



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 07:30 AM UTC

PDB ID : 2HXX / pdb_00002hxx
Title : KIF1A head-microtubule complex structure in adp-form
Authors : Kikkawa, M.; Hirokawa, N.
Deposited on : 2006-08-03
Resolution : 11.00 Å(reported)
Based on initial models : 1JFF, 1I5S

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

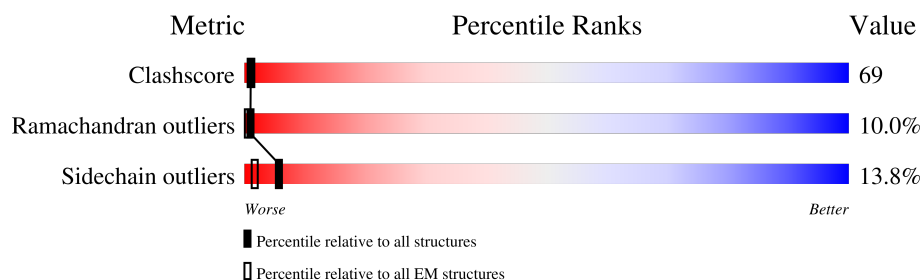
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 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 9388 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	330	Total	C	N	O	S	8	0
			2659	1645	467	532	15		

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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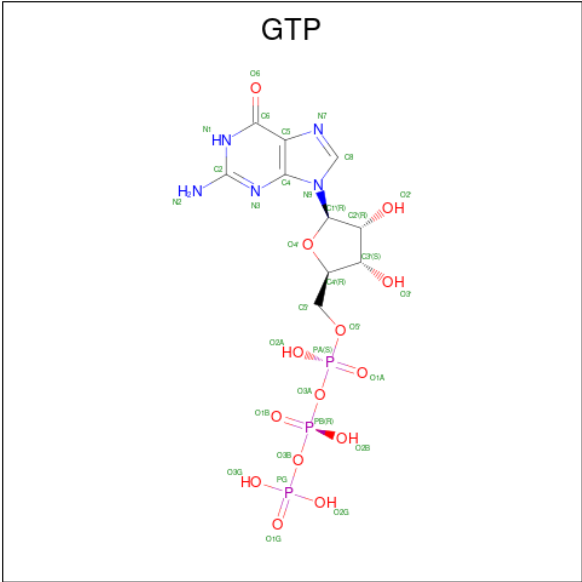
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ASN	-	cloning artifact	UNP P33173
C	1	MET	-	cloning artifact	UNP P33173
C	2	PRO	-	cloning artifact	UNP P33173
C	202	ALA	PRO	engineered mutation	UNP P33173
C	356	ASN	-	linker	UNP P33173
C	357	THR	-	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).

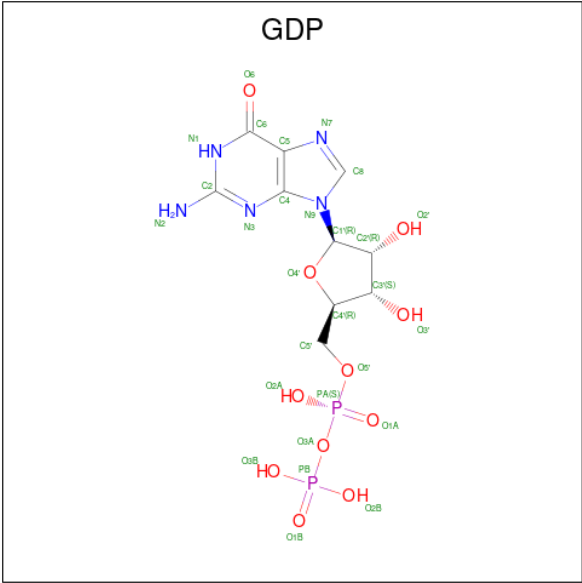
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0

