



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:28 PM UTC

PDB ID : 7E4Q / pdb_00007e4q
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

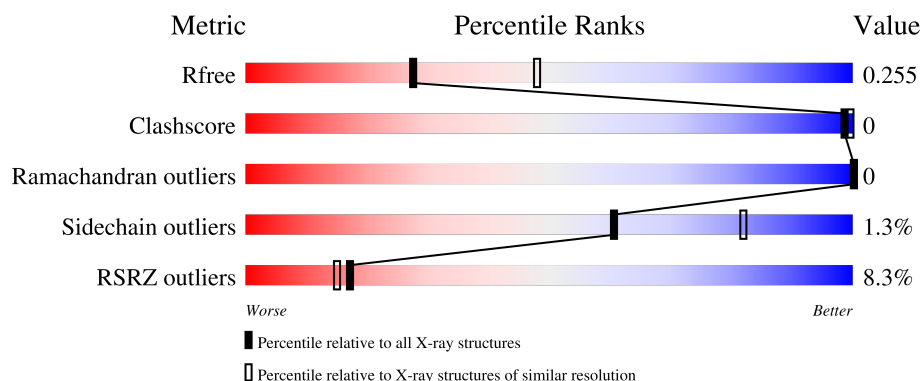
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	5% 98% ..
1	C	440	4% 99% .
2	B	431	5% 99% .
2	D	431	10% 95% ..
3	E	138	10% 86% 11%

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Mol	Chain	Length	Quality of chain
4	F	380	18% 83% • • 13%

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			

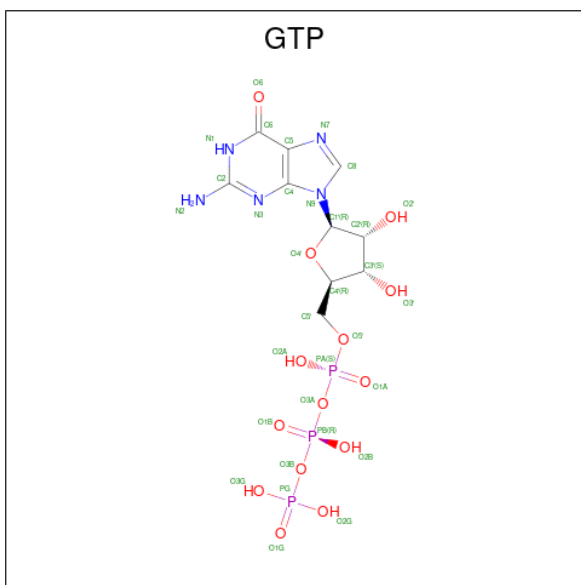
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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 (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

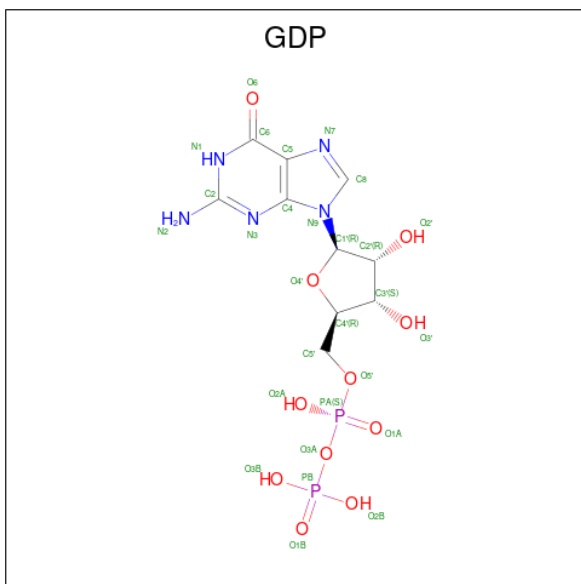
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca		
			1	1	0	0

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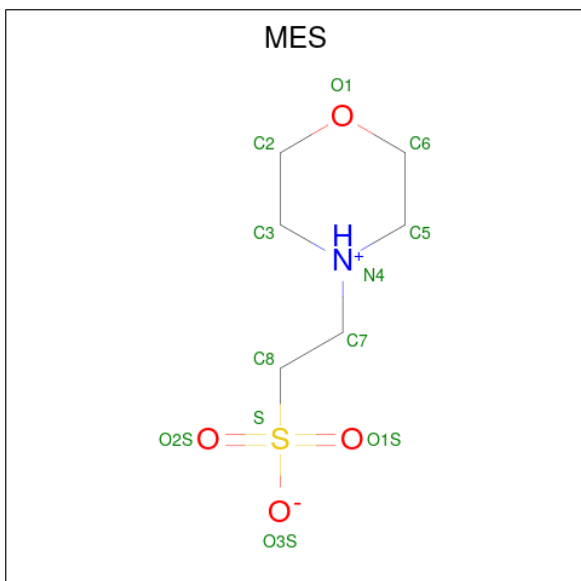
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Ca 1 1	0	0

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



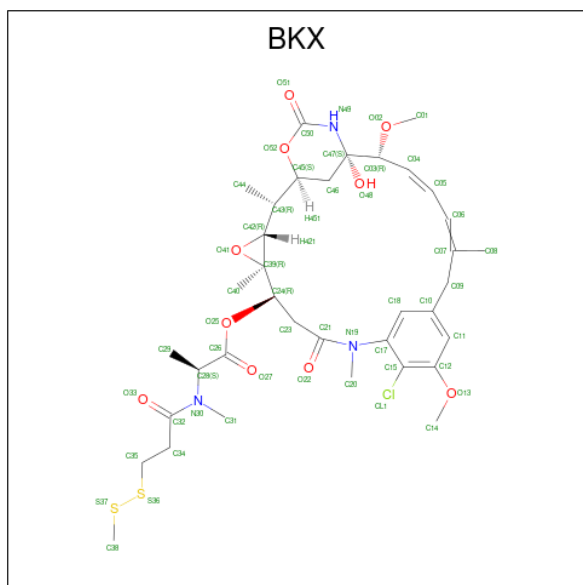
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

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



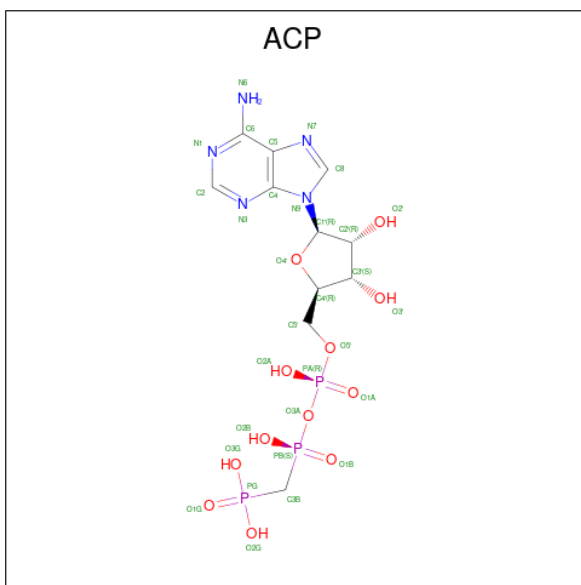
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	
			24	6	12	1	4	1	
								0	0

- 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-dioxo-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) (CCD ID: 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
			102	36	1	50	3	10	2
								0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

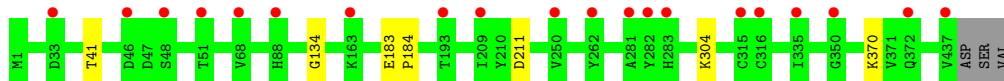
- Molecule 12 is water.

