



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:39 PM UTC

PDB ID : 8CLE / pdb_00008cle
Title : Vinblastine bound to tubulin (T2R-TTL) complex
Authors : Wranik, M.; Bertrand, Q.; Kepa, M.W.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on : 2023-02-16
Resolution : 3.20 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

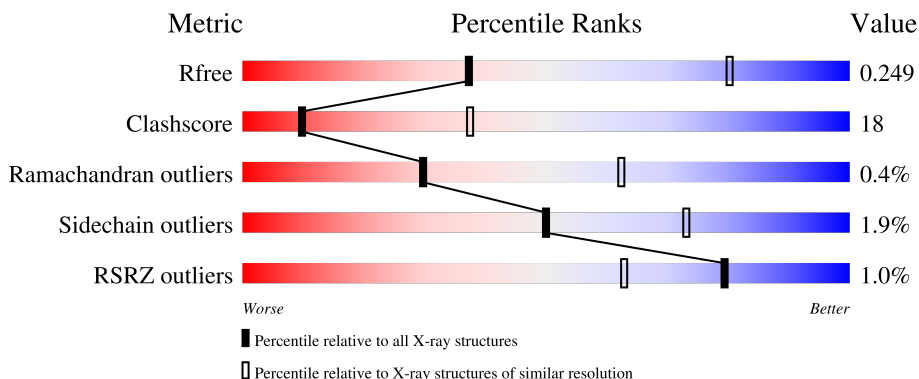
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	440	 69% 30%
1	C	440	 64% 32%
2	B	431	 73% 26%
2	D	431	 61% 36%
3	E	120	 75% 25%

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Mol	Chain	Length	Quality of chain
4	F	331	 4% 63% 35% ..

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17637 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	Total	C	N	O	S	5	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-2B chain.

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

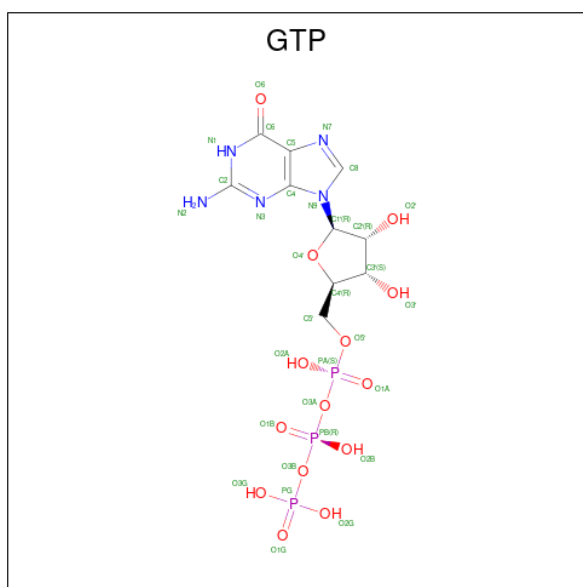
- Molecule 3 is a protein called Stathmin-4.

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

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	331	Total	C	N	O	S	5	4	0
			2729	1762	457	496	14			

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



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		

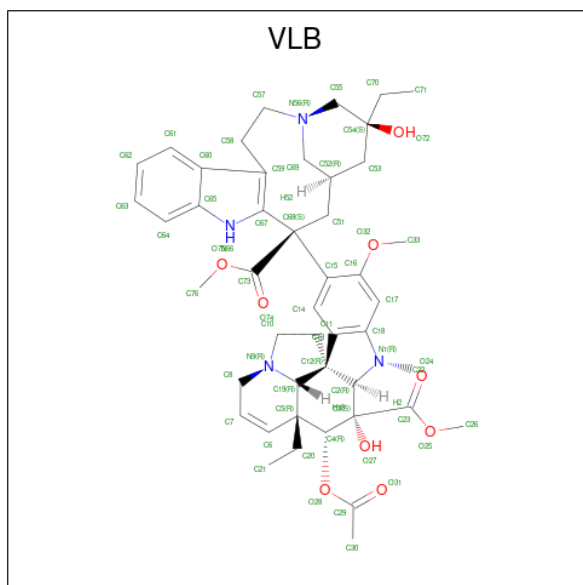
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

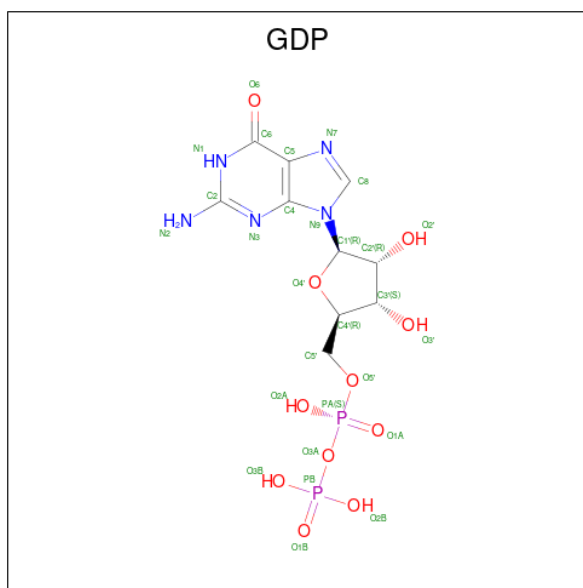
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (CCD ID: VLB) (formula: C₄₆H₅₈N₄O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
8	C	1	117	46	58	4	9	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

