



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2022 – 06:16 PM JST

PDB ID : 7VMJ
Title : Crystal structure of tubulin with 17a
Authors : Jifa, Z.; Lun, T.
Deposited on : 2021-10-08
Resolution : 2.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

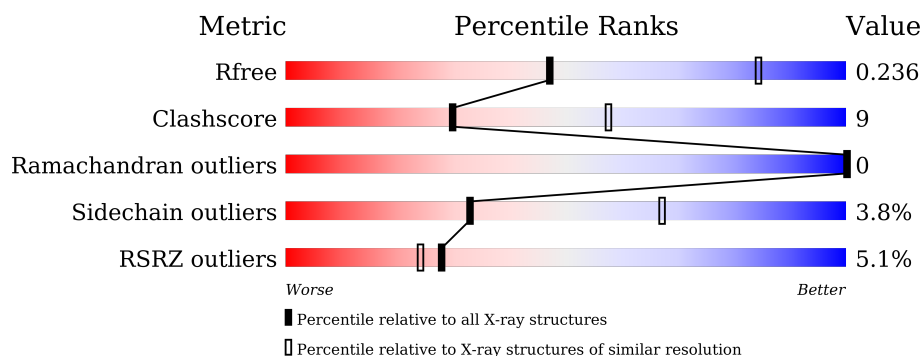
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	<div> <div>76%</div> <div>21%</div> <div>•</div> </div>
1	C	450	<div> <div>80%</div> <div>17%</div> <div>•</div> </div>
2	B	445	<div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>
2	D	445	<div> <div>7%</div> <div>65%</div> <div>28%</div> <div>• 6%</div> </div>
3	E	143	<div> <div>4%</div> <div>66%</div> <div>18%</div> <div>• 14%</div> </div>
4	F	384	<div> <div>18%</div> <div>63%</div> <div>25%</div> <div>• 10%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17608 atoms, of which 0 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3427	2170	580	653	24			
1	C	440	Total	C	N	O	S	0	8	0
			3465	2193	585	662	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	4	0
			3364	2116	575	647	26			
2	D	420	Total	C	N	O	S	0	1	0
			3291	2069	557	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	633	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	5	0
			2856	1835	487	519	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

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

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

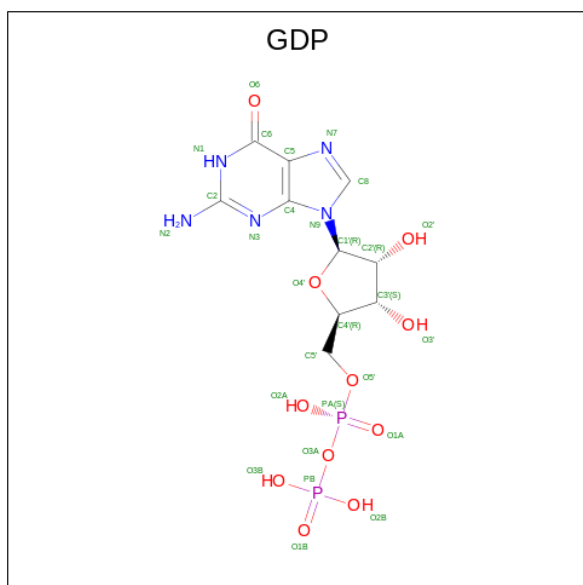
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

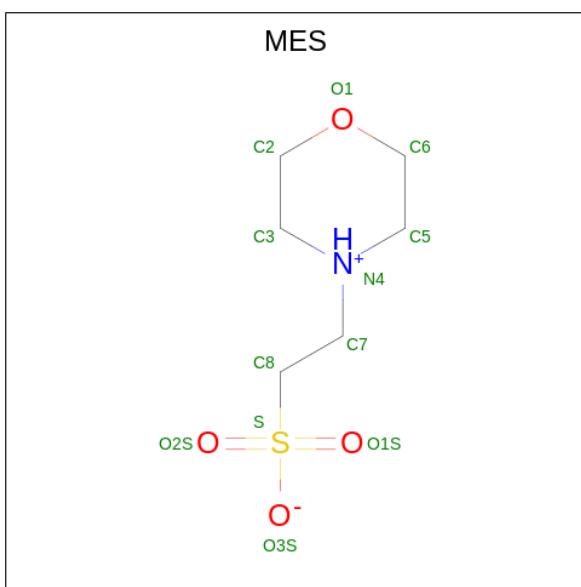
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	1	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	1	0
			1	1		