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



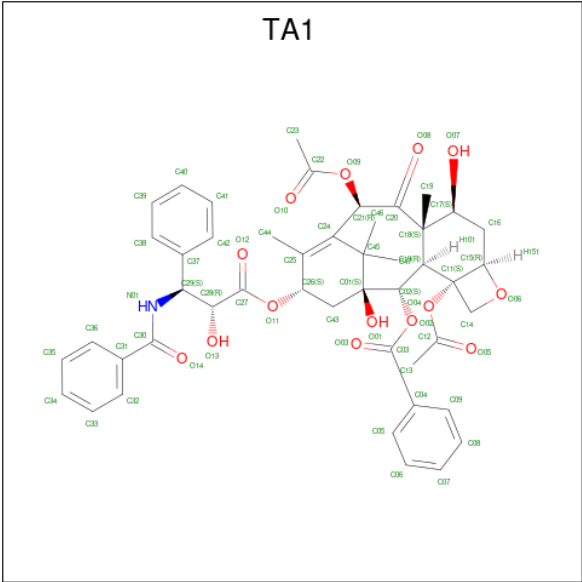
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	32	10	5	14	3	0

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



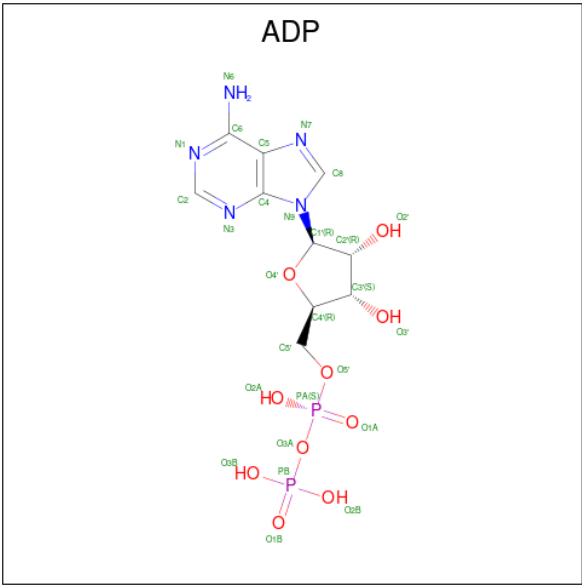
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	B	1	28	10	5	11	2	0

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



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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

