Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 10:57 AM JST

PDB ID	:	5XP3
Title	:	Crystal structure of apo T2R-TTL
Authors	:	Wang, Y.; Yang, J.; Wang, T.; Chen, L.
Deposited on	:	2017-05-31
Resolution	:	2.30 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:

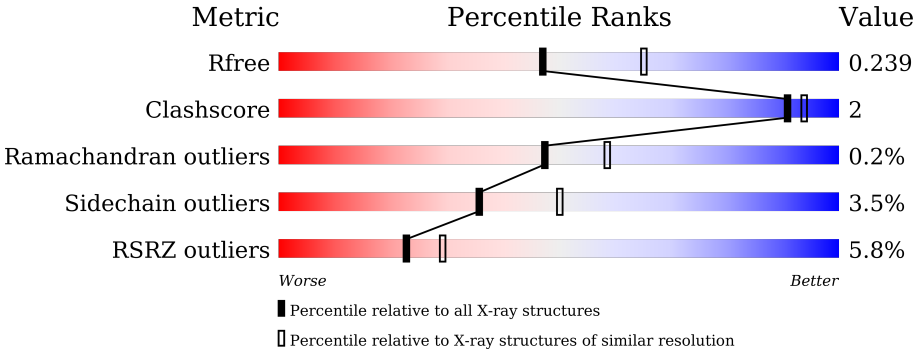
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	451	3%, 90%, 6% • •
1	C	451	92%, 5% •
2	B	445	3%, 89%, 6% •
2	D	445	9%, 87%, 7%, 5%
3	E	143	7%, 77%, 7% •, 15%
4	F	384	13%, 79%, 8%, 13%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17758 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3369	2115	577	650	27	0	0	0
2	D	421	3309	2080	562	640	27	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLY	GLU	conflict	UNP F2Z5B2
B	441	GLU	GLY	conflict	UNP F2Z5B2
D	440	GLY	GLU	conflict	UNP F2Z5B2
D	441	GLU	GLY	conflict	UNP F2Z5B2

- 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	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

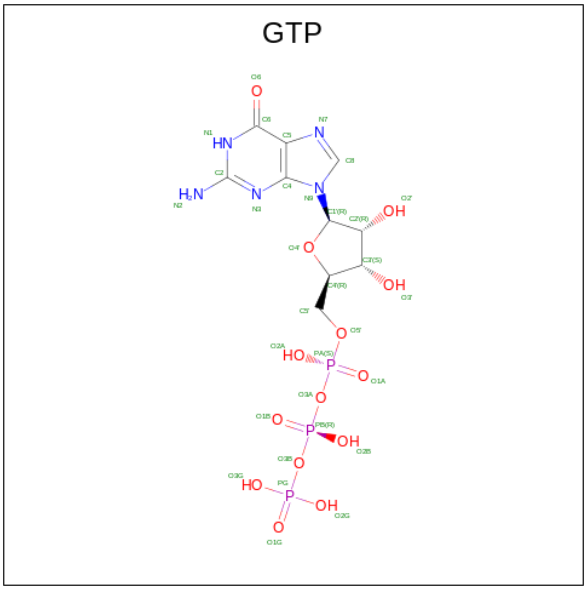
- Molecule 4 is a protein called Uncharacterized protein.

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
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	D	1	32	10	5	14	3	0	0

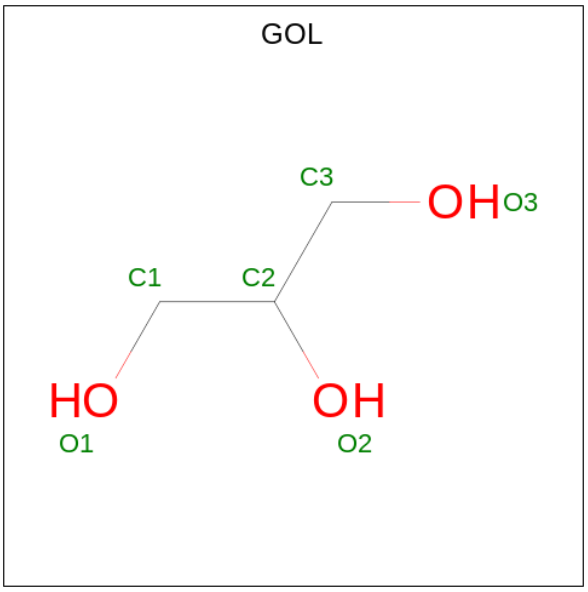
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

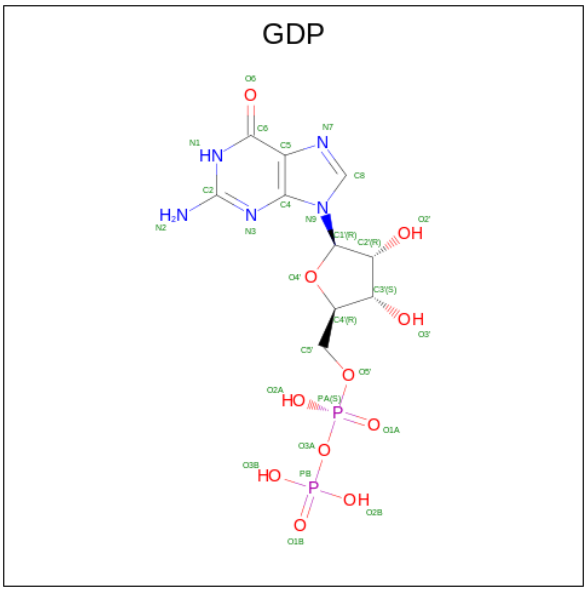
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



