wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2022 – 10:25 am BST

PDB ID	:	7Z2P
Title	:	Tubulin-nocodazole complex
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Deposited on	:	2022-02-28
Resolution	:	2.00 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

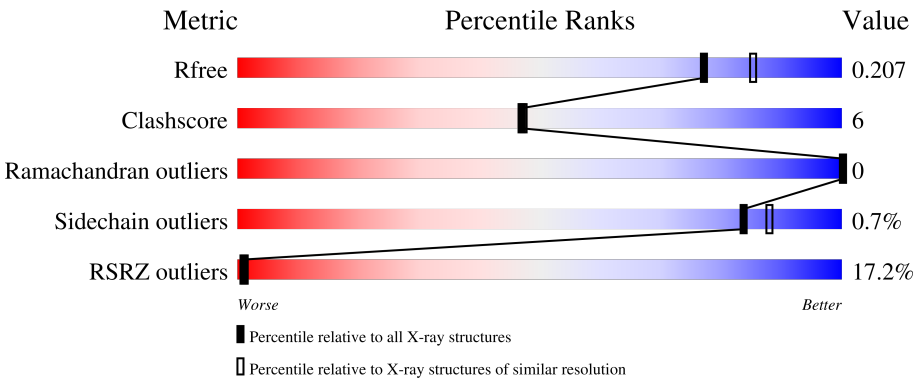
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	13% 85% 12% •
1	C	451	8% 82% 15% •
2	B	445	11% 80% 15% 5%
2	D	445	18% 79% 15% • 5%
3	E	143	16% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	35% 78% 12% 10%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18454 atoms, of which 22 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	439	3462	2199	583	655	25	0	8	0
1	C	440	3473	2203	585	660	25	0	10	0

- 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	3339	2101	565	646	27	0	4	0
2	D	421	3320	2088	562	642	28	0	3	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1021	630	185	201	5	0	1	0

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

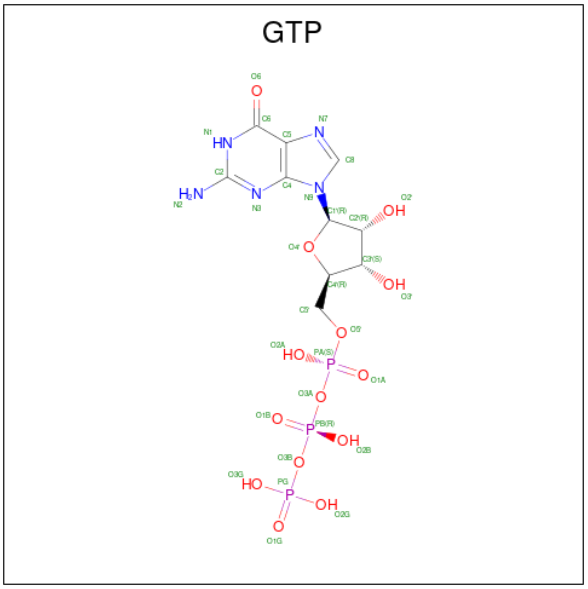
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	344	2818	1807	479	518	14	0	0	0

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
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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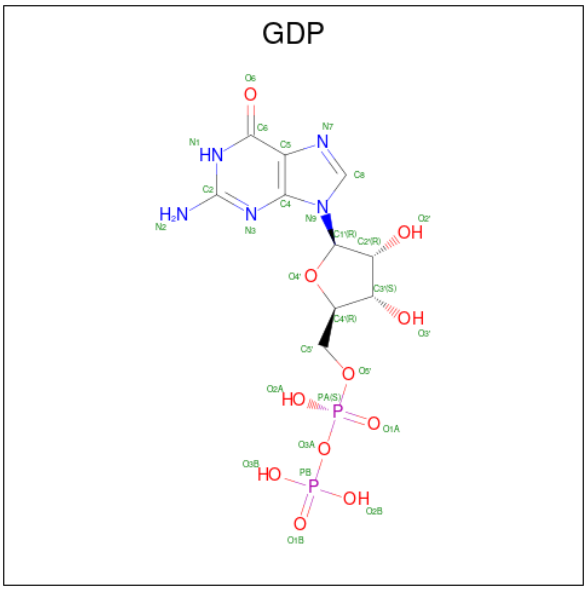
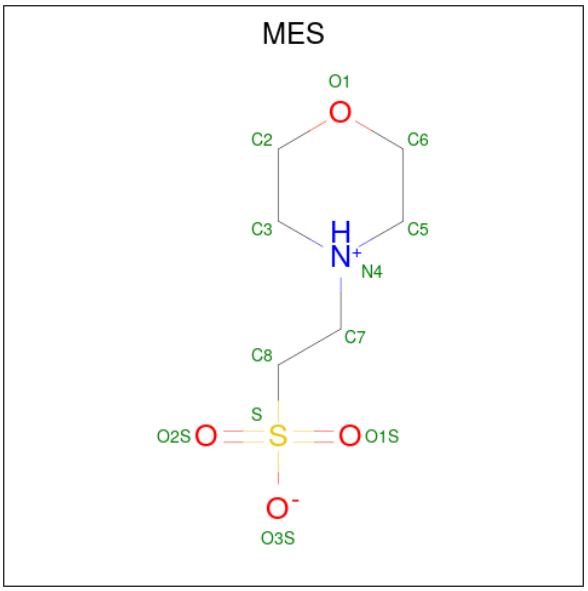
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



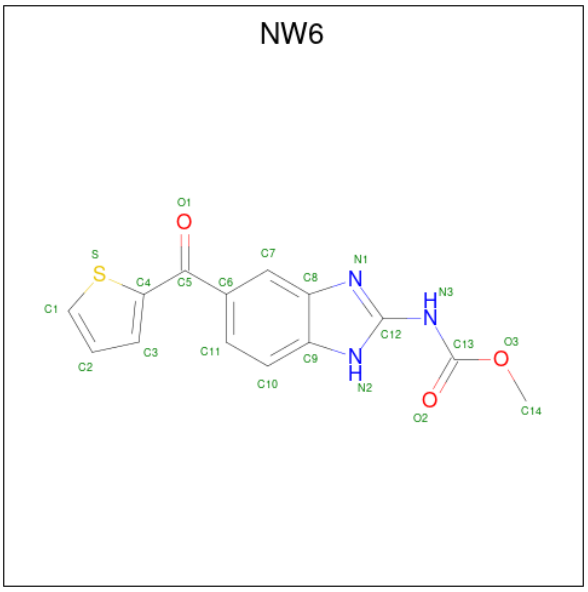
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
7	D	1	28	10	5	11	2	0	0

- Molecule 8 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		
8	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
8	D	1	12	6	1	4	1	0	0

- Molecule 9 is nocodazole (three-letter code: NW6) (formula: $C_{14}H_{11}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
9	B	1	32	14	11	3	3	1	0	0

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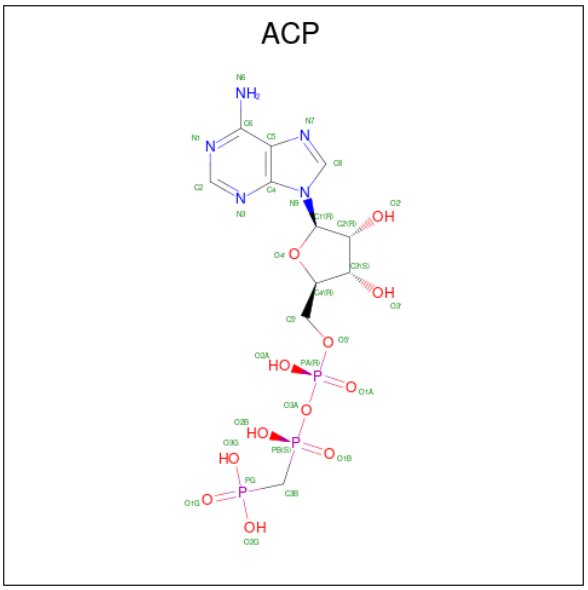
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
9	D	1	32	14	11	3	3	1	0	0

- Molecule 10 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
			Total	C	N	O	P		
10	F	1	31	11	5	12	3	0	0

- Molecule 11 is water.

