Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 12:48 AM JST

PDB ID	:	7E4Z
Title	:	Crystal structure of tubulin in complex with Maytansinol
Authors	:	Wang, Y.; Li, W.
Deposited on	:	2021-02-16
Resolution	:	2.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

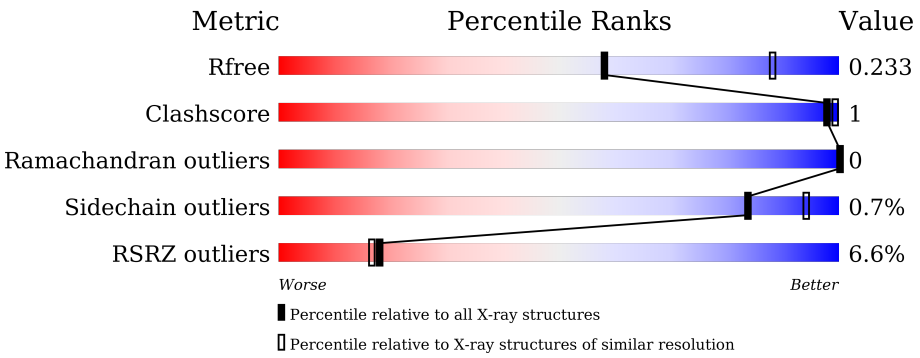
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	440	2%, 98%
1	C	440	2%, 97%
2	B	431	3%, 97%
2	D	431	7%, 95%
3	E	138	10%, 87%, 11%
4	F	384	19%, 88%, 9%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 35521 atoms, of which 17355 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	440	6869	2194	3402	589	660	24	0	6	0
1	C	440	6890	2201	3414	586	664	25	0	10	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	425	6668	2126	3286	579	650	27	0	6	0
2	D	421	6513	2085	3196	562	644	26	0	4	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	2072	632	1048	184	202	6	0	2	0

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	348	5765	1855	2879	494	521	16	0	5	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

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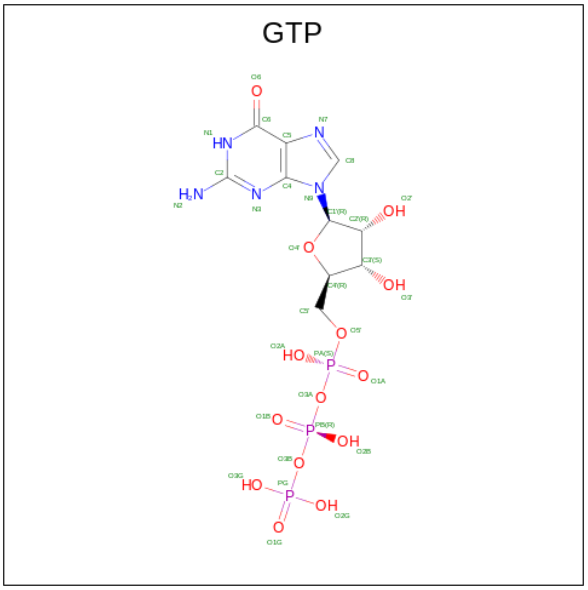
Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- 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
5	C	1	42	10	10	5	14	3	0	0
5	D	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
6	B	2	2	2	0	0
6	C	1	1	1	0	0
6	D	1	1	1	0	0

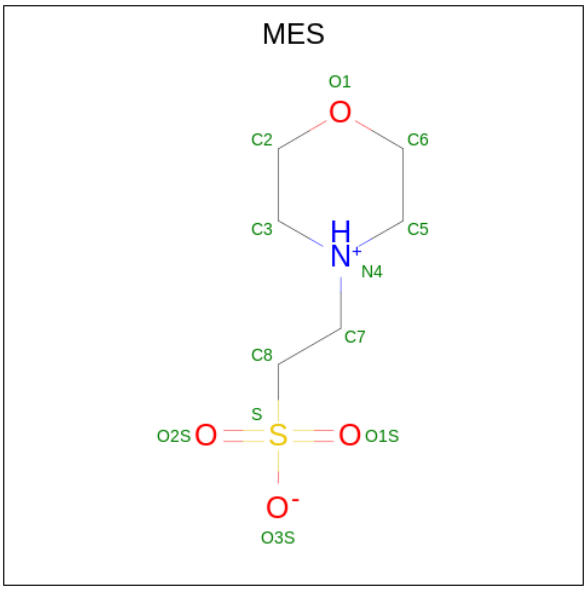
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

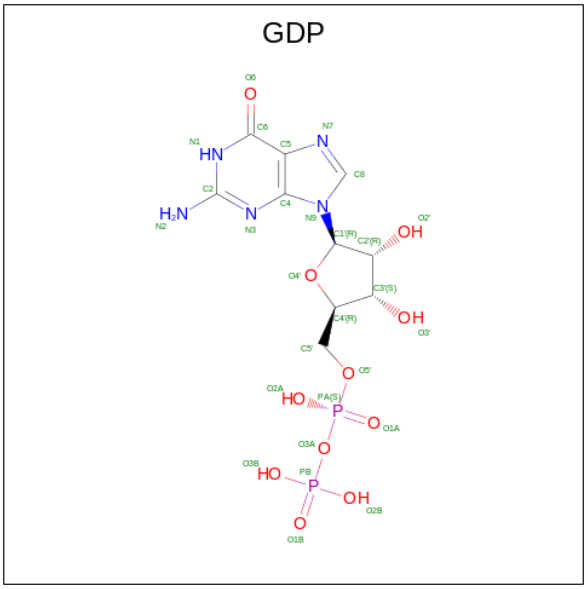
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



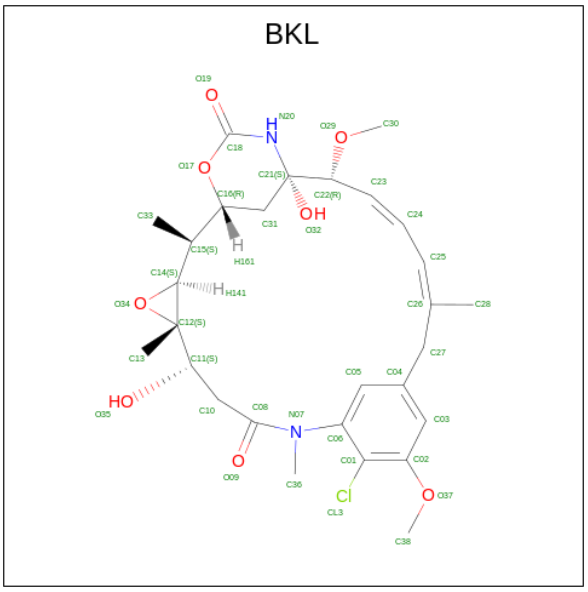
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C H N O S 25 6 13 1 4 1	0	0
9	B	1	Total C H N O S 25 6 13 1 4 1	0	0
9	B	1	Total C H N O S 25 6 13 1 4 1	0	0

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



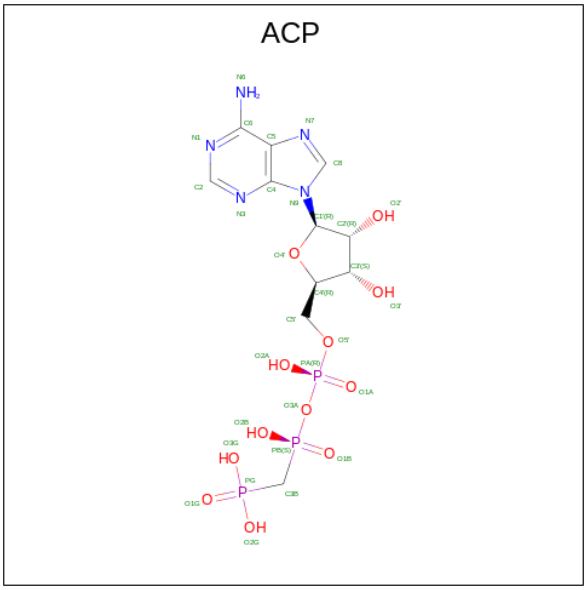
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
10	B	1	38	10	10	5	11	2	0	0

- Molecule 11 is (1R,2S,3S,5S,6S,16E,18E,20R,21S)-11-chloro-6,21-dihydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16,18-pentaene-8,23-dione (three-letter code: BKL) (formula: $C_{28}H_{37}ClN_2O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	H	N	O		
11	D	1	76	28	1	37	2	8	0	0

- 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
			Total	C	H	N	O	P		
12	F	1	45	11	14	5	12	3	0	0

- Molecule 13 is water.

