



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2021 – 04:12 PM JST

PDB ID : 7E4R  
Title : Crystal structure of tubulin in complex with D-DM1-SMe  
Authors : Wang, Y.; Li, W.  
Deposited on : 2021-02-15  
Resolution : 2.60 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 : 2.20  
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) : 2.20

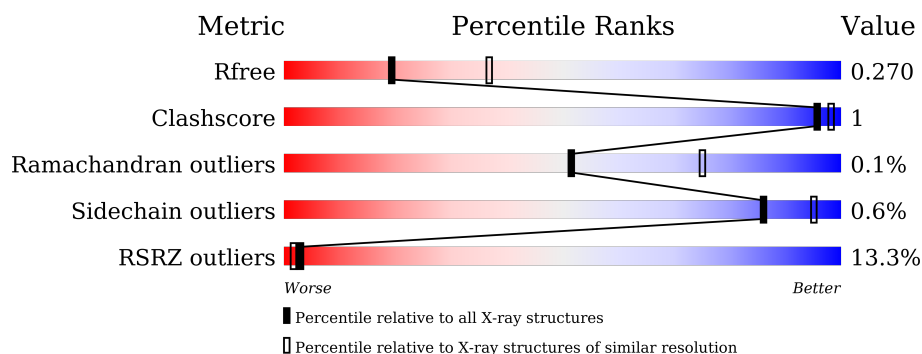
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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>99%</div> <div>.</div> </div>
2	B	431	<div> <div>8%</div> <div>96%</div> <div>..</div> </div>
2	D	431	<div> <div>18%</div> <div>93%</div> <div>5% .</div> </div>
3	E	138	<div> <div>15%</div> <div>87%</div> <div>12%</div> </div>
4	F	380	<div> <div>33%</div> <div>82%</div> <div>6% 12%</div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 34660 atoms, of which 16846 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	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6583	2110	3222	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2014	617	1014	181	197	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

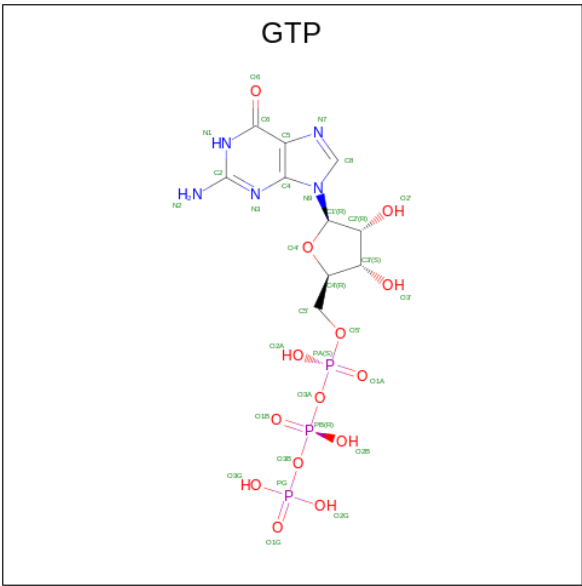
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	0	0
			5442	1761	2698	470	499	14			

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	H	N	O	P	0	0
			42	10	10	5	14	3		

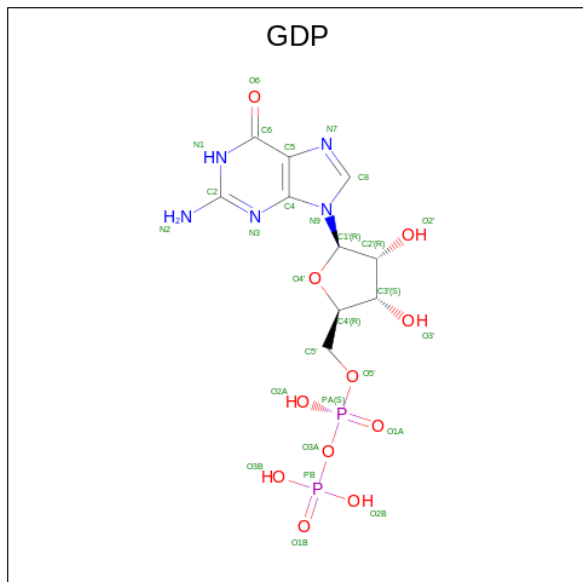
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

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

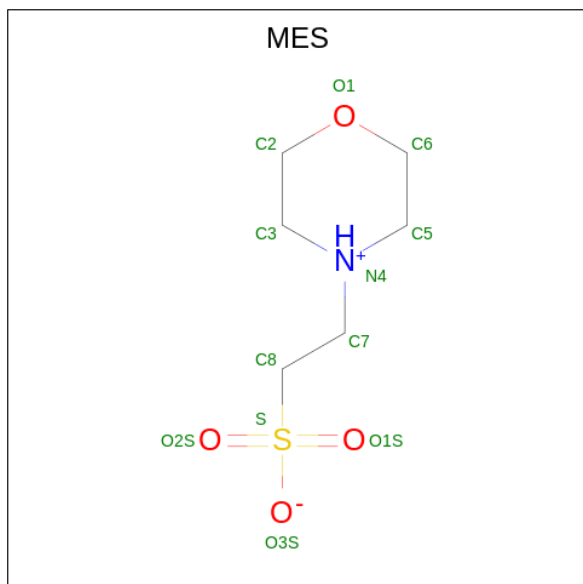
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



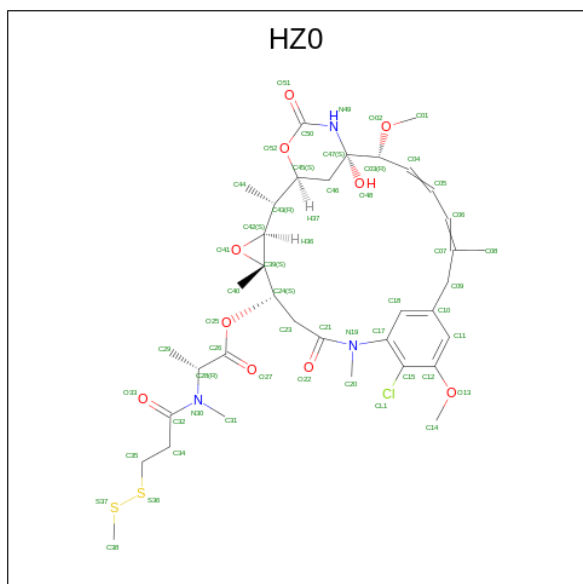
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O	P	
8	B	1	38	10	10	5	11	2	0

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



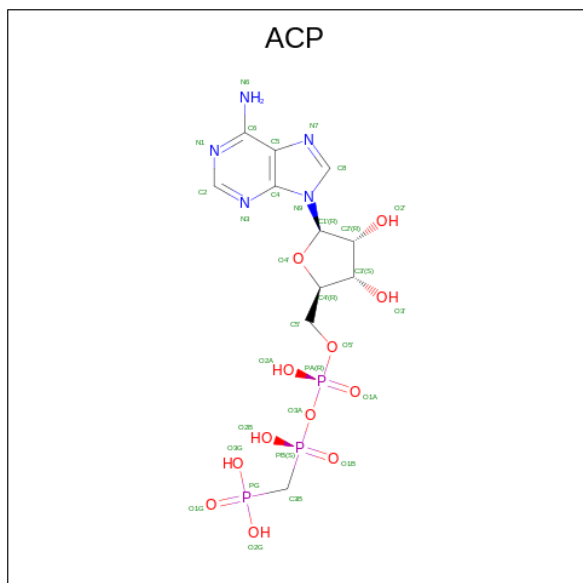
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O	S	
9	B	1	24	6	12	1	4	1	0

- Molecule 10 is (10E,12E)-86-chloro-14-hydroxy-85,14-dimethoxy-33,2,7,10-tetramethyl-12,6-dioxo-7-aza-1(6,4)-oxazinana-3(2,3)-oxirana-8(1,3)-benzenacyclotetradecaphane-10,12-dien-4-yl N-methyl-N-(3-(methylsulfinothioyl)propanoyl)-D-alaninate (three-letter code: HZ0) (formula:  $C_{36}H_{50}ClN_3O_{10}S_2$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	H	N	O	S	
10	D	1	66	36	1	14	3	10	2	0

- 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	0	0
			45	11	14	5	12	3		

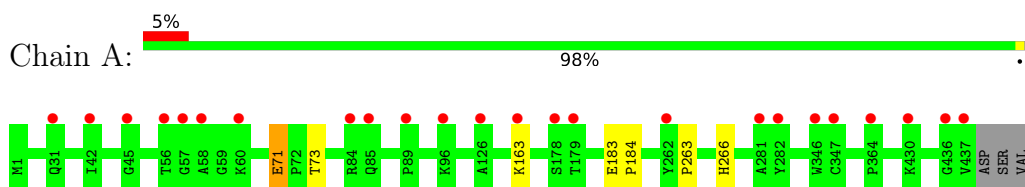
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	58	Total	O	0	0
			58	58		
12	B	68	Total	O	0	0
			68	68		
12	C	113	Total	O	0	0
			113	113		
12	D	31	Total	O	0	0
			31	31		
12	E	14	Total	O	0	0
			14	14		
12	F	38	Total	O	0	0
			38	38		

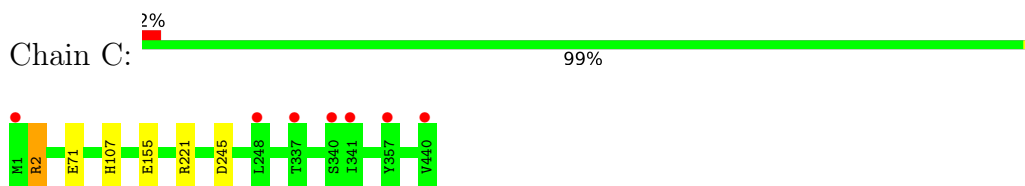
### 3 Residue-property plots [i](#)

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.

