



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 25, 2017 – 08:32 PM EDT

PDB ID : 5ND4
EMDB ID: : EMD-3622
Title : Microtubule-bound MKLP2 motor domain in the presence of ADP.AIFx
Authors : Atherton, J.; Yu, I.-M.; Cook, A.; Muretta, J.M.; Joseph, A.P.; Major, J.; Sourigues, Y.; Clause, J.; Topf, M.; Rosenfeld, S.S.; Houdusse, A.; Moores, C.A.
Deposited on : unknown
Resolution : 4.40 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

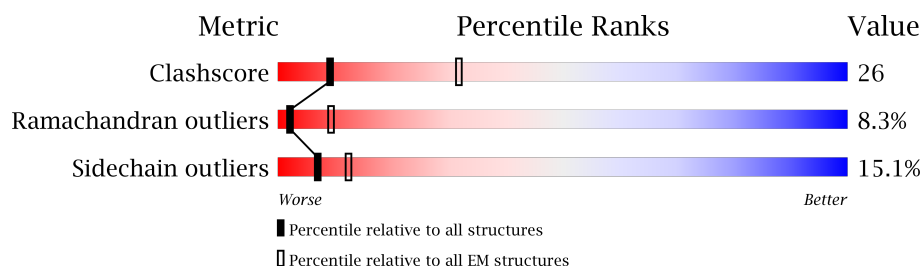
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	C	501	
2	A	412	
3	B	426	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	C	601	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9435 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 Kinesin-like protein KIF20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	337	Total	C	N	O	S	0	0
			2701	1704	487	498	12		

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP F2Z4C1
A	?	-	MET	deletion	UNP F2Z4C1
A	?	-	PRO	deletion	UNP F2Z4C1
A	?	-	SER	deletion	UNP F2Z4C1
A	?	-	ASP	deletion	UNP F2Z4C1
A	?	-	LYS	deletion	UNP F2Z4C1
A	?	-	THR	deletion	UNP F2Z4C1
A	?	-	ILE	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	ASP	deletion	UNP F2Z4C1
A	?	-	ASP	deletion	UNP F2Z4C1
A	?	-	SER	deletion	UNP F2Z4C1
A	?	-	PHE	deletion	UNP F2Z4C1
A	?	-	ASN	deletion	UNP F2Z4C1
A	?	-	THR	deletion	UNP F2Z4C1
A	?	-	PHE	deletion	UNP F2Z4C1
A	?	-	PHE	deletion	UNP F2Z4C1
A	?	-	SER	deletion	UNP F2Z4C1
A	?	-	GLU	deletion	UNP F2Z4C1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	ALA	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	LYS	deletion	UNP F2Z4C1
A	136	SER	LEU	conflict	UNP F2Z4C1
A	265	GLY	ILE	conflict	UNP F2Z4C1
A	358	GLU	GLN	conflict	UNP F2Z4C1

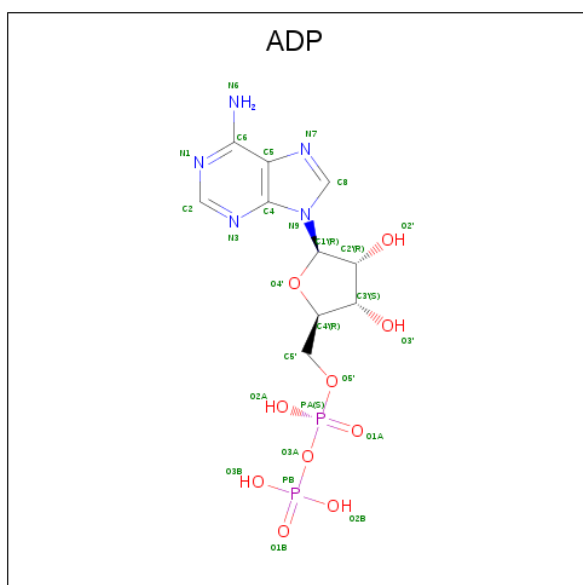
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	ALA	THR	conflict	UNP Q6B856
B	172	VAL	MET	conflict	UNP Q6B856
B	298	ALA	SER	conflict	UNP Q6B856
B	318	VAL	ILE	conflict	UNP Q6B856

