



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 12:13 AM UTC

PDB ID : 2HXF / pdb_00002hxf
Title : KIF1A head-microtubule complex structure in amppnp-form
Authors : Kikkawa, M.; Hirokawa, N.
Deposited on : 2006-08-03
Resolution : 10.00 Å(reported)
Based on initial models : 1VFV, 1JFF

This is a wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

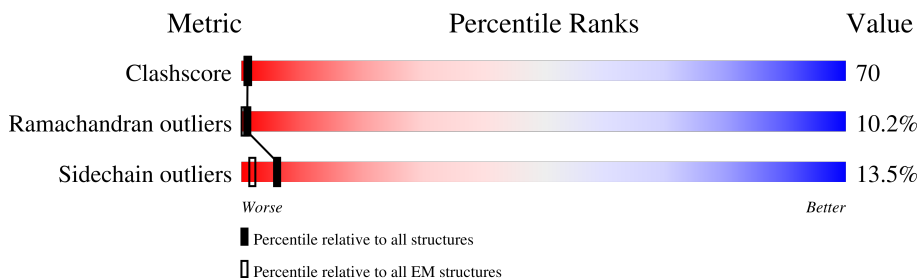
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	451	
2	B	445	
3	C	394	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9279 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
1	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

- Molecule 2 is a protein called Tubulin beta chain.

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

- Molecule 3 is a protein called Kinesin-like protein KIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2546	1581	446	505	14		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	MET	-	cloning artifact	UNP P33173
C	-14	ALA	-	cloning artifact	UNP P33173
C	-13	SER	-	cloning artifact	UNP P33173
C	-12	MET	-	cloning artifact	UNP P33173
C	-11	THR	-	cloning artifact	UNP P33173
C	-10	GLY	-	cloning artifact	UNP P33173
C	-9	GLY	-	cloning artifact	UNP P33173
C	-8	GLN	-	cloning artifact	UNP P33173
C	-7	GLN	-	cloning artifact	UNP P33173
C	-6	MET	-	cloning artifact	UNP P33173
C	-5	GLY	-	cloning artifact	UNP P33173
C	-4	ARG	-	cloning artifact	UNP P33173
C	-3	ASP	-	cloning artifact	UNP P33173
C	-2	PRO	-	cloning artifact	UNP P33173
C	-1	ILE	-	cloning artifact	UNP P33173

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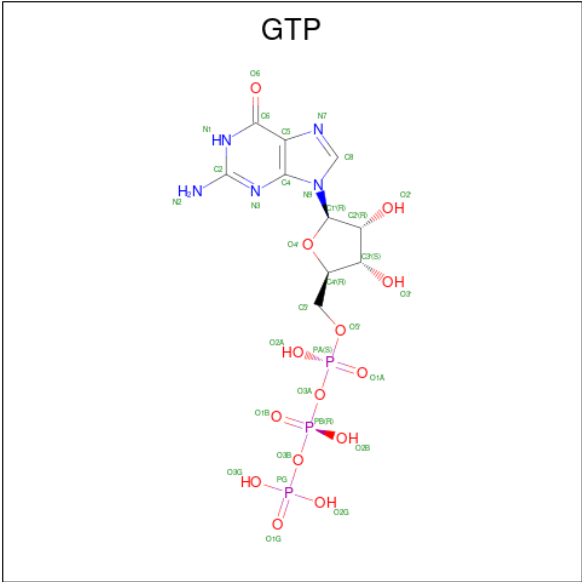
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ASN	-	cloning artifact	UNP P33173
C	1	MET	-	cloning artifact	UNP P33173
C	2	PRO	-	cloning artifact	UNP P33173
C	202	ALA	PRO	engineered mutation	UNP P33173
C	356	ASN	-	linker	UNP P33173
C	357	THR	-	linker	UNP P33173
C	358	VAL	-	linker	UNP P33173
C	359	SER	-	linker	UNP P33173
C	360	VAL	-	linker	UNP P33173
C	361	ASN	-	linker	UNP P33173
C	362	LEU	-	linker	UNP P33173
C	363	GLU	-	linker	UNP P33173
C	364	LEU	-	linker	UNP P33173
C	365	THR	-	linker	UNP P33173
C	366	ALA	-	linker	UNP P33173
C	367	GLU	-	linker	UNP P33173
C	368	GLU	-	linker	UNP P33173
C	369	TRP	-	linker	UNP P33173
C	370	LYS	-	linker	UNP P33173
C	371	LYS	-	linker	UNP P33173
C	372	LYS	-	linker	UNP P33173
C	373	HIS	-	expression tag	UNP P33173
C	374	HIS	-	expression tag	UNP P33173
C	375	HIS	-	expression tag	UNP P33173
C	376	HIS	-	expression tag	UNP P33173
C	377	HIS	-	expression tag	UNP P33173
C	378	HIS	-	expression tag	UNP P33173