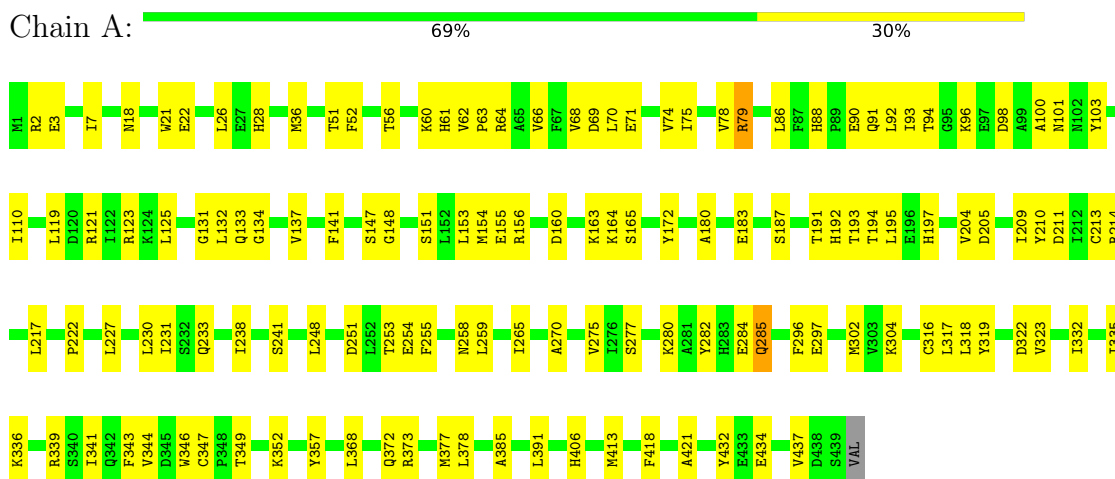
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total O 2 2	0	0
10	C	6	Total O 6 6	0	0
10	D	5	Total O 5 5	0	0
10	E	1	Total O 1 1	0	0
10	F	8	Total O 8 8	0	0
10	B	10	Total O 10 10	0	0

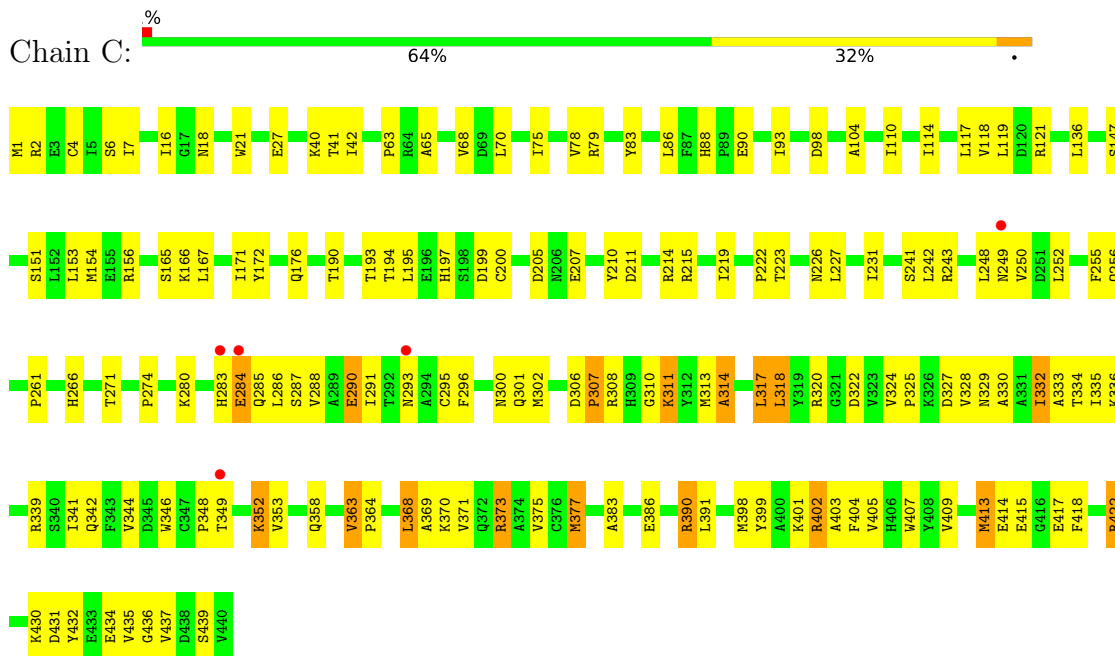
3 Residue-property plots

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.

