



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2025 – 04:10 PM JST

PDB ID : 9LNW / pdb_00009lnw
Title : Crystal structure of T2R-TTL-YQVB8 Complex
Authors : Wu, C.Y.; Wang, Y.X.; Chen, Q.F.
Deposited on : 2025-01-22
Resolution : 2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

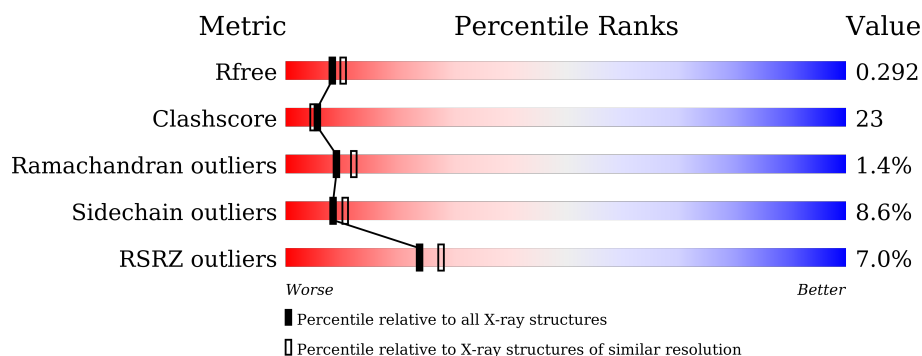
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	
1	C	450	
2	B	445	
2	D	445	
3	E	143	
4	F	384	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17615 atoms, of which 58 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	9	0
			3465	2200	584	657	24			
1	C	440	Total	C	N	O	S	4	7	0
			3466	2197	584	662	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	14	4	0
			3343	2102	567	646	28			
2	B	428	Total	C	N	O	S	6	2	0
			3370	2118	576	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

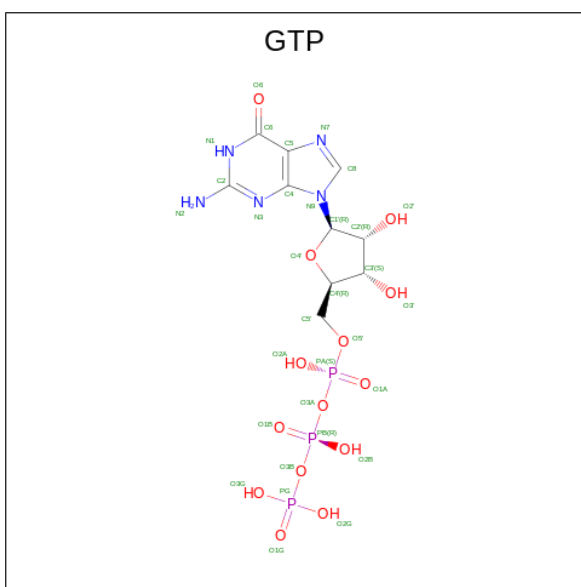
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	9	4	0
			2729	1762	457	496	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

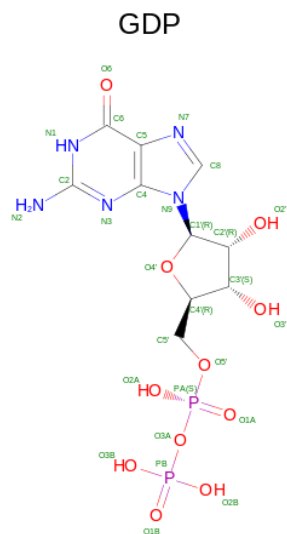
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	1	0
6	C	1	Total Mg 1 1	1	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

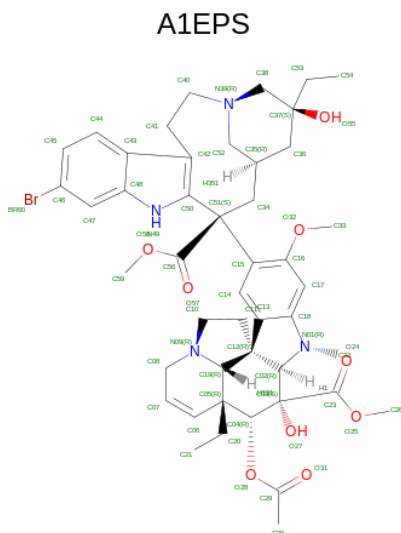
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	1	0
7	C	1	Total Ca 1 1	1	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 9 is 10'-bromovinblastine (CCD ID: A1EPS) (formula: $C_{46}H_{57}BrN_4O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	Br	C	H	N	O	0	0
			118	1	46	58	4	9		

