W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2023 – 03:09 PM JST

PDB ID	:	5JCB
Title	:	Microtubule depolymerizing agent podophyllotoxin derivative YJTSF1
Authors	:	Guan, Z.; Zhao, W.; Yin, P.
Deposited on	:	2016-04-14
Resolution	:	2.30 Å(reported)

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

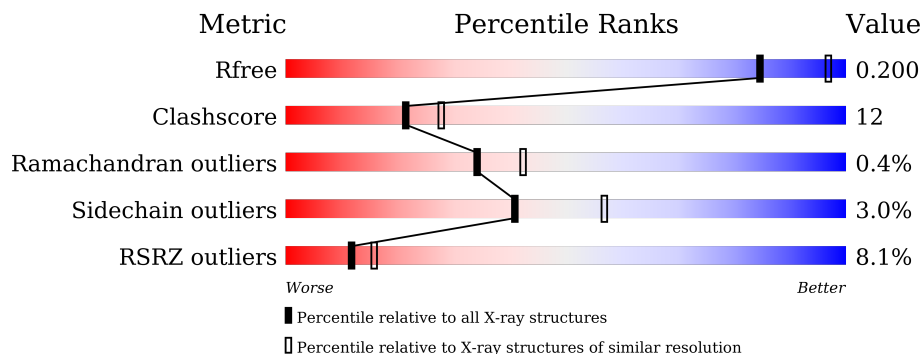|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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		0.200
Clashscore		12
Ramachandran outliers		0.4%
Sidechain outliers		3.0%
RSRZ outliers		8.1%

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	3% · 79% · 17% · ·
1	C	451	2% · 77% · 20% ·
2	B	445	5% · 73% · 20% · 5%
2	D	445	10% · 70% · 23% · 6%
3	E	152	6% · 66% · 13% · 20%
4	F	388	19% · 56% · 21% · 20%

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
13	NV4	D	507	-	-	X	-
7	GOL	C	501	-	-	X	X
7	GOL	C	504	-	-	X	-
8	IMD	A	505	-	-	X	-

2 Entry composition ⓘ

There are 16 unique types of molecules in this entry. The entry contains 18127 atoms, of which 13 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
			3482	2213	585	659	25			
1	C	440	Total	C	N	O	S	0	9	0
			3481	2204	587	667	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	11	0
			3382	2129	570	657	26			
2	D	418	Total	C	N	O	S	0	5	0
			3316	2089	561	638	28			

- Molecule 3 is a protein called Stathmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1010	624	182	198	6			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP F2Z508
E	146	LEU	-	expression tag	UNP F2Z508
E	147	GLU	-	expression tag	UNP F2Z508
E	148	HIS	-	expression tag	UNP F2Z508
E	149	HIS	-	expression tag	UNP F2Z508
E	150	HIS	-	expression tag	UNP F2Z508
E	151	HIS	-	expression tag	UNP F2Z508
E	152	HIS	-	expression tag	UNP F2Z508
E	153	HIS	-	expression tag	UNP F2Z508
E	154	HIS	-	expression tag	UNP F2Z508

Continued on next page...

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	155	HIS	-	expression tag	UNP F2Z508

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	312	2577	1673	428	462	14	0	4	0

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

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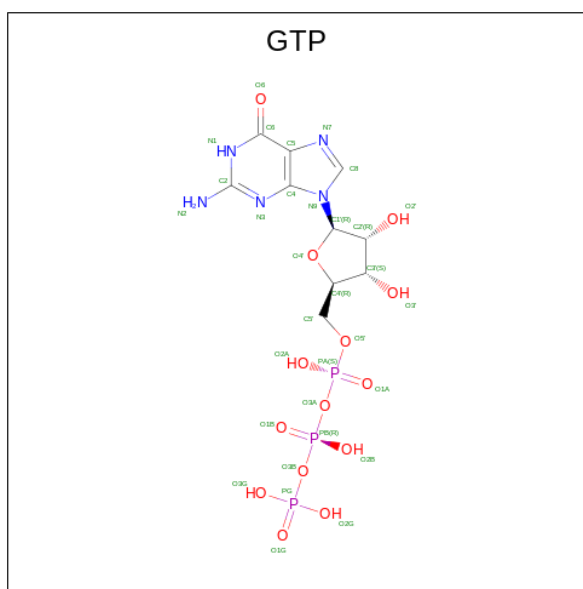
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0
			Total	Mg		
6	B	1	1	1	0	0
			Total	Mg		
6	C	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total 2	Mg 2	0	0
6	F	1	Total 1	Mg 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
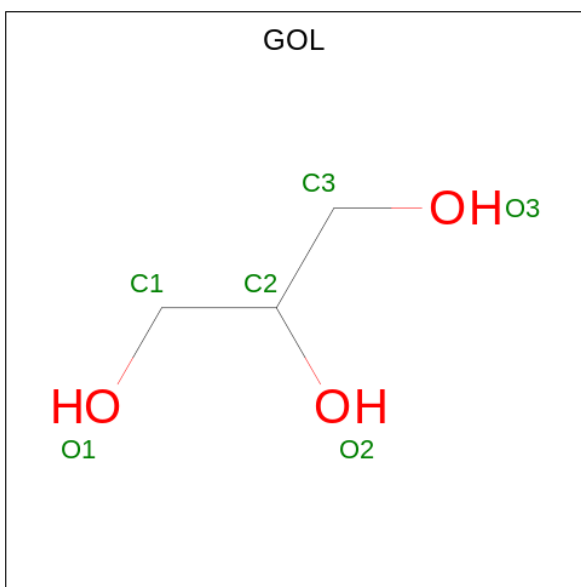
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3		0	0
7	A	1	Total 6	C 3	O 3		0	0
7	C	1	Total 6	C 3	O 3		0	0
7	C	1	Total 6	C 3	O 3		0	0
7	C	1	Total 14	C 3	H 8	O 3	0	0
7	D	1	Total 6	C 3	O 3		0	0
7	D	1	Total 6	C 3	O 3		0	0
7	D	1	Total 6	C 3	O 3		0	0

- Molecule 8 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).
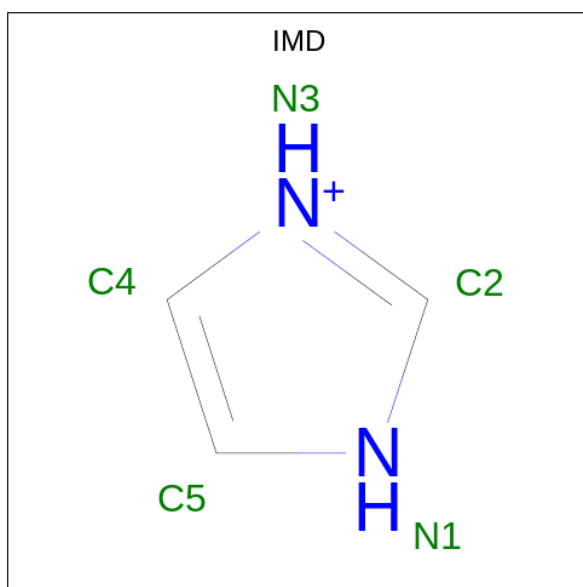
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 10	C 3	H 5	N 2	0	0
8	C	1	Total 5	C 3	N 2		0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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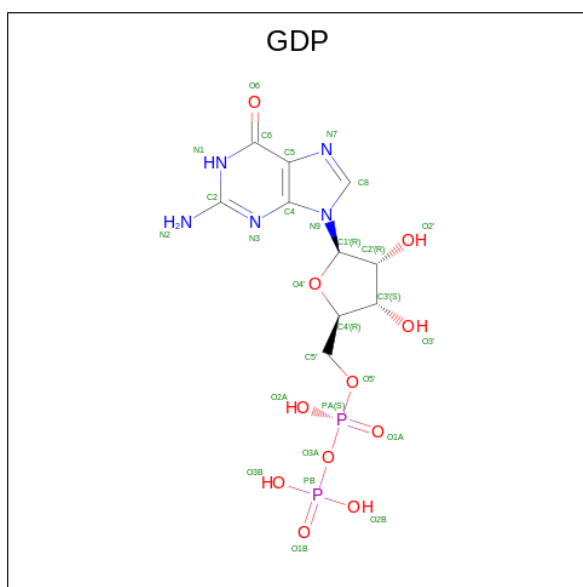
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Na	0	0
			1	1		
11	C	1	Total	Na	0	0
			1	1		

