



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 25, 2017 – 11:50 AM EST

PDB ID : 5SYF
EMDB ID: : EMD-8322
Title : High-resolution cryo-EM reconstruction of Taxol-stabilized microtubule
Authors : Kellogg, E.H.; Nogales, E.
Deposited on : 2016-08-11
Resolution : 3.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

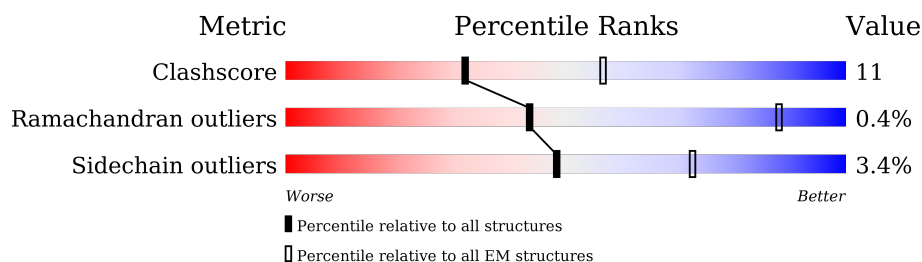
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	437	
2	B	426	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6818 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.

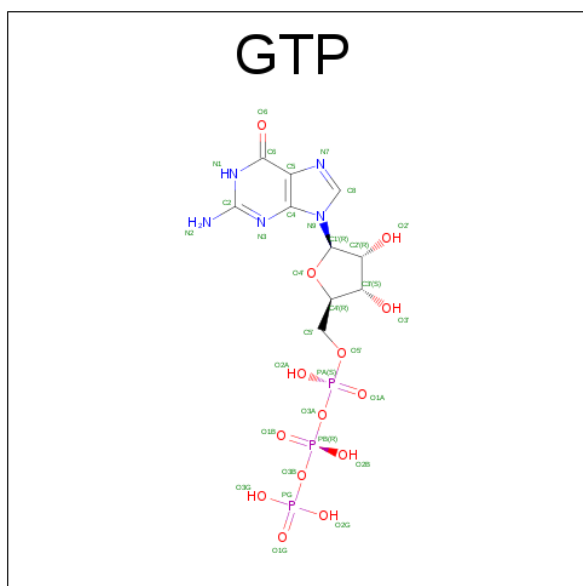
- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	426	3343	2121	569	631	22	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3352	2106	575	645	26	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

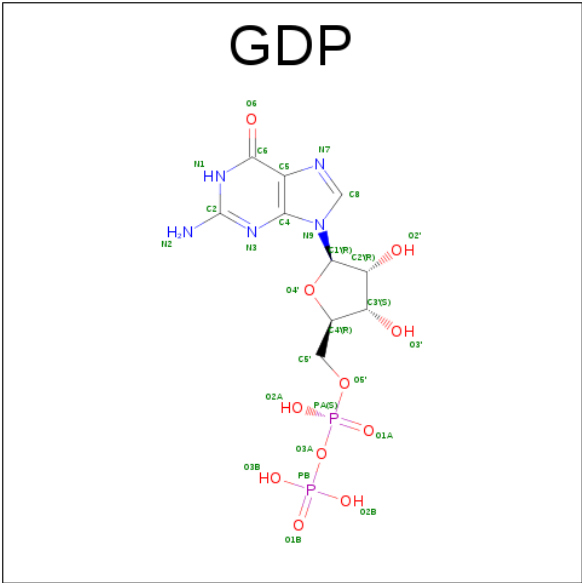


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	32	10	5	14	3	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

