



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:16 AM UTC

PDB ID : 6QUS / pdb_00006qus
EMDB ID : EMD-4643
Title : HsCKK (human CAMSAP1) decorated 13pf taxol-GDP microtubule
Authors : Atherton, J.M.; Luo, Y.; Xiang, S.; Yang, C.; Jiang, K.; Stangier, M.; Vemu, A.; Cook, A.; Wang, S.; Roll-Mecak, A.; Steinmetz, M.O.; Akhmanova, A.; Baldus, M.; Moores, C.A.
Deposited on : 2019-02-28
Resolution : 3.70 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:

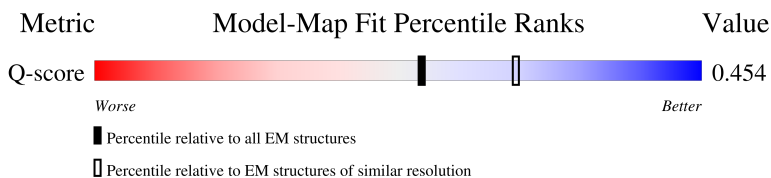
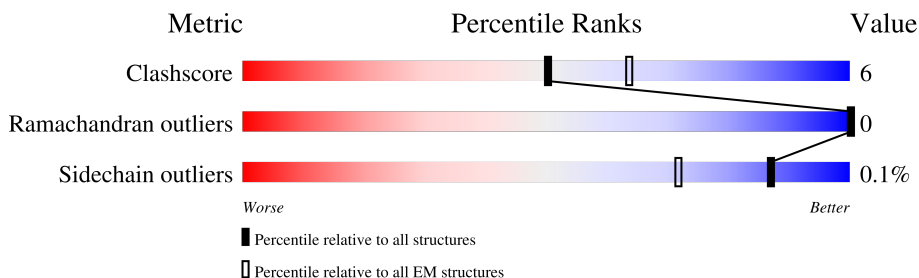
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 Å.

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



Metric	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	11569 (3.20 - 4.20)

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	O	451	
1	X	451	
2	I	174	
3	S	444	

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Mol	Chain	Length	Quality of chain
3	U	444	 79%18%•

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14715 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 alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		
1	O	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		

- Molecule 2 is a protein called Calmodulin-regulated spectrin-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	118	Total	C	N	O	S	0	0
			951	605	164	175	7		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1440	MET	-	initiating methionine	UNP Q5T5Y3
I	1441	GLY	-	expression tag	UNP Q5T5Y3
I	1442	SER	-	expression tag	UNP Q5T5Y3
I	1443	SER	-	expression tag	UNP Q5T5Y3
I	1444	HIS	-	expression tag	UNP Q5T5Y3
I	1445	HIS	-	expression tag	UNP Q5T5Y3
I	1446	HIS	-	expression tag	UNP Q5T5Y3
I	1447	HIS	-	expression tag	UNP Q5T5Y3
I	1448	HIS	-	expression tag	UNP Q5T5Y3
I	1449	HIS	-	expression tag	UNP Q5T5Y3
I	1450	SER	-	expression tag	UNP Q5T5Y3
I	1451	SER	-	expression tag	UNP Q5T5Y3
I	1452	GLY	-	expression tag	UNP Q5T5Y3
I	1453	LEU	-	expression tag	UNP Q5T5Y3
I	1454	VAL	-	expression tag	UNP Q5T5Y3
I	1455	PRO	-	expression tag	UNP Q5T5Y3
I	1456	ARG	-	expression tag	UNP Q5T5Y3
I	1457	GLY	-	expression tag	UNP Q5T5Y3
I	1458	SER	-	expression tag	UNP Q5T5Y3

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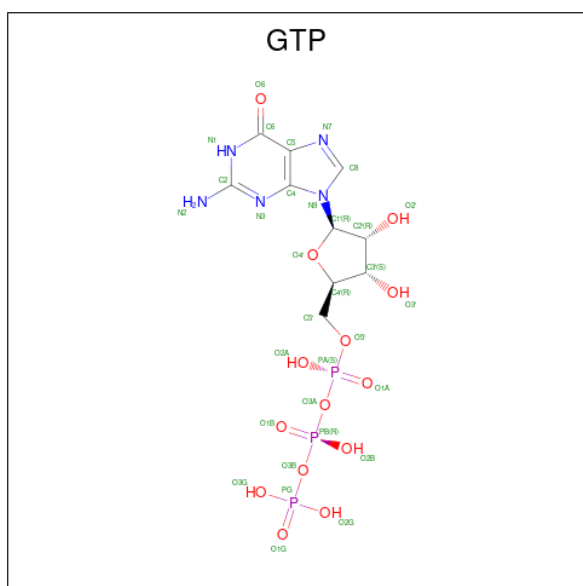
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Chain	Residue	Modelled	Actual	Comment	Reference
I	1459	HIS	-	expression tag	UNP Q5T5Y3
I	1460	MET	-	expression tag	UNP Q5T5Y3
I	1461	ALA	-	expression tag	UNP Q5T5Y3
I	1462	SER	-	expression tag	UNP Q5T5Y3
I	1463	MET	-	expression tag	UNP Q5T5Y3
I	1464	THR	-	expression tag	UNP Q5T5Y3
I	1465	GLY	-	expression tag	UNP Q5T5Y3
I	1466	GLY	-	expression tag	UNP Q5T5Y3
I	1467	GLN	-	expression tag	UNP Q5T5Y3
I	1468	GLN	-	expression tag	UNP Q5T5Y3
I	1469	MET	-	expression tag	UNP Q5T5Y3
I	1470	GLY	-	expression tag	UNP Q5T5Y3
I	1471	ARG	-	expression tag	UNP Q5T5Y3
I	1472	GLY	-	expression tag	UNP Q5T5Y3
I	1473	SER	THR	conflict	UNP Q5T5Y3

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	431	Total	C	N	O	S	0	0
			3377	2123	578	652	24		
3	S	431	Total	C	N	O	S	0	0
			3377	2123	578	652	24		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

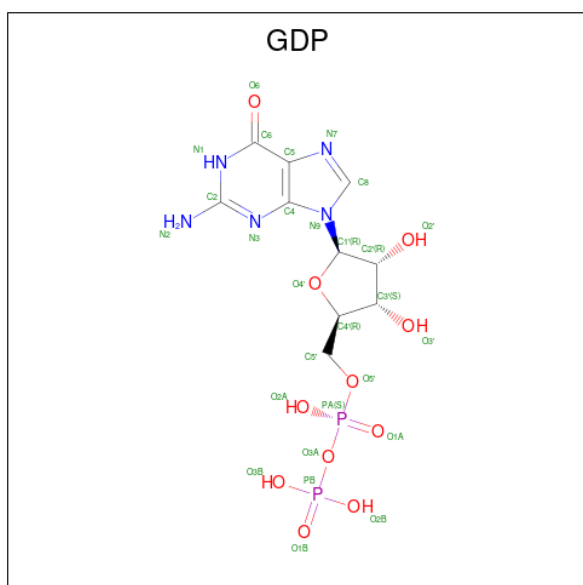


Mol	Chain	Residues	Atoms					AltConf
4	X	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

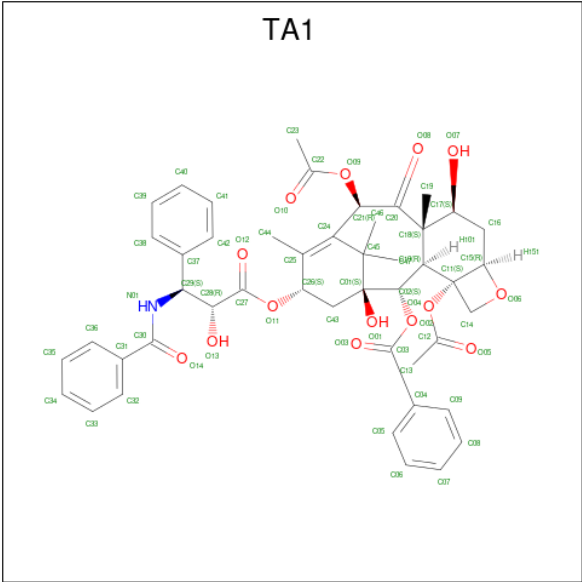
Mol	Chain	Residues	Atoms		AltConf
5	X	1	Total	Mg	0
			1	1	
5	O	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 7 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).

