



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2021 – 04:12 PM JST

PDB ID : 7E4Q
Title : Crystal structure of tubulin in complex with L-DM1-SMe
Authors : Wang, Y.; Li, W.
Deposited on : 2021-02-14
Resolution : 2.50 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 ⓘ symbol.

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

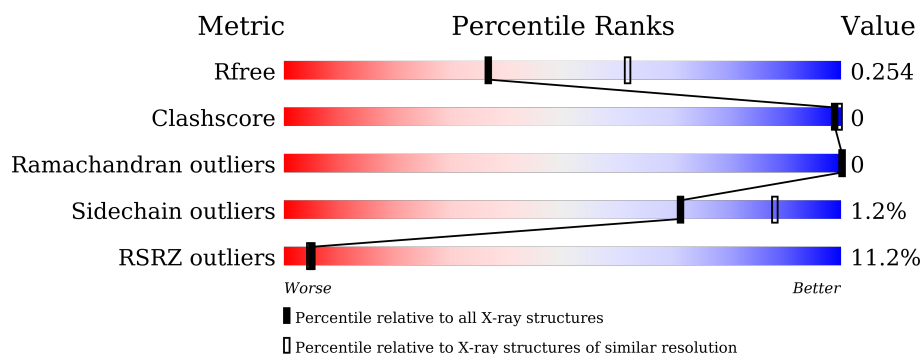
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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>4%</div> <div>98%</div> <div>.</div> </div>
2	B	431	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
2	D	431	<div> <div>13%</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>29%</div> <div>83%</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ACP	F	402	-	-	-	X
6	MG	F	401	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 35056 atoms, of which 17125 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	3	0
			6764	2171	3336	582	651	24			
1	C	440	Total	C	H	N	O	S	0	11	0
			6875	2204	3399	585	662	25			

- 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	0	12	0
			6753	2155	3324	584	662	28			
2	D	424	Total	C	H	N	O	S	0	3	0
			6560	2099	3216	570	648	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	3	0
			2064	633	1037	186	203	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

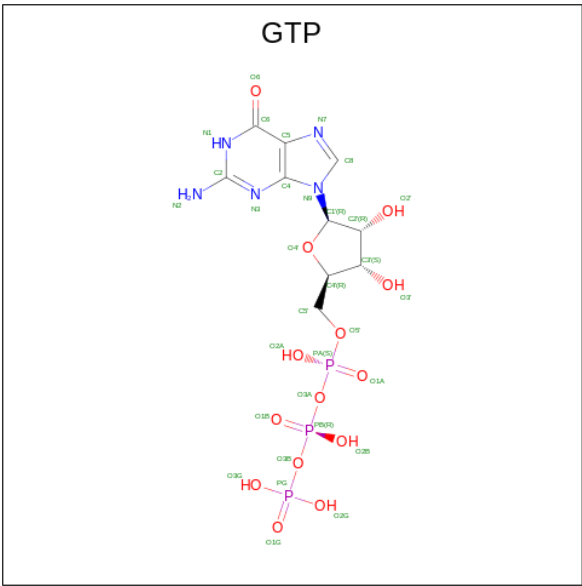
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	330	Total	C	H	N	O	S	0	3	0
			5418	1755	2697	460	492	14			

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:

C₁₀H₁₆N₅O₁₄P₃).



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		
6	F	1	Total	Mg	0	0
			1	1		

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

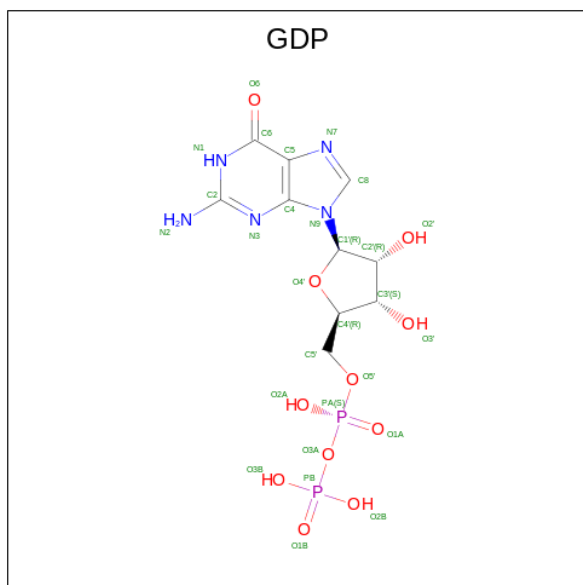
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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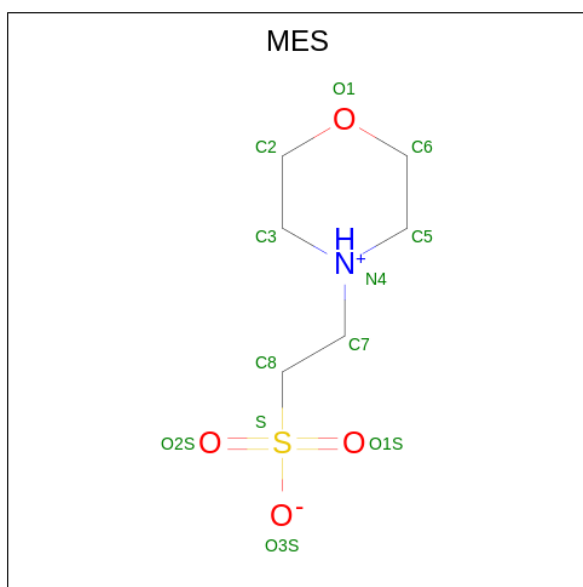
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

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



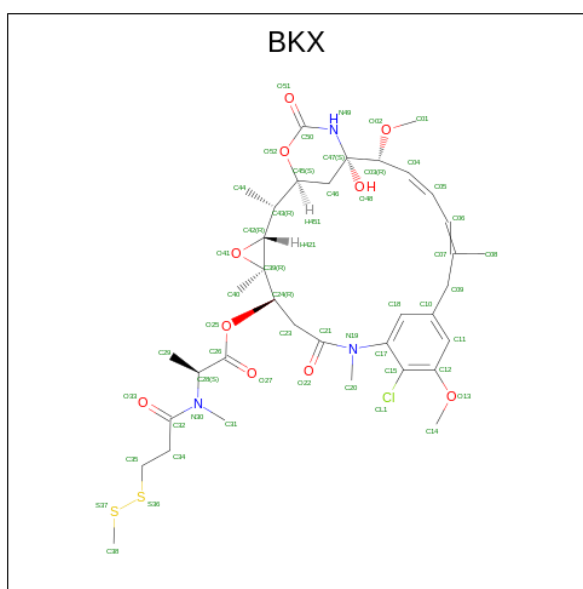
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

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



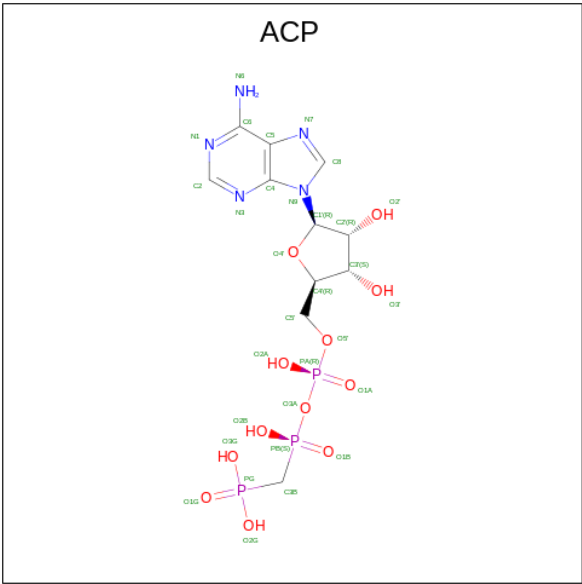
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 10 is (1S,2R,3R,5R,6R,16E,18E,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16,18-pentaen-6-yl (2S)-2-{methyl[3-(methyldisulfanyl)propanoyl]amino}propanoate (non-preferred name) (three-letter code: BKX) (formula: C₃₆H₅₀ClN₃O₁₀S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	D	1	Total	C	Cl	H	N	O	S	0	0
			102	36	1	50	3	10	2		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	F	1	Total 45	C 11	H 14	N 5	O 12	P 3	0	0

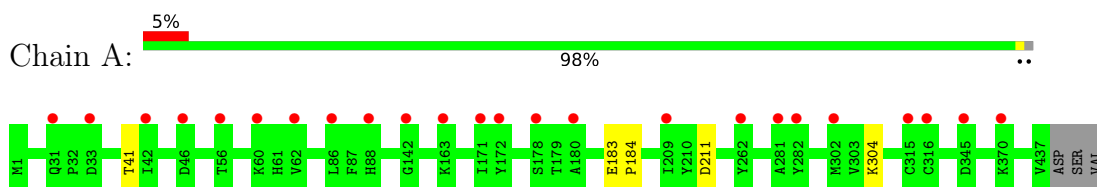
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	45	Total	O	0	0
			45	45		
12	B	61	Total	O	0	0
			61	61		
12	C	106	Total	O	0	0
			106	106		
12	D	29	Total	O	0	0
			29	29		
12	E	15	Total	O	0	0
			15	15		
12	F	24	Total	O	0	0
			24	24		

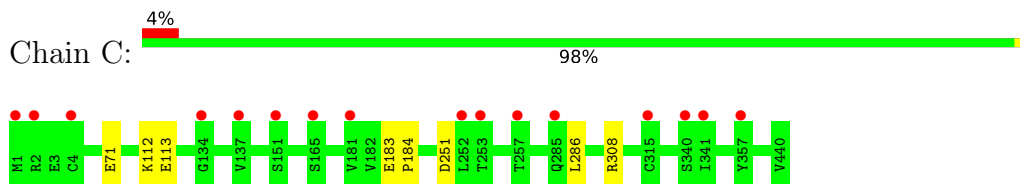
3 Residue-property plots

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.