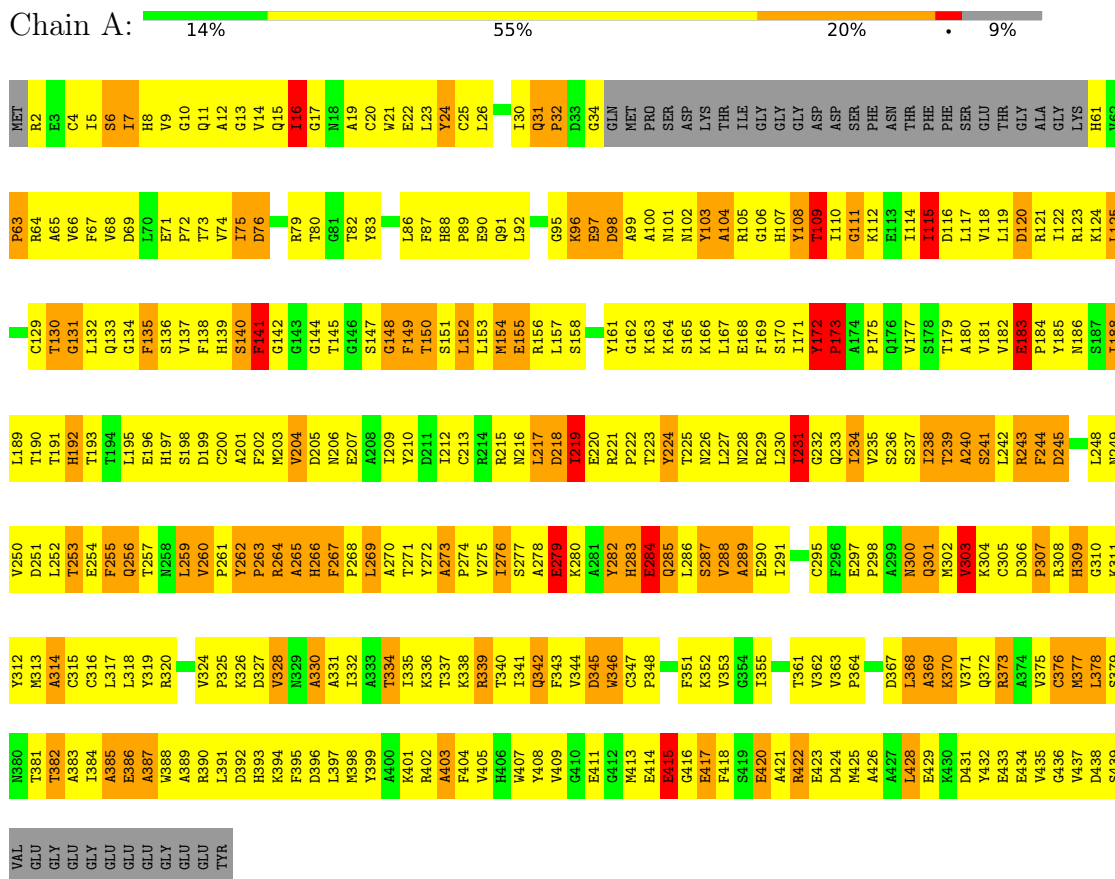


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	C	1	27	10	5	10	2	0

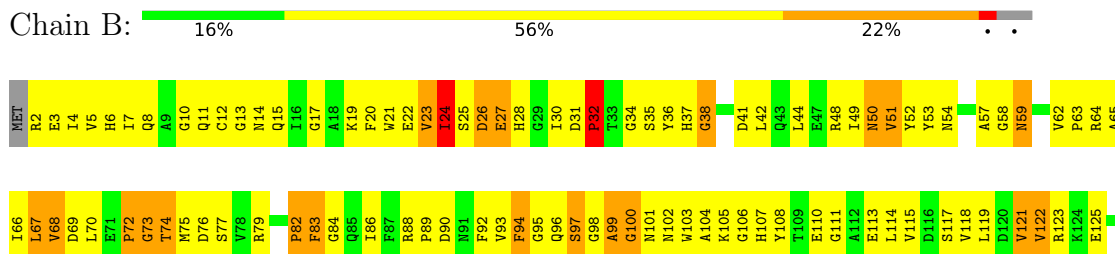
3 Residue-property plots

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



S128	S190	R253	L313	Q385	GLY
Q129	V191	K254	T314	E386	GLU
L132	H192	L255	V315	L387	GLU
L133	Q193	A256		F388	ASP
Q133	L194	V257	V318	K389	GLU
G134	V195	N258	F319	R390	ALA
F135	E196	M259	R320	I391	
Q136	N197	V260	G321		
L137	T198	P261	R322	F395	
T138	D199	F262	N323	T396	
H139	E200	P263	S324		
	T201	R264	M325	F399	
S140	Y202	L265	K326	R400	
L141	C203	H266	E327	R401	
G142	C203	F267	V328	K402	
G143	I204	F268	D329	A403	
G144	D205	M269	E330		
T145	N206	P270	Q331	W407	
G146	E207	M271	M332	Y408	
S147	A208	F272	L333	T409	
G148	L209	A273	N334	G410	
M149	Y210	P274	Q335	E411	
G150	D211	L275	Q336	G412	
T151	I212	T276	M413	M413	
L152	C213	S277	D414	D414	
L153	F214	R278		E415	
I154	R215	G279	Y342	M416	
S155	T216	S280	F343	E417	
K156	L217	K281	Y344	F418	
I157	K218	Q282	E345	T419	
R158	L219	Y283	W346	E420	
E159		R284	I347	A421	
E160	T223	A285	P348	E422	
Y161	Y224	L286	N349	S423	
P162	G225	T287	N350	M425	
D163	D226	V288	K352	N426	
R164	L227	P289	T353	D427	
I165	N228	E290	A354	L428	
M166	H229	L291	V355	V429	
M167	L230	T292	D357	S430	
T168	V231	Q293	I358	E431	
	A232	M295	P359	Y432	
V171	T234	F296	Q360	Q433	
V172	M235	D297	E389	Q434	
P173	S236	A298	G370	Y435	
S174	G237	K299	L371	Q436	
P175	V238	N300	K372	D437	
K176	T239	M301	N373	ALA	
V177	C240	K302	S374	THR	
S178	D179	A303	A375	ALA	
D179	L242	A304	T376	ASP	
V181	R243	C305	F377	GLU	
V182	F244	D306	I378	GLN	
E183		P307	G379	GLY	
P184	Q247	R308	N380	GLU	
Y185	L248	H309	S381	PHE	
N186	N249	G310	T382	GLU	
A187	A250	R311	A383	GLU	
T188	D251		I384	GLU	
L189	L252				