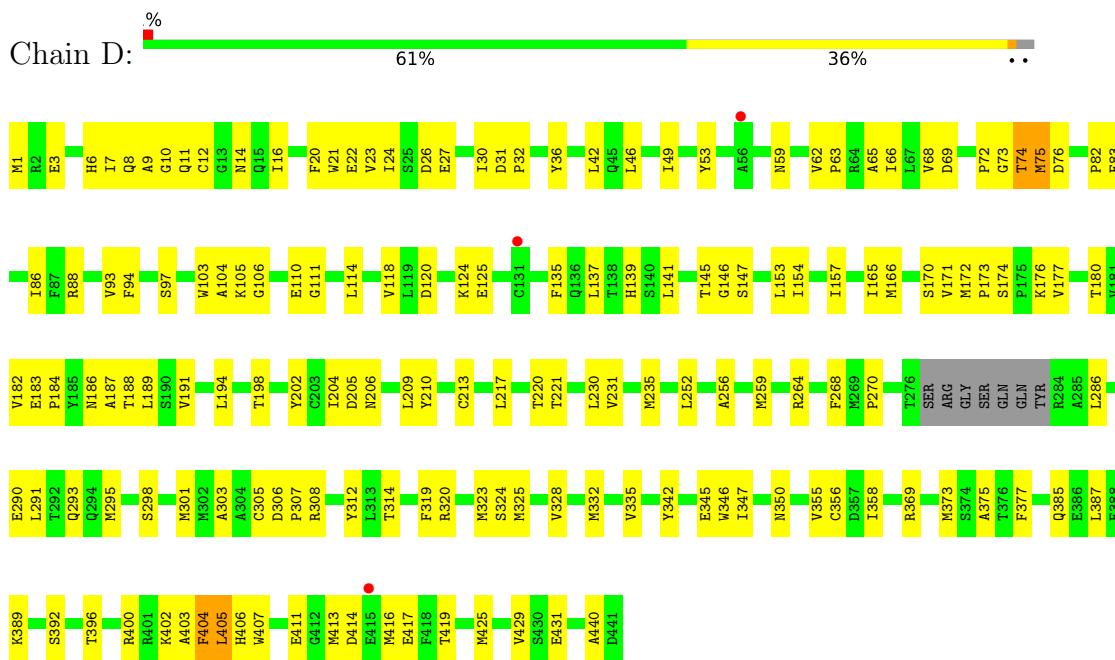
- Molecule 1: Tubulin alpha-1B chain



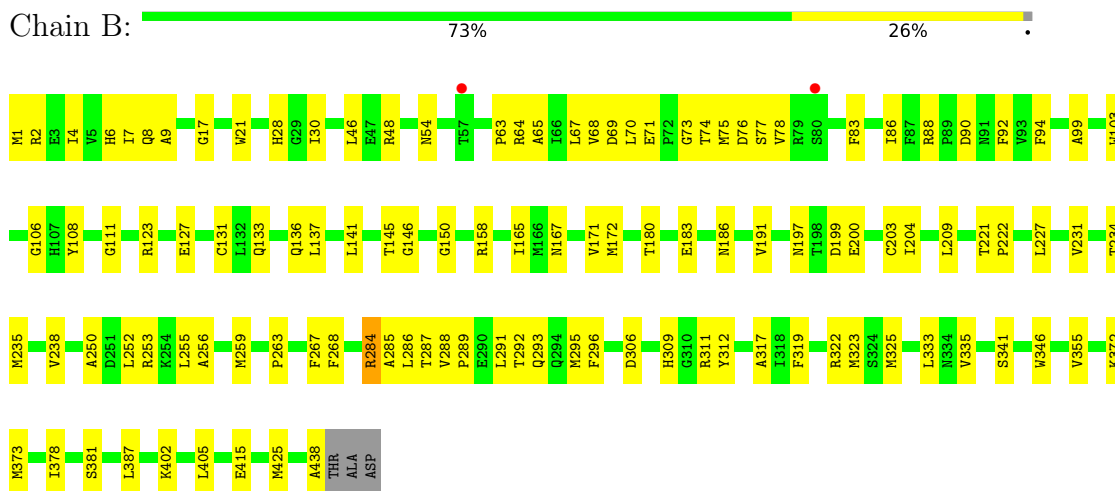
- Molecule 1: Tubulin alpha-1B chain



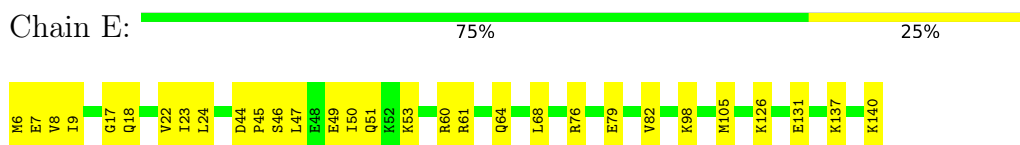
- Molecule 2: Tubulin beta-2B chain



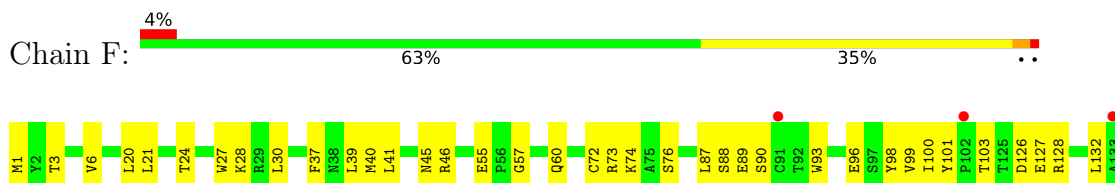
- Molecule 2: Tubulin beta-2B chain

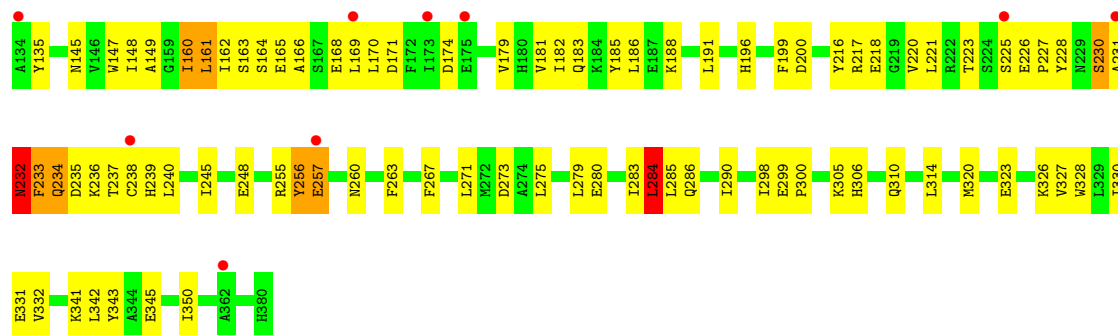


- Molecule 3: Stathmin-4



- Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.39Å 159.74Å 182.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.13 – 3.20 15.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.13-3.20) 98.8 (15.13-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.200 , 0.248 0.205 , 0.249	Depositor DCC
R_{free} test set	1999 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 142.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17637	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, VLB, 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	0.27	0/3571	0.58	0/4849
1	C	0.63	0/3565	0.96	3/4842 (0.1%)
2	B	0.29	0/3451	0.62	0/4675
2	D	0.31	0/3428	0.62	2/4645 (0.0%)
3	E	0.31	0/999	0.65	0/1325
4	F	0.42	3/2802 (0.1%)	0.71	4/3789 (0.1%)
All	All	0.40	3/17816 (0.0%)	0.71	9/24125 (0.0%)

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
1	A	0	1
1	C	0	5
2	B	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	310	GLN	C-O	6.99	1.32	1.23
4	F	284[A]	LEU	C-O	6.31	1.31	1.24
4	F	284[B]	LEU	C-O	6.31	1.31	1.24

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	284[A]	LEU	CA-C-O	7.23	129.02	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	284[B]	LEU	CA-C-O	7.23	129.02	120.92
1	C	348	PRO	N-CA-C	-6.88	101.09	111.41
1	C	363[A]	VAL	CA-C-O	6.56	125.81	119.71
1	C	363[B]	VAL	CA-C-O	6.56	125.81	119.71

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain
1	C	243	ARG	Sidechain
1	C	373	ARG	Sidechain
1	C	390	ARG	Sidechain
1	C	402	ARG	Sidechain

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	3465	0	3402	124	0
1	C	3466	0	3393	125	1
2	B	3370	0	3250	93	0
2	D	3343	0	3231	147	0
3	E	991	0	1012	28	1
4	F	2729	0	2715	97	0
5	A	32	0	12	0	0
5	C	32	0	12	1	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	C	59	58	58	16	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	A	2	0	0	0	0
10	B	10	0	0	0	0
10	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	5	0	0	1	0
10	E	1	0	0	0	0
10	F	8	0	0	1	0
All	All	17579	58	17109	607	1

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 18.

