wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2020 – 12:55 AM BST

PDB ID	:	5M7G
Title	:	Tubulin-MTD147 complex
Authors	:	Bohnacker, T.; Prota, A.E.; Steinmetz, M.O.; Wymann, M.P.
Deposited on	:	2016-10-27
Resolution	:	2.25 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

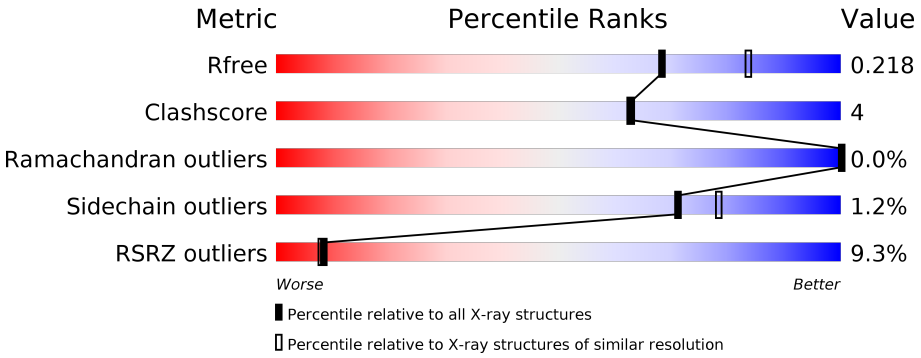
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	5% 83% 13% •
1	C	451	2% 88% 10% •
2	B	445	3% 82% 12% • 5%
2	D	445	10% 82% 11% 6%
3	E	143	9% 79% 7% 14%
4	F	384	27% 76% 9% 15%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17780 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
1	A	436	Total	C	N	O	S	0	0	0
			3409	2158	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- 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	0	0	0
			3325	2091	567	641	26			
2	D	418	Total	C	N	O	S	0	0	0
			3284	2065	557	636	26			

- 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

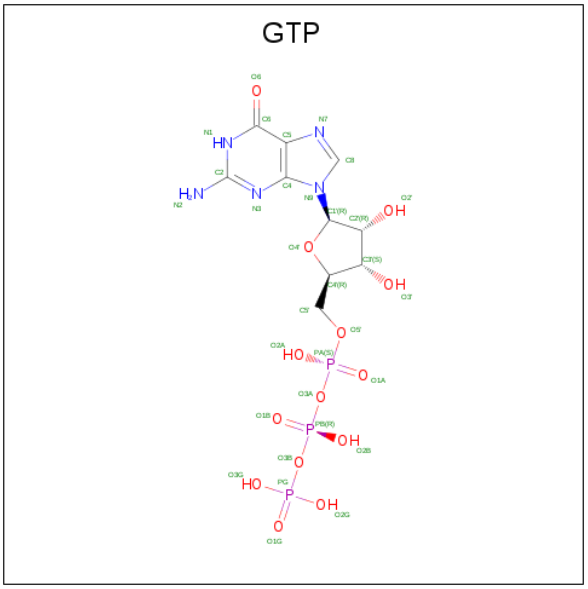
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	326	Total	C	N	O	S	0	0	0
			2647	1707	444	482	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 (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	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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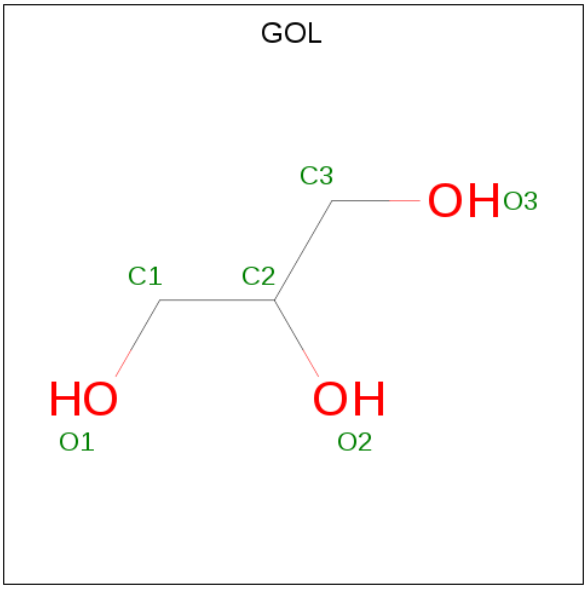
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

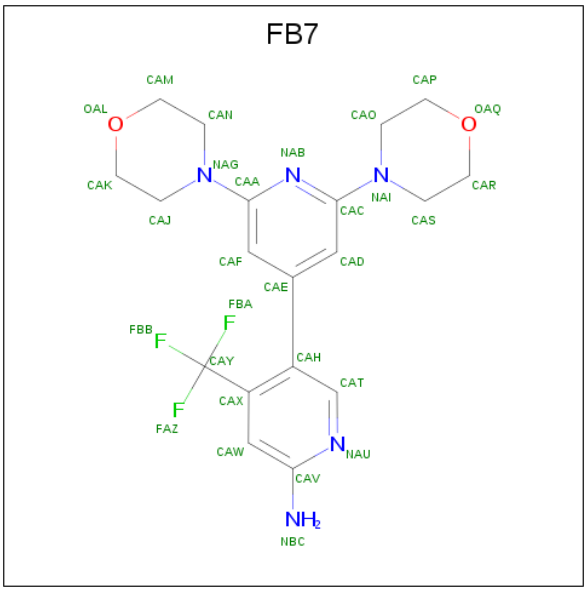
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	2	Total Ca 2 2	0	0
7	C	2	Total Ca 2 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



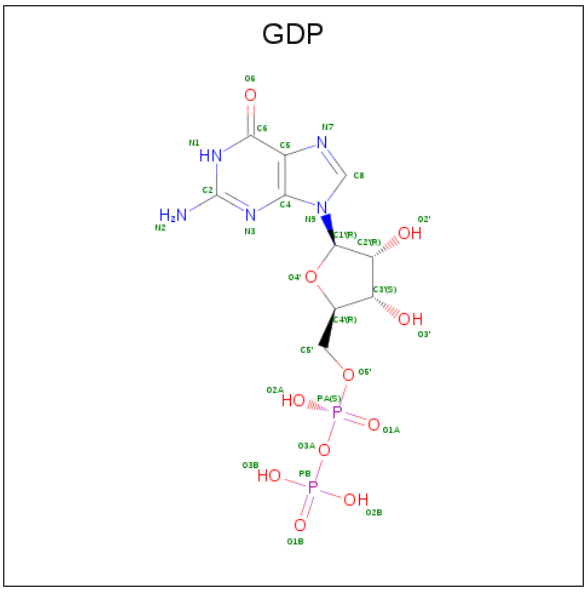
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0

- Molecule 9 is 5-(2,6-dimorpholin-4-ylpyridin-4-yl)-4-(trifluoromethyl)pyridin-2-amine (three-letter code: FB7) (formula: $C_{19}H_{22}F_3N_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	F	N	O	0	0
			29	19	3	5	2		
9	D	1	Total	C	F	N	O	0	0
			29	19	3	5	2		

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



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

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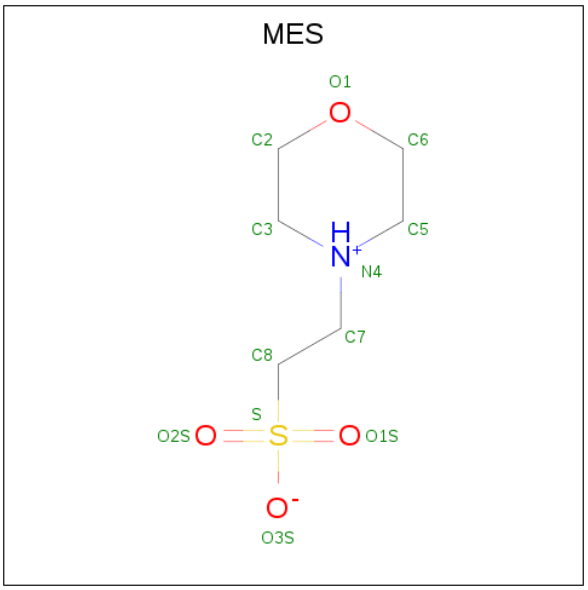
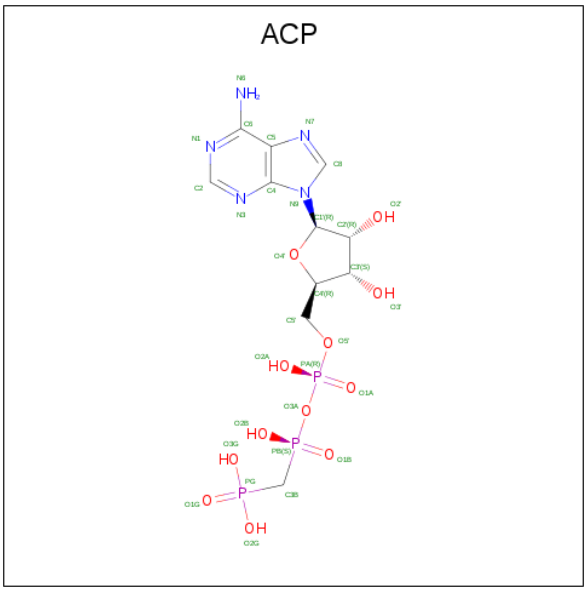
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

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



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

- Molecule 13 is water.

