



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 09:58 PM UTC

PDB ID : 8RHH / pdb_00008rhh
EMDB ID : EMD-19176
Title : Microtubule-associated kinesin-1 tail complex bound to AMPPNP, two-headed state
Authors : Atherton, J.; Chegkazi, M.S.; Steiner, R.A.
Deposited on : 2023-12-15
Resolution : 3.00 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:

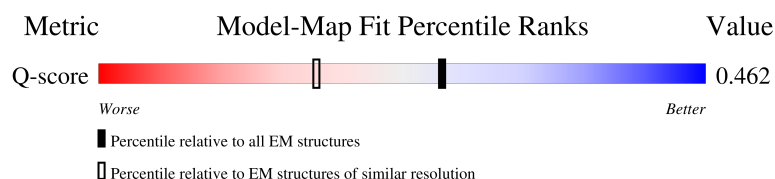
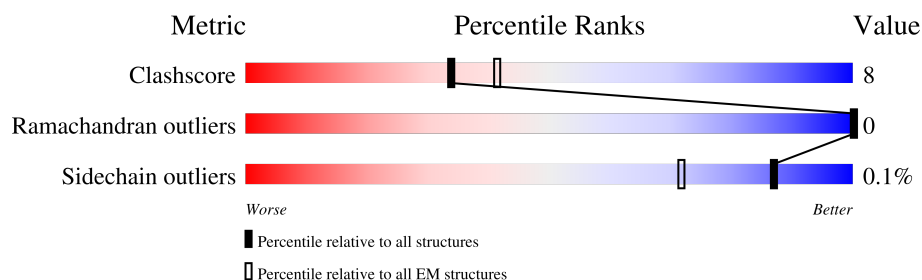
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

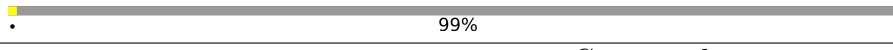
The reported resolution of this entry is 3.00 Å.

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	14081 (2.50 - 3.50)

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	B	445	
2	K	963	
2	L	963	
2	T	963	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	t	963	 99%
3	A	451	 77% 18% 5%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12261 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 Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	426	Total	C	N	O	S	0	0
			3351	2106	575	644	26		

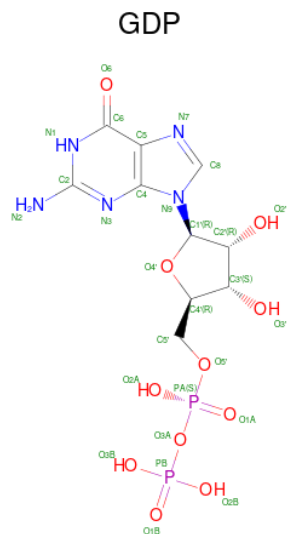
- Molecule 2 is a protein called Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	344	Total	C	N	O	S	0	0
			2710	1691	464	539	16		
2	L	317	Total	C	N	O	S	0	0
			2517	1577	430	495	15		
2	T	9	Total	C	N	O		9	0
			69	45	14	10			
2	t	9	Total	C	N	O		9	0
			69	45	14	10			

- Molecule 3 is a protein called Tubulin alpha-1B chain.

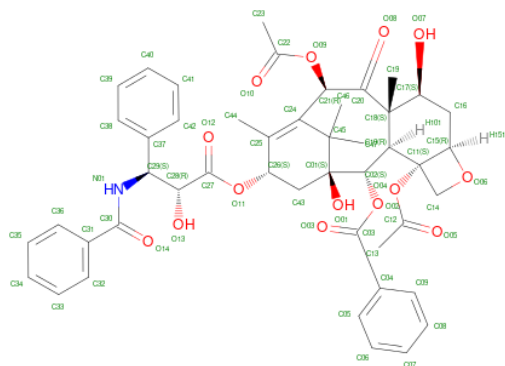
Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	428	Total	C	N	O	S	0	0
			3358	2130	571	635	22		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



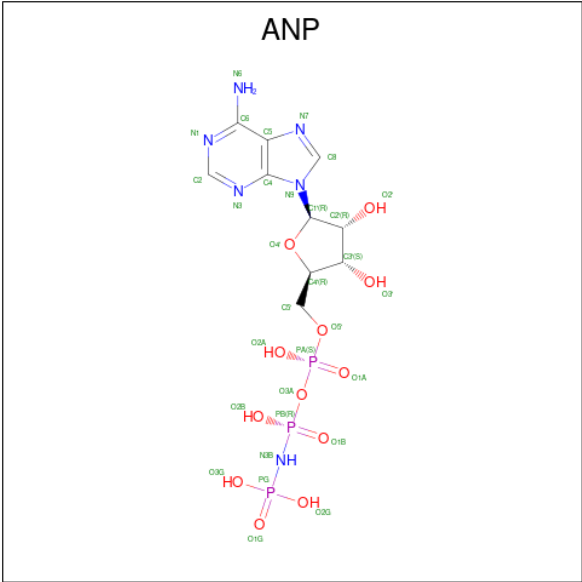
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

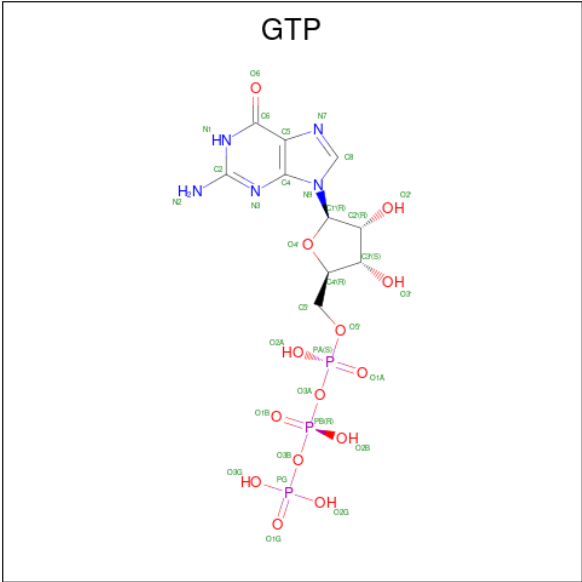
- Molecule 5 is TAXOL (CCD ID: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			62	47	1	14	

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



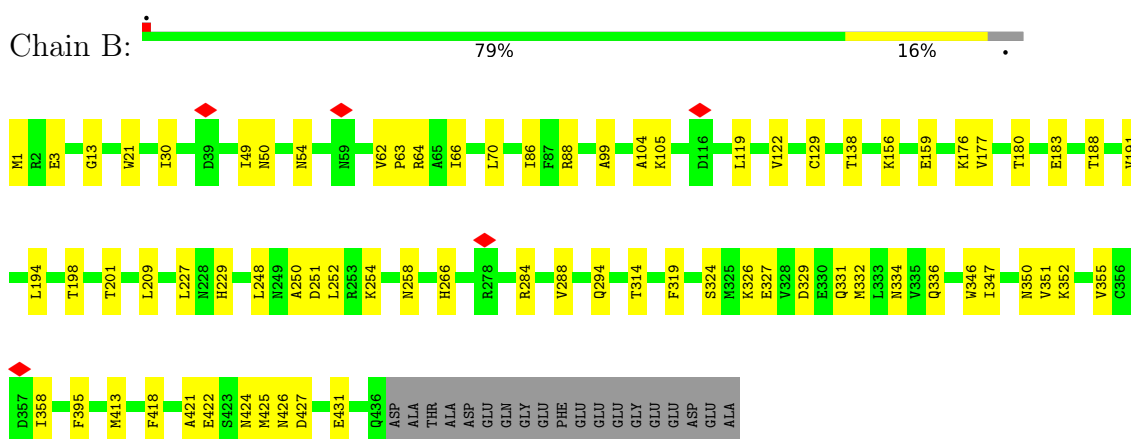


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	A	1	32	10	5	14	3	0

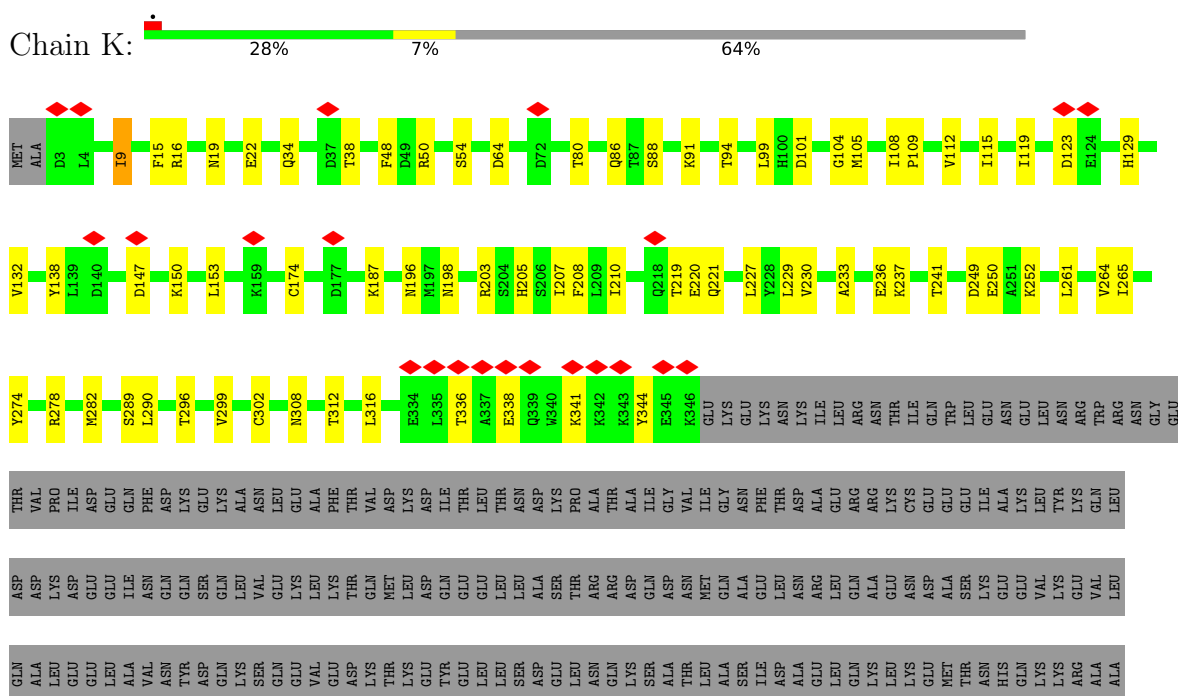
3 Residue-property plots [i](#)

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.