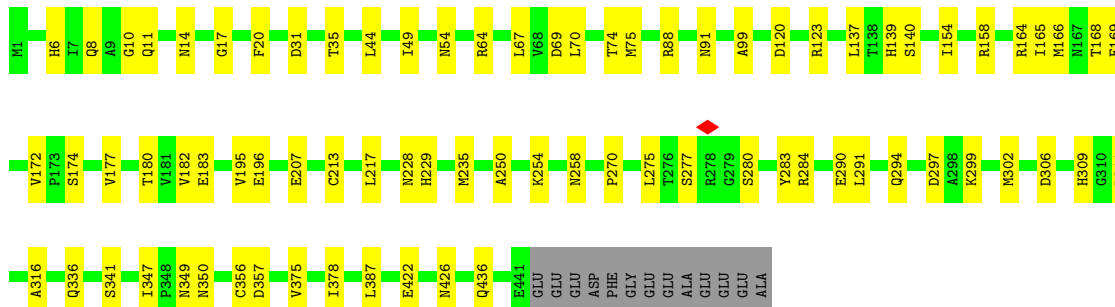


Mol	Chain	Residues	Atoms				AltConf
7	U	1	Total	C	N	O	0
			62	47	1	14	
7	S	1	Total	C	N	O	0
			62	47	1	14	

PRO
ALA
VAL
PRO
LYS
LYS
ALA
GLN
THR
ARG
LYS

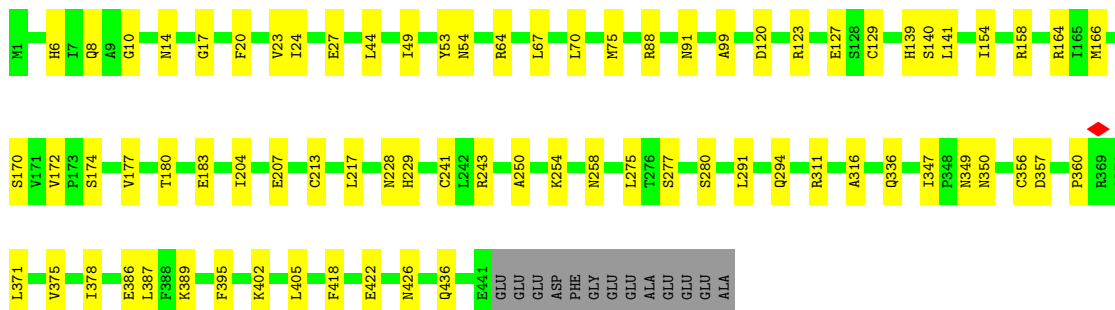
• Molecule 3: Tubulin beta chain

Chain U:  79% 18%



• Molecule 3: Tubulin beta chain

Chain S:  80% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	134.83, 90.35, 133.44	wwPDB
Map dimensions	97, 65, 96	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	O	0.35	0/3459	0.52	0/4697
1	X	0.35	0/3459	0.52	0/4697
2	I	0.19	0/973	0.53	0/1313
3	S	0.35	0/3452	0.53	0/4681
3	U	0.34	0/3452	0.51	0/4681
All	All	0.34	0/14795	0.52	0/20069

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	O	3382	0	3292	32	0
1	X	3382	0	3292	29	0
2	I	951	0	951	13	0
3	S	3377	0	3259	50	0
3	U	3377	0	3259	48	0
4	O	32	0	12	0	0
4	X	32	0	12	0	0
5	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	X	1	0	0	0	0
6	S	28	0	12	3	0
6	U	28	0	12	3	0
7	S	62	0	51	2	0
7	U	62	0	51	1	0
All	All	14715	0	14203	162	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 6.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:154:ILE:HG12	3:S:166:MET:HE2	1.78	0.65
1:X:414:GLU:HB3	1:X:417:GLU:HB2	1.79	0.65
3:S:360:PRO:HB2	3:S:371:LEU:HD13	1.78	0.65
1:X:414:GLU:HG2	1:X:416:GLY:H	1.62	0.63
3:S:275:LEU:H	3:S:294:GLN:HE22	1.48	0.62
3:U:154:ILE:HG12	3:U:166:MET:HE2	1.82	0.61
1:O:414:GLU:HB3	1:O:417:GLU:HB2	1.80	0.61
3:U:291:LEU:HD23	3:U:375:VAL:HG23	1.82	0.60
3:S:24:ILE:HD12	3:S:243:ARG:HH12	1.66	0.60
3:S:172:VAL:HG11	3:S:387:LEU:HD21	1.84	0.60
1:O:414:GLU:HG2	1:O:416:GLY:H	1.67	0.59
3:U:356:CYS:SG	3:U:357:ASP:N	2.75	0.59
1:X:213:CYS:HA	1:X:217:LEU:HD12	1.83	0.59
3:S:356:CYS:SG	3:S:357:ASP:N	2.76	0.59
3:S:291:LEU:HD23	3:S:375:VAL:HG23	1.84	0.58
3:U:172:VAL:HG11	3:U:387:LEU:HD21	1.85	0.58
1:X:64:ARG:NH2	1:X:129:CYS:SG	2.77	0.57
1:O:180:ALA:HB3	1:O:183:GLU:HB2	1.87	0.56
3:S:54:ASN:OD1	3:S:64:ARG:NH2	2.35	0.56
3:U:174:SER:HB2	3:U:207:GLU:HB2	1.86	0.56
1:X:215:ARG:NH2	1:X:299:ALA:O	2.39	0.56
3:U:229:HIS:NE2	7:U:502:TA1:O14	2.34	0.56
3:U:311:ARG:NH2	3:U:436:GLN:O	2.34	0.56
3:U:250:ALA:HA	3:U:254:LYS:HE3	1.88	0.56
3:S:229:HIS:NE2	7:S:502:TA1:O14	2.34	0.55
1:O:64:ARG:NH2	1:O:129:CYS:SG	2.80	0.55
3:U:67:LEU:HB3	3:U:75:MET:HE1	1.88	0.55
1:X:180:ALA:HB3	1:X:183:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:228:ASN:HD21	6:S:501:GDP:HN1	1.53	0.55
3:S:311:ARG:NH2	3:S:436:GLN:O	2.35	0.55
3:U:283:TYR:O	3:S:88:ARG:NH1	2.41	0.54
3:U:195:VAL:HG23	3:U:196:GLU:HG3	1.89	0.54
1:O:213:CYS:HA	1:O:217:LEU:HD12	1.88	0.54
3:U:169:PHE:HD2	3:U:235:MET:HE2	1.73	0.54
1:X:288:VAL:HA	1:X:291:ILE:HG12	1.90	0.53
2:I:1573:ARG:NH1	3:S:127:GLU:O	2.34	0.53
3:U:316:ALA:HB3	3:U:378:ILE:HB	1.90	0.53
1:X:101:ASN:HD22	3:U:258:ASN:HD21	1.55	0.53
1:X:71:GLU:HB3	1:X:98:ASP:HB3	1.90	0.53
2:I:1504:ASN:ND2	3:U:341:SER:OG	2.40	0.53
3:U:422:GLU:OE2	3:U:426:ASN:ND2	2.42	0.52
3:S:10:GLY:O	3:S:14:ASN:ND2	2.42	0.52
3:U:213:CYS:HA	3:U:217:LEU:HD12	1.92	0.52
3:S:174:SER:HB2	3:S:207:GLU:HB2	1.91	0.52
1:X:88:HIS:HB3	1:X:91:GLN:HG2	1.92	0.51
3:U:180:THR:HB	3:U:183:GLU:HB3	1.92	0.51
3:U:228:ASN:HD21	6:U:501:GDP:HN1	1.57	0.51
1:X:154:MET:HE1	1:X:166:LYS:HB3	1.93	0.51
3:U:10:GLY:O	3:U:14:ASN:ND2	2.44	0.51
3:U:139:HIS:ND1	3:U:140:SER:O	2.40	0.51
1:X:311:LYS:NZ	1:X:342:GLN:OE1	2.44	0.50
3:S:277:SER:HB3	3:S:280:SER:HB3	1.93	0.50
3:U:174:SER:OG	3:U:177:VAL:O	2.28	0.50
3:U:336:GLN:HE22	3:U:349:ASN:HA	1.77	0.50
3:S:17:GLY:HA2	3:S:20:PHE:HB3	1.93	0.50
2:I:1526:LEU:HB3	2:I:1536:ALA:HB3	1.94	0.50
1:O:88:HIS:HB3	1:O:91:GLN:HG2	1.94	0.49
2:I:1549:LYS:NZ	2:I:1554:GLY:O	2.43	0.49
1:X:295:CYS:O	1:X:301:GLN:NE2	2.46	0.49
1:O:240:ALA:O	1:O:356:ASN:ND2	2.45	0.49
3:U:277:SER:HB3	3:U:280:SER:HB3	1.94	0.49
1:O:215:ARG:NH2	1:O:299:ALA:O	2.46	0.49
2:I:1494:ILE:HG23	2:I:1499:LEU:HD13	1.94	0.49
3:S:158:ARG:NH1	3:S:164:ARG:O	2.45	0.49
1:X:27:GLU:OE1	1:X:243:ARG:NH1	2.37	0.48
1:O:27:GLU:OE1	1:O:243:ARG:NH1	2.41	0.48
3:S:44:LEU:HA	3:S:49:ILE:HB	1.94	0.48
1:X:395:PHE:HZ	1:X:418:PHE:HB3	1.78	0.48
1:O:101:ASN:HD22	3:S:258:ASN:HD21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:54:ASN:OD1	3:U:64:ARG:NH2	2.37	0.48
1:X:288:VAL:HG11	1:X:323:VAL:HG13	1.95	0.48
3:S:139:HIS:ND1	3:S:140:SER:O	2.39	0.48
3:S:422:GLU:OE2	3:S:426:ASN:ND2	2.47	0.48
3:U:158:ARG:NH1	3:U:164:ARG:O	2.47	0.48
3:U:180:THR:HG22	3:U:182:VAL:H	1.79	0.47
3:S:120:ASP:OD1	3:S:123:ARG:NH1	2.47	0.47
3:U:275:LEU:H	3:U:294:GLN:HE22	1.62	0.47
1:O:211:ASP:OD1	1:O:215:ARG:NH1	2.48	0.47
1:O:2:ARG:HB3	1:O:133:GLN:HE21	1.79	0.47
1:O:226:ASN:ND2	1:O:367:ASP:OD2	2.48	0.47
3:S:174:SER:OG	3:S:177:VAL:O	2.31	0.47
3:S:228:ASN:HD21	6:S:501:GDP:HN21	1.63	0.47
2:I:1573:ARG:NH2	3:S:129:CYS:O	2.47	0.47
3:S:213:CYS:HA	3:S:217:LEU:HD12	1.97	0.47
3:U:137:LEU:HB3	3:U:168:THR:HG22	1.97	0.46
1:O:154:MET:HE1	1:O:166:LYS:HB3	1.97	0.46
3:S:395:PHE:HZ	3:S:418:PHE:HB3	1.81	0.46
2:I:1579:ILE:HG22	2:I:1581:ALA:H	1.81	0.46
3:U:17:GLY:HA2	3:U:20:PHE:HB3	1.97	0.46
3:S:67:LEU:HB3	3:S:75:MET:HE1	1.97	0.46
2:I:1522:HIS:HD2	2:I:1540:TYR:HB3	1.80	0.46
3:S:53:TYR:O	3:S:64:ARG:NH2	2.49	0.46
3:U:306:ASP:HB2	3:U:309:HIS:HD2	1.80	0.46
1:X:271:THR:OG1	1:X:301:GLN:OE1	2.30	0.45
1:O:195:LEU:HD21	1:O:264:ARG:HE	1.81	0.45
3:U:11:GLN:HG3	3:U:74:THR:HG21	1.99	0.45
3:S:27:GLU:OE1	3:S:243:ARG:NH2	2.49	0.45
3:U:347:ILE:HG22	3:U:350:ASN:HB3	1.98	0.45
3:S:347:ILE:HG22	3:S:350:ASN:HB3	1.98	0.45
1:O:313:MET:HG2	1:O:344:VAL:HG21	1.99	0.45
1:O:237:SER:OG	1:O:320:ARG:NH1	2.49	0.45
1:O:288:VAL:HA	1:O:291:ILE:HG12	1.98	0.45
1:O:121:ARG:HA	1:O:121:ARG:HD2	1.78	0.45
3:U:31:ASP:OD1	3:U:35:THR:N	2.49	0.45
3:S:6:HIS:CD2	3:S:8:GLN:HE21	2.35	0.45
3:S:402:LYS:HB2	3:S:405:LEU:HD22	1.97	0.44
3:S:228:ASN:ND2	6:S:501:GDP:HN1	2.15	0.44
1:X:121:ARG:HA	1:X:121:ARG:HD2	1.79	0.44
1:X:226:ASN:ND2	1:X:367:ASP:OD2	2.50	0.44
1:O:187:SER:HA	1:O:190:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:69:ASP:HB2	3:U:75:MET:HE2	1.98	0.44
3:S:250:ALA:HA	3:S:254:LYS:HE3	1.99	0.44
3:S:88:ARG:HB2	3:S:91:ASN:ND2	2.33	0.44
3:S:70:LEU:HD12	3:S:99:ALA:HB2	2.00	0.43
2:I:1490:ILE:HG13	2:I:1523:TYR:HB2	2.00	0.43
3:U:297:ASP:HB3	3:U:299:LYS:HG2	2.00	0.43
2:I:1483:SER:OG	2:I:1484:LYS:N	2.51	0.43
1:X:265:ILE:HG21	1:X:313:MET:HE1	2.01	0.43
3:U:228:ASN:ND2	6:U:501:GDP:HN1	2.16	0.43
1:X:53:PHE:HB3	1:X:61:HIS:HB3	1.99	0.43
3:U:169:PHE:CE2	3:U:235:MET:HG3	2.54	0.43
1:O:84:ARG:HE	1:O:85:GLN:HE21	1.65	0.42
1:O:398:MET:HG2	3:S:347:ILE:HD13	2.00	0.42
2:I:1567:TYR:HB2	2:I:1590:ALA:HB3	2.00	0.42
2:I:1572:ASP:HB2	3:S:164:ARG:HH21	1.84	0.42
1:X:288:VAL:O	1:X:292:THR:OG1	2.35	0.42
3:S:241:CYS:SG	3:S:250:ALA:N	2.84	0.42
3:U:270:PRO:HG2	3:U:302:MET:HB2	2.01	0.42
1:X:168:GLU:OE2	1:X:194:THR:OG1	2.34	0.42
1:X:136:LEU:HD23	1:X:167:LEU:HB2	2.01	0.42
3:U:44:LEU:HA	3:U:49:ILE:HB	2.02	0.42
3:S:23:VAL:HG13	7:S:502:TA1:H411	2.00	0.42
3:U:284:ARG:NH1	3:U:290:GLU:OE2	2.53	0.42
1:X:35:GLN:NE2	1:X:59:GLY:O	2.53	0.42
1:X:195:LEU:HD21	1:X:264:ARG:HE	1.85	0.42
1:O:246:GLY:H	1:O:249:ASN:HD21	1.66	0.42
1:O:178:SER:HB2	3:S:349:ASN:HB3	2.01	0.42
1:O:276:ILE:HD11	1:O:286:LEU:HD11	2.02	0.42
3:U:6:HIS:CD2	3:U:8:GLN:HE21	2.37	0.42
3:U:70:LEU:HD12	3:U:99:ALA:HB2	2.02	0.42
3:S:172:VAL:N	3:S:204:ILE:O	2.48	0.42
3:S:316:ALA:HB3	3:S:378:ILE:HB	2.01	0.41
1:X:187:SER:HA	1:X:190:THR:HG22	2.00	0.41
3:S:336:GLN:HE22	3:S:349:ASN:HA	1.86	0.41
1:X:286:LEU:O	1:X:373:ARG:NH1	2.42	0.41
3:S:254:LYS:O	3:S:258:ASN:ND2	2.54	0.41
3:U:88:ARG:HB2	3:U:91:ASN:ND2	2.35	0.41
3:S:386:GLU:HA	3:S:389:LYS:HB3	2.03	0.41
1:O:191:THR:HA	1:O:194:THR:HG22	2.02	0.41
3:U:228:ASN:HD21	6:U:501:GDP:HN21	1.69	0.41
3:U:120:ASP:OD1	3:U:123:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:71:GLU:HB3	1:O:98:ASP:HB3	2.02	0.41
1:O:138:PHE:HZ	1:O:235:VAL:HG11	1.86	0.41
3:U:165:ILE:H	3:U:165:ILE:HG13	1.75	0.41
1:X:172:TYR:OH	1:X:387:ALA:O	2.39	0.41
2:I:1503:VAL:HG21	3:U:311:ARG:HG3	2.03	0.41
3:S:180:THR:HB	3:S:183:GLU:HB3	2.03	0.41
1:O:62:VAL:HA	1:O:63:PRO:HD3	1.92	0.40
3:S:141:LEU:HG	3:S:170:SER:HB2	2.04	0.40
1:O:328:VAL:HG11	1:O:353:VAL:HG11	2.02	0.40
1:O:215:ARG:HH11	1:O:215:ARG:HD3	1.77	0.40
1:O:264:ARG:O	1:O:266:HIS:ND1	2.54	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	O	428/451 (95%)	402 (94%)	26 (6%)	0	100	100
1	X	428/451 (95%)	400 (94%)	28 (6%)	0	100	100
2	I	116/174 (67%)	108 (93%)	8 (7%)	0	100	100
3	S	429/444 (97%)	405 (94%)	24 (6%)	0	100	100
3	U	429/444 (97%)	402 (94%)	27 (6%)	0	100	100
All	All	1830/1964 (93%)	1717 (94%)	113 (6%)	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	O	364/379 (96%)	363 (100%)	1 (0%)	86	83
1	X	364/379 (96%)	363 (100%)	1 (0%)	86	83
2	I	107/152 (70%)	107 (100%)	0	100	100
3	S	368/379 (97%)	368 (100%)	0	100	100
3	U	368/379 (97%)	368 (100%)	0	100	100
All	All	1571/1668 (94%)	1569 (100%)	2 (0%)	87	88