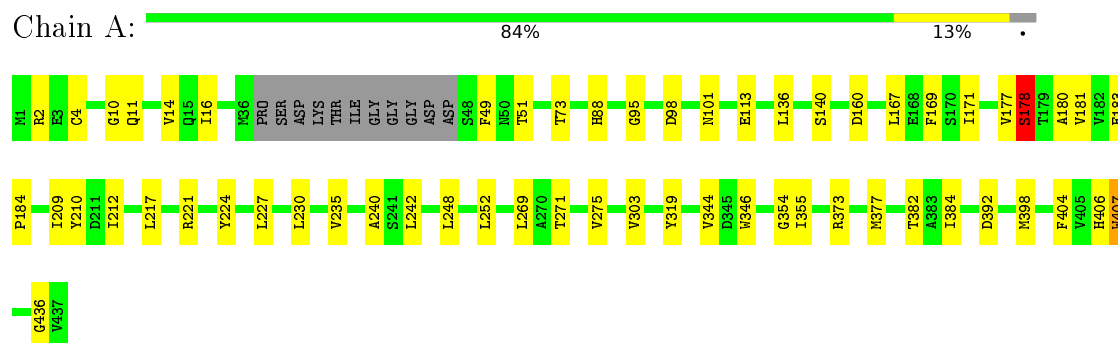


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			62	47	1	14	

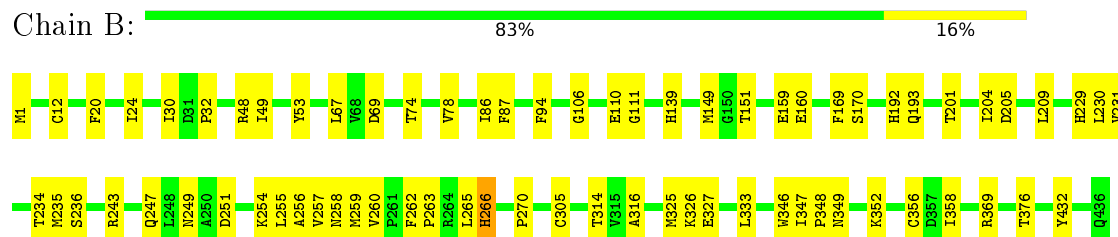
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 alpha chain



• Molecule 2: Tubulin beta chain



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	17069	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	27500	Depositor
Image detector	Not provided	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, GTP, MG, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.40	0/3419	0.66	1/4639 (0.0%)
2	B	0.41	0/3427	0.66	0/4641
All	All	0.41	0/6846	0.66	1/9280 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	SER	N-CA-CB	6.32	119.98	110.50

