



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:30 AM UTC

PDB ID : 9EDS / pdb\_00009eds  
EMDB ID : EMD-47948  
Title : Tubulin cofactors D,E,G,C bound to tubulin dimer – TBCC N terminus unbound  
Authors : Taheri, A.; Al-bassam, J.  
Deposited on : 2024-11-18  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

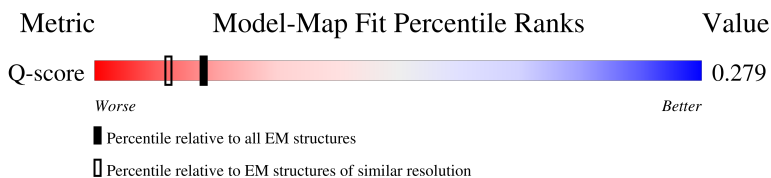
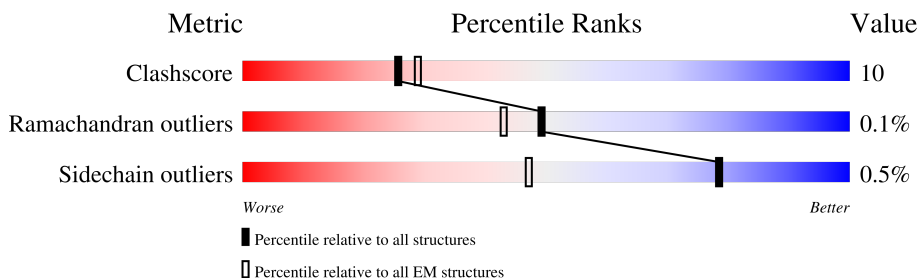
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.80 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	10198 ( 3.30 - 4.30 )

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

Mol	Chain	Length	Quality of chain
1	D	1021	
2	E	469	
3	G	191	
4	A	451	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	B	445	 74% 22%
6	I	170	 70% 22% 8%
7	C	268	 10% 54% 11% 35%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 39102 atoms, of which 18145 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 Chromosome instability protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	987	Total	C	H	N	O	S	0	0
			16156	5173	8132	1365	1455	31		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP P40987
D	-5	HIS	-	expression tag	UNP P40987
D	-4	HIS	-	expression tag	UNP P40987
D	-3	HIS	-	expression tag	UNP P40987
D	-2	HIS	-	expression tag	UNP P40987
D	-1	HIS	-	expression tag	UNP P40987
D	0	HIS	-	expression tag	UNP P40987

- Molecule 2 is a protein called Protein PAC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	456	Total	C	H	N	O	S	0	0
			3231	1558	692	488	491	2		

- Molecule 3 is a protein called GTP-binding protein CIN4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	191	Total	C	H	N	O	S	0	0
			3133	974	1591	268	288	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	73	LEU	GLN	engineered mutation	UNP P39110

- Molecule 4 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	428	Total	C	H	N	O	S	0	0
			6612	2122	3261	570	637	22		

- Molecule 5 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	427	Total	C	H	N	O	S	0	0
			6602	2110	3243	576	647	26		

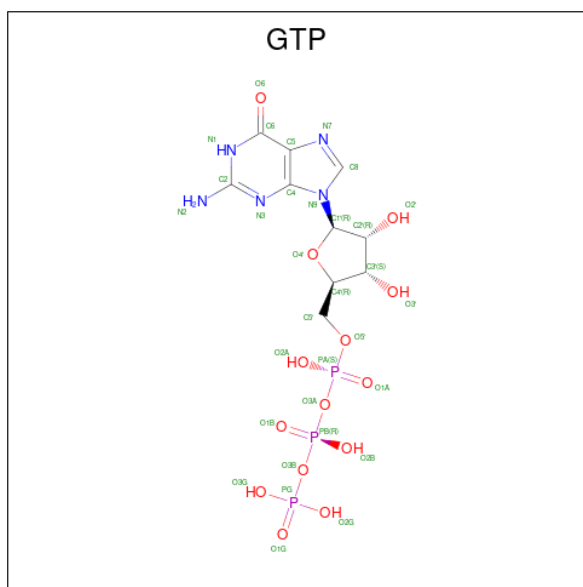
- Molecule 6 is a protein called iih5 Alpha Repeating.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	156	Total	C	H	N	O	S	0	0
			2391	746	1202	212	229	2		

- Molecule 7 is a protein called Tubulin-specific chaperone C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	C	173	Total	C	N	O	0	0
			861	515	173	173		

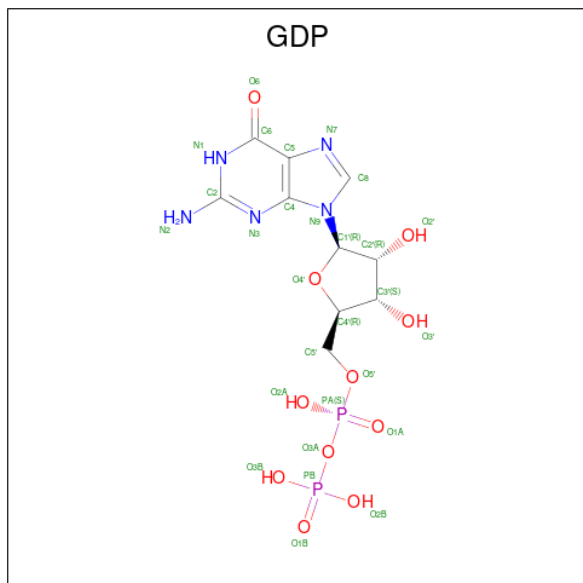
- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	
8	A	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).

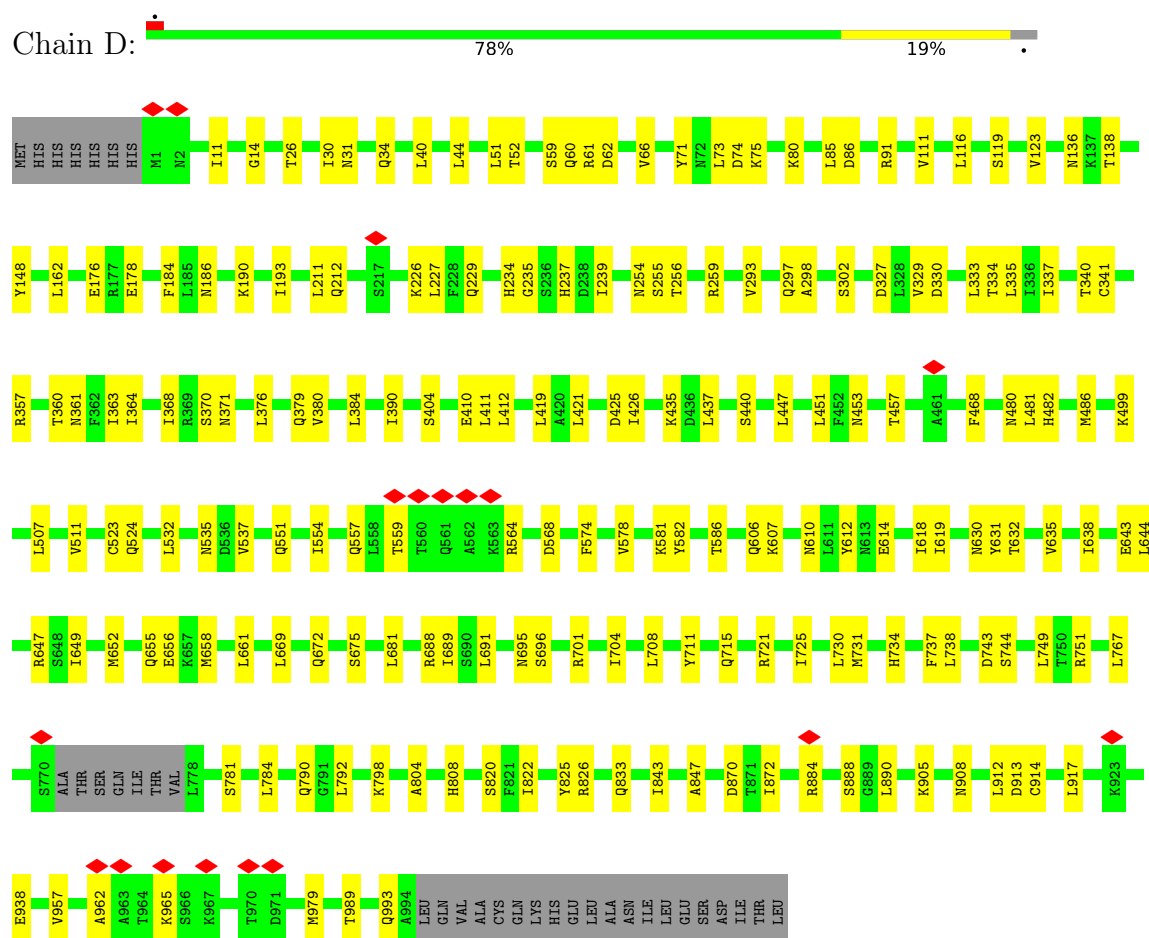


Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

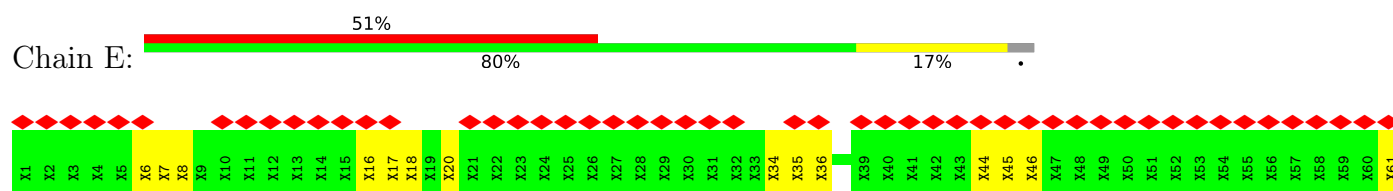
### 3 Residue-property plots

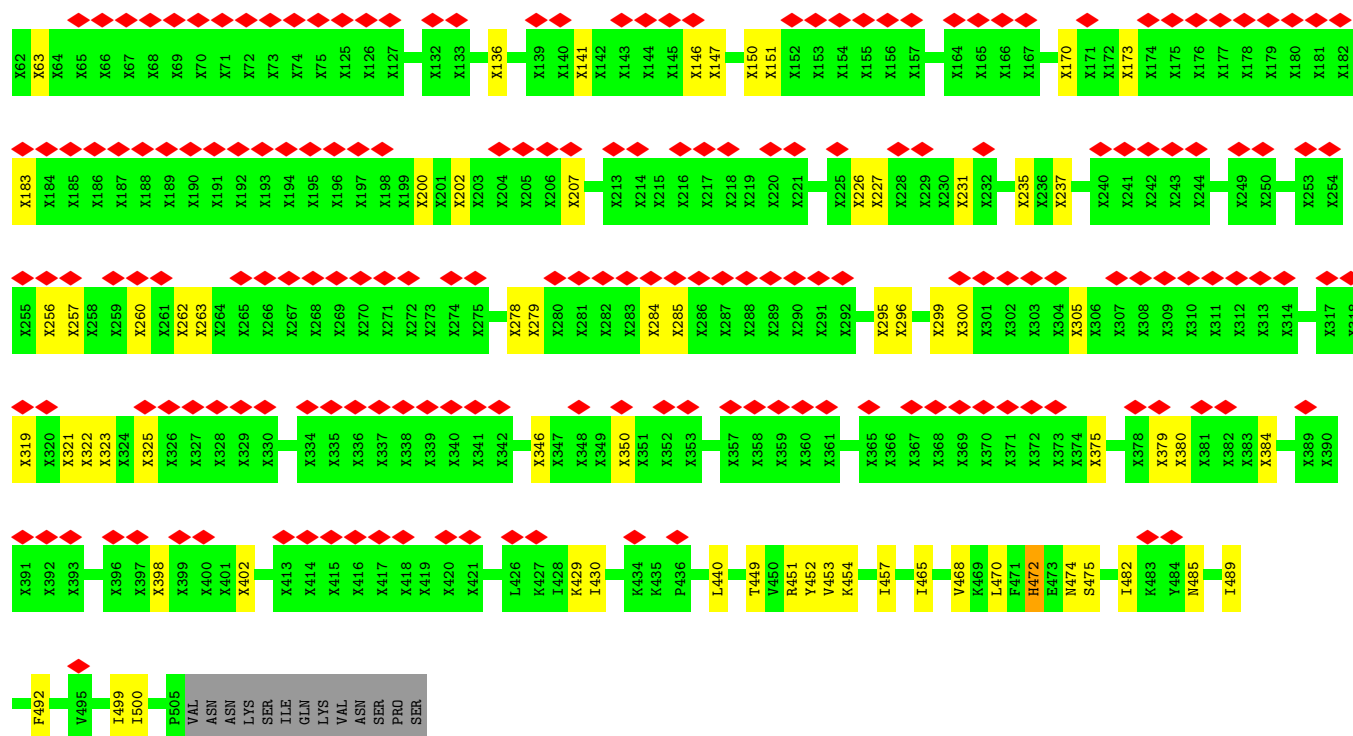
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Chromosome instability protein 1