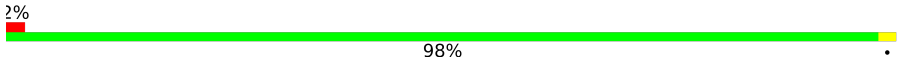
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	92	92	92	0	0
13	B	72	72	72	0	0
13	C	142	142	142	0	0
13	D	31	31	31	0	0
13	E	11	11	11	0	0
13	F	26	26	26	0	0

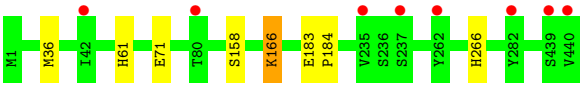
3 Residue-property plots (i)

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

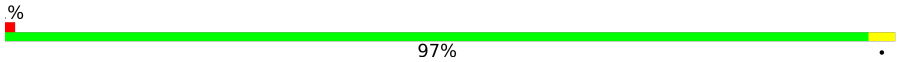
Chain A:

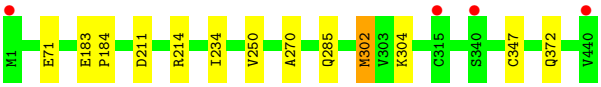




- Molecule 1: Tubulin alpha-1B chain

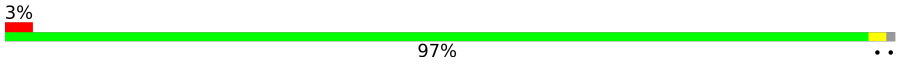
Chain C:

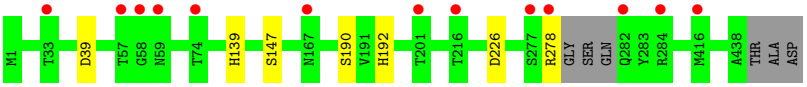




- Molecule 2: Tubulin beta-2B chain

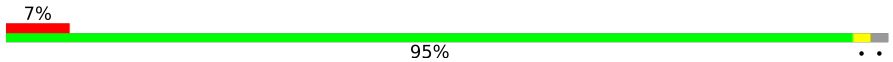
Chain B:

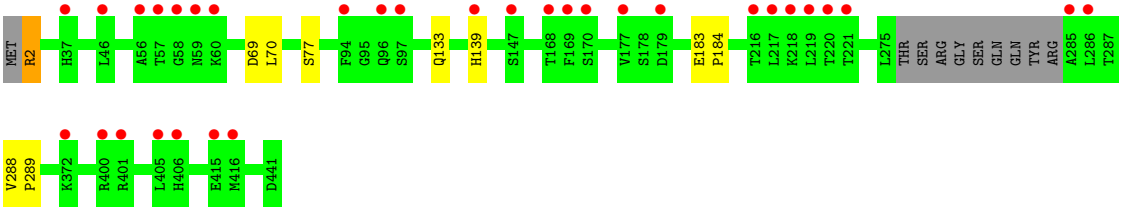




- Molecule 2: Tubulin beta-2B chain

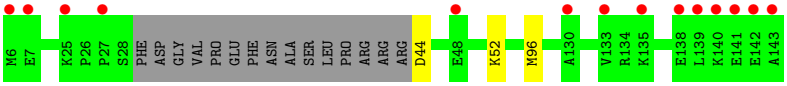
Chain D:





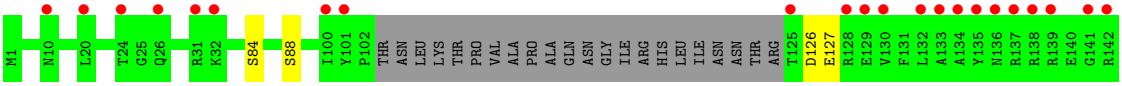
- Molecule 3: Stathmin-4

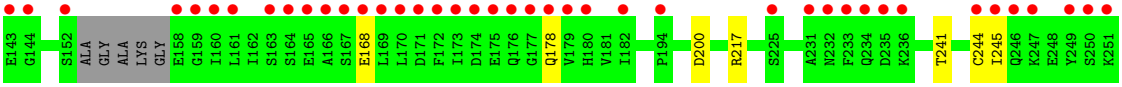
Chain E:

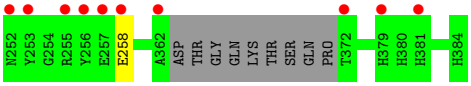


- Molecule 4: Tubulin tyrosine ligase

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	104.43Å 156.63Å 182.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.28 – 2.69 38.29 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.28-2.69) 99.5 (38.29-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.192 , 0.228 0.196 , 0.233	Depositor DCC
R_{free} test set	4059 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 45.8	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	0.94	EDS
Total number of atoms	35521	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: CA, GDP, CL, MG, BKL, ACP, GTP, 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	0.22	0/3563	0.39	0/4836
1	C	0.22	0/3581	0.39	0/4861
2	B	0.22	0/3481	0.37	0/4713
2	D	0.22	0/3401	0.38	0/4608
3	E	0.21	0/1038	0.32	0/1377
4	F	0.22	0/2969	0.39	1/4010 (0.0%)
All	All	0.22	0/18033	0.38	1/24405 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	258	GLU	C-N-CA	8.21	139.54	122.30

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	3467	3402	3390	4	0
1	C	3476	3414	3400	6	0
2	B	3382	3286	3266	3	0
2	D	3317	3196	3196	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1024	1048	1044	2	0
4	F	2886	2879	2863	6	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	12	13	13	0	0
9	B	24	26	25	0	0
10	B	28	10	12	0	0
11	D	39	37	0	0	0
12	F	31	14	14	1	0
13	A	92	0	0	0	0
13	B	72	0	0	0	0
13	C	142	0	0	1	0
13	D	31	0	0	0	0
13	E	11	0	0	2	0
13	F	26	0	0	1	0
All	All	18166	17355	17259	26	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 1.

All (26) 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)
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.12	0.67
3:E:44:ASP:N	13:E:301:HOH:O	2.32	0.63
1:C:214:ARG:NH2	13:C:603:HOH:O	2.33	0.61
4:F:168:GLU:O	13:F:501:HOH:O	2.17	0.59
2:B:226:ASP:OD1	2:B:278:ARG:NH1	2.37	0.58
4:F:126:ASP:OD2	4:F:127:GLU:N	2.38	0.57
1:A:158:SER:OG	1:A:166:LYS:NZ	2.35	0.57
3:E:52:LYS:NZ	13:E:302:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.48	0.54
1:C:211[A]:ASP:OD1	1:C:304:LYS:NZ	2.43	0.52
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.42	0.52
1:A:266:HIS:O	1:A:266:HIS:ND1	2.44	0.50
2:B:147:SER:HG	2:B:190:SER:HG	1.57	0.49
2:D:183:GLU:OE2	5:D:602:GTP:O3'	2.20	0.48
4:F:244:CYS:SG	4:F:245:ILE:N	2.88	0.47
4:F:84:SER:O	4:F:88:SER:N	2.40	0.46
4:F:200:ASP:OD2	12:F:401:ACP:O3'	2.34	0.45
2:B:39:ASP:OD1	2:B:39:ASP:N	2.50	0.45
2:D:183:GLU:N	2:D:184:PRO:CD	2.81	0.44
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.58	0.43
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.02	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.84	0.41
1:C:183:GLU:N	1:C:184:PRO:CD	2.84	0.41
2:D:2:ARG:HG3	2:D:133:GLN:CG	2.51	0.40
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.57	0.40
2:D:69:ASP:OD1	2:D:70:LEU:N	2.54	0.40