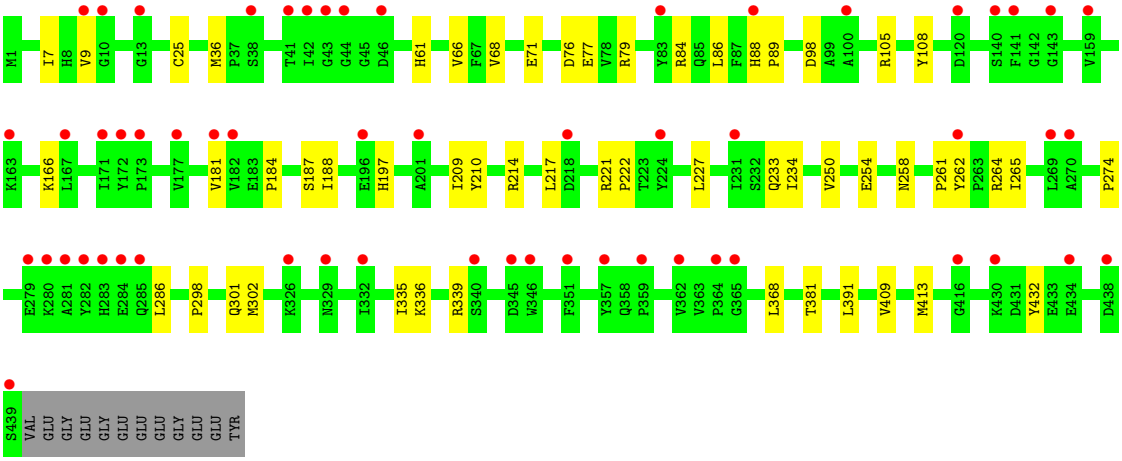
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	150	150	150	0	0
11	B	169	169	169	0	0
11	C	280	280	280	0	0
11	D	85	85	85	0	0
11	E	34	34	34	0	0
11	F	59	59	59	0	0

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.

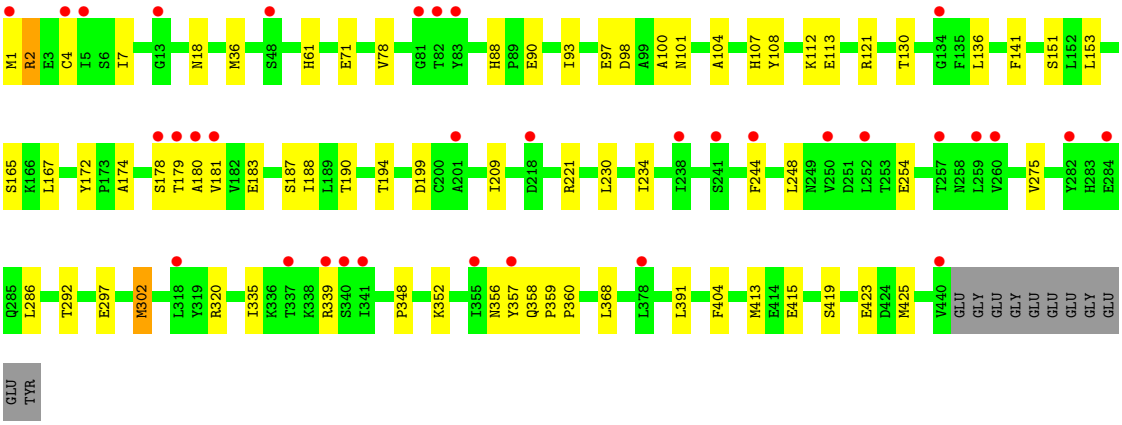
• Molecule 1: Tubulin alpha-1B chain

Chain A:



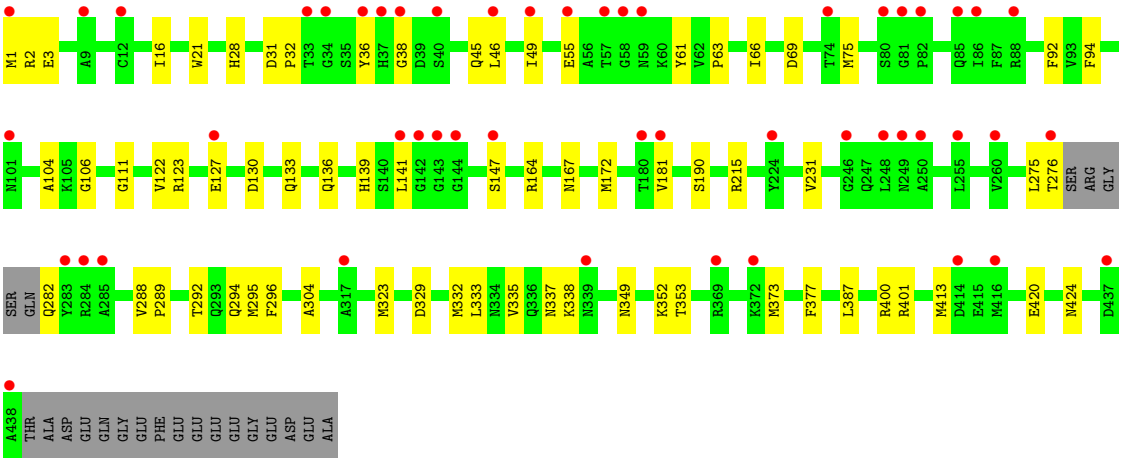
• Molecule 1: Tubulin alpha-1B chain

Chain C:



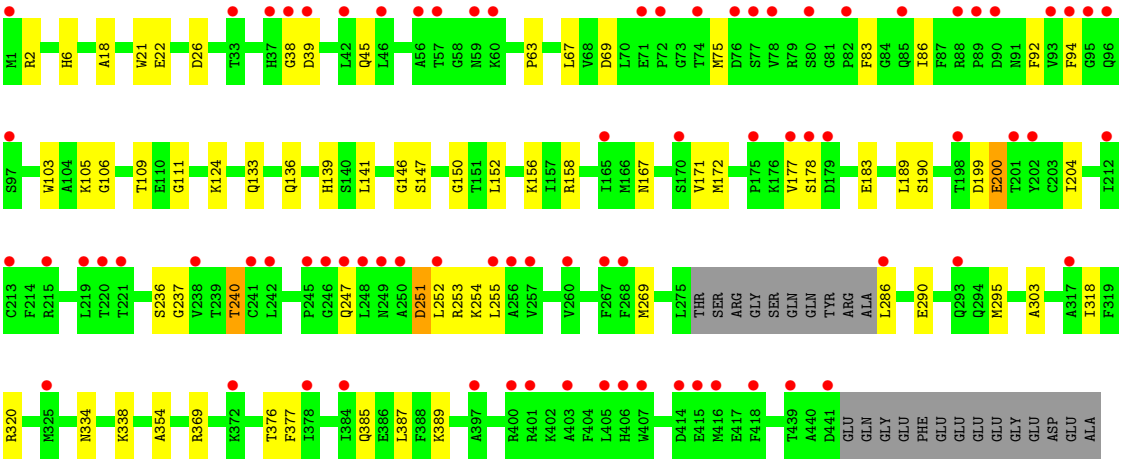
• Molecule 2: Tubulin beta-2B chain

Chain B:



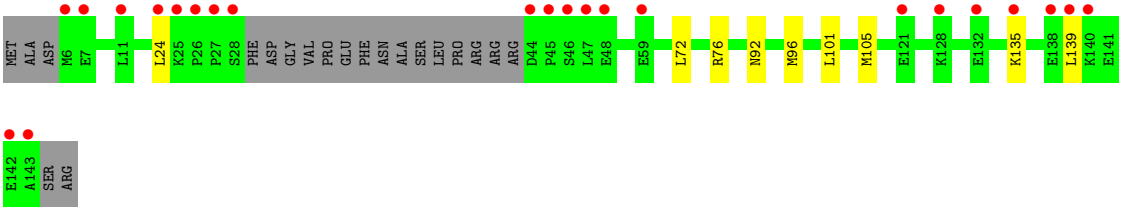
- Molecule 2: Tubulin beta-2B chain

Chain D:



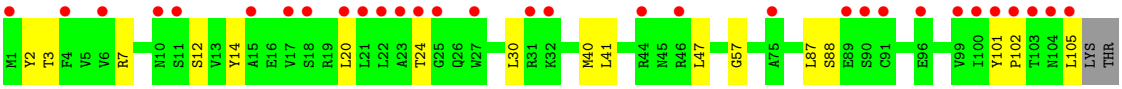
- Molecule 3: Stathmin-4

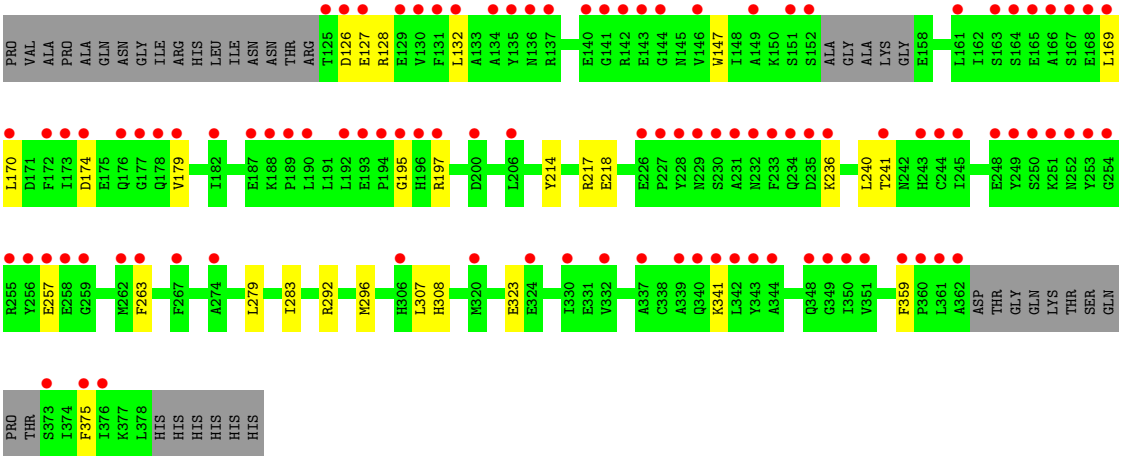
Chain E:



- Molecule 4: Tubulin beta-2B chain

Chain F:




PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG T125 D126 E127 R128 E129 V130 F131 L132 A133 A134 Y135 N136 R137 E140 G141 R142 E143 G144 N145 V146 W147 I148 A149 K150 S151 S152 ALA GLY ALA LYS GLY E158 L161 I162 S163 S164 E165 A166 S167 E168 L169
L170 D171 F172 I173 D174 E175 Q176 G177 Q178 V179 I182 E187 K188 P189 L190 L191 L192 E193 P194 G195 H196 R197 D200 L206 Y214 R217 E218 E226 P227 Y228 N229 S230 A231 N232 F233 Q234 D235 K236 L240 T241 N242 H243 C244 I245 E248 Y249 S250 K251 N252 Y253 G254
R255 Y256 E257 E258 G259 M262 F263 F267 A274 L279 I283 R292 M296 H306 L307 H308 M320 E323 E324 I330 E331 V332 A337 C338 A339 Q340 K341 L342 Y343 A344 Q348 G349 I350 V351 F359 P360 L361 A362 ASP THR GLY GLN LYS THR SER GLN
PRO THR S373 I374 F375 I376 K377 L378 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.73Å 158.09Å 179.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.00 49.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.37-2.00) 99.8 (49.37-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.178 , 0.209 0.176 , 0.207	Depositor DCC
R_{free} test set	10017 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18454	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, GDP, MG, NW6, MES, GTP

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	0.26	0/3564	0.49	0/4839
1	C	0.28	0/3582	0.50	0/4865
2	B	0.27	0/3425	0.49	0/4639
2	D	0.26	0/3402	0.49	0/4608
3	E	0.26	0/1033	0.43	0/1371
4	F	0.25	0/2880	0.47	0/3890
All	All	0.27	0/17886	0.48	0/24212

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	3462	0	3406	36	0
1	C	3473	0	3412	49	0
2	B	3339	0	3224	51	0
2	D	3320	0	3208	51	0
3	E	1021	0	1036	7	0
4	F	2818	0	2789	29	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	B	28	0	12	0	0
7	D	28	0	12	0	0
8	B	12	0	12	1	0
8	D	12	0	12	3	0
9	B	21	11	0	0	0
9	D	21	11	0	4	0
10	F	31	0	14	1	0
11	A	150	0	0	3	0
11	B	169	0	0	6	0
11	C	280	0	0	6	0
11	D	85	0	0	0	0
11	E	34	0	0	1	0
11	F	59	0	0	1	0
All	All	18432	22	17161	214	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 6.