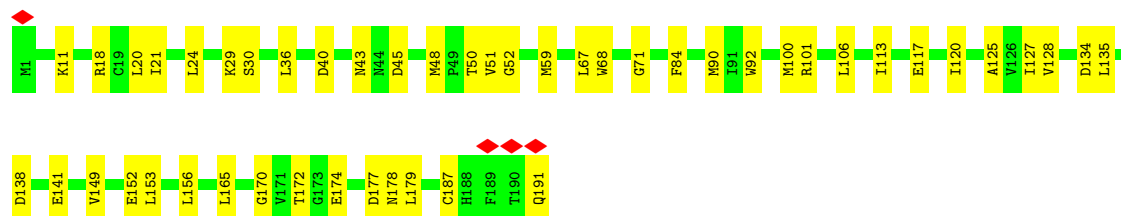
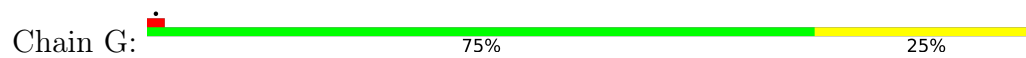


#### • Molecule 2: Protein PAC2

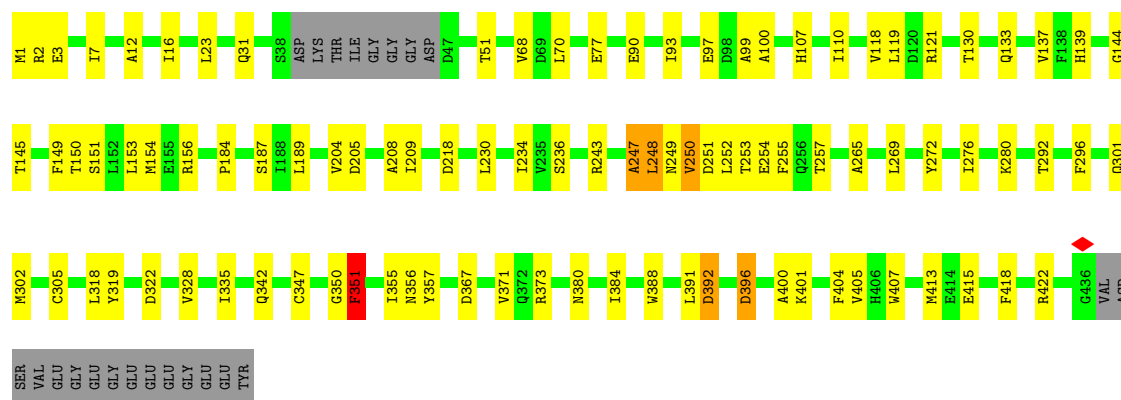




• Molecule 3: GTP-binding protein CIN4



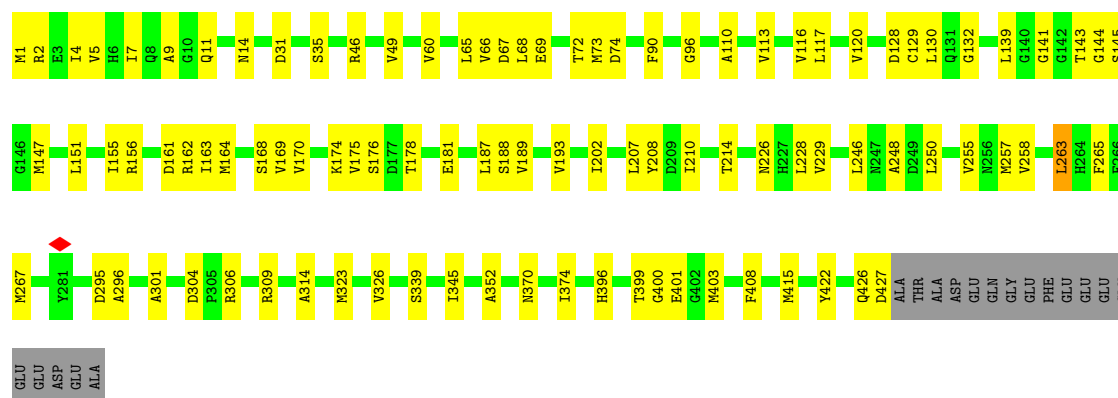
• Molecule 4: Tubulin alpha-1A chain



• Molecule 5: Tubulin beta chain

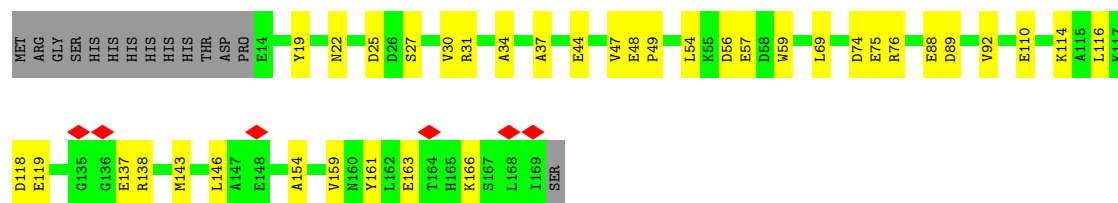


Chain B:  74% 22% .



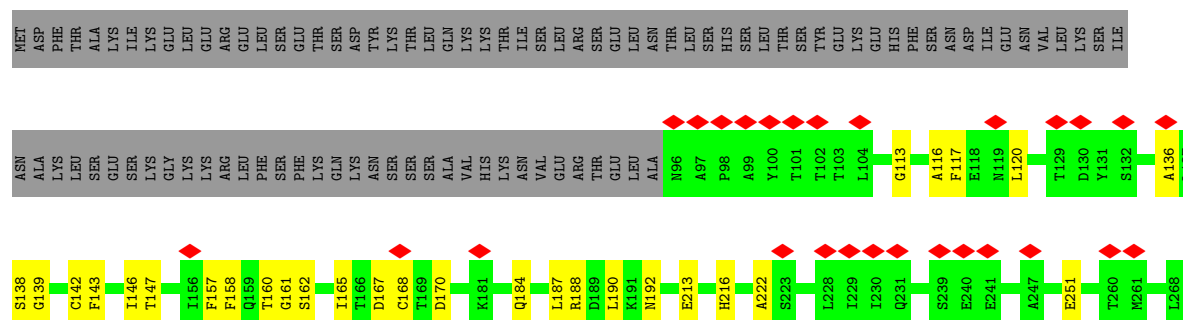
- Molecule 6: iih5 Alpha Repeating

Chain I:  70% 22% 8%



- Molecule 7: Tubulin-specific chaperone C

Chain C:  10% 54% 11% 35%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	370000, 370000, 370000, 370000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.00	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.235	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0201	Depositor
Map size ( $\text{\AA}$ )	352.0, 352.0, 352.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.88, 0.88, 0.88	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	D	0.27	0/8201	0.48	0/11110
2	E	0.21	0/694	0.44	0/938
3	G	0.28	0/1562	0.54	0/2100
4	A	0.36	0/3428	0.70	5/4653 (0.1%)
5	B	0.29	0/3434	0.49	0/4652
6	I	0.24	0/1203	0.52	0/1622
7	C	0.15	0/860	0.36	0/1200
All	All	0.28	0/19382	0.53	5/26275 (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
4	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	250	VAL	N-CA-C	18.76	132.07	108.06
4	A	250	VAL	N-CA-CB	-14.28	91.91	111.19
4	A	250	VAL	CB-CA-C	-6.88	101.20	111.80
4	A	247	ALA	N-CA-C	-5.43	105.37	111.28
4	A	351	PHE	CA-CB-CG	5.23	119.03	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	243	ARG	Sidechain

## 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	D	8024	8132	8131	136	0
2	E	2539	692	1084	55	0
3	G	1542	1591	1591	33	0
4	A	3351	3261	3259	85	0
5	B	3359	3243	3241	70	0
6	I	1189	1202	1201	25	0
7	C	861	0	369	16	0
8	A	32	12	12	5	0
8	G	32	12	12	3	0
9	B	28	0	12	5	0
All	All	20957	18145	18912	410	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 10.