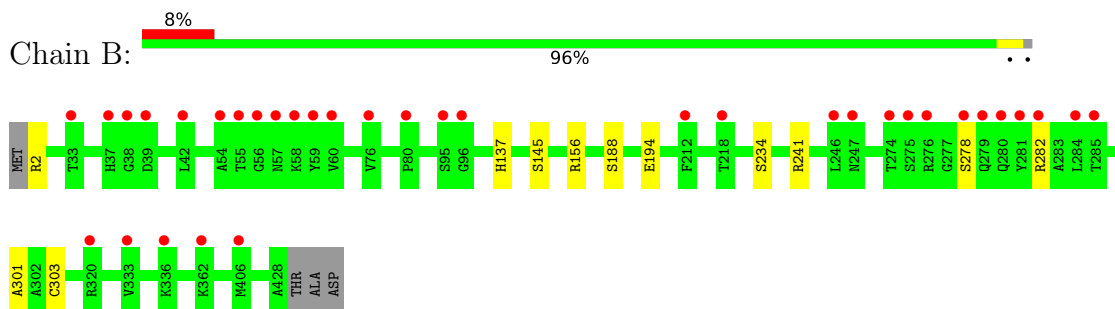
- Molecule 1: Tubulin alpha-1B chain



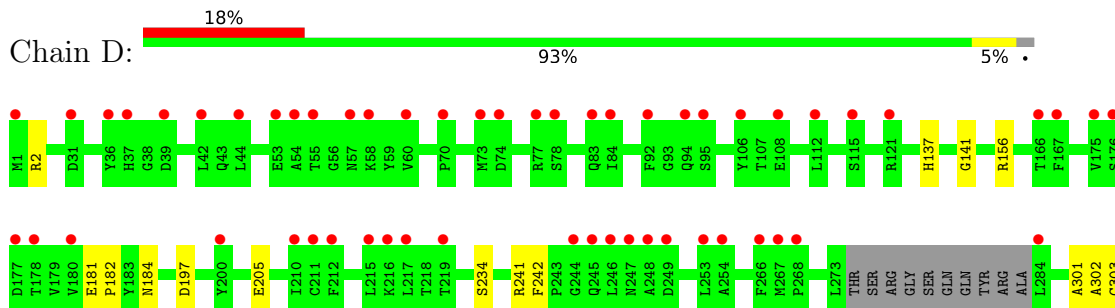
- Molecule 1: Tubulin alpha-1B chain



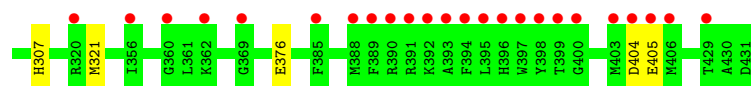
- Molecule 2: Tubulin beta-2B chain



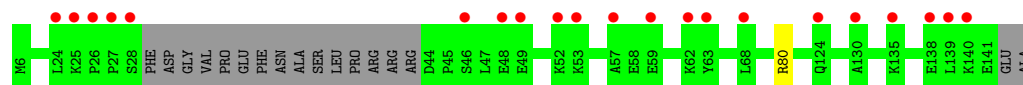
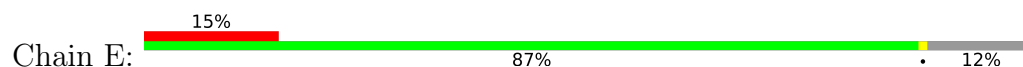
- Molecule 2: Tubulin beta-2B chain



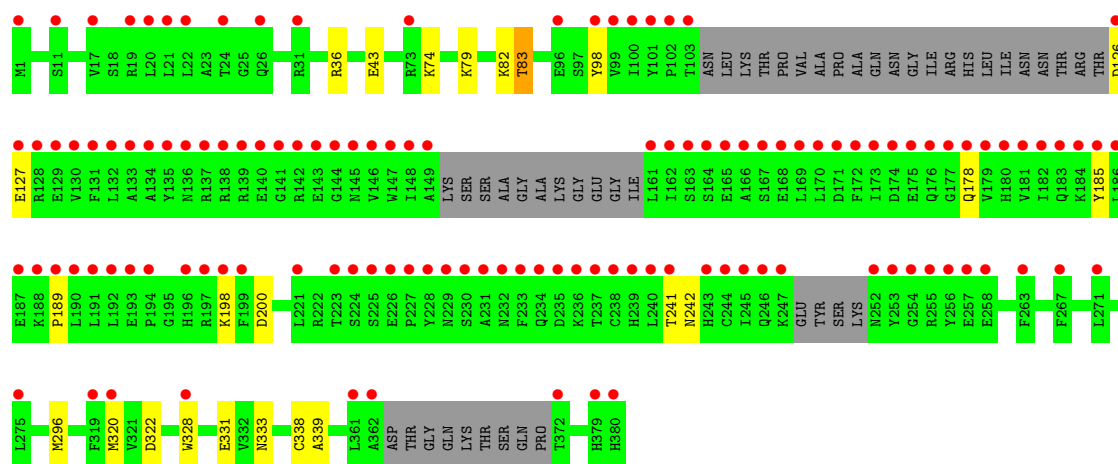
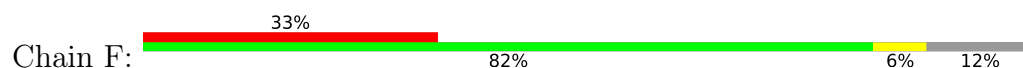




• Molecule 3: Stathmin-4



• 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, $\alpha$ , $\beta$ , $\gamma$	104.98Å 157.23Å 182.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 2.60 45.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.45-2.60) 97.9 (45.45-2.60)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.224 , 0.265 0.228 , 0.270	Depositor DCC
$R_{free}$ test set	1465 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	34660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: GDP, GTP, ACP, HZ0, 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	0.22	0/3494	0.38	0/4743
1	C	0.21	0/3515	0.37	0/4772
2	B	0.21	0/3436	0.37	0/4654
2	D	0.22	0/3382	0.36	0/4581
3	E	0.21	0/1008	0.32	0/1337
4	F	0.21	0/2806	0.36	0/3791
All	All	0.21	0/17641	0.37	0/23878

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	3330	4	0
1	C	3437	3335	3348	3	0
2	B	3361	3222	3238	6	0
2	D	3309	3179	3189	9	0
3	E	1000	1014	1018	1	0
4	F	2744	2698	2709	13	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	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
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	52	14	0	1	0
11	F	31	14	14	1	0
12	A	58	0	0	1	0
12	B	68	0	0	3	0
12	C	113	0	0	2	0
12	D	31	0	0	2	0
12	E	14	0	0	1	0
12	F	38	0	0	1	0
All	All	17814	16846	16906	38	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 (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:N	12:B:603:HOH:O	2.28	0.66
4:F:79:LYS:O	4:F:83:THR:OG1	2.15	0.65
4:F:333:ASN:ND2	11:F:401:ACP:O1G	2.33	0.62
9:B:503:MES:O2S	12:B:601:HOH:O	2.15	0.62
1:C:107:HIS:NE2	12:C:601:HOH:O	2.31	0.61
1:C:155:GLU:OE1	12:C:601:HOH:O	2.17	0.59
1:A:163:LYS:NZ	12:A:601:HOH:O	2.35	0.59
2:D:404:ASP:OD1	2:D:405:GLU:N	2.35	0.59
4:F:178:GLN:N	4:F:178:GLN:OE1	2.37	0.58
3:E:80:ARG:NH1	12:E:203:HOH:O	2.36	0.58
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.18	0.56
2:B:145:SER:HG	2:B:188:SER:HG	1.54	0.55
4:F:126:ASP:OD1	4:F:127:GLU:N	2.38	0.55
4:F:338:CYS:SG	4:F:339:ALA:N	2.80	0.55
2:D:2:ARG:NH1	12:D:611:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:36:ARG:NH2	12:F:506:HOH:O	2.43	0.51
2:B:282:ARG:NH2	12:B:611:HOH:O	2.43	0.51
2:D:301:ALA:O	2:D:303:CYS:N	2.45	0.49
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.45	0.48
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.35	0.48
1:A:71:GLU:OE1	1:A:73:THR:N	2.48	0.47
1:A:263:PRO:O	1:A:266:HIS:ND1	2.38	0.46
2:B:156:ARG:NH1	2:B:194:GLU:O	2.48	0.46
2:D:307:HIS:ND1	2:D:376:GLU:OE1	2.40	0.46
2:B:301:ALA:O	2:B:303:CYS:N	2.50	0.45
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.44	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.33	0.44
2:D:234:SER:O	2:D:241:ARG:NH2	2.51	0.44
2:D:141:GLY:O	2:D:184:ASN:ND2	2.51	0.43
2:B:234:SER:O	2:B:241:ARG:NH2	2.49	0.43
10:D:502:HZ0:C29	10:D:502:HZ0:C34	2.97	0.42
2:D:242:PHE:O	12:D:601:HOH:O	2.21	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
1:C:2:ARG:HA	1:C:2:ARG:HE	1.84	0.41
4:F:189:PRO:HA	4:F:322:ASP:HA	2.02	0.41
4:F:320:MET:O	4:F:328:TRP:N	2.47	0.41
4:F:43:GLU:OE2	4:F:43:GLU:N	2.52	0.40
4:F:82:LYS:HZ2	4:F:98:TYR:HA	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%)	421 (97%)	14 (3%)	0	100	100
1	C	438/440 (100%)	429 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	425/431 (99%)	412 (97%)	12 (3%)	1 (0%)	47	71
2	D	417/431 (97%)	403 (97%)	13 (3%)	1 (0%)	47	71
3	E	117/138 (85%)	116 (99%)	1 (1%)	0	100	100
4	F	324/380 (85%)	310 (96%)	14 (4%)	0	100	100
All	All	2156/2260 (95%)	2091 (97%)	63 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	302	ALA
2	B	278	SER