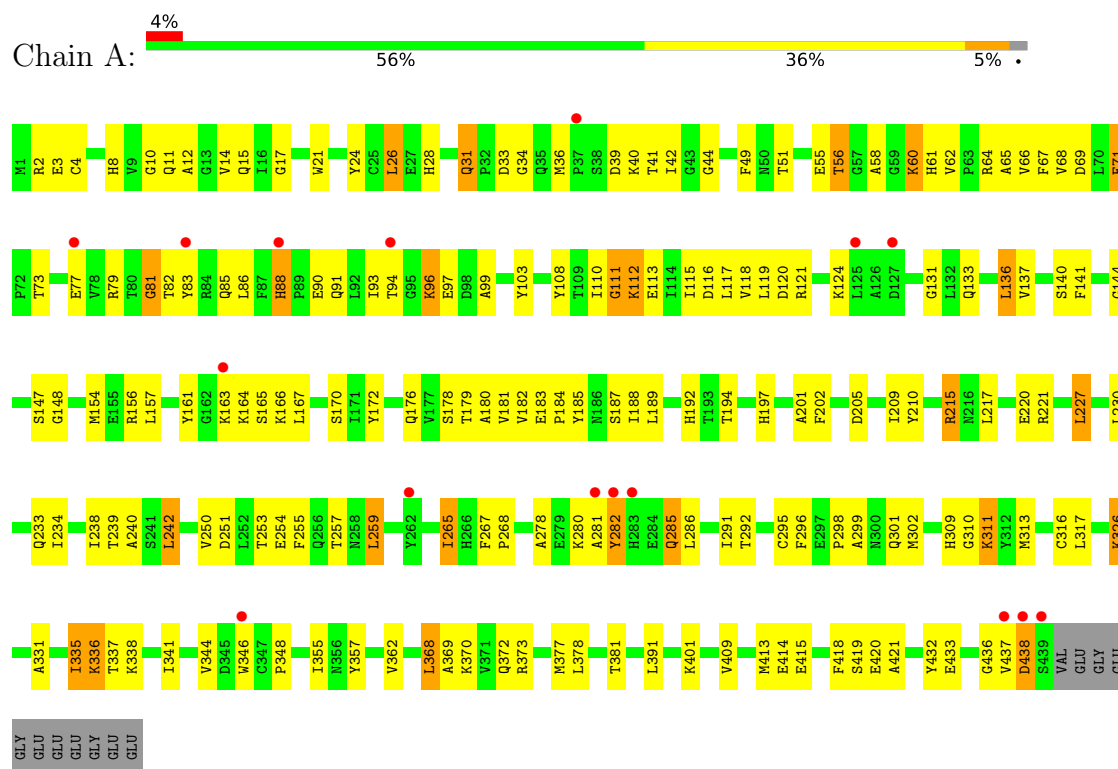
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	4	Total 4	O 4	0	0
10	B	5	Total 5	O 5	0	0

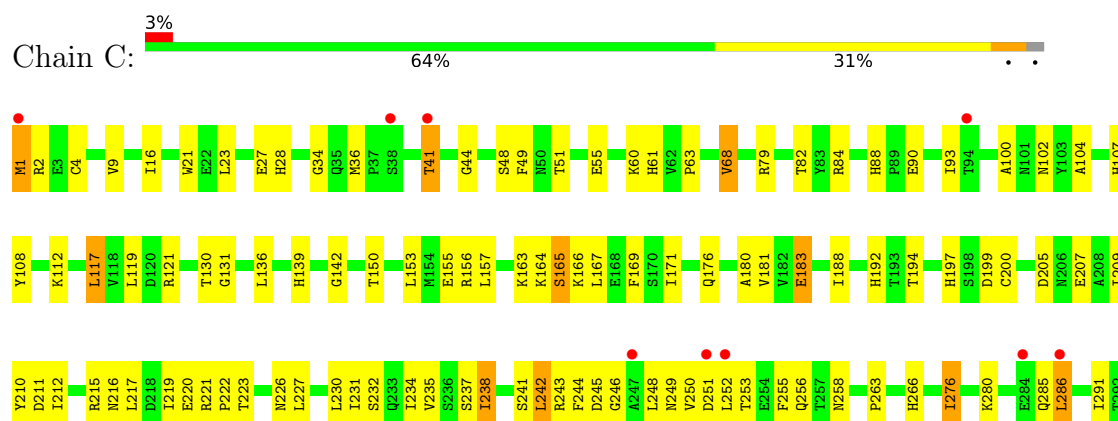
3 Residue-property plots

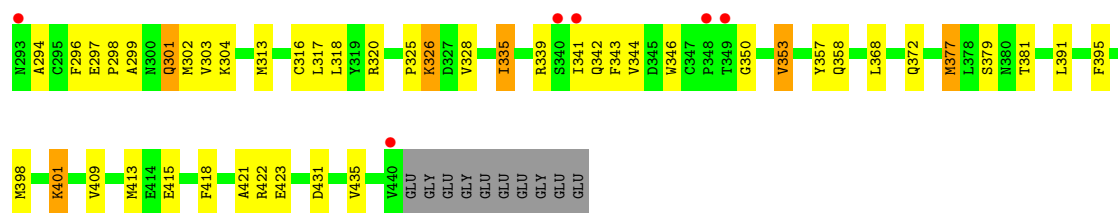
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Detyrosinated tubulin alpha-1B chain

