



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:11 AM UTC

PDB ID : 8CLH / pdb_00008clh
Title : Drug cocktail (Colchicine, Etoposide, Peloruside, Ansamitocin P3, 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 : 2.50 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

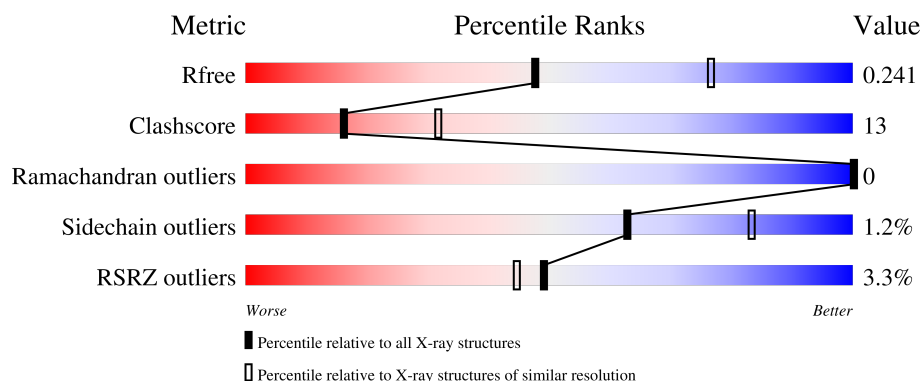
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	3% 74% 26%
1	C	440	2% 84% 16%
2	B	430	3% 78% 22%
2	D	430	3% 75% 25%

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Mol	Chain	Length	Quality of chain
3	E	138	
4	F	381	

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
10	EP	B	504	X	-	-	-
10	EP	D	503	X	-	-	-
11	POU	B	505	X	-	-	-
13	BKF	D	504	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18174 atoms, of which 252 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	2	0
			3441	2175	585	658	23			
1	C	440	Total	C	N	O	S	0	4	0
			3464	2190	590	661	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	2	3	0
			3386	2125	579	655	27			
2	D	430	Total	C	N	O	S	2	1	0
			3376	2117	577	656	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	1	0
			1020	628	184	202	6			

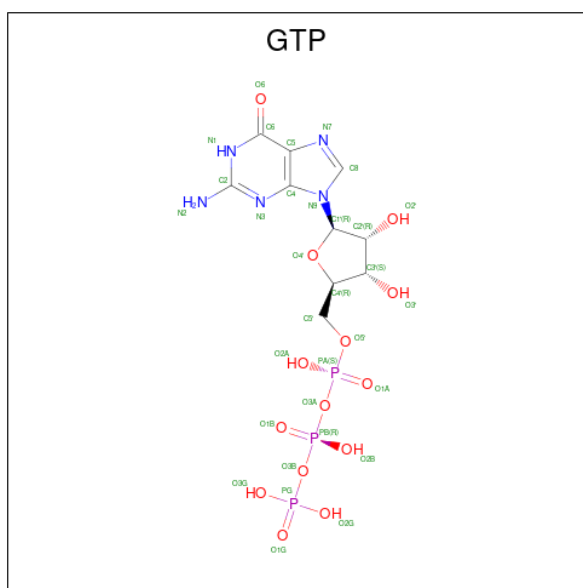
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	1	0
			2714	1740	464	495	15			

There are 3 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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	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		

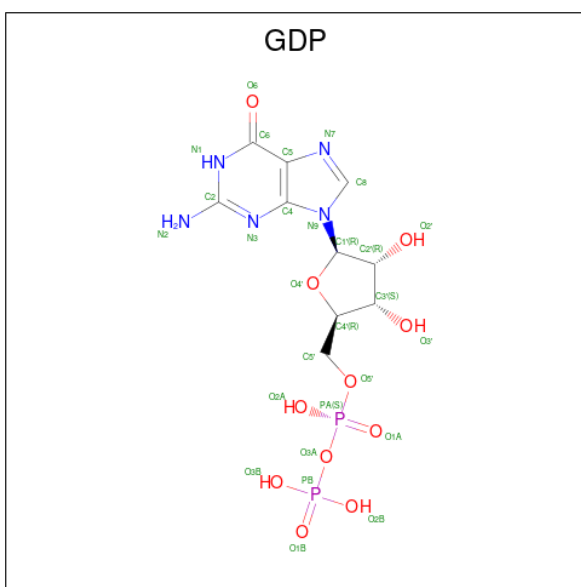
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

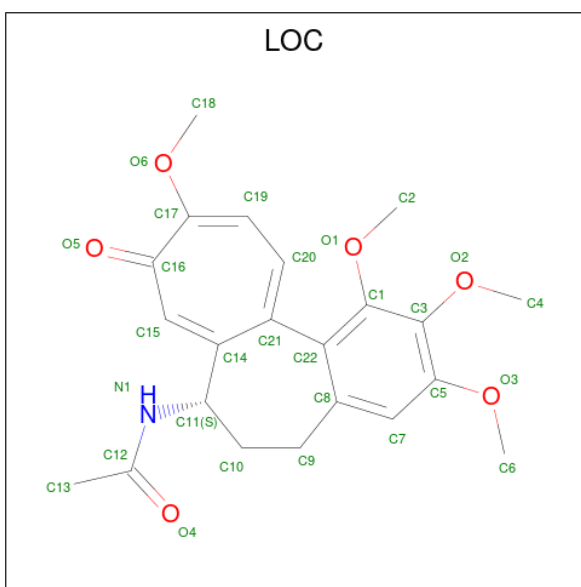
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: 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 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).

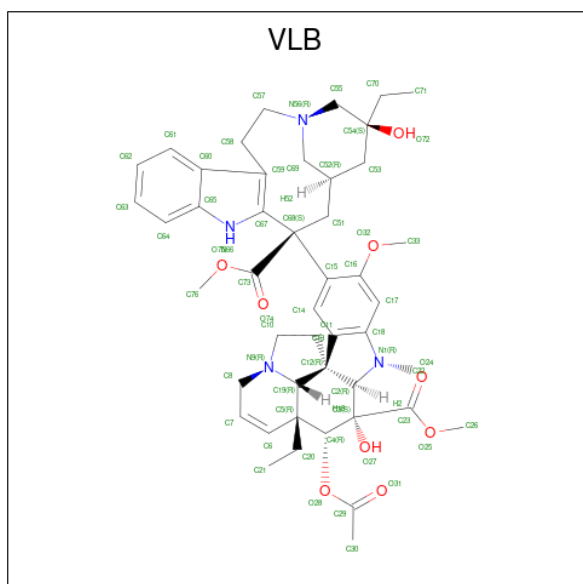


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			54	22	25	1	6		

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- Chemical structure of EP (Ergosterol) showing the steroid nucleus, side chain, and functional groups. The structure is labeled with atom names (C, O, S, N, H) and bond types (solid, dashed, wedged).

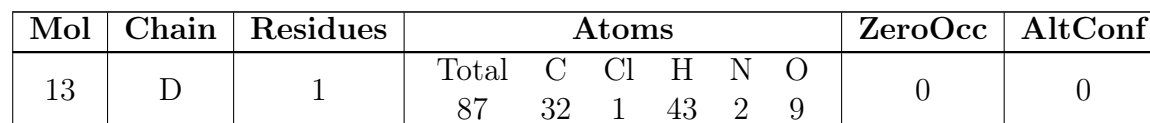
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			86	27	48	11		

- Molecule 12 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (CCD ID: VLB) (formula: $C_{46}H_{58}N_4O_9$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is (1S,2S,3S,5S,6S,16Z,18Z,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5] hexacosa-10(26),11,13,16,18-pentaen-6-yl 2-methylpropanoate (CCD ID: BKF) (formula: $C_{32}H_{43}ClN_2O_9$) (labeled as "Ligand of Interest" by depositor).



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

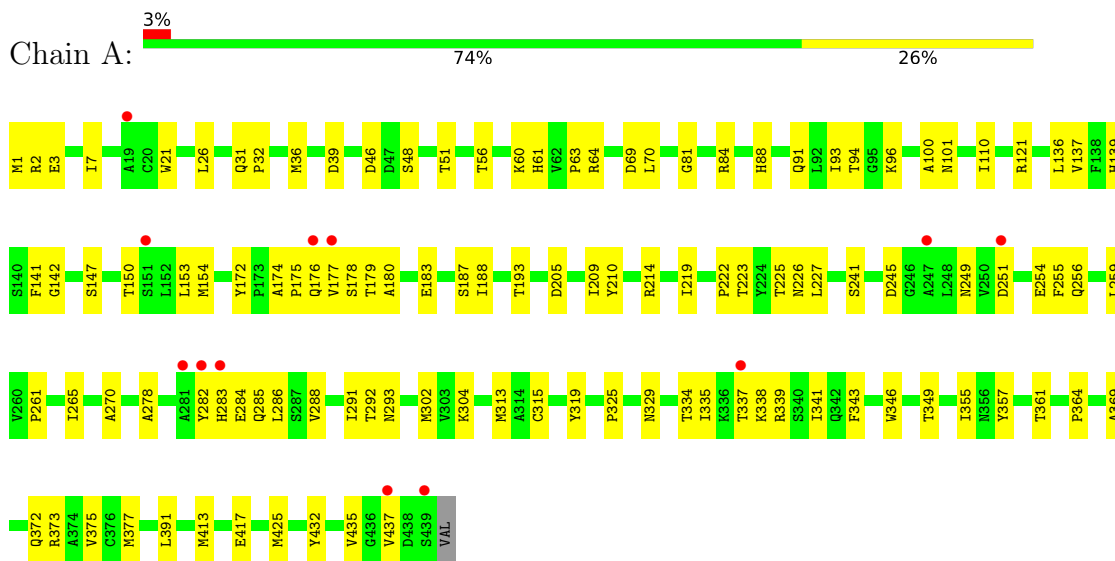
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	28	Total 28	O 28	0	0
15	B	25	Total 25	O 25	0	0
15	C	54	Total 54	O 54	0	0
15	D	10	Total 10	O 10	0	0
15	E	3	Total 3	O 3	0	0
15	F	6	Total 6	O 6	0	0

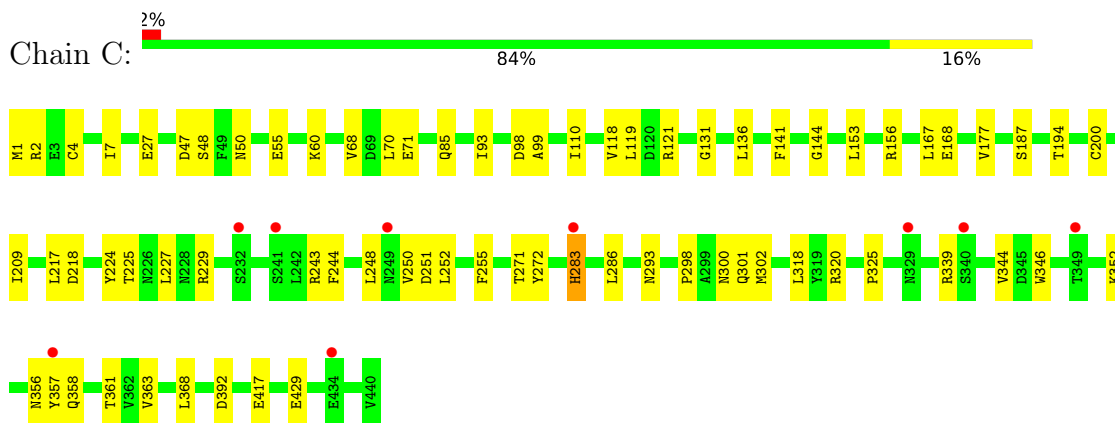
3 Residue-property plots [i](#)

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.