All (410) 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:E:231:UNK:HA	2:E:256:UNK:HA	1.54	0.89
1:D:211:LEU:HD22	1:D:227:LEU:HD13	1.55	0.88
1:D:333:LEU:HD22	1:D:384:LEU:HD21	1.57	0.86
4:A:249:ASN:HD21	4:A:318:LEU:HG	1.41	0.86
4:A:204:VAL:HG22	4:A:302:MET:HE1	1.56	0.86
2:E:237:UNK:N	2:E:262:UNK:O	2.10	0.84
2:E:7:UNK:O	2:E:18:UNK:N	2.12	0.82
2:E:20:UNK:O	2:E:34:UNK:N	2.14	0.81
1:D:334:THR:HG23	1:D:335:LEU:HD23	1.63	0.80
1:D:612:TYR:OH	1:D:643:GLU:OE1	1.98	0.80
3:G:172:THR:OG1	3:G:174:GLU:OE1	2.00	0.80
6:I:146:LEU:HD11	6:I:154:ALA:HB1	1.64	0.80
2:E:235:UNK:N	2:E:260:UNK:O	2.15	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:CYS:HA	1:D:360:THR:HG21	1.64	0.79
5:B:145:SER:OG	5:B:188:SER:OG	2.00	0.78
2:E:296:UNK:O	2:E:322:UNK:HA	1.88	0.72
4:A:249:ASN:OD1	4:A:250:VAL:HG22	1.90	0.72
4:A:209:ILE:HG23	4:A:230:LEU:HD23	1.72	0.72
1:D:825:TYR:O	1:D:833:GLN:NE2	2.23	0.71
1:D:86:ASP:OD2	1:D:91:ARG:NH1	2.24	0.71
7:C:190:LEU:O	7:C:216:HIS:N	2.20	0.71
1:D:574:PHE:O	1:D:578:VAL:HG23	1.90	0.71
6:I:138:ARG:O	6:I:138:ARG:NH1	2.24	0.71
1:D:425:ASP:OD1	1:D:451:LEU:HD12	1.92	0.70
4:A:7:ILE:HG21	4:A:153:LEU:HD21	1.73	0.70
2:E:147:UNK:O	2:E:151:UNK:N	2.25	0.69
4:A:250:VAL:HG21	4:A:255:PHE:HD1	1.57	0.69
1:D:435:LYS:NZ	5:B:400:GLY:O	2.14	0.69
3:G:48:MET:N	3:G:48:MET:HE2	2.06	0.69
5:B:1:MET:N	5:B:128:ASP:OD1	2.22	0.68
5:B:67:ASP:OD2	5:B:72:THR:OG1	2.09	0.68
3:G:134:ASP:OD1	3:G:135:LEU:N	2.26	0.68
1:D:480:ASN:OD1	1:D:482:HIS:N	2.26	0.68
5:B:210:ILE:O	5:B:214:THR:OG1	2.08	0.67
2:E:295:UNK:CB	2:E:321:UNK:HA	2.23	0.67
4:A:253:THR:O	4:A:257:THR:HG23	1.94	0.67
1:D:40:LEU:HD23	1:D:40:LEU:O	1.95	0.67
1:D:938:GLU:OE2	1:D:938:GLU:N	2.28	0.67
1:D:711:TYR:OH	1:D:751:ARG:NH1	2.26	0.67
1:D:808:HIS:NE2	5:B:427:ASP:OD1	2.28	0.66
6:I:25:ASP:O	6:I:31:ARG:NE	2.27	0.66
1:D:715:GLN:NE2	4:A:400:ALA:O	2.28	0.66
6:I:19:TYR:CE1	6:I:37:ALA:HB3	2.31	0.66
4:A:322:ASP:OD1	4:A:373:ARG:NH2	2.28	0.65
1:D:557:GLN:N	1:D:557:GLN:OE1	2.29	0.65
3:G:177:ASP:OD1	3:G:178:ASN:N	2.30	0.65
4:A:249:ASN:ND2	4:A:318:LEU:HG	2.10	0.65
4:A:415:GLU:N	4:A:415:GLU:OE1	2.30	0.64
1:D:656:GLU:OE1	1:D:656:GLU:N	2.31	0.64
5:B:66:VAL:HG11	5:B:147:MET:HE1	1.80	0.64
2:E:36:UNK:HA	2:E:63:UNK:HA	1.80	0.64
5:B:67:ASP:OD1	5:B:68:LEU:N	2.31	0.64
2:E:296:UNK:N	2:E:321:UNK:O	2.31	0.63
2:E:451:ARG:N	2:E:485:ASN:O	2.31	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:30:SER:N	8:G:501:GTP:O2B	2.30	0.63
6:I:75:GLU:N	6:I:75:GLU:OE2	2.32	0.63
7:C:113:GLY:HA2	7:C:157:PHE:CB	2.29	0.63
6:I:137:GLU:OE1	6:I:137:GLU:N	2.31	0.63
6:I:110:GLU:OE1	6:I:114:LYS:NZ	2.32	0.63
4:A:204:VAL:HG22	4:A:302:MET:CE	2.29	0.63
1:D:743:ASP:OD1	1:D:744:SER:N	2.32	0.62
4:A:396:ASP:OD2	4:A:422:ARG:NH2	2.31	0.62
1:D:11:ILE:HD11	1:D:30:ILE:HD12	1.80	0.62
2:E:136:UNK:CB	2:E:141:UNK:HA	2.30	0.62
2:E:200:UNK:O	2:E:226:UNK:HA	1.98	0.62
2:E:380:UNK:O	2:E:384:UNK:N	2.32	0.62
5:B:155:ILE:HG22	5:B:164:MET:HE2	1.82	0.62
5:B:176:SER:OG	5:B:178:THR:O	2.17	0.62
2:E:430:ILE:HD13	2:E:457:ILE:HG12	1.82	0.62
1:D:532:LEU:HD22	1:D:537:VAL:HG21	1.82	0.61
1:D:390:ILE:HD11	1:D:468:PHE:HA	1.82	0.61
5:B:161:ASP:OD2	5:B:162:ARG:NH2	2.33	0.61
4:A:137:VAL:HG21	4:A:154:MET:HE1	1.83	0.61
7:C:116:ALA:HA	7:C:142:CYS:O	2.00	0.61
1:D:254:ASN:O	1:D:259:ARG:NH1	2.34	0.61
1:D:730:LEU:HD12	1:D:734:HIS:HD2	1.65	0.61
4:A:3:GLU:OE1	4:A:3:GLU:N	2.34	0.61
7:C:146:ILE:N	7:C:167:ASP:O	2.34	0.60
1:D:293:VAL:O	1:D:297:GLN:NE2	2.34	0.60
4:A:1:MET:SD	4:A:2:ARG:N	2.72	0.60
1:D:193:ILE:HD11	1:D:229:GLN:OE1	2.02	0.60
2:E:202:UNK:C	2:E:227:UNK:HA	2.31	0.60
4:A:209:ILE:HD12	4:A:209:ILE:H	1.66	0.60
2:E:147:UNK:HA	2:E:150:UNK:CB	2.32	0.60
5:B:309:ARG:NH1	5:B:426:GLN:O	2.35	0.60
4:A:249:ASN:HD21	4:A:318:LEU:CG	2.13	0.59
5:B:202:ILE:HG21	5:B:229:VAL:HG22	1.84	0.59
4:A:1:MET:N	4:A:130:THR:OG1	2.36	0.59
4:A:107:HIS:ND1	4:A:151:SER:OG	2.35	0.59
4:A:265:ALA:O	4:A:380:ASN:ND2	2.35	0.59
1:D:235:GLY:O	1:D:237:HIS:ND1	2.35	0.59
5:B:226:ASN:OD1	9:B:501:GDP:N1	2.35	0.59
6:I:116:LEU:O	6:I:116:LEU:HD23	2.02	0.59
5:B:226:ASN:ND2	9:B:501:GDP:O6	2.36	0.59
4:A:187:SER:HB2	4:A:391:LEU:HD21	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:GLU:OE2	1:D:647:ARG:NE	2.34	0.58
1:D:333:LEU:HD23	1:D:337:ILE:HD12	1.85	0.58
4:A:97:GLU:N	4:A:97:GLU:OE1	2.36	0.58
5:B:141:GLY:CA	9:B:501:GDP:H5'	2.34	0.58
4:A:250:VAL:HG21	4:A:255:PHE:CD1	2.37	0.58
4:A:401:LYS:NZ	5:B:427:ASP:O	2.34	0.58
4:A:68:VAL:HG11	4:A:149:PHE:CE2	2.39	0.57
5:B:66:VAL:HG11	5:B:147:MET:SD	2.44	0.57
2:E:202:UNK:N	2:E:226:UNK:O	2.37	0.57
4:A:90:GLU:O	4:A:121:ARG:NE	2.37	0.57
1:D:437:LEU:O	1:D:440:SER:OG	2.18	0.57
3:G:170:GLY:N	8:G:501:GTP:O6	2.37	0.57
4:A:145:THR:N	8:A:501:GTP:O1G	2.35	0.57
4:A:249:ASN:C	4:A:250:VAL:HG13	2.29	0.57
5:B:246:LEU:HD23	5:B:352:ALA:HB2	1.85	0.57
4:A:100:ALA:N	8:A:501:GTP:O2G	2.37	0.57
1:D:486:MET:HE1	1:D:574:PHE:CE1	2.40	0.57
5:B:2:ARG:NH2	5:B:248:ALA:O	2.37	0.57
1:D:804:ALA:O	1:D:884:ARG:NH1	2.38	0.57
5:B:73:MET:HE3	5:B:73:MET:HA	1.86	0.56
5:B:401:GLU:OE1	5:B:403:MET:N	2.38	0.56
4:A:12:ALA:O	4:A:16:ILE:HG22	2.05	0.56
4:A:269:LEU:HB2	4:A:384:ILE:HD11	1.87	0.56
1:D:327:ASP:OD1	1:D:327:ASP:N	2.36	0.56
1:D:507:LEU:O	1:D:511:VAL:HG23	2.05	0.56
1:D:638:ILE:CG2	1:D:669:LEU:HD21	2.36	0.56
1:D:957:VAL:HG21	1:D:979:MET:HE2	1.87	0.56
2:E:398:UNK:O	2:E:402:UNK:N	2.38	0.56
3:G:135:LEU:HD11	7:C:139:GLY:HA2	1.87	0.56
5:B:46:ARG:O	5:B:49:VAL:HG12	2.05	0.56
1:D:52:THR:HG21	1:D:85:LEU:CD2	2.36	0.56
1:D:612:TYR:HE1	1:D:644:LEU:HD21	1.70	0.56
5:B:139:LEU:HD13	5:B:170:VAL:HG22	1.88	0.56
4:A:189:LEU:HD11	4:A:418:PHE:CE2	2.41	0.56
1:D:681:LEU:HD11	1:D:689:ILE:HD11	1.88	0.55
1:D:564:ARG:O	1:D:606:GLN:NE2	2.40	0.55
1:D:652:MET:O	1:D:688:ARG:NH2	2.38	0.55
1:D:738:LEU:HD21	1:D:767:LEU:HD11	1.88	0.55
7:C:138:SER:HA	7:C:160:THR:O	2.06	0.55
4:A:319:TYR:CE1	4:A:328:VAL:HG13	2.40	0.55
2:E:44:UNK:N	2:E:63:UNK:O	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:202:UNK:O	2:E:227:UNK:HA	2.07	0.55
1:D:822:ILE:HD11	1:D:888:SER:HB3	1.89	0.55
4:A:405:VAL:HG13	4:A:418:PHE:CE1	2.42	0.55
1:D:361:ASN:ND2	1:D:404:SER:OG	2.39	0.55
4:A:119:LEU:HD21	4:A:156:ARG:CG	2.36	0.55
5:B:65:LEU:HD12	5:B:90:PHE:CE1	2.42	0.55
1:D:333:LEU:HD23	1:D:337:ILE:CD1	2.36	0.54
4:A:70:LEU:HD22	4:A:110:ILE:HG22	1.90	0.54
1:D:695:ASN:OD1	1:D:696:SER:N	2.40	0.54
4:A:248:LEU:HD13	4:A:355:ILE:H	1.73	0.54
1:D:635:VAL:HG22	1:D:661:LEU:HD21	1.90	0.54
4:A:301:GLN:NE2	4:A:305:CYS:O	2.39	0.54
5:B:257:MET:HE1	5:B:314:ALA:HB2	1.89	0.54
7:C:222:ALA:N	7:C:251:GLU:O	2.33	0.54
5:B:257:MET:HE1	5:B:314:ALA:CB	2.38	0.54
4:A:189:LEU:HD13	4:A:413:MET:HE1	1.90	0.54
1:D:957:VAL:HG21	1:D:979:MET:CE	2.38	0.53
4:A:144:GLY:N	8:A:501:GTP:O3G	2.41	0.53
1:D:412:LEU:HD23	1:D:426:ILE:HG23	1.91	0.53
3:G:51:VAL:HG13	3:G:51:VAL:O	2.07	0.53
4:A:276:ILE:HD11	4:A:371:VAL:HG22	1.89	0.53
1:D:31:ASN:OD1	1:D:34:GLN:NE2	2.42	0.53
3:G:59:MET:SD	3:G:59:MET:N	2.81	0.53
5:B:263:LEU:O	5:B:370:ASN:ND2	2.37	0.53
1:D:499:LYS:NZ	1:D:535:ASN:O	2.38	0.53
5:B:66:VAL:HG11	5:B:147:MET:CE	2.38	0.53
4:A:118:VAL:HG11	4:A:149:PHE:HZ	1.71	0.53
1:D:989:THR:O	1:D:993:GLN:NE2	2.42	0.53
2:E:257:UNK:HA	2:E:278:UNK:HA	1.90	0.53
4:A:218:ASP:OD1	4:A:280:LYS:NZ	2.40	0.52
6:I:118:ASP:OD1	6:I:119:GLU:N	2.43	0.52
1:D:631:TYR:O	1:D:635:VAL:HG23	2.09	0.52
3:G:106:LEU:HD11	3:G:152:GLU:OE2	2.09	0.52
4:A:250:VAL:HG12	4:A:254:GLU:OE1	2.09	0.52
1:D:453:ASN:OD1	1:D:453:ASN:N	2.42	0.52
1:D:559:THR:O	1:D:564:ARG:NH2	2.42	0.52
1:D:790:GLN:OE1	1:D:792:LEU:N	2.42	0.52
2:E:429:LYS:CE	2:E:499:ILE:HG23	2.39	0.52
2:E:470:LEU:HD11	2:E:500:ILE:CG2	2.40	0.52
1:D:186:ASN:OD1	1:D:226:LYS:NZ	2.29	0.52
1:D:486:MET:HE2	1:D:524:GLN:HE22	1.75	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:139:LEU:HD11	5:B:168:SER:HB3	1.91	0.52
1:D:708:LEU:HD21	1:D:731:MET:HE1	1.92	0.52
2:E:449:THR:HG23	2:E:452:TYR:H	1.75	0.52
6:I:44:GLU:O	6:I:47:VAL:HG23	2.09	0.52
1:D:672:GLN:O	1:D:675:SER:OG	2.26	0.52
5:B:68:LEU:O	5:B:96:GLY:N	2.43	0.52
1:D:825:TYR:HE2	1:D:890:LEU:HD12	1.74	0.51
7:C:120:LEU:O	7:C:147:THR:N	2.43	0.51
1:D:256:THR:OG1	1:D:259:ARG:NH2	2.43	0.51
2:E:45:UNK:C	2:E:61:UNK:HA	2.40	0.51
5:B:110:ALA:O	5:B:113:VAL:HG12	2.10	0.51
5:B:396:HIS:HA	5:B:399:THR:HG22	1.92	0.51
4:A:249:ASN:OD1	4:A:250:VAL:CG2	2.59	0.51
4:A:342:GLN:N	4:A:342:GLN:OE1	2.44	0.51
5:B:4:ILE:HD12	5:B:132:GLY:O	2.11	0.51
7:C:117:PHE:O	7:C:143:PHE:HA	2.11	0.50
1:D:212:GLN:CD	1:D:239:ILE:HG23	2.35	0.50
2:E:263:UNK:HA	2:E:285:UNK:CB	2.41	0.50
7:C:188:ARG:HA	7:C:213:GLU:O	2.11	0.50
1:D:691:LEU:HD23	1:D:691:LEU:O	2.12	0.50
3:G:187:CYS:SG	3:G:191:GLN:NE2	2.85	0.50
1:D:119:SER:O	1:D:123:VAL:HG23	2.11	0.50
5:B:189:VAL:HG11	5:B:415:MET:SD	2.52	0.50
2:E:472:HIS:HB2	2:E:482:ILE:HD11	1.94	0.50
1:D:532:LEU:HD22	1:D:537:VAL:HG11	1.94	0.50
1:D:71:TYR:O	1:D:74:ASP:N	2.45	0.49
3:G:24:LEU:HD13	3:G:101:ARG:HH21	1.76	0.49
2:E:453:VAL:HG21	2:E:489:ILE:CD1	2.42	0.49
4:A:205:ASP:O	4:A:209:ILE:HD12	2.12	0.49
1:D:61:ARG:NH1	1:D:62:ASP:OD1	2.45	0.49
1:D:136:ASN:N	1:D:136:ASN:OD1	2.43	0.49
6:I:56:ASP:OD1	6:I:57:GLU:N	2.45	0.49
5:B:267:MET:HG3	5:B:374:ILE:HD13	1.94	0.49
1:D:630:ASN:OD1	1:D:632:THR:OG1	2.27	0.49
