



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 22, 2025 – 04:10 PM JST

PDB ID : 9IXB / pdb_00009ixb
Title : Structure of tubulin and nitrogen-containing heterocyclic substituted podophyllotoxin derivatives complex
Authors : Bi, J.; Zhao, W.
Deposited on : 2024-07-27
Resolution : 3.48 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

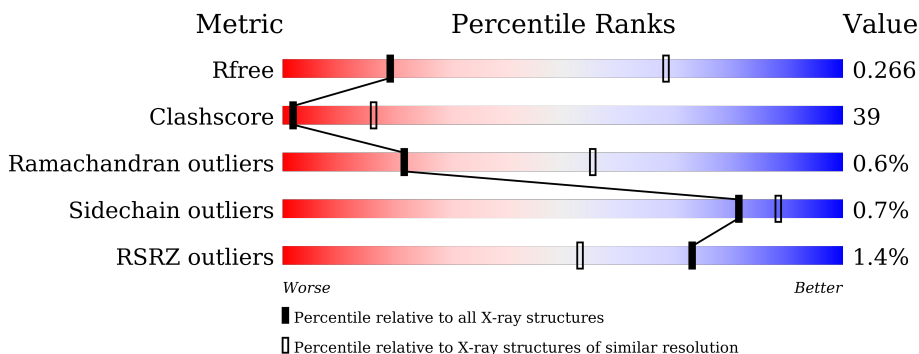
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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}	164625	1099 (3.54-3.42)
Clashscore	180529	1048 (3.52-3.44)
Ramachandran outliers	177936	1033 (3.52-3.44)
Sidechain outliers	177891	1034 (3.52-3.44)
RSRZ outliers	164620	1098 (3.54-3.42)

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	440	% 45% 54% .
1	C	440	% 48% 52% .
2	B	430	% 43% 53% ..
2	D	430	3% 46% 51% ..
3	E	138	% 49% 37% . 13%
4	F	380	% 35% 35% . 29%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15871 atoms, of which 27 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	9	0
			3273	2083	548	619	23			
1	C	439	Total	C	N	O	S	0	5	0
			3303	2096	551	634	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	7	0
			3153	1999	525	604	25			
2	D	426	Total	C	N	O	S	0	4	0
			3082	1948	521	592	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	279	THR	GLY	conflict	UNP A0A480UE93
B	285	GLY	ALA	conflict	UNP A0A480UE93
B	298	SER	ALA	conflict	UNP A0A480UE93
B	318	ILE	VAL	conflict	UNP A0A480UE93
D	279	THR	GLY	conflict	UNP A0A480UE93
D	285	GLY	ALA	conflict	UNP A0A480UE93
D	298	SER	ALA	conflict	UNP A0A480UE93
D	318	ILE	VAL	conflict	UNP A0A480UE93

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	1	0
			807	498	150	156	3			

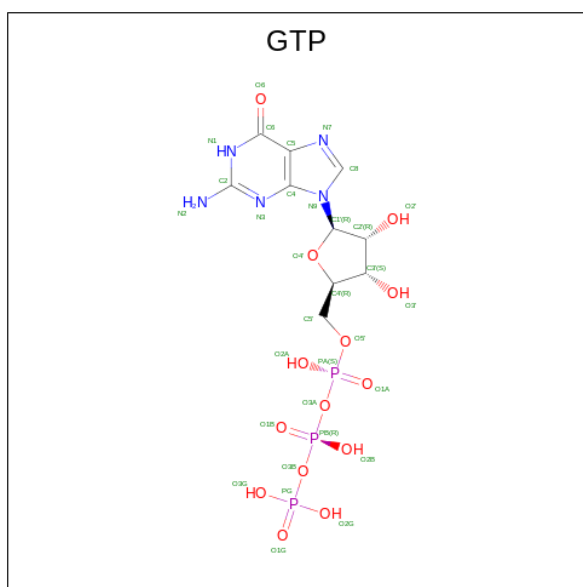
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	141	LYS	-	expression tag	UNP P63043
E	142	ASP	-	expression tag	UNP P63043
E	143	LYS	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	268	Total	C	N	O	S	0	4	0
			1996	1302	329	355	10			

- 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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

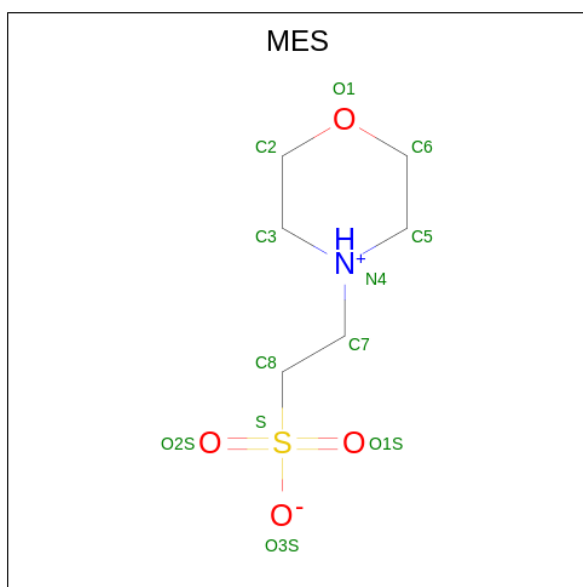
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

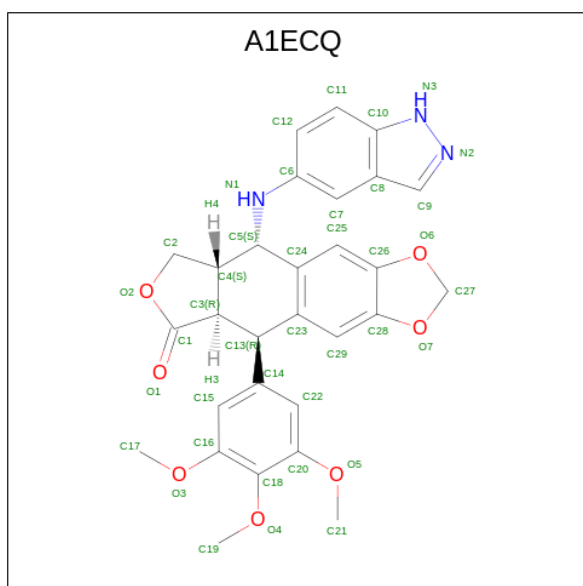
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Na	0	0
			1	1		

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



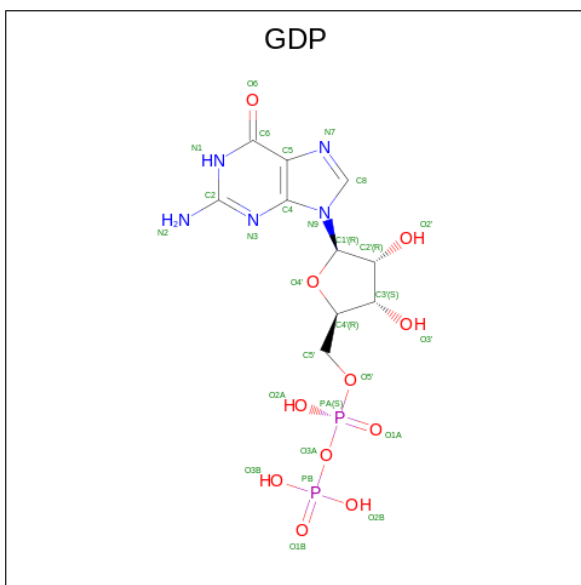
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (5 {S},5 {a} {S},8 {a} {R},9 {R})-5-(1 {H}-indazol-5-ylamino)-9-(3,4,5-trimethoxyphenyl)-5 {a},6,8 {a},9-tetrahydro-5 {H}-[2]benzofuro[6,5-f][1,3]benzodioxol-8-one (CCD ID: A1ECQ) (formula: C₂₉H₂₇N₃O₇) (labeled as "Ligand of Interest" by depositor).