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

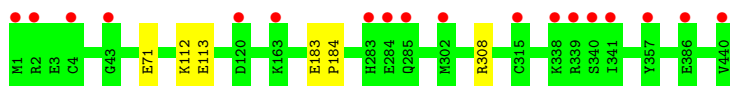
3 Residue-property plots [i](#)

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.

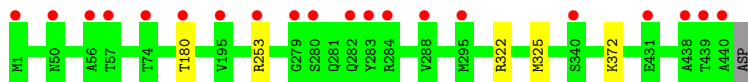
- Molecule 1: Tubulin alpha-1B chain



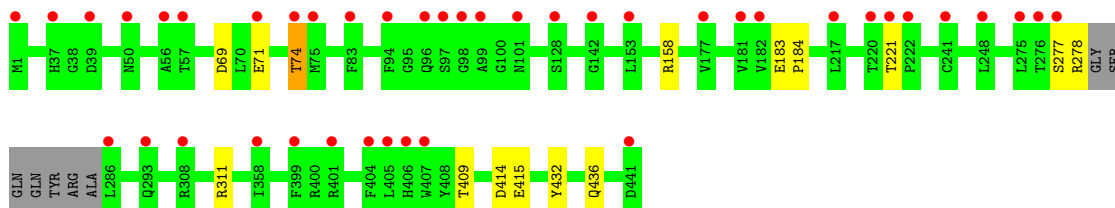
- Molecule 1: Tubulin alpha-1B chain



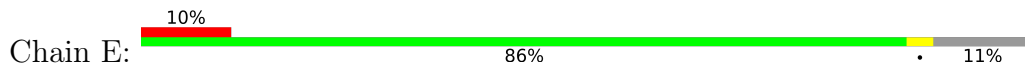
- Molecule 2: Tubulin beta-2B chain

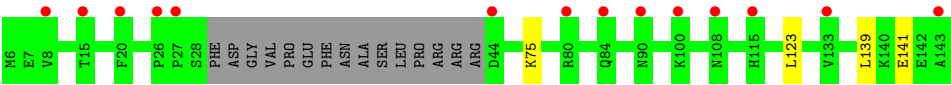


- Molecule 2: Tubulin beta-2B chain

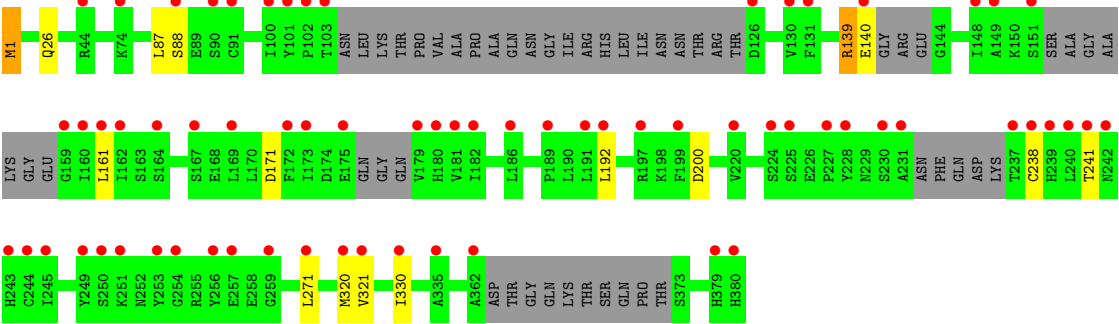
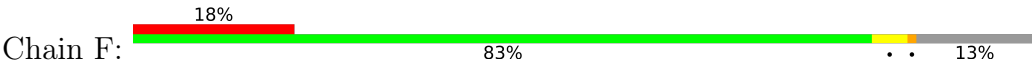


- Molecule 3: Stathmin-4





● 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, 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) 97.4 (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 0.213 , 0.255	Depositor DCC
R_{free} test set	2080 reflections (2.00%)	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)	0.38 , 44.1	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

5.1 Standard geometry

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

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	0.31	0/3515	0.65	1/4771 (0.0%)
1	C	0.32	0/3587	0.63	0/4873
2	B	0.31	0/3550	0.61	0/4807
2	D	0.30	0/3427	0.62	0/4642
3	E	0.29	0/1047	0.58	0/1390
4	F	0.27	0/2790	0.59	0/3767
All	All	0.30	0/17916	0.62	1/24250 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	GLY	N-CA-C	5.11	117.09	110.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1027	1037	1030	1	0
4	F	2721	2697	2709	5	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	1	0
6	A	1	0	0	0	0
6	B	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	17	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 (17) 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:69:ASP:OD2	2:D:74:THR:OG1	2.26	0.48
2:D:311:ARG:NH1	2:D:436:GLN:O	2.45	0.48
4:F:1:MET:HE2	4:F:26:GLN:HA	1.97	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	369 (100%)	2 (0%)	81	92
1	C	382/371 (103%)	380 (100%)	2 (0%)	81	92
2	B	383/372 (103%)	379 (99%)	4 (1%)	68	86
2	D	370/372 (100%)	364 (98%)	6 (2%)	55	79
3	E	113/123 (92%)	110 (97%)	3 (3%)	39	67
4	F	301/338 (89%)	292 (97%)	9 (3%)	36	64
All	All	1920/1947 (99%)	1894 (99%)	26 (1%)	61	81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	370	LYS
2	B	180	THR
2	B	322	ARG
2	B	325	MET
2	B	372	LYS
1	C	71	GLU
1	C	308	ARG
2	D	71	GLU
2	D	74	THR
2	D	221	THR
2	D	277	SER
2	D	278	ARG
2	D	409	THR
3	E	75	LYS
3	E	139	LEU
3	E	141	GLU
4	F	1	MET
4	F	139	ARG
4	F	161	LEU
4	F	171	ASP
4	F	192	LEU
4	F	238	CYS
4	F	271[A]	LEU
4	F	271[B]	LEU
4	F	321	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	258	ASN
1	A	393	HIS
2	B	300	ASN
2	B	349	ASN
1	C	356	ASN
2	D	331	GLN
3	E	12	ASN
3	E	90	ASN
4	F	252	ASN
4	F	310	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	33,34,34	0.95	2 (6%)	50,54,54	1.55	10 (20%)
5	GTP	D	502	6	33,34,34	0.96	2 (6%)	50,54,54	1.58	8 (16%)
5	GTP	C	501	6	33,34,34	0.93	2 (6%)	50,54,54	1.50	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BKX	D	503	-	53,55,55	2.24	14 (26%)	61,81,81	2.41	20 (32%)
8	GDP	B	501	6	29,30,30	1.18	2 (6%)	45,47,47	1.69	5 (11%)
11	ACP	F	402	6	31,33,33	4.45	10 (32%)	47,52,52	1.63	9 (19%)
9	MES	B	503	-	12,12,12	2.36	1 (8%)	15,16,16	2.29	4 (26%)