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

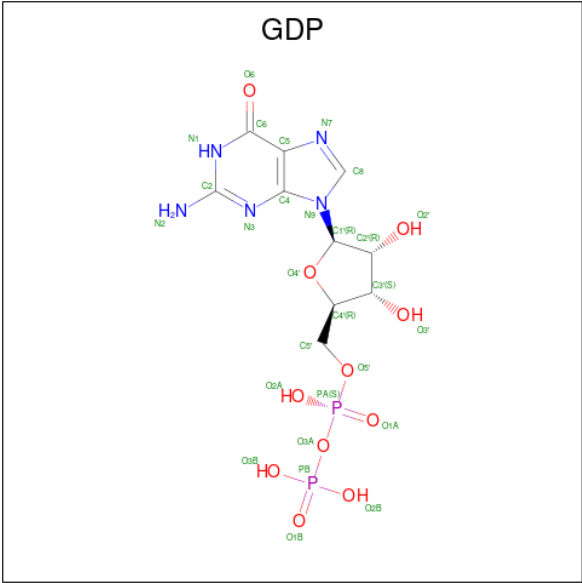
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



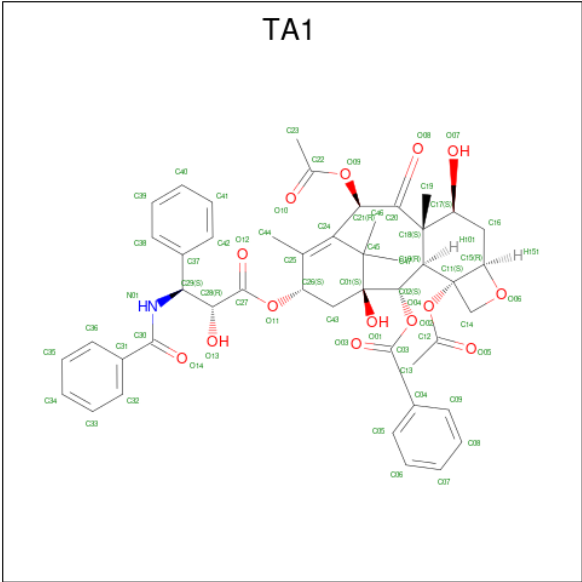
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



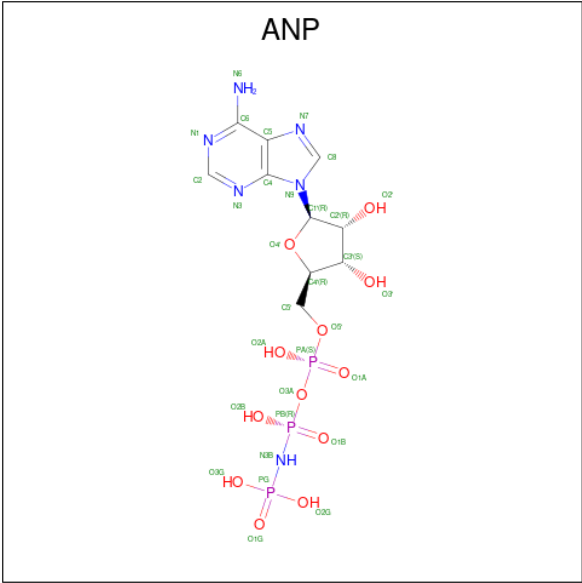
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).



