wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:52 PM BST

PDB ID	:	3JAO
EMDB ID:	:	EMD-6312
Title	:	Ciliary microtubule doublet
Authors	:	Maheshwari, A.; Obbineni, J.M.; Bui, K.H.; Shibata, K.; Toyoshima, Y.Y.; Ishikawa, T.
Deposited on	:	2015-06-18
Resolution	:	23.00 Å(reported)
Based on PDB ID	:	3J6E

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

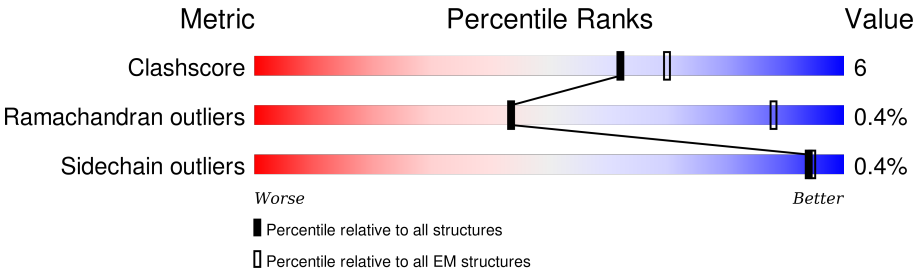
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 23.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=5%

Mol	Chain	Length	Quality of chain
1	A	451	79% 14% • 5%
2	B	445	77% 17% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6774 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.

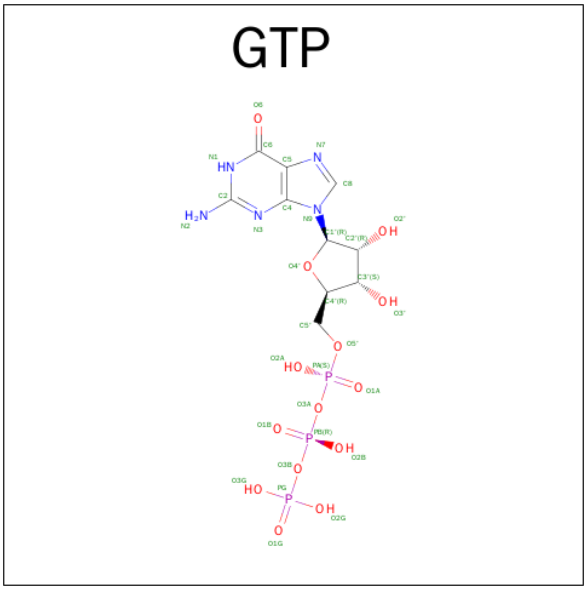
- Molecule 1 is a protein called Tubulin alpha 1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	428	3349	2121	570	637	21	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	3351	2105	575	646	25	0	0

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

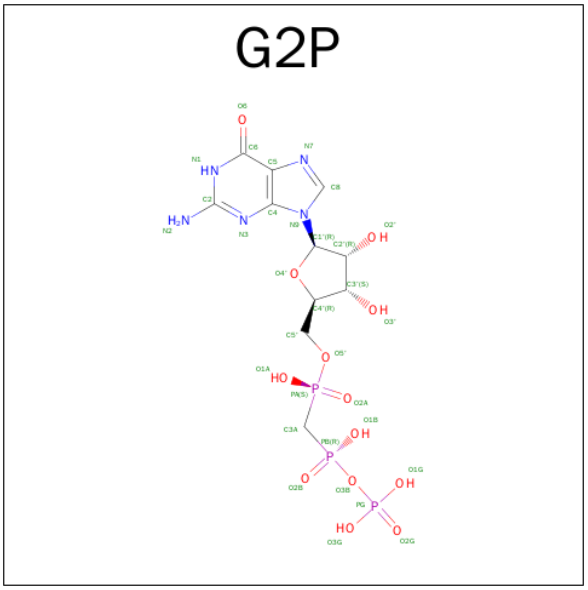


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	32	10	5	14	3	0

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

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

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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

- Molecule 6 is water.

