



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:25 AM UTC

PDB ID : 5S4P / pdb_00005s4p
Title : Tubulin-Z275165822-complex
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Deposited on : 2020-11-08
Resolution : 2.29 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

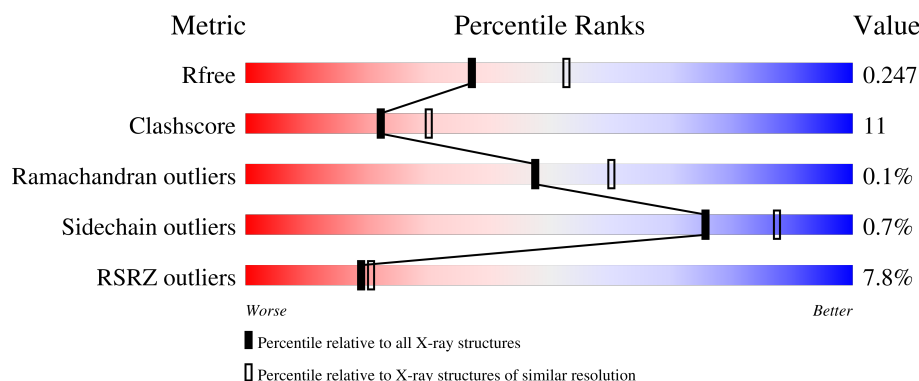
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	451	6% 76% 21% .
1	C	451	5% 77% 21% .
2	B	445	6% 69% 26% 5%
2	D	445	6% 74% 21% .
3	E	143	13% 78% 7% . 14%

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Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18111 atoms, of which 75 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	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	2	0
			3452	2183	586	660	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	3	0	0
			3324	2090	567	640	27			
2	D	426	Total	C	N	O	S	5	0	0
			3343	2098	570	648	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

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

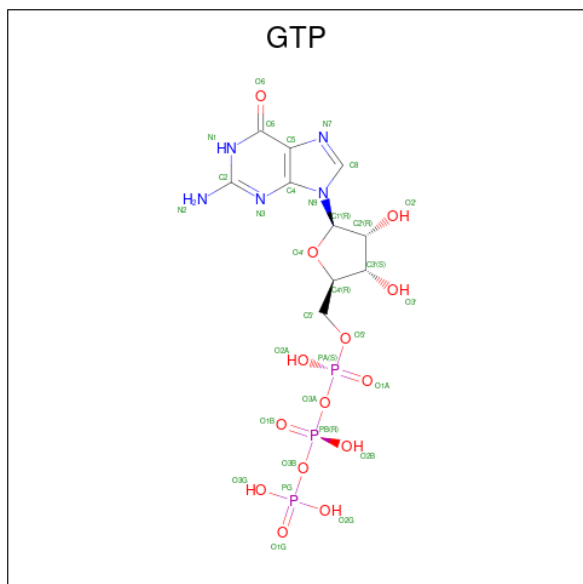
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	0	0
			2854	1829	491	520	14			

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: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

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

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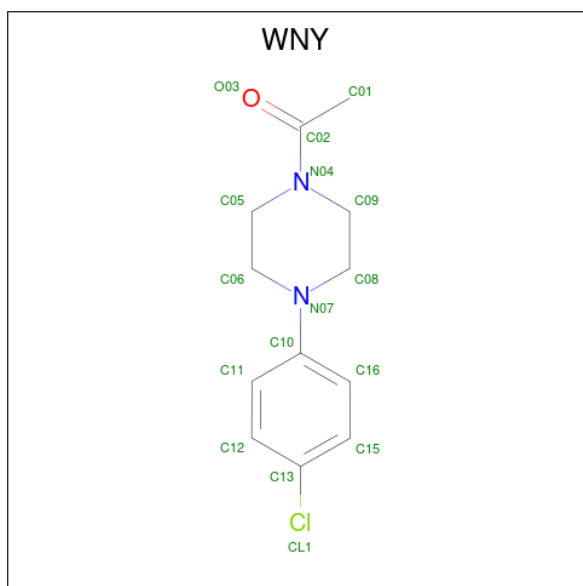
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 8 is 1-[4-(4-chlorophenyl)piperazin-1-yl]ethan-1-one (CCD ID: WNY) (formula: C₁₂H₁₅ClN₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	Cl	H	N	O	0	0
			31	12	1	15	2	1		
8	B	1	Total	C	Cl	H	N	O	0	0
			31	12	1	15	2	1		
8	B	1	Total	C	Cl	H	N	O	0	0
			31	12	1	15	2	1		
8	C	1	Total	C	Cl	H	N	O	0	0
			31	12	1	15	2	1		
8	C	1	Total	C	Cl	H	N	O	0	0
			31	12	1	15	2	1		

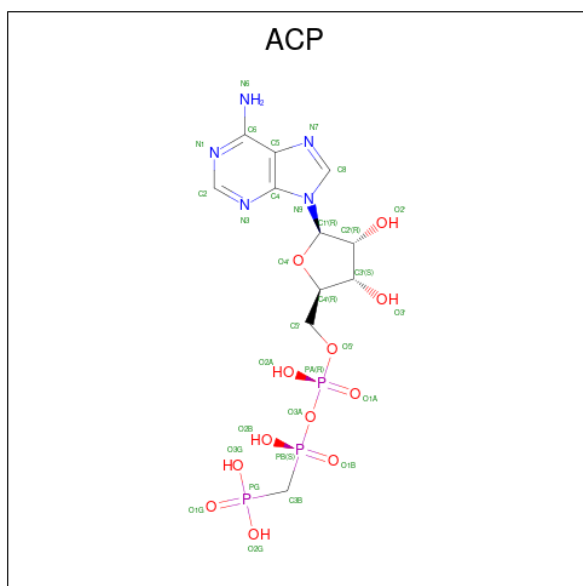
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- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including an amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group being the terminal one. The structure is labeled with various atoms and bonds, including the guanine base, ribose sugar, and the two phosphate groups.

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

- MES
-
- The chemical structure of MES (3-(3-sulfamoylpropyl)carbazole) is shown. It consists of a carbazole ring system (a benzene ring fused to a five-membered nitrogen-containing ring) with a propyl chain attached to the nitrogen atom. The propyl chain is terminated by a sulfamoyl group (SO₂OH). The atoms are labeled: O1, C2, C6, C3, C5, N4, C7, C8, S, O2S, O1S, and O3S.

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

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



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

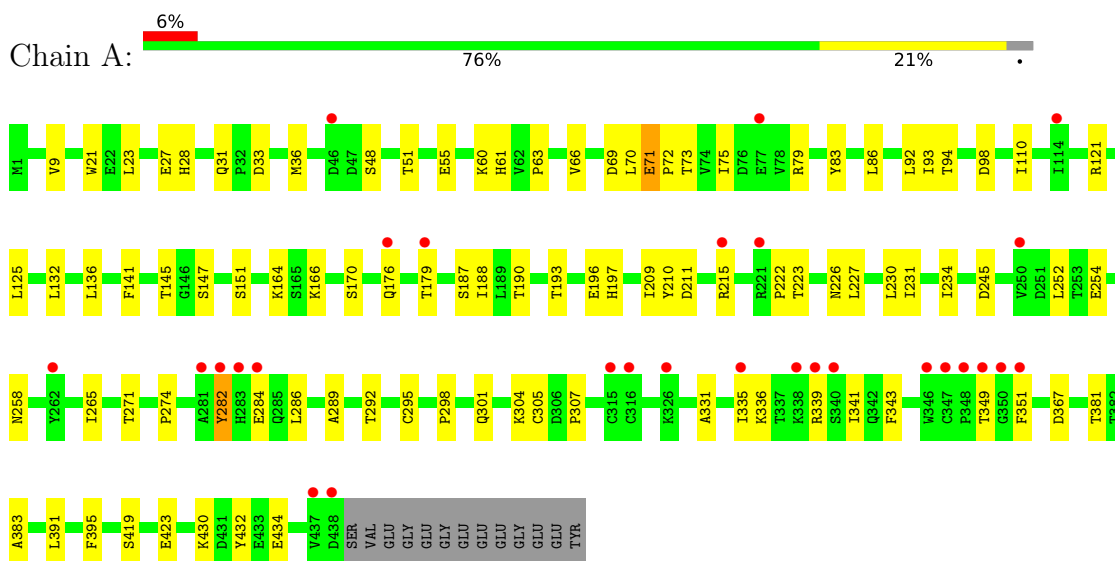
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	68	Total	O	0	0
			68	68		
12	B	70	Total	O	0	0
			70	70		
12	C	178	Total	O	0	0
			178	178		
12	D	32	Total	O	0	0
			32	32		
12	E	10	Total	O	0	0
			10	10		
12	F	15	Total	O	0	0
			15	15		