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

Mol	Chain	Res	Type
1	X	275	VAL
1	O	275	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	8	HIS
1	X	15	GLN
1	X	176	GLN
1	X	186	ASN
1	X	197	HIS
1	X	226	ASN
1	X	258	ASN
1	X	293	ASN
1	X	358	GLN
1	O	18	ASN
1	O	85	GLN
1	O	88	HIS
1	O	91	GLN
1	O	133	GLN
1	O	186	ASN
1	O	197	HIS
1	O	226	ASN
1	O	249	ASN
1	O	256	GLN
1	O	258	ASN

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Mol	Chain	Res	Type
1	O	293	ASN
1	O	358	GLN
2	I	1504	ASN
2	I	1557	ASN
3	U	8	GLN
3	U	14	ASN
3	U	37	HIS
3	U	228	ASN
3	U	258	ASN
3	U	294	GLN
3	U	309	HIS
3	U	331	GLN
3	U	336	GLN
3	U	337	ASN
3	U	433	GLN
3	S	8	GLN
3	S	37	HIS
3	S	107	HIS
3	S	228	ASN
3	S	249	ASN
3	S	258	ASN
3	S	331	GLN
3	S	336	GLN
3	S	337	ASN
3	S	433	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

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
4	GTP	X	501	5	33,34,34	0.53	0	50,54,54	0.40	0
7	TA1	U	502	-	68,68,68	1.22	8 (11%)	105,105,105	1.49	17 (16%)
7	TA1	S	502	-	68,68,68	1.22	8 (11%)	105,105,105	1.49	17 (16%)
4	GTP	O	501	5	33,34,34	0.51	0	50,54,54	0.40	0
6	GDP	U	501	-	29,30,30	0.60	0	45,47,47	0.55	0
6	GDP	S	501	-	29,30,30	0.60	0	45,47,47	0.55	0

