Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2022 – 01:05 PM EDT

PDB ID	:	5H7O
Title	:	Crystal structure of DJ-101 in complex with tubulin protein
Authors	:	Arnst, K.; Wang, Y.; Hwang, D.-J.; Xue, Y.; Costello, T.; Hamilton, D.; Chen, Q.; Yang, J.; Park, F.; Dalton, J.T.; Miller, D.D.; Li, W.
Deposited on	:	2016-11-20
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

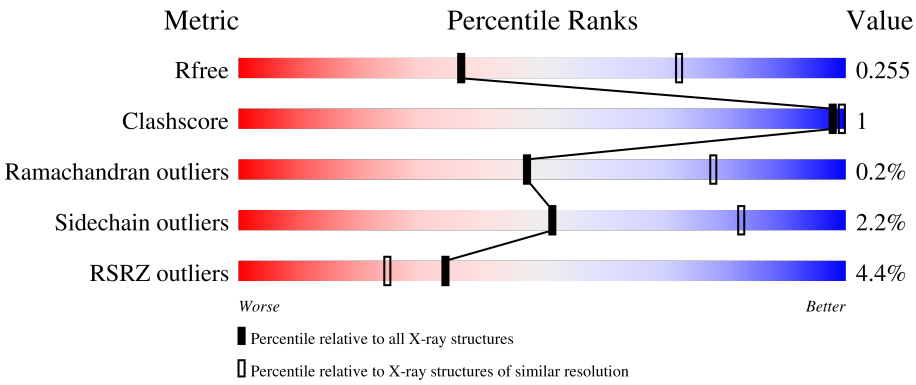
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	2% 93%
1	C	450	95%
2	B	445	2% 93%
2	D	445	7% 92% 5%
3	E	143	3% 81% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	11% 83% • 13%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 17517 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3416	2163	581	650	22	0	0	0
1	C	440	3437	2175	584	656	22	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	3350	2104	572	648	26	0	0	0
2	D	421	3309	2080	562	640	27	0	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	1000	617	181	197	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

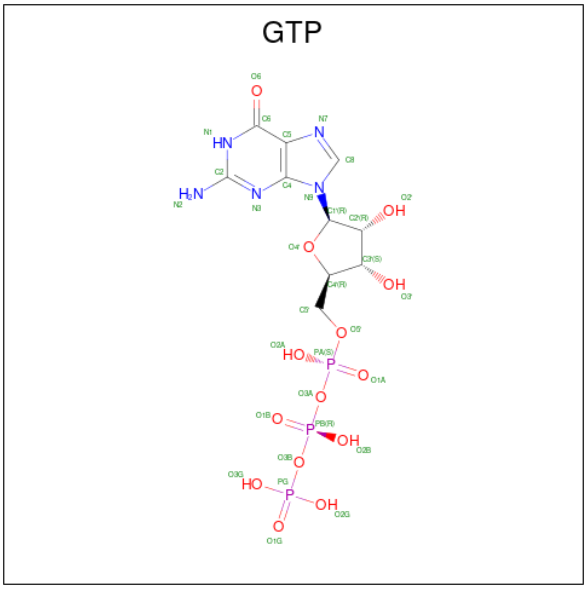
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	334	2744	1761	470	499	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

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

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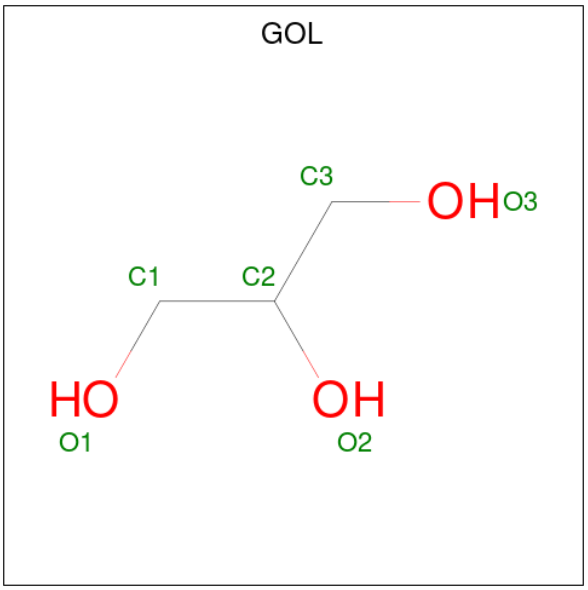
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	D	1	1	1	0	0

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

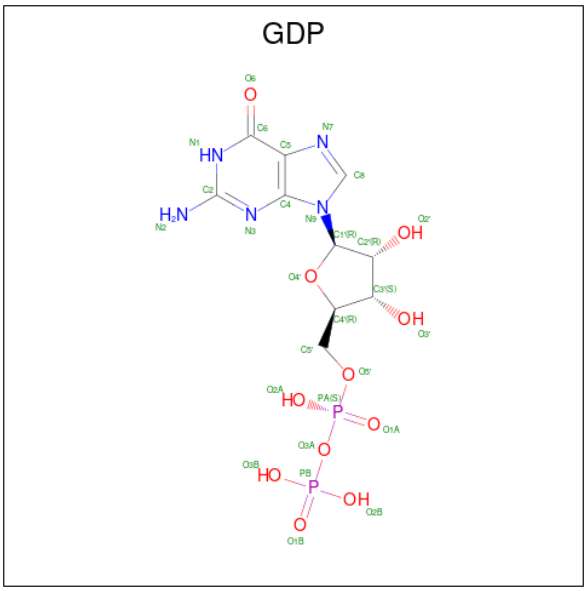
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



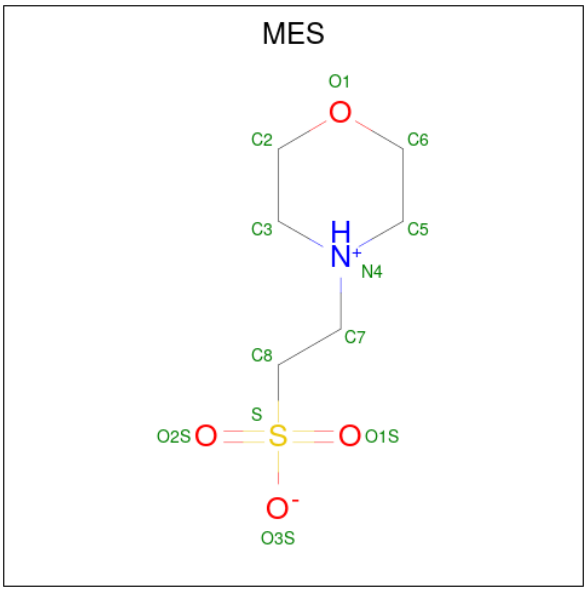
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



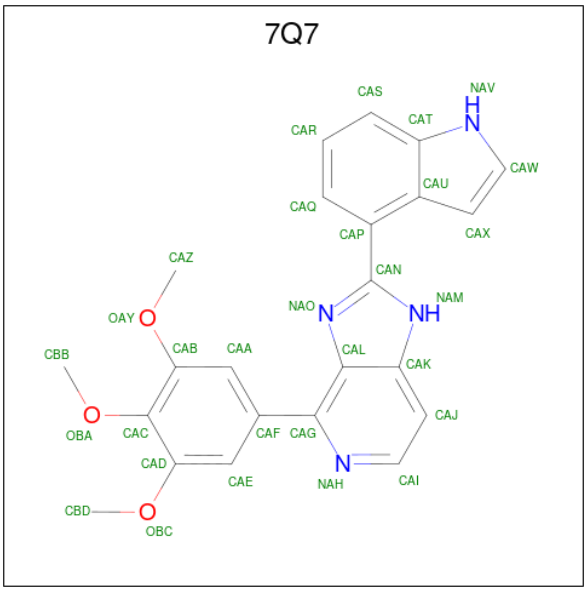
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



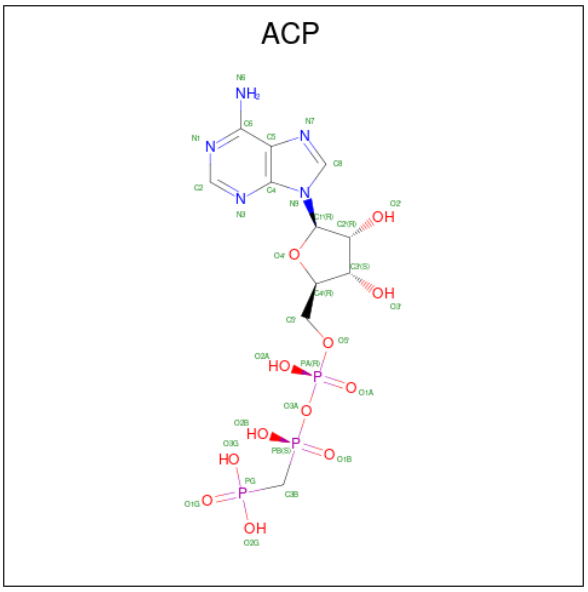
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is 2-(1H-indol-4-yl)-4-(3,4,5-trimethoxyphenyl)-1H-imidazo[4,5-c]pyridine (three-letter code: 7Q7) (formula: $C_{23}H_{20}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	B	1	30	23	4	3	0	0
			Total	C	N	O		
11	D	1	30	23	4	3	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	F	1	31	11	5	12	3	0	0

- Molecule 13 is water.