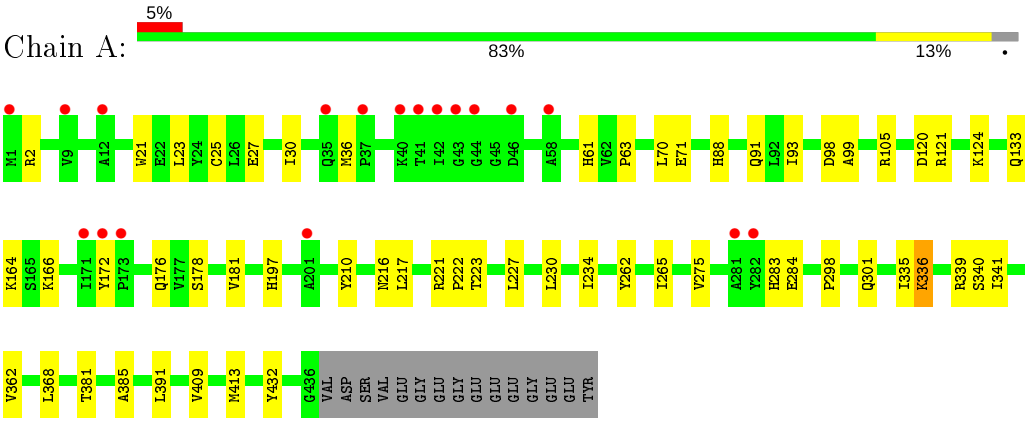
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	82	Total	O	0	0
			82	82		
13	B	76	Total	O	0	0
			76	76		
13	C	175	Total	O	0	0
			175	175		
13	D	45	Total	O	0	0
			45	45		
13	E	15	Total	O	0	0
			15	15		
13	F	28	Total	O	0	0
			28	28		

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.

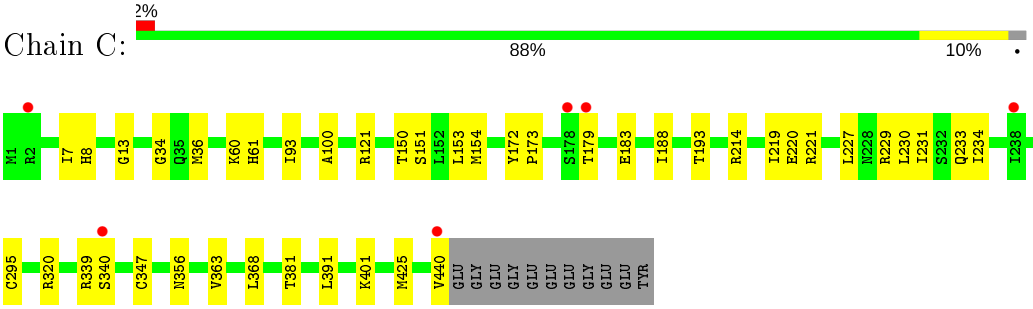
- Molecule 1: Tubulin alpha-1B chain

Chain A:



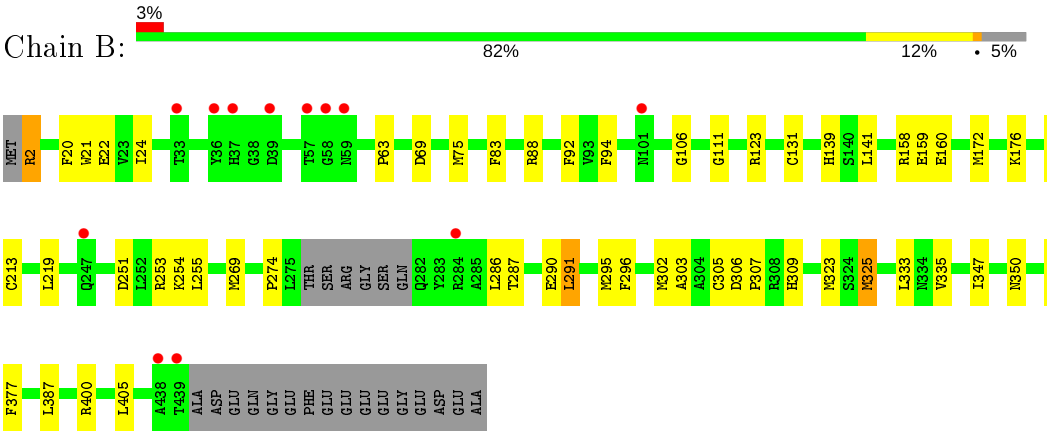
- Molecule 1: Tubulin alpha-1B chain

Chain C:



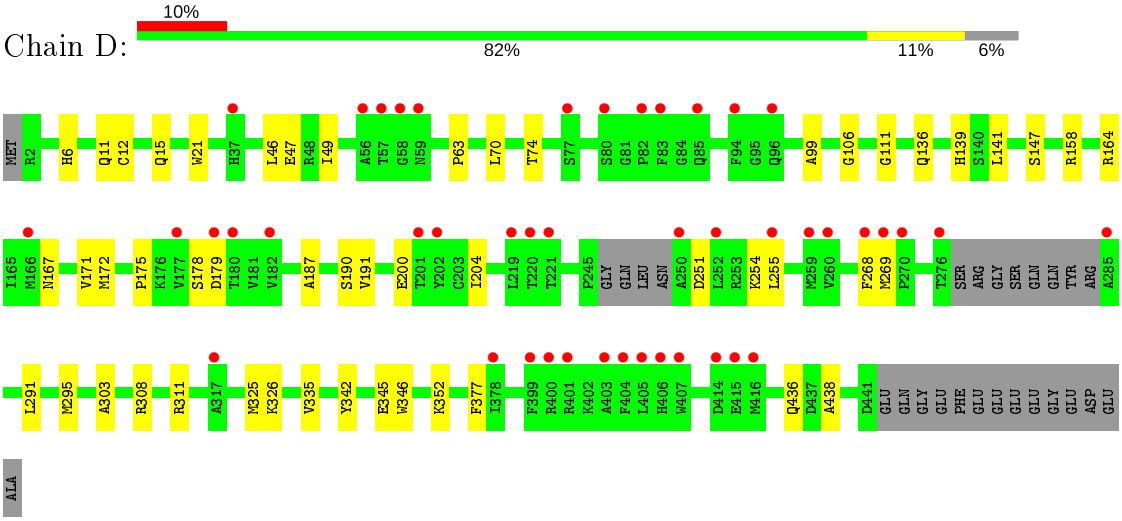
- Molecule 2: Tubulin beta-2B chain

Chain B:



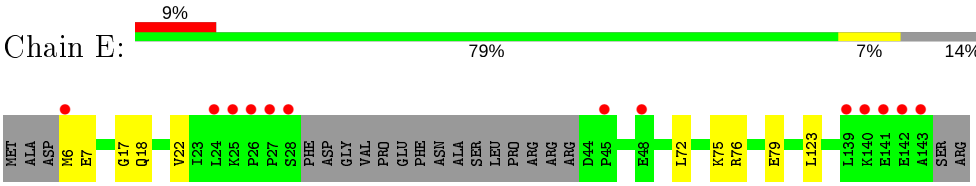
• Molecule 2: Tubulin beta-2B chain

Chain D:



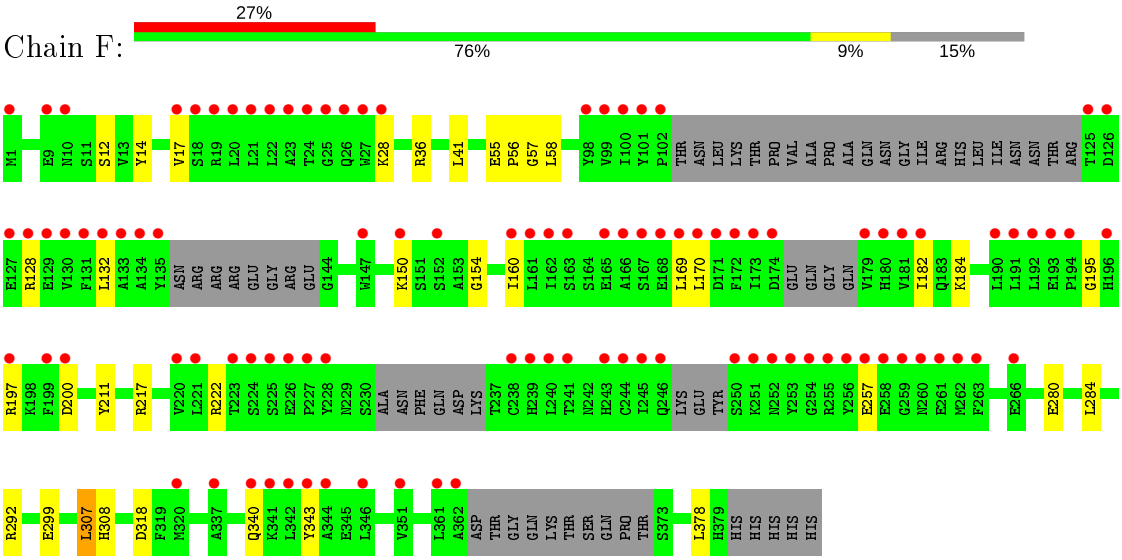
• Molecule 3: Stathmin-4

Chain E:



• Molecule 4: Tubulin-Tyrosine Ligase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.08Å 156.86Å 179.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.72 – 2.25 49.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.72-2.25) 99.1 (49.28-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.172 , 0.217 0.174 , 0.218	Depositor DCC
R_{free} test set	6944 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17780	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, FB7, CA, GTP, ACP, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/3487	0.54	0/4733
1	C	0.49	1/3515 (0.0%)	0.62	0/4772
2	B	0.42	0/3399	0.56	0/4604
2	D	0.37	0/3356	0.51	0/4546
3	E	0.40	0/1022	0.46	0/1356
4	F	0.35	0/2705	0.50	0/3653
All	All	0.41	1/17484 (0.0%)	0.55	0/23664

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-6.26	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3409	0	3322	37	0
1	C	3437	0	3348	25	0
2	B	3325	0	3203	39	0
2	D	3284	0	3160	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1014	0	1029	6	0
4	F	2647	0	2627	21	0
5	A	32	0	12	0	0
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	2	0	0	0	0
8	A	6	0	8	1	0
8	F	6	0	8	0	0
9	B	29	0	0	0	0
9	D	29	0	0	2	0
10	B	28	0	12	0	0
10	D	28	0	12	2	0
11	B	12	0	12	3	0
12	F	31	0	14	2	0
13	A	82	0	0	1	0
13	B	76	0	0	2	0
13	C	175	0	0	1	0
13	D	45	0	0	3	0
13	E	15	0	0	0	0
13	F	28	0	0	1	0
All	All	17780	0	16779	147	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 147 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ARG:NH1	11:B:505:MES:O2S	2.11	0.82
4:F:318:ASP:OD2	12:F:403:ACP:O3G	2.00	0.80
2:B:88:ARG:NH1	13:B:601:HOH:O	2.18	0.75
1:A:221:ARG:HD3	2:B:325:MET:HG3	1.70	0.74
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.69	0.73

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	434/451 (96%)	426 (98%)	7 (2%)	1 (0%)	47 53
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100 100
2	B	418/445 (94%)	407 (97%)	11 (3%)	0	100 100
2	D	412/445 (93%)	405 (98%)	7 (2%)	0	100 100
3	E	119/143 (83%)	119 (100%)	0	0	100 100
4	F	312/384 (81%)	307 (98%)	5 (2%)	0	100 100
All	All	2133/2319 (92%)	2093 (98%)	39 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	367/379 (97%)	364 (99%)	3 (1%)	81 87
1	C	371/379 (98%)	368 (99%)	3 (1%)	81 87
2	B	365/383 (95%)	359 (98%)	6 (2%)	62 70
2	D	361/383 (94%)	356 (99%)	5 (1%)	67 74
3	E	110/127 (87%)	109 (99%)	1 (1%)	78 84
4	F	291/342 (85%)	286 (98%)	5 (2%)	60 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1865/1993 (94%)	1842 (99%)	23 (1%)	71 78

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	347	CYS
2	D	47	GLU
4	F	257	GLU
1	C	381	THR
2	D	139	HIS

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

Mol	Chain	Res	Type
2	B	394	GLN
4	F	239	HIS
4	F	269	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
10	GDP	B	502	6	24,30,30	1.27	4 (16%)	31,47,47	1.95	9 (29%)
9	FB7	B	501	-	32,32,32	1.69	4 (12%)	44,46,46	1.97	13 (29%)
10	GDP	D	501	6	24,30,30	1.15	1 (4%)	31,47,47	1.99	7 (22%)
5	GTP	C	501	6	26,34,34	1.02	1 (3%)	33,54,54	1.94	7 (21%)
5	GTP	A	501	6	26,34,34	0.89	1 (3%)	33,54,54	1.80	6 (18%)
12	ACP	F	403	6	27,33,33	1.97	7 (25%)	32,52,52	1.33	5 (15%)
8	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.56	0
9	FB7	D	500	-	32,32,32	1.80	4 (12%)	44,46,46	2.05	11 (25%)
11	MES	B	505	-	12,12,12	2.33	1 (8%)	14,16,16	2.50	5 (35%)
8	GOL	F	401	-	5,5,5	0.40	0	5,5,5	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
10	GDP	B	502	6	-	5/12/32/32	0/3/3/3
9	FB7	B	501	-	-	0/18/34/34	0/4/4/4
10	GDP	D	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
12	ACP	F	403	6	-	5/15/38/38	0/3/3/3
8	GOL	A	505	-	-	4/4/4/4	-
9	FB7	D	500	-	-	2/18/34/34	0/4/4/4
11	MES	B	505	-	-	5/6/14/14	0/1/1/1
8	GOL	F	401	-	-	0/4/4/4	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	MES	C8-S	-7.85	1.66	1.77
9	D	500	FB7	CAH-CAE	-6.08	1.38	1.49
12	F	403	ACP	PG-O1G	5.47	1.61	1.50
9	B	501	FB7	CAH-CAE	-4.95	1.40	1.49
9	B	501	FB7	CAY-CAX	-4.56	1.40	1.50

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	505	MES	C5-N4-C3	7.57	125.88	108.83
9	D	500	FB7	CAE-CAD-CAC	6.97	120.71	118.25
5	C	501	GTP	N3-C2-N1	-6.61	118.40	127.22
9	B	501	FB7	CAE-CAD-CAC	6.29	120.47	118.25
5	A	501	GTP	N3-C2-N1	-5.46	119.94	127.22

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	505	GOL	O1-C1-C2-C3
10	D	501	GDP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G

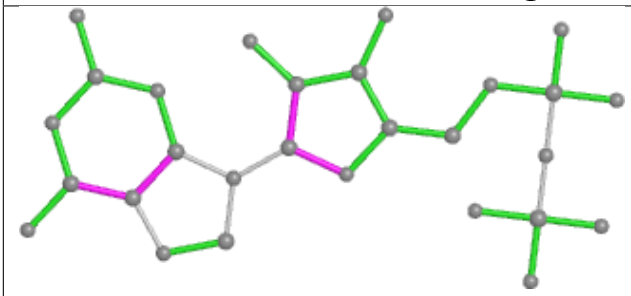
There are no ring outliers.