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
4	GTP	X	501	5	-	5/22/38/38	0/3/3/3
7	TA1	U	502	-	-	8/41/127/127	0/7/7/7
7	TA1	S	502	-	-	8/41/127/127	0/7/7/7
4	GTP	O	501	5	-	5/22/38/38	0/3/3/3
6	GDP	U	501	-	-	3/16/32/32	0/3/3/3
6	GDP	S	501	-	-	3/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	502	TA1	C45-C24	4.20	1.61	1.54
7	U	502	TA1	C45-C24	4.16	1.61	1.54
7	U	502	TA1	C18-C10	4.04	1.66	1.57
7	S	502	TA1	C18-C10	4.02	1.66	1.57
7	U	502	TA1	C01-C45	3.59	1.70	1.56
7	S	502	TA1	C01-C45	3.57	1.70	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	502	TA1	C01-C02	3.36	1.69	1.57
7	S	502	TA1	C01-C02	3.35	1.69	1.57
7	U	502	TA1	C11-C10	2.79	1.60	1.54
7	S	502	TA1	C11-C10	2.71	1.60	1.54
7	S	502	TA1	C43-C26	2.57	1.57	1.52
7	U	502	TA1	C43-C26	2.53	1.57	1.52
7	S	502	TA1	C21-C24	2.24	1.56	1.51
7	U	502	TA1	C18-C20	2.17	1.61	1.55
7	U	502	TA1	C21-C24	2.16	1.56	1.51
7	S	502	TA1	C18-C20	2.14	1.61	1.55

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	502	TA1	C47-C45-C46	-5.16	91.65	106.29
7	U	502	TA1	C47-C45-C46	-5.16	91.65	106.29
7	U	502	TA1	O11-C26-C25	4.44	120.40	109.85
7	S	502	TA1	O11-C26-C25	4.39	120.28	109.85
7	S	502	TA1	O08-C20-C21	-3.80	114.72	119.28
7	U	502	TA1	O08-C20-C21	-3.69	114.85	119.28
7	S	502	TA1	C19-C18-C20	-3.67	97.06	106.56
7	U	502	TA1	C19-C18-C20	-3.66	97.08	106.56
7	S	502	TA1	C05-C04-C03	3.54	128.20	120.40
7	U	502	TA1	C05-C04-C03	3.54	128.20	120.40
7	U	502	TA1	C09-C04-C03	-3.30	113.12	120.40
7	S	502	TA1	C09-C04-C03	-3.27	113.19	120.40
7	S	502	TA1	C47-C45-C24	3.12	125.24	112.78
7	U	502	TA1	C47-C45-C24	3.12	125.23	112.78
7	U	502	TA1	C45-C01-C02	3.11	115.35	111.93
7	S	502	TA1	C21-O09-C22	3.11	122.36	115.95
7	S	502	TA1	C45-C01-C02	3.09	115.32	111.93
7	U	502	TA1	C21-O09-C22	3.08	122.30	115.95
7	S	502	TA1	O04-C11-C14	-3.01	101.74	108.13
7	U	502	TA1	O04-C11-C14	-2.97	101.83	108.13
7	U	502	TA1	C10-C18-C20	2.68	120.72	116.30
7	S	502	TA1	C10-C18-C20	2.68	120.71	116.30
7	U	502	TA1	C11-O04-C12	2.53	125.58	119.17
7	S	502	TA1	C11-O04-C12	2.50	125.50	119.17
7	U	502	TA1	O01-C01-C43	2.29	112.90	107.04
7	S	502	TA1	O01-C01-C43	2.28	112.87	107.04
7	U	502	TA1	C01-C43-C26	2.25	119.13	114.98
7	S	502	TA1	C01-C43-C26	2.22	119.08	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	502	TA1	O04-C11-C10	2.18	112.62	109.24
7	U	502	TA1	C11-C10-C02	2.14	115.81	111.70
7	S	502	TA1	C11-C10-C02	2.11	115.77	111.70
7	U	502	TA1	O04-C11-C10	2.11	112.51	109.24
7	S	502	TA1	C46-C45-C01	2.10	115.57	111.13
7	U	502	TA1	C46-C45-C01	2.07	115.50	111.13

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	501	GTP	PB-O3B-PG-O3G
4	X	501	GTP	C5'-O5'-PA-O3A
4	X	501	GTP	C5'-O5'-PA-O1A
4	X	501	GTP	C5'-O5'-PA-O2A
4	O	501	GTP	PB-O3B-PG-O3G
4	O	501	GTP	C5'-O5'-PA-O3A
4	O	501	GTP	C5'-O5'-PA-O1A
4	O	501	GTP	C5'-O5'-PA-O2A
6	U	501	GDP	C5'-O5'-PA-O3A
6	U	501	GDP	C5'-O5'-PA-O1A
6	U	501	GDP	C5'-O5'-PA-O2A
6	S	501	GDP	C5'-O5'-PA-O3A
6	S	501	GDP	C5'-O5'-PA-O1A
6	S	501	GDP	C5'-O5'-PA-O2A
7	U	502	TA1	O03-C03-C04-C09
7	S	502	TA1	O03-C03-C04-C09
7	U	502	TA1	O02-C03-C04-C09
7	S	502	TA1	O02-C03-C04-C09
7	S	502	TA1	N01-C30-C31-C36
7	U	502	TA1	N01-C30-C31-C36
7	U	502	TA1	O14-C30-C31-C36
7	S	502	TA1	O03-C03-C04-C05
7	U	502	TA1	O03-C03-C04-C05
7	S	502	TA1	O14-C30-C31-C36
7	S	502	TA1	N01-C30-C31-C32
7	U	502	TA1	N01-C30-C31-C32
7	U	502	TA1	O14-C30-C31-C32
7	S	502	TA1	O14-C30-C31-C32
7	S	502	TA1	O02-C03-C04-C05
7	U	502	TA1	O02-C03-C04-C05
4	X	501	GTP	PB-O3A-PA-O2A

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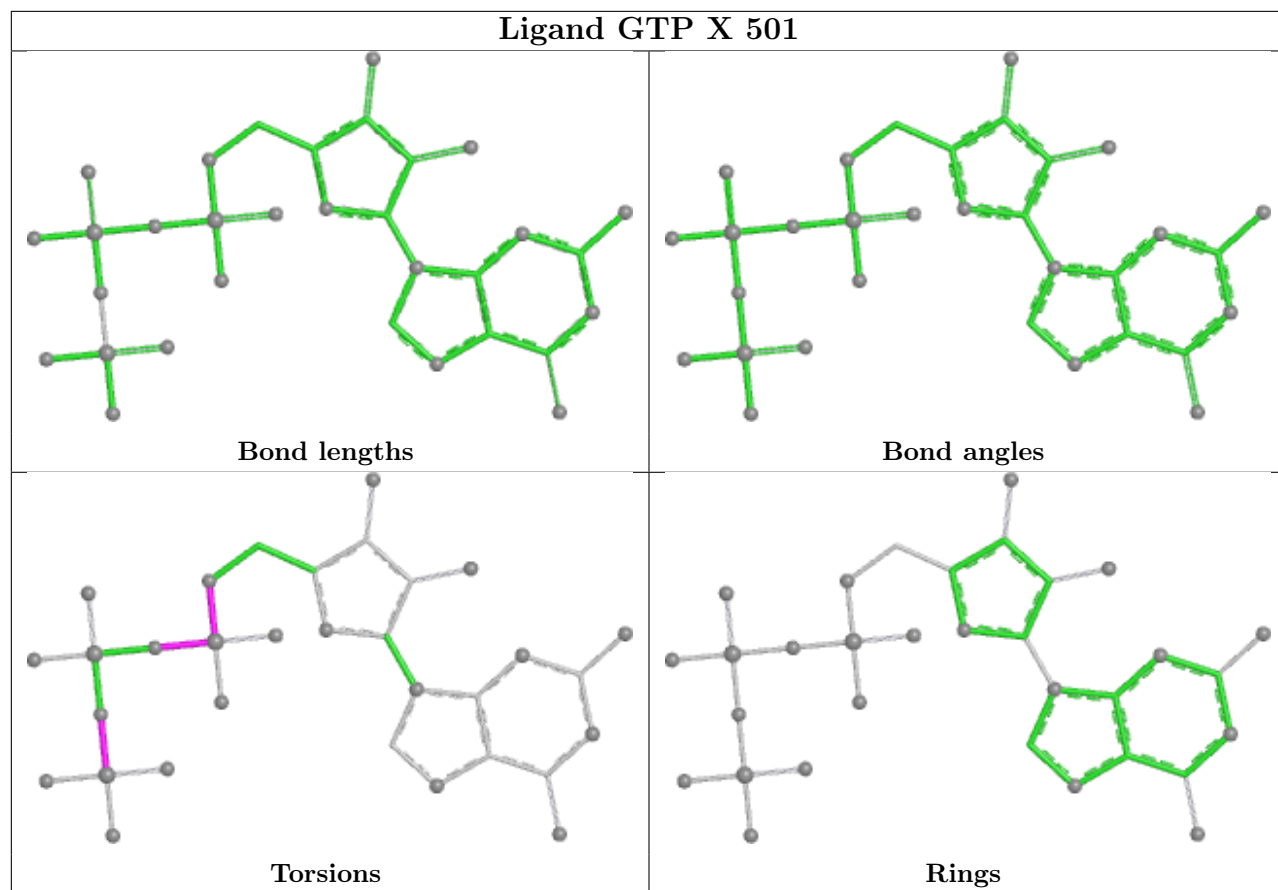
Mol	Chain	Res	Type	Atoms
4	O	501	GTP	PB-O3A-PA-O2A