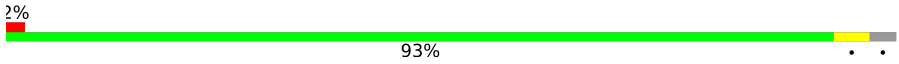
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	6	6	6	0	0
			Total	O		
13	B	8	8	8	0	0
			Total	O		
13	C	8	8	8	0	0

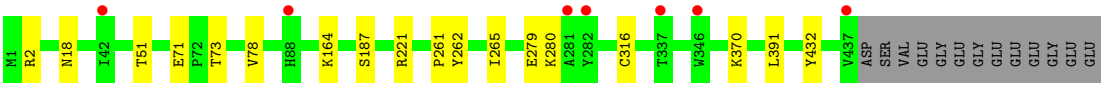
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha-1B chain

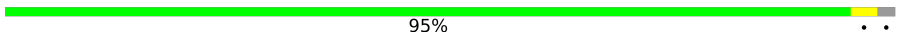
Chain A:





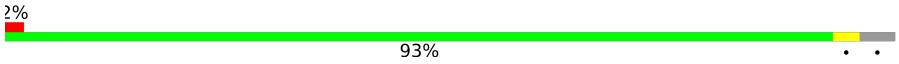
• Molecule 1: Tubulin alpha-1B chain

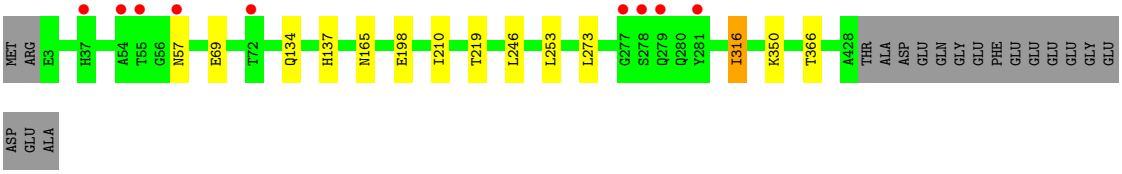
Chain C:



• Molecule 2: Tubulin beta-2B chain

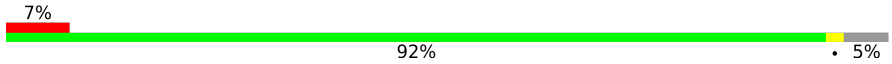
Chain B:

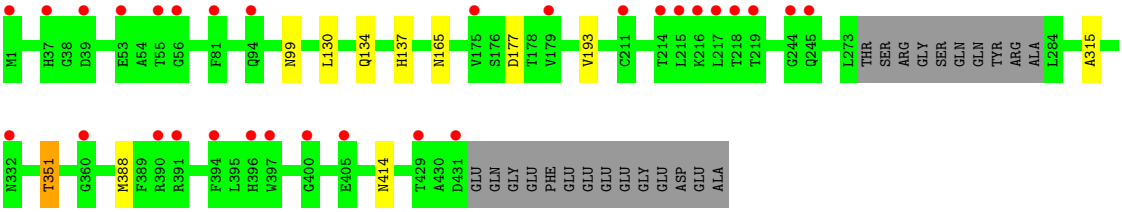




• Molecule 2: Tubulin beta-2B chain

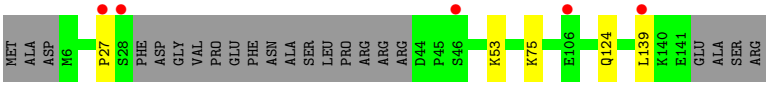
Chain D:





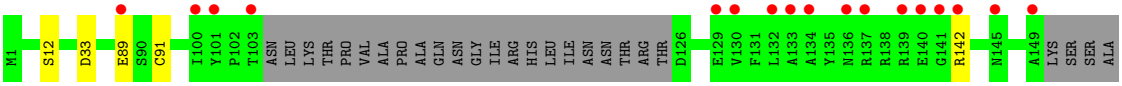
• Molecule 3: Stathmin-4

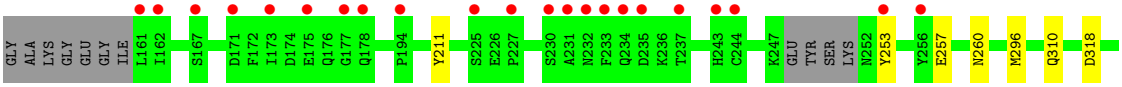
Chain E:

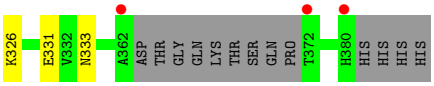


• Molecule 4: Tubulin tyrosine ligase

Chain F:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.20Å 157.03Å 182.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.80) 99.9 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.214 , 0.256 0.216 , 0.255	Depositor DCC
R_{free} test set	3809 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17517	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MES, GDP, CA, MG, ACP, GOL, 7Q7

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	0.37	0/3494	0.59	0/4743
1	C	0.37	0/3515	0.61	0/4772
2	B	0.38	0/3425	0.58	0/4640
2	D	0.39	0/3382	0.56	0/4581
3	E	0.38	0/1008	0.52	0/1337
4	F	0.39	0/2806	0.57	0/3791
All	All	0.38	0/17630	0.58	0/23864

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	0	3331	4	0
1	C	3437	0	3348	4	0
2	B	3350	0	3225	5	0
2	D	3309	0	3189	6	0
3	E	1000	0	1018	0	0
4	F	2744	0	2709	5	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	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	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	0	0
11	B	30	0	0	0	0
11	D	30	0	0	0	0
12	F	31	0	14	6	0
13	A	6	0	0	0	0
13	B	8	0	0	0	0
13	C	8	0	0	0	0
All	All	17517	0	16903	24	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 (24) 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:318:ASP:OD2	12:F:401:ACP:O1G	1.56	1.24
4:F:331:GLU:OE2	12:F:401:ACP:O1G	1.93	0.87
4:F:331:GLU:OE2	12:F:401:ACP:PG	2.34	0.85
4:F:331:GLU:OE2	12:F:401:ACP:O2G	2.01	0.79
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.81	0.61
2:D:193:VAL:HG11	2:D:414:ASN:HD21	1.70	0.57
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.70	0.55
2:B:316:ILE:HG23	2:B:366:THR:HB	1.89	0.54
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.53
12:F:401:ACP:H3B2	12:F:401:ACP:O2A	2.11	0.50
2:D:315:ALA:HB3	2:D:351:THR:CG2	2.44	0.48
4:F:331:GLU:OE1	12:F:401:ACP:O2B	2.31	0.48
2:B:210:ILE:HG23	2:B:273:LEU:HD13	1.96	0.48
2:B:219:THR:HG21	1:C:326:LYS:HA	1.98	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.99	0.43
1:A:2:ARG:O	1:A:51:THR:HG23	2.18	0.43
1:C:71:GLU:HB2	1:C:98:ASP:HB3	2.01	0.42
2:D:99:ASN:HD22	2:D:99:ASN:N	2.18	0.42
2:B:134:GLN:HA	2:B:165:ASN:O	2.20	0.42
2:D:193:VAL:CG1	2:D:414:ASN:HD21	2.34	0.41
2:B:198:GLU:OE1	2:B:253:LEU:HD23	2.21	0.41