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

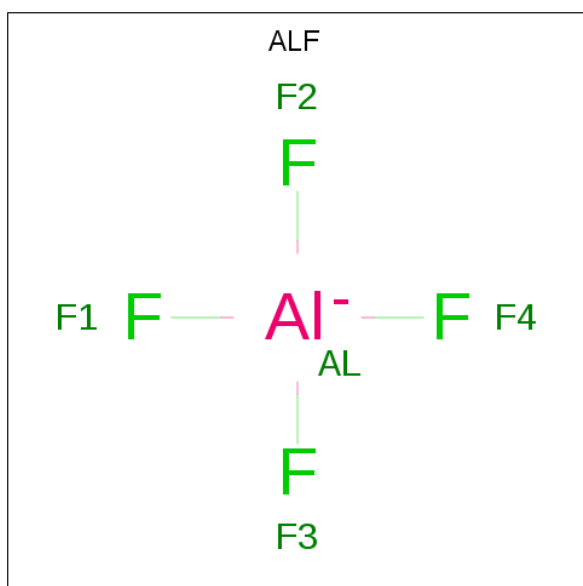


Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

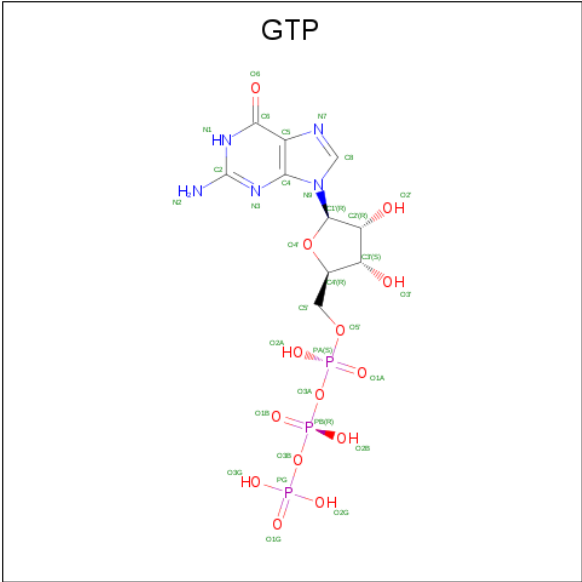
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	

- Molecule 6 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



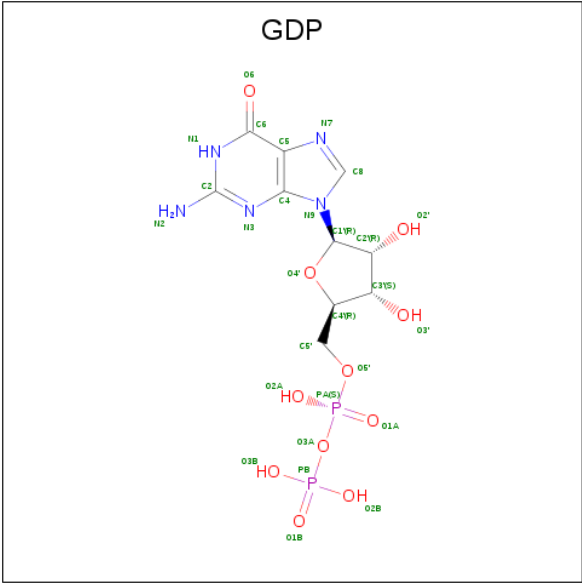
Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	Al	F	0
			5	1	4	