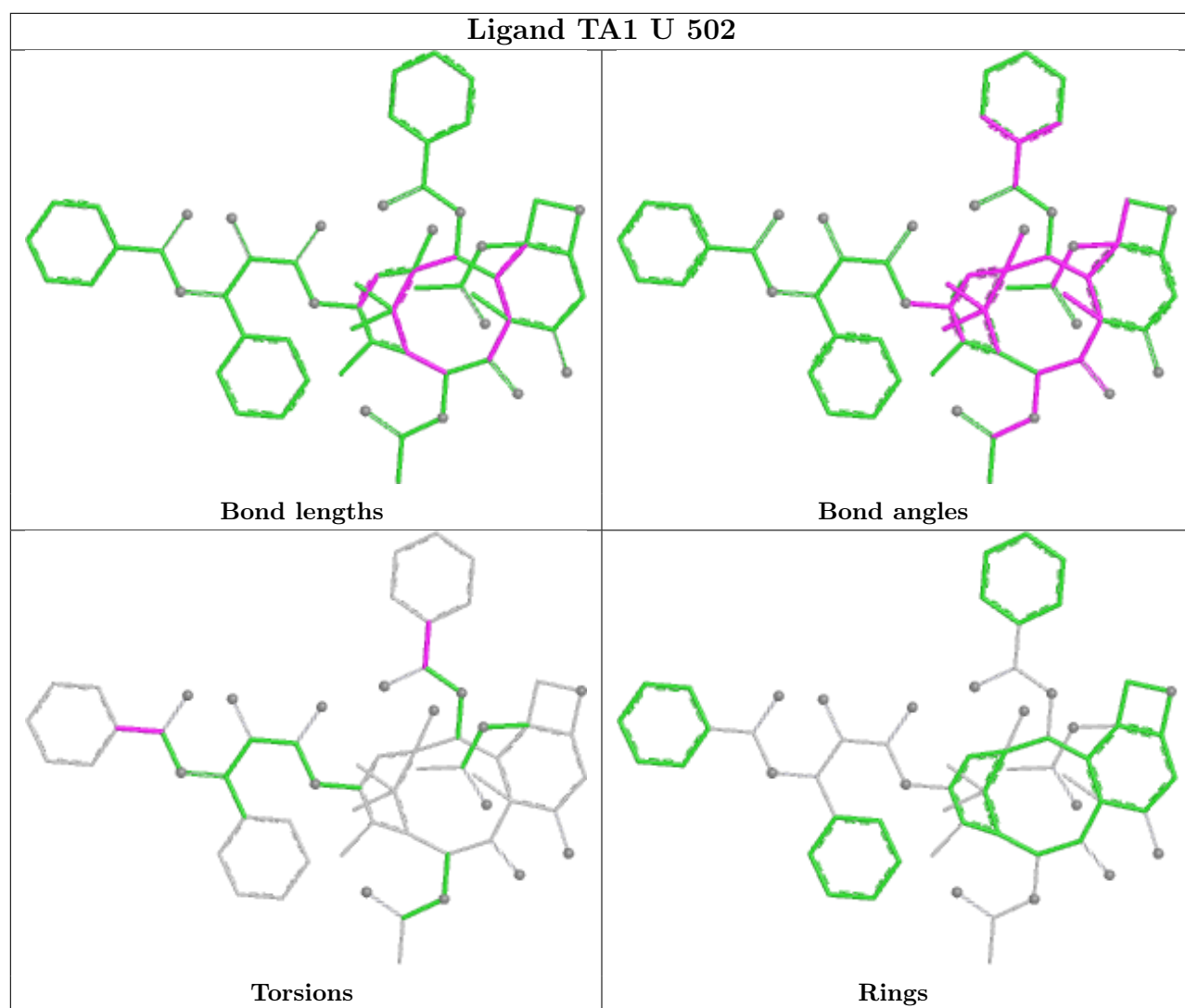
There are no ring outliers.

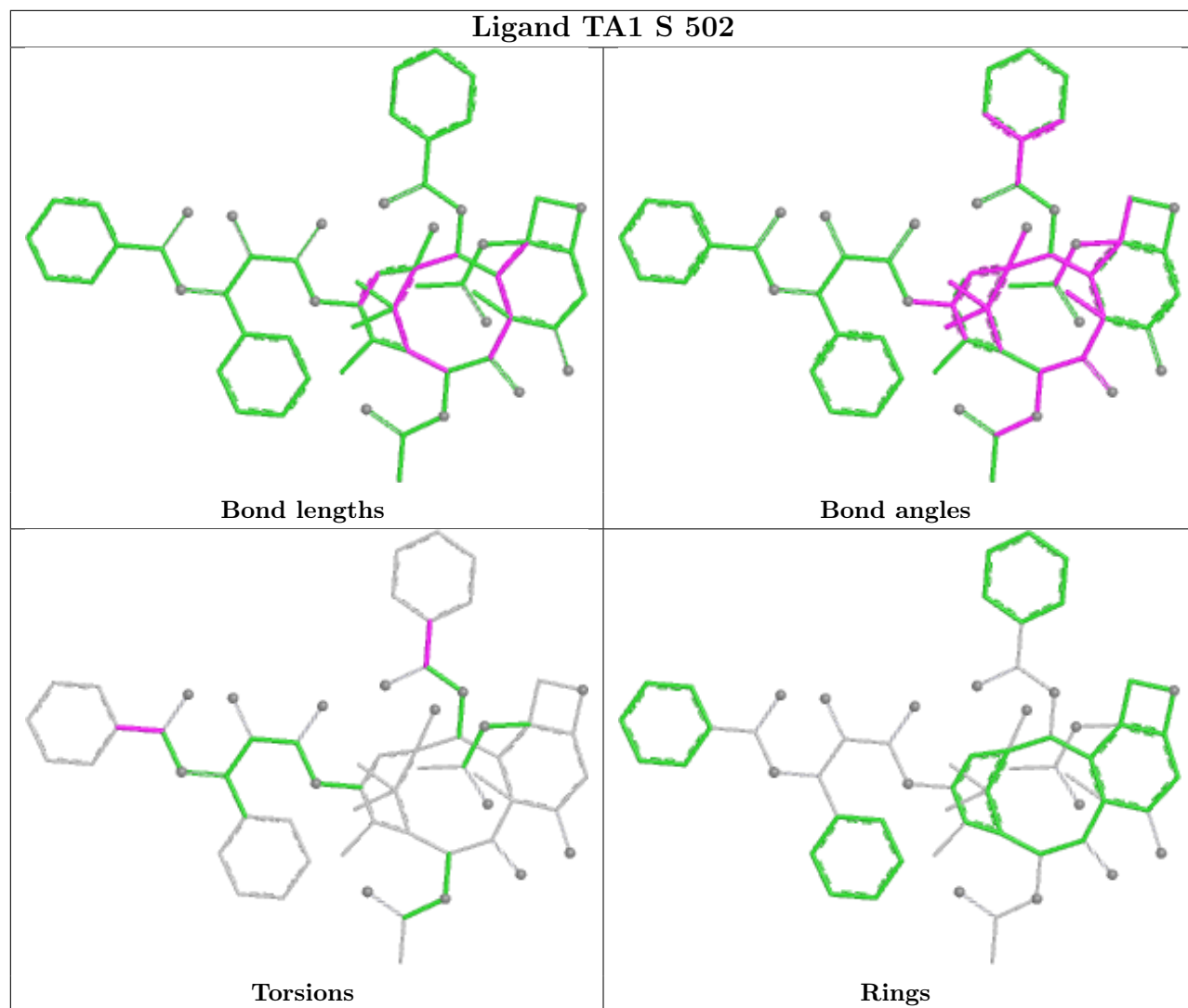
4 monomers are involved in 9 short contacts:

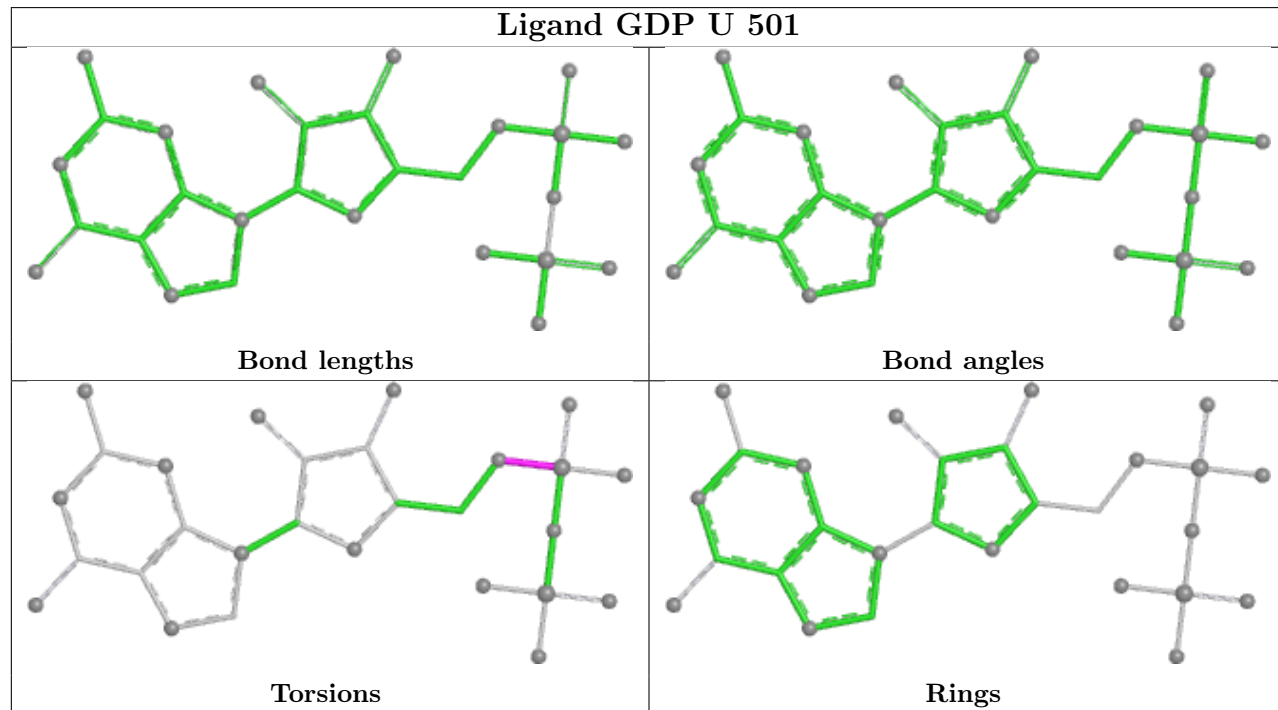
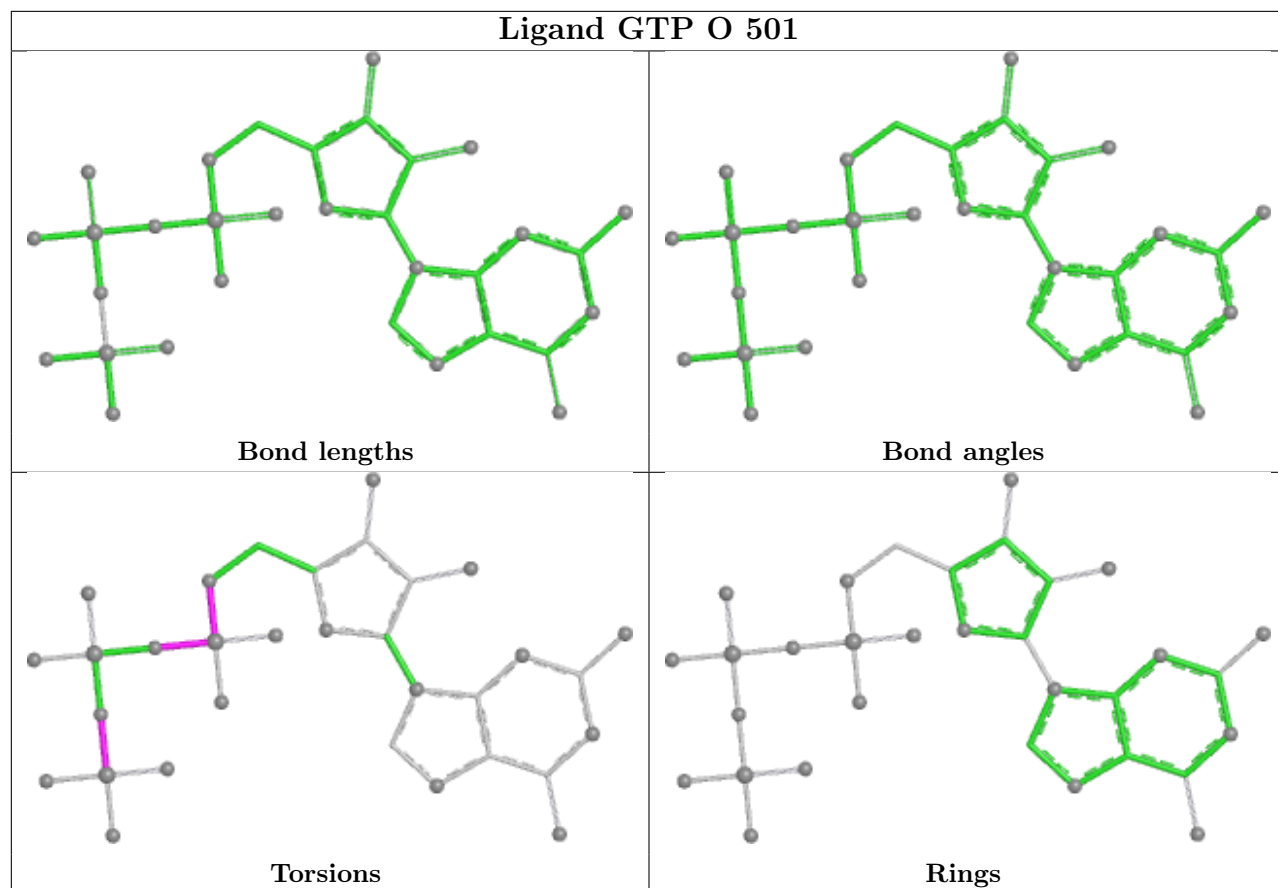
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	502	TA1	1	0
7	S	502	TA1	2	0
6	U	501	GDP	3	0
6	S	501	GDP	3	0

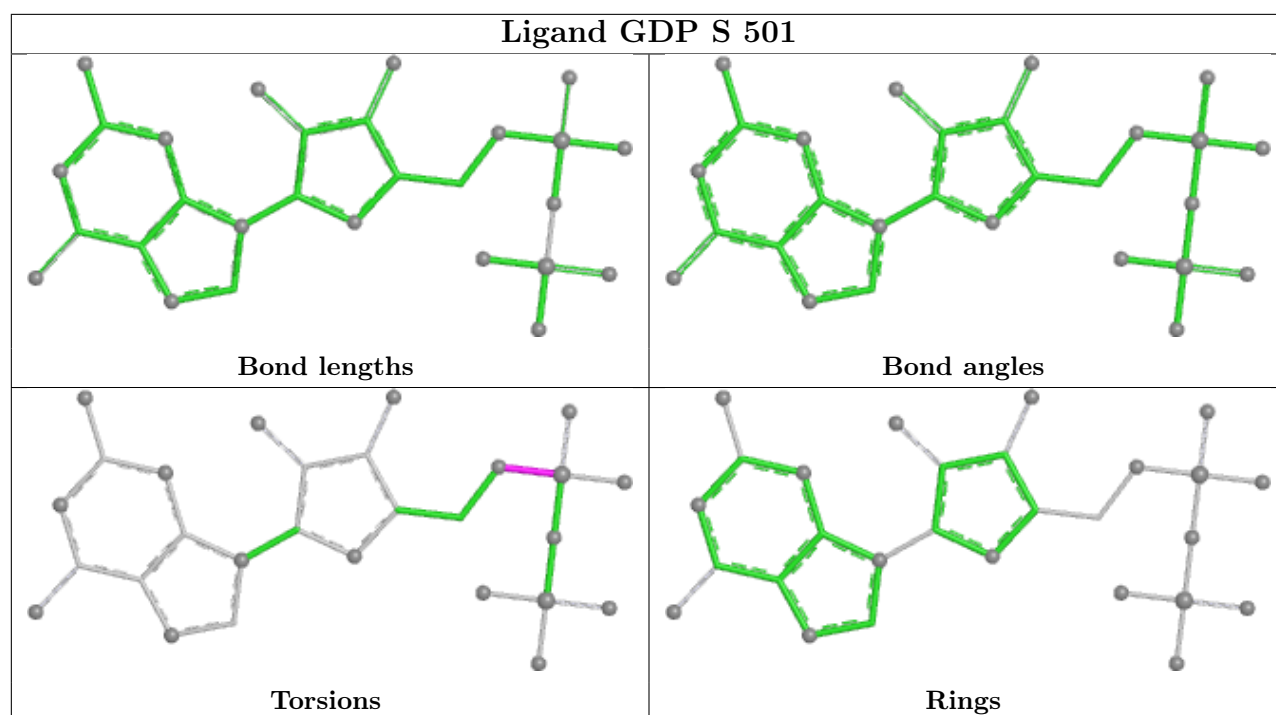
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

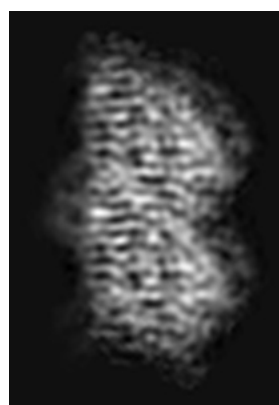
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4643. These allow visual inspection of the internal detail of the map and identification of artifacts.