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	A	3343	0	3262	119	0
2	B	3352	0	3235	127	0
3	A	32	0	12	0	0
4	A	1	0	0	0	0
5	B	28	0	12	0	0
6	B	62	0	51	9	0
All	All	6818	0	6572	151	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 11.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TRP:CG	2:B:257:VAL:HG22	1.18	1.66
1:A:210:TYR:CG	2:B:326:LYS:HD3	1.40	1.52
1:A:177:VAL:HG22	2:B:333:LEU:CD1	1.40	1.47
1:A:398:MET:SD	2:B:348:PRO:HD2	1.52	1.46
1:A:407:TRP:CD2	2:B:257:VAL:HG22	1.56	1.38
1:A:224:TYR:CE2	2:B:325:MET:HG3	1.62	1.33
1:A:407:TRP:CD1	2:B:257:VAL:HG22	1.34	1.33
2:B:229:HIS:NE2	6:B:502:TA1:O14	1.63	1.30
1:A:177:VAL:CG2	2:B:333:LEU:HD11	1.62	1.28
1:A:407:TRP:CG	2:B:257:VAL:CG2	2.13	1.27
1:A:407:TRP:HZ2	2:B:256:ALA:C	1.40	1.24
1:A:407:TRP:CD2	2:B:257:VAL:CG2	2.19	1.24
1:A:224:TYR:CD2	2:B:325:MET:HG3	1.73	1.23
1:A:210:TYR:CD1	2:B:326:LYS:HD3	1.76	1.19
1:A:398:MET:HG3	2:B:346:TRP:O	1.42	1.16
1:A:210:TYR:HB3	2:B:326:LYS:CE	1.76	1.15
1:A:407:TRP:CD1	2:B:257:VAL:HG13	1.82	1.13
1:A:210:TYR:HB3	2:B:326:LYS:HE2	1.23	1.11
1:A:210:TYR:CG	2:B:326:LYS:CD	2.34	1.10
1:A:407:TRP:CE2	2:B:257:VAL:CG2	2.21	1.10
1:A:407:TRP:CZ2	2:B:256:ALA:C	2.28	1.05
1:A:407:TRP:CD1	2:B:257:VAL:CG2	2.07	1.03
1:A:398:MET:SD	2:B:348:PRO:CD	2.47	1.02
1:A:224:TYR:CE2	2:B:325:MET:CG	2.42	1.01
1:A:407:TRP:CD1	2:B:257:VAL:CG1	2.41	1.01
1:A:404:PHE:CE2	2:B:257:VAL:O	2.15	0.99
1:A:210:TYR:CD1	2:B:326:LYS:CD	2.45	0.99
1:A:398:MET:CG	2:B:346:TRP:O	2.10	0.99
1:A:404:PHE:CD2	2:B:257:VAL:O	2.17	0.97
1:A:407:TRP:HD1	2:B:257:VAL:HG13	1.28	0.95
2:B:229:HIS:HB3	6:B:502:TA1:HC71	1.50	0.94
1:A:181:VAL:HG23	2:B:258:ASN:OD1	1.69	0.92
1:A:407:TRP:CE2	2:B:257:VAL:HG23	2.05	0.91
1:A:407:TRP:CZ2	2:B:257:VAL:N	2.30	0.90
1:A:210:TYR:CB	2:B:326:LYS:CE	2.50	0.89
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.08	0.88
1:A:177:VAL:CG2	2:B:333:LEU:CD1	2.36	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TRP:HZ2	2:B:256:ALA:O	1.60	0.84
1:A:98:ASP:OD2	2:B:251:ASP:OD2	1.96	0.83
1:A:16:ILE:HD11	1:A:171:ILE:HD11	1.60	0.81
1:A:269:LEU:HD22	1:A:303:VAL:HG21	1.62	0.81
1:A:224:TYR:HE2	2:B:325:MET:SD	2.03	0.81
1:A:210:TYR:CB	2:B:326:LYS:HD3	2.09	0.80
1:A:406:HIS:ND1	2:B:263:PRO:HD3	1.96	0.80
1:A:210:TYR:CD2	2:B:326:LYS:HD3	2.15	0.80
2:B:204:ILE:HD13	2:B:231:VAL:HG22	1.66	0.76
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.65	0.76
1:A:406:HIS:CE1	2:B:260:VAL:HG12	2.22	0.75
1:A:101:ASN:HD21	2:B:254:LYS:NZ	1.81	0.75
1:A:73:THR:N	2:B:48:ARG:HH22	1.84	0.75
1:A:95:GLY:O	2:B:1:MET:HE1	1.84	0.75
1:A:404:PHE:HE2	2:B:257:VAL:O	1.70	0.74
2:B:32:PRO:HA	2:B:86:ILE:HD11	1.69	0.74
1:A:210:TYR:HB3	2:B:326:LYS:CD	2.18	0.74
1:A:224:TYR:OH	2:B:325:MET:CE	2.35	0.74
1:A:406:HIS:NE2	2:B:260:VAL:HG12	2.03	0.74
6:B:502:TA1:H261	6:B:502:TA1:H463	1.68	0.73
1:A:73:THR:OG1	2:B:48:ARG:NH2	2.21	0.73
1:A:224:TYR:CE2	2:B:325:MET:CE	2.71	0.73
1:A:73:THR:CA	2:B:48:ARG:HH22	2.02	0.72
1:A:210:TYR:CB	2:B:326:LYS:CD	2.68	0.72
1:A:224:TYR:OH	2:B:325:MET:HE1	1.89	0.71
1:A:177:VAL:HG22	2:B:333:LEU:HD11	0.72	0.70
2:B:229:HIS:HB3	6:B:502:TA1:C07	2.21	0.70
1:A:73:THR:N	2:B:48:ARG:NH2	2.39	0.69
1:A:73:THR:CA	2:B:48:ARG:NH2	2.56	0.68
1:A:404:PHE:HD2	2:B:257:VAL:O	1.75	0.68
1:A:180:ALA:O	2:B:349:ASN:ND2	2.28	0.67
1:A:177:VAL:HA	2:B:333:LEU:HD21	1.77	0.67
1:A:73:THR:HA	2:B:48:ARG:HH22	1.60	0.67
1:A:11:GLN:NE2	2:B:247:GLN:O	2.28	0.66
2:B:229:HIS:CE1	6:B:502:TA1:O14	2.47	0.66
1:A:406:HIS:HE2	2:B:260:VAL:HG12	1.60	0.66
1:A:11:GLN:HE22	2:B:249:ASN:HD22	1.45	0.65
1:A:177:VAL:HG22	2:B:333:LEU:HD13	1.65	0.65
1:A:407:TRP:CZ2	2:B:256:ALA:O	2.44	0.64
1:A:210:TYR:CB	2:B:326:LYS:NZ	2.61	0.64