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

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

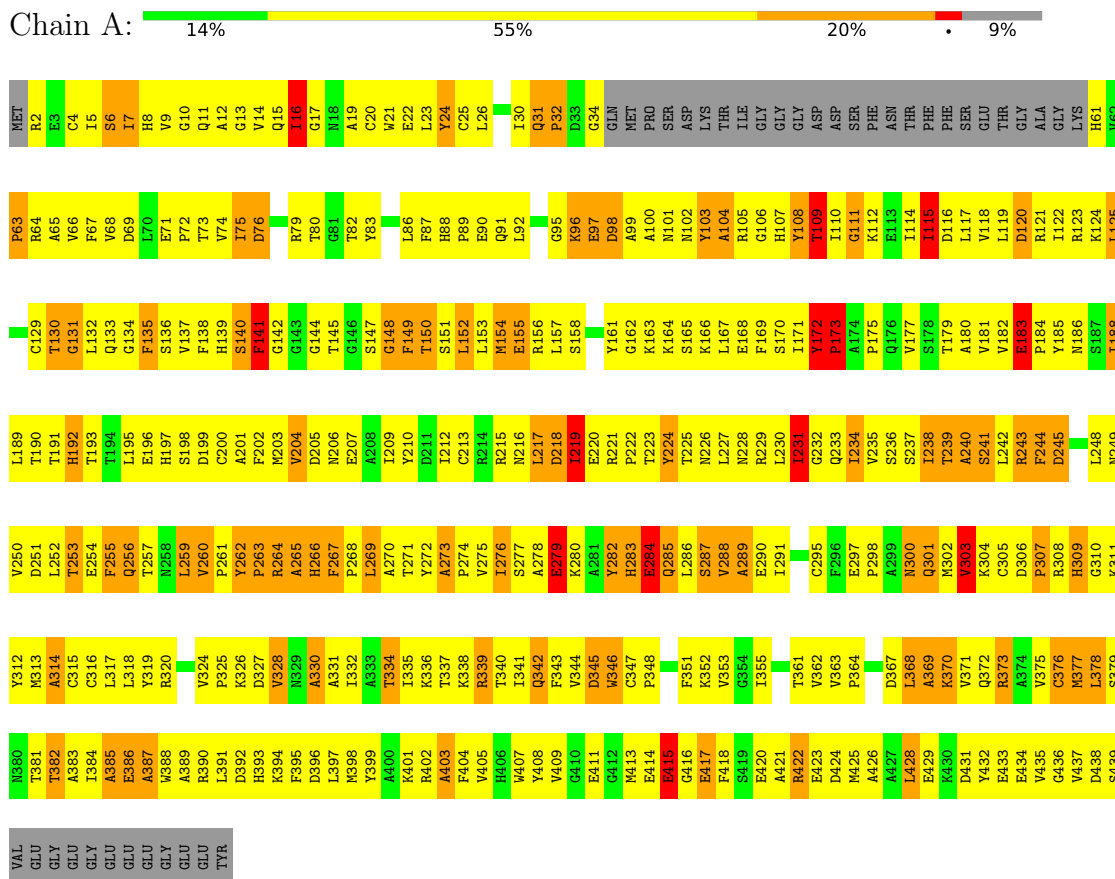


Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

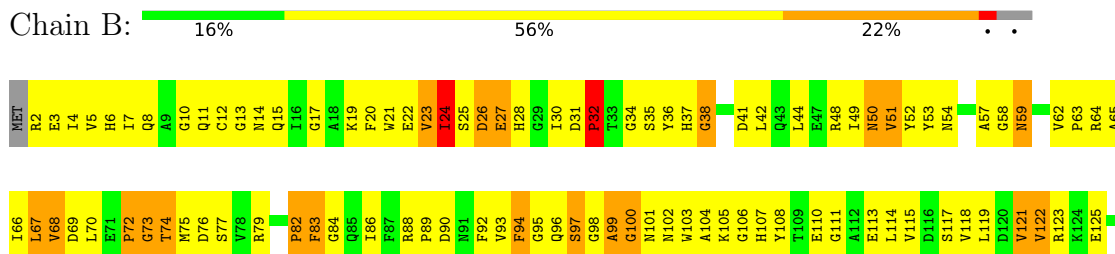
3 Residue-property plots

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: Tubulin alpha chain



- Molecule 2: Tubulin beta chain



GLY GLU GLU ASP GLU ALA	Q385	L313	R253	S190	C129
	C386	T314	K254	V191	
	L387	V315	L255	H192	
	F388		A256	Q193	L132
	F389	V318	V257	L194	Q133
	K389	F319	N258	V195	G134
	R390	R320	M259	E196	F135
	L391		V260	N197	Q136
	G321	G321	P261	T198	L137
	R322	K323	F262	D199	T138
	T396	S324	P263	E200	H139
	F399	M325	R264	T201	S140
	R400	K326	L265	Y202	L141
	R401	E327	H266	C203	G142
	K402	V328	F267	I204	G143
	A403	D329	F268	D205	G144
		E330	M269	N206	T145
	W407	Q331	P270	E207	G146
	Y408	M332	G271	A208	S147
	T409	L333	F272	L209	G148
	G410	N334	A273	Y210	M149
	E411	V335	P274	D211	G150
	G412	Q336	L275	I212	T151
	D414	N337	T276	C213	L152
			S277	F214	L153
	E415	Y342	R278	R215	N154
	M416	F343	G279	T216	S155
	A417	V344	S280	L217	S156
	F418	E345	Q281	K218	K156
	T419	W346	Q282	L219	L157
	E420	L347	Y283		R158
	A421	P348	R284	T223	E159
	E422	N349	A285	Y224	E160
	S423	K350	L286	G225	P162
	N424	V351	T287	D226	D163
	M425	K352	V288	L227	R164
	N426	T353	P289	N228	I165
	D427	A354	E290	H229	M166
	L428	V355	L291	L230	M167
	V429	C356	T292	V231	T168
	S430	D357	Q293	S232	
	E431	L358	Q294	A233	V171
	Y432	P359	M295	T234	V172
	Q433	P360	F296	M235	P173
	Q434	R369	D297	S236	S174
	Y435	G370	A298	G237	P175
	Q436	L371	K299	V238	K176
	D437	K372	N300	T239	V177
