



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:06 AM UTC

PDB ID : 7DP8 / pdb_00007dp8
Title : Crystal structure of T2R-TTL-Cevipabulin-eribulin complex
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on : 2020-12-18
Resolution : 2.45 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

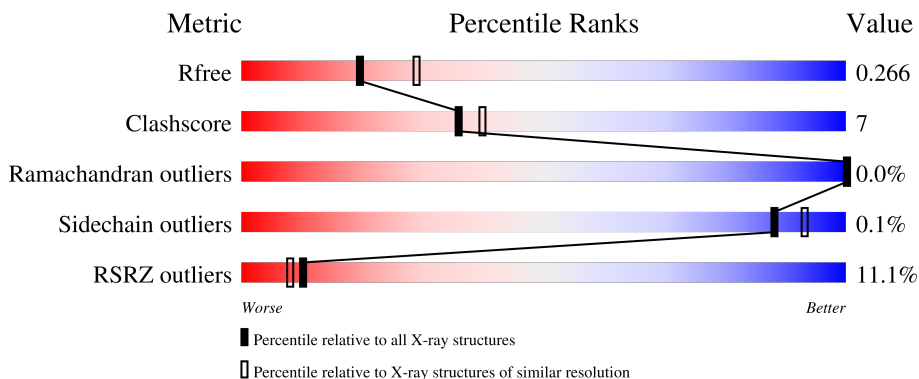
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



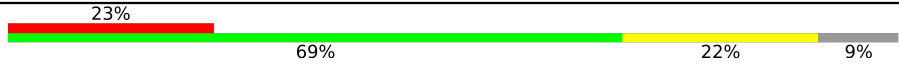
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	450	 5% 82% 15%
1	C	450	 2% 87% 10%
2	B	445	 8% 78% 16% 6%
2	D	445	 14% 82% 14%
3	E	143	 17% 70% 15% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart showing the quality of chain. The bar is divided into four segments: red (23%), green (69%), yellow (22%), and grey (9%).</p>

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 35012 atoms, of which 17101 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	438	Total	C	H	N	O	S	0	4	0
			6802	2182	3351	588	657	24			
1	C	440	Total	C	H	N	O	S	0	8	0
			6844	2201	3369	589	662	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	418	Total	C	H	N	O	S	0	4	0
			6498	2080	3185	565	639	29			
2	D	426	Total	C	H	N	O	S	0	1	0
			6563	2100	3217	570	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	E	123	Total	C	H	N	O	S	0	2	0
			2069	635	1037	188	204	5			

There are 2 discrepancies between the modelled and reference sequences:

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

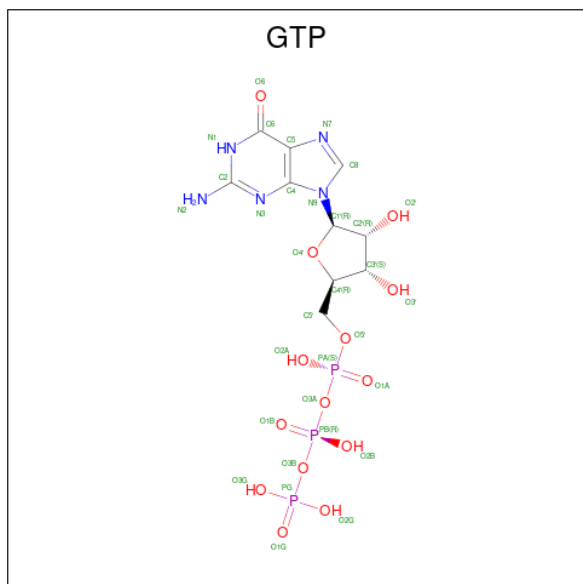
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	F	351	Total	C	H	N	O	S	0	1	0
			5696	1838	2824	491	528	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	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		

Continued on next page...

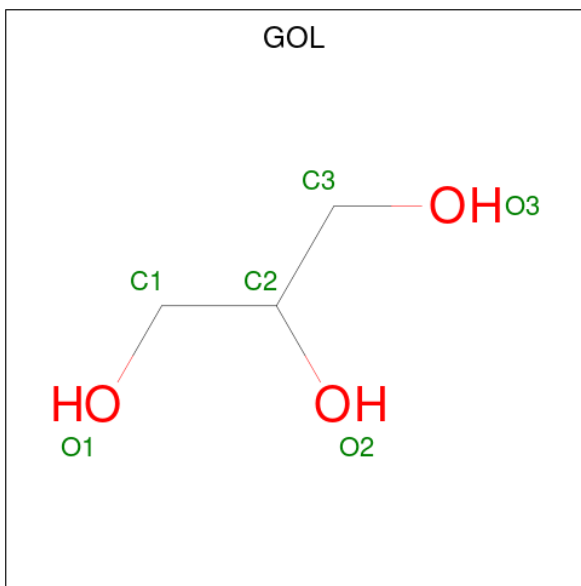
Continued from previous page...

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

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

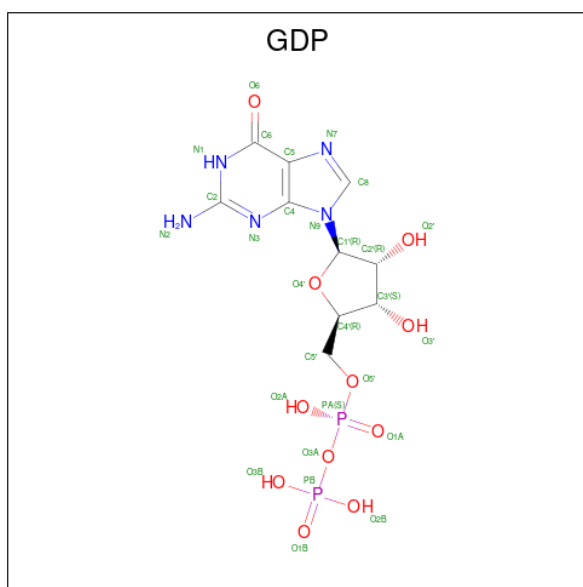
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0
7	B	2	Total Ca 2 2	0	0
7	C	2	Total Ca 2 2	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



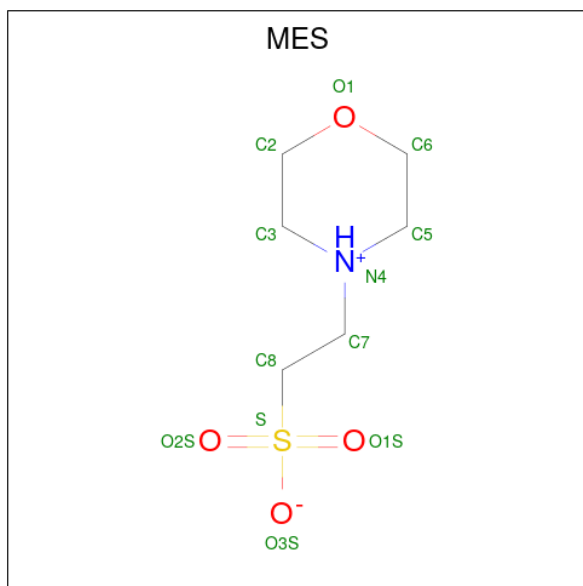
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 14 3 8 3	0	0
8	A	1	Total C H O 14 3 8 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
9	B	1	38	10	10	5	11	2	0	0