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	444/440 (101%)	430 (97%)	14 (3%)	0	100	100
1	C	447/440 (102%)	435 (97%)	12 (3%)	0	100	100
2	B	427/431 (99%)	417 (98%)	10 (2%)	0	100	100
2	D	420/431 (97%)	407 (97%)	13 (3%)	0	100	100
3	E	121/138 (88%)	119 (98%)	2 (2%)	0	100	100
4	F	345/384 (90%)	326 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2204/2264 (97%)	2134 (97%)	70 (3%)	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	377/371 (102%)	375 (100%)	2 (0%)	88	96
1	C	380/371 (102%)	375 (99%)	5 (1%)	69	87
2	B	374/372 (100%)	372 (100%)	2 (0%)	88	96
2	D	366/372 (98%)	363 (99%)	3 (1%)	81	93
3	E	112/123 (91%)	111 (99%)	1 (1%)	78	92
4	F	319/342 (93%)	317 (99%)	2 (1%)	86	95
All	All	1928/1951 (99%)	1913 (99%)	15 (1%)	84	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	166	LYS
2	B	139	HIS
2	B	192	HIS
1	C	71	GLU
1	C	250	VAL
1	C	302[A]	MET
1	C	302[B]	MET
1	C	347	CYS
2	D	2	ARG
2	D	77	SER
2	D	139	HIS
3	E	96	MET
4	F	178	GLN

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Mol	Chain	Res	Type
4	F	217	ARG

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

Mol	Chain	Res	Type
1	A	309	HIS
3	E	18	GLN
4	F	209	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.45	7 (21%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.50	7 (21%)
5	GTP	D	602	6	26,34,34	1.10	2 (7%)	32,54,54	1.62	6 (18%)
12	ACP	F	401	-	27,33,33	4.30	7 (25%)	32,52,52	1.65	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	BKL	D	603	-	40,42,42	1.66	5 (12%)	44,64,64	2.14	8 (18%)
9	MES	A	505	-	12,12,12	2.28	1 (8%)	14,16,16	1.43	3 (21%)
9	MES	B	504	-	12,12,12	2.25	1 (8%)	14,16,16	1.82	4 (28%)
10	GDP	B	501	6	24,30,30	0.98	1 (4%)	30,47,47	1.18	4 (13%)
9	MES	B	505	-	12,12,12	2.27	1 (8%)	14,16,16	1.78	6 (42%)

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	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
5	GTP	D	602	6	-	0/18/38/38	0/3/3/3
12	ACP	F	401	-	-	5/15/38/38	0/3/3/3
11	BKL	D	603	-	-	17/41/68/68	0/2/4/4
9	MES	A	505	-	-	3/6/14/14	0/1/1/1
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	GDP	B	501	6	-	4/12/32/32	0/3/3/3
9	MES	B	505	-	-	2/6/14/14	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PB-O3A	19.56	1.80	1.58
9	A	505	MES	C8-S	-7.66	1.66	1.77
9	B	505	MES	C8-S	-7.61	1.66	1.77
9	B	504	MES	C8-S	-7.56	1.66	1.77
12	F	401	ACP	PA-O5'	7.28	1.88	1.59
11	D	603	BKL	C12-C14	5.13	1.53	1.47
11	D	603	BKL	C08-N07	4.43	1.44	1.35
5	C	501	GTP	C5-C6	-4.02	1.39	1.47
5	A	501	GTP	C5-C6	-3.96	1.39	1.47
5	D	602	GTP	C5-C6	-3.95	1.39	1.47
12	F	401	ACP	C5'-C4'	3.64	1.63	1.51
11	D	603	BKL	O34-C12	-3.59	1.41	1.45
11	D	603	BKL	O17-C16	-3.15	1.42	1.46
12	F	401	ACP	O5'-C5'	-3.10	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	501	GDP	C6-N1	-2.74	1.33	1.37
12	F	401	ACP	C2-N1	2.74	1.39	1.33
11	D	603	BKL	C10-C11	2.62	1.56	1.53
12	F	401	ACP	C4-N3	2.57	1.39	1.35
5	C	501	GTP	C2-N3	2.21	1.38	1.33
12	F	401	ACP	C2-N3	2.20	1.35	1.32
5	A	501	GTP	C2-N3	2.19	1.38	1.33
5	D	602	GTP	C2-N3	2.11	1.38	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	603	BKL	C12-O34-C14	7.34	65.20	60.79
11	D	603	BKL	O37-C02-C01	4.98	121.43	115.53
11	D	603	BKL	O34-C14-C12	-4.37	56.72	59.83
11	D	603	BKL	C01-C06-N07	4.34	125.16	120.71
12	F	401	ACP	O1B-PB-C3B	4.03	119.73	109.07
11	D	603	BKL	O37-C02-C03	-3.99	117.25	124.12
5	D	602	GTP	PB-O3B-PG	-3.93	119.35	132.83
11	D	603	BKL	C05-C06-C01	-3.86	117.61	122.53
12	F	401	ACP	O5'-PA-O1A	-3.84	94.05	109.07
9	B	504	MES	O3S-S-C8	3.67	111.70	105.77
11	D	603	BKL	O35-C11-C12	-3.64	104.82	110.33
5	D	602	GTP	PA-O3A-PB	-3.60	120.46	132.83
12	F	401	ACP	PB-O3A-PA	-3.22	122.36	132.56
5	C	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
5	D	602	GTP	C5-C6-N1	3.20	119.60	113.95
5	A	501	GTP	C5-C6-N1	3.17	119.56	113.95
5	C	501	GTP	C5-C6-N1	3.17	119.54	113.95
9	B	505	MES	C5-N4-C3	3.11	115.82	108.83
10	B	501	GDP	PA-O3A-PB	-3.10	122.20	132.83
5	D	602	GTP	C8-N7-C5	3.09	108.88	102.99
5	C	501	GTP	C8-N7-C5	3.04	108.79	102.99
9	B	504	MES	C2-C3-N4	-3.04	105.49	110.10
5	A	501	GTP	C8-N7-C5	3.02	108.73	102.99
5	C	501	GTP	PB-O3B-PG	-2.99	122.55	132.83
9	B	505	MES	C2-C3-N4	-2.90	105.71	110.10
5	A	501	GTP	PA-O3A-PB	-2.86	123.02	132.83
5	A	501	GTP	C2-N1-C6	-2.79	119.96	125.10
5	C	501	GTP	C2-N1-C6	-2.77	119.99	125.10
5	D	602	GTP	C3'-C2'-C1'	2.68	105.01	100.98
9	A	505	MES	O3S-S-C8	2.68	110.10	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	602	GTP	C2-N1-C6	-2.67	120.17	125.10
5	A	501	GTP	PB-O3B-PG	-2.64	123.77	132.83
9	B	504	MES	C5-N4-C3	2.57	114.60	108.83
9	A	505	MES	C5-N4-C3	2.56	114.59	108.83
5	C	501	GTP	C3'-C2'-C1'	2.55	104.82	100.98
12	F	401	ACP	O2A-PA-O5'	-2.54	95.94	107.75
10	B	501	GDP	C3'-C2'-C1'	2.47	104.70	100.98
10	B	501	GDP	C8-N7-C5	2.39	107.54	102.99
9	B	505	MES	O3S-S-C8	2.39	109.63	105.77
10	B	501	GDP	C5-C6-N1	2.38	118.15	113.95
5	A	501	GTP	C3'-C2'-C1'	2.36	104.53	100.98
12	F	401	ACP	O1G-PG-C3B	-2.28	106.33	111.24
9	B	504	MES	C7-N4-C5	2.27	117.04	111.23
9	B	505	MES	O1S-S-C8	2.26	109.63	106.92
9	B	505	MES	O2S-S-C8	2.23	109.61	106.92
12	F	401	ACP	O2B-PB-C3B	2.18	115.49	106.58
9	A	505	MES	O2S-S-C8	2.18	109.54	106.92
11	D	603	BKL	C04-C27-C26	2.12	122.82	114.47
5	C	501	GTP	O6-C6-C5	-2.11	120.25	124.37
5	A	501	GTP	O6-C6-C5	-2.08	120.30	124.37
9	B	505	MES	C7-N4-C5	2.07	116.52	111.23
12	F	401	ACP	O3'-C3'-C4'	2.02	116.88	111.05