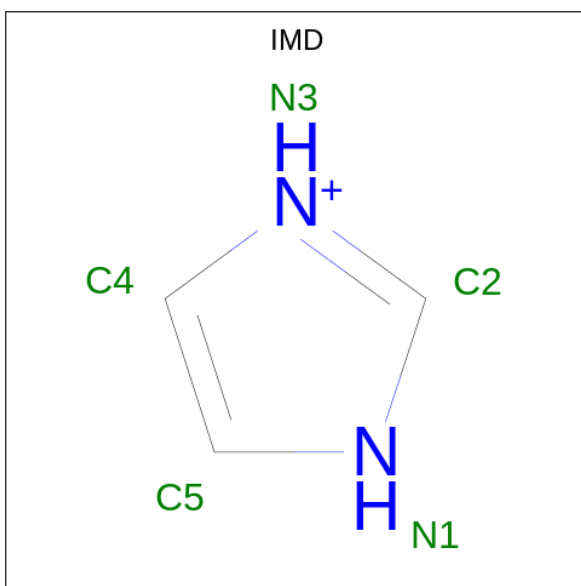
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	0	0
			66	29	27	3	7		

- Molecule 12 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

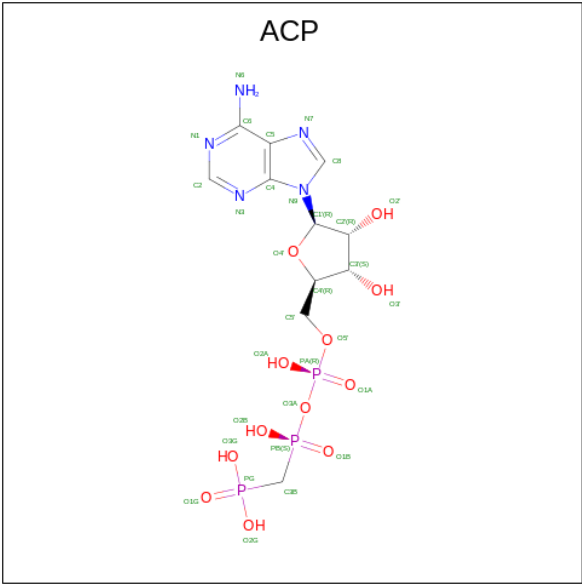
- Molecule 13 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	N	0	0
			5	3	2		

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD

ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

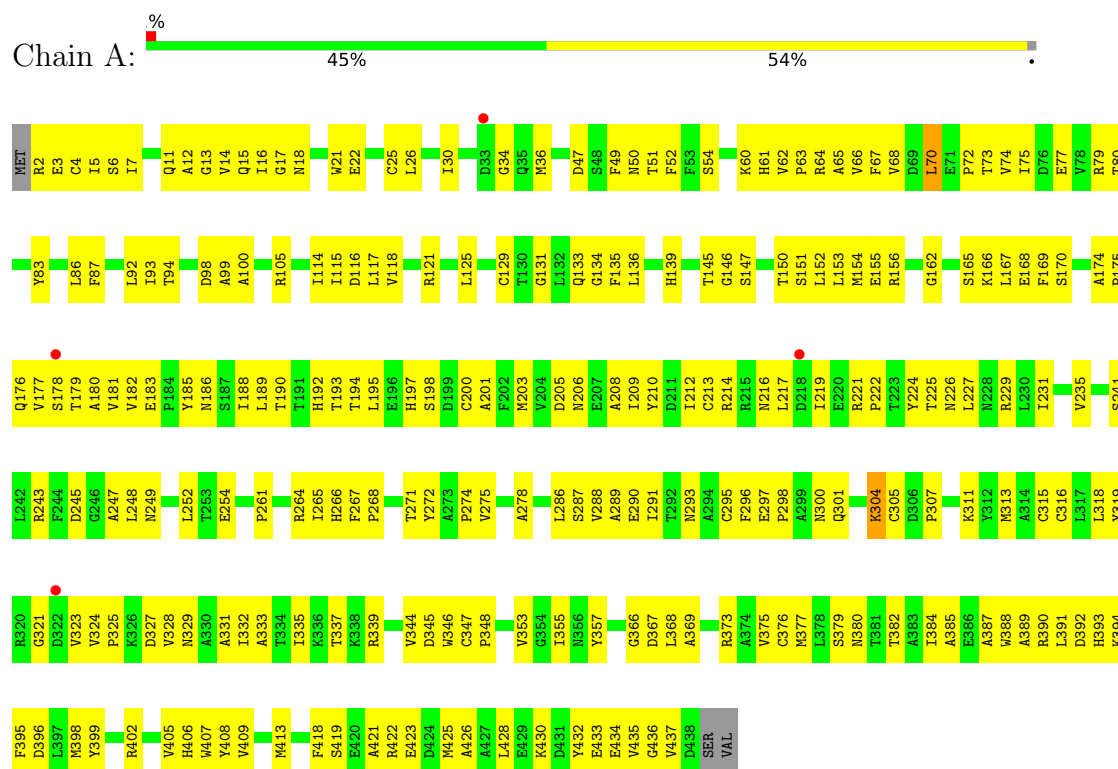
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	5	Total	O	0	0
			5	5		
15	C	4	Total	O	0	0
			4	4		
15	D	2	Total	O	0	0
			2	2		
15	F	3	Total	O	0	0
			3	3		

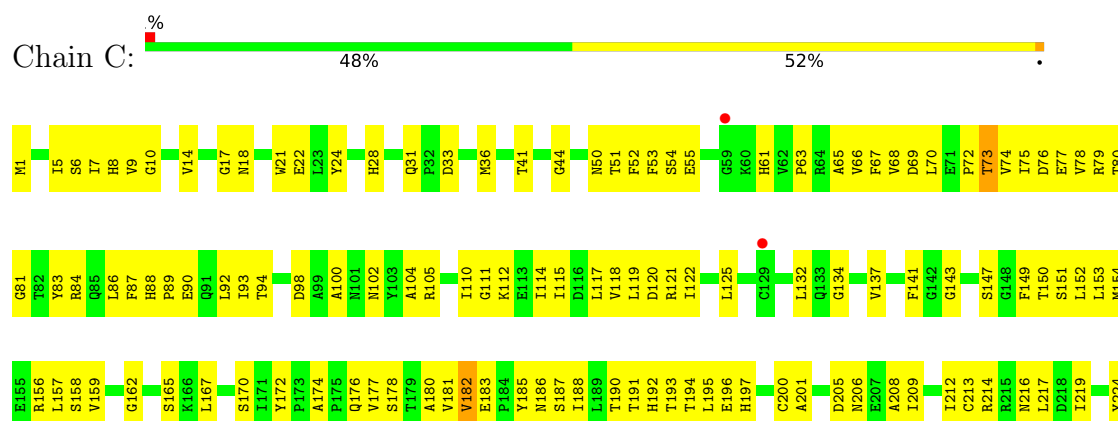
3 Residue-property plots

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: Detyrosinated tubulin alpha-1B chain