● Molecule 3: Kinesin-like protein KIF1A



MET	K113	A219	THR
ALA	D114		ASP
GLY	Q115	T224	PHE
THR		F225	I304
GLY	D125	T226	P305
GLY	L126	Q227	Y306
GLN	F127	K228	E307
GLN	S128	R229	D308
GLN	I129	H230	
MET	I130	D231	R316
GLY		A232	E317
ARG	T133	E233	N318
ASP	T134	T234	
PRO	N135	M235	N322
ILE	D136	T236	S323
ASN	N137	T237	R324
MET	S145	E238	T325
PRO	E148	K240	A326
GLY	C151	K243	S332
A4	E152	V247	P333
	R153	D248	A334
	V154		D335
	R155		I336
	D156		
	K161	R254	L342
	K25	A255	R346
	T34	SER	
	T35	THR	R350
	T36	GLY	A351
	K41	ALA	K352
	Q42	K261	GLN
	P43	G262	ILE
	K44	R263	ARG
	E45	L265	ASN
	P47	K266	THR
	H59	E267	VAL
	T60	N272	SER
	S61	K273	VAL
	I77		ASN
	M81		LEU
	H84		GLU
	Y89	A284	LEU
	C92	L285	THR
	M108	A286	ALA
	Q111	E287	GLU
	E112	M288	GLU
		Q193	TRP
		M196	LYS
		N200	LYS
		V205	PRO
		T208	GLY
		R216	ASN
			LYS
			LYS
			LYS
			LYS

4 Data and refinement statistics

Xtriage (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) – 11.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-11.00)	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.	Xtriage
Total number of atoms	9388	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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: MG, ADP, GDP, GTP, TA1

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	0.58	0/2700	1.08	14/3643 (0.4%)
All	All	0.61	1/9426 (0.0%)	1.10	58/12767 (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	1

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 58 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
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
1	A	283	HIS	N-CA-C	-8.23	101.27	113.61

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	47	PRO	Mainchain

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	3141	602	0
2	B	3351	0	3229	608	0
3	C	2659	0	2604	122	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	27	0	12	0	0
All	All	9388	0	9061	1271	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 69.

