Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 12:20 pm GMT

PDB ID	:	7Z2A
EMDB ID	:	EMD-14459
Title	:	P. berghei kinesin-8B motor domain in no nucleotide state bound to tubulin dimer
Authors	:	Liu, T.; Shilliday, F.; Cook, A.D.; Moores, C.A.
Deposited on	:	2022-02-26
Resolution	:	4.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

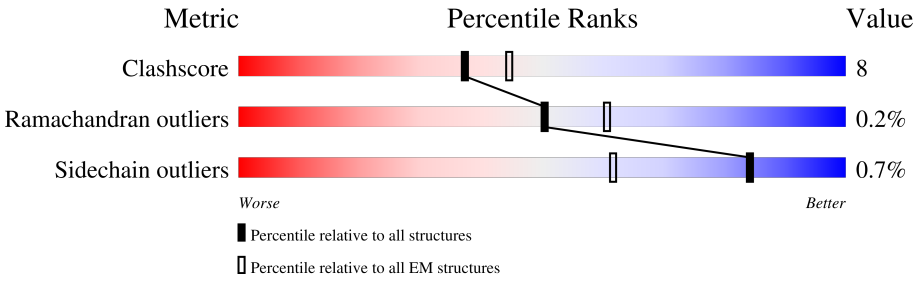
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	428	93% 7%
2	H	426	93% 7%
3	K	347	90% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12244 atoms, of which 2765 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	428	3342	2122	571	628	21	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q2XVP4
A	?	-	ASP	deletion	UNP Q2XVP4
A	?	-	LYS	deletion	UNP Q2XVP4
A	?	-	THR	deletion	UNP Q2XVP4
A	?	-	ILE	deletion	UNP Q2XVP4
A	?	-	GLY	deletion	UNP Q2XVP4
A	?	-	GLY	deletion	UNP Q2XVP4
A	?	-	GLY	deletion	UNP Q2XVP4
A	?	-	ASP	deletion	UNP Q2XVP4

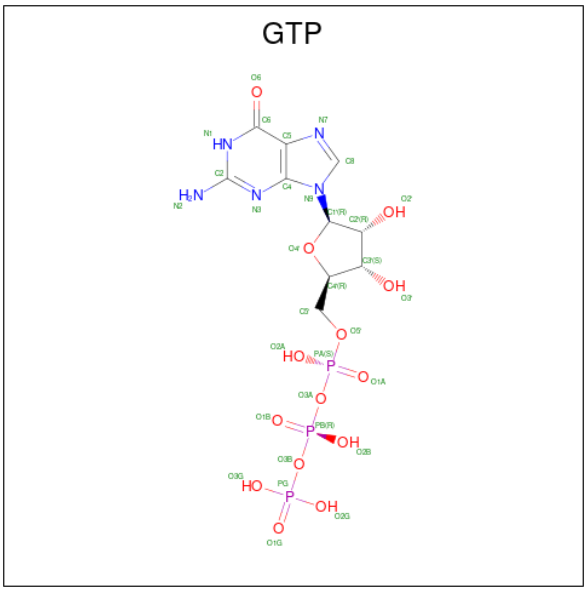
- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	426	3342	2101	572	644	25	0	0

- Molecule 3 is a protein called Kinesin-8, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	K	347	5494	1693	2765	482	535	19	0	0