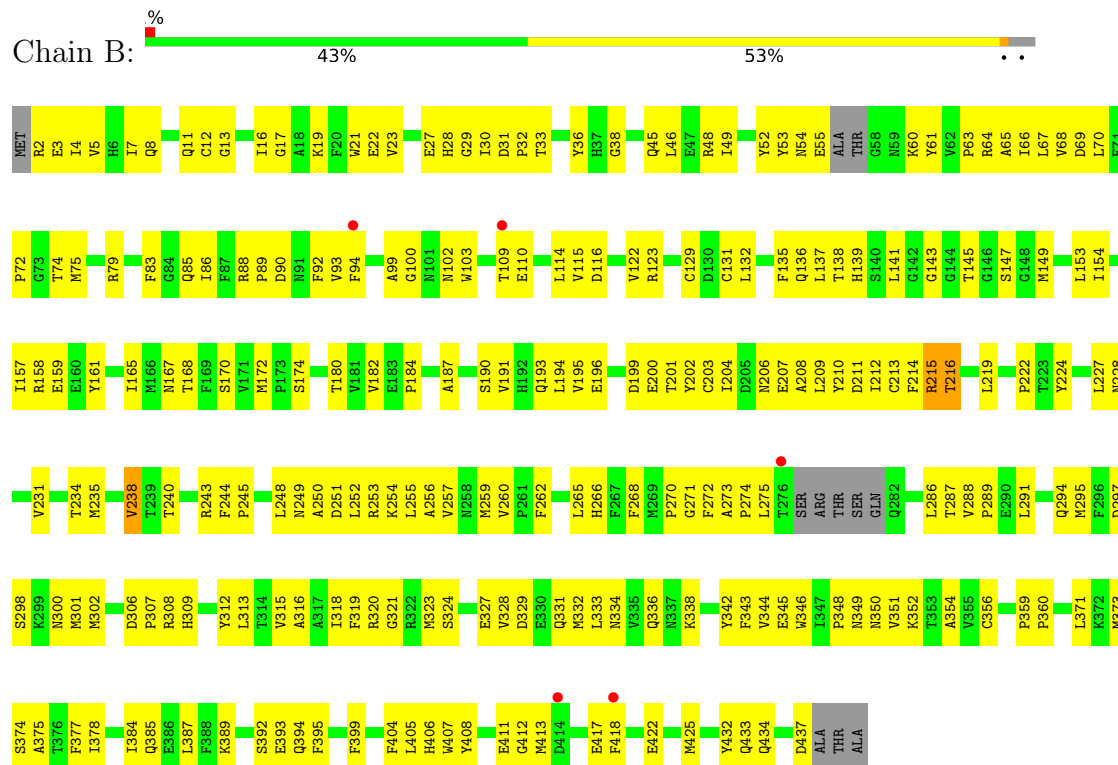


• Molecule 1: Detyrosinated tubulin alpha-1B chain

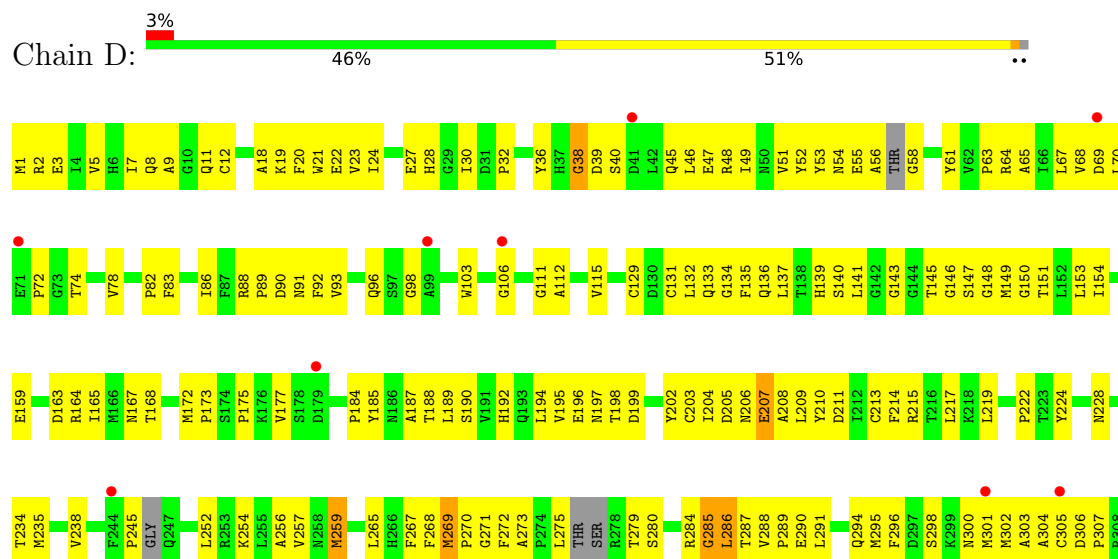


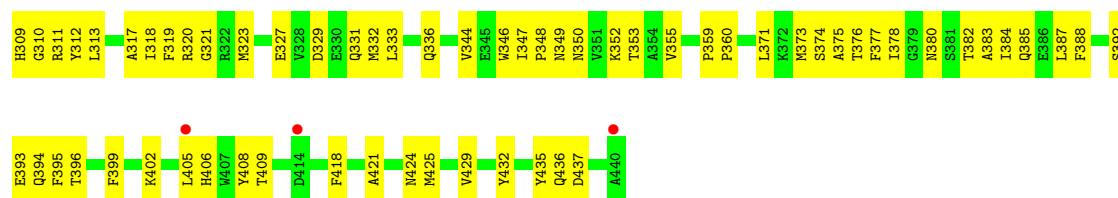


• Molecule 2: Tubulin beta chain

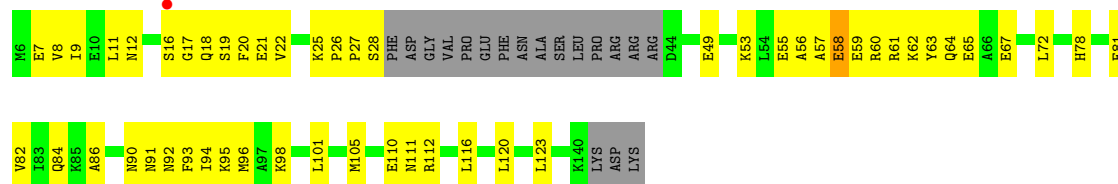


• Molecule 2: Tubulin beta chain

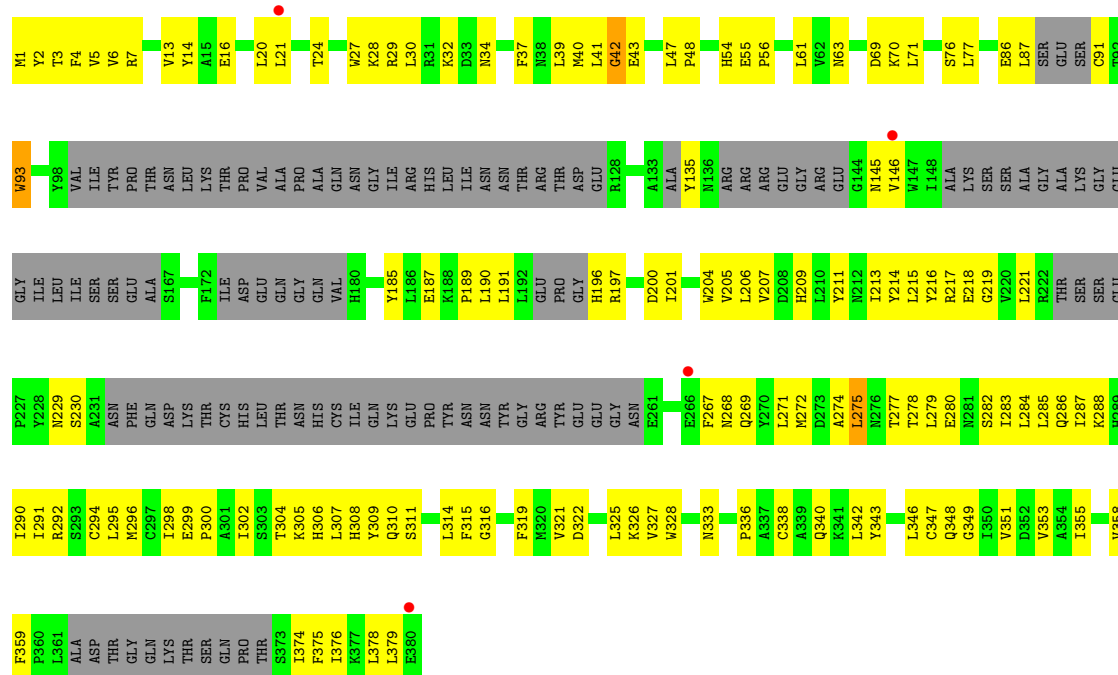




• Molecule 3: Stathmin-4



• 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	104.60Å 155.89Å 181.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.98 – 3.48 25.98 – 3.48	Depositor EDS
% Data completeness (in resolution range)	97.5 (25.98-3.48) 97.2 (25.98-3.48)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.46Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.267 0.222 , 0.266	Depositor DCC
R_{free} test set	1917 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	91.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15871	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, NA, GTP, A1ECQ, IMD, EDO, GDP, ACP, MG, CA