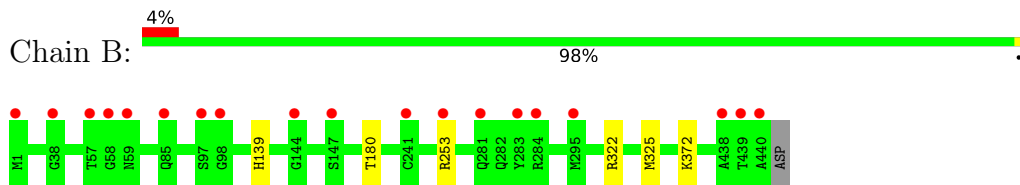
- Molecule 1: Tubulin alpha-1B chain



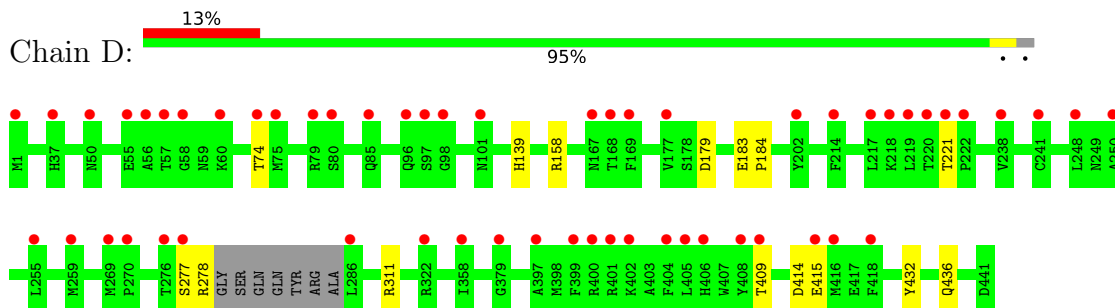
- Molecule 1: Tubulin alpha-1B chain



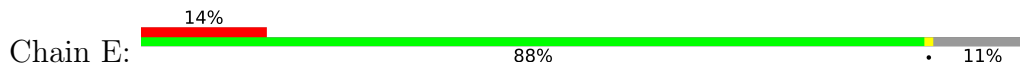
- Molecule 2: Tubulin beta-2B chain

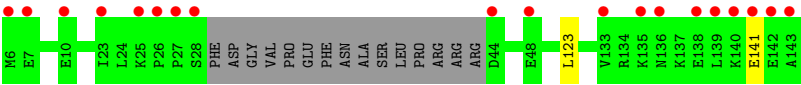


- Molecule 2: Tubulin beta-2B chain

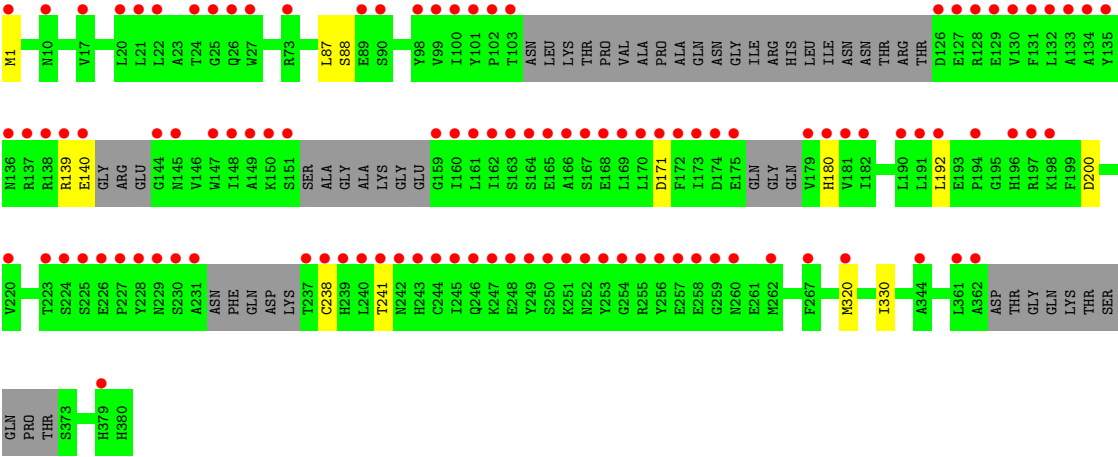
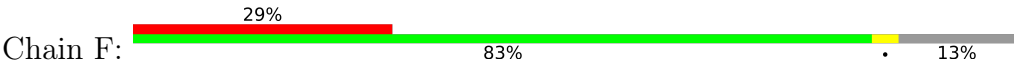


- Molecule 3: Stathmin-4





● 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, α , β , γ	104.89Å 157.21Å 181.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.88 – 2.50 46.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.88-2.50) 97.5 (46.88-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.205 , 0.252 0.212 , 0.254	Depositor DCC
R_{free} test set	2076 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35056	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, GDP, MG, ACP, BKX, 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	0.23	0/3515	0.41	0/4771
1	C	0.24	0/3587	0.41	0/4873
2	B	0.24	0/3550	0.39	0/4807
2	D	0.23	0/3427	0.39	0/4642
3	E	0.22	0/1047	0.34	0/1390
4	F	0.23	0/2790	0.39	0/3767
All	All	0.23	0/17916	0.39	0/24250

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	3428	3336	3349	2	0
1	C	3476	3399	3406	2	0
2	B	3429	3324	3311	1	0
2	D	3344	3216	3216	6	0
3	E	1027	1037	1030	1	0
4	F	2721	2697	2709	4	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	1	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	52	50	0	0	0
11	F	31	14	14	0	0
12	A	45	0	0	0	0
12	B	61	0	0	0	0
12	C	106	0	0	0	0
12	D	29	0	0	1	0
12	E	15	0	0	0	0
12	F	24	0	0	0	0
All	All	17931	17125	17095	15	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 0.

All (15) 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:139:ARG:NH2	4:F:140:GLU:OE2	2.29	0.64
2:D:183:GLU:OE2	5:D:502:GTP:O3'	2.13	0.61
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.20	0.60
2:D:414:ASP:OD1	2:D:415:GLU:N	2.37	0.58
2:B:253[B]:ARG:NH1	9:B:503:MES:O3S	2.36	0.56
2:D:311:ARG:NH1	2:D:436:GLN:O	2.45	0.48
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.49	0.46
1:C:183:GLU:N	1:C:184:PRO:CD	2.82	0.43
4:F:87:LEU:O	4:F:88:SER:OG	2.28	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
2:D:183:GLU:N	2:D:184:PRO:HD2	2.34	0.42
2:D:432:TYR:OH	12:D:601:HOH:O	2.21	0.41
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.53	0.41
4:F:320:MET:HG2	4:F:330:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ARG:HG2	3:E:123:LEU:HD11	2.03	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	438/440 (100%)	423 (97%)	15 (3%)	0	100	100
1	C	449/440 (102%)	441 (98%)	8 (2%)	0	100	100
2	B	440/431 (102%)	432 (98%)	8 (2%)	0	100	100
2	D	423/431 (98%)	413 (98%)	10 (2%)	0	100	100
3	E	122/138 (88%)	121 (99%)	1 (1%)	0	100	100
4	F	319/380 (84%)	311 (98%)	8 (2%)	0	100	100
All	All	2191/2260 (97%)	2141 (98%)	50 (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	371/371 (100%)	370 (100%)	1 (0%)	92	97
1	C	382/371 (103%)	378 (99%)	4 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	383/372 (103%)	378 (99%)	5 (1%)	69	87
2	D	370/372 (100%)	363 (98%)	7 (2%)	57	80
3	E	113/123 (92%)	112 (99%)	1 (1%)	78	92
4	F	301/338 (89%)	296 (98%)	5 (2%)	60	82
All	All	1920/1947 (99%)	1897 (99%)	23 (1%)	71	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
2	B	139	HIS
2	B	180	THR
2	B	322	ARG
2	B	325	MET
2	B	372	LYS
1	C	71	GLU
1	C	251	ASP
1	C	286	LEU
1	C	308	ARG
2	D	74	THR
2	D	139	HIS
2	D	179	ASP
2	D	221	THR
2	D	277	SER
2	D	278	ARG
2	D	409	THR
3	E	141	GLU
4	F	1	MET
4	F	171	ASP
4	F	180	HIS
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$
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.68	7 (21%)
9	MES	B	503	-	12,12,12	2.31	1 (8%)	14,16,16	2.40	5 (35%)
11	ACP	F	402	6	27,33,33	4.64	7 (25%)	32,52,52	1.60	7 (21%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.72	6 (18%)
5	GTP	D	502	6	26,34,34	0.98	1 (3%)	33,54,54	1.82	6 (18%)
8	GDP	B	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.95	7 (22%)
10	BKX	D	503	-	53,55,55	2.18	13 (24%)	61,81,81	2.27	19 (31%)