The worst 5 of 214 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:247:GLN:HE21	2:D:354:ALA:HA	1.41	0.84
1:A:77:GLU:OE1	11:A:601:HOH:O	1.99	0.81
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.63	0.80
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.63	0.80
2:D:167:ASN:OD1	2:D:200:GLU:HG3	1.82	0.79

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	445/451 (99%)	437 (98%)	8 (2%)	0	100	100
1	C	448/451 (99%)	441 (98%)	7 (2%)	0	100	100
2	B	423/445 (95%)	418 (99%)	5 (1%)	0	100	100
2	D	420/445 (94%)	409 (97%)	11 (3%)	0	100	100
3	E	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
4	F	336/384 (88%)	328 (98%)	8 (2%)	0	100	100
All	All	2192/2319 (94%)	2150 (98%)	42 (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	378/379 (100%)	374 (99%)	4 (1%)	73	78
1	C	381/379 (100%)	378 (99%)	3 (1%)	81	86
2	B	369/383 (96%)	368 (100%)	1 (0%)	92	95
2	D	367/383 (96%)	362 (99%)	5 (1%)	67	72
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	310/342 (91%)	309 (100%)	1 (0%)	92	95
All	All	1916/1993 (96%)	1902 (99%)	14 (1%)	84	88

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	302	MET
2	D	39	ASP
4	F	12	SER
2	D	240	THR
2	D	251	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	356	ASN
2	D	15	GLN
2	D	247	GLN
3	E	92	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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NW6	D	504	-	23,23,23	1.86	4 (17%)	20,32,32	1.62	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.10	3 (10%)
9	NW6	B	504	-	23,23,23	1.74	5 (21%)	20,32,32	1.70	5 (25%)
5	GTP	A	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.30	5 (15%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.32	5 (15%)
7	GDP	B	501	6	24,30,30	0.94	2 (8%)	30,47,47	1.12	4 (13%)
8	MES	D	503	-	12,12,12	2.18	1 (8%)	14,16,16	1.96	6 (42%)
8	MES	B	503	-	12,12,12	1.96	1 (8%)	14,16,16	1.89	3 (21%)
10	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.37	4 (12%)

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	NW6	D	504	-	-	0/8/14/14	0/3/3/3
7	GDP	D	501	6	-	4/12/32/32	0/3/3/3
9	NW6	B	504	-	-	0/8/14/14	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
7	GDP	B	501	6	-	5/12/32/32	0/3/3/3
8	MES	D	503	-	-	4/6/14/14	0/1/1/1
8	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	ACP	F	401	6	-	3/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	MES	C8-S	-7.28	1.67	1.77
8	B	503	MES	C8-S	-6.51	1.68	1.77
9	D	504	NW6	C12-N2	4.92	1.41	1.34
9	B	504	NW6	C12-N2	4.46	1.41	1.34
9	D	504	NW6	C12-N3	4.08	1.44	1.38

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	503	MES	C5-N4-C3	4.30	118.50	108.83
9	B	504	NW6	C11-C10-C9	-3.78	116.08	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	401	ACP	PB-O3A-PA	-3.64	121.00	132.56
9	D	504	NW6	C11-C10-C9	-3.62	116.28	120.84
8	D	503	MES	C5-N4-C3	3.34	116.35	108.83

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

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

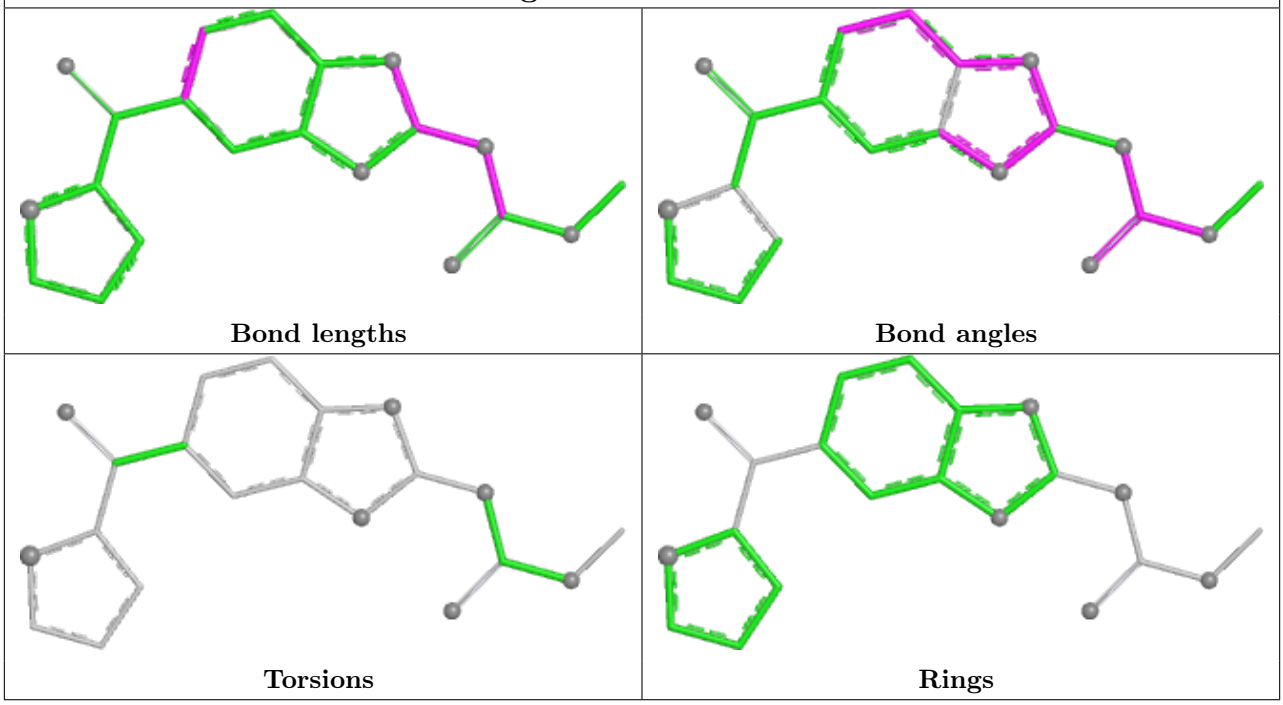
There are no ring outliers.

4 monomers are involved in 9 short contacts:

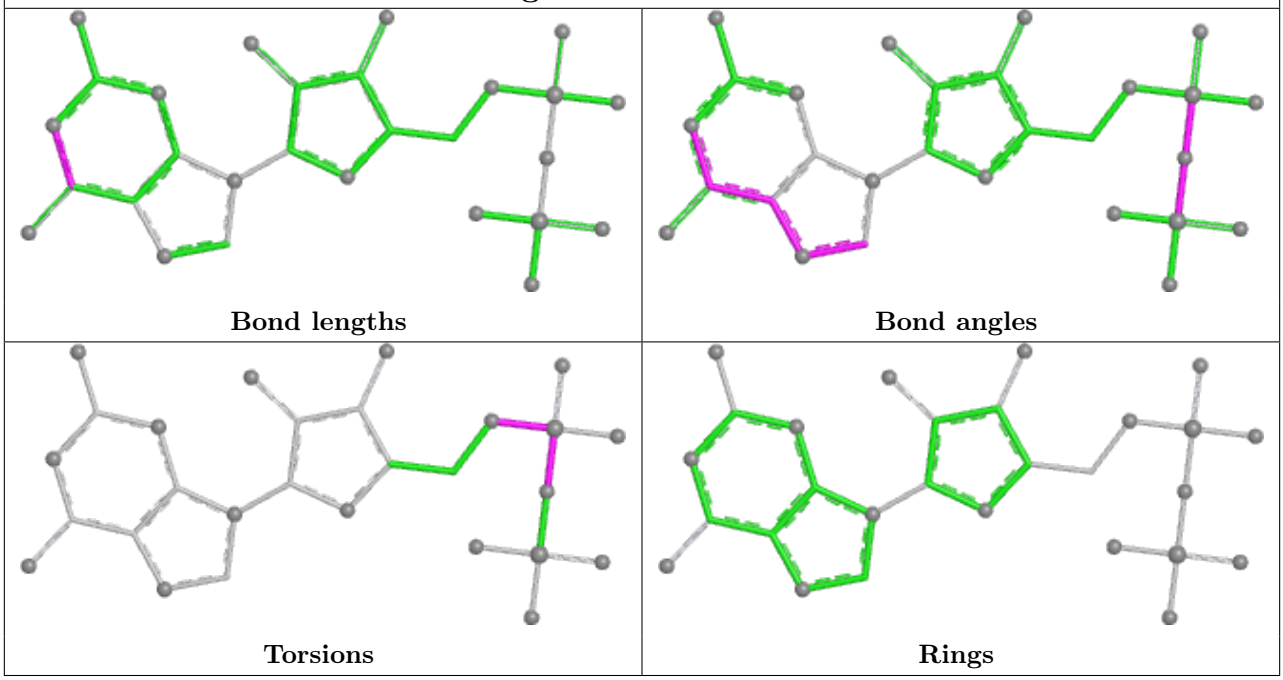
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	504	NW6	4	0
8	D	503	MES	3	0
8	B	503	MES	1	0
10	F	401	ACP	1	0

