



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2024 – 04:27 pm GMT

PDB ID : 8RIW
Title : T2R-TTL-1-L01 complex
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Deposited on : 2023-12-19
Resolution : 2.57 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

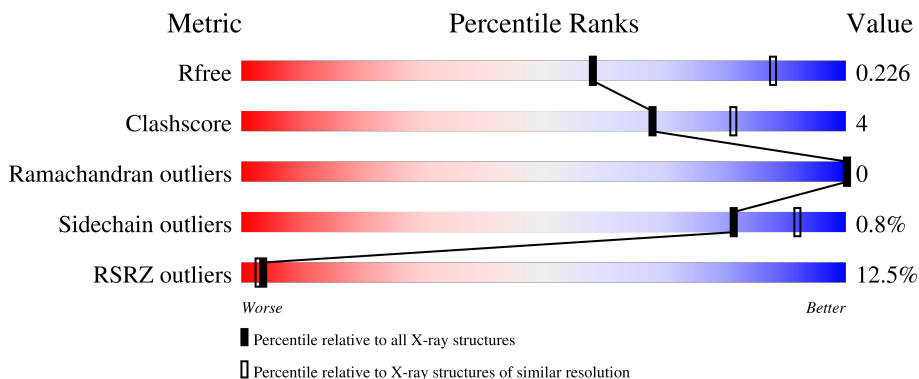
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	 7% 86% 11% •
1	C	451	 % 88% 10% •
2	B	445	 5% 84% 11% 5%
2	D	445	 13% 83% 13% •
3	E	142	 13% 85% • 13%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment labeled '38%', a green segment labeled '80%', a yellow segment labeled '9%', and a grey segment labeled '10%'. The segments are stacked from left to right in the order: red, green, yellow, grey.</p>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17779 atoms, of which 0 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	N	O	S			
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
			3449	2181	586	658	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	Total	C	N	O	S	0	1	0
			3345	2102	572	644	27			
2	D	427	Total	C	N	O	S	0	0	0
			3348	2101	571	649	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 3 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
E	?	-	GLY	deletion	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	344	Total	C	N	O	S	0	0	0
			2812	1803	482	513	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: 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 (three-letter code: 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		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

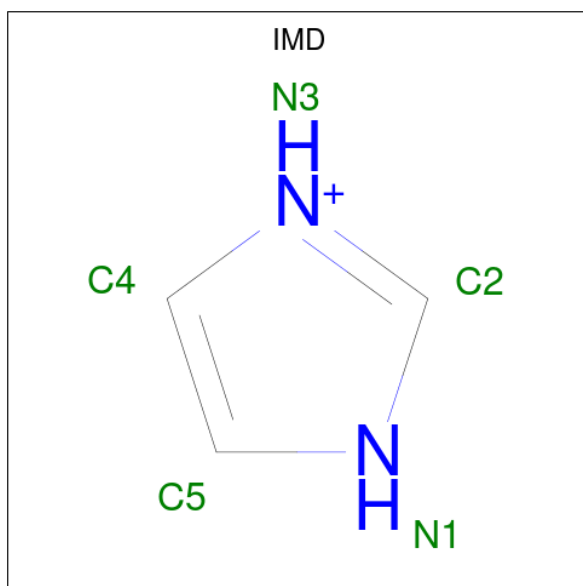
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		

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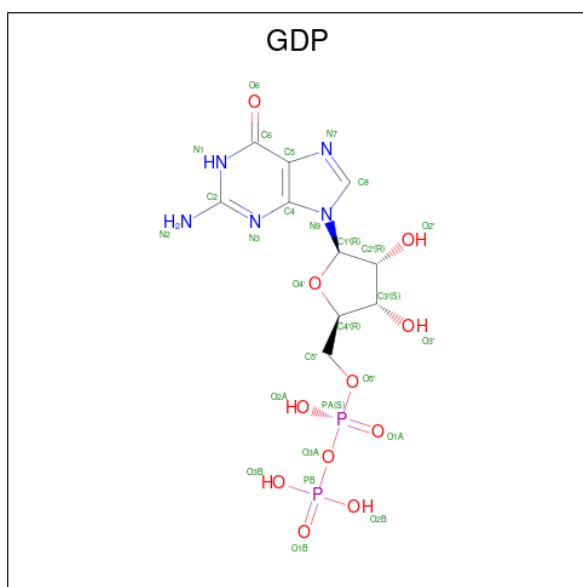
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



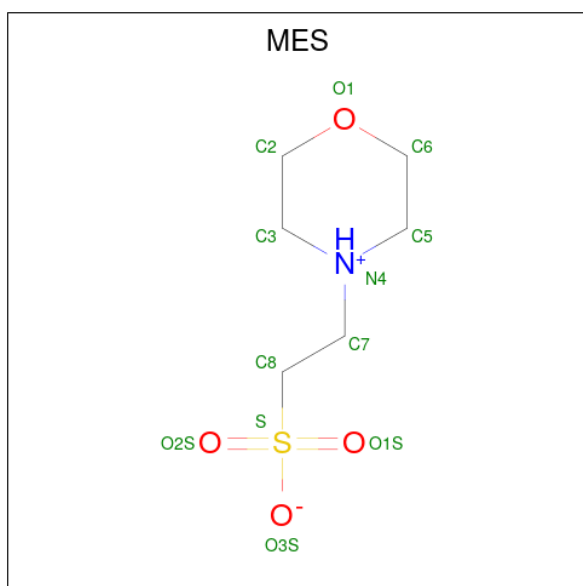
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N 5 3 2	0	0
8	B	1	Total C N 5 3 2	0	0
8	B	1	Total C N 5 3 2	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



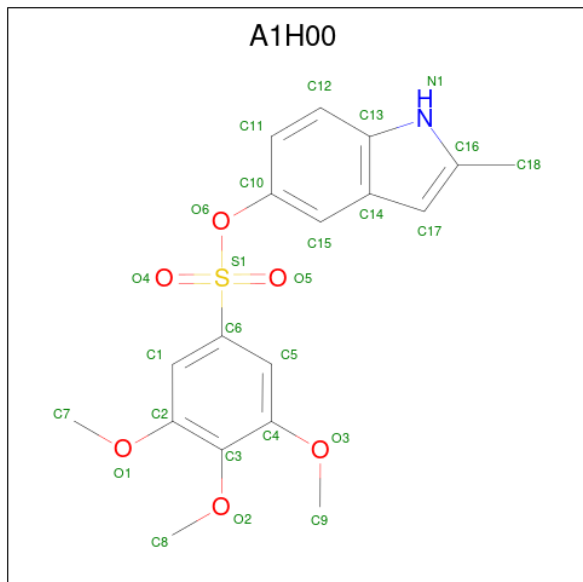
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0
9	D	1	28	10	5	11	2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



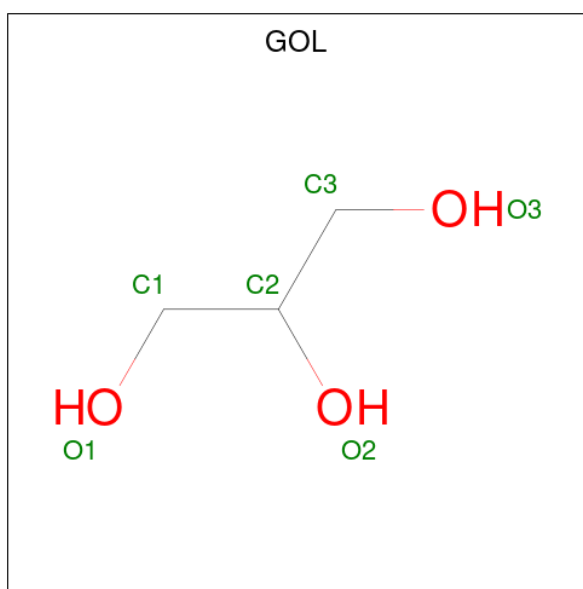
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is (2-methyl-1 {H}-indol-5-yl) 3,4,5-trimethoxybenzenesulfonate (three-letter code: A1H00) (formula: C₁₈H₁₉NO₆S) (labeled as "Ligand of Interest" by depositor).



