



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:22 am GMT

PDB ID : 3EDL
EMDB ID: : EMD-5027
Title : Kinesin13-Microtubule Ring complex
Authors : Tan, D.; Rice, W.J.; Sosa, H.
Deposited on : 2008-09-03
Resolution : 28.00 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) : recalc29047

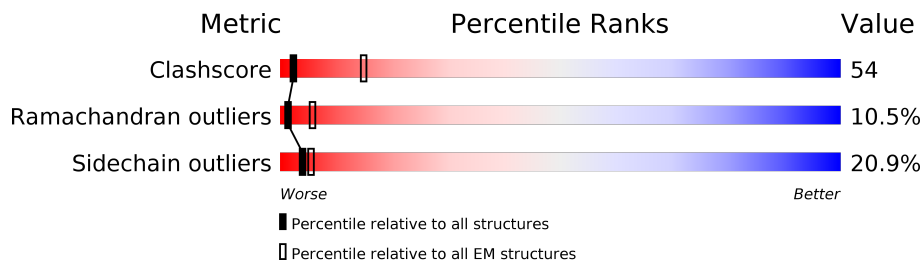
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 28.00 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	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	A	451	
2	B	445	
2	G	445	
3	D	331	
4	F	451	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 15757 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 Alpha-tubulin.

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

- Molecule 2 is a protein called Beta tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
2	G	419	Total	C	N	O	S	0	0
			3237	2037	544	631	25		

- Molecule 3 is a protein called Kinesin13 Motor domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	301	Total	C	N	O	S	0	0
			2368	1496	416	438	18		

- Molecule 4 is a protein called Alpha-tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	421	Total	C	N	O	S	0	0
			3220	2043	544	612	21		

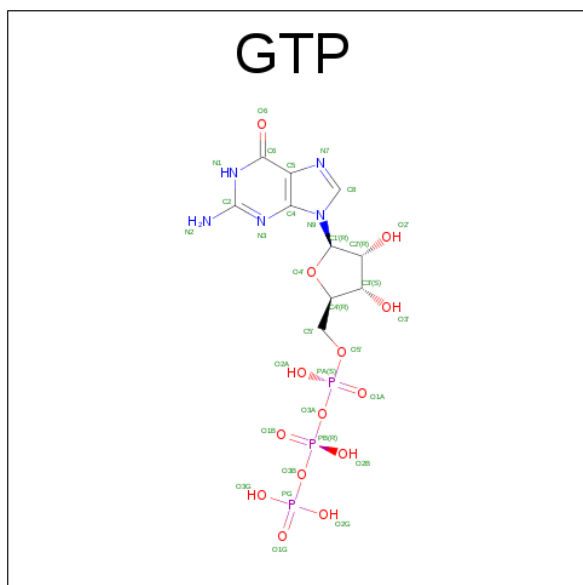
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

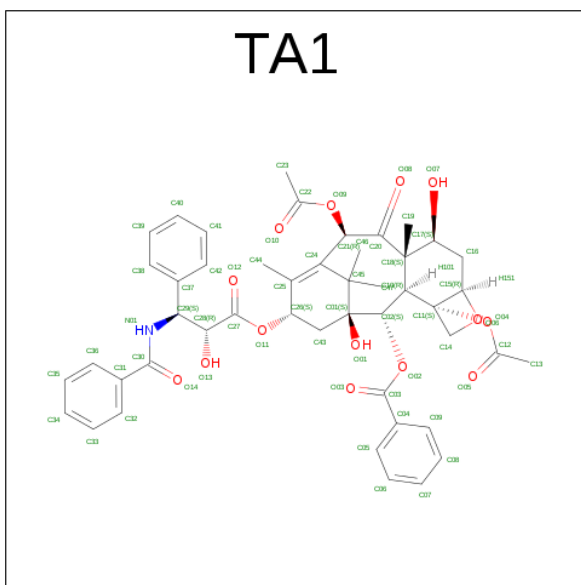
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP, GDP) (formula: $C_{10}H_{16}N_5O_{14}P_3$, $C_{10}H_{15}N_5O_{11}P_2$).