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	435/450 (97%)	419 (96%)	15 (3%)	1 (0%)	47	78
1	C	438/450 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	406 (97%)	11 (3%)	0	100	100
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	17	46
4	F	324/384 (84%)	304 (94%)	18 (6%)	2 (1%)	25	56
All	All	2155/2317 (93%)	2084 (97%)	67 (3%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	253	TYR
3	E	27	PRO
4	F	91	CYS
1	A	261	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/378 (97%)	359 (98%)	9 (2%)	49	81
1	C	371/378 (98%)	365 (98%)	6 (2%)	62	88
2	B	368/383 (96%)	362 (98%)	6 (2%)	62	88
2	D	364/383 (95%)	359 (99%)	5 (1%)	67	90
3	E	109/127 (86%)	105 (96%)	4 (4%)	34	68
4	F	301/342 (88%)	290 (96%)	11 (4%)	34	68
All	All	1881/1991 (94%)	1840 (98%)	41 (2%)	52	83

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	73	THR
1	A	164	LYS
1	A	221	ARG
1	A	262	TYR
1	A	279	GLU
1	A	280	LYS
1	A	316	CYS
1	A	370	LYS
2	B	57	ASN
2	B	69	GLU
2	B	137	HIS
2	B	246	LEU
2	B	316	ILE
2	B	350	LYS
1	C	2	ARG
1	C	190	THR
1	C	221	ARG
1	C	284	GLU
1	C	302	MET
1	C	381	THR
2	D	130	LEU

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Mol	Chain	Res	Type
2	D	137	HIS
2	D	177	ASP
2	D	351	THR
2	D	388	MET
3	E	53	LYS
3	E	75	LYS
3	E	124	GLN
3	E	139	LEU
4	F	12	SER
4	F	33	ASP
4	F	89	GLU
4	F	142	ARG
4	F	211	TYR
4	F	257	GLU
4	F	260	ASN
4	F	296	MET
4	F	310	GLN
4	F	326	LYS
4	F	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	301	GLN
2	B	375	GLN
1	C	11	GLN
1	C	358	GLN
2	D	99	ASN
2	D	414	ASN
3	E	92	ASN
4	F	176	GLN
4	F	310	GLN

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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	0.91	0	32,54,54	1.14	4 (12%)
10	MES	B	503	-	12,12,12	2.17	1 (8%)	14,16,16	1.44	3 (21%)
11	7Q7	D	503	-	30,34,34	2.35	10 (33%)	36,49,49	1.44	4 (11%)
8	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.26	0
5	GTP	D	501	6	26,34,34	0.90	0	32,54,54	1.30	5 (15%)
5	GTP	C	501	6	26,34,34	0.89	1 (3%)	32,54,54	1.15	5 (15%)
12	ACP	F	401	-	27,33,33	2.16	8 (29%)	32,52,52	2.31	8 (25%)
11	7Q7	B	504	-	30,34,34	2.34	10 (33%)	36,49,49	1.70	4 (11%)
9	GDP	B	501	6	24,30,30	0.91	0	30,47,47	1.12	3 (10%)

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	-	6/18/38/38	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	7Q7	D	503	-	-	4/14/14/14	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	D	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
12	ACP	F	401	-	-	9/15/38/38	0/3/3/3
11	7Q7	B	504	-	-	4/14/14/14	0/5/5/5
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.04	1.67	1.77
11	D	503	7Q7	CAF-CAG	-6.42	1.40	1.49
11	B	504	7Q7	CAF-CAG	-6.21	1.40	1.49
11	B	504	7Q7	CAP-CAN	-5.50	1.35	1.48
11	D	503	7Q7	CAP-CAN	-5.41	1.35	1.48
12	F	401	ACP	PB-O1B	5.28	1.64	1.51
12	F	401	ACP	PG-O1G	5.27	1.61	1.50
12	F	401	ACP	PB-O2B	4.58	1.67	1.56
11	D	503	7Q7	CAJ-CAK	-4.50	1.34	1.41
11	B	504	7Q7	CAS-CAT	-4.45	1.34	1.41
11	B	504	7Q7	CAJ-CAK	-4.43	1.34	1.41
11	D	503	7Q7	CAS-CAT	-4.40	1.34	1.41
12	F	401	ACP	PB-O3A	3.27	1.62	1.58
12	F	401	ACP	PG-O2G	-3.07	1.47	1.54
11	D	503	7Q7	CAU-CAT	-2.80	1.35	1.42
11	B	504	7Q7	CAU-CAT	-2.77	1.35	1.42
11	B	504	7Q7	CAI-NAH	2.70	1.40	1.34
11	D	503	7Q7	CAI-NAH	2.69	1.40	1.34
11	D	503	7Q7	CAP-CAU	-2.65	1.36	1.42
11	B	504	7Q7	CAP-CAU	-2.58	1.36	1.42
12	F	401	ACP	C5-C4	2.57	1.47	1.40
12	F	401	ACP	PG-O3G	2.42	1.60	1.54
11	D	503	7Q7	CAK-CAL	-2.20	1.35	1.42
11	B	504	7Q7	CAK-CAL	-2.18	1.35	1.42
11	D	503	7Q7	CAN-NAM	-2.07	1.33	1.35
12	F	401	ACP	C2-N3	2.07	1.35	1.32
5	C	501	GTP	C6-N1	-2.05	1.34	1.37
11	D	503	7Q7	CAG-NAH	2.03	1.34	1.32
11	B	504	7Q7	CAN-NAO	-2.03	1.33	1.35
11	B	504	7Q7	CAG-NAH	2.03	1.34	1.32

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	401	ACP	O1B-PB-C3B	8.04	130.34	109.07
11	B	504	7Q7	CAJ-CAI-NAH	-6.25	117.65	123.81
11	D	503	7Q7	CAJ-CAI-NAH	-5.12	118.76	123.81
11	B	504	7Q7	CAI-NAH-CAG	4.62	121.32	117.99
12	F	401	ACP	O2B-PB-O1B	-4.12	96.30	110.07
12	F	401	ACP	N3-C2-N1	-3.83	122.70	128.68
12	F	401	ACP	O2B-PB-C3B	3.72	121.79	106.58
10	B	503	MES	O3S-S-C8	3.29	111.09	105.77
12	F	401	ACP	C3'-C2'-C1'	3.27	105.90	100.98
11	D	503	7Q7	CAI-NAH-CAG	3.16	120.27	117.99
12	F	401	ACP	PB-O3A-PA	-3.09	122.75	132.56
11	B	504	7Q7	CAZ-OAY-CAB	-3.07	112.89	117.53
5	D	501	GTP	PA-O3A-PB	-2.91	122.84	132.83
12	F	401	ACP	C4-C5-N7	-2.90	106.37	109.40
11	B	504	7Q7	CAP-CAN-NAM	2.71	127.13	123.67
5	D	501	GTP	PB-O3B-PG	-2.52	124.19	132.83
12	F	401	ACP	O3G-PG-C3B	2.47	112.39	106.40
5	D	501	GTP	C8-N7-C5	2.35	107.46	102.99
9	B	501	GDP	C5-C6-N1	2.34	118.08	113.95
11	D	503	7Q7	CAZ-OAY-CAB	-2.32	114.02	117.53
5	C	501	GTP	C8-N7-C5	2.32	107.40	102.99
5	D	501	GTP	C5-C6-N1	2.30	118.01	113.95
10	B	503	MES	O2S-S-C8	2.28	109.67	106.92
5	A	501	GTP	C8-N7-C5	2.26	107.29	102.99
5	C	501	GTP	O3G-PG-O2G	2.25	116.25	107.64
9	B	501	GDP	C8-N7-C5	2.22	107.21	102.99
5	A	501	GTP	O6-C6-C5	-2.18	120.11	124.37
9	B	501	GDP	O6-C6-C5	-2.15	120.18	124.37
10	B	503	MES	O1S-S-C8	2.13	109.48	106.92
5	C	501	GTP	C5-C6-N1	2.12	117.70	113.95
5	C	501	GTP	PA-O3A-PB	-2.10	125.63	132.83
11	D	503	7Q7	CAN-NAM-CAK	2.02	107.79	103.78
5	A	501	GTP	C5-C6-N1	2.02	117.51	113.95
5	D	501	GTP	O6-C6-C5	-2.01	120.44	124.37
5	A	501	GTP	PA-O3A-PB	-2.01	125.94	132.83
5	C	501	GTP	PB-O3B-PG	-2.00	125.96	132.83

There are no chirality outliers.

