wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 04:57 AM EDT

PDB ID	:	4I4T
Title	:	Crystal structure of tubulin-RB3-TTL-Zampanolide complex
Authors	:	Prota, A.E.; Steinmetz, M.O.
Deposited on	:	2012-11-28
Resolution	:	1.80 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:

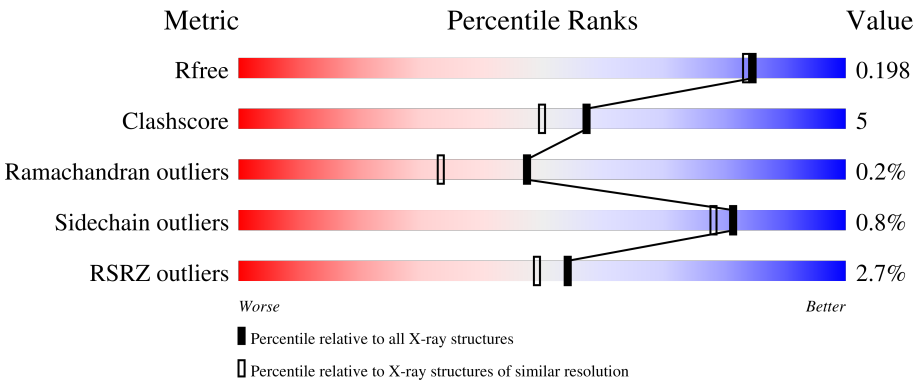
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	450	2%, 89%, 10%, •
1	C	450	87%, 10%, •
2	B	445	.%, 82%, 12%, 6%
2	D	445	2%, 88%, 9%, •
3	E	143	.%, 77%, 9%, 14%

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Mol	Chain	Length	Quality of chain
4	F	384	8% 84% 9% 7%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 37713 atoms, of which 17968 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	H	N	O	S			
1	A	447	7106	2266	3537	599	679	25	0	17	0
1	C	440	7045	2249	3503	588	678	27	0	24	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	420	6753	2149	3350	569	656	29	0	22	0
2	D	431	6752	2151	3330	580	662	29	0	8	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	123	2131	649	1082	188	206	6	0	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

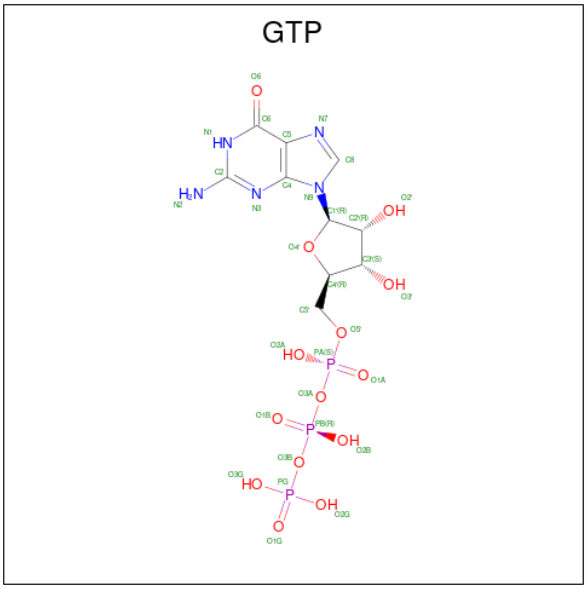
- Molecule 4 is a protein called Tubulin Tyrosine ligase, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	357	5964	1914	2991	508	536	15	0	11	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	H	N	O	P		
5	A	1	42	10	10	5	14	3	0	0
			Total	C	H	N	O	P		
5	C	1	42	10	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	2	2	2	0	0

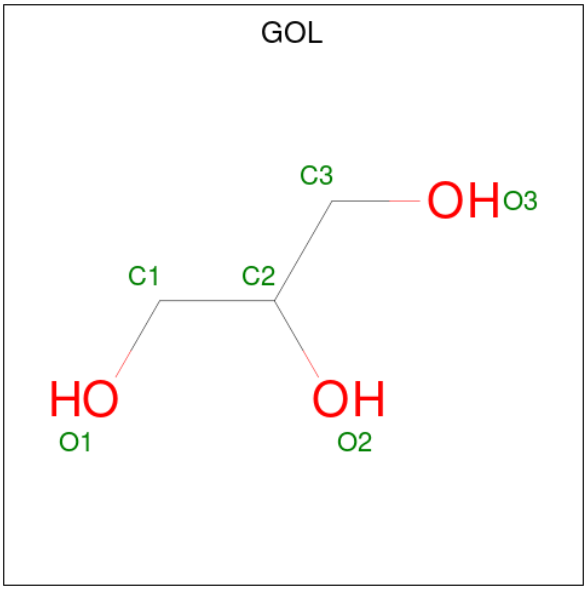
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	A	1	14	3	8	3	0	0
			Total	C	H	O		
9	A	1	14	3	8	3	0	0

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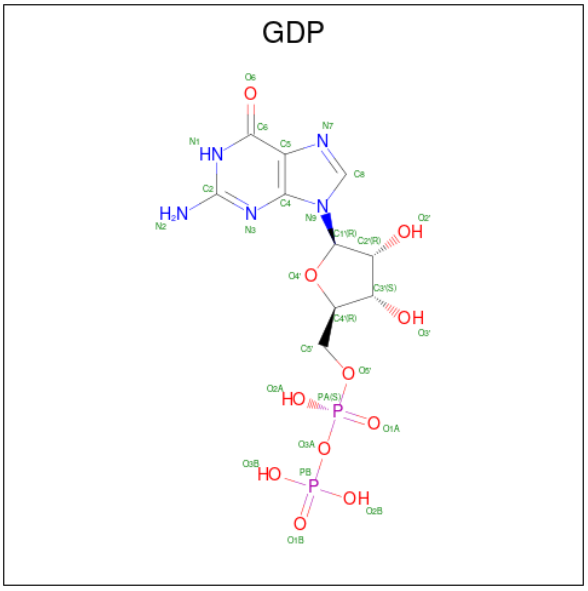
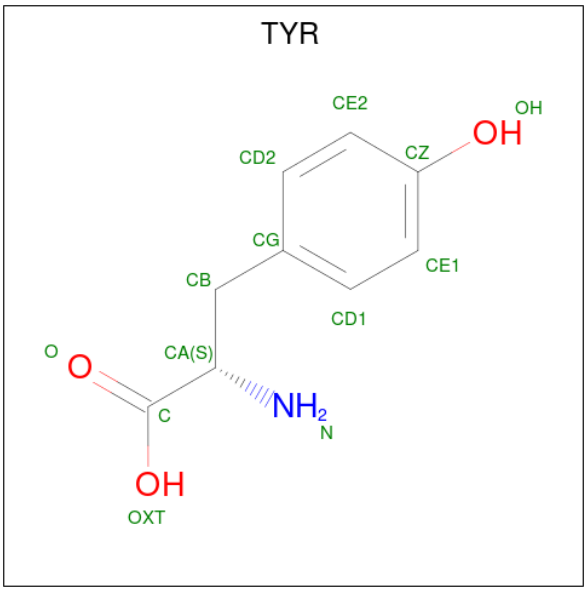
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	A	1	14	3	8	3	0	0
			Total	C	H	O		
9	B	1	14	3	8	3	0	0
			Total	C	H	O		
9	B	1	14	3	8	3	0	0
			Total	C	H	O		
9	F	1	14	3	8	3	0	0
			Total	C	H	O		
9	F	1	14	3	8	3	0	0