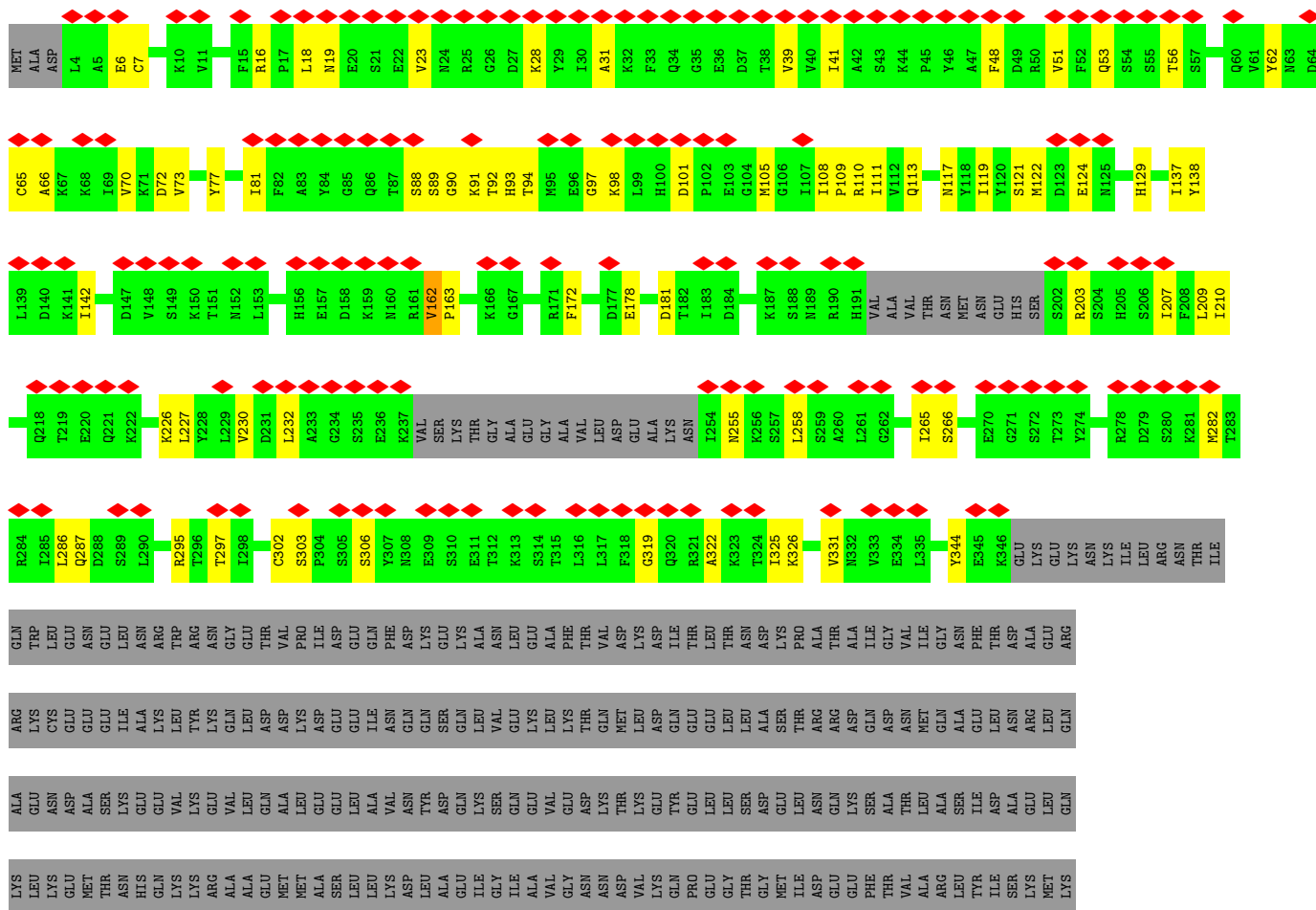
- Molecule 1: Tubulin beta chain



- Molecule 2: Kinesin-1 heavy chain



- Molecule 2: Kinesin-1 heavy chain



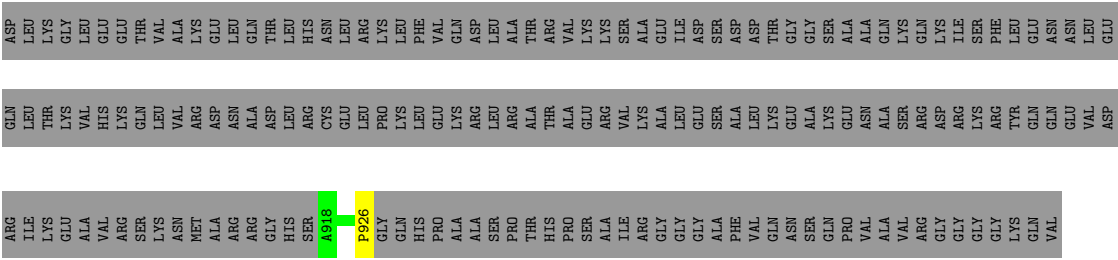
GLY	VAL	LEU	ARG	LEU	ARG	GLN	LEU	GLN	SER
	ASP	GLU	GLN	GLN	ASP	GLN	LEU	LEU	GLU
GLY	ASP	GLN	GLN	GLN	ASP	GLN	GLU	GLU	VAL
LYS	ILE	THR	THR	LYS	GLY	LYS	VAL	SER	GLY
GLN	GLU	LYS	VAL	VAL	LEU	GLY	GLU	VAL	VAL
	ALA	HIS	HIS	VAL	LEU	GLU	ALA	ASP	VAL
VAL	VAL	ARG	LYS	HIS	GLU	GLU	LYS	LYS	LYS
	ARG	GLN	GLN	GLN	GLU	GLU	ALA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

- Molecule 2: Kinesin-1 heavy chain

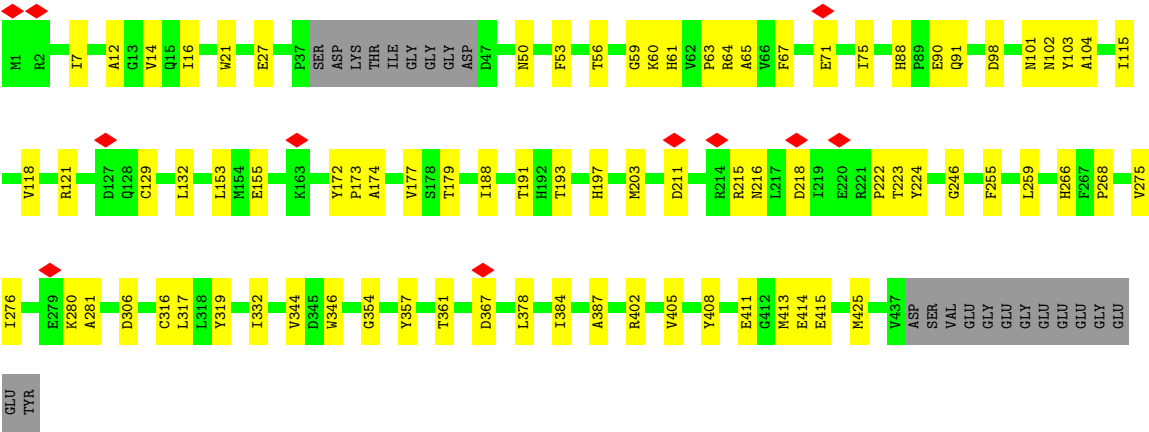
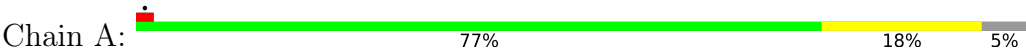
Chain T: 99%

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





● Molecule 3: Tubulin alpha-1B chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	570836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	259.91998, 259.91998, 259.91998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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: GDP, ANP, GTP, TA1, 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	B	0.16	0/3426	0.29	0/4641
2	K	0.15	0/2752	0.28	0/3709
2	L	0.11	0/2556	0.30	0/3440
2	T	0.12	0/70	0.27	0/94
2	t	0.12	0/70	0.20	0/94
3	A	0.17	0/3435	0.29	0/4663
All	All	0.15	0/12309	0.29	0/16641

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	B	3351	0	3237	49	0
2	K	2710	0	2687	52	0
2	L	2517	0	2503	54	0
2	T	69	0	70	8	0
2	t	69	0	73	2	0
3	A	3358	0	3277	53	0
4	B	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	62	0	51	3	0
6	K	31	0	13	0	0
6	L	31	0	13	5	0
7	A	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
8	A	32	0	12	0	0
All	All	12261	0	11948	198	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 8.