	ALA	M373	X301	T240	S178
	THR	S374	R302	C241	D179
	ALA	A375	A303	L242	T180
	ASP	T376	A304	R243	V181
	GLU	F377	C305	F244	E182
	GLN	L378	D306		E183
	GLY	G379	P307	Q247	P184
	GLU	N380	R308	L248	Y185
	PHE	S381	H309	N249	M186
	GLU	T382	G310	A250	A187
	GLU	A383	R311	D251	T188
	GLU	L384	Y312	L252	L189

● Molecule 3: Kinesin-like protein KIF1A



HIS	THR	ASP	N222	D114	MET	ALA
	F303	I304	T226	I118	SER	MET
	P305	Y306	T26	I119	THR	GLY
	R307	R230	R229	I130	GLY	GLN
	D308	D231	H230	M138	GLN	GLN
	S309	A232	D231	S139	MET	MET
	V310	E233	E233	Y140	GLY	GLY
	L314	T234	R235	S141	ARG	ARG
	L315	R235	I236	Y150	ASP	ASP
	R316	S242	S242	C151	PRO	PRO
	G320	S245	S245	E152	ILE	ILE
	G321	L246	L246	R153	ASN	ASN
	N322	V247	V247	R154	MET	MET
	A326	S252	S252	R155	PRO	PRO
	R327	E253	ARG	D156	G3	G3
	V328	ALA	ALA	N159	K7	K7
	S332	ASP	ASP	P160	V8	V8
	D335	SER	SER	N162	A9	A9
	I336	THR	THR	K163	K25	K25
	N337	GLY	GLY	G164	S33	S33
	Y338	ALA	ALA	N165	V38	V38
	S343	LYS	LYS	L166	N39	N39
	R346	GLY	GLY	R167	P40	P40
	Y347	THR	THR	V168	K41	K41
	R350	LEU	LEU	R169	Q42	Q42
	R355	LYS	LYS	E170	P43	P43
	N356	GLU	GLU	H171	R44	R44
	T357	GLY	GLY	P172	E45	E45
	V358	A269	A269	L173	F52	F52
	S359	N270	N270	L174	D53	D53
	V360	I271	I271	P176	Y54	Y54
	N361	K273	K273	Y189	D64	D64
	L362	T276	T276	I192	Y67	Y67
	GLU	K280	K280	A202	Y74	Y74
	LEU	R288	R288	R203	R75	R75
	THR	ALA	ASP	T204	D76	D76
	ALA	SER	THR	V205	I77	I77
	GLU	ASP	GLY	ALA	G78	G78
	GLU	GLY	GLY	ALA	E79	E79
	TRP	PRO	PRO	THR	E80	E80
	LYS	ASN	ASN	ASN	C92	C92
	LYS	LYS	LYS	ASN	T106	T106
	LYS	LYS	LYS	GLU	Q111	Q111
	HIS	LYS	LYS	T213	E112	E112
	HIS	LYS	LYS	S214	K113	K113
	HIS	LYS	LYS	R215		
	HIS	LYS	LYS	S217		