The worst 5 of 1271 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)
1:A:409:VAL:HG12	3:C:272:ASN:CG	1.22	1.52
2:B:419:THR:CG2	3:C:172:PRO:O	1.65	1.44
1:A:409:VAL:CG1	3:C:272:ASN:OD1	1.65	1.43
1:A:409:VAL:HG12	3:C:272:ASN:ND2	1.21	1.43
1:A:409:VAL:CG1	3:C:272:ASN:CG	2.01	1.33

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	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	332/394 (84%)	317 (96%)	14 (4%)	1 (0%)	36	72
All	All	1164/1290 (90%)	856 (74%)	192 (16%)	116 (10%)	1	7

5 of 116 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	298/345 (86%)	271 (91%)	27 (9%)	9	27
All	All	1012/1103 (92%)	871 (86%)	141 (14%)	6	14

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	25	LYS
3	C	112[B]	GLU
3	C	239[A]	GLU
1	A	417	GLU
1	A	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	406	HIS
3	C	222	ASN
2	B	434	GLN
3	C	115	GLN
3	C	235	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	$\# Z > 2$
6	GDP	B	600	-	29,30,30	2.86	11 (37%)	45,47,47	3.47	16 (35%)
8	ADP	C	2000	4	28,29,29	2.38	9 (32%)	43,45,45	2.43	12 (27%)
7	TA1	B	601	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
5	GTP	A	500	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)

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	GDP	B	600	-	-	4/16/32/32	0/3/3/3
8	ADP	C	2000	4	-	4/16/32/32	0/3/3/3
7	TA1	B	601	-	-	9/41/127/127	0/7/7/7
5	GTP	A	500	4	-	4/22/38/38	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2000	ADP	PA-O3A	8.09	1.68	1.59
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

The worst 5 of 44 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
6	B	600	GDP	C6-C5-N7	8.57	145.90	130.29
8	C	2000	ADP	O5'-PA-O1A	-8.33	75.93	108.94
8	C	2000	ADP	O2A-PA-O5'	-6.81	76.69	107.57

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

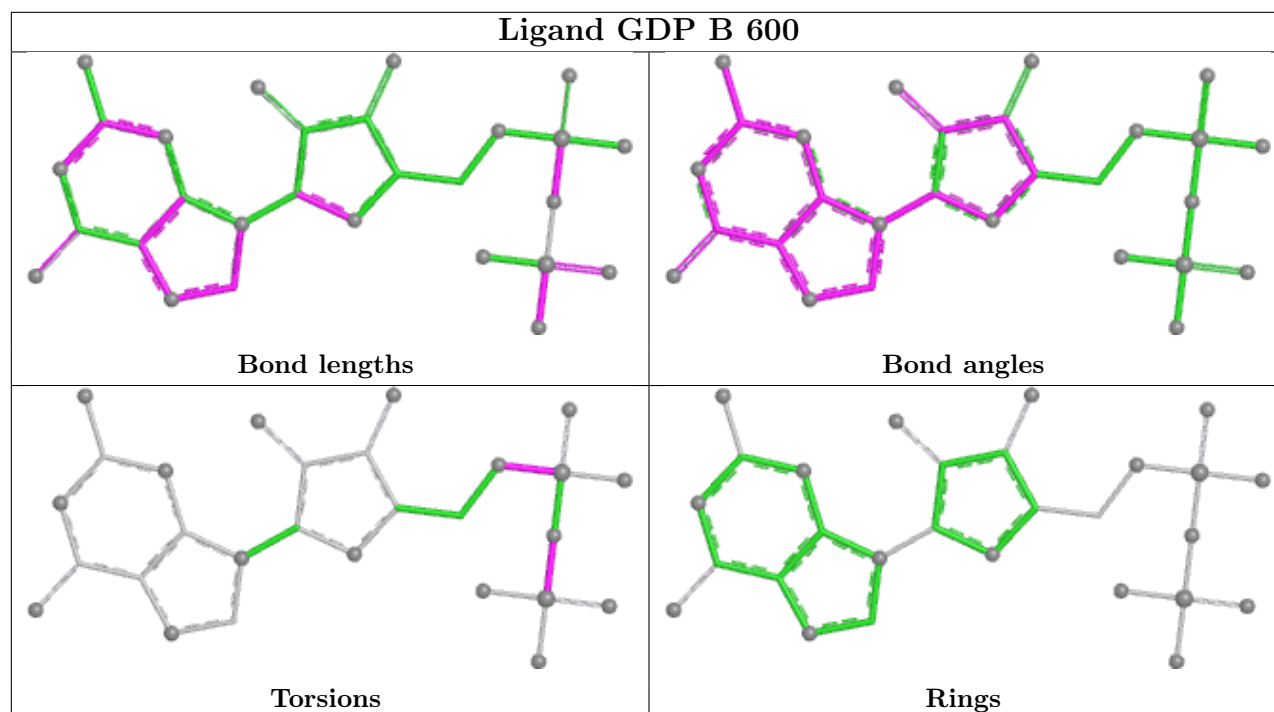
Mol	Chain	Res	Type	Atoms
6	B	600	GDP	PA-O3A-PB-O2B
6	B	600	GDP	C5'-O5'-PA-O3A
6	B	600	GDP	C5'-O5'-PA-O1A
7	B	601	TA1	O02-C03-C04-C05
7	B	601	TA1	O02-C03-C04-C09