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	0.61	0/3375	0.81	3/4612 (0.1%)
1	C	0.70	2/3390 (0.1%)	0.92	5/4629 (0.1%)
2	B	0.66	0/3246	0.88	1/4424 (0.0%)
2	D	0.54	0/3160	0.79	4/4315 (0.1%)
3	E	0.54	0/817	0.73	0/1114
4	F	0.48	1/2049 (0.0%)	0.68	0/2790
All	All	0.61	3/16037 (0.0%)	0.82	13/21884 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315[A]	CYS	C-O	5.97	1.31	1.23
1	C	315[B]	CYS	C-O	5.97	1.31	1.23
4	F	93	TRP	C-N	5.33	1.42	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315[A]	CYS	CA-C-O	7.09	129.06	120.27
1	C	315[B]	CYS	CA-C-O	7.09	129.06	120.27
1	C	182	VAL	N-CA-C	-6.33	106.57	112.83
2	D	38	GLY	CA-C-N	5.98	131.61	121.14
2	D	38	GLY	C-N-CA	5.98	131.61	121.14

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	3273	0	3064	259	0
1	C	3303	0	3088	230	0
2	B	3153	0	2912	226	0
2	D	3082	0	2768	235	0
3	E	807	0	658	51	0
4	F	1996	0	1808	210	0
5	A	32	0	12	3	0
5	C	32	0	12	7	0
6	A	4	0	6	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	1	0	0	0	0
10	B	12	0	13	0	0
11	B	39	27	0	7	0
12	B	28	0	12	5	0
12	D	28	0	12	7	0
13	C	5	0	5	0	0
14	F	31	0	14	0	0
15	B	5	0	0	0	0
15	C	4	0	0	0	0
15	D	2	0	0	0	0
15	F	3	0	0	0	0
All	All	15844	27	14384	1165	0

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 39.

The worst 5 of 1165 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)
11:B:503:A1ECQ:C2	11:B:503:A1ECQ:O2	1.63	1.33
4:F:271:LEU:HA	4:F:275[A]:LEU:HD23	1.31	1.09
2:B:8:GLN:HE21	2:B:67:LEU:HG	1.19	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.46	0.98
2:B:115:VAL:HG23	2:B:153:LEU:HD23	1.47	0.96

There are no symmetry-related clashes.

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	444/440 (101%)	417 (94%)	25 (6%)	2 (0%)	25	59
1	C	440/440 (100%)	410 (93%)	27 (6%)	3 (1%)	19	53
2	B	420/430 (98%)	393 (94%)	24 (6%)	3 (1%)	19	53
2	D	422/430 (98%)	388 (92%)	30 (7%)	4 (1%)	14	48
3	E	117/138 (85%)	114 (97%)	3 (3%)	0	100	100
4	F	250/380 (66%)	238 (95%)	11 (4%)	1 (0%)	30	64
All	All	2093/2258 (93%)	1960 (94%)	120 (6%)	13 (1%)	22	55

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	215	ARG
1	C	404	PHE
1	A	162	GLY
2	B	109	THR
1	C	73	THR

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	331/371 (89%)	330 (100%)	1 (0%)	91	96
1	C	338/371 (91%)	336 (99%)	2 (1%)	84	91
2	B	326/372 (88%)	323 (99%)	3 (1%)	75	85
2	D	299/372 (80%)	296 (99%)	3 (1%)	73	84
3	E	61/124 (49%)	60 (98%)	1 (2%)	58	76
4	F	189/338 (56%)	187 (99%)	2 (1%)	70	82
All	All	1544/1948 (79%)	1532 (99%)	12 (1%)	81	87

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	259	MET
2	D	437	ASP
4	F	275[B]	LEU
3	E	58	GLU
2	B	437	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	266	HIS
2	D	14	ASN
2	D	8	GLN
2	D	136	GLN
2	B	11	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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
12	GDP	B	504	7	24,30,30	1.20	2 (8%)	30,47,47	2.17	12 (40%)
5	GTP	C	501	7	26,34,34	1.50	4 (15%)	32,54,54	2.38	13 (40%)
10	MES	B	502	-	12,12,12	2.29	1 (8%)	14,16,16	1.28	2 (14%)
6	EDO	A	502	-	3,3,3	0.41	0	2,2,2	0.39	0
12	GDP	D	501	-	24,30,30	1.06	3 (12%)	30,47,47	1.88	8 (26%)
11	A1ECQ	B	503	-	43,45,45	3.56	18 (41%)	61,67,67	1.95	15 (24%)
5	GTP	A	501	7	26,34,34	1.58	5 (19%)	32,54,54	2.94	10 (31%)
14	ACP	F	401	-	27,33,33	1.32	5 (18%)	32,52,52	1.48	4 (12%)
13	IMD	C	502	-	3,5,5	0.44	0	4,5,5	0.43	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
12	GDP	B	504	7	-	2/12/32/32	0/3/3/3
5	GTP	C	501	7	-	3/18/38/38	0/3/3/3
10	MES	B	502	-	-	5/6/14/14	0/1/1/1
6	EDO	A	502	-	-	0/1/1/1	-
12	GDP	D	501	-	-	1/12/32/32	0/3/3/3
11	A1ECQ	B	503	-	-	6/14/55/55	0/7/7/7
5	GTP	A	501	7	-	6/18/38/38	0/3/3/3
14	ACP	F	401	-	-	5/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	IMD	C	502	-	-	-	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	503	A1ECQ	C24-C23	11.42	1.59	1.40
11	B	503	A1ECQ	O2-C2	8.89	1.63	1.45
11	B	503	A1ECQ	O2-C1	8.13	1.53	1.35
10	B	502	MES	C8-S	-7.76	1.66	1.77
11	B	503	A1ECQ	C4-C5	-7.72	1.45	1.53

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N1-C6	-8.74	109.00	125.10
5	A	501	GTP	C5-C6-N1	7.78	127.69	113.95
5	A	501	GTP	N2-C2-N3	-6.38	107.32	119.74
5	A	501	GTP	O6-C6-C5	-6.10	112.46	124.37
11	B	503	A1ECQ	C2-C4-C3	6.03	110.51	101.79

There are no chirality outliers.

5 of 28 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	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
10	B	502	MES	C8-C7-N4-C5

