WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2023 – 03:28 pm GMT

PDB ID	:	8BDE
Title	:	Tubulin-baccatin III complex
Authors	:	Prota, A.E.; Lucena-Agell, D.; Ma, Y.; Estevez-Gallego, J.; Li, S.; Bargsten, K.; Altmann, K.H.; Gaillard, N.; Kamimura, S.; Muehlethaler, T.; Gago, F.; Oliva, M.A.; Steinmetz, M.O.; Fang, W.S.; Diaz, J.F.
Deposited on	:	2022-10-19
Resolution	:	1.90 Å(reported)

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

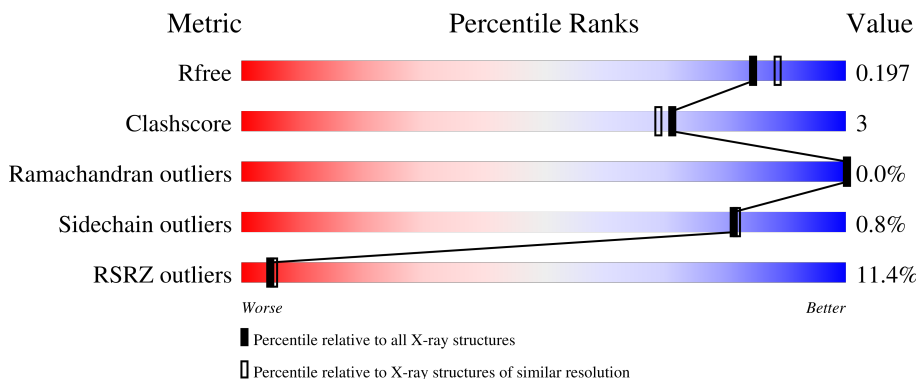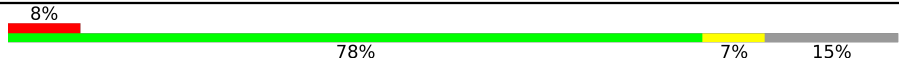|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 1.90 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	Percentile Ranks	Value
Rfree		0.197
Clashscore		3
Ramachandran outliers		0.0%
Sidechain outliers		0.8%
RSRZ outliers		11.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	451	4% / 88% / 8% ·
1	C	451	2% / 91% / 6% ·
2	B	445	8% / 86% / 9% ·
2	D	445	11% / 83% / 12% / 5%

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Mol	Chain	Length	Quality of chain
3	E	143	8% / 78% / 7% / 15%
4	F	384	32% / 77% / 10% / 13%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18429 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	434	Total 3412	C 2165	N 576	O 647	S 24	0	6	0
1	C	440	Total 3484	C 2208	N 586	O 665	S 25	0	10	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total 3385	C 2125	N 582	O 651	S 27	0	5	0
2	D	424	Total 3340	C 2098	N 568	O 646	S 28	0	2	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total 1000	C 617	N 181	O 197	S 5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total 2737	C 1760	N 466	O 497	S 14	0	0	0

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	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total 1	Mg 1	0	0

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

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
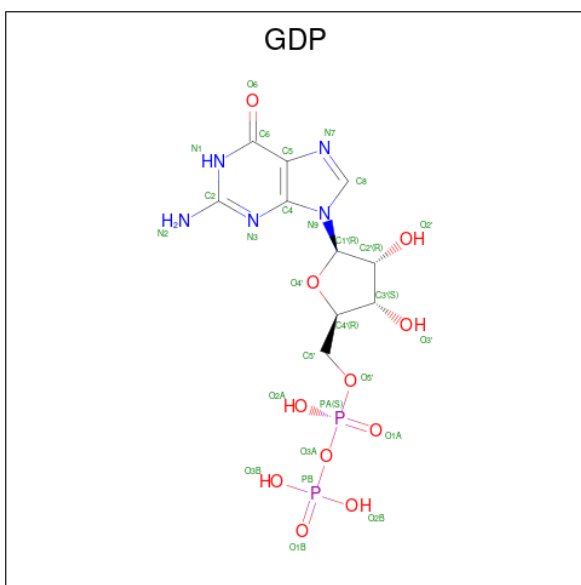
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

MES

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

- Molecule 10 is [(1 {S},2 {S},3 {R},4 {S},7 {R},9 {S},10 {S},12 {R},15 {S})-4,12-diacetyloxy-10,14,16,16-tetramethyl-1,9,15-tris(oxidanyl)-11-oxidanylidene-6-oxatetracyclo[11.3.1.0^{3,10}.0^{4,7}]heptadec-13-en-2-yl] benzoate (three-letter code: R3Q) (formula: $C_{31}H_{38}O_{11}$) (labeled as "Ligand of Interest" by depositor).

