



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:17 PM UTC

PDB ID : 8CLG / pdb_00008clg
Title : Epothilone A and Colchicine 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 : 2.80 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)
Xtriage (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

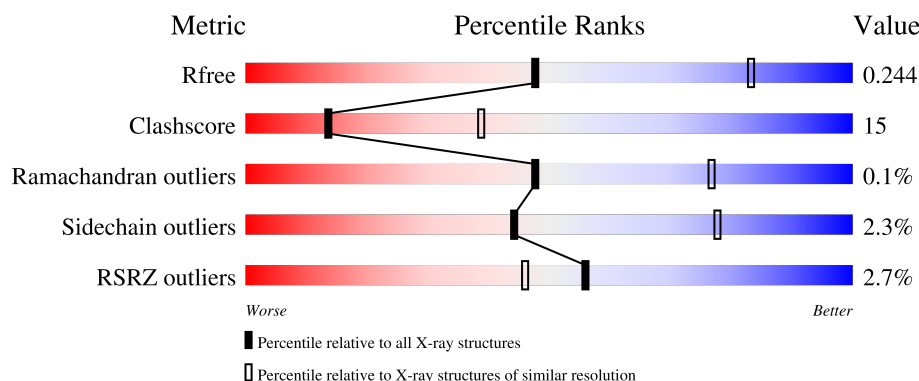
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	82% 18%
1	C	440	84% 16%
2	B	431	3% 70% 28% ..
2	D	431	2% 74% 25% .
3	E	123	3% 82% 16% .

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Mol	Chain	Length	Quality of chain
4	F	351	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EP	B	503	X	-	-	-
8	EP	D	501	X	-	-	-
9	LOC	B	504	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18186 atoms, of which 103 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	439	Total	C	N	O	S	0	12	0
			3480	2211	584	661	24			
1	C	440	Total	C	N	O	S	0	18	0
			3519	2231	588	674	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	7	15	0
			3441	2167	581	664	29			
2	D	431	Total	C	N	O	S	0	6	0
			3411	2143	580	660	28			

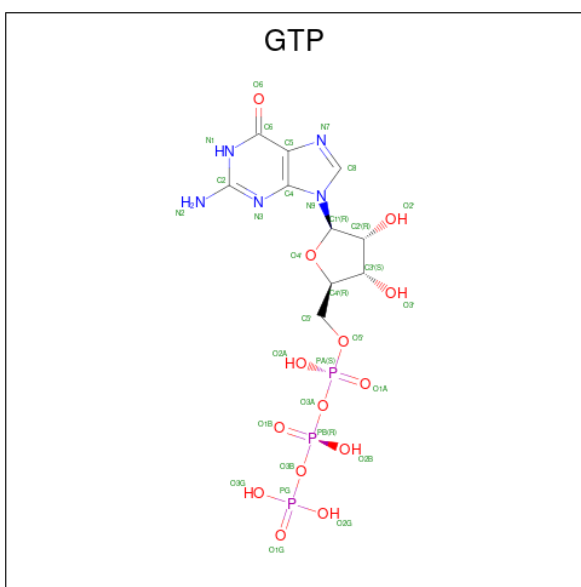
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	5	0
			1042	644	188	204	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	18	8	0
			2890	1861	488	527	14			

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



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

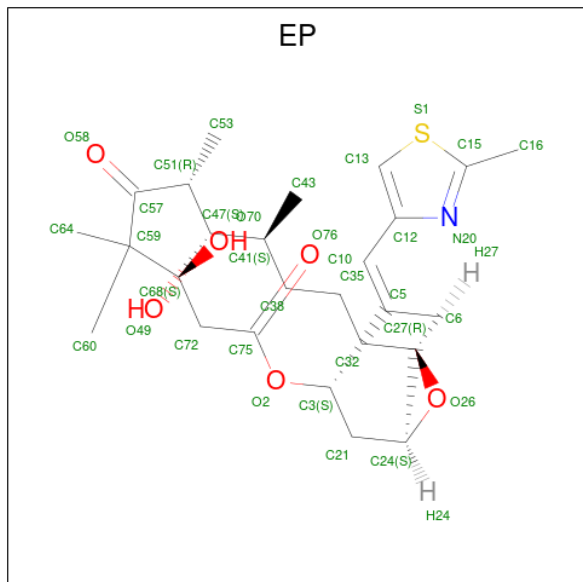
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

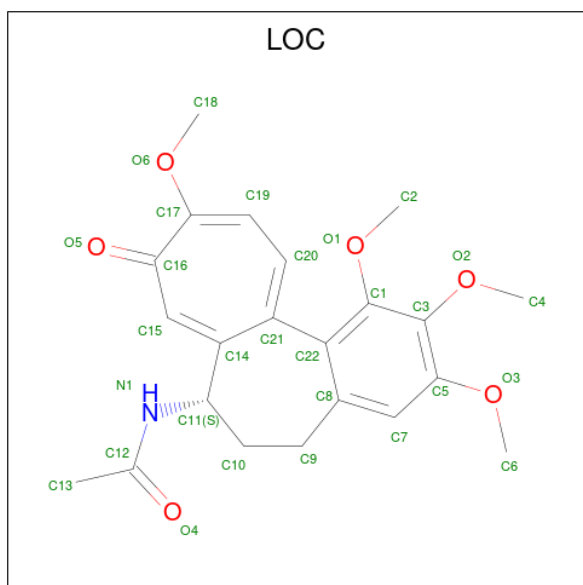
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	2	Total Ca 2 2	2	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is EPOTHILONE A (CCD ID: EP) (formula: $C_{26}H_{39}NO_6S$) (labeled as "Ligand of Interest" by depositor).



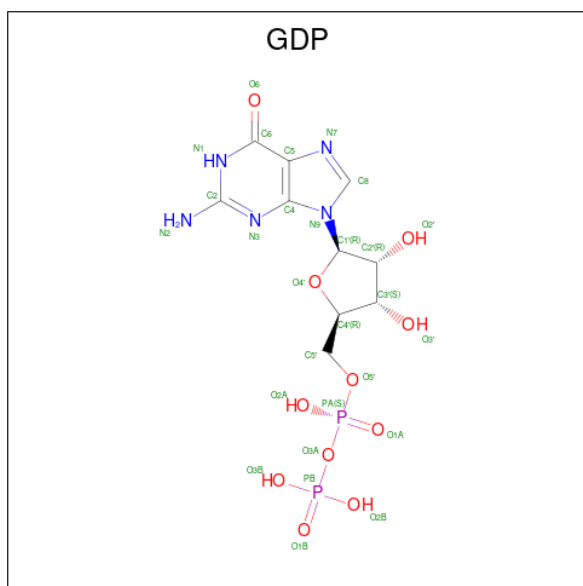
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		
8	D	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		

- Molecule 9 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (CCD ID: LOC) (formula: $C_{22}H_{25}NO_6$) (labeled as "Ligand of Interest" by depositor).



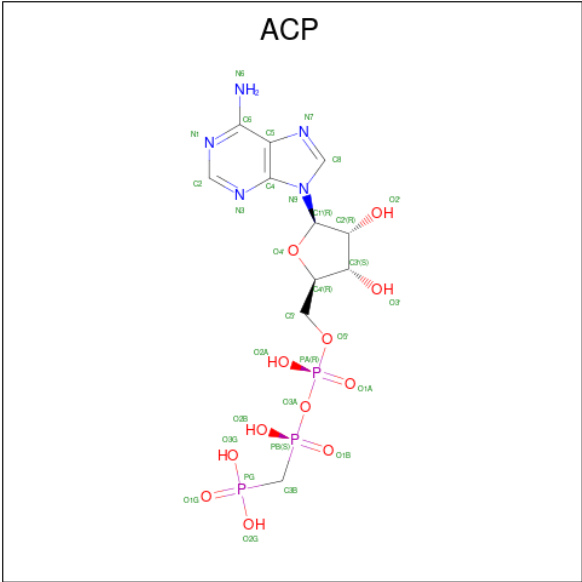
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			54	22	25	1	6		

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



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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