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



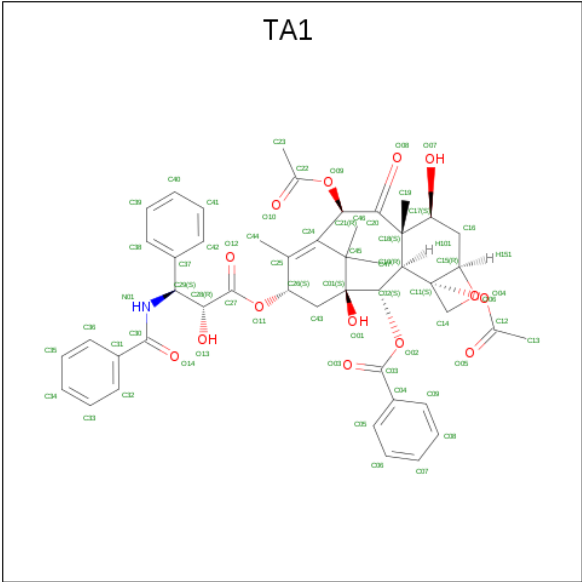
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 9 is TAXOL (three-letter code: TA1) (formula: C₄₇H₅₁NO₁₄).

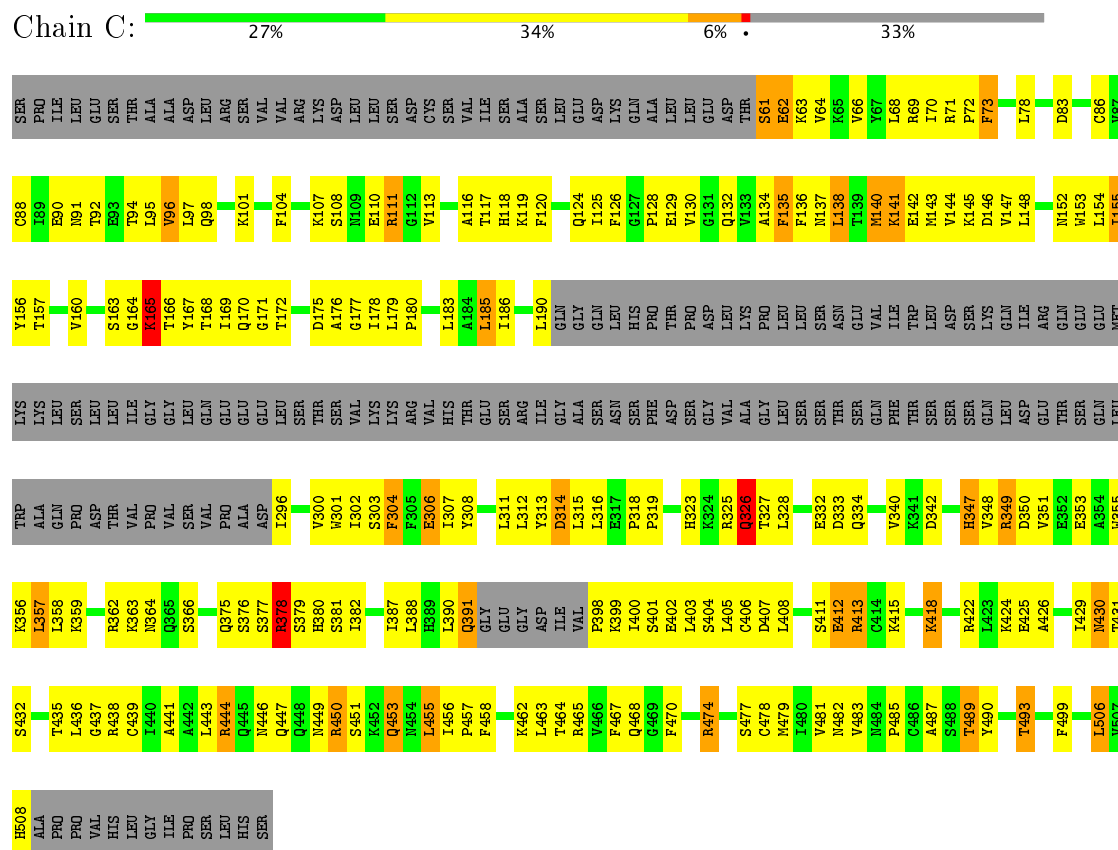


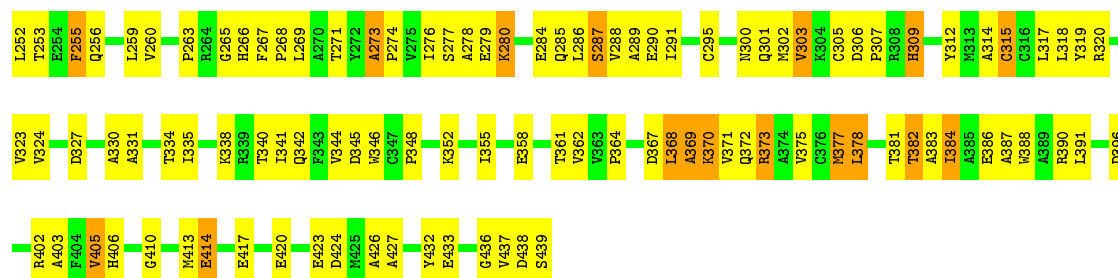
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	62	47	1	14	0

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 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.

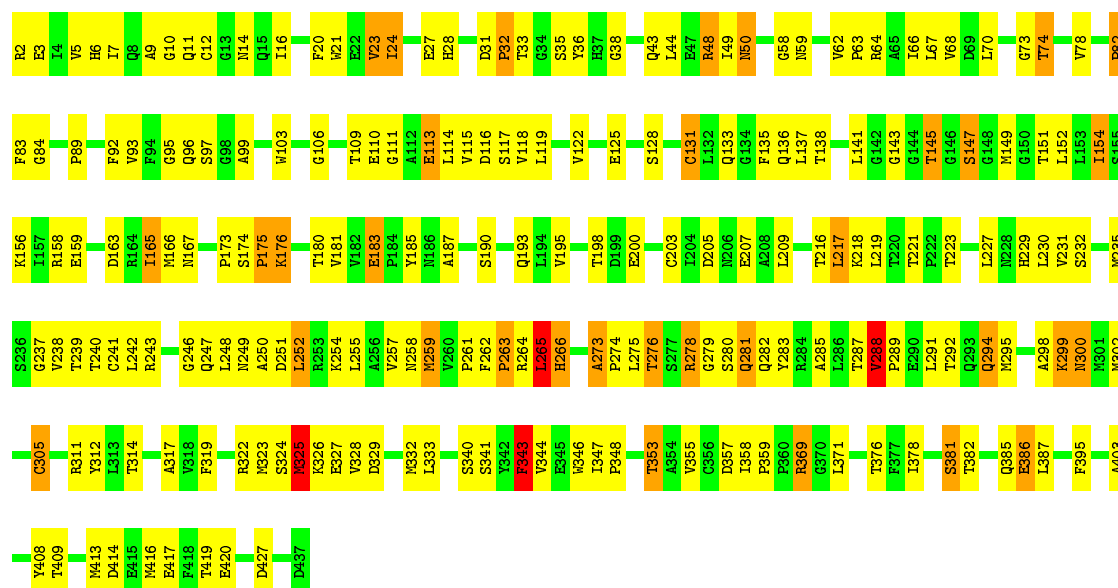
• Molecule 1: Kinesin-like protein KIF20A





• Molecule 3: Tubulin beta-2B chain

Chain B: 50% 41% 8%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	21239	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	C	0.47	1/2753 (0.0%)	0.65	4/3709 (0.1%)
2	A	0.35	1/3300 (0.0%)	0.59	2/4482 (0.0%)
3	B	0.31	0/3426	0.50	0/4642
All	All	0.37	2/9479 (0.0%)	0.58	6/12833 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0
2	A	0	1
3	B	1	0
All	All	2	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	ARG	NE-CZ	5.79	1.40	1.33
1	C	430	ASN	CB-CG	5.00	1.62	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	ARG	NE-CZ-NH2	-17.59	111.50	120.30
1	C	165	LYS	CB-CG-CD	-8.73	88.91	111.60
2	A	2	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	C	412	GLU	C-N-CA	8.01	141.73	121.70
1	C	378	ARG	CD-NE-CZ	-5.06	116.51	123.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	472	THR	CA
3	B	280	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2	ARG	Sidechain