4 Data and refinement statistics

Xtrriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 10.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-10.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9279	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, TA1, MG, ANP, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	1/3300 (0.0%)	1.09	22/4482 (0.5%)
2	B	0.63	0/3426	1.11	22/4642 (0.5%)
3	C	0.56	0/2585	1.08	20/3491 (0.6%)
All	All	0.61	1/9311 (0.0%)	1.10	64/12615 (0.5%)

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	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	TYR	CA-C	-5.48	1.48	1.53

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	CA-C-N	10.69	133.20	119.84
1	A	172	TYR	C-N-CA	10.69	133.20	119.84
3	C	213	THR	CA-CB-CG2	-10.07	93.38	110.50
2	B	262	PHE	CA-C-N	10.02	132.36	119.84
2	B	262	PHE	C-N-CA	10.02	132.36	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	155	ARG	Sidechain
3	C	74	TYR	Sidechain

5.2 Too-close contacts

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	3141	605	0
2	B	3351	0	3227	610	0
3	C	2546	0	2507	136	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	5	0
6	B	28	0	12	1	0
7	B	62	0	51	5	0
8	C	31	0	13	0	0
All	All	9279	0	8963	1285	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 70.

The worst 5 of 1285 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:C:204:THR:CA	3:C:205:VAL:HB	1.63	1.27
1:A:414:GLU:HB2	3:C:253:GLU:O	1.32	1.25
1:A:409:VAL:HG12	3:C:272:ASN:CB	1.69	1.23
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.17
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.14

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	3
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	4
3	C	316/394 (80%)	309 (98%)	5 (2%)	2 (1%)	21	59
All	All	1148/1290 (89%)	848 (74%)	183 (16%)	117 (10%)	1	7

5 of 117 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%)	294 (85%)	53 (15%)	3	12
2	B	367/381 (96%)	306 (83%)	61 (17%)	2	10
3	C	286/345 (83%)	265 (93%)	21 (7%)	13	34
All	All	1000/1103 (91%)	865 (86%)	135 (14%)	6	14

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	25	LYS
3	C	113	LYS
3	C	253	GLU
1	A	417	GLU
1	A	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	406	HIS
2	B	436	GLN
3	C	171	HIS
2	B	43	GLN
2	B	14	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
5	GTP	A	500	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
7	TA1	B	601	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
8	ANP	C	1500	4	33,33,33	2.04	11 (33%)	45,52,52	2.92	15 (33%)
6	GDP	B	600	-	29,30,30	2.86	11 (37%)	45,47,47	3.47	16 (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
5	GTP	A	500	4	-	4/22/38/38	0/3/3/3
7	TA1	B	601	-	-	9/41/127/127	0/7/7/7
8	ANP	C	1500	4	-	9/18/38/38	0/3/3/3
6	GDP	B	600	-	-	4/16/32/32	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	GDP	PA-O3A	7.54	1.67	1.59
7	B	601	TA1	C06-C05	6.52	1.50	1.38
5	A	500	GTP	PA-O3A	-6.04	1.53	1.59
6	B	600	GDP	O6-C6	5.99	1.34	1.23
6	B	600	GDP	C8-N9	5.88	1.50	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	N9-C8-N7	-10.74	93.48	113.40
6	B	600	GDP	C8-N7-C5	9.22	120.68	104.26
8	C	1500	ANP	O2B-PB-O1B	8.96	129.08	109.87
6	B	600	GDP	C6-C5-N7	8.57	145.90	130.29
8	C	1500	ANP	O5'-PA-O1A	-7.96	77.41	108.94