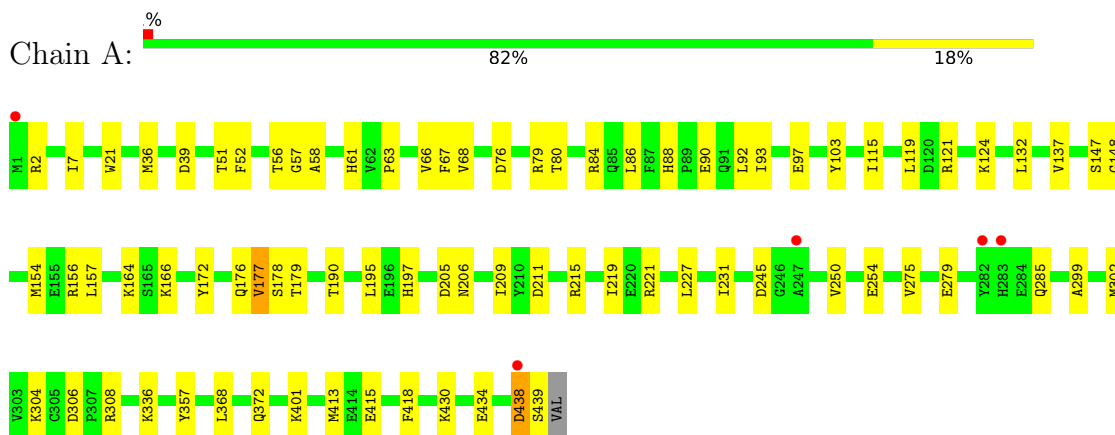
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	O	0	0
			8	8		
12	B	9	Total	O	0	0
			9	9		
12	C	21	Total	O	0	0
			21	21		
12	D	4	Total	O	0	0
			4	4		
12	E	1	Total	O	0	0
			1	1		
12	F	1	Total	O	0	0
			1	1		

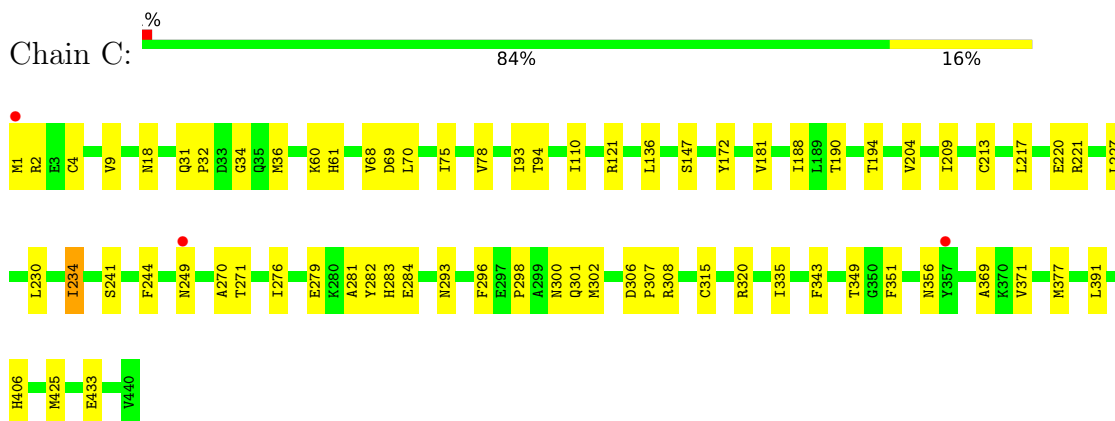
3 Residue-property plots [i](#)

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.

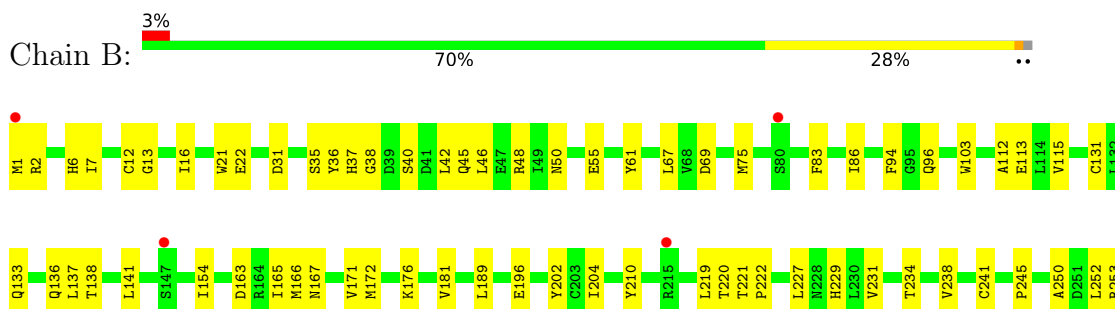
- Molecule 1: Tubulin alpha-1B chain

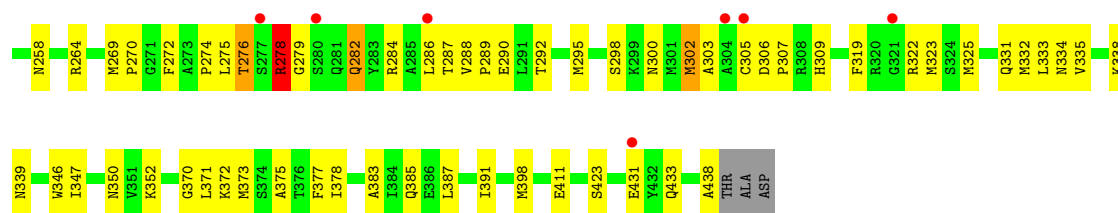


- Molecule 1: Tubulin alpha-1B chain

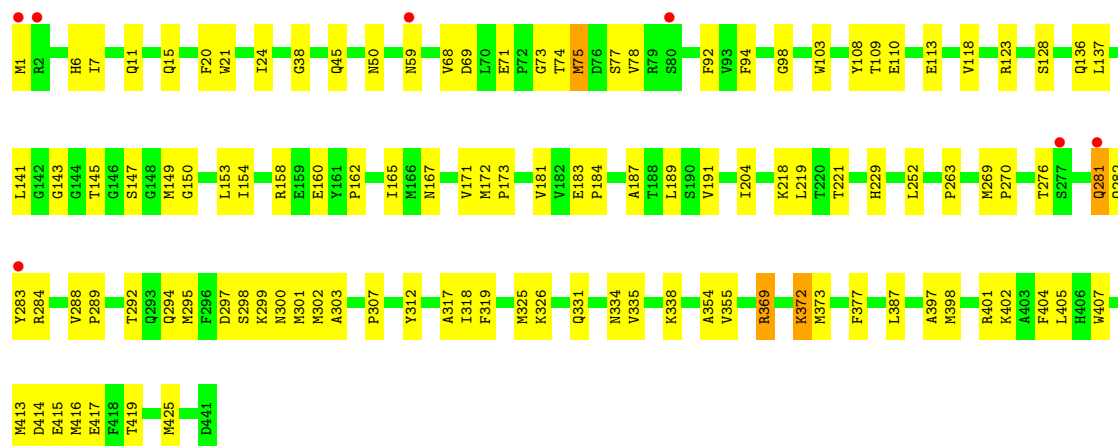
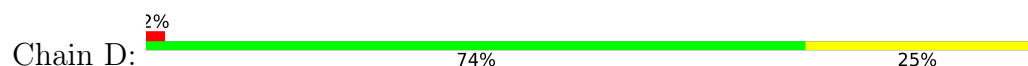


- Molecule 2: Tubulin beta-2B chain

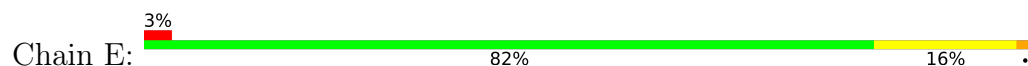




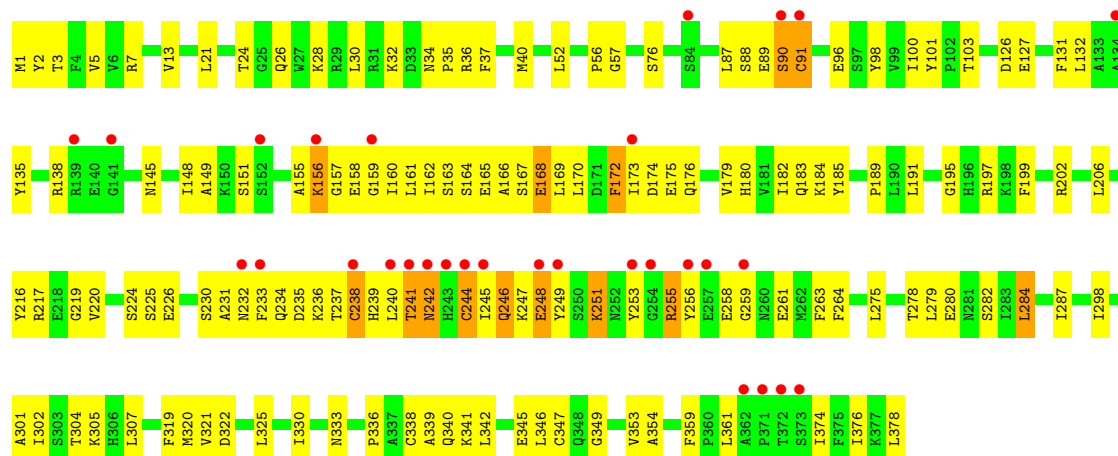
• Molecule 2: Tubulin beta-2B chain



• 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	106.76Å 160.76Å 180.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.26 – 2.80 15.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.26-2.80) 99.2 (15.26-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.178 , 0.227 (Not available) , 0.244	Depositor DCC
R_{free} test set	2000 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18186	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, MG, ACP, GDP, GTP, EP, LOC