5 monomers are involved in 10 short contacts:

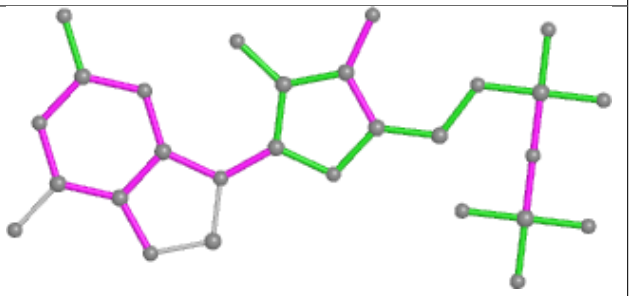
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	501	GDP	2	0
12	F	403	ACP	2	0
8	A	505	GOL	1	0
9	D	500	FB7	2	0
11	B	505	MES	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

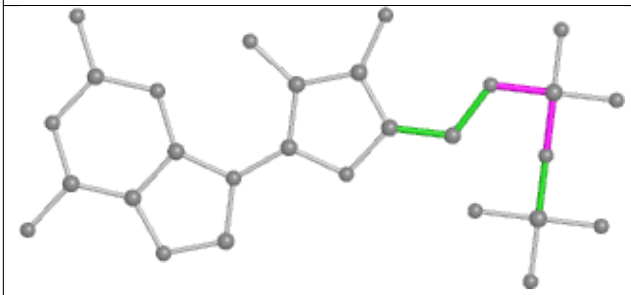
Ligand GDP B 502



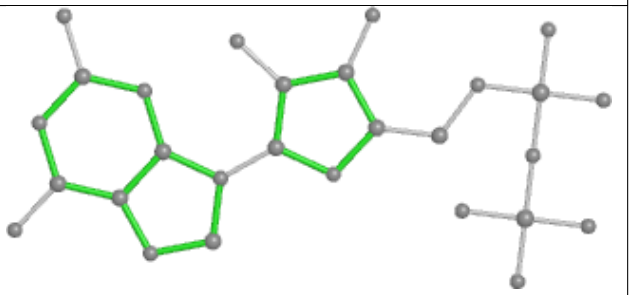
Bond lengths



Bond angles

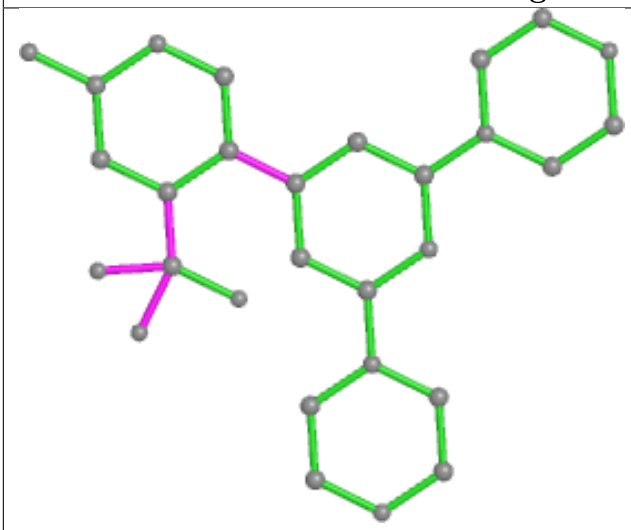


Torsions

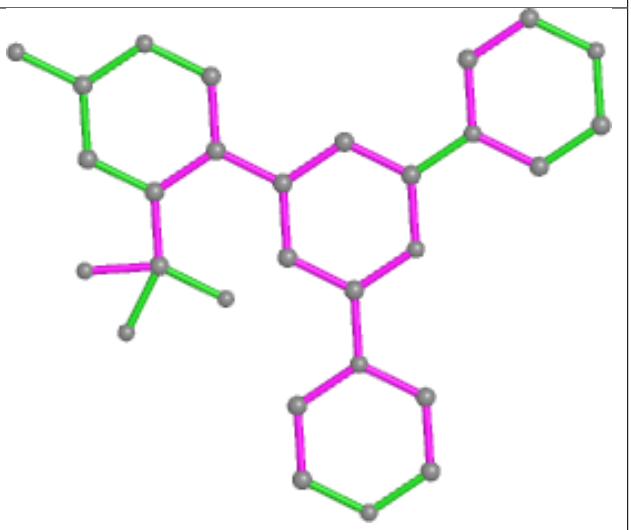


Rings

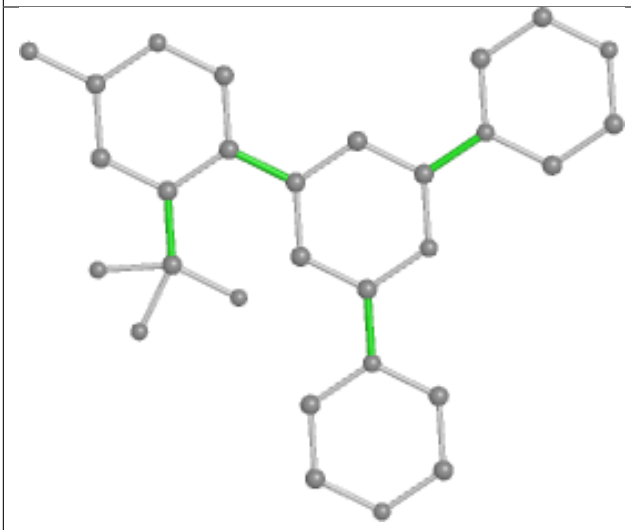
Ligand FB7 B 501



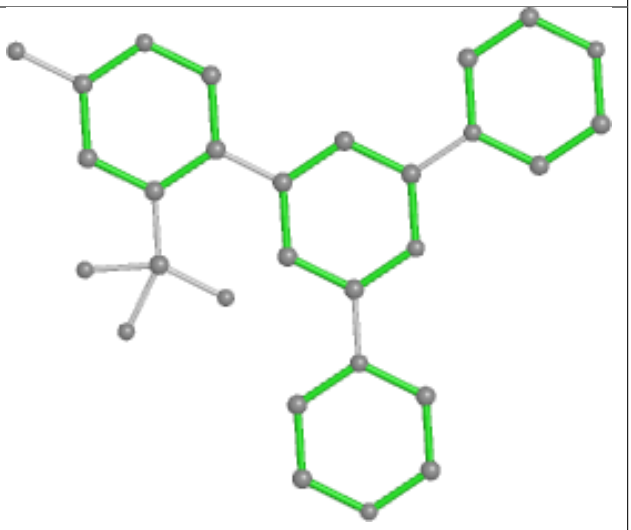
Bond lengths



Bond angles

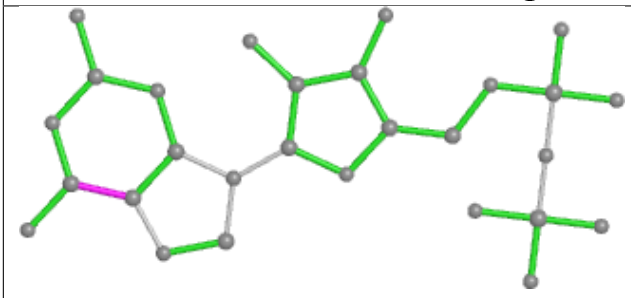


Torsions

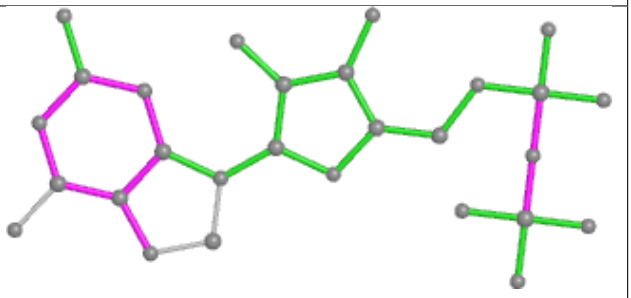


Rings

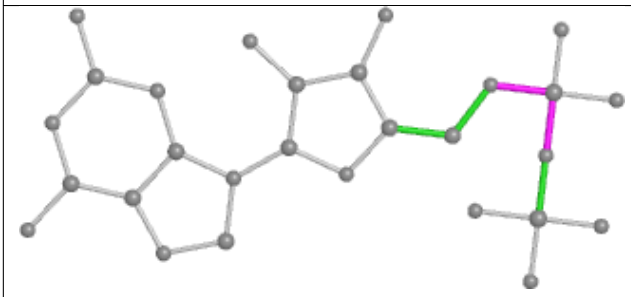
Ligand GDP D 501