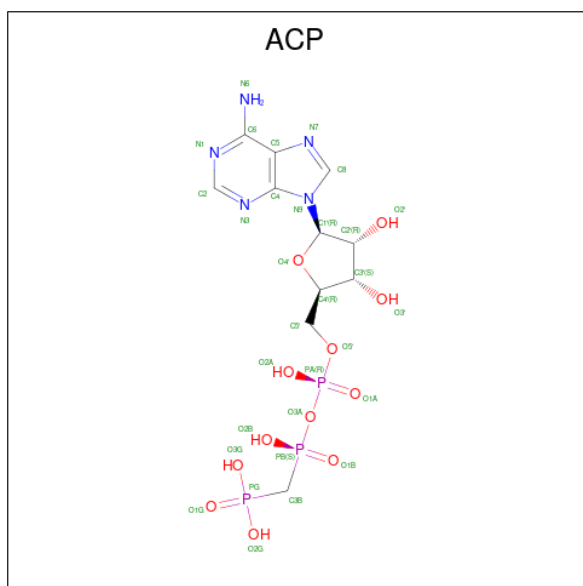
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
11	B	1	26	18	1	6	1	0	0
11	D	1	26	18	1	6	1	0	0

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

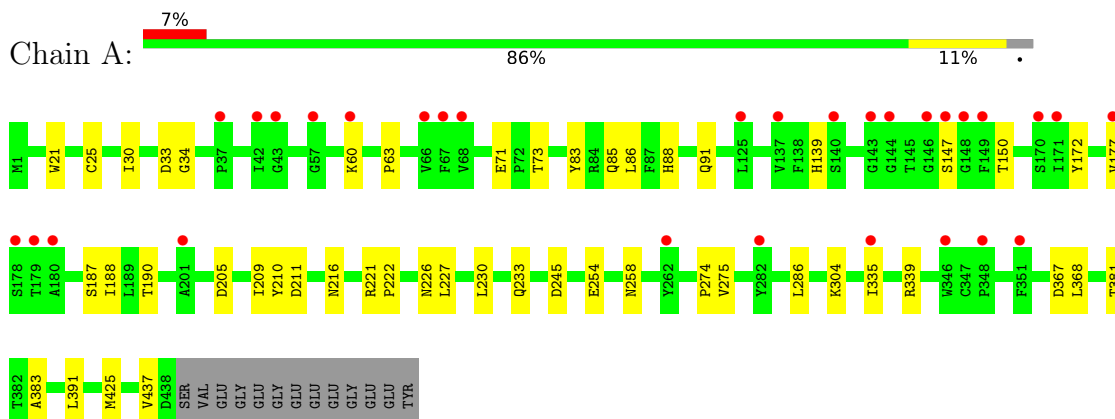
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	17	Total	O	0	0
			17	17		
14	B	38	Total	O	0	0
			38	38		
14	C	76	Total	O	0	0
			76	76		
14	D	5	Total	O	0	0
			5	5		
14	E	3	Total	O	0	0
			3	3		
14	F	3	Total	O	0	0
			3	3		

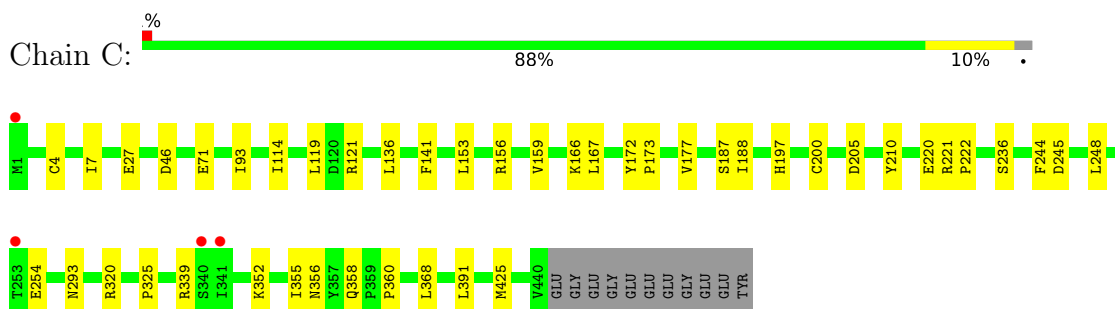
3 Residue-property plots [i](#)

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.