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
9	A	505	MES	C7-C8-S-O2S
9	A	505	MES	C7-C8-S-O3S
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
9	B	505	MES	C8-C7-N4-C5
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
11	D	603	BKL	C12-C14-C15-C16
11	D	603	BKL	O34-C14-C15-C16
11	D	603	BKL	O34-C14-C15-C33
11	D	603	BKL	C14-C15-C16-C31

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Mol	Chain	Res	Type	Atoms
11	D	603	BKL	C21-C22-C23-C24
11	D	603	BKL	O29-C22-C23-C24
11	D	603	BKL	C21-C22-O29-C30
11	D	603	BKL	C23-C24-C25-C26
11	D	603	BKL	C24-C25-C26-C28
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
12	F	401	ACP	C3'-C4'-C5'-O5'
11	D	603	BKL	C01-C02-O37-C38
11	D	603	BKL	C03-C02-O37-C38
11	D	603	BKL	C23-C22-O29-C30
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
9	A	505	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O1S
11	D	603	BKL	O35-C11-C12-C14
11	D	603	BKL	O09-C08-C10-C11
11	D	603	BKL	C33-C15-C16-C31
5	A	501	GTP	PB-O3A-PA-O2A
10	B	501	GDP	PB-O3A-PA-O2A
11	D	603	BKL	N07-C08-C10-C11
9	B	505	MES	C8-C7-N4-C3
12	F	401	ACP	PG-C3B-PB-O1B
11	D	603	BKL	C25-C26-C27-C04
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	C4'-C5'-O5'-PA

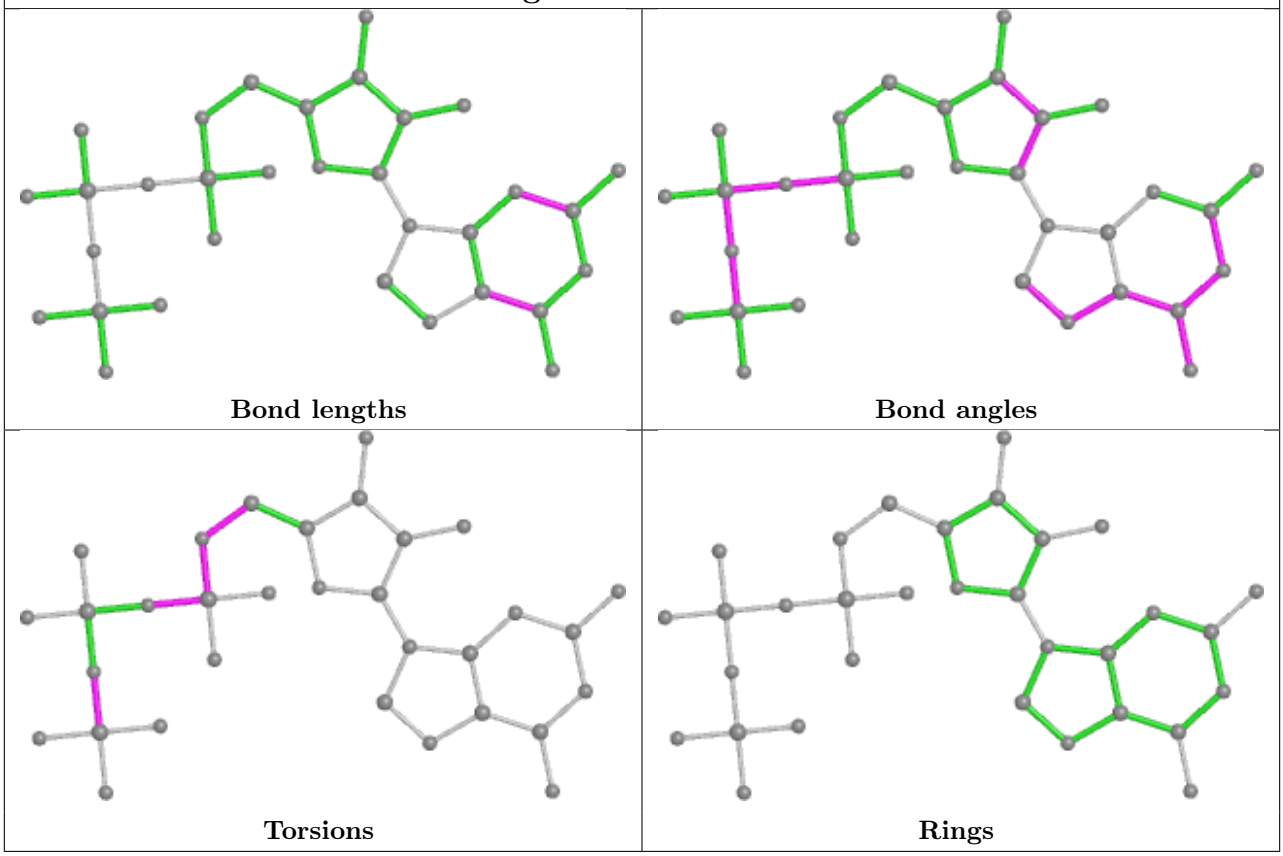
There are no ring outliers.

2 monomers are involved in 2 short contacts:

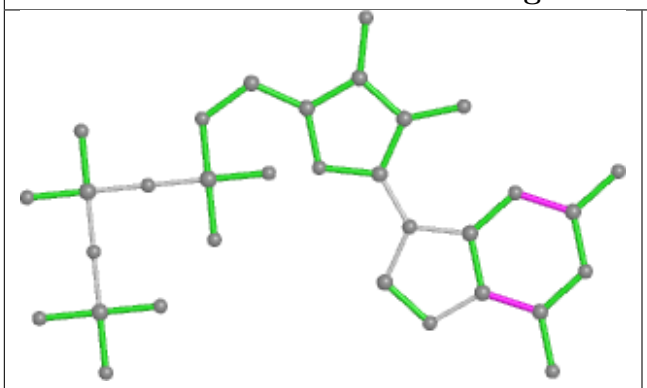
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	602	GTP	1	0
12	F	401	ACP	1	0

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.

