



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 02:13 PM JST

PDB ID : 7E4Y  
Title : Crystal structure of tubulin in complex with L-DM4-SMe  
Authors : Wang, Y.; Li, W.  
Deposited on : 2021-02-16  
Resolution : 2.71 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.26  
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) : 2.26

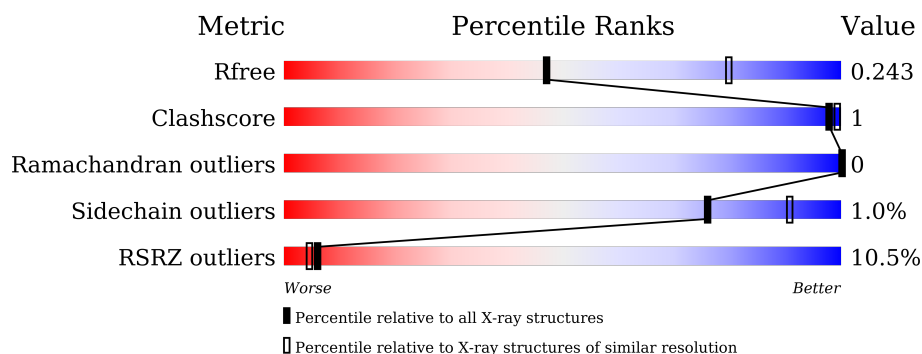
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>5%</div> <div>98%</div> <div>..</div> </div>
1	C	440	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
2	B	431	<div> <div>6%</div> <div>97%</div> <div>.</div> </div>
2	D	431	<div> <div>18%</div> <div>95%</div> <div>..</div> </div>
3	E	138	<div> <div>14%</div> <div>88%</div> <div>11%</div> </div>
4	F	380	<div> <div>20%</div> <div>83%</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 34556 atoms, of which 16907 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6734	2163	3318	581	650	22			
1	C	439	Total	C	H	N	O	S	0	0	0
			6758	2171	3328	583	654	22			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	430	Total	C	H	N	O	S	3	0	0
			6632	2122	3251	579	653	27			
2	D	423	Total	C	H	N	O	S	4	0	0
			6526	2090	3199	567	643	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	0	0
			2039	625	1025	183	201	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

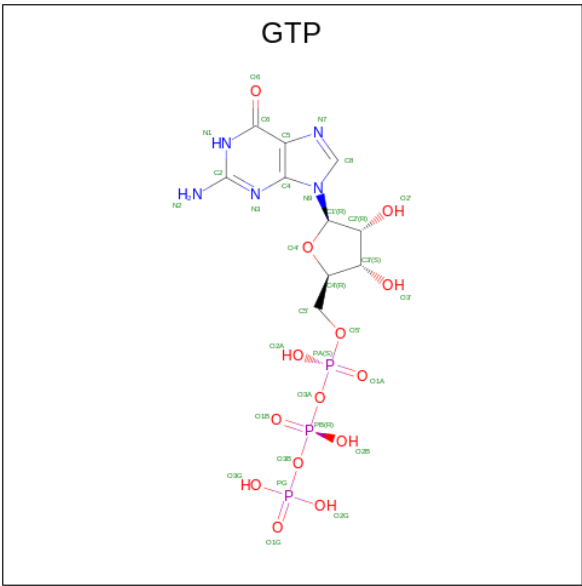
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	331	Total	C	H	N	O	S	0	0	0
			5389	1746	2676	461	492	14			

There are 2 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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0	
			32	10	5	14	3			

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

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

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

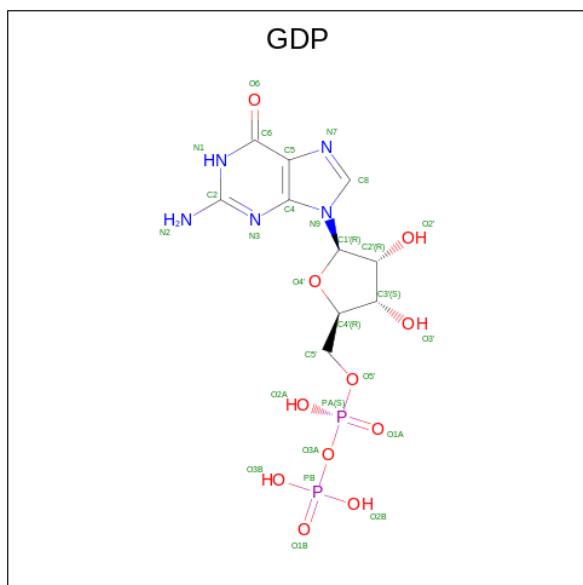
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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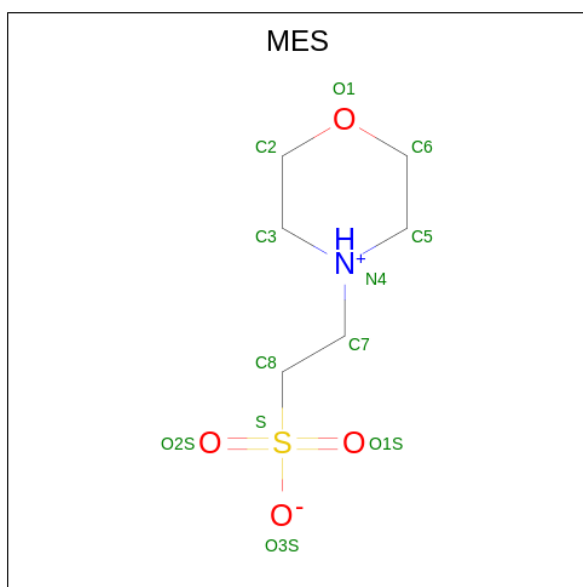
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



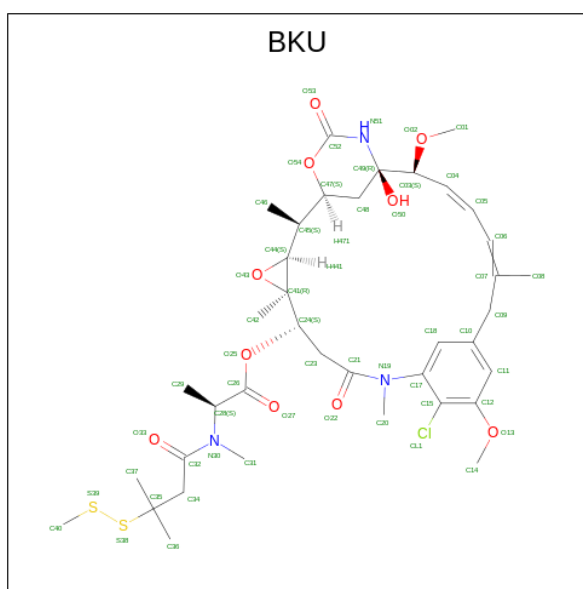
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

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

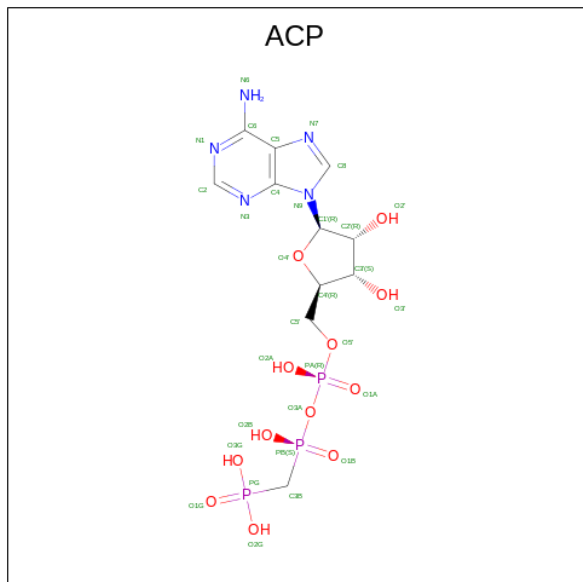


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 10 is (1S,2S,3S,5R,6S,16E,18E,20S,21R)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxo-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5 ]hexacosan-10(26),11,13,16,18-pentaen-6-yl (2S)-2-{methyl[3-methyl-3-(methyldisulfanyl)butanoyl]amino}propanoate (non-preferred name) (three-letter code: BKU) (formula: C<sub>38</sub>H<sub>54</sub>ClN<sub>3</sub>O<sub>10</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

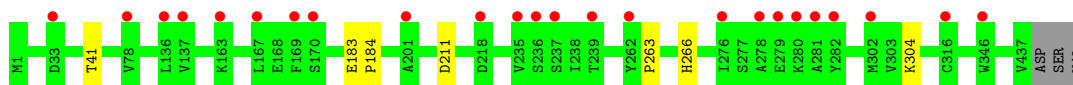
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	23	Total	O		
			23	23	0	0
12	B	30	Total	O		
			30	30	0	0
12	C	59	Total	O		
			59	59	0	0
12	D	11	Total	O		
			11	11	0	0
12	E	4	Total	O		
			4	4	0	0
12	F	13	Total	O		
			13	13	0	0

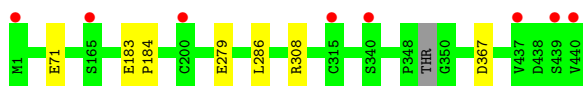
### 3 Residue-property plots [i](#)

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.