### 5.3.2 Protein sidechains ⓘ

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	371/371 (100%)	367 (99%)	4 (1%)	73	88
2	B	369/372 (99%)	368 (100%)	1 (0%)	92	98
2	D	364/372 (98%)	361 (99%)	3 (1%)	81	92
3	E	109/123 (89%)	109 (100%)	0	100	100
4	F	301/338 (89%)	298 (99%)	3 (1%)	76	90
All	All	1882/1947 (97%)	1870 (99%)	12 (1%)	86	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
2	B	137	HIS
1	C	2	ARG
1	C	71	GLU
1	C	221	ARG

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Mol	Chain	Res	Type
1	C	245	ASP
2	D	137	HIS
2	D	205	GLU
2	D	321	MET
4	F	83	THR
4	F	242	ASN
4	F	296	MET

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

### 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 13 ligands modelled in this entry, 6 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	$\# Z  > 2$
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.78	7 (21%)
10	HZ0	D	502	-	53,55,55	2.28	15 (28%)	61,81,81	4.27	28 (45%)
11	ACP	F	401	-	27,33,33	4.38	8 (29%)	32,52,52	1.63	7 (21%)

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	1.13	2 (8%)	31,47,47	1.96	8 (25%)
9	MES	B	503	-	12,12,12	2.32	1 (8%)	14,16,16	2.36	7 (50%)
5	GTP	C	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.78	7 (21%)
5	GTP	D	501	6	26,34,34	0.93	1 (3%)	33,54,54	1.75	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
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3
10	HZ0	D	502	-	-	22/61/89/89	0/2/4/4
11	ACP	F	401	-	-	2/15/38/38	0/3/3/3
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
5	GTP	D	501	6	-	6/18/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	20.00	1.80	1.58
9	B	503	MES	C8-S	-7.80	1.66	1.77
10	D	502	HZ0	C32-N30	7.41	1.47	1.35
11	F	401	ACP	PA-O5'	7.31	1.88	1.59
10	D	502	HZ0	O52-C45	-5.55	1.38	1.46
10	D	502	HZ0	C21-N19	5.32	1.46	1.35
10	D	502	HZ0	O25-C26	4.22	1.44	1.34
10	D	502	HZ0	O25-C24	-3.99	1.39	1.46
8	B	501	GDP	C6-C5	3.98	1.48	1.41
10	D	502	HZ0	C06-C07	3.85	1.38	1.34
11	F	401	ACP	C5'-C4'	3.77	1.63	1.51
10	D	502	HZ0	O41-C39	3.72	1.50	1.45
10	D	502	HZ0	C05-C06	3.60	1.54	1.43
10	D	502	HZ0	O13-C12	3.41	1.42	1.37
11	F	401	ACP	O5'-C5'	-3.04	1.33	1.44
5	C	501	GTP	C6-N1	3.03	1.38	1.33
5	A	501	GTP	C6-N1	3.02	1.38	1.33
5	D	501	GTP	C6-N1	2.98	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	HZ0	C09-C07	2.93	1.55	1.51
11	F	401	ACP	C2-N1	2.69	1.38	1.33
10	D	502	HZ0	C50-N49	2.69	1.40	1.34
10	D	502	HZ0	C09-C10	2.65	1.55	1.51
11	F	401	ACP	C4-N3	2.48	1.39	1.35
10	D	502	HZ0	C46-C45	2.46	1.57	1.52
10	D	502	HZ0	C17-N19	2.36	1.47	1.44
8	B	501	GDP	C5-C4	2.28	1.47	1.40
11	F	401	ACP	C2-N3	2.24	1.35	1.32
10	D	502	HZ0	C47-N49	-2.20	1.43	1.46
11	F	401	ACP	C2'-C1'	2.01	1.56	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	HZ0	O41-C39-C40	-20.58	84.63	114.17
10	D	502	HZ0	C40-C39-C24	-10.01	86.76	114.51
10	D	502	HZ0	O48-C47-N49	-9.57	86.33	110.21
10	D	502	HZ0	O41-C39-C24	9.34	132.43	115.00
10	D	502	HZ0	O48-C47-C46	-7.99	87.76	109.98
10	D	502	HZ0	C24-O25-C26	-5.62	108.18	118.18
9	B	503	MES	C5-N4-C3	5.48	121.16	108.83
10	D	502	HZ0	C23-C24-C39	-5.40	103.21	114.60
10	D	502	HZ0	O13-C12-C15	5.37	121.89	115.53
5	C	501	GTP	N3-C2-N1	-5.34	120.10	127.22
5	A	501	GTP	N3-C2-N1	-5.24	120.23	127.22
10	D	502	HZ0	O25-C24-C39	5.23	117.29	105.48
10	D	502	HZ0	C18-C17-C15	-4.88	116.31	122.53
5	D	501	GTP	N3-C2-N1	-4.76	120.87	127.22
10	D	502	HZ0	C40-C39-C42	4.73	131.76	121.05
8	B	501	GDP	C2-N3-C4	4.71	120.74	115.36
5	C	501	GTP	C2-N3-C4	4.27	120.23	115.36
5	A	501	GTP	C2-N3-C4	4.24	120.20	115.36
8	B	501	GDP	C6-C5-C4	-4.18	116.81	120.80
10	D	502	HZ0	O25-C26-C28	4.17	119.85	110.80
8	B	501	GDP	C6-N1-C2	4.13	122.49	115.93
5	D	501	GTP	C2-N3-C4	4.06	119.99	115.36
11	F	401	ACP	O1B-PB-C3B	3.97	119.57	109.07
11	F	401	ACP	O5'-PA-O1A	-3.95	93.64	109.07
8	B	501	GDP	C5-C6-N1	-3.84	118.17	123.43
9	B	503	MES	C7-N4-C5	3.84	121.05	111.23
5	D	501	GTP	PA-O3A-PB	-3.78	119.86	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	PB-O3B-PG	-3.41	121.12	132.83
8	B	501	GDP	N3-C2-N1	-3.41	122.68	127.22
10	D	502	HZ0	O25-C26-O27	-3.40	117.58	123.94
5	C	501	GTP	PA-O3A-PB	-3.26	121.65	132.83
10	D	502	HZ0	C17-C18-C10	3.25	124.71	120.23
5	A	501	GTP	PA-O3A-PB	-3.25	121.68	132.83
10	D	502	HZ0	C20-N19-C17	3.17	121.15	116.72
10	D	502	HZ0	C28-N30-C32	3.12	128.65	117.64
11	F	401	ACP	PA-O3A-PB	-3.12	122.67	132.56
10	D	502	HZ0	O13-C12-C11	-3.05	118.87	124.12
10	D	502	HZ0	C31-N30-C32	-3.03	115.01	122.01
5	A	501	GTP	PB-O3B-PG	-3.02	122.48	132.83
5	D	501	GTP	C5-C6-N1	-3.00	119.33	123.43
5	C	501	GTP	PB-O3B-PG	-2.89	122.90	132.83
5	A	501	GTP	C5-C6-N1	-2.88	119.49	123.43
5	C	501	GTP	C5-C6-N1	-2.88	119.49	123.43
10	D	502	HZ0	C29-C28-N30	2.87	116.65	111.94
8	B	501	GDP	PA-O3A-PB	-2.81	123.17	132.83
10	D	502	HZ0	C15-C17-N19	2.80	123.59	120.71
9	B	503	MES	C6-C5-N4	-2.65	106.09	110.10
10	D	502	HZ0	C44-C43-C45	-2.62	107.60	111.43
5	C	501	GTP	C6-N1-C2	2.60	120.07	115.93
8	B	501	GDP	C3'-C2'-C1'	2.60	104.89	100.98
11	F	401	ACP	O2A-PA-O5'	-2.54	95.96	107.75
10	D	502	HZ0	O33-C32-N30	-2.53	117.45	121.88
10	D	502	HZ0	C45-C43-C42	2.52	117.67	111.19
8	B	501	GDP	C4-C5-N7	-2.52	106.77	109.40
5	A	501	GTP	C6-N1-C2	2.51	119.92	115.93
5	C	501	GTP	C3'-C2'-C1'	2.42	104.62	100.98
10	D	502	HZ0	O41-C42-C39	2.42	61.54	59.83
5	D	501	GTP	C3'-C2'-C1'	2.41	104.61	100.98
9	B	503	MES	O2S-S-C8	2.40	109.81	106.92
10	D	502	HZ0	C14-O13-C12	-2.40	113.91	117.53
5	D	501	GTP	C6-N1-C2	2.33	119.62	115.93
9	B	503	MES	O1S-S-C8	2.27	109.65	106.92
11	F	401	ACP	O1G-PG-C3B	-2.26	106.36	111.24
10	D	502	HZ0	C44-C43-C42	-2.23	107.73	112.55
5	A	501	GTP	C3'-C2'-C1'	2.21	104.31	100.98
11	F	401	ACP	O2B-PB-C3B	2.16	115.40	106.58
9	B	503	MES	C7-N4-C3	2.09	116.59	111.23
9	B	503	MES	O3S-S-C8	2.05	109.09	105.77
10	D	502	HZ0	O41-C39-C42	-2.05	58.00	59.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	O3'-C3'-C4'	2.03	116.91	111.05
10	D	502	HZ0	C38-S37-S36	2.02	109.56	102.58

There are no chirality outliers.