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	600	GDP	PA-O3A-PB-O2B
6	B	600	GDP	C5'-O5'-PA-O3A

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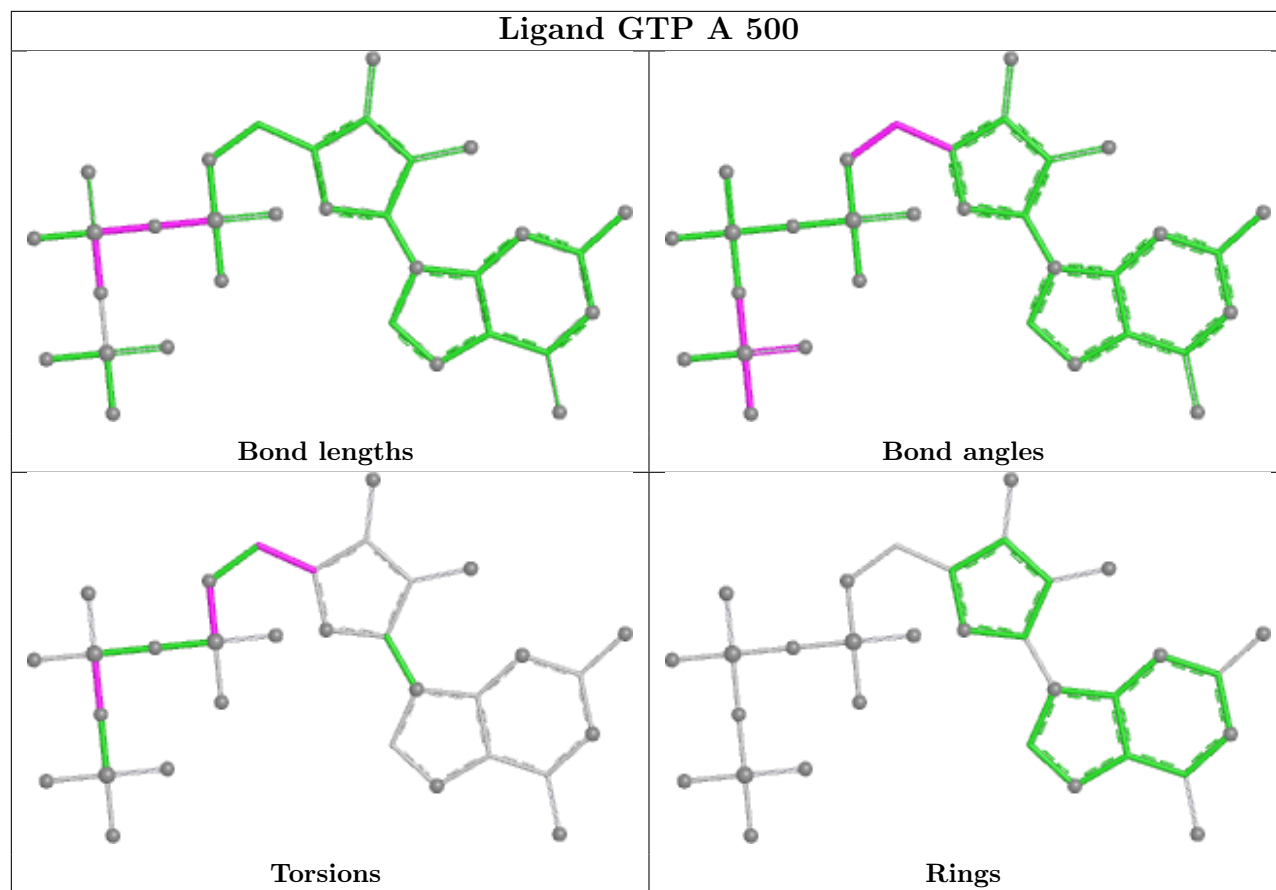
Mol	Chain	Res	Type	Atoms
6	B	600	GDP	C5'-O5'-PA-O1A
8	C	1500	ANP	PG-N3B-PB-O1B
8	C	1500	ANP	PA-O3A-PB-O2B

There are no ring outliers.