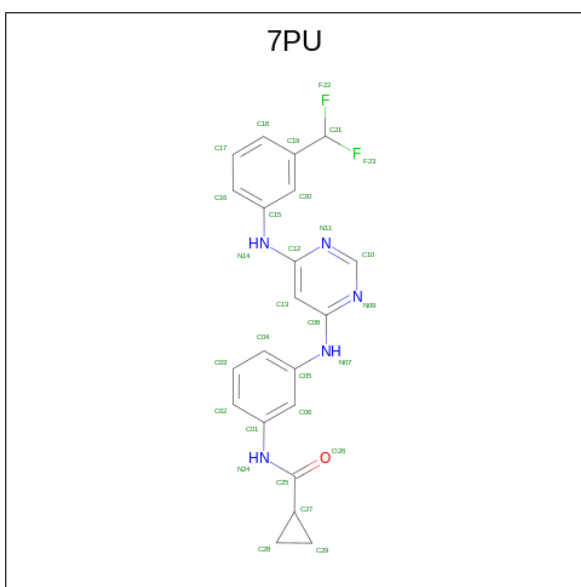
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is N-[3-[[6-[[3-[bis(fluoranyl)methyl]phenyl]amino]pyrimidin-4-yl]amino]phenyl]cyclopropanecarboxamide (three-letter code: 7PU) (formula: C₂₁H₁₉F₂N₅O) (labeled as "Ligand of Interest" by depositor).

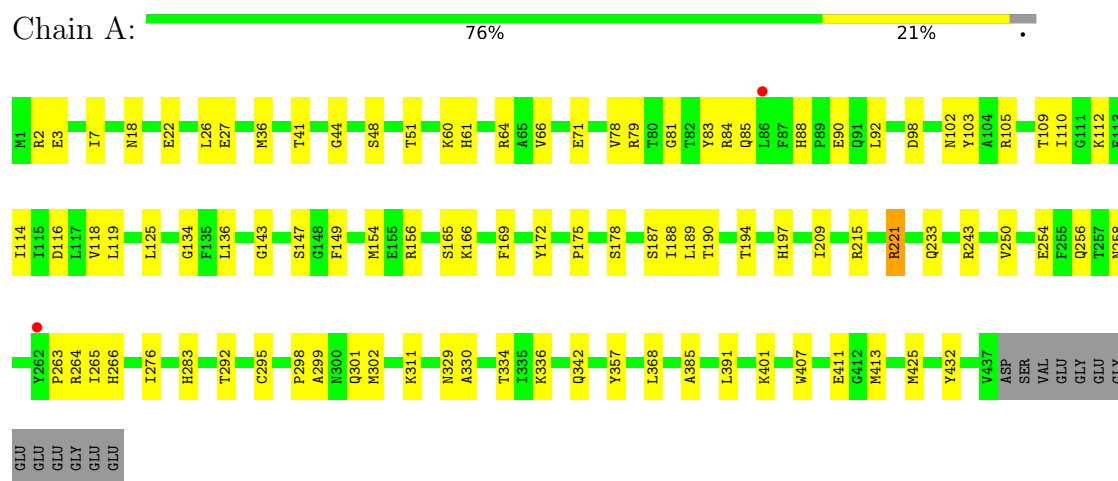


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	F	N	O	0	0
			29	21	2	5	1		

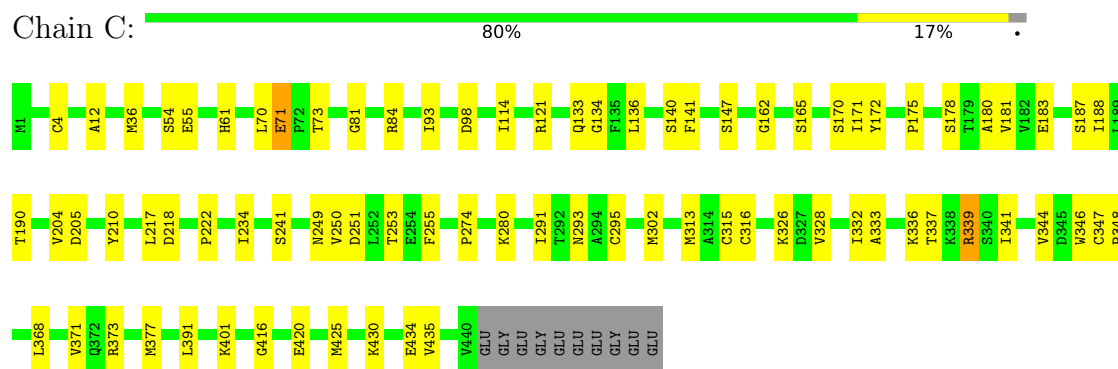
3 Residue-property plots

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.