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	-	8/22/38/38	0/3/3/3
5	GTP	D	502	6	-	1/22/38/38	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
10	BKX	D	503	-	-	28/62/89/89	0/2/4/4
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
11	ACP	F	402	6	-	7/19/38/38	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	PB-O3A	21.46	1.82	1.58
11	F	402	ACP	PA-O5'	8.03	1.90	1.59
9	B	503	MES	C8-S	-7.91	1.66	1.77
10	D	503	BKX	C32-N30	7.13	1.46	1.35
10	D	503	BKX	C21-N19	5.81	1.46	1.35
10	D	503	BKX	C39-C42	5.61	1.54	1.47
10	D	503	BKX	O52-C45	-4.91	1.39	1.46
11	F	402	ACP	C5'-C4'	4.00	1.63	1.51
10	D	503	BKX	C20-N19	3.82	1.52	1.46
10	D	503	BKX	C23-C21	3.50	1.57	1.51
10	D	503	BKX	C23-C24	3.45	1.57	1.52
10	D	503	BKX	O41-C39	-3.30	1.42	1.46
10	D	503	BKX	C50-N49	3.13	1.41	1.34
8	B	501	GDP	C5-C4	2.99	1.46	1.38
11	F	402	ACP	O5'-C5'	-2.93	1.33	1.44
11	F	402	ACP	C2-N1	2.86	1.39	1.33
11	F	402	ACP	C8-N9	2.82	1.42	1.37
11	F	402	ACP	C8-N7	2.79	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C6-N1	-2.67	1.33	1.38
11	F	402	ACP	C4-N3	2.58	1.39	1.34
10	D	503	BKX	C34-C32	2.44	1.56	1.51
11	F	402	ACP	PA-O3A	-2.41	1.56	1.59
10	D	503	BKX	O41-C42	-2.40	1.41	1.45
10	D	503	BKX	C09-C07	-2.39	1.50	1.52
11	F	402	ACP	C5-C4	2.38	1.43	1.39
10	D	503	BKX	O25-C26	2.30	1.39	1.34
5	C	501	GTP	PA-O3A	2.24	1.61	1.59
10	D	503	BKX	O13-C12	2.17	1.40	1.37
5	A	501	GTP	C2-N3	2.10	1.38	1.33
5	C	501	GTP	C2-N3	2.09	1.38	1.33
5	D	502	GTP	PB-O3A	2.06	1.61	1.59
5	D	502	GTP	C2-N3	2.05	1.38	1.33
5	A	501	GTP	PB-O3B	2.02	1.61	1.59

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	BKX	C39-O41-C42	9.08	65.96	60.81
9	B	503	MES	C5-N4-C3	6.53	122.91	108.84
10	D	503	BKX	C18-C17-C15	-6.17	115.05	122.54
8	B	501	GDP	C5-C4-N3	-5.56	119.55	128.39
11	F	402	ACP	O2A-PA-O3A	4.92	120.57	107.27
5	A	501	GTP	C5-C4-N3	-4.83	120.71	128.39
8	B	501	GDP	C2-N3-C4	4.75	120.48	112.30
5	C	501	GTP	C5-C4-N3	-4.71	120.90	128.39
10	D	503	BKX	O25-C26-C28	4.68	120.40	110.82
5	D	502	GTP	C5-C4-N3	-4.68	120.94	128.39
5	D	502	GTP	C2-N3-C4	4.55	120.14	112.30
5	A	501	GTP	C2-N3-C4	4.44	119.94	112.30
5	C	501	GTP	C2-N3-C4	4.42	119.91	112.30
10	D	503	BKX	O25-C26-O27	-4.21	116.34	123.95
8	B	501	GDP	N9-C4-N3	4.18	134.32	125.95
11	F	402	ACP	O1B-PB-C3B	4.11	119.87	109.05
10	D	503	BKX	O41-C42-C39	-4.09	57.05	59.82
11	F	402	ACP	O5'-PA-O1A	-3.78	93.94	108.94
10	D	503	BKX	O41-C39-C42	-3.76	56.99	59.38
10	D	503	BKX	C34-C32-N30	3.62	125.28	119.14
8	B	501	GDP	C6-C5-N7	3.50	136.67	130.29
10	D	503	BKX	O13-C12-C15	3.29	119.05	115.44
10	D	503	BKX	C17-C15-CL1	3.26	123.13	120.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	BKX	C20-N19-C17	3.12	121.13	116.74
10	D	503	BKX	C12-C15-CL1	-3.11	114.53	120.27
5	A	501	GTP	N9-C4-N3	3.07	132.10	125.95
5	C	501	GTP	N9-C4-N3	2.95	131.86	125.95
5	D	502	GTP	N9-C4-N3	2.91	131.77	125.95
5	A	501	GTP	C2-N1-C6	-2.90	119.85	125.11
5	D	502	GTP	C2-N1-C6	-2.90	119.85	125.11
5	D	502	GTP	N9-C8-N7	-2.90	108.02	113.40
10	D	503	BKX	C17-C18-C10	2.86	124.74	120.28
11	F	402	ACP	PB-O3A-PA	-2.82	123.16	132.37
9	B	503	MES	O1S-S-C8	2.76	110.90	106.73
10	D	503	BKX	C40-C39-C42	-2.76	115.14	121.17
5	C	501	GTP	N9-C8-N7	-2.73	108.33	113.40
5	C	501	GTP	C2-N1-C6	-2.72	120.17	125.11
5	A	501	GTP	N9-C8-N7	-2.68	108.43	113.40
10	D	503	BKX	C08-C07-C09	-2.66	113.29	115.53
9	B	503	MES	C7-N4-C5	2.65	118.29	111.24
5	D	502	GTP	C8-N7-C5	2.59	108.87	104.26
10	D	503	BKX	O33-C32-N30	-2.58	117.59	121.92
8	B	501	GDP	C4-C5-N7	-2.55	106.62	110.67
5	C	501	GTP	C8-N7-C5	2.52	108.75	104.26
5	D	502	GTP	C5-C6-N1	2.52	119.66	113.25
10	D	503	BKX	C05-C06-C07	-2.51	124.16	127.69
5	A	501	GTP	C8-N7-C5	2.50	108.71	104.26
10	D	503	BKX	C26-C28-N30	2.44	115.83	110.92
5	A	501	GTP	C5-C6-N1	2.43	119.44	113.25
11	F	402	ACP	O1G-PG-C3B	-2.42	106.10	111.37
5	D	502	GTP	O6-C6-C5	-2.41	120.17	126.53
5	A	501	GTP	O6-C6-C5	-2.38	120.25	126.53
5	C	501	GTP	C5-C6-N1	2.35	119.25	113.25
11	F	402	ACP	C5-C4-N3	-2.35	123.48	126.72
11	F	402	ACP	O2A-PA-O5'	-2.33	96.99	107.57
5	C	501	GTP	O2A-PA-O3A	2.23	113.31	107.27
5	C	501	GTP	O6-C6-C5	-2.23	120.65	126.53
10	D	503	BKX	C14-O13-C12	2.20	120.75	117.51
10	D	503	BKX	C24-O25-C26	2.20	122.05	118.20
5	A	501	GTP	O3G-PG-O3B	2.18	111.94	104.64
9	B	503	MES	C2-C3-N4	2.16	113.41	110.12
11	F	402	ACP	O3'-C3'-C4'	2.14	117.22	111.08
10	D	503	BKX	O22-C21-C23	-2.05	118.25	122.07
5	A	501	GTP	O2A-PA-O3A	2.04	112.78	107.27
11	F	402	ACP	O2B-PB-C3B	2.04	115.16	106.73

There are no chirality outliers.