All (198) 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)
2:L:73:VAL:HG11	2:L:227:LEU:HD23	1.57	0.87
1:B:229:HIS:NE2	5:B:502:TA1:O14	2.14	0.79
1:B:332:MET:HB3	1:B:351:VAL:HG21	1.67	0.76
2:L:137:ILE:HD11	2:L:282:MET:HG2	1.66	0.76
2:L:124:GLU:HA	2:t:926[B]:PRO:HG2	1.68	0.76
2:K:132:VAL:HG22	2:K:210:ILE:HG22	1.68	0.76
2:K:9:ILE:HG23	2:K:296:THR:HG23	1.70	0.73
2:K:16:ARG:NH1	2:K:88:SER:O	2.24	0.70
2:L:255:ASN:HD21	2:L:258:LEU:HD23	1.56	0.70
2:K:210:ILE:HD11	2:K:227:LEU:HD23	1.73	0.69
3:A:50:ASN:O	3:A:64:ARG:NH1	2.26	0.68
2:L:129:HIS:HD2	2:T:923[A]:PRO:HG3	1.58	0.67
1:B:30:ILE:HD11	1:B:49:ILE:HD11	1.76	0.66
2:L:209:LEU:HD21	2:L:226:LYS:HB3	1.77	0.65
1:B:99:ALA:HA	1:B:105:LYS:HG2	1.77	0.65
3:A:211:ASP:HB3	3:A:215:ARG:HH12	1.64	0.62
1:B:248:LEU:HD21	3:A:179:THR:HG21	1.80	0.62
2:K:22:GLU:OE2	2:K:308:ASN:ND2	2.33	0.61
3:A:218:ASP:OD2	3:A:280:LYS:NZ	2.32	0.61
3:A:102:ASN:ND2	3:A:411:GLU:OE1	2.34	0.61
1:B:54:ASN:OD1	1:B:64:ARG:NH2	2.34	0.61
2:K:237:LYS:NZ	3:A:414:GLU:OE1	2.32	0.61
2:L:7:CYS:SG	2:L:295:ARG:NH2	2.74	0.60
2:L:93:HIS:HA	2:L:97:GLY:HA2	1.84	0.59
2:L:72:ASP:HB3	2:L:77:TYR:HB2	1.82	0.59
2:L:28:LYS:HG2	2:L:306:SER:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:88:SER:H	6:L:1002:ANP:HNB1	1.48	0.59
2:K:50:ARG:NH1	2:K:64:ASP:OD2	2.35	0.57
2:K:147:ASP:OD2	2:K:150:LYS:NZ	2.37	0.57
2:L:98:LYS:HB3	2:L:101:ASP:HB3	1.86	0.57
2:L:172:PHE:CD2	2:T:923[A]:PRO:HG2	2.40	0.57
2:L:6:GLU:HB2	2:L:326:LYS:HD2	1.86	0.57
2:L:31:ALA:HB2	2:L:41:ILE:HD12	1.87	0.57
1:B:201:THR:HG22	1:B:266:HIS:HD2	1.70	0.57
2:K:138:TYR:HE1	2:K:250:GLU:HG2	1.70	0.56
1:B:324:SER:OG	3:A:222:PRO:O	2.24	0.55
3:A:56:THR:HG21	3:A:60:LYS:HB3	1.89	0.55
1:B:250:ALA:HA	1:B:254:LYS:HD3	1.89	0.55
2:L:70:VAL:HG22	2:L:111:ILE:HG13	1.89	0.55
1:B:191:VAL:HG11	1:B:425:MET:HE1	1.88	0.55
2:L:18:LEU:HD23	2:L:23:VAL:HG12	1.89	0.54
2:L:53:GLN:HB2	2:L:56:THR:HG23	1.88	0.54
2:K:80:THR:HG21	2:K:289:SER:HB3	1.88	0.54
3:A:317:LEU:HD12	3:A:332:ILE:HD11	1.89	0.54
3:A:90:GLU:HG3	3:A:121:ARG:HD3	1.89	0.53
1:B:104:ALA:HB2	1:B:413:MET:HE2	1.89	0.53
3:A:53:PHE:O	3:A:64:ARG:NH1	2.40	0.53
2:L:163:PRO:HD2	2:L:287:GLN:HG3	1.91	0.53
2:L:113:GLN:O	2:L:117:ASN:ND2	2.32	0.53
2:L:119:ILE:HG21	2:T:920[A]:ILE:HD11	1.91	0.53
1:B:427:ASP:OD2	2:K:278:ARG:NH1	2.37	0.53
2:L:16:ARG:HE	2:L:89:SER:HA	1.74	0.53
2:K:302:CYS:HB3	2:K:312:THR:HG23	1.91	0.52
2:K:207:ILE:HG12	2:K:230:VAL:HG13	1.90	0.52
2:L:230:VAL:HG21	2:L:286:LEU:HD11	1.91	0.52
2:L:92:THR:HG23	6:L:1002:ANP:O1B	2.10	0.52
2:K:338:GLU:HA	2:K:341:LYS:HE3	1.91	0.52
2:K:207:ILE:HD11	2:K:282:MET:HE1	1.90	0.52
2:L:39:VAL:HB	2:L:51:VAL:HG11	1.92	0.52
1:B:1:MET:N	1:B:50:ASN:OD1	2.42	0.52
3:A:71:GLU:HG2	3:A:98:ASP:HB3	1.92	0.51
2:K:123:ASP:O	2:T:926[A]:PRO:HG2	2.11	0.51
3:A:367:ASP:N	3:A:367:ASP:OD1	2.44	0.51
2:K:203:ARG:NH1	2:K:236:GLU:OE2	2.43	0.51
3:A:172:TYR:HE2	3:A:387:ALA:HB1	1.75	0.51
2:K:99:LEU:HD21	2:K:187:LYS:HD3	1.93	0.50
3:A:223:THR:OG1	3:A:224:TYR:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLN:HA	1:B:334:ASN:ND2	2.25	0.50
1:B:425:MET:HA	1:B:425:MET:HE3	1.94	0.50
2:L:90:GLY:HA2	6:L:1002:ANP:H8	1.93	0.49
2:L:91:LYS:NZ	2:L:232:LEU:O	2.42	0.49
3:A:319:TYR:N	3:A:354:GLY:O	2.45	0.49
2:K:344:TYR:HB2	2:L:344:TYR:HB2	1.93	0.49
2:L:124:GLU:HA	2:T:918[A]:ALA:HA	1.92	0.49
2:K:344:TYR:HD1	2:L:344:TYR:HA	1.78	0.49
2:K:236:GLU:HB3	2:K:241:THR:HG21	1.94	0.49
3:A:316:CYS:SG	3:A:378:LEU:HB2	2.52	0.49
3:A:344:VAL:HG11	3:A:346:TRP:CE2	2.48	0.49
1:B:329:ASP:CG	3:A:177:VAL:HG13	2.38	0.49
1:B:63:PRO:HD3	1:B:86:ILE:HG12	1.95	0.49
2:L:90:GLY:O	2:L:94:THR:OG1	2.30	0.49
1:B:62:VAL:HG21	1:B:88:ARG:HH21	1.78	0.48
1:B:319:PHE:HB2	1:B:355:VAL:HG22	1.95	0.48
2:L:210:ILE:HG12	2:L:227:LEU:HG	1.95	0.48
3:A:408:TYR:HB3	3:A:413:MET:HE3	1.95	0.48
2:L:66:ALA:O	2:L:70:VAL:HG23	2.14	0.48
2:L:265:ILE:HG13	2:L:266:SER:N	2.29	0.48
3:A:216:ASN:HB3	3:A:275:VAL:O	2.13	0.48
1:B:180:THR:OG1	1:B:183:GLU:HG3	2.14	0.47
1:B:251:ASP:OD1	1:B:252:LEU:N	2.43	0.47
3:A:104:ALA:HB2	3:A:413:MET:HE2	1.96	0.47
2:K:150:LYS:HB3	2:K:153:LEU:HD21	1.97	0.47
2:K:108:ILE:HG12	2:K:229:LEU:HD13	1.95	0.47
2:L:48:PHE:HE1	2:L:319:GLY:HA3	1.79	0.47
1:B:258:ASN:O	1:B:314:THR:HG21	2.15	0.47
2:L:65:CYS:SG	2:L:66:ALA:N	2.87	0.47
2:K:112:VAL:O	2:K:115:ILE:HG22	2.14	0.47
1:B:21:TRP:CZ3	1:B:63:PRO:HB3	2.50	0.47
2:K:196:ASN:ND2	2:K:241:THR:O	2.39	0.47
3:A:191:THR:HG23	3:A:425:MET:HE1	1.96	0.47
1:B:326:LYS:HG2	3:A:222:PRO:HD2	1.96	0.47
2:K:261:LEU:O	2:K:264:VAL:HG12	2.15	0.47
2:K:34:GLN:HG3	2:K:38:THR:HG23	1.96	0.46
2:L:105:MET:HB2	2:L:110:ARG:NH2	2.29	0.46
2:L:138:TYR:HE1	2:L:203:ARG:HB2	1.81	0.46
1:B:70:LEU:HD12	1:B:99:ALA:HB2	1.97	0.46
3:A:88:HIS:HB3	3:A:91:GLN:HG3	1.98	0.46
1:B:209:LEU:HD13	1:B:227:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:129:HIS:CD2	2:T:923[A]:PRO:HB3	2.51	0.46
2:L:207:ILE:HA	2:L:230:VAL:HG12	1.97	0.46
3:A:255:PHE:O	3:A:259:LEU:HB2	2.15	0.46
2:K:174:CYS:SG	2:T:922[A]:LYS:HB3	2.56	0.45
3:A:12:ALA:O	3:A:16:ILE:HG13	2.16	0.45
2:K:86:GLN:O	2:K:91:LYS:NZ	2.29	0.45
5:B:502:TA1:H463	5:B:502:TA1:H261	1.97	0.45
2:K:15:PHE:O	2:K:54:SER:HA	2.17	0.45
2:L:137:ILE:HG22	2:L:142:ILE:HA	1.99	0.45
3:A:174:ALA:HB3	3:A:177:VAL:O	2.17	0.45
1:B:13:GLY:HA2	1:B:138:THR:HG22	1.99	0.45
2:K:205:HIS:HB3	2:K:282:MET:HE3	1.98	0.45
1:B:431:GLU:HB2	2:K:274:TYR:CE1	2.52	0.45
2:L:178:GLU:HA	2:L:181:ASP:OD2	2.17	0.45
2:L:302:CYS:SG	2:L:303:SER:N	2.90	0.45
2:K:219:THR:HG23	2:K:221:GLN:H	1.82	0.44
2:L:108:ILE:O	2:L:111:ILE:HG22	2.17	0.44
3:A:402:ARG:HG3	3:A:405:VAL:HG21	1.99	0.44
3:A:103:TYR:HD2	3:A:413:MET:HE1	1.83	0.44
1:B:424:ASN:OD1	2:K:278:ARG:NE	2.50	0.44
3:A:21:TRP:CZ2	3:A:65:ALA:HB2	2.53	0.44
2:K:48:PHE:CE2	2:K:316:LEU:HD13	2.53	0.44
3:A:21:TRP:CZ3	3:A:63:PRO:HB3	2.52	0.44
1:B:331:GLN:HA	1:B:334:ASN:HD21	1.82	0.44
2:K:115:ILE:O	2:K:119:ILE:HG12	2.18	0.44
2:K:94:THR:HG21	2:K:299:VAL:HG11	2.00	0.44
2:K:208:PHE:HB3	2:K:229:LEU:HB2	2.00	0.43
3:A:246:GLY:HA2	3:A:357:TYR:CE2	2.52	0.43
1:B:431:GLU:HB2	2:K:274:TYR:CZ	2.54	0.43
1:B:66:ILE:HD13	1:B:122:VAL:HG22	2.00	0.43
2:K:220:GLU:HG3	2:K:336:THR:HB	2.01	0.43
2:L:91:LYS:HG2	6:L:1002:ANP:PB	2.58	0.43
1:B:176:LYS:HG3	1:B:177:VAL:HG23	1.99	0.43
2:K:119:ILE:O	2:T:926[A]:PRO:HB3	2.18	0.43
2:K:19:ASN:OD1	2:K:19:ASN:N	2.47	0.43
3:A:59:GLY:O	3:A:61:HIS:ND1	2.51	0.43
3:A:14:VAL:HG11	3:A:75:ILE:HD11	2.01	0.43
3:A:7:ILE:HG21	3:A:153:LEU:HD21	2.00	0.43
3:A:211:ASP:HB3	3:A:215:ARG:NH1	2.32	0.43
1:B:50:ASN:O	1:B:64:ARG:NH1	2.49	0.43
1:B:194:LEU:O	1:B:198:THR:OG1	2.23	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ARG:HA	1:B:284:ARG:HD3	1.81	0.43
3:A:276:ILE:HD12	3:A:281:ALA:HA	1.99	0.43
1:B:395:PHE:HZ	1:B:418:PHE:HB3	1.84	0.43
3:A:98:ASP:OD1	3:A:98:ASP:N	2.51	0.43
2:K:208:PHE:HD2	2:K:229:LEU:HD12	1.84	0.42
2:L:16:ARG:NH1	2:L:19:ASN:OD1	2.53	0.42
3:A:203:MET:HE2	3:A:384:ILE:HD11	2.01	0.42
1:B:422:GLU:OE2	1:B:426:ASN:ND2	2.51	0.42
3:A:266:HIS:C	3:A:268:PRO:HD3	2.45	0.42
5:B:502:TA1:C25	5:B:502:TA1:H101	2.50	0.42
2:K:108:ILE:HB	2:K:109:PRO:HD3	2.01	0.42
3:A:172:TYR:CE2	3:A:387:ALA:HB1	2.54	0.42
3:A:155:GLU:HG2	3:A:197:HIS:NE2	2.35	0.42
1:B:188:THR:HG22	1:B:421:ALA:HB1	2.00	0.42
1:B:288:VAL:HB	1:B:327:GLU:HG2	2.02	0.42
1:B:294:GLN:HE21	1:B:294:GLN:HB2	1.60	0.42
2:L:119:ILE:O	2:t:926[B]:PRO:HB3	2.20	0.42
3:A:129:CYS:SG	3:A:132:LEU:HB2	2.59	0.42
2:L:108:ILE:HB	2:L:109:PRO:HD3	2.02	0.42
3:A:67:PHE:HB3	3:A:75:ILE:HD12	2.02	0.42
1:B:3:GLU:OE1	1:B:129:CYS:HB3	2.20	0.42
1:B:254:LYS:HG2	1:B:352:LYS:HE3	2.02	0.41
2:K:249:ASP:HA	2:K:252:LYS:HD3	2.01	0.41
3:A:27:GLU:HG2	3:A:361:THR:HG21	2.01	0.41
2:K:88:SER:HB3	2:K:198:ASN:HB2	2.02	0.41
2:L:162:VAL:HG23	2:L:287:GLN:NE2	2.36	0.41
1:B:336:GLN:NE2	1:B:350:ASN:OD1	2.53	0.41
3:A:306:ASP:OD1	3:A:306:ASP:N	2.41	0.41
1:B:346:TRP:CE3	1:B:347:ILE:HG13	2.55	0.41
3:A:103:TYR:OH	3:A:193:THR:HG21	2.20	0.41
1:B:254:LYS:HE3	3:A:101:ASN:CG	2.46	0.41
2:K:105:MET:HE2	2:K:109:PRO:HB2	2.03	0.41
2:K:210:ILE:HG13	2:K:227:LEU:HB3	2.03	0.41
2:K:265:ILE:HD11	2:K:290:LEU:HD22	2.03	0.41
3:A:402:ARG:HD3	3:A:415:GLU:OE2	2.20	0.41
1:B:156:LYS:O	1:B:159:GLU:HG3	2.20	0.41
1:B:358:ILE:HD13	1:B:358:ILE:HA	1.92	0.41
1:B:119:LEU:HD11	1:B:156:LYS:HB3	2.03	0.40
2:L:81:ILE:HG22	2:L:297:THR:OG1	2.21	0.40
2:L:121:SER:O	2:L:122:MET:HG2	2.21	0.40
3:A:188:ILE:HG23	3:A:425:MET:HE3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:62:TYR:CD1	2:L:66:ALA:HB3	2.57	0.40
2:L:90:GLY:CA	6:L:1002:ANP:H8	2.51	0.40
3:A:172:TYR:CD1	3:A:173:PRO:HD2	2.57	0.40
2:K:101:ASP:OD2	2:K:104:GLY:N	2.51	0.40
2:L:322:ALA:O	2:L:325:ILE:HG22	2.21	0.40
3:A:115:ILE:HA	3:A:118:VAL:HG12	2.04	0.40
2:K:205:HIS:HE1	2:K:233:ALA:HB3	1.86	0.40
2:L:77:TYR:CE1	2:L:331:VAL:HG22	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	K	342/963 (36%)	335 (98%)	7 (2%)	0	100	100
2	L	311/963 (32%)	298 (96%)	13 (4%)	0	100	100
2	T	7/963 (1%)	7 (100%)	0	0	100	100
2	t	7/963 (1%)	6 (86%)	1 (14%)	0	100	100
3	A	424/451 (94%)	407 (96%)	17 (4%)	0	100	100
All	All	1515/4748 (32%)	1467 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	367/381 (96%)	367 (100%)	0	100	100
2	K	308/854 (36%)	307 (100%)	1 (0%)	86	91
2	L	287/854 (34%)	286 (100%)	1 (0%)	86	91
2	T	7/854 (1%)	7 (100%)	0	100	100
2	t	7/854 (1%)	7 (100%)	0	100	100
3	A	362/379 (96%)	362 (100%)	0	100	100
All	All	1338/4176 (32%)	1336 (100%)	2 (0%)	87	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	9	ILE
2	L	162	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	GLN
1	B	281	GLN
2	K	205	HIS
2	K	211	ASN
2	L	100	HIS
2	L	216	ASN
2	L	255	ASN
3	A	31	GLN
3	A	102	ASN
3	A	258	ASN
3	A	300	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z > 2$
5	TA1	B	502	-	68,68,68	0.67	1 (1%)	105,105,105	1.14	9 (8%)
6	ANP	L	1002	7	33,33,33	1.13	3 (9%)	45,52,52	1.77	10 (22%)
4	GDP	B	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	7 (15%)
6	ANP	K	1001	7	33,33,33	1.72	4 (12%)	45,52,52	1.68	10 (22%)
8	GTP	A	501	7	33,34,34	0.79	1 (3%)	50,54,54	1.53	8 (16%)

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
5	TA1	B	502	-	-	8/41/127/127	0/7/7/7
6	ANP	L	1002	7	-	8/18/38/38	0/3/3/3
4	GDP	B	501	-	-	3/16/32/32	0/3/3/3
6	ANP	K	1001	7	-	3/18/38/38	0/3/3/3
8	GTP	A	501	7	-	8/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1001	ANP	PA-O3A	-6.97	1.52	1.59
6	K	1001	ANP	PB-O3A	-4.90	1.53	1.59
6	L	1002	ANP	PB-O3A	-4.57	1.53	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	GDP	C5-C4	3.02	1.47	1.38
6	K	1001	ANP	O5'-C5'	-2.88	1.33	1.44
4	B	501	GDP	C6-N1	-2.62	1.33	1.38
6	L	1002	ANP	PG-O1G	2.42	1.49	1.46
5	B	502	TA1	C18-C10	2.32	1.62	1.57
6	K	1001	ANP	PG-O1G	2.27	1.49	1.46
8	A	501	GTP	C2-N3	2.10	1.38	1.33
4	B	501	GDP	C5-N7	-2.08	1.34	1.39
6	L	1002	ANP	PG-N3B	2.04	1.68	1.63