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

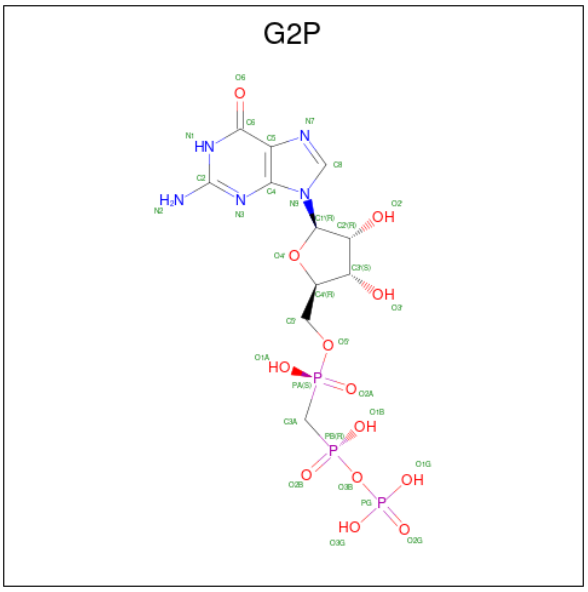


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



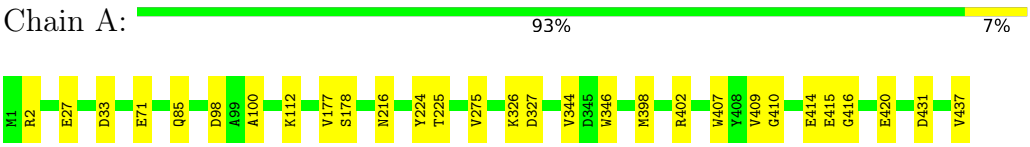
Mol	Chain	Residues	Atoms					AltConf
6	H	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots (i)

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

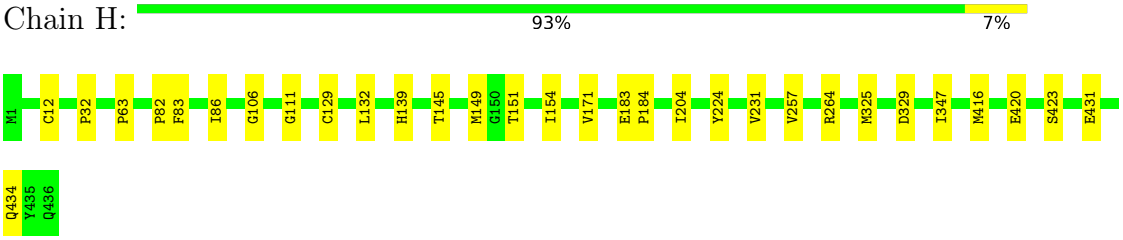
- Molecule 1: Detyrosinated tubulin alpha-1B chain

Chain A:



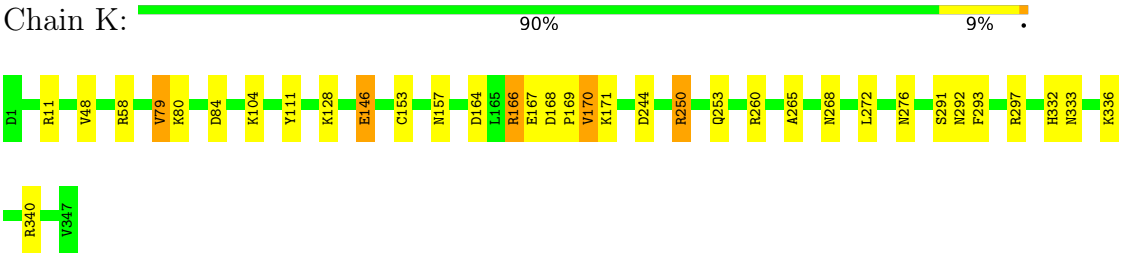
- Molecule 2: Tubulin beta chain

Chain H:



- Molecule 3: Kinesin-8, putative

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196084	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, G2P

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	A	0.45	0/3419	0.71	0/4643
2	H	0.45	0/3417	0.70	0/4631
3	K	0.86	2/2763 (0.1%)	0.87	7/3719 (0.2%)
All	All	0.59	2/9599 (0.0%)	0.76	7/12993 (0.1%)

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
3	K	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	79	VAL	CB-CG2	-6.06	1.40	1.52
3	K	146	GLU	CB-CG	-5.10	1.42	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	58	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	K	11	ARG	NE-CZ-NH2	-6.06	117.27	120.30
3	K	166	ARG	NE-CZ-NH2	-5.91	117.35	120.30
3	K	250	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	K	260	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	K	11	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	K	260	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	170	VAL	Peptide