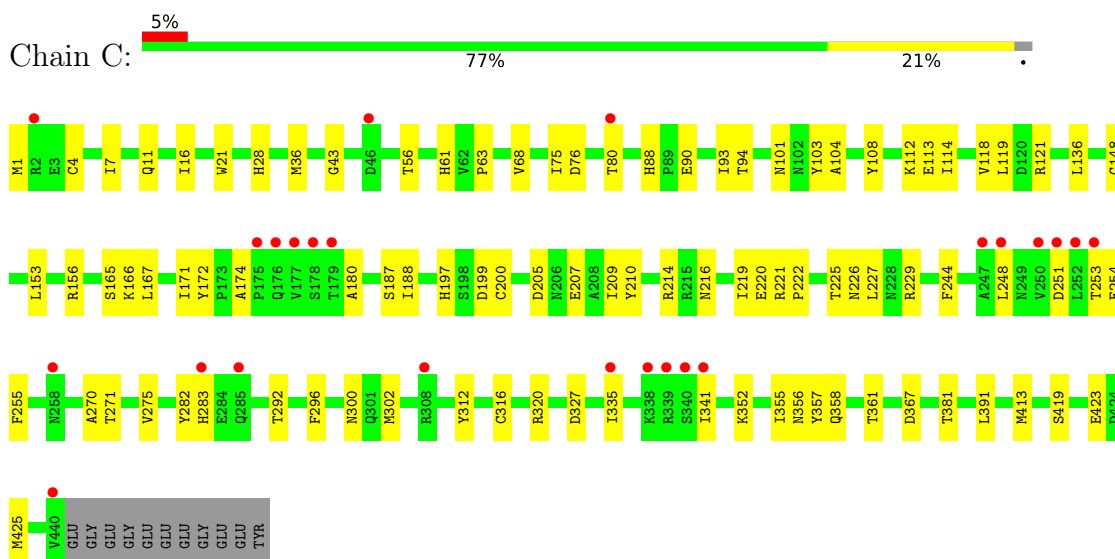
3 Residue-property plots

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.