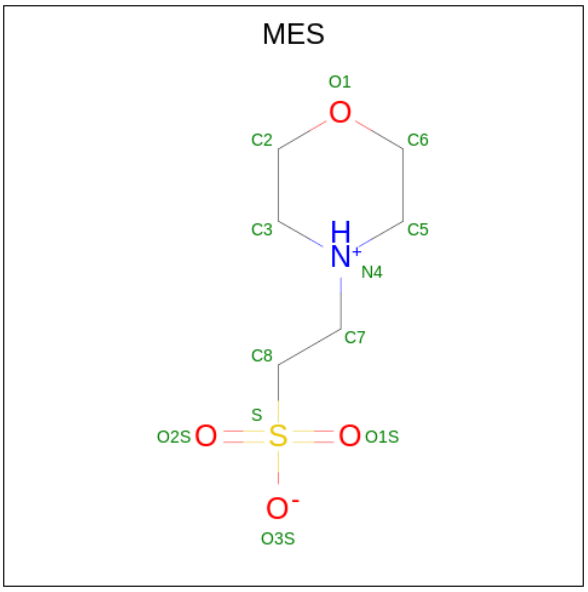
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

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



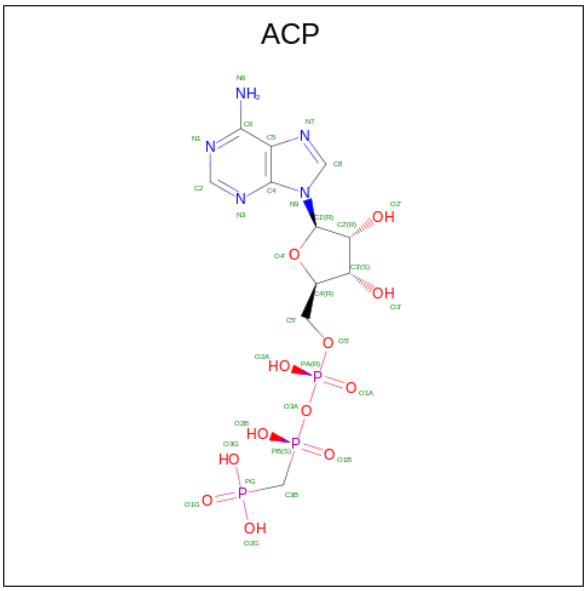
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0

- 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 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		
11	F	1	31	11	5	12	3	0	0

- Molecule 12 is water.

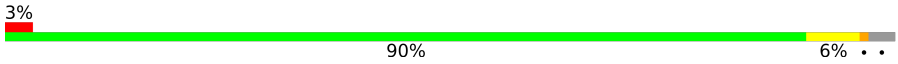
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	62	62	62	0	0
12	B	69	69	69	0	0
12	C	131	131	131	0	0
12	D	19	19	19	0	0
12	E	10	10	10	0	0
12	F	13	13	13	0	0

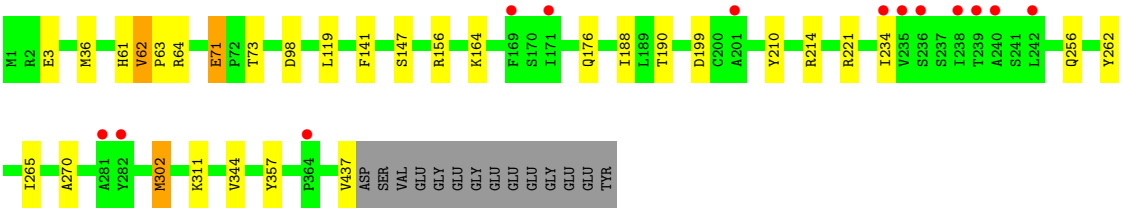
3 Residue-property plots (i)

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

• Molecule 1: Tubulin alpha-1B chain

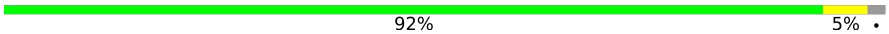
Chain A:

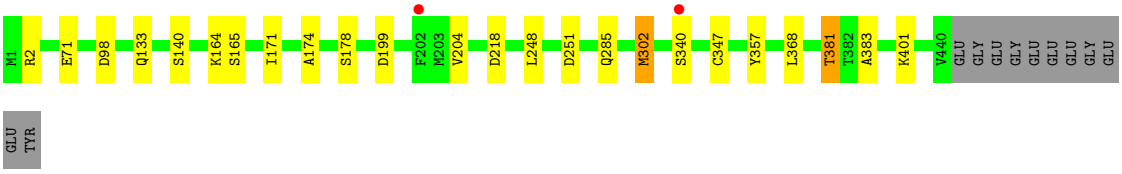




• Molecule 1: Tubulin alpha-1B chain

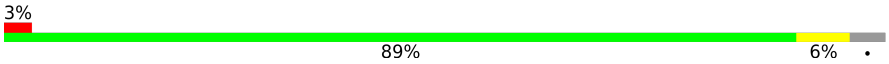
Chain C:

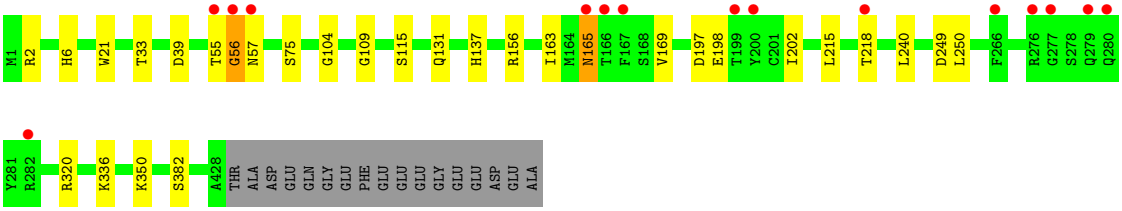




• Molecule 2: Tubulin beta chain

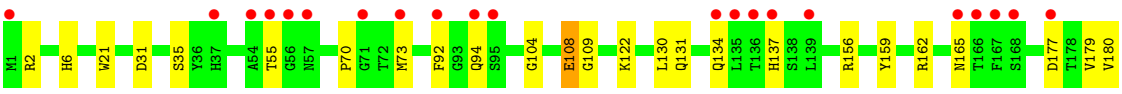
Chain B:

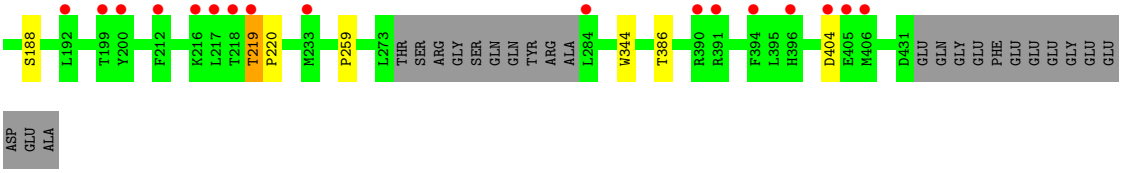




• Molecule 2: Tubulin beta chain

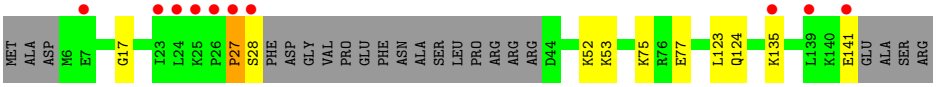
Chain D:





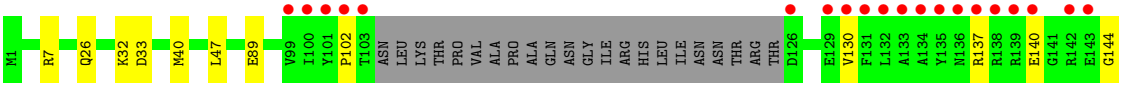
- Molecule 3: Stathmin-4

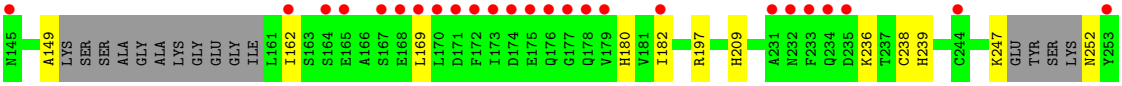
Chain E:

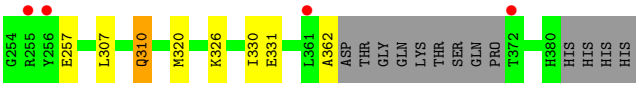


- Molecule 4: Uncharacterized protein

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	105.17Å 157.96Å 181.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 39.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.30) 99.6 (39.33-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.189 , 0.240 0.189 , 0.239	Depositor DCC
R_{free} test set	6607 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17758	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, GDP, GOL, MG, MES, CA, ACP

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	0.61	0/3494	0.73	0/4743
1	C	0.67	0/3515	0.79	2/4772 (0.0%)
2	B	0.63	0/3444	0.74	0/4664
2	D	0.55	0/3382	0.70	0/4581
3	E	0.59	0/1008	0.76	0/1337
4	F	0.55	0/2806	0.73	1/3791 (0.0%)
All	All	0.61	0/17649	0.74	3/23888 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	302	MET	CB-CG-SD	-5.76	95.13	112.40
4	F	307	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	381	THR	CB-CA-C	-5.20	97.56	111.60

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	14	0
1	C	3437	0	3348	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3369	0	3250	13	0
2	D	3309	0	3189	12	0
3	E	1000	0	1018	3	0
4	F	2744	0	2709	9	0
5	A	32	0	12	0	0
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	4	0
11	F	31	0	14	0	0
12	A	62	0	0	0	0
12	B	69	0	0	0	0
12	C	131	0	0	1	0
12	D	19	0	0	0	0
12	E	10	0	0	0	0
12	F	13	0	0	0	0
All	All	17758	0	16928	59	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 2.