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	GDP	C5-C4-N3	-6.69	117.74	128.39
4	B	501	GDP	C2-N3-C4	5.40	121.60	112.30
8	A	501	GTP	C5-C4-N3	-5.32	119.93	128.39
5	B	502	TA1	O08-C20-C21	-5.20	113.04	119.28
6	L	1002	ANP	O2B-PB-O1B	5.19	120.99	109.87
4	B	501	GDP	N9-C4-N3	5.09	136.12	125.95
8	A	501	GTP	C2-N3-C4	4.54	120.12	112.30
6	K	1001	ANP	C5'-C4'-C3'	-4.24	99.94	115.21
6	L	1002	ANP	O1B-PB-N3B	4.22	117.98	111.77
6	L	1002	ANP	O5'-PA-O1A	-4.21	92.27	108.94
6	K	1001	ANP	PA-O5'-C5'	-3.90	99.01	121.35
6	L	1002	ANP	O1G-PG-N3B	-3.86	106.08	111.77
6	K	1001	ANP	O2A-PA-O3A	3.83	117.61	107.27
5	B	502	TA1	C18-C20-C21	3.69	129.29	121.38
6	K	1001	ANP	O5'-C5'-C4'	3.62	121.32	108.99
6	K	1001	ANP	O3A-PB-N3B	-3.41	97.14	106.59
6	L	1002	ANP	O2A-PA-O5'	-3.22	92.96	107.57
8	A	501	GTP	N9-C4-N3	3.19	132.33	125.95
6	L	1002	ANP	O2A-PA-O3A	3.13	115.72	107.27
5	B	502	TA1	C11-O04-C12	3.00	126.79	119.17
4	B	501	GDP	C6-C5-N7	2.99	135.73	130.29
6	L	1002	ANP	O2B-PB-O3A	-2.98	94.69	104.64
5	B	502	TA1	C47-C45-C46	-2.98	97.84	106.29
6	L	1002	ANP	O3A-PB-N3B	-2.86	98.67	106.59
6	L	1002	ANP	O2A-PA-O1A	2.82	125.56	112.44
5	B	502	TA1	C21-O09-C22	2.81	121.75	115.95
8	A	501	GTP	C2-N1-C6	-2.78	120.08	125.11
6	K	1001	ANP	O3'-C3'-C4'	2.70	118.82	111.08
6	K	1001	ANP	O2B-PB-O3A	2.64	113.46	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	501	GTP	C8-N7-C5	2.60	108.89	104.26
5	B	502	TA1	O11-C26-C25	2.54	115.88	109.85
4	B	501	GDP	C4-C5-N7	-2.46	106.77	110.67
5	B	502	TA1	C24-C21-C20	-2.45	107.96	113.31
6	K	1001	ANP	C2'-C1'-N9	-2.43	107.27	113.30
8	A	501	GTP	N9-C8-N7	-2.32	109.10	113.40
8	A	501	GTP	C5-C6-N1	2.31	119.14	113.25
4	B	501	GDP	O6-C6-C5	-2.30	120.45	126.53
5	B	502	TA1	C02-O02-C03	2.29	121.98	117.80
8	A	501	GTP	C4-C5-N7	-2.24	107.11	110.67
5	B	502	TA1	C45-C01-C02	2.16	114.31	111.93
6	K	1001	ANP	O4'-C1'-N9	2.13	112.18	108.09
4	B	501	GDP	C5-C6-N1	2.11	118.63	113.25
6	K	1001	ANP	O2A-PA-O1A	2.09	122.17	112.44
6	L	1002	ANP	O3G-PG-O1G	-2.02	108.38	113.45

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	GDP	C5'-O5'-PA-O3A
4	B	501	GDP	C5'-O5'-PA-O1A
4	B	501	GDP	C5'-O5'-PA-O2A
6	K	1001	ANP	PB-N3B-PG-O1G
6	K	1001	ANP	PG-N3B-PB-O1B
6	K	1001	ANP	PG-N3B-PB-O3A
6	L	1002	ANP	PG-N3B-PB-O1B
6	L	1002	ANP	PA-O3A-PB-O2B
6	L	1002	ANP	C5'-O5'-PA-O1A
6	L	1002	ANP	C5'-O5'-PA-O2A
6	L	1002	ANP	C5'-O5'-PA-O3A
8	A	501	GTP	PB-O3B-PG-O3G
8	A	501	GTP	C5'-O5'-PA-O3A
8	A	501	GTP	C5'-O5'-PA-O1A
8	A	501	GTP	C5'-O5'-PA-O2A
5	B	502	TA1	O02-C03-C04-C05
5	B	502	TA1	O02-C03-C04-C09
5	B	502	TA1	N01-C30-C31-C36
5	B	502	TA1	O03-C03-C04-C09
5	B	502	TA1	O03-C03-C04-C05
5	B	502	TA1	O14-C30-C31-C36
6	L	1002	ANP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

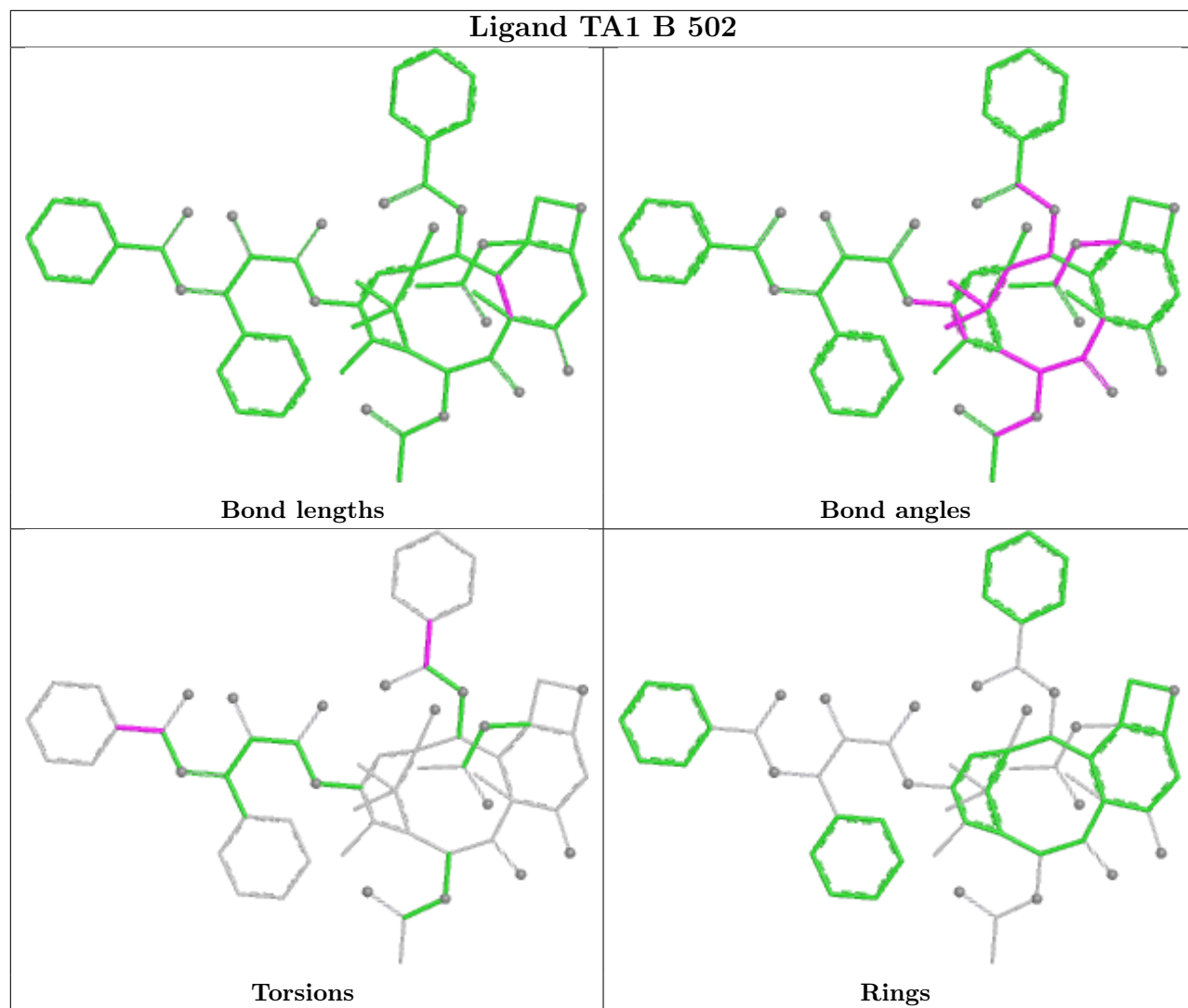
Mol	Chain	Res	Type	Atoms
6	L	1002	ANP	C3'-C4'-C5'-O5'
5	B	502	TA1	N01-C30-C31-C32
5	B	502	TA1	O14-C30-C31-C32
8	A	501	GTP	PB-O3A-PA-O2A
8	A	501	GTP	PB-O3B-PG-O1G
8	A	501	GTP	PB-O3B-PG-O2G
6	L	1002	ANP	PA-O3A-PB-O1B
8	A	501	GTP	PB-O3A-PA-O1A

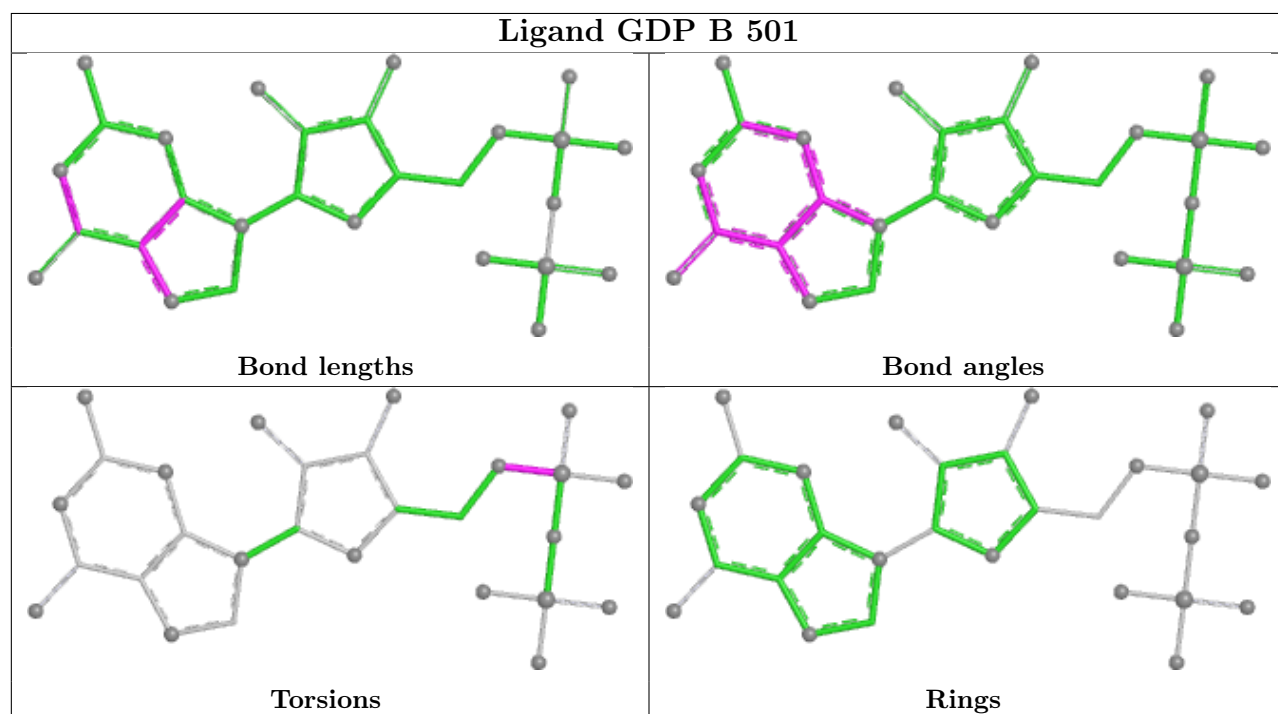
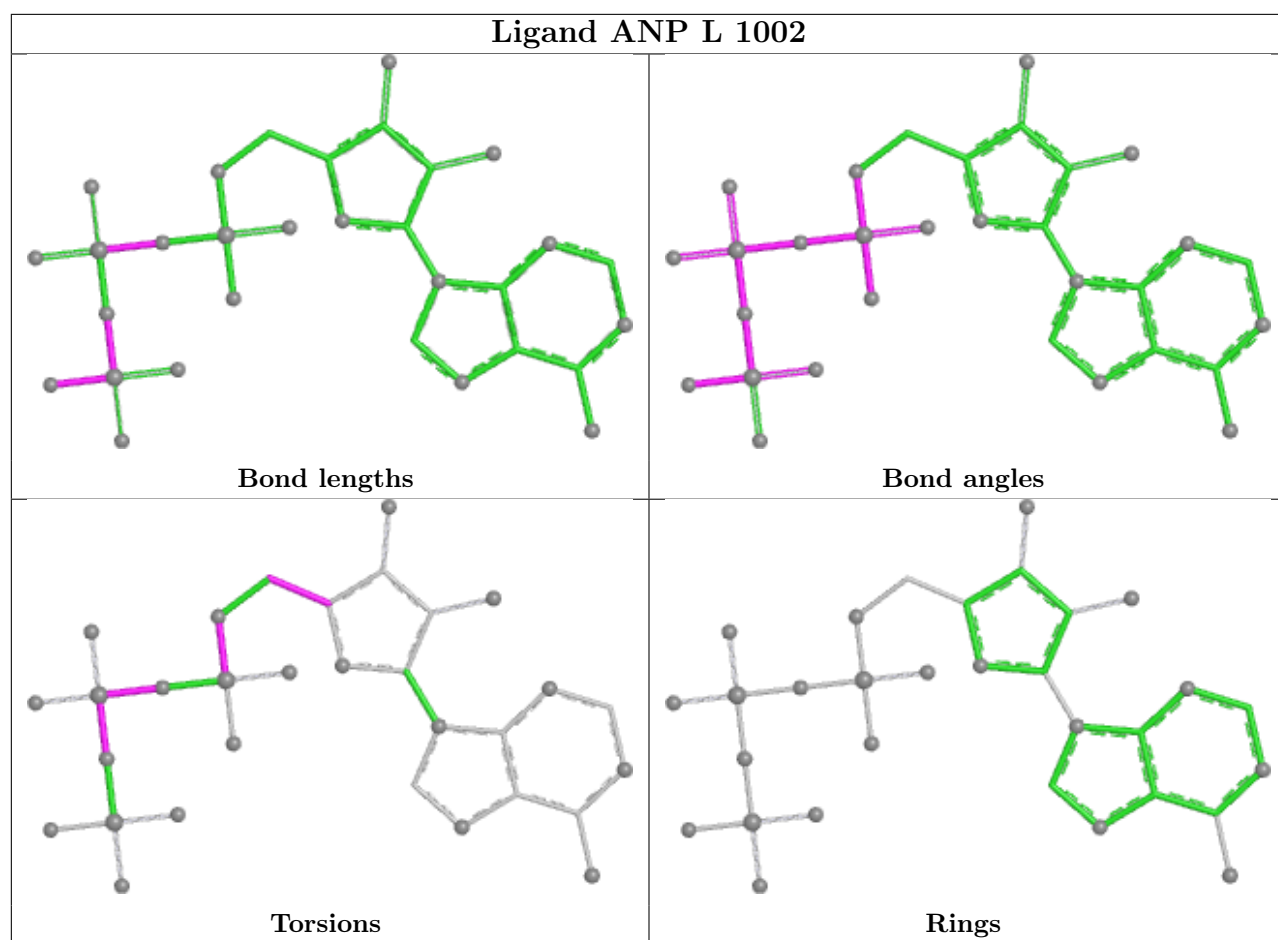
There are no ring outliers.