All (59) 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-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
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	O02-C03-C47-O48
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
10	D	503	BKX	C15-C12-O13-C14
11	F	402	ACP	O4'-C4'-C5'-O5'
9	B	503	MES	C7-C8-S-O3S
10	D	503	BKX	C11-C12-O13-C14
10	D	503	BKX	C04-C05-C06-C07
10	D	503	BKX	C44-C43-C45-C46
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
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

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Mol	Chain	Res	Type	Atoms
10	D	503	BKX	N19-C21-C23-C24
10	D	503	BKX	O02-C03-C04-C05
11	F	402	ACP	C3'-C4'-C5'-O5'
11	F	402	ACP	PB-C3B-PG-O2G
10	D	503	BKX	C29-C28-N30-C31
10	D	503	BKX	C34-C35-S36-S37
10	D	503	BKX	O27-C26-C28-C29
10	D	503	BKX	C29-C28-N30-C32
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	D	502	GTP	C4'-C5'-O5'-PA
10	D	503	BKX	C21-C23-C24-C39
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
10	D	503	BKX	O27-C26-C28-N30
10	D	503	BKX	O25-C26-C28-C29
10	D	503	BKX	O22-C21-C23-C24
5	C	501	GTP	C4'-C5'-O5'-PA

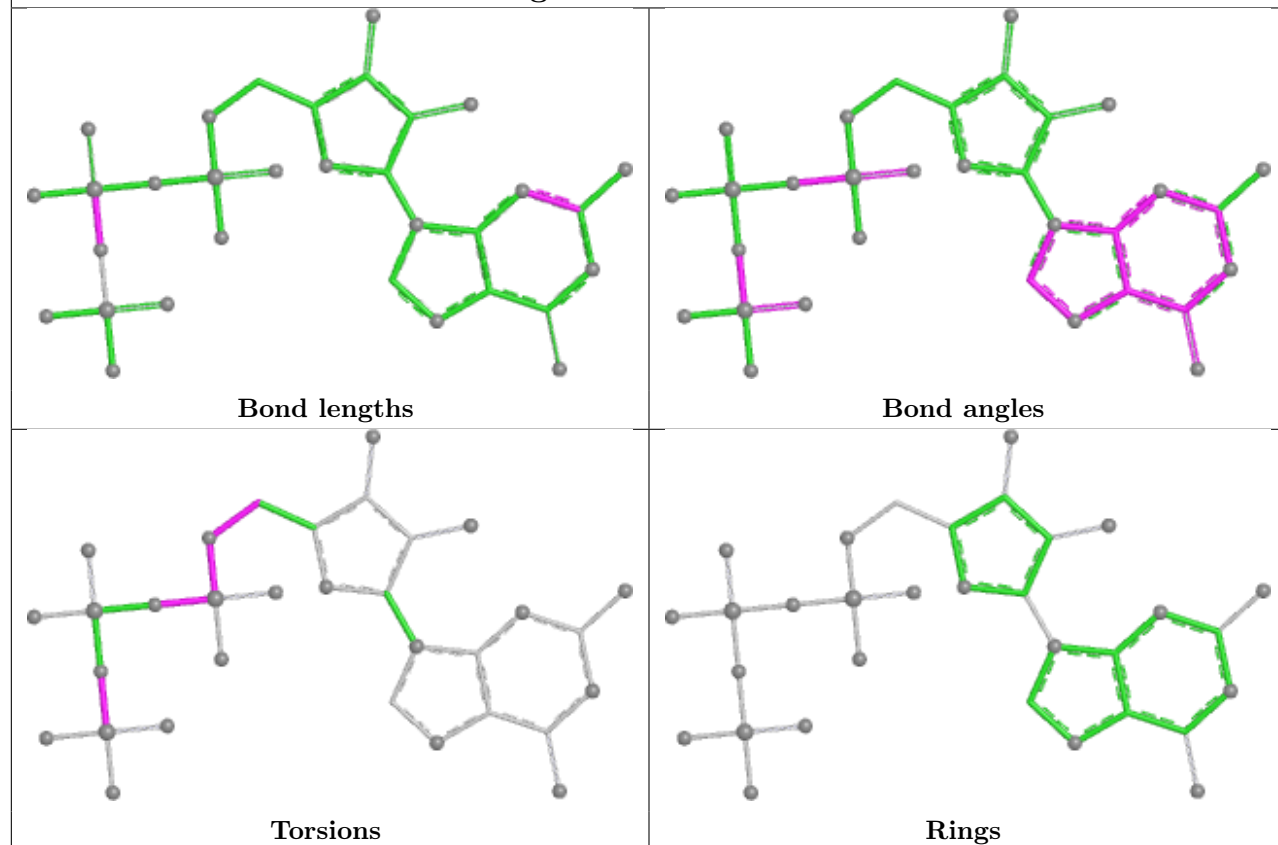
There are no ring outliers.

2 monomers are involved in 2 short contacts:

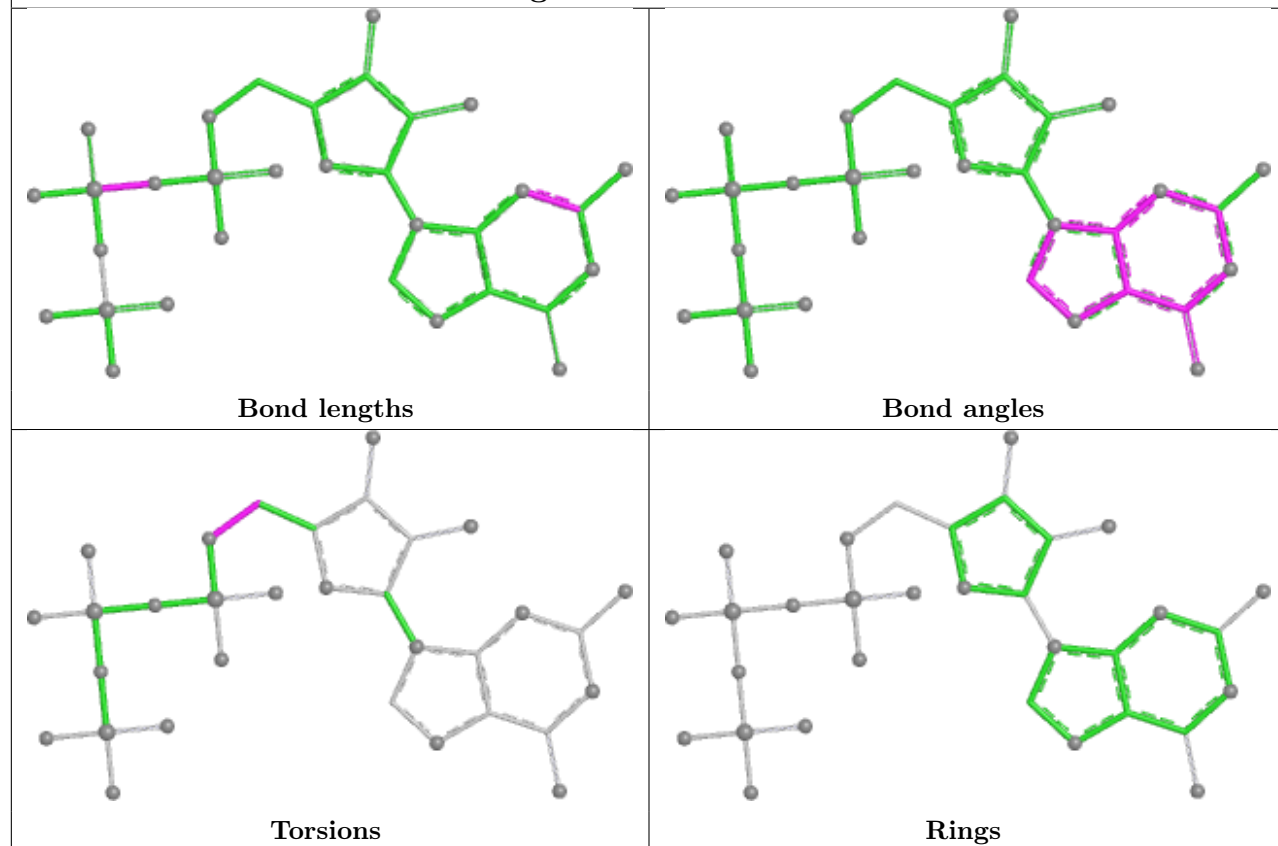
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	GTP	1	0
9	B	503	MES	1	0

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.