1:D:781:SER:N	1:D:820:SER:OG	2.45	0.49
5:B:263:LEU:HD22	5:B:422:TYR:CE1	2.48	0.49
4:A:350:GLY:O	4:A:351:PHE:C	2.55	0.49
2:E:279:UNK:HA	2:E:299:UNK:HA	1.94	0.49
4:A:392:ASP:OD1	4:A:422:ARG:NH1	2.46	0.48
7:C:139:GLY:O	7:C:161:GLY:HA3	2.14	0.48
3:G:100:MET:SD	3:G:100:MET:N	2.83	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD22	1:D:44:LEU:HD21	1.94	0.48
4:A:119:LEU:HD21	4:A:156:ARG:HG3	1.96	0.48
1:D:872:ILE:HD11	1:D:917:LEU:HB2	1.95	0.48
3:G:92:TRP:N	3:G:127:ILE:O	2.43	0.48
5:B:181:GLU:OE2	9:B:501:GDP:H3'	2.14	0.48
1:D:333:LEU:CD1	1:D:380:VAL:HG13	2.44	0.48
1:D:607:LYS:HA	1:D:612:TYR:CD2	2.48	0.48
5:B:309:ARG:NE	5:B:339:SER:O	2.45	0.48
2:E:429:LYS:HE3	2:E:499:ILE:HG23	1.95	0.48
5:B:11:GLN:NE2	5:B:72:THR:HG22	2.28	0.48
1:D:357:ARG:O	1:D:360:THR:HG22	2.13	0.48
4:A:139:HIS:CG	4:A:150:THR:HG21	2.49	0.48
1:D:111:VAL:HG22	1:D:148:TYR:CE2	2.49	0.47
1:D:337:ILE:HD11	1:D:363:ILE:HG21	1.96	0.47
4:A:139:HIS:CD2	4:A:150:THR:HG21	2.49	0.47
1:D:638:ILE:HD11	1:D:649:ILE:HD11	1.95	0.47
4:A:99:ALA:HB3	8:A:501:GTP:O1G	2.14	0.47
4:A:292:THR:HG23	4:A:335:ILE:HD11	1.96	0.47
3:G:138:ASP:OD2	3:G:141:GLU:HB3	2.14	0.47
3:G:138:ASP:OD2	3:G:138:ASP:O	2.31	0.47
3:G:149:VAL:O	3:G:153:LEU:HD23	2.15	0.47
4:A:7:ILE:HG21	4:A:153:LEU:CD2	2.43	0.47
4:A:367:ASP:OD1	4:A:367:ASP:N	2.48	0.47
2:E:482:ILE:HG23	2:E:492:PHE:CZ	2.50	0.47
1:D:798:LYS:HD2	1:D:843:ILE:HG23	1.96	0.47
1:D:211:LEU:HD23	1:D:211:LEU:O	2.14	0.47
1:D:330:ASP:O	1:D:334:THR:HG22	2.15	0.47
1:D:523:CYS:SG	1:D:554:ILE:HD12	2.53	0.47
4:A:2:ARG:O	4:A:51:THR:HG23	2.14	0.47
4:A:187:SER:CB	4:A:391:LEU:HD21	2.45	0.47
4:A:119:LEU:HD21	4:A:156:ARG:HG2	1.96	0.47
5:B:128:ASP:OD2	5:B:129:CYS:N	2.48	0.47
5:B:304:ASP:OD1	5:B:306:ARG:NE	2.47	0.47
2:E:46:UNK:CA	2:E:61:UNK:HA	2.44	0.46
7:C:136:ALA:O	7:C:158:PHE:HA	2.15	0.46
1:D:410:GLU:OE2	3:G:11:LYS:NZ	2.36	0.46
3:G:106:LEU:HD22	3:G:156:LEU:HD11	1.97	0.46
4:A:276:ILE:HD11	4:A:371:VAL:CG2	2.45	0.46
2:E:8:UNK:HA	2:E:17:UNK:HA	1.97	0.46
2:E:474:ASN:OD1	2:E:475:SER:N	2.47	0.46
4:A:251:ASP:OD1	4:A:252:LEU:N	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ILE:CD1	1:D:384:LEU:HD22	2.44	0.46
5:B:69:GLU:OE2	5:B:72:THR:HG23	2.16	0.46
5:B:207:LEU:HD12	5:B:228:LEU:HB2	1.97	0.46
5:B:323:MET:HA	5:B:326:VAL:HG12	1.97	0.46
1:D:211:LEU:HD22	1:D:227:LEU:CD1	2.37	0.46
2:E:257:UNK:O	2:E:279:UNK:N	2.49	0.46
1:D:568:ASP:OD2	1:D:610:ASN:ND2	2.45	0.46
2:E:46:UNK:N	2:E:61:UNK:HA	2.31	0.46
4:A:133:GLN:NE2	4:A:251:ASP:OD1	2.47	0.46
6:I:74:ASP:OD1	6:I:76:ARG:HG3	2.15	0.46
1:D:614:GLU:O	1:D:618:ILE:HG22	2.15	0.46
3:G:128:VAL:CG2	3:G:165:LEU:HD23	2.46	0.46
5:B:187:LEU:HD11	5:B:408:PHE:CE1	2.51	0.46
4:A:70:LEU:HD13	4:A:110:ILE:CG2	2.46	0.45
1:D:371:ASN:OD1	1:D:371:ASN:O	2.33	0.45
3:G:43:ASN:OD1	3:G:45:ASP:N	2.47	0.45
3:G:113:ILE:O	3:G:117:GLU:N	2.49	0.45
1:D:190:LYS:O	1:D:193:ILE:HG22	2.15	0.45
5:B:5:VAL:HG11	5:B:120:VAL:HG23	1.98	0.45
6:I:44:GLU:OE2	6:I:76:ARG:NH2	2.49	0.45
1:D:337:ILE:HA	1:D:340:THR:HG22	1.97	0.45
3:G:21:ILE:CD1	3:G:67:LEU:HD12	2.46	0.45
1:D:364:ILE:HD12	1:D:384:LEU:HD22	1.98	0.45
3:G:90:MET:N	3:G:125:ALA:O	2.47	0.45
5:B:7:ILE:HD13	5:B:151:LEU:HD21	1.99	0.45
3:G:36:LEU:HD21	3:G:179:LEU:HD22	1.98	0.45
1:D:847:ALA:HB1	1:D:912:LEU:HD21	1.98	0.45
1:D:872:ILE:HD11	1:D:914:CYS:SG	2.57	0.45
3:G:106:LEU:HD11	3:G:152:GLU:CD	2.41	0.45
2:E:430:ILE:HD12	2:E:440:LEU:HD11	1.99	0.45
5:B:258:VAL:HG12	5:B:258:VAL:O	2.17	0.45
3:G:84:PHE:CZ	3:G:120:ILE:HD11	2.51	0.45
4:A:70:LEU:HD13	4:A:110:ILE:HB	1.99	0.45
6:I:54:LEU:HD21	6:I:69:LEU:HD12	1.99	0.45
6:I:88:GLU:OE1	6:I:88:GLU:N	2.37	0.45
1:D:870:ASP:OD1	1:D:872:ILE:HG22	2.17	0.44
2:E:146:UNK:O	2:E:150:UNK:N	2.50	0.44
4:A:93:ILE:HD11	4:A:121:ARG:HG3	1.99	0.44
1:D:329:VAL:HG11	1:D:376:LEU:HD22	1.98	0.44
6:I:74:ASP:OD1	6:I:76:ARG:N	2.46	0.44
2:E:375:UNK:O	2:E:379:UNK:N	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:205:ASP:O	4:A:208:ALA:N	2.51	0.44
4:A:392:ASP:OD1	4:A:422:ARG:CZ	2.65	0.44
5:B:31:ASP:OD1	5:B:35:SER:N	2.46	0.44
1:D:44:LEU:HD13	1:D:80:LYS:HB3	1.99	0.44
1:D:71:TYR:OH	5:B:74:ASP:OD2	2.28	0.44
2:E:284:UNK:HA	2:E:305:UNK:O	2.18	0.44
4:A:209:ILE:HD12	4:A:209:ILE:N	2.32	0.44
4:A:296:PHE:CE1	4:A:335:ILE:HD13	2.52	0.44
7:C:146:ILE:O	7:C:168:CYS:HA	2.17	0.44
1:D:329:VAL:O	1:D:333:LEU:HG	2.18	0.44
1:D:447:LEU:O	1:D:451:LEU:HD23	2.18	0.44
1:D:551:GLN:OE1	1:D:551:GLN:HA	2.18	0.44
2:E:136:UNK:CA	2:E:141:UNK:HA	2.48	0.44
3:G:20:LEU:HD13	3:G:68:TRP:HB2	1.99	0.44
4:A:247:ALA:HB3	6:I:59:TRP:NE1	2.33	0.44
4:A:250:VAL:HG23	4:A:250:VAL:O	2.18	0.44
5:B:14:ASN:N	5:B:14:ASN:OD1	2.49	0.44
5:B:202:ILE:HG22	5:B:207:LEU:HD21	1.99	0.44
1:D:825:TYR:CE2	1:D:890:LEU:HD12	2.52	0.44
1:D:480:ASN:OD1	1:D:481:LEU:N	2.51	0.43
2:E:6:UNK:N	2:E:18:UNK:O	2.51	0.43
1:D:59:SER:OG	1:D:60:GLN:N	2.52	0.43
1:D:457:THR:HG22	1:D:457:THR:O	2.17	0.43
1:D:704:ILE:HD12	1:D:730:LEU:CD2	2.47	0.43
4:A:404:PHE:HE2	5:B:345:ILE:HD12	1.83	0.43
6:I:19:TYR:HE1	6:I:37:ALA:HB3	1.81	0.43
1:D:701:ARG:NH2	1:D:737:PHE:O	2.44	0.43
2:E:278:UNK:O	2:E:299:UNK:HA	2.19	0.43
4:A:407:TRP:CD2	5:B:255:VAL:HG22	2.52	0.43
1:D:116:LEU:C	1:D:116:LEU:HD23	2.43	0.43
2:E:453:VAL:HG21	2:E:489:ILE:HD11	2.00	0.43
3:G:40:ASP:OD1	3:G:40:ASP:N	2.49	0.43
2:E:300:UNK:HA	2:E:325:UNK:HA	1.99	0.43
4:A:405:VAL:HG13	4:A:418:PHE:HE1	1.81	0.43
5:B:263:LEU:HD22	5:B:422:TYR:CZ	2.53	0.43
1:D:333:LEU:HD12	1:D:380:VAL:HG13	2.01	0.43
2:E:183:UNK:N	2:E:207:UNK:O	2.52	0.43
6:I:27:SER:OG	6:I:30:VAL:HG23	2.18	0.43
1:D:368:ILE:CG2	1:D:411:LEU:HD13	2.48	0.43
2:E:482:ILE:HG23	2:E:492:PHE:CE1	2.54	0.43
3:G:18:ARG:HE	3:G:68:TRP:NE1	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:LYS:N	8:G:501:GTP:O2B	2.52	0.43
4:A:371:VAL:HG12	4:A:373:ARG:H	1.83	0.43
7:C:165:ILE:O	7:C:187:LEU:HA	2.19	0.43
7:C:170:ASP:HA	7:C:192:ASN:O	2.19	0.43
1:D:364:ILE:HD11	1:D:384:LEU:O	2.19	0.43
1:D:962:ALA:O	1:D:965:LYS:NZ	2.51	0.43
6:I:22:ASN:OD1	6:I:34:ALA:HB2	2.19	0.43
1:D:655:GLN:HA	1:D:658:MET:HE2	2.00	0.42
1:D:721:ARG:O	1:D:725:ILE:HD12	2.19	0.42
4:A:184:PRO:HA	4:A:391:LEU:HD11	2.00	0.42
1:D:234:HIS:O	1:D:234:HIS:ND1	2.52	0.42
4:A:249:ASN:C	4:A:250:VAL:CG1	2.93	0.42
4:A:356:ASN:OD1	4:A:357:TYR:N	2.53	0.42
5:B:9:ALA:HB1	5:B:144:GLY:HA2	2.01	0.42
6:I:89:ASP:HB3	6:I:92:VAL:HG12	2.02	0.42
1:D:178:GLU:HB3	1:D:184:PHE:CE1	2.54	0.42
5:B:267:MET:HG2	5:B:301:ALA:HB3	2.01	0.42
1:D:905:LYS:O	1:D:908:ASN:OD1	2.38	0.42
2:E:465:ILE:HD12	2:E:465:ILE:H	1.84	0.42
5:B:141:GLY:N	9:B:501:GDP:H5'	2.34	0.42
5:B:193:VAL:HG22	5:B:265:PHE:CE1	2.55	0.42
1:D:749:LEU:HD13	1:D:767:LEU:HG	2.02	0.42
2:E:8:UNK:HA	2:E:16:UNK:O	2.20	0.42
2:E:17:UNK:O	2:E:35:UNK:HA	2.20	0.42
5:B:139:LEU:HD12	5:B:169:VAL:C	2.45	0.42
1:D:176:GLU:OE2	1:D:176:GLU:N	2.48	0.42
1:D:582:TYR:HE1	1:D:586:THR:HG21	1.86	0.41
5:B:163:ILE:HG21	5:B:250:LEU:HB3	2.02	0.41
1:D:581:LYS:HA	1:D:618:ILE:HD11	2.02	0.41
2:E:454:LYS:NZ	2:E:468:VAL:O	2.53	0.41
4:A:23:LEU:HD23	4:A:236:SER:CB	2.51	0.41
5:B:68:LEU:HD23	5:B:143:THR:HG23	2.01	0.41
5:B:295:ASP:OD1	5:B:296:ALA:N	2.53	0.41
1:D:254:ASN:OD1	1:D:255:SER:N	2.53	0.41
3:G:30:SER:OG	3:G:50:THR:OG1	2.33	0.41
4:A:249:ASN:HD21	4:A:318:LEU:CD2	2.33	0.41
1:D:51:LEU:HD22	1:D:66:VAL:HG23	2.01	0.41
1:D:71:TYR:CD1	1:D:71:TYR:C	2.98	0.41
1:D:138:THR:HB	1:D:162:LEU:HD21	2.01	0.41
5:B:116:VAL:HG21	5:B:151:LEU:HD11	2.02	0.41
6:I:159:VAL:HG12	6:I:163:GLU:OE1	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:145:THR:OG1	8:A:501:GTP:O1G	2.34	0.41
6:I:48:GLU:CD	6:I:49:PRO:HD3	2.45	0.41
1:D:507:LEU:O	1:D:507:LEU:HD23	2.20	0.41
1:D:784:LEU:HD12	1:D:820:SER:HB3	2.03	0.41
2:E:319:UNK:O	2:E:323:UNK:HA	2.21	0.41
1:D:190:LYS:HB2	1:D:226:LYS:HZ3	1.86	0.41
1:D:419:LEU:HD12	1:D:421:LEU:HD12	2.02	0.41
4:A:384:ILE:HG22	4:A:388:TRP:HD1	1.86	0.41
5:B:117:LEU:HA	5:B:120:VAL:HG12	2.01	0.41
5:B:175:VAL:O	5:B:175:VAL:HG12	2.20	0.41
6:I:143:MET:HE3	6:I:161:TYR:CG	2.56	0.41
3:G:52:GLY:O	3:G:71:GLY:N	2.53	0.41
5:B:130:LEU:HD21	5:B:162:ARG:HH11	1.86	0.41
6:I:116:LEU:HD22	6:I:154:ALA:HB2	2.03	0.41
1:D:379:GLN:OE1	1:D:380:VAL:N	2.54	0.40
1:D:913:ASP:OD1	1:D:913:ASP:N	2.54	0.40
1:D:826:ARG:HA	1:D:826:ARG:HE	1.86	0.40
2:E:170:UNK:O	2:E:173:UNK:N	2.54	0.40
4:A:31:GLN:HA	4:A:31:GLN:OE1	2.21	0.40
5:B:174:LYS:HD3	5:B:208:TYR:CD2	2.57	0.40
1:D:14:GLY:HA3	1:D:26:THR:HG21	2.02	0.40
2:E:346:UNK:O	2:E:350:UNK:N	2.54	0.40
1:D:30:ILE:HD11	1:D:73:LEU:HG	2.03	0.40
1:D:298:ALA:HB1	1:D:302:SER:OG	2.21	0.40
4:A:234:ILE:HG12	4:A:272:TYR:HB2	2.02	0.40
5:B:156:ARG:HD2	5:B:164:MET:HE1	2.03	0.40
1:D:618:ILE:HG23	1:D:619:ILE:N	2.37	0.40
7:C:162:SER:HA	7:C:184:GLN:O	2.22	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	D	983/1021 (96%)	947 (96%)	36 (4%)	0	100	100
2	E	83/469 (18%)	81 (98%)	2 (2%)	0	100	100
3	G	189/191 (99%)	182 (96%)	7 (4%)	0	100	100
4	A	424/451 (94%)	413 (97%)	10 (2%)	1 (0%)	43	73
5	B	425/445 (96%)	410 (96%)	15 (4%)	0	100	100
6	I	154/170 (91%)	152 (99%)	1 (1%)	1 (1%)	21	54
7	C	171/268 (64%)	163 (95%)	8 (5%)	0	100	100
All	All	2429/3015 (81%)	2348 (97%)	79 (3%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	351	PHE
6	I	166	LYS