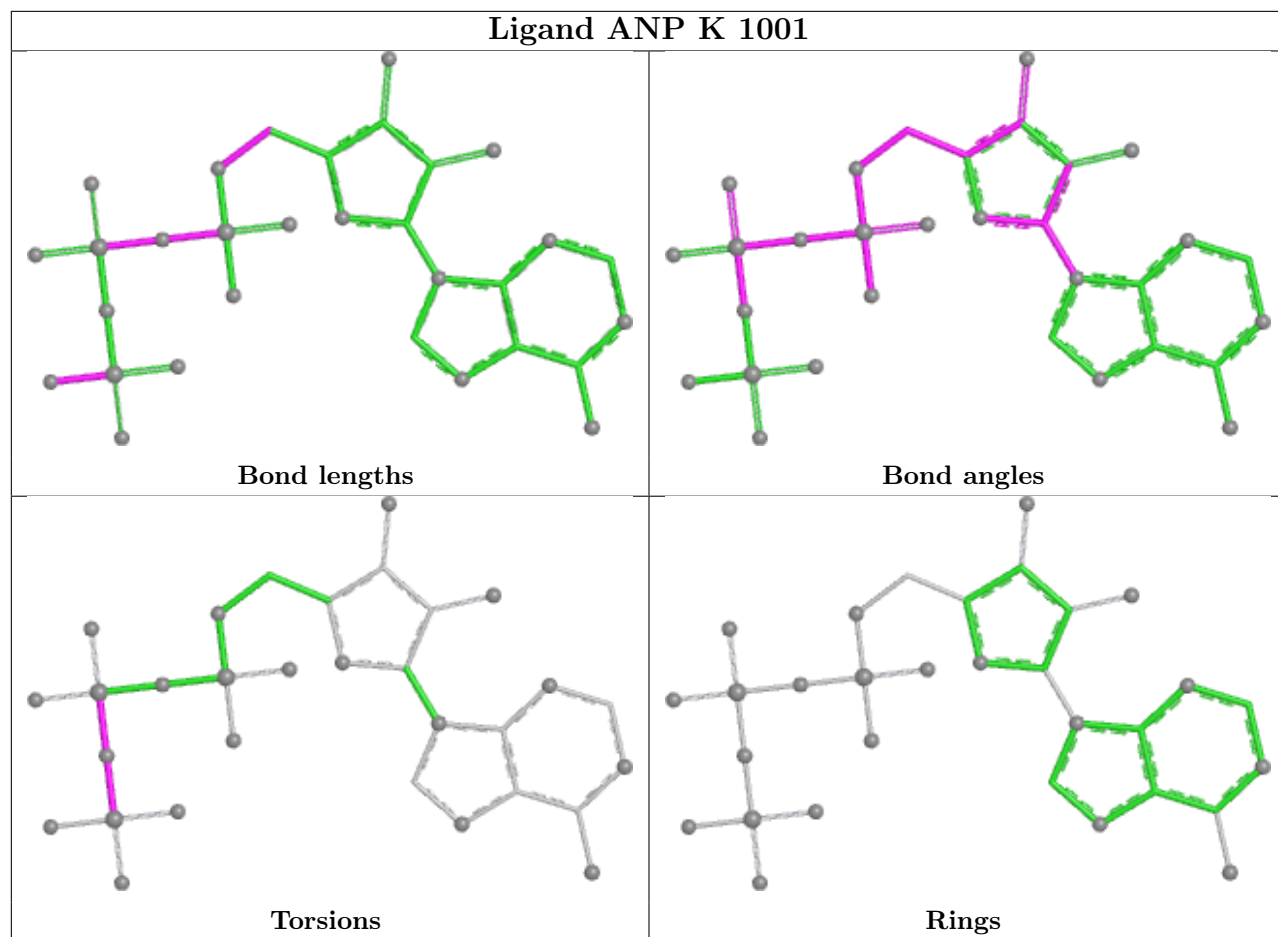
2 monomers are involved in 8 short contacts:

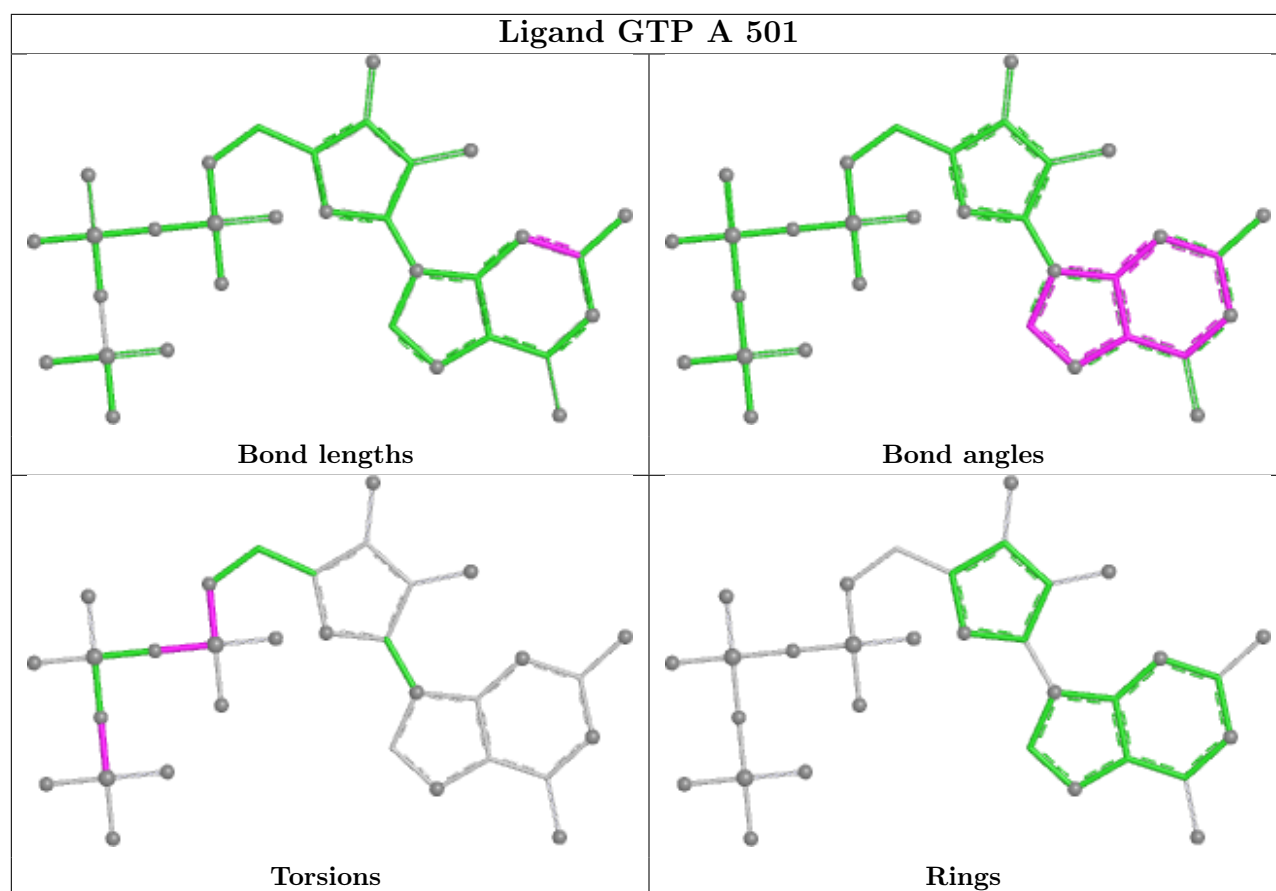
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	TA1	3	0
6	L	1002	ANP	5	0

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 than 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.









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.

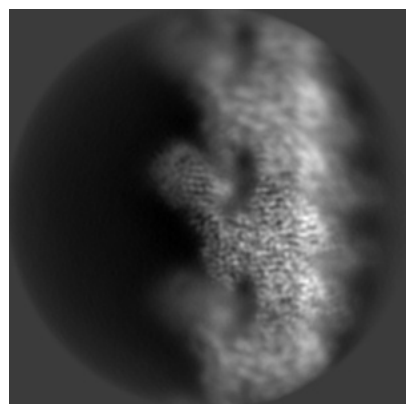
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19176. These allow visual inspection of the internal detail of the map and identification of artifacts.