All (40) 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	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	C1-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	N4-C7-C8-S
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O3G
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O3A
11	B	504	7Q7	CAC-CAB-OAY-CAZ
11	D	503	7Q7	CAC-CAD-OBC-CBD
11	B	504	7Q7	CAA-CAB-OAY-CAZ
11	D	503	7Q7	CAE-CAD-OBC-CBD
11	D	503	7Q7	CAC-CAB-OAY-CAZ
11	B	504	7Q7	CAC-CAD-OBC-CBD
12	F	401	ACP	O4'-C4'-C5'-O5'
11	D	503	7Q7	CAA-CAB-OAY-CAZ
11	B	504	7Q7	CAE-CAD-OBC-CBD
12	F	401	ACP	PB-O3A-PA-O1A
8	A	504	GOL	O2-C2-C3-O3
12	F	401	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
12	F	401	ACP	PB-C3B-PG-O2G
5	D	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PB-O3A-PA-O1A
12	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
9	B	501	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G

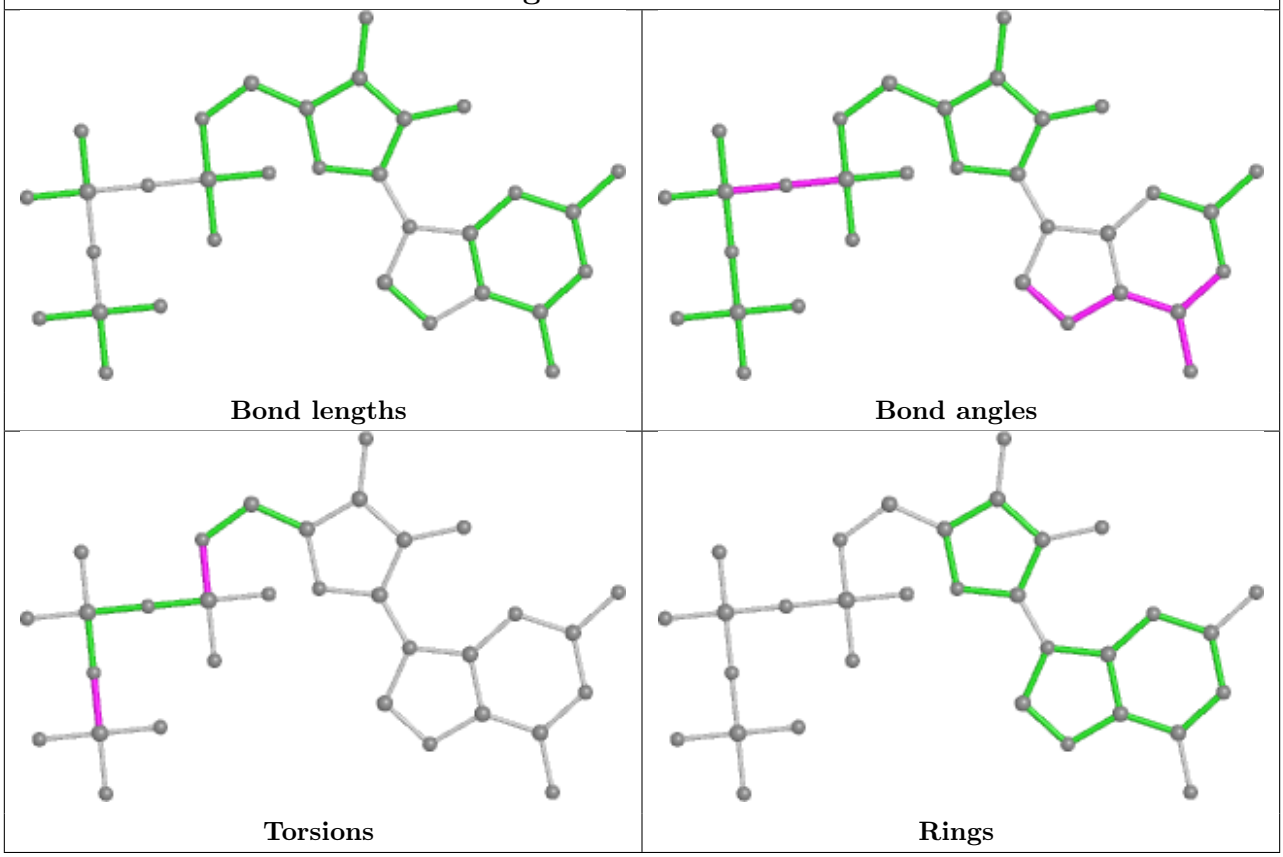
There are no ring outliers.

1 monomer is involved in 6 short contacts:

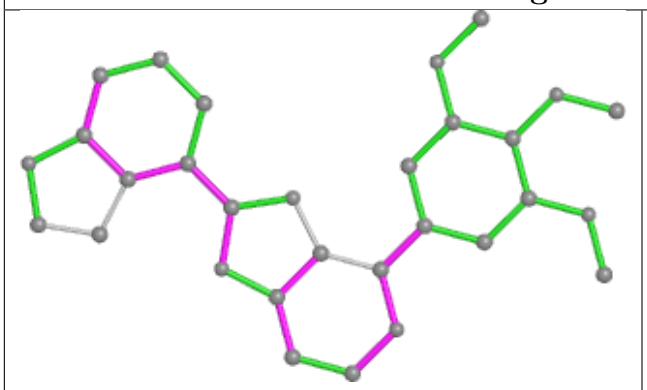
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