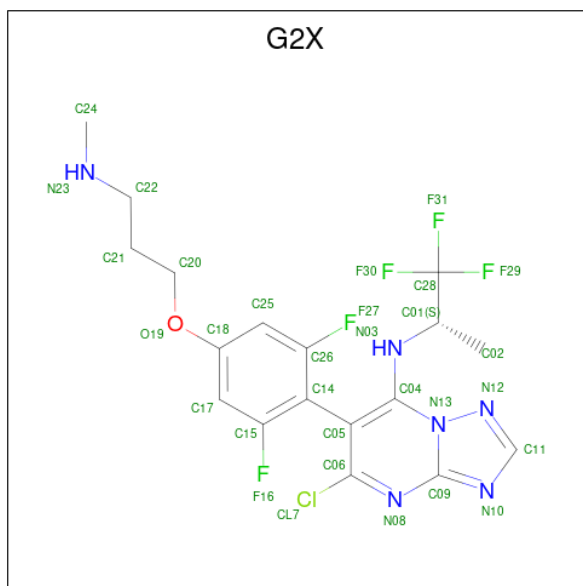
- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
10	B	1	24	6	12	1	4	1	0	0

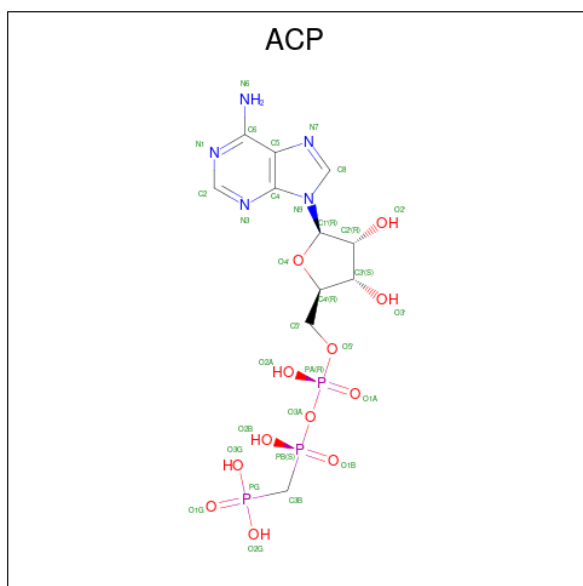
- Molecule 11 is 6-[2,6-bis(fluoranyl)-4-[3-(methylamino)propoxy]phenyl]-5-chloranyl-N-[(2S)-1,1,1-tris(fluoranyl)propan-2-yl]-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (CCD ID: G2X)

(formula: $C_{18}H_{18}ClF_5N_6O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	D	1	52	40	1	11	0	0

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
13	F	1	45	11	14	5	12	3	0	0

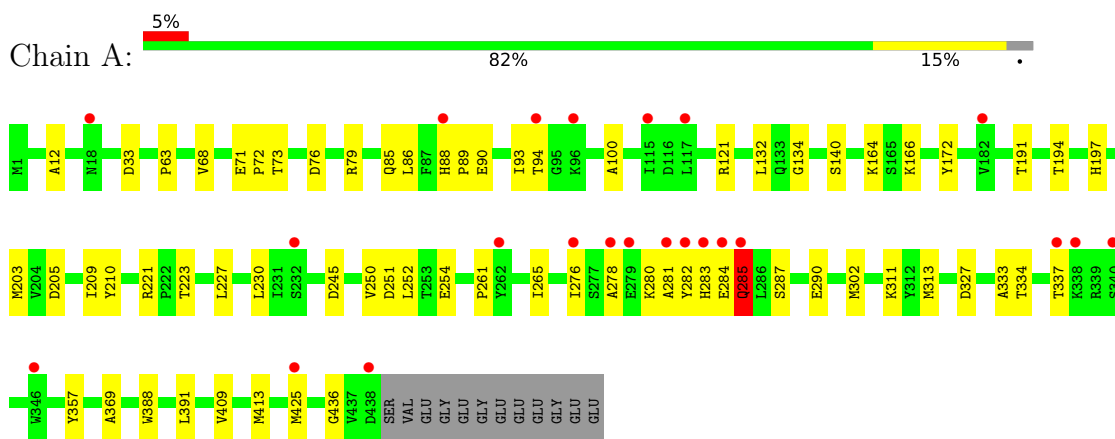
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	18	Total	O	0	0
			18	18		
14	B	29	Total	O	0	0
			29	29		
14	C	57	Total	O	0	0
			57	57		
14	D	7	Total	O	0	0
			7	7		
14	E	4	Total	O	0	0
			4	4		
14	F	3	Total	O	0	0
			3	3		

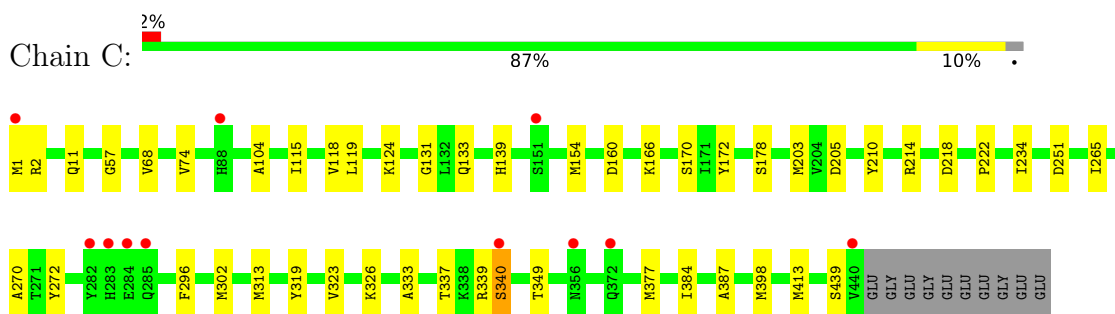
3 Residue-property plots [i](#)

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.