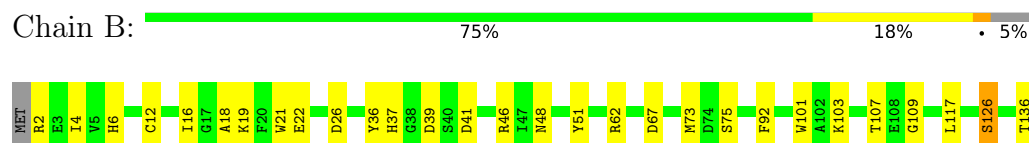
• Molecule 1: Tubulin alpha-1B chain

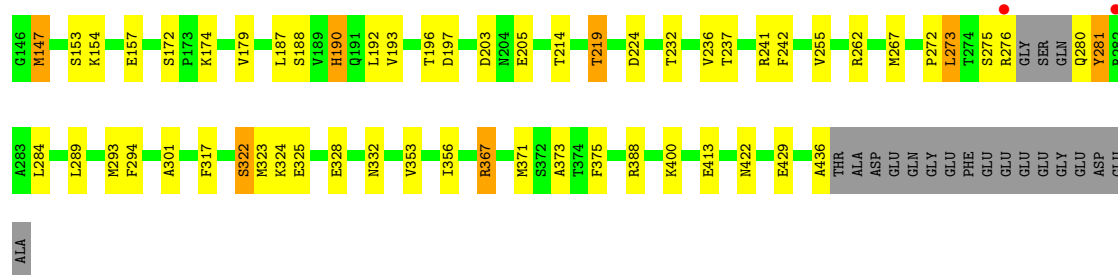


• Molecule 1: Tubulin alpha-1B chain

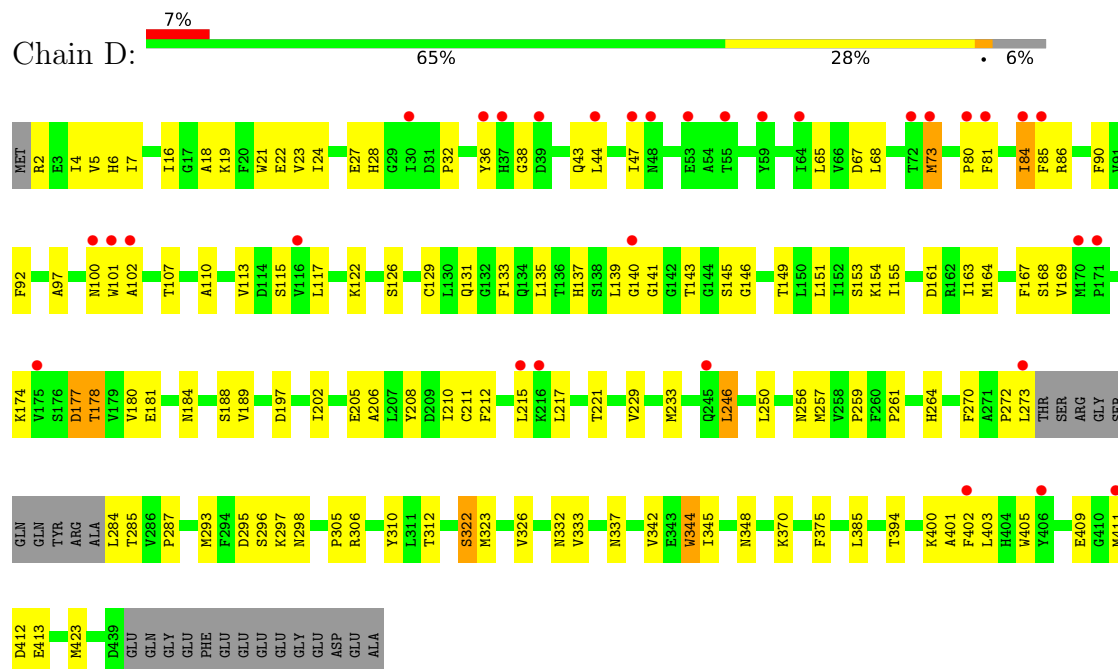


• Molecule 2: Tubulin beta-2B chain

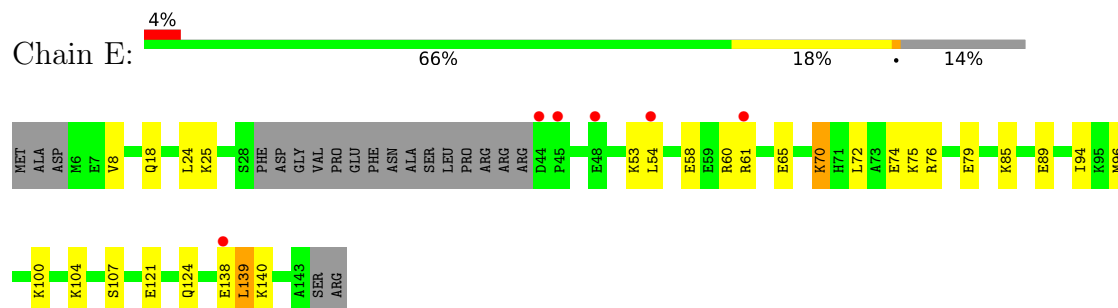




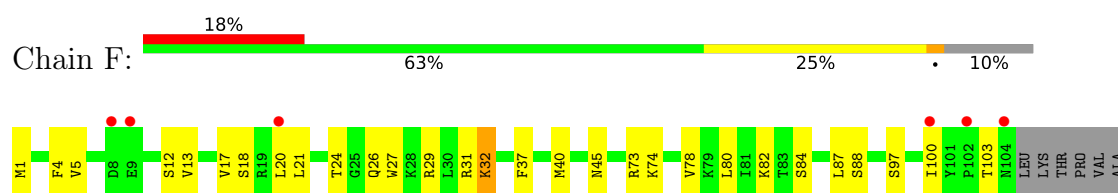
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