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



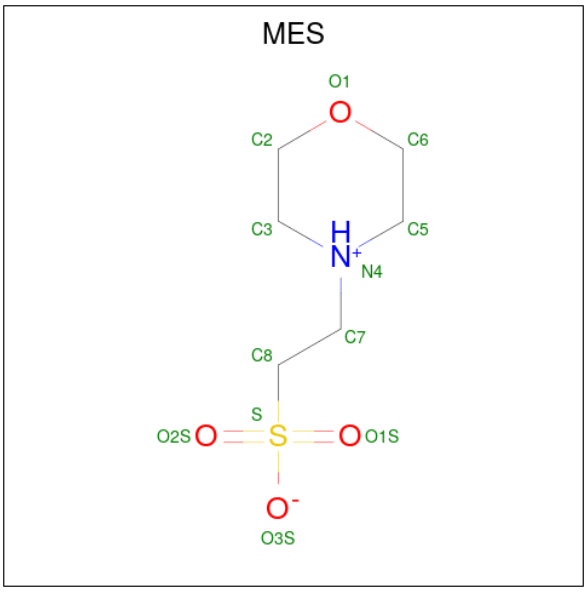
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
10	B	1	38	10	10	5	11	2	0	0
			Total	C	H	N	O	P		
10	D	1	38	10	10	5	11	2	0	0

- Molecule 11 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
11	B	1	24	9	11	1	3	0	0

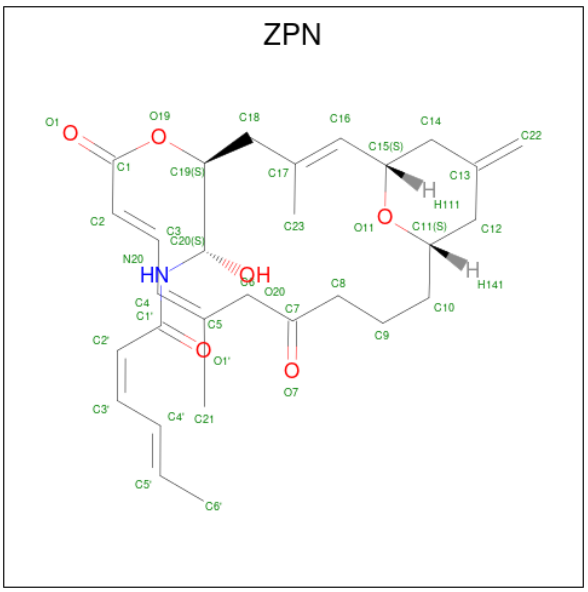
- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
12	B	1	25	6	13	1	4	1	0	0

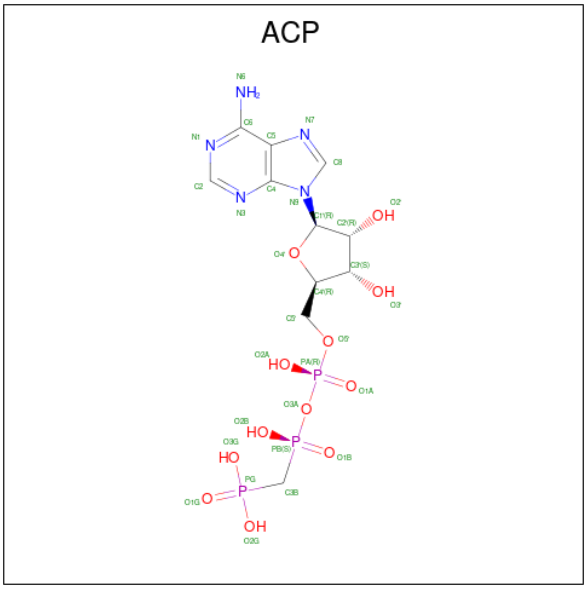
- Molecule 13 is (2Z,4E)-N-[(S)-[(1S,2E,5S,8E,10Z,17S)-3,11-dimethyl-19-methylidene-7,13-dioxo-6,21-dioxabicyclo[15.3.1]henicosa-2,8,10-trien-5-yl](hydroxy)methyl]hexa-2,4-dienamide

(three-letter code: ZPN) (formula: $C_{29}H_{39}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
13	D	1	74	29	38	1	6	0	0

- Molecule 14 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	H	N	O	P		
14	F	1	48	11	17	5	12	3	0	0

- Molecule 15 is water.

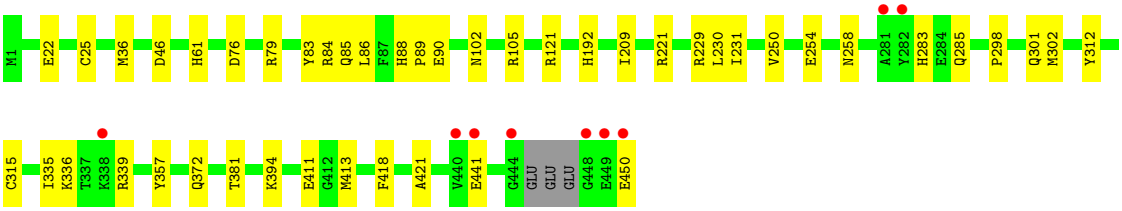
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	316	Total O 316 316	0	0
15	B	235	Total O 235 235	0	0
15	C	417	Total O 417 417	0	0
15	D	265	Total O 265 265	0	0
15	E	81	Total O 81 81	0	0
15	F	208	Total O 208 208	0	0

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.

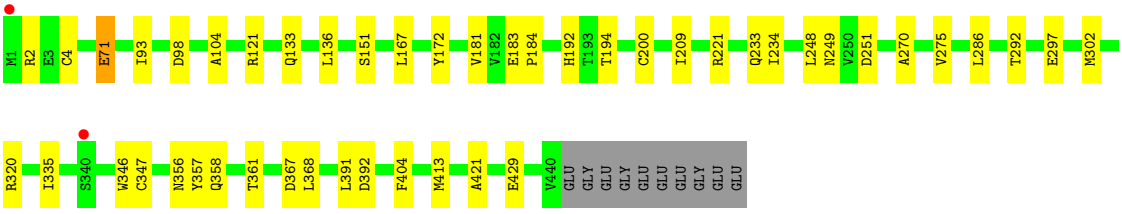
• Molecule 1: Tubulin alpha-1B chain

Chain A:



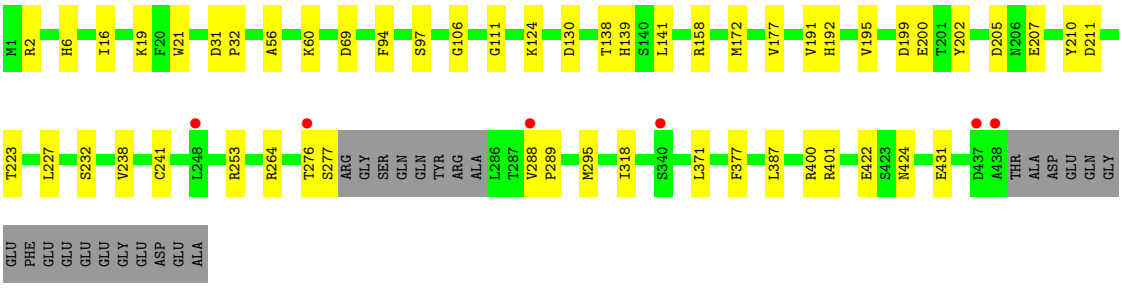
• Molecule 1: Tubulin alpha-1B chain

Chain C:



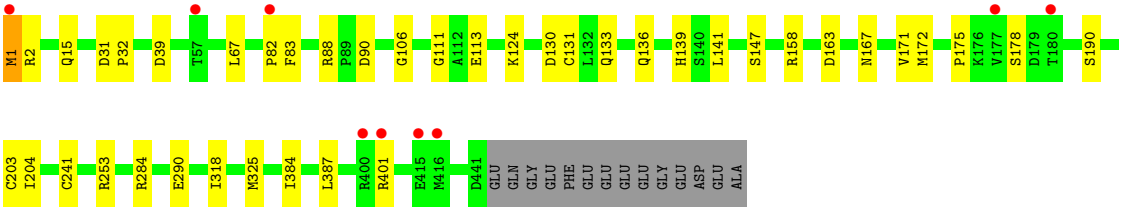
• Molecule 2: Tubulin beta-2B chain

Chain B:



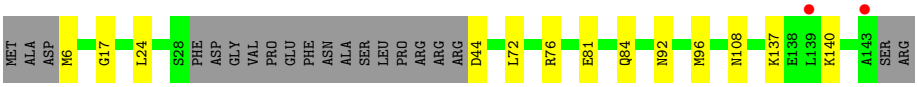
• Molecule 2: Tubulin beta-2B chain

Chain D:



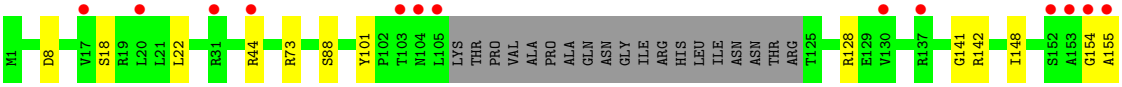
- Molecule 3: Stathmin-4

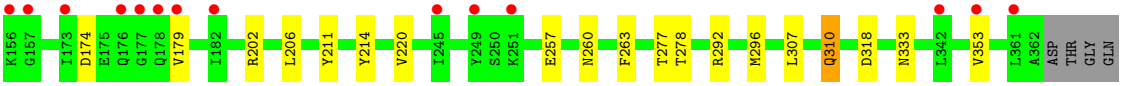
Chain E:

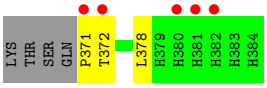


- Molecule 4: Tubulin Tyrosine ligase, TTL

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	104.77Å 158.64Å 179.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.32 – 1.80 79.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (79.32-1.80) 99.8 (79.32-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.171 , 0.204 0.165 , 0.198	Depositor DCC
R_{free} test set	13945 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	37713	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: GOL, ACP, CL, CA, MG, ZPN, GTP, GDP, 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	0/3698	0.57	0/5015
1	C	0.49	0/3695	0.60	0/5020
2	B	0.44	0/3549	0.56	0/4805
2	D	0.36	0/3521	0.52	0/4771
3	E	0.39	0/1079	0.47	0/1433
4	F	0.38	0/3076	0.52	0/4157
All	All	0.42	0/18618	0.55	0/25201

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	3569	3537	3524	44	0
1	C	3542	3503	3480	32	0
2	B	3403	3350	3330	40	0
2	D	3422	3330	3321	27	0
3	E	1049	1082	1077	10	0
4	F	2973	2991	2978	32	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	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	2	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	1	0	0	0	0
9	A	18	24	24	2	0
9	B	12	16	16	1	0
9	F	12	16	16	1	0
10	B	28	10	12	0	0
10	D	28	10	12	0	0
11	B	13	11	8	0	0
12	B	12	13	13	4	0
13	D	36	38	38	2	0
14	F	31	17	14	1	0
15	A	316	0	0	9	0
15	B	235	0	0	9	0
15	C	417	0	0	6	0
15	D	265	0	0	6	0
15	E	81	0	0	2	0
15	F	208	0	0	2	0
All	All	19745	17968	17887	178	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 5.

The worst 5 of 178 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.07	0.94
2:D:241[B]:CYS:SG	15:D:792:HOH:O	2.30	0.89
2:B:241[B]:CYS:SG	15:B:768:HOH:O	2.31	0.88
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.21	0.81
2:B:253[A]:ARG:NH1	12:B:507:MES:O2S	2.17	0.77

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	460/450 (102%)	448 (97%)	12 (3%)	0	100	100
1	C	462/450 (103%)	448 (97%)	13 (3%)	1 (0%)	47	33
2	B	438/445 (98%)	432 (99%)	6 (1%)	0	100	100
2	D	437/445 (98%)	429 (98%)	8 (2%)	0	100	100
3	E	126/143 (88%)	126 (100%)	0	0	100	100
4	F	362/384 (94%)	352 (97%)	7 (2%)	3 (1%)	19	7
All	All	2285/2317 (99%)	2235 (98%)	46 (2%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ARG
4	F	155	ALA
4	F	88	SER
4	F	154	GLY

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	392/378 (104%)	390 (100%)	2 (0%)	88	87
1	C	395/378 (104%)	393 (100%)	2 (0%)	88	87
2	B	386/383 (101%)	383 (99%)	3 (1%)	81	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	380/383 (99%)	375 (99%)	5 (1%)	69	62
3	E	117/127 (92%)	117 (100%)	0	100	100
4	F	330/342 (96%)	327 (99%)	3 (1%)	78	75
All	All	2000/1991 (100%)	1985 (99%)	15 (1%)	81	78