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	-	8/18/38/38	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
11	ACP	F	402	6	-	9/15/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
5	GTP	D	502	6	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
10	BKX	D	503	-	-	27/61/89/89	0/2/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	PB-O3A	21.43	1.82	1.58
11	F	402	ACP	PA-O5'	7.79	1.90	1.59
9	B	503	MES	C8-S	-7.75	1.66	1.77
10	D	503	BKX	C32-N30	6.93	1.46	1.35
10	D	503	BKX	C39-C42	5.81	1.54	1.47
10	D	503	BKX	C21-N19	5.57	1.46	1.35
10	D	503	BKX	O52-C45	-4.91	1.39	1.46
8	B	501	GDP	C6-C5	3.96	1.48	1.41
11	F	402	ACP	C5'-C4'	3.84	1.63	1.51
10	D	503	BKX	C20-N19	3.63	1.52	1.46
10	D	503	BKX	C23-C24	3.40	1.57	1.52
10	D	503	BKX	C23-C21	3.32	1.57	1.51
10	D	503	BKX	O41-C39	-3.22	1.42	1.45
5	D	502	GTP	C6-N1	3.19	1.38	1.33
10	D	503	BKX	C50-N49	3.11	1.41	1.34
5	C	501	GTP	C6-N1	3.09	1.38	1.33
5	A	501	GTP	C6-N1	3.09	1.38	1.33
11	F	402	ACP	O5'-C5'	-2.93	1.33	1.44
11	F	402	ACP	C2-N1	2.74	1.39	1.33
11	F	402	ACP	C4-N3	2.61	1.39	1.35
10	D	503	BKX	O41-C42	-2.37	1.41	1.45
10	D	503	BKX	C34-C32	2.35	1.56	1.51
8	B	501	GDP	C5-C4	2.27	1.46	1.40
10	D	503	BKX	O25-C26	2.26	1.39	1.34
10	D	503	BKX	O13-C12	2.22	1.40	1.37
11	F	402	ACP	C2-N3	2.05	1.35	1.32

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	BKX	C39-O41-C42	8.59	65.96	60.79
9	B	503	MES	C5-N4-C3	6.26	122.91	108.83
10	D	503	BKX	C18-C17-C15	-5.86	115.05	122.53
5	D	502	GTP	N3-C2-N1	-5.30	120.16	127.22
5	C	501	GTP	N3-C2-N1	-5.24	120.24	127.22
5	A	501	GTP	N3-C2-N1	-5.11	120.41	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C2-N3-C4	4.49	120.48	115.36
10	D	503	BKX	O25-C26-C28	4.42	120.40	110.80
8	B	501	GDP	C6-N1-C2	4.32	122.80	115.93
8	B	501	GDP	C6-C5-C4	-4.28	116.71	120.80
5	D	502	GTP	C2-N3-C4	4.19	120.14	115.36
8	B	501	GDP	C5-C6-N1	-4.09	117.84	123.43
11	F	402	ACP	O1B-PB-C3B	4.09	119.87	109.07
10	D	503	BKX	O25-C26-O27	-4.07	116.34	123.94
5	A	501	GTP	C2-N3-C4	4.01	119.94	115.36
5	C	501	GTP	C2-N3-C4	3.98	119.91	115.36
10	D	503	BKX	O41-C42-C39	-3.91	57.05	59.83
11	F	402	ACP	O5'-PA-O1A	-3.87	93.94	109.07
10	D	503	BKX	O41-C39-C42	-3.55	56.99	59.38
8	B	501	GDP	N3-C2-N1	-3.45	122.62	127.22
5	D	502	GTP	PB-O3B-PG	-3.34	121.36	132.83
5	D	502	GTP	PA-O3A-PB	-3.32	121.43	132.83
9	B	503	MES	O1S-S-C8	3.31	110.90	106.92
10	D	503	BKX	C17-C18-C10	3.28	124.74	120.23
10	D	503	BKX	C23-C21-N19	3.26	122.57	118.89
10	D	503	BKX	C20-N19-C17	3.16	121.13	116.72
5	C	501	GTP	PA-O3A-PB	-3.08	122.26	132.83
5	C	501	GTP	C5-C6-N1	-3.06	119.25	123.43
10	D	503	BKX	O13-C12-C15	2.97	119.05	115.53
11	F	402	ACP	PA-O3A-PB	-2.96	123.16	132.56
5	C	501	GTP	PB-O3B-PG	-2.92	122.79	132.83
5	A	501	GTP	C5-C6-N1	-2.92	119.44	123.43
10	D	503	BKX	C12-C15-CL1	-2.87	114.53	119.84
10	D	503	BKX	C17-C15-CL1	2.86	123.13	120.09
5	A	501	GTP	PB-O3B-PG	-2.77	123.32	132.83
9	B	503	MES	C7-N4-C5	2.76	118.29	111.23
5	D	502	GTP	C5-C6-N1	-2.76	119.66	123.43
5	C	501	GTP	C6-N1-C2	2.67	120.17	115.93
8	B	501	GDP	C4-C5-N7	-2.66	106.62	109.40
5	A	501	GTP	PA-O3A-PB	-2.63	123.79	132.83
8	B	501	GDP	PA-O3A-PB	-2.62	123.83	132.83
10	D	503	BKX	C40-C39-C42	-2.61	115.14	121.05
5	D	502	GTP	C6-N1-C2	2.47	119.85	115.93
5	A	501	GTP	C6-N1-C2	2.47	119.85	115.93
10	D	503	BKX	O33-C32-N30	-2.45	117.59	121.88
11	F	402	ACP	O1G-PG-C3B	-2.38	106.10	111.24
11	F	402	ACP	O2A-PA-O5'	-2.32	96.99	107.75
9	B	503	MES	O3S-S-C8	2.27	109.44	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	BKX	C15-C17-N19	2.25	123.02	120.71
10	D	503	BKX	O22-C21-C23	-2.19	118.25	122.20
9	B	503	MES	C2-C3-N4	2.18	113.41	110.10
5	A	501	GTP	O3G-PG-O3B	2.18	111.94	104.64
10	D	503	BKX	C24-O25-C26	2.18	122.05	118.18
11	F	402	ACP	O3'-C3'-C4'	2.13	117.22	111.05
10	D	503	BKX	C14-O13-C12	2.13	120.75	117.53
11	F	402	ACP	O2B-PB-C3B	2.10	115.16	106.58
10	D	503	BKX	C38-S37-S36	2.06	109.68	102.58

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
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	503	BKX	C21-C23-C24-O25
10	D	503	BKX	C39-C24-O25-C26
10	D	503	BKX	C23-C24-C39-C40
10	D	503	BKX	C23-C24-C39-O41
10	D	503	BKX	O25-C24-C39-C40
10	D	503	BKX	C47-C03-O02-C01
10	D	503	BKX	C47-C03-C04-C05
10	D	503	BKX	C03-C04-C05-C06
10	D	503	BKX	C05-C06-C07-C09
10	D	503	BKX	C39-C42-C43-C44
10	D	503	BKX	O41-C42-C43-C44
10	D	503	BKX	C42-C43-C45-C46
11	F	402	ACP	PB-C3B-PG-O1G
11	F	402	ACP	PB-C3B-PG-O3G
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	503	BKX	C15-C12-O13-C14
9	B	503	MES	C7-C8-S-O3S
10	D	503	BKX	C11-C12-O13-C14