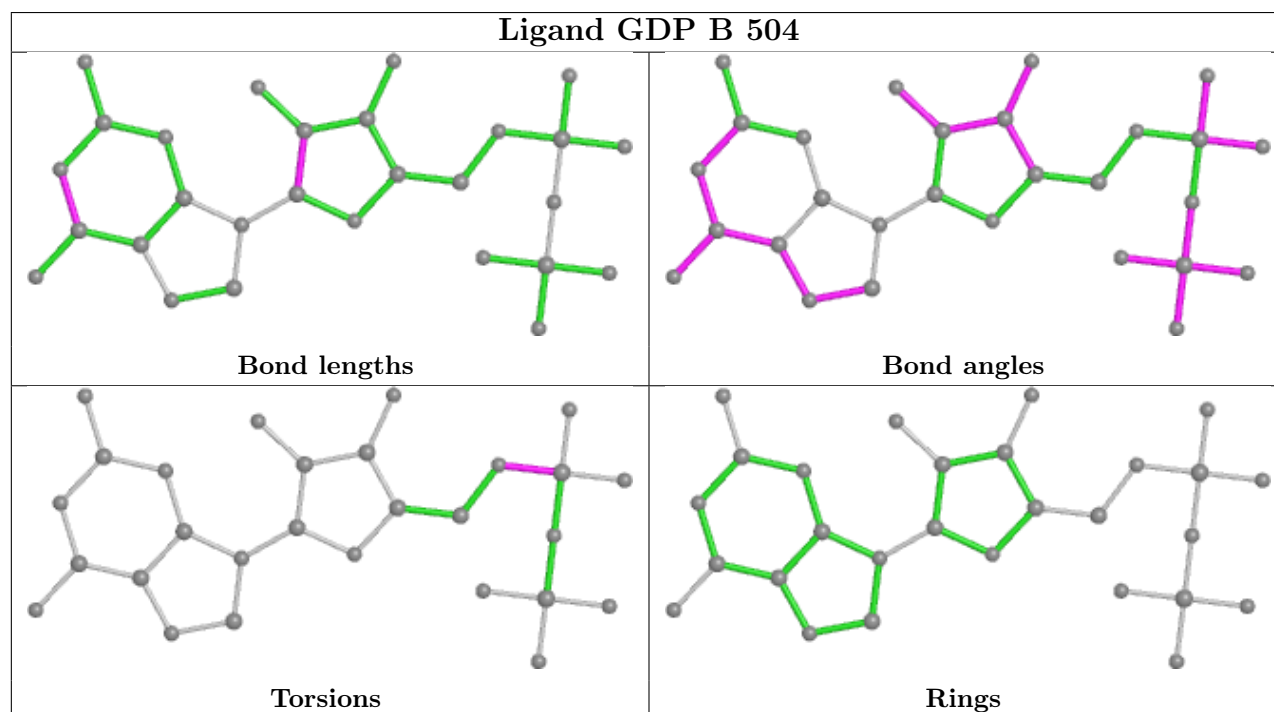
There are no ring outliers.

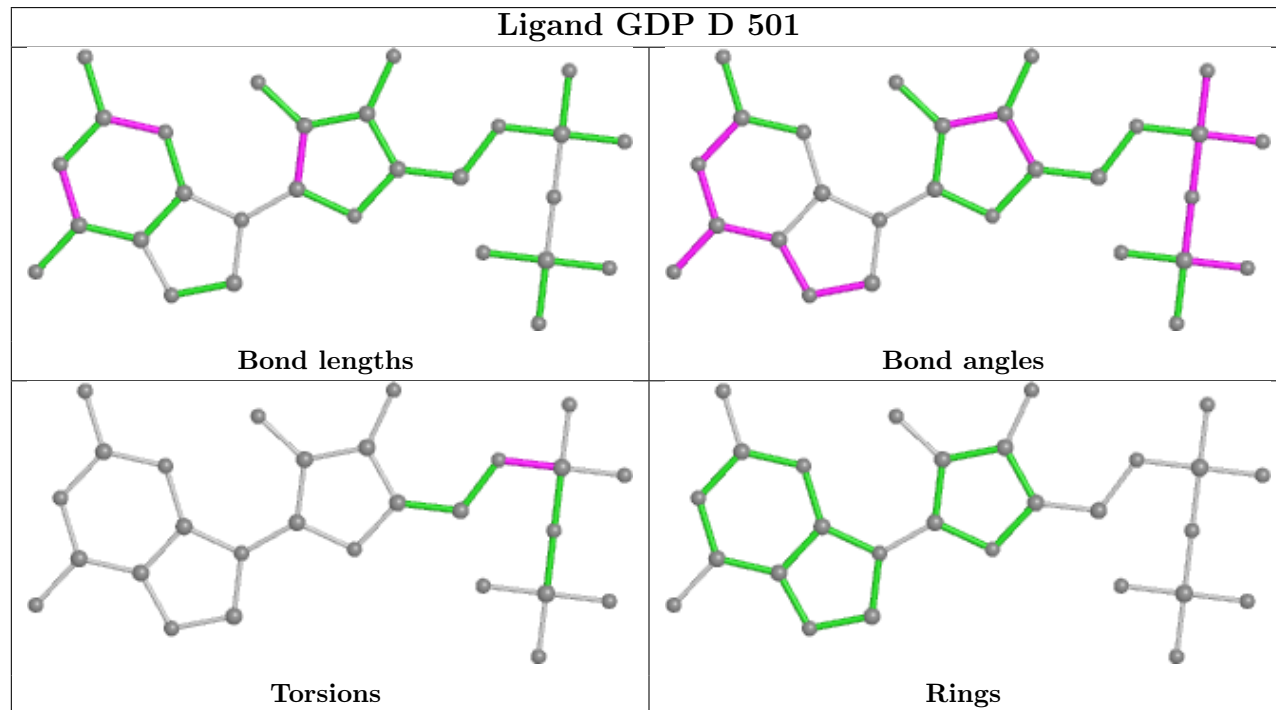
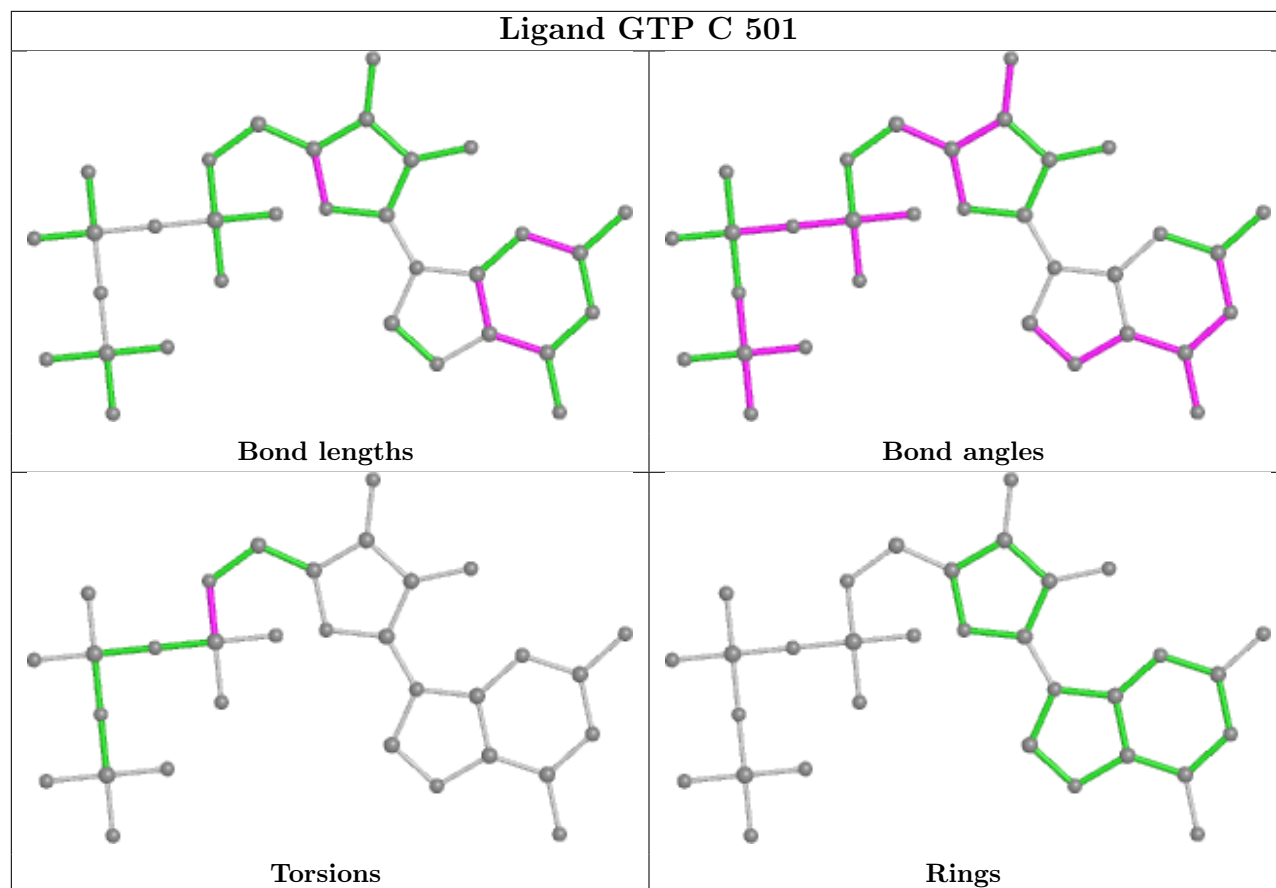
5 monomers are involved in 28 short contacts:

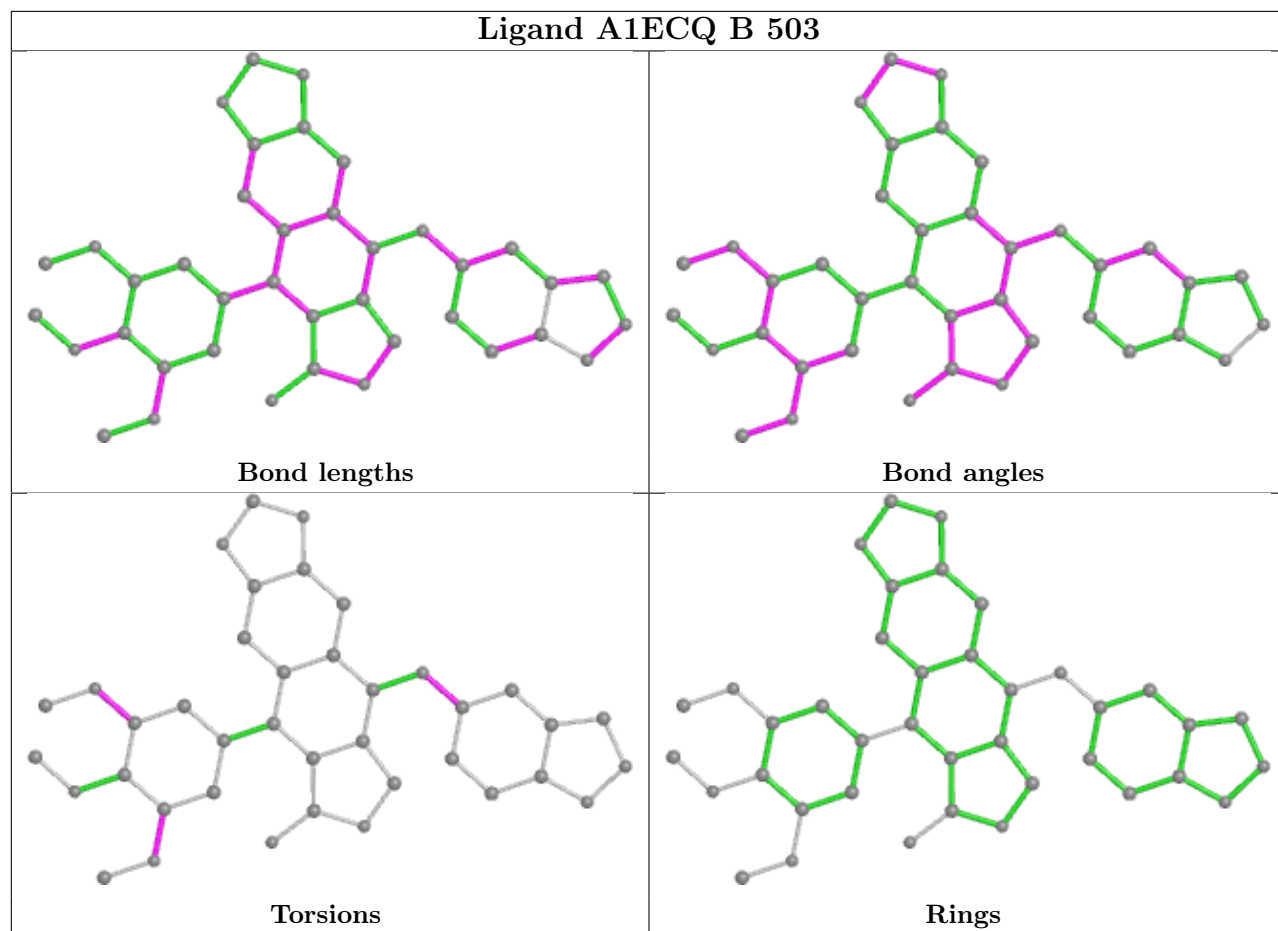
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	504	GDP	5	0
5	C	501	GTP	7	0
12	D	501	GDP	7	0
11	B	503	A1ECQ	7	0
5	A	501	GTP	3	0

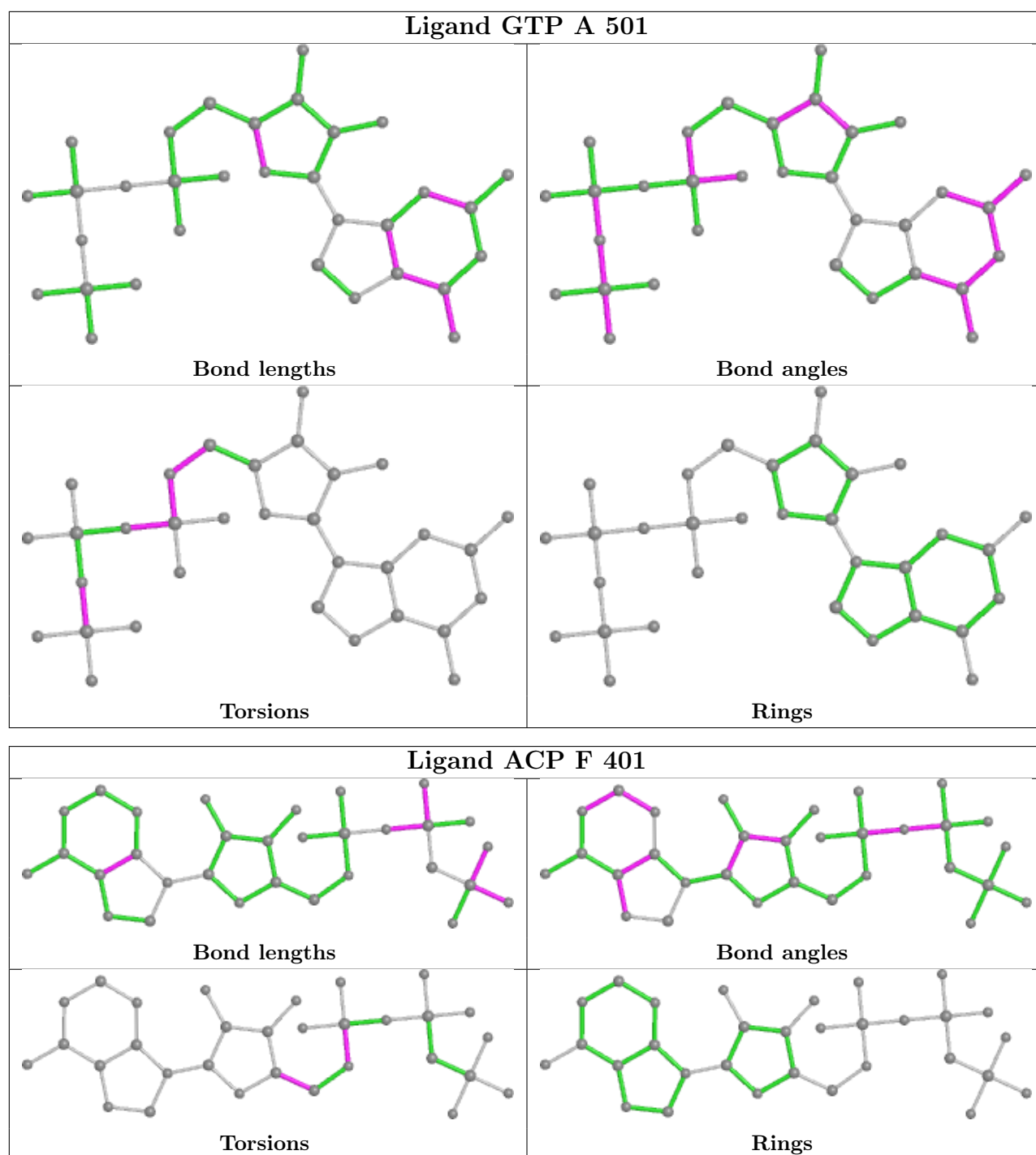
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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	437/440 (99%)	0.06	4 (0%) 81 64	45, 86, 108, 116	9 (2%)
1	C	439/440 (99%)	0.02	4 (0%) 81 64	38, 73, 95, 106	5 (1%)
2	B	419/430 (97%)	0.00	5 (1%) 76 57	41, 74, 97, 112	9 (2%)
2	D	426/430 (99%)	0.20	12 (2%) 55 37	53, 92, 111, 122	5 (1%)
3	E	120/138 (86%)	-0.17	1 (0%) 82 67	46, 84, 112, 117	1 (0%)
4	F	268/380 (70%)	0.35	4 (1%) 71 53	60, 102, 125, 142	4 (1%)
All	All	2109/2258 (93%)	0.09	30 (1%) 73 53	38, 84, 112, 142	33 (1%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	CYS	3.8
2	B	109	THR	3.8
4	F	146	VAL	3.2
2	D	99	ALA	3.1
1	C	59	GLY	3.0