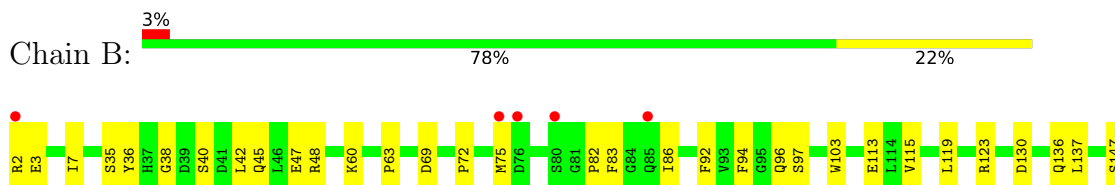
- Molecule 1: Tubulin alpha-1B chain

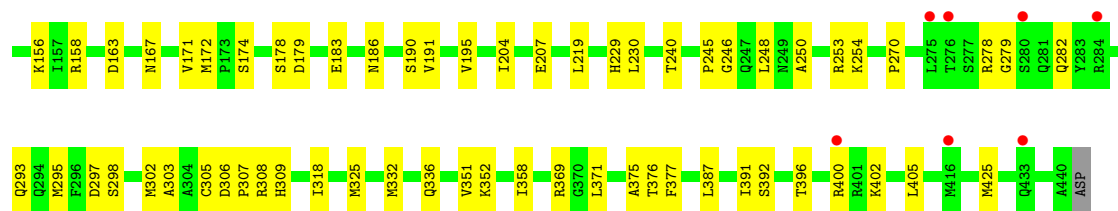


- Molecule 1: Tubulin alpha-1B chain

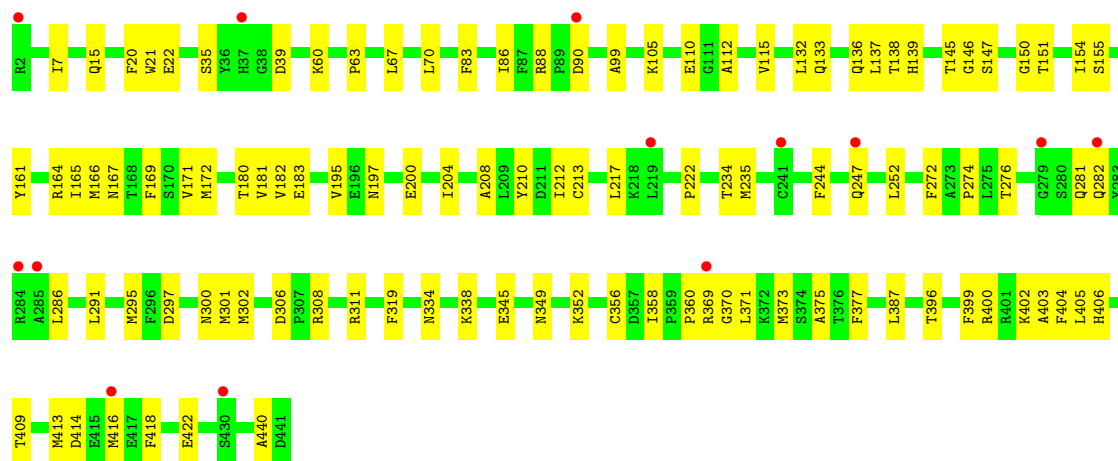
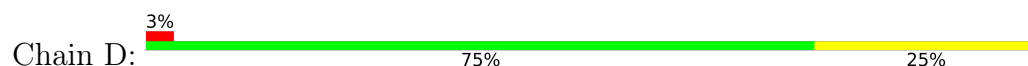


- Molecule 2: Tubulin beta-2B chain

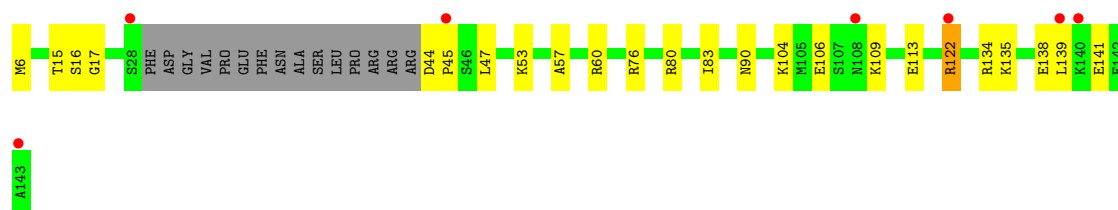




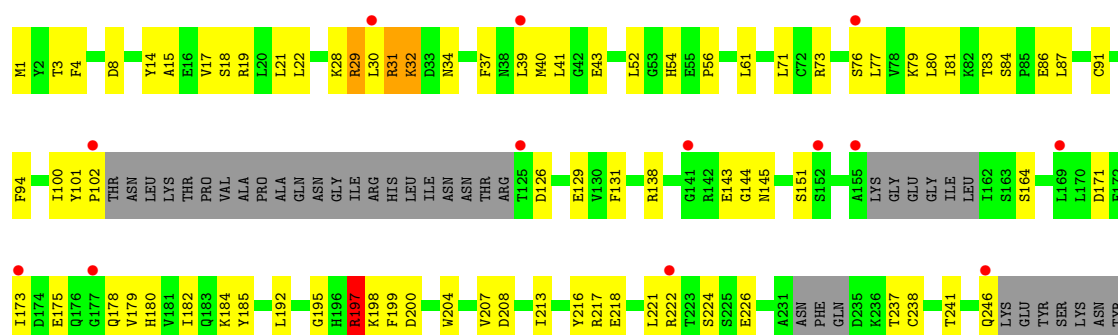
• Molecule 2: Tubulin beta-2B chain

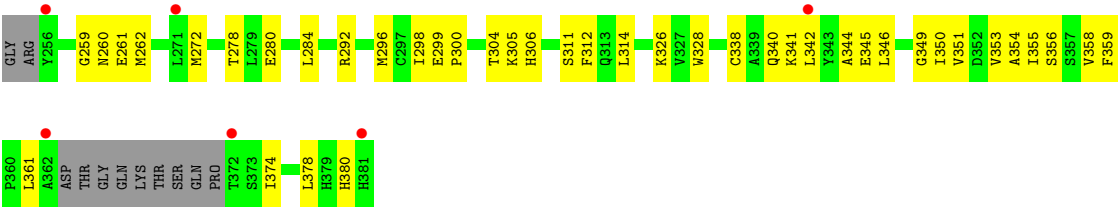


• Molecule 3: Stathmin-4



• 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	107.00Å 160.34Å 181.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.29 – 2.50 15.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.29-2.50) 99.4 (15.29-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.04 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.185 , 0.239 0.187 , 0.241	Depositor DCC
R_{free} test set	1990 reflections (1.08%)	wwPDB-VP
Wilson B-factor (Å ²)	-7.5	Xtriage
Anisotropy	-0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 114.9	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	0.94	EDS
Total number of atoms	18174	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, CA, GDP, BKF, POU, EP, MG, VLB, ACP, 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	0.25	0/3517	0.45	0/4772
1	C	0.29	0/3550	0.46	0/4817
2	B	0.28	0/3463	0.48	0/4690
2	D	0.27	0/3449	0.44	0/4671
3	E	0.17	0/1028	0.32	0/1364
4	F	0.28	0/2777	0.44	1/3750 (0.0%)
All	All	0.27	0/17784	0.45	1/24064 (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
2	D	0	1
3	E	0	1
4	F	0	3
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	31	ARG	CB-CA-C	-5.10	109.16	115.89

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	311	ARG	Sidechain
3	E	122	ARG	Sidechain
4	F	197	ARG	Sidechain
4	F	29	ARG	Sidechain
4	F	31	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	3441	0	3340	105	0
1	C	3464	0	3364	60	1
2	B	3386	0	3254	86	1
2	D	3376	0	3241	92	0
3	E	1020	0	1033	21	0
4	F	2714	0	2682	103	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	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	29	25	25	6	0
10	B	34	39	37	10	0
10	D	34	39	37	6	0
11	B	38	48	48	6	0
12	C	59	58	58	5	0
13	D	44	43	0	3	0
14	F	31	0	14	0	0
15	A	28	0	0	1	0
15	B	25	0	0	2	0
15	C	54	0	0	5	0
15	D	10	0	0	0	0
15	E	3	0	0	0	0
15	F	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17922	252	17181	458	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 13.