1:A:101:ASN:ND2	2:B:254:LYS:NZ	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:MET:SD	2:B:347:ILE:HA	2.39	0.62
1:A:209:ILE:HG21	1:A:227:LEU:HG	1.81	0.62
1:A:221:ARG:CZ	2:B:327:GLU:OE1	2.49	0.61
1:A:224:TYR:CE2	2:B:325:MET:SD	2.86	0.61
1:A:177:VAL:CB	2:B:333:LEU:HD11	2.32	0.59
1:A:210:TYR:HB2	2:B:326:LYS:NZ	2.17	0.59
1:A:210:TYR:HD1	2:B:326:LYS:HZ3	1.50	0.59
1:A:224:TYR:CZ	2:B:325:MET:CE	2.87	0.58
6:B:502:TA1:C26	6:B:502:TA1:H463	2.33	0.58
1:A:11:GLN:NE2	2:B:249:ASN:HD22	2.01	0.58
1:A:224:TYR:OH	2:B:325:MET:HE2	2.02	0.58
1:A:224:TYR:HE2	2:B:325:MET:CE	2.13	0.58
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.85	0.57
1:A:269:LEU:HD21	1:A:384:ILE:HD12	1.86	0.57
1:A:181:VAL:CG2	2:B:258:ASN:OD1	2.49	0.56
1:A:224:TYR:CD2	2:B:325:MET:CG	2.68	0.56
1:A:11:GLN:HE22	2:B:249:ASN:ND2	2.03	0.55
1:A:224:TYR:CZ	2:B:325:MET:HE2	2.41	0.55
2:B:265:LEU:HD22	2:B:432:TYR:CZ	2.41	0.55
1:A:404:PHE:CZ	2:B:258:ASN:O	2.60	0.54
2:B:20:PHE:CE1	2:B:24:ILE:HD11	2.43	0.53
1:A:210:TYR:CD1	2:B:326:LYS:HD2	2.42	0.52
1:A:98:ASP:OD2	2:B:251:ASP:HB2	2.10	0.52
1:A:73:THR:HA	2:B:48:ARG:NH2	2.22	0.51
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.44	0.51
1:A:210:TYR:HB2	2:B:326:LYS:HZ3	1.75	0.51
2:B:236:SER:O	2:B:243:ARG:NH2	2.43	0.51
1:A:2:ARG:O	1:A:51:THR:HG22	2.11	0.50
1:A:136:LEU:CD2	1:A:167:LEU:HD12	2.41	0.50
1:A:212:ILE:CG2	1:A:275:VAL:HG11	2.41	0.50
1:A:101:ASN:HD21	2:B:254:LYS:HZ2	1.57	0.49
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.95	0.49
2:B:259:MET:SD	2:B:316:ALA:HB2	2.52	0.49
1:A:406:HIS:HE2	2:B:260:VAL:CG1	2.24	0.49
2:B:151:THR:HG23	2:B:193:GLN:HB2	1.95	0.49
1:A:210:TYR:CB	2:B:326:LYS:HZ3	2.26	0.48
2:B:263:PRO:O	2:B:266:HIS:CD2	2.67	0.48
1:A:407:TRP:CH2	2:B:256:ALA:HB1	2.50	0.47
2:B:254:LYS:HE2	2:B:352:LYS:HE2	1.96	0.47
1:A:404:PHE:CE2	2:B:258:ASN:C	2.88	0.47
6:B:502:TA1:H101	6:B:502:TA1:C25	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD11	2:B:87:PHE:CD2	2.51	0.46
1:A:10:GLY:O	1:A:14:VAL:HG23	2.15	0.46
1:A:224:TYR:CE2	2:B:325:MET:HE2	2.50	0.46
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.50	0.46
2:B:209:LEU:HD22	2:B:230:LEU:HD23	1.97	0.45
1:A:248:LEU:HD12	1:A:355:ILE:HD12	1.99	0.44
2:B:74:THR:O	2:B:78:VAL:HG23	2.18	0.44
1:A:183:GLU:N	1:A:184:PRO:CD	2.81	0.43
1:A:406:HIS:CE1	2:B:262:PHE:C	2.92	0.43
1:A:181:VAL:HG21	2:B:258:ASN:O	2.18	0.43
1:A:136:LEU:HD21	1:A:167:LEU:HD12	2.00	0.43
1:A:224:TYR:CE2	2:B:325:MET:HE1	2.53	0.43
6:B:502:TA1:H101	6:B:502:TA1:C24	2.49	0.42
1:A:271:THR:HG23	1:A:377:MET:HB3	2.02	0.42
2:B:229:HIS:CG	6:B:502:TA1:C07	3.02	0.42
1:A:217:LEU:HG	1:A:275:VAL:HG12	2.02	0.42
2:B:234:THR:HG21	2:B:270:PRO:CB	2.50	0.42
1:A:11:GLN:NE2	2:B:249:ASN:ND2	2.66	0.42
2:B:30:ILE:HD13	2:B:53:TYR:CE2	2.55	0.42
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.55	0.42
1:A:319:TYR:N	1:A:354:GLY:O	2.53	0.41
1:A:407:TRP:HH2	2:B:256:ALA:HB1	1.83	0.41
2:B:204:ILE:CD1	2:B:231:VAL:HG13	2.50	0.41
2:B:265:LEU:HD22	2:B:432:TYR:CE2	2.55	0.41
1:A:242:LEU:HD11	1:A:252:LEU:HG	2.01	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.20	0.41
1:A:269:LEU:CD2	1:A:384:ILE:HD12	2.50	0.41
2:B:20:PHE:CZ	2:B:24:ILE:HD11	2.55	0.41
2:B:358:ILE:O	2:B:358:ILE:HG23	2.21	0.41
1:A:178:SER:HB2	2:B:349:ASN:HD22	0.90	0.40
2:B:69:ASP:O	2:B:94:PHE:HA	2.21	0.40
1:A:382:THR:HG21	1:A:436:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/437 (97%)	389 (92%)	31 (7%)	2 (0%)	34	78
2	B	424/426 (100%)	412 (97%)	11 (3%)	1 (0%)	52	88
All	All	846/863 (98%)	801 (95%)	42 (5%)	3 (0%)	43	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	369	ARG
1	A	113	GLU
1	A	240	ALA