The worst 5 of 607 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:277:SER:HB3	1:A:280:LYS:HG3	1.35	1.07
2:B:2:ARG:HD3	2:B:133:GLN:HG2	1.41	1.02
2:D:141:LEU:HD11	2:D:170:SER:HB3	1.46	0.95
2:D:319:PHE:HB3	2:D:323:MET:HE1	1.48	0.95
4:F:233:PHE:HA	4:F:239:HIS:CE1	2.02	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ASP:OD2	3:E:98:LYS:NZ[4_455]	1.92	0.28

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	446/440 (101%)	426 (96%)	18 (4%)	2 (0%)	30 62
1	C	445/440 (101%)	415 (93%)	27 (6%)	3 (1%)	18 52
2	B	428/431 (99%)	415 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	424/431 (98%)	402 (95%)	20 (5%)	2 (0%)	24	59
3	E	116/120 (97%)	113 (97%)	3 (3%)	0	100	100
4	F	323/331 (98%)	295 (91%)	26 (8%)	2 (1%)	21	56
All	All	2182/2193 (100%)	2066 (95%)	107 (5%)	9 (0%)	30	62

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	THR
1	C	284	GLU
2	D	404	PHE
4	F	230	SER
1	A	284	GLU

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	378/371 (102%)	377 (100%)	1 (0%)	86	88
1	C	378/371 (102%)	358 (95%)	20 (5%)	20	53
2	B	369/372 (99%)	366 (99%)	3 (1%)	73	82
2	D	369/372 (99%)	367 (100%)	2 (0%)	81	85
3	E	108/108 (100%)	107 (99%)	1 (1%)	70	81
4	F	303/299 (101%)	292 (96%)	11 (4%)	31	63
All	All	1905/1893 (101%)	1867 (98%)	38 (2%)	50	72

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	233	PHE
2	B	71	GLU
4	F	234	GLN
4	F	257	GLU

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Mol	Chain	Res	Type
2	B	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	45	GLN
4	F	260	ASN
4	F	229	ASN
4	F	333	ASN
1	C	256	GLN

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 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	A	501	6	33,34,34	0.56	0	50,54,54	0.50	0
5	GTP	C	502	6	33,34,34	0.58	0	50,54,54	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	VLB	C	501	-	66,67,67	3.20	23 (34%)	82,108,108	2.77	35 (42%)
9	GDP	B	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.64	5 (11%)
9	GDP	D	501	-	29,30,30	1.19	5 (17%)	45,47,47	1.71	7 (15%)

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	501	6	-	6/22/38/38	0/3/3/3
5	GTP	C	502	6	-	7/22/38/38	0/3/3/3
8	VLB	C	501	-	-	15/40/131/131	0/7/9/9
9	GDP	B	501	-	-	2/16/32/32	0/3/3/3
9	GDP	D	501	-	-	3/16/32/32	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	VLB	C68-C73	15.80	1.74	1.53
8	C	501	VLB	C58-C59	-8.95	1.37	1.51
8	C	501	VLB	C57-N56	6.52	1.62	1.47
8	C	501	VLB	O75-C76	-5.81	1.32	1.45
8	C	501	VLB	O32-C33	-5.55	1.27	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	VLB	O32-C16-C15	7.39	123.91	116.59
8	C	501	VLB	O25-C23-C3	7.23	124.10	112.21
8	C	501	VLB	O72-C54-C70	-5.70	99.11	108.74
8	C	501	VLB	C3-C2-N1	-5.58	105.13	112.81
8	C	501	VLB	C57-C58-C59	5.57	122.65	113.65

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A

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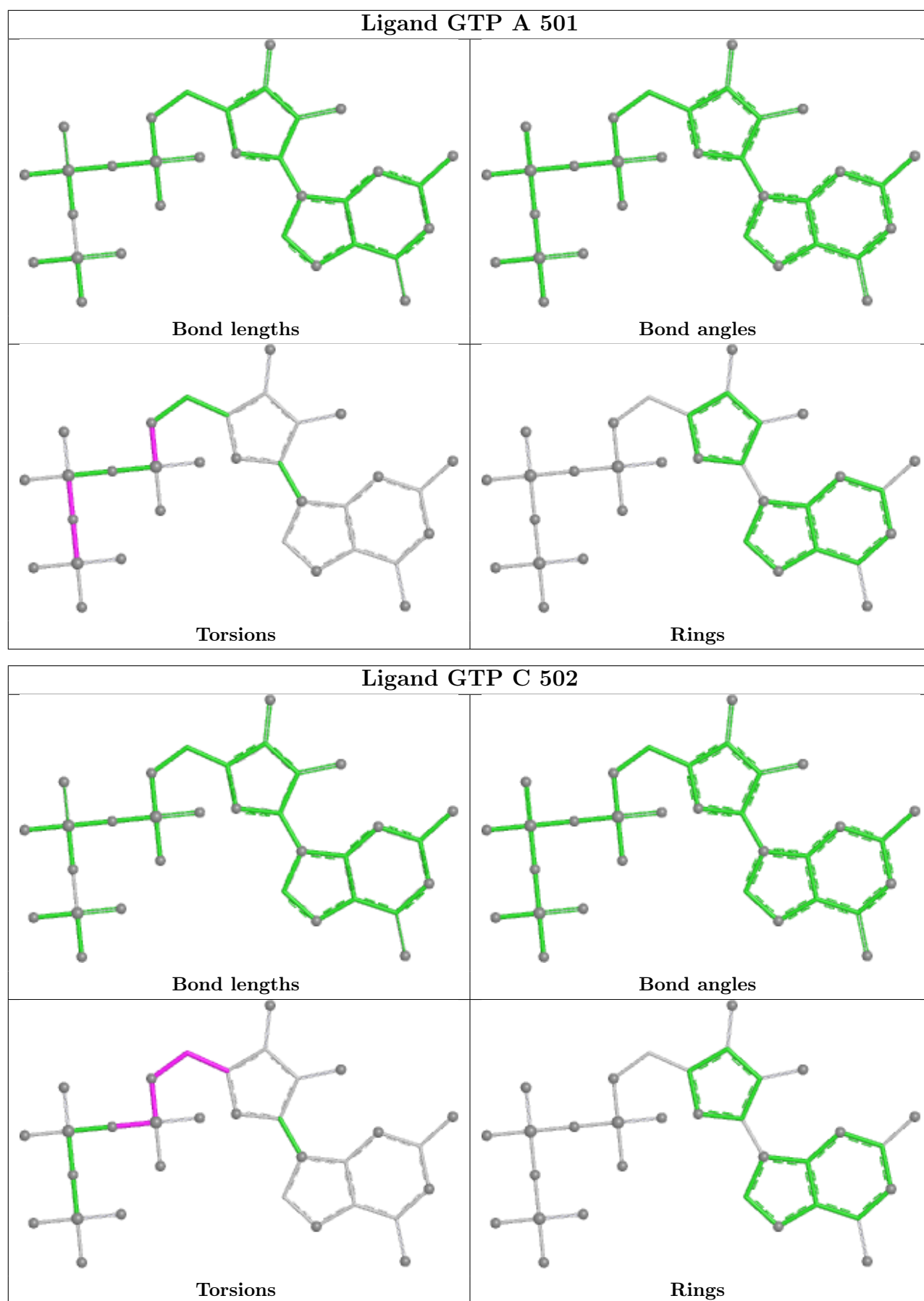
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O1A