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	C	2701	0	2700	182	0
2	A	3227	0	3143	172	0
3	B	3351	0	3229	136	0
4	C	27	0	12	23	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	C	5	0	0	0	0
7	A	32	0	12	7	0
8	B	28	0	12	8	0
9	B	62	0	51	7	0
All	All	9435	0	9159	478	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 26.

The worst 5 of 478 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:A:2:ARG:CZ	2:A:133:GLN:HG2	1.66	1.24
2:A:11:GLN:HB3	7:A:500:GTP:O2B	1.44	1.18
1:C:164:GLY:HA2	4:C:601:ADP:O5'	1.52	1.09
3:B:12:CYS:SG	8:B:600:GDP:C4	2.45	1.09
1:C:164:GLY:HA3	4:C:601:ADP:H8	1.14	1.05

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	C	331/501 (66%)	317 (96%)	11 (3%)	3 (1%)	20	63
2	A	408/412 (99%)	283 (69%)	76 (19%)	49 (12%)	0	8
3	B	424/426 (100%)	297 (70%)	82 (19%)	45 (11%)	0	11
All	All	1163/1339 (87%)	897 (77%)	169 (14%)	97 (8%)	2	17

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	GLN
2	A	97	GLU
2	A	109	THR
2	A	141	PHE
2	A	183	GLU

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	C	301/447 (67%)	243 (81%)	58 (19%)	1	12
2	A	347/347 (100%)	300 (86%)	47 (14%)	4	26
3	B	367/367 (100%)	319 (87%)	48 (13%)	5	27
All	All	1015/1161 (87%)	862 (85%)	153 (15%)	7	22

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	141	PHE
2	A	305	CYS
3	B	325	MET
2	A	149	PHE
2	A	219	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	375	GLN
3	B	406	HIS
2	A	11	GLN
1	C	326	GLN
1	C	434	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
7	GTP	A	500	5	27,34,34	1.54	3 (11%)	27,54,54	2.16	5 (18%)
8	GDP	B	600	-	25,30,30	2.61	8 (32%)	26,47,47	3.64	9 (34%)
9	TA1	B	601	-	68,68,68	1.97	20 (29%)	105,105,105	1.32	8 (7%)
4	ADP	C	601	5	25,29,29	0.57	0	24,45,45	0.83	0
6	ALF	C	603	-	0,4,4	0.00	-	0,6,6	0.00	-

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
7	GTP	A	500	5	-	0/18/38/38	0/3/3/3
8	GDP	B	600	-	-	0/12/32/32	0/3/3/3
9	TA1	B	601	-	-	0/41/127/127	0/5/7/7
4	ADP	C	601	5	-	0/12/32/32	0/3/3/3
6	ALF	C	603	-	-	0/0/0/0	0/0/0/0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	TA1	C08-C07	-5.10	1.25	1.38
8	B	600	GDP	PB-O2B	-3.55	1.40	1.54
9	B	601	TA1	C04-C03	-2.36	1.44	1.49
7	A	500	GTP	C8-N7	-2.02	1.30	1.34
9	B	601	TA1	C10-C02	2.03	1.62	1.57

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	600	GDP	C6-C5-C4	-11.40	109.51	120.84
7	A	500	GTP	C5-C6-N1	-7.09	113.39	123.48
8	B	600	GDP	N2-C2-N1	-5.89	107.83	117.24
8	B	600	GDP	C4-C5-N7	-5.02	104.56	109.41
8	B	600	GDP	N3-C2-N1	-4.94	120.24	127.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	500	GTP	7	0
8	B	600	GDP	8	0
9	B	601	TA1	7	0
4	C	601	ADP	23	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	34:GLY	C	61:HIS	N	3.53