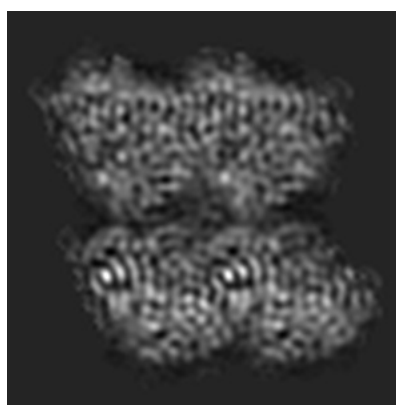
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

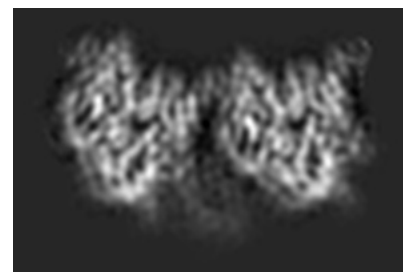
6.1.1 Primary map



X



Y

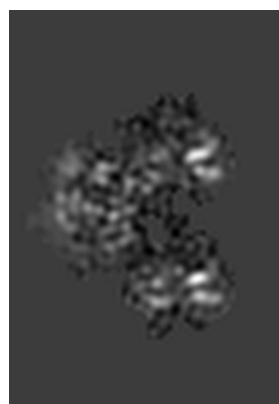


Z

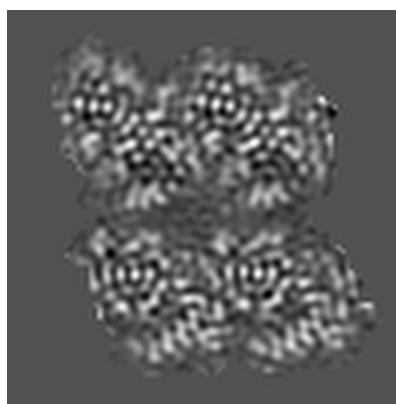
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

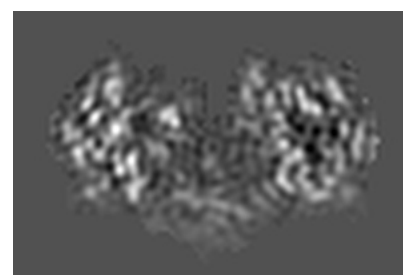
6.2.1 Primary map



X Index: 48



Y Index: 32

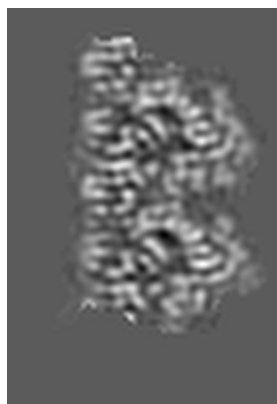


Z Index: 48

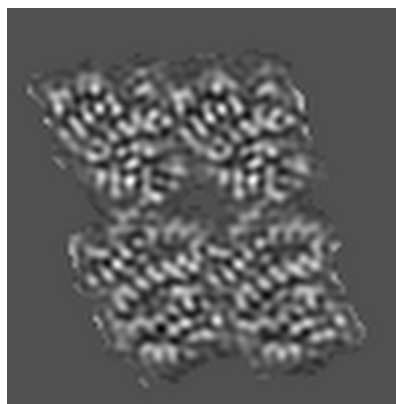
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

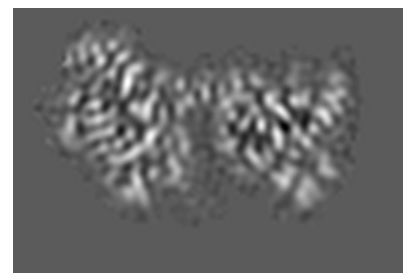
6.3.1 Primary map



X Index: 27



Y Index: 42

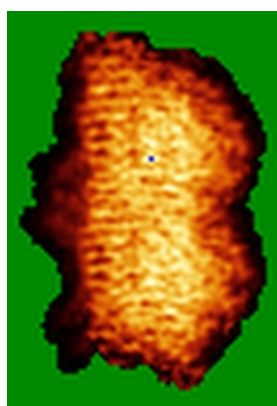


Z Index: 34

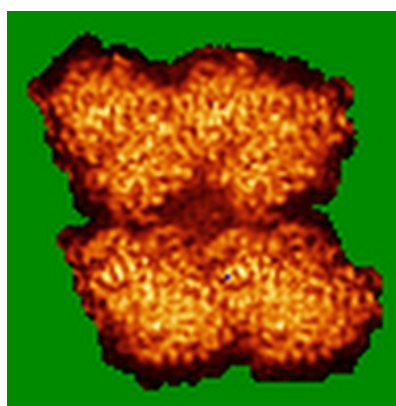
The images above show the largest variance slices of the map in three orthogonal directions.

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

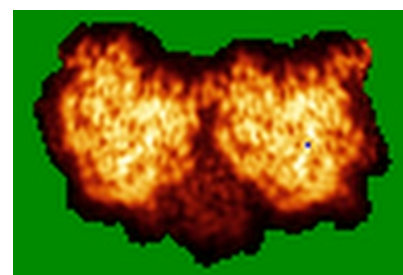
6.4.1 Primary map



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

This section was not generated.