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Mol	Chain	Res	Type	Atoms
10	D	503	BKX	C04-C05-C06-C07
10	D	503	BKX	C29-C28-N30-C31
10	D	503	BKX	C29-C28-N30-C32
10	D	503	BKX	C44-C43-C45-C46
5	A	501	GTP	PB-O3B-PG-O2G
10	D	503	BKX	C23-C24-O25-C26
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
10	D	503	BKX	O41-C42-C43-C45
10	D	503	BKX	O02-C03-C04-C05
11	F	402	ACP	PB-C3B-PG-O2G
11	F	402	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	D	502	GTP	C4'-C5'-O5'-PA
10	D	503	BKX	O27-C26-C28-N30
10	D	503	BKX	C34-C35-S36-S37
5	C	501	GTP	PB-O3B-PG-O1G
10	D	503	BKX	O27-C26-C28-C29
10	D	503	BKX	C26-C28-N30-C31
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	402	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C4'-C5'-O5'-PA
10	D	503	BKX	C21-C23-C24-C39
11	F	402	ACP	C5'-O5'-PA-O1A
10	D	503	BKX	N19-C21-C23-C24

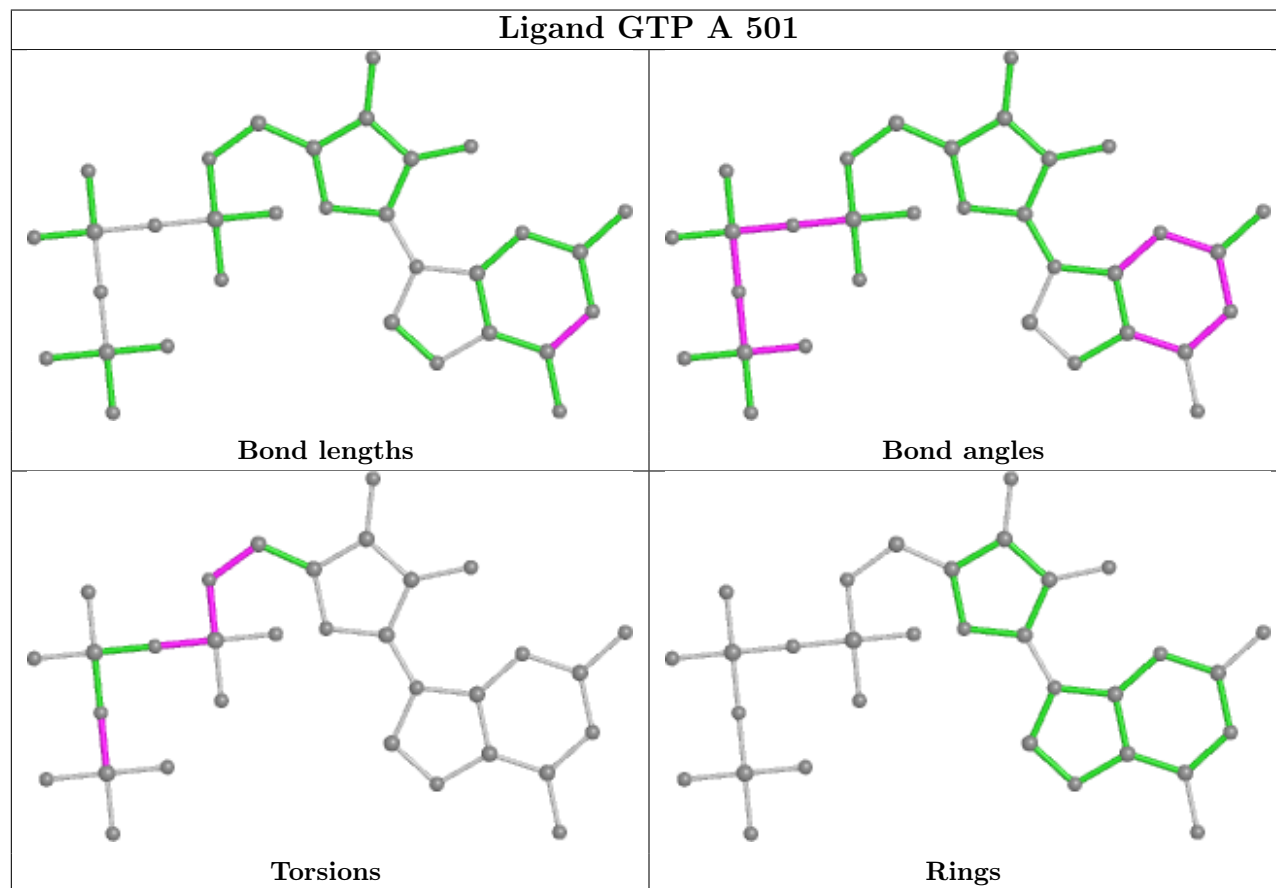
There are no ring outliers.

2 monomers are involved in 2 short contacts:

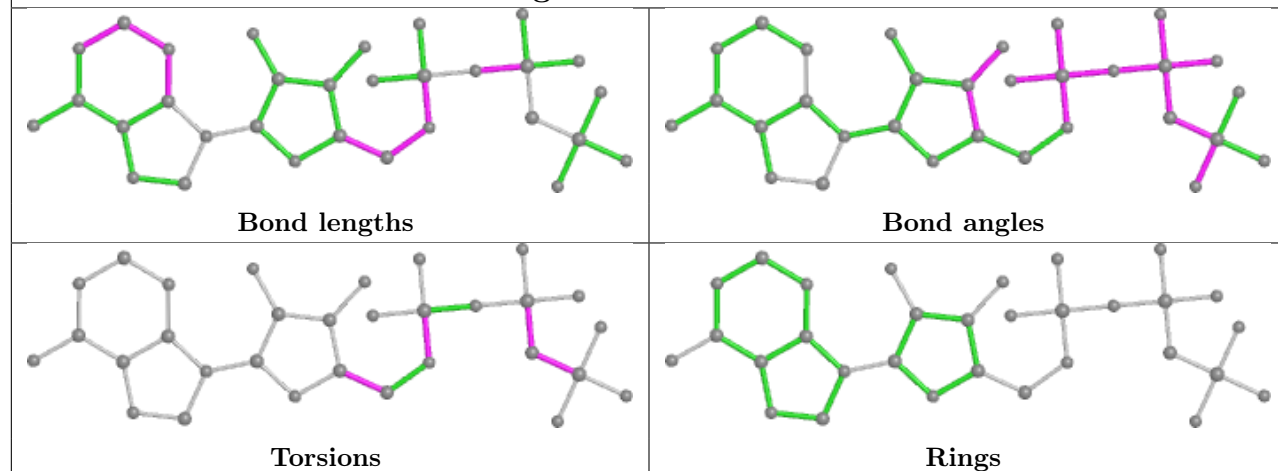
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	1	0
5	D	502	GTP	1	0

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

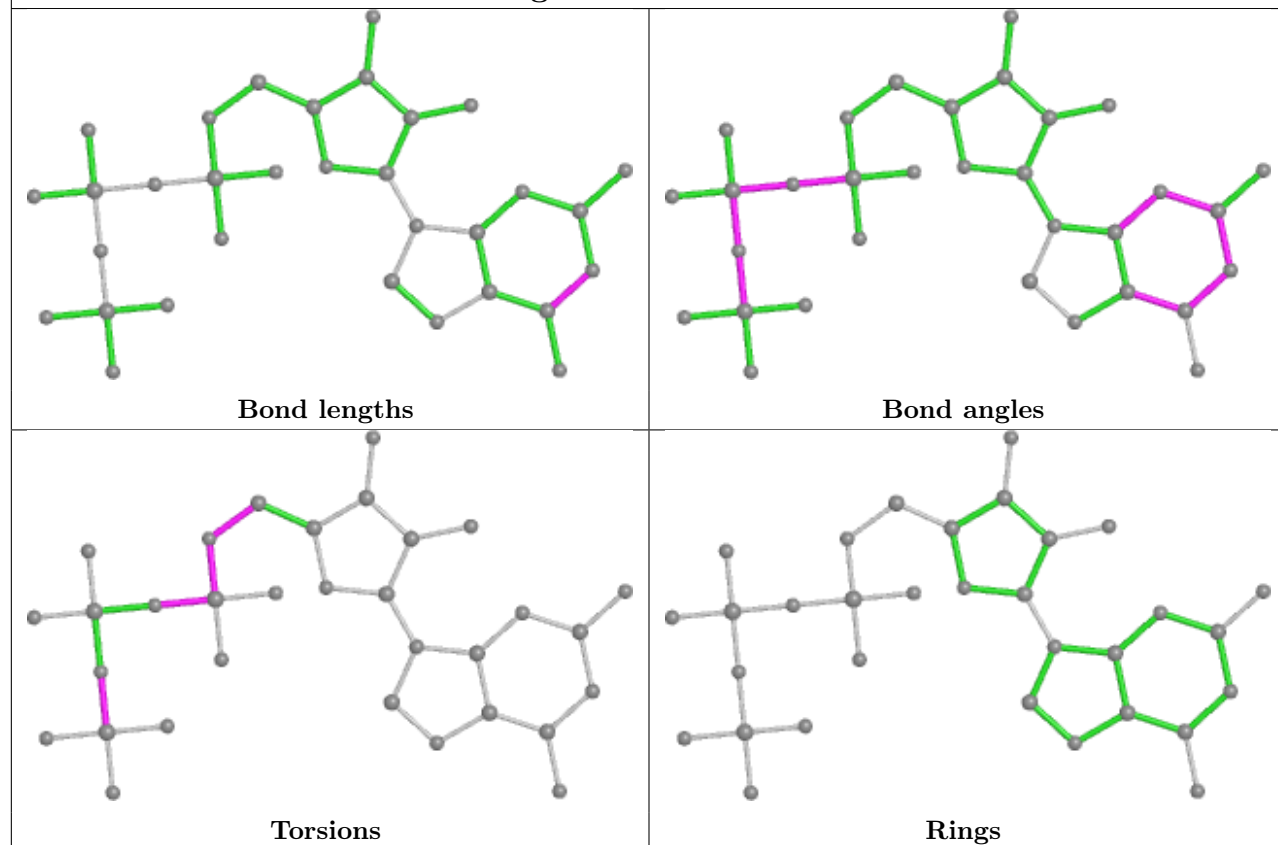
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