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

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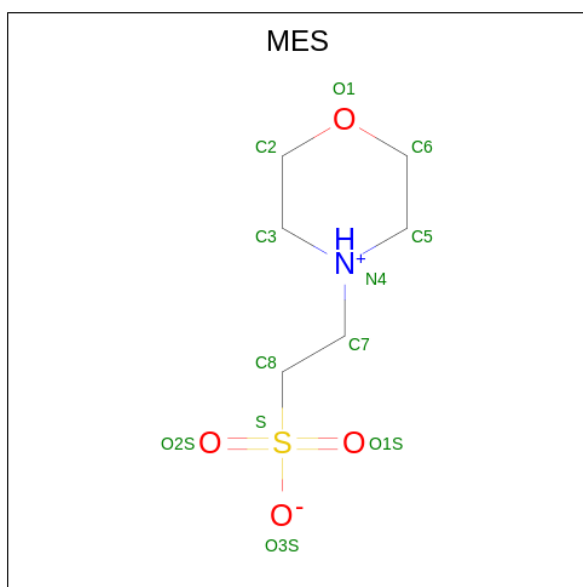
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 13 is (5R,5aR,8aS,9R)-9-[(4H-1,2,4-triazol-3-yl)sulfanyl]-5-(3,4,5-trimethoxyphenyl)-5,8,8a,9-tetrahydro-2H-furo[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one (three-letter code: NV4) (formula: $C_{24}H_{23}N_3O_7S$).
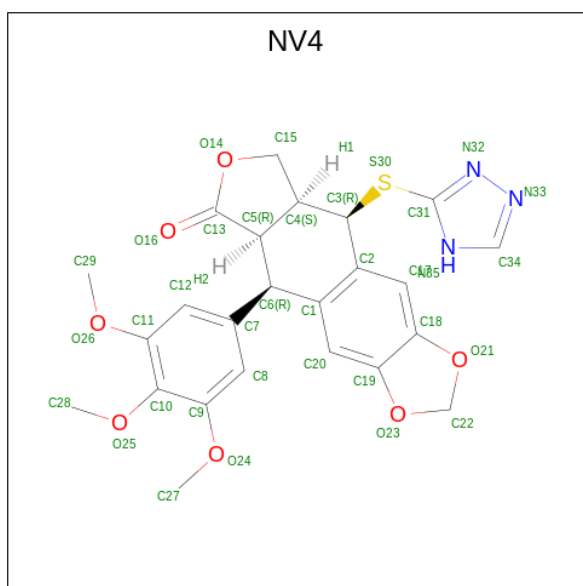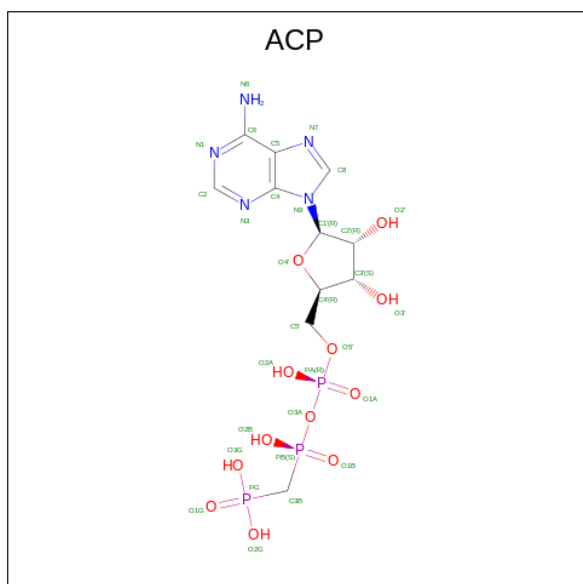
NV4

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	N	O	S	0	0
			35	24	3	7	1		
13	D	1	Total	C	N	O	S	0	0
			35	24	3	7	1		

- Molecule 14 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
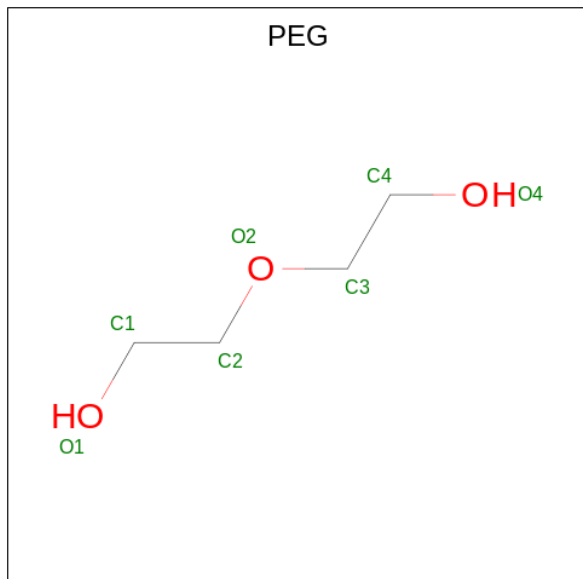
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	C	1	7	4	3	0	0

- Molecule 15 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
			Total	C	N	O	P		
15	F	1	31	11	5	12	3	0	0

• Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	115	Total 115	O 115	0	0
16	B	84	Total 84	O 84	0	0
16	C	199	Total 199	O 199	0	0
16	D	66	Total 66	O 66	0	0
16	E	28	Total 28	O 28	0	0
16	F	65	Total 65	O 65	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.
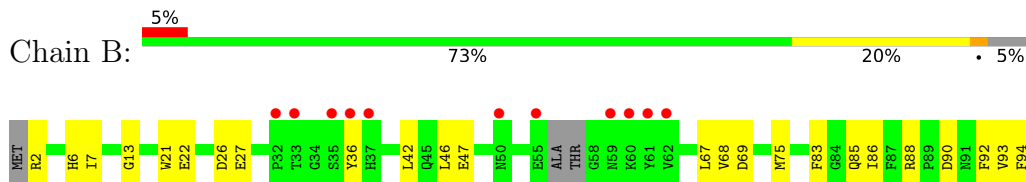
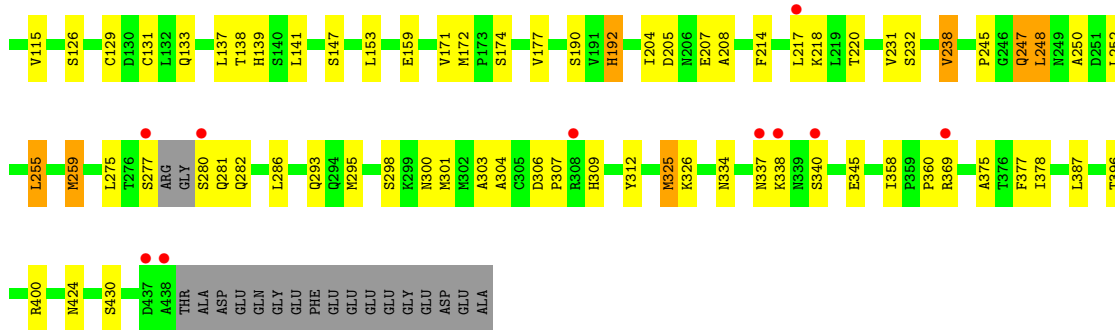- Molecule 1: Tubulin alpha-1B chain
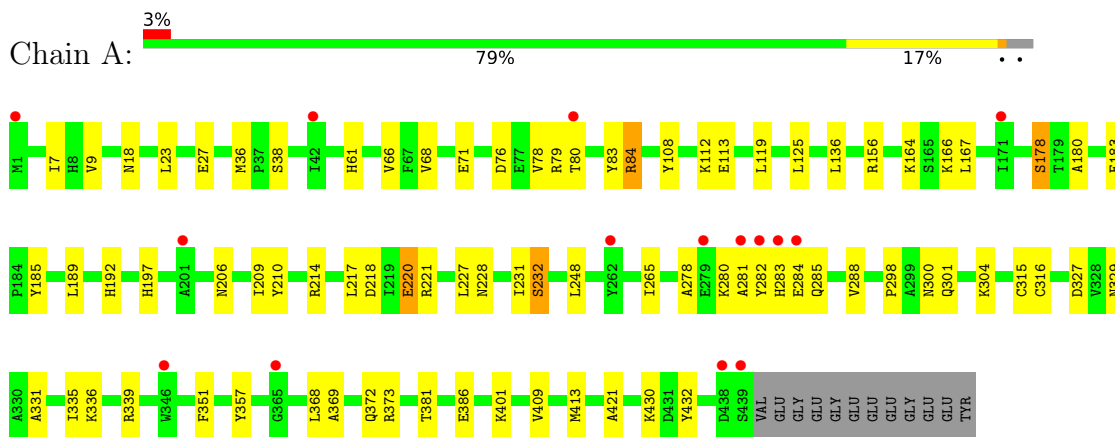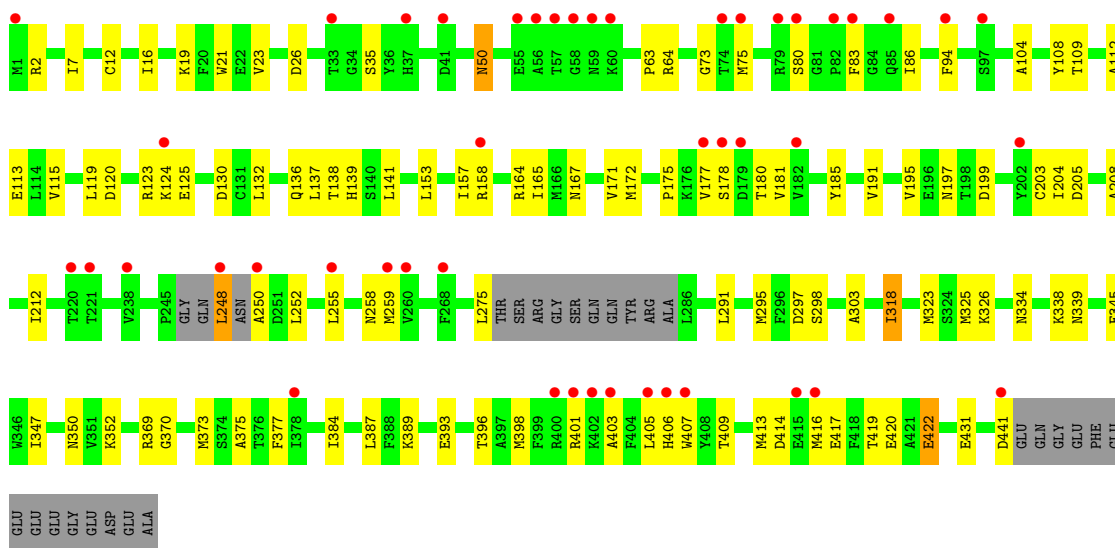

- Molecule 1: Tubulin alpha-1B chain
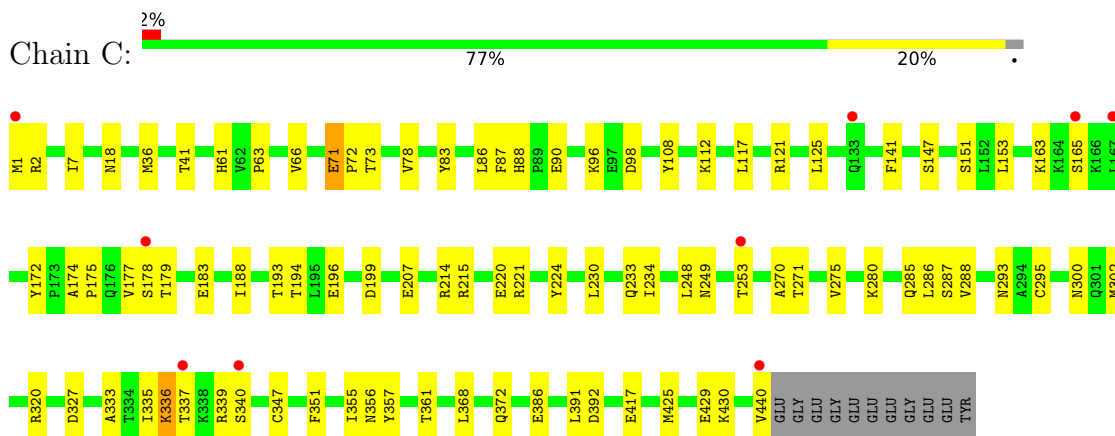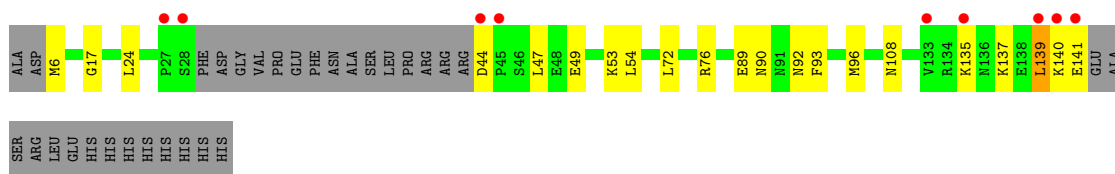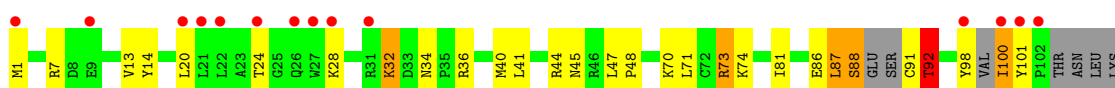

- Molecule 2: Tubulin beta chain

• Molecule 2: Tubulin beta chain

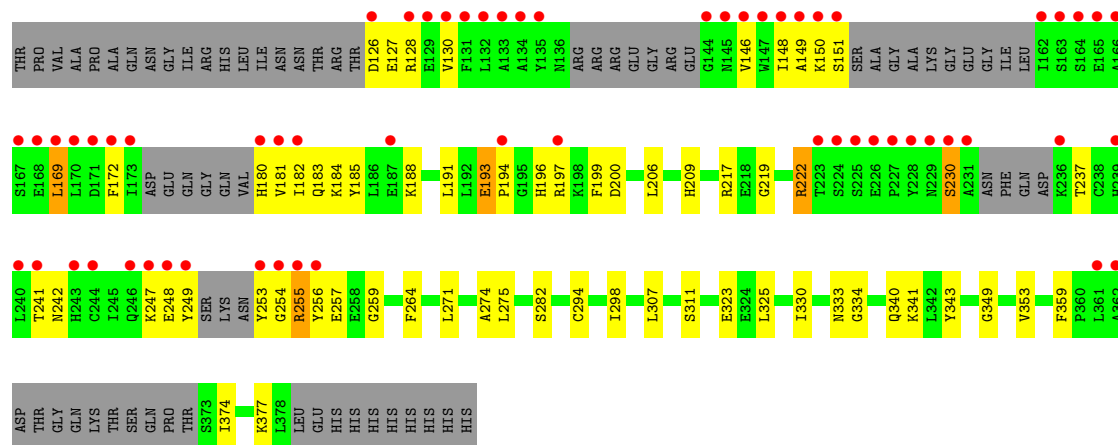• Molecule 3: Stathmin

• 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	104.36Å 157.25Å 179.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 2.30 47.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.64-2.30) 99.8 (47.64-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.181 , 0.200 0.181 , 0.200	Depositor DCC
R_{free} test set	6500 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18127	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: IMD, CA, MG, ACP, MES, NA, GTP, GDP, NV4, GOL, PEG