All (53) 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	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
10	D	502	HZ0	C23-C24-C39-C42
10	D	502	HZ0	O25-C26-C28-N30
10	D	502	HZ0	O27-C26-C28-N30
10	D	502	HZ0	C28-C26-O25-C24
10	D	502	HZ0	C29-C28-N30-C31
10	D	502	HZ0	C29-C28-N30-C32
10	D	502	HZ0	C04-C03-O02-C01
10	D	502	HZ0	O02-C03-C47-C46
10	D	502	HZ0	C03-C04-C05-C06
10	D	502	HZ0	C05-C06-C07-C08
10	D	502	HZ0	C05-C06-C07-C09
10	D	502	HZ0	C15-C12-O13-C14
10	D	502	HZ0	C32-C34-C35-S36
10	D	502	HZ0	C44-C43-C45-C46
10	D	502	HZ0	O27-C26-O25-C24
10	D	502	HZ0	C04-C05-C06-C07
10	D	502	HZ0	C11-C12-O13-C14
5	A	501	GTP	C3'-C4'-C5'-O5'
10	D	502	HZ0	C44-C43-C45-O52
5	A	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A

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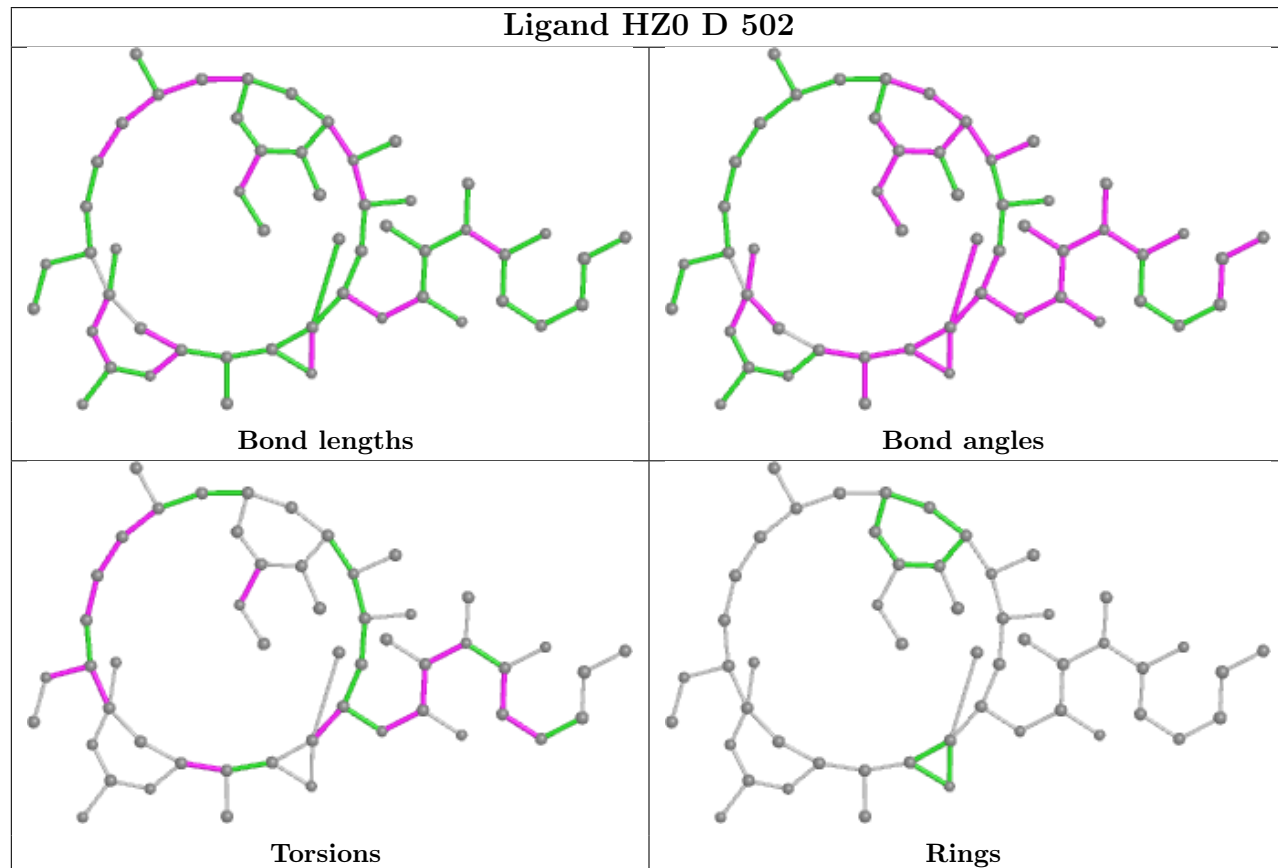
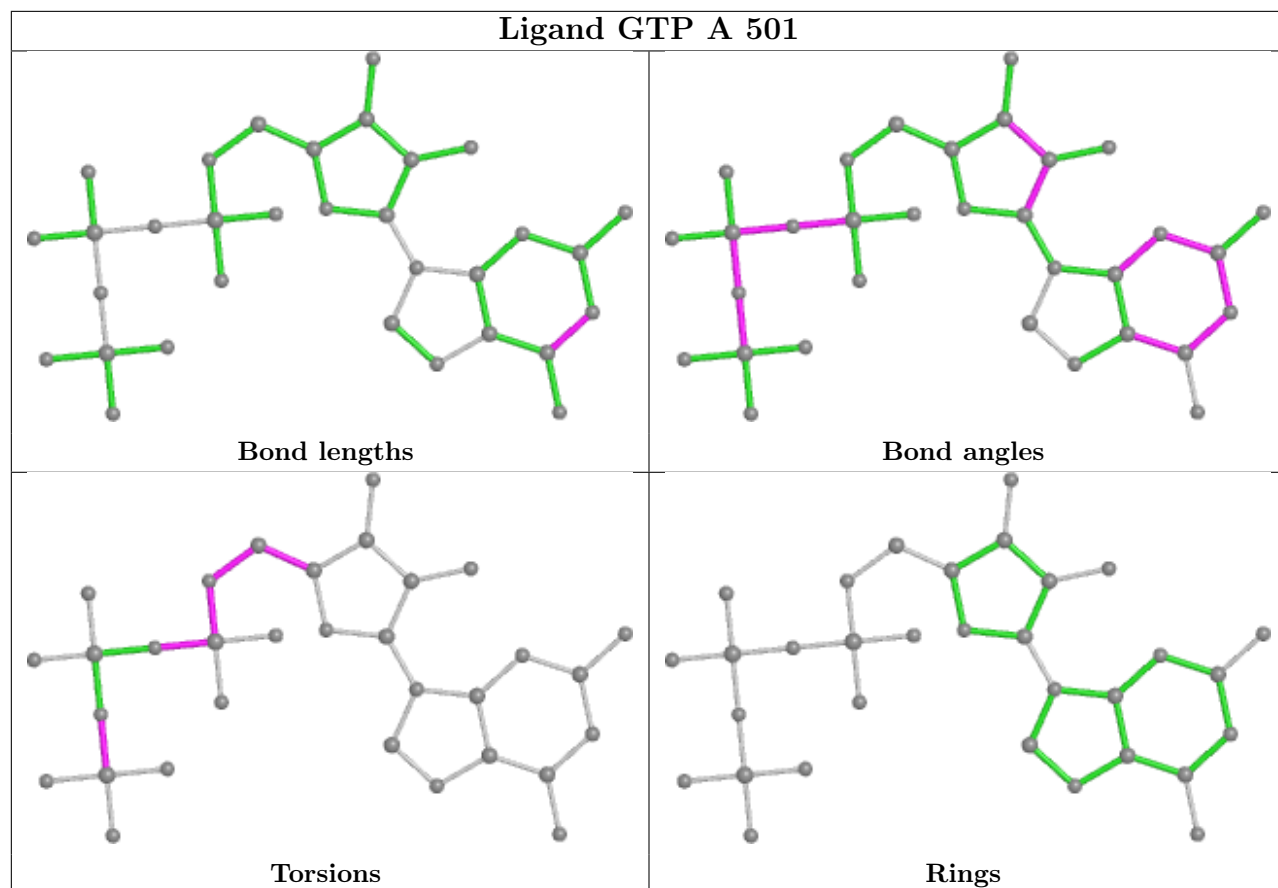
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
10	D	502	HZ0	O25-C26-C28-C29
5	A	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	PB-O3A-PA-O2A
5	D	501	GTP	C4'-C5'-O5'-PA
10	D	502	HZ0	O33-C32-C34-C35
10	D	502	HZ0	O27-C26-C28-C29
10	D	502	HZ0	N30-C32-C34-C35
5	D	501	GTP	PB-O3B-PG-O2G
8	B	501	GDP	PA-O3A-PB-O3B
5	D	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