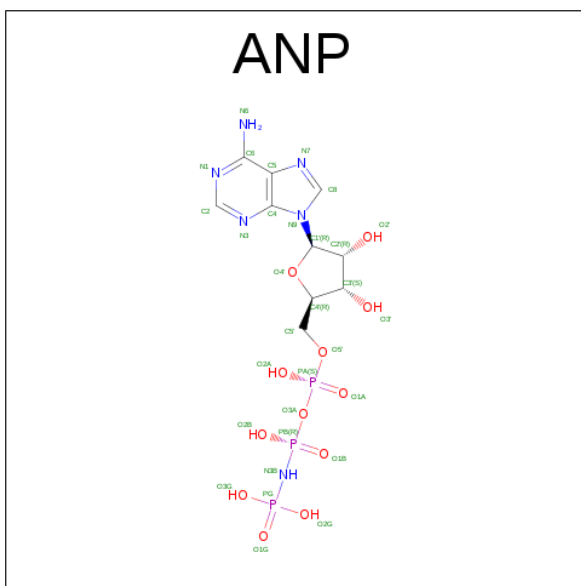
Mol	Chain	Residues	Atoms					AltConf
7	B	2	Total	C	N	O	P	0
			60	20	10	25	5	
7	F	2	Total	C	N	O	P	0
			60	20	10	25	5	

- Molecule 8 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



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

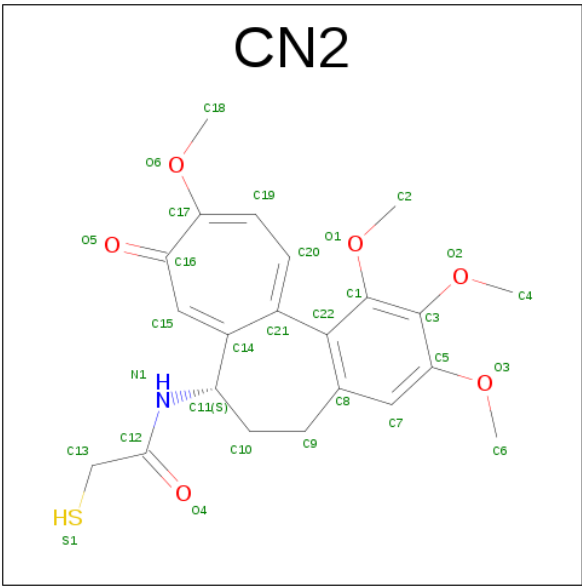
- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 10 is 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRAHYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula:

C₂₂H₂₅NO₆S).

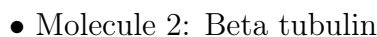


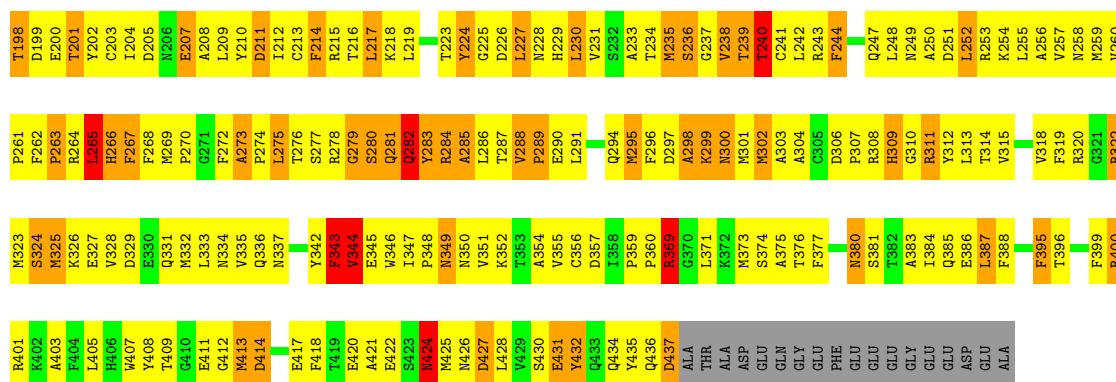
Mol	Chain	Residues	Atoms					AltConf
10	G	1	Total	C	N	O	S	0
			30	22	1	6	1	

- Molecule 11 is water.