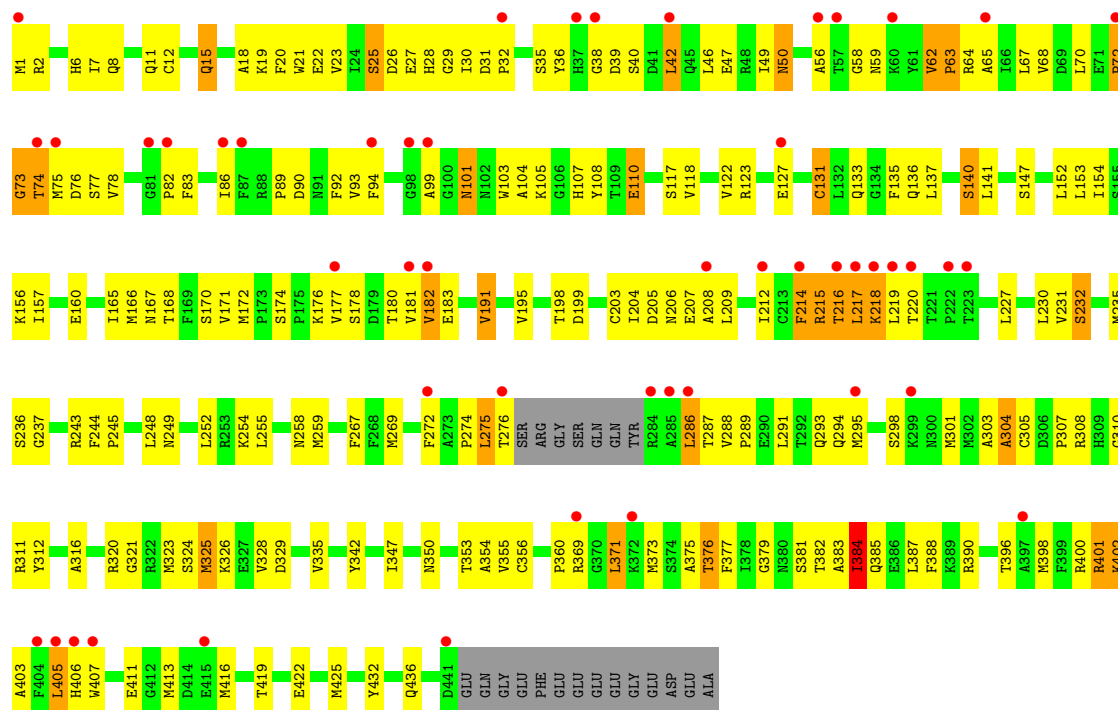


• Molecule 1: Detyrosinated tubulin alpha-1B chain

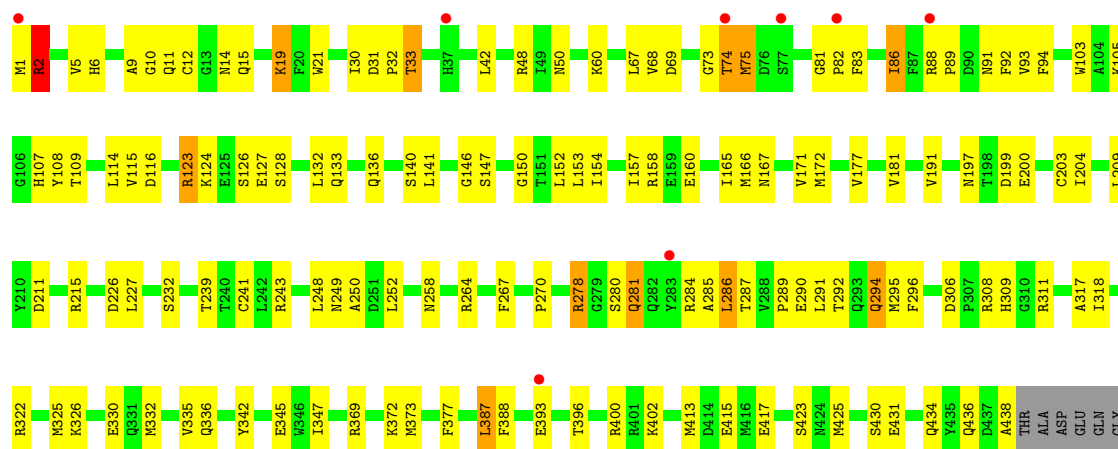




● Molecule 2: Tubulin beta chain



● Molecule 2: Tubulin beta chain



GLU
PHE
GLU
GLU
GLU
GLU
GLY
GLY
ASP
GLU
ALA

● Molecule 3: Stathmin-4



RET ALA ASP N6 E7 V8 T9 E10 C14 T15 S16 G17 Q18 S19 V22 V23 L24 V25 P26 P27 S28 PHE ASP GLY VAL L123 PRO Q124 PHE ASN K126 ALA D127 SER LEU A130 PRO ARG E132 ARG D44 P45 S46 L47 I50 Q51 K52 K53 L54 E55 E59 R60 R61 K62 E65 L68 R76