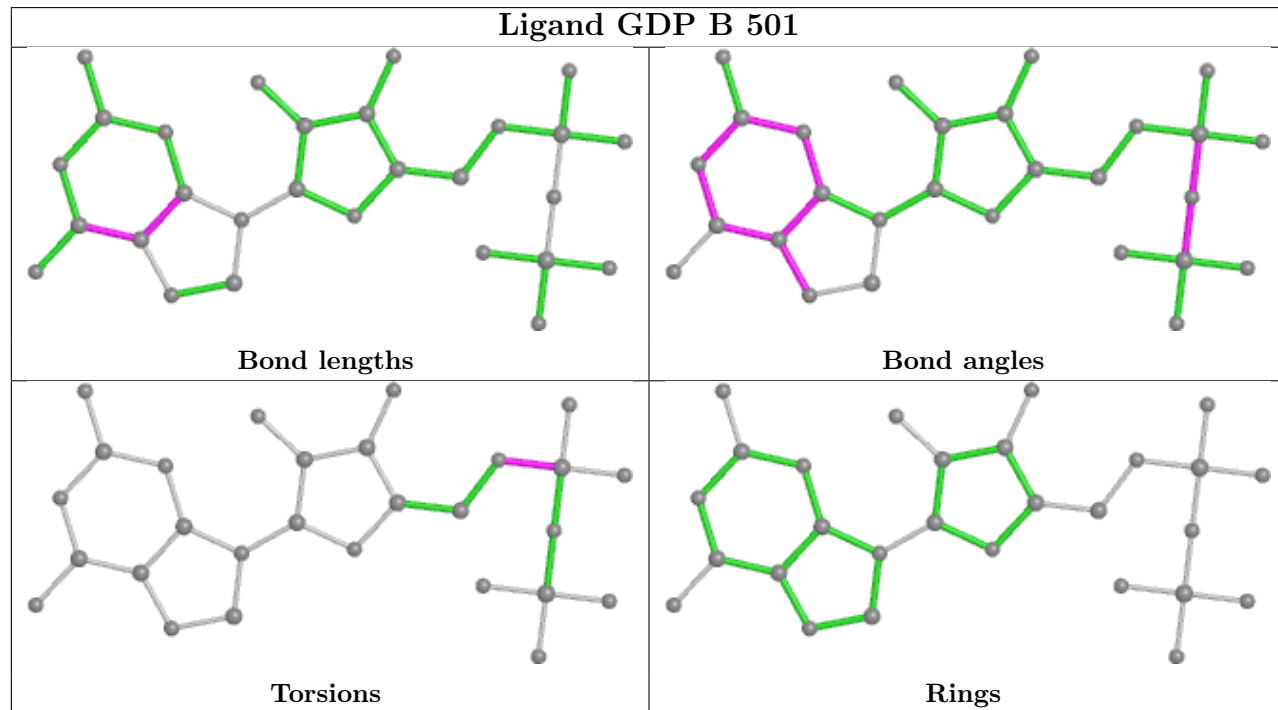
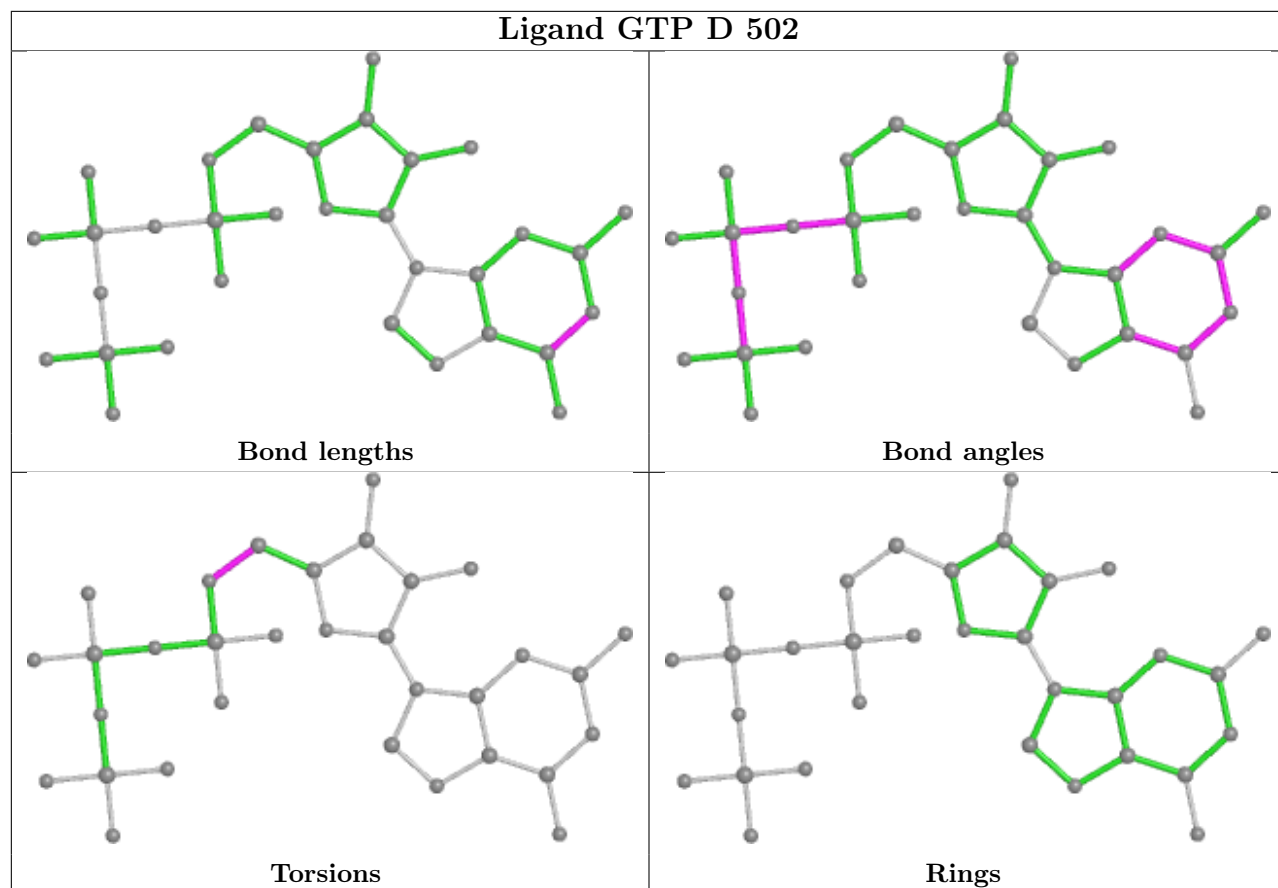