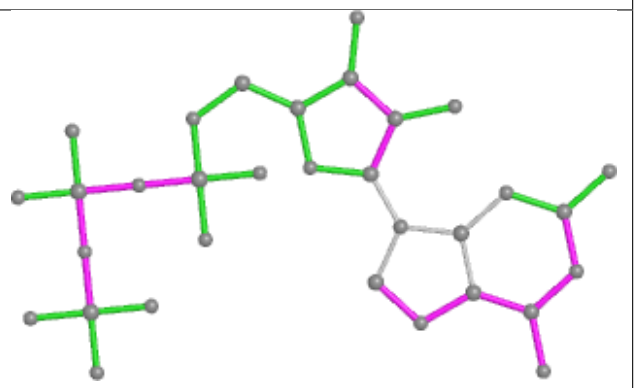
Ligand GTP A 501



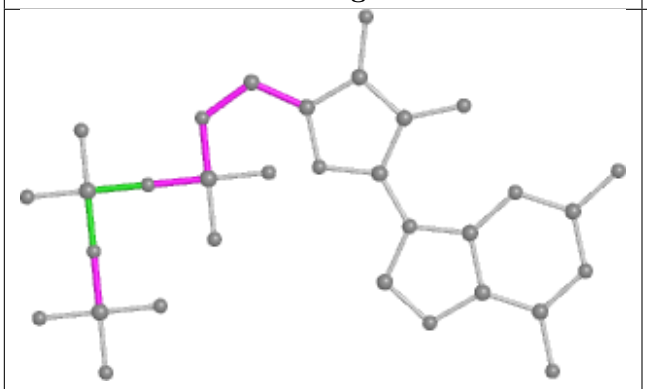
Ligand GTP C 501



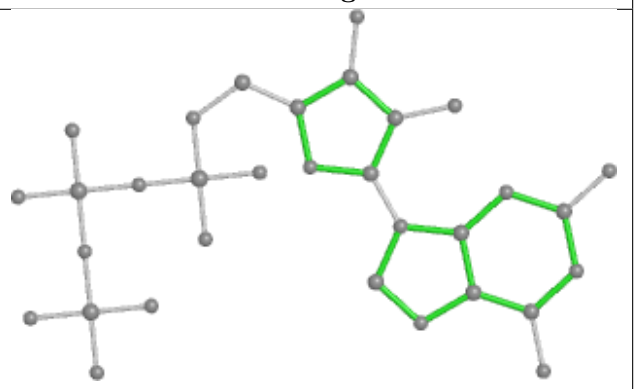
Bond lengths



Bond angles

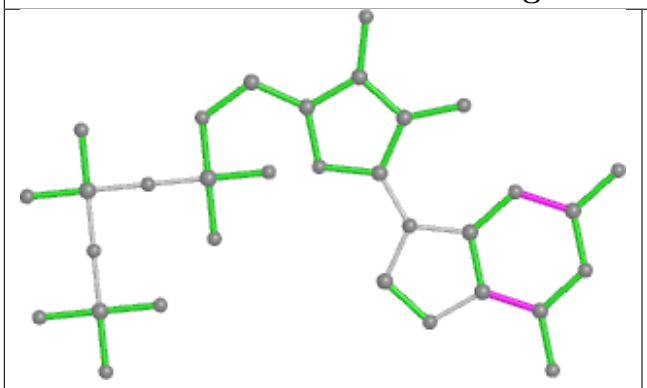


Torsions

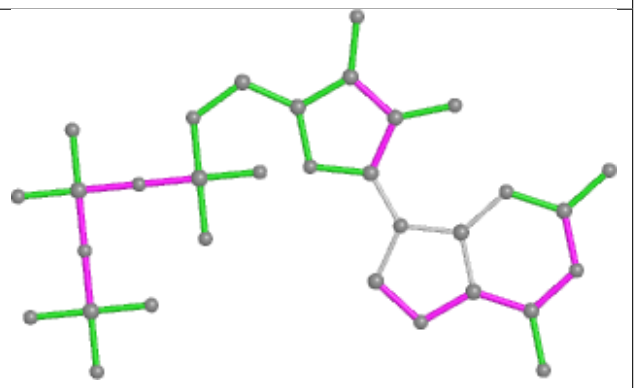


Rings

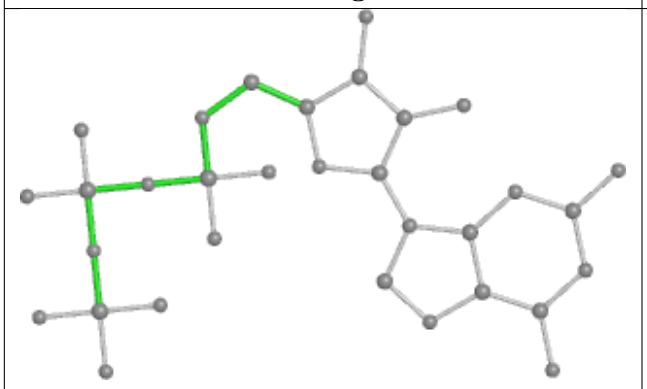
Ligand GTP D 602



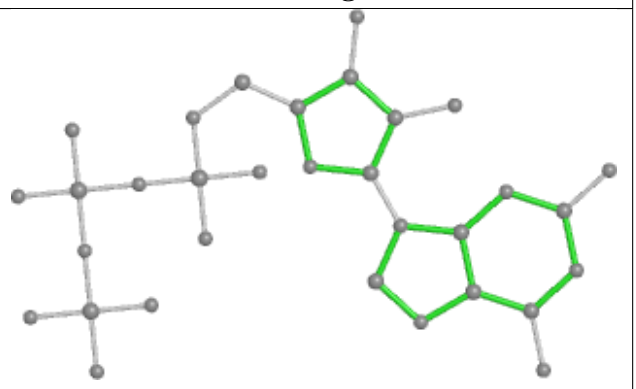
Bond lengths



Bond angles

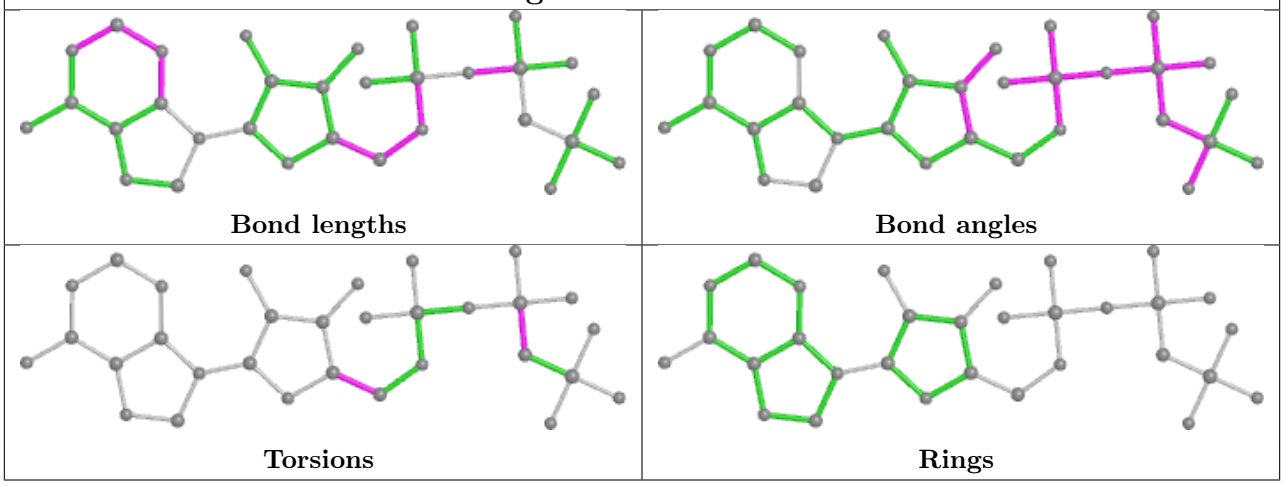


Torsions

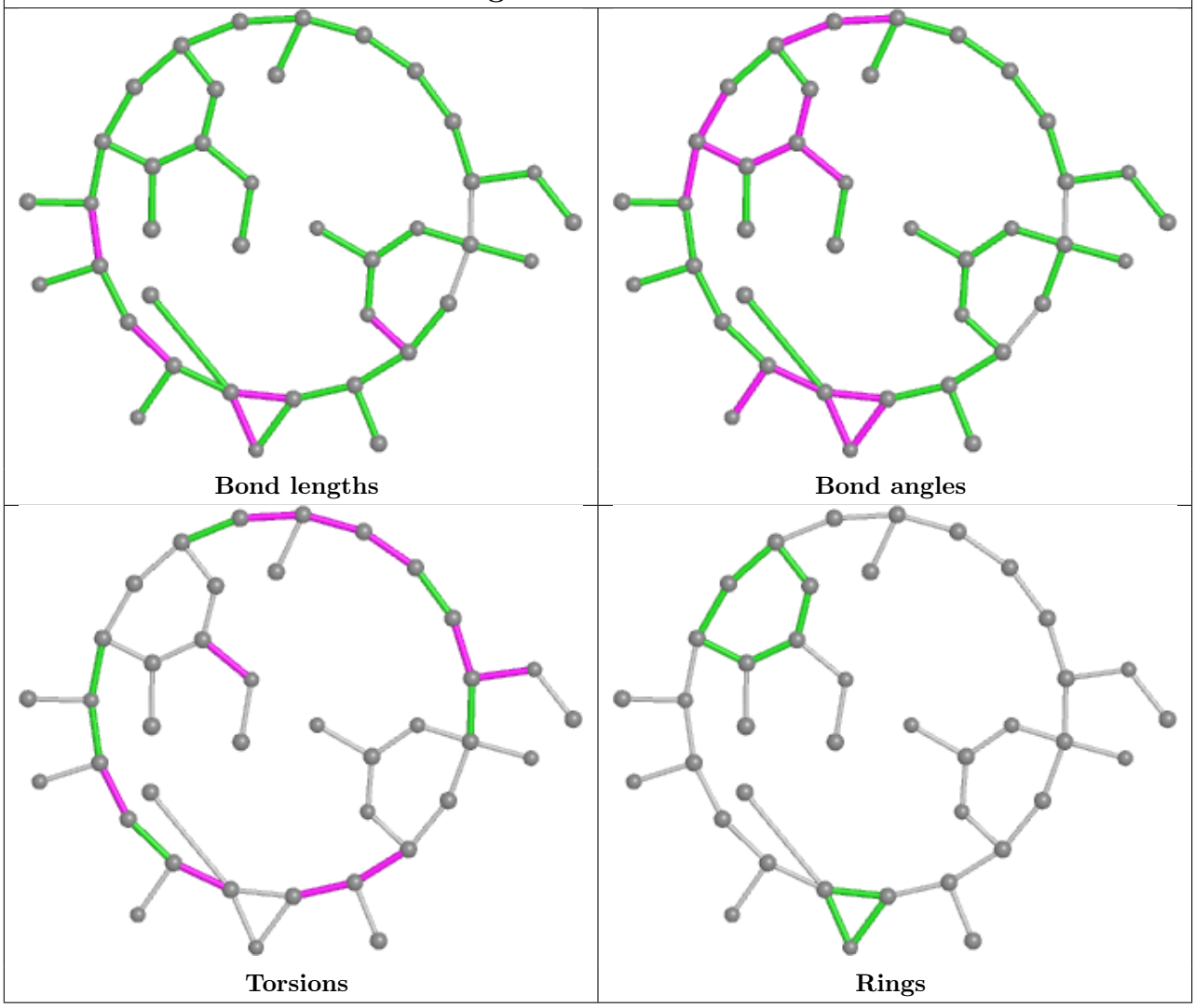


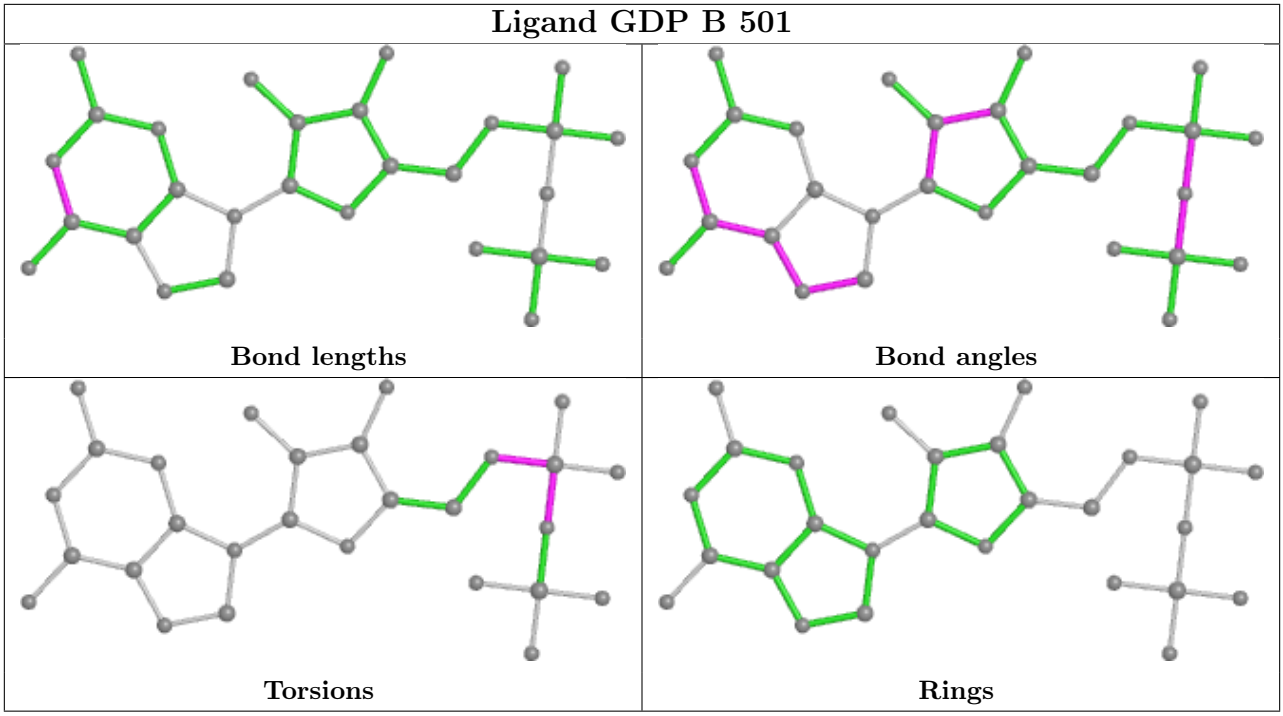
Rings

Ligand ACP F 401



Ligand BKL D 603





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	440/440 (100%)	0.06	8 (1%)	68	70	22, 37, 69, 140	0
1	C	440/440 (100%)	-0.19	4 (0%)	84	85	17, 30, 57, 91	0
2	B	425/431 (98%)	0.08	13 (3%)	49	49	16, 37, 69, 125	0
2	D	421/431 (97%)	0.53	32 (7%)	13	12	26, 54, 93, 129	3 (0%)
3	E	123/138 (89%)	0.55	14 (11%)	5	4	27, 55, 97, 125	0
4	F	348/384 (90%)	0.99	73 (20%)	1	0	30, 68, 139, 166	0
All	All	2197/2264 (97%)	0.28	144 (6%)	18	16	16, 43, 99, 166	3 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	VAL	10.8
4	F	173	ILE	9.8
4	F	176	GLN	6.4
2	D	405	LEU	6.3
4	F	130	VAL	6.0
4	F	169	LEU	5.9
4	F	170	LEU	5.7
4	F	249	TYR	5.5
2	D	285	ALA	5.4
2	D	57	THR	5.3
4	F	372	THR	5.1
2	D	400	ARG	5.1
2	D	218	LYS	5.1
4	F	164	SER	5.1
4	F	125	THR	5.1
4	F	101	TYR	4.8
4	F	177	GLY	4.7
4	F	179	VAL	4.7
2	B	284	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
4	F	178	GLN	4.6
1	C	340	SER	4.4
4	F	136	ASN	4.4
4	F	182	ILE	4.4
2	D	94	PHE	4.4
2	B	57	THR	4.2
2	D	217	LEU	4.2
4	F	174	ASP	4.2
4	F	133	ALA	4.1
2	D	37	HIS	4.1