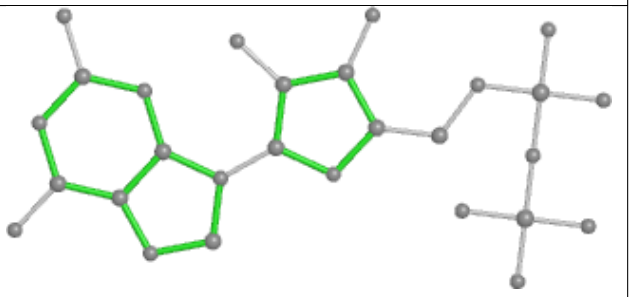
Bond lengths



Bond angles

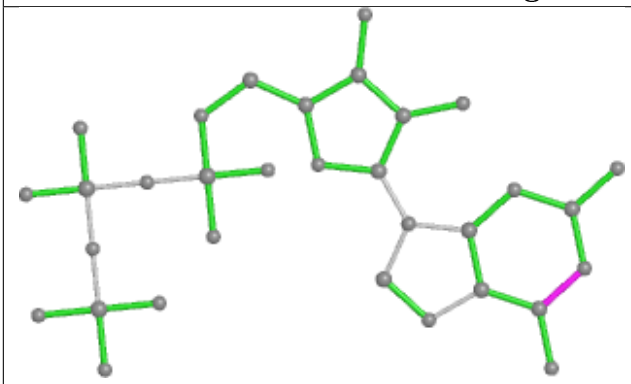


Torsions

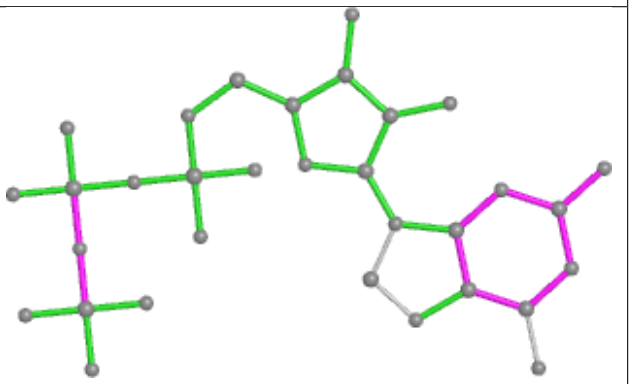


Rings

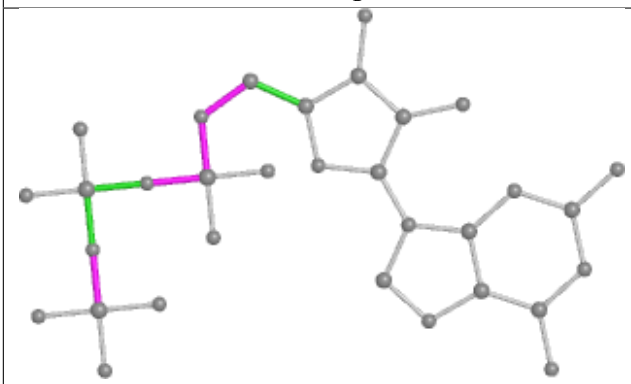
Ligand GTP C 501



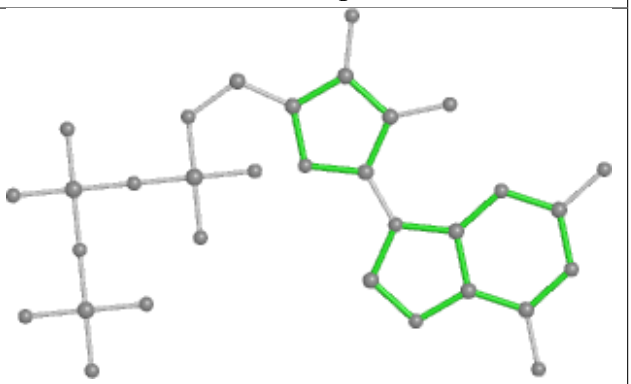
Bond lengths



Bond angles

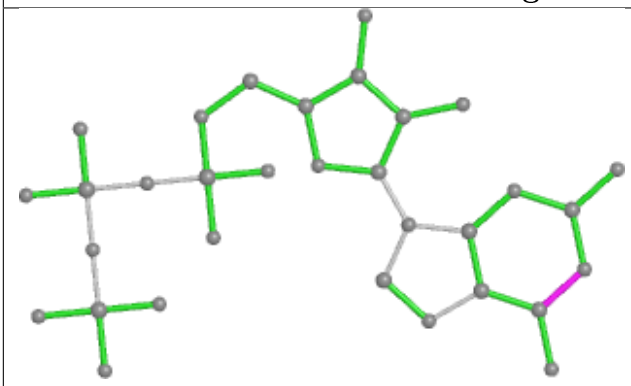


Torsions

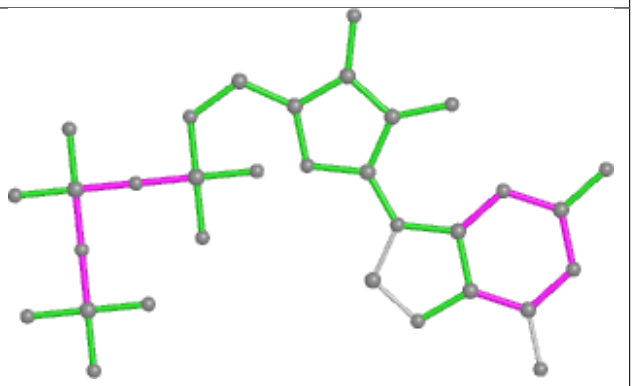


Rings

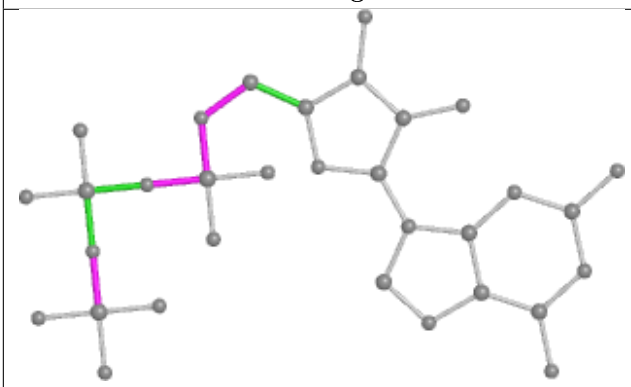
Ligand GTP A 501



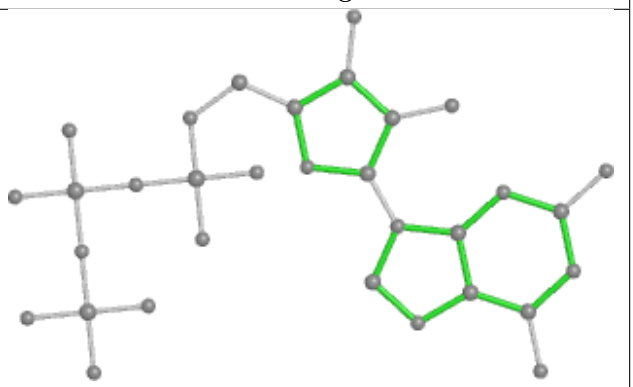
Bond lengths



Bond angles

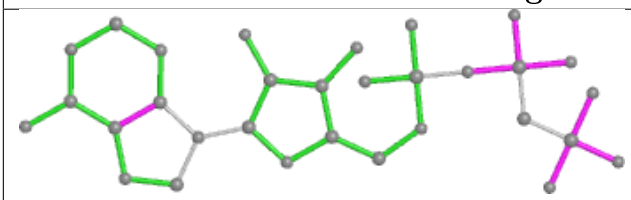


Torsions

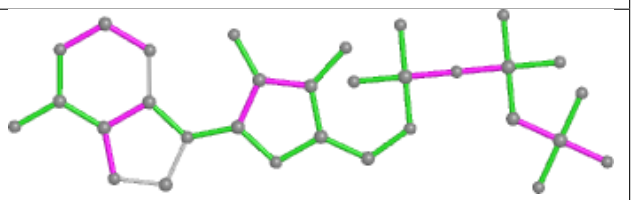


Rings

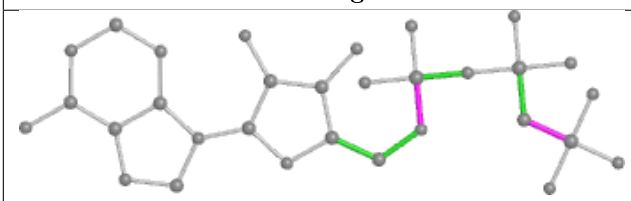
Ligand ACP F 403



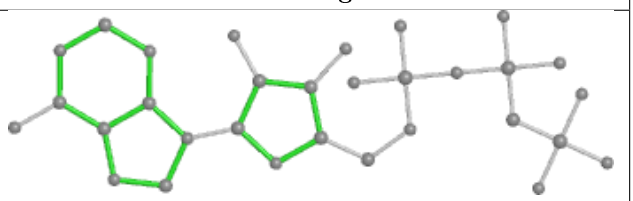
Bond lengths



Bond angles

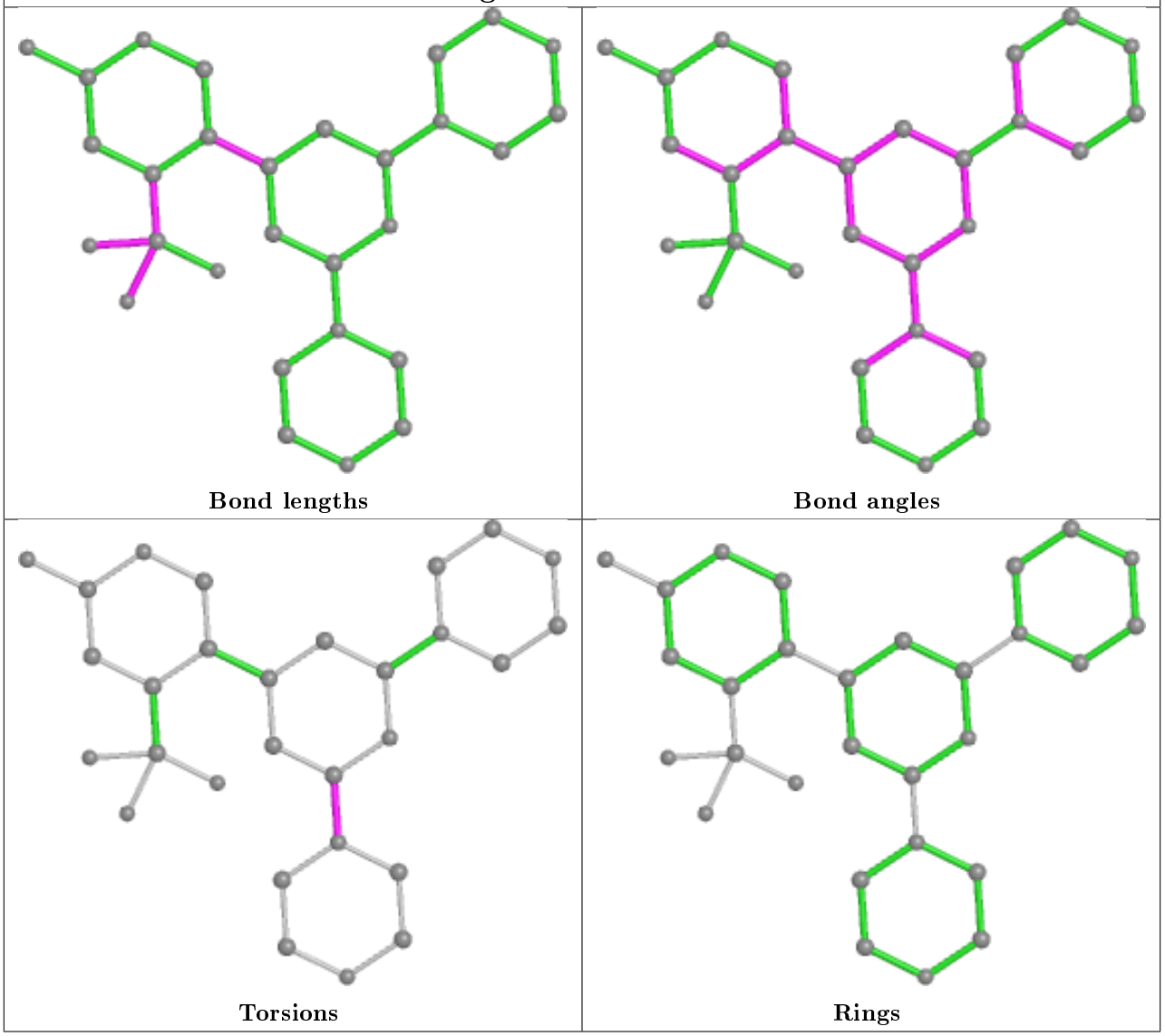