All (59) 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)
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.66	0.75
2:B:197:ASP:OD1	10:B:503:MES:H32	1.92	0.69
4:F:209:HIS:HB2	4:F:310:GLN:HG3	1.74	0.68
1:C:381:THR:HG23	12:C:618:HOH:O	1.95	0.66
1:C:381:THR:HG22	1:C:383:ALA:H	1.62	0.65
2:B:197:ASP:OD2	10:B:503:MES:H52	1.97	0.64
1:C:204:VAL:HG22	1:C:302:MET:CE	2.28	0.63
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.81	0.63
2:B:165:ASN:HB2	2:B:198:GLU:HG3	1.80	0.62
4:F:40:MET:HE1	4:F:47:LEU:HG	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG22	1:A:265:ILE:O	2.04	0.58
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.03	0.58
2:D:31:ASP:HB2	2:D:35:SER:H	1.68	0.58
2:B:131:GLN:HE22	2:B:250:LEU:H	1.53	0.57
2:B:131:GLN:NE2	2:B:250:LEU:H	2.03	0.55
4:F:149:ALA:O	4:F:180:HIS:CD2	2.60	0.55
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.41	0.54
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.91	0.53
2:B:156:ARG:HG3	10:B:503:MES:H62	1.90	0.53
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.52
2:B:104:GLY:O	2:B:109:GLY:HA3	2.10	0.52
1:A:234:ILE:HD13	1:A:302:MET:SD	2.49	0.52
1:C:204:VAL:HG22	1:C:302:MET:HE2	1.91	0.52
2:B:156:ARG:CZ	10:B:503:MES:H21	2.40	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.51
4:F:137:ARG:HA	4:F:140:GLU:HG3	1.94	0.50
4:F:320:MET:HB2	4:F:330:ILE:HD11	1.94	0.50
1:C:165:SER:HA	1:C:199:ASP:OD2	2.13	0.49
2:B:56:GLY:N	2:B:57:ASN:HA	2.27	0.49
2:D:2:ARG:HB3	2:D:131:GLN:HG2	1.95	0.49
2:D:104:GLY:O	2:D:109:GLY:HA3	2.14	0.48
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.96	0.47
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.97	0.47
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.51	0.46
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.46
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.46	0.46
2:D:108:GLU:H	2:D:108:GLU:HG2	1.58	0.46
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.98	0.45
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.51	0.45
2:B:131:GLN:NE2	2:B:249:ASP:HB2	2.32	0.45
4:F:169:LEU:HD13	4:F:182:ILE:HD11	1.98	0.45
1:A:141:PHE:O	1:A:147:SER:HB3	2.17	0.45
1:A:270:ALA:HB3	1:A:302:MET:HG2	2.00	0.44
1:C:174:ALA:O	1:C:178:SER:HB3	2.18	0.44
2:D:70:PRO:HD3	2:D:94:GLN:HA	2.00	0.44
4:F:26:GLN:HE22	4:F:362:ALA:H	1.66	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.43
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.54	0.43
2:D:219:THR:HA	2:D:220:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:TYR:HB3	2:D:162:ARG:HG3	2.01	0.42
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.02	0.41
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.41
1:A:311:LYS:HD3	1:A:344:VAL:HG12	2.02	0.41
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.97	0.41
4:F:7:ARG:HD3	4:F:40:MET:HE2	2.03	0.41
1:C:285:GLN:H	1:C:285:GLN:HG3	1.75	0.40
3:E:27:PRO:HB2	3:E:28:SER:H	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	427 (98%)	8 (2%)	0	100	100
1	C	438/451 (97%)	430 (98%)	8 (2%)	0	100	100
2	B	426/445 (96%)	413 (97%)	12 (3%)	1 (0%)	47	58
2	D	417/445 (94%)	402 (96%)	15 (4%)	0	100	100
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	17	20
4	F	324/384 (84%)	307 (95%)	14 (4%)	3 (1%)	17	20
All	All	2157/2319 (93%)	2094 (97%)	58 (3%)	5 (0%)	47	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27	PRO
4	F	32	LYS
4	F	144	GLY
4	F	102	PRO
2	B	56	GLY

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	368/379 (97%)	358 (97%)	10 (3%)	44	61
1	C	371/379 (98%)	363 (98%)	8 (2%)	52	69
2	B	370/383 (97%)	355 (96%)	15 (4%)	30	43
2	D	364/383 (95%)	351 (96%)	13 (4%)	35	49
3	E	109/127 (86%)	102 (94%)	7 (6%)	17	23
4	F	301/342 (88%)	289 (96%)	12 (4%)	31	44
All	All	1883/1993 (94%)	1818 (96%)	65 (4%)	36	50

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	71	GLU
1	A	73	THR
1	A	164	LYS
1	A	176	GLN
1	A	188	ILE
1	A	221	ARG
1	A	262	TYR
1	A	302	MET
1	A	437	VAL
2	B	2	ARG
2	B	33	THR
2	B	39	ASP
2	B	55	THR
2	B	75	SER
2	B	115	SER
2	B	137	HIS
2	B	165	ASN
2	B	215	LEU
2	B	218	THR
2	B	240	LEU
2	B	320	ARG

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Mol	Chain	Res	Type
2	B	336	LYS
2	B	350	LYS
2	B	382	SER
1	C	2	ARG
1	C	133	GLN
1	C	164	LYS
1	C	218	ASP
1	C	251	ASP
1	C	340	SER
1	C	347	CYS
1	C	368	LEU
2	D	55	THR
2	D	108	GLU
2	D	122	LYS
2	D	130	LEU
2	D	137	HIS
2	D	177	ASP
2	D	179	VAL
2	D	180	VAL
2	D	188	SER
2	D	219	THR
2	D	259	PRO
2	D	386	THR
2	D	404	ASP
3	E	52	LYS
3	E	53	LYS
3	E	75	LYS
3	E	77	GLU
3	E	124	GLN
3	E	135	LYS
3	E	141	GLU
4	F	33	ASP
4	F	89	GLU
4	F	130	VAL
4	F	162	ILE
4	F	236	LYS
4	F	238	CYS
4	F	239	HIS
4	F	247	LYS
4	F	252	ASN
4	F	310	GLN
4	F	326	LYS

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Mol	Chain	Res	Type
4	F	331	GLU

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	329	ASN
2	B	57	ASN
2	B	131	GLN
2	B	375	GLN
1	C	101	ASN
1	C	356	ASN
2	D	165	ASN
3	E	18	GLN
3	E	92	ASN
4	F	26	GLN
4	F	180	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	C	501	6	26,34,34	1.09	2 (7%)	32,54,54	1.15	2 (6%)
5	GTP	A	501	6	26,34,34	1.04	2 (7%)	32,54,54	1.32	5 (15%)
8	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.34	0
10	MES	B	503	-	12,12,12	2.11	2 (16%)	14,16,16	6.60	7 (50%)
9	GDP	B	501	6	24,30,30	1.05	1 (4%)	30,47,47	1.23	3 (10%)
5	GTP	D	501	6	26,34,34	0.87	0	32,54,54	1.22	4 (12%)
11	ACP	F	401	-	27,33,33	1.62	7 (25%)	32,52,52	1.36	3 (9%)