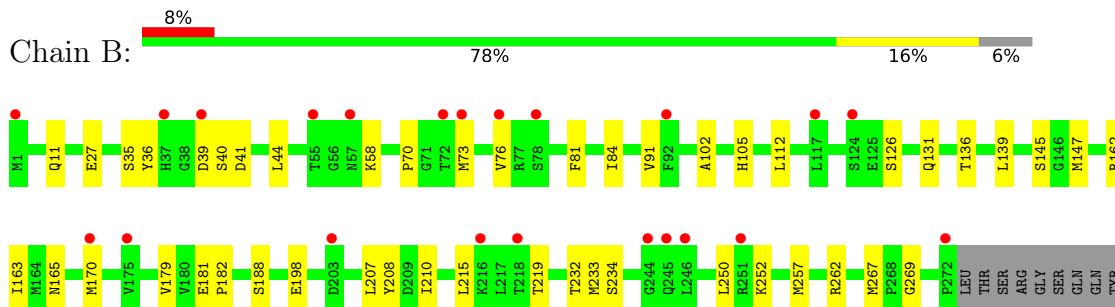
- Molecule 1: Tubulin alpha-1B chain

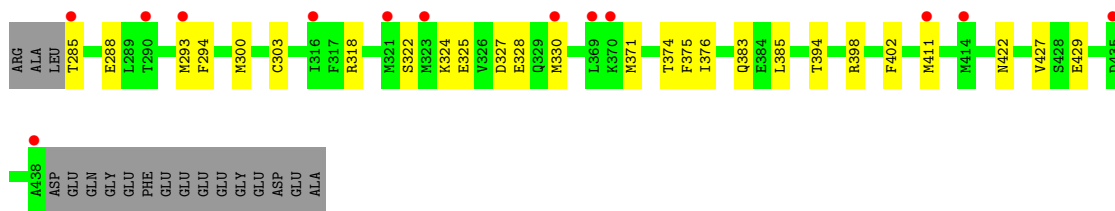


- Molecule 1: Tubulin alpha-1B chain

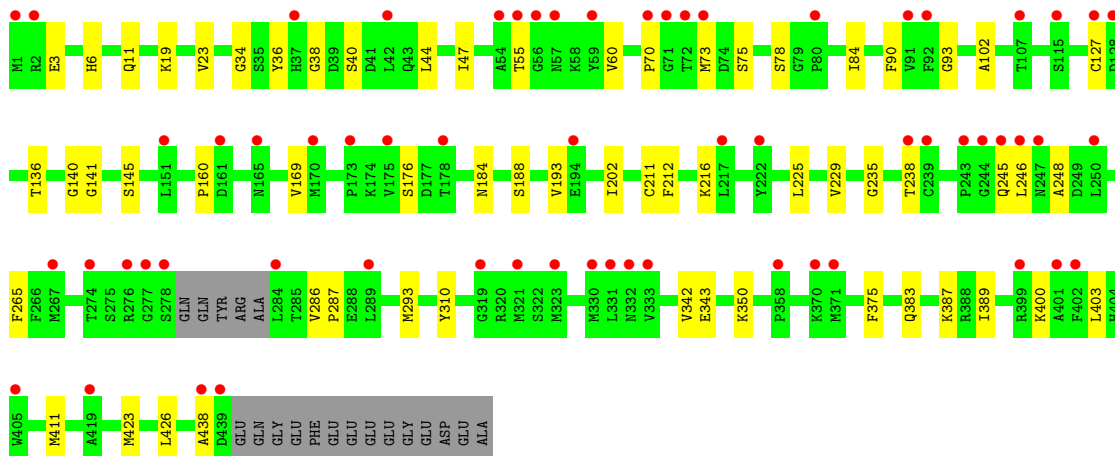
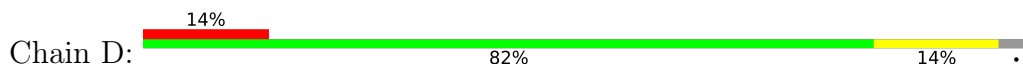


- Molecule 2: Tubulin beta chain

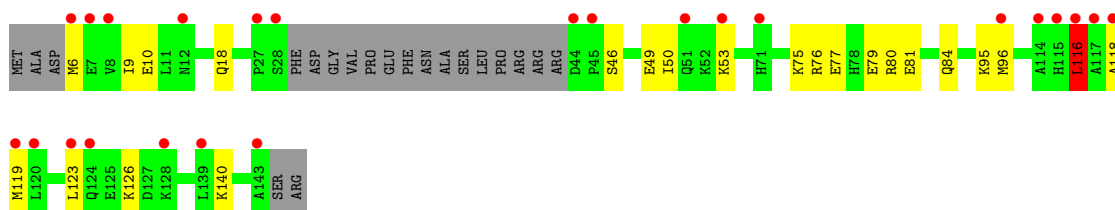




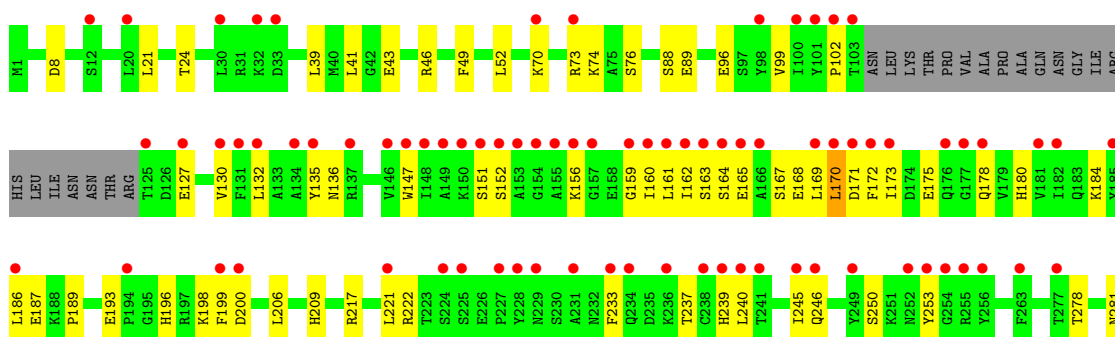
- Molecule 2: Tubulin beta chain



- 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	103.94Å 159.07Å 176.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.46 – 2.45 59.46 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.0 (59.46-2.45) 95.0 (59.46-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.227 , 0.264 0.230 , 0.266	Depositor DCC
R_{free} test set	5153 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35012	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: MES, G2X, CA, MG, ACP, GTP, GOL, 6K9, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	2/3532 (0.1%)	0.45	2/4794 (0.0%)
1	C	0.26	2/3577 (0.1%)	0.55	6/4859 (0.1%)
2	B	0.18	0/3389	0.37	0/4588
2	D	0.18	0/3422	0.40	0/4634
3	E	0.22	0/1041	0.45	1/1382 (0.1%)
4	F	0.17	0/2937	0.45	0/3967
All	All	0.22	4/17898 (0.0%)	0.45	9/24224 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	D	0	1
3	E	0	1
4	F	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	339	ARG	C-N	7.36	1.44	1.33
1	A	285	GLN	CB-CG	-6.62	1.32	1.52
1	C	340	SER	CB-OG	5.79	1.53	1.42
1	A	285	GLN	CA-CB	-5.42	1.44	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	SER	CA-CB-OG	19.10	149.30	111.10
1	C	340	SER	N-CA-C	-10.38	100.03	112.89
1	A	285	GLN	CB-CG-CD	-9.75	96.02	112.60
1	C	340	SER	CA-C-O	7.02	128.02	119.31
1	C	340	SER	CB-CA-C	-6.88	95.61	109.99

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	GLN	Sidechain
1	C	340	SER	Mainchain
2	D	55	THR	Peptide
3	E	116	LEU	Peptide
4	F	170	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3451	3351	3362	46	1
1	C	3475	3369	3384	31	1
2	B	3313	3185	3192	54	0
2	D	3346	3217	3227	43	0
3	E	1032	1037	1040	25	0
4	F	2872	2824	2835	65	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
8	A	12	16	16	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	28	10	12	2	0
10	B	12	12	12	0	0
11	C	62	36	0	0	0
12	D	52	0	0	2	0
13	F	31	14	14	1	0
14	A	18	0	0	1	0
14	B	29	0	0	4	0
14	C	57	0	0	3	0
14	D	7	0	0	0	0
14	E	4	0	0	2	0
14	F	3	0	0	0	0
All	All	17911	17101	17130	256	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 7.

The worst 5 of 256 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:162:ARG:NH1	14:B:601:HOH:O	1.93	1.00
3:E:116:LEU:HA	3:E:119:MET:H	1.47	0.80
2:D:75:SER:O	2:D:78:SER:OG	1.99	0.79
1:A:276:ILE:HG21	1:A:283:HIS:CE1	2.19	0.77
4:F:168:GLU:HA	4:F:171:ASP:HB3	1.68	0.76