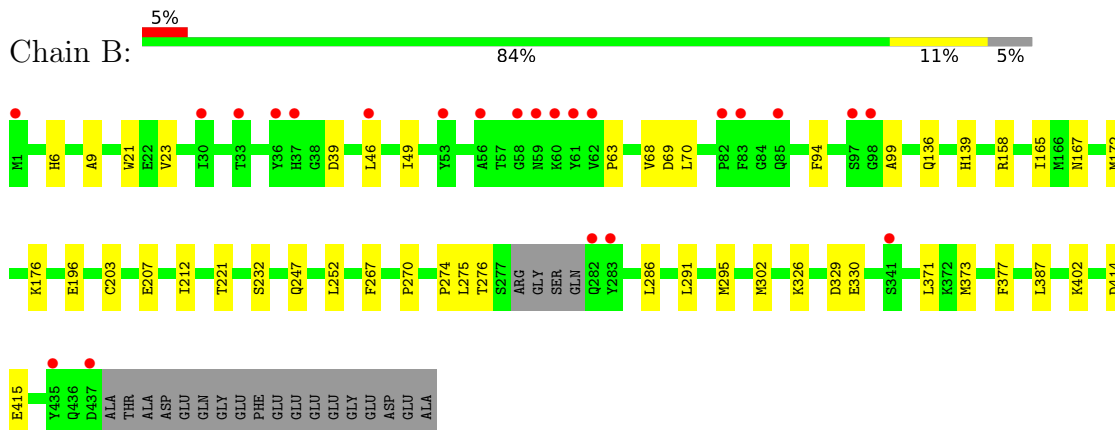
- Molecule 1: Tubulin alpha-1B chain



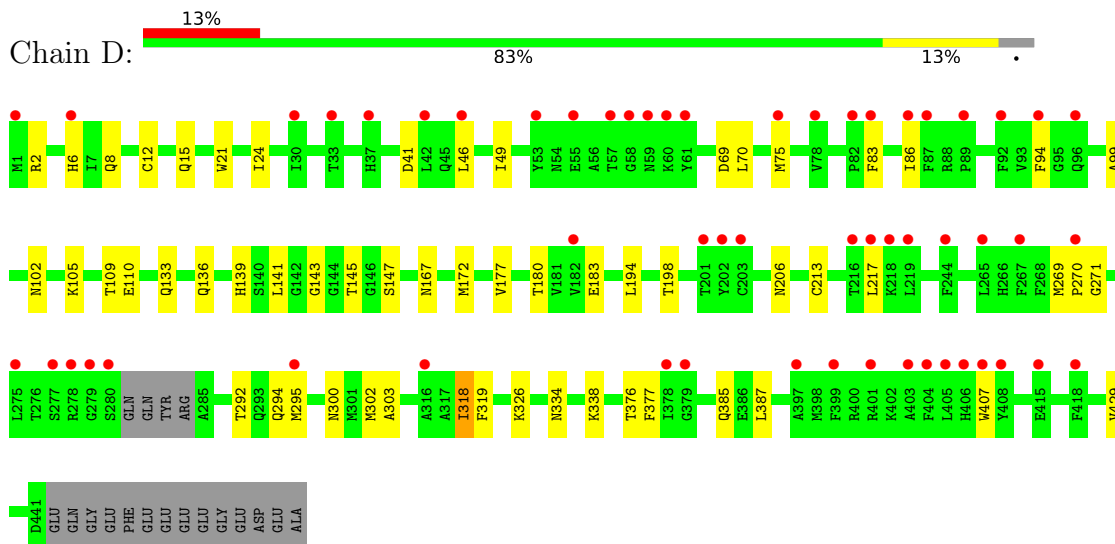
- Molecule 1: Tubulin alpha-1B chain



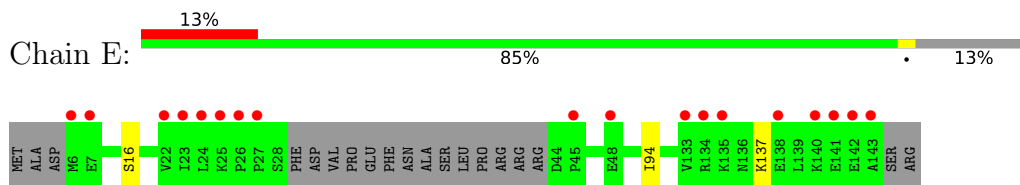
- Molecule 2: Tubulin beta-2B chain



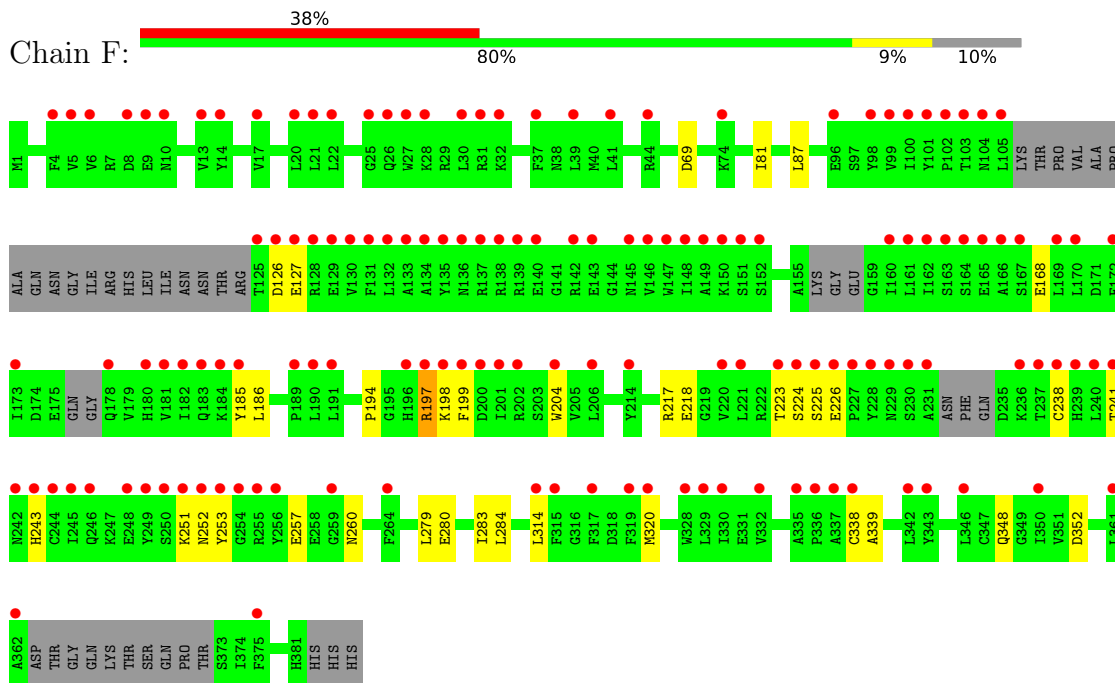
- Molecule 2: Tubulin beta-2B chain



- 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	104.69Å 156.10Å 182.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.99 – 2.57 49.63 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.99-2.57) 99.3 (49.63-2.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.21rc1_5058	Depositor
R, R_{free}	0.189 , 0.228 0.186 , 0.226	Depositor DCC
R_{free} test set	4735 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtrriage
Anisotropy	0.136	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17779	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GOL, IMD, MES, GDP, MG, A1H00, CA, ACP

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	0.24	0/3502	0.46	0/4754
1	C	0.25	0/3527	0.47	0/4789
2	B	0.24	0/3419	0.46	0/4629
2	D	0.24	0/3421	0.45	0/4633
3	E	0.23	0/1022	0.41	0/1356
4	F	0.24	0/2874	0.45	0/3880
All	All	0.24	0/17765	0.46	0/24041

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

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	3334	27	0
1	C	3449	0	3357	23	0
2	B	3345	0	3227	26	0
2	D	3348	0	3227	36	0
3	E	1014	0	1029	3	0
4	F	2812	0	2781	20	0
5	A	32	0	12	0	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	5	0	5	2	0
8	B	10	0	10	1	0
9	B	28	0	12	0	0
9	D	28	0	12	2	0
10	B	12	0	13	0	0
11	B	26	0	0	0	0
11	D	26	0	0	0	0
12	C	6	0	8	0	0
13	F	31	0	14	0	0
14	A	17	0	0	0	0
14	B	38	0	0	0	0
14	C	76	0	0	0	0
14	D	5	0	0	0	0
14	E	3	0	0	0	0
14	F	3	0	0	0	0
All	All	17779	0	17053	130	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 4.

The worst 5 of 130 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:D:318:ILE:HD12	2:D:376:THR:HB	1.70	0.74
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.74	0.69
4:F:194:PRO:O	4:F:197:ARG:NH1	2.27	0.68
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.28	0.67
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.77	0.67

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	436/451 (97%)	429 (98%)	7 (2%)	0	100	100
1	C	440/451 (98%)	434 (99%)	6 (1%)	0	100	100
2	B	420/445 (94%)	412 (98%)	8 (2%)	0	100	100
2	D	423/445 (95%)	419 (99%)	4 (1%)	0	100	100
3	E	119/142 (84%)	119 (100%)	0	0	100	100
4	F	332/384 (86%)	324 (98%)	8 (2%)	0	100	100
All	All	2170/2318 (94%)	2137 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	369/379 (97%)	368 (100%)	1 (0%)	92	97
1	C	373/379 (98%)	368 (99%)	5 (1%)	69	85
2	B	368/383 (96%)	366 (100%)	2 (0%)	88	96
2	D	368/383 (96%)	363 (99%)	5 (1%)	67	84
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	308/342 (90%)	306 (99%)	2 (1%)	86	94
All	All	1896/1993 (95%)	1881 (99%)	15 (1%)	81	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	368	LEU
4	F	197	ARG
2	D	8	GLN
4	F	251	LYS
2	D	139	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	300	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	IMD	A	505	-	3,5,5	0.15	0	4,5,5	0.97	0
9	GDP	B	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.09	3 (10%)
5	GTP	C	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.45	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	GOL	C	504	-	5,5,5	0.33	0	5,5,5	0.29	0
9	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.27	4 (13%)
13	ACP	F	401	6	27,33,33	2.31	3 (11%)	32,52,52	1.09	3 (9%)
10	MES	B	504	-	12,12,12	1.10	1 (8%)	14,16,16	0.89	1 (7%)
8	IMD	B	506	-	3,5,5	0.16	0	4,5,5	1.00	0
11	A1H00	D	503	-	26,28,28	1.02	2 (7%)	36,41,41	1.33	6 (16%)
8	IMD	B	507	-	3,5,5	0.17	0	4,5,5	0.99	0
5	GTP	A	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.46	7 (21%)
11	A1H00	B	505	-	26,28,28	1.05	2 (7%)	36,41,41	1.39	6 (16%)