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	C	501	6	-	5/18/38/38	0/3/3/3
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
10	MES	B	503	-	-	5/6/14/14	0/1/1/1
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
5	GTP	D	501	6	-	6/18/38/38	0/3/3/3
11	ACP	F	401	-	-	8/15/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-6.34	1.68	1.77
11	F	401	ACP	PB-O3A	4.11	1.62	1.58
11	F	401	ACP	PG-O3G	2.93	1.61	1.54
11	F	401	ACP	C5-C4	2.87	1.48	1.40
5	C	501	GTP	C6-N1	-2.74	1.33	1.37
11	F	401	ACP	PG-O2G	2.68	1.61	1.54
5	A	501	GTP	C6-N1	-2.62	1.34	1.37
5	A	501	GTP	O4'-C1'	2.53	1.44	1.41
5	C	501	GTP	O4'-C1'	2.48	1.44	1.41
10	B	503	MES	O2S-S	2.41	1.52	1.45
9	B	501	GDP	C2'-C1'	-2.37	1.50	1.53
11	F	401	ACP	C2-N3	2.31	1.35	1.32
11	F	401	ACP	PB-O2B	2.21	1.61	1.56
11	F	401	ACP	O4'-C1'	2.01	1.43	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	503	MES	O3S-S-C8	-12.84	85.01	105.77
10	B	503	MES	O3S-S-O2S	-11.55	83.05	111.27
10	B	503	MES	O2S-S-C8	10.78	119.89	106.92
10	B	503	MES	O3S-S-O1S	-9.94	87.00	111.27
10	B	503	MES	O1S-S-C8	8.65	117.33	106.92
11	F	401	ACP	N3-C2-N1	-3.48	123.25	128.68
11	F	401	ACP	C3'-C2'-C1'	3.15	105.73	100.98
10	B	503	MES	C6-O1-C2	3.01	119.92	109.89
5	C	501	GTP	C8-N7-C5	2.96	108.62	102.99
9	B	501	GDP	O6-C6-C5	-2.86	118.78	124.37
9	B	501	GDP	C5-C6-N1	2.55	118.45	113.95
5	A	501	GTP	C8-N7-C5	2.51	107.78	102.99
5	D	501	GTP	PA-O3A-PB	-2.45	124.43	132.83
5	C	501	GTP	O3G-PG-O1G	2.44	120.23	110.68
10	B	503	MES	C5-N4-C3	2.43	114.31	108.83
5	D	501	GTP	C8-N7-C5	2.38	107.53	102.99
5	D	501	GTP	C5-C6-N1	2.35	118.10	113.95
5	A	501	GTP	O3G-PG-O3B	-2.23	97.15	104.64
5	A	501	GTP	O2A-PA-O1A	2.13	122.76	112.24
5	D	501	GTP	O6-C6-C5	-2.12	120.22	124.37
11	F	401	ACP	C4-C5-N7	-2.11	107.20	109.40
9	B	501	GDP	PA-O3A-PB	-2.07	125.72	132.83
5	A	501	GTP	O3G-PG-O2G	2.01	115.31	107.64
5	A	501	GTP	C5-C6-N1	2.01	117.50	113.95

There are no chirality outliers.

All (34) 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	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
8	A	504	GOL	C1-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O1A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	N4-C7-C8-S
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	O4'-C4'-C5'-O5'
8	A	504	GOL	O2-C2-C3-O3
10	B	503	MES	C7-C8-S-O3S
10	B	503	MES	C8-C7-N4-C3
11	F	401	ACP	PB-O3A-PA-O5'
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O1S
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A

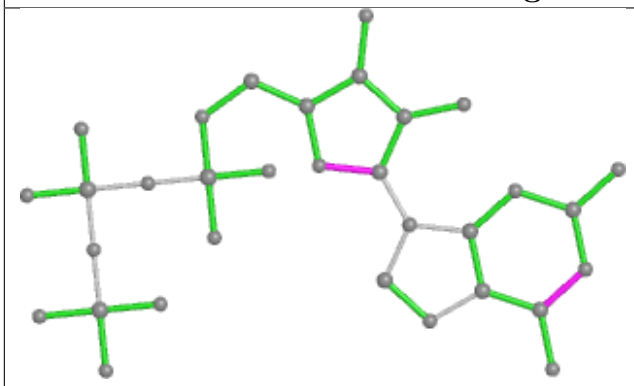
There are no ring outliers.

1 monomer is involved in 4 short contacts:

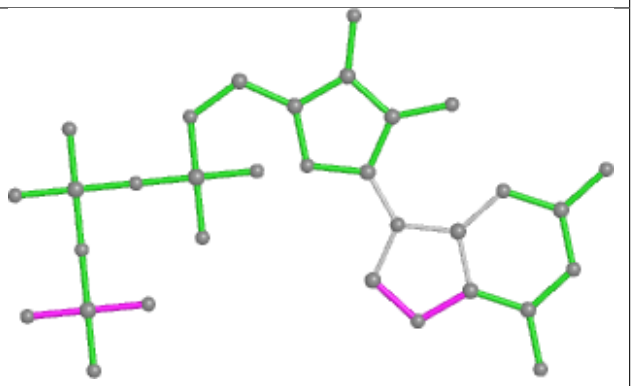
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	4	0

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.