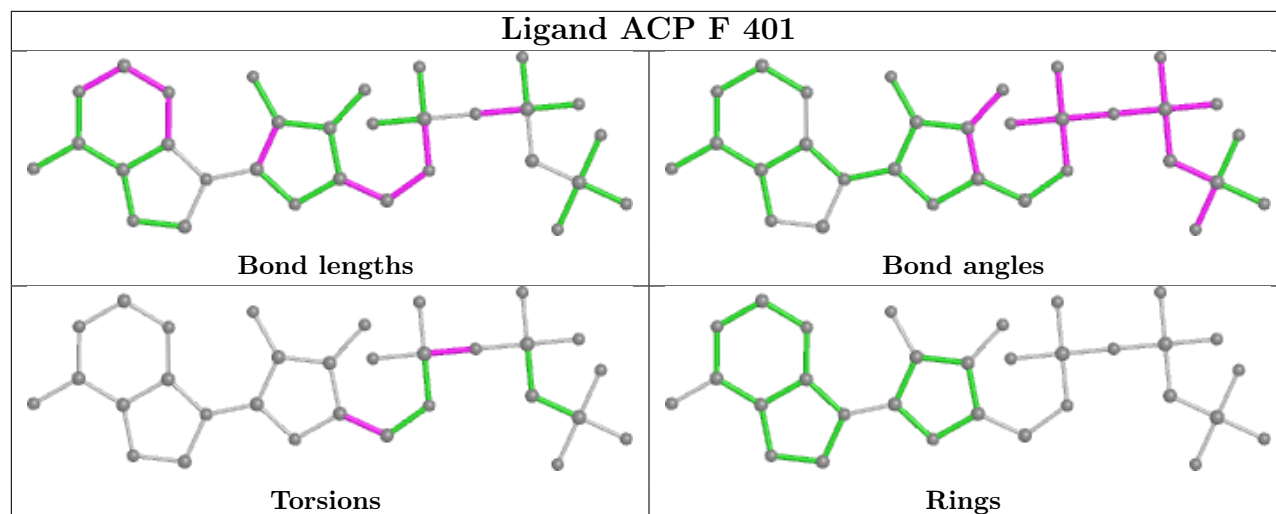
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	HZ0	1	0
11	F	401	ACP	1	0
9	B	503	MES	1	0

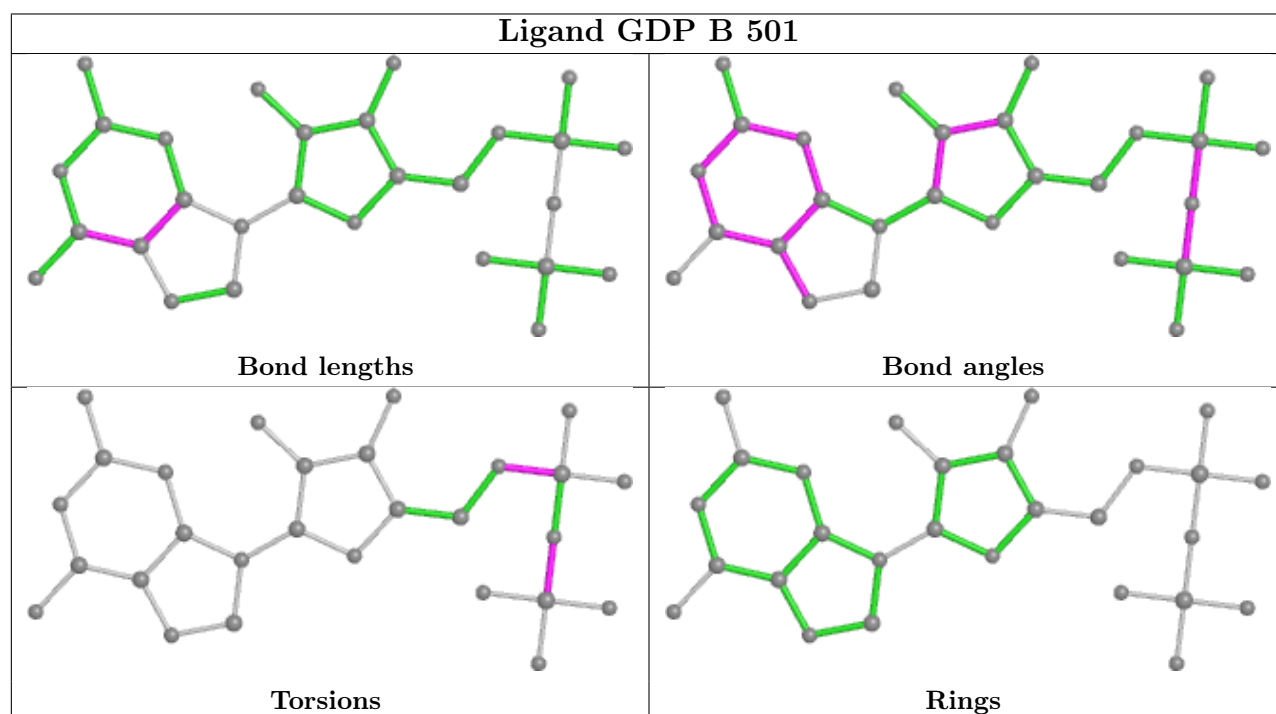
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