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:OD1	1:C:57:GLY:H[2_565]	1.50	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/450 (98%)	426 (97%)	14 (3%)	0	100	100
1	C	446/450 (99%)	431 (97%)	15 (3%)	0	100	100
2	B	418/445 (94%)	402 (96%)	16 (4%)	0	100	100
2	D	423/445 (95%)	409 (97%)	14 (3%)	0	100	100
3	E	121/143 (85%)	118 (98%)	3 (2%)	0	100	100
4	F	346/384 (90%)	329 (95%)	16 (5%)	1 (0%)	36	44
All	All	2194/2317 (95%)	2115 (96%)	78 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	88	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/378 (99%)	373 (100%)	0	100	100
1	C	379/378 (100%)	378 (100%)	1 (0%)	86	91
2	B	365/383 (95%)	365 (100%)	0	100	100
2	D	369/383 (96%)	369 (100%)	0	100	100
3	E	112/127 (88%)	112 (100%)	0	100	100
4	F	314/342 (92%)	314 (100%)	0	100	100
All	All	1912/1991 (96%)	1911 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	128	GLN
4	F	180	HIS
1	C	356	ASN
4	F	242	ASN
3	E	18	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 22 ligands modelled in this entry, 11 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	$\# Z > 2$
5	GTP	D	502	6	33,34,34	0.85	1 (3%)	50,54,54	1.63	11 (22%)
5	GTP	C	602	6	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
13	ACP	F	402	6	31,33,33	2.52	9 (29%)	47,52,52	2.51	16 (34%)
5	GTP	A	501	6	33,34,34	0.90	2 (6%)	50,54,54	1.58	10 (20%)
9	GDP	B	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	10 (22%)
11	G2X	C	601	-	30,33,33	2.22	13 (43%)	37,48,48	1.99	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	504	-	5,5,5	0.82	0	5,5,5	0.82	0
11	G2X	C	605	-	30,33,33	2.40	16 (53%)	37,48,48	1.86	10 (27%)
10	MES	B	503	-	12,12,12	2.08	1 (8%)	15,16,16	1.66	3 (20%)
12	6K9	D	503	-	57,60,60	2.22	14 (24%)	61,92,92	1.74	15 (24%)
8	GOL	A	505	-	5,5,5	0.54	0	5,5,5	0.80	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	D	502	6	-	5/22/38/38	0/3/3/3
5	GTP	C	602	6	-	7/22/38/38	0/3/3/3
13	ACP	F	402	6	-	1/19/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
9	GDP	B	501	-	-	3/16/32/32	0/3/3/3
11	G2X	C	601	-	-	3/20/20/20	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
11	G2X	C	605	-	-	4/20/20/20	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
12	6K9	D	503	-	-	3/31/131/131	-
8	GOL	A	505	-	-	4/4/4/4	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	6K9	C18-C19	-7.35	1.40	1.51
12	D	503	6K9	C02-C01	-7.07	1.41	1.51
10	B	503	MES	C8-S	-6.86	1.68	1.77
13	F	402	ACP	PB-O3A	5.74	1.64	1.58
12	D	503	6K9	C39-C01	-5.54	1.43	1.51

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	402	ACP	C4-N9-C8	9.16	115.36	105.74
11	C	601	G2X	C11-N12-N13	6.24	105.95	100.86
9	B	501	GDP	C5-C4-N3	-5.98	118.86	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	605	G2X	C11-N12-N13	5.89	105.66	100.86
13	F	402	ACP	N3-C4-N9	5.11	135.85	127.17

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

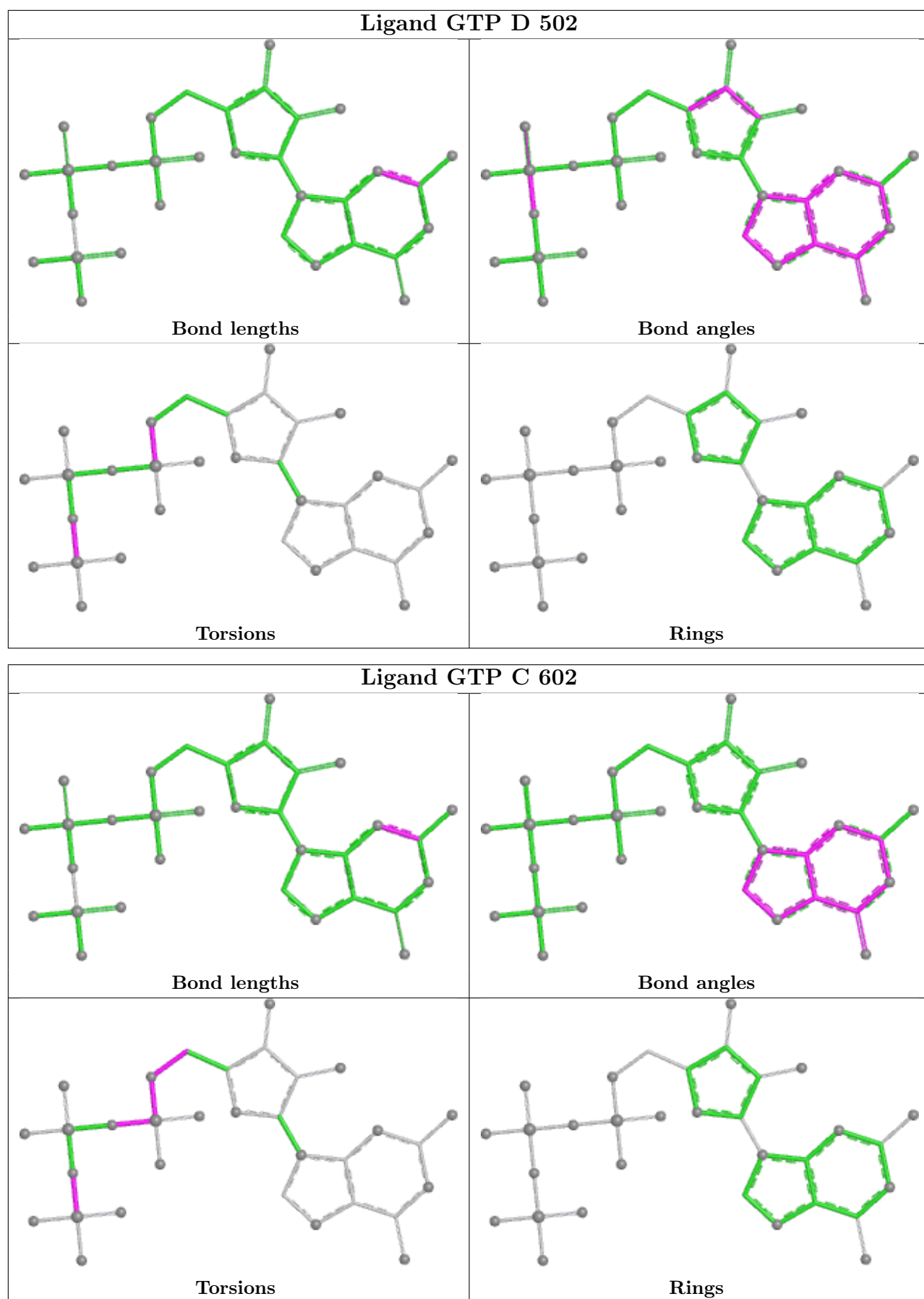
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	602	GTP	PB-O3B-PG-O2G