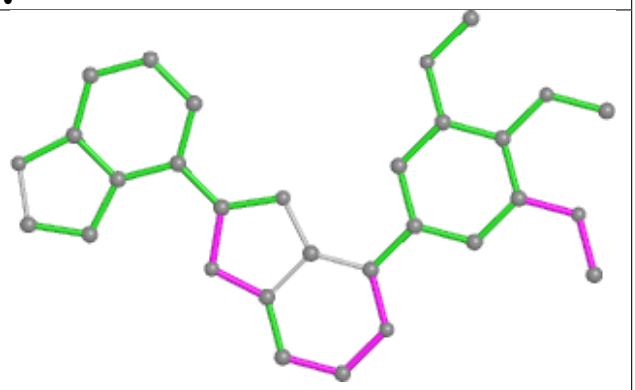
Ligand GTP A 501



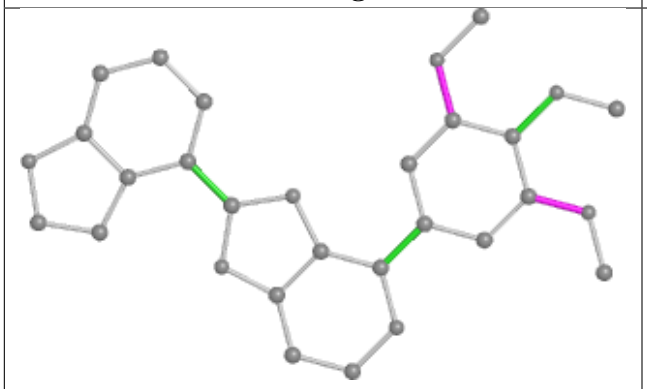
Ligand 7Q7 D 503



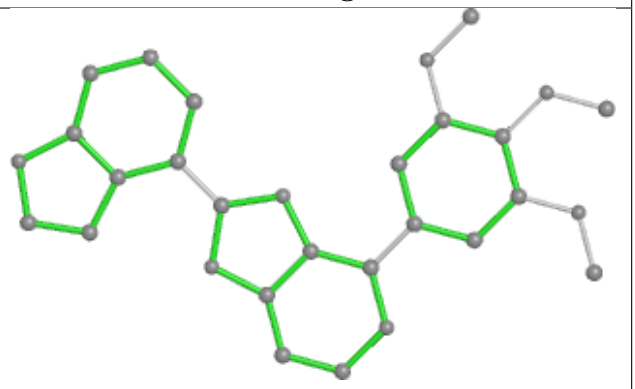
Bond lengths



Bond angles

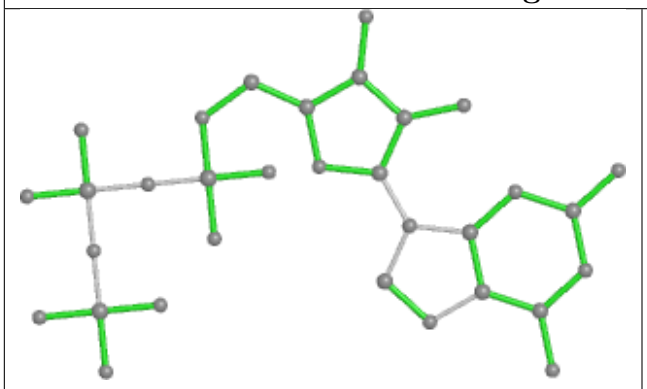


Torsions

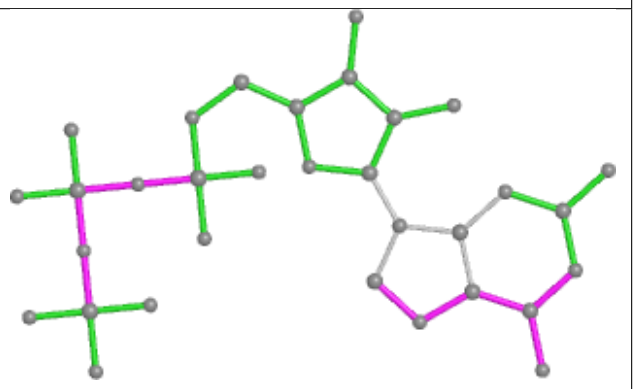


Rings

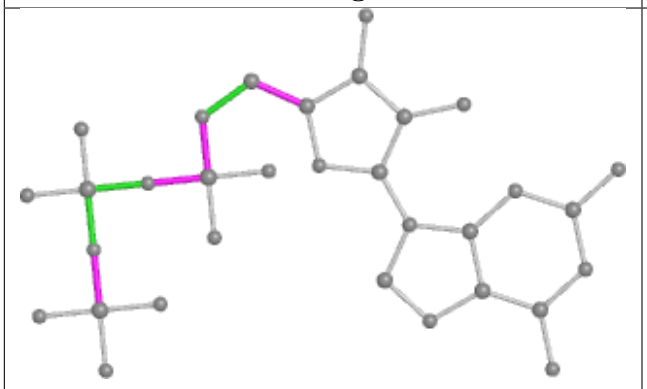
Ligand GTP D 501



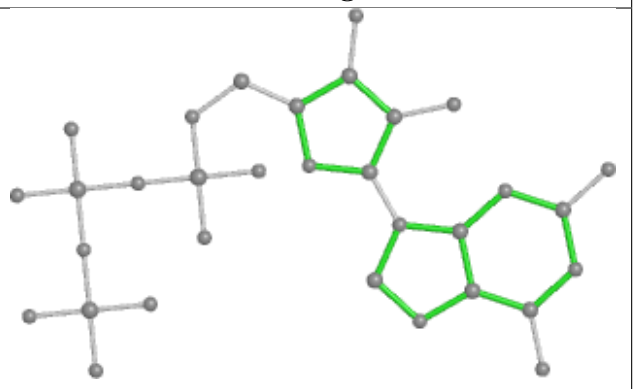
Bond lengths



Bond angles

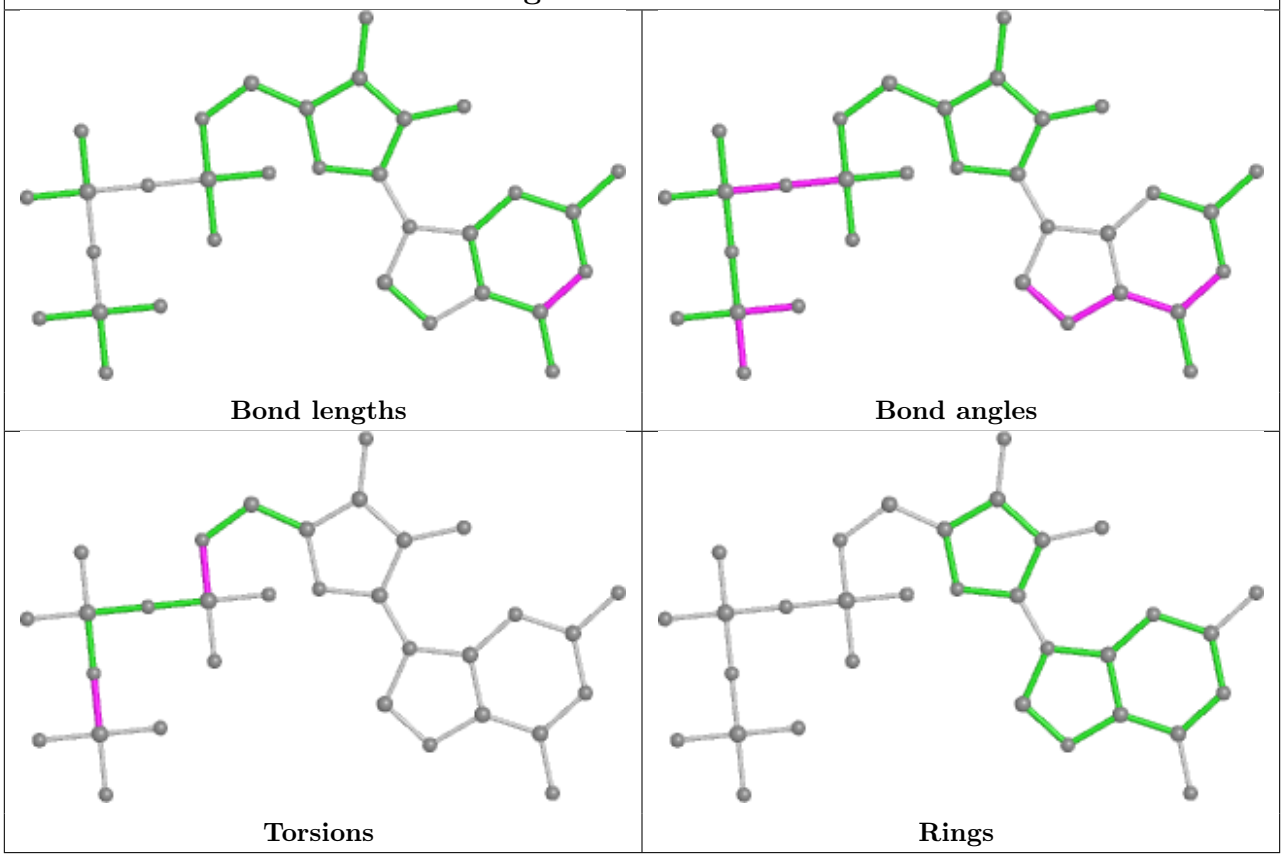


Torsions

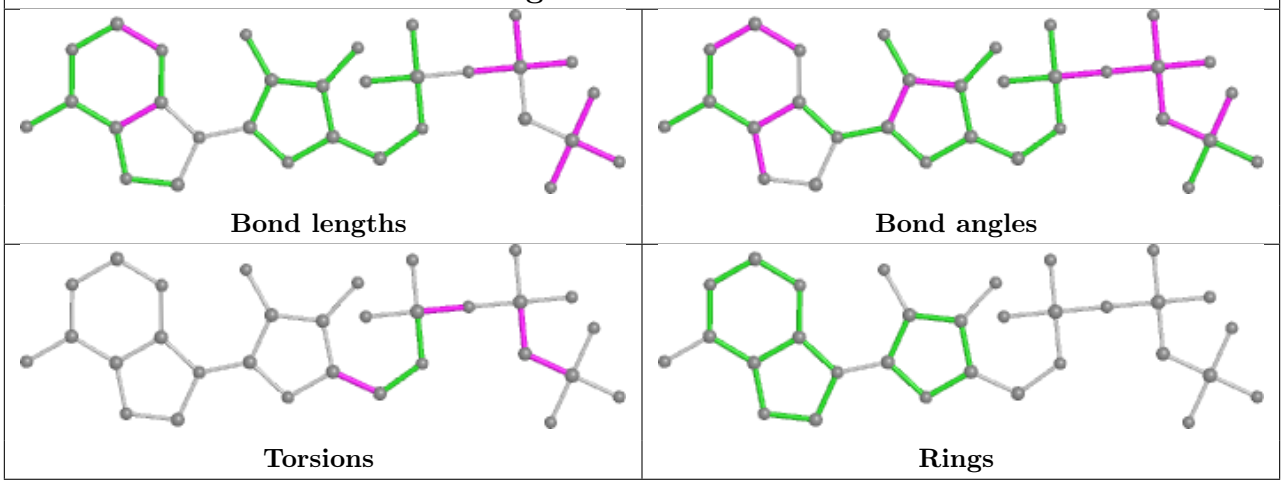


Rings

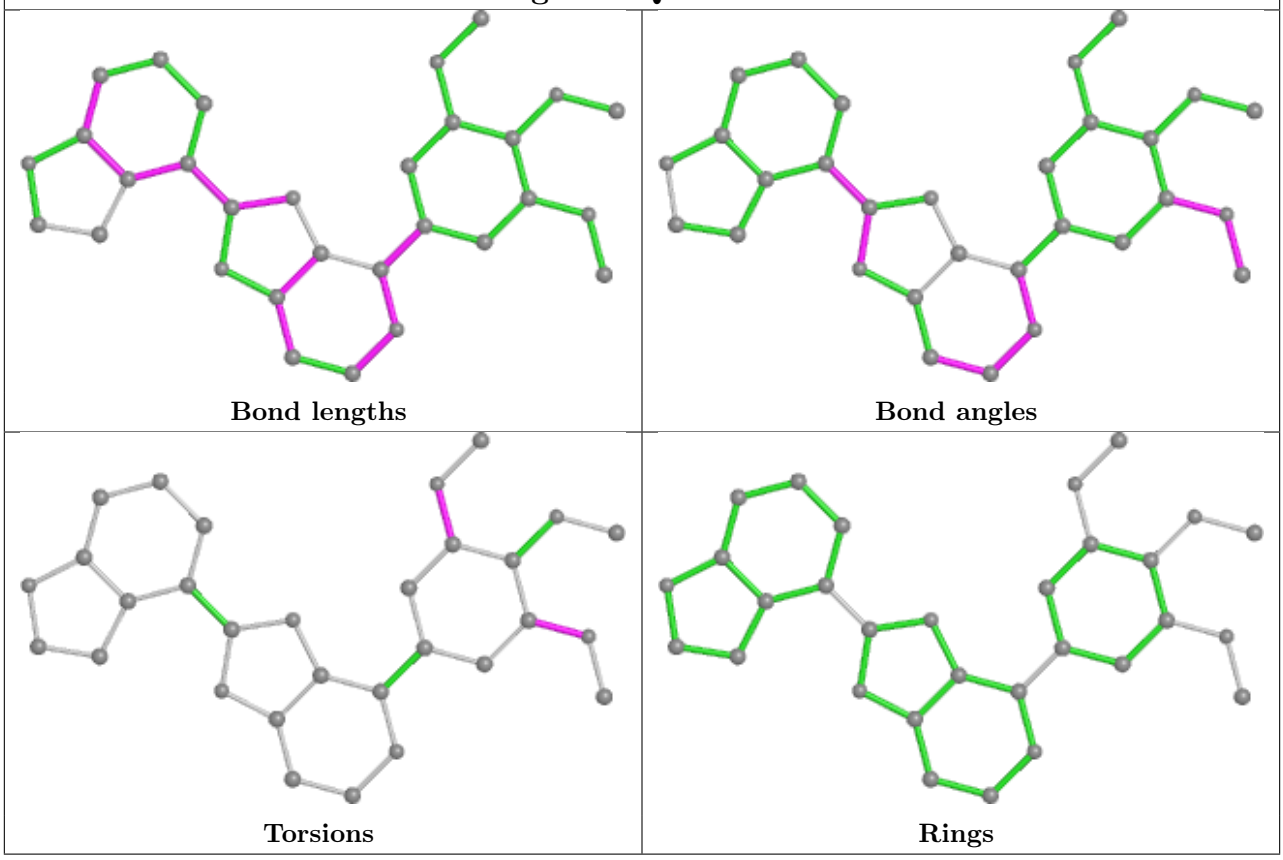
Ligand GTP C 501



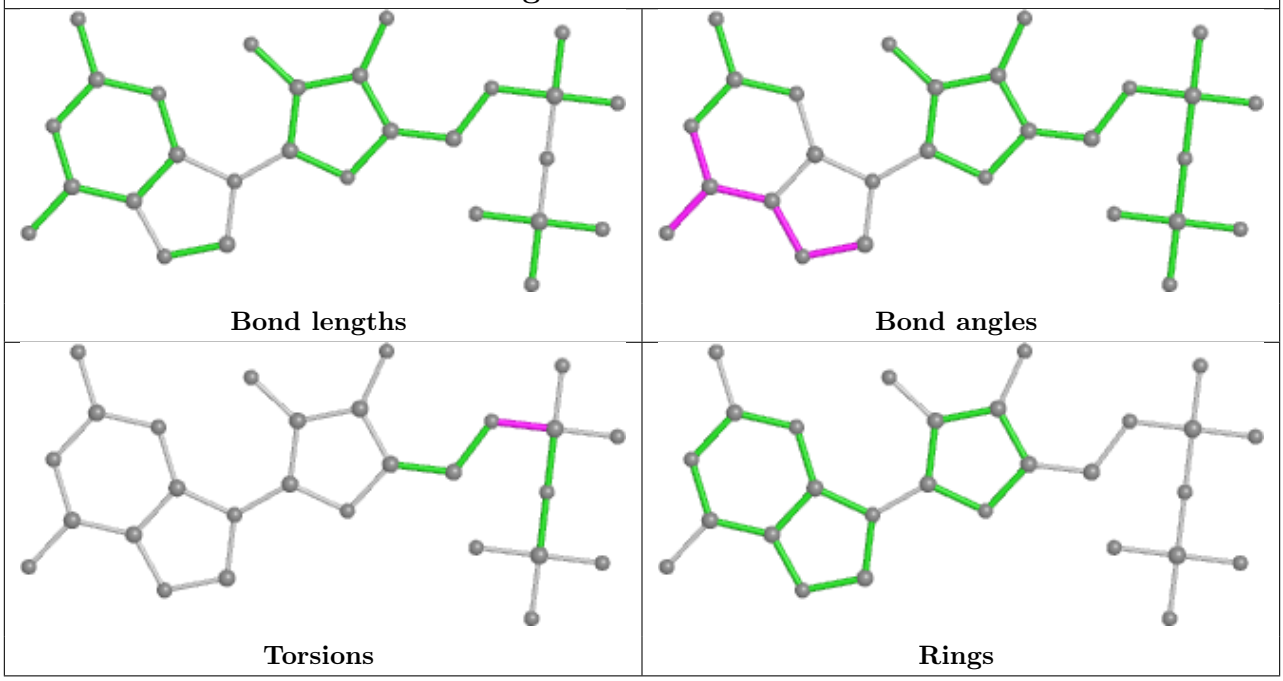
Ligand ACP F 401



Ligand 7Q7 B 504



Ligand GDP B 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	437/450 (97%)	-0.14	7 (1%)	72	66	26, 46, 74, 96	0
1	C	440/450 (97%)	-0.37	2 (0%)	91	88	20, 36, 60, 78	0
2	B	426/445 (95%)	-0.14	9 (2%)	63	54	23, 43, 79, 112	0
2	D	421/445 (94%)	0.36	30 (7%)	16	9	33, 64, 101, 120	0
3	E	121/143 (84%)	0.44	5 (4%)	37	27	38, 65, 92, 105	0
4	F	334/384 (86%)	0.57	42 (12%)	3	2	35, 74, 129, 145	0
All	All	2179/2317 (94%)	0.05	95 (4%)	34	24	20, 52, 101, 145	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	8.0
4	F	231	ALA	6.5
2	D	37	HIS	6.1
4	F	233	PHE	5.7
4	F	232	ASN	5.7
2	D	245	GLN	5.4
4	F	178	GLN	5.0
2	B	279	GLN	4.7
2	D	1	MET	4.6
4	F	161	LEU	4.5
2	B	55	THR	4.4
2	D	244	GLY	4.4
4	F	140	GLU	4.2
2	D	219	THR	4.1
4	F	133	ALA	4.0