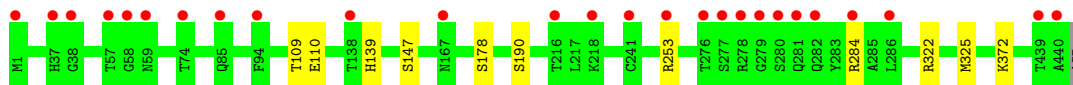
- Molecule 1: Tubulin alpha-1B chain



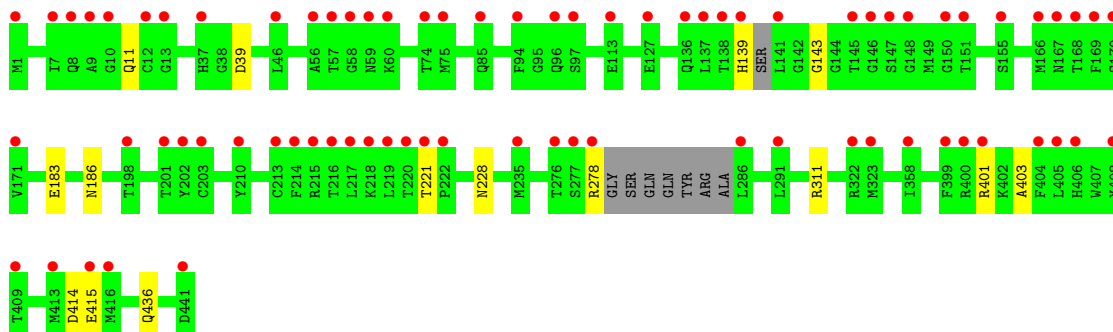
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain

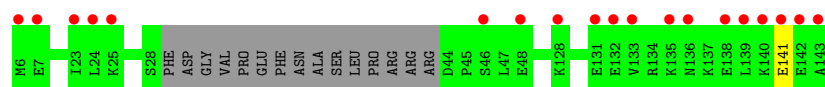
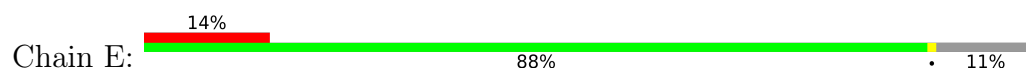


- Molecule 2: Tubulin beta-2B chain

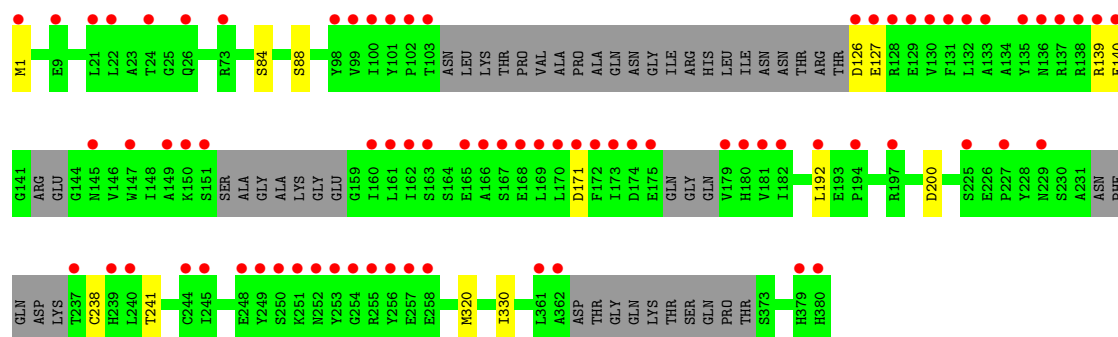
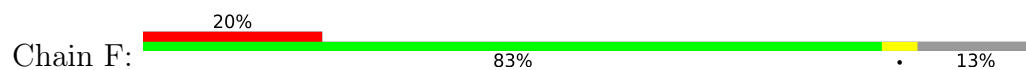


- Molecule 3: Stathmin-4





● Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.99Å 156.03Å 182.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.71 39.51 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.51-2.71) 99.5 (39.51-2.71)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.196 , 0.239 0.200 , 0.243	Depositor DCC
$R_{free}$ test set	3956 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.23	0/3494	0.39	0/4743
1	C	0.25	0/3507	0.39	0/4759
2	B	0.24	0/3456	0.39	0/4681
2	D	0.23	0/3399	0.38	0/4602
3	E	0.22	0/1022	0.32	0/1356
4	F	0.22	0/2773	0.38	0/3743
All	All	0.23	0/17651	0.38	0/23884

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	3416	3318	3331	3	0
1	C	3430	3328	3340	3	0
2	B	3381	3251	3262	4	0
2	D	3327	3199	3208	8	0
3	E	1014	1025	1029	0	0
4	F	2713	2676	2687	5	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
5	D	32	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
9	B	12	12	12	1	0
10	D	54	54	0	0	0
11	F	31	14	14	0	0
12	A	23	0	0	0	0
12	B	30	0	0	0	0
12	C	59	0	0	1	0
12	D	11	0	0	1	0
12	E	4	0	0	0	0
12	F	13	0	0	0	0
All	All	17649	16907	16931	23	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 (23) 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	2.10	0.68
4:F:139:ARG:NH2	4:F:140:GLU:OE2	2.30	0.63
2:D:11:GLN:NE2	12:D:602:HOH:O	2.34	0.59
2:D:228:ASN:OD1	5:D:501:GTP:N1	2.29	0.58
2:B:147:SER:OG	2:B:190:SER:OG	2.22	0.56
2:D:414:ASP:OD1	2:D:415:GLU:N	2.38	0.56
2:B:147:SER:HG	2:B:190:SER:HG	1.51	0.55
2:B:253:ARG:NH1	9:B:503:MES:O3S	2.42	0.52
2:D:311:ARG:NH1	2:D:436:GLN:O	2.43	0.48
1:C:367:ASP:O	12:C:601:HOH:O	2.20	0.48
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.47	0.48
2:B:109:THR:OG1	2:B:110:GLU:N	2.50	0.43
2:D:183:GLU:OE2	5:D:501:GTP:O3'	2.13	0.43
2:D:143:GLY:O	2:D:186:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:84:SER:O	4:F:88:SER:N	2.46	0.43
1:A:263:PRO:O	1:A:266:HIS:ND1	2.35	0.42
4:F:320:MET:HG2	4:F:330:ILE:HD11	2.00	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
4:F:126:ASP:OD1	4:F:127:GLU:N	2.54	0.41
1:C:183:GLU:N	1:C:184:PRO:CD	2.84	0.41
1:C:279:GLU:OE1	1:C:279:GLU:N	2.53	0.40
2:D:39:ASP:OD1	2:D:39:ASP:N	2.53	0.40
2:D:401:ARG:HE	2:D:403:ALA:HB2	1.86	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	435/440 (99%)	425 (98%)	10 (2%)	0	100	100
1	C	435/440 (99%)	426 (98%)	9 (2%)	0	100	100
2	B	428/431 (99%)	419 (98%)	9 (2%)	0	100	100
2	D	417/431 (97%)	408 (98%)	9 (2%)	0	100	100
3	E	119/138 (86%)	118 (99%)	1 (1%)	0	100	100
4	F	317/380 (83%)	309 (98%)	8 (2%)	0	100	100
All	All	2151/2260 (95%)	2105 (98%)	46 (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	368/371 (99%)	367 (100%)	1 (0%)	92	98
1	C	370/371 (100%)	367 (99%)	3 (1%)	81	93
2	B	371/372 (100%)	365 (98%)	6 (2%)	62	85
2	D	366/372 (98%)	363 (99%)	3 (1%)	81	93
3	E	110/123 (89%)	109 (99%)	1 (1%)	78	92
4	F	298/338 (88%)	294 (99%)	4 (1%)	69	87
All	All	1883/1947 (97%)	1865 (99%)	18 (1%)	76	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
2	B	139	HIS
2	B	178	SER
2	B	284	ARG
2	B	322	ARG
2	B	325	MET
2	B	372	LYS
1	C	71	GLU
1	C	286	LEU
1	C	308	ARG
2	D	139	HIS
2	D	221	THR
2	D	278	ARG
3	E	141	GLU
4	F	1	MET
4	F	171	ASP
4	F	192	LEU
4	F	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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, 7 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	GDP	B	501	6	24,30,30	1.08	2 (8%)	31,47,47	1.90	7 (22%)
10	BKU	D	502	-	54,57,57	3.81	34 (62%)	63,86,86	2.97	31 (49%)
5	GTP	D	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.83	7 (21%)
11	ACP	F	402	6	27,33,33	4.35	7 (25%)	32,52,52	1.64	6 (18%)
9	MES	B	503	-	12,12,12	2.33	1 (8%)	14,16,16	2.59	5 (35%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.69	7 (21%)
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.71	7 (21%)