HIS	E257	Q178	PRO
HIS	E261	V179	ALA
HIS	E262	H180	GLN
	M262	V181	ASN
	F263	I182	GLY
	F267	I183	ILE
	L271	K184	ARG
		Y185	HIS
		L186	LEU
		L190	ILE
	T277	L191	ASN
	T278		THR
	L279	G195	ARG
	E280	H196	T125
	M281	R197	R128
	S282	K198	F131
	I283	F199	L132
	L284	D200	A133
		I201	A134
			Y135
		Y211	N136
	I287	V220	R137
	K288	L221	R138
	M296	R222	
	E299	T223	N145
	L307	S224	V146
		S225	W147
	F319	E226	I148
	N320	P227	A149
	V321	Y228	A150
		N229	S151
	L325	A231	S152
	K326	N232	ALA
	V327	P233	GLY
	N328	Q234	ALA
	E331	D235	LYS
		K236	GLY
	A339	T237	E158
	Q340	C238	G159
	K341	H239	I160
	L342	L240	L161
	Y343	T241	I162
		S242	S163
	A362	H243	S164
	ASP	C244	E165
	THR	I245	A166
	GLY	Q246	S167
	GLN	K247	E168
	LYS	E248	L169
	THR	Y249	L170
	SER	S250	D171
	GLN	K251	I172
	PRO	N252	I173
	T372	Y253	D174
		G254	E175
	H379	R255	Q176
	H380	Y256	G177
	HIS		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.98Å 157.93Å 182.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.43 – 2.90 87.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (87.43-2.90) 99.7 (87.43-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.199 , 0.243 0.191 , 0.236	Depositor DCC
R_{free} test set	1995 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17608	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MES, CL, 7PU, MG, CA, 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	0.48	0/3517	0.66	0/4776
1	C	0.58	1/3564 (0.0%)	0.71	0/4839
2	B	0.48	0/3447	0.69	1/4667 (0.0%)
2	D	0.45	0/3364	0.63	0/4560
3	E	0.51	0/1041	0.69	1/1382 (0.1%)
4	F	0.47	1/2935 (0.0%)	0.66	0/3966
All	All	0.50	2/17868 (0.0%)	0.67	2/24190 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	238	CYS	CB-SG	-9.16	1.66	1.82
1	C	295	CYS	CB-SG	-7.10	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	139	LEU	CA-CB-CG	6.04	129.18	115.30
2	B	273	LEU	CA-CB-CG	-5.12	103.53	115.30

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	3427	0	3340	64	0
1	C	3465	0	3383	47	0
2	B	3364	0	3250	59	0
2	D	3291	0	3155	84	0
3	E	1026	0	1042	23	0
4	F	2856	0	2837	66	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	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	A	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	24	0	24	2	0
11	B	29	0	0	0	0
All	All	17608	0	17079	326	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 9.

The worst 5 of 326 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:139:LEU:HD11	2:D:168:SER:HB3	1.38	1.04
1:C:234:ILE:HD13	1:C:302:MET:SD	2.18	0.84
1:A:154:MET:HG3	1:A:194:THR:HG23	1.63	0.80
2:D:65:LEU:HD11	2:D:85:PHE:HD2	1.47	0.78
4:F:135:TYR:OH	4:F:165:GLU:HA	1.84	0.78

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 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	439/450 (98%)	421 (96%)	18 (4%)	0	100	100
1	C	445/450 (99%)	436 (98%)	9 (2%)	0	100	100
2	B	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
2	D	416/445 (94%)	390 (94%)	26 (6%)	0	100	100
3	E	121/143 (85%)	118 (98%)	3 (2%)	0	100	100
4	F	343/384 (89%)	328 (96%)	15 (4%)	0	100	100
All	All	2188/2317 (94%)	2099 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 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	371/378 (98%)	365 (98%)	6 (2%)	62	86
1	C	378/378 (100%)	369 (98%)	9 (2%)	49	79
2	B	370/383 (97%)	358 (97%)	12 (3%)	39	73
2	D	361/383 (94%)	339 (94%)	22 (6%)	18	48
3	E	112/127 (88%)	107 (96%)	5 (4%)	27	61
4	F	315/342 (92%)	294 (93%)	21 (7%)	16	43
All	All	1907/1991 (96%)	1832 (96%)	75 (4%)	33	66