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

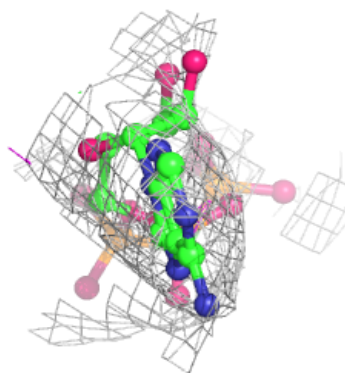
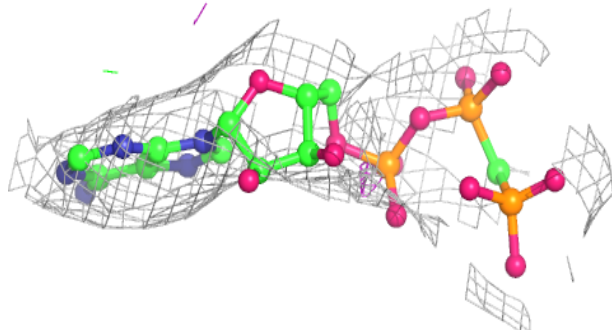
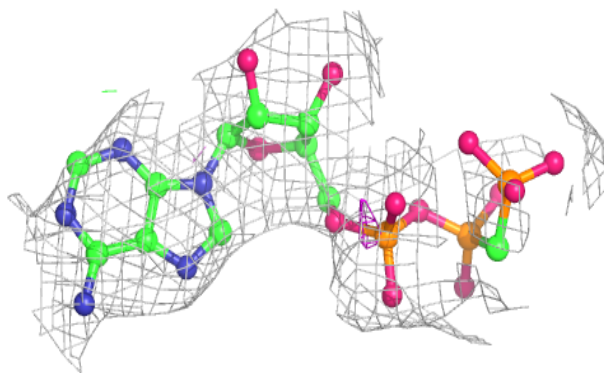
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	502	4/4	0.59	0.22	99,99,104,107	0
7	MG	C	503	1/1	0.68	0.32	67,67,67,67	0
7	MG	A	503	1/1	0.70	0.28	68,68,68,68	0
7	MG	B	505	1/1	0.73	0.26	69,69,69,69	0
13	IMD	C	502	5/5	0.73	0.35	83,85,98,102	0
14	ACP	F	401	31/31	0.77	0.11	99,119,143,152	0
10	MES	B	502	12/12	0.79	0.16	59,72,83,86	0
11	A1ECQ	B	503	39/39	0.81	0.14	58,92,116,137	0
8	CA	A	504	1/1	0.82	0.16	124,124,124,124	0
9	NA	B	501	1/1	0.82	0.18	70,70,70,70	0
12	GDP	D	501	28/28	0.85	0.11	87,93,113,120	0
5	GTP	C	501	32/32	0.89	0.12	64,69,79,81	0
12	GDP	B	504	28/28	0.93	0.09	55,61,73,77	0
5	GTP	A	501	32/32	0.93	0.09	66,72,86,92	0

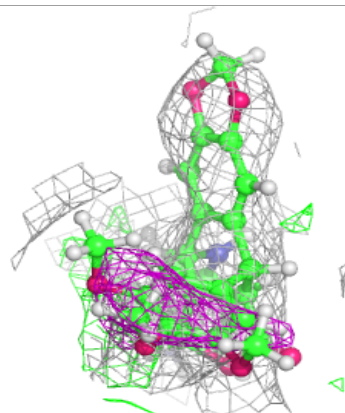
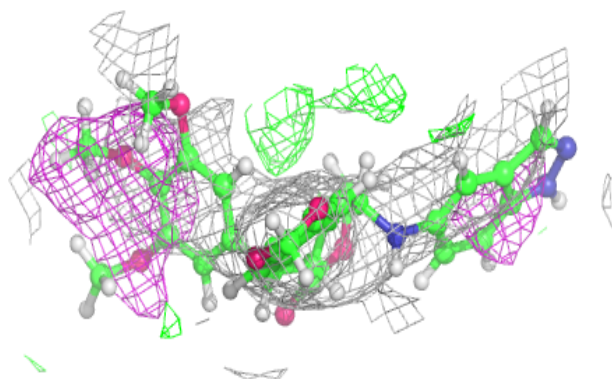
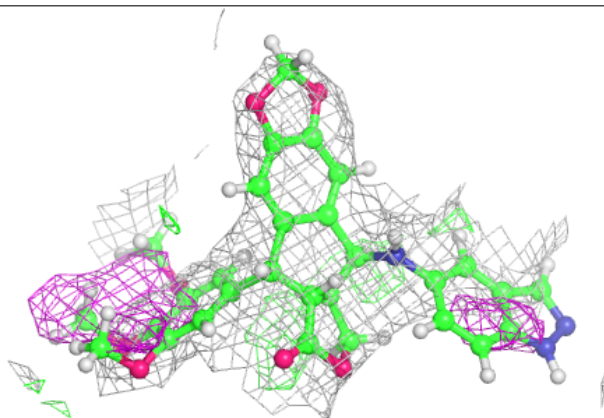
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

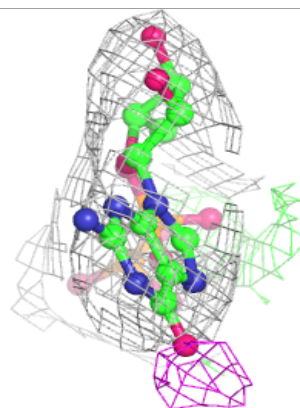
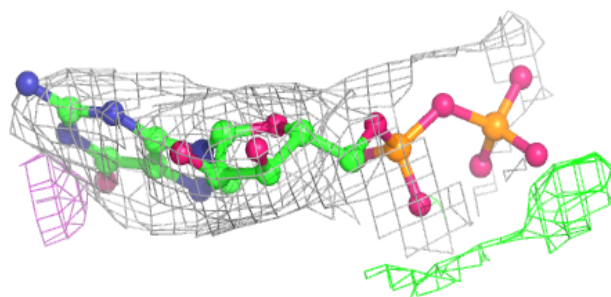
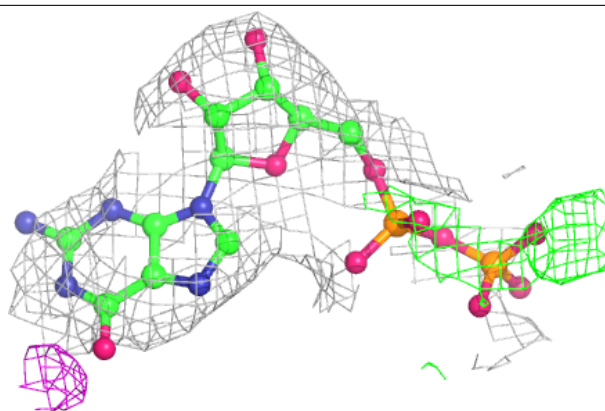
**Electron density around A1ECQ B 503:**