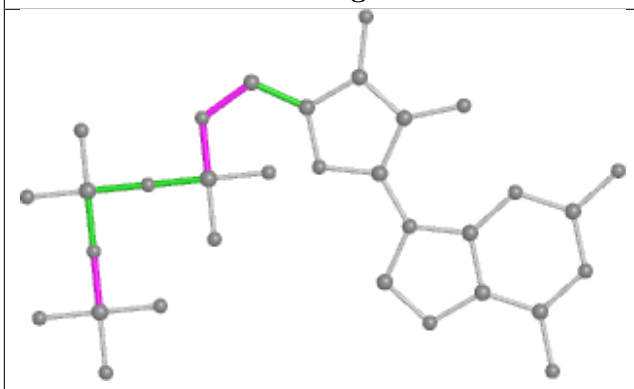
Ligand GTP C 501



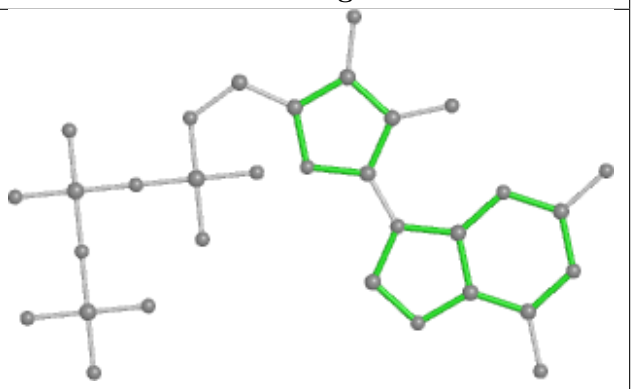
Bond lengths



Bond angles

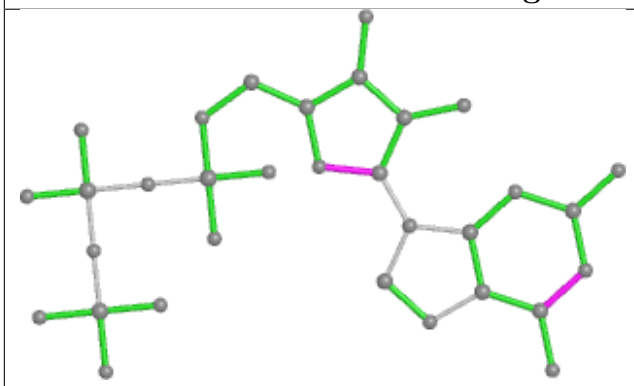


Torsions



Rings

Ligand GTP A 501



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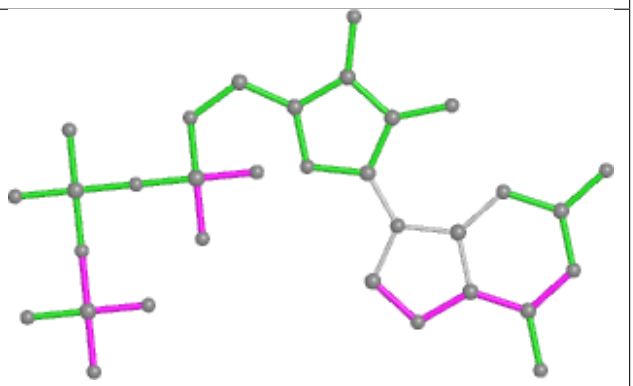

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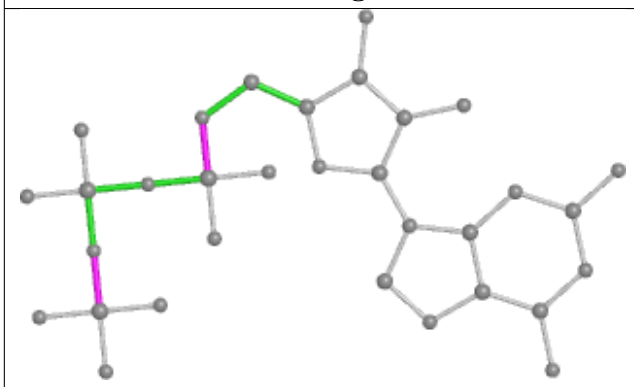
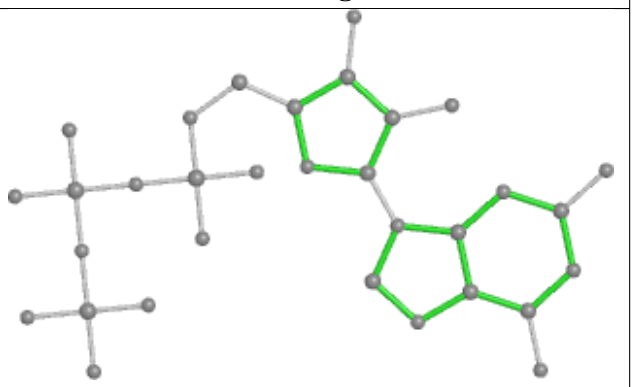
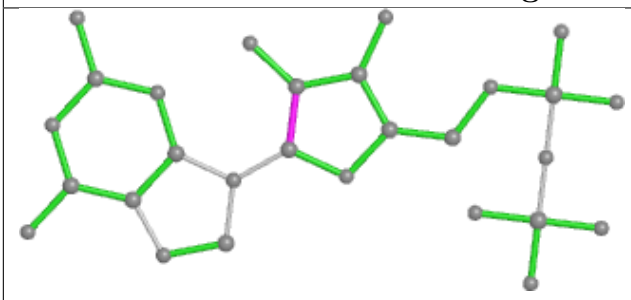