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	32	LYS
4	F	296[A]	MET
4	F	73	ARG
4	F	230	SER
1	C	339	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	18	GLN
4	F	26	GLN
4	F	243	HIS
4	F	145	ASN
2	B	332	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 6 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	$\# Z > 2$
10	MES	B	503	-	12,12,12	1.83	2 (16%)	14,16,16	3.14	10 (71%)
9	GDP	D	501	-	24,30,30	1.04	2 (8%)	30,47,47	1.17	3 (10%)
11	7PU	B	505	-	31,32,32	1.79	8 (25%)	39,44,44	1.54	5 (12%)
5	GTP	A	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.39	4 (12%)
5	GTP	C	501	6	26,34,34	1.36	3 (11%)	32,54,54	1.51	7 (21%)
10	MES	B	504	-	12,12,12	1.80	1 (8%)	14,16,16	2.79	8 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GDP	B	501	6	24,30,30	1.00	1 (4%)	30,47,47	1.26	5 (16%)

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
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3
11	7PU	B	505	-	-	2/20/22/22	0/4/4/4
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
10	MES	B	504	-	-	2/6/14/14	0/1/1/1
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-5.87	1.69	1.77
10	B	503	MES	C8-S	-5.73	1.69	1.77
11	B	505	7PU	C25-N24	5.20	1.47	1.35
5	C	501	GTP	C5-C6	-4.29	1.38	1.47
11	B	505	7PU	C12-N14	4.21	1.46	1.38

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	505	7PU	N11-C10-N09	-5.48	120.04	128.60
10	B	503	MES	C5-N4-C3	5.06	120.22	108.83
10	B	503	MES	C2-C3-N4	-4.96	102.58	110.10
10	B	504	MES	C2-C3-N4	-4.84	102.76	110.10
10	B	503	MES	O3S-S-C8	4.77	113.48	105.77