R3Q
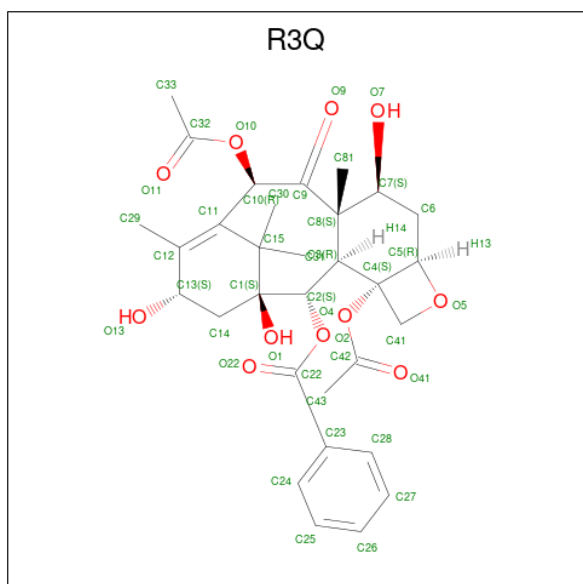
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	D	1	42	31	11	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).
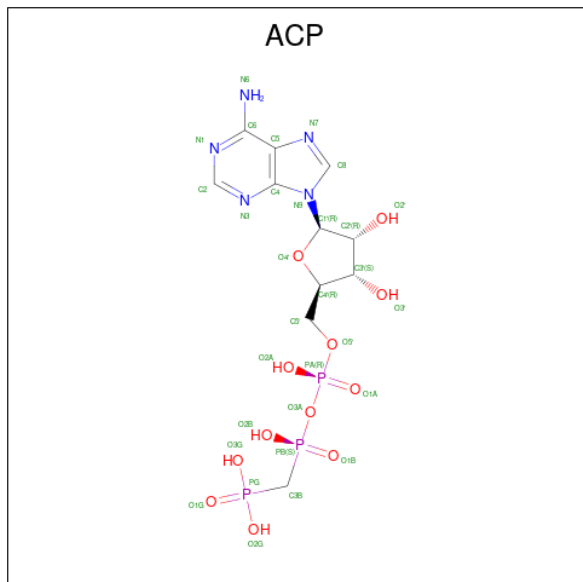
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	181	Total 181	O 181	0	0
12	B	153	Total 153	O 153	0	0
12	C	300	Total 300	O 300	0	0
12	D	121	Total 121	O 121	0	0
12	E	47	Total 47	O 47	0	0
12	F	57	Total 57	O 57	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
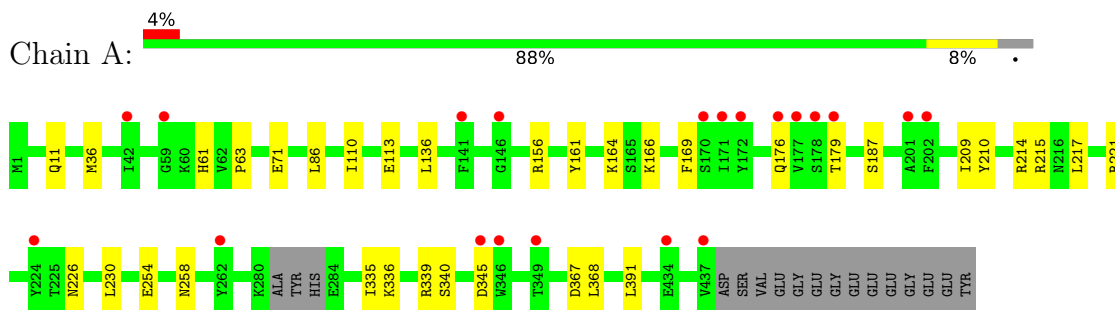
- Molecule 1: Tubulin alpha-1B chain
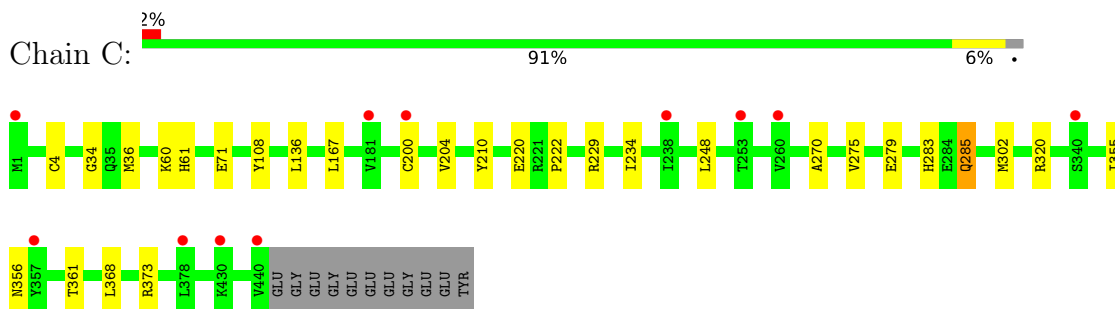
- Molecule 2: Tubulin beta-2B chain
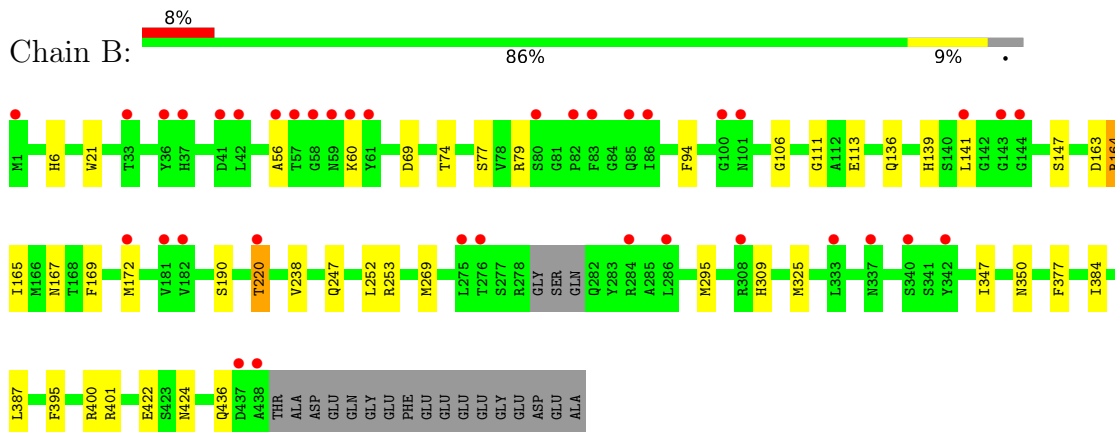
- Molecule 2: Tubulin beta-2B chain
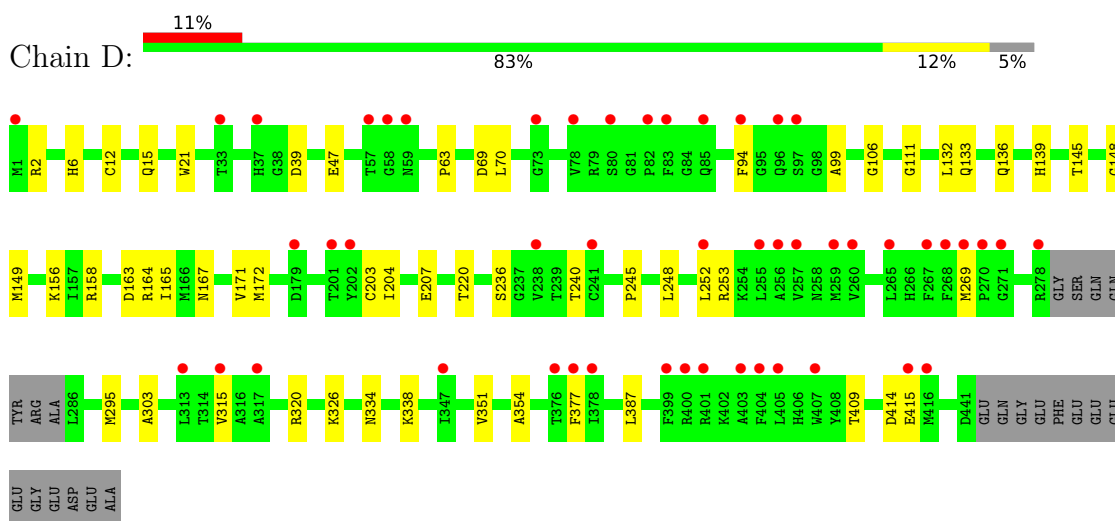
Chain D:

• Molecule 3: Stathmin-4
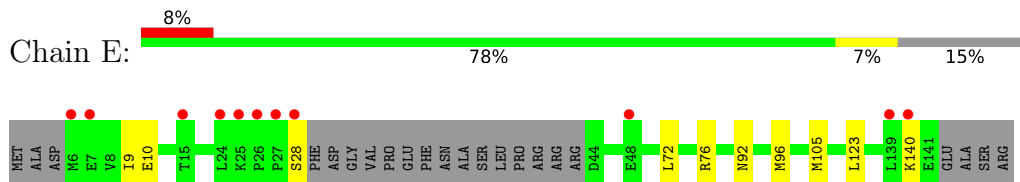
Chain E:

• Molecule 4: Tubulin beta-2B chain

Chain F:
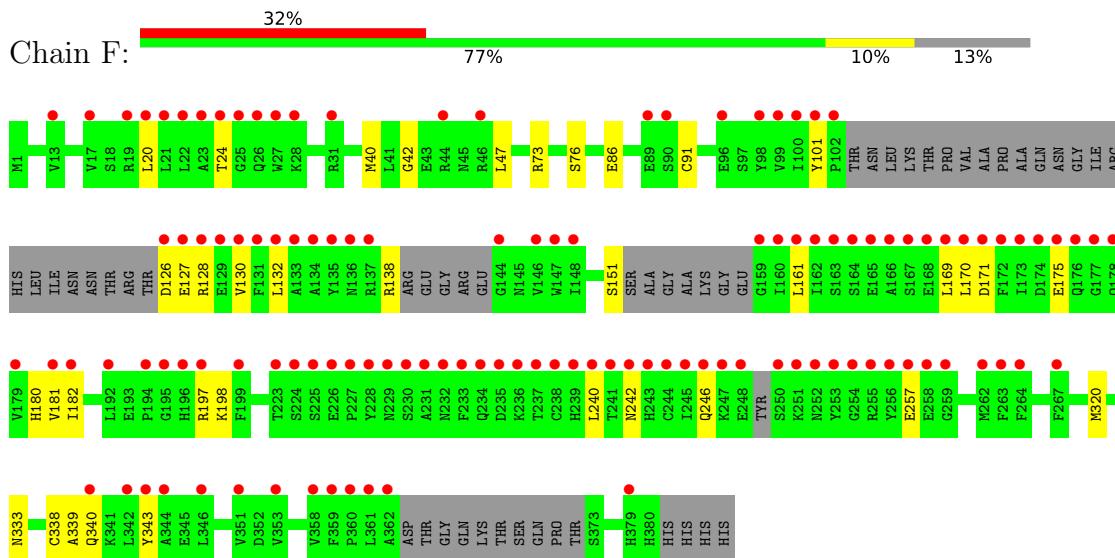
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.10Å 157.15Å 179.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 1.90 49.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.20-1.90) 100.0 (49.20-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.192 , 0.218 0.194 , 0.197	Depositor DCC
R_{free} test set	11325 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18429	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: MES, GTP, ACP, CA, R3Q, GDP, MG

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	0/3505	0.45	0/4757
1	C	0.29	0/3586	0.47	0/4871
2	B	0.38	0/3465	0.50	0/4690
2	D	0.26	0/3419	0.44	0/4631
3	E	0.26	0/1008	0.37	0/1337
4	F	0.25	0/2798	0.42	0/3777
All	All	0.29	0/17781	0.45	0/24063

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
2	B	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	163	ASP	Mainchain
2	B	164[A]	ARG	Mainchain
2	B	164[B]	ARG	Mainchain
2	B	253[A]	ARG	Mainchain
2	B	253[B]	ARG	Mainchain

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	3412	0	3354	22	0
1	C	3484	0	3413	18	1
2	B	3385	0	3273	24	1
2	D	3340	0	3226	36	0
3	E	1000	0	1018	9	0
4	F	2737	0	2709	20	0
5	A	32	0	12	0	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
6	D	1	0	0	0	0
6	F	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	1	0
9	B	12	0	13	0	0
10	D	42	0	0	0	0
11	F	31	0	14	2	0
12	A	181	0	0	5	0
12	B	153	0	0	3	0
12	C	300	0	0	3	0
12	D	121	0	0	7	0
12	E	47	0	0	0	0
12	F	57	0	0	0	0
All	All	18429	0	17068	120	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 3.

The worst 5 of 120 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:B:79:ARG:NH1	12:B:601:HOH:O	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ARG:NH1	12:D:601:HOH:O	2.11	0.84
2:D:149:MET:N	12:D:602:HOH:O	2.12	0.79
2:B:220:THR:O	12:B:602:HOH:O	2.07	0.71
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.72	0.71

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)
2:B:113:GLU:OE2	1:C:283:HIS:NE2[4_555]	2.13	0.07

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	436/451 (97%)	431 (99%)	5 (1%)	0	100	100
1	C	448/451 (99%)	438 (98%)	10 (2%)	0	100	100
2	B	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
2	D	422/445 (95%)	417 (99%)	5 (1%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	322/384 (84%)	308 (96%)	13 (4%)	1 (0%)	41	31
All	All	2171/2319 (94%)	2132 (98%)	38 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	91	CYS

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	372/379 (98%)	369 (99%)	3 (1%)	81	82
1	C	381/379 (100%)	377 (99%)	4 (1%)	76	76
2	B	373/383 (97%)	371 (100%)	2 (0%)	88	89
2	D	369/383 (96%)	365 (99%)	4 (1%)	73	73
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	301/342 (88%)	298 (99%)	3 (1%)	76	76
All	All	1905/1993 (96%)	1889 (99%)	16 (1%)	81	82

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	181	VAL
4	F	138	ARG
1	C	361[B]	THR
2	D	220	THR
1	C	361[A]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	C	107	HIS
1	C	285	GLN
2	D	334	ASN
3	E	124	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 7 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	$\#|Z| > 2$
9	MES	B	503	-	12,12,12	0.72	0	14,16,16	0.46	0
8	GDP	B	501	6	24,30,30	0.86	0	30,47,47	1.15	4 (13%)
5	GTP	A	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.33	5 (15%)
11	ACP	F	402	6	27,33,33	1.42	5 (18%)	32,52,52	1.29	4 (12%)
8	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.17	4 (13%)
10	R3Q	D	503	-	46,46,46	0.87	1 (2%)	74,75,75	1.24	8 (10%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.34	5 (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
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
11	ACP	F	402	6	-	6/15/38/38	0/3/3/3
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	R3Q	D	503	-	-	6/17/103/103	0/5/5/5
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C5-C6	-4.05	1.39	1.47
5	A	501	GTP	C5-C6	-4.04	1.39	1.47
11	F	402	ACP	PB-O3A	3.28	1.62	1.58
11	F	402	ACP	PG-O2G	2.87	1.61	1.54
11	F	402	ACP	PG-O3G	2.81	1.61	1.54

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	R3Q	C15-C1-C2	3.30	115.53	111.91
5	C	501	GTP	C5-C6-N1	3.21	119.62	113.95
11	F	402	ACP	C3'-C2'-C1'	3.21	105.81	100.98
11	F	402	ACP	N3-C2-N1	-3.08	123.86	128.68
10	D	503	R3Q	C3-C8-C9	2.97	121.42	116.31

There are no chirality outliers.