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	3342	0	3252	62	0
2	H	3342	0	3219	92	0
3	K	2729	2765	2760	131	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0
5	H	1	0	0	0	0
6	H	32	0	14	0	0
All	All	9479	2765	9257	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (154) 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:H:431:GLU:CB	3:K:297:ARG:HH12	1.11	1.64
2:H:431:GLU:CG	3:K:297:ARG:NH1	1.74	1.50
2:H:431:GLU:CB	3:K:297:ARG:NH1	1.75	1.46
2:H:431:GLU:OE2	3:K:293:PHE:CD2	1.67	1.46
2:H:431:GLU:CD	3:K:293:PHE:HD2	1.28	1.34
2:H:420:GLU:OE2	3:K:166:ARG:CA	1.75	1.32
2:H:431:GLU:HG3	3:K:297:ARG:NH1	1.34	1.24
2:H:434:GLN:OE1	3:K:291:SER:O	1.57	1.22
2:H:264:ARG:NE	3:K:297:ARG:HD2	1.54	1.20
2:H:416:MET:HE2	3:K:167:GLU:O	1.39	1.20
2:H:416:MET:CE	3:K:169:PRO:HD3	1.73	1.18
2:H:420:GLU:OE2	3:K:166:ARG:CB	1.90	1.18
2:H:431:GLU:CD	3:K:293:PHE:CD2	2.13	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLY:HA2	3:K:336:LYS:HD3	1.16	1.15
2:H:431:GLU:OE2	3:K:293:PHE:HD2	1.07	1.15
1:A:414:GLU:OE2	3:K:250:ARG:HD3	1.44	1.14
2:H:431:GLU:OE2	3:K:293:PHE:HB3	1.48	1.11
1:A:415:GLU:HB3	3:K:340:ARG:HH22	1.10	1.10
1:A:409:VAL:HG13	3:K:268:ASN:HB3	1.28	1.09
2:H:431:GLU:OE2	3:K:293:PHE:CG	2.05	1.08
2:H:431:GLU:OE2	3:K:293:PHE:CB	2.02	1.07
2:H:420:GLU:OE2	3:K:166:ARG:HB3	1.49	1.07
2:H:264:ARG:HE	3:K:297:ARG:HD2	0.90	1.06
2:H:416:MET:CE	3:K:167:GLU:O	2.05	1.03
2:H:431:GLU:HB3	3:K:297:ARG:HH12	0.86	1.03
2:H:416:MET:HE1	3:K:169:PRO:HD3	1.03	1.02
2:H:434:GLN:CD	3:K:292:ASN:HA	1.79	1.01
2:H:423:SER:OG	3:K:171:LYS:NZ	1.94	1.00
2:H:420:GLU:OE2	3:K:167:GLU:N	1.94	1.00
2:H:420:GLU:OE2	3:K:166:ARG:HA	1.54	0.99
2:H:416:MET:HE1	3:K:169:PRO:CD	1.93	0.99
2:H:420:GLU:OE1	3:K:166:ARG:CD	2.11	0.98
1:A:409:VAL:CG1	3:K:268:ASN:HB3	1.94	0.96
2:H:420:GLU:OE1	3:K:166:ARG:HD3	1.64	0.96
2:H:431:GLU:HB2	3:K:297:ARG:HH12	1.26	0.96
2:H:431:GLU:HB2	3:K:297:ARG:NH1	1.79	0.93
2:H:423:SER:OG	3:K:171:LYS:CE	2.16	0.93
1:A:410:GLY:O	3:K:265:ALA:HB2	1.69	0.92
1:A:410:GLY:O	3:K:265:ALA:CB	2.16	0.92
2:H:420:GLU:OE2	3:K:166:ARG:C	2.10	0.90
2:H:431:GLU:HG3	3:K:297:ARG:HH11	0.92	0.88
2:H:423:SER:CB	3:K:167:GLU:OE1	2.22	0.87
1:A:416:GLY:HA2	3:K:336:LYS:CD	2.05	0.85
1:A:431:ASP:CB	3:K:48:VAL:HG21	2.05	0.85
2:H:431:GLU:CG	3:K:293:PHE:CD2	2.60	0.83
1:A:415:GLU:CB	3:K:340:ARG:HH22	1.90	0.82
1:A:420:GLU:OE2	3:K:332:HIS:CD2	2.34	0.81
2:H:420:GLU:OE1	3:K:166:ARG:HD2	1.80	0.81