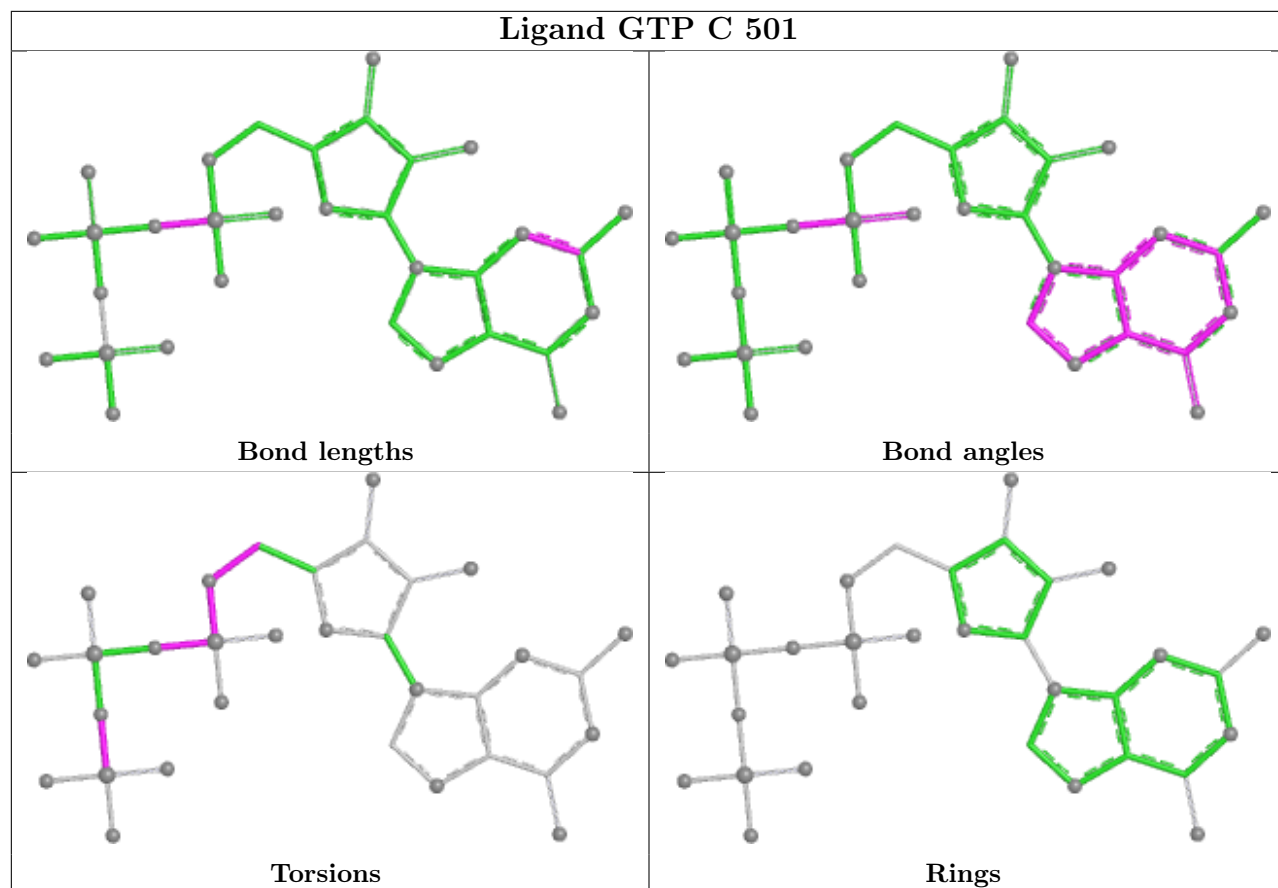
Ligand GTP A 501



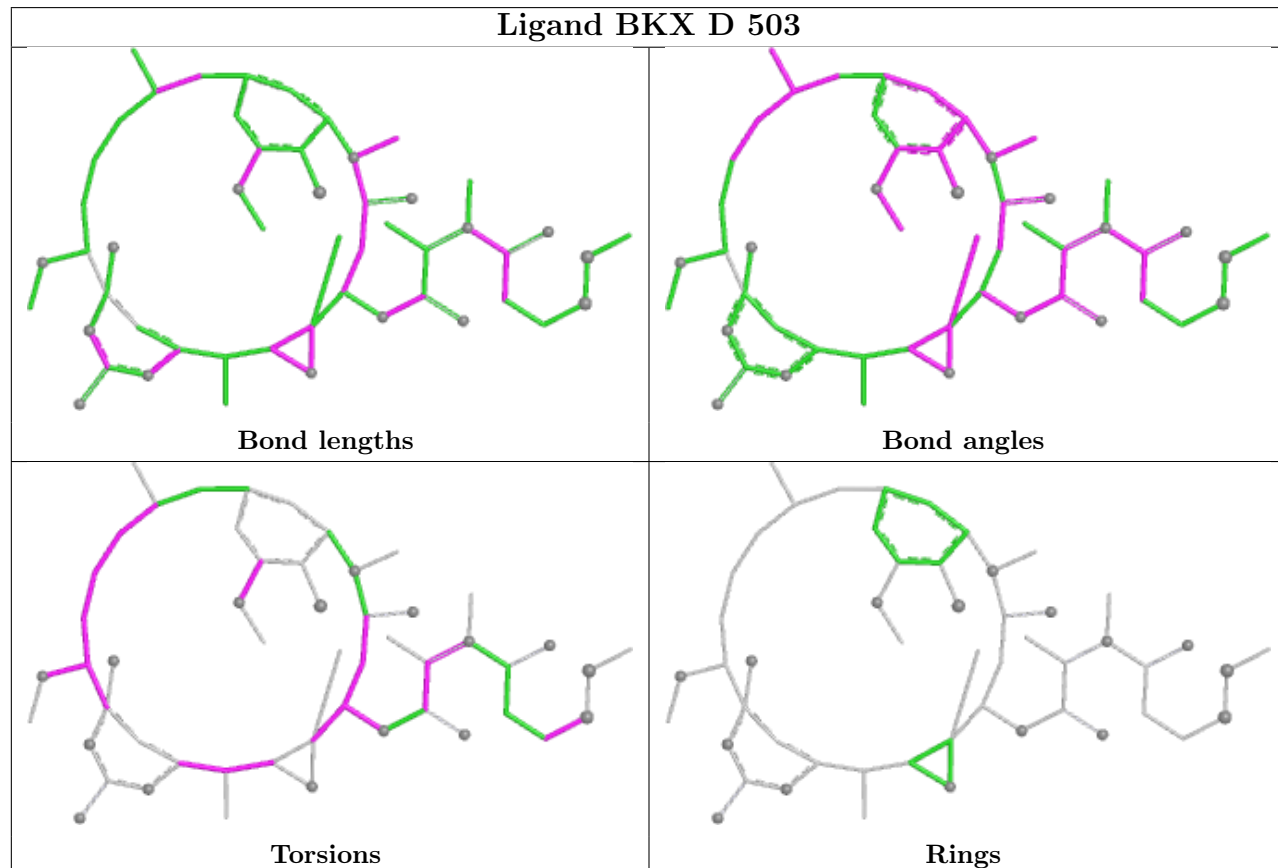
Ligand GTP D 502

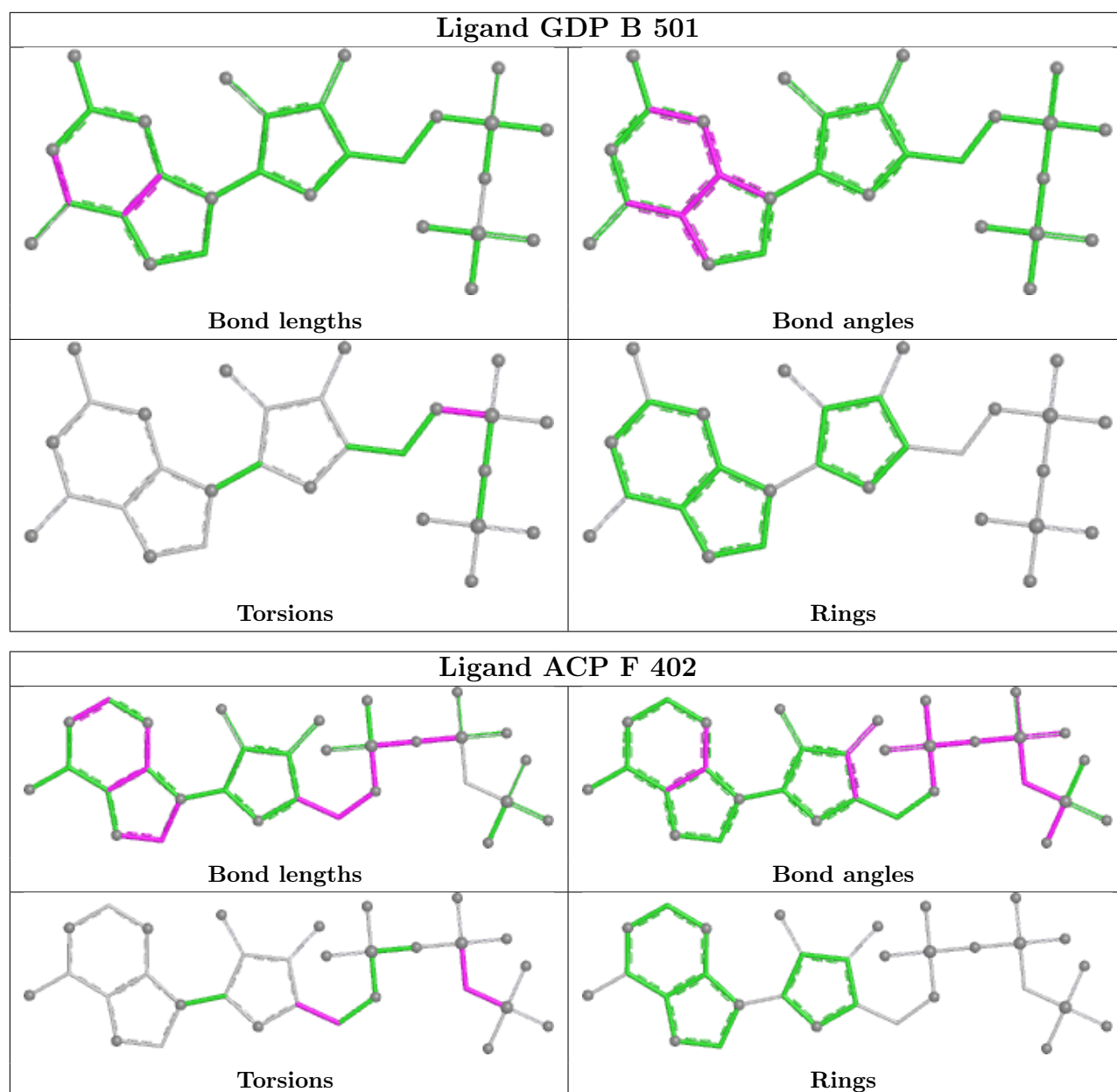


Ligand GTP C 501



Ligand BKX D 503





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%)	0.52	20 (4%)	37	33	41, 64, 95, 111	3 (0%)
1	C	440/440 (100%)	0.10	18 (4%)	41	37	27, 49, 77, 116	10 (2%)
2	B	430/431 (99%)	0.38	20 (4%)	36	32	31, 58, 94, 151	10 (2%)
2	D	424/431 (98%)	0.79	42 (9%)	13	11	43, 72, 105, 129	2 (0%)
3	E	123/138 (89%)	1.08	14 (11%)	10	8	45, 76, 120, 156	2 (1%)
4	F	330/380 (86%)	1.19	68 (20%)	2	2	49, 86, 154, 175	3 (0%)
All	All	2184/2260 (96%)	0.59	182 (8%)	17	15	27, 65, 117, 175	30 (1%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	115[A]	HIS	11.7
2	B	253[A]	ARG	6.5
1	C	315[A]	CYS	6.3
4	F	245	ILE	6.0
1	A	315[A]	CYS	5.7
3	E	143	ALA	5.4
1	A	316[A]	CYS	5.2
4	F	161	LEU	5.1
2	D	50[A]	ASN	5.0
2	D	98	GLY	4.8
1	A	372[A]	GLN	4.8
4	F	240	LEU	4.7
4	F	244	CYS	4.7
3	E	90	ASN	4.6
4	F	103	THR	4.6
2	B	431[A]	GLU	4.5
4	F	243	HIS	4.5
2	B	295	MET	4.5
4	F	151	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	386	GLU	4.3
1	A	437	VAL	4.2
4	F	239	HIS	4.2
3	E	15	THR	4.1
2	B	440	ALA	4.0
1	C	440	VAL	4.0
2	B	1	MET	3.9
4	F	159	GLY	3.9
4	F	90	SER	3.9
4	F	101	TYR	3.8
2	B	57	THR	3.8
2	B	50	ASN	3.8
4	F	241	THR	3.7
4	F	102	PRO	3.7
4	F	181	VAL	3.7
4	F	237	THR	3.7
2	D	286	LEU	3.7
3	E	84	GLN	3.7
4	F	192	LEU	3.7
1	A	193	THR	3.6
2	D	276	THR	3.6
3	E	108	ASN	3.6
1	C	340	SER	3.6
4	F	169	LEU	3.6
1	C	4[A]	CYS	3.5
2	B	74	THR	3.5
4	F	231	ALA	3.5
4	F	179	VAL	3.4
4	F	249	TYR	3.4
4	F	253	TYR	3.4
4	F	256	TYR	3.4
2	B	56	ALA	3.3
4	F	224	SER	3.3
4	F	321	VAL	3.3
4	F	228	TYR	3.2
4	F	182	ILE	3.2
1	C	43	GLY	3.2
2	D	74	THR	3.2
2	B	283	TYR	3.2
4	F	259	GLY	3.2
4	F	335	ALA	3.1
4	F	257	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	380	HIS	3.1
1	C	339	ARG	3.1
1	A	46	ASP	3.1
4	F	271[A]	LEU	3.0
3	E	8	VAL	3.0
4	F	100	ILE	3.0
2	D	222	PRO	3.0
4	F	238	CYS	3.0