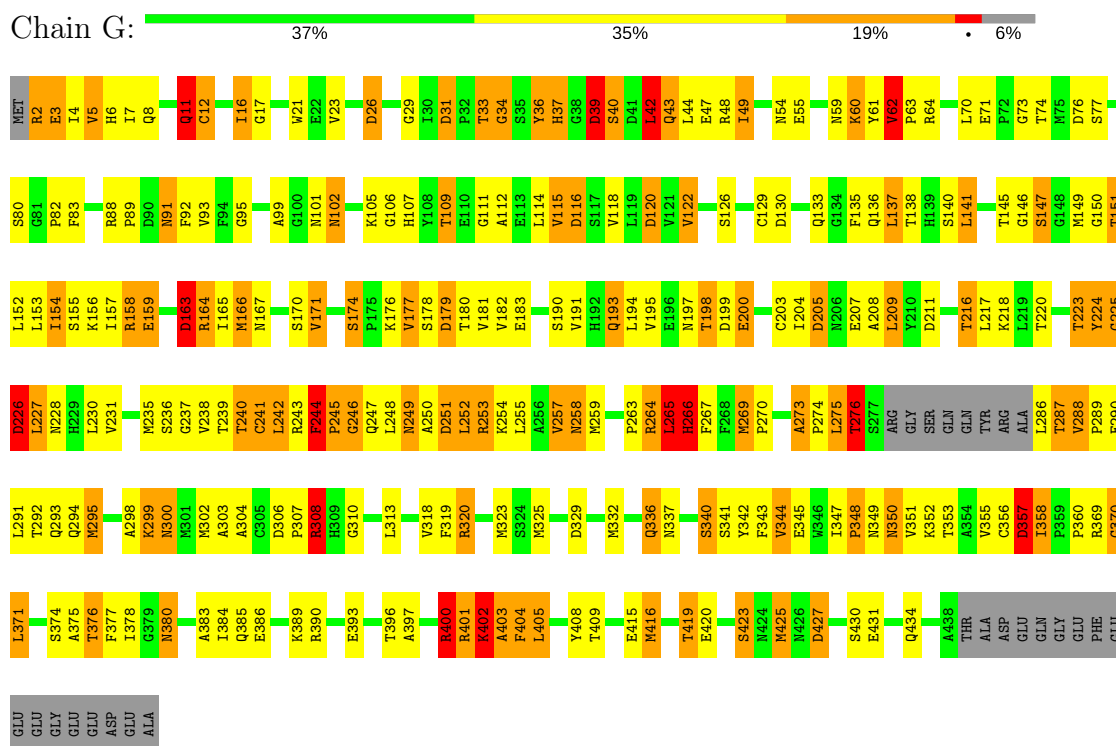
Mol	Chain	Residues	Atoms		AltConf
11	D	98	Total	O	0
			98	98	
11	F	9	Total	O	0
			9	9	