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

Mol	Chain	Res	Type
2	D	1	MET
4	F	307	LEU
2	D	39	ASP
4	F	310	GLN
2	D	401	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
4	F	333	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 26 ligands modelled in this entry, 11 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.21	2 (7%)	32,54,54	1.14	3 (9%)
9	GOL	F	705	-	5,5,5	0.39	0	5,5,5	0.19	0
12	MES	B	507	-	12,12,12	2.36	1 (8%)	14,16,16	1.19	1 (7%)
9	GOL	A	506	-	5,5,5	0.13	0	5,5,5	0.48	0
9	GOL	B	504	-	5,5,5	0.47	0	5,5,5	0.71	0
10	GDP	B	501	6	24,30,30	1.21	2 (8%)	30,47,47	1.25	3 (10%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.16	2 (6%)
11	TYR	B	506	-	12,13,13	0.69	1 (8%)	16,17,17	0.91	2 (12%)
9	GOL	B	505	-	5,5,5	0.31	0	5,5,5	0.54	0
9	GOL	A	508	-	5,5,5	0.36	0	5,5,5	0.49	0
13	ZPN	D	503	2	36,37,37	0.81	1 (2%)	35,48,48	1.61	5 (14%)
10	GDP	D	501	6	24,30,30	1.17	1 (4%)	30,47,47	1.06	2 (6%)
14	ACP	F	703	6	27,33,33	1.12	2 (7%)	32,52,52	1.65	7 (21%)
9	GOL	F	704	-	5,5,5	0.36	0	5,5,5	0.28	0
9	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.25	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
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
9	GOL	F	705	-	-	2/4/4/4	-
12	MES	B	507	-	-	5/6/14/14	0/1/1/1
9	GOL	A	506	-	-	2/4/4/4	-
9	GOL	B	504	-	-	4/4/4/4	-
10	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
11	TYR	B	506	-	-	4/8/8/8	0/1/1/1
9	GOL	B	505	-	-	2/4/4/4	-
9	GOL	A	508	-	-	2/4/4/4	-
13	ZPN	D	503	2	-	6/41/53/53	0/1/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GDP	D	501	6	-	3/12/32/32	0/3/3/3
14	ACP	F	703	6	-	2/15/38/38	0/3/3/3
9	GOL	F	704	-	-	1/4/4/4	-
9	GOL	A	507	-	-	2/4/4/4	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	507	MES	C8-S	-8.00	1.66	1.77
5	C	501	GTP	C5-C6	-3.89	1.39	1.47
10	B	501	GDP	O4'-C1'	3.88	1.46	1.41
5	A	501	GTP	C6-N1	-3.11	1.33	1.37
13	D	503	ZPN	C20-N20	3.05	1.47	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	503	ZPN	O19-C19-C18	5.96	122.19	107.05
14	F	703	ACP	PB-O3A-PA	-4.07	119.65	132.56
14	F	703	ACP	N3-C2-N1	-3.90	122.58	128.68
13	D	503	ZPN	O1'-C1'-N20	-3.10	118.26	122.35
5	C	501	GTP	C8-N7-C5	3.06	108.81	102.99

There are no chirality outliers.

5 of 51 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	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	507	MES	4	0
9	A	506	GOL	2	0
9	B	505	GOL	1	0

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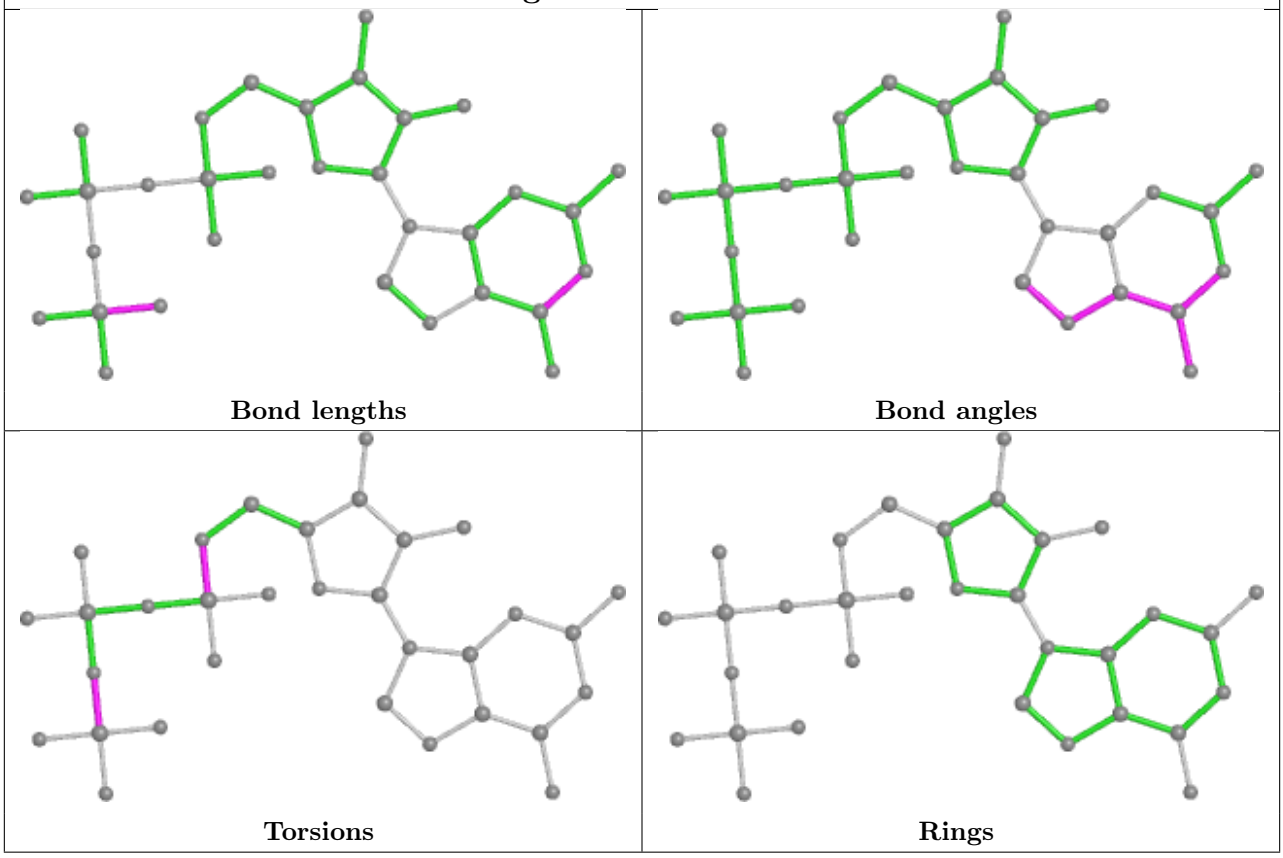
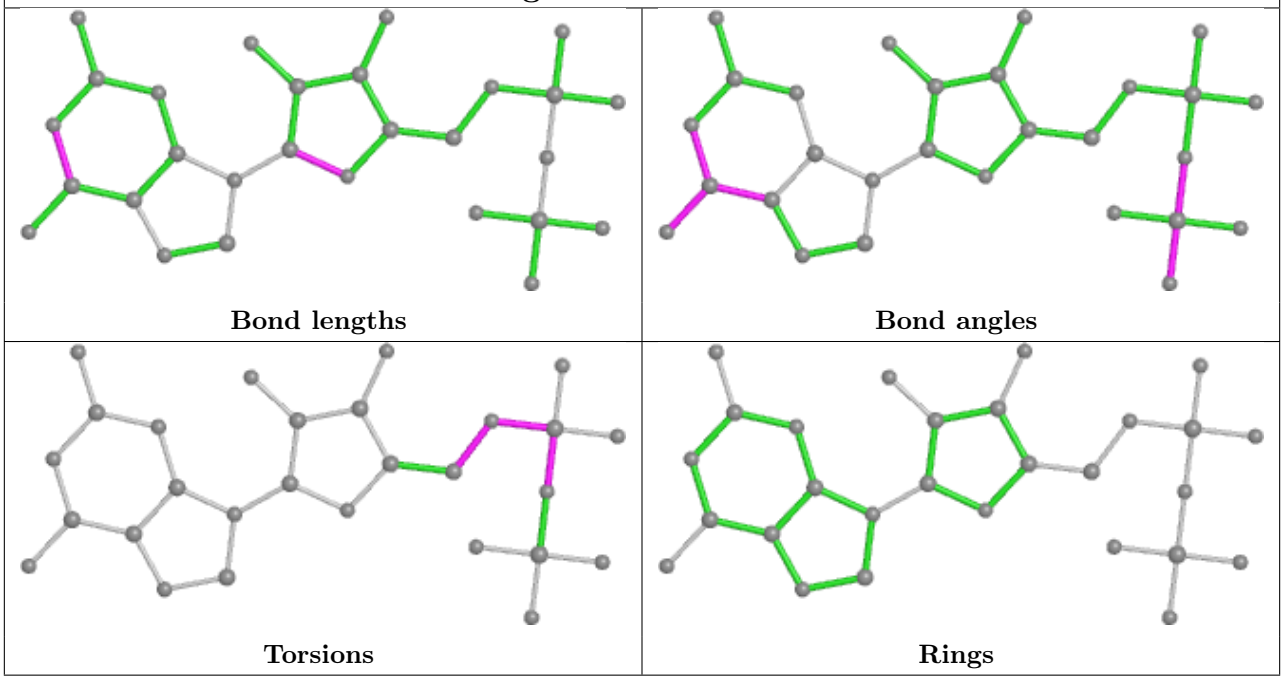
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	503	ZPN	2	0
14	F	703	ACP	1	0
9	F	704	GOL	1	0