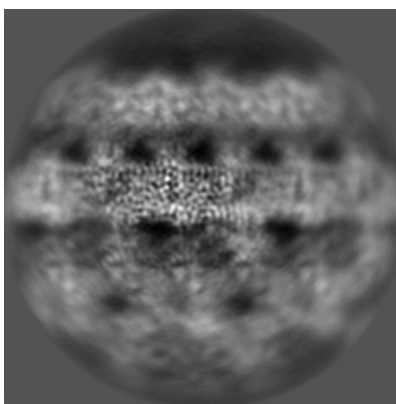
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

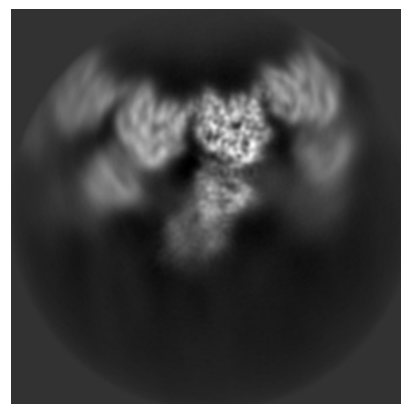
6.1.1 Primary map



X

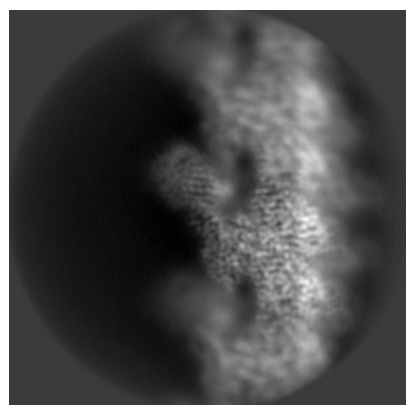


Y

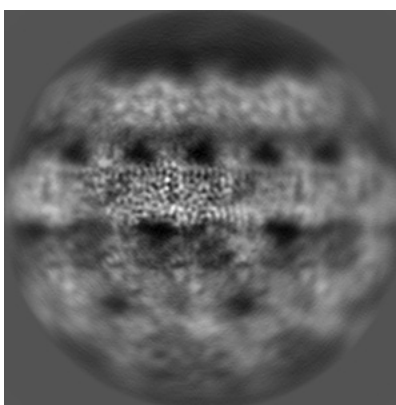


Z

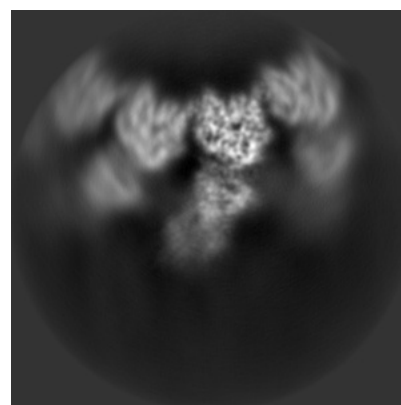
6.1.2 Raw map



X



Y

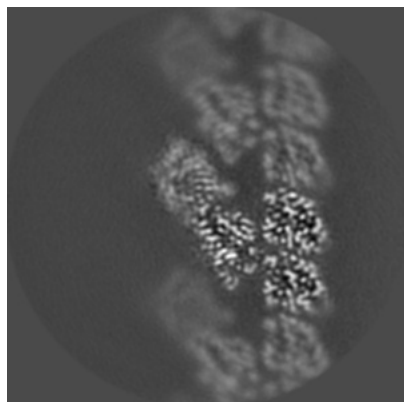


Z

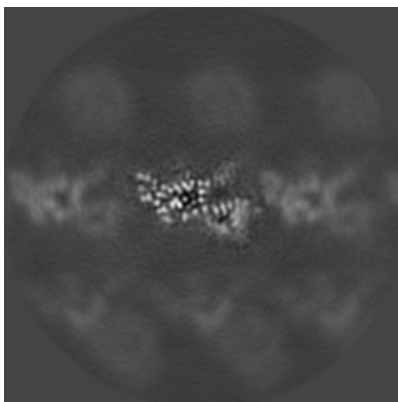
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

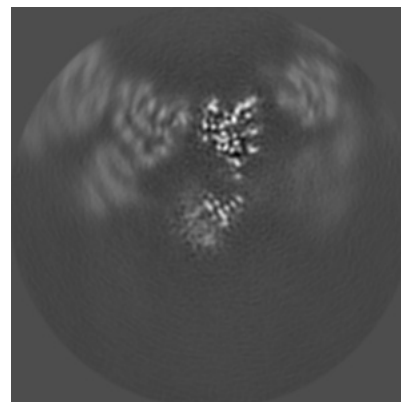
6.2.1 Primary map



X Index: 120

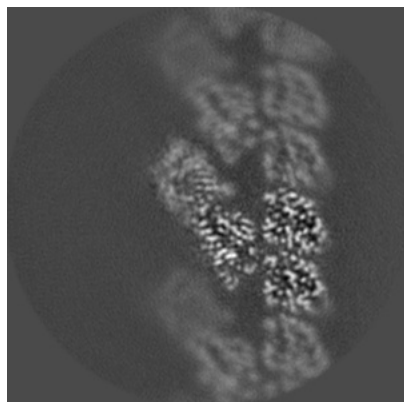


Y Index: 120

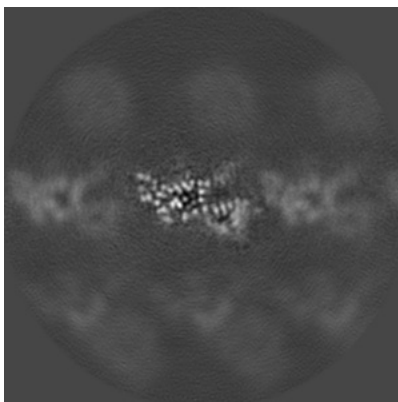


Z Index: 120

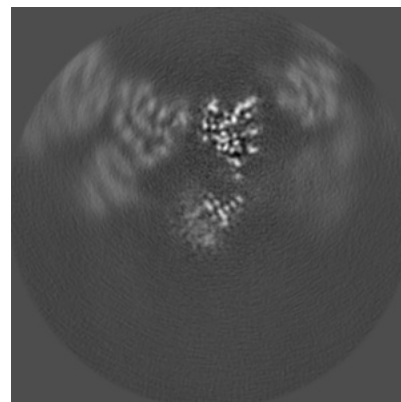
6.2.2 Raw map



X Index: 120



Y Index: 120

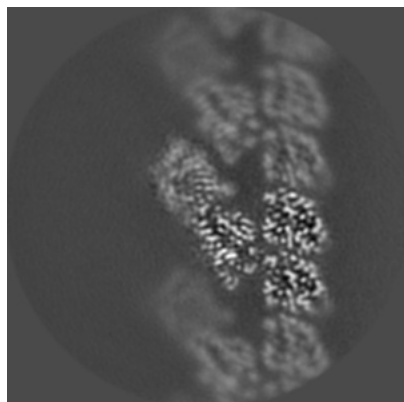


Z Index: 120

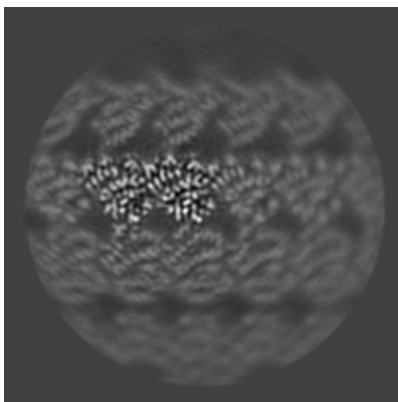
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

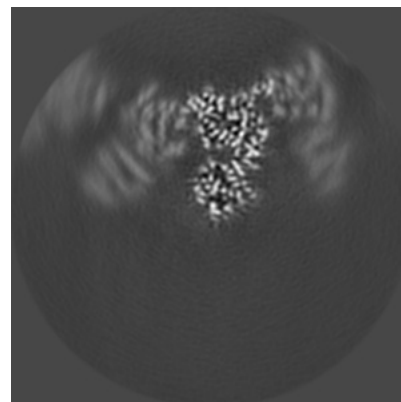
6.3.1 Primary map



X Index: 120

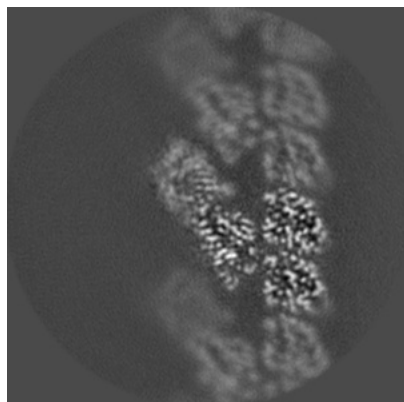


Y Index: 176

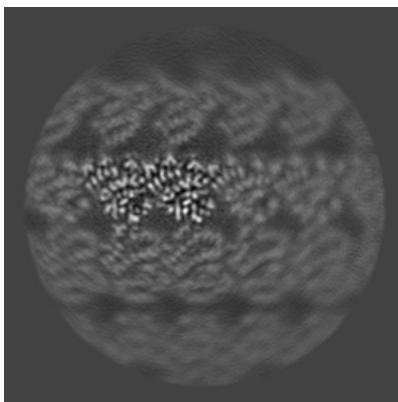


Z Index: 105

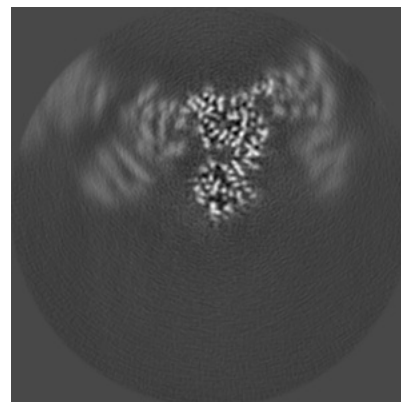
6.3.2 Raw map



X Index: 120



Y Index: 176

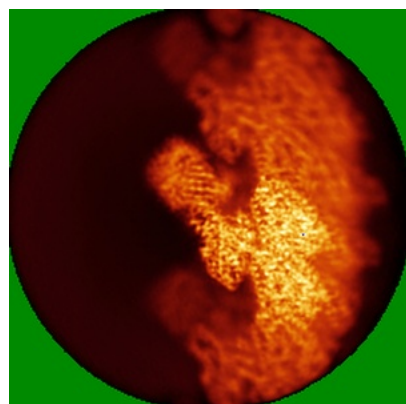


Z Index: 105

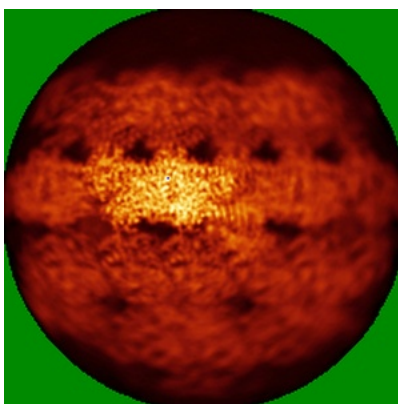
The images above show the largest variance slices of the map in three orthogonal directions.

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

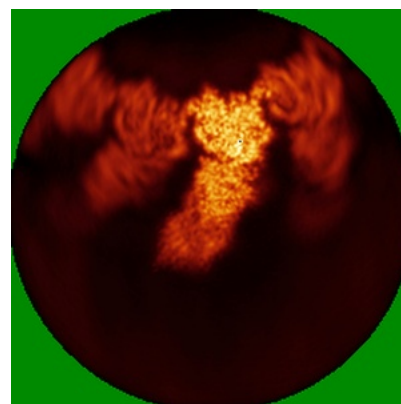
6.4.1 Primary map



X

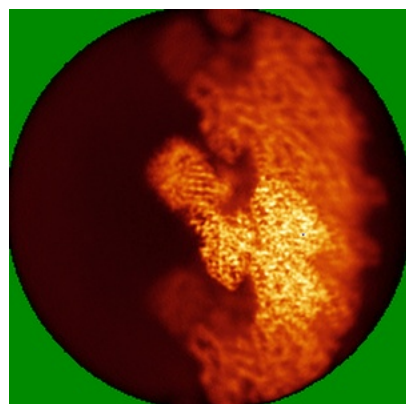


Y

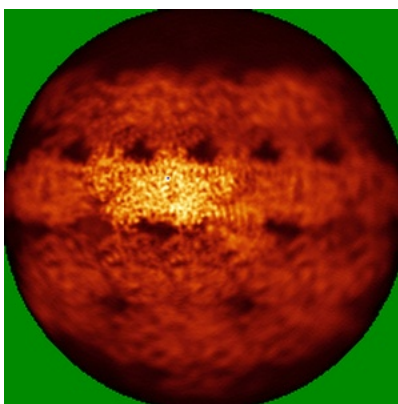


Z

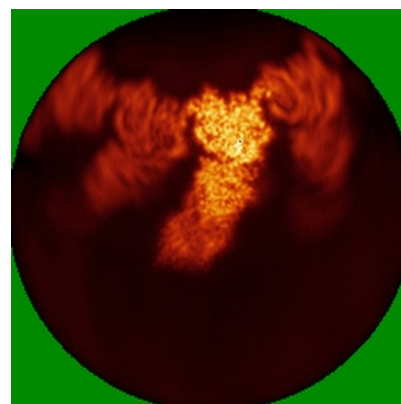
6.4.2 Raw map



X



Y

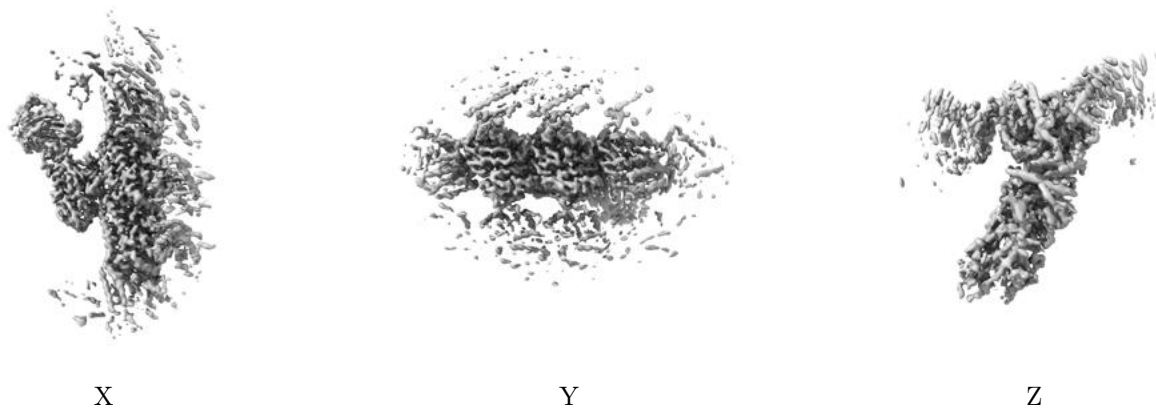


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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



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.