### 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	D	919/950 (97%)	917 (100%)	2 (0%)	87	87
2	E	78/93 (84%)	77 (99%)	1 (1%)	61	71
3	G	178/178 (100%)	178 (100%)	0	100	100
4	A	360/377 (96%)	354 (98%)	6 (2%)	53	67
5	B	368/381 (97%)	366 (100%)	2 (0%)	81	81
6	I	117/135 (87%)	117 (100%)	0	100	100
All	All	2020/2114 (96%)	2009 (100%)	11 (0%)	78	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	75	LYS
1	D	370	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	472	HIS
4	A	77	GLU
4	A	248	LEU
4	A	347	CYS
4	A	351	PHE
4	A	392	ASP
4	A	396	ASP
5	B	60	VAL
5	B	263	LEU

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

Mol	Chain	Res	Type
1	D	34	GLN
1	D	166	ASN
1	D	561	GLN
1	D	621	GLN
1	D	734	HIS
1	D	766	GLN
1	D	993	GLN
3	G	191	GLN
4	A	192	HIS
5	B	396	HIS
6	I	60	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 oligosaccharides in this entry.



## 5.6 Ligand geometry

3 ligands are modelled in this entry.

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
9	GDP	B	501	-	29,30,30	1.63	5 (17%)	45,47,47	1.63	7 (15%)
8	GTP	A	501	-	33,34,34	2.26	8 (24%)	50,54,54	1.78	12 (24%)
8	GTP	G	501	-	33,34,34	2.29	6 (18%)	50,54,54	1.80	12 (24%)

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
9	GDP	B	501	-	-	3/16/32/32	0/3/3/3
8	GTP	A	501	-	-	6/22/38/38	0/3/3/3
8	GTP	G	501	-	-	0/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	501	GTP	PA-O5'	6.07	1.83	1.59
8	G	501	GTP	PB-O3B	-6.03	1.53	1.59
8	A	501	GTP	PB-O3A	5.87	1.65	1.59
8	A	501	GTP	PA-O5'	5.71	1.81	1.59
8	A	501	GTP	PB-O3B	-5.70	1.53	1.59
8	G	501	GTP	PB-O3A	5.35	1.65	1.59
8	G	501	GTP	PA-O3A	-5.10	1.54	1.59
9	B	501	GDP	PA-O3A	-5.06	1.54	1.59
8	A	501	GTP	PA-O3A	-4.99	1.54	1.59
9	B	501	GDP	PA-O5'	3.56	1.73	1.59
8	G	501	GTP	O5'-C5'	-2.66	1.34	1.44
8	A	501	GTP	O4'-C4'	-2.47	1.39	1.45
8	A	501	GTP	O5'-C5'	-2.39	1.35	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	501	GTP	C2-N2	2.31	1.39	1.34
9	B	501	GDP	O4'-C1'	-2.26	1.36	1.42
9	B	501	GDP	O5'-C5'	-2.25	1.36	1.44
8	G	501	GTP	O4'-C1'	-2.25	1.36	1.42
8	A	501	GTP	O4'-C1'	-2.22	1.36	1.42
9	B	501	GDP	O3'-C3'	-2.06	1.37	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	O2A-PA-O3A	5.86	123.11	107.27
8	G	501	GTP	O2B-PB-O3A	-5.45	92.53	107.27
8	A	501	GTP	O2B-PB-O3A	-5.39	92.70	107.27
8	A	501	GTP	O3A-PA-O1A	3.90	122.45	110.70
8	G	501	GTP	O5'-PA-O1A	-3.55	94.86	108.94
8	G	501	GTP	O3A-PA-O1A	3.53	121.34	110.70
8	A	501	GTP	O5'-PA-O1A	-3.48	95.15	108.94
8	A	501	GTP	O2B-PB-O3B	3.28	116.15	107.27
8	G	501	GTP	O2B-PB-O3B	3.28	116.14	107.27
8	G	501	GTP	O2A-PA-O3A	3.27	116.12	107.27
9	B	501	GDP	C3'-C2'-C1'	-3.03	95.73	101.46
8	G	501	GTP	C3'-C2'-C1'	-2.85	96.07	101.46
9	B	501	GDP	O3A-PB-O1B	-2.83	96.12	111.04
8	A	501	GTP	O2A-PA-O3A	2.75	114.70	107.27
9	B	501	GDP	O6-C6-N1	-2.56	115.30	120.11
8	A	501	GTP	C3'-C2'-C1'	-2.54	96.65	101.46
9	B	501	GDP	O5'-PA-O1A	-2.52	98.93	108.94
8	G	501	GTP	C2-N1-C6	-2.48	120.61	125.11
8	G	501	GTP	N1-C2-N3	2.47	127.85	123.32
8	G	501	GTP	O6-C6-N1	-2.46	115.48	120.11
8	A	501	GTP	O6-C6-N1	-2.43	115.54	120.11
8	A	501	GTP	O2A-PA-O5'	-2.39	96.72	107.57
8	A	501	GTP	N1-C2-N3	2.36	127.64	123.32
8	A	501	GTP	O3'-C3'-C4'	-2.35	104.34	111.08
8	G	501	GTP	O2A-PA-O5'	-2.30	97.14	107.57
9	B	501	GDP	O6-C6-C5	2.26	132.50	126.53
8	G	501	GTP	O3'-C3'-C4'	-2.25	104.62	111.08
8	A	501	GTP	C2-N1-C6	-2.25	121.04	125.11
9	B	501	GDP	N1-C2-N3	2.18	127.31	123.32
8	G	501	GTP	C2'-C1'-N9	-2.18	107.19	113.25
8	A	501	GTP	O3A-PB-O1B	-2.14	104.28	110.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