Torsions

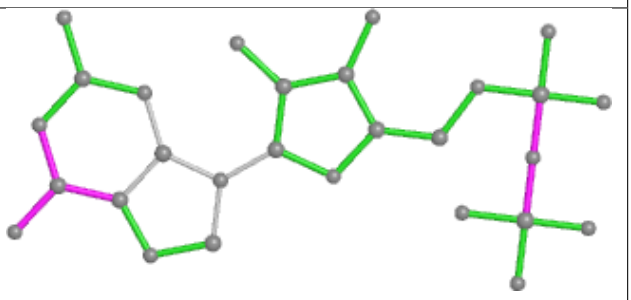


Rings

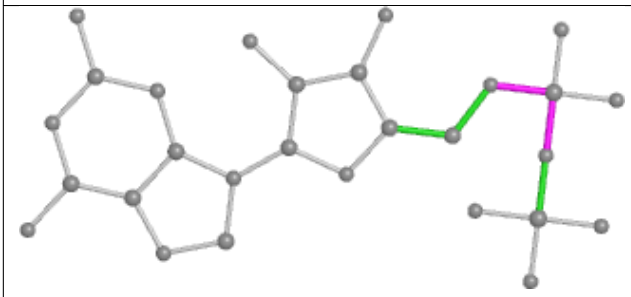
Ligand GDP B 501



Bond lengths



Bond angles



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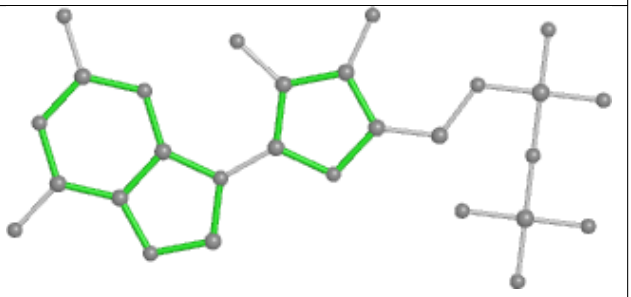

Rings

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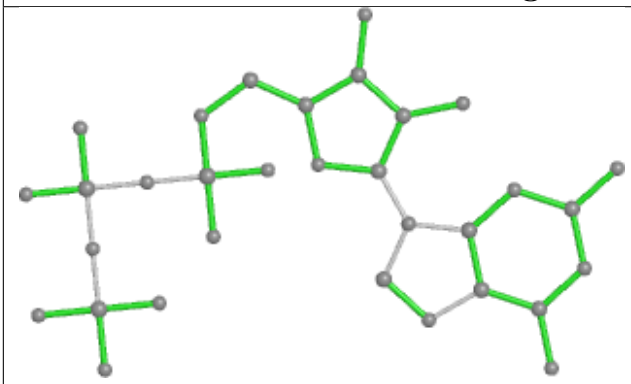
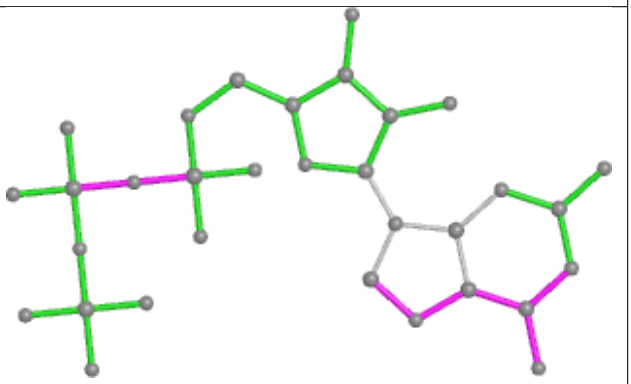
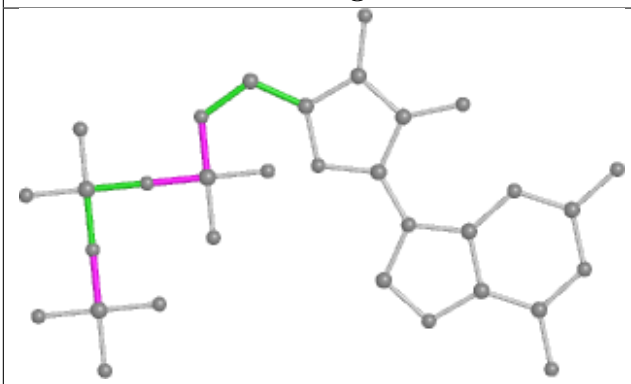