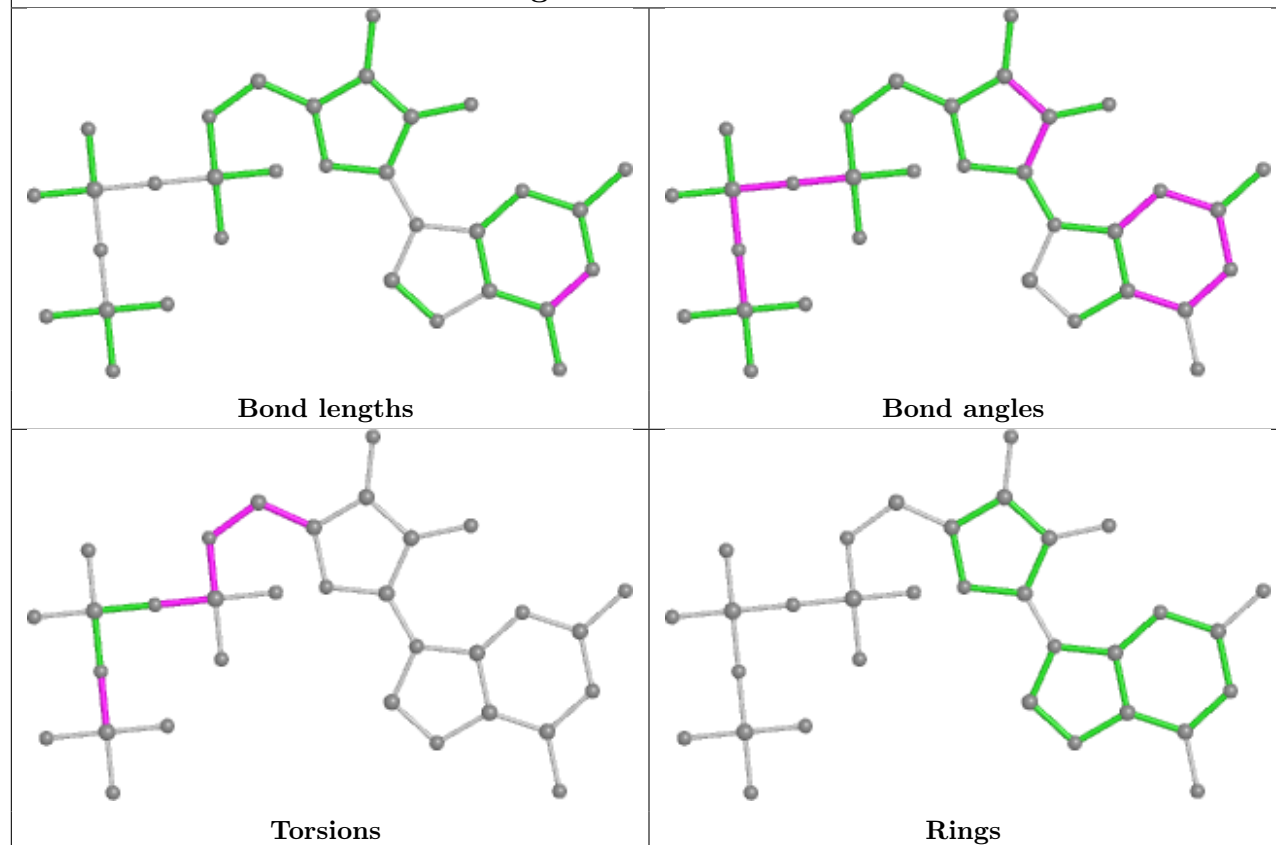
## Ligand ACP F 401



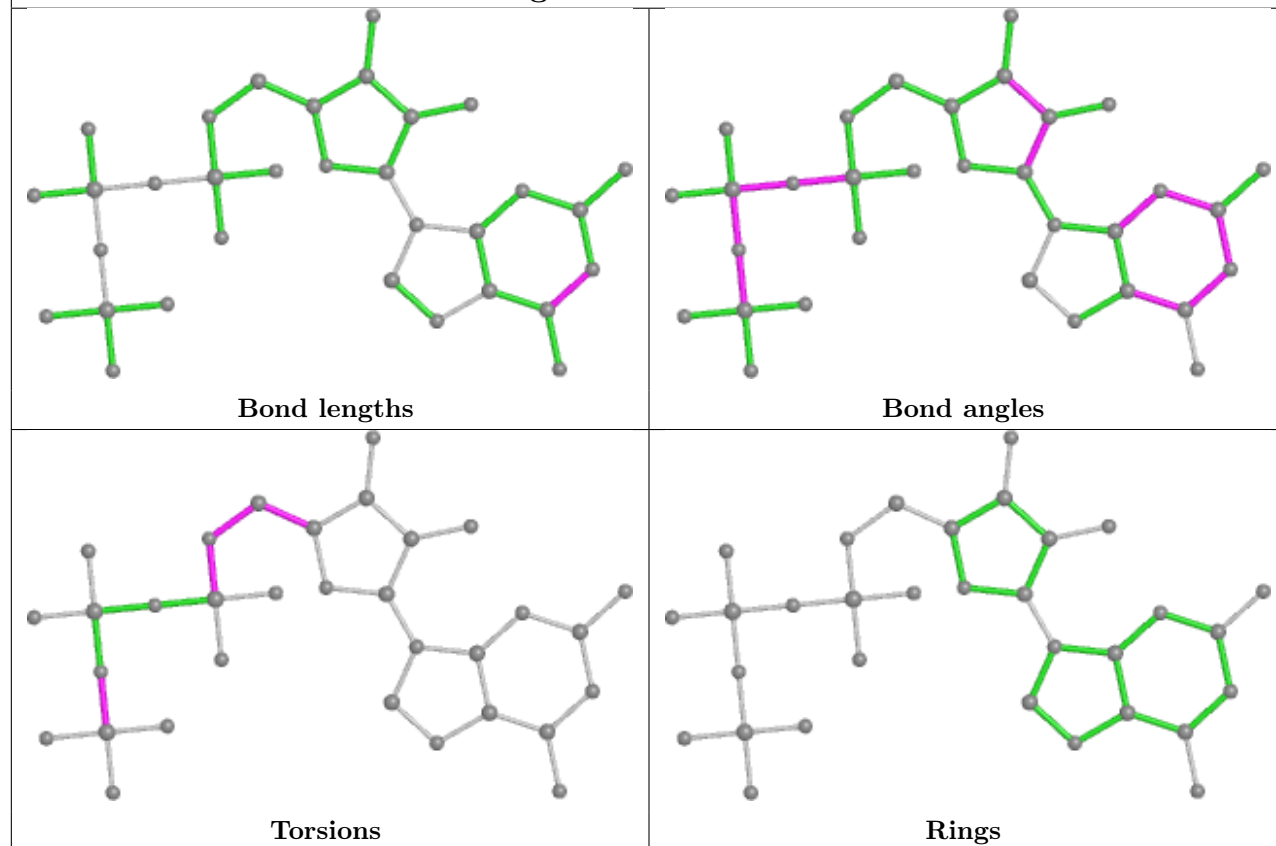
## Ligand GDP B 501



## Ligand GTP C 501



## Ligand GTP D 501



## 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%)	0.50	24 (5%)	25 19	23, 40, 70, 88	0
1	C	440/440 (100%)	0.08	7 (1%)	72 68	16, 31, 57, 83	0
2	B	427/431 (99%)	0.65	35 (8%)	11 8	19, 41, 74, 124	0
2	D	421/431 (97%)	1.19	79 (18%)	1 0	29, 58, 93, 120	0
3	E	121/138 (87%)	1.03	21 (17%)	1 0	31, 56, 88, 106	0
4	F	334/380 (87%)	1.96	124 (37%)	0 0	32, 67, 138, 154	0
All	All	2180/2260 (96%)	0.83	290 (13%)	3 2	16, 46, 102, 154	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	133	ALA	10.7
4	F	169	LEU	10.6
4	F	173	ILE	10.4
4	F	130	VAL	9.0
2	B	57	ASN	7.7
4	F	233	PHE	7.6
4	F	236	LYS	7.5
4	F	245	ILE	7.4
4	F	164	SER	7.1
4	F	101	TYR	7.0
4	F	142	ARG	7.0
4	F	182	ILE	7.0
4	F	231	ALA	6.8
4	F	230	SER	6.7
4	F	134	ALA	6.7
4	F	143	GLU	6.6
4	F	170	LEU	6.6
4	F	244	CYS	6.6
4	F	138	ARG	6.5