4	F	101	TYR	3.9
2	D	55	THR	3.7
2	D	360	GLY	3.7
4	F	89	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	177	GLY	3.6
4	F	230	SER	3.5
2	D	396	HIS	3.5
2	D	397	TRP	3.4
2	B	37	HIS	3.4
4	F	234	GLN	3.4
4	F	372	THR	3.4
2	B	278	SER	3.4
4	F	175	GLU	3.3
4	F	141	GLY	3.3
4	F	142	ARG	3.2
4	F	253	TYR	3.2
2	D	216	LYS	3.0
1	A	281	ALA	3.0
4	F	137	ARG	3.0
2	B	57	ASN	3.0
4	F	136	ASN	3.0
4	F	132	LEU	3.0
3	E	28	SER	3.0
4	F	130	VAL	2.9
4	F	256	TYR	2.9
2	D	218	THR	2.9
2	D	332	ASN	2.9
3	E	46	SER	2.8
4	F	362	ALA	2.8
4	F	173	ILE	2.8
4	F	134	ALA	2.8
2	D	94	GLN	2.8
4	F	129	GLU	2.8
2	D	214	THR	2.7
1	A	437	VAL	2.7
4	F	103	THR	2.7
4	F	243	HIS	2.7
2	B	54	ALA	2.6
2	D	394	PHE	2.6
4	F	171	ASP	2.6
2	D	179	VAL	2.5
2	D	391	ARG	2.5
4	F	149	ALA	2.5
2	B	72	THR	2.5
1	A	337	THR	2.5
4	F	225	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	106	GLU	2.5
4	F	100	ILE	2.5
2	D	39	ASP	2.4
2	D	211	CYS	2.4
1	A	282	TYR	2.4
4	F	235	ASP	2.4
3	E	27	PRO	2.3
4	F	139	ARG	2.3
2	D	400	GLY	2.3
2	B	281	TYR	2.3
4	F	237	THR	2.2
2	D	175	VAL	2.2
2	D	217	LEU	2.2
4	F	380	HIS	2.2
1	C	440	VAL	2.2
1	C	283	HIS	2.2
2	B	277	GLY	2.2
2	D	56	GLY	2.2
4	F	145	ASN	2.1
3	E	139	LEU	2.1
4	F	227	PRO	2.1
2	D	53	GLU	2.1
2	D	390	ARG	2.1
2	D	431	ASP	2.1
4	F	167	SER	2.1
1	A	88	HIS	2.1
1	A	346	TRP	2.1
1	A	42	ILE	2.1
2	D	405	GLU	2.1
4	F	194	PRO	2.1
2	D	215	LEU	2.0
4	F	162	ILE	2.0
2	D	429	THR	2.0
2	D	81	PHE	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)