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A

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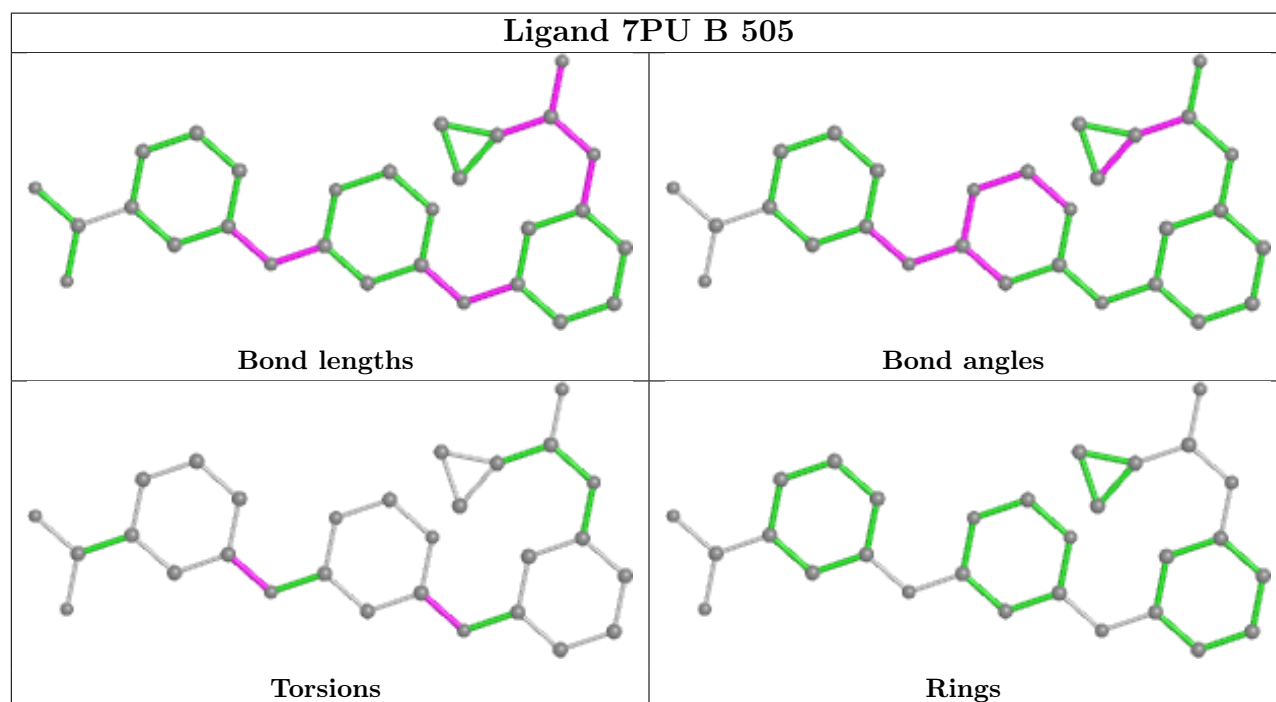
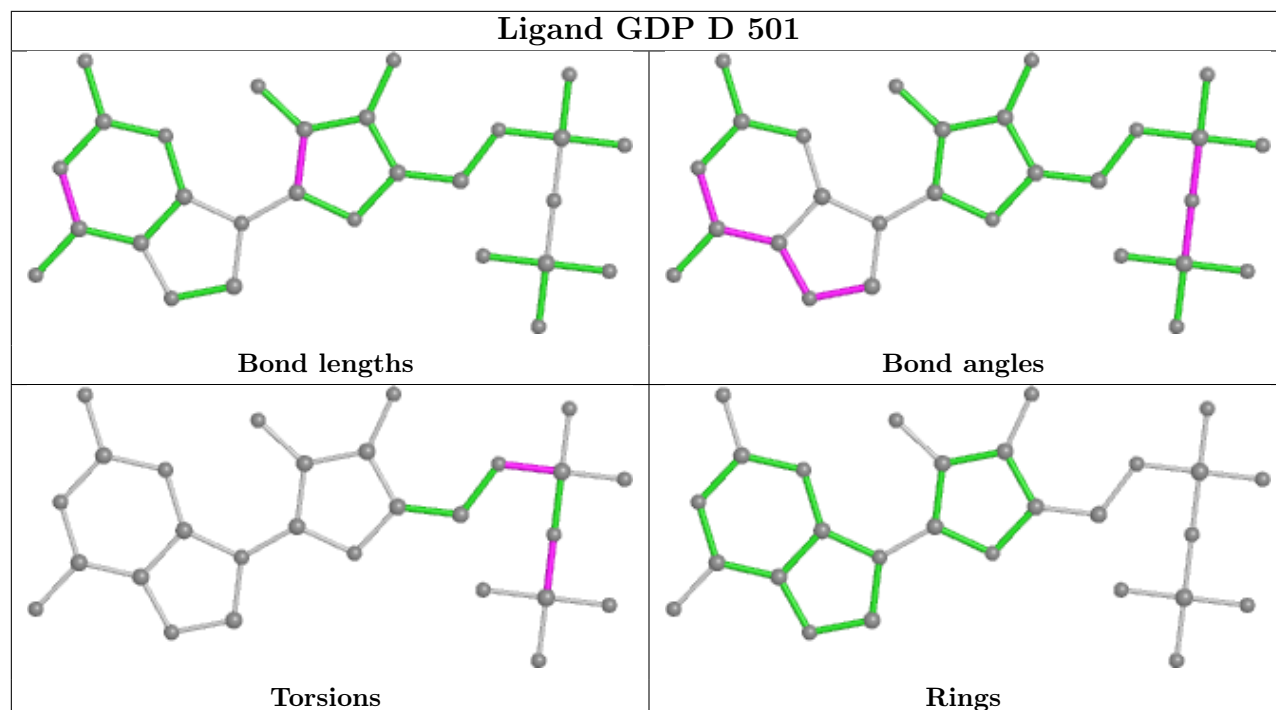
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