2:H:423:SER:HB2	3:K:167:GLU:OE1	1.81	0.80
2:H:431:GLU:CG	3:K:297:ARG:HH11	1.63	0.80
1:A:416:GLY:CA	3:K:336:LYS:HD3	2.07	0.80
1:A:415:GLU:HB3	3:K:340:ARG:NH2	1.94	0.78
2:H:151:THR:O	2:H:154:ILE:HG22	1.84	0.78
2:H:434:GLN:CD	3:K:292:ASN:CA	2.52	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ASP:HA	3:K:48:VAL:CG2	2.15	0.76
1:A:431:ASP:HA	3:K:48:VAL:HG21	1.70	0.73
2:H:264:ARG:NE	3:K:297:ARG:CD	2.45	0.73
2:H:431:GLU:HG3	3:K:297:ARG:CZ	2.17	0.72
2:H:431:GLU:HB3	3:K:297:ARG:NH1	1.65	0.72
1:A:409:VAL:CG1	3:K:268:ASN:CB	2.68	0.72
1:A:431:ASP:CA	3:K:48:VAL:HG21	2.20	0.71
1:A:112:LYS:HE2	3:K:253:GLN:HA	1.72	0.71
2:H:420:GLU:HG2	3:K:167:GLU:H	1.57	0.70
2:H:423:SER:OG	3:K:167:GLU:OE1	2.10	0.70
2:H:416:MET:CE	3:K:169:PRO:CD	2.58	0.70
2:H:431:GLU:CG	3:K:297:ARG:CZ	2.68	0.69
2:H:434:GLN:CD	3:K:291:SER:O	2.32	0.67
1:A:112:LYS:HE2	3:K:253:GLN:CA	2.25	0.67
2:H:431:GLU:HG2	3:K:293:PHE:CD2	2.31	0.66
2:H:420:GLU:HG2	3:K:167:GLU:HB2	1.75	0.66
1:A:409:VAL:CG1	3:K:268:ASN:C	2.64	0.66
2:H:420:GLU:CG	3:K:167:GLU:H	2.09	0.66
2:H:416:MET:CE	3:K:168:ASP:HA	2.25	0.65
1:A:420:GLU:OE2	3:K:332:HIS:HD2	1.79	0.65
2:H:416:MET:HE3	3:K:168:ASP:C	2.16	0.65
1:A:177:VAL:HG13	2:H:329:ASP:HB3	1.79	0.64
2:H:431:GLU:OE1	3:K:297:ARG:CZ	2.46	0.64
2:H:420:GLU:CD	3:K:167:GLU:H	2.00	0.64
2:H:434:GLN:HG3	3:K:293:PHE:H	1.62	0.62
2:H:434:GLN:HG3	3:K:293:PHE:N	2.14	0.62
1:A:416:GLY:HA3	3:K:333:ASN:OD1	1.99	0.62
1:A:414:GLU:OE2	3:K:250:ARG:CD	2.36	0.62
2:H:423:SER:OG	3:K:171:LYS:HE2	1.97	0.62
2:H:423:SER:HB2	3:K:167:GLU:CD	2.21	0.61
1:A:112:LYS:HE2	3:K:253:GLN:CB	2.32	0.60
1:A:414:GLU:CD	3:K:250:ARG:HD3	2.20	0.60
1:A:409:VAL:HG11	3:K:268:ASN:C	2.24	0.58
2:H:416:MET:HE1	3:K:168:ASP:HA	1.85	0.58
1:A:420:GLU:CG	3:K:332:HIS:NE2	2.67	0.57
2:H:416:MET:HE3	3:K:167:GLU:O	2.00	0.57
1:A:402:ARG:NH1	3:K:340:ARG:HH11	2.03	0.56
2:H:416:MET:CE	3:K:168:ASP:CA	2.83	0.56
1:A:409:VAL:HG11	3:K:268:ASN:O	2.06	0.56
3:K:84:ASP:OD1	3:K:128:LYS:NZ	2.36	0.56
1:A:431:ASP:CG	3:K:48:VAL:HG21	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:CG1	2:H:329:ASP:HB3	2.36	0.55
1:A:100:ALA:O	2:H:257:VAL:HG11	2.07	0.54
2:H:420:GLU:CD	3:K:166:ARG:HA	2.26	0.53
1:A:431:ASP:HB3	3:K:48:VAL:HG21	1.85	0.53
2:H:264:ARG:CZ	3:K:297:ARG:HD2	2.31	0.53
2:H:434:GLN:OE1	3:K:292:ASN:CB	2.57	0.53
1:A:326:LYS:HG3	1:A:327:ASP:N	2.24	0.52
2:H:423:SER:HB2	3:K:167:GLU:OE2	2.10	0.52
1:A:420:GLU:HG3	3:K:332:HIS:NE2	2.25	0.52