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	0.43	0/3594	0.74	1/4881 (0.0%)
1	C	0.47	0/3648	0.73	1/4955 (0.0%)
2	B	0.47	0/3555	0.84	4/4813 (0.1%)
2	D	0.45	0/3504	0.78	1/4748 (0.0%)
3	E	0.52	1/1066 (0.1%)	0.88	2/1415 (0.1%)
4	F	0.46	0/2975	0.86	2/4022 (0.0%)
All	All	0.46	1/18342 (0.0%)	0.80	11/24834 (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
2	B	0	1
2	D	0	1
4	F	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	15	THR	C-O	6.49	1.32	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	303	ALA	CA-C-N	-7.99	111.80	122.42
2	B	303	ALA	C-N-CA	-7.99	111.80	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	15	THR	CA-C-O	7.49	128.63	119.79
4	F	238	CYS	N-CA-C	-6.95	104.93	113.41
4	F	89	GLU	N-CA-C	-5.54	106.22	112.87

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
2	B	278	ARG	Sidechain
2	D	369	ARG	Sidechain
4	F	255	ARG	Sidechain

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	3480	0	3427	72	0
1	C	3519	0	3458	63	2
2	B	3441	0	3356	145	2
2	D	3411	0	3306	95	0
3	E	1042	0	1065	17	0
4	F	2890	0	2894	150	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
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	B	34	39	37	14	0
8	D	34	39	37	8	0
9	B	29	25	25	9	0
10	B	28	0	12	1	0
10	D	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	31	0	14	4	0
12	A	8	0	0	0	0
12	B	9	0	0	0	0
12	C	21	0	0	0	0
12	D	4	0	0	0	0
12	E	1	0	0	0	0
12	F	1	0	0	1	0
All	All	18083	103	17667	521	2

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 15.

The worst 5 of 521 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:221:ARG:HH21	2:B:325:MET:HE2	1.11	1.15
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.33	1.06
2:B:274:PRO:HG2	8:B:503:EP:H62	1.39	1.03
2:B:338:LYS:O	2:B:338:LYS:NZ	1.90	1.02
2:D:284:ARG:HH22	2:D:294:GLN:HE22	1.05	0.96

All (2) 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:OE1	1:C:283:HIS:NE2[4_555]	1.57	0.63
2:B:411:GLU:OE1	1:C:282:TYR:OH[4_555]	2.08	0.12

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	449/440 (102%)	432 (96%)	16 (4%)	1 (0%)	43	72
1	C	456/440 (104%)	448 (98%)	8 (2%)	0	100	100
2	B	441/431 (102%)	429 (97%)	12 (3%)	0	100	100
2	D	435/431 (101%)	419 (96%)	16 (4%)	0	100	100
3	E	124/123 (101%)	121 (98%)	3 (2%)	0	100	100
4	F	353/351 (101%)	322 (91%)	29 (8%)	2 (1%)	21	51
All	All	2258/2216 (102%)	2171 (96%)	84 (4%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	248	GLU
4	F	346	LEU
1	A	177	VAL

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	381/371 (103%)	377 (99%)	4 (1%)	68	88
1	C	389/371 (105%)	386 (99%)	3 (1%)	73	90
2	B	385/372 (104%)	374 (97%)	11 (3%)	37	73
2	D	378/372 (102%)	372 (98%)	6 (2%)	55	83
3	E	115/110 (104%)	110 (96%)	5 (4%)	26	60
4	F	319/313 (102%)	297 (93%)	22 (7%)	14	41
All	All	1967/1909 (103%)	1916 (97%)	51 (3%)	44	75

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	108[B]	ASN
4	F	168	GLU

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Mol	Chain	Res	Type
4	F	284[A]	LEU
4	F	76[A]	SER
4	F	90	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	331	GLN
4	F	242	ASN
3	E	92	ASN
4	F	34	ASN
2	B	424	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	33,34,34	0.63	0	50,54,54	0.50	0

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	0.99	3 (9%)	50,54,54	1.61	12 (24%)
10	GDP	B	505	6	29,30,30	1.19	3 (10%)	45,47,47	1.78	10 (22%)
8	EP	D	501	-	36,36,36	0.25	0	48,53,53	0.87	2 (4%)
9	LOC	B	504	-	31,31,31	0.77	0	44,44,44	0.89	1 (2%)
10	GDP	D	502	6	29,30,30	1.30	4 (13%)	45,47,47	1.67	6 (13%)
8	EP	B	503	-	36,36,36	0.31	0	48,53,53	0.84	3 (6%)
11	ACP	F	401	-	31,33,33	0.72	1 (3%)	47,52,52	0.59	0

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	-	6/22/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
10	GDP	B	505	6	-	3/16/32/32	0/3/3/3
8	EP	D	501	-	4/4/12/12	21/50/55/55	1/3/3/3
9	LOC	B	504	-	-	4/12/25/25	0/3/3/3
10	GDP	D	502	6	-	8/16/32/32	0/3/3/3
8	EP	B	503	-	4/4/12/12	29/50/55/55	1/3/3/3
11	ACP	F	401	-	-	7/19/38/38	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)
10	D	502	GDP	C5-C4	3.31	1.47	1.38
10	D	502	GDP	C6-N1	-3.00	1.33	1.38
10	B	505	GDP	C5-C4	2.87	1.46	1.38
5	A	501	GTP	PB-O3A	2.60	1.62	1.59
10	B	505	GDP	PA-O3A	2.40	1.62	1.59

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	GDP	C5-C4-N3	-5.67	119.37	128.39
10	B	505	GDP	C5-C4-N3	-5.41	119.79	128.39
10	B	505	GDP	C2-N3-C4	4.55	120.14	112.30
5	A	501	GTP	C2-N3-C4	4.49	120.03	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	GDP	N9-C4-N3	4.31	134.57	125.95

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	503	EP	C27
8	B	503	EP	C3
8	B	503	EP	C41
8	B	503	EP	C24
8	D	501	EP	C27

5 of 84 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
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A

All (2) ring outliers are listed below:

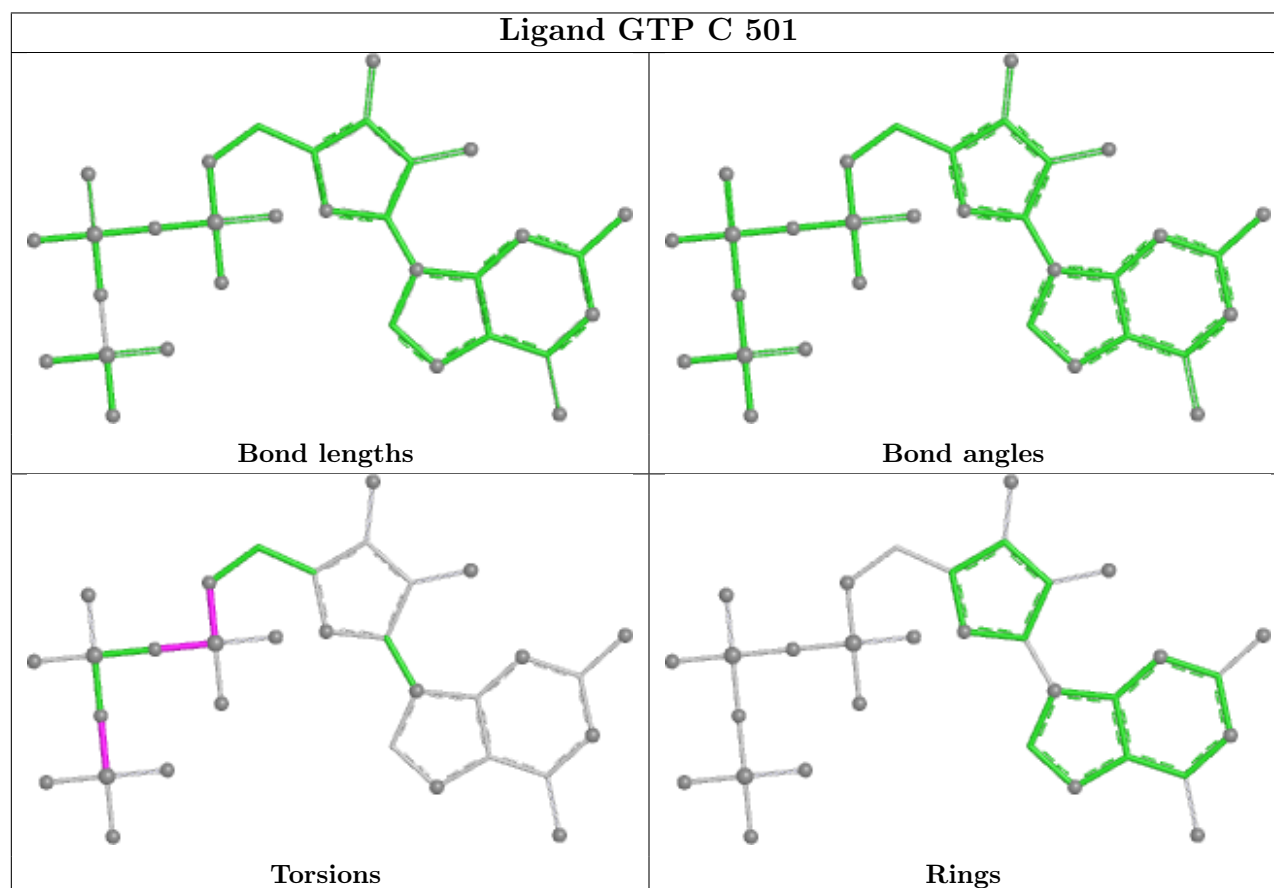
Mol	Chain	Res	Type	Atoms
8	D	501	EP	C21-C24-C27-C3-C32-C35-C38-C41-C47-C51-C57-C59-C68-C72-C75-O2
8	B	503	EP	C21-C24-C27-C3-C32-C35-C38-C41-C47-C51-C57-C59-C68-C72-C75-O2

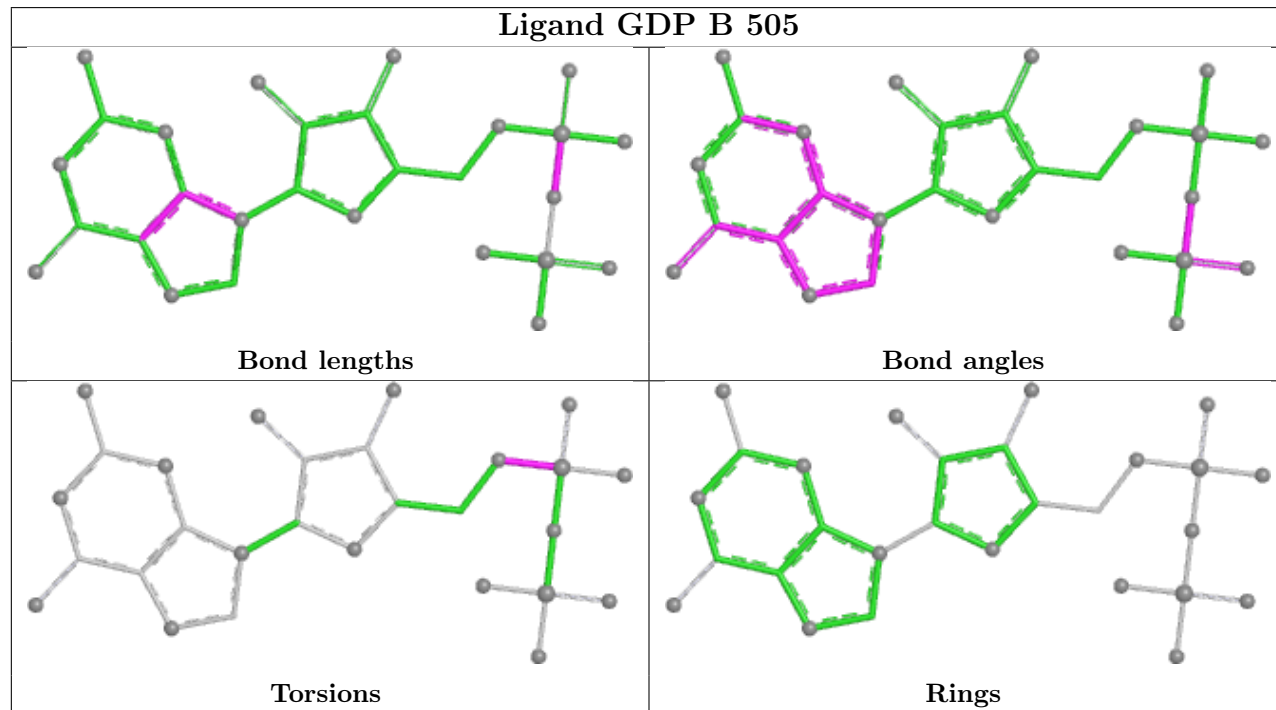
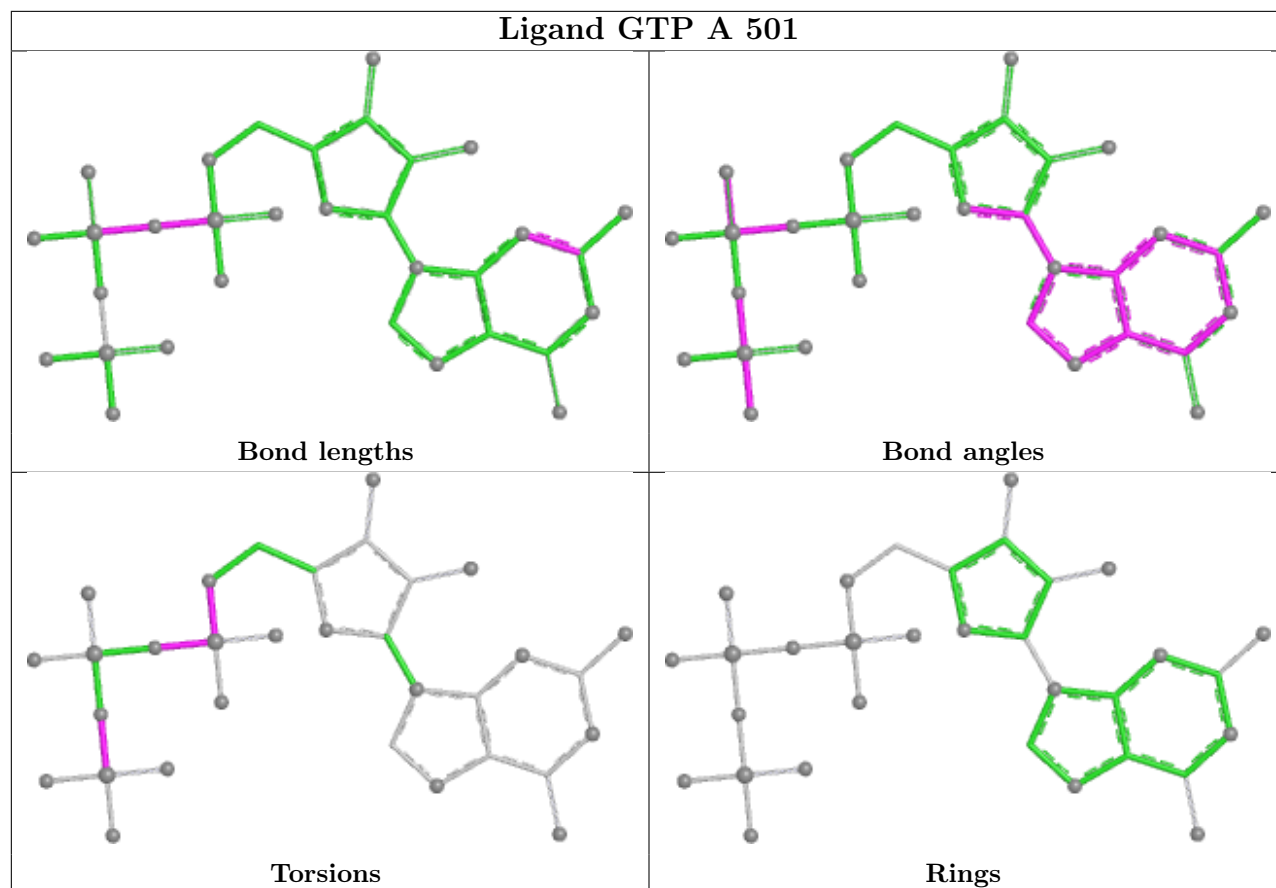
6 monomers are involved in 38 short contacts:

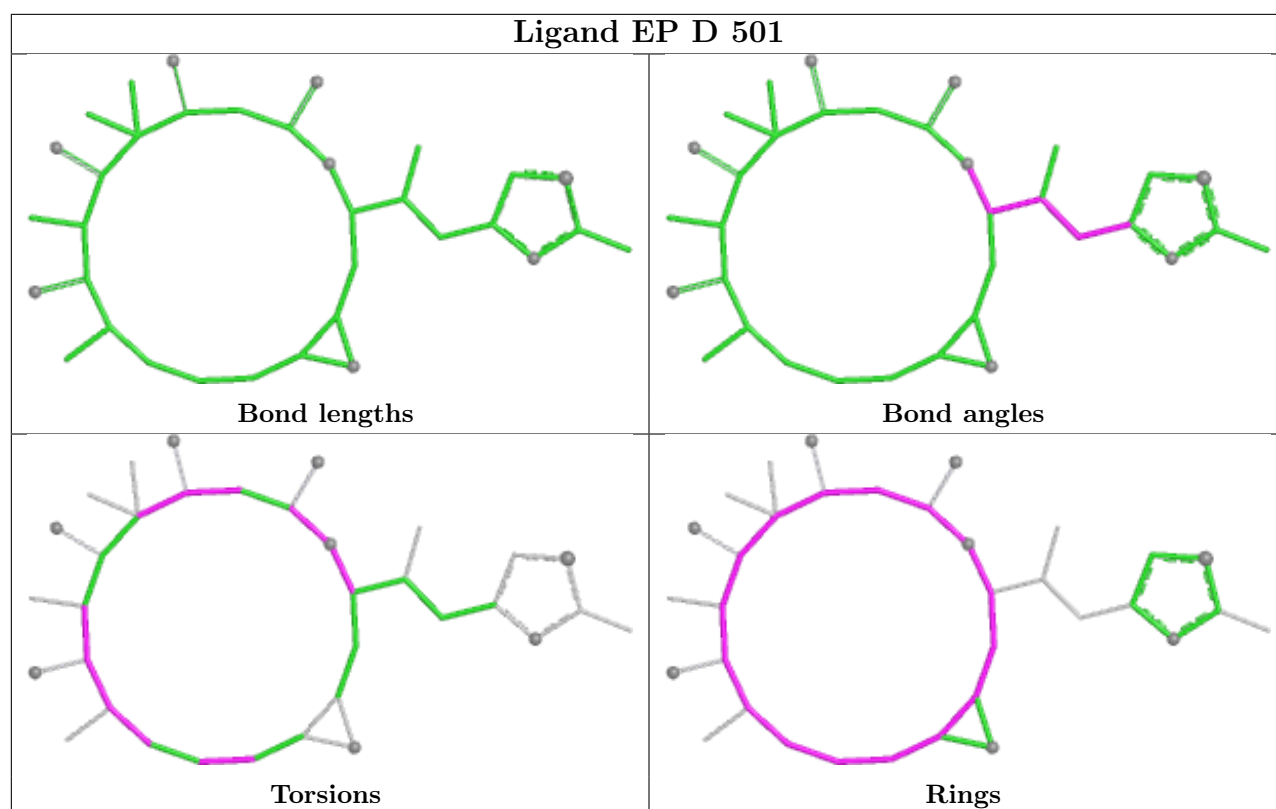
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	GDP	1	0
8	D	501	EP	8	0
9	B	504	LOC	9	0
10	D	502	GDP	2	0
8	B	503	EP	14	0
11	F	401	ACP	4	0

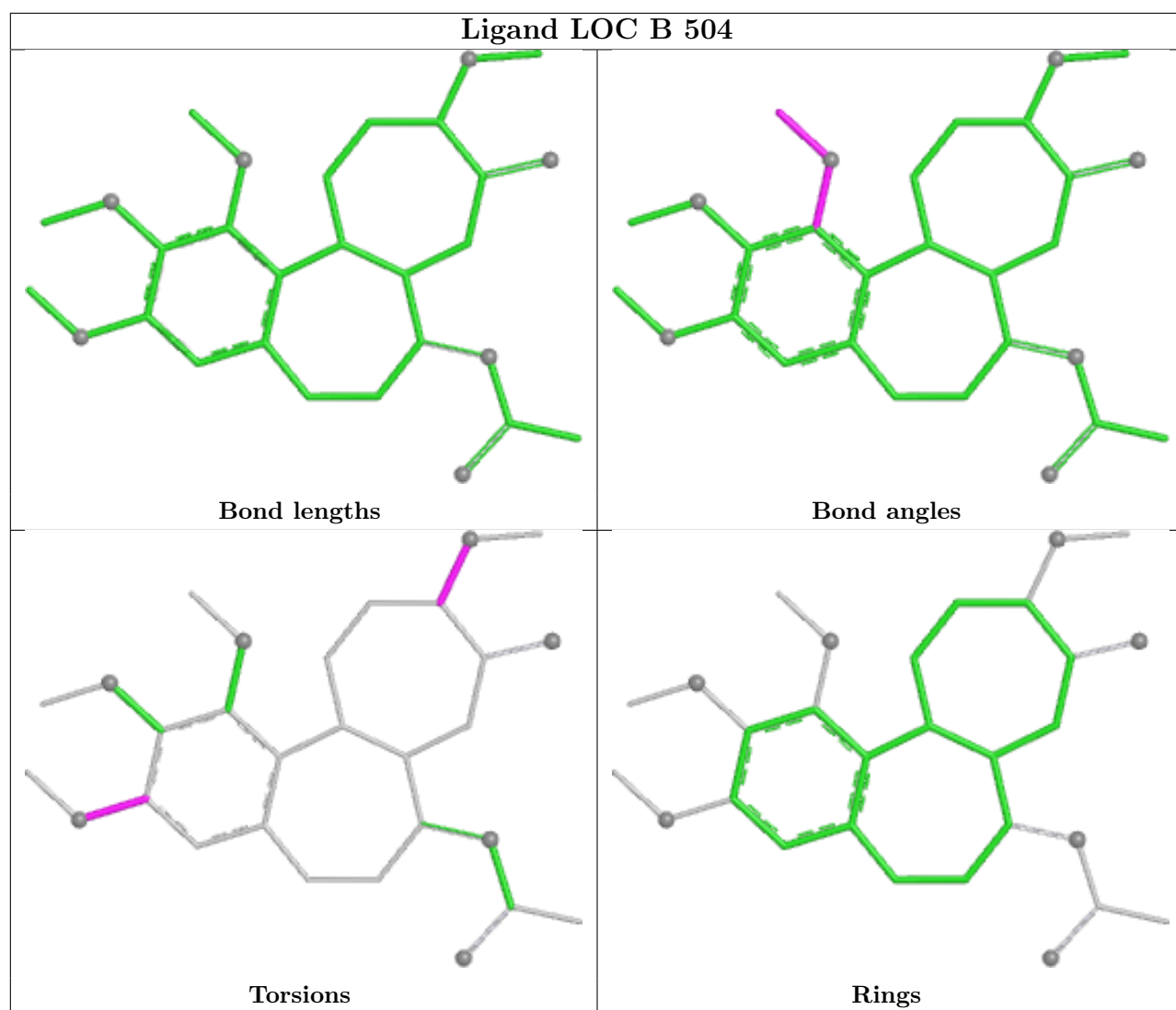
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