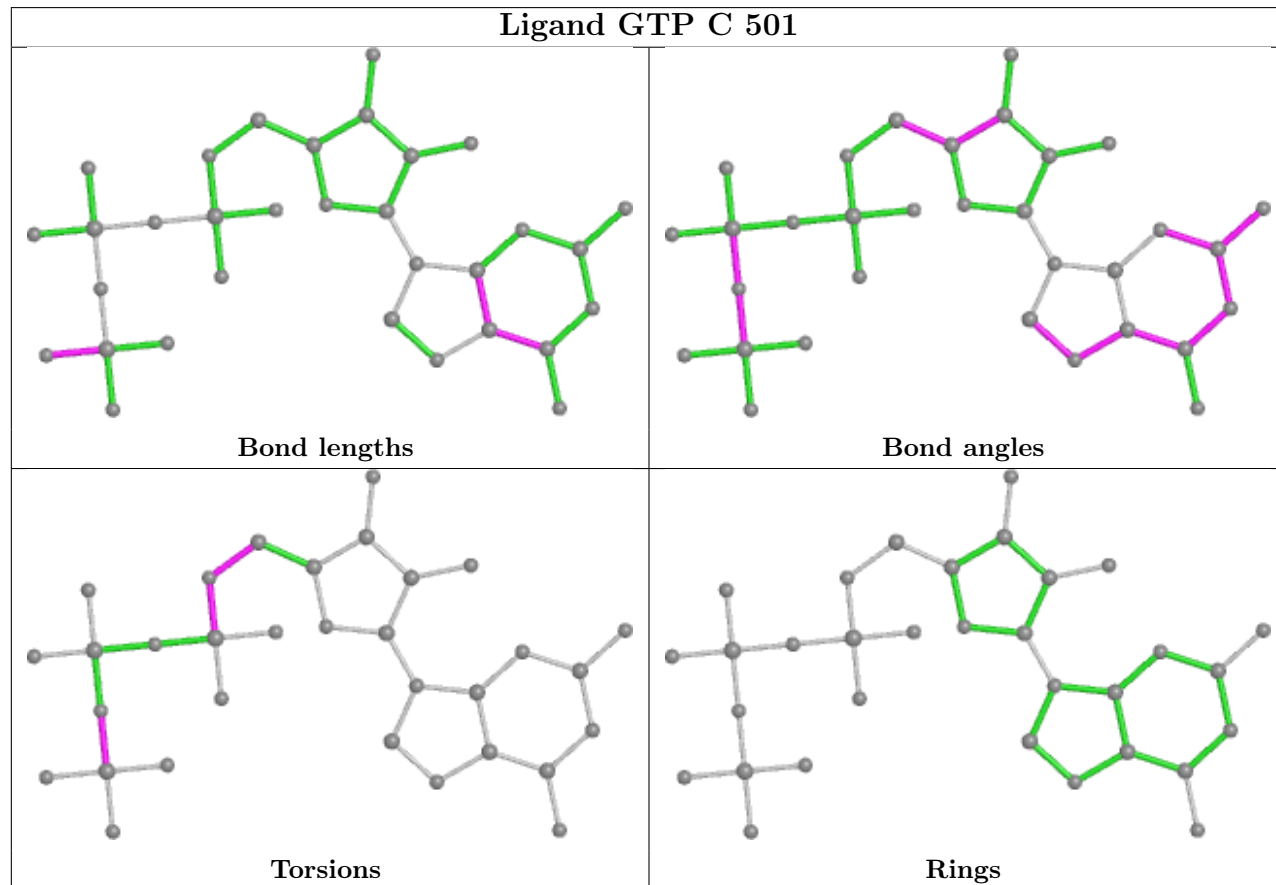
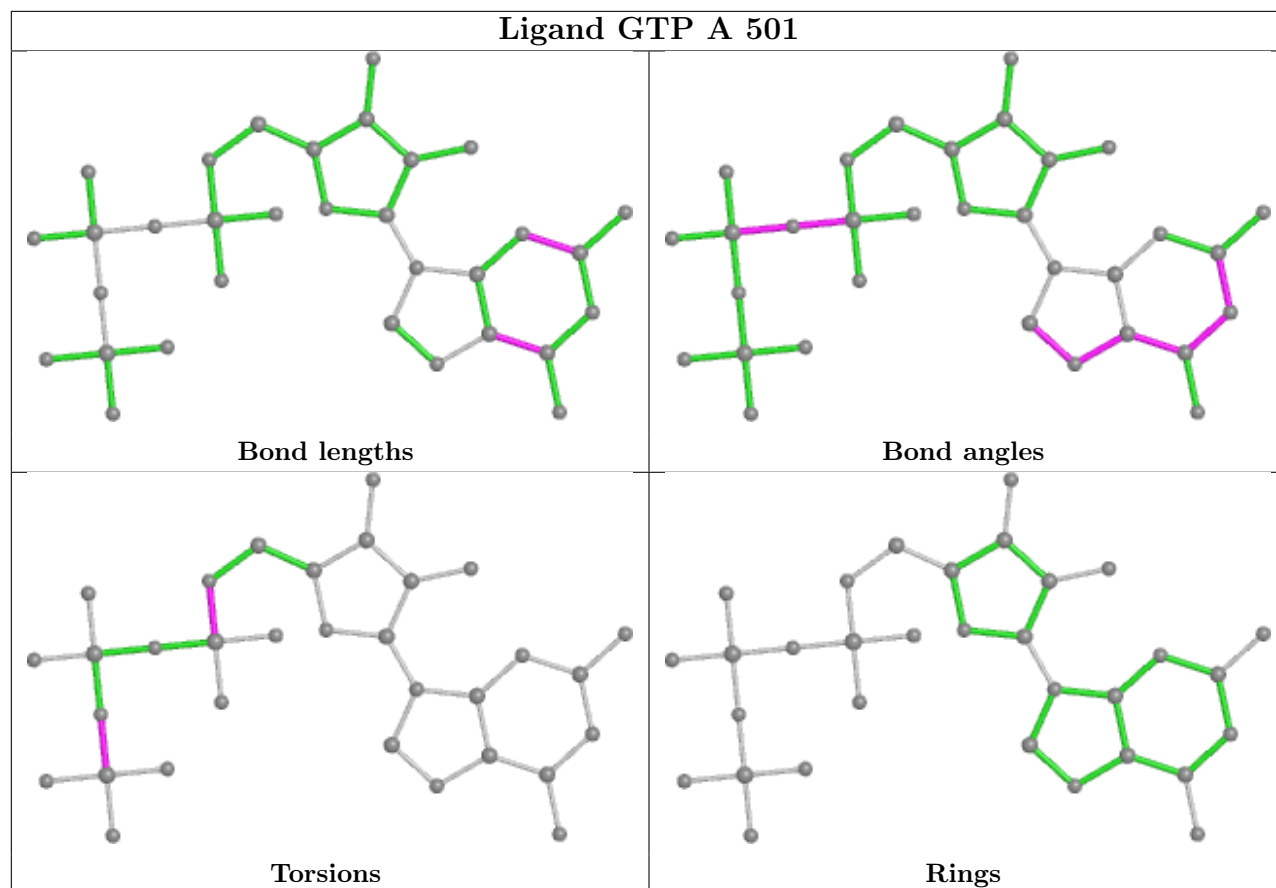
There are no ring outliers.