The worst 5 of 458 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:40:SER:OG	2:B:42:LEU:HD13	1.56	1.05
4:F:304:THR:HG21	4:F:311:SER:HB2	1.40	1.03
4:F:100:ILE:HG13	4:F:182:ILE:HD12	1.41	1.01
2:B:396:THR:O	2:B:400:ARG:HG3	1.58	1.01
4:F:14:TYR:HA	4:F:17:VAL:HG12	1.49	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)
2:B:113:GLU:OE2	1:C:283:HIS:NE2[4_555]	1.62	0.58

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	436/440 (99%)	420 (96%)	16 (4%)	0	100	100
1	C	442/440 (100%)	426 (96%)	16 (4%)	0	100	100
2	B	428/430 (100%)	413 (96%)	15 (4%)	0	100	100
2	D	427/430 (99%)	414 (97%)	13 (3%)	0	100	100
3	E	120/138 (87%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	321/381 (84%)	304 (95%)	17 (5%)	0	100	100
All	All	2174/2259 (96%)	2096 (96%)	78 (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	371/371 (100%)	364 (98%)	7 (2%)	50	76
1	C	375/371 (101%)	373 (100%)	2 (0%)	81	92
2	B	371/371 (100%)	370 (100%)	1 (0%)	86	94
2	D	369/371 (100%)	363 (98%)	6 (2%)	55	79
3	E	111/123 (90%)	111 (100%)	0	100	100
4	F	298/339 (88%)	292 (98%)	6 (2%)	48	75
All	All	1895/1946 (97%)	1873 (99%)	22 (1%)	63	83

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	282	GLN
4	F	164	SER
4	F	32	LYS
4	F	197	ARG
1	A	437	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	249	ASN
2	D	406	HIS
2	D	349	ASN

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Mol	Chain	Res	Type
3	E	84	GLN
2	B	436	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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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
8	GDP	B	501	6	29,30,30	0.55	0	45,47,47	0.44	0
13	BKF	D	504	-	45,47,47	0.88	1 (2%)	53,71,71	0.67	1 (1%)
5	GTP	C	502	6	33,34,34	0.59	0	50,54,54	0.49	0
8	GDP	D	501	6	29,30,30	0.51	0	45,47,47	0.43	0
5	GTP	A	501	6	33,34,34	0.59	0	50,54,54	0.49	0
10	EP	B	504	-	36,36,36	0.25	0	48,53,53	0.86	2 (4%)
14	ACP	F	401	-	31,33,33	0.73	1 (3%)	47,52,52	0.57	1 (2%)
12	VLB	C	501	-	66,67,67	1.79	18 (27%)	82,108,108	2.32	26 (31%)
10	EP	D	503	-	36,36,36	0.29	0	48,53,53	0.93	1 (2%)
9	LOC	B	503	-	31,31,31	0.52	0	44,44,44	0.36	0
11	POU	B	505	-	38,39,39	0.29	0	44,57,57	0.49	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
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3
13	BKF	D	504	-	4/4/17/17	22/50/76/76	0/2/4/4
5	GTP	C	502	6	-	6/22/38/38	0/3/3/3
8	GDP	D	501	6	-	4/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
10	EP	B	504	-	4/4/12/12	12/50/55/55	1/3/3/3
14	ACP	F	401	-	-	0/19/38/38	0/3/3/3
12	VLB	C	501	-	-	16/40/131/131	0/7/9/9
10	EP	D	503	-	3/3/12/12	8/50/55/55	1/3/3/3
9	LOC	B	503	-	-	0/12/25/25	0/3/3/3
11	POU	B	505	-	4/4/14/14	24/54/76/76	1/1/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	504	BKF	C27-C26	-5.31	1.48	1.52
12	C	501	VLB	C57-N56	5.18	1.59	1.47
12	C	501	VLB	C58-C59	-3.69	1.45	1.51
12	C	501	VLB	C67-N66	3.56	1.43	1.38
12	C	501	VLB	C19-N9	3.26	1.52	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	VLB	C57-C58-C59	6.98	124.94	113.65
12	C	501	VLB	O25-C23-C3	6.61	123.08	112.21
12	C	501	VLB	C52-C69-N56	5.88	121.05	111.20
10	D	503	EP	C5-C10-C12	4.98	142.43	128.86
12	C	501	VLB	O72-C54-C70	-4.97	100.35	108.74

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	504	EP	C24
10	B	504	EP	C41
10	B	504	EP	C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	B	504	EP	C27
10	D	503	EP	C24

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	PB-O3B-PG-O3G

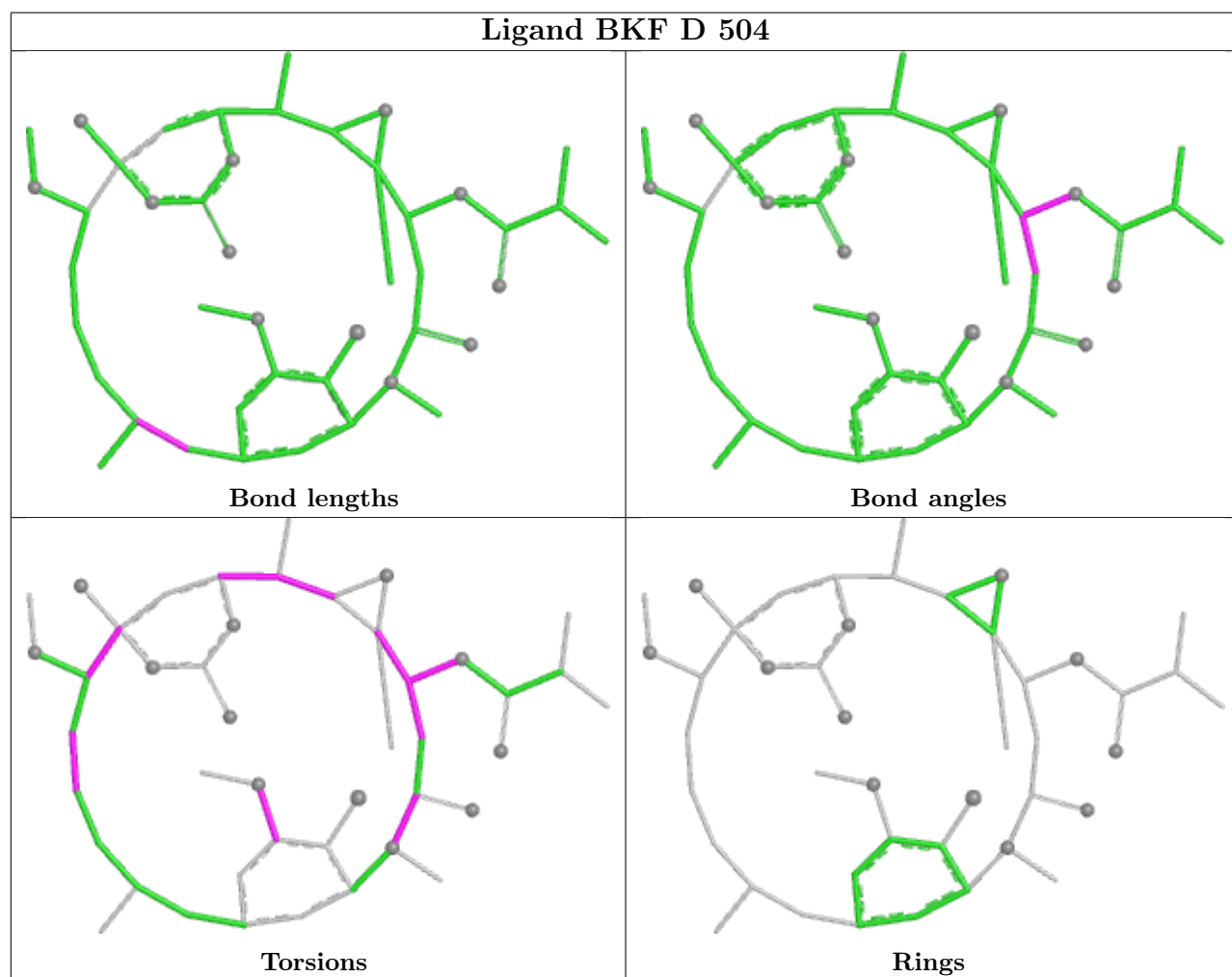
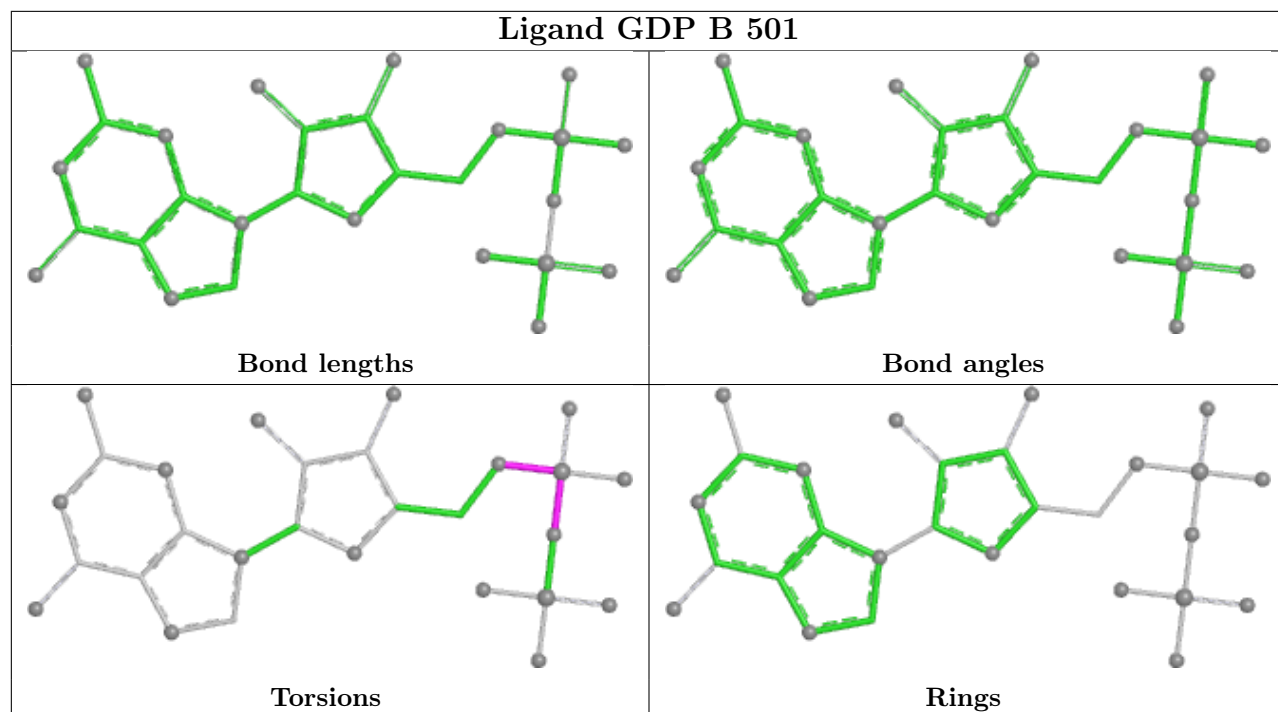
All (3) ring outliers are listed below:

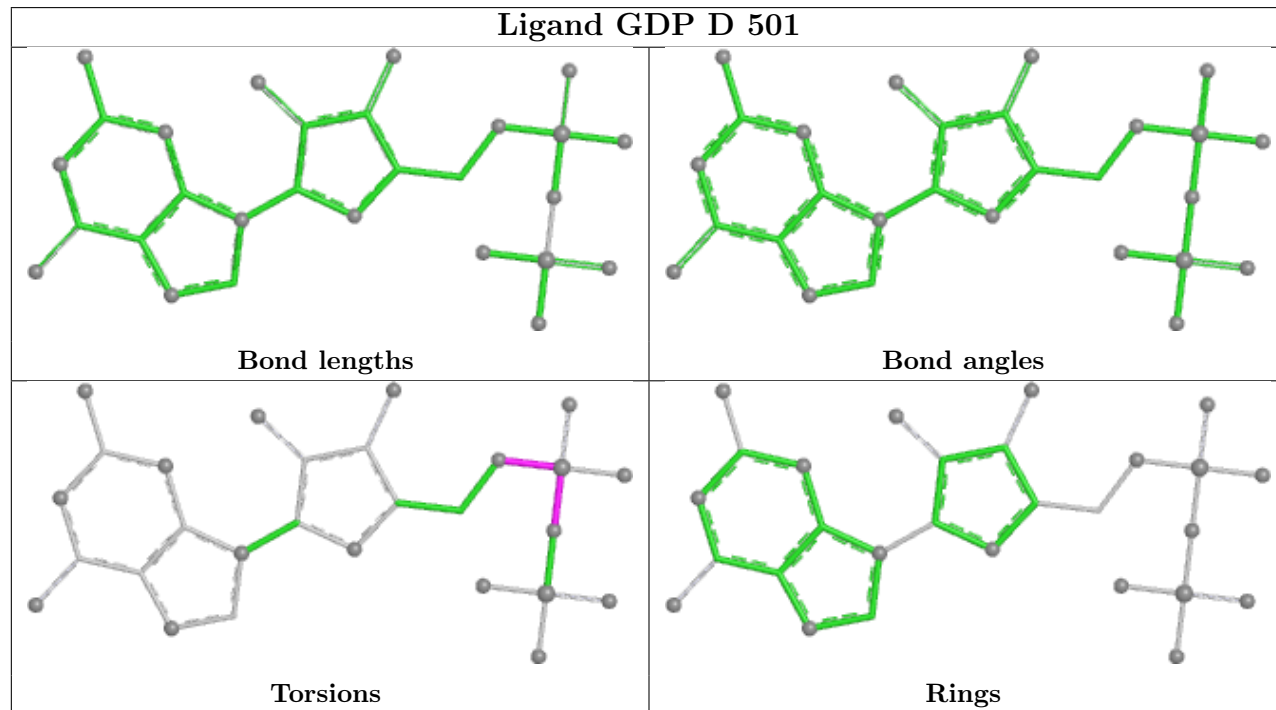
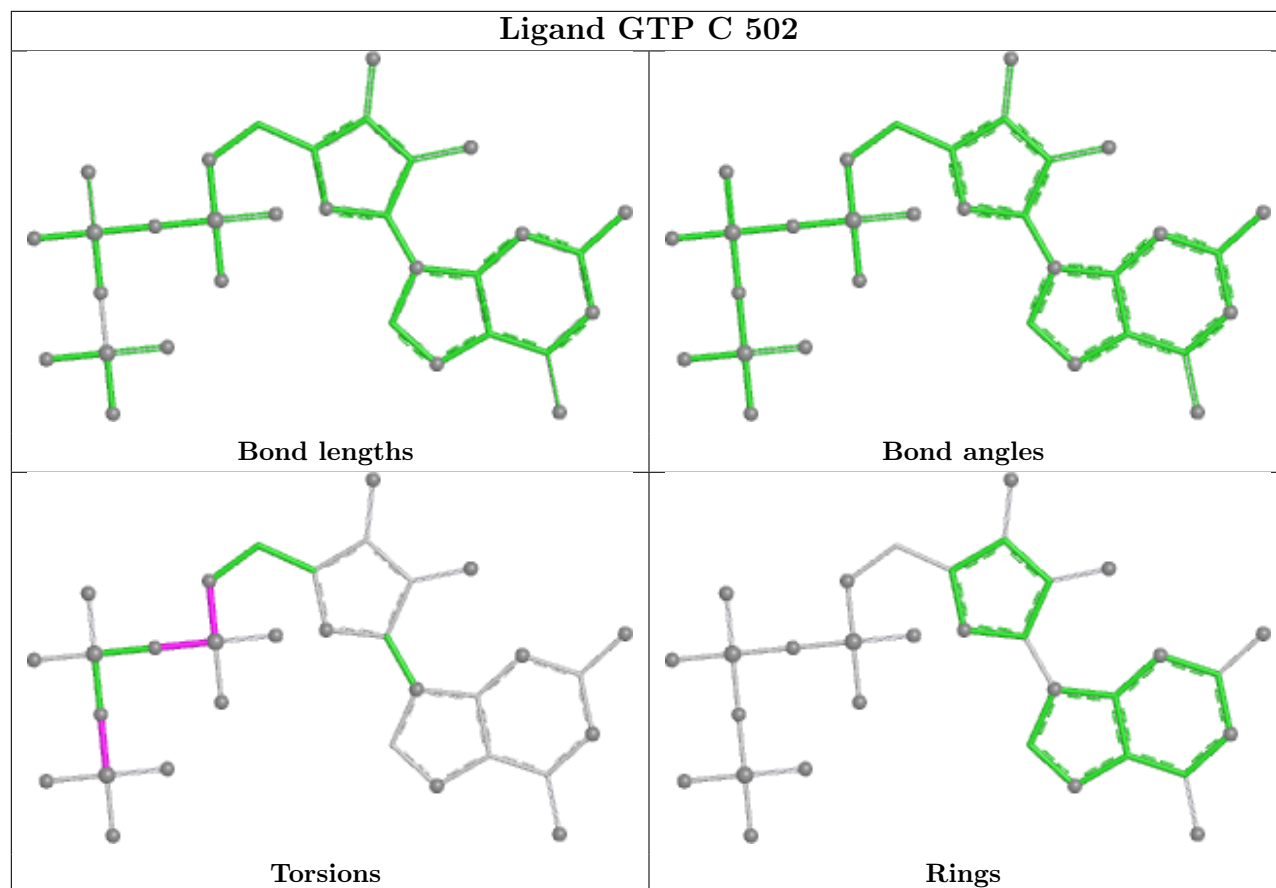
Mol	Chain	Res	Type	Atoms
11	B	505	POU	C5-C6-C7-C8-C9-O9
10	D	503	EP	C21-C24-C27-C3-C32-C35-C38-C41-C47-C51-C57-C59-C68-C72-C75-O2
10	B	504	EP	C21-C24-C27-C3-C32-C35-C38-C41-C47-C51-C57-C59-C68-C72-C75-O2

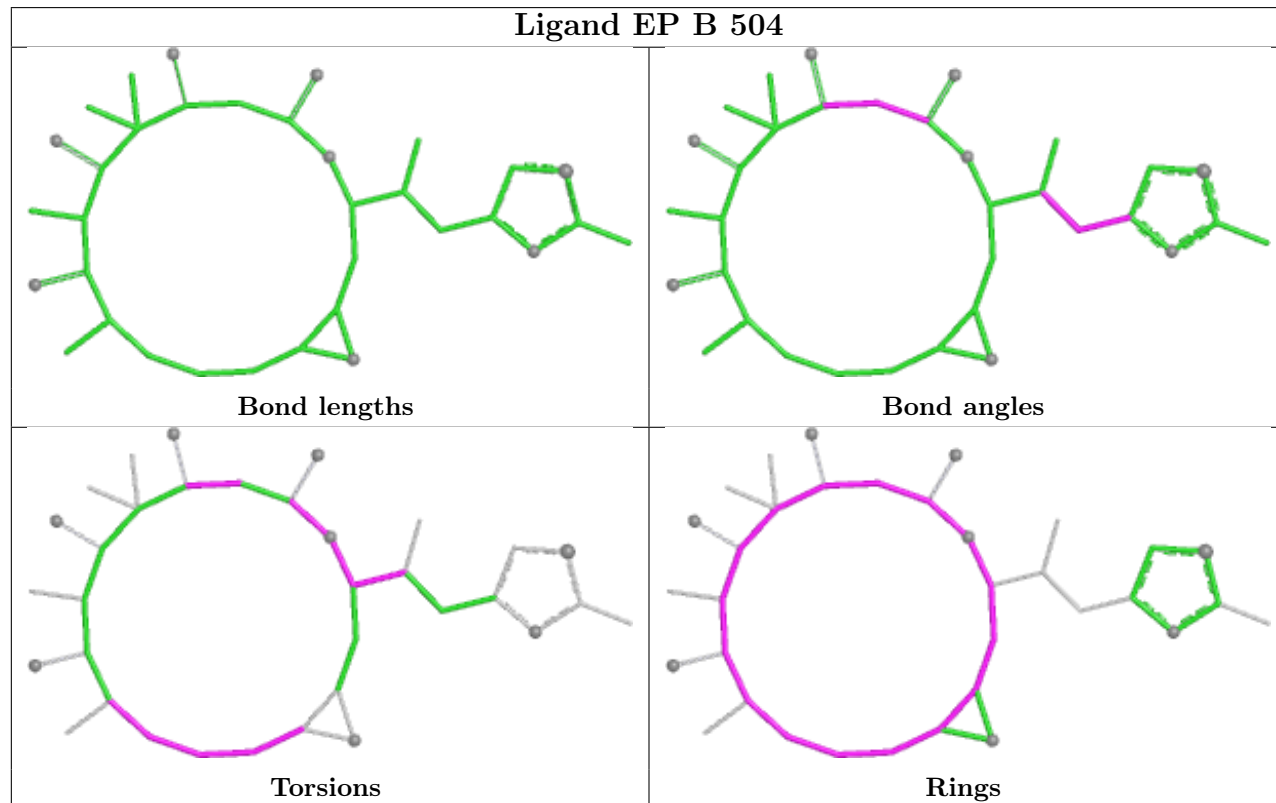
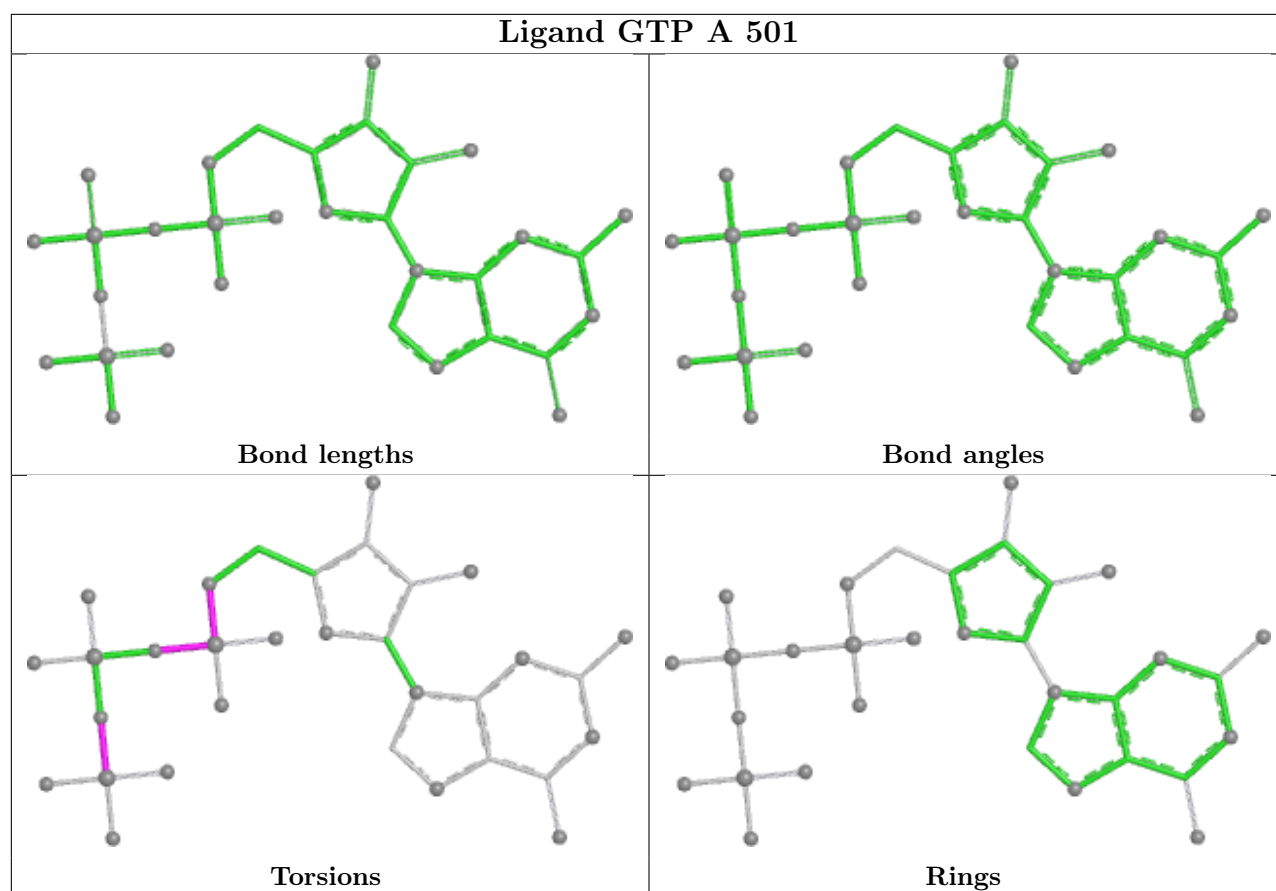
6 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	504	BKF	3	0
10	B	504	EP	10	0
12	C	501	VLB	5	0
10	D	503	EP	6	0
9	B	503	LOC	6	0
11	B	505	POU	6	0