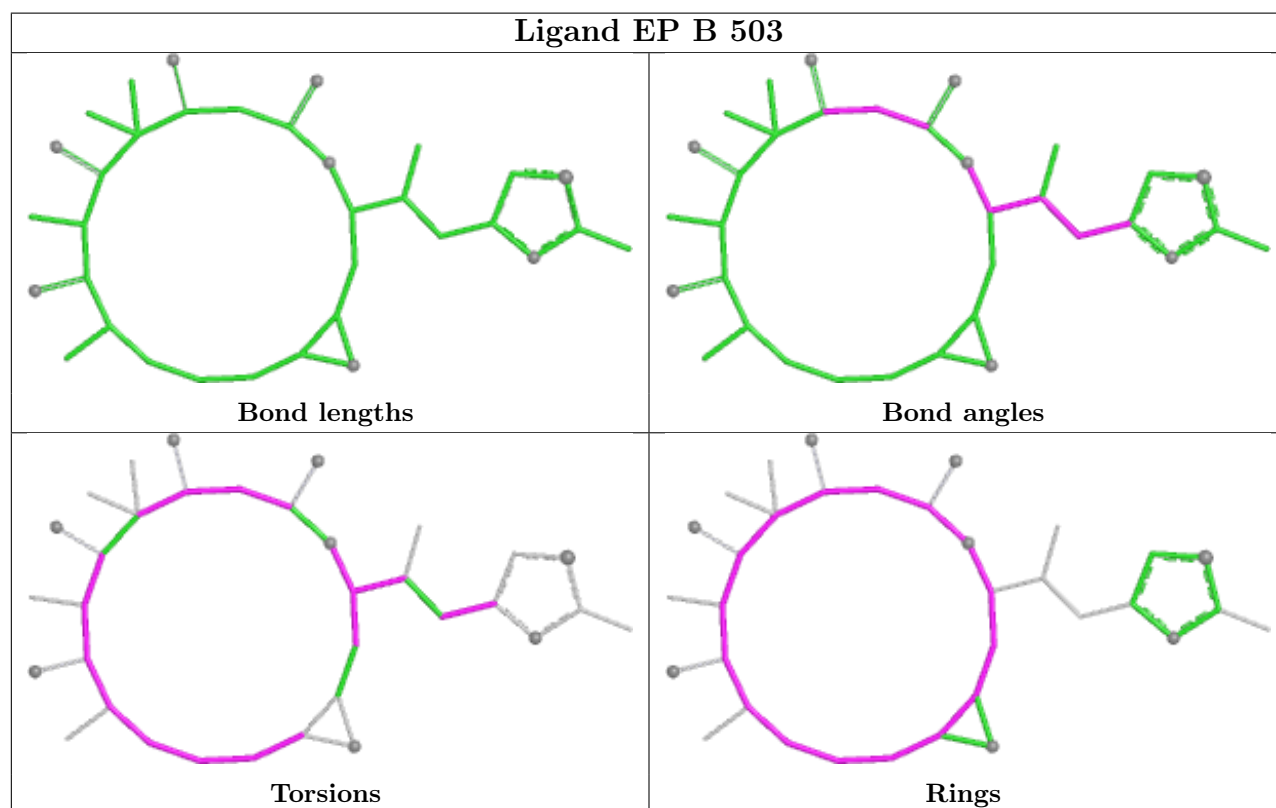
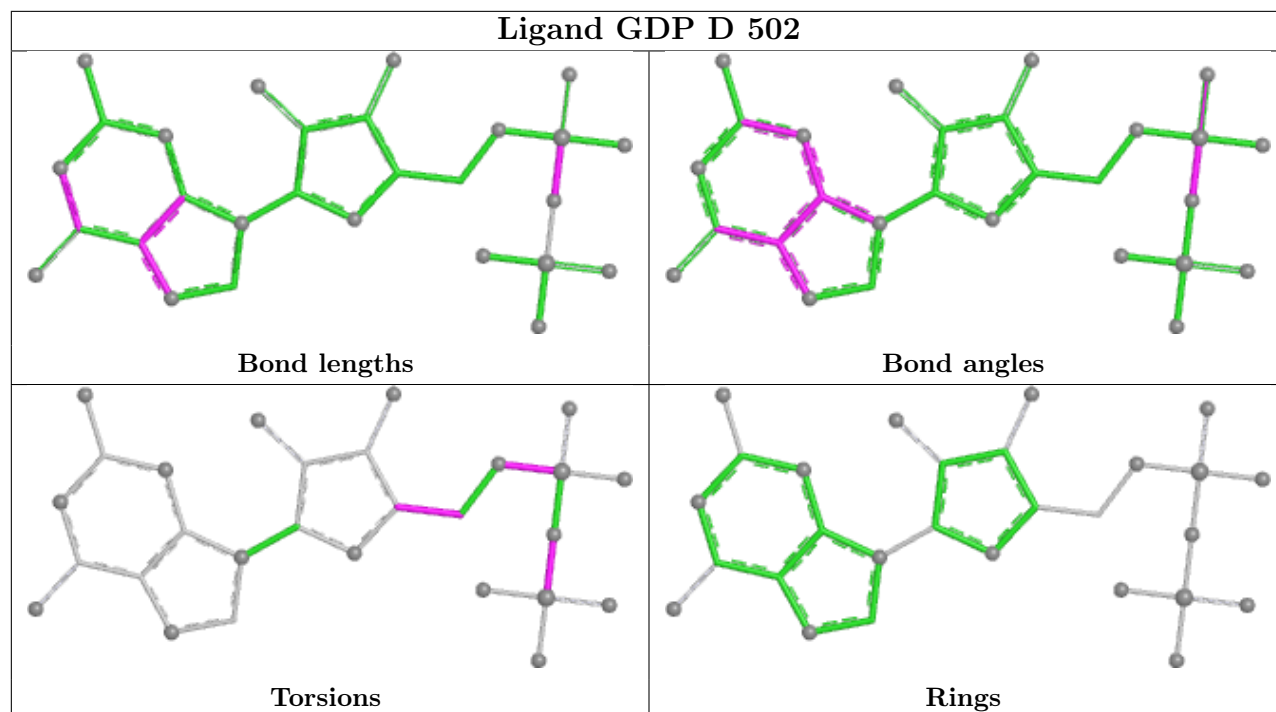
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

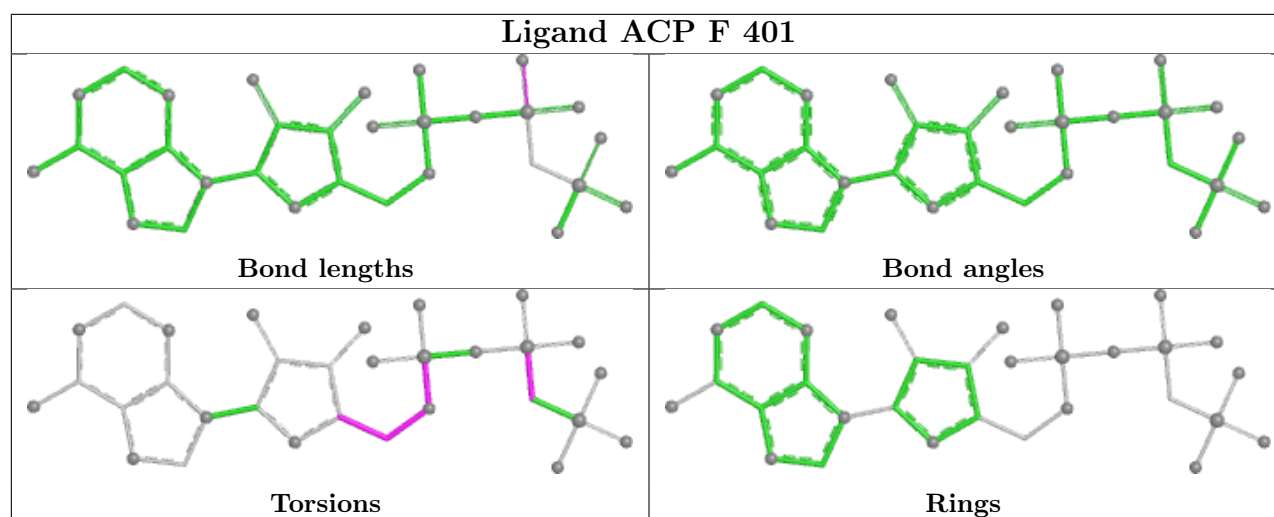












5.7 Other polymers [i](#)

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	2
3	E	1

All 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	34.14
1	F	362:ALA	C	371:PRO	N	14.08
1	F	105:LEU	C	125:THR	N	12.54

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%)	-0.36	5 (1%) 78 70	25, 55, 97, 179	12 (2%)
1	C	440/440 (100%)	-0.50	3 (0%) 84 77	20, 44, 79, 115	18 (4%)
2	B	428/431 (99%)	-0.18	11 (2%) 57 47	21, 53, 105, 163	19 (4%)
2	D	431/431 (100%)	-0.21	7 (1%) 70 61	28, 64, 108, 170	9 (2%)
3	E	123/123 (100%)	0.17	4 (3%) 49 39	28, 72, 124, 184	5 (4%)
4	F	351/351 (100%)	0.44	30 (8%) 16 12	26, 88, 184, 219	8 (2%)
All	All	2212/2216 (99%)	-0.17	60 (2%) 56 46	20, 59, 128, 219	71 (3%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	305	CYS	6.6
4	F	240	LEU	4.5
4	F	254	GLY	4.4
4	F	362	ALA	3.9
4	F	372	THR	3.9