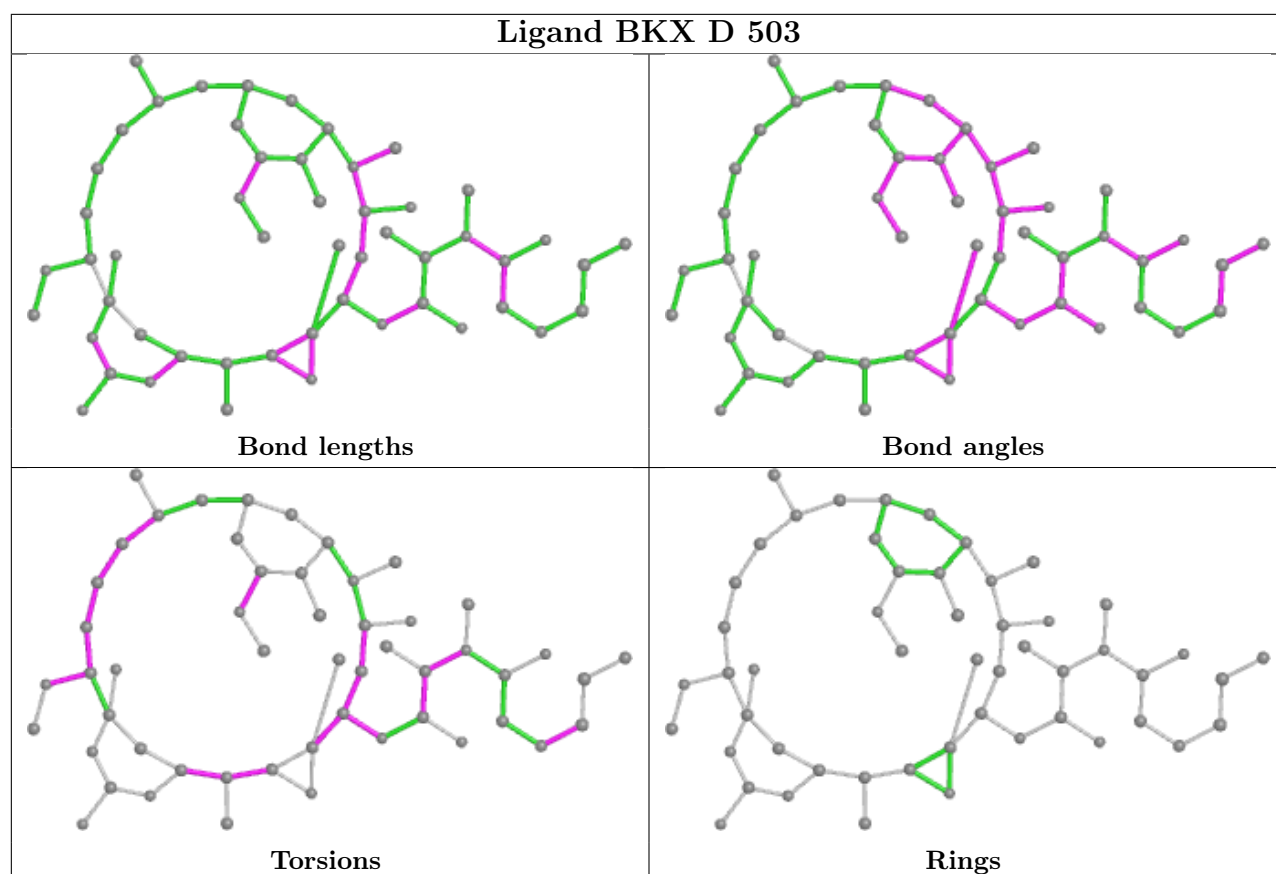
Ligand ACP F 402



Ligand GTP C 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, 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	437/440 (99%)	0.51	24 (5%)	25 26	38, 58, 87, 105	0
1	C	440/440 (100%)	0.27	16 (3%)	42 46	30, 45, 72, 106	0
2	B	430/431 (99%)	0.45	19 (4%)	34 37	32, 53, 88, 134	0
2	D	424/431 (98%)	0.80	56 (13%)	3 3	42, 67, 96, 116	0
3	E	123/138 (89%)	0.92	19 (15%)	2 1	44, 71, 109, 134	0
4	F	330/380 (86%)	1.83	110 (33%)	0 0	46, 79, 142, 161	0
All	All	2184/2260 (96%)	0.73	244 (11%)	5 4	30, 60, 108, 161	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	12.4
4	F	245	ILE	11.0
4	F	250	SER	10.6
4	F	256	TYR	10.2
4	F	244	CYS	10.0
4	F	241	THR	9.6
4	F	251	LYS	9.3
4	F	169	LEU	9.3
4	F	240	LEU	9.3
4	F	253	TYR	9.1
4	F	101	TYR	9.1
4	F	161	LEU	9.0
4	F	239	HIS	8.7
4	F	231	ALA	8.7
4	F	173	ILE	8.6
4	F	248	GLU	8.2
4	F	257	GLU	8.1
2	B	1	MET	7.8
4	F	102	PRO	7.6