- Molecule 1: Alpha-tubulin

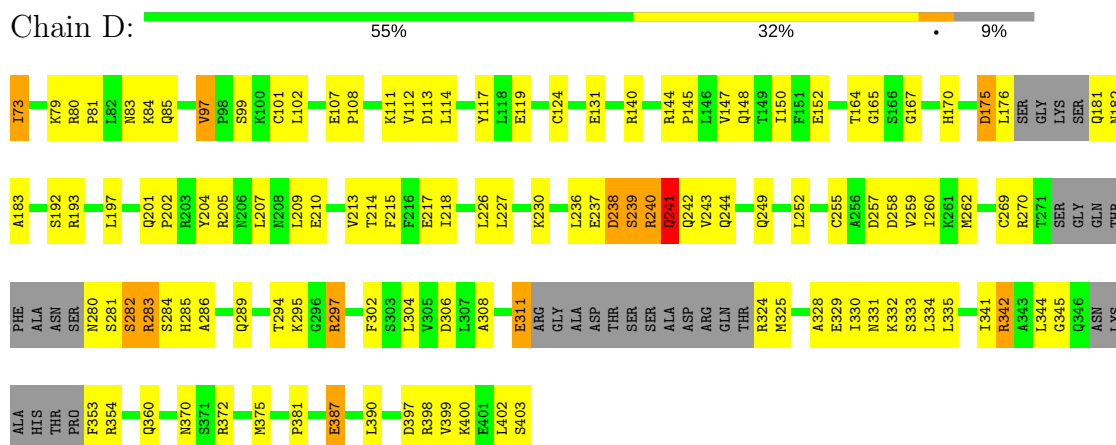




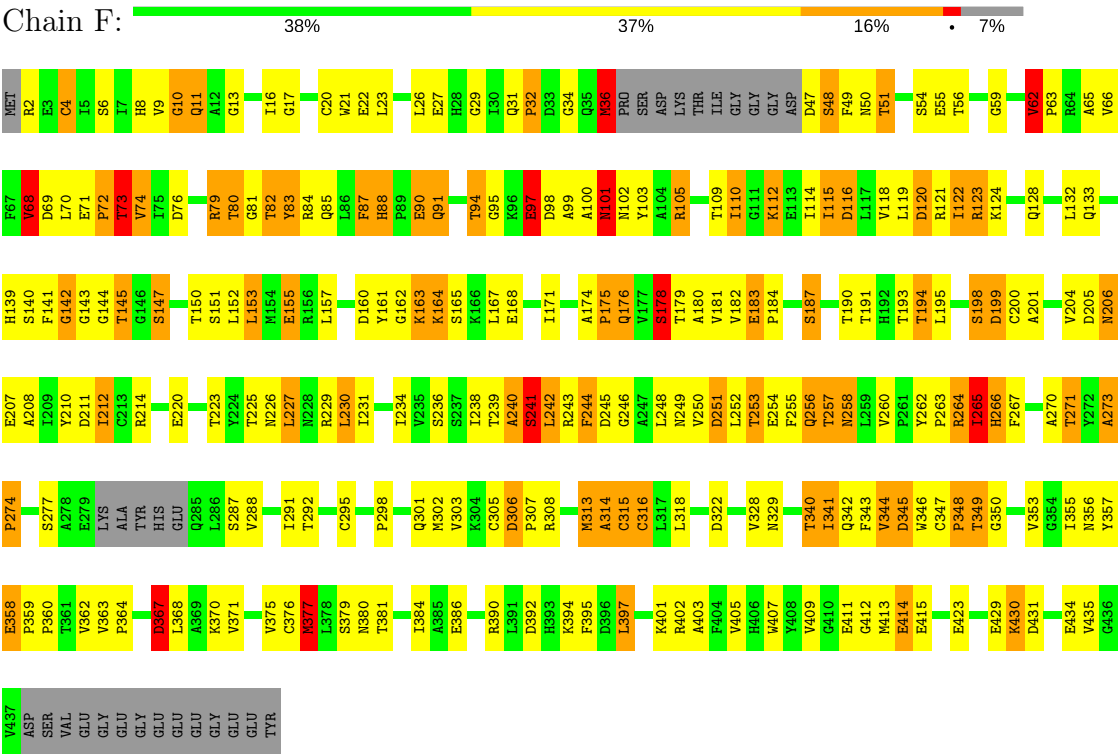
• Molecule 2: Beta tubulin



• Molecule 3: Kinesin13 Motor domain



● Molecule 4: Alpha-tubulin



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Each particle	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Film Kodak SO163	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, MG, CN2, TA1, ZN, GTP, ANP

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	0.51	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
2	G	0.61	0/3309	1.00	20/4494 (0.4%)
3	D	0.46	0/2398	0.71	2/3217 (0.1%)
4	F	0.66	2/3292 (0.1%)	0.95	15/4479 (0.3%)
All	All	0.56	2/15725 (0.0%)	0.84	39/21314 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	97	GLU	CD-OE1	-6.53	1.18	1.25
4	F	97	GLU	CD-OE2	-5.40	1.19	1.25

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	160	ASP	CB-CG-OD2	6.88	124.49	118.30
2	G	205	ASP	CB-CG-OD2	6.84	124.45	118.30
2	G	163	ASP	CB-CG-OD2	6.73	124.36	118.30
4	F	244	PHE	N-CA-C	6.73	129.17	111.00
2	G	116	ASP	CB-CG-OD2	6.32	123.99	118.30

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	3227	0	3143	548	0
2	B	3351	0	3229	545	0
2	G	3237	0	3060	269	0
3	D	2368	0	2410	219	0
4	F	3220	0	3074	232	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	60	0	24	5	0
7	F	60	0	24	3	0
8	B	62	0	51	6	0
9	D	31	0	13	3	0
10	G	30	0	23	8	0
11	D	98	0	0	4	0
11	F	9	0	0	10	0
All	All	15757	0	15051	1665	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 54.