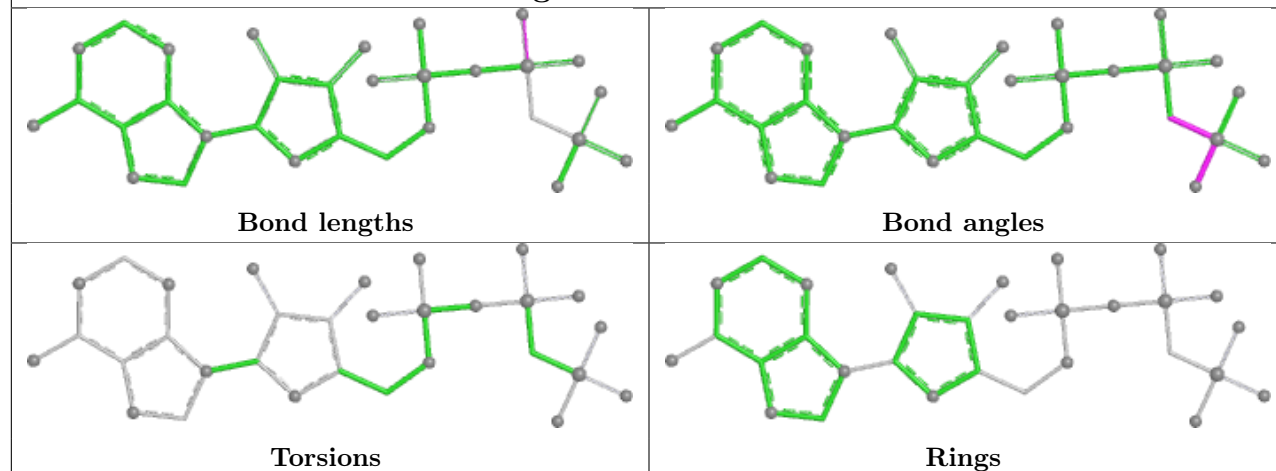
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