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 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.

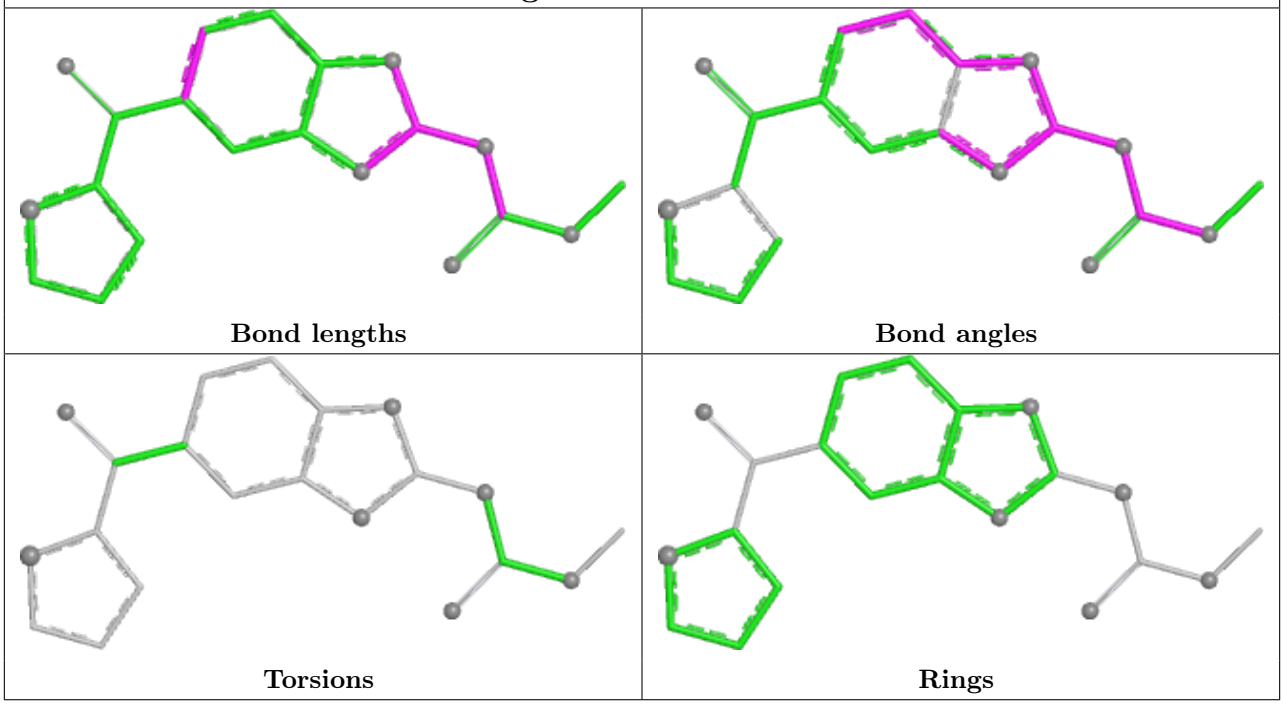
Ligand NW6 D 504



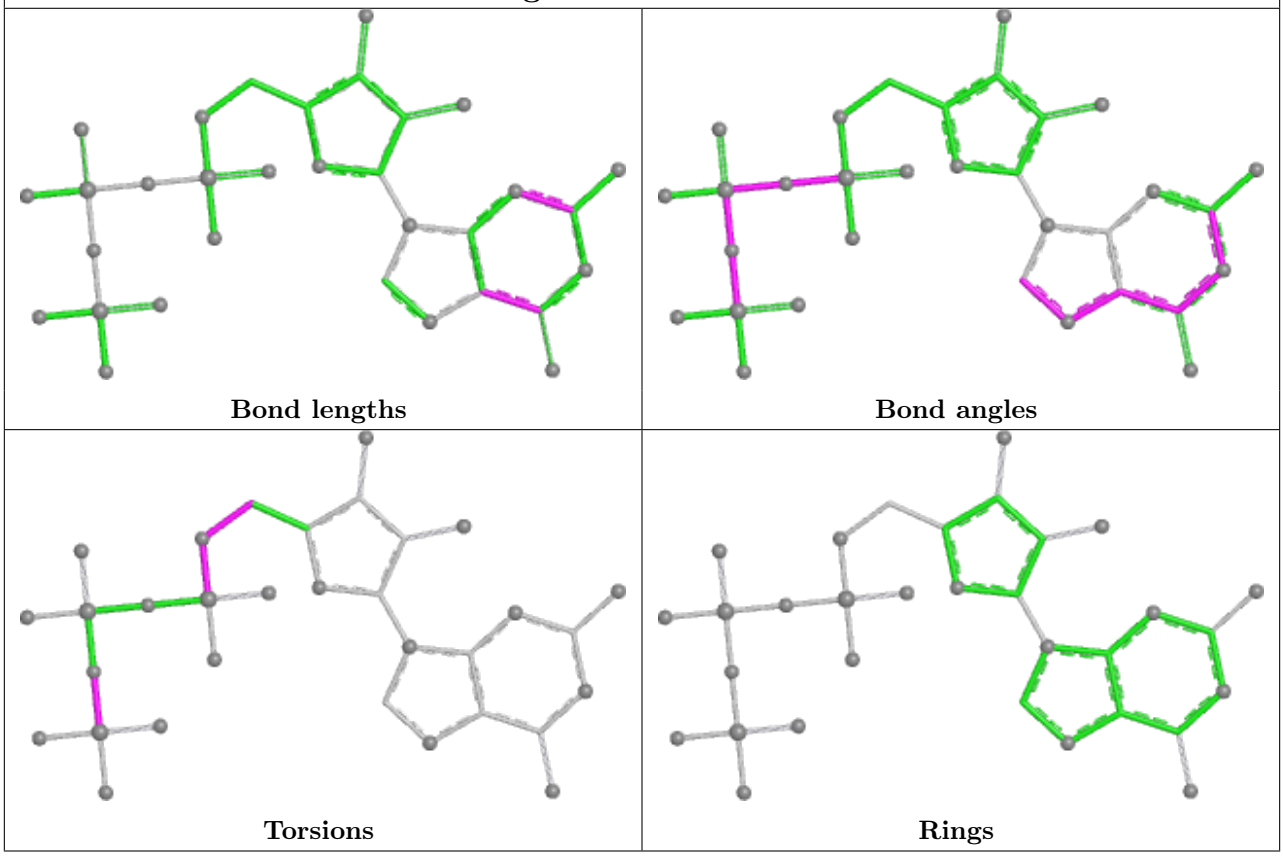
Ligand GDP D 501



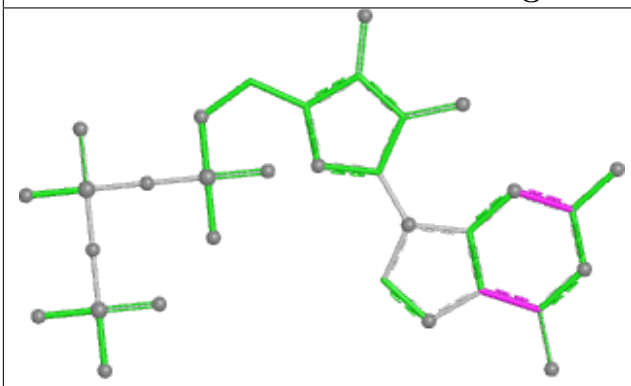
Ligand NW6 B 504



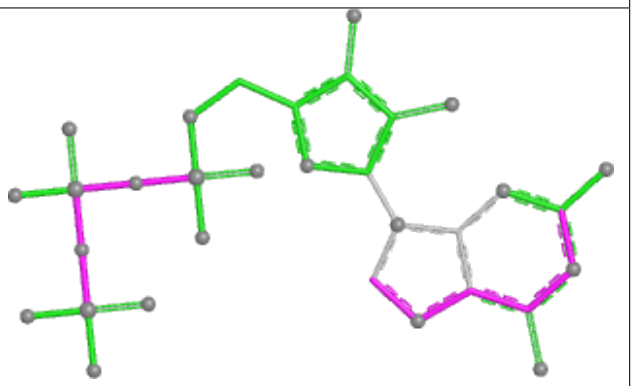
Ligand GTP A 501



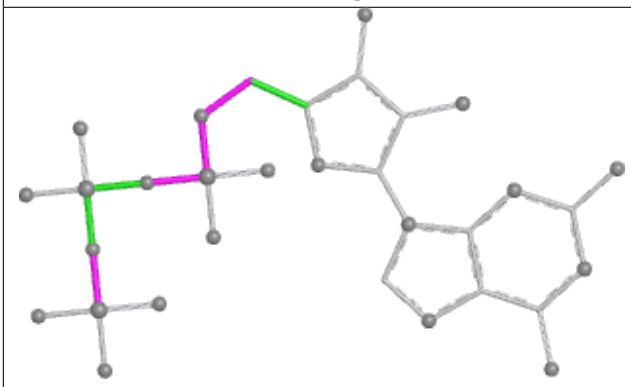
Ligand GTP C 501



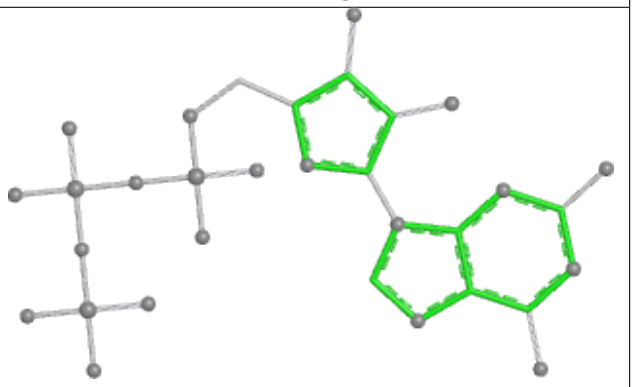