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	0.41	0/3596	0.56	0/4883
1	C	0.51	1/3583 (0.0%)	0.60	0/4866
2	B	0.42	0/3485	0.57	0/4718
2	D	0.37	0/3399	0.53	0/4602
3	E	0.38	0/1024	0.51	0/1358
4	F	0.42	0/2644	0.53	0/3566
All	All	0.43	1/17731 (0.0%)	0.56	0/23993

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-6.82	1.70	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3482	0	3434	66	0
1	C	3481	0	3401	82	0
2	B	3382	0	3270	82	0
2	D	3316	0	3213	81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1010	0	1033	25	0
4	F	2577	0	2576	100	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	F	1	0	0	0	0
7	A	12	0	16	2	0
7	C	18	8	24	10	0
7	D	18	0	23	2	0
8	A	5	5	5	4	0
8	C	5	0	5	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
12	B	12	0	12	0	0
13	B	35	0	0	3	0
13	D	35	0	0	9	0
14	C	7	0	10	0	0
15	F	31	0	13	3	0
16	A	115	0	0	10	1
16	B	84	0	0	4	0
16	C	199	0	0	17	1
16	D	66	0	0	7	0
16	E	28	0	0	6	0
16	F	65	0	0	9	0
All	All	18114	13	17083	416	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 12.

The worst 5 of 416 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:C:221:ARG:HD2	2:D:325:MET:HB3	1.29	1.09
4:F:100:ILE:HD11	4:F:127:GLU:H	1.15	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLU:HB3	2:D:326:LYS:HE3	1.46	0.98
2:B:27:GLU:HA	2:B:369:ARG:HH22	1.27	0.98
4:F:32:LYS:H	4:F:32:LYS:HD2	1.24	0.98

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)
16:A:665:HOH:O	16:C:677:HOH:O[3_554]	1.70	0.50

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	449/451 (100%)	437 (97%)	10 (2%)	2 (0%)	34	42
1	C	447/451 (99%)	434 (97%)	12 (3%)	1 (0%)	47	58
2	B	428/445 (96%)	414 (97%)	12 (3%)	2 (0%)	29	35
2	D	416/445 (94%)	407 (98%)	8 (2%)	1 (0%)	47	58
3	E	119/152 (78%)	118 (99%)	1 (1%)	0	100	100
4	F	296/388 (76%)	288 (97%)	6 (2%)	2 (1%)	22	26
All	All	2155/2332 (92%)	2098 (97%)	49 (2%)	8 (0%)	34	42

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA
2	D	73	GLY
4	F	92	THR
4	F	255	ARG
1	A	178	SER

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	382/379 (101%)	372 (97%)	10 (3%)	46	63
1	C	380/379 (100%)	374 (98%)	6 (2%)	62	78
2	B	377/383 (98%)	364 (97%)	13 (3%)	37	51
2	D	367/383 (96%)	357 (97%)	10 (3%)	44	61
3	E	111/136 (82%)	110 (99%)	1 (1%)	78	89
4	F	285/346 (82%)	270 (95%)	15 (5%)	22	31
All	All	1902/2006 (95%)	1847 (97%)	55 (3%)	41	58

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	430	LYS
2	D	259	MET
4	F	377	LYS
4	F	169	LEU
2	D	35	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
2	B	101	ASN
4	F	196	HIS

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 30 ligands modelled in this entry, 11 are monoatomic - leaving 19 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	#$|Z| > 2$
7	GOL	D	504	-	5,5,5	0.34	0	5,5,5	0.79	0
7	GOL	A	504	-	5,5,5	0.43	0	5,5,5	0.48	0
5	GTP	C	502	6	26,34,34	1.26	2 (7%)	32,54,54	1.35	3 (9%)
5	GTP	A	501	6	26,34,34	1.17	1 (3%)	32,54,54	1.41	7 (21%)
7	GOL	D	505	2	5,5,5	0.35	0	5,5,5	0.52	0
13	NV4	D	507	-	34,40,40	2.06	7 (20%)	49,59,59	2.53	19 (38%)
7	GOL	C	504	-	5,5,5	0.40	0	5,5,5	0.22	0
7	GOL	C	501	-	5,5,5	0.36	0	5,5,5	0.39	0
8	IMD	C	508	-	3,5,5	0.48	0	4,5,5	0.37	0
14	PEG	C	505	-	6,6,6	0.50	0	5,5,5	0.40	0
7	GOL	C	509	-	5,5,5	0.40	0	5,5,5	0.50	0
10	GDP	D	501	6	24,30,30	1.10	2 (8%)	30,47,47	1.16	3 (10%)
8	IMD	A	505	-	3,5,5	0.32	0	4,5,5	0.75	0
10	GDP	B	501	6	24,30,30	1.25	3 (12%)	30,47,47	1.33	3 (10%)
12	MES	B	504	-	12,12,12	2.09	1 (8%)	14,16,16	2.23	5 (35%)
7	GOL	D	506	-	5,5,5	0.40	0	5,5,5	0.73	0
7	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.25	0
15	ACP	F	402	6	27,33,33	4.93	9 (33%)	32,52,52	2.68	5 (15%)
13	NV4	B	505	-	34,40,40	2.11	8 (23%)	49,59,59	2.21	12 (24%)

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
7	GOL	D	504	-	-	2/4/4/4	-
7	GOL	A	504	-	-	4/4/4/4	-
5	GTP	C	502	6	-	7/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
7	GOL	D	505	2	-	2/4/4/4	-
13	NV4	D	507	-	-	3/12/49/49	0/6/6/6
7	GOL	C	504	-	-	2/4/4/4	-
7	GOL	C	501	-	-	2/4/4/4	-
8	IMD	C	508	-	-	-	0/1/1/1
14	PEG	C	505	-	-	1/4/4/4	-
7	GOL	C	509	-	-	2/4/4/4	-
10	GDP	D	501	6	-	5/12/32/32	0/3/3/3
8	IMD	A	505	-	-	-	0/1/1/1
10	GDP	B	501	6	-	4/12/32/32	0/3/3/3
12	MES	B	504	-	-	1/6/14/14	0/1/1/1
7	GOL	D	506	-	-	2/4/4/4	-
7	GOL	A	507	-	-	3/4/4/4	-
15	ACP	F	402	6	-	8/15/38/38	0/3/3/3
13	NV4	B	505	-	-	1/12/49/49	0/6/6/6

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	402	ACP	O4'-C1'	15.05	1.62	1.41
15	F	402	ACP	C2'-C1'	-14.85	1.31	1.53
15	F	402	ACP	PB-O3A	7.87	1.67	1.58
12	B	504	MES	C8-S	-7.12	1.67	1.77
15	F	402	ACP	O4'-C4'	-7.12	1.29	1.45

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	402	ACP	C5-C6-N6	10.51	136.33	120.35
15	F	402	ACP	N6-C6-N1	-7.01	104.03	118.57
13	D	507	NV4	C9-C10-C11	-6.65	112.76	119.57
13	D	507	NV4	O25-C10-C11	-6.63	110.58	120.12
13	B	505	NV4	C9-C10-C11	-6.11	113.31	119.57