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
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	IMD	A	505	-	-	-	0/1/1/1
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
12	GOL	C	504	-	-	2/4/4/4	-
9	GDP	D	501	6	-	2/12/32/32	0/3/3/3
13	ACP	F	401	6	-	3/15/38/38	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
11	A1H00	D	503	-	-	4/17/17/17	0/3/3/3
8	IMD	B	506	-	-	-	0/1/1/1
8	IMD	B	507	-	-	-	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
11	A1H00	B	505	-	-	4/17/17/17	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	401	ACP	PB-O3A	10.87	1.70	1.58
5	A	501	GTP	C5-C6	-4.07	1.39	1.47
5	C	501	GTP	C5-C6	-4.06	1.39	1.47
10	B	504	MES	C8-S	2.94	1.81	1.77
9	B	501	GDP	C6-N1	-2.38	1.34	1.37

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	PA-O3A-PB	-3.26	121.63	132.83
5	A	501	GTP	C5-C6-N1	3.22	119.63	113.95
5	C	501	GTP	PB-O3B-PG	-3.10	122.19	132.83
5	C	501	GTP	C5-C6-N1	3.08	119.38	113.95
5	A	501	GTP	C8-N7-C5	3.00	108.70	102.99

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

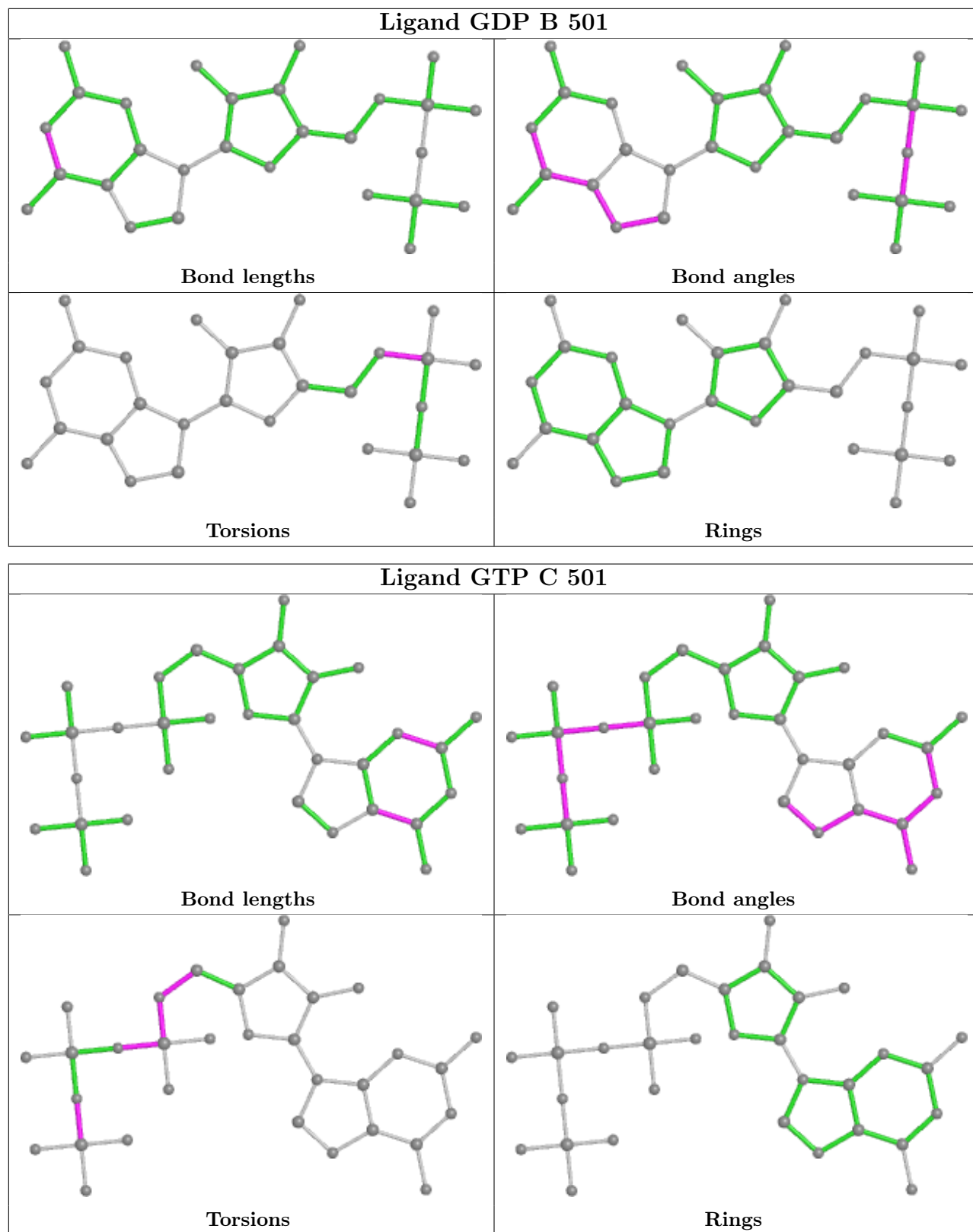
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A

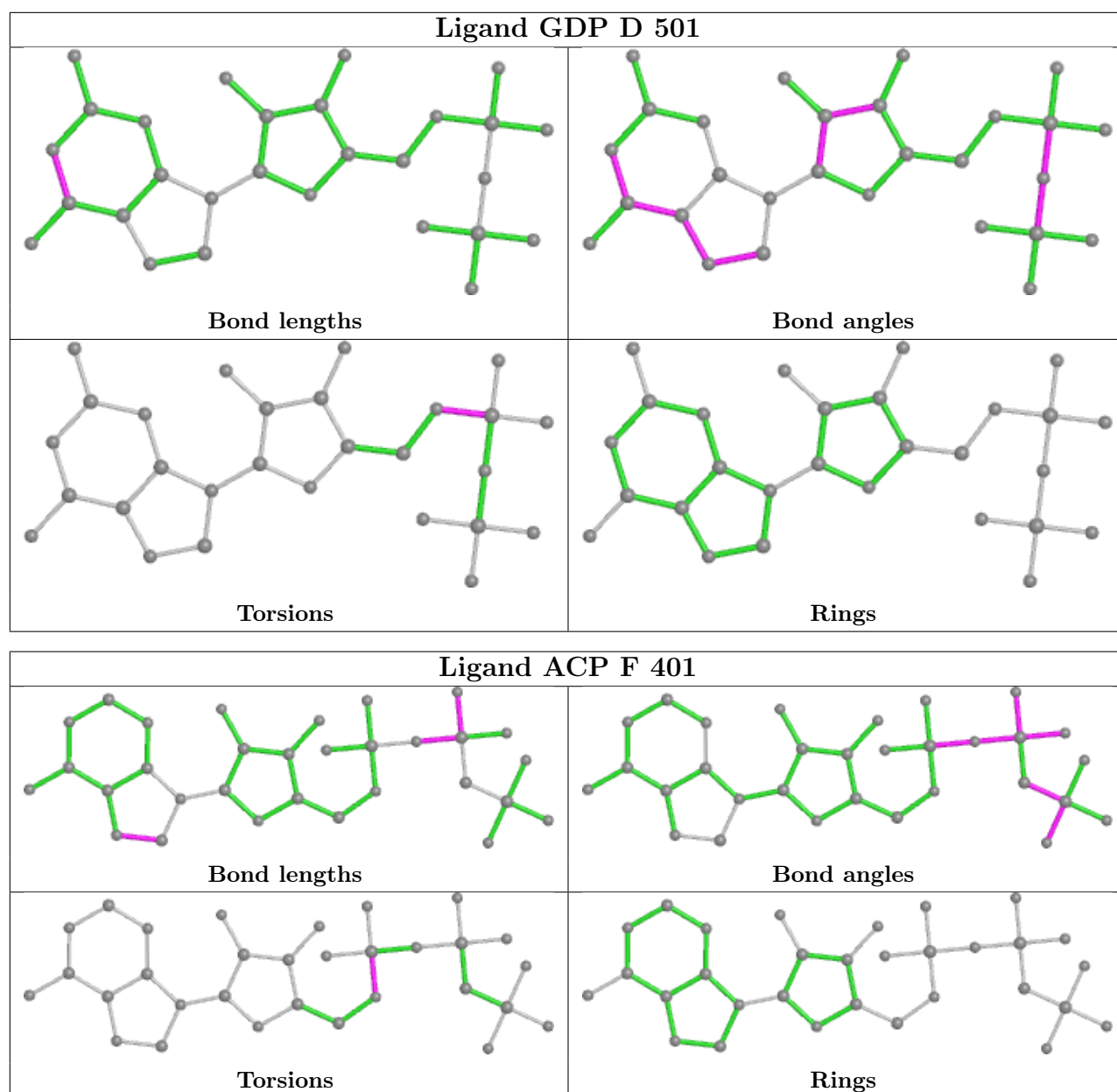
There are no ring outliers.