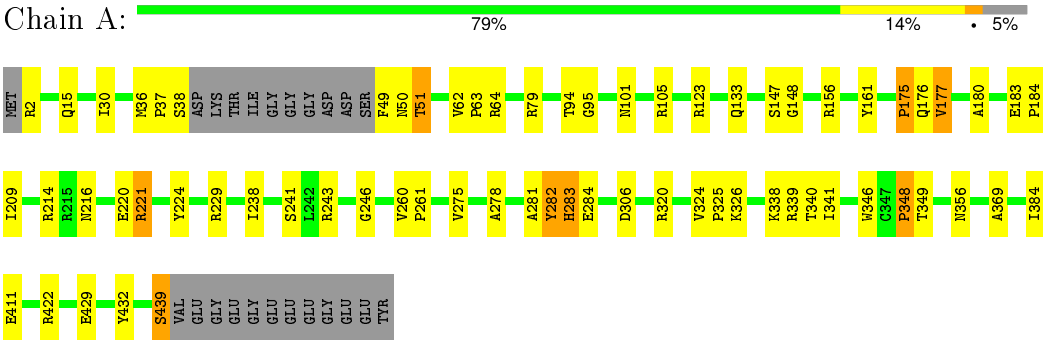
Mol	Chain	Residues	Atoms	AltConf
6	A	4	Total O 4 4	0
6	B	4	Total O 4 4	0

3 Residue-property plots (i)

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.

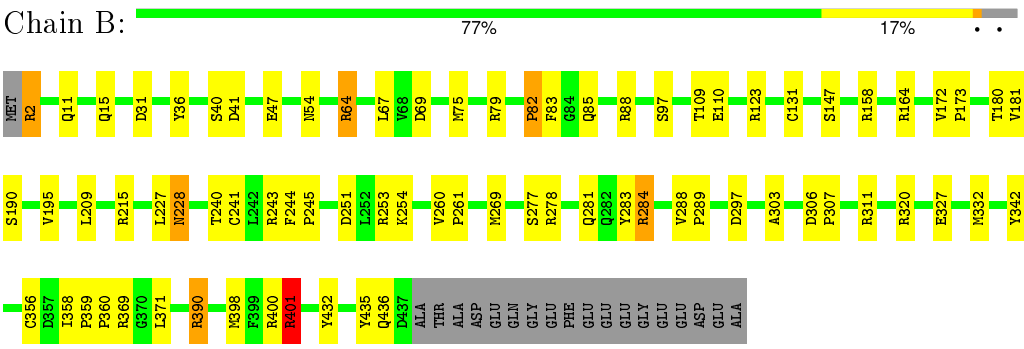
- Molecule 1: Tubulin alpha 1A chain

Chain A:



- Molecule 2: Tubulin beta chain

Chain B:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	10700	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	67000	Depositor
Image detector	CCD	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, MG, 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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	1.13	15/3426 (0.4%)	1.42	37/4651 (0.8%)
2	B	0.94	1/3426 (0.0%)	1.45	44/4642 (0.9%)
All	All	1.04	16/6852 (0.2%)	1.44	81/9293 (0.9%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ASN	N-CA	-10.24	1.25	1.46
1	A	349	THR	CA-C	-8.04	1.32	1.52
1	A	340	THR	N-CA	-7.79	1.30	1.46
1	A	37	PRO	N-CA	-6.96	1.35	1.47
1	A	339	ARG	CA-C	-6.60	1.35	1.52
1	A	283	HIS	CA-C	-6.32	1.36	1.52
1	A	339	ARG	N-CA	-6.03	1.34	1.46
1	A	284	GLU	N-CA	-5.93	1.34	1.46
1	A	51	THR	N-CA	-5.81	1.34	1.46
1	A	38	SER	CA-C	-5.62	1.38	1.52
1	A	283	HIS	N-CA	-5.58	1.35	1.46
1	A	338	LYS	CA-C	-5.51	1.38	1.52
1	A	348	PRO	CA-C	-5.38	1.42	1.52
1	A	282	TYR	CA-C	-5.32	1.39	1.52
1	A	175	PRO	N-CA	-5.26	1.38	1.47
2	B	82	PRO	CA-C	-5.01	1.42	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	88	ARG	NE-CZ-NH1	18.64	129.62	120.30
2	B	401	ARG	NE-CZ-NH1	16.80	128.70	120.30
1	A	105	ARG	NE-CZ-NH2	-14.72	112.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	ARG	NE-CZ-NH2	-14.23	113.18	120.30
2	B	253	ARG	NE-CZ-NH1	14.01	127.31	120.30
1	A	123	ARG	NE-CZ-NH2	-12.44	114.08	120.30
2	B	88	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	A	402	ARG	NE-CZ-NH2	11.10	125.85	120.30
2	B	64	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	A	339	ARG	CA-C-N	-10.60	93.88	117.20
2	B	369	ARG	NE-CZ-NH1	9.75	125.18	120.30
2	B	123	ARG	NE-CZ-NH2	-9.65	115.47	120.30
2	B	320	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	214	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	432	TYR	CB-CG-CD2	-8.79	115.73	121.00
2	B	311	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	243	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	64	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	A	282	TYR	CB-CG-CD2	-8.58	115.85	121.00
2	B	2	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	A	79	ARG	NE-CZ-NH2	-8.29	116.16	120.30
2	B	283	TYR	CB-CG-CD1	-8.23	116.06	121.00
2	B	123	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	B	243	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	A	229	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	A	123	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	221	ARG	NE-CZ-NH1	-7.92	116.34	120.30
2	B	311	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	320	ARG	NE-CZ-NH2	7.49	124.04	120.30
2	B	306	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	283	HIS	C-N-CA	-7.31	103.42	121.70
1	A	320	ARG	NE-CZ-NH1	7.19	123.89	120.30
2	B	390	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	A	338	LYS	C-N-CA	-7.12	103.89	121.70
2	B	253	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	339	ARG	O-C-N	6.81	133.59	122.70
1	A	422	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	B	284	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	B	2	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	320	ARG	NH1-CZ-NH2	-6.67	112.06	119.40
2	B	243	ARG	NH1-CZ-NH2	-6.62	112.11	119.40
1	A	185	TYR	CB-CG-CD2	-6.59	117.05	121.00
2	B	243	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	B	215	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	B	320	ARG	NE-CZ-NH2	-6.41	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	164	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	37	PRO	CA-N-CD	6.32	120.54	111.70
2	B	158	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	B	436	GLN	C-N-CA	-5.97	106.78	121.70
2	B	88	ARG	CD-NE-CZ	5.96	131.94	123.60
1	A	339	ARG	CA-C-O	5.90	132.48	120.10
1	A	79	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	282	TYR	CA-C-N	-5.75	104.54	117.20
2	B	332	MET	CG-SD-CE	5.71	109.33	100.20
2	B	69	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	342	TYR	CB-CG-CD1	-5.68	117.59	121.00
2	B	297	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	177	VAL	CB-CA-C	-5.64	100.69	111.40
2	B	228	ASN	CA-CB-CG	-5.63	101.02	113.40
2	B	432	TYR	CB-CG-CD2	-5.58	117.65	121.00
2	B	400	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	A	156	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	161	TYR	CA-CB-CG	-5.45	103.05	113.40
2	B	435	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	439	SER	N-CA-C	5.42	125.64	111.00
1	A	51	THR	CA-CB-CG2	-5.38	104.87	112.40
2	B	401	ARG	CD-NE-CZ	-5.37	116.08	123.60
1	A	432	TYR	CB-CG-CD1	5.34	124.20	121.00
1	A	64	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	B	36	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	281	ALA	C-N-CA	-5.26	108.56	121.70
1	A	224	TYR	CB-CG-CD1	-5.22	117.87	121.00
2	B	79	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	75	MET	CG-SD-CE	-5.18	91.92	100.20
2	B	251	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	339	ARG	N-CA-C	5.14	124.87	111.00
2	B	284	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	B	185	TYR	CA-CB-CG	5.12	123.12	113.40
1	A	411	GLU	CA-CB-CG	5.06	124.54	113.40
1	A	105	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	B	240	THR	CA-CB-CG2	-5.02	105.37	112.40