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
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3
10	BKU	D	502	-	-	26/64/93/93	0/2/4/4
5	GTP	D	501	6	-	8/18/38/38	0/3/3/3
11	ACP	F	402	6	-	8/15/38/38	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	10/18/38/38	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	PB-O3A	19.90	1.80	1.58
10	D	502	BKU	C41-C44	11.46	1.61	1.47
10	D	502	BKU	C09-C07	8.18	1.61	1.51
9	B	503	MES	C8-S	-7.83	1.66	1.77
10	D	502	BKU	C23-C24	7.83	1.63	1.52
11	F	402	ACP	PA-O5'	7.41	1.89	1.59
10	D	502	BKU	C17-N19	7.06	1.52	1.44
10	D	502	BKU	C06-C07	6.97	1.41	1.34
10	D	502	BKU	C09-C10	6.62	1.62	1.51
10	D	502	BKU	C34-C32	5.74	1.58	1.51
10	D	502	BKU	C21-N19	5.48	1.46	1.35
10	D	502	BKU	C32-N30	5.48	1.44	1.35
10	D	502	BKU	C49-N51	5.34	1.54	1.46
10	D	502	BKU	O54-C47	-4.55	1.40	1.46
10	D	502	BKU	C45-C47	4.49	1.64	1.53
10	D	502	BKU	C15-CL1	4.09	1.81	1.72
10	D	502	BKU	O43-C44	3.86	1.50	1.45
10	D	502	BKU	C42-C41	-3.76	1.42	1.52
11	F	402	ACP	C5'-C4'	3.64	1.63	1.51
8	B	501	GDP	C5-C6	3.63	1.47	1.41
10	D	502	BKU	S38-S39	3.61	2.10	2.04
10	D	502	BKU	C52-N51	3.56	1.42	1.34
10	D	502	BKU	C45-C44	-3.31	1.46	1.55
10	D	502	BKU	C05-C06	3.08	1.53	1.43
5	D	501	GTP	C6-N1	3.03	1.38	1.33
11	F	402	ACP	O5'-C5'	-3.03	1.33	1.44
10	D	502	BKU	C35-S38	2.96	1.88	1.85
10	D	502	BKU	C11-C10	2.95	1.44	1.39
10	D	502	BKU	C20-N19	2.94	1.51	1.46
5	A	501	GTP	C6-N1	2.93	1.38	1.33
10	D	502	BKU	C23-C21	2.91	1.56	1.51
5	C	501	GTP	C6-N1	2.91	1.38	1.33
10	D	502	BKU	C28-N30	2.89	1.52	1.47
10	D	502	BKU	O53-C52	2.83	1.26	1.21
10	D	502	BKU	O54-C52	-2.70	1.30	1.35
11	F	402	ACP	C2-N1	2.69	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	BKU	C17-C15	2.63	1.43	1.40
10	D	502	BKU	C03-C04	2.62	1.59	1.50
10	D	502	BKU	C11-C12	2.57	1.43	1.38
10	D	502	BKU	C18-C17	2.49	1.43	1.39
11	F	402	ACP	C4-N3	2.43	1.39	1.35
10	D	502	BKU	O43-C41	2.24	1.48	1.45
8	B	501	GDP	C5-C4	2.23	1.46	1.40
10	D	502	BKU	C12-C15	2.22	1.44	1.40
10	D	502	BKU	O13-C12	2.22	1.40	1.37
10	D	502	BKU	C05-C04	2.17	1.41	1.33
11	F	402	ACP	C2-N3	2.12	1.35	1.32

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	BKU	C41-O43-C44	7.82	65.49	60.79
10	D	502	BKU	C15-C17-N19	7.52	128.42	120.71
10	D	502	BKU	C23-C21-N19	7.44	127.28	118.89
9	B	503	MES	C5-N4-C3	6.81	124.16	108.83
10	D	502	BKU	O13-C12-C15	5.34	121.86	115.53
5	C	501	GTP	N3-C2-N1	-5.30	120.15	127.22
5	D	501	GTP	N3-C2-N1	-5.28	120.18	127.22
5	A	501	GTP	N3-C2-N1	-5.17	120.33	127.22
10	D	502	BKU	C35-C34-C32	5.14	123.00	114.84
10	D	502	BKU	C18-C17-C15	-5.11	116.01	122.53
10	D	502	BKU	C42-C41-C44	-5.01	109.69	121.05
10	D	502	BKU	O25-C26-O27	-4.69	115.18	123.94
10	D	502	BKU	O25-C26-C28	4.59	120.77	110.80
8	B	501	GDP	C2-N1-C6	4.46	123.02	115.93
8	B	501	GDP	C2-N3-C4	4.25	120.22	115.36
10	D	502	BKU	O43-C44-C41	-4.20	56.84	59.83
5	D	501	GTP	C2-N3-C4	4.19	120.14	115.36
10	D	502	BKU	O25-C24-C41	4.19	114.94	105.48
8	B	501	GDP	C5-C6-N1	-4.15	117.76	123.43
5	C	501	GTP	C2-N3-C4	4.09	120.02	115.36
11	F	402	ACP	O5'-PA-O1A	-4.07	93.15	109.07
8	B	501	GDP	C4-C5-C6	-4.05	116.93	120.80
11	F	402	ACP	O1B-PB-C3B	4.04	119.74	109.07
5	A	501	GTP	C2-N3-C4	4.00	119.92	115.36
10	D	502	BKU	C35-S38-S39	3.99	112.14	107.08
10	D	502	BKU	O33-C32-N30	-3.90	115.06	121.88
10	D	502	BKU	O22-C21-C23	-3.78	115.37	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	PB-O3B-PG	-3.70	120.12	132.83
10	D	502	BKU	C09-C10-C11	3.60	126.08	120.38
9	B	503	MES	O1S-S-C8	3.56	111.21	106.92
10	D	502	BKU	C17-C18-C10	3.53	125.08	120.23
8	B	501	GDP	N3-C2-N1	-3.53	122.52	127.22
11	F	402	ACP	PB-O3A-PA	-3.28	122.17	132.56
10	D	502	BKU	O54-C52-N51	3.12	124.59	118.78
9	B	503	MES	C7-N4-C5	3.04	119.01	111.23
5	D	501	GTP	PA-O3A-PB	-2.96	122.68	132.83
5	A	501	GTP	C5-C6-N1	-2.91	119.45	123.43
5	C	501	GTP	C5-C6-N1	-2.87	119.50	123.43
5	A	501	GTP	PB-O3B-PG	-2.81	123.19	132.83
5	D	501	GTP	C5-C6-N1	-2.81	119.59	123.43
5	C	501	GTP	PA-O3A-PB	-2.75	123.38	132.83
5	D	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98
10	D	502	BKU	O54-C47-C45	2.66	111.28	105.76
10	D	502	BKU	O22-C21-N19	-2.65	117.30	121.90
5	C	501	GTP	C2-N1-C6	2.63	120.11	115.93
9	B	503	MES	C2-C3-N4	2.61	114.06	110.10
5	C	501	GTP	PB-O3B-PG	-2.59	123.93	132.83
5	A	501	GTP	C2-N1-C6	2.57	120.01	115.93
10	D	502	BKU	C17-C15-CL1	-2.56	117.37	120.09
10	D	502	BKU	O43-C41-C44	-2.55	57.67	59.38
5	D	501	GTP	C2-N1-C6	2.52	119.94	115.93
5	A	501	GTP	O3G-PG-O3B	2.40	112.70	104.64
9	B	503	MES	O3S-S-C8	2.39	109.63	105.77
11	F	402	ACP	O2A-PA-O5'	-2.36	96.79	107.75
11	F	402	ACP	O1G-PG-C3B	-2.34	106.19	111.24
10	D	502	BKU	C42-C41-C24	2.34	120.99	114.51
10	D	502	BKU	O13-C12-C11	-2.31	120.14	124.12
10	D	502	BKU	C28-N30-C32	2.27	125.66	117.64
10	D	502	BKU	C31-N30-C32	-2.27	116.77	122.01
10	D	502	BKU	O54-C52-O53	-2.27	114.58	117.87
8	B	501	GDP	O3B-PB-O3A	2.26	112.23	104.64
8	B	501	GDP	C4-C5-N7	-2.23	107.08	109.40
5	A	501	GTP	PA-O3A-PB	-2.22	125.21	132.83
10	D	502	BKU	C11-C12-C15	-2.22	117.99	120.76
11	F	402	ACP	O2B-PB-C3B	2.18	115.51	106.58
10	D	502	BKU	O27-C26-C28	-2.13	115.47	122.81
10	D	502	BKU	O33-C32-C34	-2.12	117.56	121.65
10	D	502	BKU	O50-C49-N51	2.04	115.30	110.21
5	C	501	GTP	C3'-C2'-C1'	2.02	104.01	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
10	D	502	BKU	O50-C49-C48	-2.01	104.40	109.98