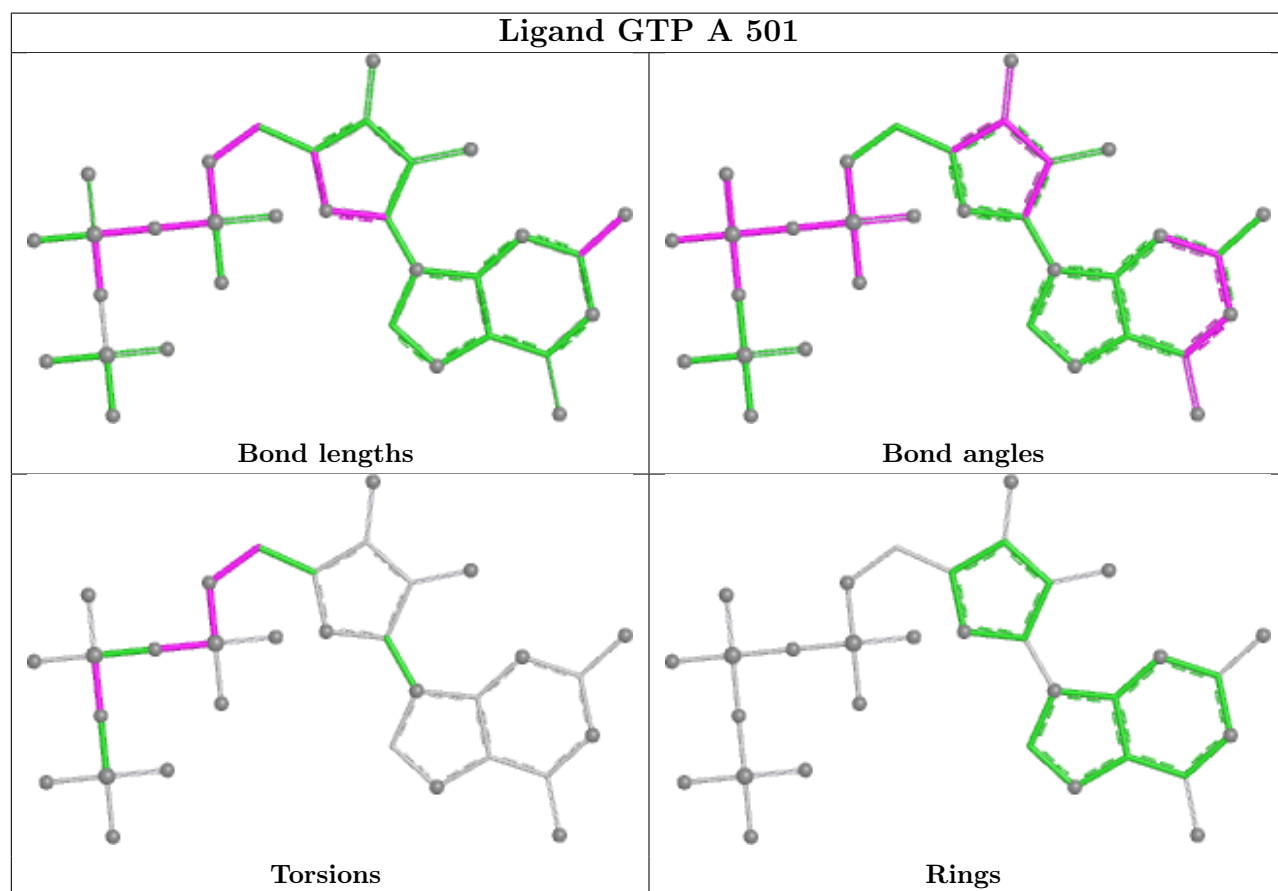
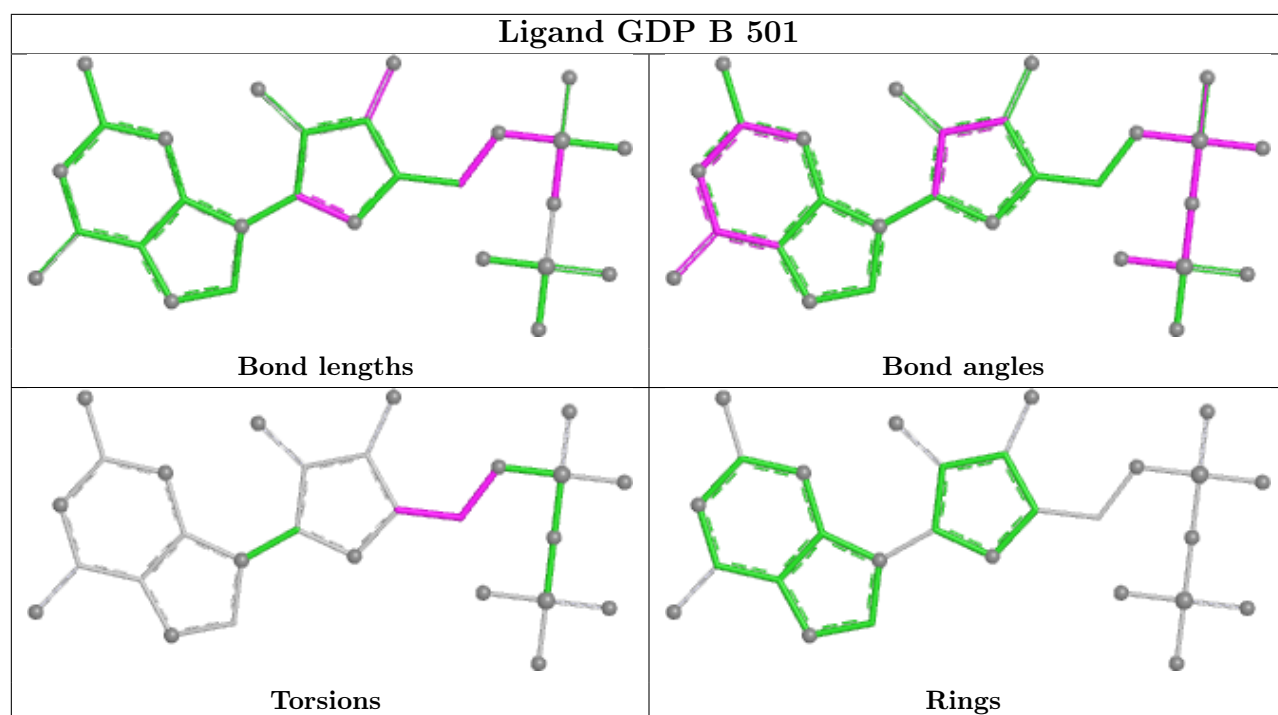
Mol	Chain	Res	Type	Atoms
8	A	501	GTP	C5'-O5'-PA-O3A
8	A	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	O4'-C4'-C5'-O5'
9	B	501	GDP	C3'-C4'-C5'-O5'
8	A	501	GTP	PB-O3A-PA-O1A
8	A	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C4'-C5'-O5'-PA
8	A	501	GTP	C4'-C5'-O5'-PA
8	A	501	GTP	PG-O3B-PB-O1B

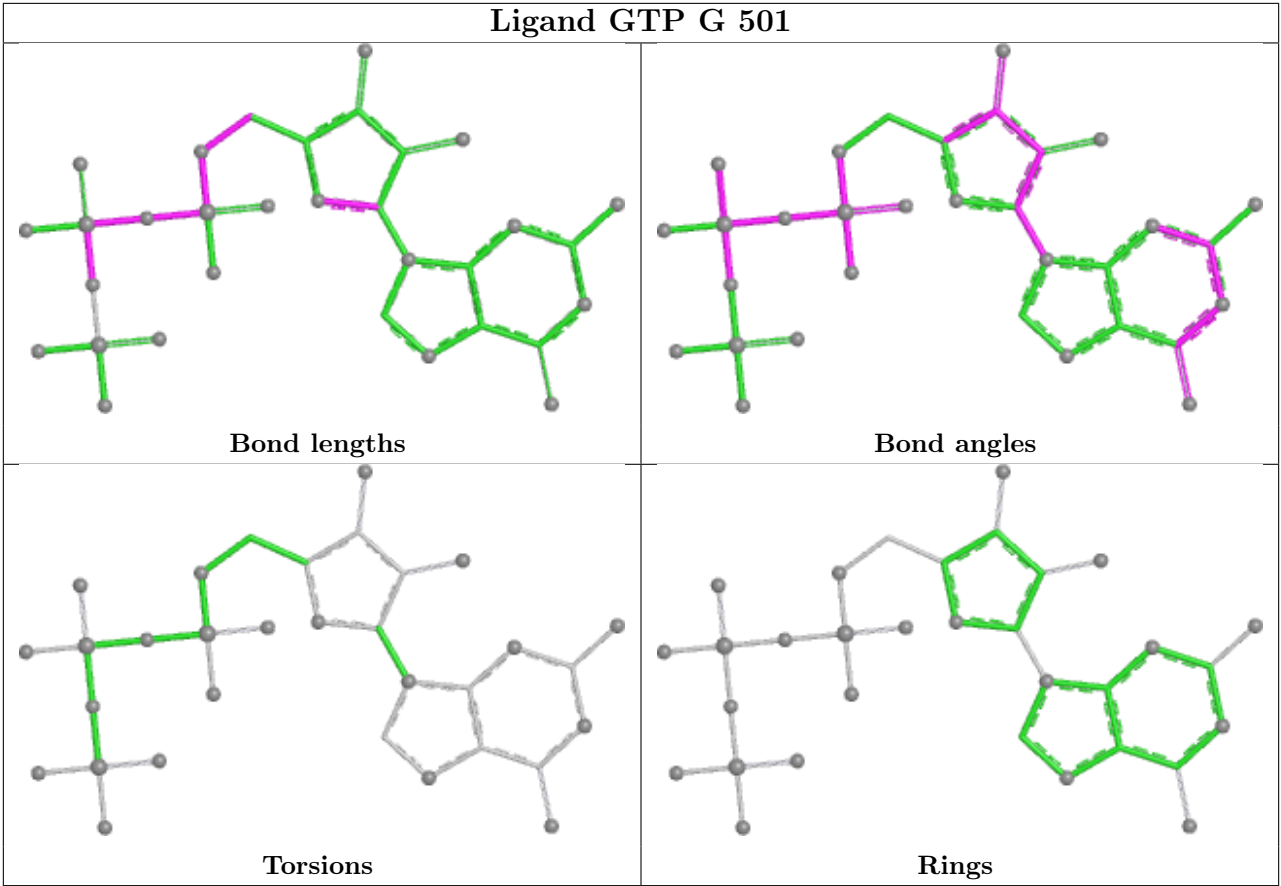
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	GDP	5	0
8	A	501	GTP	5	0
8	G	501	GTP	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	75:UNK	C	125:UNK	N	26.74

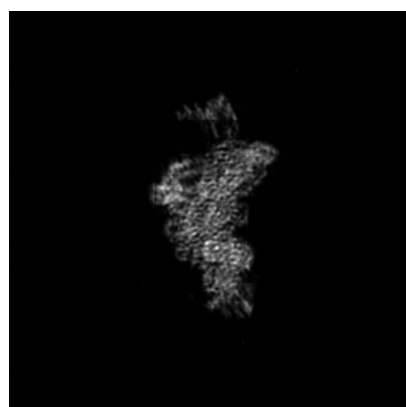
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47948. These allow visual inspection of the internal detail of the map and identification of artifacts.

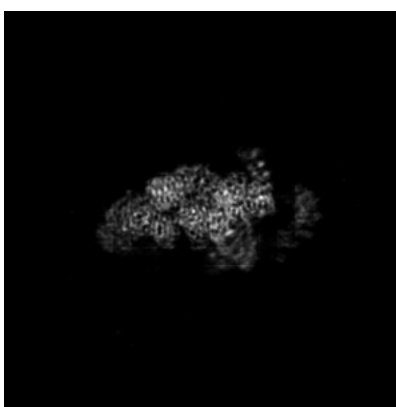
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

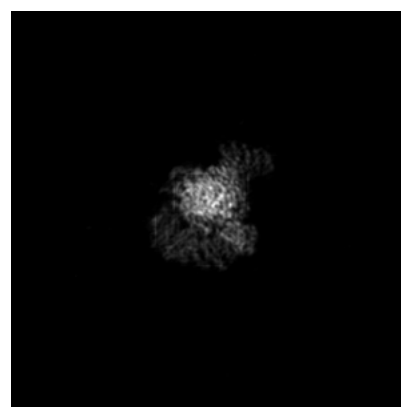
#### 6.1.1 Primary map



X



Y



Z

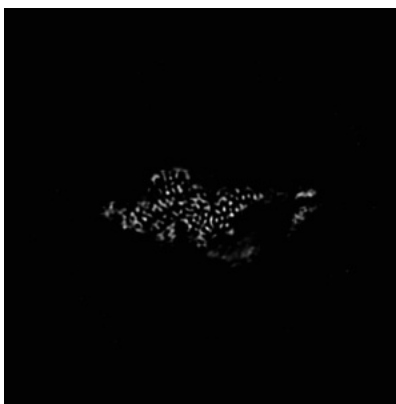
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

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: 198



Y Index: 206

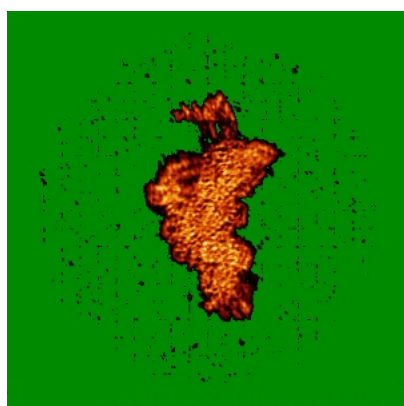


Z Index: 222

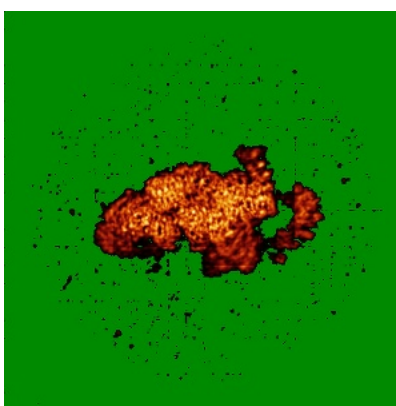
The images above show the largest variance slices of the map in three orthogonal directions.