Torsions



Rings

Ligand FB7 D 500



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	436/451 (96%)	0.21	21 (4%) 30 30	40, 58, 96, 124	0
1	C	440/451 (97%)	-0.09	7 (1%) 72 73	34, 46, 77, 111	1 (0%)
2	B	422/445 (94%)	0.09	12 (2%) 53 53	35, 56, 96, 139	2 (0%)
2	D	418/445 (93%)	0.43	45 (10%) 5 5	40, 67, 102, 132	5 (1%)
3	E	123/143 (86%)	0.48	13 (10%) 6 5	46, 74, 116, 127	0
4	F	326/384 (84%)	1.26	103 (31%) 0 0	47, 84, 135, 155	0
All	All	2165/2319 (93%)	0.34	201 (9%) 8 8	34, 61, 111, 155	8 (0%)

The worst 5 of 201 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	100	ILE	8.9
4	F	173	ILE	7.6
4	F	253	TYR	7.5
4	F	132	LEU	7.4
4	F	130	VAL	7.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

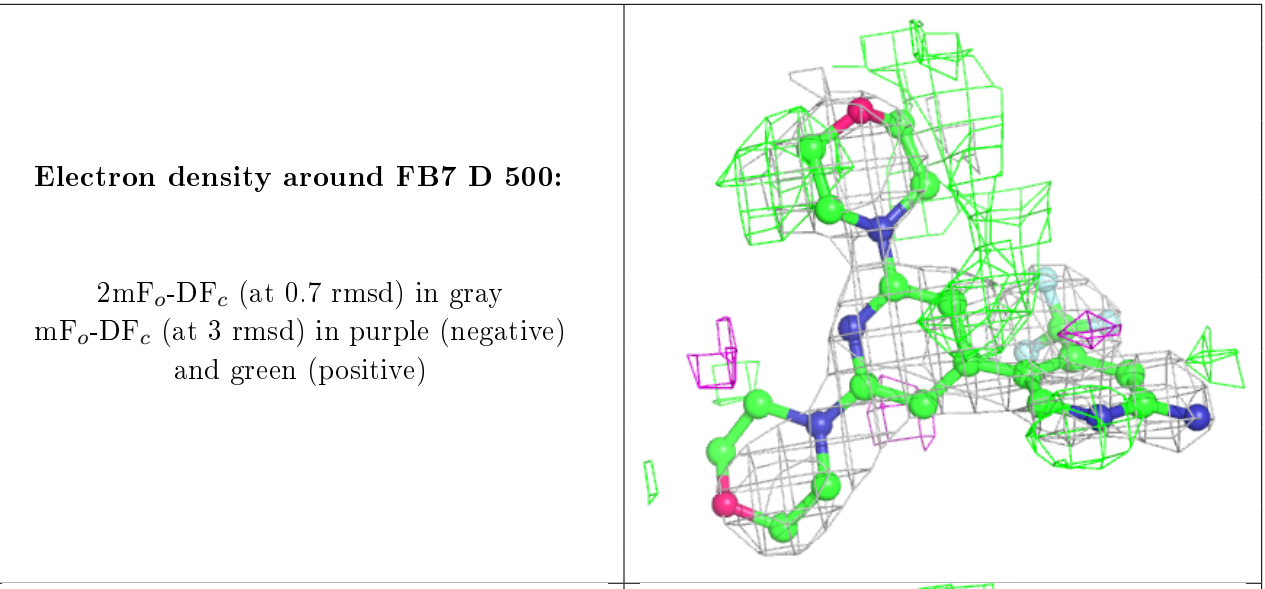
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