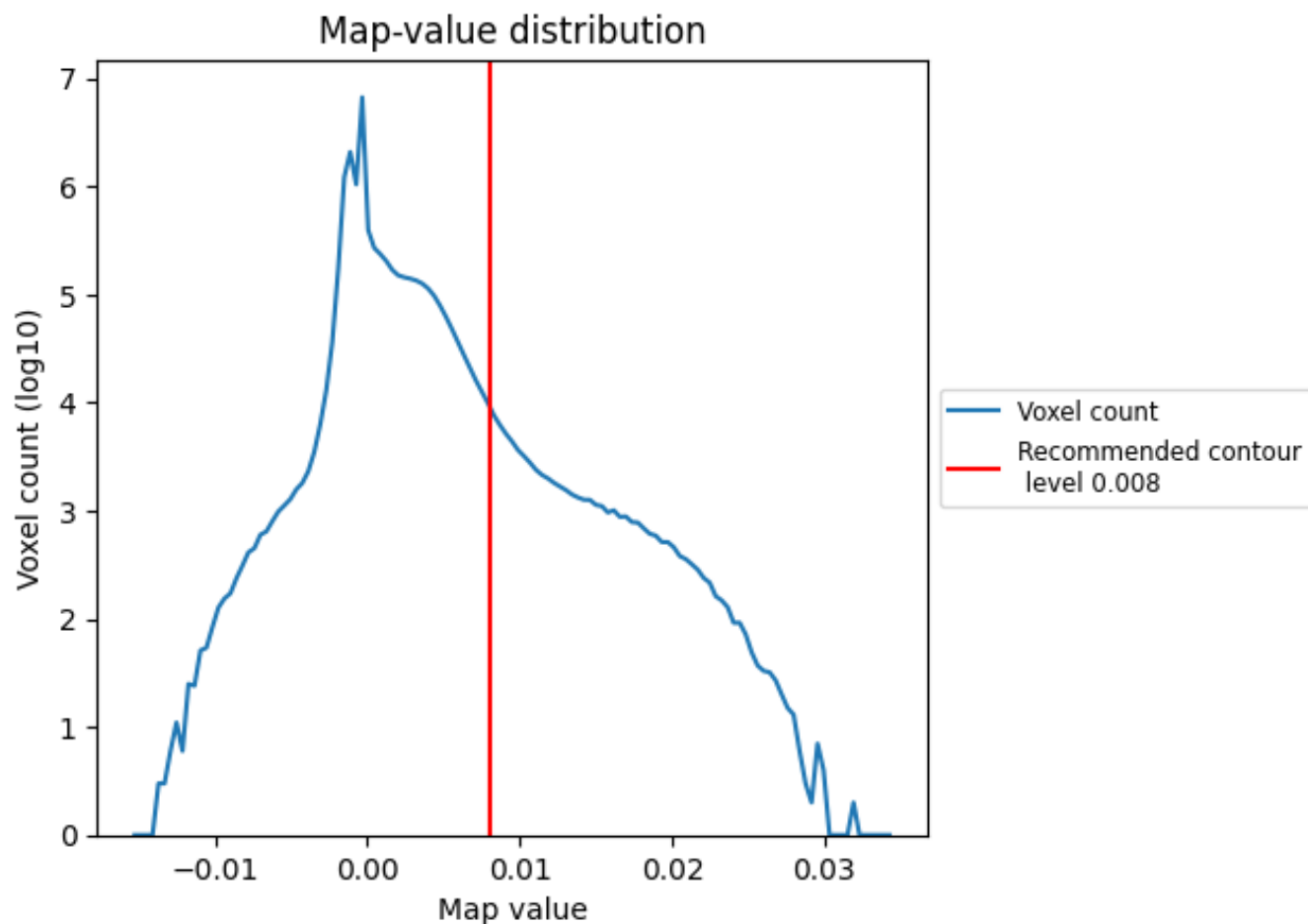
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

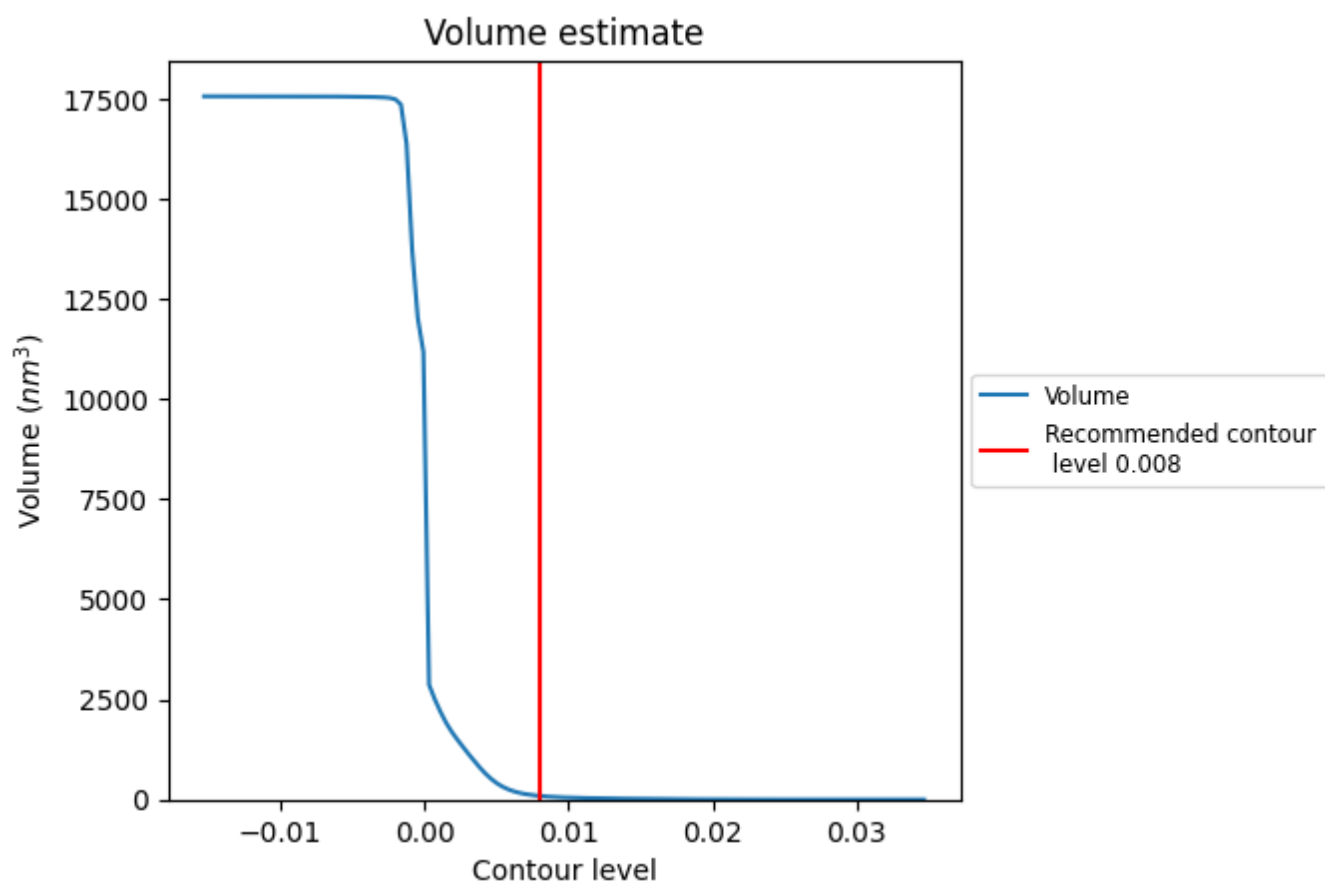
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

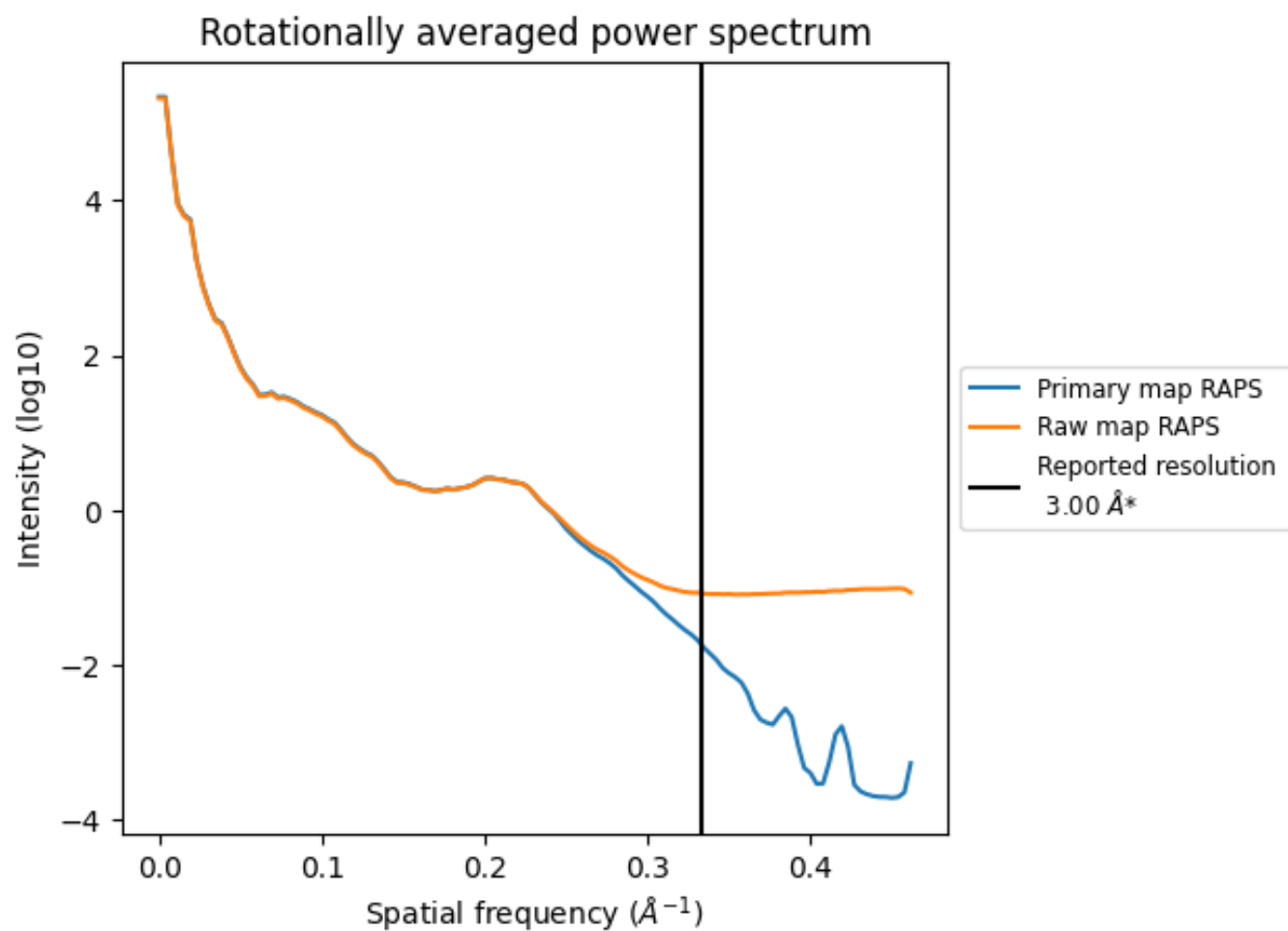
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm³; this corresponds to an approximate mass of 82 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 ⓘ