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

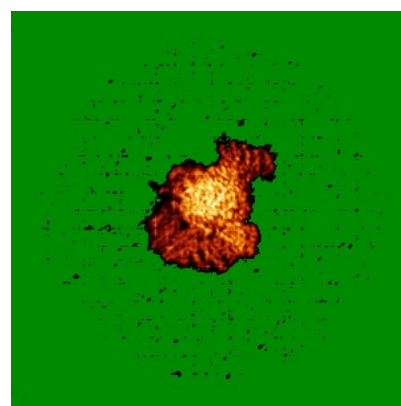
### 6.4.1 Primary map



X



Y

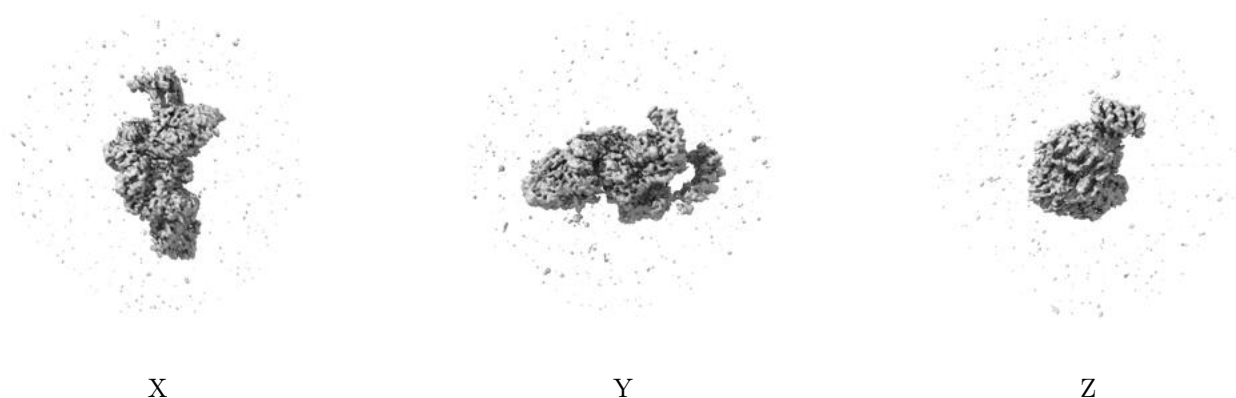


Z

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 0.0201. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

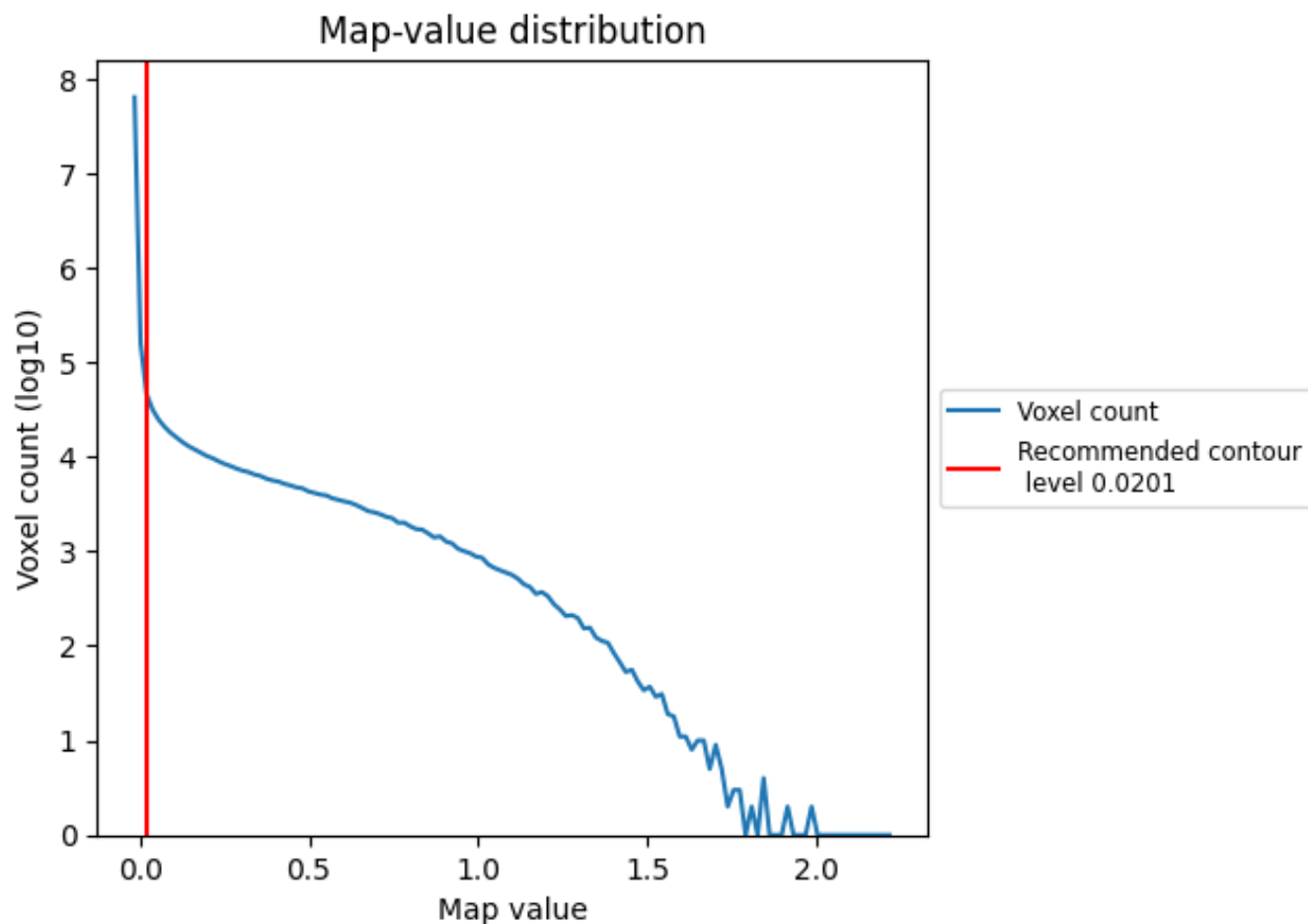
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

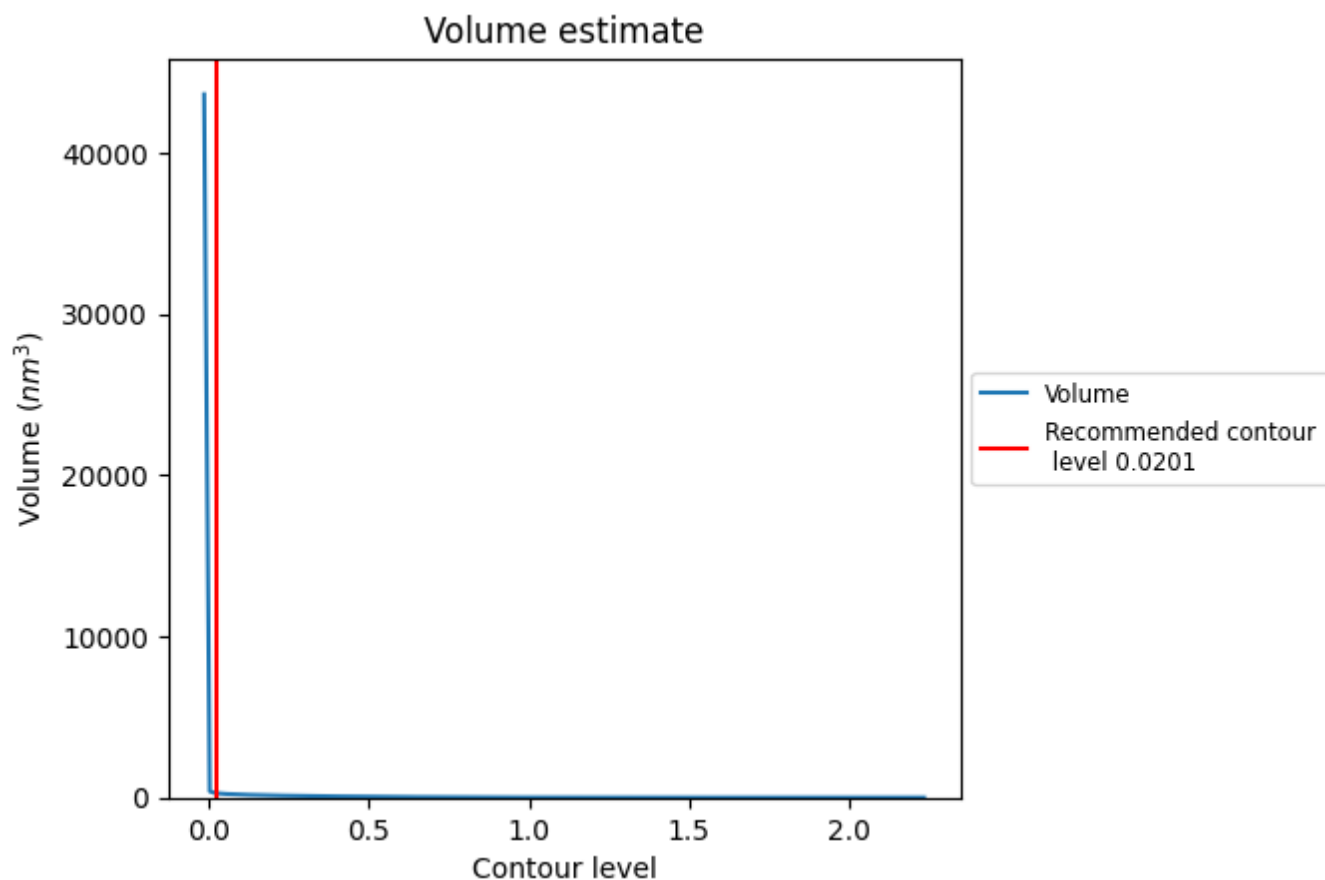
This section contains the results of statistical analysis of the map.