There are no chirality outliers.
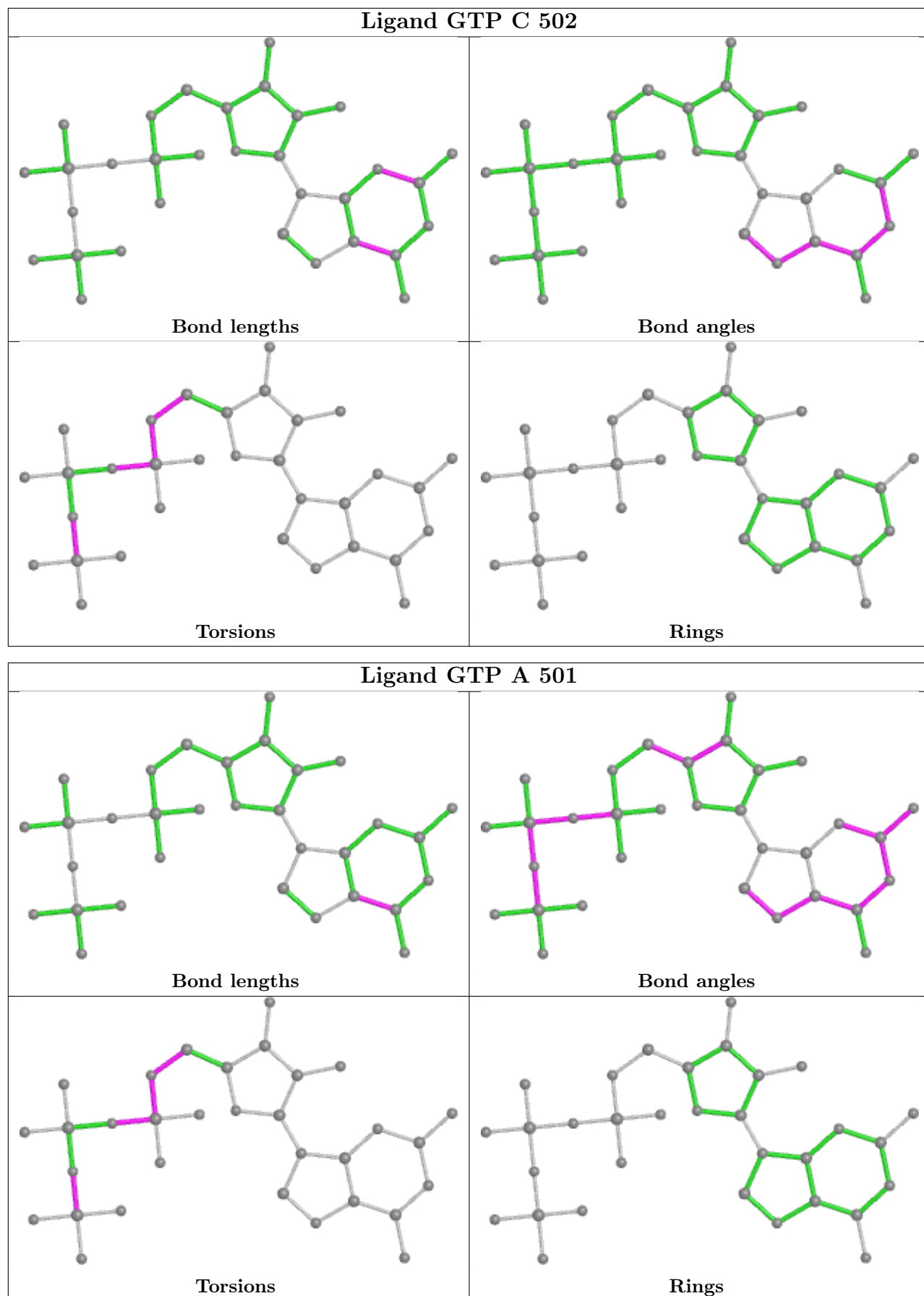
5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

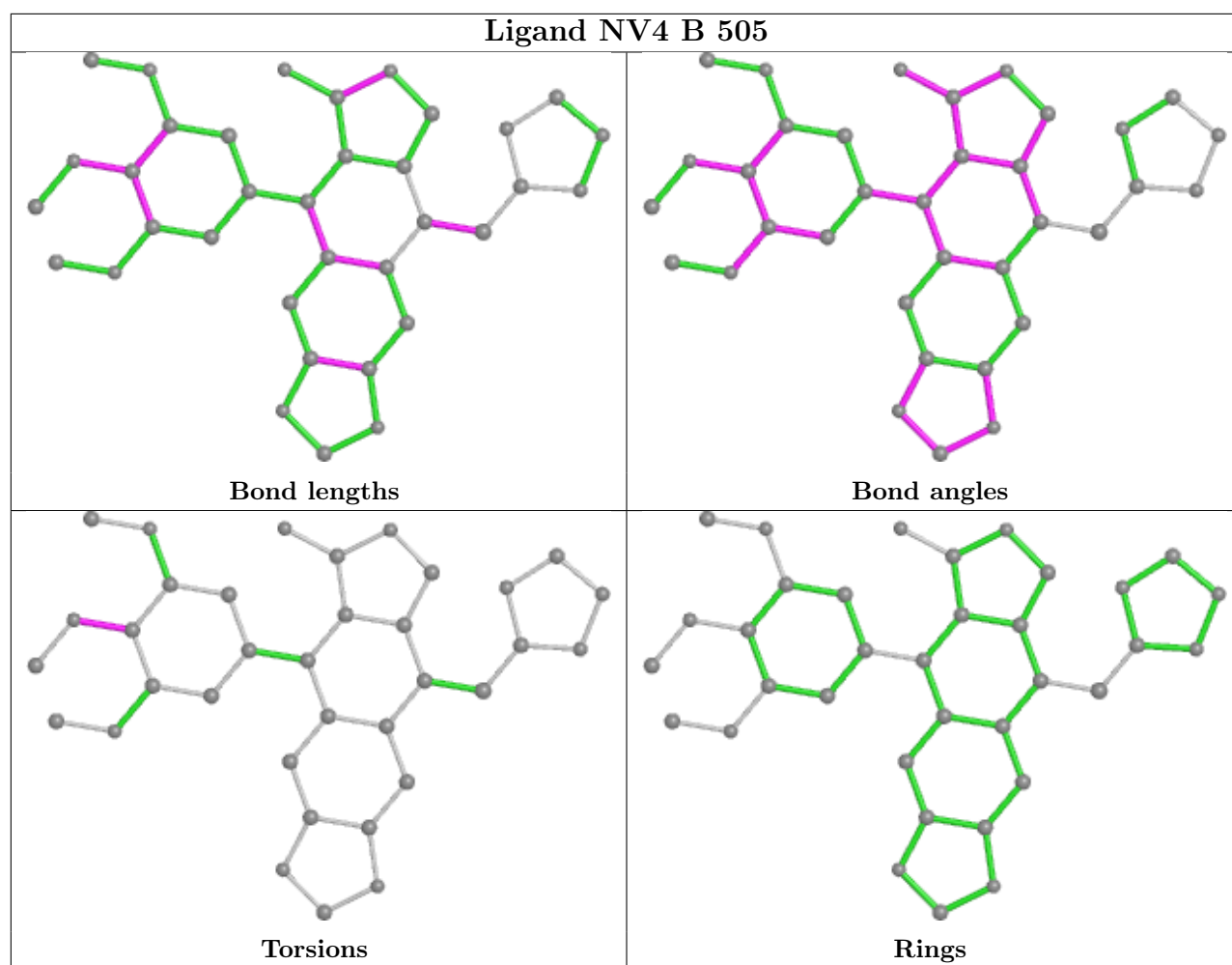10 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	504	GOL	1	0
13	D	507	NV4	9	0
7	C	504	GOL	6	0
7	C	501	GOL	4	0
10	D	501	GDP	1	0
8	A	505	IMD	4	0
7	D	506	GOL	2	0
7	A	507	GOL	1	0
15	F	402	ACP	3	0
13	B	505	NV4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 GTP C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NV4 D 507

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP F 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NV4 B 505