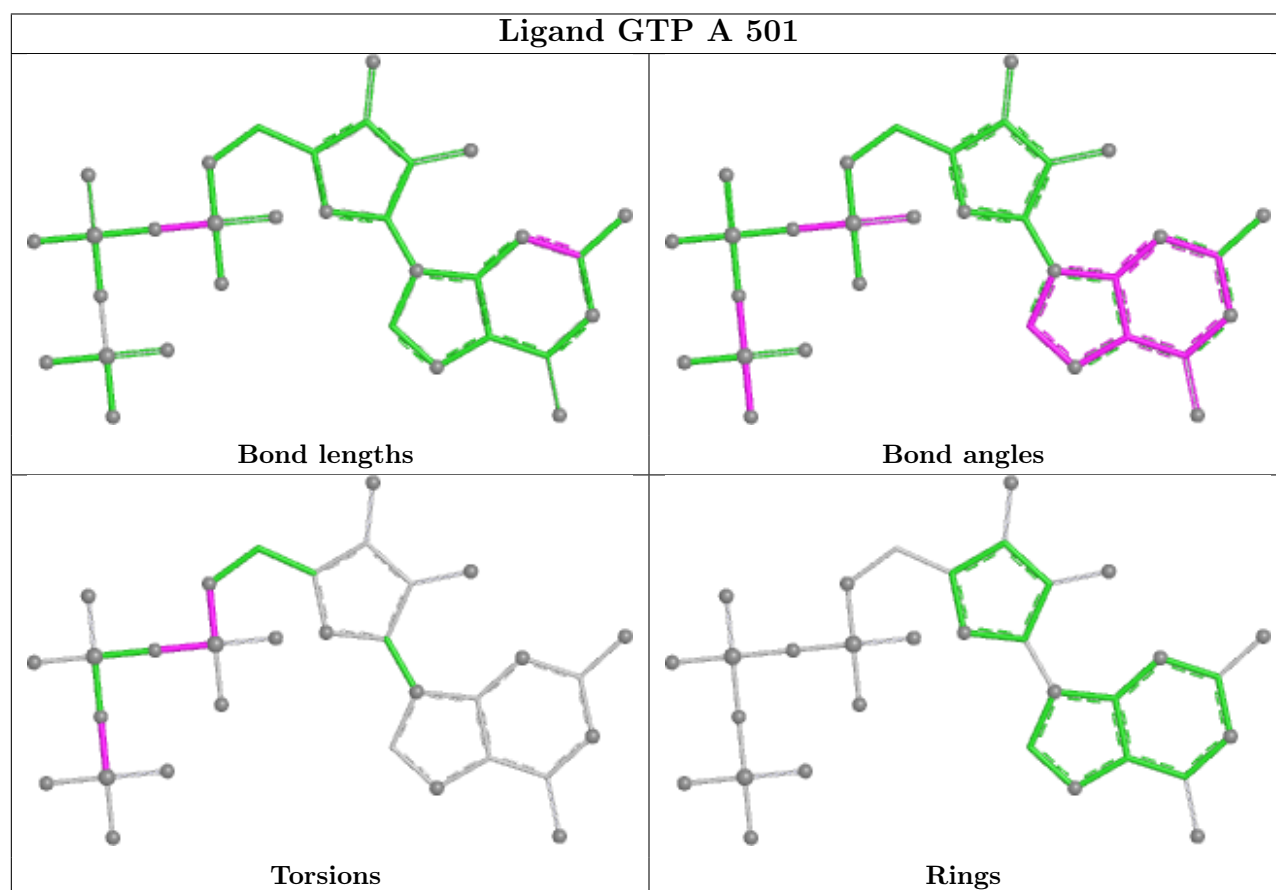
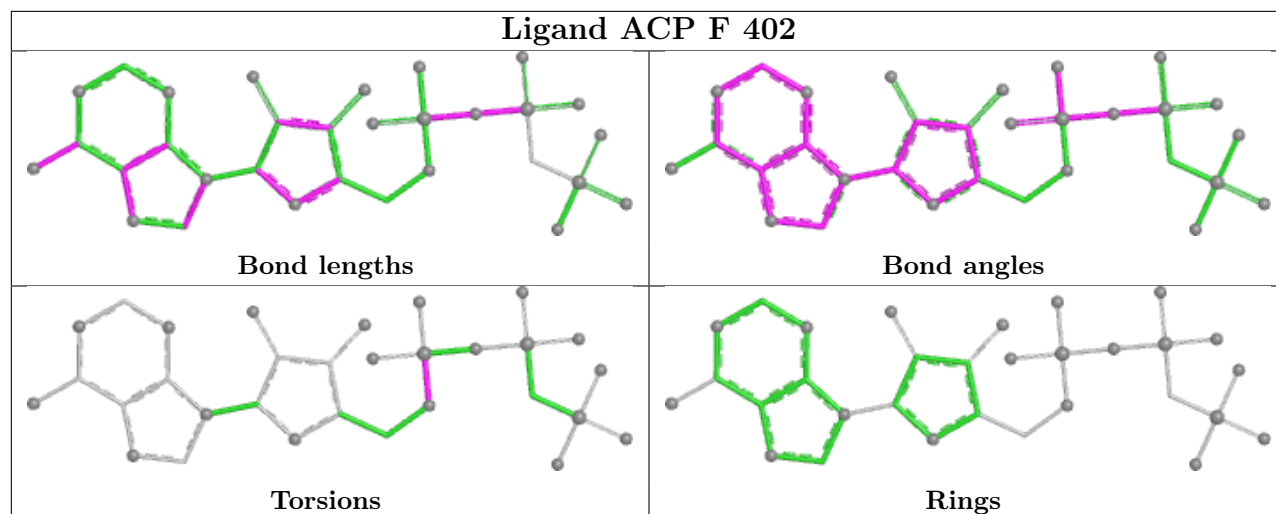
There are no ring outliers.

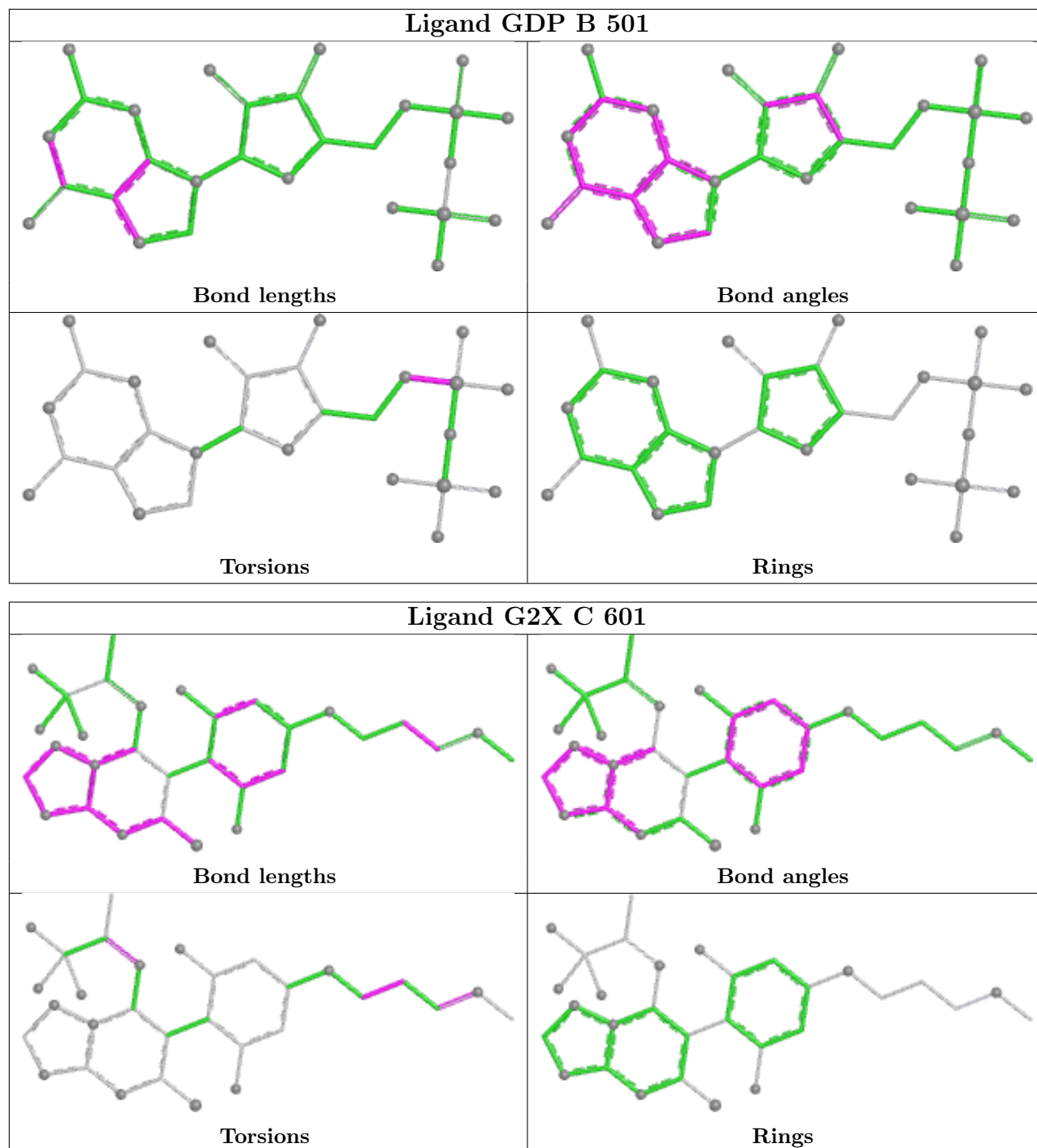
4 monomers are involved in 6 short contacts:

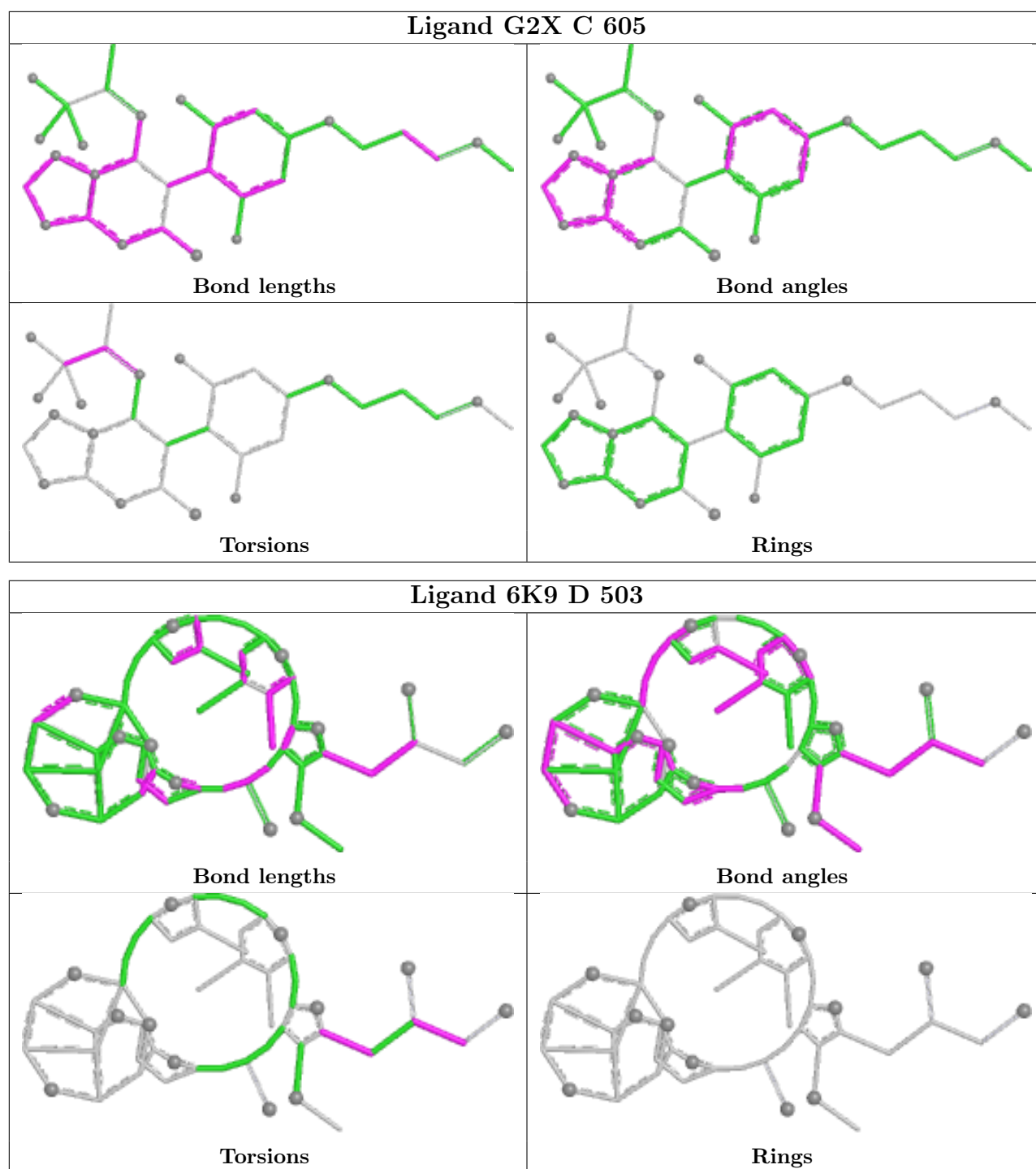
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	402	ACP	1	0
9	B	501	GDP	2	0
8	A	504	GOL	1	0
12	D	503	6K9	2	0

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 [\(i\)](#)

There are no chain breaks in this entry.

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	438/450 (97%)	0.70	23 (5%) 32 29	31, 66, 86, 117	4 (0%)
1	C	440/450 (97%)	0.38	11 (2%) 58 59	26, 54, 71, 97	7 (1%)
2	B	418/445 (93%)	0.72	35 (8%) 17 14	32, 62, 84, 99	4 (0%)
2	D	426/445 (95%)	1.07	62 (14%) 6 4	39, 71, 90, 110	1 (0%)
3	E	123/143 (86%)	1.26	24 (19%) 3 2	30, 74, 99, 104	2 (1%)
4	F	351/384 (91%)	1.48	89 (25%) 1 1	34, 81, 120, 126	1 (0%)
All	All	2196/2317 (94%)	0.86	244 (11%) 10 8	26, 66, 99, 126	19 (0%)

The worst 5 of 244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	6.9
4	F	103	THR	6.5
1	A	283	HIS	5.6
1	A	346	TRP	5.5
1	C	151[A]	SER	5.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

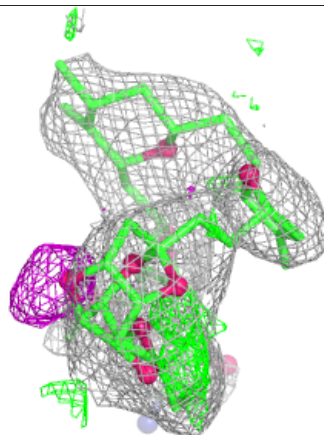
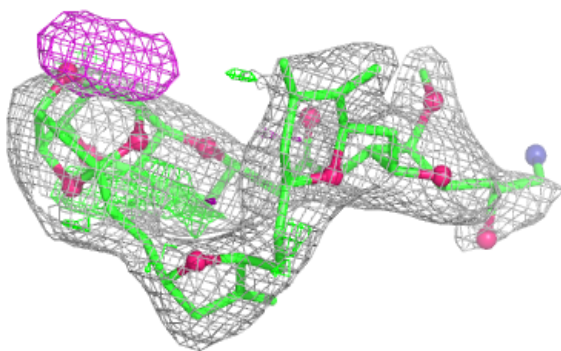
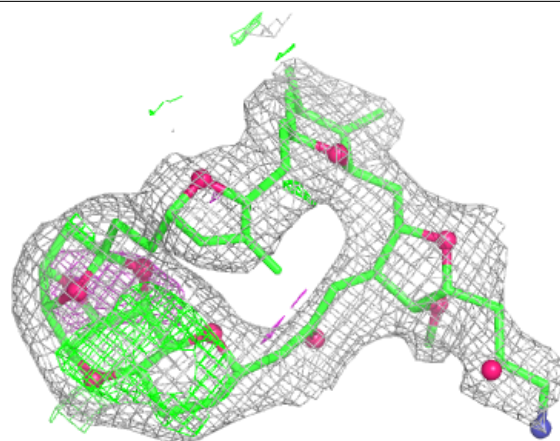
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	505	1/1	0.65	0.20	94,94,94,94	0
8	GOL	A	504	6/6	0.77	0.17	65,78,85,90	0
12	6K9	D	503	52/52	0.82	0.23	63,84,94,96	0
7	CA	B	504	1/1	0.85	0.13	101,101,101,101	0
6	MG	F	401	1/1	0.85	0.16	79,79,79,79	0
11	G2X	C	605	31/31	0.86	0.15	43,58,74,77	0
7	CA	A	506	1/1	0.87	0.17	96,96,96,96	0
6	MG	D	501	1/1	0.88	0.25	63,63,63,63	0
8	GOL	A	505	6/6	0.88	0.14	77,92,101,110	0
13	ACP	F	402	31/31	0.88	0.13	80,88,105,112	0
11	G2X	C	601	31/31	0.89	0.14	51,58,76,80	0
5	GTP	D	502	32/32	0.92	0.12	55,64,81,87	0
6	MG	B	502	1/1	0.94	0.12	65,65,65,65	0
7	CA	C	604	1/1	0.94	0.28	75,75,75,75	0
5	GTP	C	602	32/32	0.95	0.09	31,49,64,78	0
5	GTP	A	501	32/32	0.96	0.08	43,51,67,82	0
7	CA	A	503	1/1	0.96	0.07	82,82,82,82	0
9	GDP	B	501	28/28	0.96	0.10	31,55,77,92	0
10	MES	B	503	12/12	0.96	0.09	48,59,71,73	0
6	MG	C	603	1/1	0.98	0.05	40,40,40,40	0
6	MG	A	502	1/1	0.99	0.05	47,47,47,47	0
7	CA	C	606	1/1	0.99	0.03	47,47,47,47	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.