4	F	167	SER	4.1
2	D	221	THR	4.1
4	F	233	PHE	4.1
4	F	171	ASP	4.0
4	F	139	ARG	4.0
4	F	161	LEU	4.0
4	F	143	GLU	4.0
4	F	158	GLU	3.9
3	E	48	GLU	3.9
2	D	416	MET	3.8
4	F	234	GLN	3.8
4	F	231	ALA	3.7
4	F	137	ARG	3.7
4	F	32	LYS	3.7
2	D	46	LEU	3.7
3	E	140	LYS	3.7
3	E	142	GLU	3.7
2	D	96	GLN	3.6
4	F	251	LYS	3.6
4	F	172	PHE	3.5
4	F	152	SER	3.5
2	B	59	ASN	3.5
1	C	440	VAL	3.5
3	E	135	LYS	3.4
4	F	253	TYR	3.4
2	D	97	SER	3.4
3	E	139	LEU	3.4
3	E	141	GLU	3.4
4	F	255	ARG	3.4
4	F	256	TYR	3.3
4	F	235	ASP	3.3
4	F	165	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	282	GLN	3.3
1	C	315[A]	CYS	3.3
1	A	439	SER	3.2
2	D	219	LEU	3.2
4	F	142	ARG	3.2
4	F	362	ALA	3.2
4	F	381	HIS	3.1
4	F	10	ASN	3.1
2	B	278	ARG	3.1
2	D	177	VAL	3.1
4	F	24	THR	3.0
2	D	56	ALA	3.0
4	F	100	ILE	3.0
3	E	138	GLU	3.0
1	C	1	MET	3.0
4	F	232	ASN	3.0
4	F	225	SER	3.0
4	F	135	TYR	2.9
3	E	27	PRO	2.9
4	F	236	LYS	2.9
4	F	166	ALA	2.9
4	F	138	ARG	2.8
4	F	245	ILE	2.8
4	F	194	PRO	2.8
2	D	168	THR	2.8
1	A	262	TYR	2.8
2	D	59	ASN	2.8
4	F	141	GLY	2.8
2	D	170	SER	2.8
3	E	25	LYS	2.8
2	D	139	HIS	2.7
2	D	406	HIS	2.7
4	F	129	GLU	2.7
2	B	416	MET	2.7
4	F	250	SER	2.6
4	F	132	LEU	2.6
4	F	163	SER	2.6
2	D	286	LEU	2.5
2	D	216	THR	2.5
2	D	415	GLU	2.5
2	D	401	ARG	2.5
4	F	258	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	2.5
4	F	246	GLN	2.5
4	F	31	ARG	2.5
4	F	134	ALA	2.4
4	F	20	LEU	2.4
4	F	252	ASN	2.4
3	E	6	MET	2.4
2	D	147[A]	SER	2.4
2	D	58	GLY	2.4
4	F	144	GLY	2.4
4	F	160	ILE	2.4
4	F	257	GLU	2.3
4	F	175	GLU	2.3
2	B	33	THR	2.3
4	F	247	LYS	2.3
4	F	128	ARG	2.3
4	F	379	HIS	2.2
4	F	168	GLU	2.2
4	F	159	GLY	2.2
2	D	169	PHE	2.2
1	A	42	ILE	2.2
1	A	282	TYR	2.2
2	D	179	ASP	2.2
1	A	235	VAL	2.2