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	PA-O3A-PB-O3B
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
10	D	502	BKU	C49-C03-O02-C01
10	D	502	BKU	O02-C03-C04-C05
10	D	502	BKU	C49-C03-C04-C05
10	D	502	BKU	O02-C03-C49-C48
10	D	502	BKU	C05-C06-C07-C09
10	D	502	BKU	C21-C23-C24-O25
10	D	502	BKU	C23-C24-O25-C26
10	D	502	BKU	C23-C24-C41-C42
10	D	502	BKU	O25-C26-C28-N30
10	D	502	BKU	C34-C35-S38-S39
10	D	502	BKU	C36-C35-S38-S39
10	D	502	BKU	C37-C35-S38-S39
10	D	502	BKU	C44-C45-C47-C48
10	D	502	BKU	C44-C45-C47-O54
10	D	502	BKU	C46-C45-C47-C48
10	D	502	BKU	C46-C45-C47-O54
11	F	402	ACP	PB-C3B-PG-O1G
11	F	402	ACP	PB-C3B-PG-O3G
11	F	402	ACP	PG-C3B-PB-O1B
11	F	402	ACP	PG-C3B-PB-O2B
11	F	402	ACP	PG-C3B-PB-O3A
11	F	402	ACP	O4'-C4'-C5'-O5'
10	D	502	BKU	C04-C05-C06-C07
10	D	502	BKU	C15-C12-O13-C14
9	B	503	MES	C7-C8-S-O3S
10	D	502	BKU	C11-C12-O13-C14
10	D	502	BKU	C04-C03-O02-C01
10	D	502	BKU	O27-C26-C28-N30
10	D	502	BKU	C41-C24-O25-C26

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Mol	Chain	Res	Type	Atoms
5	D	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
11	F	402	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
10	D	502	BKU	C23-C24-C41-O43
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
5	D	501	GTP	C3'-C4'-C5'-O5'
10	D	502	BKU	C23-C24-C41-C44
11	F	402	ACP	PB-C3B-PG-O2G
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
10	D	502	BKU	N19-C21-C23-C24
8	B	501	GDP	PA-O3A-PB-O1B
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
10	D	502	BKU	O27-C26-O25-C24

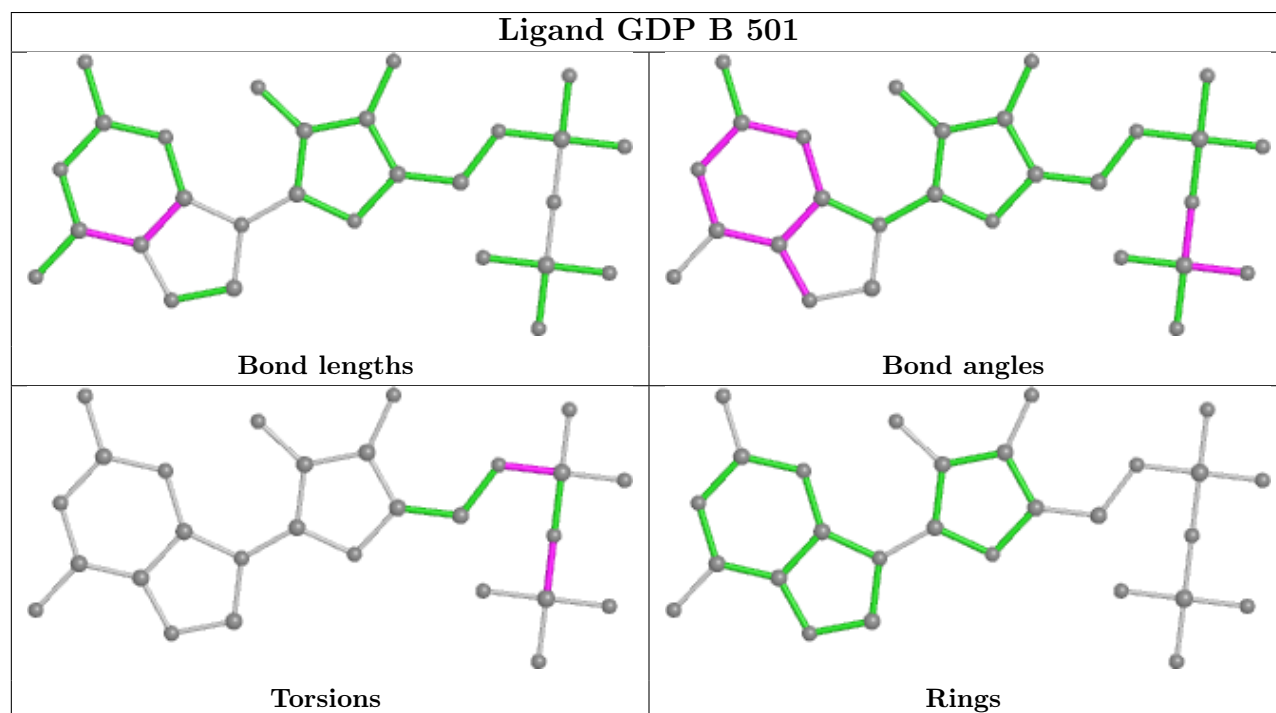
There are no ring outliers.

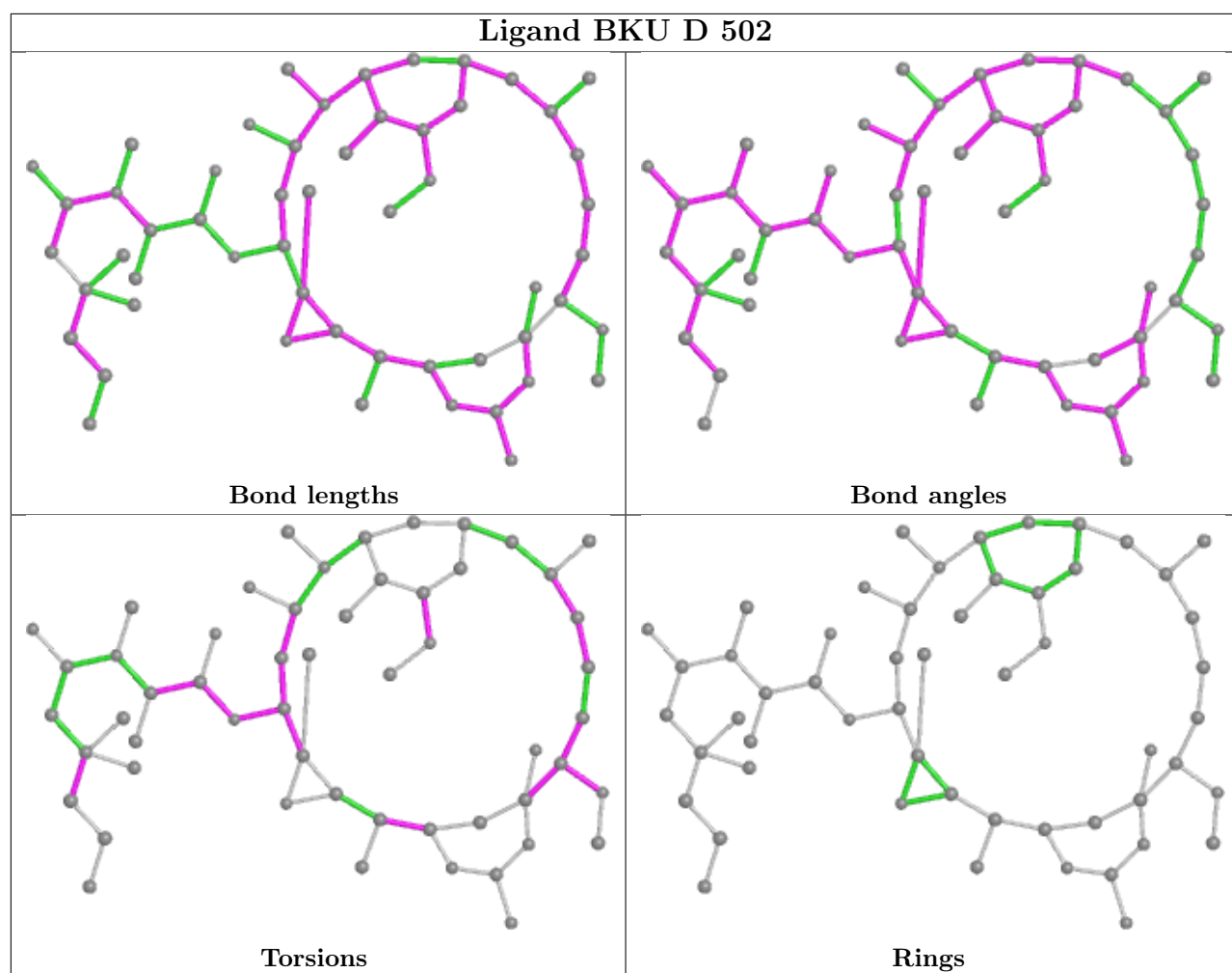
2 monomers are involved in 3 short contacts:

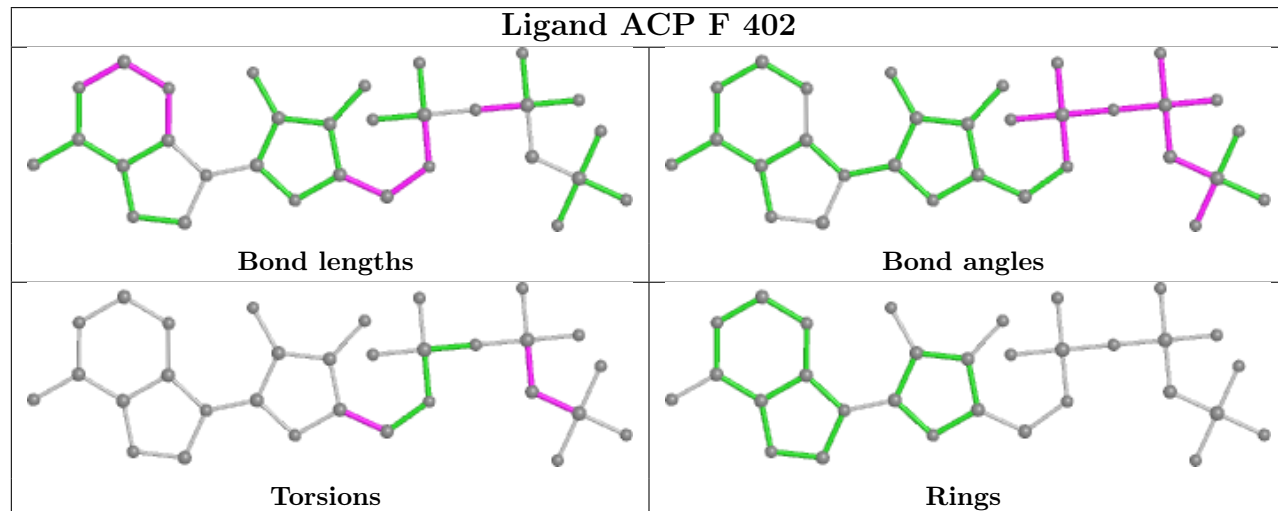
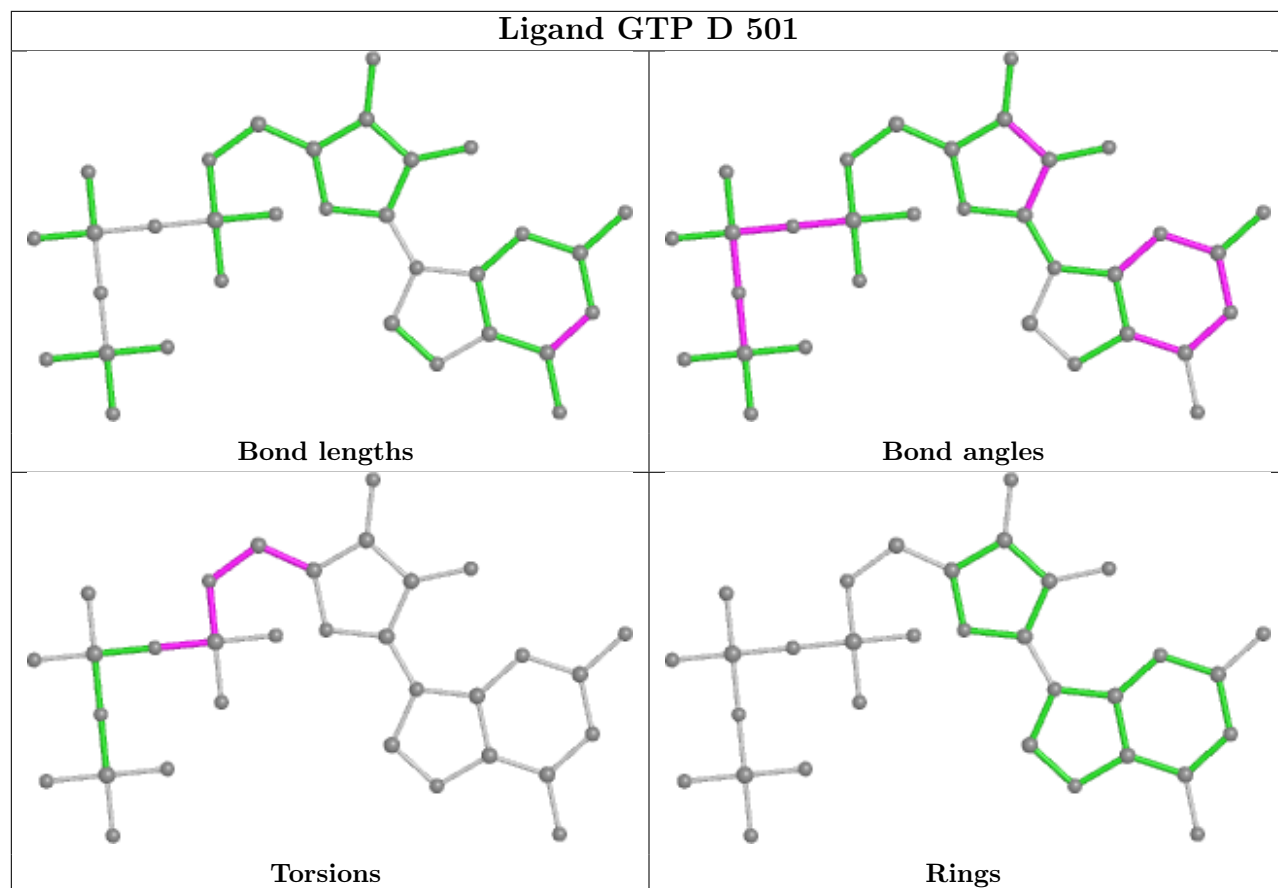
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	GTP	2	0
9	B	503	MES	1	0