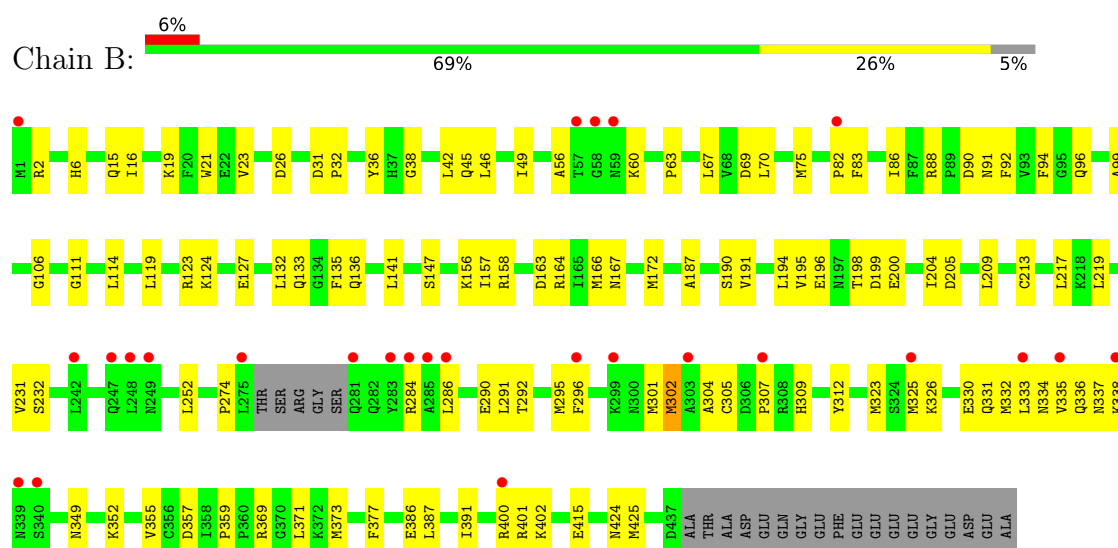
• Molecule 1: Tubulin alpha-1B chain



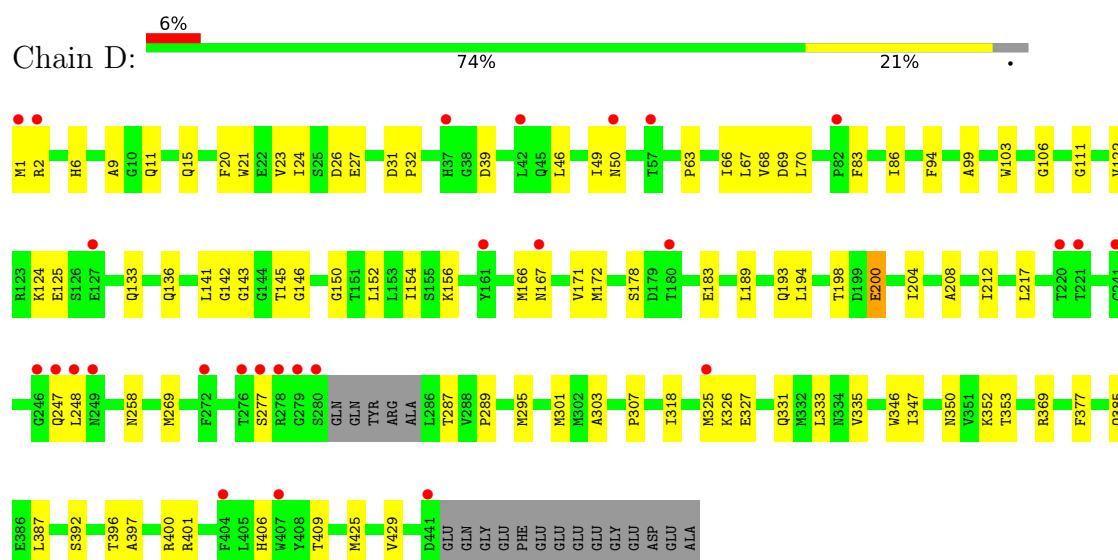
• Molecule 1: Tubulin alpha-1B chain



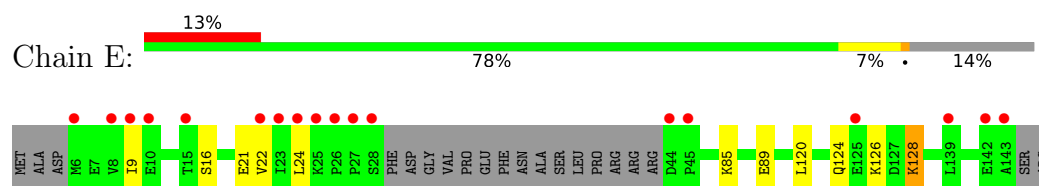
• Molecule 2: Tubulin beta-2B chain



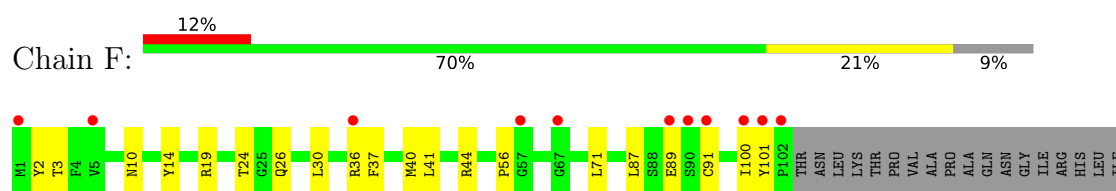
• Molecule 2: Tubulin beta-2B chain

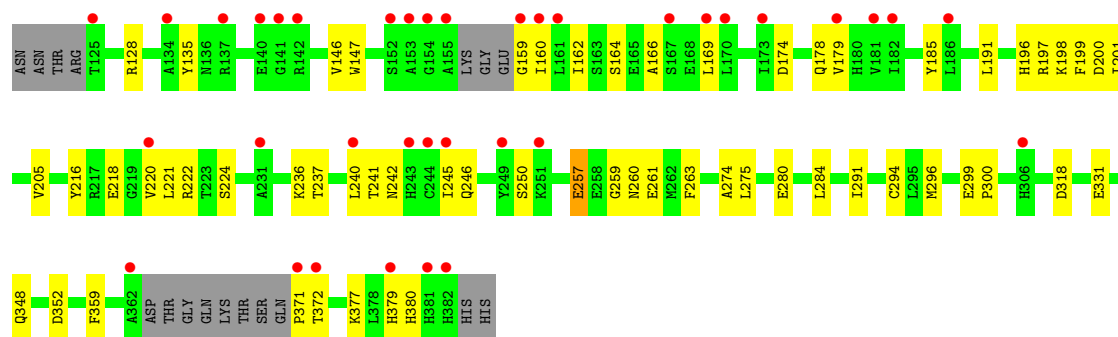


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.25Å 157.05Å 178.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.52 – 2.29 78.52 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.8 (78.52-2.29) 97.8 (78.52-2.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.208 , 0.244 0.209 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18111	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: GDP, ACP, MG, MES, WNY, GTP, 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	0.11	0/3502	0.29	0/4754
1	C	0.13	0/3530	0.31	0/4792
2	B	0.12	0/3398	0.28	0/4601
2	D	0.11	0/3416	0.29	0/4626
3	E	0.11	0/1022	0.25	0/1356
4	F	0.10	0/2921	0.29	0/3946
All	All	0.12	0/17789	0.29	0/24075

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3424	0	3335	76	0
1	C	3452	0	3357	68	0
2	B	3324	0	3198	98	0
2	D	3343	0	3222	72	0
3	E	1014	0	1029	11	0
4	F	2854	0	2815	58	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	16	15	0	0	0
8	B	32	30	0	1	0
8	C	32	30	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	12	0	12	2	0
11	F	31	0	14	4	0
12	A	68	0	0	2	0
12	B	70	0	0	3	0
12	C	178	0	0	1	0
12	D	32	0	0	1	0
12	E	10	0	0	0	0
12	F	15	0	0	0	0
All	All	18036	75	17030	366	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 11.

The worst 5 of 366 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:209:ILE:HD11	1:C:302:MET:HE3	1.48	0.92
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.57	0.87
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.57	0.86
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.57	0.86
2:D:217:LEU:HA	2:D:277:SER:HB3	1.60	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	425 (98%)	10 (2%)	1 (0%)	43	55
1	C	440/451 (98%)	431 (98%)	9 (2%)	0	100	100
2	B	418/445 (94%)	406 (97%)	11 (3%)	1 (0%)	43	55
2	D	422/445 (95%)	407 (96%)	15 (4%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	341/384 (89%)	324 (95%)	17 (5%)	0	100	100
All	All	2176/2319 (94%)	2112 (97%)	62 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
2	B	82	PRO

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	369/379 (97%)	366 (99%)	3 (1%)	73	86
1	C	373/379 (98%)	371 (100%)	2 (0%)	81	90
2	B	364/383 (95%)	363 (100%)	1 (0%)	86	93
2	D	368/383 (96%)	364 (99%)	4 (1%)	65	81
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	312/342 (91%)	310 (99%)	2 (1%)	78	89
All	All	1896/1993 (95%)	1883 (99%)	13 (1%)	76	87

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	200	GLU
2	D	333	LEU
4	F	257	GLU
3	E	128	LYS
4	F	89	GLU

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	11	GLN
4	F	242	ASN
1	C	285	GLN
4	F	306	HIS
3	E	115	HIS

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 20 ligands modelled in this entry, 9 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	A	501	6	33,34,34	1.01	4 (12%)	50,54,54	1.47	8 (16%)
9	GDP	B	501	6	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
5	GTP	C	501	6	33,34,34	0.96	2 (6%)	50,54,54	1.51	8 (16%)
8	WNY	B	506	-	17,17,17	0.27	0	23,23,23	0.92	1 (4%)
8	WNY	A	505	-	17,17,17	0.23	0	23,23,23	0.80	1 (4%)
8	WNY	C	505	-	17,17,17	0.18	0	23,23,23	0.69	0
9	GDP	D	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.72	5 (11%)
8	WNY	C	504	-	17,17,17	0.21	0	23,23,23	0.74	0
11	ACP	F	401	6	31,33,33	1.70	9 (29%)	47,52,52	1.87	10 (21%)
8	WNY	B	505	-	17,17,17	0.30	0	23,23,23	1.08	2 (8%)
10	MES	B	504	-	12,12,12	2.27	1 (8%)	15,16,16	1.84	5 (33%)

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	A	501	6	-	9/22/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
8	WNY	B	506	-	-	7/8/18/18	0/2/2/2
8	WNY	A	505	-	-	4/8/18/18	0/2/2/2
8	WNY	C	505	-	-	4/8/18/18	0/2/2/2
9	GDP	D	501	6	-	6/16/32/32	0/3/3/3
8	WNY	C	504	-	-	4/8/18/18	0/2/2/2
11	ACP	F	401	6	-	13/19/38/38	0/3/3/3
8	WNY	B	505	-	-	0/8/18/18	0/2/2/2
10	MES	B	504	-	-	4/6/14/14	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.58	1.67	1.77
11	F	401	ACP	C5-C4	4.74	1.47	1.39
9	D	501	GDP	C5-C4	3.11	1.47	1.38
9	B	501	GDP	C5-C4	3.07	1.47	1.38
11	F	401	ACP	PG-O2G	3.04	1.61	1.55

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C5-C4-N3	-5.98	118.88	128.39
11	F	401	ACP	C5-C4-N3	-5.74	118.82	126.72
9	B	501	GDP	C5-C4-N3	-5.73	119.27	128.39
9	D	501	GDP	C2-N3-C4	5.00	120.92	112.30
9	B	501	GDP	C2-N3-C4	5.00	120.92	112.30

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

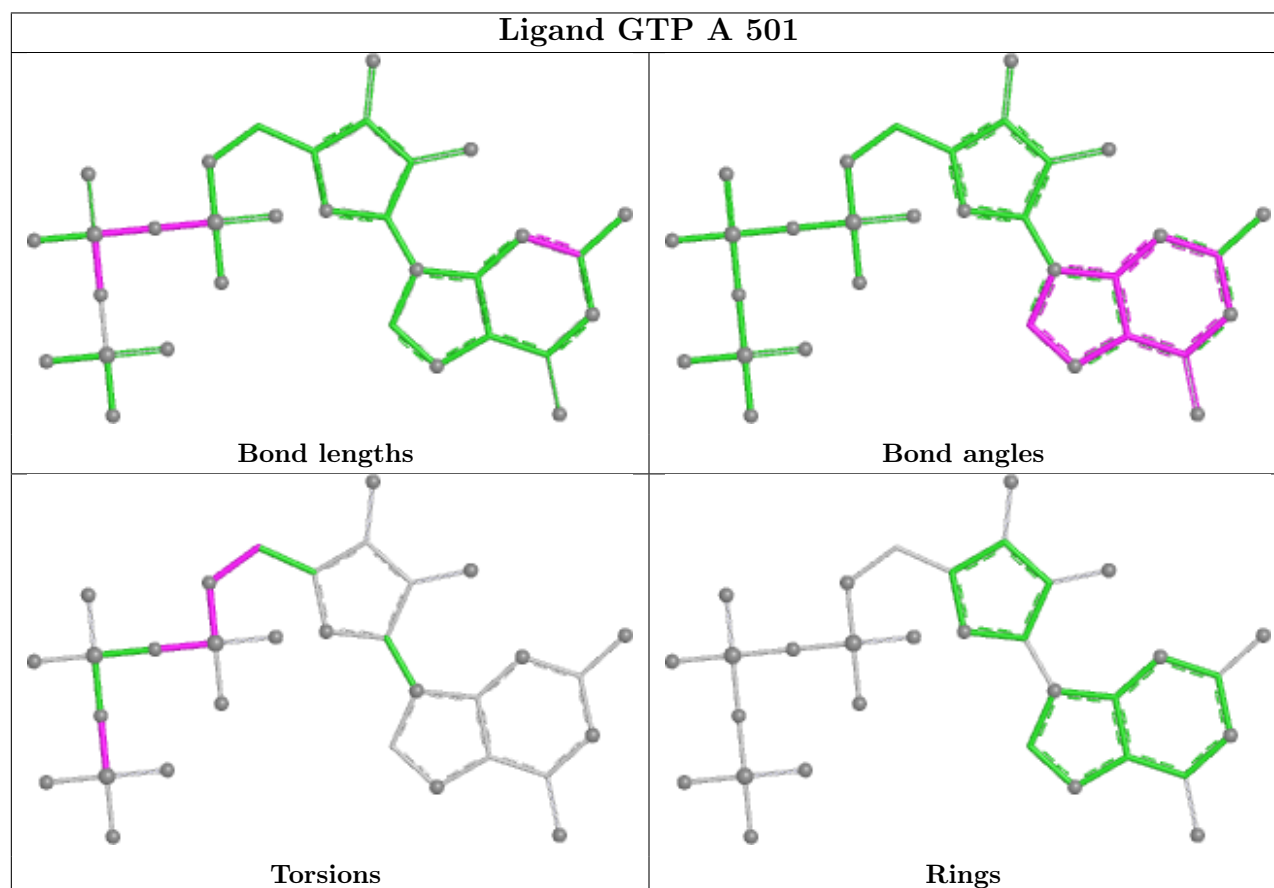
There are no ring outliers.