1	A	80	THR	2.2
2	B	167	ASN	2.2
2	B	58	GLY	2.2
2	B	277	SER	2.1
4	F	26	GLN	2.1
2	D	372	LYS	2.1
2	B	201	THR	2.1
2	D	60	LYS	2.1
4	F	244	CYS	2.1
2	B	74	THR	2.1
1	A	237	SER	2.1
2	D	220	THR	2.1
3	E	7	GLU	2.1
2	B	216	THR	2.0
3	E	133	VAL	2.0
4	F	180	HIS	2.0
3	E	130	ALA	2.0

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)

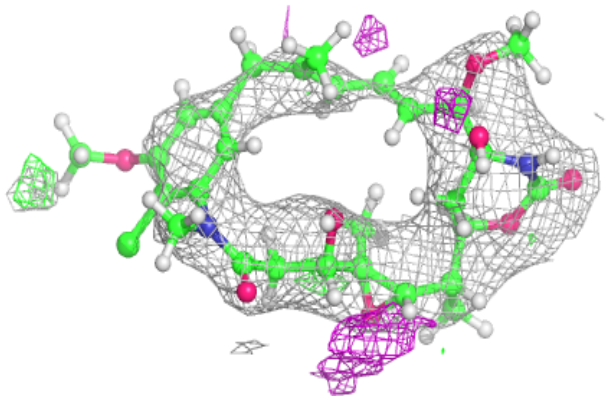
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

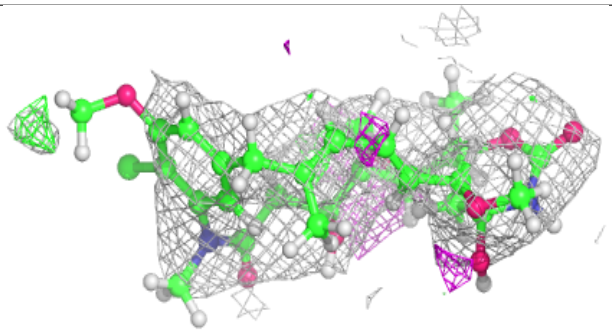
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MES	A	505	12/12	0.71	0.37	63,93,113,165	0
11	BKL	D	603	39/39	0.81	0.36	57,87,107,152	0
12	ACP	F	401	31/31	0.85	0.29	71,101,140,191	0
7	CA	A	503	1/1	0.88	0.06	49,49,49,49	0
8	CL	A	504	1/1	0.89	0.18	54,54,54,54	0
6	MG	D	601	1/1	0.90	0.07	78,78,78,78	0
6	MG	C	502	1/1	0.90	0.12	28,28,28,28	0
7	CA	B	503	1/1	0.93	0.05	70,70,70,70	0
7	CA	E	201	1/1	0.93	0.06	69,69,69,69	0
9	MES	B	504	12/12	0.95	0.18	31,46,59,63	0
6	MG	B	506	1/1	0.95	0.09	66,66,66,66	0
5	GTP	D	602	32/32	0.95	0.18	46,58,72,114	0
9	MES	B	505	12/12	0.96	0.15	46,57,77,83	0
7	CA	C	503	1/1	0.97	0.04	39,39,39,39	0
6	MG	B	502	1/1	0.97	0.12	21,21,21,21	0
10	GDP	B	501	28/28	0.97	0.20	18,28,39,43	0
5	GTP	A	501	32/32	0.97	0.17	18,26,39,46	0
6	MG	A	502	1/1	0.97	0.13	27,27,27,27	0
5	GTP	C	501	32/32	0.98	0.17	16,23,35,44	0

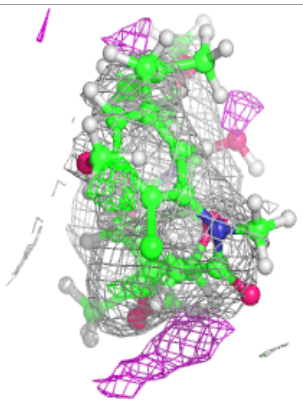
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BKL D 603:

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

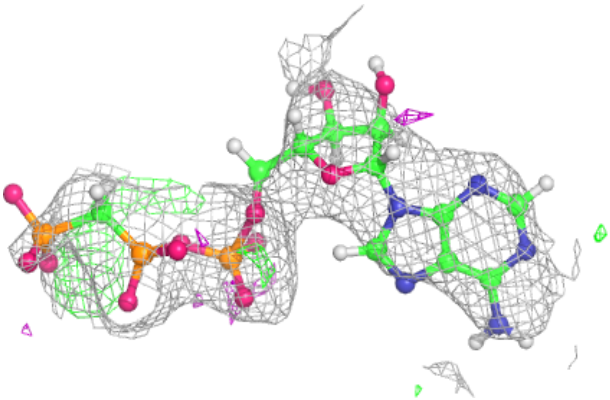


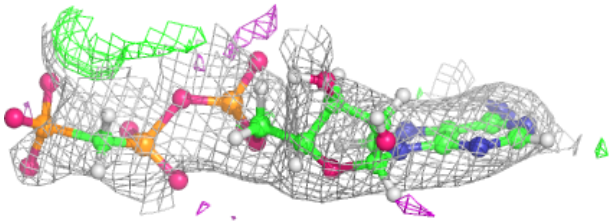


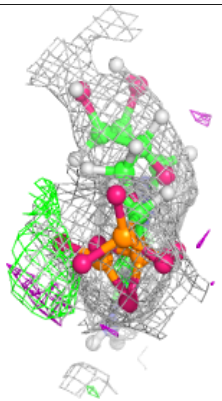


Electron density around ACP F 401:

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

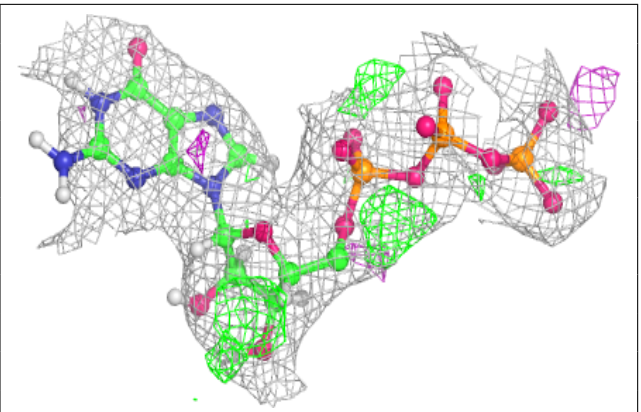


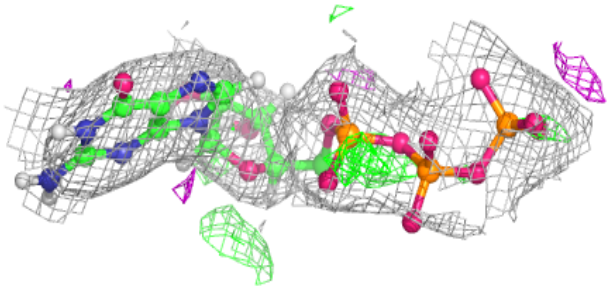


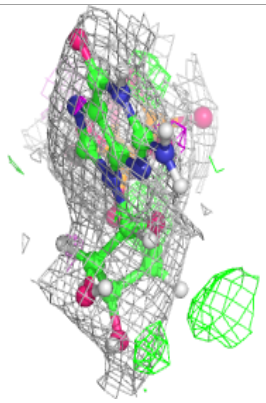


Electron density around GTP D 602:

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

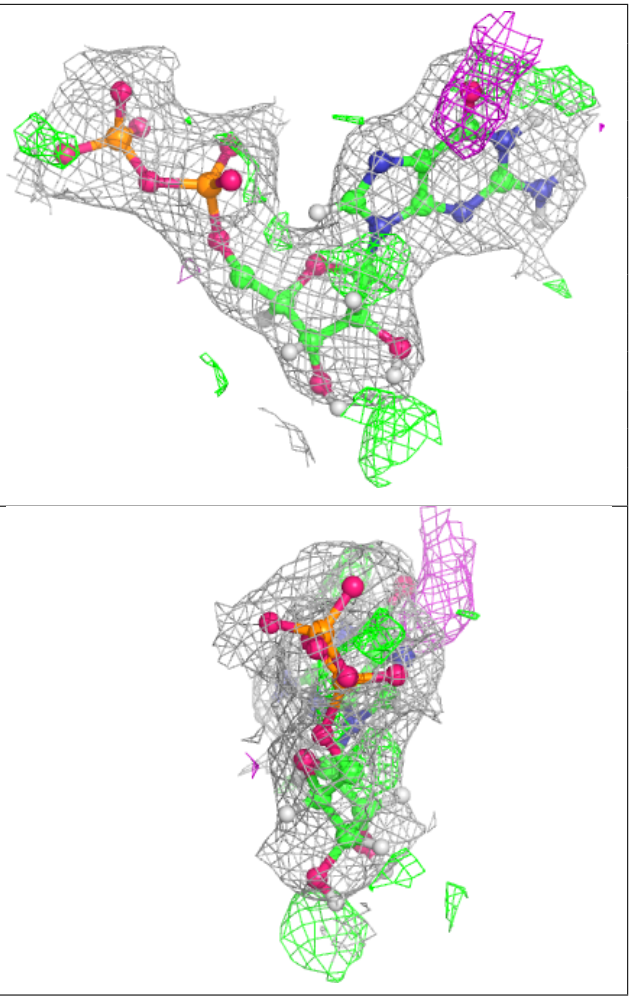






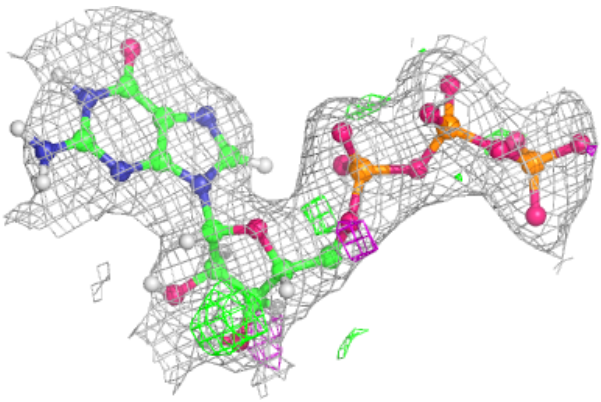
Electron density around GDP B 501:

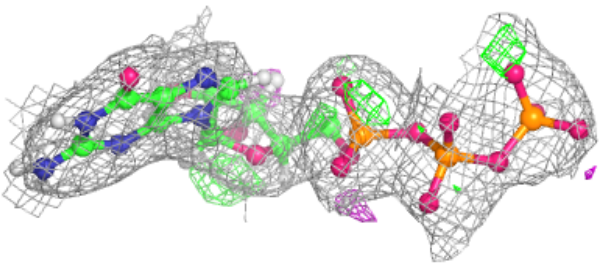
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

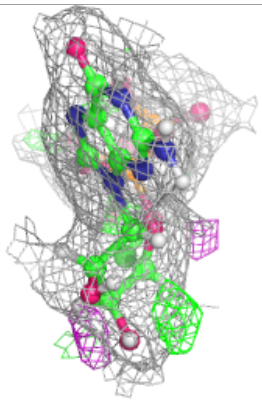


Electron density around GTP A 501:

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

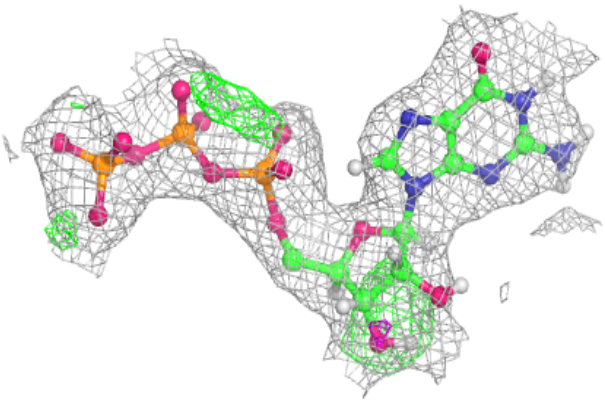


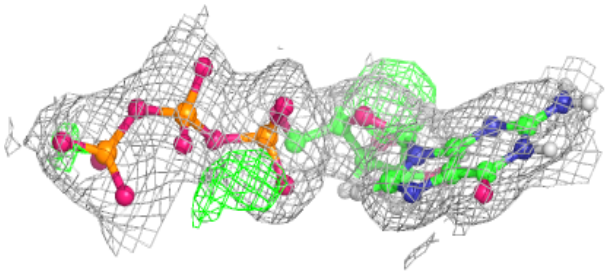


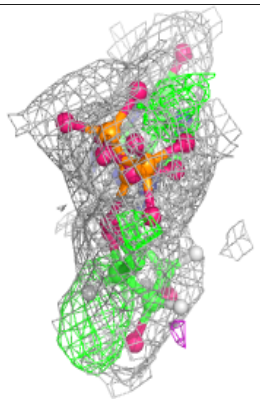


Electron density around GTP C 501:

$2mF_o$-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.