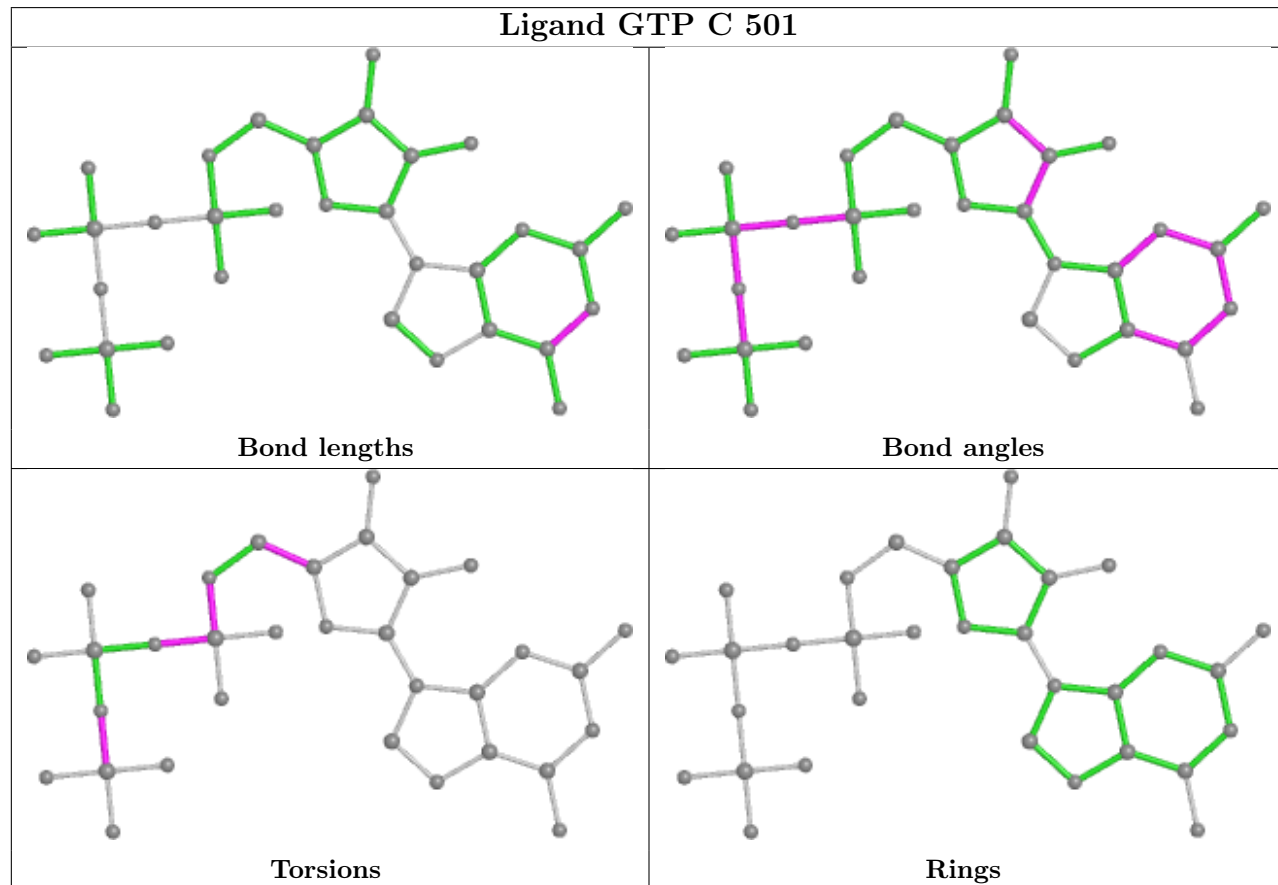
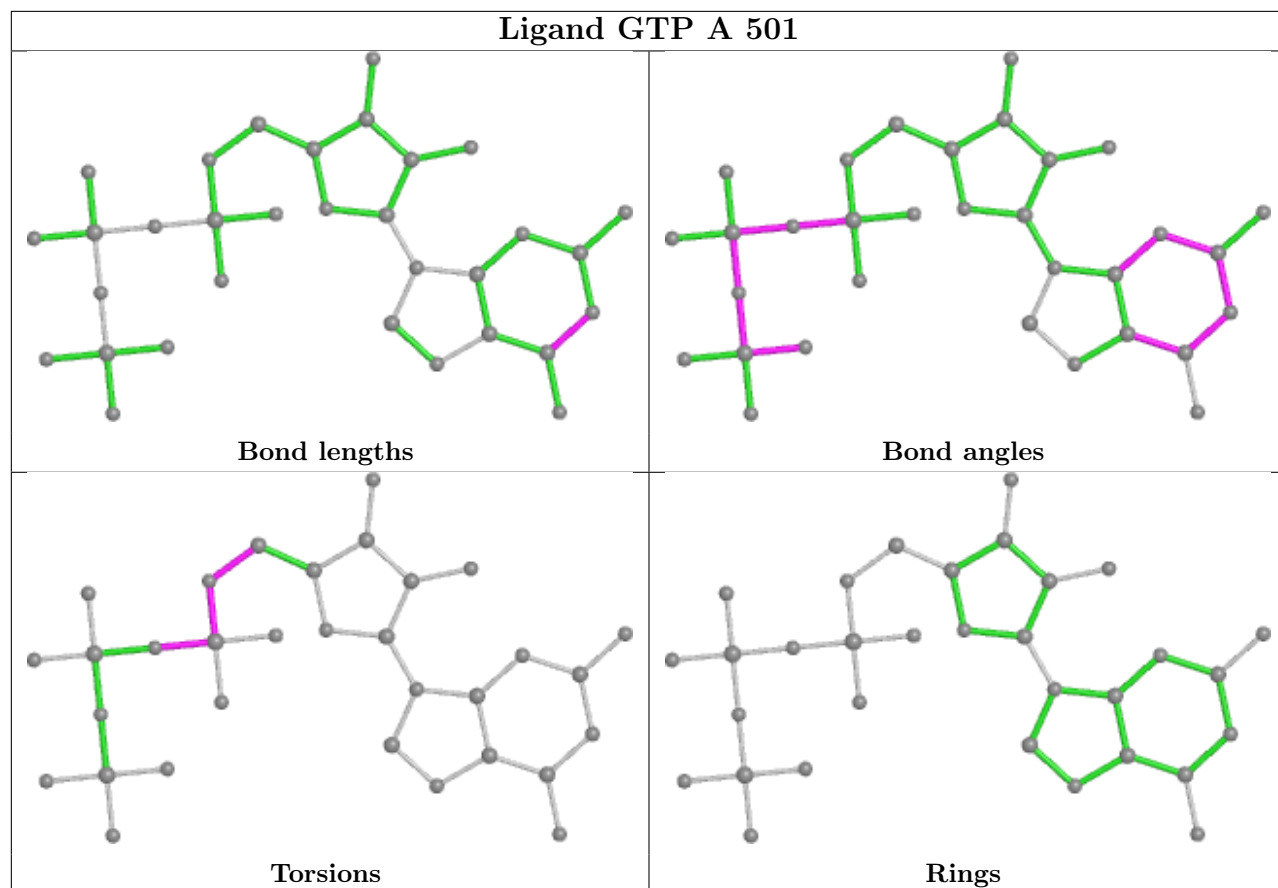
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/440 (99%)	0.40	24 (5%)	25 24	30, 50, 81, 108	0
1	C	439/440 (99%)	0.04	8 (1%)	68 70	25, 40, 70, 106	0
2	B	430/431 (99%)	0.33	26 (6%)	21 20	25, 49, 86, 132	1 (0%)
2	D	423/431 (98%)	0.95	76 (17%)	1 1	38, 69, 104, 124	2 (0%)
3	E	123/138 (89%)	0.78	19 (15%)	2 1	35, 68, 104, 130	0
4	F	331/380 (87%)	1.08	77 (23%)	0 0	41, 79, 136, 150	0
All	All	2183/2260 (96%)	0.54	230 (10%)	6 4	25, 57, 105, 150	3 (0%)

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.5
4	F	132	LEU	7.6
4	F	100	ILE	7.2
4	F	169	LEU	6.7
4	F	101	TYR	6.7
2	D	139	HIS	6.3
4	F	102	PRO	6.2
4	F	165	GLU	6.1
4	F	99	VAL	6.1
4	F	161	LEU	6.0
2	D	37	HIS	5.9
4	F	172	PHE	5.9
4	F	182	ILE	5.8
4	F	166	ALA	5.8
2	D	277	SER	5.7
2	D	168	THR	5.7
2	D	405	LEU	5.5
4	F	179	VAL	5.4
2	D	57	THR	5.4