E17 K85 E88 F83 I94 K95 E99 K100 L101 A102 Q103 M105 E106 E110 H115 L116 M119 R122 L123 Q124 E125 K126 D127 K128 H129 A130 E131 V133 R134 K135 M136 K137 E138 L139 K140 GLU ALA SER ARG

● Molecule 4: Tubulin tyrosine ligase



M1 Y2 T3 F4 S12 V13 V17 L20 L24 K28 R29 L30 D33 N34 P35 R36 F37 N38 L39 K40 L41 R44 N45 R46 E55 L61 R66 K70 L71 C72 V78 K79 L80 I81 K82 T83 S84 S88 E89 S90 C91 T92 W93 Y98 V99 I100

Y101 F102 T103 ASN LEU LYS THR PRO VAL ALA PRO F173 ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN THR ARG T125 D126 E127 R128 F131 L132 A133 A134 Y135 N136 R137 ARG ARG GLY ARG GLU G144 N145 V146 W147 I148 A149 LYS SER SER ALA GLY ALA C91 T92 W93 Y98 V99 I161

I162 S163 S164 E165 A166 S167 E168 L169 D171 F172 L173 D174 E175 V179 H180 Y181 I182 Q183 K184 Y185 L186 E187 L190 P194 R197 K198 F199 V205 L206 D207 D208 H209 Y214 L215 L216 R217 E218 G219 V220 L221 S224 S225 T228 N229 S230 A231 N232 F233 Q234 D235 K236

T237 C238 H239 L240 T241 N242 H243 C244 T245 Q246 K247 E248 Y249 S250 LYS ASN TYR GLY R255 E258 G259 N260 M261 M262 F263 E266 L275 N276 T277 T278 S282 L283 L284 L285 T290 T291 R292 L295 M296 C297 I298 I302 K305 H306 Q310 F319 M320 V321 D322

L325 E331 V332 N333 K341 L342 Y343 G349 A354 V358 F359 P360 L361 A362 ASP THR GLY GLN THR SER GLN T372 S373 I374 F375 I376 K377 H379 H380 HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.82Å 155.76Å 185.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.21 – 2.55 91.21 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.6 (91.21-2.55) 97.6 (91.21-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.55Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.225 , 0.292 0.228 , 0.292	Depositor DCC
R_{free} test set	7096 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17615	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A1EPS, MG, GTP, GDP

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	0.37	0/3571	0.54	0/4849
1	C	0.42	0/3565	0.60	0/4842
2	B	0.41	0/3451	0.57	0/4675
2	D	0.31	0/3428	0.49	0/4645
3	E	0.37	0/999	0.51	0/1325
4	F	0.31	0/2802	0.51	0/3789
All	All	0.37	0/17816	0.54	0/24125

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	E	0	1
4	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	76	ARG	Sidechain
4	F	89	GLU	Peptide

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	3465	0	3401	176	0
1	C	3466	0	3393	153	0
2	B	3370	0	3249	119	0
2	D	3343	0	3230	201	0
3	E	991	0	1012	51	0
4	F	2729	0	2715	123	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	60	58	0	7	0
10	B	5	0	0	0	0
10	C	4	0	0	0	0
All	All	17557	58	17048	790	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 23.

The worst 5 of 790 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:D:135:PHE:HB2	2:D:166:MET:HE1	1.31	1.11
2:B:1:MET:HE2	2:B:1:MET:HA	1.41	1.03
2:D:166:MET:HE3	2:D:166:MET:HA	1.42	0.97
1:C:285:GLN:NE2	1:C:372:GLN:OE1	1.97	0.97
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.46	0.96

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 X-ray entries followed by that with respect to entries of similar resolution.

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	446/450 (99%)	411 (92%)	29 (6%)	6 (1%)	10	13
1	C	445/450 (99%)	422 (95%)	22 (5%)	1 (0%)	44	56
2	B	428/445 (96%)	407 (95%)	18 (4%)	3 (1%)	19	26
2	D	424/445 (95%)	375 (88%)	36 (8%)	13 (3%)	3	2
3	E	116/143 (81%)	109 (94%)	6 (5%)	1 (1%)	14	21
4	F	323/384 (84%)	281 (87%)	35 (11%)	7 (2%)	5	5
All	All	2182/2317 (94%)	2005 (92%)	146 (7%)	31 (1%)	9	12

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	438	ASP
2	D	64	ARG
2	D	72	PRO
2	D	73	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	378/378 (100%)	337 (89%)	41 (11%)	5	6
1	C	378/378 (100%)	353 (93%)	25 (7%)	14	18
2	B	369/383 (96%)	344 (93%)	25 (7%)	13	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	369/383 (96%)	340 (92%)	29 (8%)	10	13
3	E	108/127 (85%)	95 (88%)	13 (12%)	4	4
4	F	303/342 (89%)	267 (88%)	36 (12%)	4	4
All	All	1905/1991 (96%)	1736 (91%)	169 (9%)	8	9