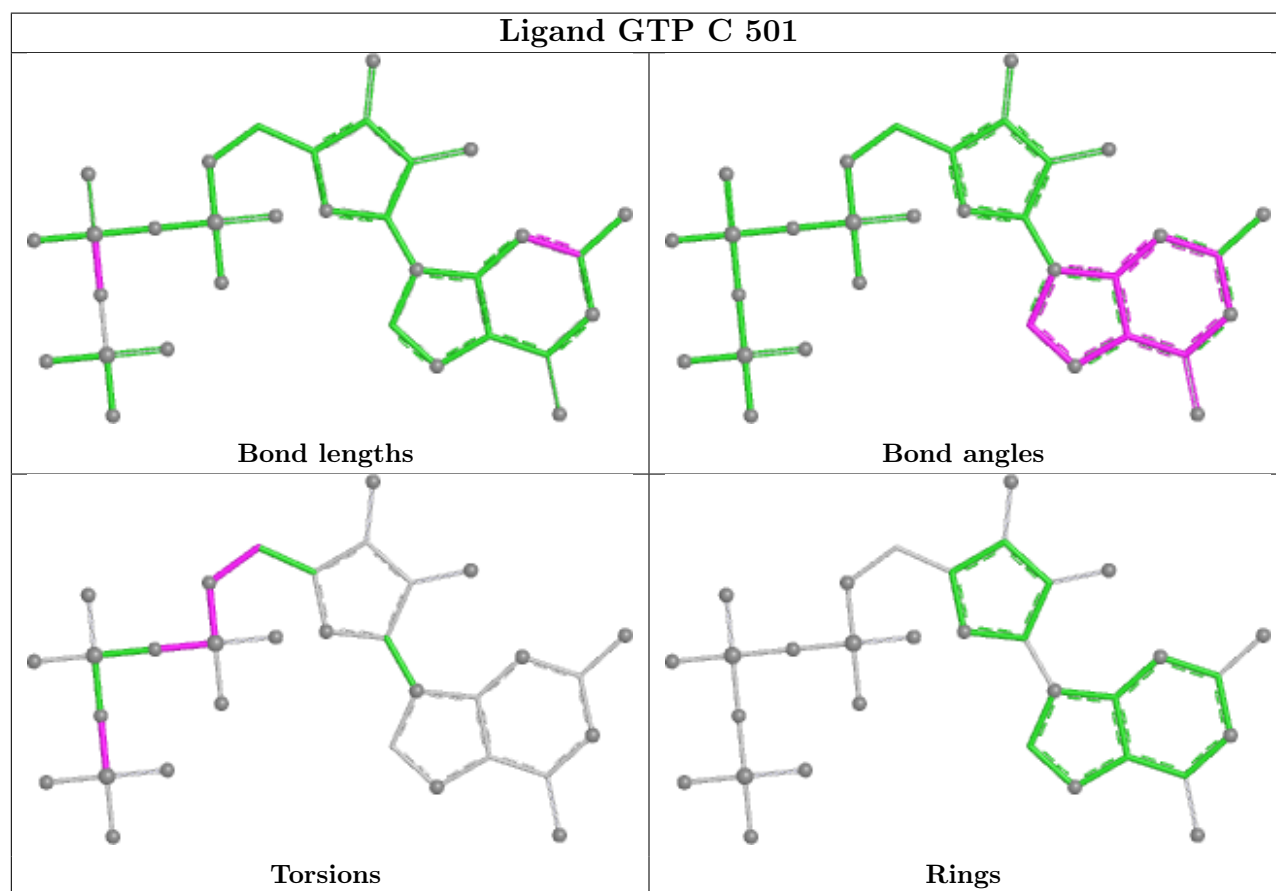
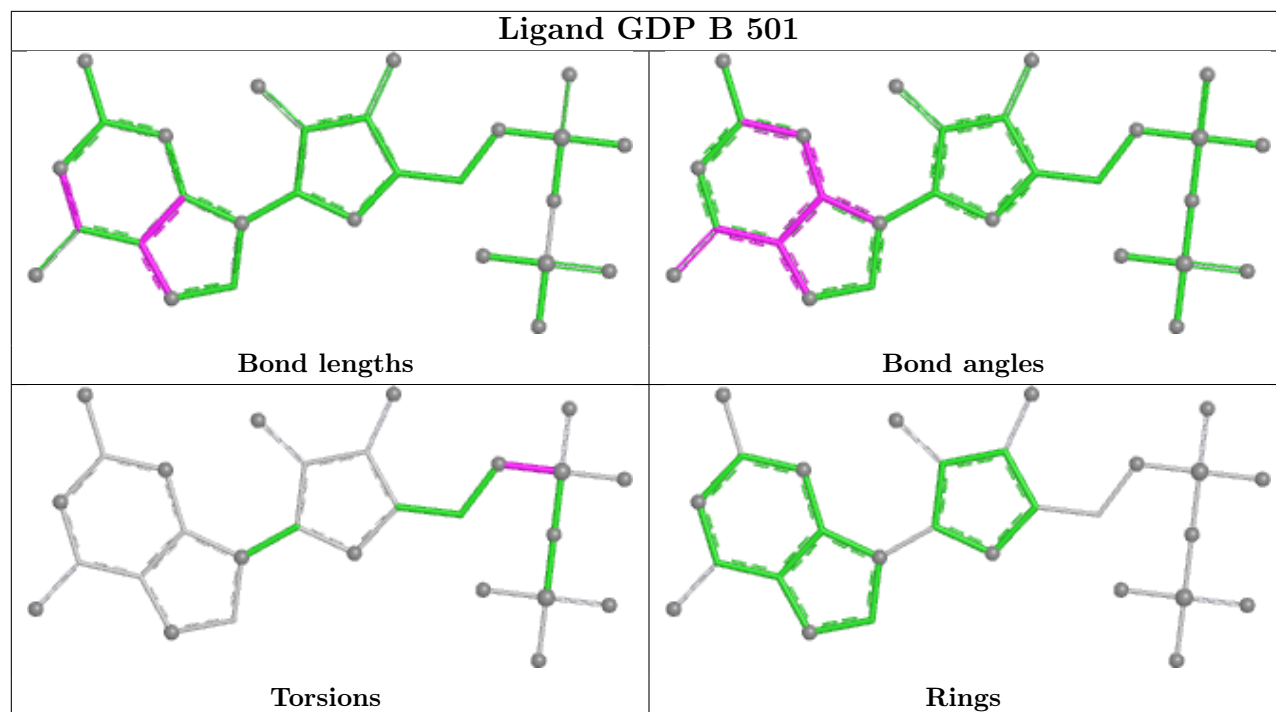
6 monomers are involved in 10 short contacts:

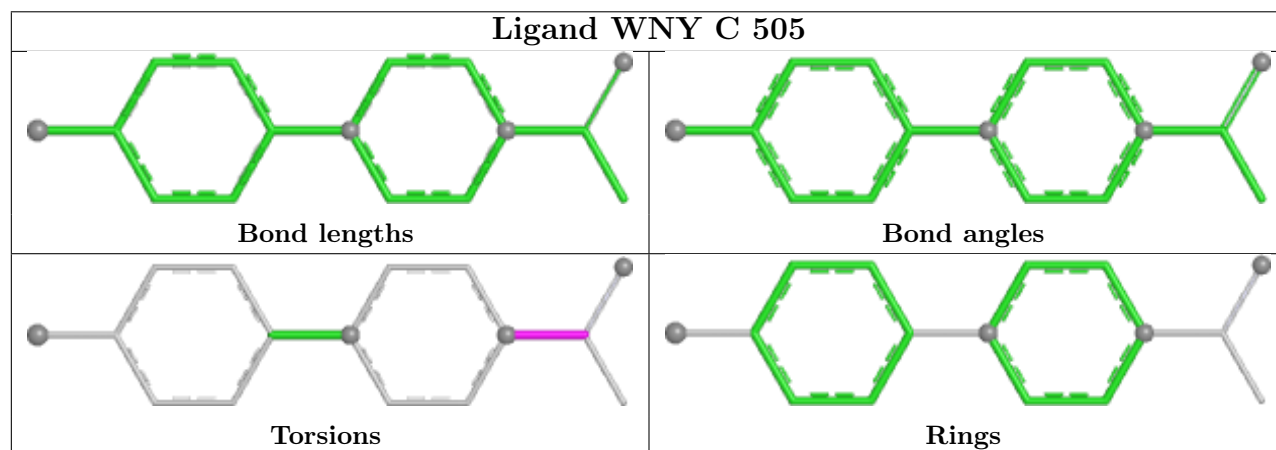
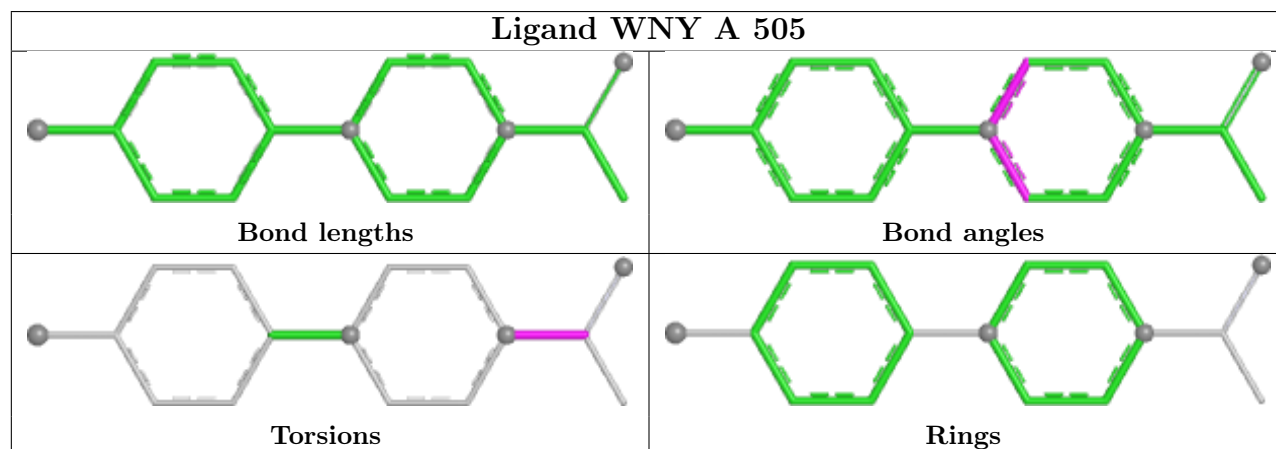
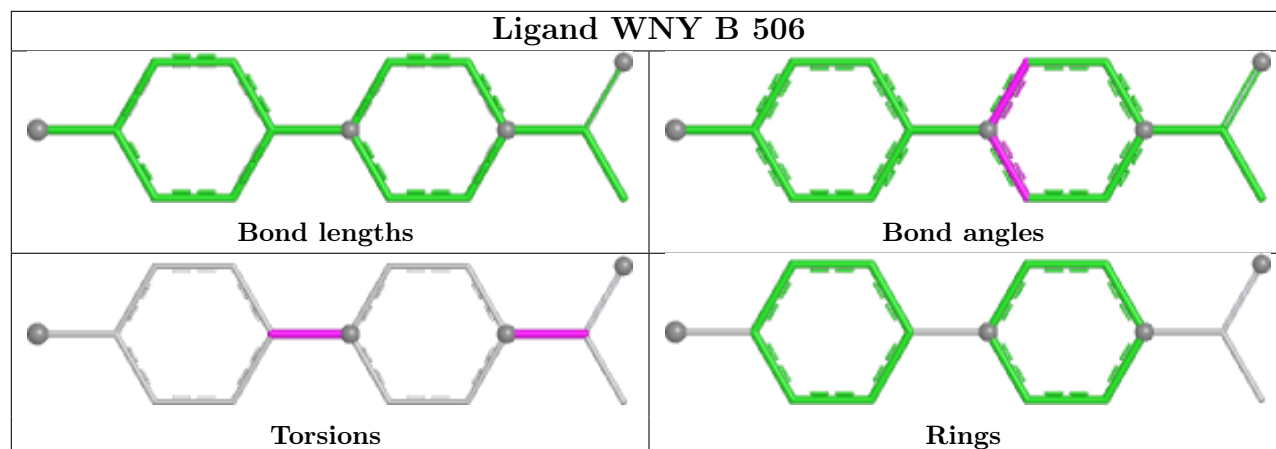
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	B	501	GDP	1	0
8	B	506	WNY	1	0
9	D	501	GDP	1	0
11	F	401	ACP	4	0
10	B	504	MES	2	0

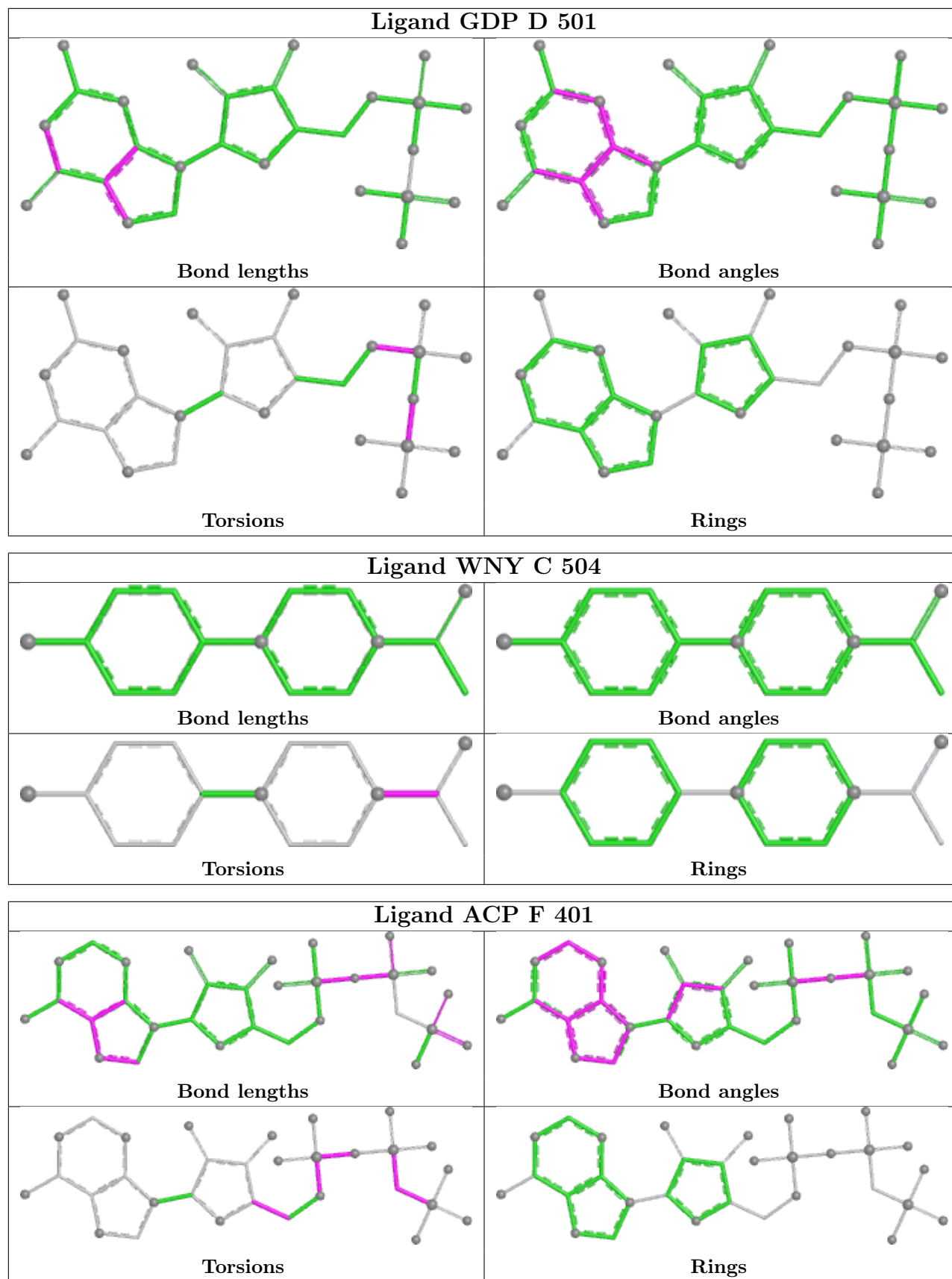
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