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	3349	0	3254	34	0
2	B	3351	0	3229	41	0
3	A	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	32	0	13	4	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	6774	0	6508	73	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 (73) 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:B:228:ASN:HD21	5:B:501:G2P:H1	1.13	0.97
1:A:341:ILE:HG13	1:A:341:ILE:O	1.67	0.92
2:B:401:ARG:HD3	2:B:401:ARG:N	2.07	0.69
1:A:439:SER:O	1:A:439:SER:OG	2.05	0.66
1:A:177:VAL:HG23	1:A:207:GLU:OE1	1.95	0.66
1:A:147:SER:OG	1:A:148:GLY:N	2.26	0.65
2:B:401:ARG:CD	2:B:401:ARG:N	2.56	0.65
2:B:85:GLN:CD	2:B:85:GLN:H	2.03	0.62
1:A:30:ILE:HG12	1:A:36:MET:SD	2.41	0.61
1:A:207:GLU:OE2	1:A:207:GLU:N	2.35	0.60
2:B:228:ASN:ND2	5:B:501:G2P:H1	1.93	0.59
2:B:390:ARG:HA	2:B:390:ARG:NE	2.18	0.59
1:A:2:ARG:HA	1:A:133:GLN:HG3	1.84	0.58
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.89	0.55
2:B:277:SER:OG	2:B:278:ARG:N	2.41	0.53
1:A:341:ILE:CG1	1:A:341:ILE:O	2.43	0.53
2:B:269:MET:SD	2:B:307:PRO:HG3	2.48	0.53
2:B:85:GLN:CD	2:B:85:GLN:N	2.64	0.51
2:B:2:ARG:N	2:B:131:CYS:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PRO:HG2	2:B:371:LEU:HB2	1.93	0.51
2:B:288:VAL:HB	2:B:327:GLU:HG2	1.91	0.51
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.94	0.50
2:B:195:VAL:O	2:B:195:VAL:HG22	2.12	0.50
1:A:282:TYR:O	1:A:283:HIS:HB2	2.11	0.50
1:A:15:GLN:HA	1:A:15:GLN:OE1	2.13	0.49
2:B:181:VAL:O	2:B:398:MET:SD	2.71	0.48
1:A:346:TRP:CD1	1:A:346:TRP:N	2.78	0.48
2:B:40:SER:OG	2:B:41:ASP:N	2.46	0.48
2:B:348:PRO:O	2:B:349:ASN:HB2	2.14	0.48
2:B:390:ARG:HA	2:B:390:ARG:HE	1.80	0.47
1:A:220:GLU:OE2	1:A:221:ARG:NH1	2.49	0.46
1:A:241:SER:O	1:A:356:ASN:ND2	2.48	0.46
2:B:180:THR:HG23	2:B:183:GLU:HB2	1.98	0.45
1:A:326:LYS:HD2	1:A:326:LYS:C	2.37	0.45
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.45
2:B:401:ARG:HA	2:B:401:ARG:HD2	1.61	0.45