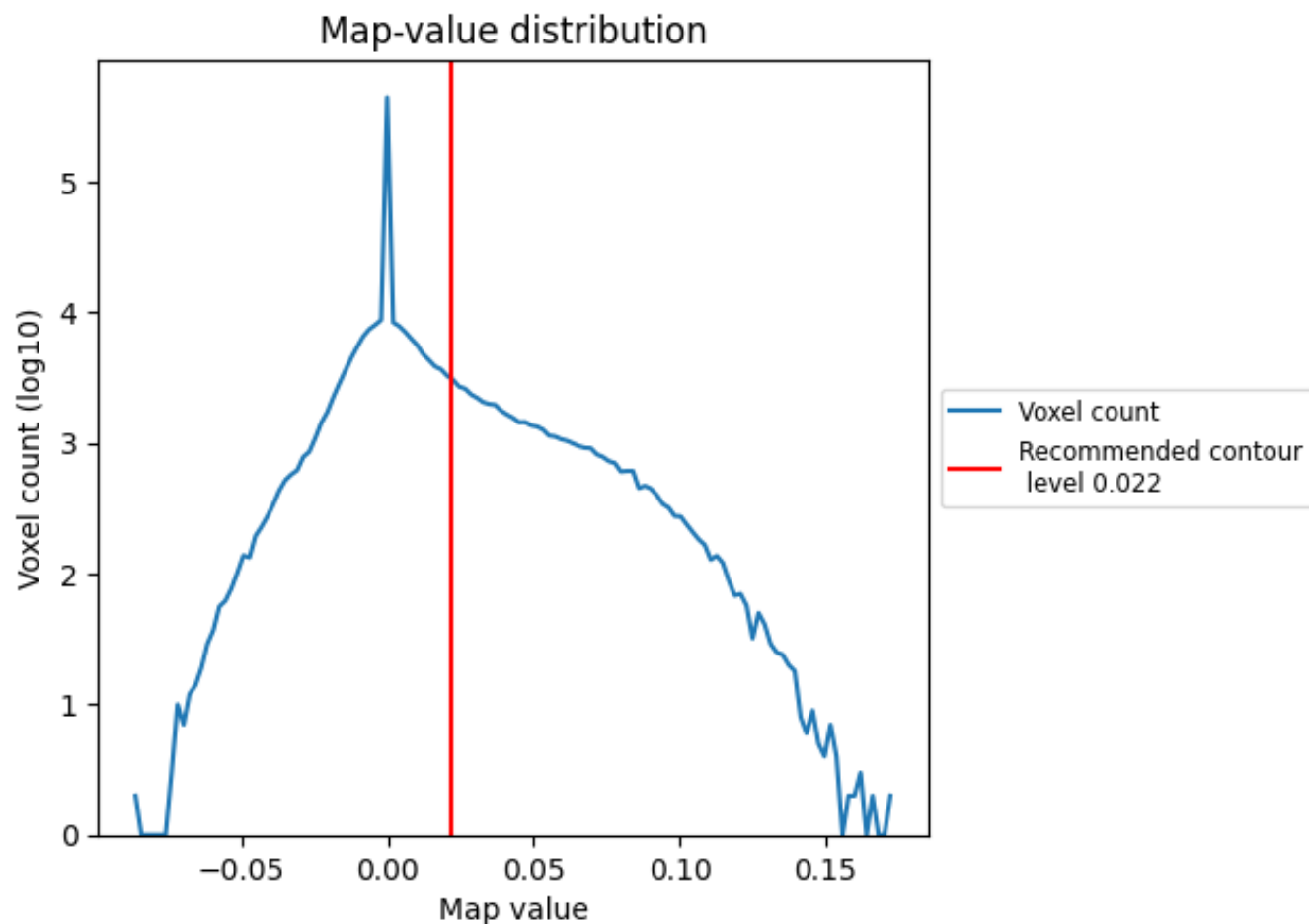
6.6 Mask visualisation

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

7 Map analysis [i](#)

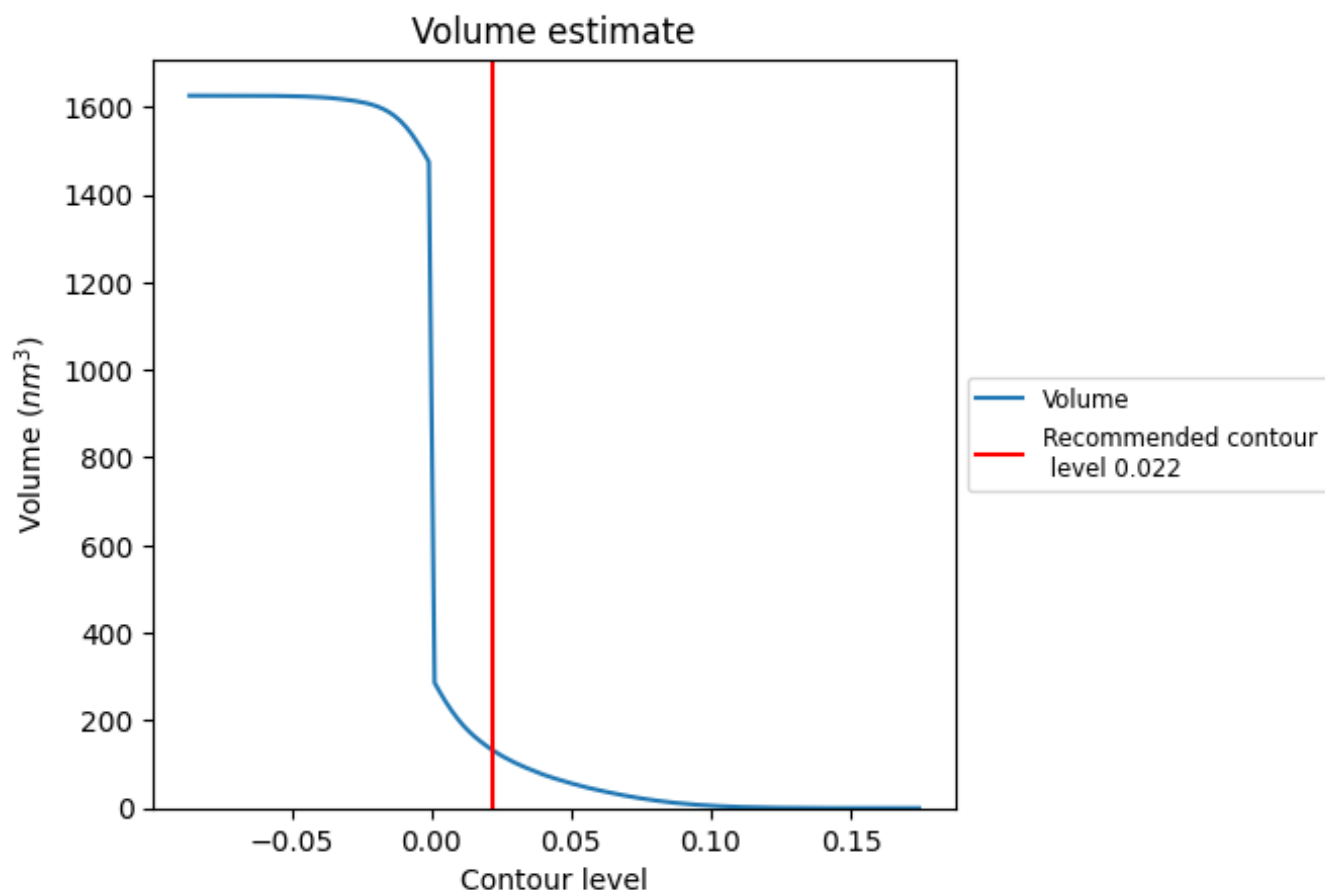
This section contains the results of statistical analysis of the map.

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 132 nm³; this corresponds to an approximate mass of 119 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

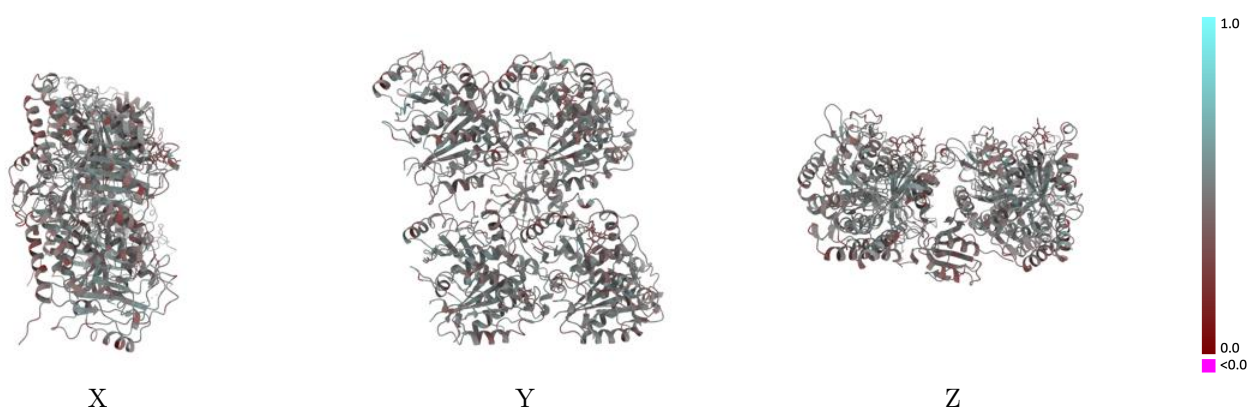
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4643 and PDB model 6QUS. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

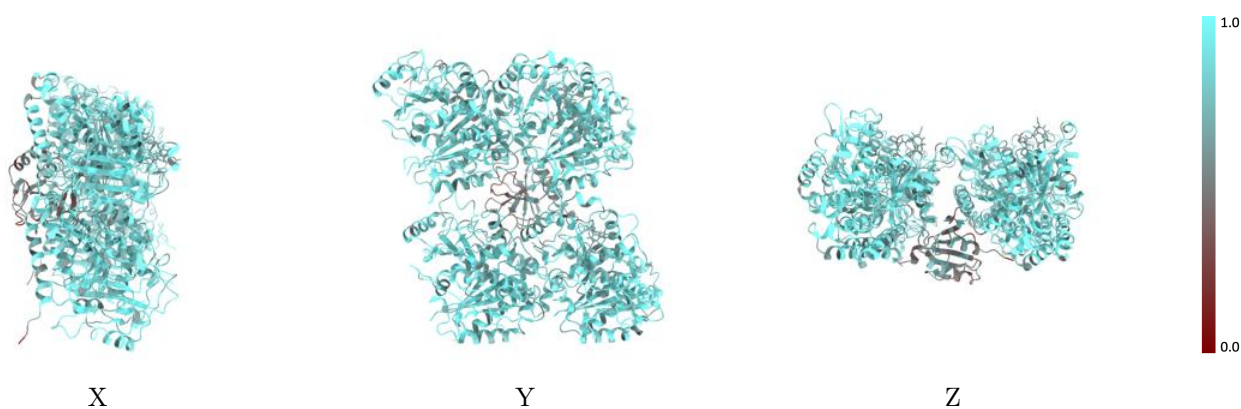
This section was not generated.

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



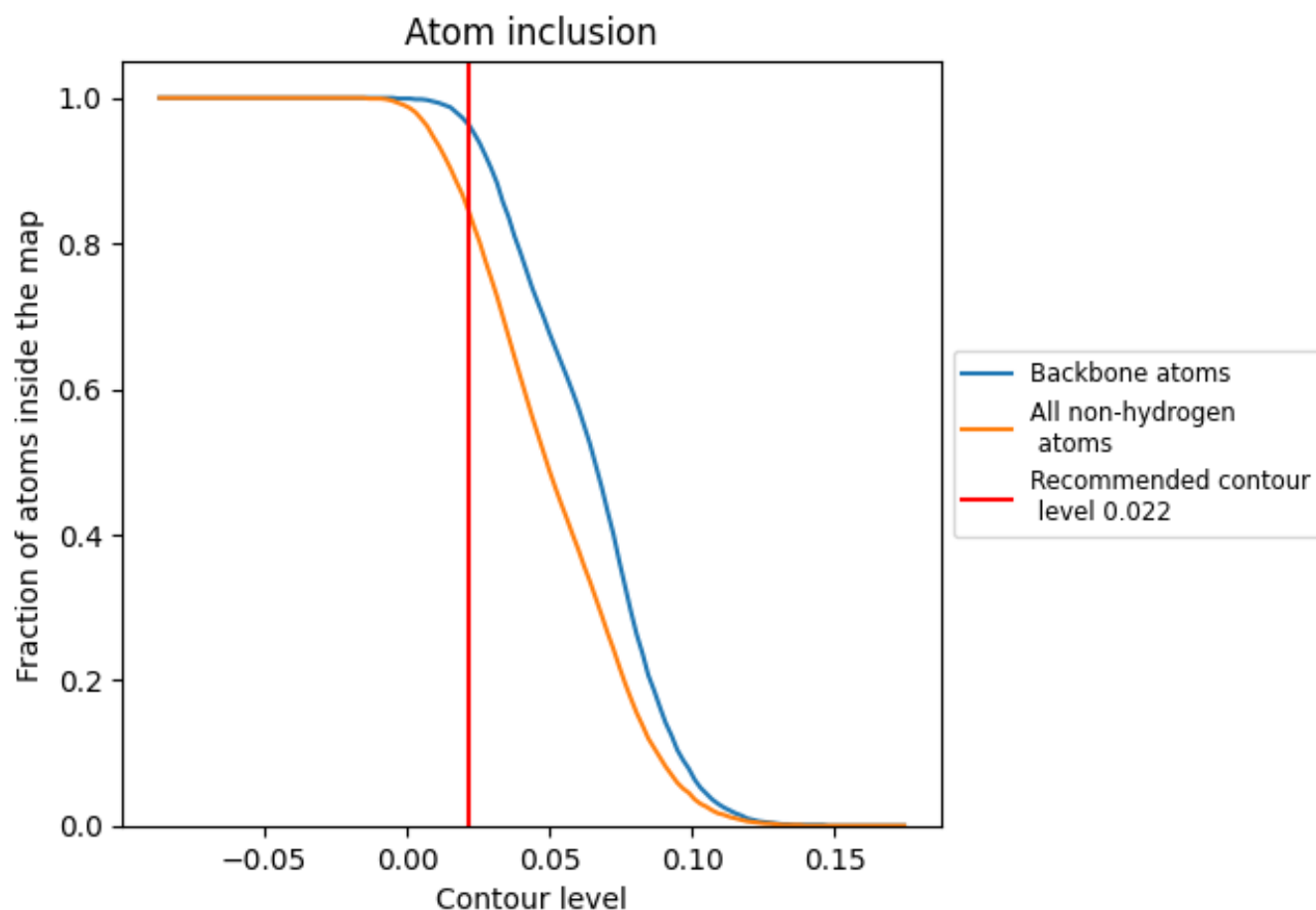
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.4540
I	0.4980	0.4050
O	0.8670	0.4570
S	0.8610	0.4570
U	0.8620	0.4560
X	0.8730	0.4620