Bond lengths



Bond angles

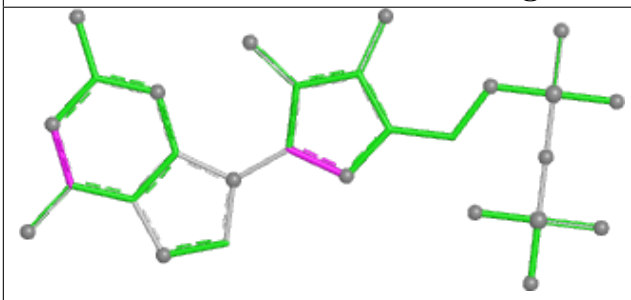


Torsions

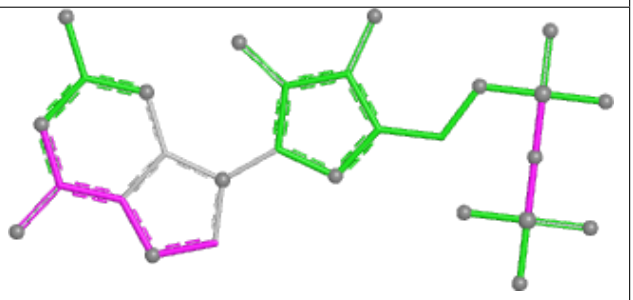


Rings

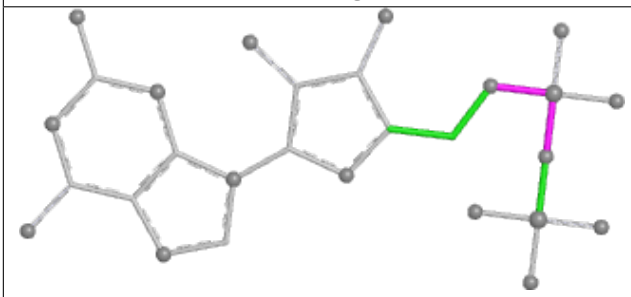
Ligand GDP B 501



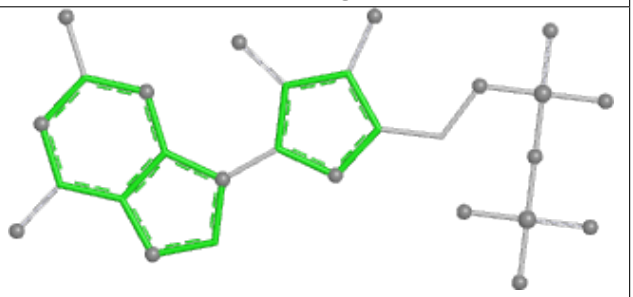
Bond lengths



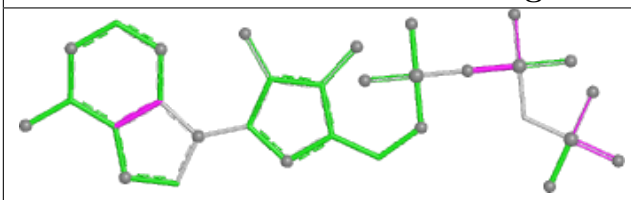
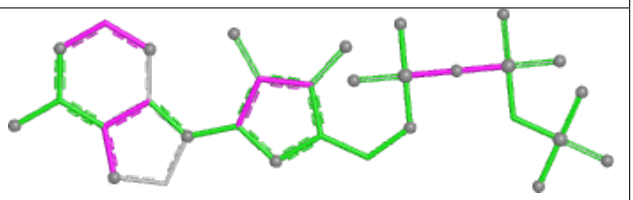
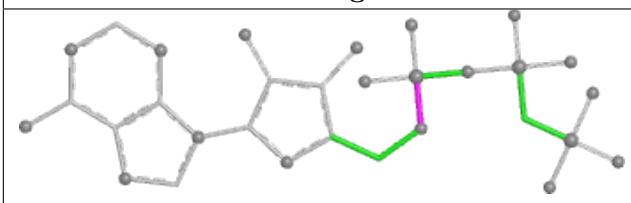
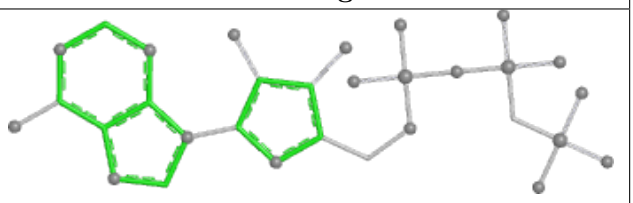
Bond angles