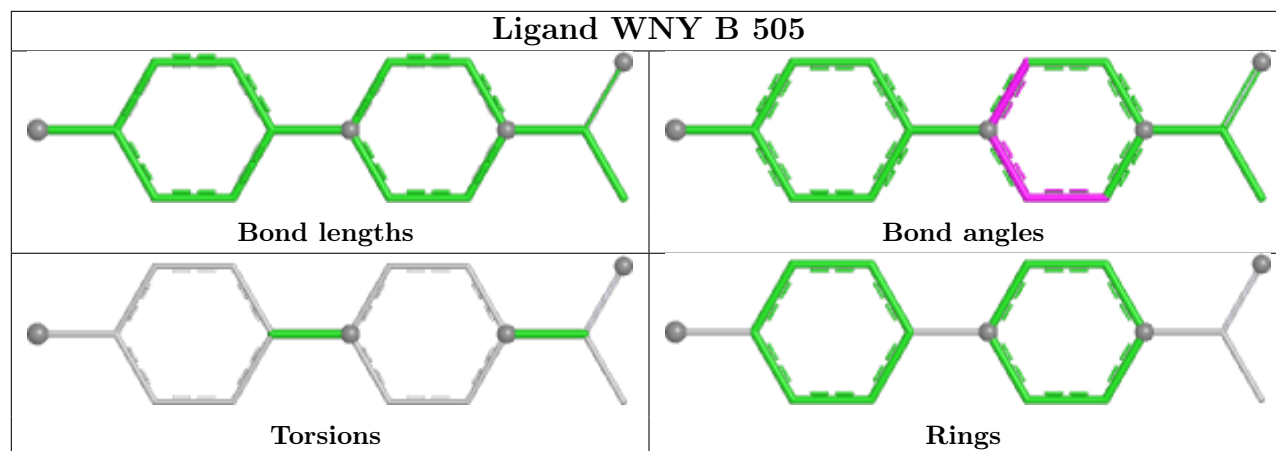
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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	438/451 (97%)	0.34	28 (6%)	25	27	34, 55, 95, 154	0
1	C	440/451 (97%)	0.19	24 (5%)	30	32	21, 45, 69, 124	2 (0%)
2	B	422/445 (94%)	0.56	26 (6%)	26	28	33, 55, 101, 145	3 (0%)
2	D	426/445 (95%)	0.52	28 (6%)	24	26	40, 63, 96, 140	4 (0%)
3	E	123/143 (86%)	0.94	18 (14%)	6	6	43, 64, 124, 161	0
4	F	349/384 (90%)	0.84	47 (13%)	7	8	48, 79, 137, 163	0
All	All	2198/2319 (94%)	0.50	171 (7%)	19	21	21, 59, 109, 163	9 (0%)

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	8.1
3	E	143	ALA	6.5
3	E	24	LEU	6.1
4	F	159	GLY	5.8
2	B	248	LEU	5.1

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

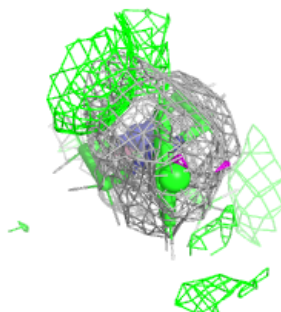
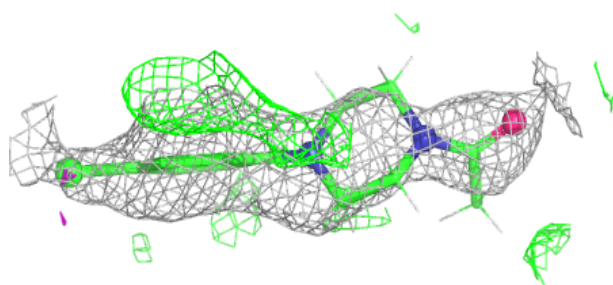
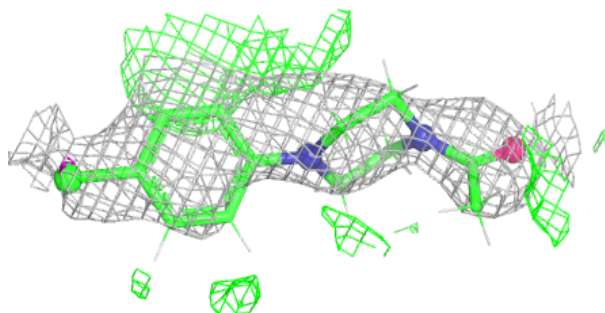
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	WNY	B	506	16/16	0.74	0.23	52,69,76,83	31
8	WNY	C	505	16/16	0.82	0.17	46,63,75,82	31
7	CA	B	503	1/1	0.83	0.13	95,95,95,95	0
8	WNY	A	505	16/16	0.83	0.17	61,82,111,111	31
6	MG	F	402	1/1	0.85	0.18	78,78,78,78	0
8	WNY	C	504	16/16	0.87	0.17	49,64,77,77	31
11	ACP	F	401	31/31	0.87	0.11	76,86,93,99	0
10	MES	B	504	12/12	0.88	0.13	57,63,77,81	0
8	WNY	B	505	16/16	0.89	0.13	51,60,69,72	31
7	CA	A	504	1/1	0.89	0.11	84,84,84,84	0
6	MG	D	502	1/1	0.91	0.08	63,63,63,63	0
9	GDP	D	501	28/28	0.92	0.11	54,59,68,74	0
6	MG	B	502	1/1	0.94	0.09	36,36,36,36	0
9	GDP	B	501	28/28	0.98	0.06	30,42,47,49	0
5	GTP	A	501	32/32	0.98	0.06	32,38,41,43	0
7	CA	A	503	1/1	0.98	0.04	73,73,73,73	0
5	GTP	C	501	32/32	0.98	0.06	29,35,40,42	0
6	MG	C	502	1/1	0.99	0.04	34,34,34,34	0
6	MG	A	502	1/1	0.99	0.02	32,32,32,32	0
7	CA	C	503	1/1	0.99	0.04	59,59,59,59	0