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	90	SER
4	F	378	LEU
4	F	136	ASN
4	F	233	PHE
2	B	75	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
4	F	242	ASN
2	D	294	GLN
4	F	239	HIS
2	D	15	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 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	$\# Z > 2$
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.55	7 (21%)
8	GDP	D	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.63	7 (21%)
8	GDP	B	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
9	A1EPS	B	502	-	64,68,68	4.98	32 (50%)	81,110,110	3.44	37 (45%)

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	C	501	6	-	7/18/38/38	0/3/3/3
8	GDP	D	501	-	-	0/12/32/32	0/3/3/3
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
8	GDP	B	501	-	-	1/12/32/32	0/3/3/3
9	A1EPS	B	502	-	-	12/38/131/131	0/7/9/9

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	A1EPS	C18-C13	12.91	1.55	1.39
9	B	502	A1EPS	C06-C07	12.32	1.55	1.32
9	B	502	A1EPS	C14-C15	11.92	1.57	1.39
9	B	502	A1EPS	C14-C13	10.88	1.55	1.39
9	B	502	A1EPS	C18-N01	9.45	1.56	1.39

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	502	A1EPS	O55-C37-C53	-16.67	79.99	108.75
9	B	502	A1EPS	C11-C12-C13	-10.43	93.33	112.35
9	B	502	A1EPS	O55-C37-C36	-7.85	88.20	109.28
9	B	502	A1EPS	C11-C12-C02	7.40	126.28	112.34
9	B	502	A1EPS	C14-C13-C18	-5.59	115.62	120.31