Torsions



Rings

Ligand ACP F 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	439/451 (97%)	0.93	57 (12%)	3	3	28, 44, 71, 130	0
1	C	440/451 (97%)	0.75	34 (7%)	13	12	23, 34, 57, 89	0
2	B	423/445 (95%)	0.96	50 (11%)	4	4	24, 40, 70, 110	0
2	D	421/445 (94%)	1.16	79 (18%)	1	1	29, 50, 79, 133	0
3	E	123/143 (86%)	1.13	23 (18%)	1	1	31, 55, 93, 113	0
4	F	344/384 (89%)	1.98	134 (38%)	0	0	36, 68, 124, 148	0
All	All	2190/2319 (94%)	1.12	377 (17%)	1	1	23, 45, 91, 148	0

The worst 5 of 377 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	249	ASN	12.3
4	F	89	GLU	11.1
4	F	169	LEU	10.4
4	F	104	ASN	10.3
1	C	440	VAL	10.2

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 (i)

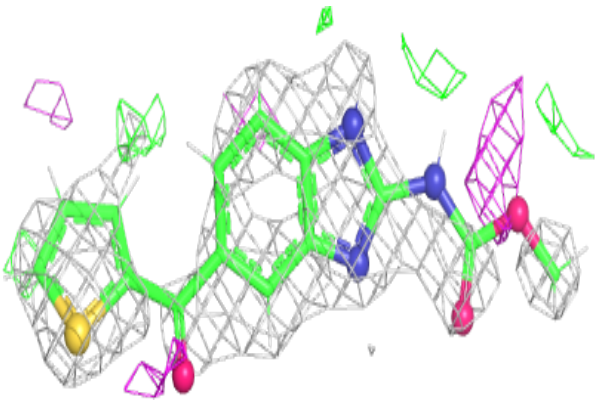
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

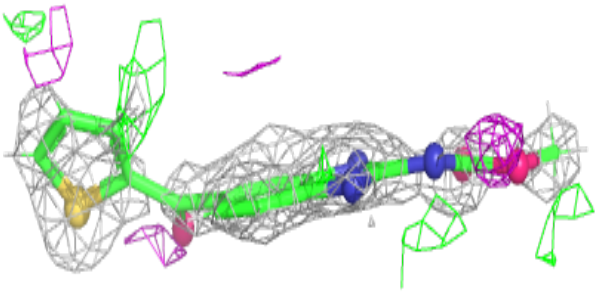
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NW6	D	504	21/21	0.77	0.37	39,48,60,62	32
8	MES	D	503	12/12	0.79	0.31	47,53,57,60	12
10	ACP	F	401	31/31	0.85	0.16	61,73,90,95	0
6	MG	D	502	1/1	0.91	0.10	52,52,52,52	0
9	NW6	B	504	21/21	0.93	0.14	30,36,41,46	0
6	MG	F	402	1/1	0.94	0.09	57,57,57,57	0
7	GDP	D	501	28/28	0.94	0.13	38,45,51,54	0
6	MG	C	502	1/1	0.94	0.11	26,26,26,26	0
6	MG	A	502	1/1	0.95	0.13	27,27,27,27	0
8	MES	B	503	12/12	0.95	0.15	34,39,48,49	0
5	GTP	A	501	32/32	0.96	0.18	23,29,34,34	0
5	GTP	C	501	32/32	0.96	0.18	19,25,29,30	0
7	GDP	B	501	28/28	0.96	0.18	23,29,31,32	0
6	MG	B	502	1/1	0.98	0.18	18,18,18,18	0

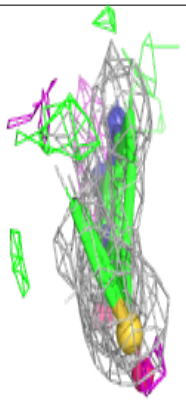
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NW6 D 504:

$2mF_o$-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 401:

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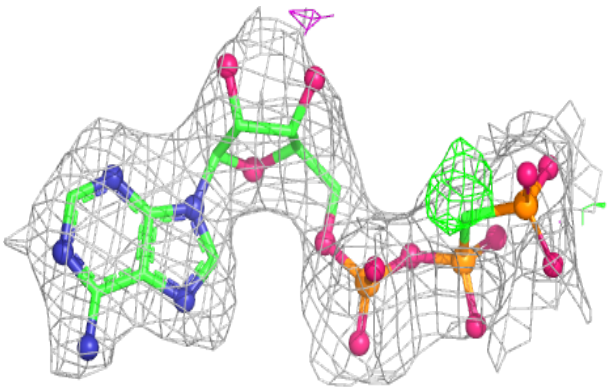
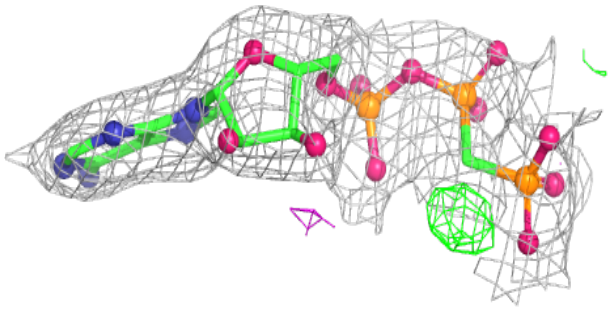
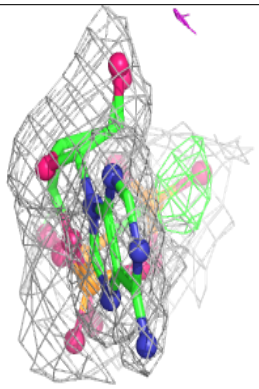
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NW6 B 504:

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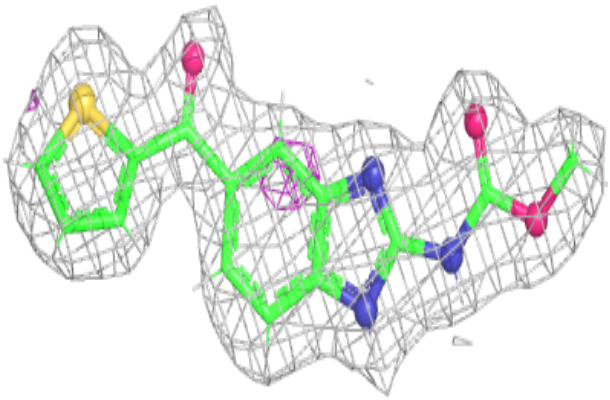
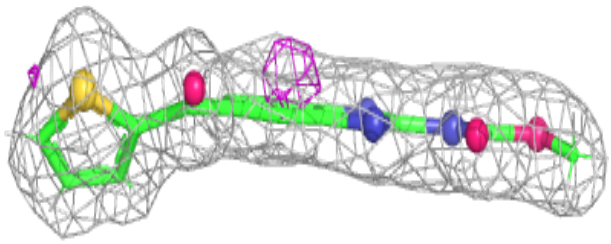
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around GDP D 501:

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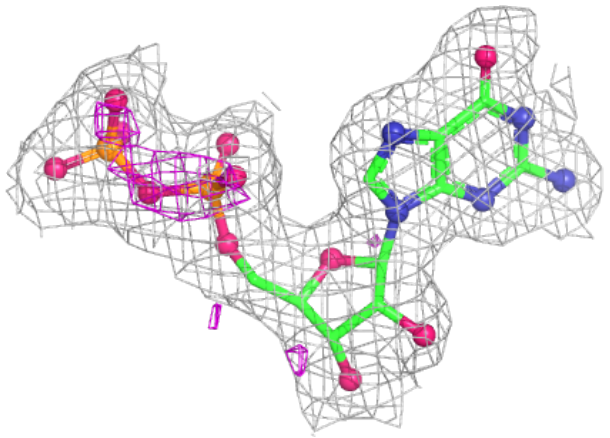
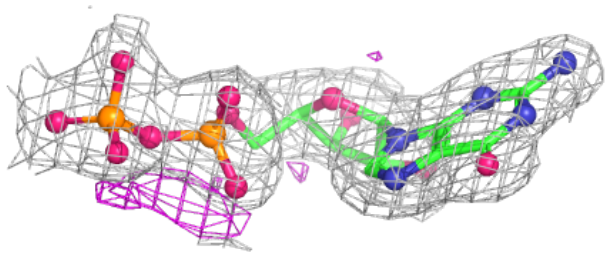
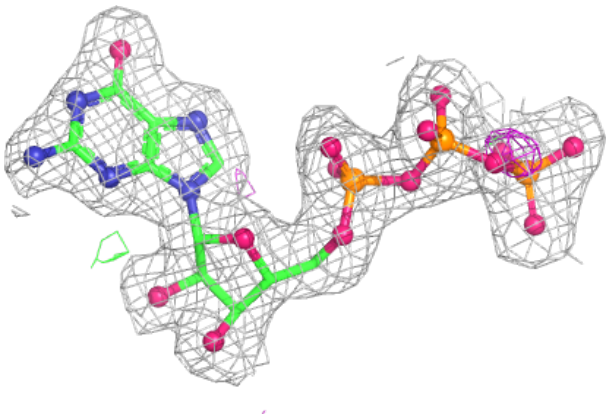
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

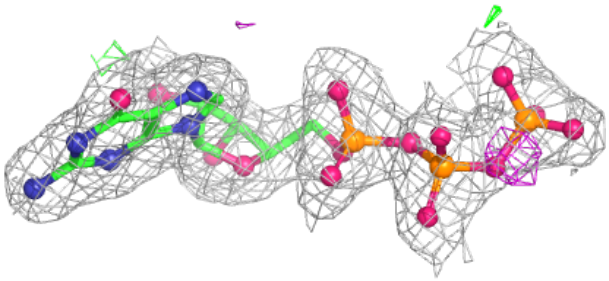


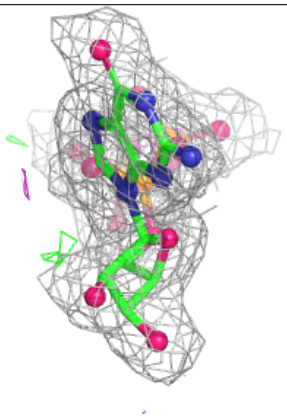


Electron density around GTP A 501:

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







Electron density around GTP C 501:

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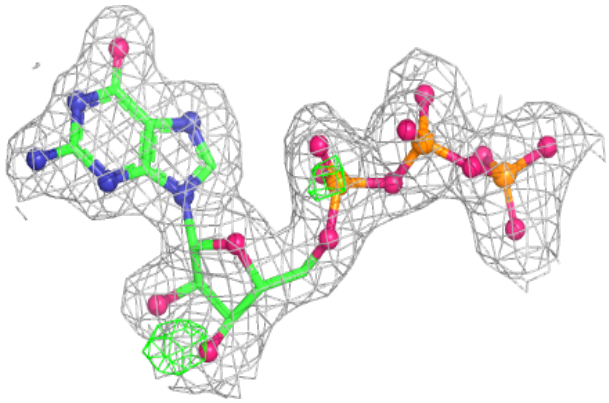
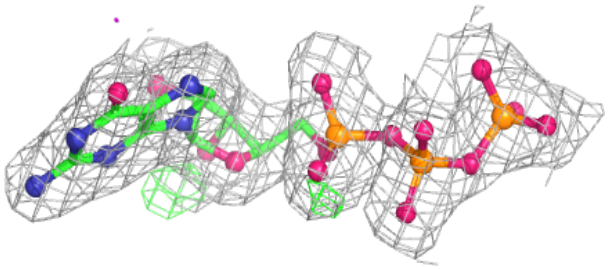
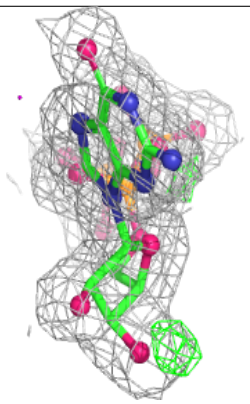
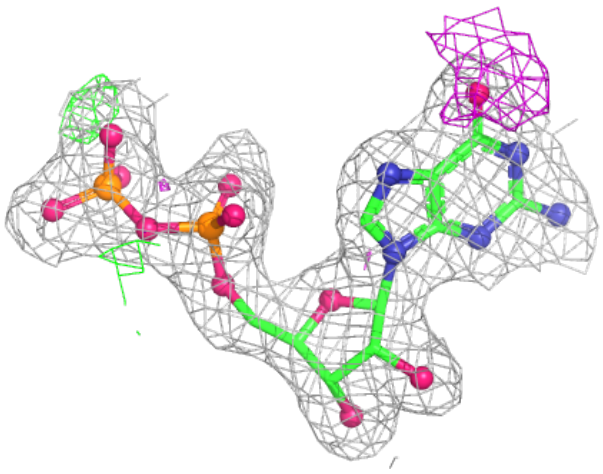
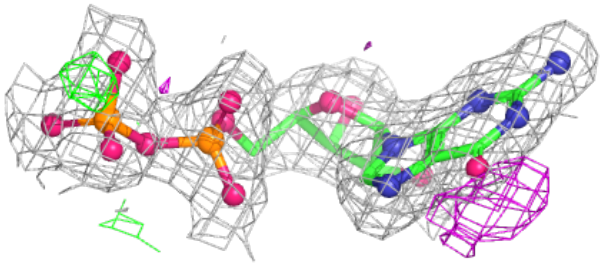
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.