1	C	338	LYS	3.0
1	A	88	HIS	3.0
4	F	230	SER	2.9
1	A	250	VAL	2.9
4	F	140	GLU	2.9
2	B	279	GLY	2.9
4	F	91	CYS	2.9
2	D	1	MET	2.9
2	D	101	ASN	2.8
2	D	406	HIS	2.8
4	F	320	MET	2.8
3	E	133	VAL	2.8
2	D	75	MET	2.8
1	C	285	GLN	2.8
2	D	94	PHE	2.8
1	C	357	TYR	2.8
4	F	330	ILE	2.8
2	B	340[A]	SER	2.8
1	A	262	TYR	2.7
1	A	282	TYR	2.7
4	F	88	SER	2.7
4	F	173	ILE	2.7
4	F	251	LYS	2.7
1	C	1	MET	2.7
2	D	56	ALA	2.7
4	F	186	LEU	2.7
1	C	341	ILE	2.6
1	C	120[A]	ASP	2.6
2	D	142	GLY	2.6
1	A	209	ILE	2.6
2	D	407	TRP	2.6
4	F	197	ARG	2.6
4	F	130	VAL	2.6
4	F	362	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	2.5
4	F	160	ILE	2.5
2	D	275	LEU	2.5
3	E	27	PRO	2.5
2	D	182	VAL	2.5
2	D	99	ALA	2.5
4	F	225	SER	2.5
4	F	126	ASP	2.5
2	D	405	LEU	2.5
2	D	404	PHE	2.5
1	C	2	ARG	2.5
1	A	281	ALA	2.5
2	D	221	THR	2.4
4	F	175	GLU	2.4
2	D	248	LEU	2.4
4	F	191	LEU	2.4
4	F	164	SER	2.4
4	F	227	PRO	2.4
2	D	308	ARG	2.4
4	F	172	PHE	2.4
2	D	358	ILE	2.4
4	F	162	ILE	2.4
2	D	441	ASP	2.4
4	F	199	PHE	2.4
2	D	153	LEU	2.3
2	B	439	THR	2.3
2	D	128	SER	2.3
4	F	167	SER	2.3
1	A	68	VAL	2.3
2	B	195[A]	VAL	2.3
4	F	149	ALA	2.3
2	D	277	SER	2.3
1	A	283	HIS	2.3
1	C	284	GLU	2.3
2	D	71	GLU	2.3
4	F	379	HIS	2.3
1	A	163	LYS	2.3
3	E	20	PHE	2.3
4	F	189	PRO	2.3
4	F	242	ASN	2.2
2	D	57	THR	2.2
1	C	283	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	180	HIS	2.2
2	D	97	SER	2.2
3	E	80	ARG	2.2
4	F	44	ARG	2.2
2	D	83	PHE	2.2
2	B	288	VAL	2.2
2	D	181	VAL	2.2
4	F	148	ILE	2.2
4	F	74	LYS	2.2
1	A	51	THR	2.2
2	B	284	ARG	2.2
2	D	399	PHE	2.2
4	F	131	PHE	2.2
2	D	37	HIS	2.1
2	B	180	THR	2.1
2	D	220	THR	2.1
3	E	100	LYS	2.1
2	D	217	LEU	2.1
1	A	48	SER	2.1
2	B	280	SER	2.1
1	C	302	MET	2.1
2	D	177	VAL	2.1
4	F	220[A]	VAL	2.1
4	F	254	GLY	2.1
2	D	39	ASP	2.1
2	D	241	CYS	2.1
3	E	26	PRO	2.1
2	D	293	GLN	2.1
2	B	438	ALA	2.1
1	A	350	GLY	2.1
1	C	163	LYS	2.1
1	A	33	ASP	2.1
4	F	250	SER	2.0
2	B	282	GLN	2.0
2	D	96	GLN	2.0
2	D	401	ARG	2.0
3	E	44	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