5 of 35 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	402	ACP	2	0
8	D	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP F 402

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand R3Q D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 501

Bond lengths

Bond angles

Torsions

Rings
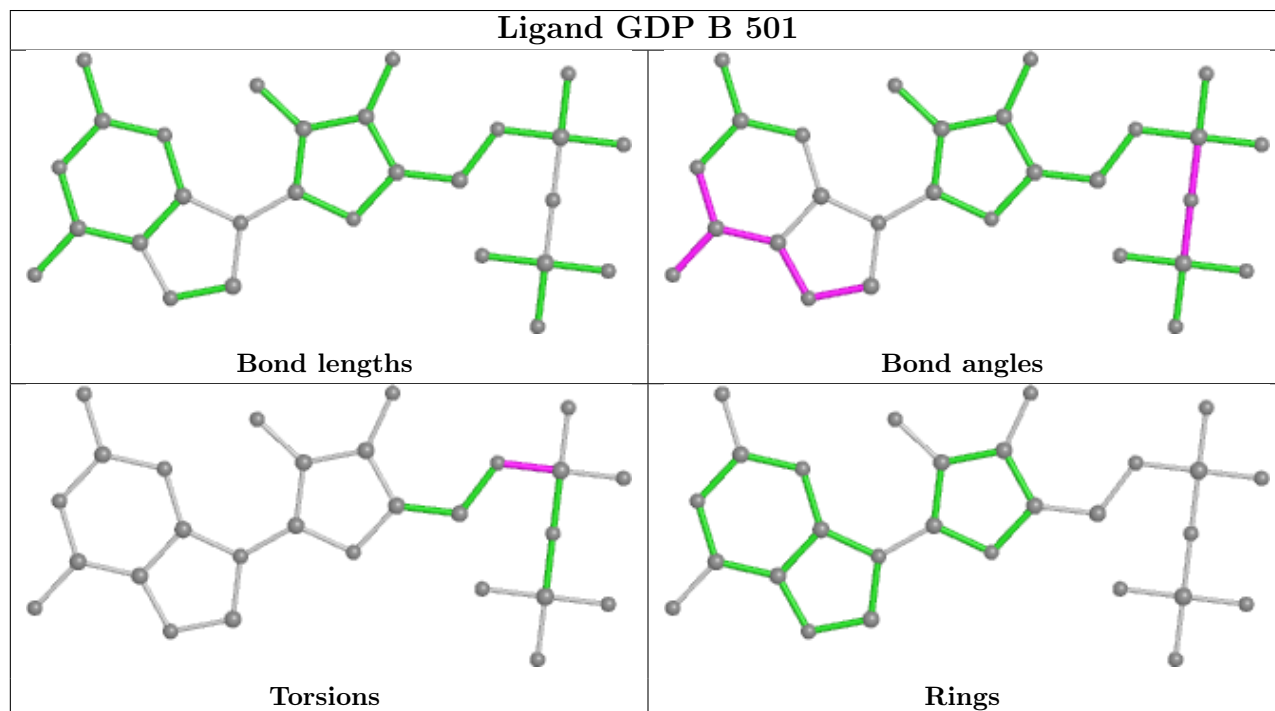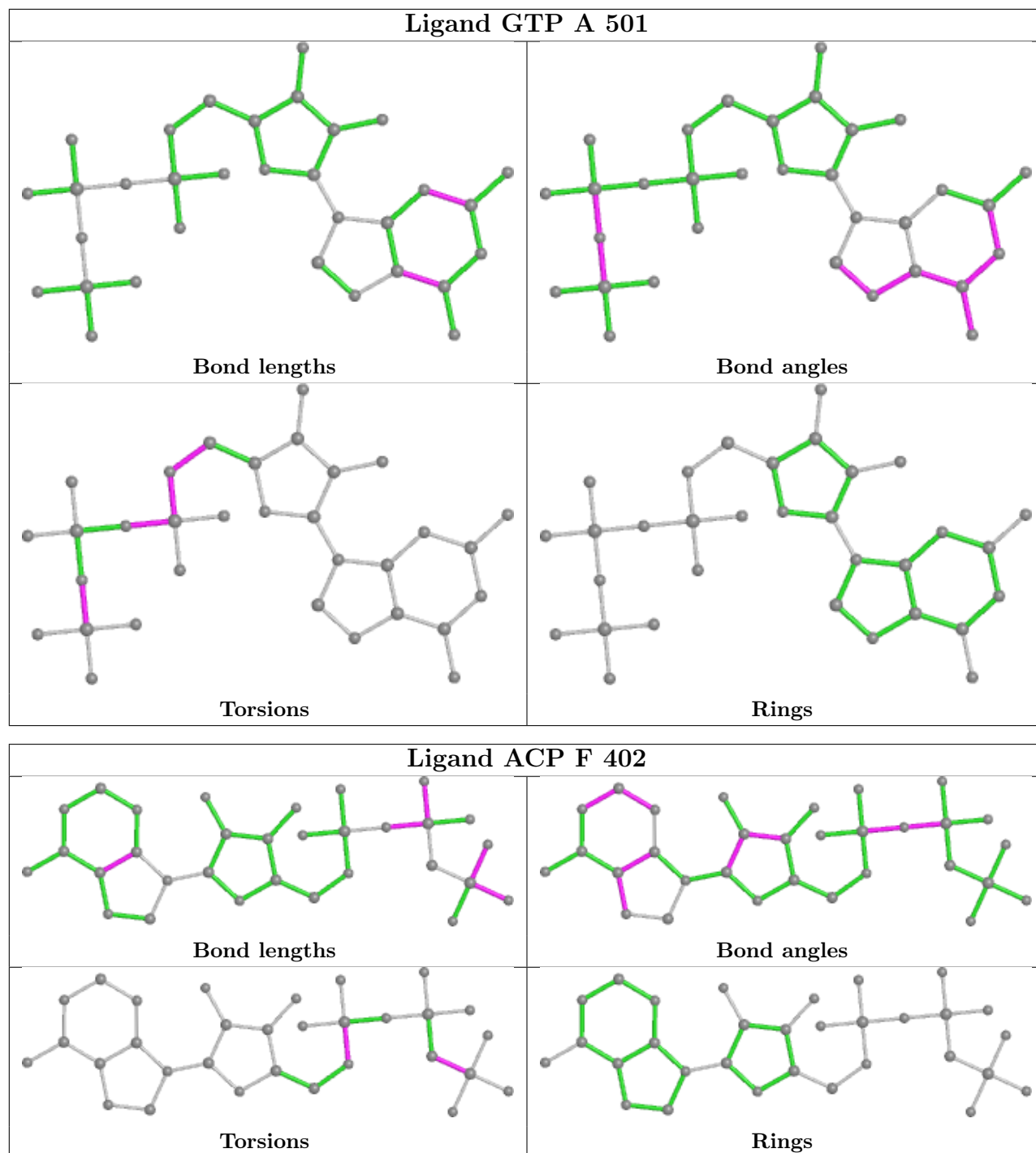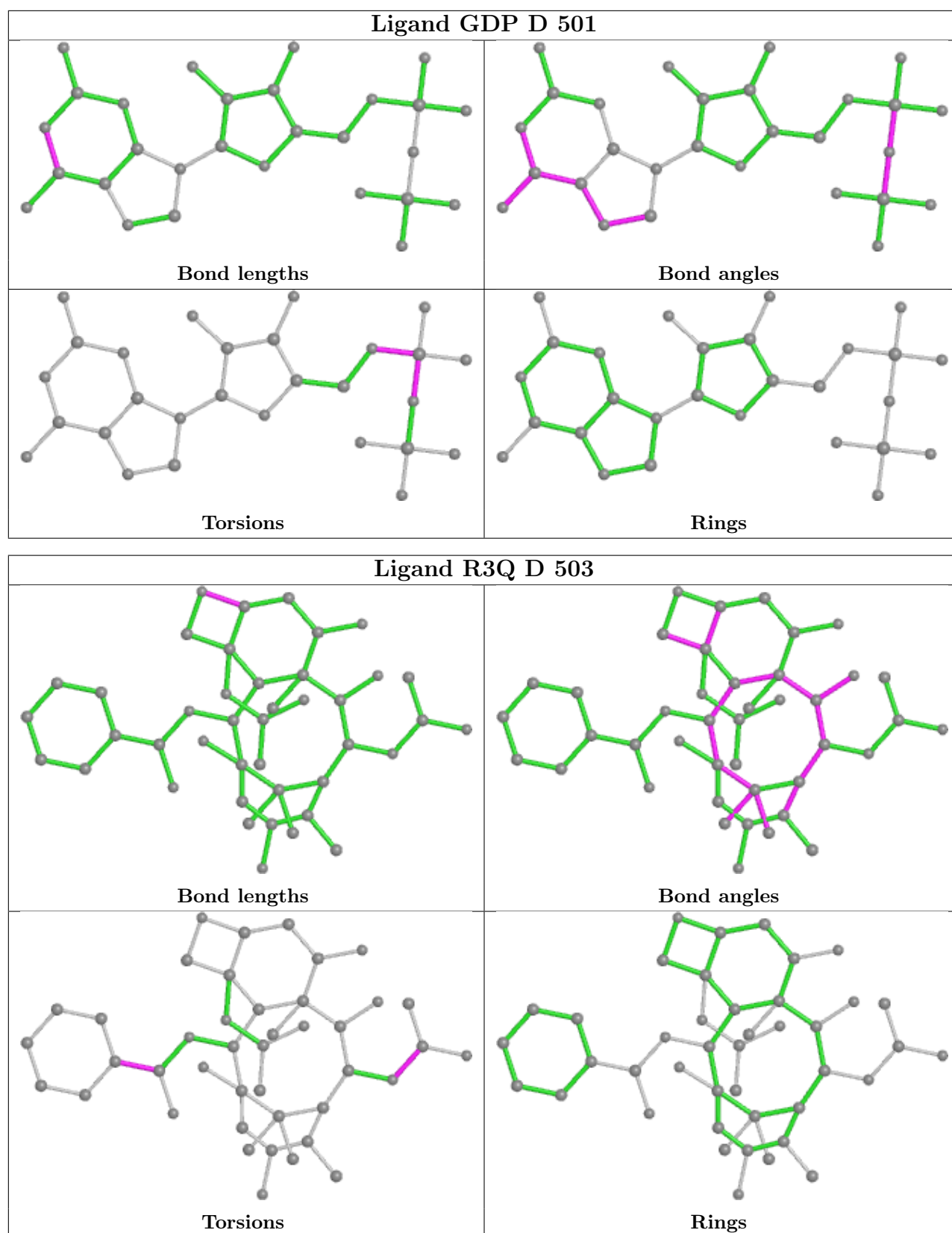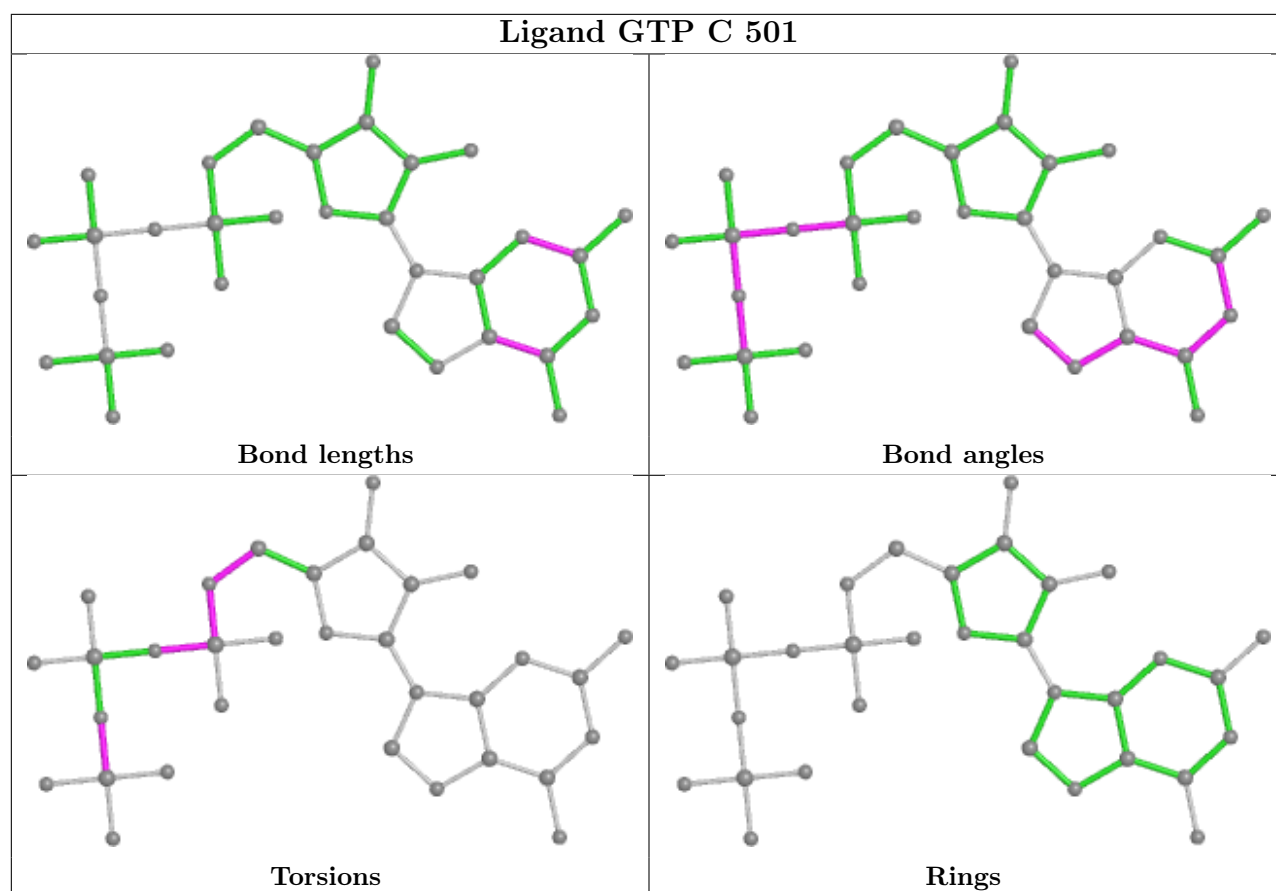
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	434/451 (96%)	0.40	20 (4%)	32	35	32, 51, 83, 107	0
1	C	440/451 (97%)	0.18	11 (2%)	57	60	28, 41, 68, 106	0
2	B	425/445 (95%)	0.52	37 (8%)	10	11	31, 50, 87, 135	0
2	D	424/445 (95%)	0.58	49 (11%)	4	5	34, 56, 89, 124	0
3	E	121/143 (84%)	0.41	11 (9%)	9	10	38, 62, 101, 123	0
4	F	334/384 (86%)	1.75	121 (36%)	0	0	44, 75, 150, 186	0