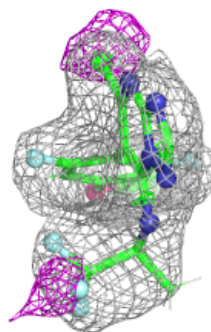
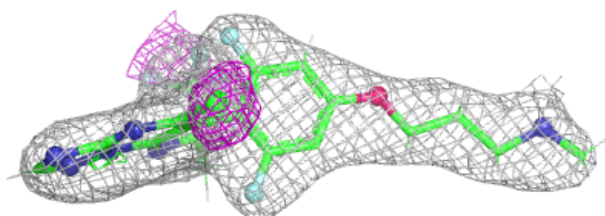
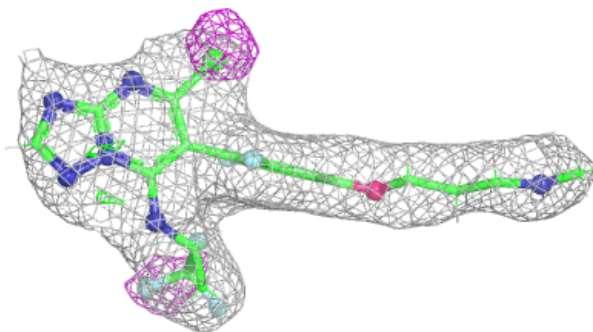
Electron density around 6K9 D 503:

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

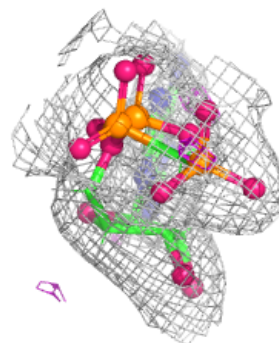
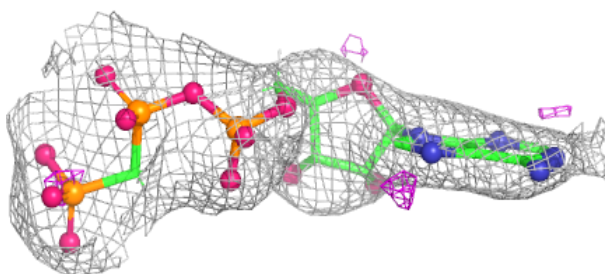
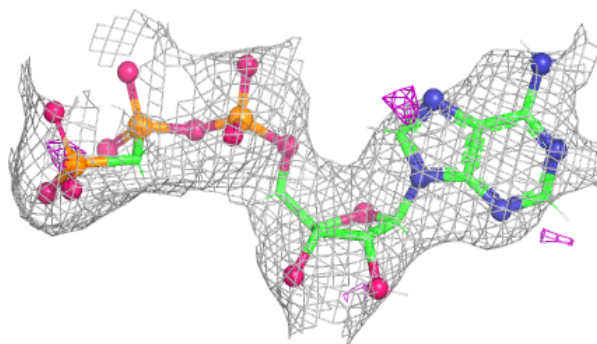


Electron density around G2X C 605:

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

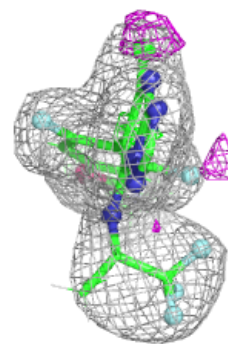
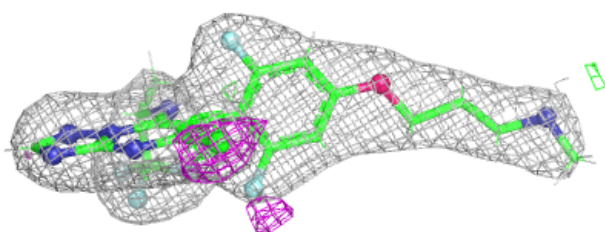
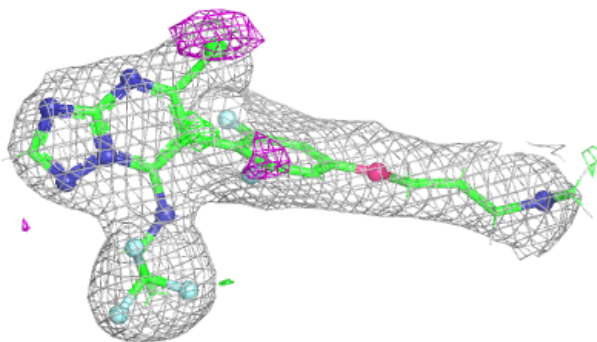
**Electron density around ACP F 402:**

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

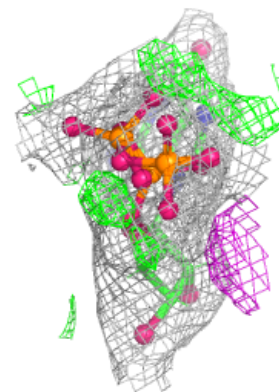
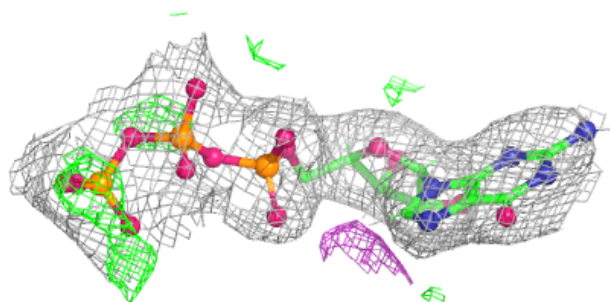
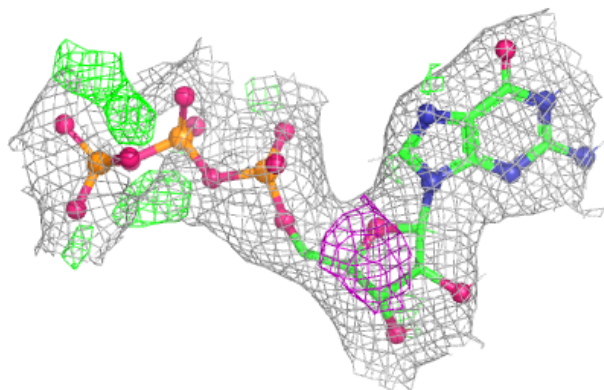