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.

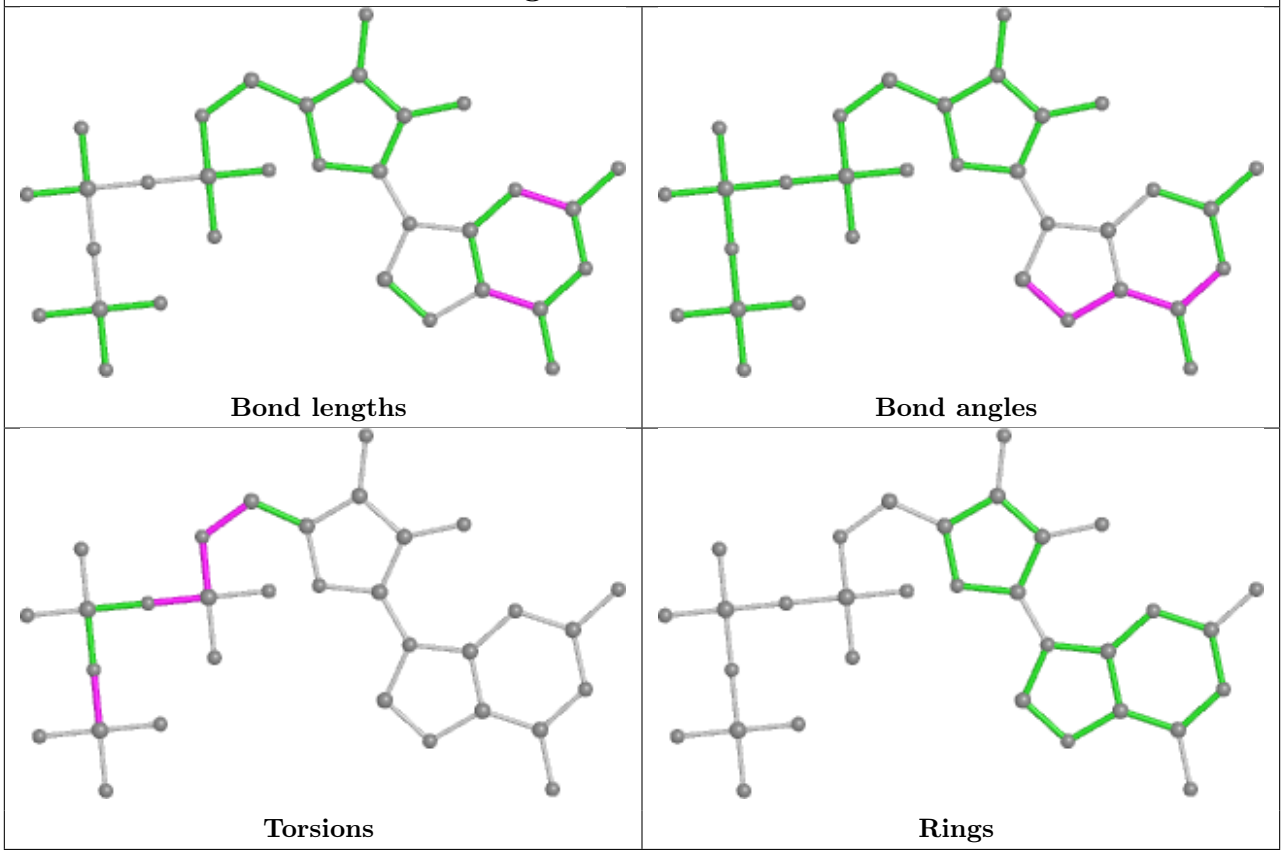
Ligand GTP A 501



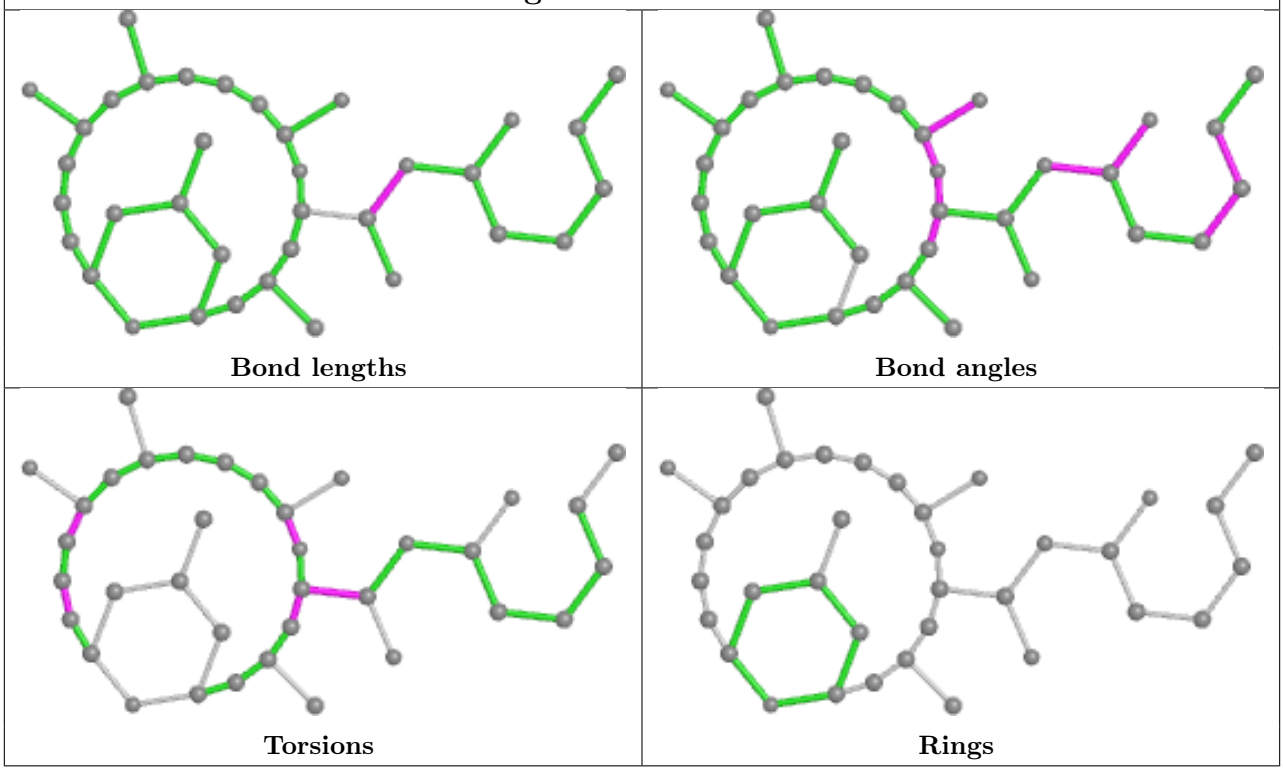
Ligand GDP B 501



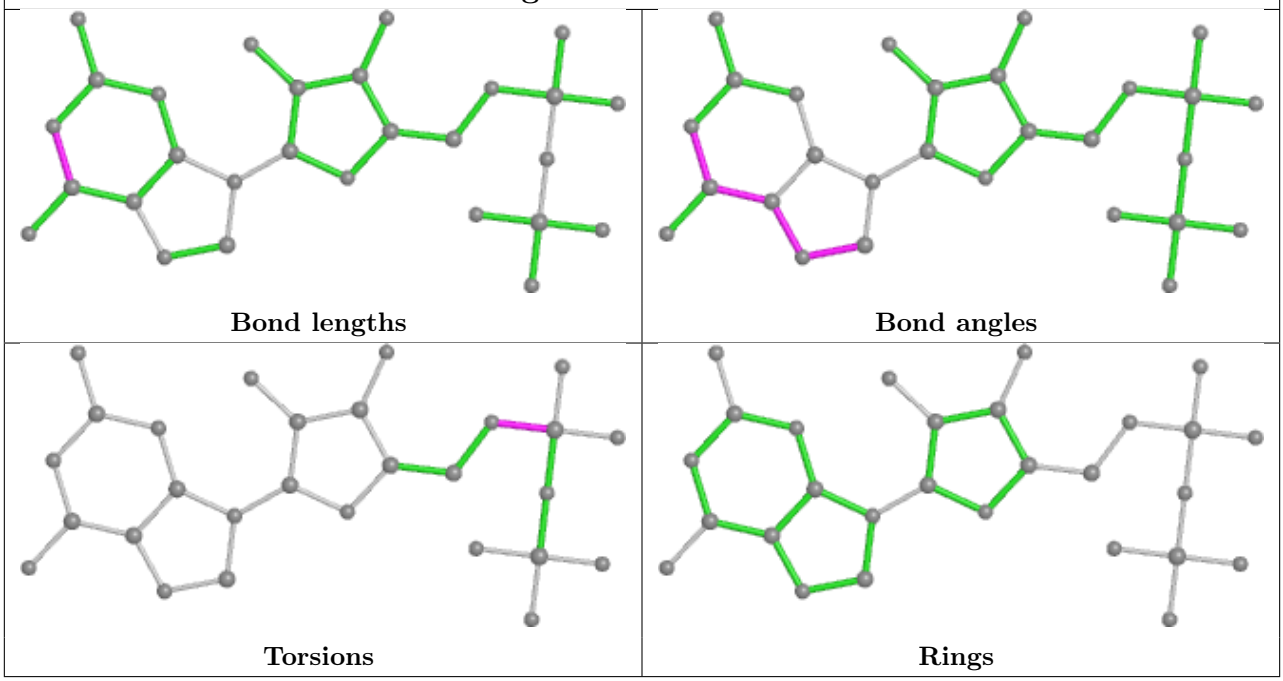
Ligand GTP C 501



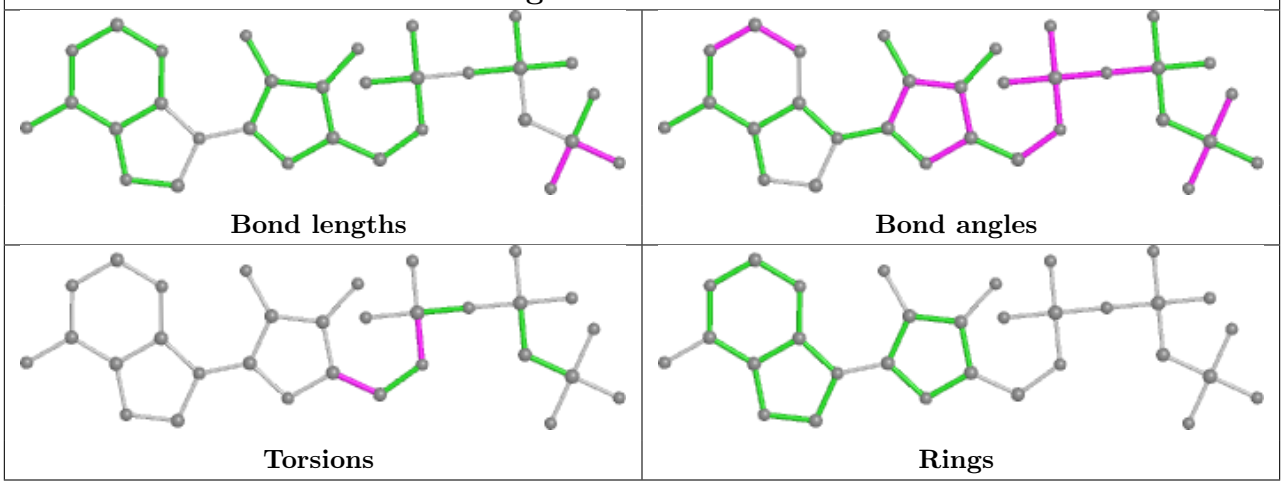
Ligand ZPN D 503



Ligand GDP D 501



Ligand ACP F 703



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	447/450 (99%)	-0.05	9 (2%)	65	61	24, 38, 69, 134	0
1	C	440/450 (97%)	0.16	2 (0%)	91	89	20, 30, 53, 84	0
2	B	420/445 (94%)	0.11	6 (1%)	75	72	23, 40, 72, 106	2 (0%)
2	D	431/445 (96%)	-0.06	9 (2%)	63	59	24, 40, 71, 105	6 (1%)
3	E	123/143 (86%)	0.19	2 (1%)	72	68	27, 52, 89, 112	0
4	F	357/384 (92%)	0.44	32 (8%)	9	7	28, 51, 100, 117	0
All	All	2218/2317 (95%)	0.11	60 (2%)	54	49	20, 40, 77, 134	8 (0%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	6.1
1	A	448	GLY	6.0
4	F	155	ALA	5.4
4	F	372	THR	5.2
2	B	276	THR	5.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