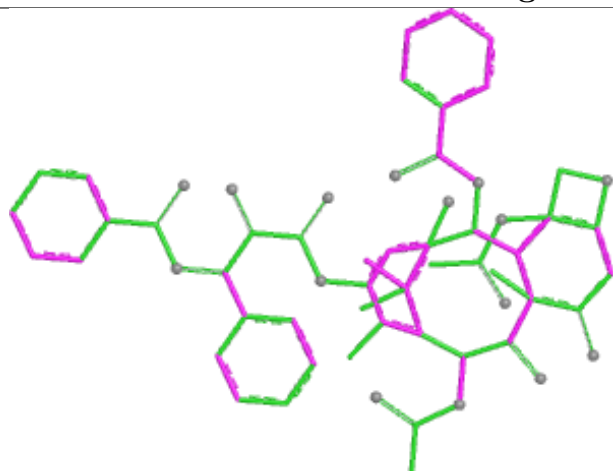
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	GTP	5	0
7	B	601	TA1	5	0
6	B	600	GDP	1	0

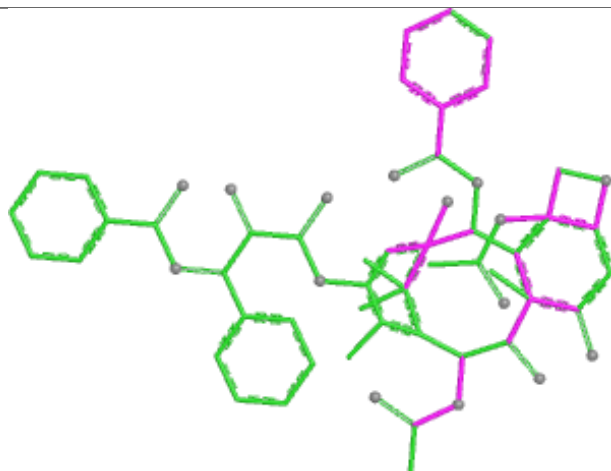
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