1:A:238:ILE:O	1:A:238:ILE:HG22	2.16	0.45
1:A:216:ASN:HB3	1:A:275:VAL:O	2.16	0.45
2:B:67:LEU:HD12	2:B:67:LEU:N	2.31	0.45
1:A:260:VAL:HA	1:A:261:PRO:HD2	1.87	0.44
2:B:54:ASN:OD1	2:B:64:ARG:NH1	2.50	0.44
2:B:269:MET:HG2	2:B:269:MET:O	2.18	0.44
1:A:385:ALA:HB1	1:A:429:GLU:HG3	1.98	0.44
2:B:183:GLU:N	2:B:184:PRO:CD	2.80	0.44
1:A:101:ASN:OD1	2:B:254:LYS:NZ	2.48	0.44
1:A:209:ILE:O	1:A:209:ILE:HG22	2.16	0.44
2:B:209:LEU:HB3	2:B:227:LEU:HD22	2.00	0.43
1:A:175:PRO:O	2:B:349:ASN:ND2	2.51	0.43
2:B:281:GLN:HA	2:B:284:ARG:HG2	2.01	0.43
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.88	0.43
2:B:31:ASP:C	2:B:31:ASP:OD1	2.58	0.43
2:B:15:GLN:NE2	5:B:501:G2P:O6	2.52	0.42
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.01	0.42
2:B:241:CYS:SG	2:B:356:CYS:HB3	2.59	0.42
2:B:358:ILE:HA	2:B:359:PRO:HD2	1.88	0.42
2:B:147:SER:HB2	2:B:190:SER:HB3	2.02	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
1:A:49:PHE:HD1	1:A:49:PHE:HA	1.72	0.42
1:A:238:ILE:O	1:A:238:ILE:CG2	2.67	0.41
2:B:109:THR:OG1	2:B:110:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:VAL:HA	2:B:173:PRO:HD3	1.82	0.41
1:A:306:ASP:C	1:A:306:ASP:OD1	2.56	0.41
1:A:94:THR:OG1	1:A:95:GLY:N	2.53	0.41
2:B:82:PRO:O	2:B:83:PHE:HB2	2.20	0.41
1:A:49:PHE:C	1:A:51:THR:N	2.73	0.41
2:B:244:PHE:HA	2:B:245:PRO:HD3	1.91	0.41
2:B:11:GLN:HB3	5:B:501:G2P:O1A	2.21	0.41
1:A:324:VAL:HA	1:A:325:PRO:HD3	1.93	0.41
1:A:384:ILE:O	1:A:384:ILE:HG12	2.21	0.41
1:A:176:GLN:HB3	1:A:207:GLU:HG2	2.03	0.40
2:B:288:VAL:N	2:B:289:PRO:CD	2.83	0.40
2:B:401:ARG:N	2:B:401:ARG:HD2	2.29	0.40
2:B:260:VAL:HA	2:B:261:PRO:HD2	1.87	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	424/451 (94%)	405 (96%)	18 (4%)	1 (0%)	52 86
2	B	424/445 (95%)	411 (97%)	11 (3%)	2 (0%)	34 77
All	All	848/896 (95%)	816 (96%)	29 (3%)	3 (0%)	43 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PRO
2	B	97	SER
2	B	47	GLU