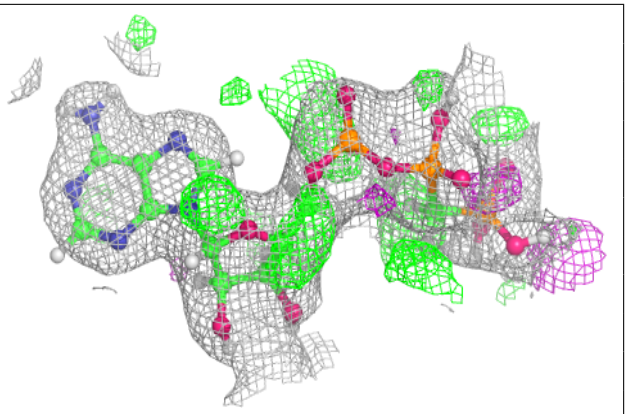
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

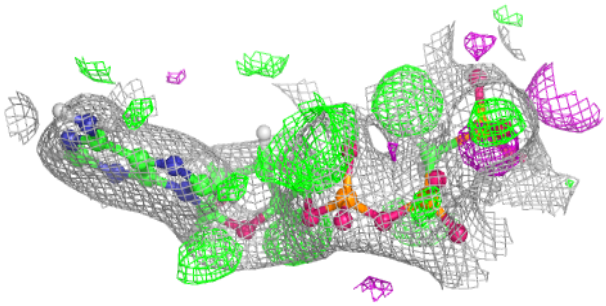
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GOL	F	705	6/6	0.71	0.22	55,84,101,116	0
11	TYR	B	506	13/13	0.81	0.23	72,94,112,113	0
6	MG	F	701	1/1	0.84	0.21	68,68,68,68	0
7	CA	B	503	1/1	0.85	0.15	76,76,76,76	0
9	GOL	B	505	6/6	0.85	0.24	55,85,113,120	0
9	GOL	F	704	6/6	0.86	0.23	50,87,105,109	0
6	MG	D	502	1/1	0.88	0.18	62,62,62,62	0
14	ACP	F	703	31/31	0.90	0.12	42,56,93,104	0
9	GOL	A	508	6/6	0.91	0.13	37,58,70,70	0
9	GOL	A	506	6/6	0.92	0.10	29,65,85,87	0
9	GOL	B	504	6/6	0.93	0.15	45,63,96,111	0
7	CA	A	505	1/1	0.93	0.13	80,80,80,80	0
8	CL	A	504	1/1	0.93	0.15	56,56,56,56	0
12	MES	B	507	12/12	0.94	0.12	35,51,67,72	0
6	MG	F	702	1/1	0.94	0.08	38,38,38,38	0
13	ZPN	D	503	36/36	0.95	0.10	29,39,73,81	0
9	GOL	A	507	6/6	0.96	0.15	53,107,124,134	0
7	CA	A	503	1/1	0.97	0.14	44,44,44,44	0
10	GDP	D	501	28/28	0.97	0.09	33,37,46,49	0
10	GDP	B	501	28/28	0.98	0.14	22,27,36,37	0
5	GTP	A	501	32/32	0.98	0.12	21,26,33,34	0
6	MG	C	502	1/1	0.99	0.17	23,23,23,23	0
7	CA	C	503	1/1	0.99	0.13	39,39,39,39	0
5	GTP	C	501	32/32	0.99	0.13	16,22,27,30	0
6	MG	A	502	1/1	0.99	0.18	27,27,27,27	0
6	MG	B	502	1/1	1.00	0.25	21,21,21,21	0

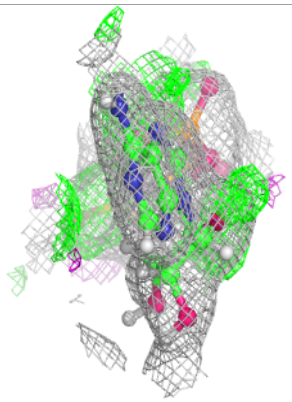
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 703:

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

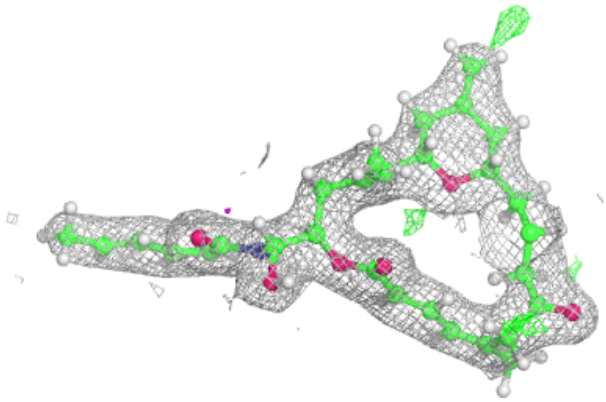


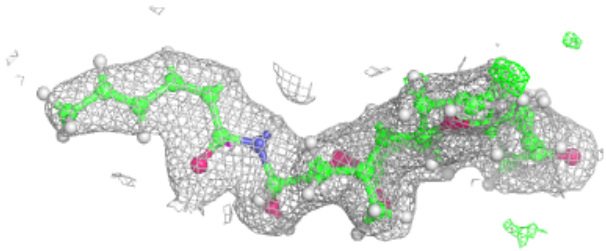


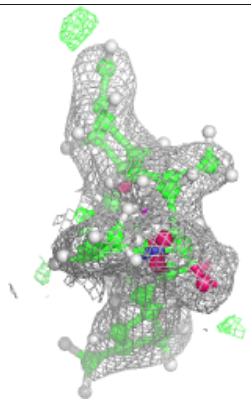


Electron density around ZPN D 503:

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

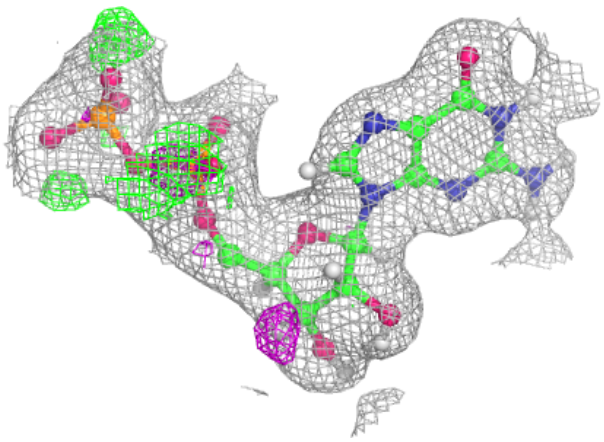


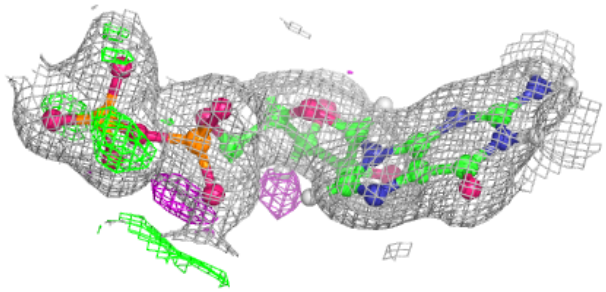


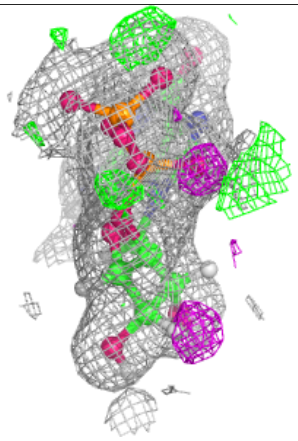


Electron density around GDP D 501:

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







Electron density around GDP B 501:

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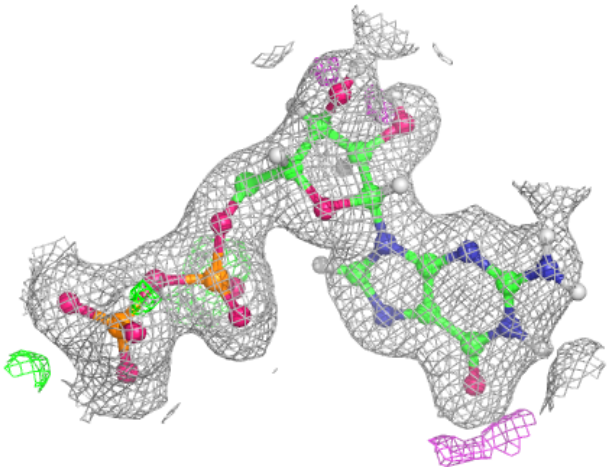
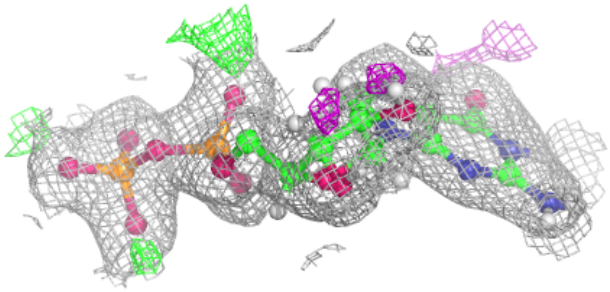
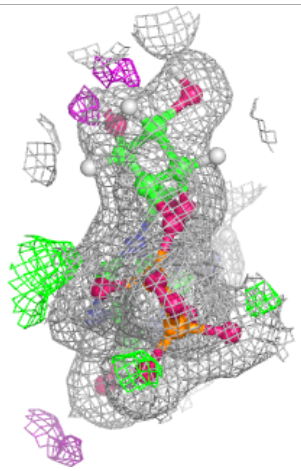
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around GTP A 501:

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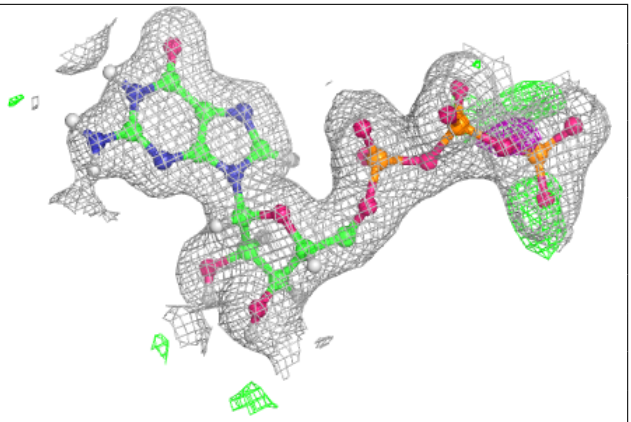
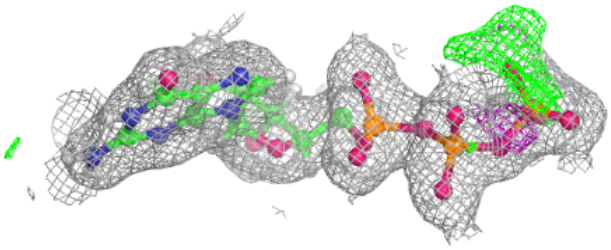
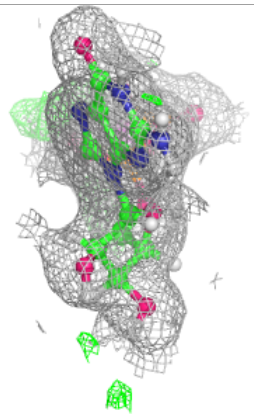
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

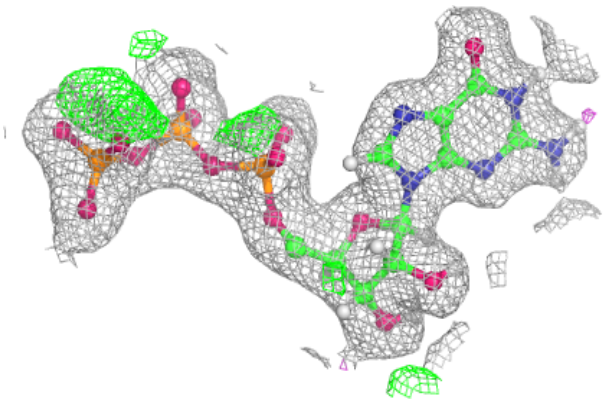


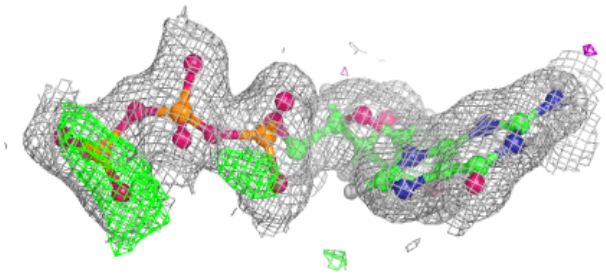


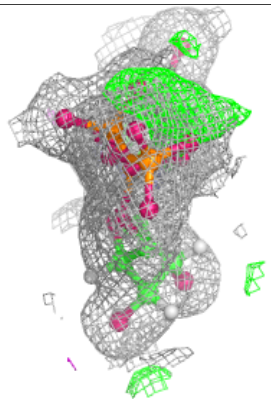


Electron density around GTP C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.