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

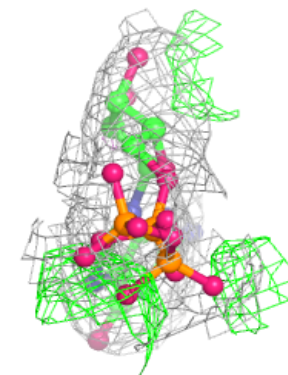
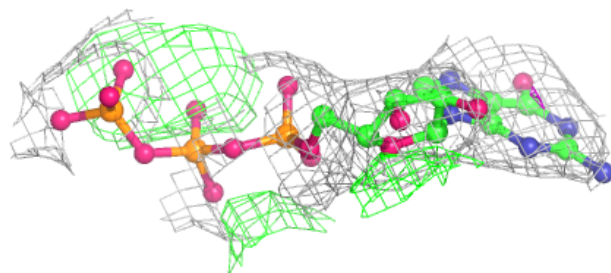
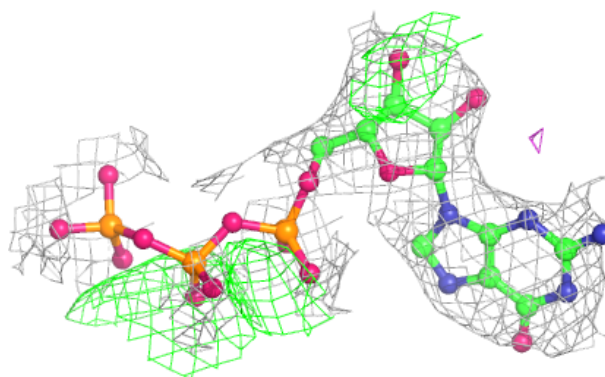


Electron density around GDP D 501:

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

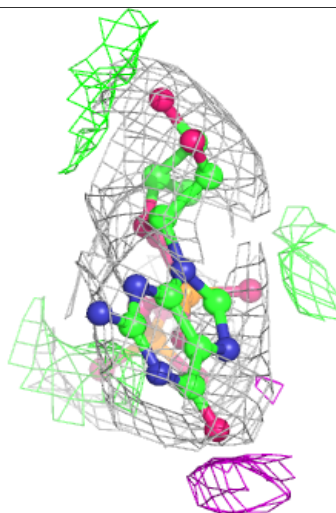
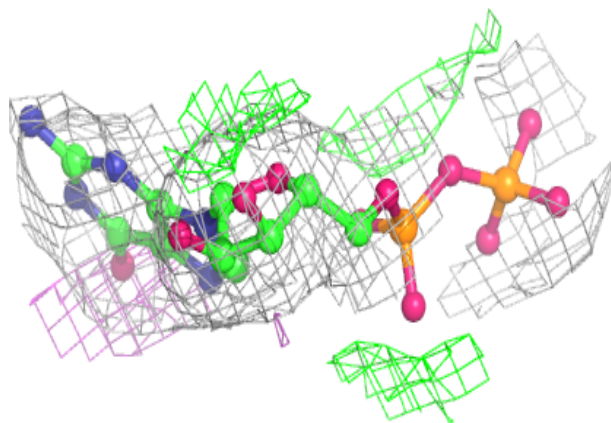
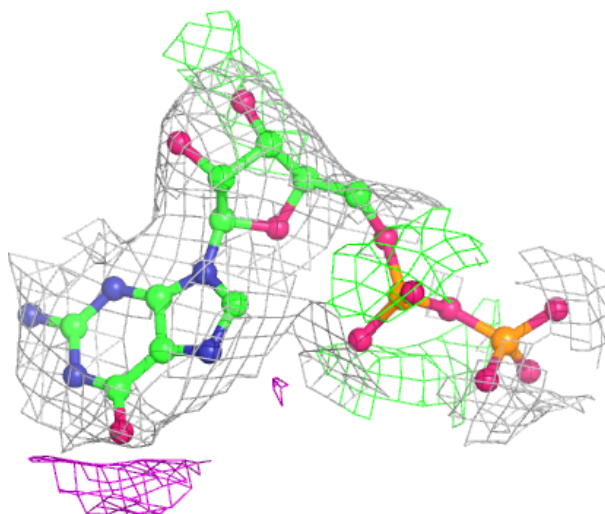
**Electron density around GTP C 501:**

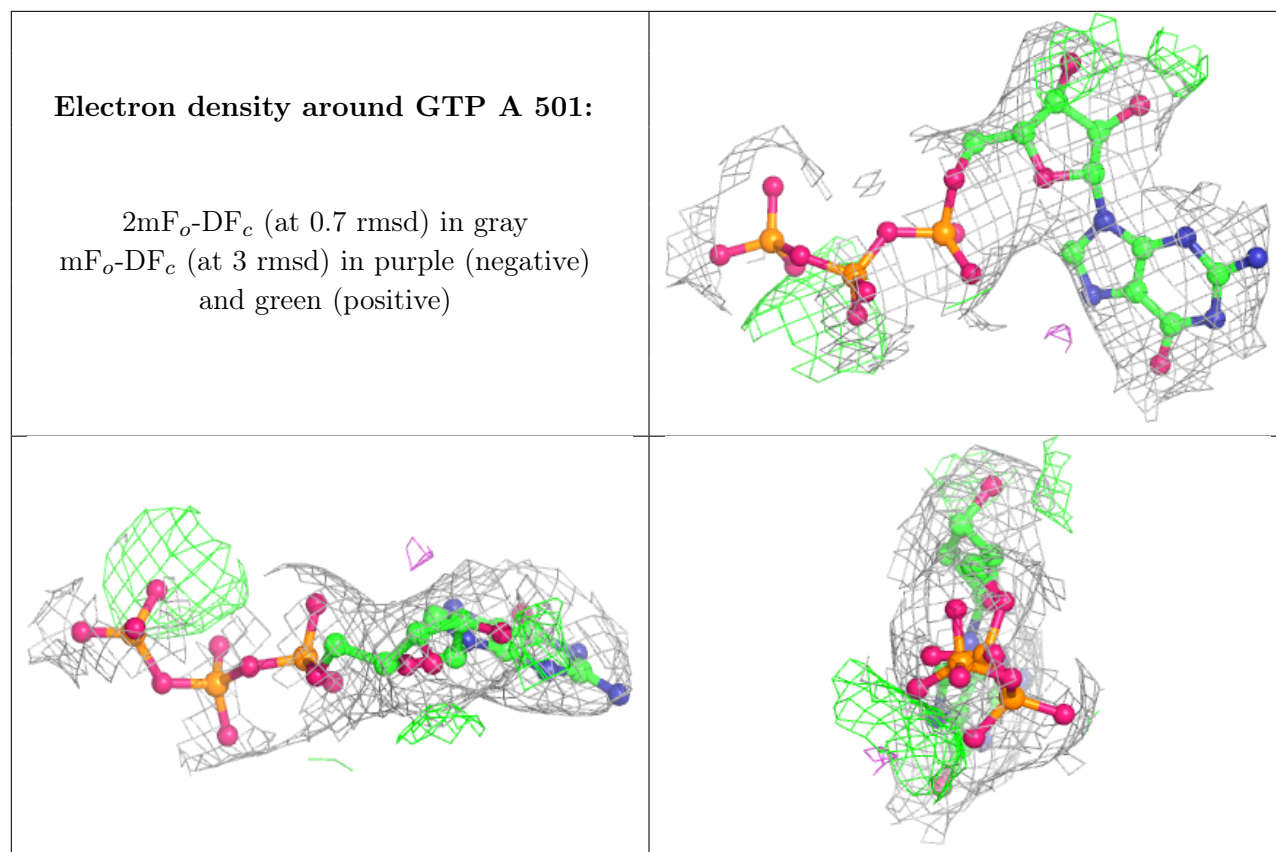
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 504:

$2mF_o-DF_c$ (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.