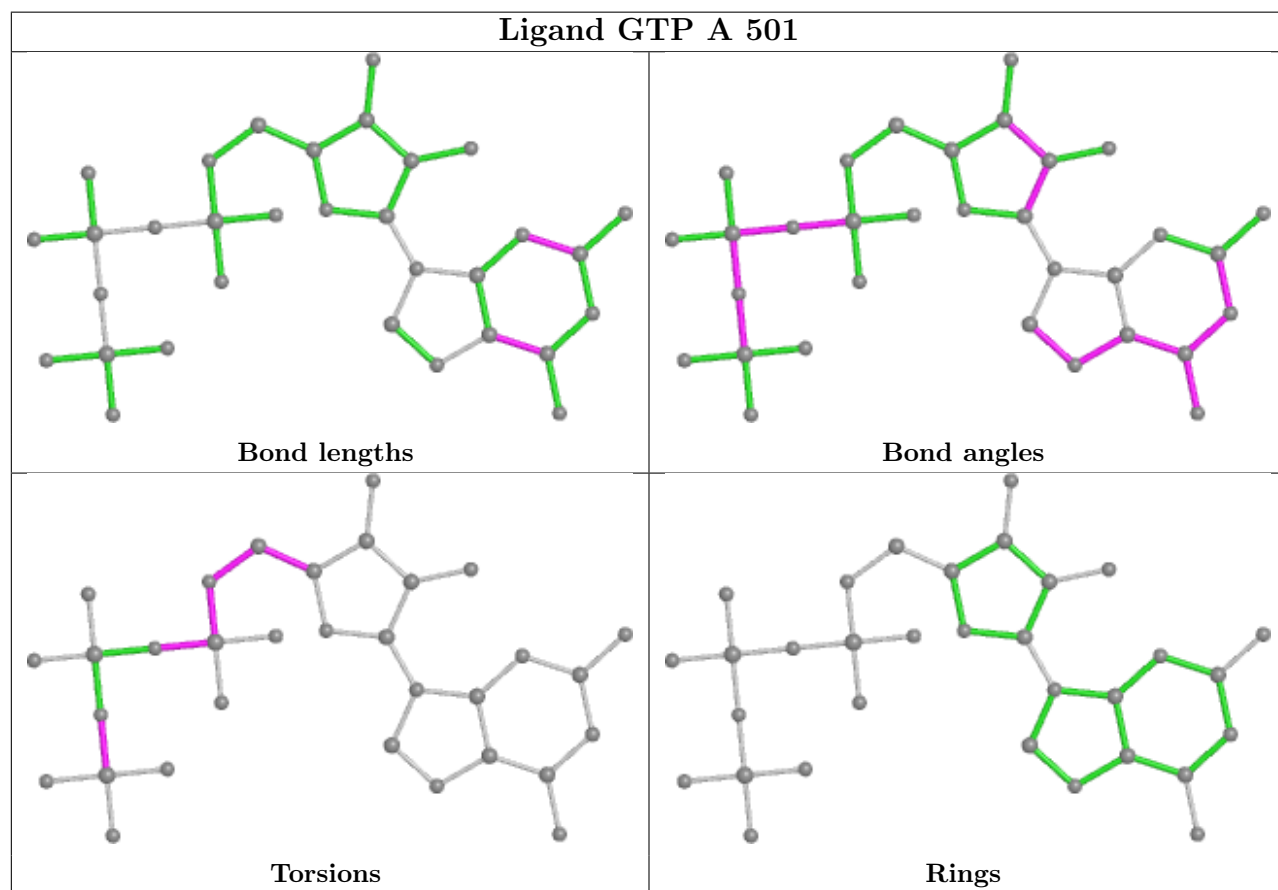
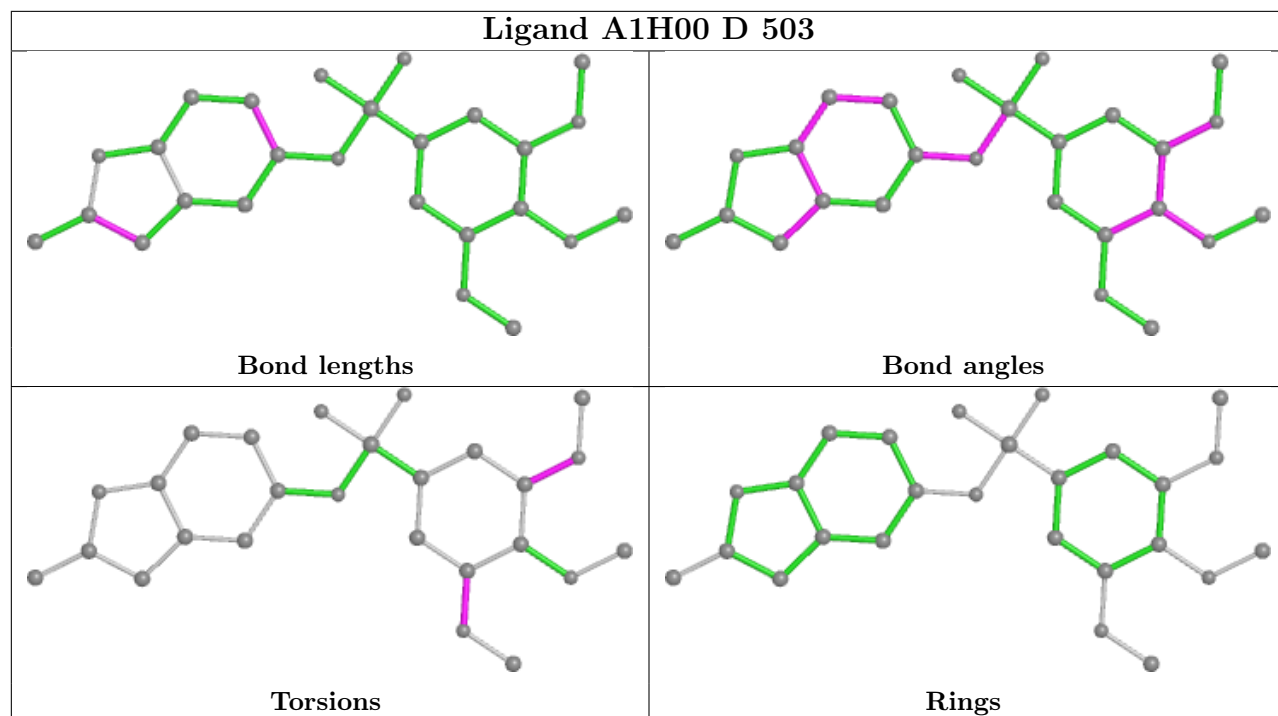
4 monomers are involved in 5 short contacts:

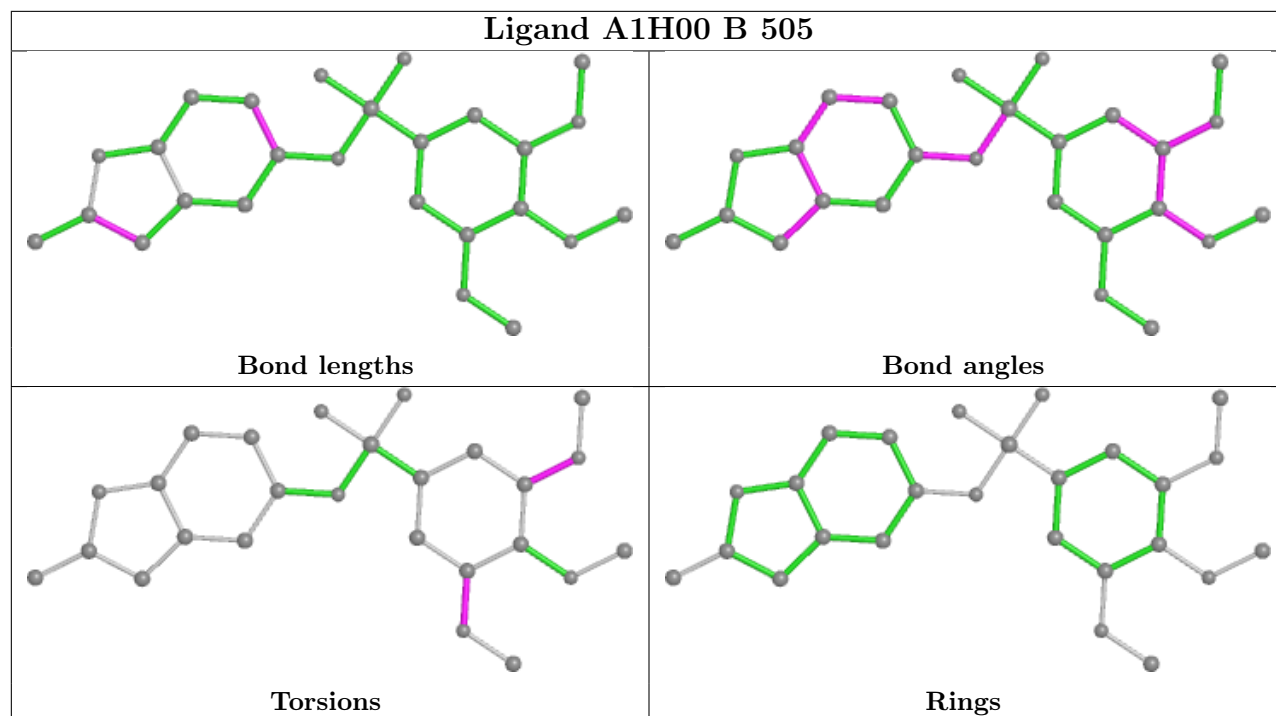
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	505	IMD	2	0
9	D	501	GDP	2	0
8	B	506	IMD	1	0
8	B	507	IMD	1	0

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%)	0.57	30 (6%) 17 14	68, 95, 139, 210	0
1	C	440/451 (97%)	0.18	4 (0%) 84 83	55, 74, 110, 137	0
2	B	423/445 (95%)	0.51	23 (5%) 25 22	59, 82, 128, 178	0
2	D	427/445 (95%)	0.78	56 (13%) 3 2	72, 115, 158, 193	0
3	E	123/142 (86%)	0.68	18 (14%) 2 1	74, 108, 161, 210	0
4	F	344/384 (89%)	2.06	144 (41%) 0 0	85, 140, 200, 254	0
All	All	2195/2318 (94%)	0.76	275 (12%) 3 3	55, 98, 170, 254	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	11.2
4	F	173	ILE	10.7
4	F	169	LEU	8.3
4	F	236	LYS	8.1
4	F	6	VAL	7.7

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 monosaccharides in this entry.

6.4 Ligands

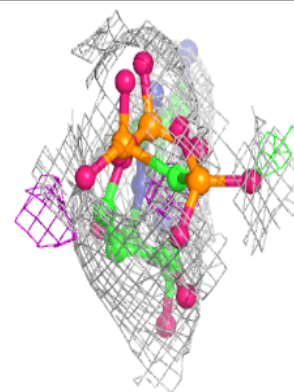
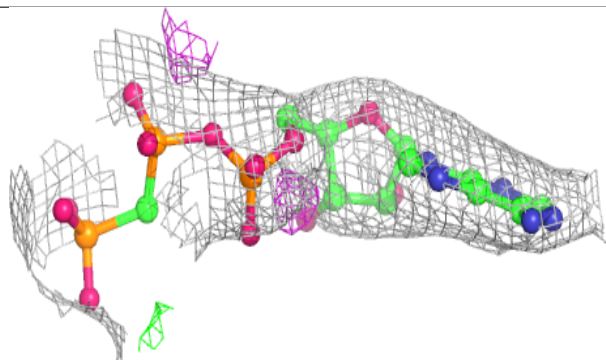
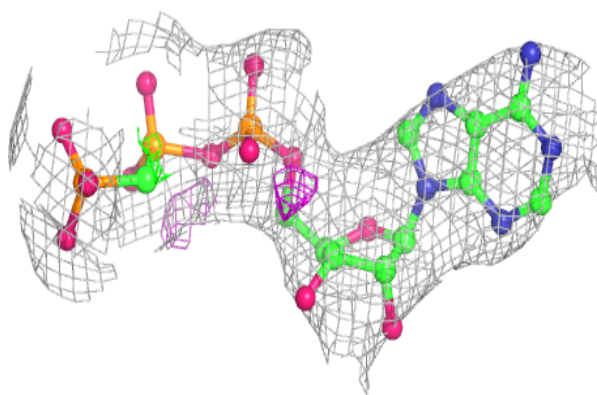
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	A	504	1/1	0.70	0.28	137,137,137,137	0
6	MG	F	402	1/1	0.77	0.26	174,174,174,174	0
12	GOL	C	504	6/6	0.82	0.33	71,84,90,99	0
8	IMD	A	505	5/5	0.83	0.28	106,108,119,122	0
13	ACP	F	401	31/31	0.84	0.20	138,158,174,182	0
8	IMD	B	506	5/5	0.86	0.18	123,123,125,127	0
11	A1H00	D	503	26/26	0.90	0.31	65,94,104,112	26
9	GDP	D	501	28/28	0.93	0.16	91,110,125,145	0
11	A1H00	B	505	26/26	0.94	0.22	70,88,101,120	0
6	MG	D	502	1/1	0.95	0.05	125,125,125,125	0
7	CA	B	503	1/1	0.95	0.27	117,117,117,117	0
6	MG	C	502	1/1	0.95	0.18	63,63,63,63	0
6	MG	B	502	1/1	0.96	0.29	80,80,80,80	0
10	MES	B	504	12/12	0.96	0.18	71,79,94,95	0
8	IMD	B	507	5/5	0.96	0.12	98,108,111,114	0
7	CA	A	503	1/1	0.97	0.06	133,133,133,133	0
5	GTP	C	501	32/32	0.97	0.18	47,62,74,85	0
9	GDP	B	501	28/28	0.97	0.22	45,65,71,77	0
5	GTP	A	501	32/32	0.98	0.28	64,72,87,93	0
7	CA	C	503	1/1	0.98	0.10	103,103,103,103	0
6	MG	A	502	1/1	0.99	0.24	74,74,74,74	0