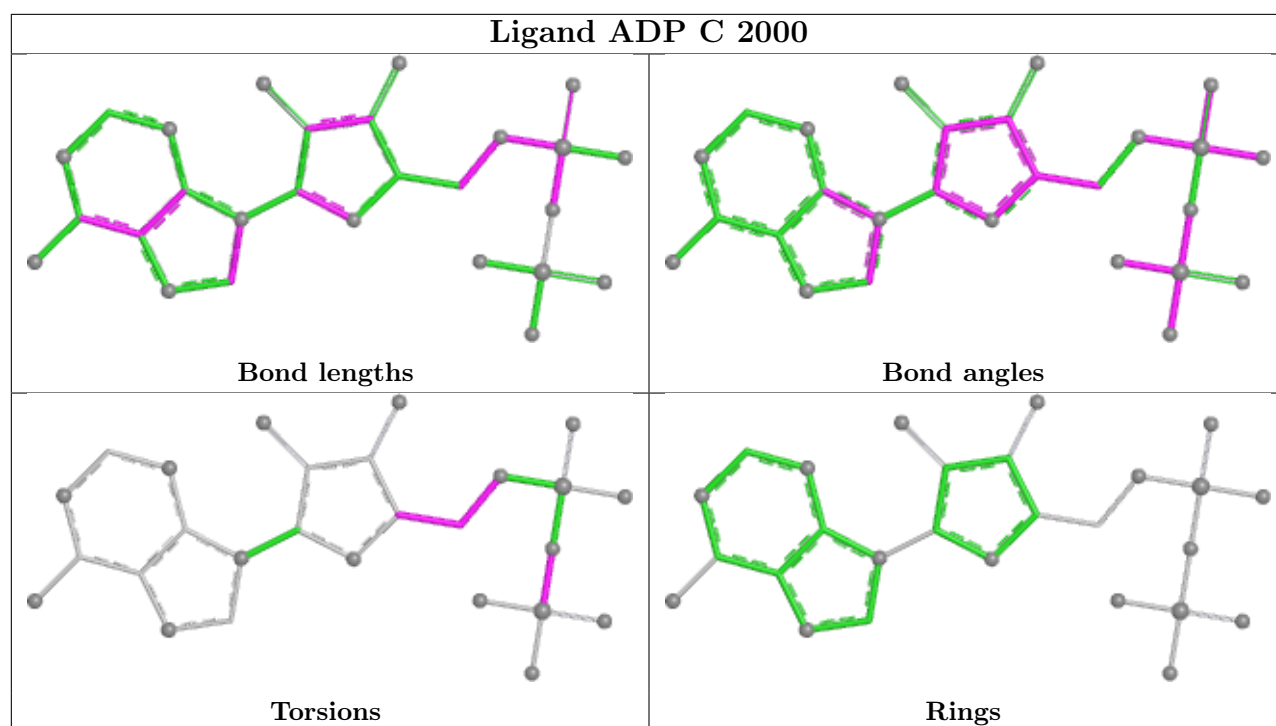
There are no ring outliers.