### 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.

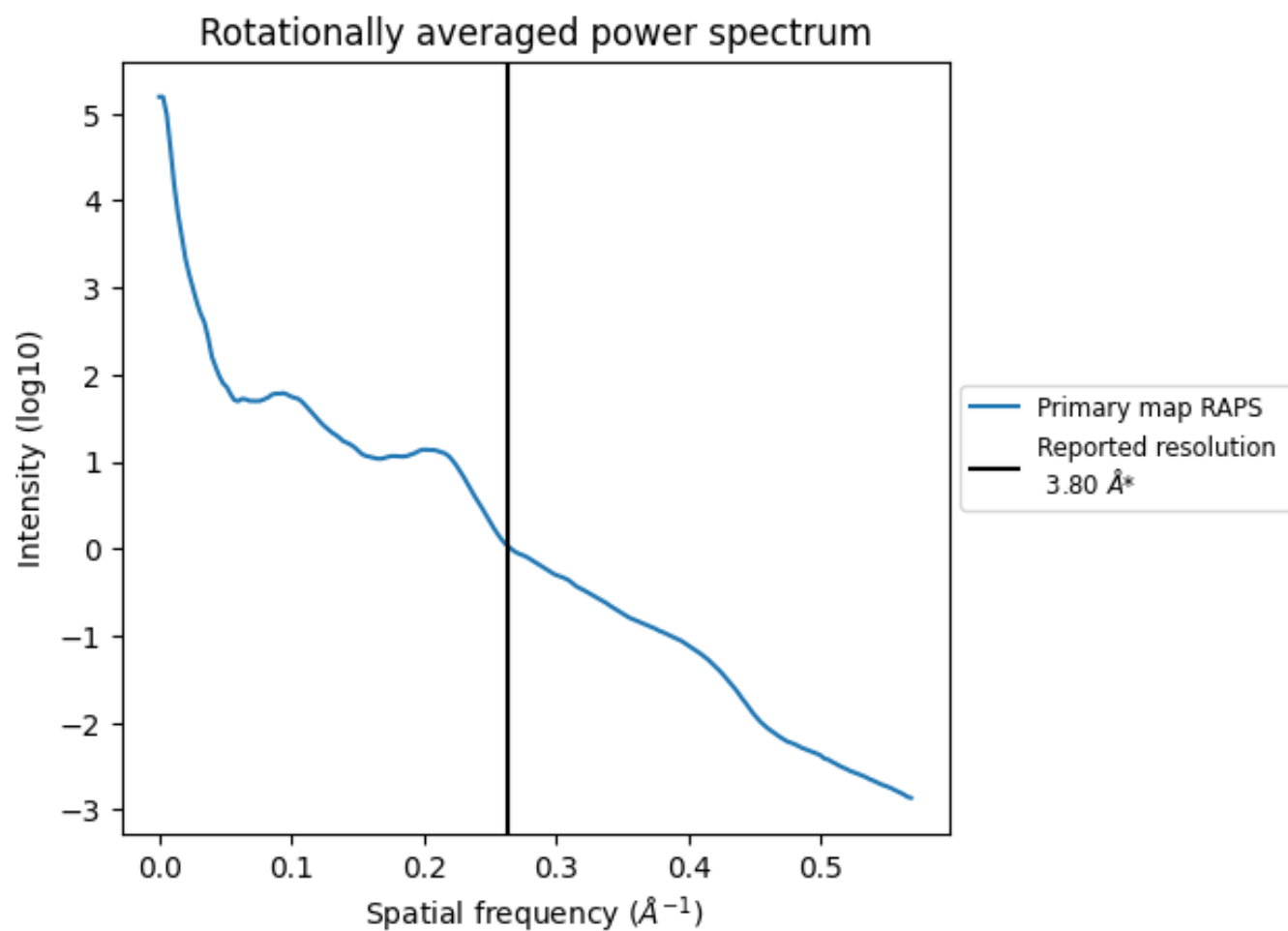
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 272 nm<sup>3</sup>; this corresponds to an approximate mass of 246 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 0.263 Å<sup>-1</sup>

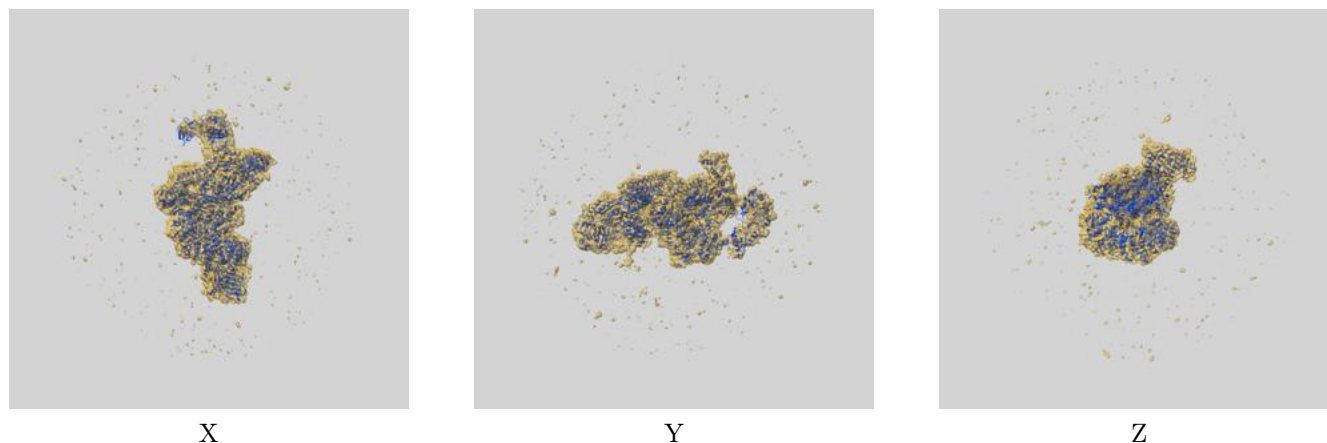
## 8 Fourier-Shell correlation ⓘ

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

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

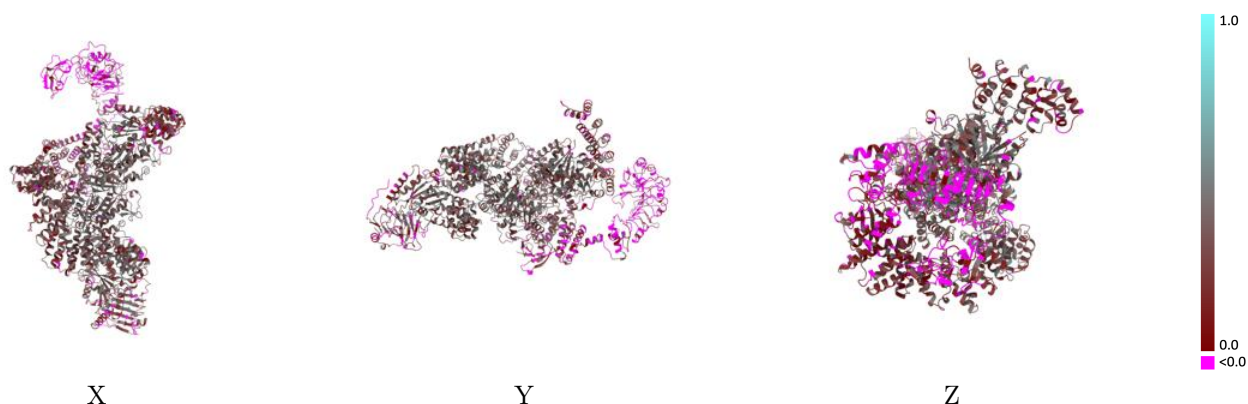
This section contains information regarding the fit between EMDB map EMD-47948 and PDB model 9EDS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



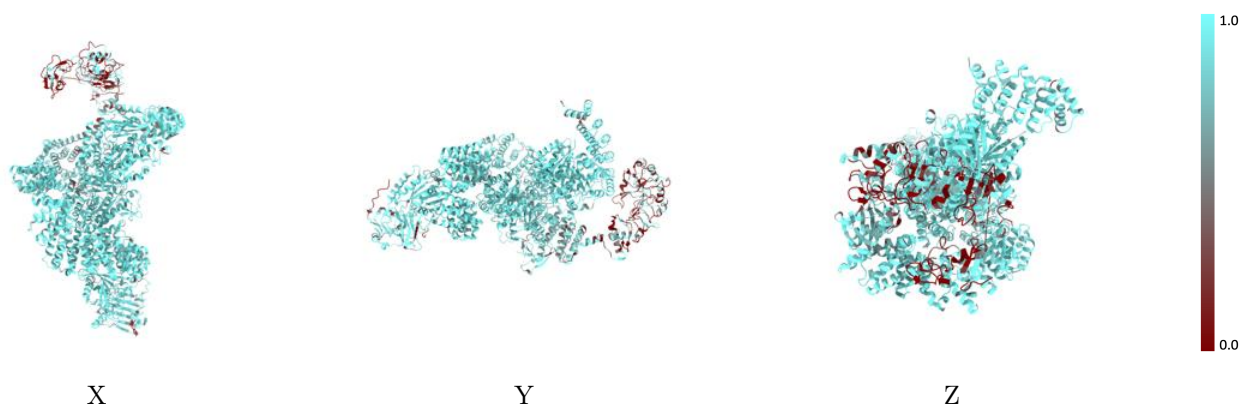
The images above show the 3D surface view of the map at the recommended contour level 0.0201 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



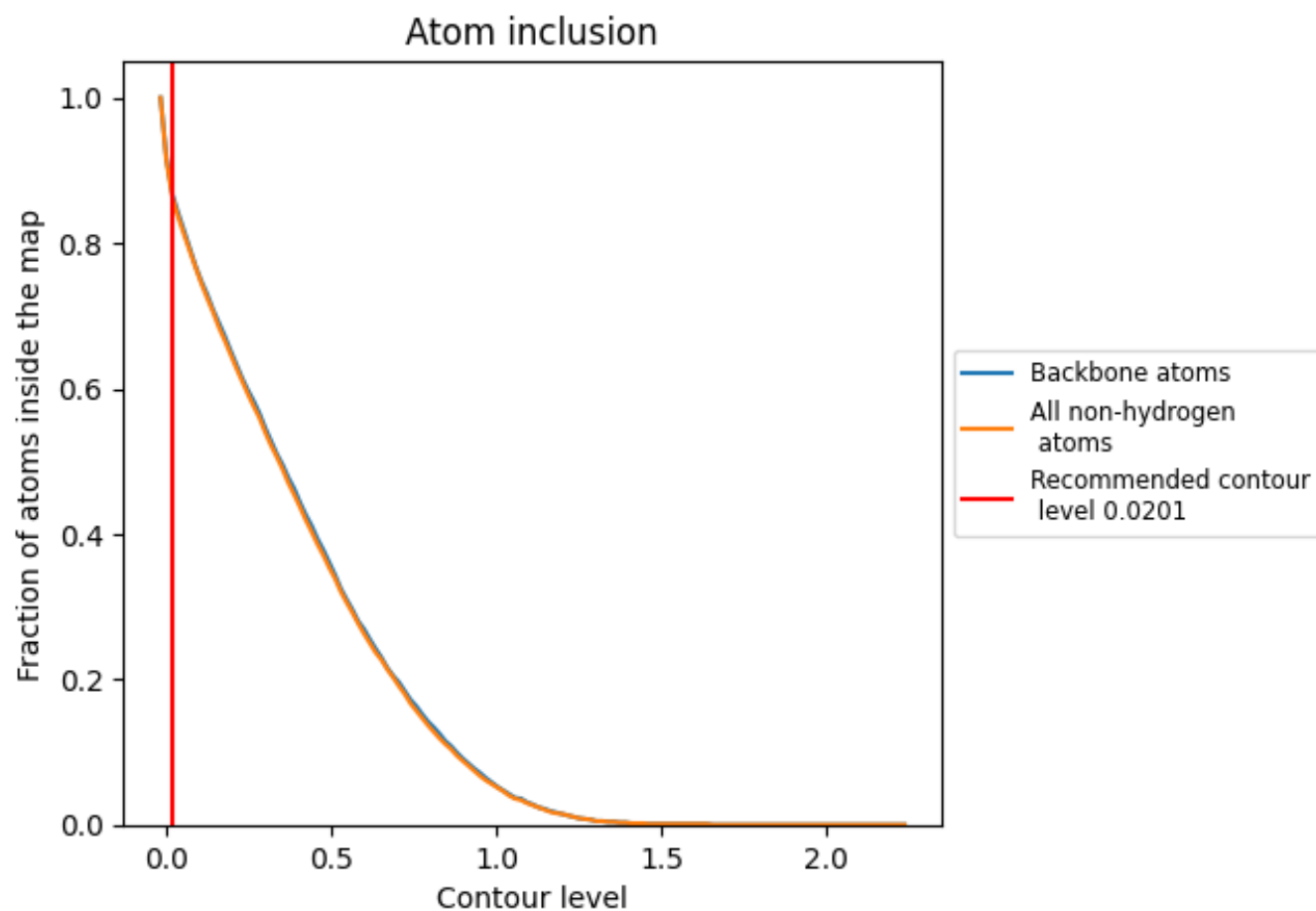
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0201).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.0201) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8620</div>	<div><div></div>0.2790</div>
A	<div><div></div>0.9460</div>	<div><div></div>0.3650</div>
B	<div><div></div>0.9300</div>	<div><div></div>0.3650</div>
C	<div><div></div>0.7840</div>	<div><div></div>0.1970</div>
D	<div><div></div>0.9030</div>	<div><div></div>0.2880</div>
E	<div><div></div>0.4920</div>	<div><div></div>0.0510</div>
G	<div><div></div>0.9090</div>	<div><div></div>0.3070</div>
I	<div><div></div>0.8830</div>	<div><div></div>0.2340</div>

1.0

0.0

<0.0