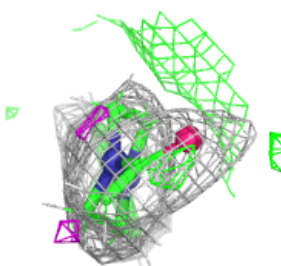
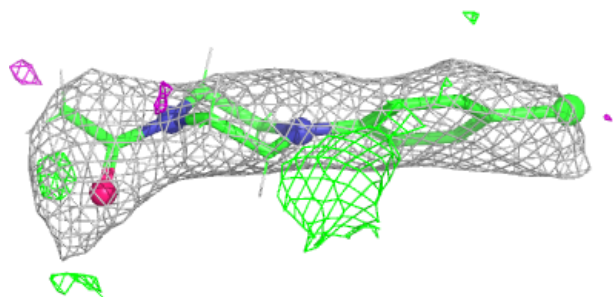
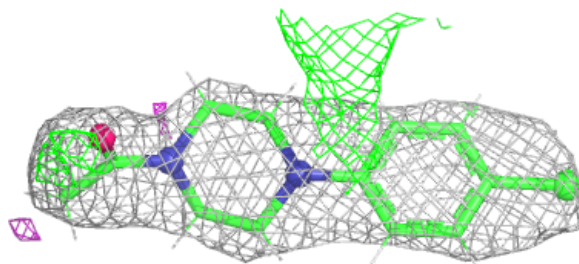
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WNY B 506:

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

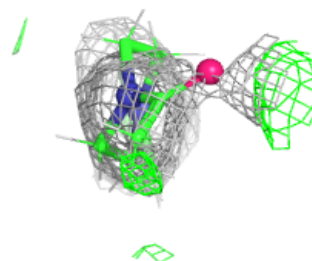
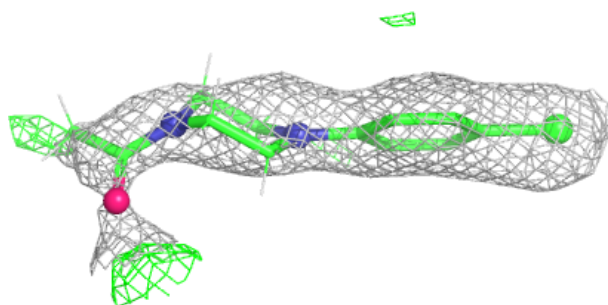
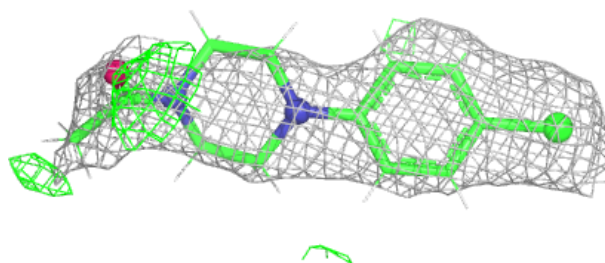
**Electron density around WNY C 505:**

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

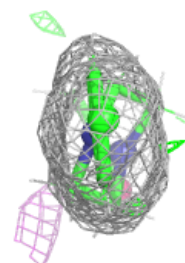
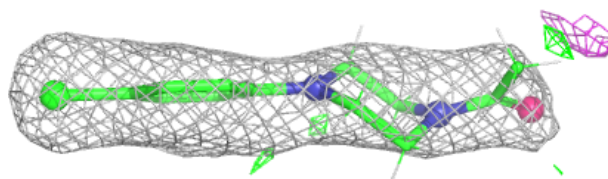
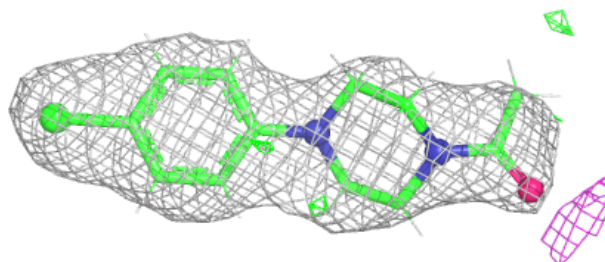


Electron density around WNY A 505:

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

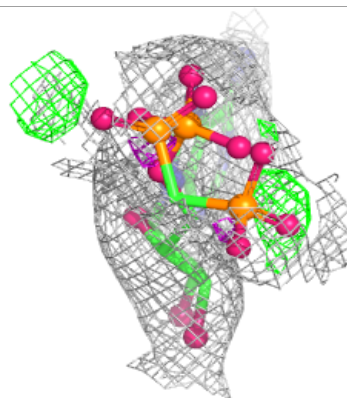
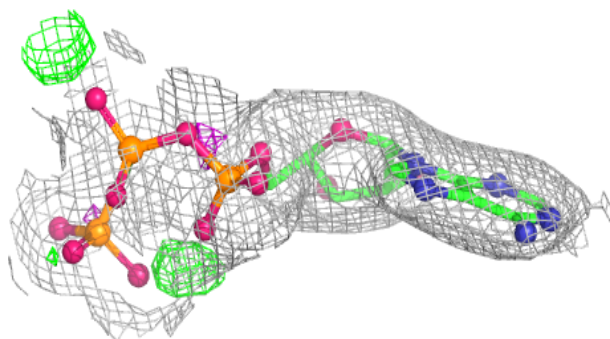
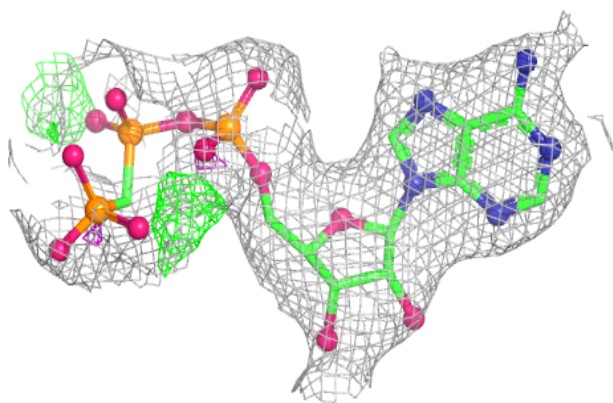
**Electron density around WNY C 504:**

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

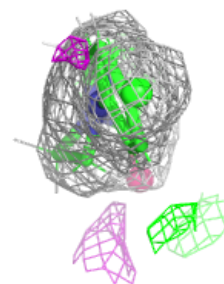
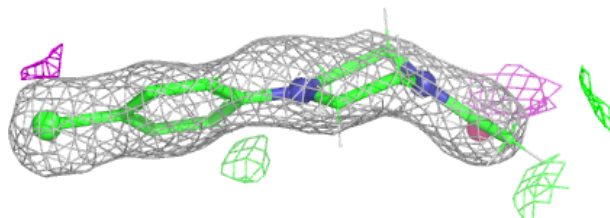
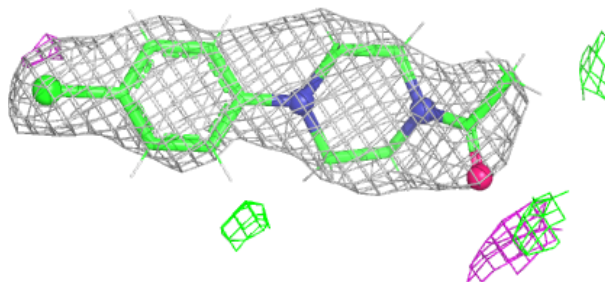


Electron density around ACP F 401:

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

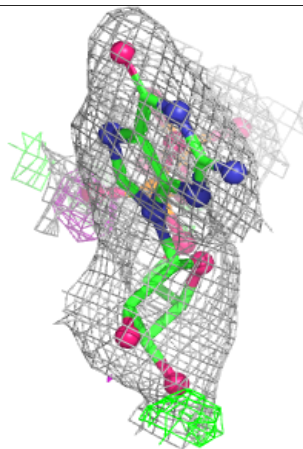
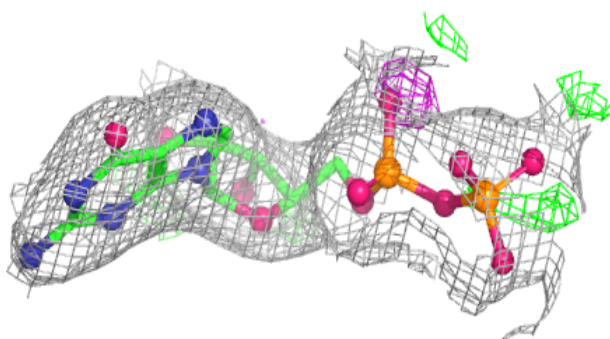
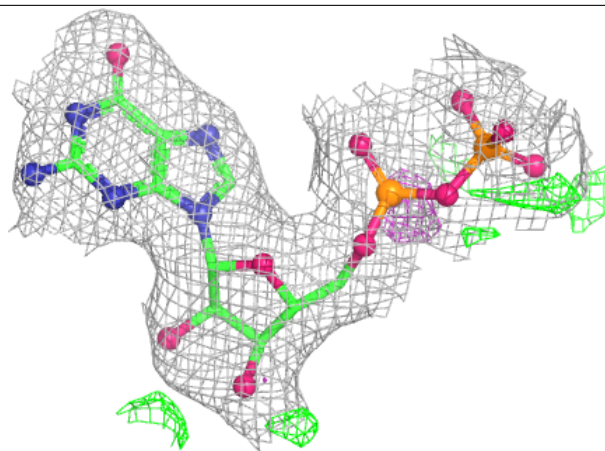
**Electron density around WNY B 505:**