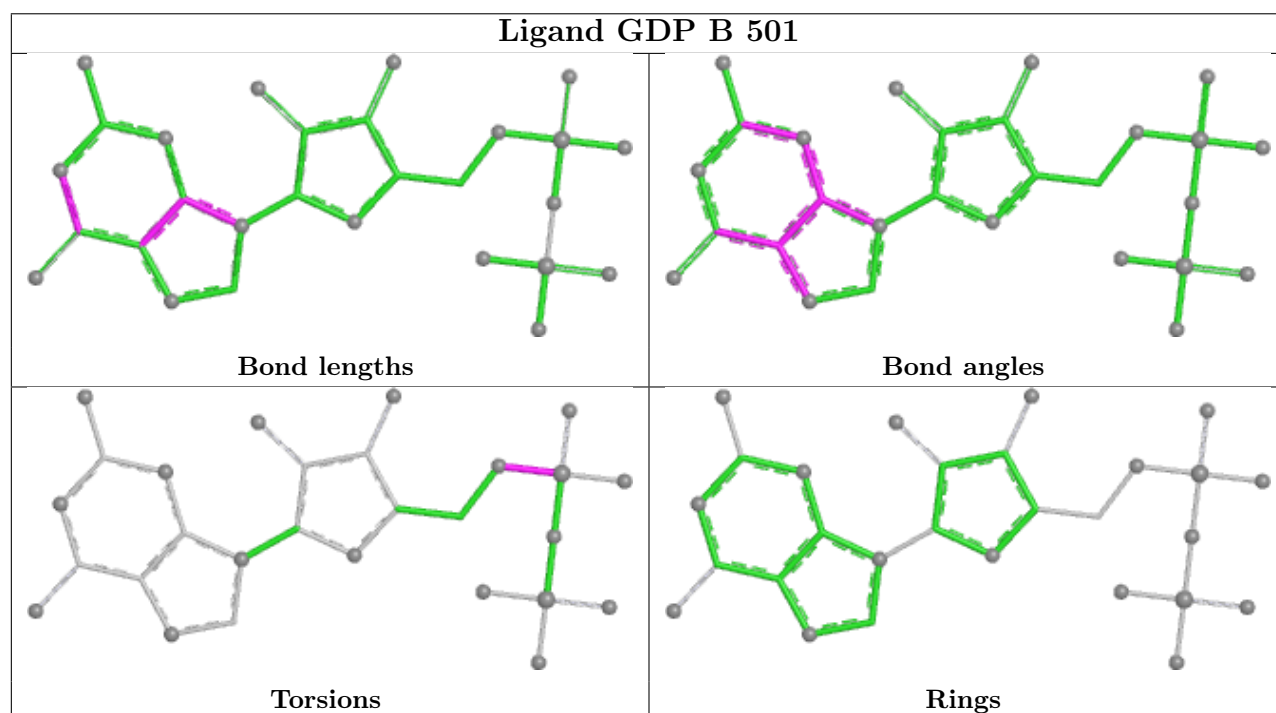
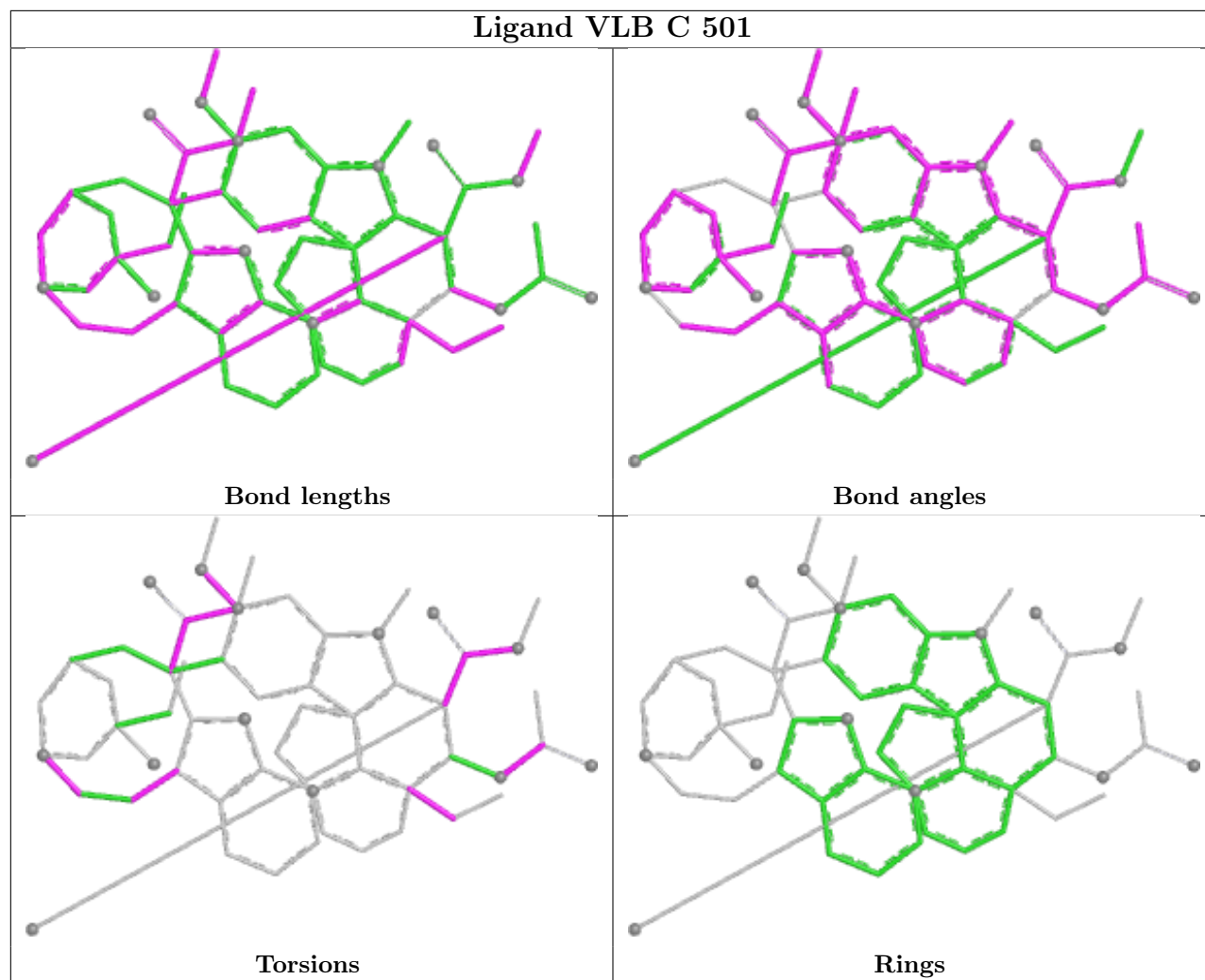
There are no ring outliers.