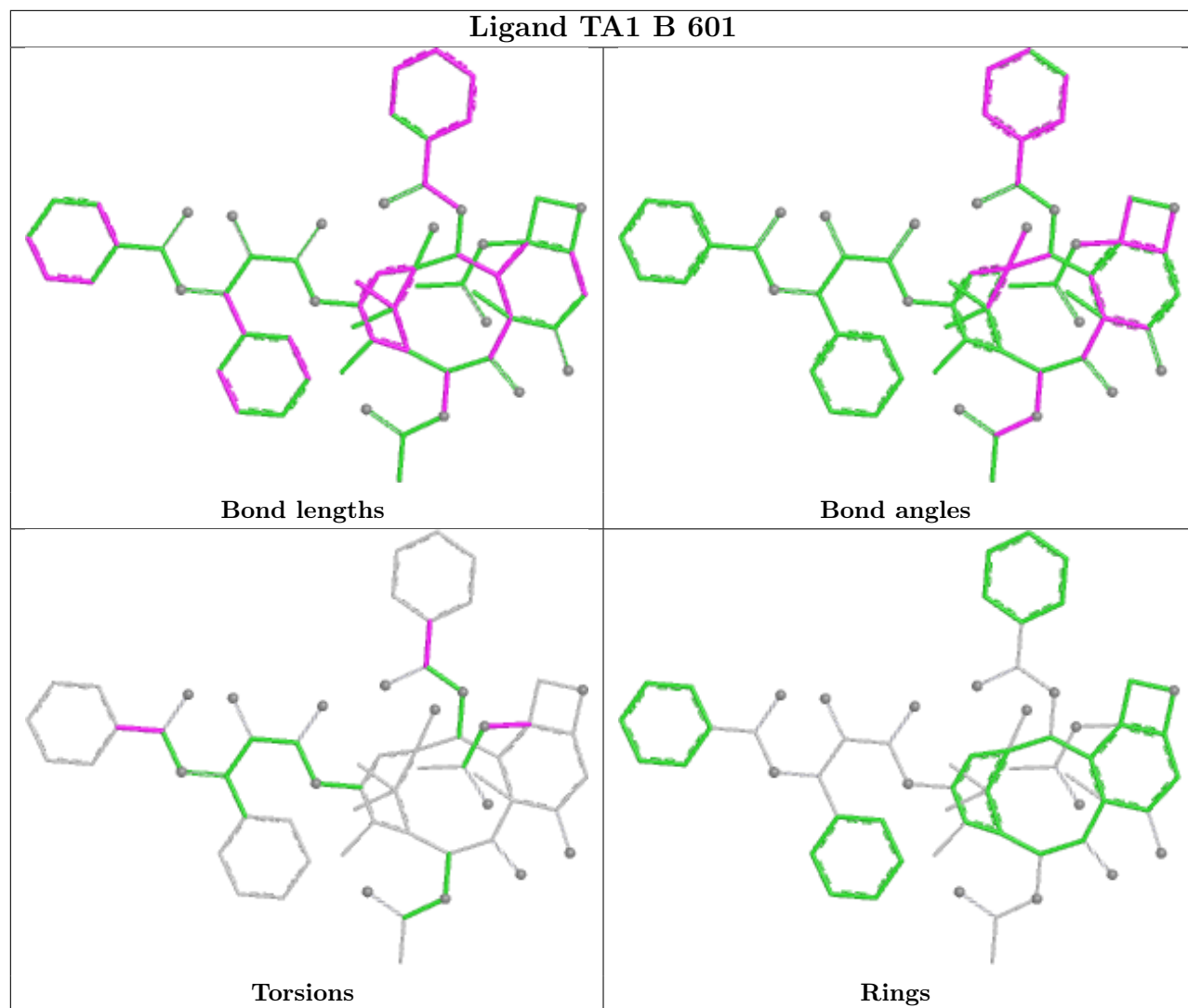
3 monomers are involved in 11 short contacts:

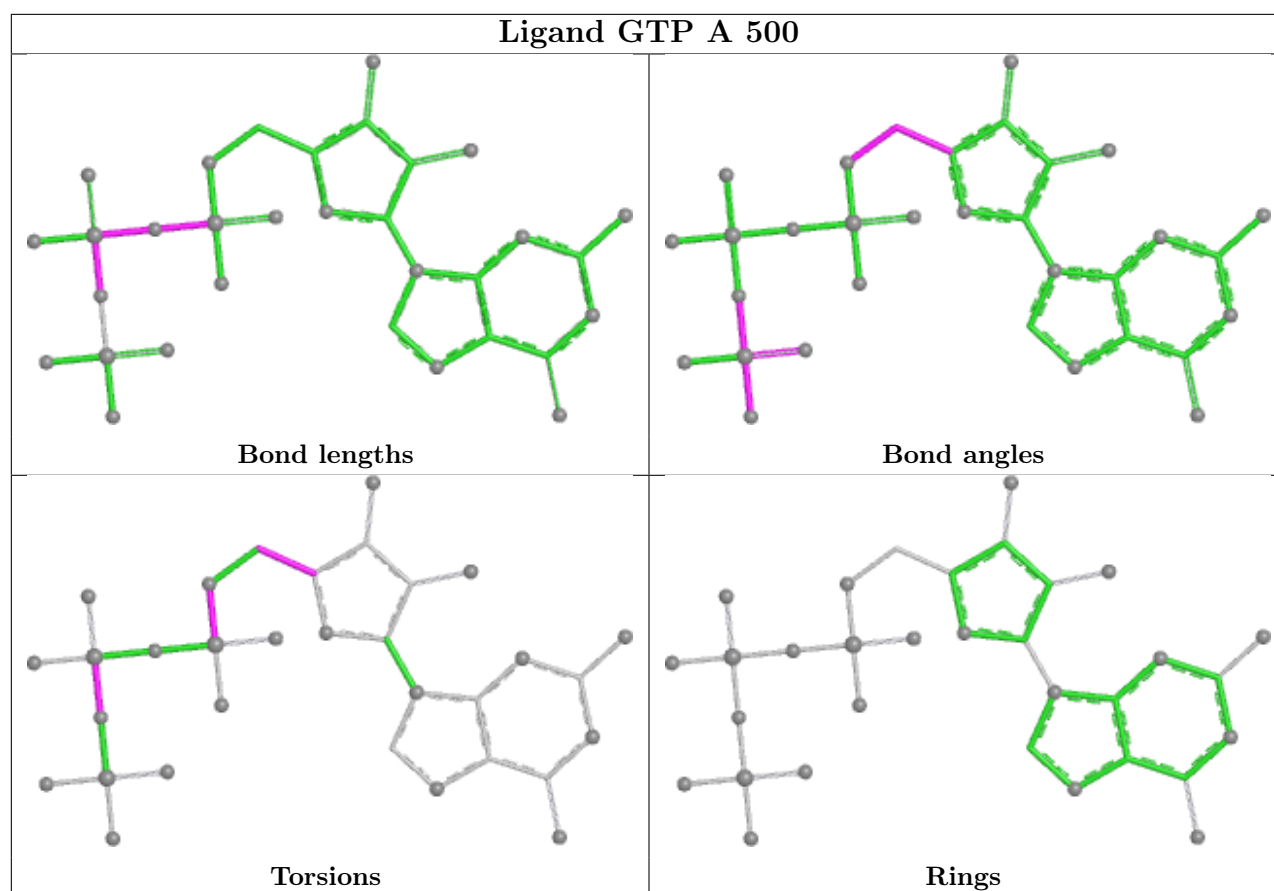
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	600	GDP	1	0
7	B	601	TA1	5	0
5	A	500	GTP	5	0

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.









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.