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	360/377 (96%)	359 (100%)	1 (0%)	94	96
2	B	367/381 (96%)	365 (100%)	2 (0%)	92	96
All	All	727/758 (96%)	724 (100%)	3 (0%)	94	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
2	B	352	LYS
2	B	401	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
2	B	8	GLN
2	B	192	HIS

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 (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	$\#\|Z\| > 2$
3	GTP	A	501	4	26,34,34	1.37	3 (11%)	29,54,54	2.33	5 (17%)
5	G2P	B	501	4	29,34,34	5.92	25 (86%)	32,54,54	4.83	20 (62%)

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	G2P	B	501	4	-	0/15/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	G2P	PB-C3A	-19.24	1.60	1.80
5	B	501	G2P	PA-O1A	-6.24	1.41	1.56
5	B	501	G2P	O2'-C2'	-6.12	1.28	1.43
5	B	501	G2P	C8-N7	-5.01	1.25	1.34
5	B	501	G2P	PA-C3A	-4.81	1.75	1.80
5	B	501	G2P	O5'-C5'	-4.32	1.27	1.44
5	B	501	G2P	PG-O3G	-3.73	1.41	1.54
5	B	501	G2P	O6-C6	-2.50	1.18	1.24
5	B	501	G2P	C2'-C3'	-2.34	1.47	1.53
3	A	501	GTP	PB-O2B	-2.09	1.46	1.55
3	A	501	GTP	O4'-C1'	2.01	1.44	1.41
5	B	501	G2P	PB-O3B	2.11	1.60	1.58
5	B	501	G2P	C2-N3	2.33	1.47	1.35
5	B	501	G2P	PG-O1G	2.60	1.63	1.54
5	B	501	G2P	O4'-C4'	2.65	1.51	1.45
5	B	501	G2P	PB-O1B	2.91	1.63	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	G2P	C3'-C4'	3.06	1.61	1.53
5	B	501	G2P	PB-O2B	3.67	1.61	1.51
5	B	501	G2P	PA-O2A	4.22	1.62	1.51
5	B	501	G2P	C6-N1	4.46	1.41	1.33
3	A	501	GTP	C6-N1	4.74	1.41	1.33
5	B	501	G2P	C4-N3	5.65	1.44	1.35
5	B	501	G2P	C6-C5	5.75	1.53	1.41
5	B	501	G2P	C2-N1	6.62	1.47	1.35
5	B	501	G2P	C2'-C1'	6.77	1.64	1.53
5	B	501	G2P	C2-N2	7.92	1.51	1.34
5	B	501	G2P	O3'-C3'	8.03	1.61	1.43
5	B	501	G2P	PA-O5'	9.62	1.67	1.57

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	501	G2P	N3-C2-N1	-11.04	112.54	127.56
3	A	501	GTP	C5-C6-N1	-7.73	113.41	123.52
5	B	501	G2P	O4'-C4'-C3'	-7.61	89.73	105.16
5	B	501	G2P	C1'-N9-C4	-6.16	119.93	126.81
5	B	501	G2P	C5-C6-N1	-5.56	116.25	123.52
5	B	501	G2P	O5'-PA-O2A	-5.44	98.99	114.05
5	B	501	G2P	O2'-C2'-C3'	-4.51	97.27	111.86
3	A	501	GTP	N3-C2-N1	-3.50	122.80	127.56
5	B	501	G2P	O2A-PA-C3A	-2.86	100.46	108.82
5	B	501	G2P	O5'-PA-C3A	-2.58	96.90	104.23
5	B	501	G2P	C6-C5-C4	-2.48	118.03	120.86
3	A	501	GTP	C6-C5-C4	-2.16	118.39	120.86
5	B	501	G2P	O1A-PA-O2A	-2.08	103.61	110.24
3	A	501	GTP	O2G-PG-O1G	-2.06	103.92	110.63
5	B	501	G2P	O3'-C3'-C4'	2.01	117.02	111.01
5	B	501	G2P	O3'-C3'-C2'	2.27	119.18	111.86
5	B	501	G2P	O2'-C2'-C1'	2.86	120.55	111.61
5	B	501	G2P	O1A-PA-C3A	3.85	125.81	107.14
5	B	501	G2P	O1B-PB-O2B	5.04	126.34	110.24
5	B	501	G2P	N2-C2-N3	6.89	130.64	117.72
5	B	501	G2P	O1A-PA-O5'	7.47	125.61	106.69
3	A	501	GTP	C6-N1-C2	7.49	124.66	115.88
5	B	501	G2P	C4'-O4'-C1'	7.71	117.81	109.64
5	B	501	G2P	PA-O5'-C5'	8.27	145.86	122.23
5	B	501	G2P	C6-N1-C2	10.62	128.33	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	G2P	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.