2:H:129:CYS:SG	2:H:132:LEU:HB3	2.50	0.52
1:A:71:GLU:CG	1:A:98:ASP:HB3	2.40	0.52
1:A:409:VAL:HG12	3:K:268:ASN:CB	2.39	0.52
1:A:402:ARG:HH12	3:K:340:ARG:HH11	1.59	0.51
2:H:63:PRO:HD3	2:H:86:ILE:HG22	1.93	0.51
1:A:420:GLU:HG3	3:K:332:HIS:HE2	1.75	0.50
3:K:104:LYS:NZ	3:K:244:ASP:OD1	2.44	0.50
1:A:112:LYS:NZ	3:K:253:GLN:HB3	2.26	0.50
2:H:12:CYS:SG	2:H:171:VAL:HG21	2.52	0.50
2:H:423:SER:CB	3:K:167:GLU:CD	2.80	0.49
2:H:423:SER:CB	3:K:171:LYS:HZ3	2.23	0.49
1:A:398:MET:SD	2:H:347:ILE:HA	2.51	0.49
2:H:423:SER:OG	3:K:171:LYS:CD	2.60	0.49
2:H:82:PRO:O	2:H:83:PHE:HB2	2.13	0.49
1:A:415:GLU:CG	3:K:340:ARG:NH2	2.75	0.48
3:K:164:ASP:OD1	3:K:164:ASP:C	2.51	0.48
2:H:145:THR:O	2:H:149:MET:HB3	2.14	0.48
1:A:410:GLY:O	3:K:265:ALA:CA	2.61	0.48
1:A:431:ASP:HA	3:K:48:VAL:HG22	1.94	0.47
3:K:146:GLU:HB3	3:K:153:CYS:HB3	1.97	0.47
2:H:106:GLY:O	2:H:111:GLY:HA3	2.13	0.47
1:A:71:GLU:HG3	1:A:98:ASP:HB3	1.96	0.47
1:A:415:GLU:HB2	3:K:272:LEU:HD21	1.97	0.46
1:A:431:ASP:CG	3:K:48:VAL:CG2	2.75	0.46
1:A:420:GLU:CG	3:K:332:HIS:CD2	2.99	0.46
2:H:431:GLU:HG3	3:K:297:ARG:HD3	1.97	0.46
2:H:32:PRO:HA	2:H:86:ILE:HD11	1.97	0.45
2:H:183:GLU:N	2:H:184:PRO:CD	2.80	0.45
2:H:423:SER:OG	3:K:171:LYS:HD3	2.17	0.45
2:H:171:VAL:HA	2:H:204:ILE:O	2.17	0.45
1:A:409:VAL:HG11	3:K:272:LEU:HD12	1.71	0.44
1:A:112:LYS:HE2	3:K:253:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:420:GLU:HG2	3:K:167:GLU:CB	2.43	0.43
3:K:157:ASN:OD1	3:K:157:ASN:C	2.57	0.43
1:A:112:LYS:CE	3:K:253:GLN:HB3	2.48	0.43
1:A:402:ARG:HG3	3:K:276:ASN:OD1	2.19	0.42
1:A:224:TYR:CD2	2:H:325:MET:HG3	2.54	0.42
2:H:420:GLU:CD	3:K:166:ARG:CD	2.83	0.42
1:A:431:ASP:OD2	3:K:48:VAL:HB	2.20	0.42
2:H:416:MET:HE3	3:K:168:ASP:CA	2.50	0.42
3:K:79:VAL:O	3:K:80:LYS:C	2.58	0.42
1:A:420:GLU:HG2	3:K:332:HIS:NE2	2.35	0.41
2:H:204:ILE:HD13	2:H:231:VAL:HG13	2.02	0.41
1:A:33:ASP:HA	1:A:85:GLN:HB2	2.02	0.41
1:A:420:GLU:CD	3:K:332:HIS:CD2	2.94	0.41
2:H:416:MET:CE	3:K:168:ASP:C	2.87	0.41
1:A:216:ASN:HB3	1:A:275:VAL:O	2.21	0.40
1:A:344:VAL:HG11	1:A:346:TRP:NE1	2.36	0.40
1:A:407:TRP:CG	2:H:257:VAL:HG23	2.57	0.40
1:A:410:GLY:O	3:K:265:ALA:HB1	2.15	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	A	424/428 (99%)	410 (97%)	13 (3%)	1 (0%)	47 81
2	H	424/426 (100%)	411 (97%)	13 (3%)	0	100 100
3	K	345/347 (99%)	336 (97%)	8 (2%)	1 (0%)	41 76
All	All	1193/1201 (99%)	1157 (97%)	34 (3%)	2 (0%)	50 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
3	K	170	VAL