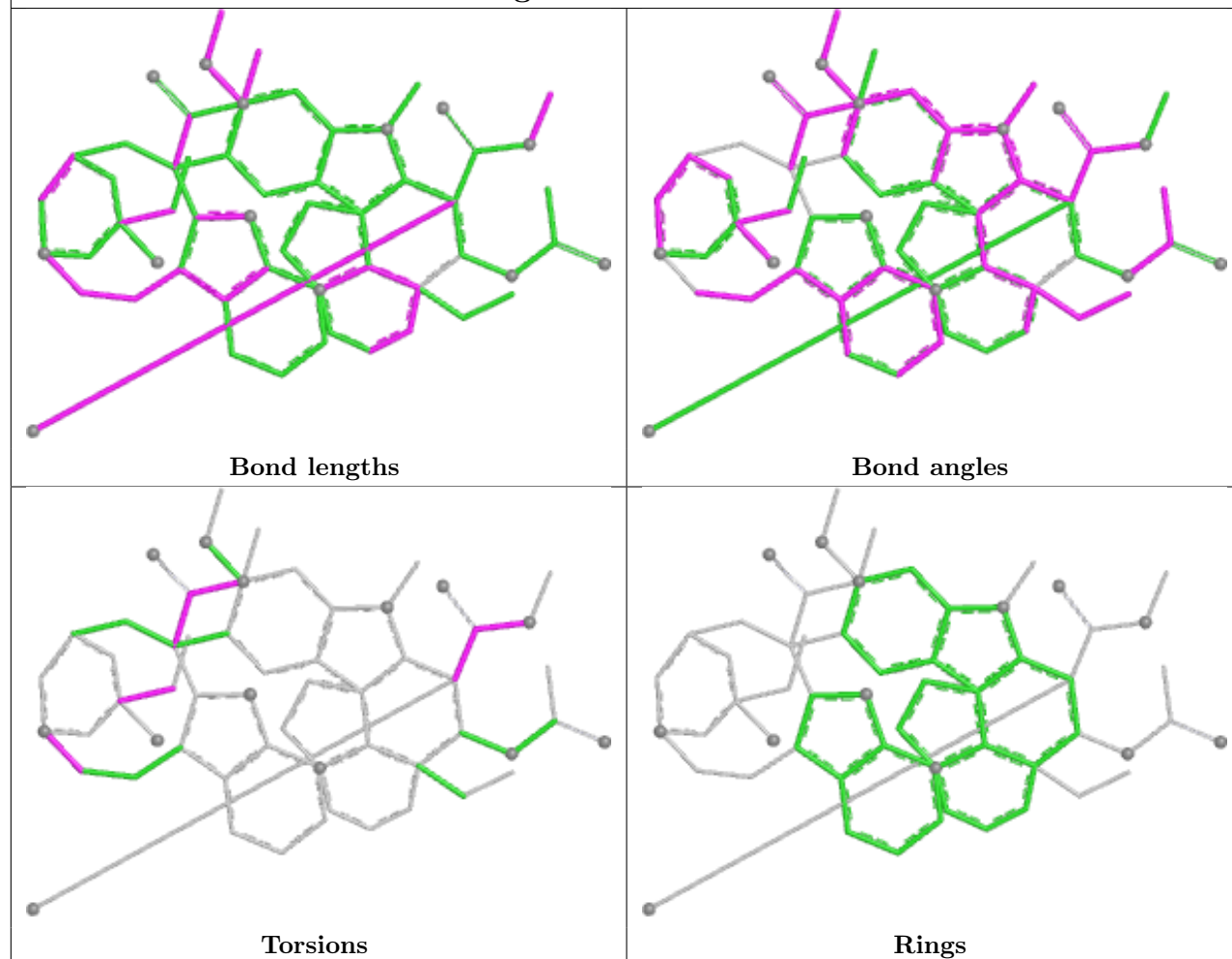


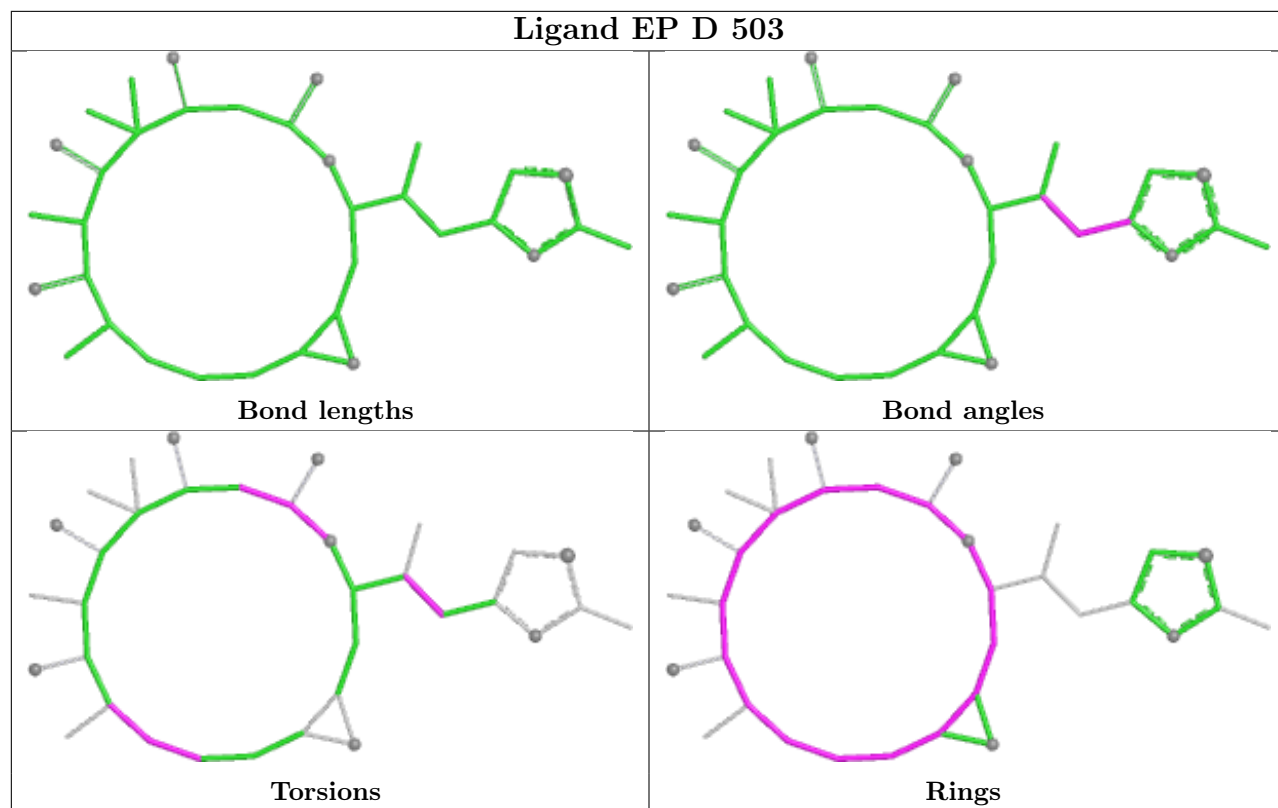


Ligand ACP F 401

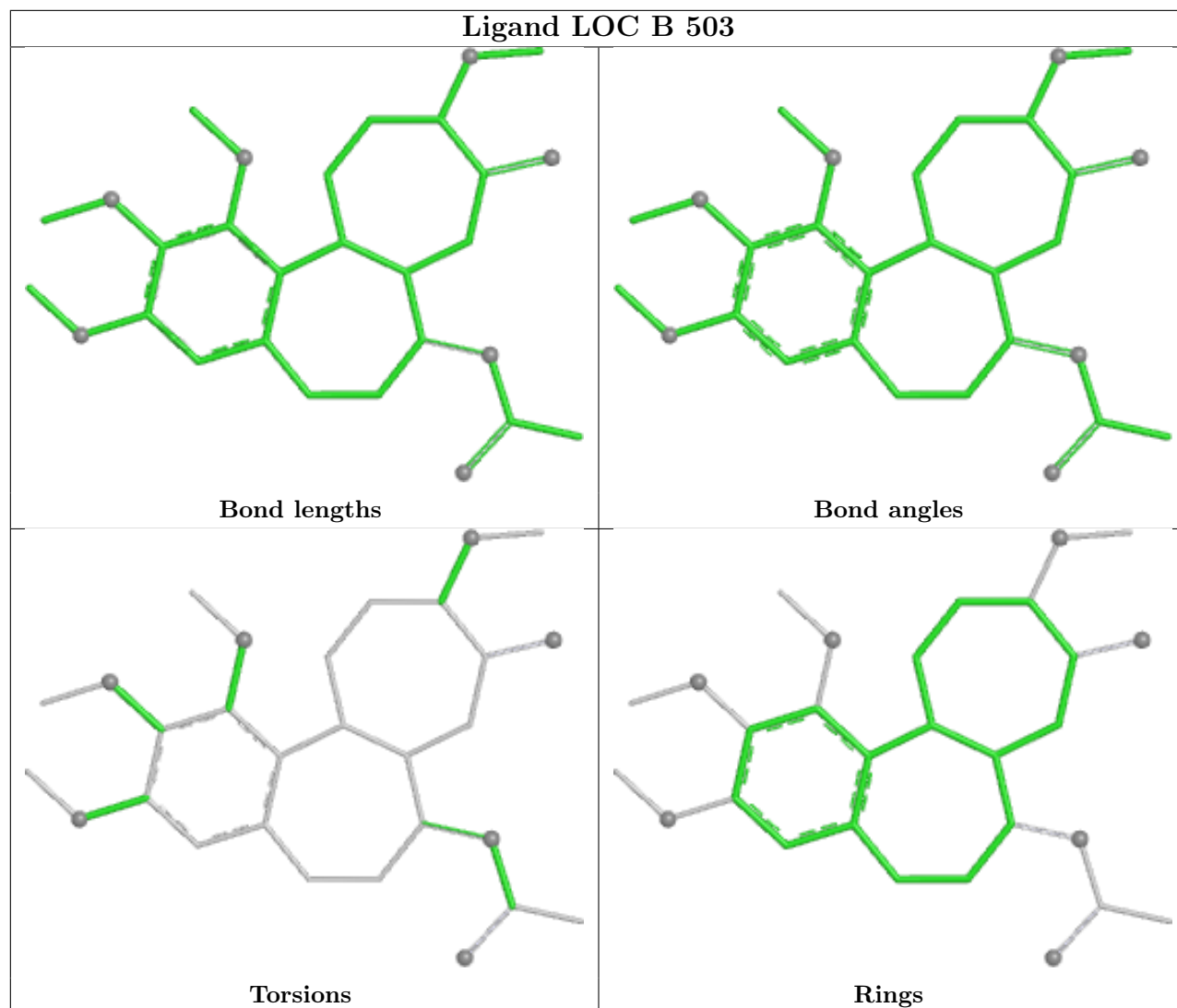


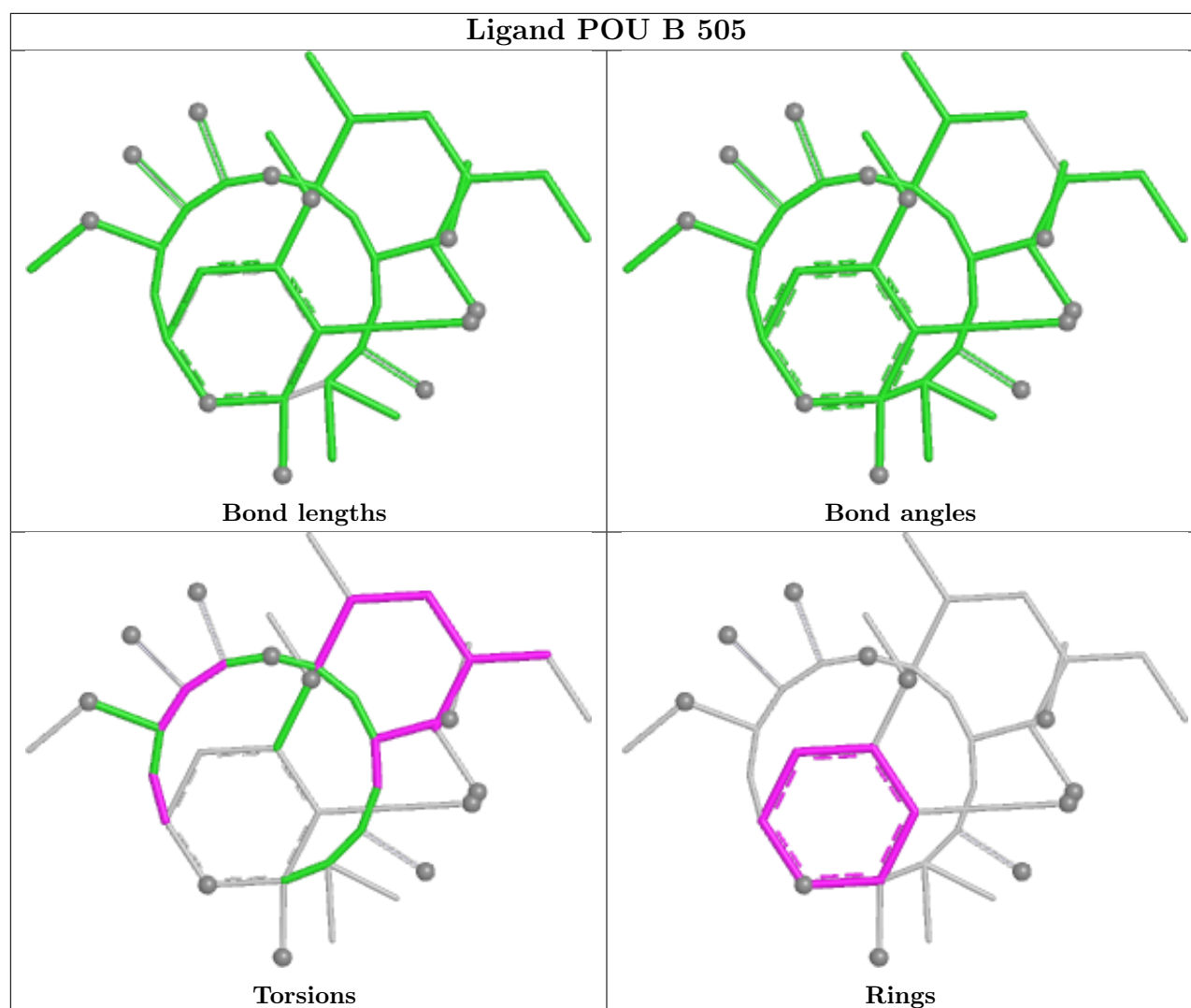
Ligand VLB C 501





Ligand LOC B 503





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
1	A	2
2	D	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	176[A]:GLN	C	177:VAL	N	5.41
1	A	176[B]:GLN	C	177:VAL	N	5.38
1	D	360:PRO	C	369:ARG	N	2.73
1	B	42:LEU	C	45:GLN	N	2.66

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%)	0.01	12 (2%) 56 51	31, 68, 115, 214	2 (0%)
1	C	440/440 (100%)	-0.11	9 (2%) 65 61	29, 57, 93, 129	4 (0%)
2	B	429/430 (99%)	0.02	12 (2%) 55 50	26, 61, 113, 179	5 (1%)
2	D	430/430 (100%)	0.15	13 (3%) 52 48	48, 78, 125, 181	3 (0%)
3	E	123/138 (89%)	0.55	7 (5%) 29 26	48, 86, 138, 179	1 (0%)
4	F	332/381 (87%)	0.60	19 (5%) 29 26	45, 103, 171, 200	1 (0%)
All	All	2193/2259 (97%)	0.13	72 (3%) 49 45	26, 71, 137, 214	16 (0%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	247[A]	GLN	6.1
4	F	362	ALA	4.4
1	C	249	ASN	4.3
4	F	173	ILE	4.2
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 ⓘ

