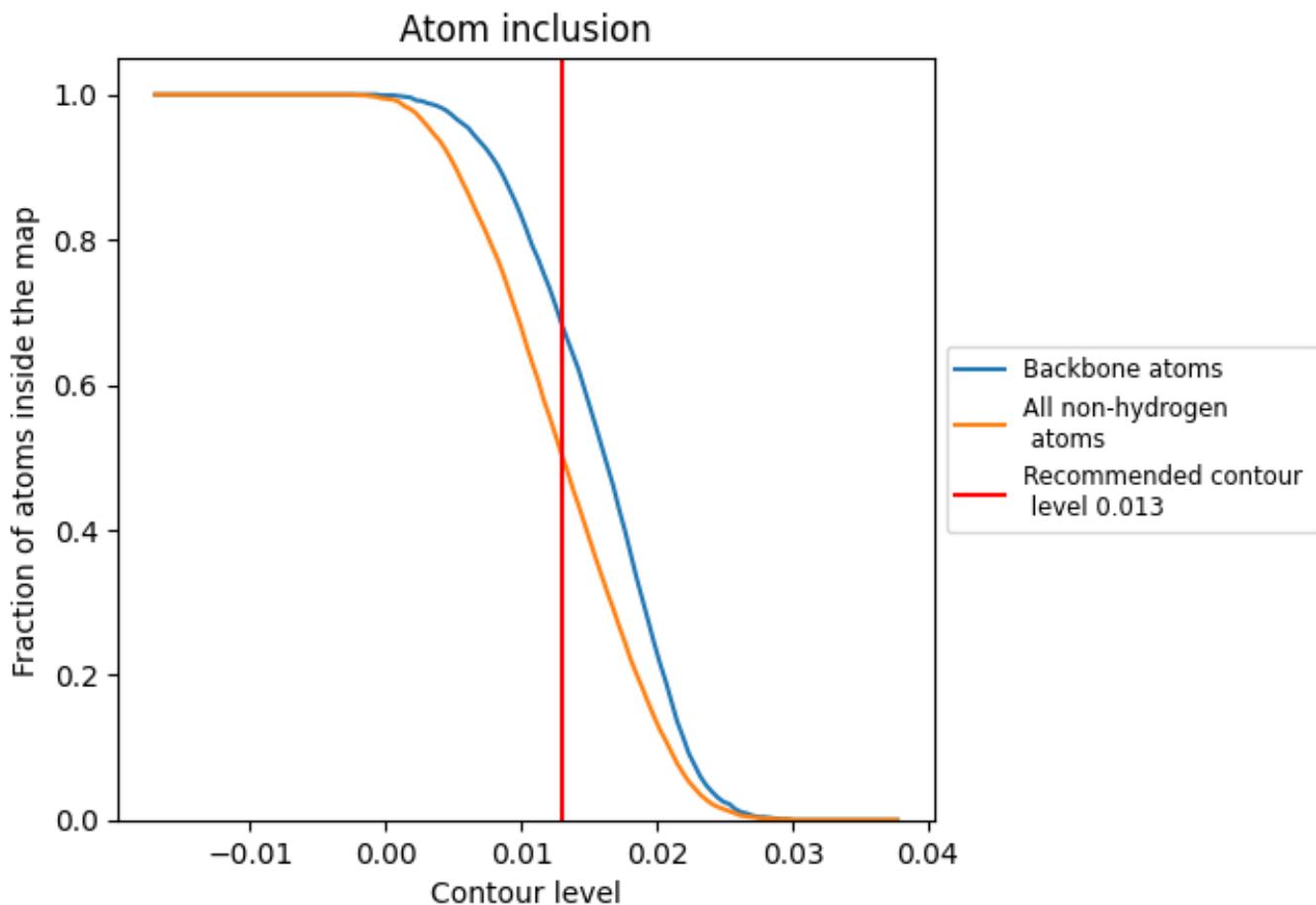
At the recommended contour level, 68% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.5020	▬ 0.4640
A	▬ 0.5610	▬ 0.4910
B	▬ 0.5760	▬ 0.5000
K	▬ 0.3340	▬ 0.3860

1.0

0.0

<0.0