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

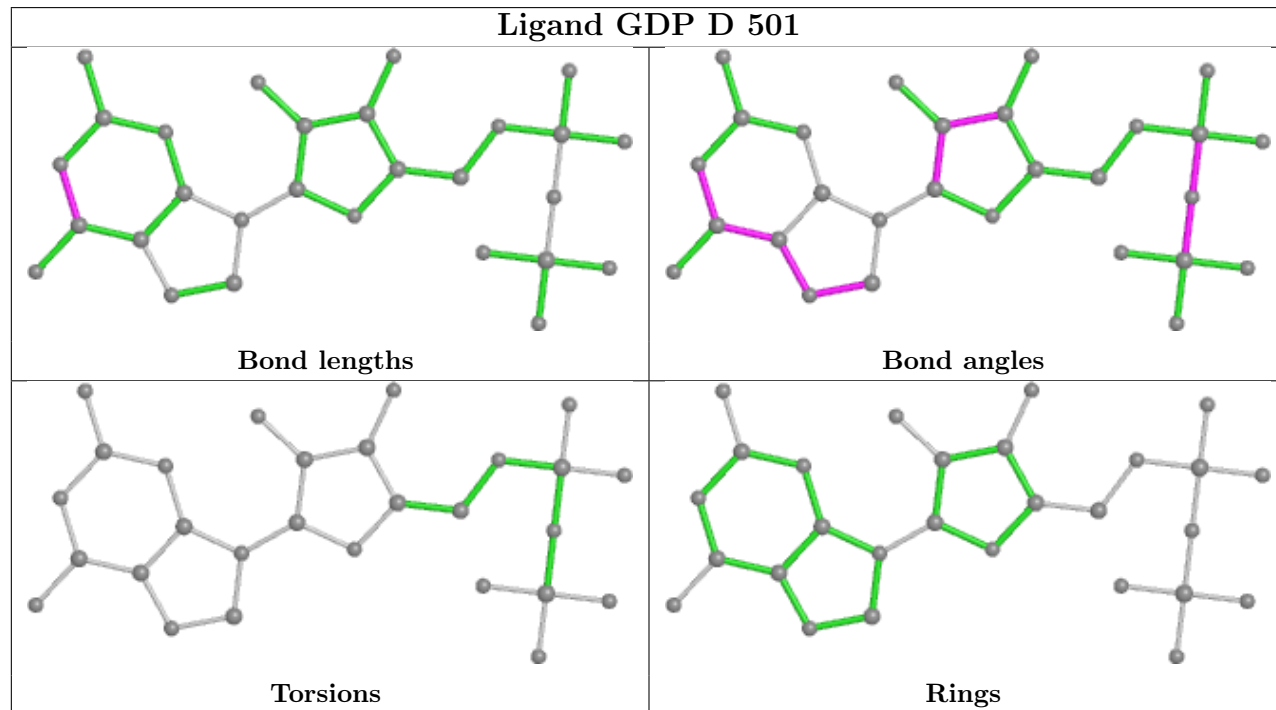
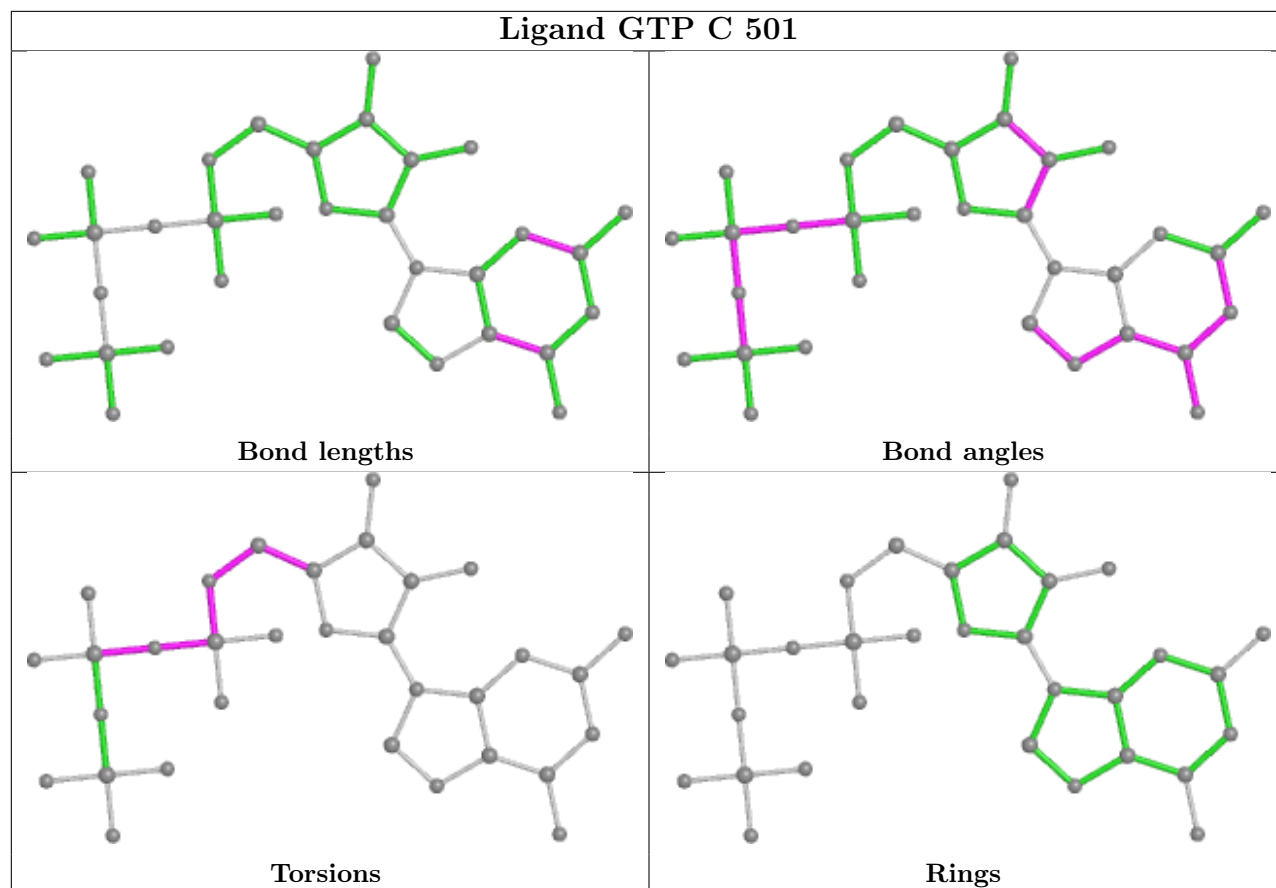
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O5'
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	502	A1EPS	C03-C23-O25-C26
9	B	502	A1EPS	O24-C23-O25-C26