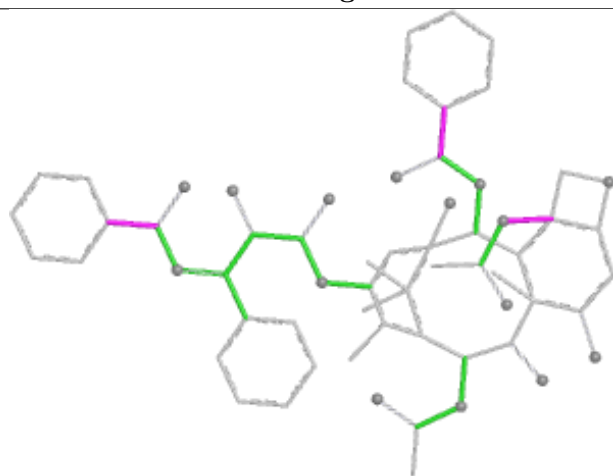
Ligand TA1 B 601



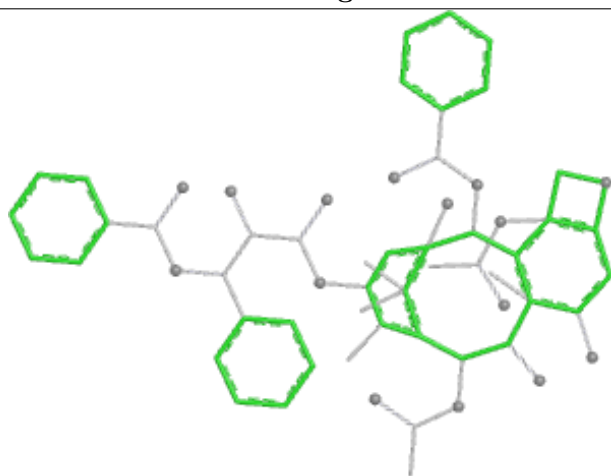
Bond lengths



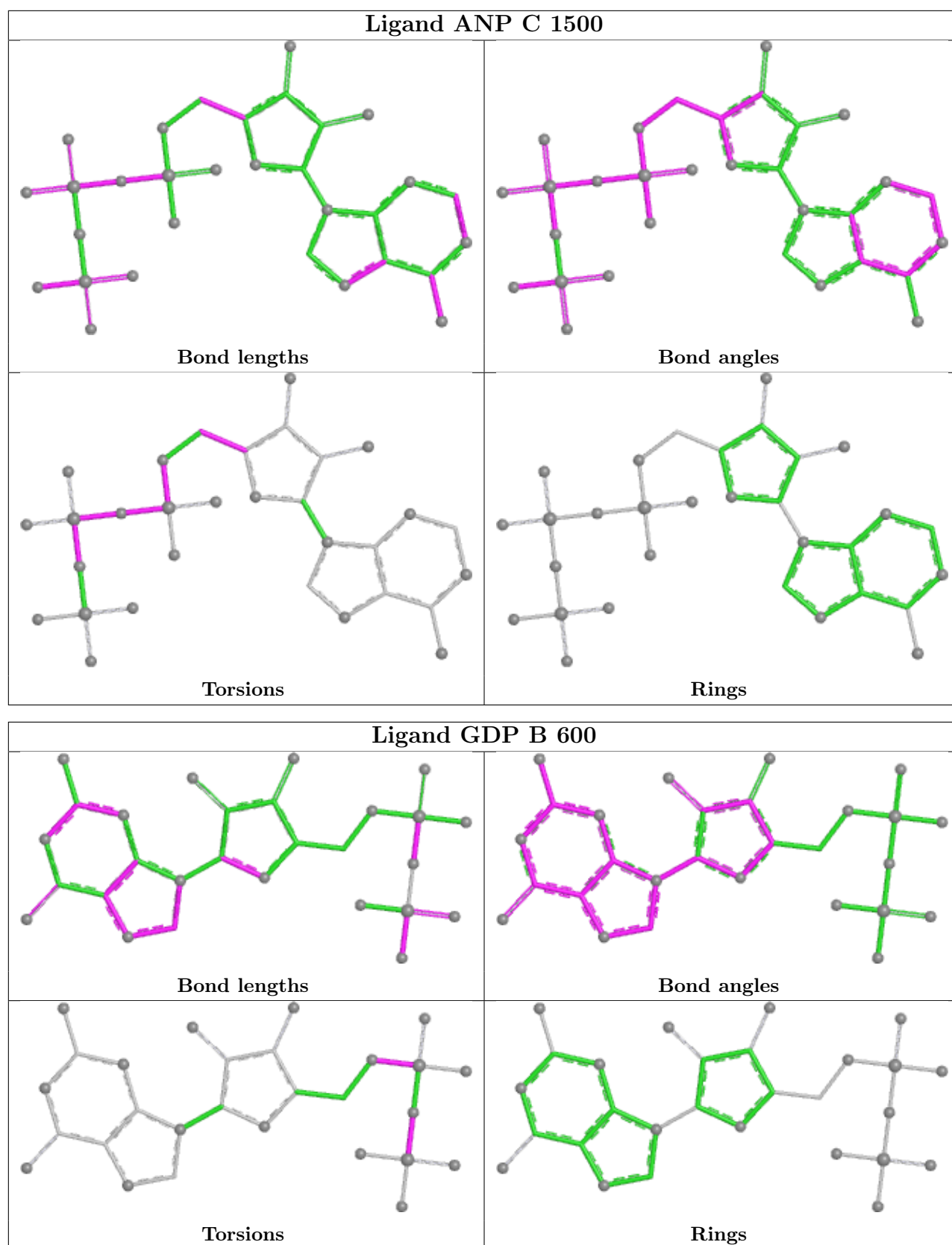
Bond angles



Torsions



Rings



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.