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Mol	Chain	Res	Type	RSRZ
4	F	170	LEU	5.3
4	F	251	LYS	5.2
4	F	128	ARG	5.1
2	D	221	THR	5.1
2	D	400	ARG	5.0
1	A	282	TYR	5.0
2	D	219	LEU	5.0
4	F	248	GLU	4.9
2	D	276	THR	4.9
4	F	136	ASN	4.8
4	F	249	TYR	4.7
4	F	180	HIS	4.6
2	D	217	LEU	4.6
4	F	135	TYR	4.5
4	F	139	ARG	4.5
2	D	58	GLY	4.5
2	B	1	MET	4.4
2	B	57	THR	4.3
3	E	139	LEU	4.3
2	D	220	THR	4.2
4	F	131	PHE	4.2
2	D	96	GLN	4.2
2	D	170	SER	4.2
2	D	415	GLU	4.2
4	F	151	SER	4.2
4	F	160	ILE	4.1
4	F	162	ILE	4.1
3	E	138	GLU	4.1
4	F	253	TYR	4.1
2	D	1	MET	4.1
4	F	361	LEU	4.0
2	D	137	LEU	4.0
4	F	127	GLU	4.0
1	A	281	ALA	4.0
4	F	174	ASP	3.9
2	D	218	LYS	3.9
3	E	7	GLU	3.9
4	F	149	ALA	3.9
4	F	168	GLU	3.9
3	E	142	GLU	3.8
3	E	143	ALA	3.8
2	D	60	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	169	PHE	3.8
4	F	255	ARG	3.8
1	C	340	SER	3.8
2	B	281	GLN	3.7
1	A	302	MET	3.7
2	D	167	ASN	3.7
2	D	138	THR	3.7
4	F	133	ALA	3.7
3	E	135	LYS	3.6
3	E	6	MET	3.6
4	F	225	SER	3.6
1	A	262	TYR	3.6
1	C	315	CYS	3.5
2	D	146	GLY	3.5
2	B	440	ALA	3.5
2	D	9	ALA	3.5
2	B	37	HIS	3.5
3	E	140	LYS	3.5
2	D	201	THR	3.5
4	F	362	ALA	3.4
2	D	358	ILE	3.4
2	D	441	ASP	3.4
2	D	59	ASN	3.4
4	F	171	ASP	3.4
2	D	214	PHE	3.4
4	F	256	TYR	3.4
4	F	240	LEU	3.4
4	F	244	CYS	3.3
1	A	136	LEU	3.3
2	D	286	LEU	3.3
2	D	213	CYS	3.3
3	E	136	ASN	3.2
2	B	279	GLY	3.2
4	F	163	SER	3.2
4	F	98	TYR	3.2
3	E	133	VAL	3.2
2	D	147	SER	3.2
2	D	150	GLY	3.2
2	B	253	ARG	3.2
3	E	48	GLU	3.2
2	B	278	ARG	3.1
2	D	210	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	138	ARG	3.1
4	F	245	ILE	3.1
2	D	202	TYR	3.1
2	B	74	THR	3.1
2	B	59	ASN	3.1
4	F	129	GLU	3.1
4	F	380	HIS	3.0
2	D	399	PHE	3.0
1	A	169	PHE	3.0
2	D	136	GLN	3.0
1	C	440	VAL	3.0
2	B	241	CYS	3.0
4	F	103	THR	3.0
2	D	56	ALA	2.9
2	B	58	GLY	2.9
2	D	141	LEU	2.9
2	D	401	ARG	2.9
2	D	12	CYS	2.9
1	A	279	GLU	2.8
3	E	46	SER	2.8
2	D	198	THR	2.8
3	E	128	LYS	2.8
2	D	215	ARG	2.8
4	F	137	ARG	2.8
2	B	218	LYS	2.8
4	F	257	GLU	2.8
2	D	46	LEU	2.8
2	D	203	CYS	2.8
4	F	130	VAL	2.7
2	D	406	HIS	2.7
3	E	141	GLU	2.7
4	F	147	TRP	2.7
3	E	24	LEU	2.7
3	E	132	GLU	2.7
2	D	151	THR	2.7
4	F	126	ASP	2.7
2	D	85	GLN	2.7
2	D	74	THR	2.7
2	D	171	VAL	2.6
2	D	13	GLY	2.6
2	D	416	MET	2.6
2	D	97	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	379	HIS	2.6
3	E	25	LYS	2.6
2	D	322	ARG	2.6
2	B	216	THR	2.6
4	F	24	THR	2.6
2	D	404	PHE	2.6
2	B	280	SER	2.6
4	F	194	PRO	2.6
2	D	127	GLU	2.5
2	D	75	MET	2.5
4	F	192	LEU	2.5
4	F	1	MET	2.5
4	F	145	ASN	2.5
1	A	33	ASP	2.5
2	B	38	GLY	2.5
2	D	113	GLU	2.5
2	B	284	ARG	2.5
2	D	155	SER	2.5
1	C	1	MET	2.5
4	F	250	SER	2.5
4	F	21	LEU	2.4
1	C	165	SER	2.4
2	D	413	MET	2.4
2	D	7	ILE	2.4
4	F	9	GLU	2.4
2	D	166	MET	2.4
2	D	222	PRO	2.4
2	B	85	GLN	2.4
2	D	8	GLN	2.4
2	D	323	MET	2.4
2	D	278	ARG	2.4
4	F	258	GLU	2.4
2	D	216	THR	2.4
4	F	197	ARG	2.4
2	B	277	SER	2.3
1	A	236	SER	2.3
1	A	346	TRP	2.3
2	B	138	THR	2.3
2	B	439	THR	2.3
3	E	131	GLU	2.3
2	B	94	PHE	2.3
2	D	291	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	237	THR	2.3
1	A	316	CYS	2.3
2	D	408	TYR	2.3
2	D	10	GLY	2.2
2	B	286	LEU	2.2
4	F	140	GLU	2.2
2	D	235	MET	2.2
2	D	409	THR	2.2
4	F	254	GLY	2.2
3	E	23	ILE	2.2
4	F	229	ASN	2.2
4	F	22	LEU	2.2
1	A	280	LYS	2.2
2	B	282	GLN	2.2
4	F	26	GLN	2.2
2	B	167	ASN	2.2
1	A	278	ALA	2.2
2	D	148	GLY	2.2
1	A	237	SER	2.1
2	D	145	THR	2.1
2	D	94	PHE	2.1
4	F	167	SER	2.1
1	A	78	VAL	2.1
1	A	163	LYS	2.1
4	F	175	GLU	2.1
1	C	439	SER	2.1
1	A	218	ASP	2.1
4	F	239	HIS	2.1
2	B	276	THR	2.1
4	F	252	ASN	2.1
4	F	150	LYS	2.1
4	F	227	PRO	2.1
4	F	181	VAL	2.1
1	A	137	VAL	2.1
4	F	73	ARG	2.1
1	A	235	VAL	2.1
1	C	437	VAL	2.0
1	A	276	ILE	2.0
1	A	170	SER	2.0
1	A	239	THR	2.0
1	A	167	LEU	2.0
1	A	201	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	200	CYS	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, 95<sup>th</sup> 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.

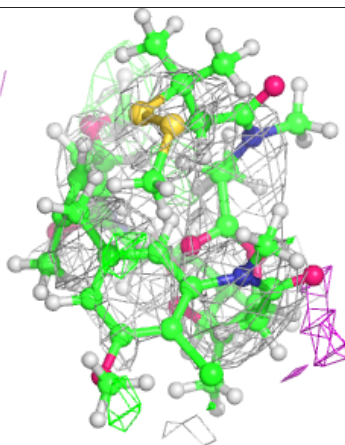
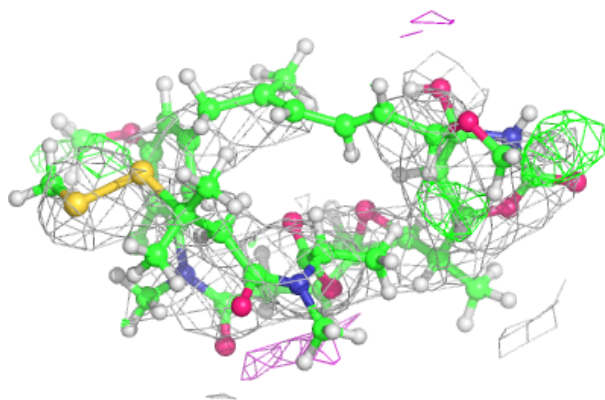
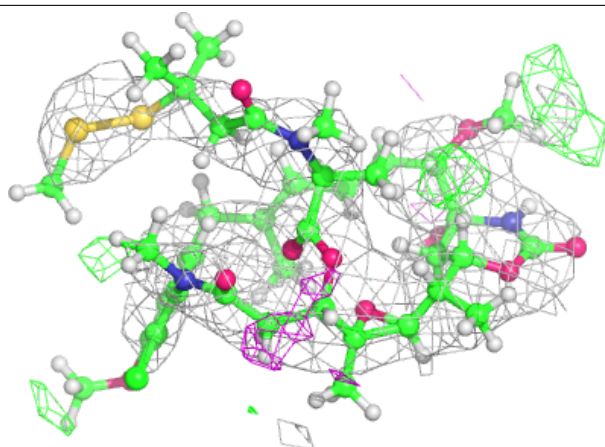
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	BKU	D	502	54/54	0.81	0.42	66,107,134,295	0
11	ACP	F	402	31/31	0.84	0.32	95,134,178,190	0
6	MG	B	502	1/1	0.86	0.21	39,39,39,39	0
6	MG	D	503	1/1	0.88	0.15	78,78,78,78	0
9	MES	B	503	12/12	0.92	0.21	50,73,91,114	0
6	MG	F	401	1/1	0.93	0.40	90,90,90,90	0
5	GTP	D	501	32/32	0.95	0.20	56,66,90,95	0
7	CA	C	503	1/1	0.95	0.06	54,54,54,54	0
8	GDP	B	501	28/28	0.95	0.23	23,37,48,58	0
7	CA	A	503	1/1	0.96	0.10	71,71,71,71	0
6	MG	A	502	1/1	0.96	0.41	39,39,39,39	0
5	GTP	A	501	32/32	0.97	0.24	23,38,50,59	0
5	GTP	C	501	32/32	0.98	0.17	20,33,49,59	0
6	MG	C	502	1/1	0.98	0.11	34,34,34,34	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.