All	All	2178/2319 (93%)	0.62	249 (11%)	5	5	28, 52, 103, 186	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	11.8
4	F	231	ALA	10.4
4	F	130	VAL	10.1
4	F	244	CYS	9.5
4	F	177	GLY	9.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
10	R3Q	D	503	42/42	0.76	0.33	94,109,117,119	0
6	MG	F	401	1/1	0.88	0.17	82,82,82,82	0
6	MG	D	502	1/1	0.88	0.12	82,82,82,82	0
11	ACP	F	402	31/31	0.88	0.17	80,96,134,135	0
7	CA	A	503	1/1	0.93	0.05	63,63,63,63	0
9	MES	B	503	12/12	0.93	0.12	47,60,69,71	0
6	MG	A	502	1/1	0.94	0.13	35,35,35,35	0
8	GDP	D	501	28/28	0.97	0.09	45,52,59,64	0
6	MG	C	502	1/1	0.98	0.10	32,32,32,32	0
5	GTP	A	501	32/32	0.98	0.17	29,36,39,40	0
7	CA	C	503	1/1	0.98	0.06	51,51,51,51	0
8	GDP	B	501	28/28	0.98	0.17	29,36,40,41	0
5	GTP	C	501	32/32	0.99	0.14	26,31,34,37	0
6	MG	B	502	1/1	0.99	0.25	29,29,29,29	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 R3Q D 503:

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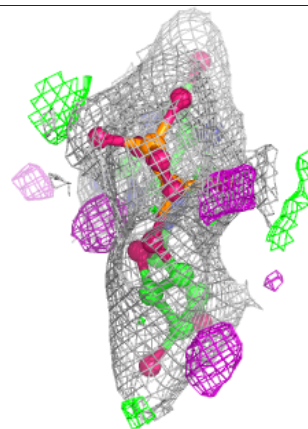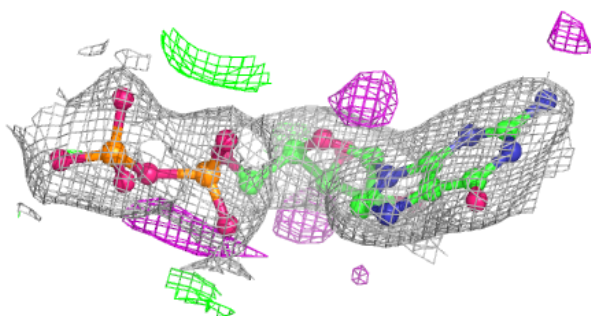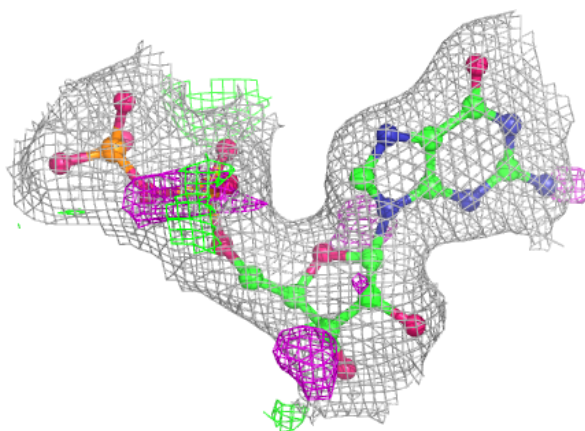and green (positive)
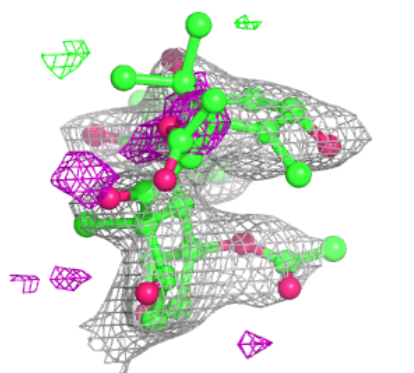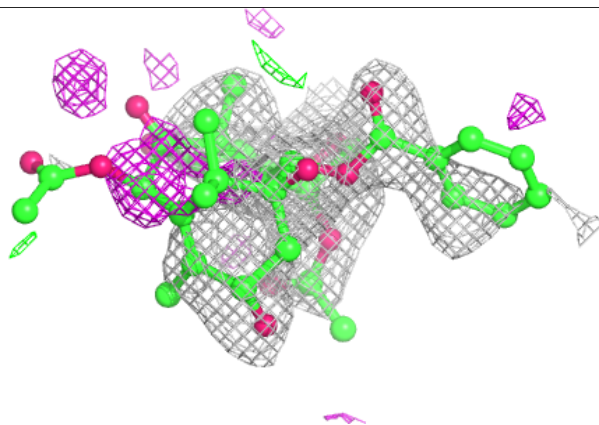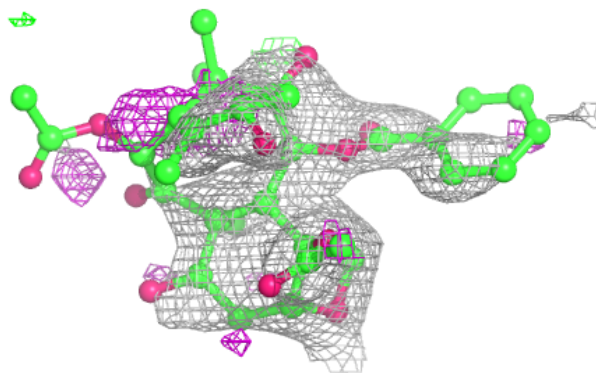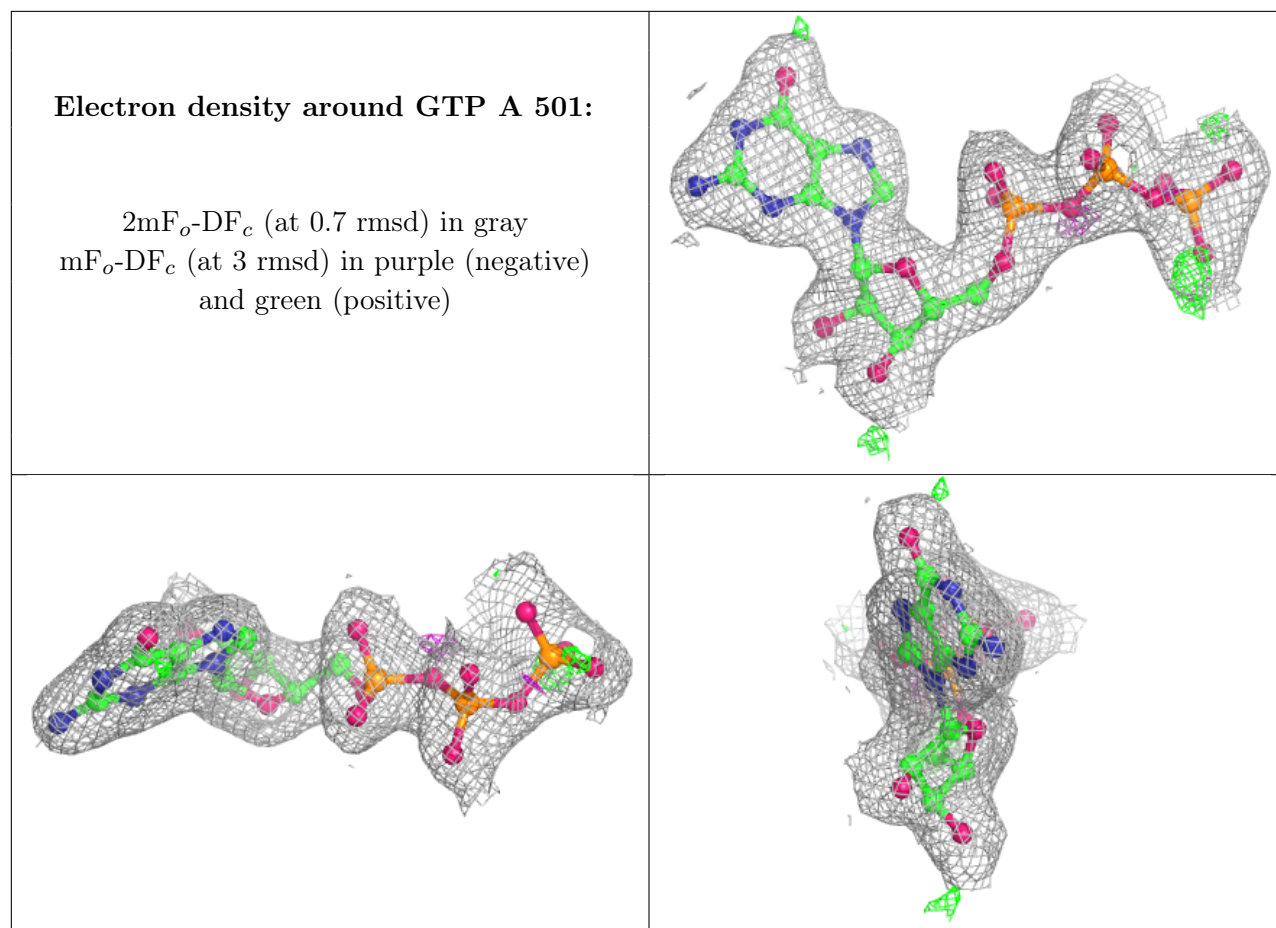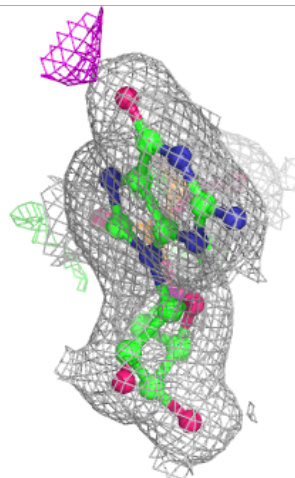