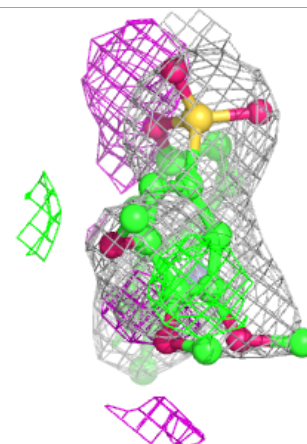
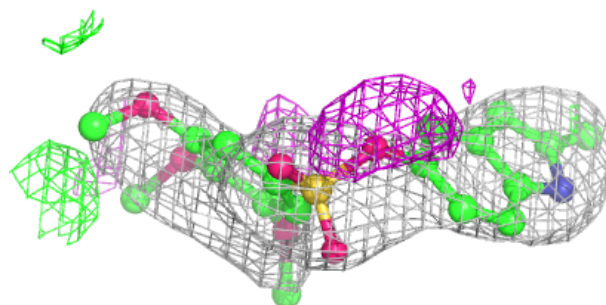
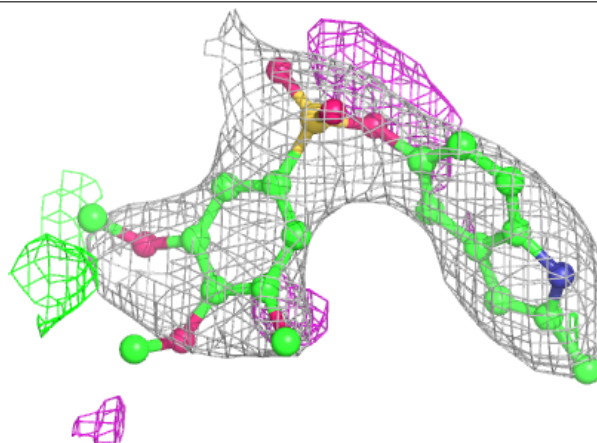
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

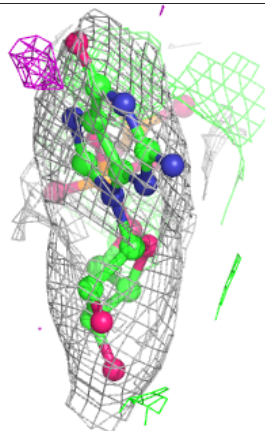
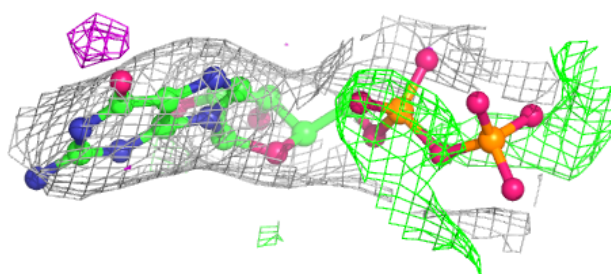
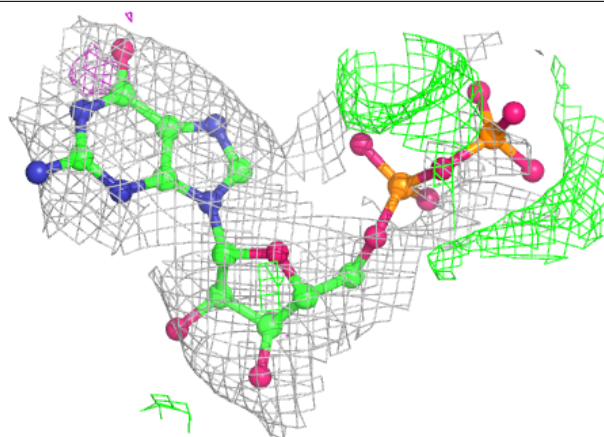
**Electron density around A1H00 D 503:**

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

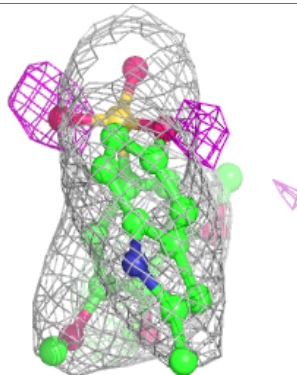
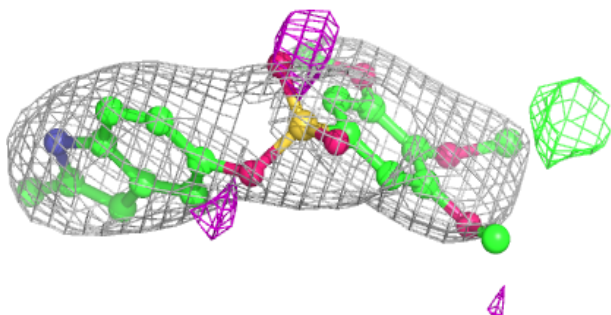
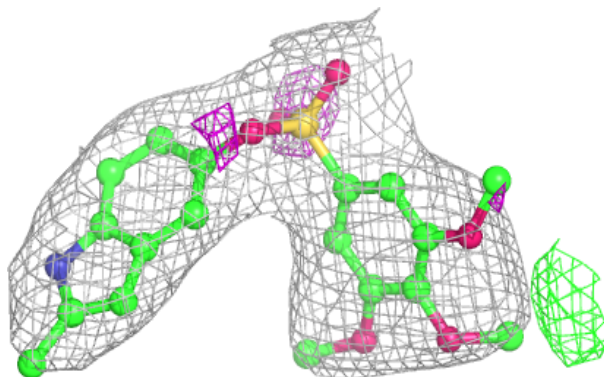