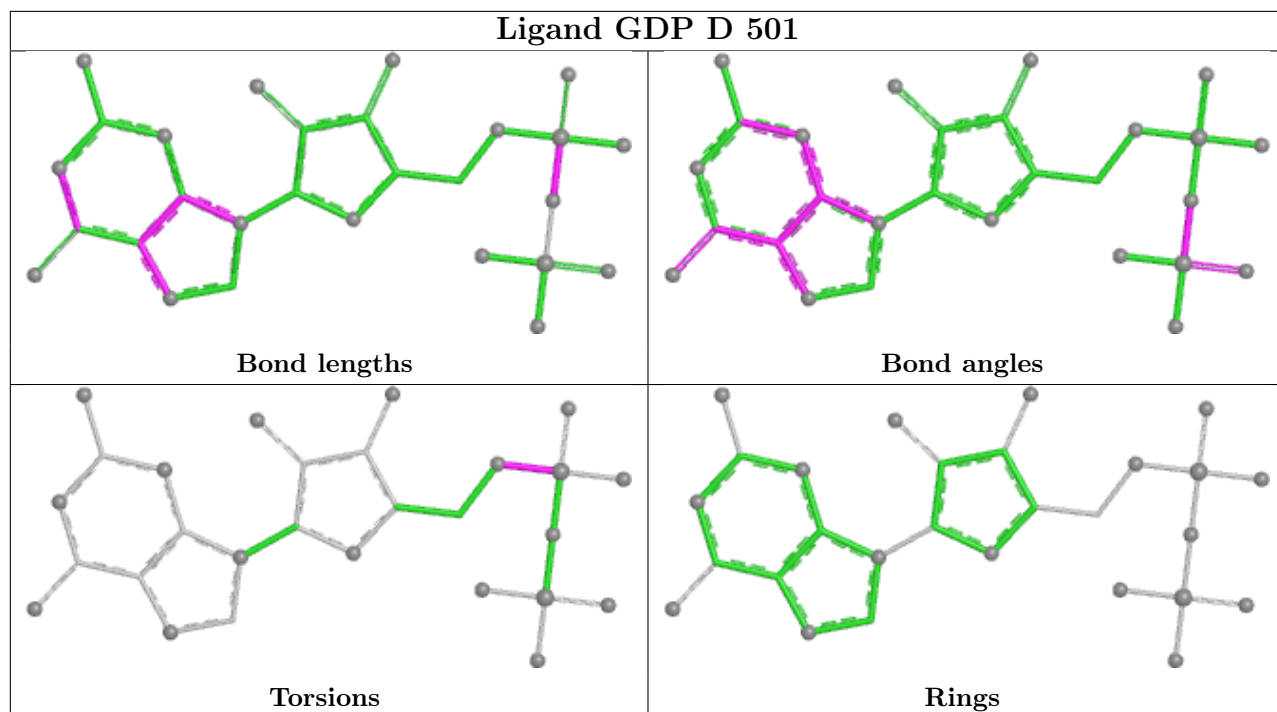
4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	GTP	1	0
8	C	501	VLB	16	0
9	B	501	GDP	1	0
9	D	501	GDP	3	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	5
3	E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.56
1	F	362:ALA	C	372:THR	N	20.09
1	F	103:THR	C	125:THR	N	13.23
1	F	250:SER	C	255:ARG	N	9.11
1	F	149:ALA	C	159:GLY	N	8.13

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	439/440 (99%)	-0.23	0 100 100	30, 65, 112, 259	9 (2%)
1	C	440/440 (100%)	-0.17	5 (1%) 78 61	24, 50, 88, 226	7 (1%)
2	B	428/431 (99%)	-0.36	2 (0%) 87 76	17, 54, 97, 150	6 (1%)
2	D	424/431 (98%)	-0.07	3 (0%) 84 69	31, 82, 130, 180	5 (1%)
3	E	120/120 (100%)	0.09	0 100 100	47, 82, 130, 153	0
4	F	331/331 (100%)	0.19	12 (3%) 46 28	40, 97, 172, 212	4 (1%)
All	All	2182/2193 (99%)	-0.13	22 (1%) 79 63	17, 68, 134, 259	31 (1%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	THR	4.0
4	F	238	CYS	3.7
4	F	175	GLU	3.1
4	F	231	ALA	3.1
4	F	257	GLU	3.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