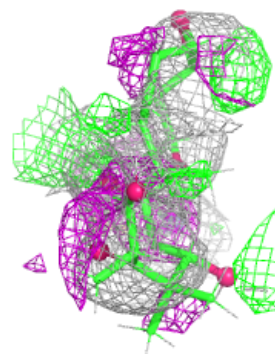
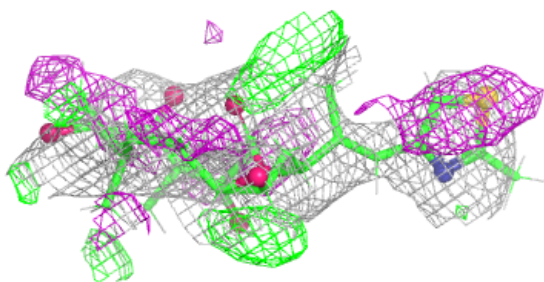
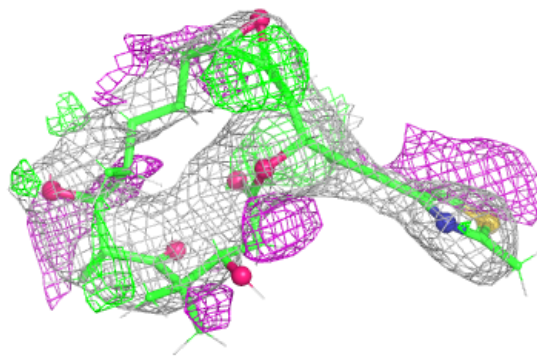
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	EP	B	504	34/34	0.65	0.19	87,119,148,155	0
6	MG	B	502	1/1	0.74	0.24	83,83,83,83	0
11	POU	B	505	38/38	0.74	0.17	69,109,151,169	0
13	BKF	D	504	44/44	0.74	0.17	89,117,144,159	0
6	MG	D	502	1/1	0.79	0.13	93,93,93,93	0
14	ACP	F	401	31/31	0.80	0.11	109,123,156,174	0
10	EP	D	503	34/34	0.83	0.14	92,113,129,139	0
9	LOC	B	503	29/29	0.93	0.09	57,74,97,98	0
8	GDP	D	501	28/28	0.94	0.10	65,75,96,114	0
12	VLB	C	501	59/59	0.95	0.08	47,63,76,77	0
5	GTP	A	501	32/32	0.96	0.08	49,59,65,75	0
8	GDP	B	501	28/28	0.97	0.07	46,51,55,63	0
5	GTP	C	502	32/32	0.97	0.07	42,51,57,60	0
7	CA	A	503	1/1	0.97	0.04	96,96,96,96	0
7	CA	C	504	1/1	0.98	0.04	89,89,89,89	0
6	MG	A	502	1/1	0.99	0.02	56,56,56,56	0
6	MG	C	503	1/1	1.00	0.04	52,52,52,52	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.

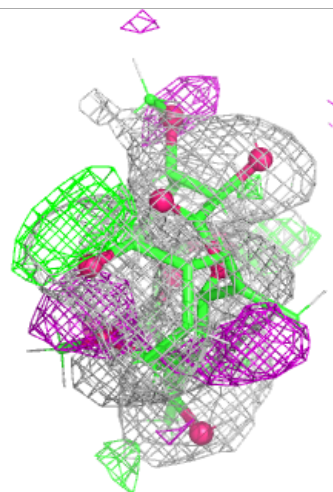
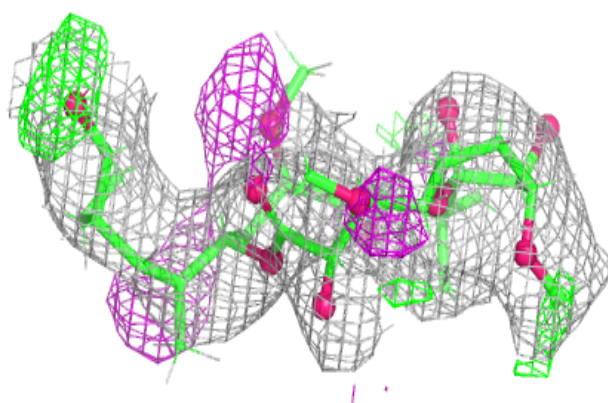
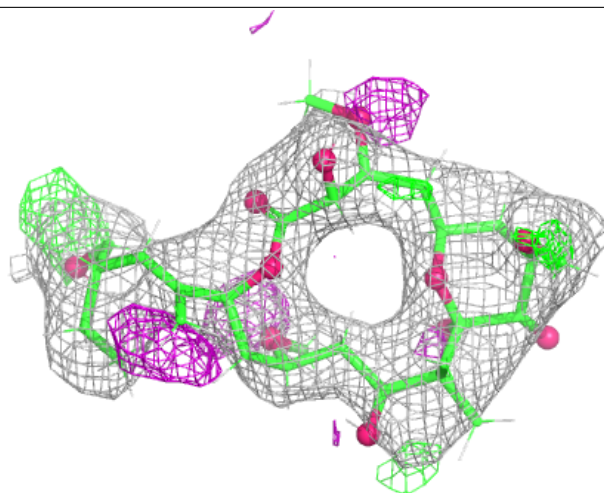
Electron density around EP B 504:

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



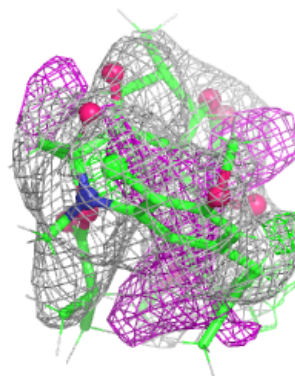
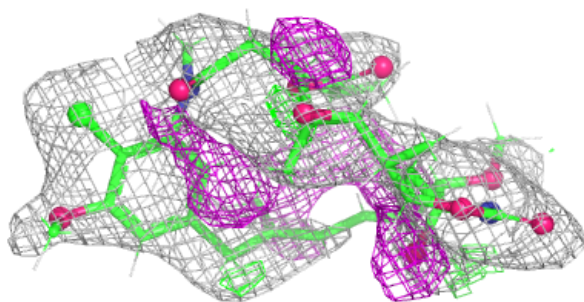
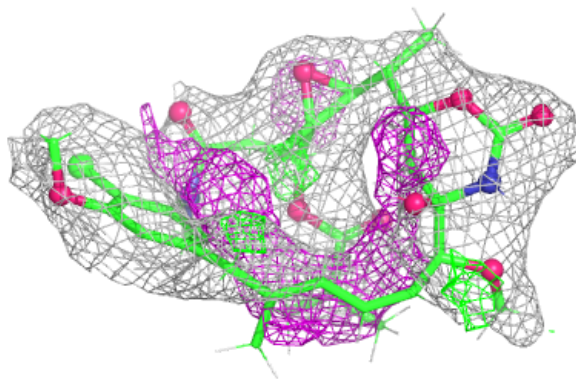
Electron density around POU B 505:

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

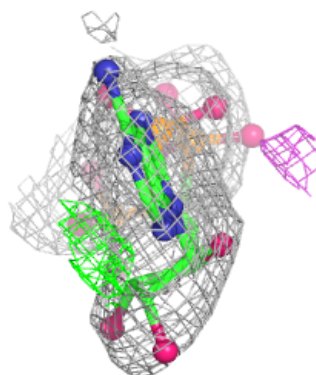
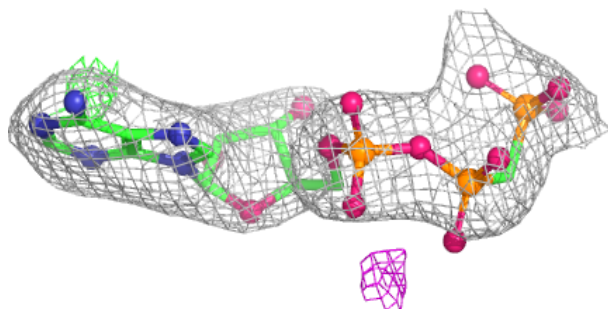
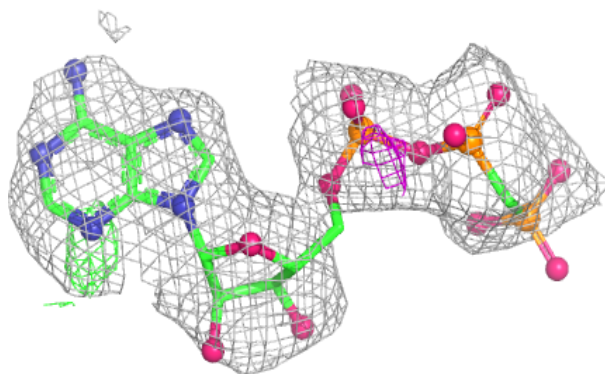


Electron density around BKF D 504:

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

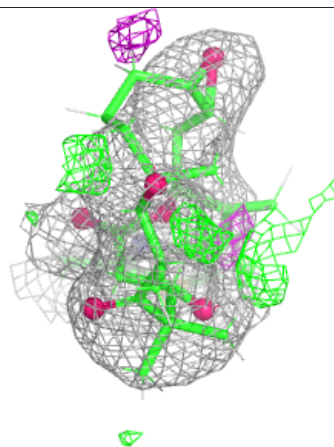
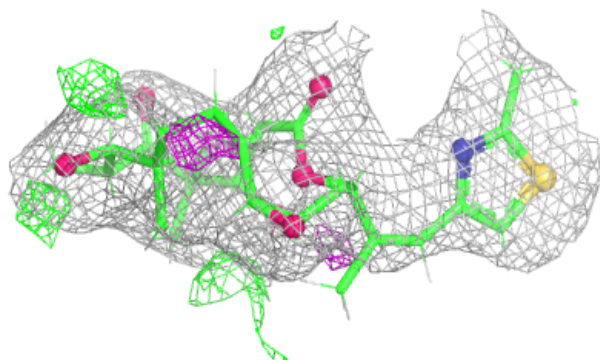
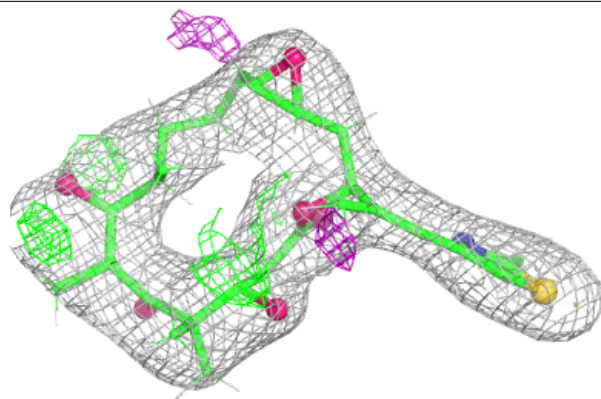
**Electron density around ACP F 401:**

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



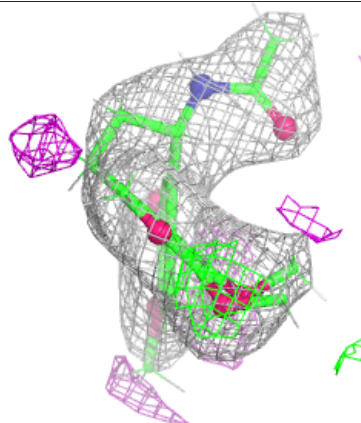
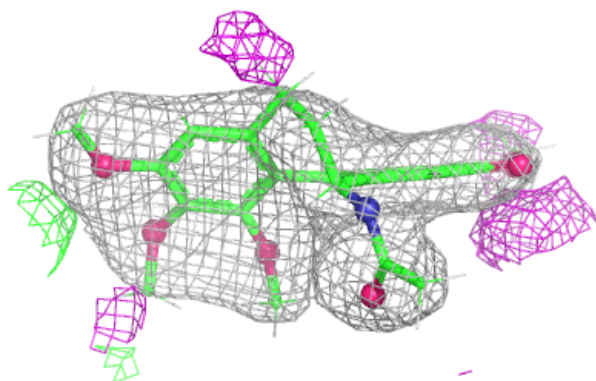
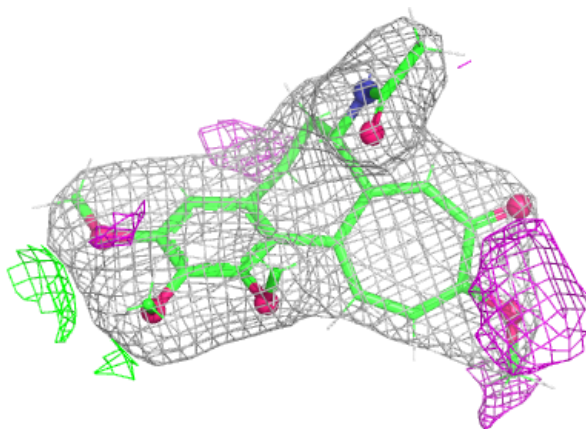
Electron density around EP D 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