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	A	357/362 (99%)	353 (99%)	4 (1%)	73 85
2	H	365/367 (100%)	363 (100%)	2 (0%)	88 93
3	K	312/312 (100%)	311 (100%)	1 (0%)	92 95
All	All	1034/1041 (99%)	1027 (99%)	7 (1%)	84 90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	178	SER
1	A	225	THR
1	A	437	VAL
2	H	139	HIS
2	H	224	TYR
3	K	111	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
3	K	51	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
6	G2P	H	501	5	26,34,34	2.86	9 (34%)	30,54,54	1.84	8 (26%)
4	GTP	A	501	5	26,34,34	1.15	2 (7%)	33,54,54	2.02	9 (27%)

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
6	G2P	H	501	5	-	3/18/38/38	0/3/3/3
4	GTP	A	501	5	-	5/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	501	G2P	C4-N9	-10.91	1.33	1.47
6	H	501	G2P	PB-O2B	4.12	1.61	1.51
4	A	501	GTP	C5-C6	4.09	1.48	1.41
6	H	501	G2P	PA-O2A	4.03	1.61	1.51
6	H	501	G2P	PB-O1B	-3.55	1.48	1.56
6	H	501	G2P	PA-O1A	-3.36	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	501	G2P	C8-N9	-3.07	1.35	1.45
6	H	501	G2P	PA-O5'	2.50	1.61	1.57
6	H	501	G2P	PB-O3B	2.36	1.61	1.58
4	A	501	GTP	C5-C4	2.15	1.46	1.40
6	H	501	G2P	C5-C6	-2.01	1.49	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	GTP	C2-N3-C4	4.88	120.93	115.36
4	A	501	GTP	C4-C5-C6	-4.29	116.71	120.80
6	H	501	G2P	O4'-C4'-C3'	-4.27	96.67	105.11
4	A	501	GTP	C2-N1-C6	4.03	122.34	115.93
4	A	501	GTP	C5-C6-N1	-3.88	118.13	123.43
4	A	501	GTP	C4-C5-N7	-3.48	105.77	109.40
4	A	501	GTP	N3-C2-N1	-3.46	122.61	127.22
6	H	501	G2P	PB-O3B-PG	-3.18	121.41	132.62
6	H	501	G2P	O2'-C2'-C1'	3.14	120.51	110.02
4	A	501	GTP	PB-O3B-PG	-3.02	122.45	132.83
6	H	501	G2P	O2'-C2'-C3'	-2.97	102.22	111.82
4	A	501	GTP	C1'-N9-C4	-2.80	121.73	126.64
6	H	501	G2P	O1B-PB-O2B	2.68	119.01	110.07
6	H	501	G2P	C3'-C2'-C1'	-2.65	96.40	101.43
6	H	501	G2P	O5'-C5'-C4'	-2.63	99.92	108.99
4	A	501	GTP	PA-O3A-PB	-2.48	124.31	132.83
6	H	501	G2P	C4-C5-N7	2.41	105.66	102.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