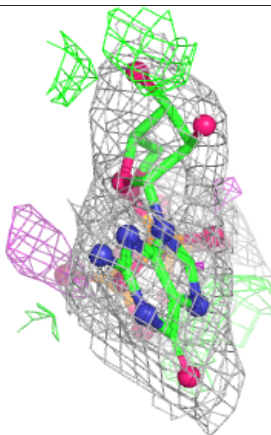
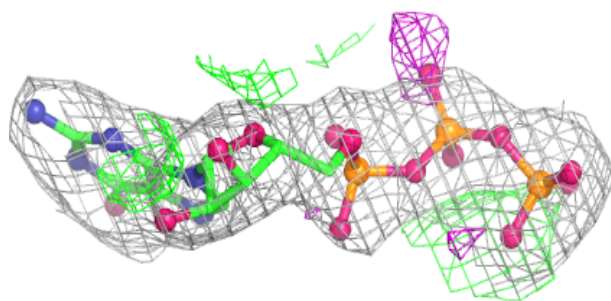
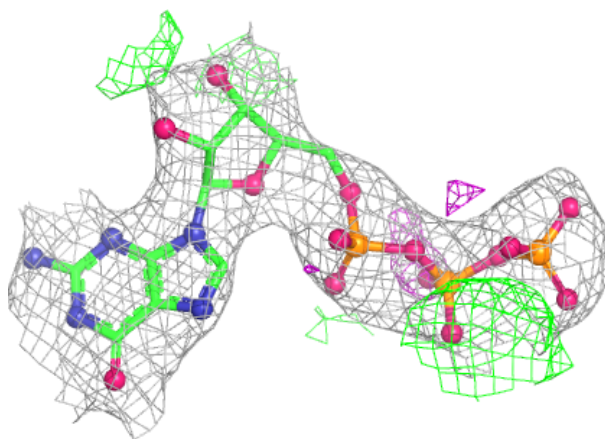
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GDP	D	501	28/28	0.84	0.12	74,78,89,101	0
6	MG	C	503	1/1	0.89	0.35	41,41,41,41	0
6	MG	A	502	1/1	0.92	0.27	45,45,45,45	0
5	GTP	C	502	32/32	0.94	0.09	41,45,48,48	0
8	VLB	C	501	59/59	0.94	0.09	38,47,55,59	0
5	GTP	A	501	32/32	0.94	0.09	49,51,55,55	0
7	CA	A	503	1/1	0.96	0.05	91,91,91,91	0
9	GDP	B	501	28/28	0.96	0.07	36,41,43,44	0
7	CA	C	504	1/1	0.98	0.15	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



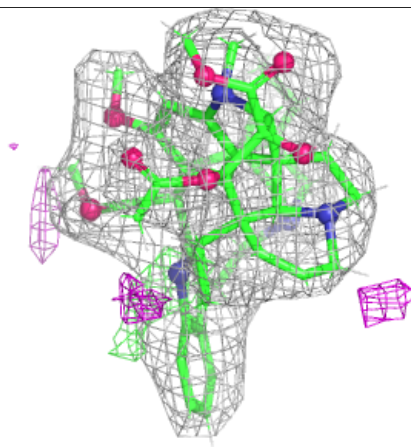
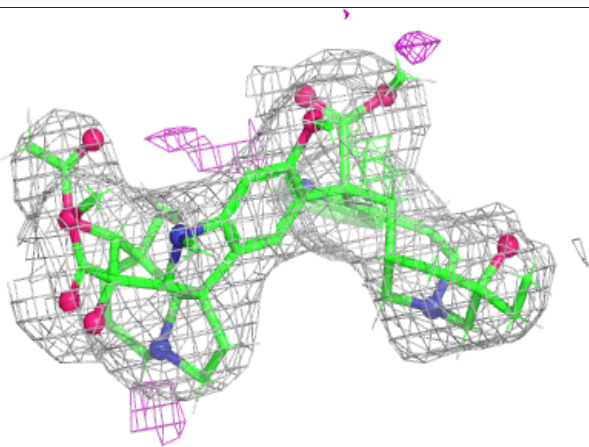
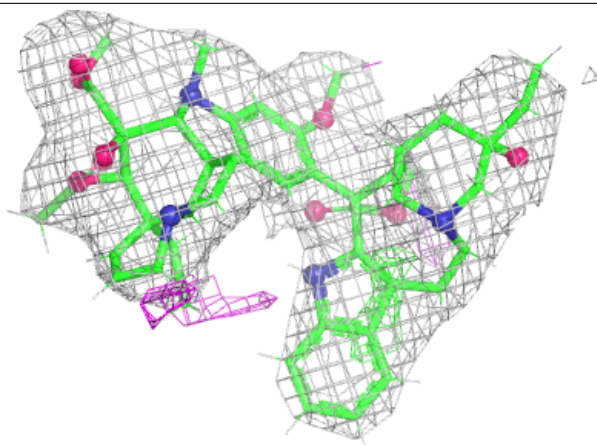
Electron density around GTP C 502:

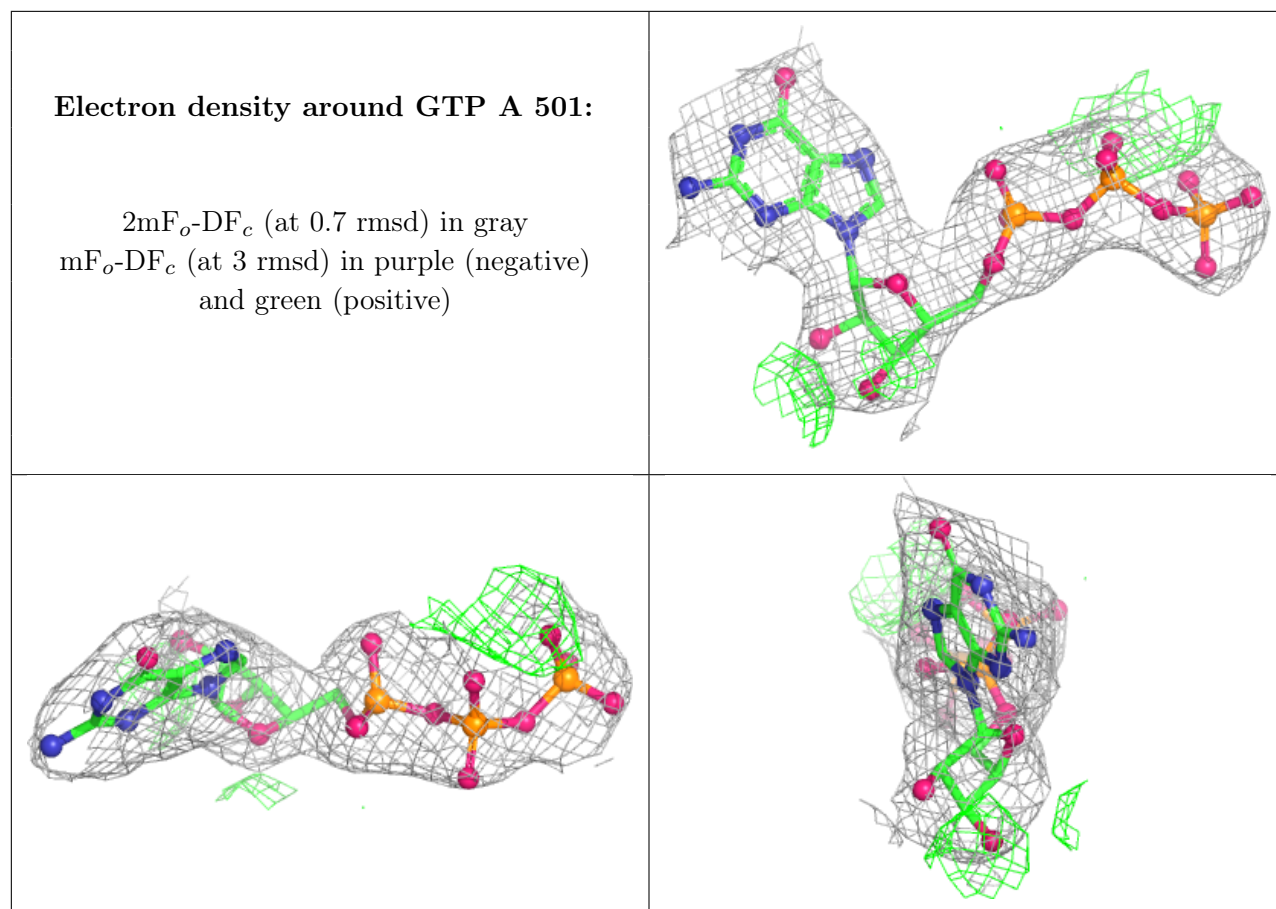
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

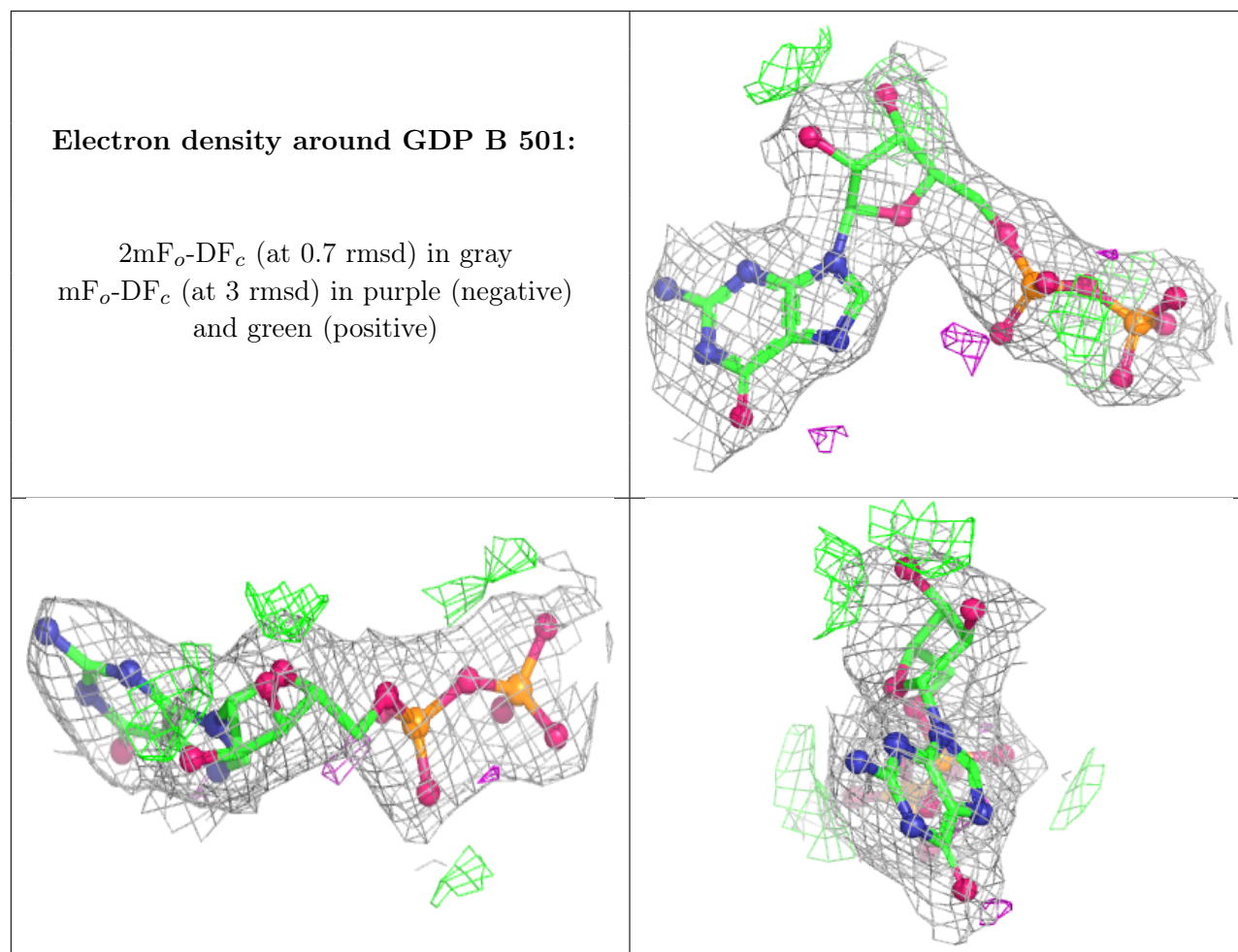


Electron density around VLB C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers [i](#)

There are no such residues in this entry.