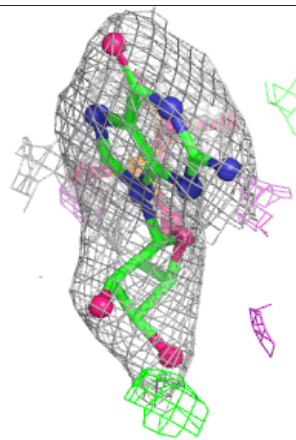
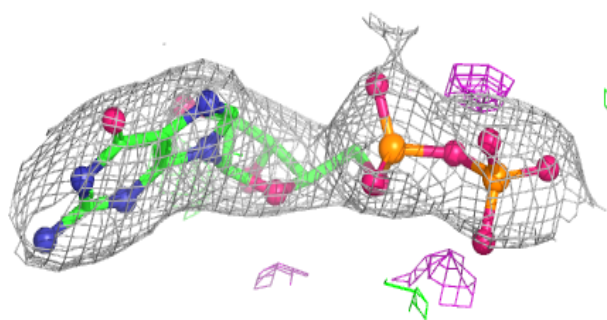
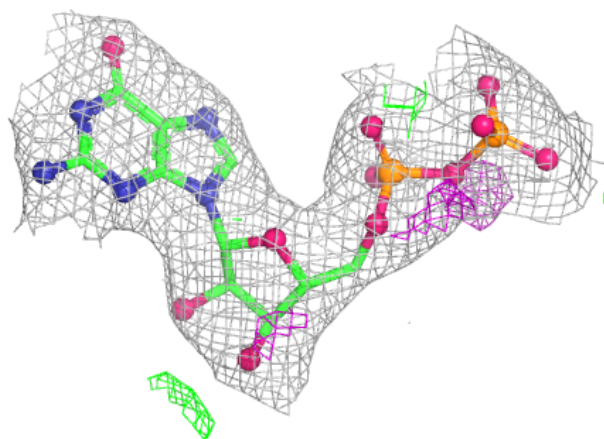
Electron density around LOC B 503:

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



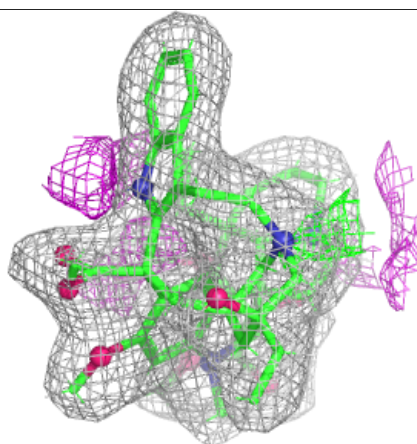
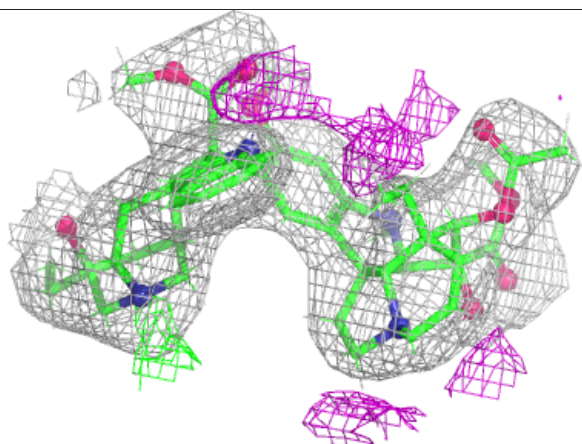
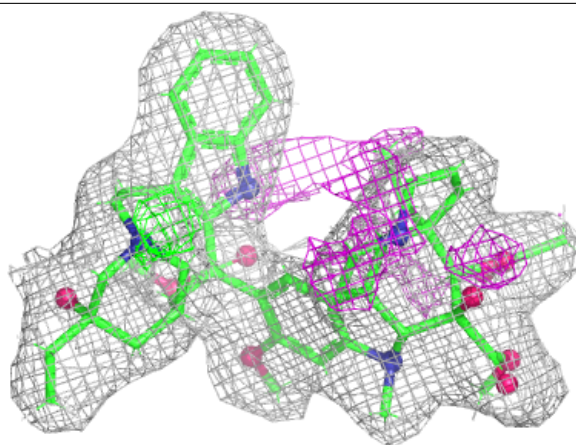
Electron density around GDP D 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

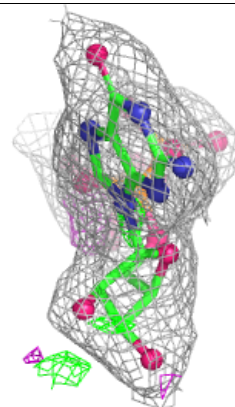
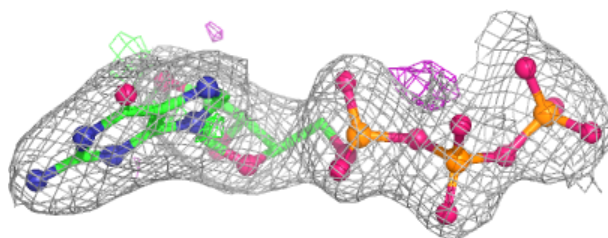
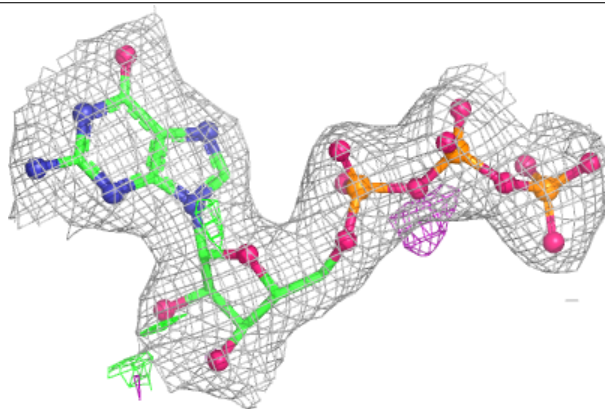


Electron density around VLB C 501:

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and green (positive)

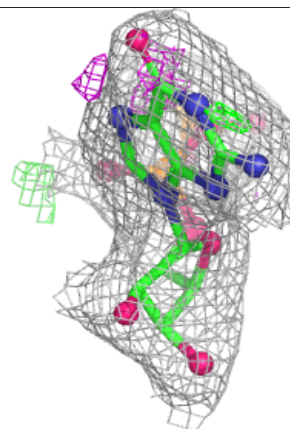
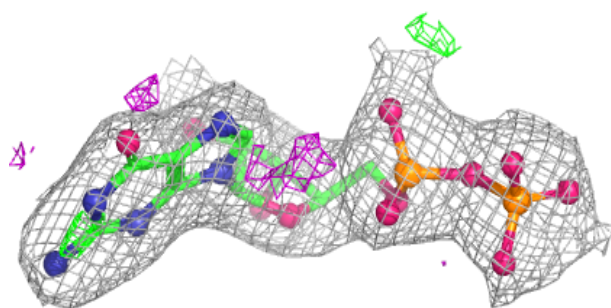
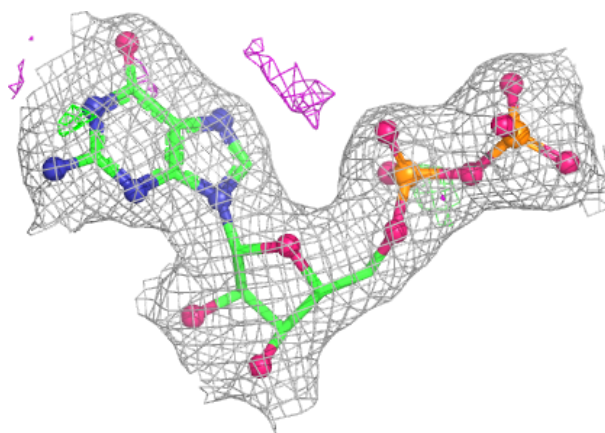
**Electron density around GTP A 501:**

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

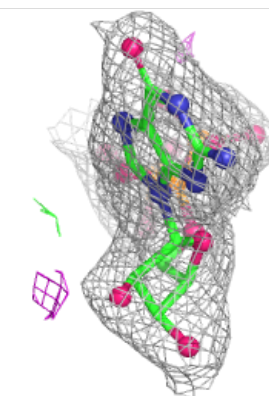
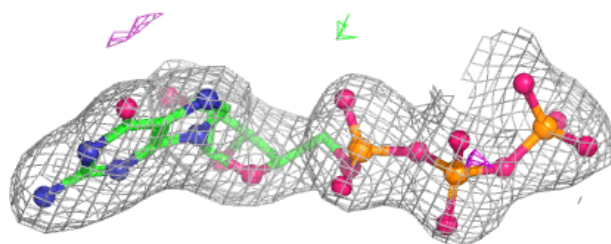
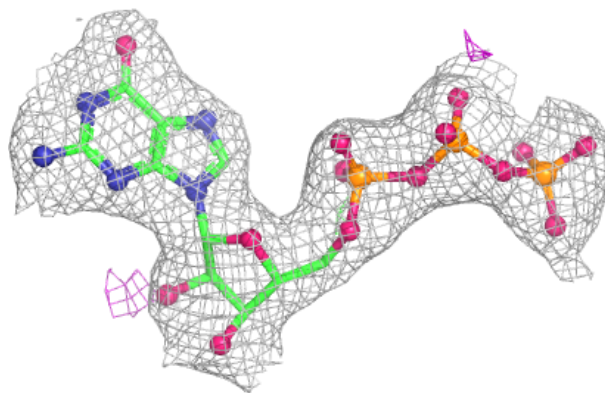


Electron density around GDP B 501:

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

**Electron density around GTP C 502:**

$2mF_o-DF_c$ (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.