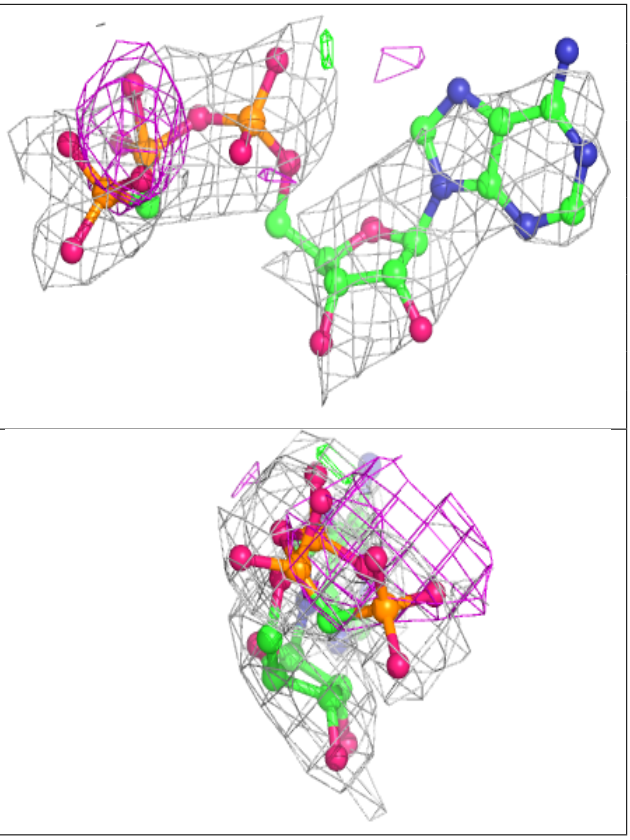
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

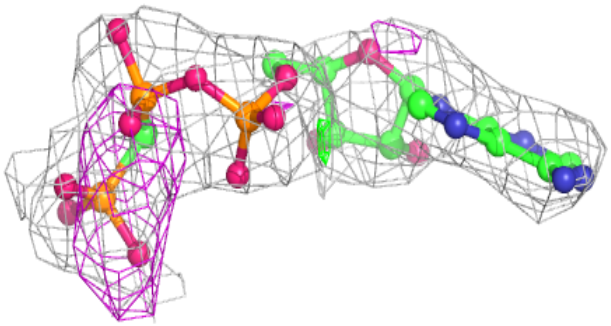
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MES	B	503	12/12	0.78	0.29	97,103,107,107	0
12	ACP	F	401	31/31	0.80	0.25	82,89,104,110	0
8	GOL	A	504	6/6	0.86	0.33	57,61,63,66	0
11	7Q7	D	503	30/30	0.88	0.25	73,78,85,88	0
7	CA	C	503	1/1	0.92	0.11	66,66,66,66	0
7	CA	A	503	1/1	0.93	0.08	73,73,73,73	0
5	GTP	D	501	32/32	0.93	0.17	50,54,64,73	0
6	MG	B	502	1/1	0.93	0.13	33,33,33,33	0
6	MG	D	502	1/1	0.94	0.20	49,49,49,49	0
11	7Q7	B	504	30/30	0.96	0.14	38,42,51,53	0
5	GTP	A	501	32/32	0.97	0.13	30,32,34,34	0
5	GTP	C	501	32/32	0.98	0.13	24,26,27,28	0
9	GDP	B	501	28/28	0.98	0.13	26,30,30,32	0
6	MG	A	502	1/1	0.98	0.17	32,32,32,32	0
6	MG	C	502	1/1	0.99	0.10	29,29,29,29	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 401:

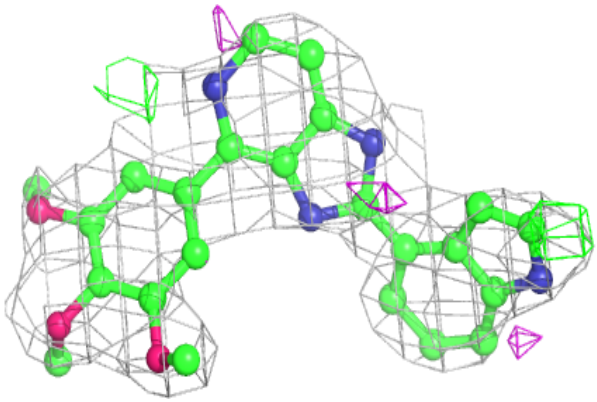
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

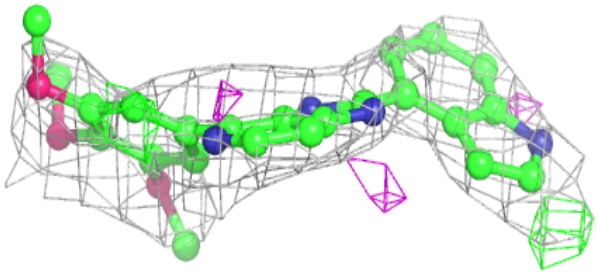


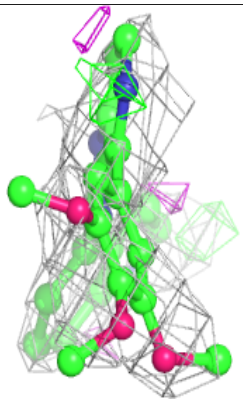


Electron density around 7Q7 D 503:

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

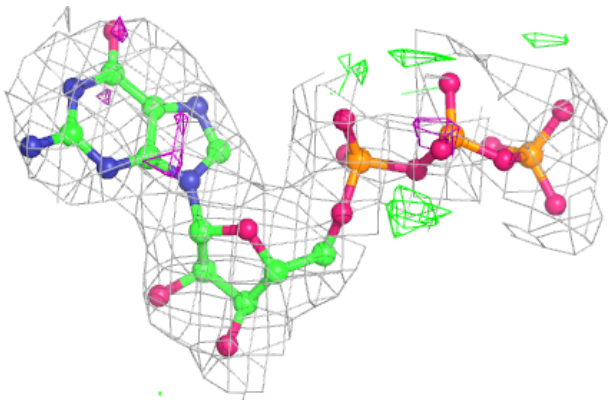


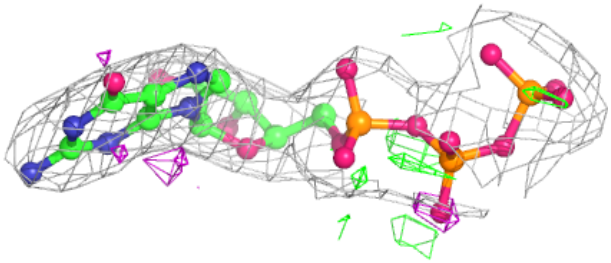


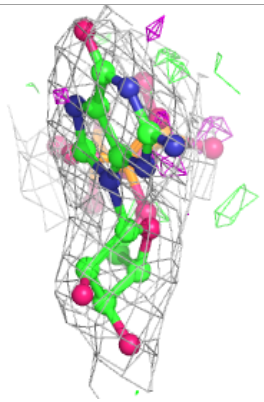


Electron density around GTP D 501:

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

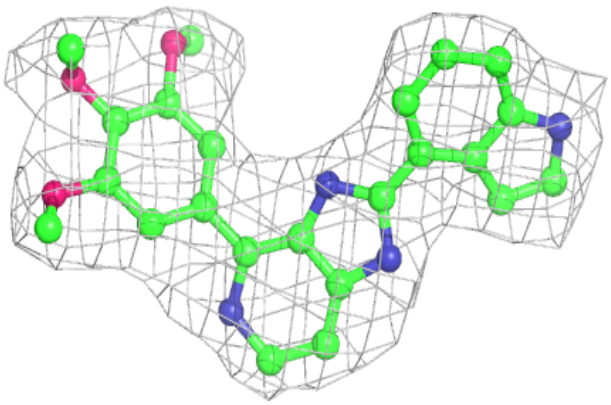


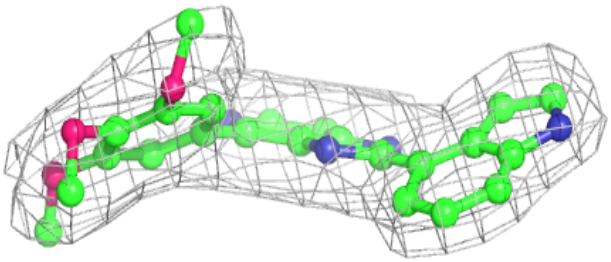


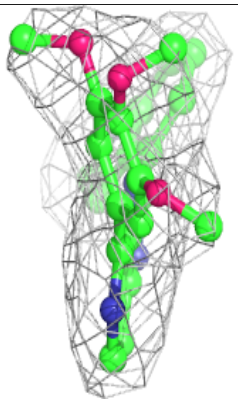


Electron density around 7Q7 B 504:

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

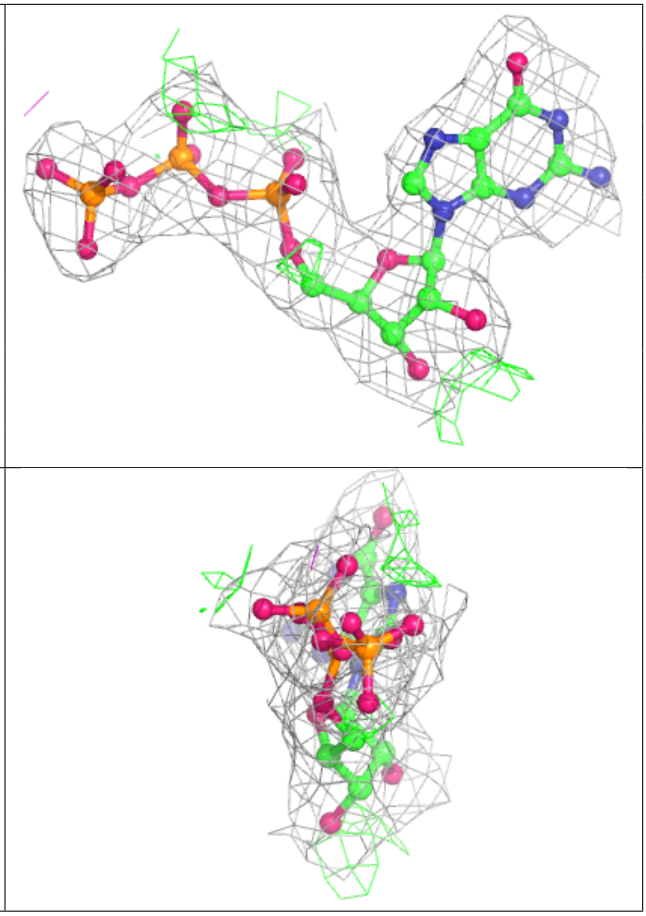






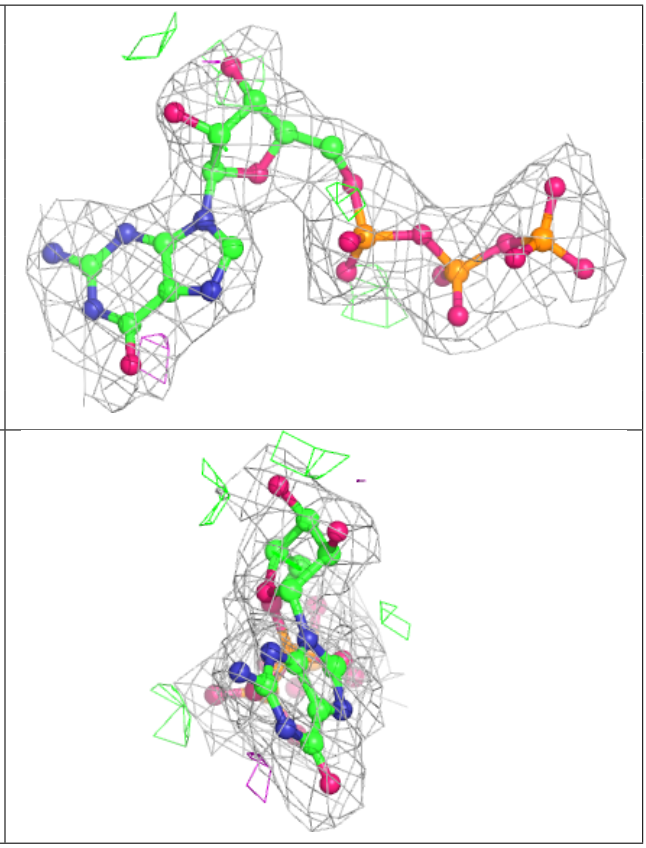
Electron density around GTP A 501:

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



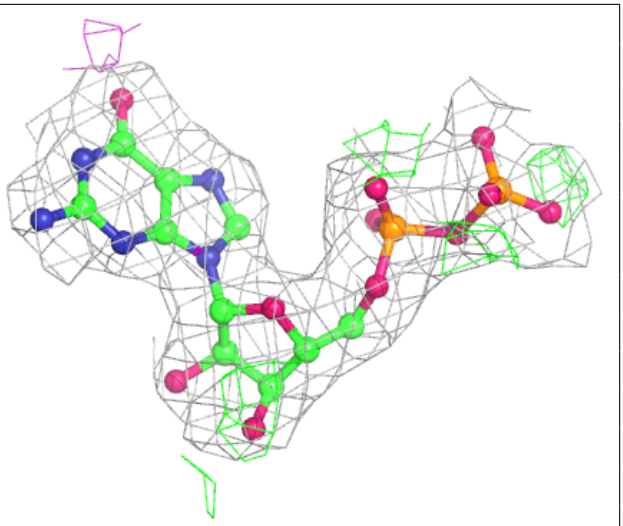
Electron density around GTP C 501:

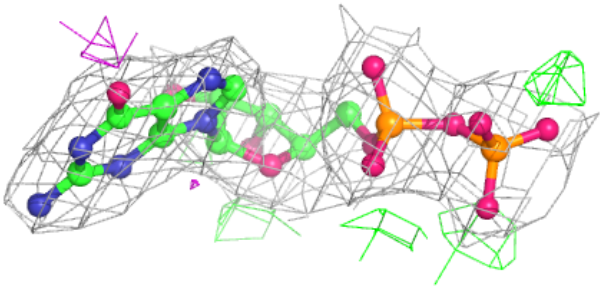
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

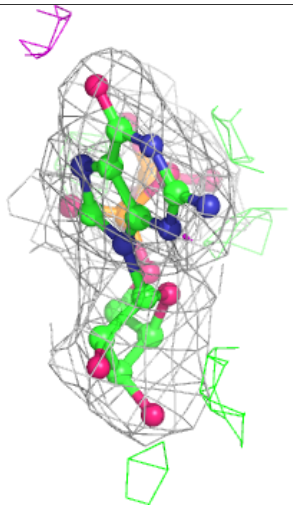


Electron density around GDP B 501:

$2mF_o$-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.