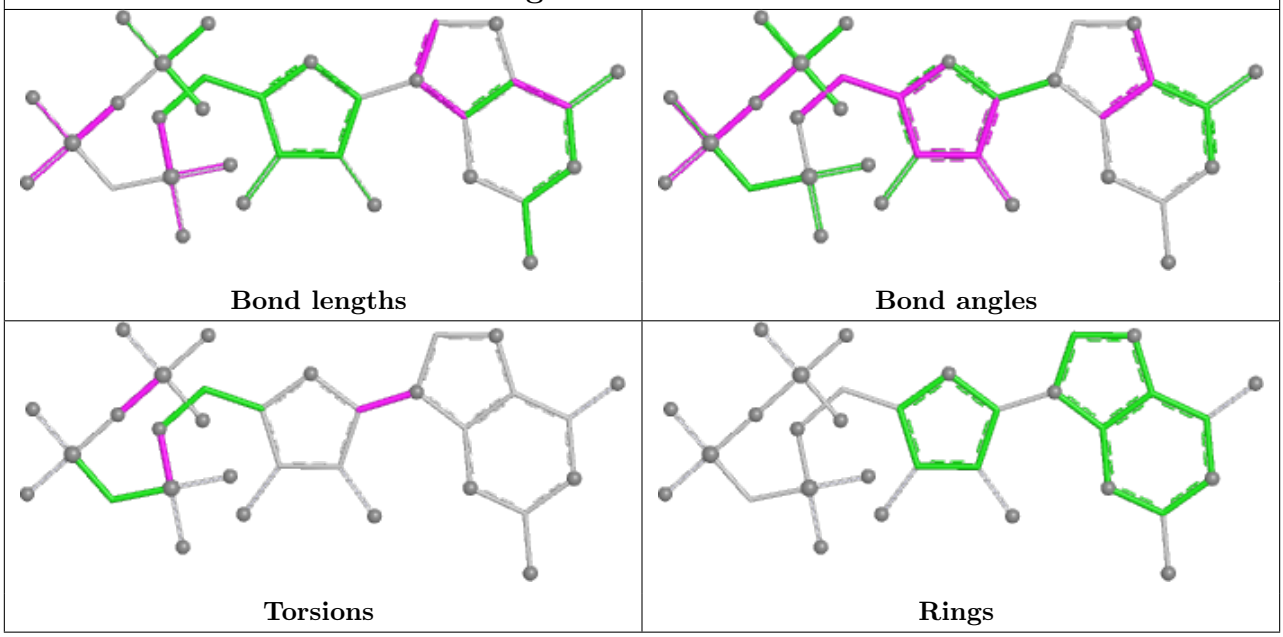
Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
6	H	501	G2P	C2'-C1'-N9-C4
6	H	501	G2P	C5'-O5'-PA-O1A
6	H	501	G2P	PB-O3B-PG-O1G
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	PB-O3A-PA-O1A