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 ⓘ

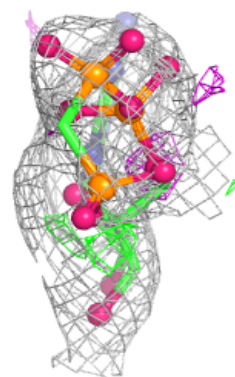
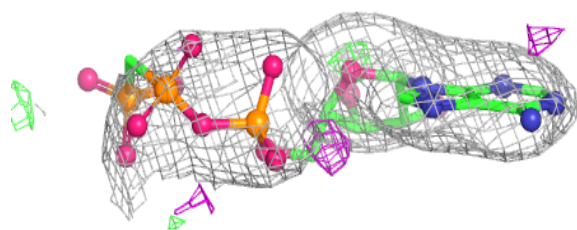
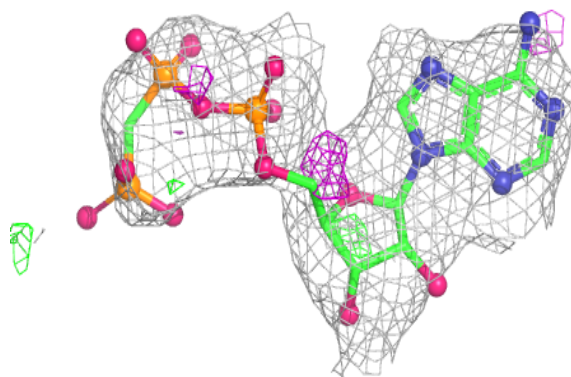
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ACP	F	401	31/31	0.76	0.14	91,123,169,178	0
8	EP	B	503	34/34	0.77	0.15	69,115,144,147	0
8	EP	D	501	34/34	0.88	0.11	58,82,102,109	0
9	LOC	B	504	29/29	0.92	0.09	41,63,82,88	0
6	MG	B	506	1/1	0.93	0.18	45,45,45,45	0
6	MG	D	503	1/1	-	-	76,76,76,76	1
6	MG	A	502	1/1	0.94	0.07	44,44,44,44	0
7	CA	B	501	1/1	-	-	77,77,77,77	1
7	CA	B	502	1/1	-	-	94,94,94,94	1
10	GDP	D	502	28/28	0.96	0.08	38,56,73,101	0
6	MG	C	502	1/1	0.97	0.05	32,32,32,32	0
5	GTP	C	501	32/32	0.97	0.06	24,36,41,48	0
7	CA	C	503	1/1	0.98	0.03	71,71,71,71	0
10	GDP	B	505	28/28	0.98	0.06	31,39,44,54	0
5	GTP	A	501	32/32	0.98	0.05	32,41,50,58	0
7	CA	A	503	1/1	0.98	0.03	79,79,79,79	0

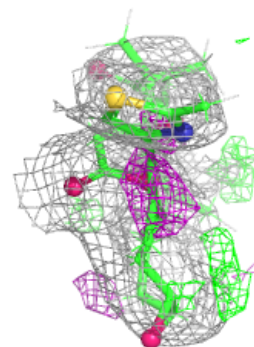
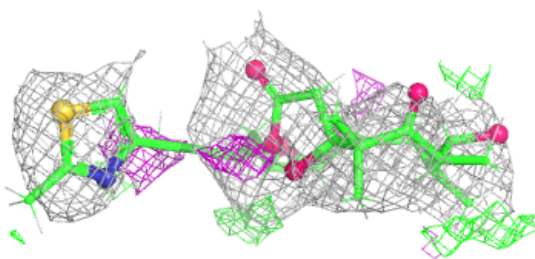
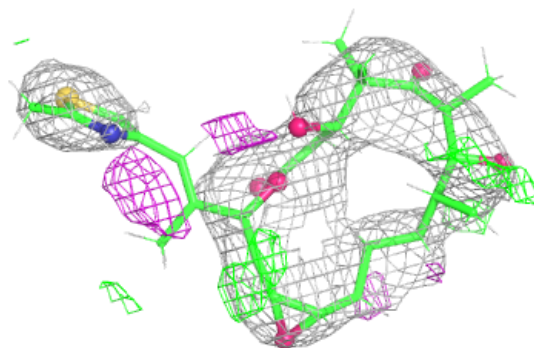
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

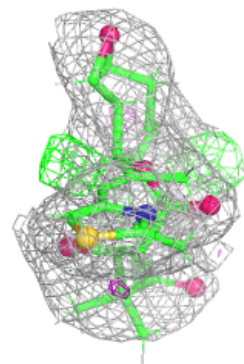
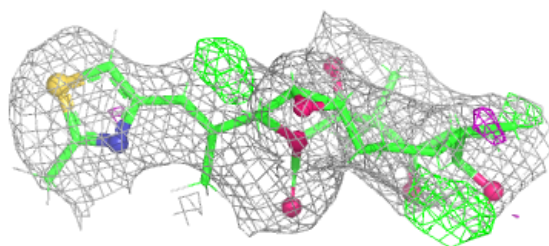
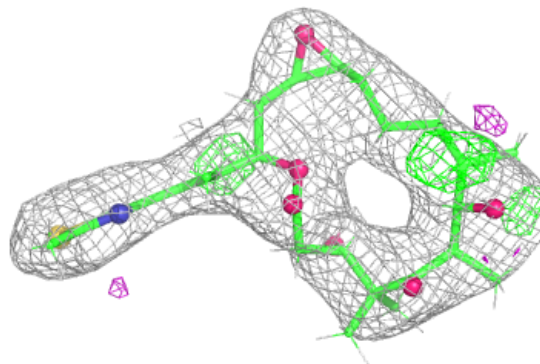
**Electron density around EP B 503:**

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

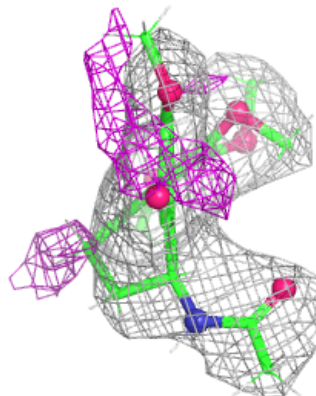
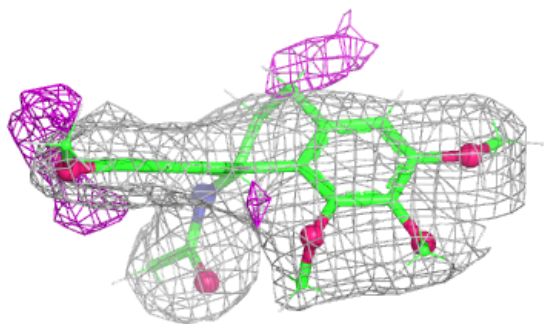
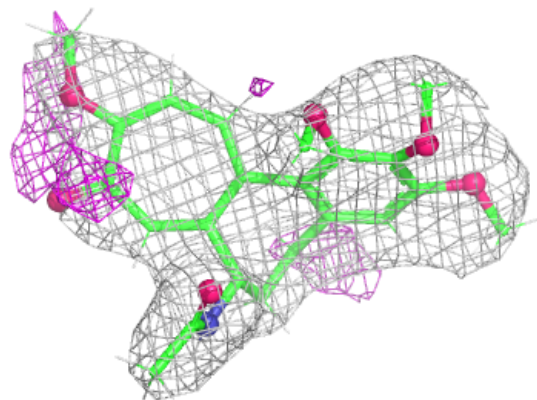


Electron density around EP D 501:

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

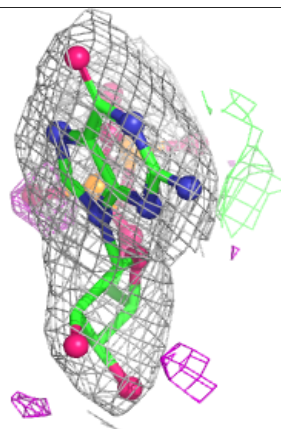
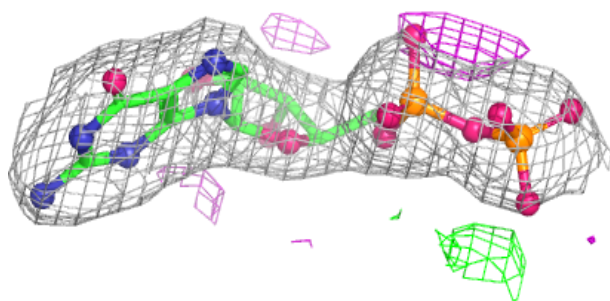
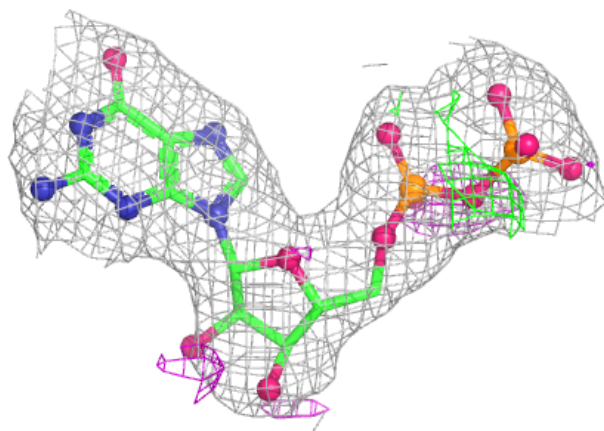
**Electron density around LOC B 504:**