Bond lengths

Bond angles

Torsions

Rings
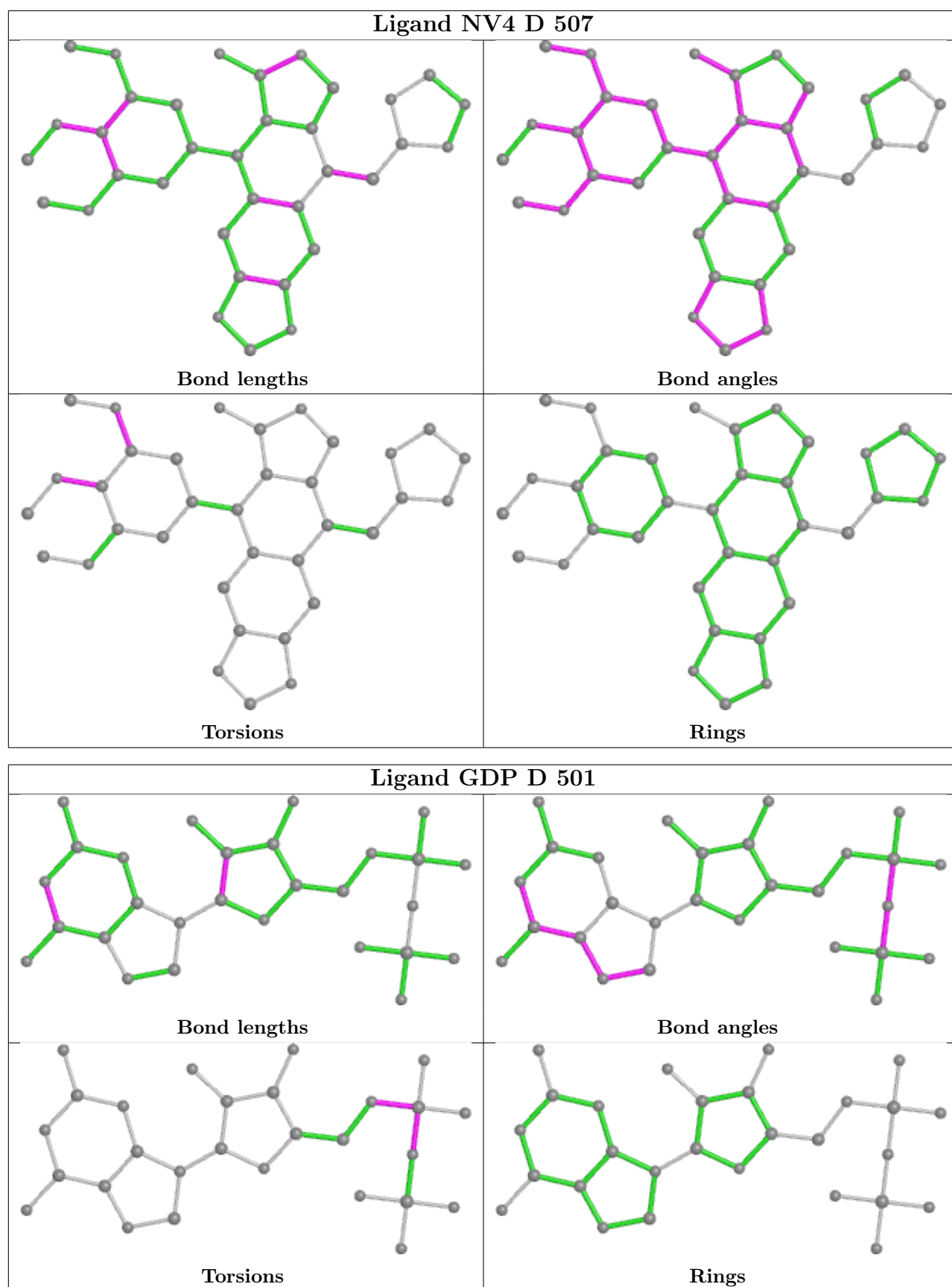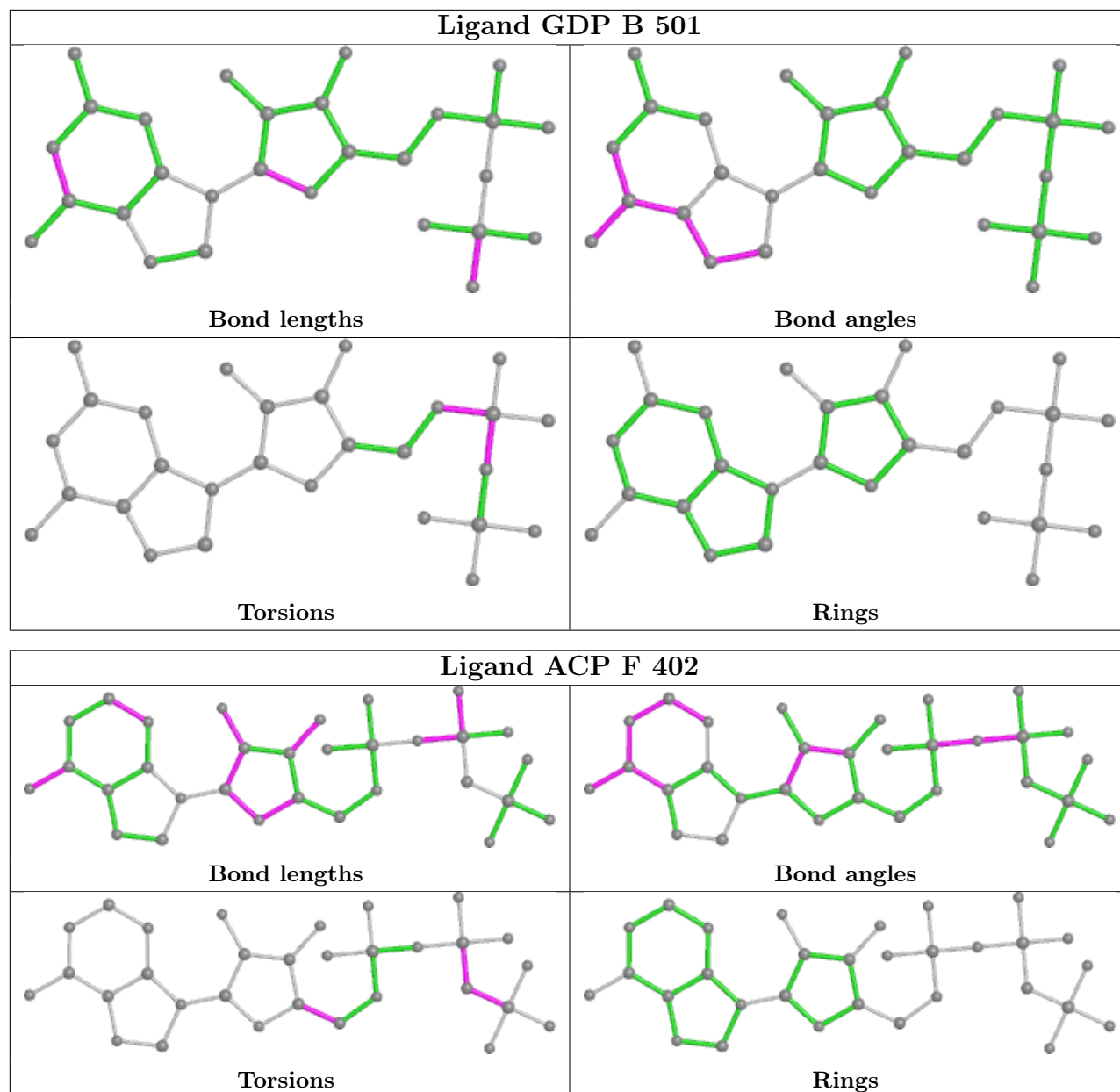
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	439/451 (97%)	0.17	15 (3%)	45	52	25, 41, 76, 126	0
1	C	440/451 (97%)	-0.05	9 (2%)	65	71	20, 32, 61, 98	0
2	B	423/445 (95%)	0.16	21 (4%)	28	35	20, 40, 80, 114	1 (0%)
2	D	418/445 (93%)	0.45	46 (11%)	5	7	27, 49, 84, 126	2 (0%)
3	E	121/152 (79%)	0.35	9 (7%)	14	19	29, 53, 90, 106	0
4	F	312/388 (80%)	0.90	74 (23%)	0	0	30, 61, 113, 144	0
All	All	2153/2332 (92%)	0.29	174 (8%)	12	16	20, 44, 87, 144	3 (0%)