There are no ring outliers.

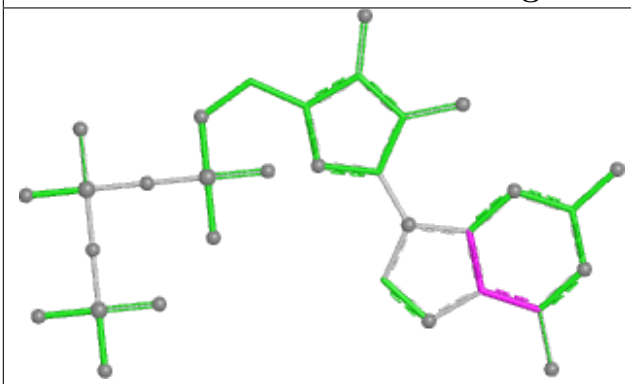
No monomer is involved in short contacts.

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

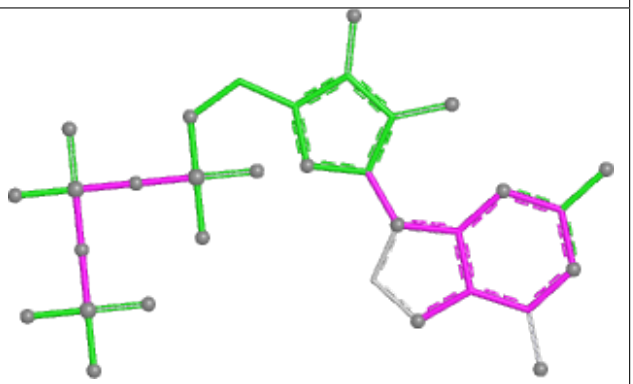
Ligand G2P H 501



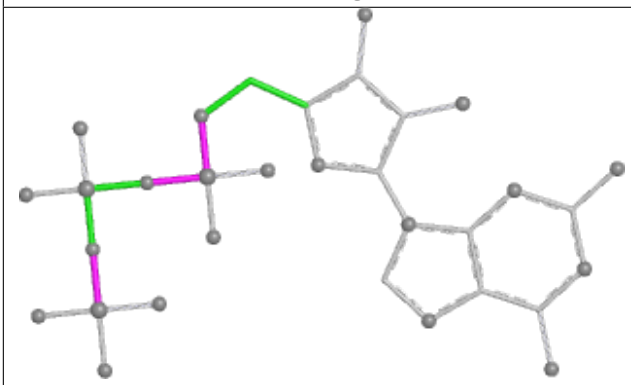
Ligand GTP A 501



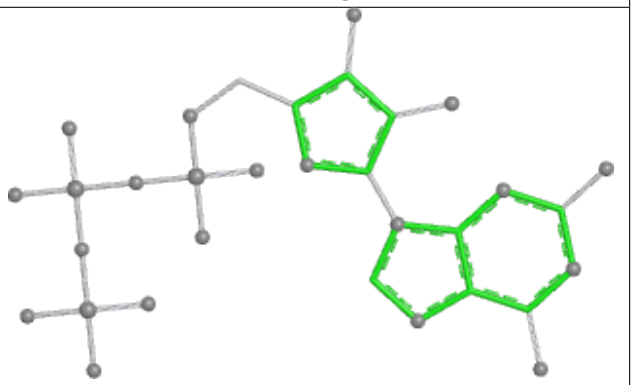
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	37:PRO	C	47:ASP	N	14.02

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14459. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.