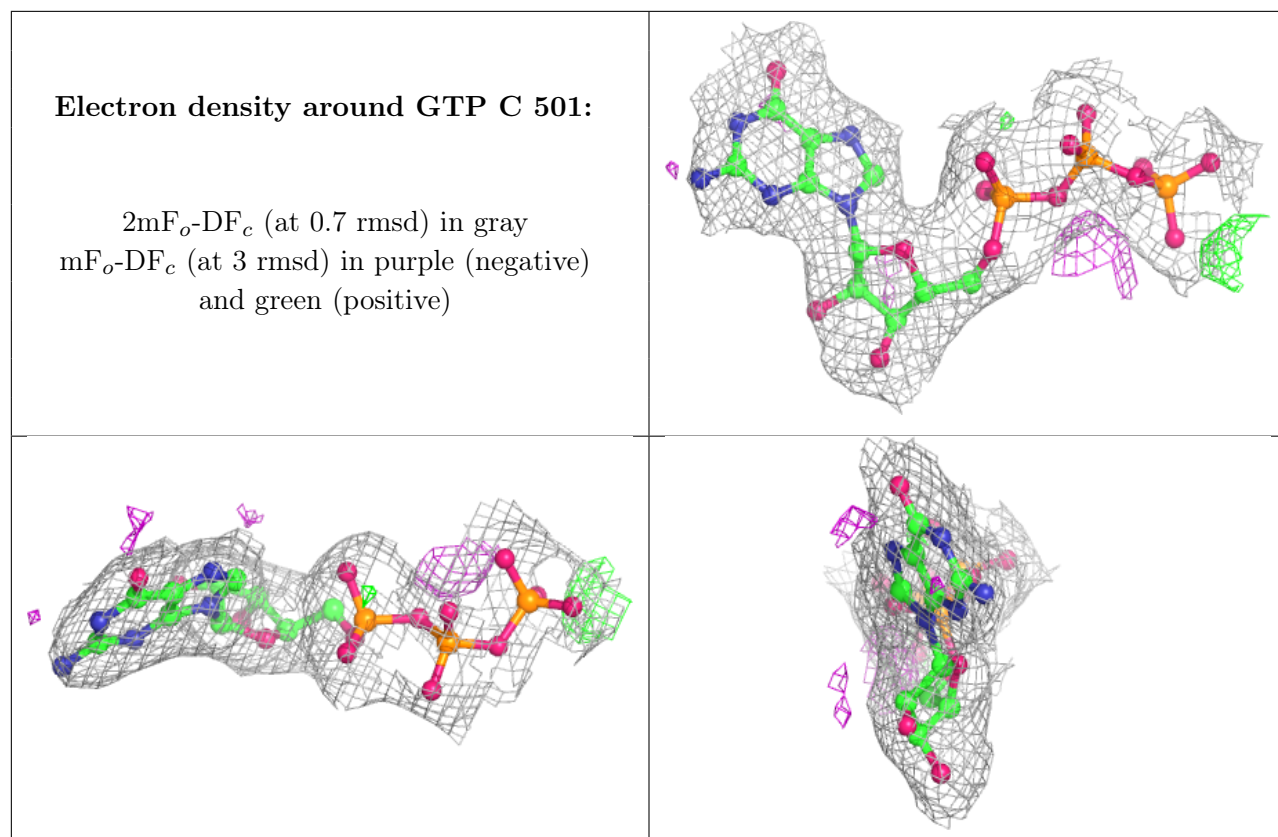
Electron density around GDP D 501:

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

**Electron density around A1H00 B 505:**

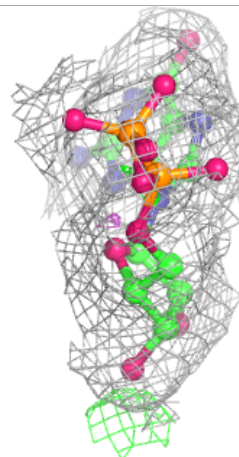
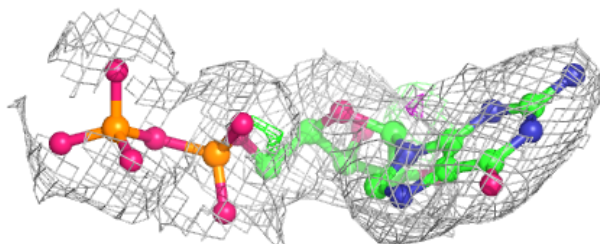
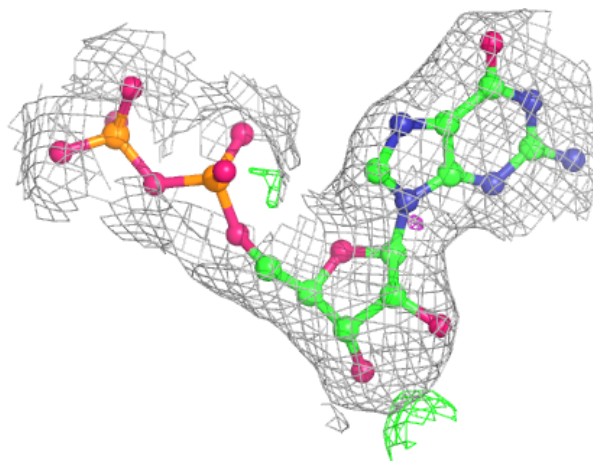
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

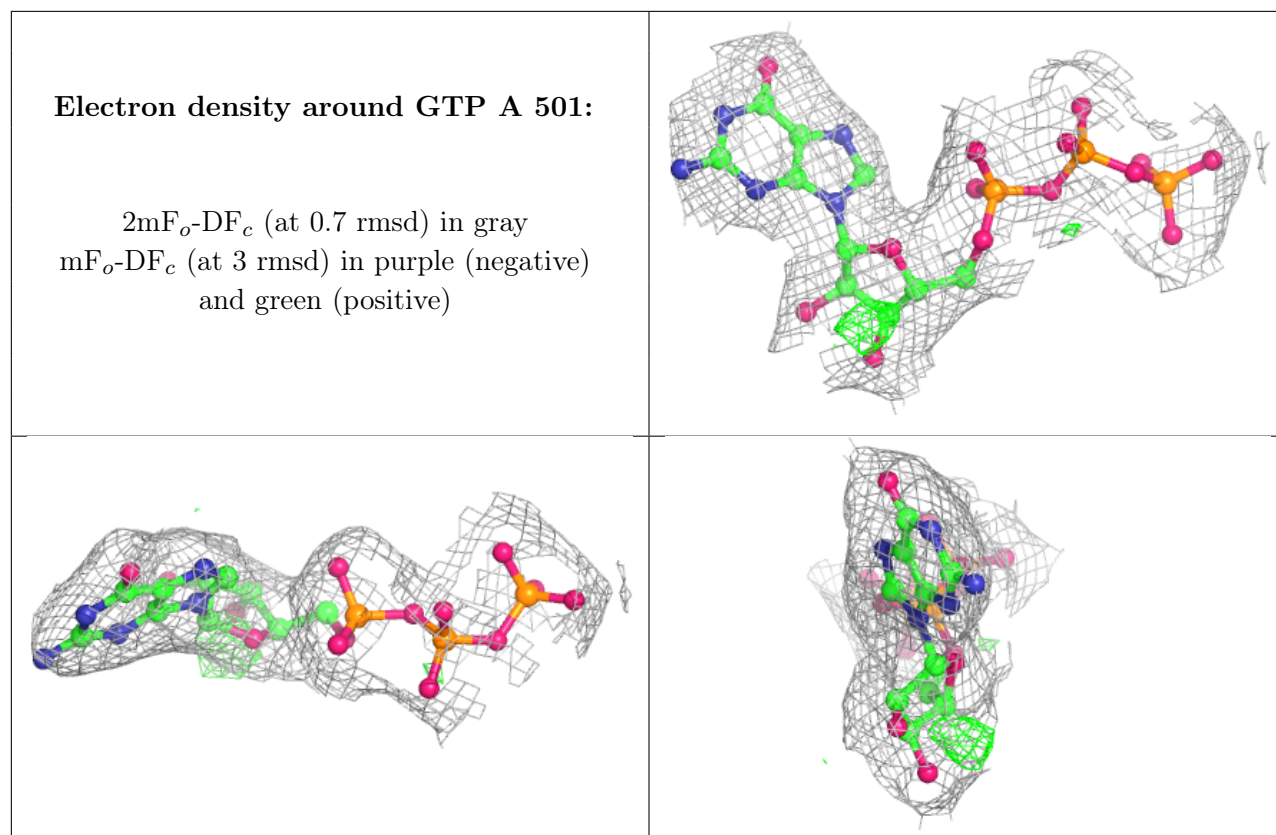




Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.