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Mol	Chain	Res	Type	RSRZ
2	D	55	THR	6.3
4	F	137	ARG	6.3
4	F	234	GLN	6.2
4	F	172	PHE	6.1
4	F	103	THR	6.0
4	F	232	ASN	6.0
4	F	256	TYR	5.9
2	D	92	PHE	5.9
4	F	235	ASP	5.8
4	F	184	LYS	5.8
4	F	176	GLN	5.8
4	F	99	VAL	5.7
4	F	175	GLU	5.6
1	C	340	SER	5.6
2	D	389	PHE	5.5
4	F	246	GLN	5.5
4	F	161	LEU	5.5
4	F	100	ILE	5.4
4	F	129	GLU	5.4
4	F	139	ARG	5.3
4	F	166	ALA	5.2
4	F	191	LEU	5.2
2	D	390	ARG	5.1
2	B	55	THR	5.1
4	F	253	TYR	5.0
4	F	131	PHE	5.0
2	B	58	LYS	5.0
4	F	255	ARG	5.0
4	F	225	SER	4.9
4	F	361	LEU	4.9
2	D	44	LEU	4.9
4	F	179	VAL	4.8
2	D	175	VAL	4.8
4	F	136	ASN	4.7
4	F	372	THR	4.7
2	D	395	LEU	4.7
2	D	356	ILE	4.5
4	F	98	TYR	4.5
4	F	146	VAL	4.5
4	F	196	HIS	4.5
4	F	186	LEU	4.5
4	F	144	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
4	F	254	GLY	4.3
4	F	127	GLU	4.3
2	B	54	ALA	4.3
2	B	282	ARG	4.3
2	D	112	LEU	4.3
1	A	262	TYR	4.2
3	E	27	PRO	4.2
4	F	177	GLY	4.2
2	D	215	LEU	4.2
2	B	56	GLY	4.1
3	E	139	LEU	4.1
4	F	148	ILE	4.1
2	B	275	SER	4.1
2	D	391	ARG	4.1
2	D	211	CYS	4.0
4	F	163	SER	4.0
2	D	216	LYS	4.0
2	D	1	MET	4.0
3	E	25	LYS	4.0
2	D	77	ARG	3.9
4	F	223	THR	3.9
4	F	194	PRO	3.9
4	F	102	PRO	3.9
4	F	192	LEU	3.9
4	F	20	LEU	3.9
4	F	135	TYR	3.8
4	F	320	MET	3.8
2	D	108	GLU	3.8
4	F	167	SER	3.8
2	D	217	LEU	3.8
4	F	178	GLN	3.8
4	F	258	GLU	3.8
4	F	221	LEU	3.7
4	F	22	LEU	3.7
2	D	219	THR	3.7
4	F	174	ASP	3.6
2	B	37	HIS	3.6
4	F	237	THR	3.6
2	D	39	ASP	3.6
2	B	280	GLN	3.6
4	F	126	ASP	3.6
4	F	188	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	3.5
2	D	180	VAL	3.5
2	D	37	HIS	3.5
4	F	247	LYS	3.5
1	A	57	GLY	3.5
2	D	94	GLN	3.5
2	D	388	MET	3.4
2	D	399	THR	3.4
2	B	279	GLN	3.4
4	F	228	TYR	3.4
4	F	362	ALA	3.4
2	D	70	PRO	3.4
4	F	21	LEU	3.3
4	F	140	GLU	3.3
2	D	398	TYR	3.3
4	F	168	GLU	3.3
4	F	147	TRP	3.3
4	F	243	HIS	3.3
4	F	239	HIS	3.2
4	F	141	GLY	3.2
1	A	42	ILE	3.2
4	F	162	ILE	3.2
2	D	320	ARG	3.2
1	A	60	LYS	3.2
2	B	284	LEU	3.2
4	F	241	THR	3.2
2	D	58	LYS	3.2
1	C	440	VAL	3.2
2	B	278	SER	3.2
3	E	48	GLU	3.2
3	E	135	LYS	3.1
4	F	171	ASP	3.1
4	F	181	VAL	3.1
4	F	257	GLU	3.1
4	F	149	ALA	3.1
2	B	247	ASN	3.1
2	D	246	LEU	3.1
4	F	379	HIS	3.1
4	F	128	ARG	3.1
4	F	190	LEU	3.1
2	B	38	GLY	3.0
3	E	26	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	392	LYS	3.0
2	D	360	GLY	3.0
4	F	238	CYS	3.0
4	F	380	HIS	3.0
2	D	54	ALA	3.0
4	F	227	PRO	3.0
2	D	83	GLN	3.0
4	F	263	PHE	2.9
1	C	1	MET	2.9
4	F	24	THR	2.9
2	D	405	GLU	2.9
3	E	59	GLU	2.9
4	F	226	GLU	2.9
1	A	56	THR	2.9
4	F	185	TYR	2.9
2	D	74	ASP	2.8
4	F	165	GLU	2.8
2	D	247	ASN	2.8
2	B	336	LYS	2.8
2	D	84	ILE	2.8
2	D	42	LEU	2.8
2	D	362	LYS	2.8
2	B	246	LEU	2.8
2	D	176	SER	2.8
1	A	346	TRP	2.8
2	D	73	MET	2.8
1	A	364	PRO	2.8
2	D	396	HIS	2.8
4	F	197	ARG	2.8
2	D	245	GLN	2.8
4	F	252	ASN	2.8
3	E	62	LYS	2.8
2	D	177	ASP	2.8
2	B	59	TYR	2.7
1	A	179	THR	2.7
2	D	267	MET	2.7
2	D	210	ILE	2.7
4	F	73	ARG	2.7
4	F	96	GLU	2.7
3	E	53	LYS	2.7
4	F	240	LEU	2.6
2	B	274	THR	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	145	ASN	2.6
2	B	406	MET	2.6
4	F	224	SER	2.6
1	C	337	THR	2.6
3	E	138	GLU	2.6
4	F	1	MET	2.6
2	D	284	LEU	2.6
1	C	341	ILE	2.6
2	D	394	PHE	2.6
2	D	31	ASP	2.6
2	D	244	GLY	2.6
2	B	212	PHE	2.5
2	D	200	TYR	2.5
2	D	212	PHE	2.5
1	A	58	ALA	2.5
2	B	281	TYR	2.5
4	F	271	LEU	2.5
1	A	430	LYS	2.5
1	A	436	GLY	2.5
2	B	42	LEU	2.5
1	A	31	GLN	2.5
4	F	31	ARG	2.5
2	D	60	VAL	2.4
2	D	406	MET	2.4
4	F	198	LYS	2.4
1	A	437	VAL	2.4
1	C	357	TYR	2.4
1	A	84	ARG	2.4
2	B	276	ARG	2.4
4	F	183	GLN	2.4
3	E	130	ALA	2.4
2	D	106	TYR	2.4
2	B	95	SER	2.4
1	A	45	GLY	2.4
4	F	193	GLU	2.4
4	F	229	ASN	2.4
2	D	248	ALA	2.4
3	E	57	ALA	2.4
1	A	163	LYS	2.3
1	A	282	TYR	2.3
2	D	53	GLU	2.3
2	D	95	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	333	VAL	2.3
4	F	275	LEU	2.3
1	A	96	LYS	2.3
2	D	403	MET	2.3
3	E	52	LYS	2.3
1	A	178	SER	2.3
2	B	80	PRO	2.3
2	B	76	VAL	2.3
2	D	397	TRP	2.3
4	F	328	TRP	2.3
2	D	253	LEU	2.3
2	B	96	GLY	2.2
2	D	254	ALA	2.2
2	D	266	PHE	2.2
1	C	248	LEU	2.2
2	D	369	GLY	2.2
2	D	178	THR	2.2
4	F	199	PHE	2.2
2	D	115	SER	2.2
4	F	267	PHE	2.2
4	F	180	HIS	2.2
4	F	187	GLU	2.2
2	D	167	PHE	2.2
3	E	68	LEU	2.2
2	D	78	SER	2.2
2	B	33	THR	2.2
2	B	218	THR	2.2
4	F	19	ARG	2.2
1	A	281	ALA	2.1
2	B	320	ARG	2.1
2	D	400	GLY	2.1
2	D	268	PRO	2.1
2	B	60	VAL	2.1
2	D	121	ARG	2.1
4	F	17	VAL	2.1
2	D	385	PHE	2.1
1	A	347	CYS	2.1
2	B	362	LYS	2.1
2	D	393	ALA	2.1
3	E	63	TYR	2.1
3	E	140	LYS	2.1
3	E	49	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	11	SER	2.1
1	A	126	ALA	2.1
2	B	285	THR	2.1
2	D	36	TYR	2.1
2	D	249	ASP	2.1
2	D	166	THR	2.1
2	D	404	ASP	2.1
3	E	46	SER	2.1
2	D	57	ASN	2.0
1	A	89	PRO	2.0
4	F	189	PRO	2.0
2	D	429	THR	2.0
3	E	124	GLN	2.0
4	F	26	GLN	2.0
3	E	24	LEU	2.0
4	F	319	PHE	2.0
3	E	28	SER	2.0
2	B	39	ASP	2.0
1	A	85	GLN	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( $\text{\AA}^2$ )	Q<0.9
6	MG	D	503	1/1	0.61	0.24	73,73,73,73	0
11	ACP	F	401	31/31	0.72	0.28	97,127,164,171	0
10	HZ0	D	502	52/52	0.83	0.36	81,104,153,186	0
5	GTP	D	501	32/32	0.90	0.21	46,68,105,129	0

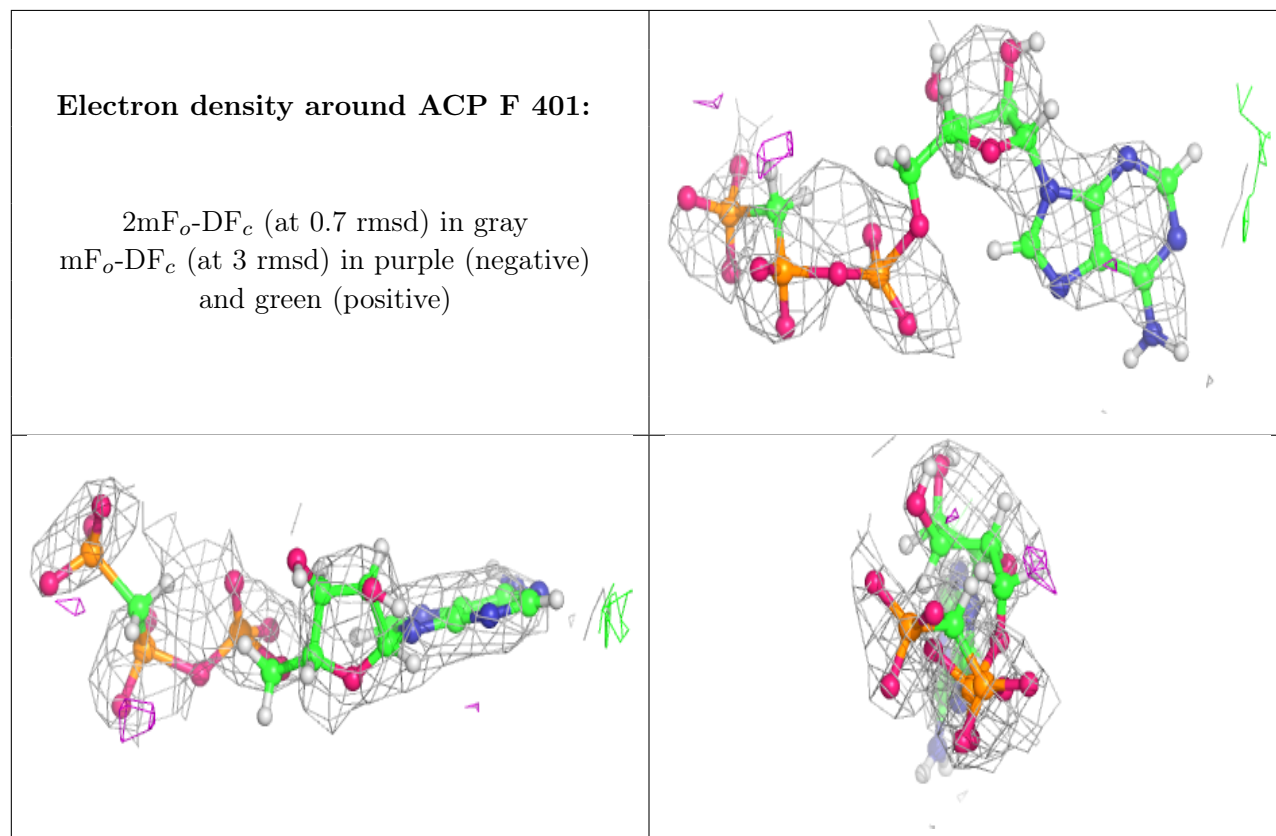
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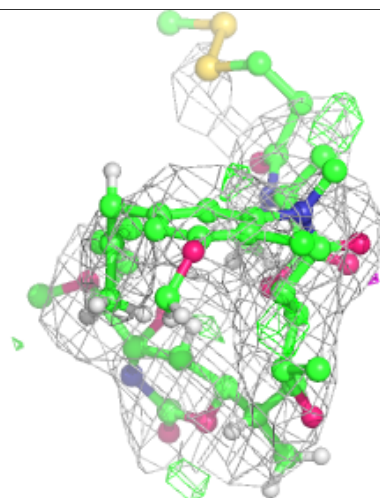
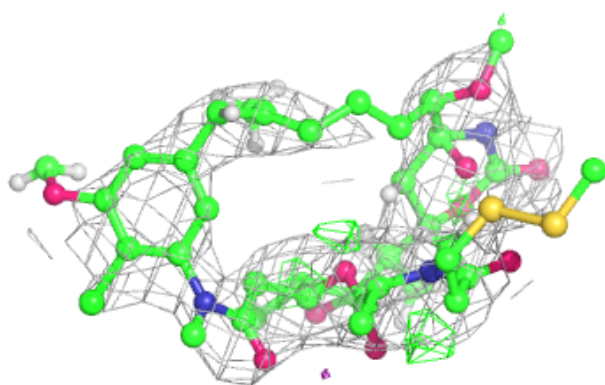
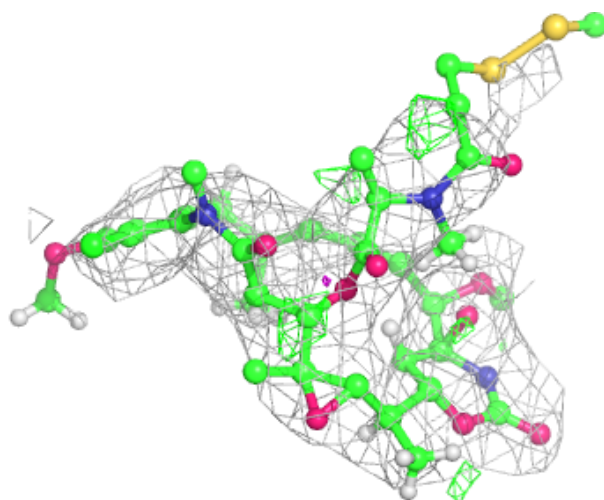
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	502	1/1	0.91	0.32	40,40,40,40	0
7	CA	A	503	1/1	0.93	0.11	67,67,67,67	0
9	MES	B	503	12/12	0.95	0.19	35,49,71,72	0
8	GDP	B	501	28/28	0.96	0.23	17,33,50,60	0
5	GTP	A	501	32/32	0.97	0.24	18,33,45,54	0
5	GTP	C	501	32/32	0.98	0.17	19,24,35,39	0
7	CA	C	503	1/1	0.98	0.08	42,42,42,42	0
6	MG	C	502	1/1	0.99	0.18	22,22,22,22	0
6	MG	A	502	1/1	0.99	0.19	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.