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



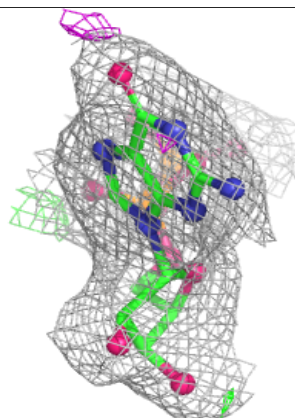
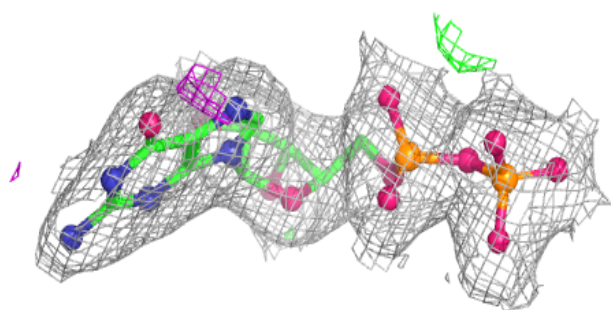
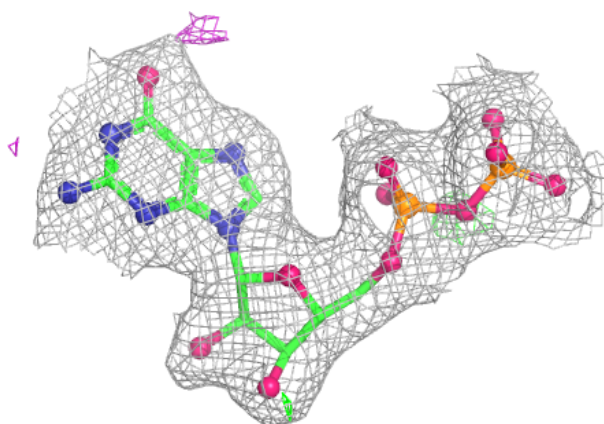
Electron density around GDP D 501:

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

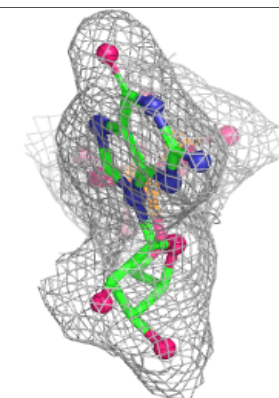
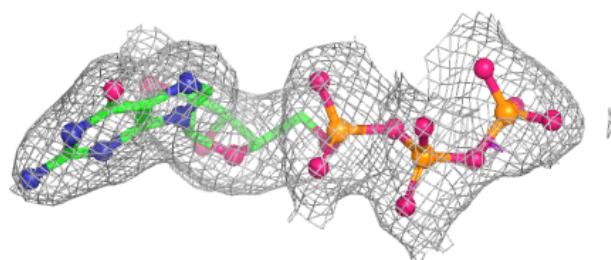
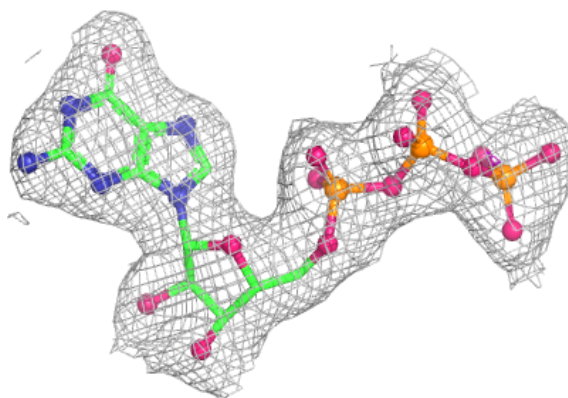


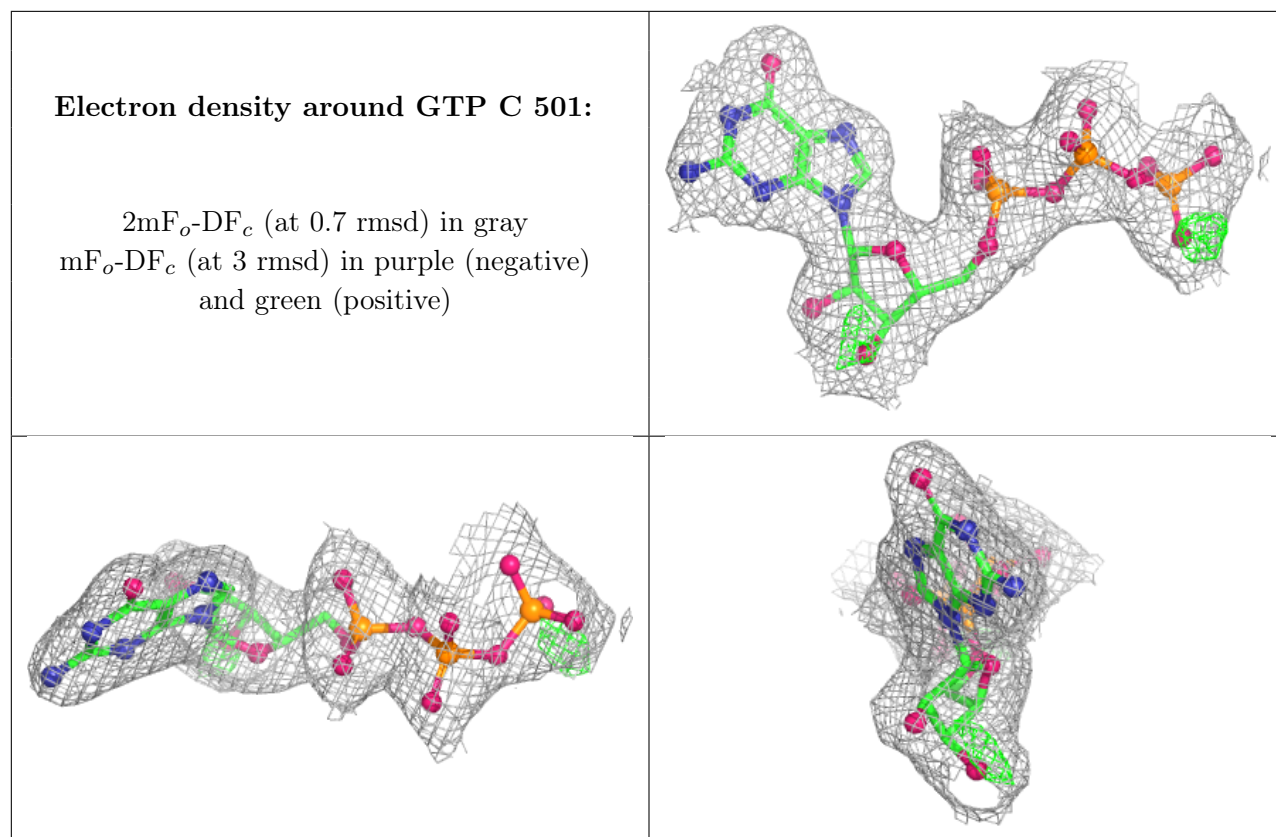
Electron density around GDP B 501:

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

**Electron density around GTP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.