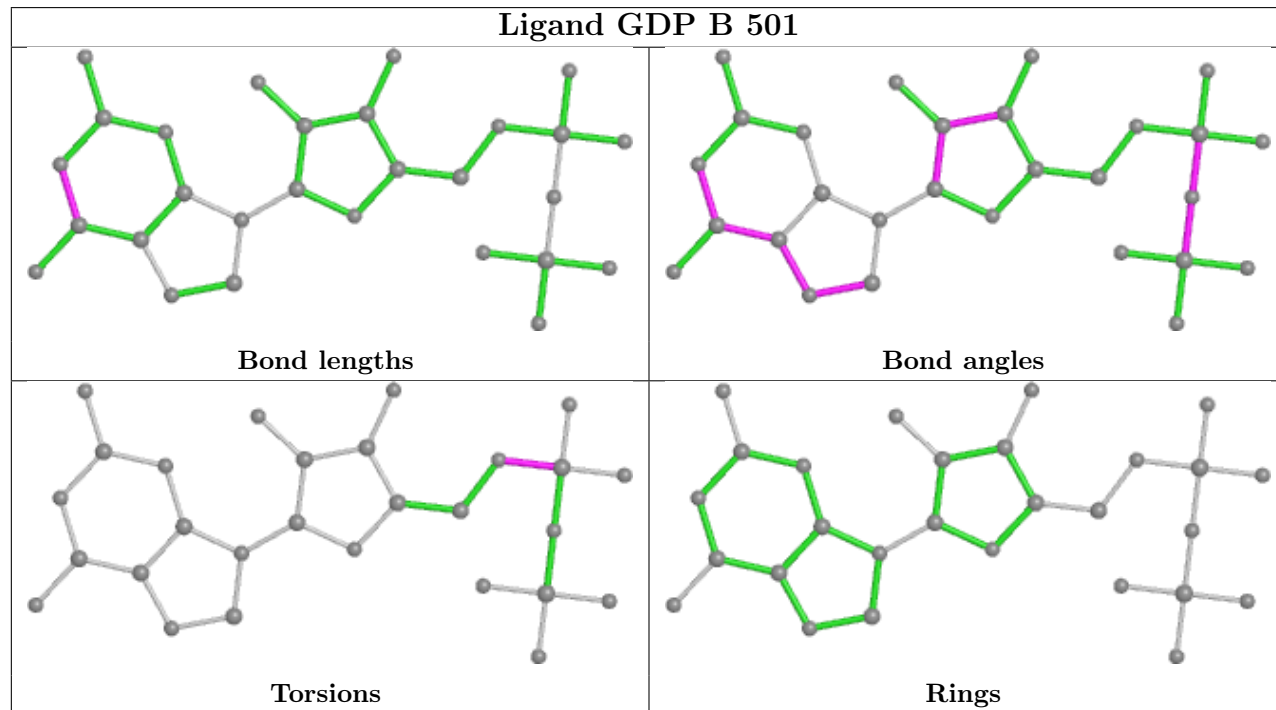
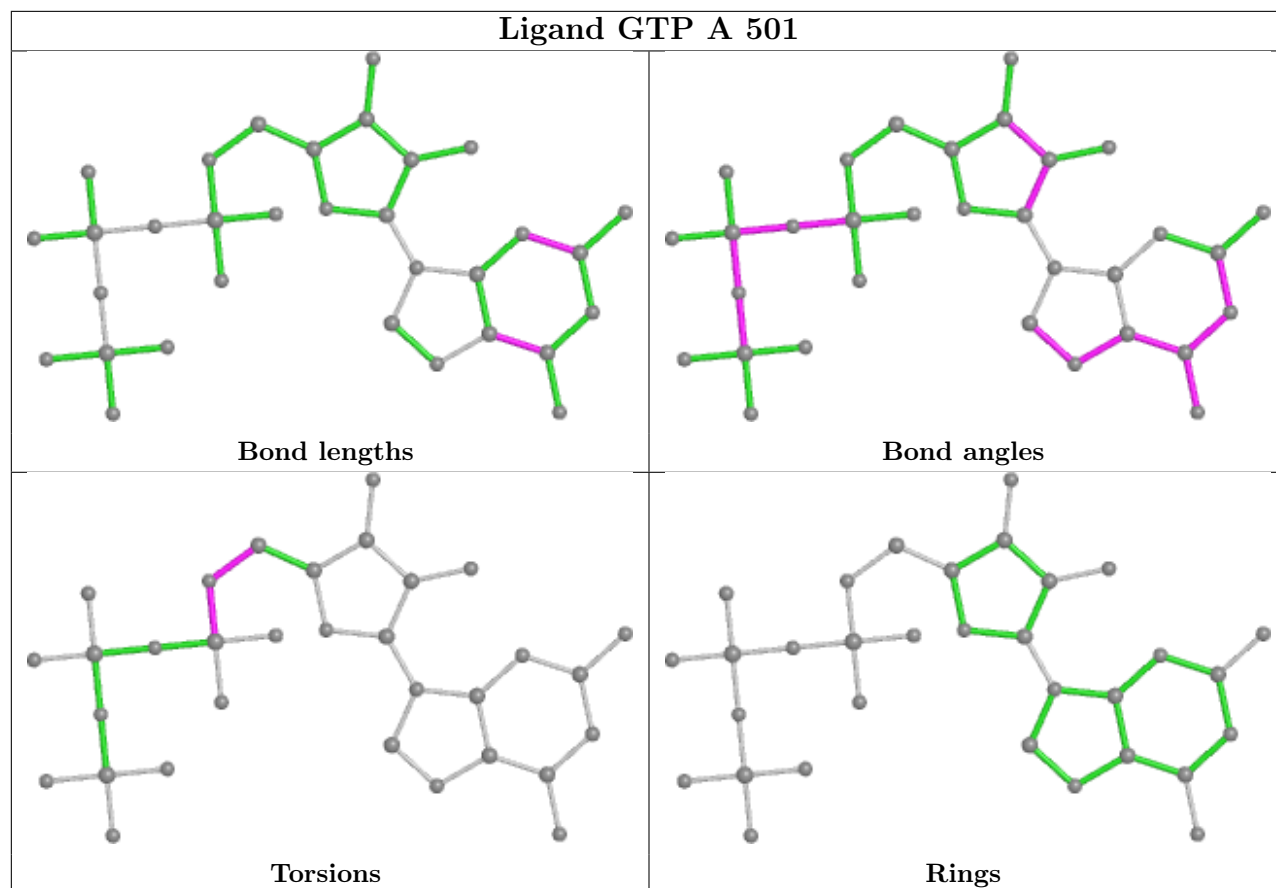
There are no ring outliers.