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	A	359/368 (98%)	350 (98%)	9 (2%)	55	84
2	B	367/367 (100%)	351 (96%)	16 (4%)	35	73
All	All	726/735 (99%)	701 (97%)	25 (3%)	48	79

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	CYS
1	A	49	PHE
1	A	88	HIS
1	A	140	SER
1	A	160	ASP
1	A	178	SER
1	A	373	ARG
1	A	392	ASP
1	A	407	TRP

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Mol	Chain	Res	Type
2	B	12	CYS
2	B	110	GLU
2	B	139	HIS
2	B	149	MET
2	B	159	GLU
2	B	160	GLU
2	B	170	SER
2	B	192	HIS
2	B	201	THR
2	B	205	ASP
2	B	255	LEU
2	B	266	HIS
2	B	305	CYS
2	B	314	THR
2	B	356	CYS
2	B	376	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	256	GLN
2	B	139	HIS
2	B	249	ASN
2	B	309	HIS
2	B	349	ASN
2	B	350	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GTP	A	501	4	26,34,34	1.00	2 (7%)	29,54,54	1.64	5 (17%)
5	GDP	B	501	-	24,30,30	1.22	3 (12%)	26,47,47	1.67	6 (23%)
6	TA1	B	502	-	68,68,68	0.51	0	102,105,105	0.66	1 (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
3	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3
6	TA1	B	502	-	-	0/41/127/127	0/5/7/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	O4'-C1'	2.16	1.44	1.41
3	A	501	GTP	C5-C4	2.77	1.46	1.40
5	B	501	GDP	C5-C4	3.03	1.47	1.40
3	A	501	GTP	C6-C5	3.18	1.47	1.41
5	B	501	GDP	C6-C5	3.80	1.49	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GTP	C5-C6-N1	-3.89	118.44	123.52
5	B	501	GDP	C5-C6-N1	-3.50	118.95	123.52
5	B	501	GDP	N3-C2-N1	-3.48	122.82	127.56
3	A	501	GTP	N3-C2-N1	-3.38	122.95	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GTP	C6-C5-C4	-2.97	117.46	120.86
5	B	501	GDP	C6-C5-C4	-2.75	117.72	120.86
6	B	502	TA1	O04-C11-C14	-2.34	102.14	108.08
3	A	501	GTP	O3G-PG-O2G	2.02	114.85	107.44
5	B	501	GDP	C4'-O4'-C1'	2.03	111.79	109.64
5	B	501	GDP	O3B-PB-O2B	2.08	115.07	107.44
5	B	501	GDP	C6-N1-C2	4.71	121.40	115.88
3	A	501	GTP	C6-N1-C2	5.08	121.84	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	TA1	9	0

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.