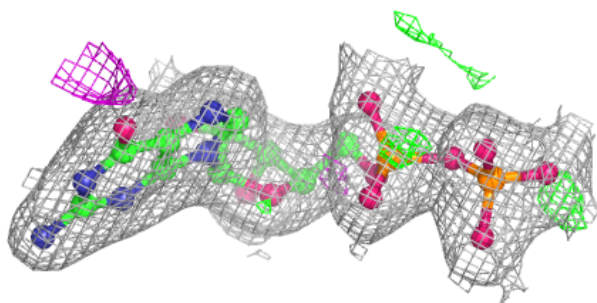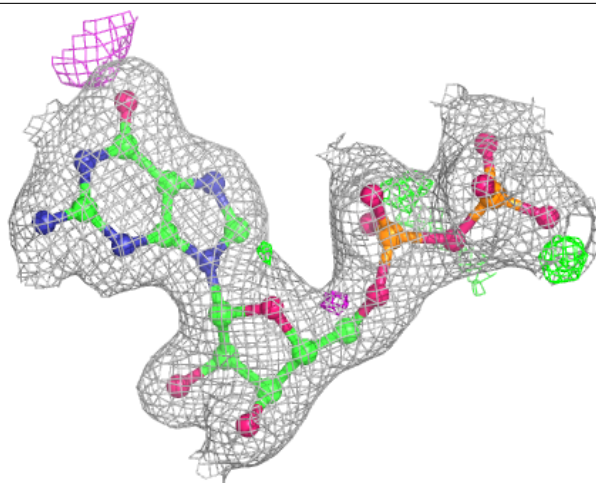**Electron density around ACP F 402:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
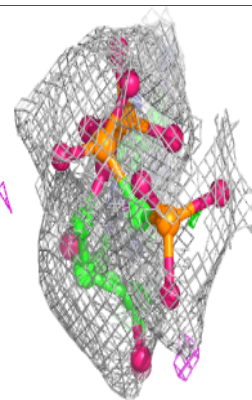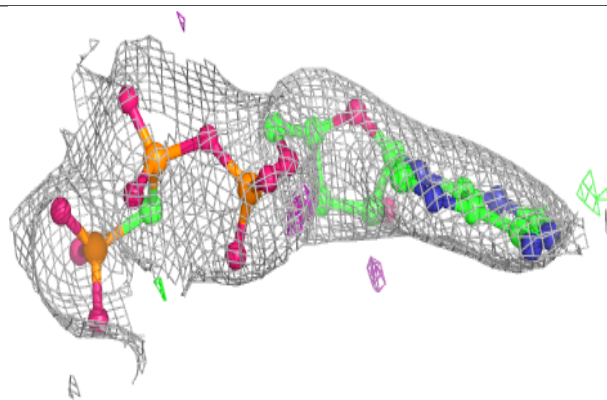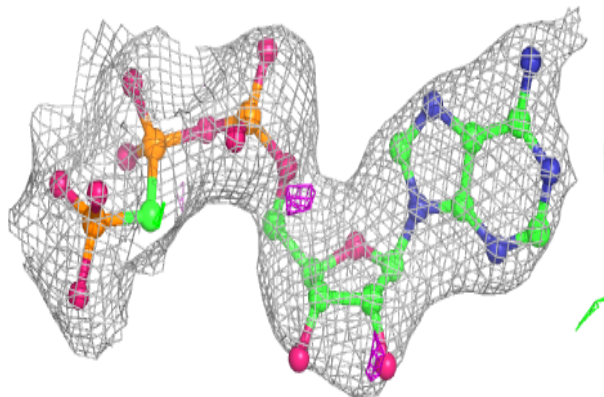
Electron density around GDP D 501:

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

Electron density around GTP A 501:

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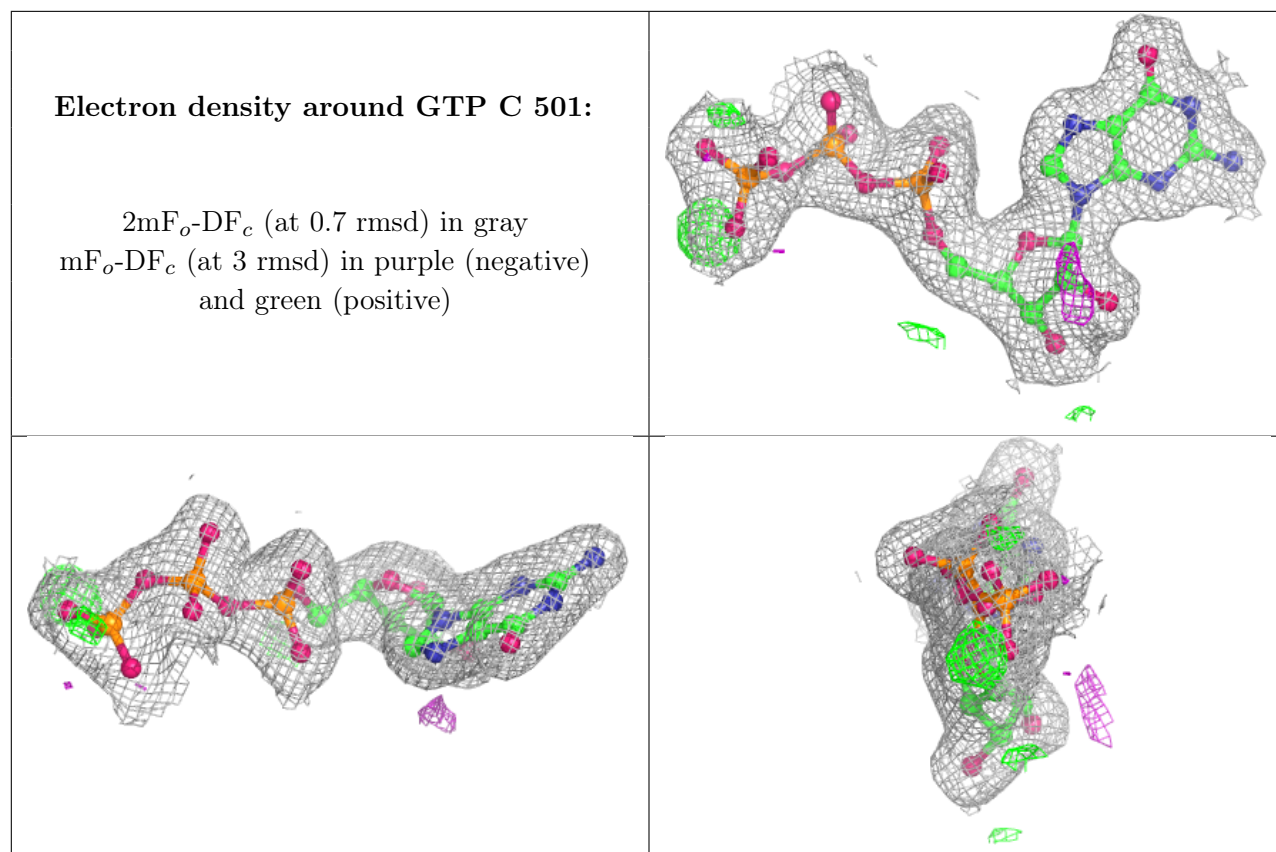$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GDP B 501:

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

Electron density around GTP C 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.