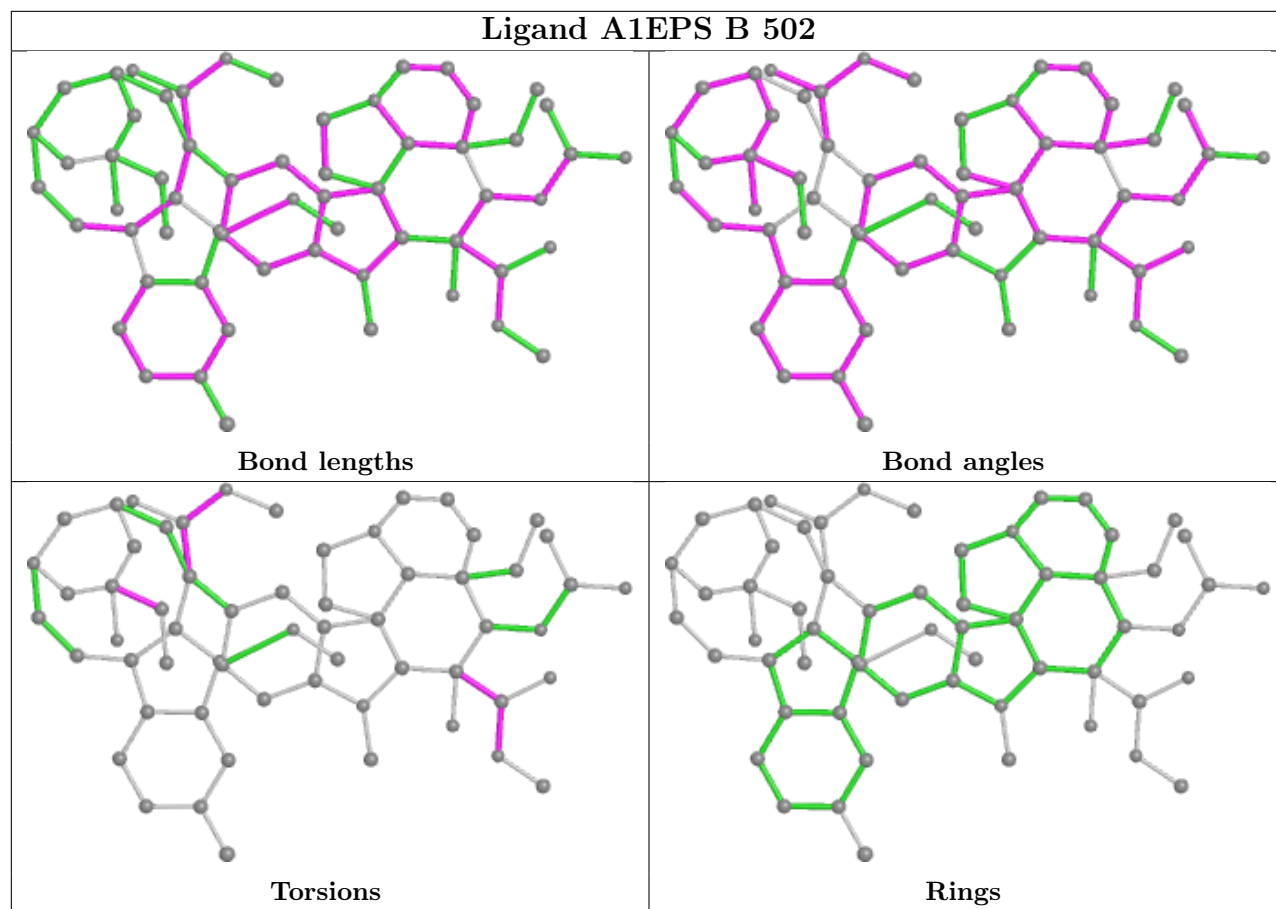
1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	A1EPS	7	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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/450 (97%)	0.25	16 (3%) 46 52	22, 41, 65, 99	9 (2%)
1	C	440/450 (97%)	0.05	15 (3%) 48 53	17, 35, 56, 72	7 (1%)
2	B	428/445 (96%)	-0.07	8 (1%) 66 69	16, 34, 62, 84	4 (0%)
2	D	424/445 (95%)	0.90	49 (11%) 11 13	29, 56, 83, 107	7 (1%)
3	E	120/143 (83%)	0.89	14 (11%) 10 13	29, 55, 79, 86	0
4	F	331/384 (86%)	0.90	51 (15%) 6 8	28, 58, 99, 114	4 (1%)
All	All	2182/2317 (94%)	0.41	153 (7%) 24 28	16, 44, 81, 114	31 (1%)

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	5.3
1	A	439	SER	5.1
4	F	125	THR	4.7
4	F	233	PHE	4.6
1	A	282	TYR	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.