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	THR	10.6
4	F	253	TYR	9.3
4	F	173	ILE	8.8
4	F	102	PRO	6.9
1	A	439	SER	6.5

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 ⓘ

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
7	GOL	C	501	6/6	0.71	0.61	78,80,88,94	0
7	GOL	C	509	6/6	0.78	0.16	80,97,100,100	0
6	MG	D	502	1/1	0.80	0.09	52,52,52,52	0
9	CA	C	507	1/1	0.82	0.14	105,105,105,105	0
7	GOL	D	505	6/6	0.84	0.30	79,81,84,86	0
6	MG	A	502	1/1	0.85	0.22	40,40,40,40	0
7	GOL	A	507	6/6	0.85	0.13	75,82,90,90	0
14	PEG	C	505	7/7	0.85	0.17	42,77,82,82	0
7	GOL	D	504	6/6	0.86	0.29	90,103,104,104	0
13	NV4	D	507	35/35	0.86	0.25	41,64,88,100	0
7	GOL	A	504	6/6	0.86	0.19	47,68,71,76	0
7	GOL	C	504	6/6	0.89	0.58	67,70,83,84	0
8	IMD	A	505	5/5	0.90	0.34	68,82,95,98	0
7	GOL	D	506	6/6	0.92	0.20	54,62,67,68	0
6	MG	F	401	1/1	0.93	0.09	75,75,75,75	0
6	MG	C	503	1/1	0.93	0.14	27,27,27,27	0
8	IMD	C	508	5/5	0.93	0.15	38,48,56,56	0
15	ACP	F	402	31/31	0.93	0.12	51,78,113,122	0
6	MG	D	503	1/1	0.95	0.10	60,60,60,60	0
6	MG	B	502	1/1	0.96	0.27	20,20,20,20	0
11	NA	B	503	1/1	0.96	0.33	78,78,78,78	0
13	NV4	B	505	35/35	0.96	0.19	30,41,78,92	0
11	NA	C	506	1/1	0.97	0.17	27,27,27,27	0
10	GDP	D	501	28/28	0.98	0.09	40,47,51,59	0
5	GTP	A	501	32/32	0.98	0.17	23,31,45,46	0
6	MG	A	503	1/1	0.98	0.39	74,74,74,74	0
12	MES	B	504	12/12	0.98	0.11	35,41,56,59	0
10	GDP	B	501	28/28	0.99	0.16	17,28,33,35	0
9	CA	A	506	1/1	0.99	0.04	53,53,53,53	0
5	GTP	C	502	32/32	0.99	0.14	21,24,32,36	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 NV4 D 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
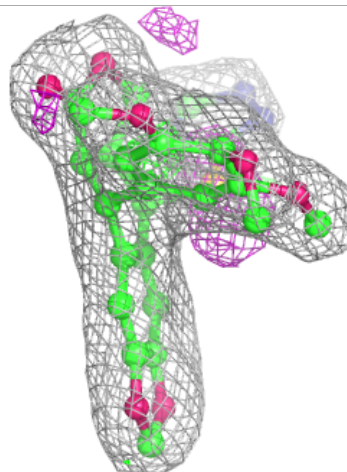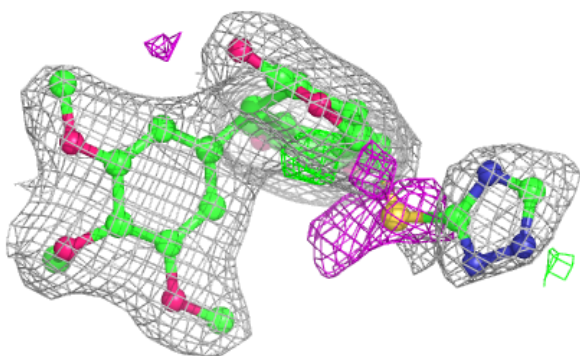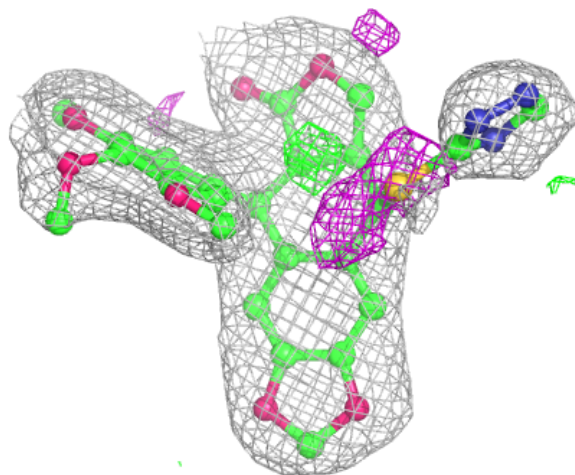and green (positive)
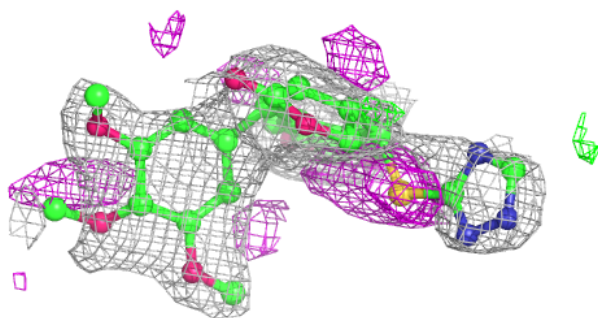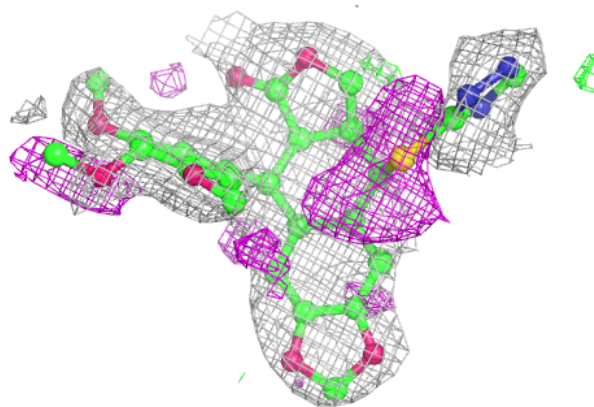
Electron density around ACP F 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
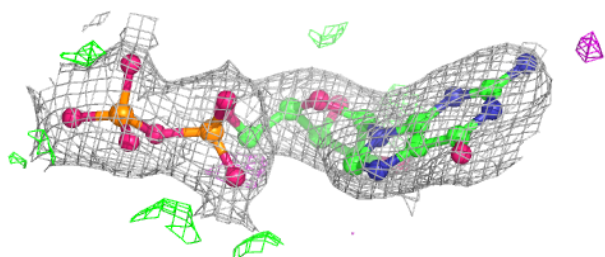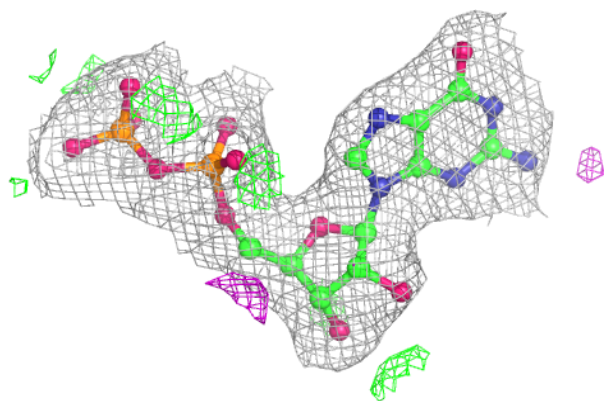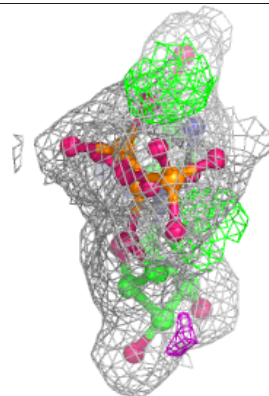mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
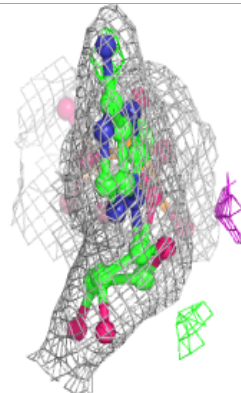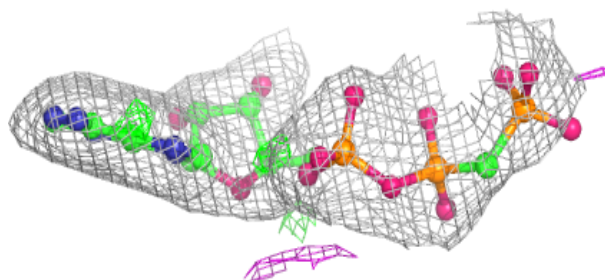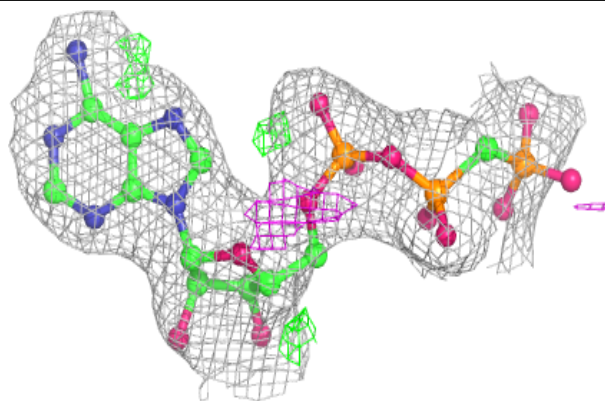
Electron density around NV4 B 505:

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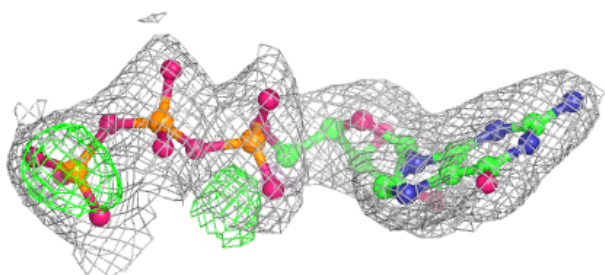mF_o-DF_c (at 3 rmsd) in purple (negative)
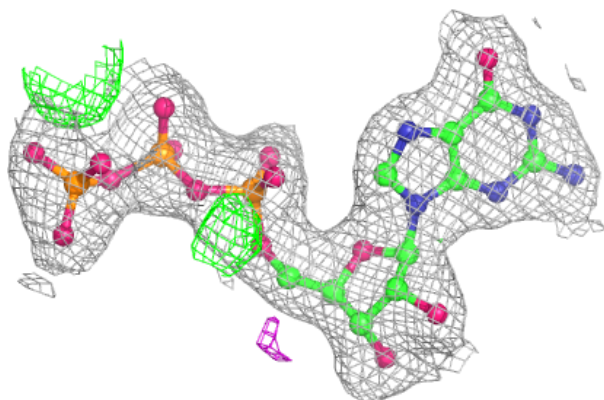and green (positive)

Electron density around GDP 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 GTP A 501:

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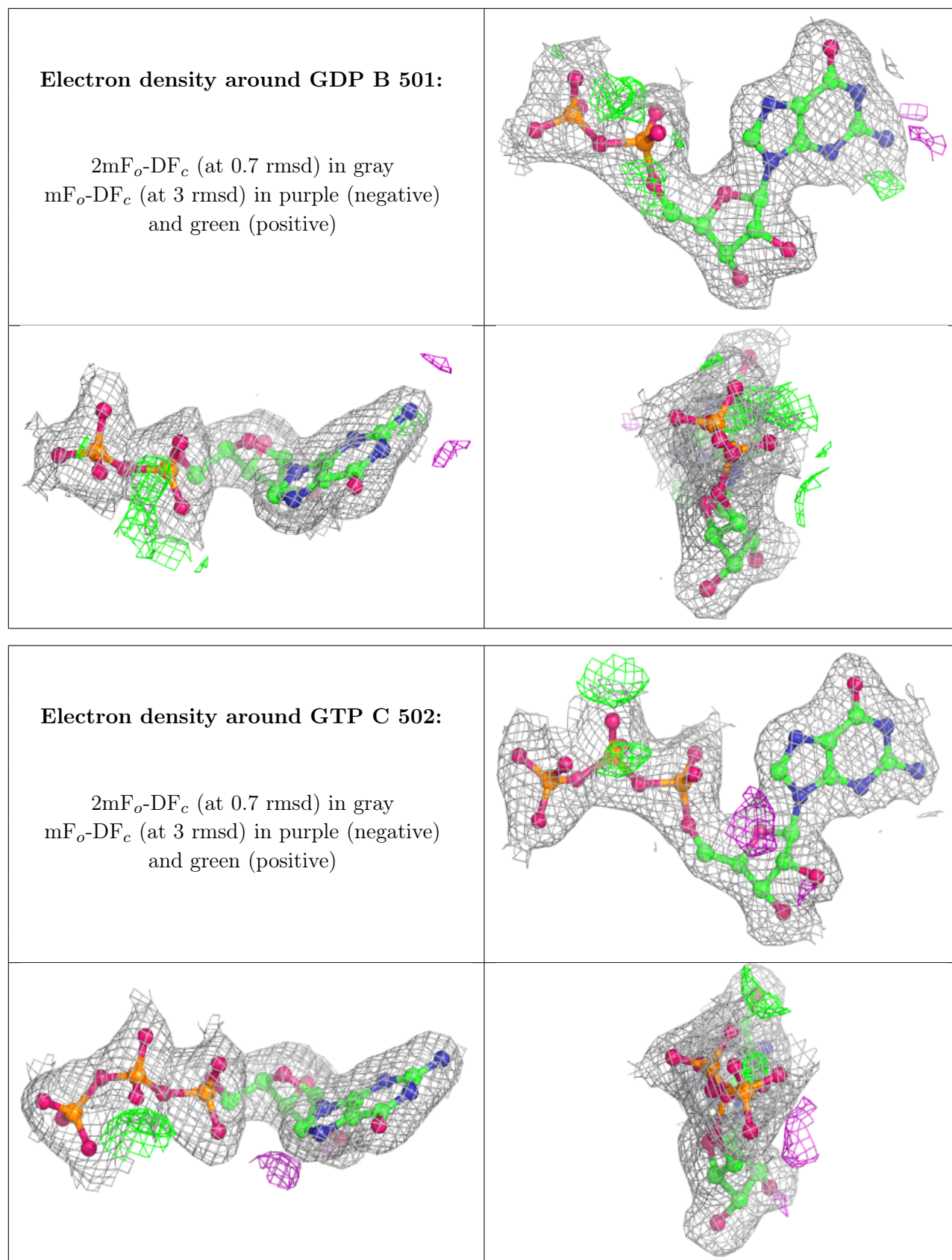mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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 ⓘ

There are no such residues in this entry.