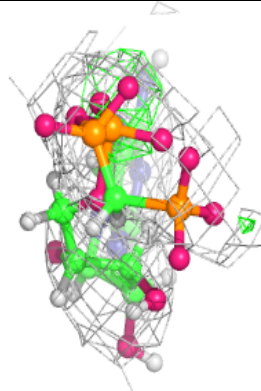
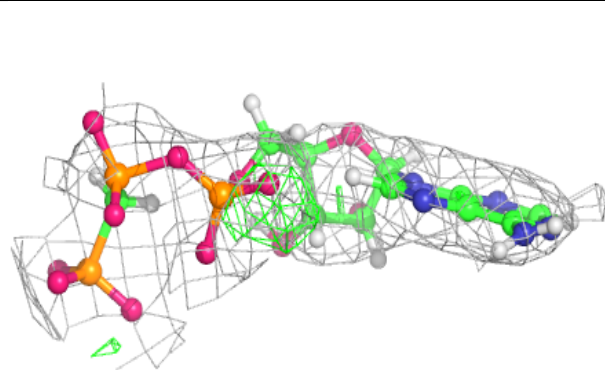
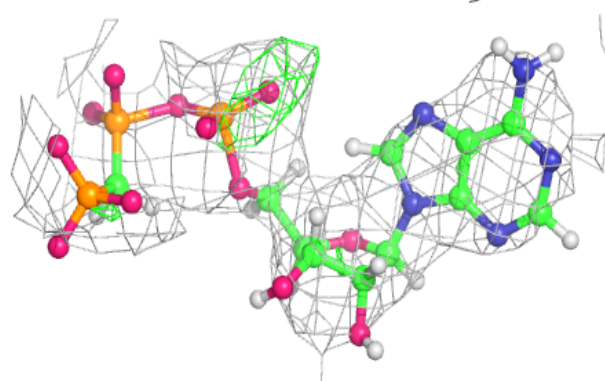


**Electron density around BKU D 502:**

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

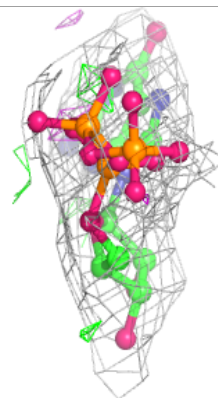
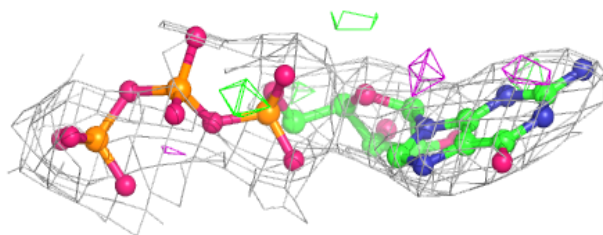
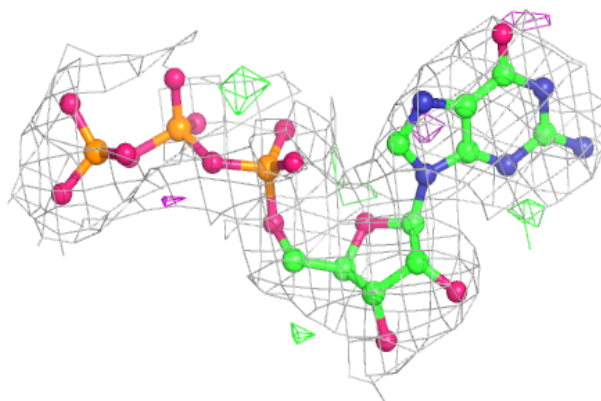
**Electron density around ACP F 402:**

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

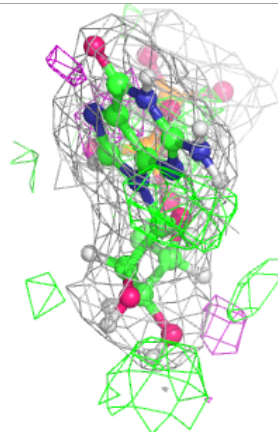
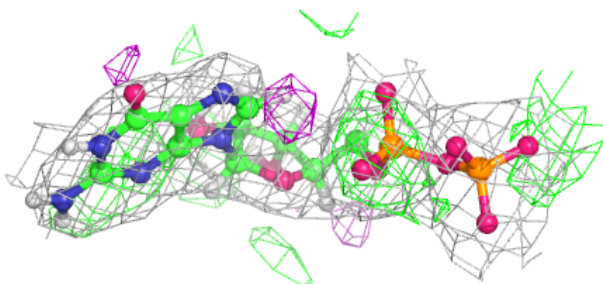
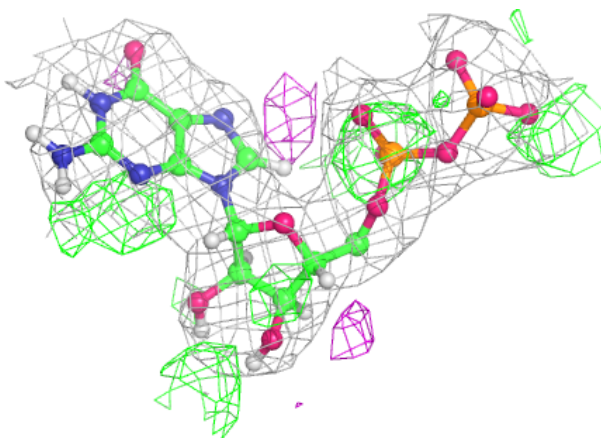


**Electron density around GTP D 501:**

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

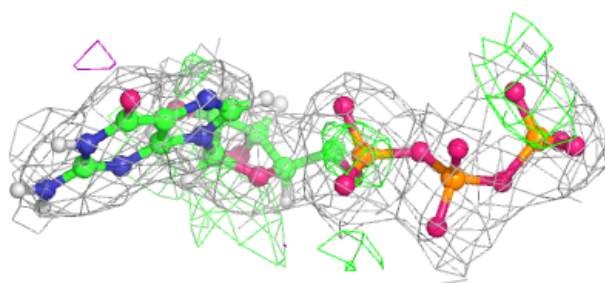
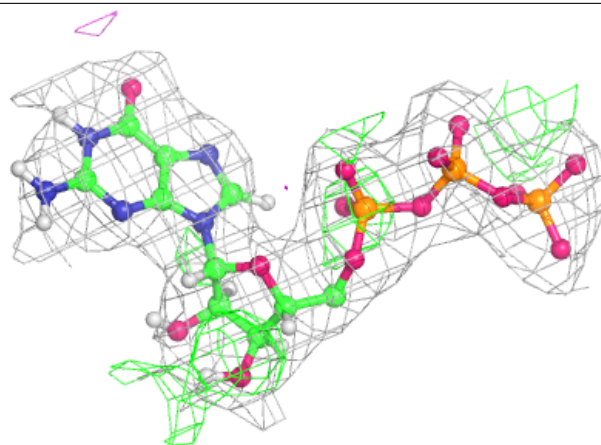
**Electron density around GDP B 501:**

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

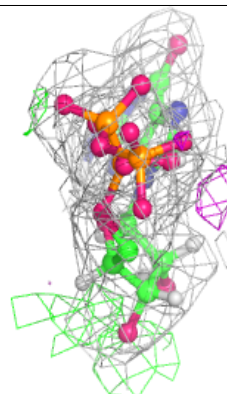
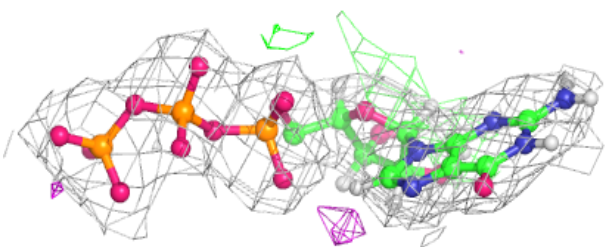
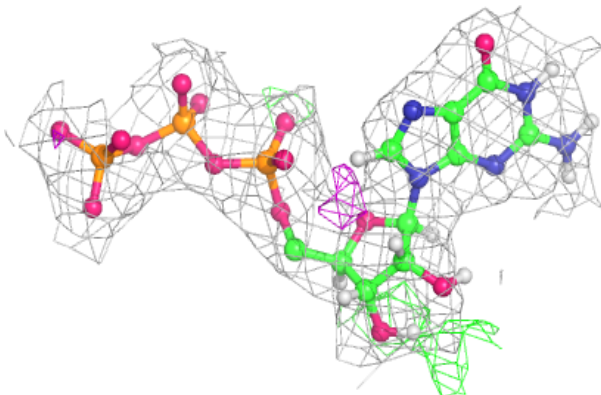


**Electron density around GTP A 501:**

$2mF_o-DF_c$  (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.