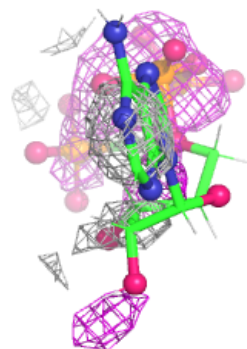
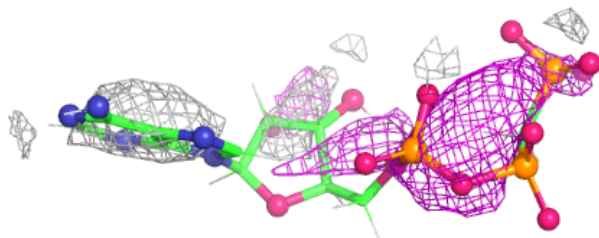
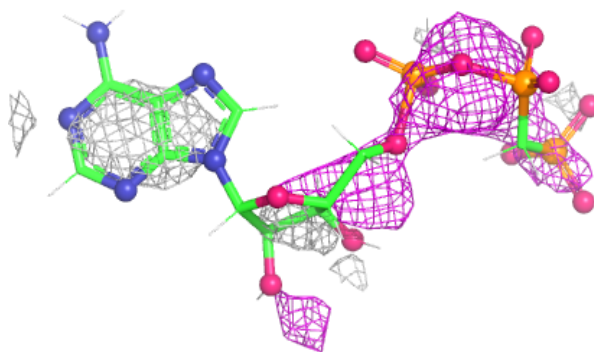
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.21	0.24	114,114,114,114	0
11	ACP	F	402	31/31	0.40	0.19	111,144,192,198	0
10	BKX	D	503	52/52	0.82	0.20	72,105,129,281	0
9	MES	B	503	12/12	0.88	0.14	51,68,88,105	0
5	GTP	D	502	32/32	0.92	0.12	50,64,87,89	0
7	CA	A	503	1/1	0.93	0.09	79,79,79,79	0
6	MG	D	501	1/1	0.95	0.11	67,67,67,67	0
8	GDP	B	501	28/28	0.96	0.09	32,45,57,68	0
5	GTP	C	501	32/32	0.96	0.08	29,40,50,53	0
5	GTP	A	501	32/32	0.97	0.07	29,47,57,59	0
6	MG	B	502	1/1	0.99	0.09	45,45,45,45	0
7	CA	C	503	1/1	0.99	0.08	61,61,61,61	0
6	MG	C	502	1/1	0.99	0.05	36,36,36,36	0
6	MG	A	502	1/1	1.00	0.08	43,43,43,43	0

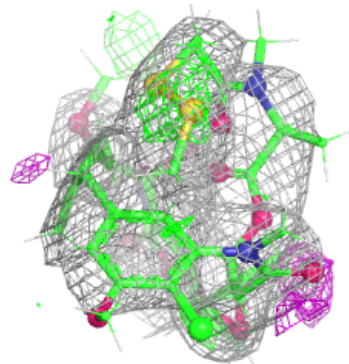
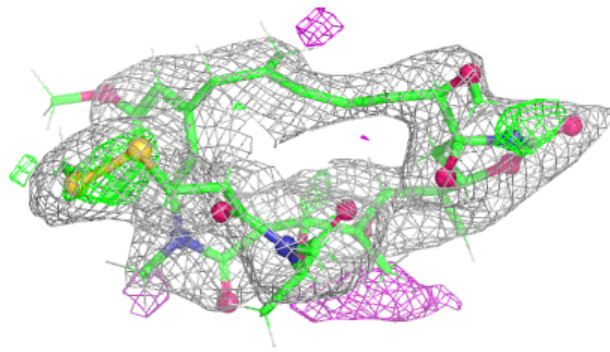
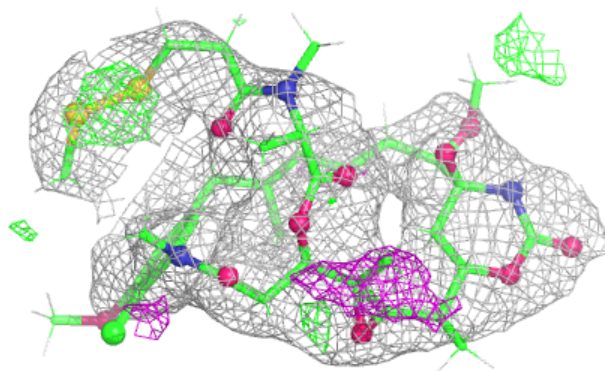
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