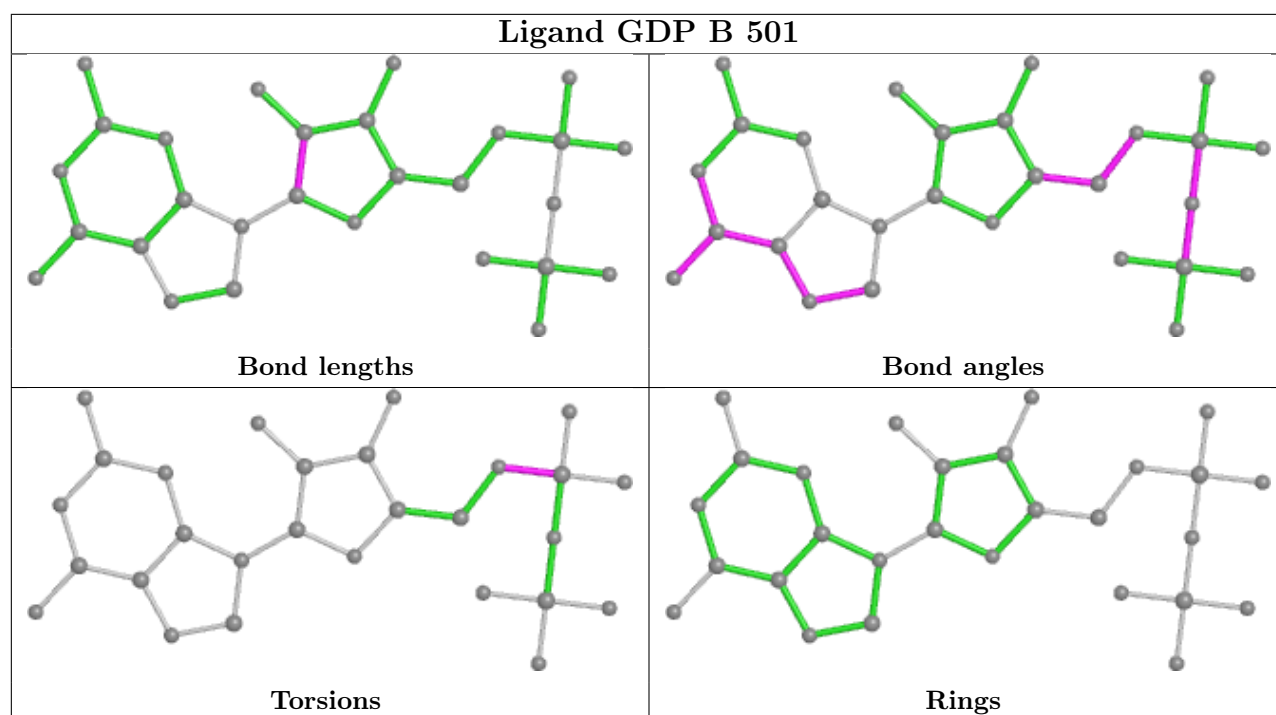
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	1	0
9	D	501	GDP	2	0
5	A	501	GTP	1	0
10	B	504	MES	1	0
9	B	501	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.







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	437/450 (97%)	0.16	2 (0%) 91 91	32, 49, 71, 90	0
1	C	440/450 (97%)	0.11	0 100 100	23, 41, 65, 85	0
2	B	424/445 (95%)	0.14	2 (0%) 91 91	28, 47, 75, 106	1 (0%)
2	D	420/445 (94%)	0.66	32 (7%) 13 10	36, 74, 103, 121	2 (0%)
3	E	123/143 (86%)	0.36	6 (4%) 29 26	40, 71, 107, 132	0
4	F	346/384 (90%)	1.16	69 (19%) 1 0	41, 75, 134, 152	0
All	All	2190/2317 (94%)	0.41	111 (5%) 28 24	23, 56, 104, 152	3 (0%)

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	7.0
4	F	233	PHE	6.5
4	F	159	GLY	5.8
4	F	152	SER	5.8
2	D	72	THR	5.5

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.