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



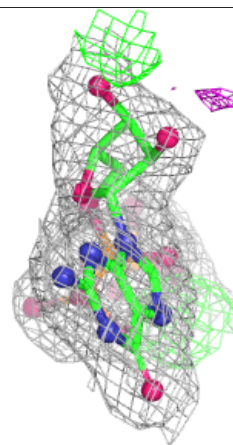
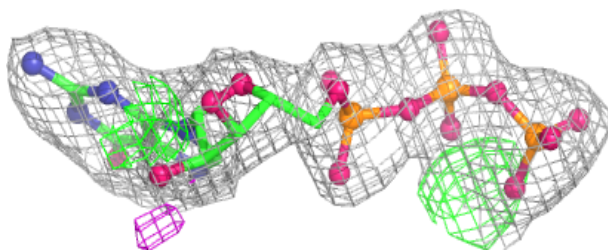
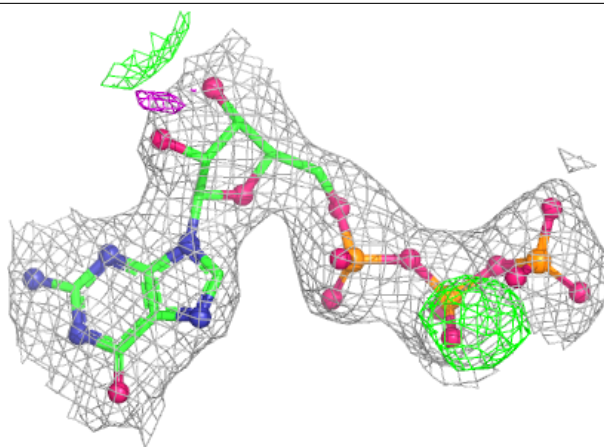
Electron density around GDP D 502:

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



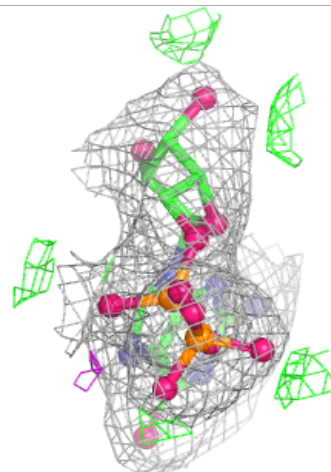
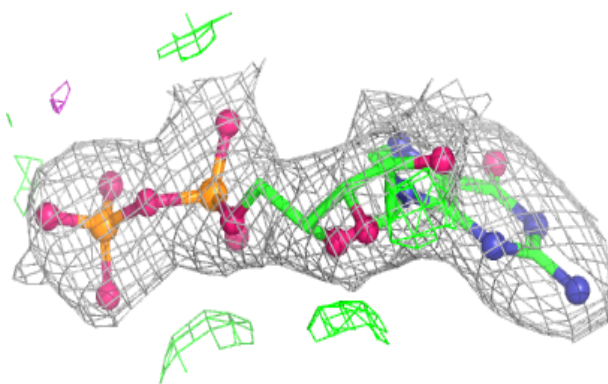
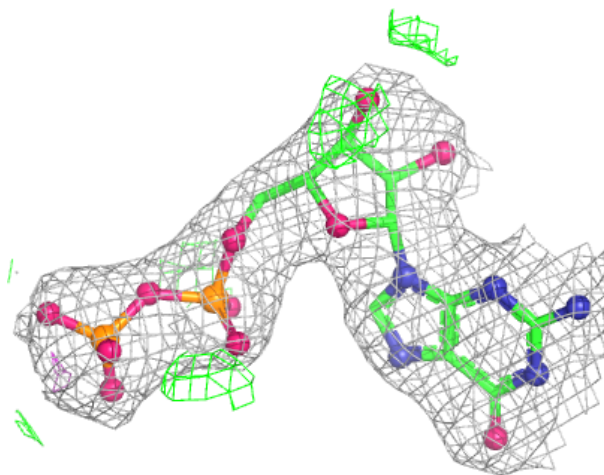
Electron density around GTP C 501:

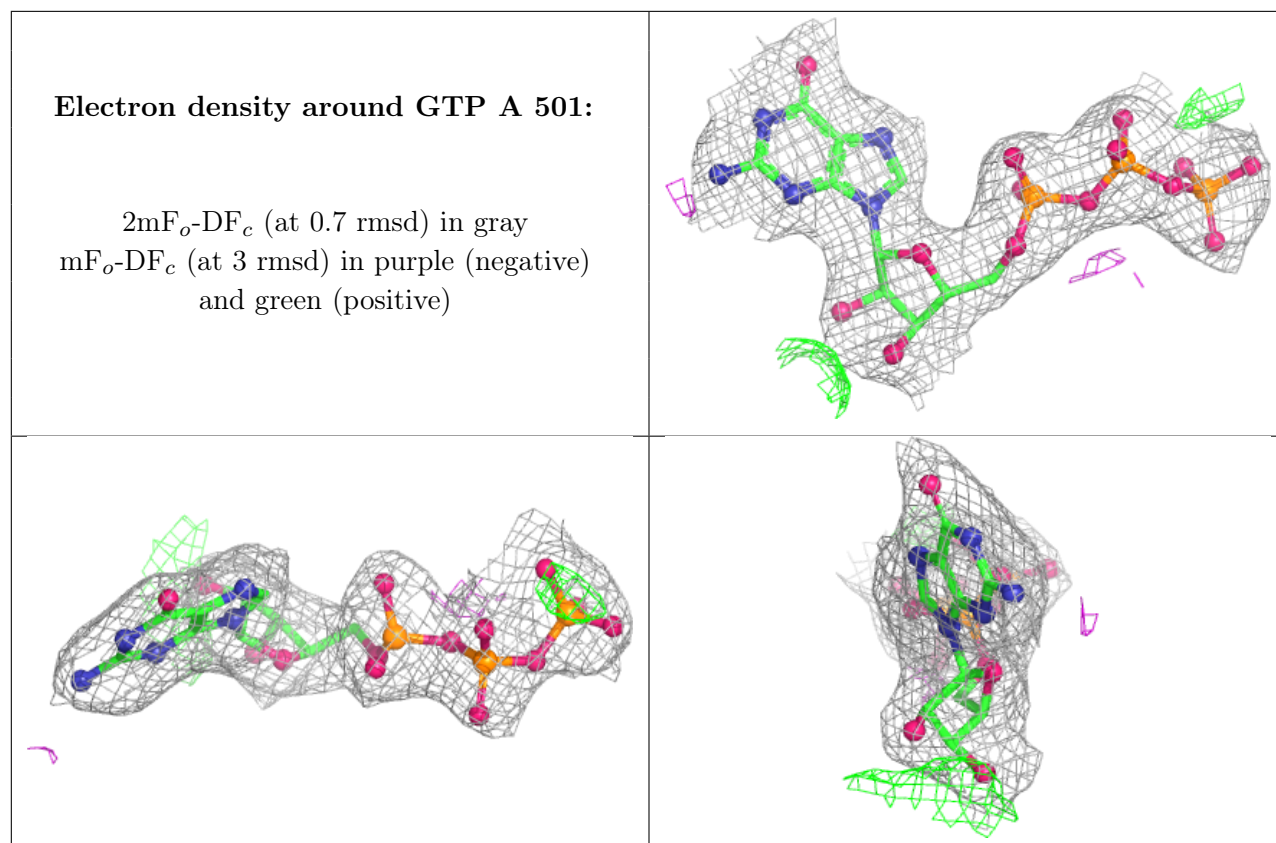
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 505:

$2mF_o-DF_c$ (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.