The worst 5 of 1665 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:D:238:ASP:CA	2:G:419:THR:HB	1.24	1.61
3:D:237:GLU:O	2:G:420:GLU:HA	1.30	1.28
3:D:236:LEU:CD2	2:G:416:MET:CE	2.11	1.28
3:D:238:ASP:CB	2:G:419:THR:HB	1.63	1.27
3:D:112:VAL:HG11	4:F:435:VAL:CG2	1.62	1.27

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	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	5
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	6
2	G	415/445 (93%)	310 (75%)	57 (14%)	48 (12%)	0	8
3	D	291/331 (88%)	275 (94%)	13 (4%)	3 (1%)	18	61
4	F	415/451 (92%)	316 (76%)	59 (14%)	40 (10%)	1	13
All	All	1953/2123 (92%)	1440 (74%)	307 (16%)	206 (10%)	1	10

5 of 206 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	97	GLU
1	A	108	TYR
1	A	109	THR
1	A	141	PHE

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	347/377 (92%)	298 (86%)	49 (14%)	4	22
2	B	367/381 (96%)	307 (84%)	60 (16%)	3	17
2	G	348/381 (91%)	241 (69%)	107 (31%)	0	2
3	D	261/286 (91%)	237 (91%)	24 (9%)	11	37
4	F	336/378 (89%)	229 (68%)	107 (32%)	0	2
All	All	1659/1803 (92%)	1312 (79%)	347 (21%)	4	8

5 of 347 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	97	GLU

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Mol	Chain	Res	Type
4	F	226	ASN
2	G	308	ARG
4	F	114	ILE
4	F	165	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	85	GLN
3	D	391	ASN
2	G	300	ASN
3	D	244	GLN
4	F	88	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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	B	500	6	27,34,34	1.52	3 (11%)	27,54,54	2.15	5 (18%)
7	GDP	B	600	-	25,30,30	2.61	8 (32%)	26,47,47	3.63	9 (34%)
8	TA1	B	601	-	68,68,68	1.97	21 (30%)	105,105,105	1.33	8 (7%)
9	ANP	D	500	6	29,33,33	1.75	4 (13%)	28,52,52	3.36	11 (39%)
7	GTP	F	601	6	27,34,34	1.20	3 (11%)	27,54,54	2.02	9 (33%)
7	GDP	F	603	-	25,30,30	1.04	1 (4%)	26,47,47	2.02	6 (23%)
10	CN2	G	701	-	31,32,32	3.12	7 (22%)	28,45,45	3.04	10 (35%)

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	B	500	6	-	0/18/38/38	0/3/3/3
7	GDP	B	600	-	-	0/12/32/32	0/3/3/3
8	TA1	B	601	-	-	0/41/127/127	0/5/7/7
9	ANP	D	500	6	-	0/13/38/38	0/3/3/3
7	GTP	F	601	6	-	0/18/38/38	0/3/3/3
7	GDP	F	603	-	-	0/12/32/32	0/3/3/3
10	CN2	G	701	-	-	0/10/27/27	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	701	CN2	C20-C21	-9.91	1.24	1.40
10	G	701	CN2	C19-C17	-7.84	1.25	1.39
10	G	701	CN2	C19-C20	-5.44	1.24	1.40
8	B	601	TA1	C08-C07	-5.15	1.25	1.38
9	D	500	ANP	PB-O2B	-3.81	1.46	1.56

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	GDP	C6-C5-C4	-11.34	109.57	120.84
10	G	701	CN2	C10-C11-N1	-8.63	93.97	110.05
9	D	500	ANP	O5'-PA-O1A	-7.47	79.12	109.25
7	B	500	GTP	C5-C6-N1	-7.12	113.34	123.48
10	G	701	CN2	C13-C12-N1	-6.61	104.90	115.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	500	GTP	4	0
7	B	600	GDP	1	0
8	B	601	TA1	6	0
9	D	500	ANP	3	0
7	F	601	GTP	2	0
7	F	603	GDP	1	0
10	G	701	CN2	8	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.