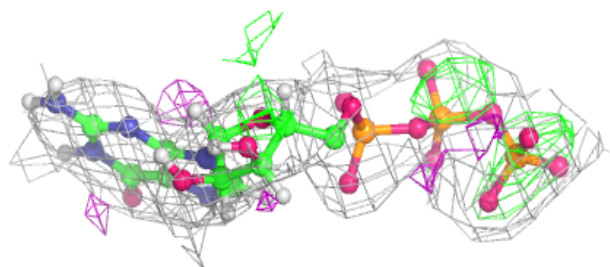
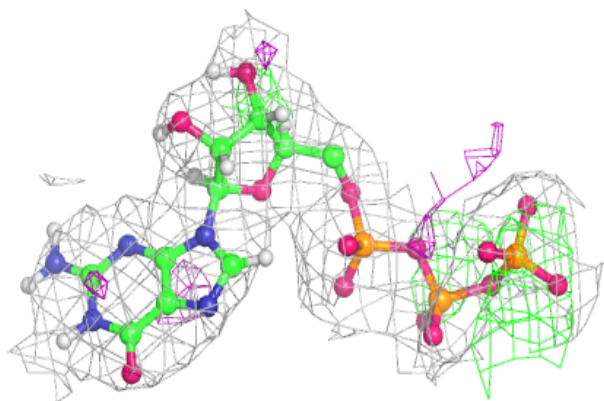
**Electron density around HZ0 D 502:**

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



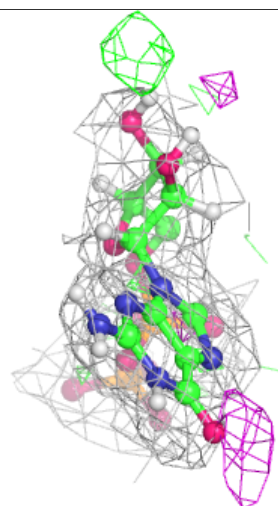
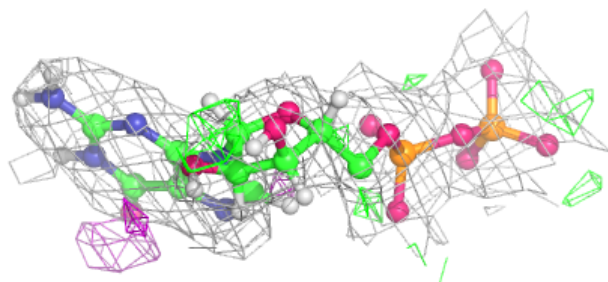
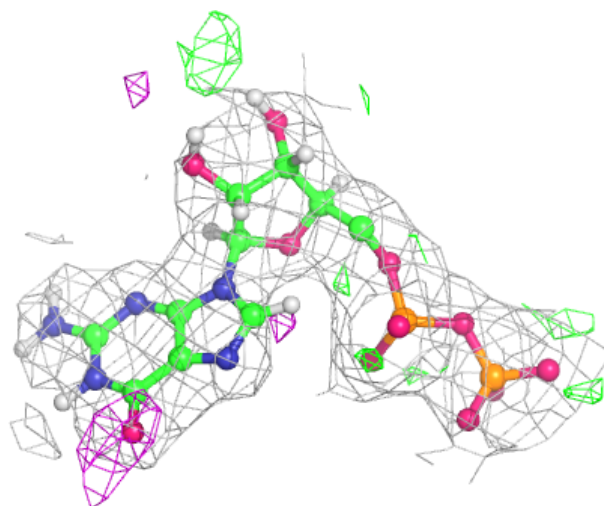
**Electron density around GTP D 501:**

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



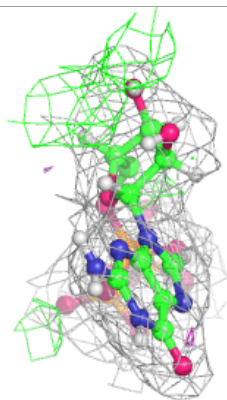
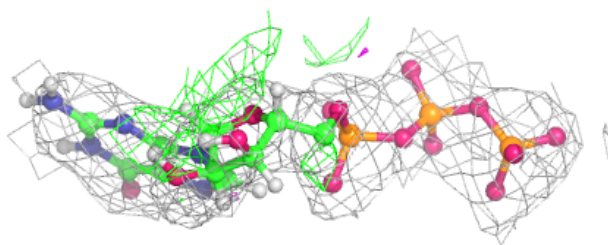
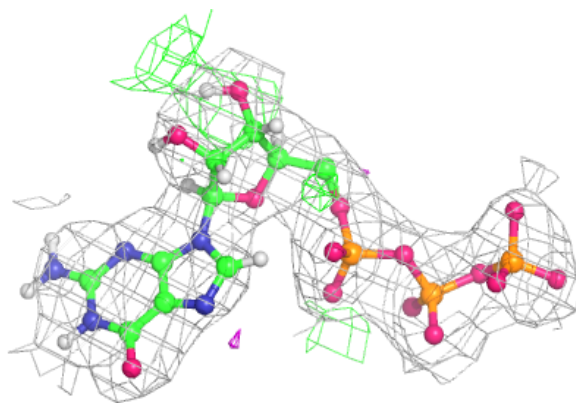
**Electron density around GDP B 501:**

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

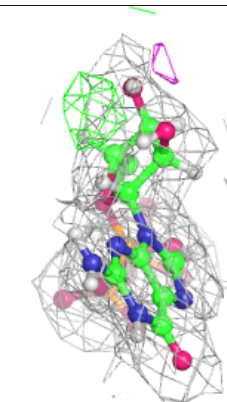
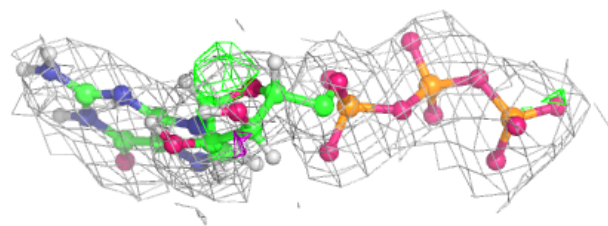
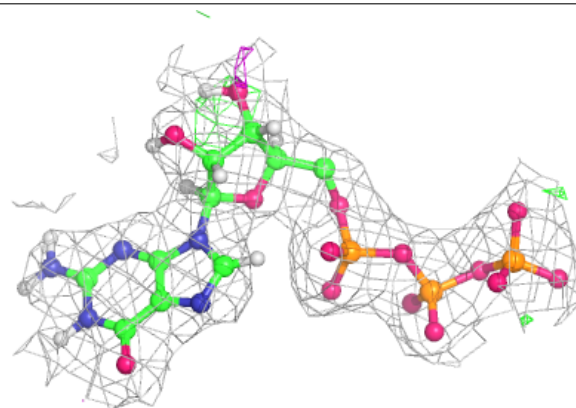


**Electron density around GTP A 501:**

$2mF_o-DF_c$  (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.