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Mol	Chain	Res	Type	RSRZ
4	F	100	ILE	7.5
4	F	242	ASN	7.5
3	E	143	ALA	7.3
4	F	255	ARG	7.2
4	F	258	GLU	6.9
4	F	225	SER	6.9
4	F	182	ILE	6.8
4	F	229	ASN	6.6
4	F	254	GLY	6.6
4	F	238	CYS	6.4
4	F	181	VAL	6.2
1	C	4[A]	CYS	6.0
2	D	405	LEU	6.0
4	F	131	PHE	5.9
2	D	277	SER	5.9
4	F	247	LYS	5.8
4	F	135	TYR	5.8
4	F	243	HIS	5.6
4	F	230	SER	5.6
4	F	252	ASN	5.6
4	F	132	LEU	5.4
4	F	172	PHE	5.4
4	F	162	ILE	5.4
2	B	440	ALA	5.3
3	E	139	LEU	5.3
2	D	1	MET	5.2
4	F	180	HIS	5.2
4	F	136	ASN	5.1
4	F	228	TYR	5.1
1	C	315[A]	CYS	5.0
4	F	224	SER	5.0
2	D	57	THR	4.9
3	E	28	SER	4.8
2	B	59	ASN	4.8
4	F	133	ALA	4.8
4	F	168	GLU	4.7
2	B	439	THR	4.7
4	F	159	GLY	4.6
4	F	160	ILE	4.6
3	E	26	PRO	4.6
4	F	163	SER	4.6
4	F	174	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
4	F	361	LEU	4.6
4	F	103	THR	4.5
3	E	133	VAL	4.4
2	D	400	ARG	4.4
4	F	227	PRO	4.4
1	A	315[A]	CYS	4.3
4	F	89	GLU	4.3
3	E	27	PRO	4.3
4	F	259	GLY	4.3
4	F	237	THR	4.3
4	F	194	PRO	4.3
2	B	57	THR	4.2
4	F	139	ARG	4.2
4	F	179	VAL	4.2
1	A	282	TYR	4.2
4	F	170	LEU	4.2
1	A	316[A]	CYS	4.2
4	F	197	ARG	4.1
4	F	175	GLU	4.1
4	F	138	ARG	4.0
2	D	56	ALA	3.9
2	D	60	LYS	3.8
4	F	149	ALA	3.8
2	D	399	PHE	3.8
4	F	191	LEU	3.8
4	F	171	ASP	3.8
4	F	166	ALA	3.8
4	F	167	SER	3.7
4	F	129	GLU	3.7
2	B	253[A]	ARG	3.7
3	E	140	LYS	3.7
4	F	128	ARG	3.7
2	D	97	SER	3.7
4	F	90	SER	3.6
4	F	137	ARG	3.6
1	A	262	TYR	3.6
4	F	140	GLU	3.5
2	D	75	MET	3.5
2	B	58	GLY	3.5
2	D	276	THR	3.5
4	F	165	GLU	3.5
1	A	42	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
3	E	7	GLU	3.4
4	F	21	LEU	3.4
4	F	196	HIS	3.4
4	F	148	ILE	3.3
4	F	164	SER	3.3
2	B	241[A]	CYS	3.3
4	F	22	LEU	3.3
4	F	192	LEU	3.2
4	F	379	HIS	3.2
4	F	130	VAL	3.2
2	D	220	THR	3.2
2	D	219	LEU	3.2
2	B	85	GLN	3.2
4	F	99	VAL	3.2
1	A	180	ALA	3.1
2	D	74	THR	3.1
4	F	127	GLU	3.0
4	F	226	GLU	3.0
4	F	10	ASN	3.0
2	D	415	GLU	3.0
1	A	281	ALA	3.0
2	B	281	GLN	3.0
3	E	142	GLU	2.9
2	D	241	CYS	2.9
1	A	86	LEU	2.9
4	F	134	ALA	2.9
4	F	145	ASN	2.9
1	C	253	THR	2.9
4	F	267	PHE	2.9
4	F	147	TRP	2.9
4	F	126	ASP	2.8
1	A	370	LYS	2.8
4	F	246	GLN	2.8
4	F	25	GLY	2.8
1	A	172	TYR	2.8
4	F	151	SER	2.8
1	C	2	ARG	2.8
2	D	37	HIS	2.8
4	F	260	ASN	2.8
2	D	406	HIS	2.8
1	C	165[A]	SER	2.8
3	E	135	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	96	GLN	2.7
2	D	416	MET	2.7
4	F	20	LEU	2.7
1	A	163	LYS	2.7
3	E	23	ILE	2.7
2	B	98	GLY	2.7
1	A	33	ASP	2.7
3	E	10	GLU	2.6
3	E	25	LYS	2.6
2	D	358	ILE	2.6
1	C	134	GLY	2.6
1	A	88	HIS	2.6
2	D	221	THR	2.6
1	C	181[A]	VAL	2.6
2	D	50[A]	ASN	2.6
1	C	357	TYR	2.6
4	F	320	MET	2.6
1	A	56	THR	2.6
2	D	202	TYR	2.6
4	F	362	ALA	2.6
2	D	217	LEU	2.6
1	C	1	MET	2.6
2	D	218	LYS	2.6
1	A	171	ILE	2.6
2	B	295	MET	2.6
2	D	55	GLU	2.5
2	D	58	GLY	2.5
4	F	344	ALA	2.5
1	A	60	LYS	2.5
3	E	141	GLU	2.5
4	F	17	VAL	2.5
4	F	190	LEU	2.5
2	B	438	ALA	2.5
2	D	98	GLY	2.5
2	D	397	ALA	2.4
4	F	1	MET	2.4
2	D	168	THR	2.4
1	A	178	SER	2.4
2	D	409	THR	2.4
2	D	79	ARG	2.4
2	D	255	LEU	2.4
2	B	283	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	401	ARG	2.4
3	E	136	ASN	2.3
1	A	62	VAL	2.3
1	C	252	LEU	2.3
2	D	248	LEU	2.3
2	D	418	PHE	2.3
4	F	262	MET	2.3
2	D	408	TYR	2.3
2	D	402	LYS	2.3
1	A	302	MET	2.3
2	D	259	MET	2.3
2	D	85	GLN	2.3
2	D	404	PHE	2.3
2	D	286	LEU	2.3
3	E	6	MET	2.2
2	D	169	PHE	2.2
2	D	379	GLY	2.2
1	A	46	ASP	2.2
1	C	257	THR	2.2
4	F	73	ARG	2.2
4	F	144	GLY	2.2
4	F	150	LYS	2.2
2	B	284	ARG	2.2
2	D	177	VAL	2.2
1	C	285	GLN	2.2
1	C	137	VAL	2.2
2	D	269	MET	2.2
4	F	26	GLN	2.2
1	C	341	ILE	2.2
3	E	138	GLU	2.2
2	D	80	SER	2.2
2	B	38	GLY	2.1
2	D	214	PHE	2.1
1	C	340	SER	2.1
2	B	97	SER	2.1
2	B	147[A]	SER	2.1
1	A	345	ASP	2.1
2	D	322	ARG	2.1
1	A	142	GLY	2.1
1	A	209	ILE	2.1
3	E	48	GLU	2.1
2	D	167	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	151[A]	SER	2.1
3	E	44	ASP	2.1
1	A	31	GLN	2.1
4	F	27	TRP	2.1
2	D	270	PRO	2.1
2	D	238	VAL	2.0
4	F	24	THR	2.0
4	F	220[A]	VAL	2.0
4	F	223	THR	2.0
2	B	144	GLY	2.0
4	F	98	TYR	2.0
2	D	222	PRO	2.0
2	D	250	ALA	2.0
2	D	101	ASN	2.0
4	F	198	LYS	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
6	MG	F	401	1/1	0.23	1.02	114,114,114,114	0
11	ACP	F	402	31/31	0.44	0.77	111,144,192,198	0
10	BKX	D	503	52/52	0.85	0.27	72,105,129,281	0
6	MG	D	501	1/1	0.87	0.09	67,67,67,67	0
7	CA	A	503	1/1	0.93	0.06	79,79,79,79	0
9	MES	B	503	12/12	0.94	0.16	51,68,88,105	0
5	GTP	D	502	32/32	0.96	0.14	50,64,87,89	0
5	GTP	C	501	32/32	0.96	0.22	29,40,50,53	0

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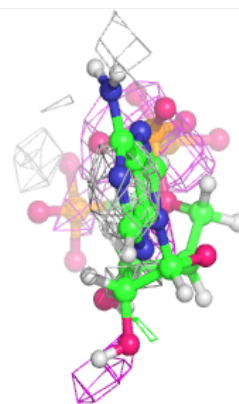
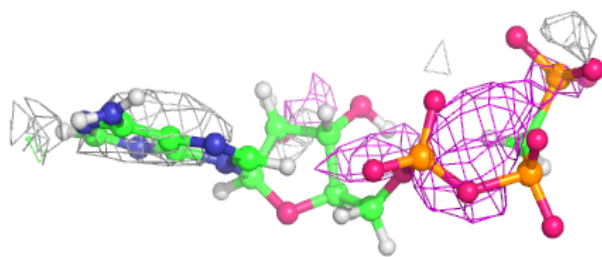
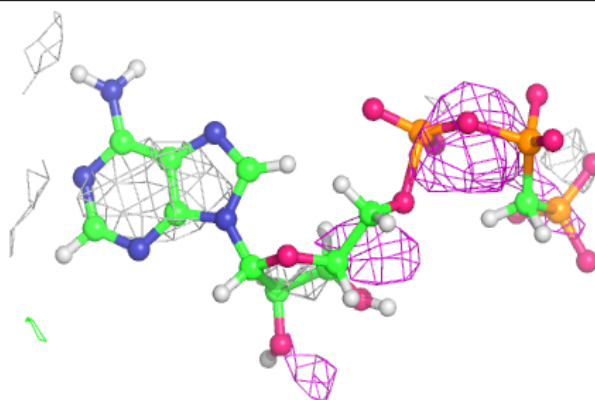
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	C	503	1/1	0.96	0.19	61,61,61,61	0
8	GDP	B	501	28/28	0.97	0.24	32,45,57,68	0
6	MG	B	502	1/1	0.97	0.30	45,45,45,45	0
5	GTP	A	501	32/32	0.98	0.27	29,47,57,59	0
6	MG	C	502	1/1	0.98	0.23	36,36,36,36	0
6	MG	A	502	1/1	0.99	0.28	43,43,43,43	0

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

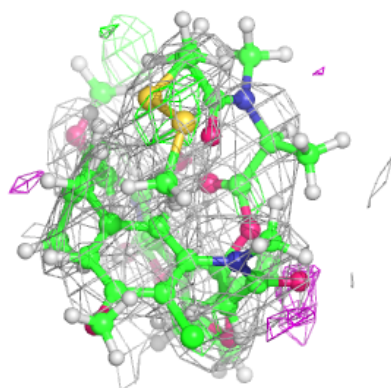
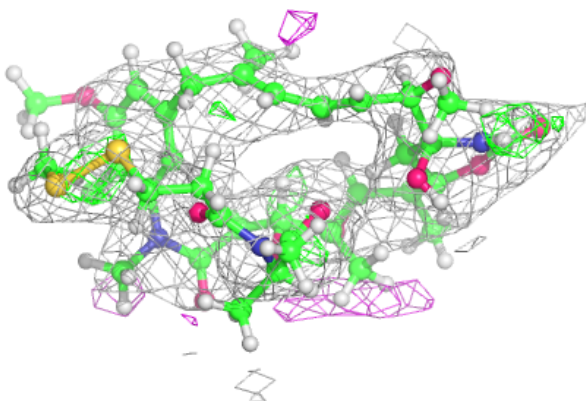
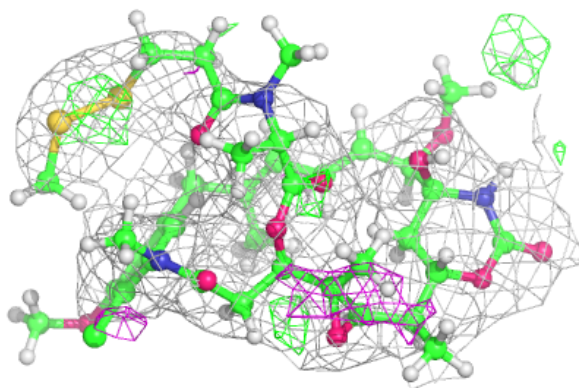
Electron density around ACP F 402:

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

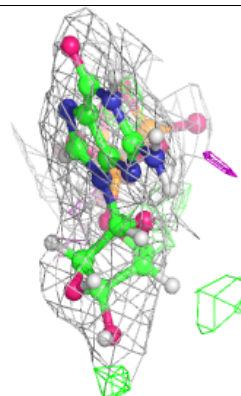
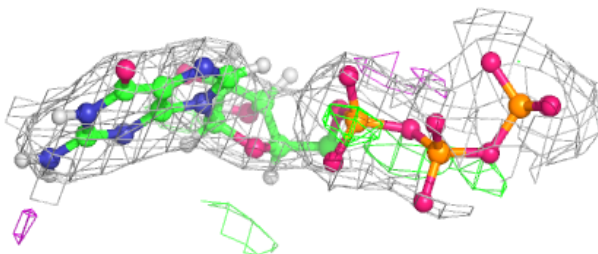
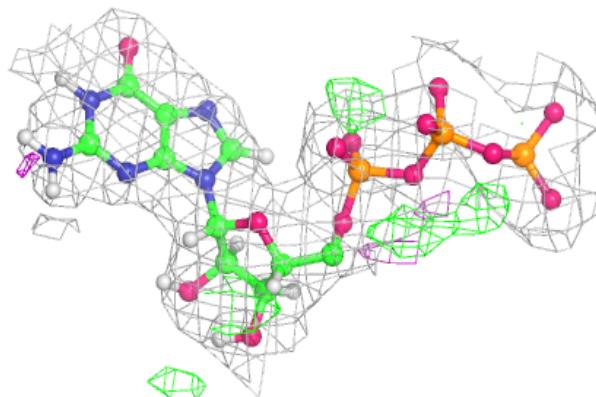


Electron density around BKX D 503:

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

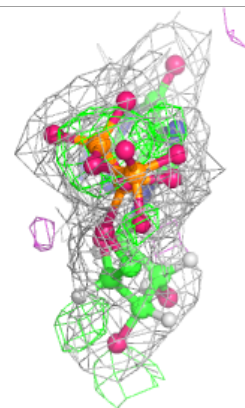
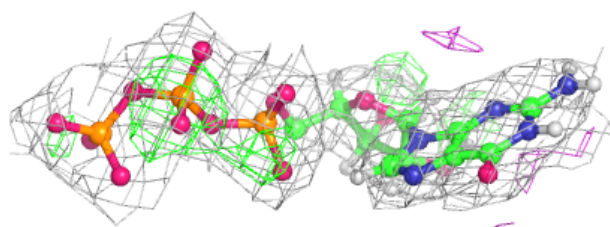
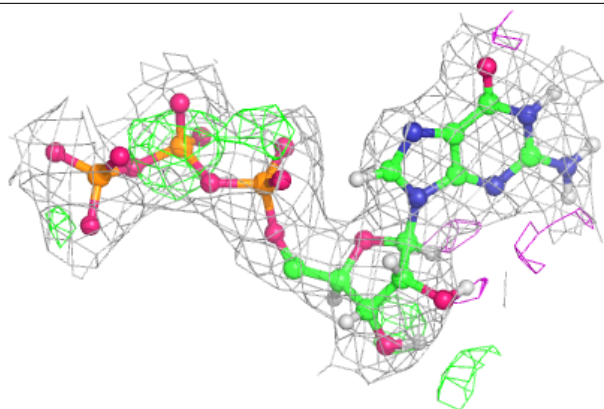
**Electron density around GTP D 502:**

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



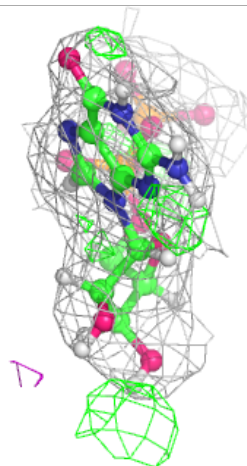
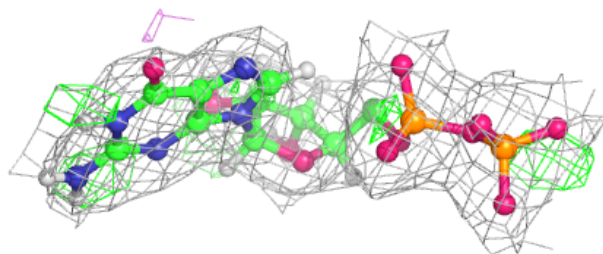
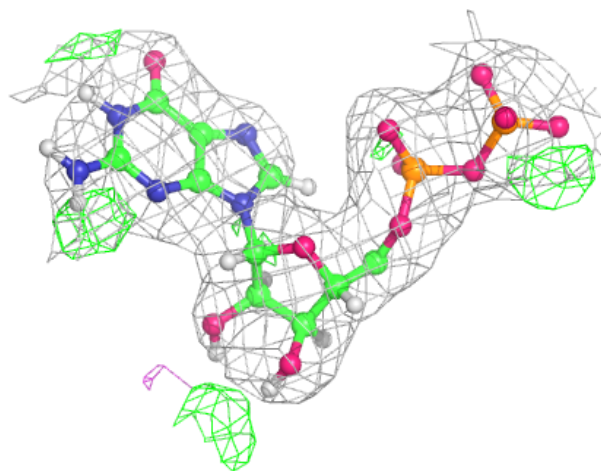
Electron density around GTP C 501:

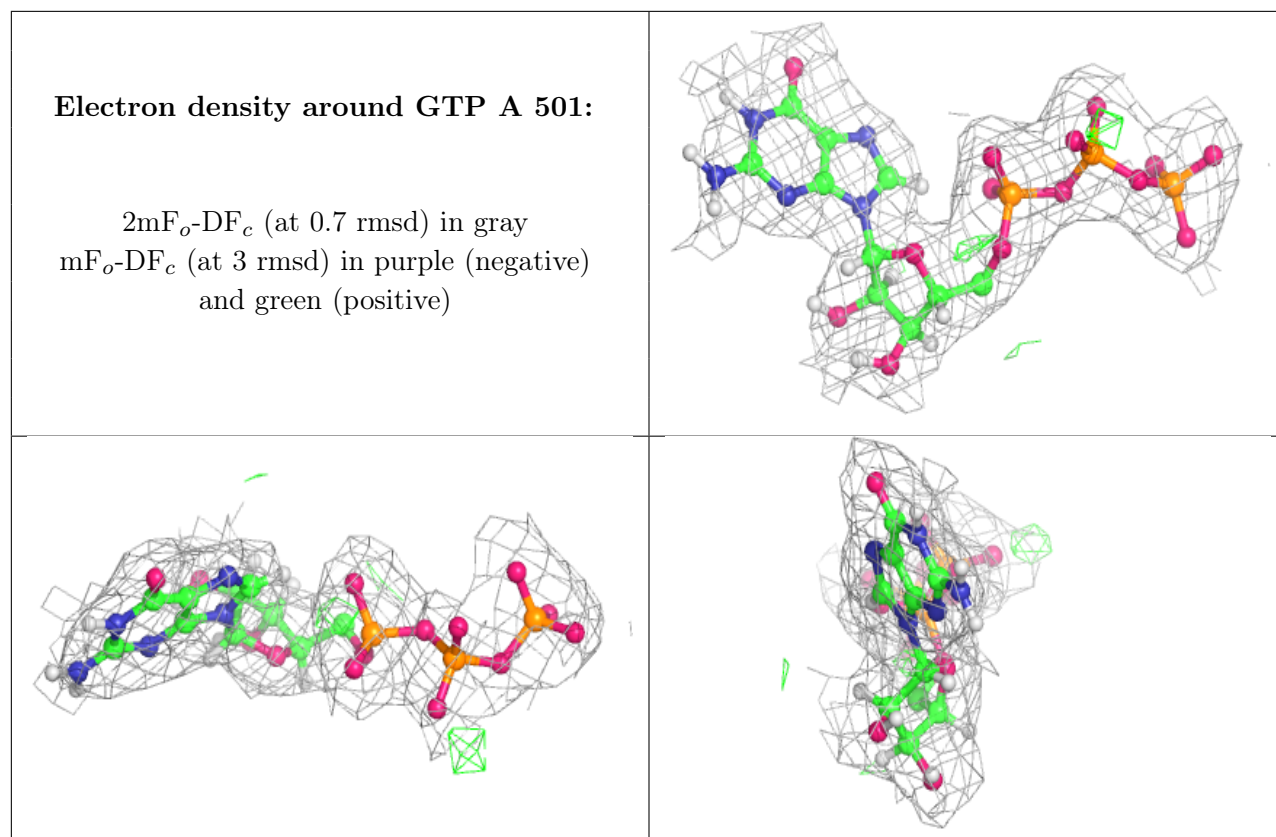
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.