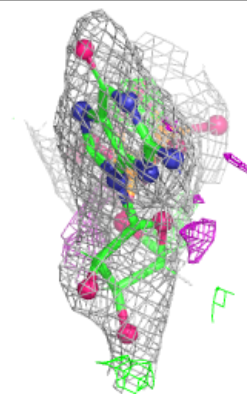
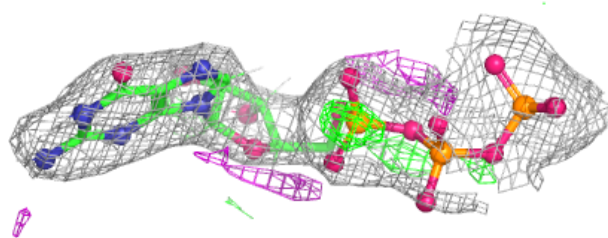
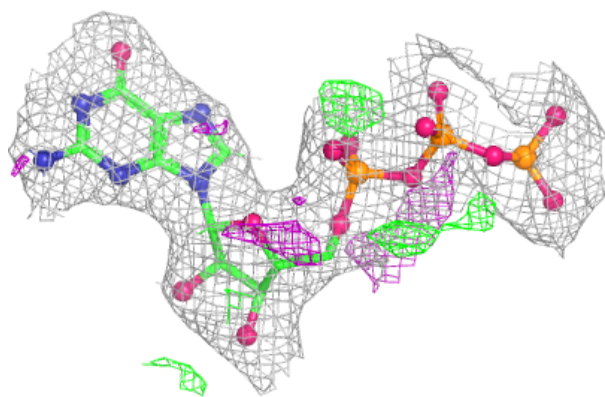
**Electron density around BKX D 503:**

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



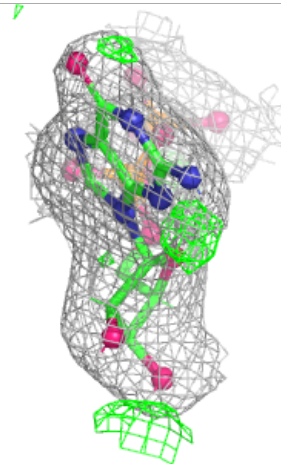
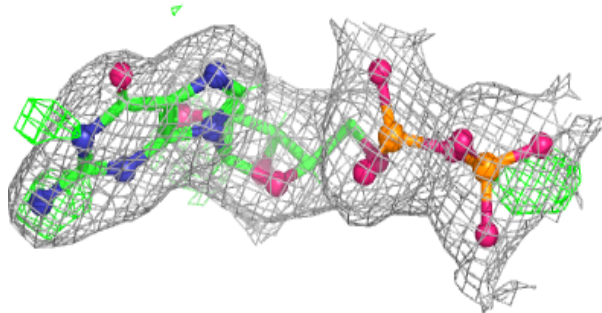
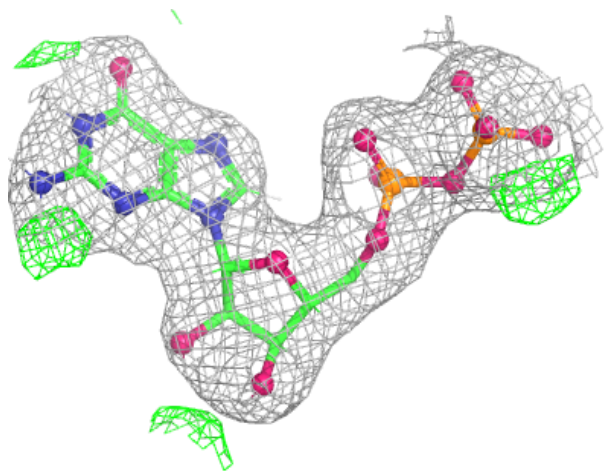
Electron density around GTP D 502:

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



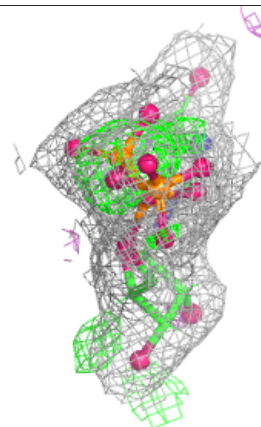
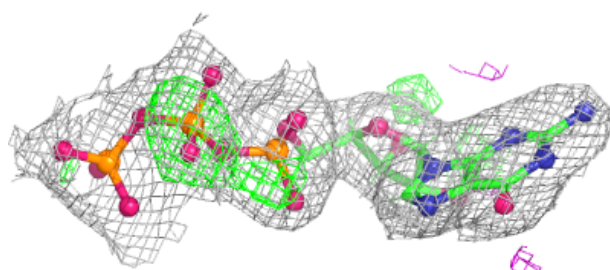
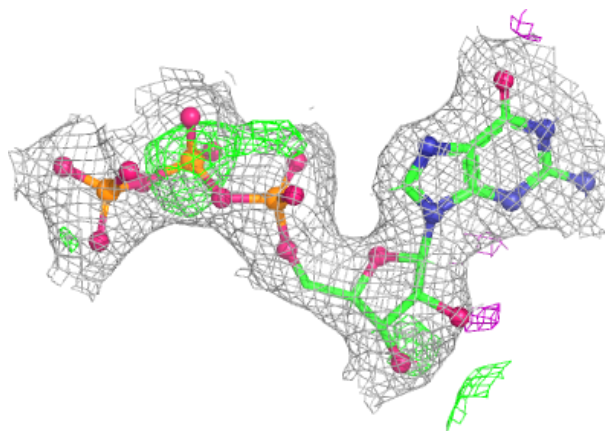
Electron density around GDP B 501:

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

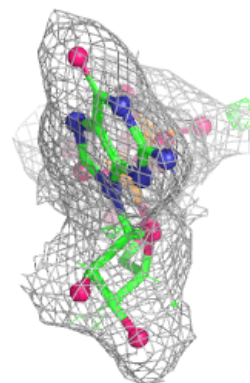
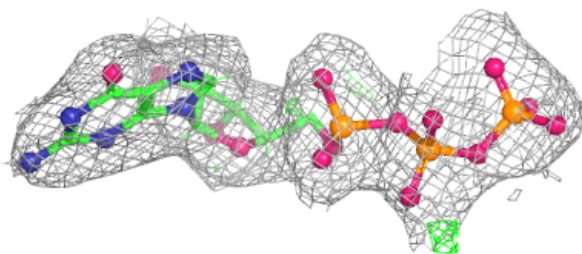
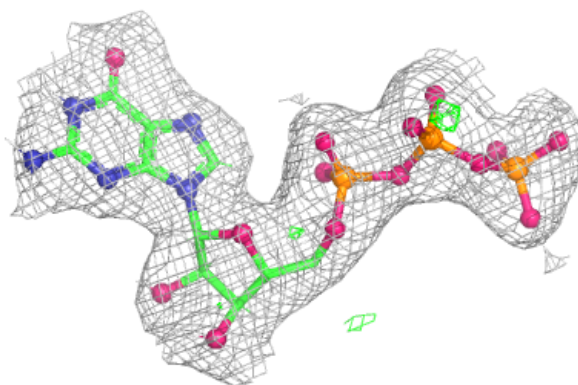


Electron density around GTP C 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.