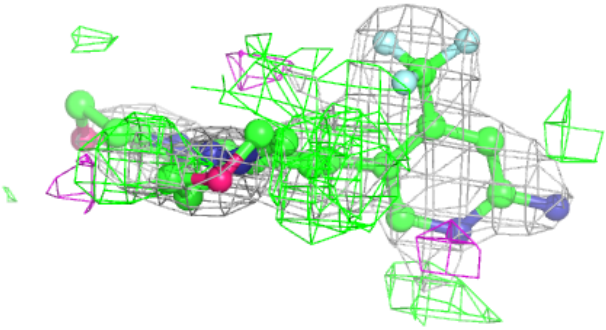
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	C	504	1/1	0.81	0.04	127,127,127,127	0
6	MG	A	502	1/1	0.81	0.38	74,74,74,74	0
8	GOL	F	401	6/6	0.81	0.14	76,84,89,94	0
9	FB7	D	500	29/29	0.82	0.45	33,50,65,66	29
7	CA	A	504	1/1	0.85	0.14	100,100,100,100	0
6	MG	F	402	1/1	0.89	0.10	82,82,82,82	0
12	ACP	F	403	31/31	0.91	0.12	86,97,122,134	0
8	GOL	A	505	6/6	0.91	0.15	79,83,84,84	0
6	MG	D	502	1/1	0.92	0.11	58,58,58,58	0
6	MG	C	502	1/1	0.95	0.17	40,40,40,40	0
7	CA	B	504	1/1	0.95	0.10	83,83,83,83	0
6	MG	B	503	1/1	0.95	0.24	34,34,34,34	0
11	MES	B	505	12/12	0.96	0.13	56,66,84,88	0
9	FB7	B	501	29/29	0.96	0.15	35,49,68,70	0
10	GDP	D	501	28/28	0.97	0.12	45,59,69,74	0
7	CA	A	503	1/1	0.98	0.06	81,81,81,81	0
5	GTP	C	501	32/32	0.99	0.14	32,37,43,51	0
7	CA	C	503	1/1	0.99	0.07	67,67,67,67	0
5	GTP	A	501	32/32	0.99	0.20	35,43,49,49	0
10	GDP	B	502	28/28	0.99	0.18	29,40,45,50	0

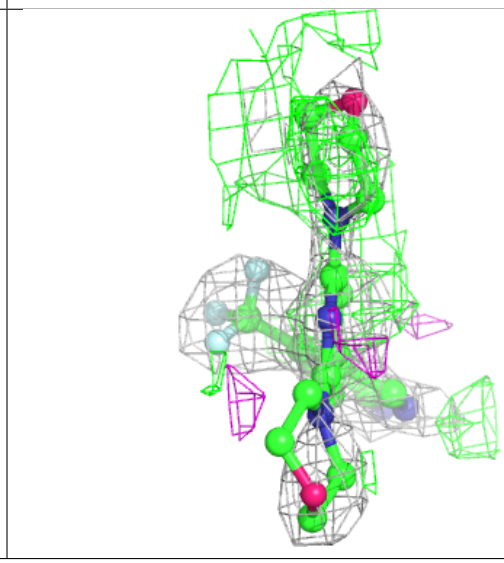
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FB7 D 500:

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







Electron density around ACP F 403:

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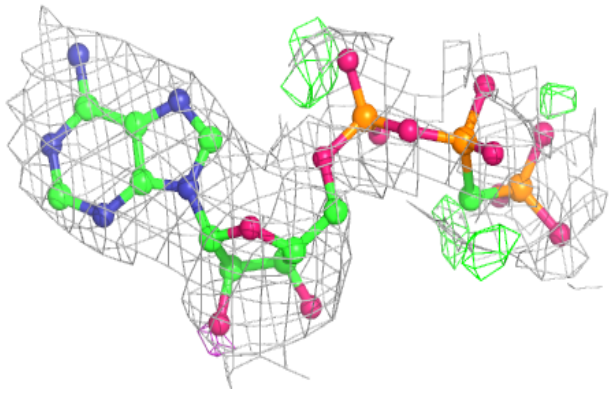
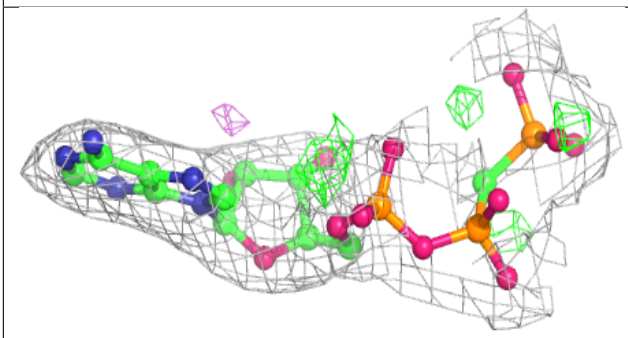
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around FB7 B 501:

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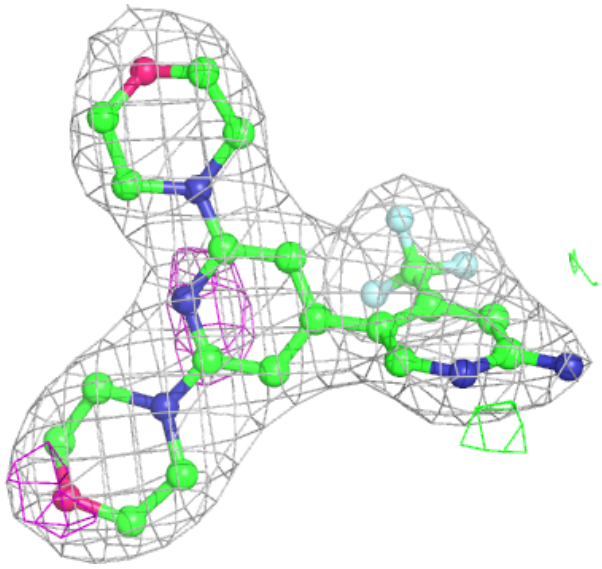
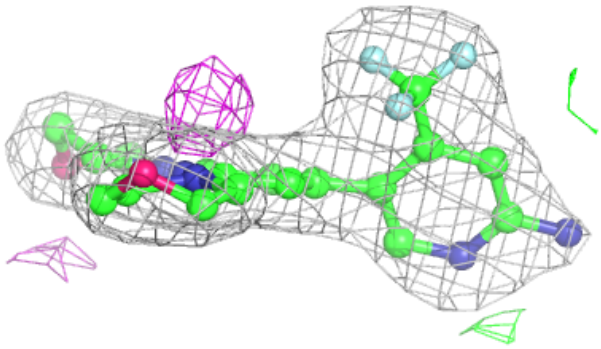
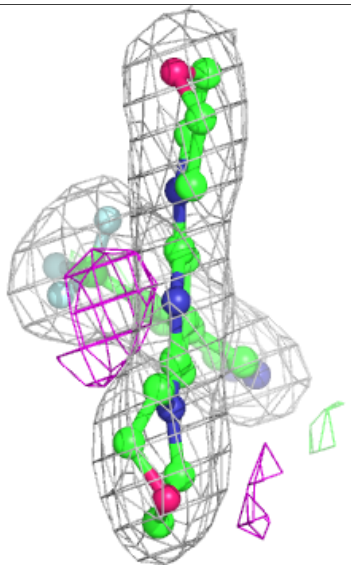
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around GDP D 501:

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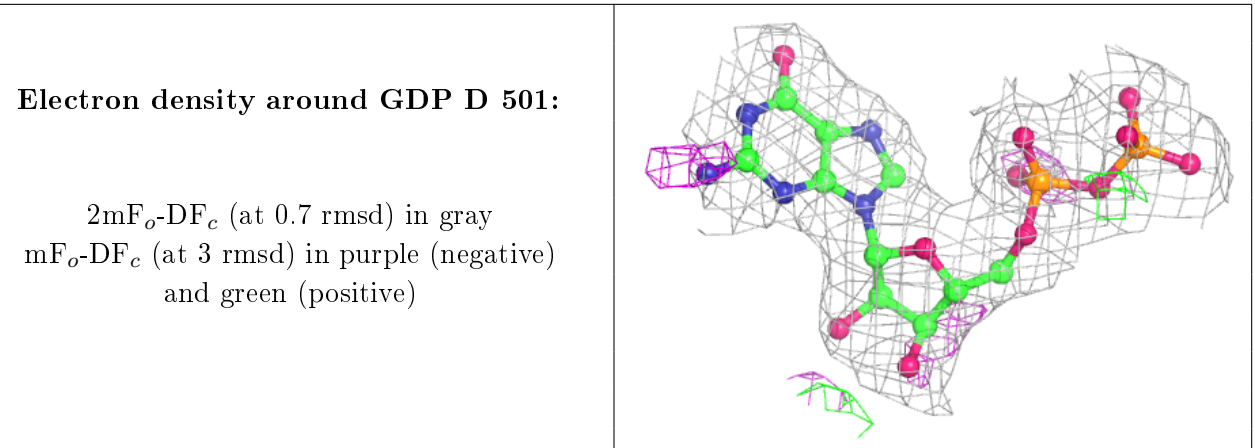
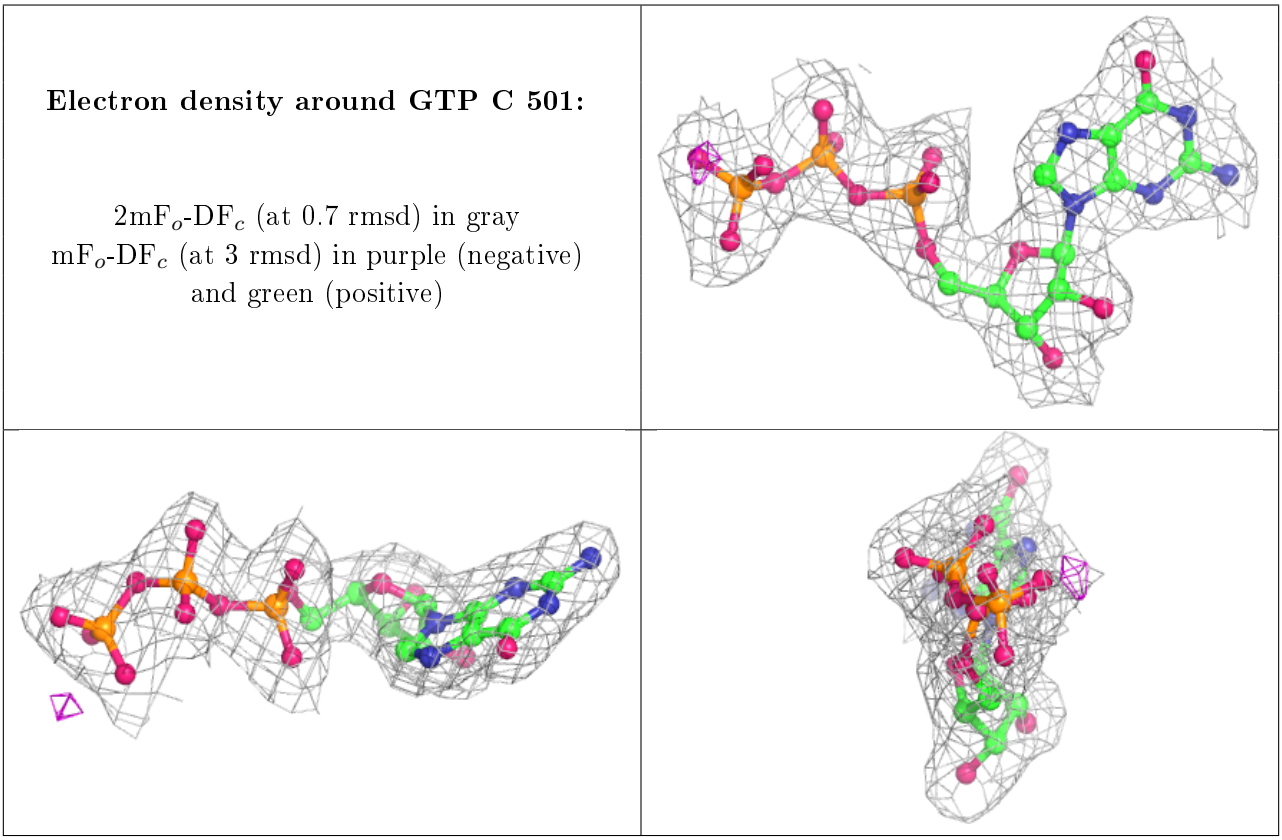
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



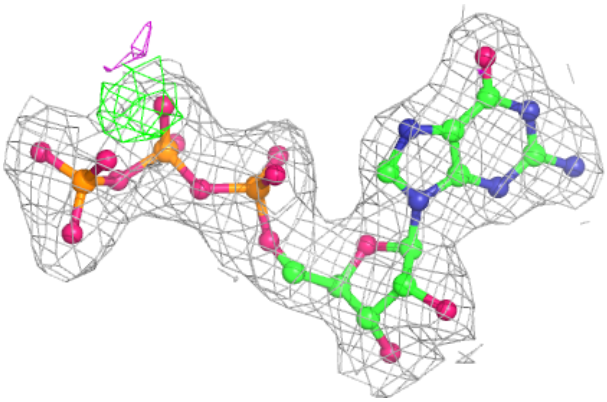
Electron density around GTP C 501:

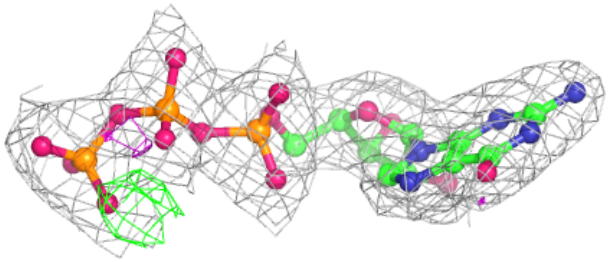
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

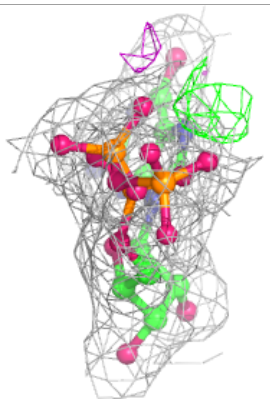


Electron density around GTP A 501:

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

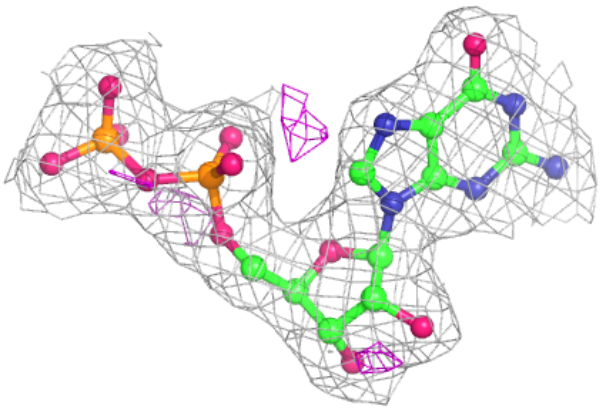


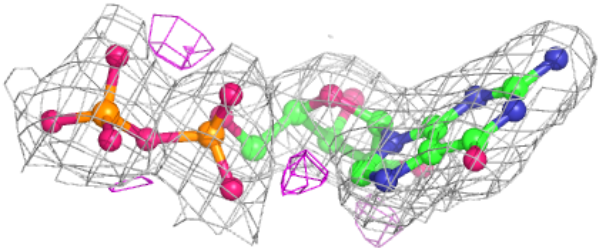


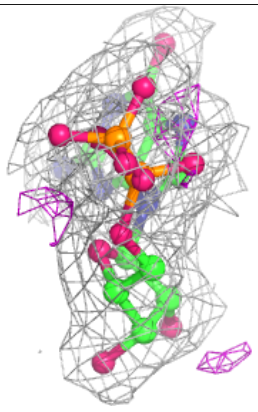


Electron density around GDP B 502:

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







6.5 Other polymers (i)

There are no such residues in this entry.