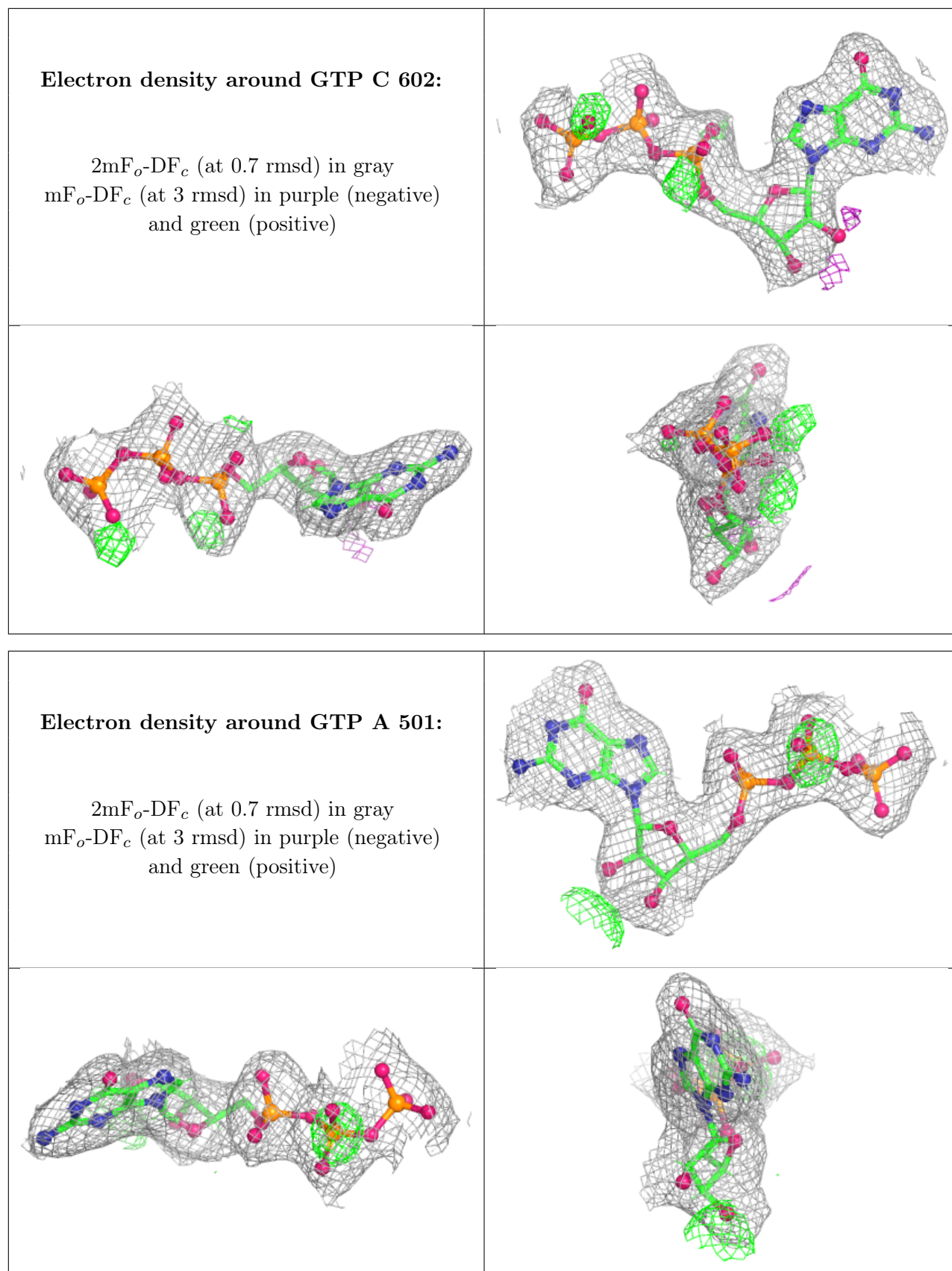
Electron density around G2X C 601:

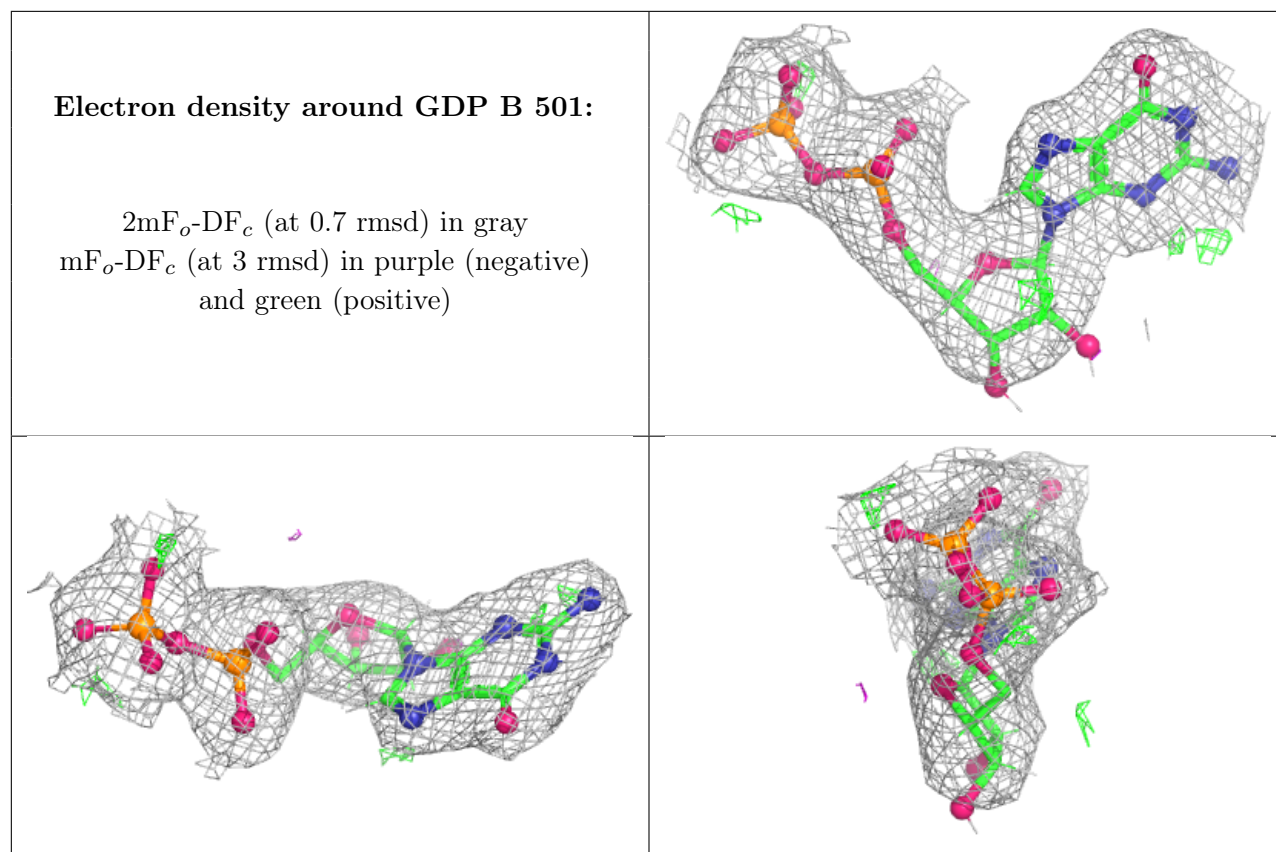
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GTP 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)







6.5 Other polymers [i](#)

There are no such residues in this entry.