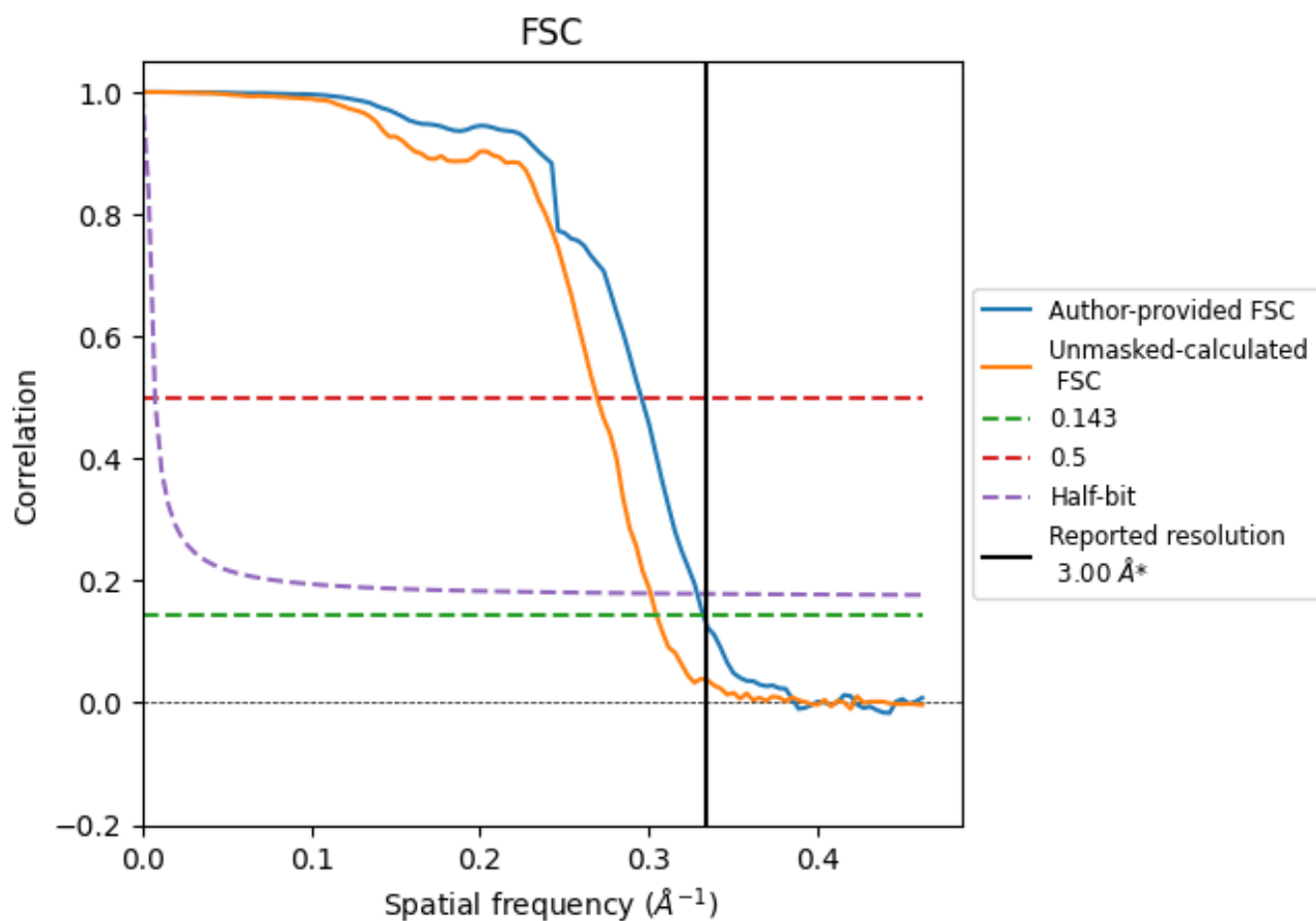


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

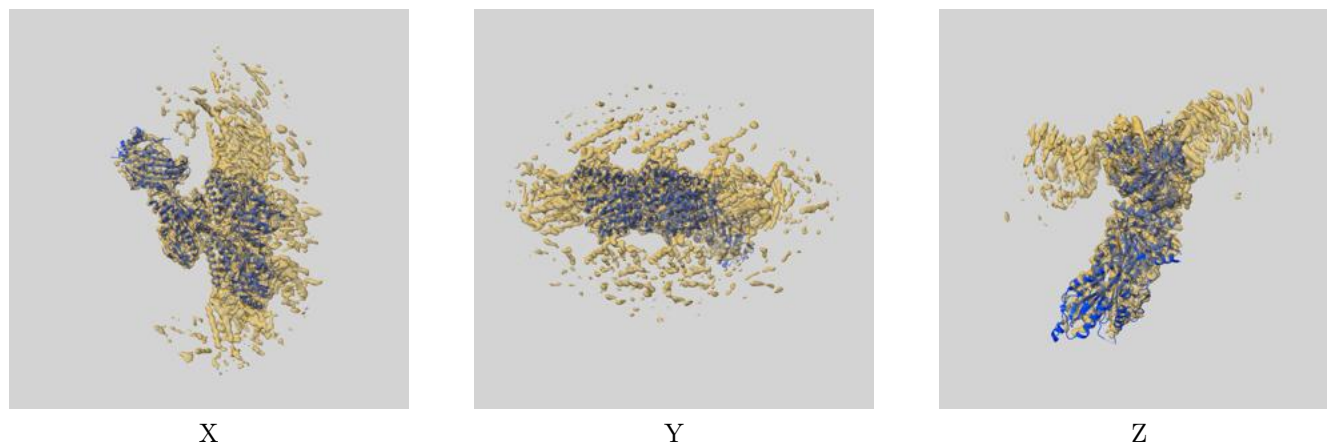
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.38	3.04
Unmasked-calculated*	3.28	3.71	3.32

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

9 Map-model fit [i](#)

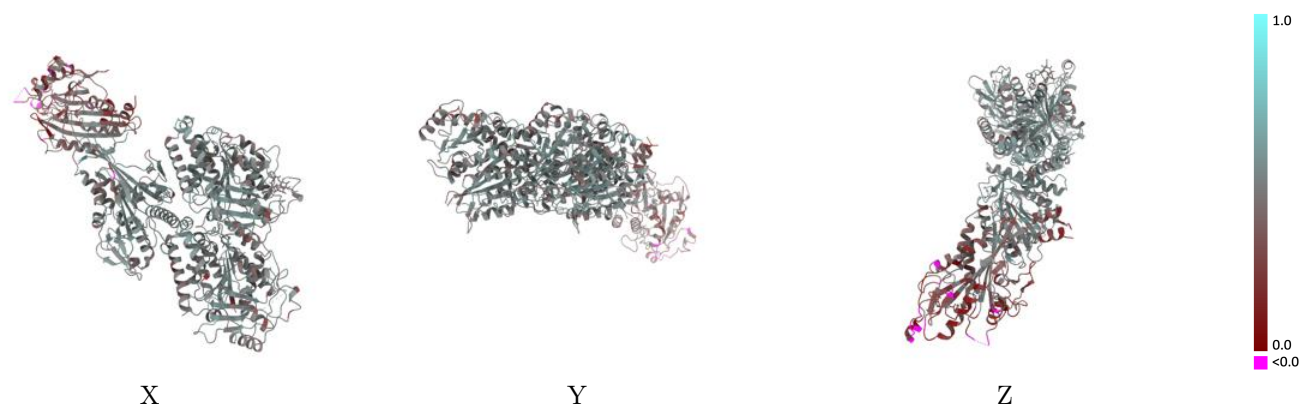
This section contains information regarding the fit between EMDB map EMD-19176 and PDB model 8RHH. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



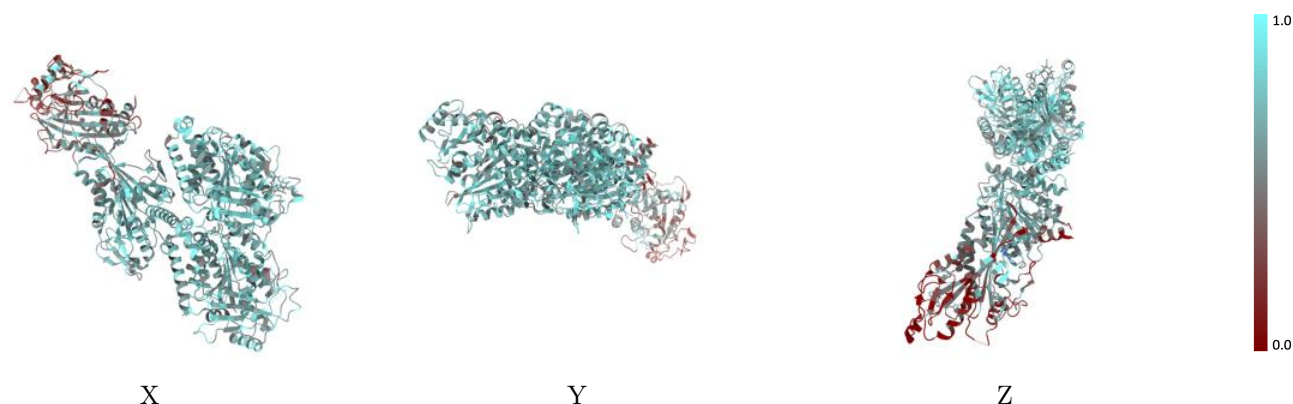
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



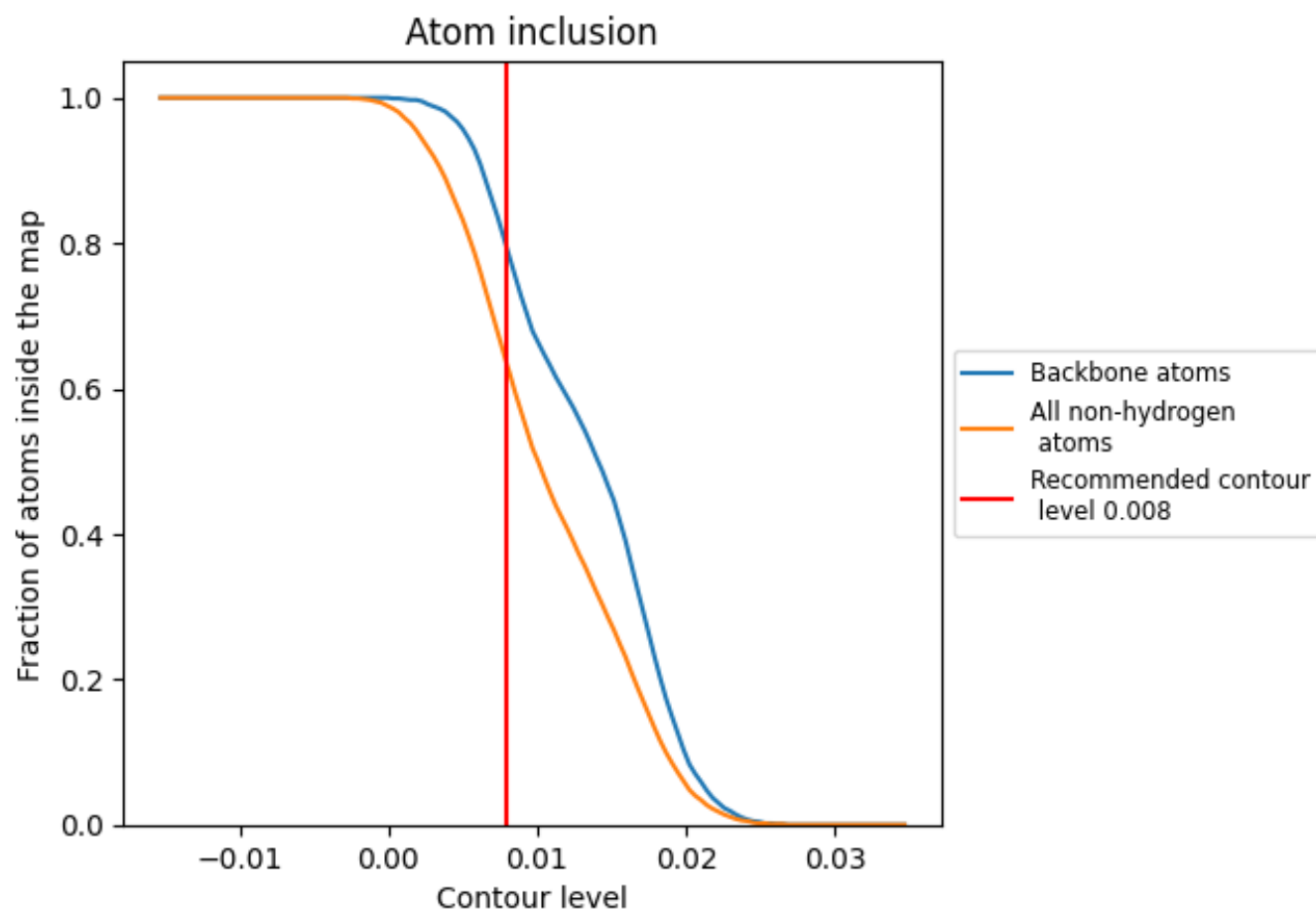
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 63% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6310	0.4620
A	0.6990	0.4970
B	0.7250	0.5100
K	0.6640	0.4960
L	0.3790	0.3080
T	0.6120	0.5990