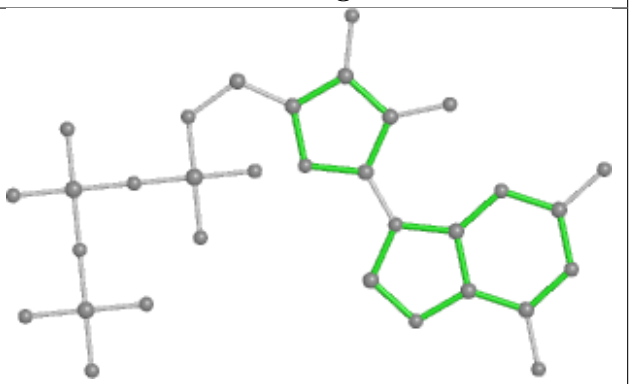
Bond lengths



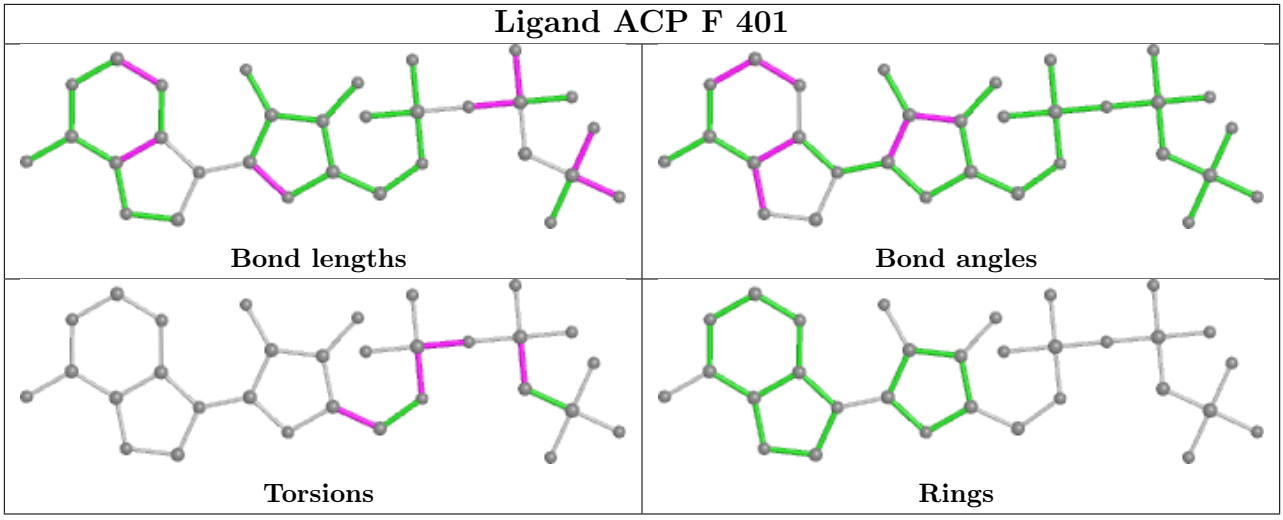
Bond angles



Torsions



Rings



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	437/451 (96%)	-0.03	13 (2%) 50 57	36, 51, 78, 98	0
1	C	440/451 (97%)	-0.29	2 (0%) 91 94	30, 42, 67, 92	0
2	B	428/445 (96%)	0.04	15 (3%) 44 51	32, 50, 83, 129	0
2	D	421/445 (94%)	0.29	38 (9%) 9 12	38, 62, 99, 119	0
3	E	121/143 (84%)	0.21	10 (8%) 11 15	37, 64, 96, 131	0
4	F	334/384 (86%)	0.51	49 (14%) 2 3	40, 71, 134, 150	0
All	All	2181/2319 (94%)	0.09	127 (5%) 23 29	30, 54, 100, 150	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	176	GLN	6.8
4	F	133	ALA	6.3
4	F	169	LEU	6.2
4	F	172	PHE	5.8
4	F	102	PRO	5.6
4	F	132	LEU	5.4
4	F	173	ILE	5.3
4	F	179	VAL	5.2
2	D	1	MET	5.1
4	F	182	ILE	5.1
4	F	101	TYR	4.9
4	F	177	GLY	4.8
4	F	130	VAL	4.7
4	F	134	ALA	4.7
4	F	137	ARG	4.6
2	B	277	GLY	4.6
4	F	234	GLN	4.6
4	F	135	TYR	4.5
4	F	136	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
3	E	139	LEU	4.3
4	F	170	LEU	4.2
2	B	279	GLN	4.1
4	F	100	ILE	4.1
4	F	103	THR	4.1
4	F	131	PHE	4.1
4	F	174	ASP	3.8
2	B	282	ARG	3.8
4	F	142	ARG	3.7
4	F	143	GLU	3.7
4	F	231	ALA	3.7
4	F	140	GLU	3.7
4	F	175	GLU	3.7
2	D	390	ARG	3.7
2	D	55	THR	3.6
4	F	233	PHE	3.5
4	F	232	ASN	3.5
4	F	178	GLN	3.5
4	F	256	TYR	3.4
4	F	171	ASP	3.3
2	D	57	ASN	3.2
4	F	372	THR	3.2
2	D	167	PHE	3.2
2	D	168	SER	3.1
2	D	216	LYS	3.1
1	A	281	ALA	3.1
4	F	167	SER	3.1
2	B	57	ASN	3.1
2	D	37	HIS	3.1
3	E	141	GLU	3.1
4	F	138	ARG	3.0
2	D	135	LEU	3.0
4	F	361	LEU	2.9
3	E	26	PRO	2.9
1	A	282	TYR	2.9
3	E	24	LEU	2.9
2	D	94	GLN	2.8
2	D	92	PHE	2.8
2	D	54	ALA	2.8
1	A	242	LEU	2.8
4	F	235	ASP	2.8
3	E	7	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	239	THR	2.7
3	E	25	LYS	2.6
2	B	55	THR	2.6
2	D	218	THR	2.6
2	D	219	THR	2.6
2	B	280	GLN	2.6
2	D	217	LEU	2.5
2	D	73	MET	2.5
2	D	166	THR	2.5
3	E	28	SER	2.5
4	F	162	ILE	2.5
2	B	276	ARG	2.4
2	D	212	PHE	2.4
2	D	137	HIS	2.4
2	D	405	GLU	2.4
2	B	165	ASN	2.4
2	D	396	HIS	2.4
2	B	166	THR	2.4
2	D	139	LEU	2.4
1	A	235	VAL	2.4
4	F	99	VAL	2.4
2	D	165	ASN	2.4
2	D	199	THR	2.3
4	F	168	GLU	2.3
1	A	238	ILE	2.3
4	F	255	ARG	2.3
2	D	404	ASP	2.3
1	A	201	ALA	2.3
1	C	340	SER	2.3
2	B	56	GLY	2.3
2	D	177	ASP	2.3
2	D	134	GLN	2.2
4	F	165	GLU	2.2
2	B	200	TYR	2.2
2	D	406	MET	2.2
2	B	199	THR	2.2
1	A	364	PRO	2.2
3	E	27	PRO	2.2
2	D	394	PHE	2.2
2	D	200	TYR	2.2
2	B	167	PHE	2.1
4	F	129	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	164	SER	2.1
2	D	71	GLY	2.1
2	D	391	ARG	2.1
1	C	202	PHE	2.1
3	E	135	LYS	2.1
4	F	126	ASP	2.1
2	D	136	THR	2.1
1	A	171	ILE	2.1
4	F	145	ASN	2.1
2	D	192	LEU	2.1
4	F	244	CYS	2.1
4	F	253	TYR	2.1
2	D	56	GLY	2.1
4	F	139	ARG	2.1
2	B	266	PHE	2.1
1	A	240	ALA	2.0
1	A	236	SER	2.0
3	E	23	ILE	2.0
2	D	233	MET	2.0
2	B	218	THR	2.0
2	D	95	SER	2.0
1	A	169	PHE	2.0
1	A	234	ILE	2.0
2	D	284	LEU	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)

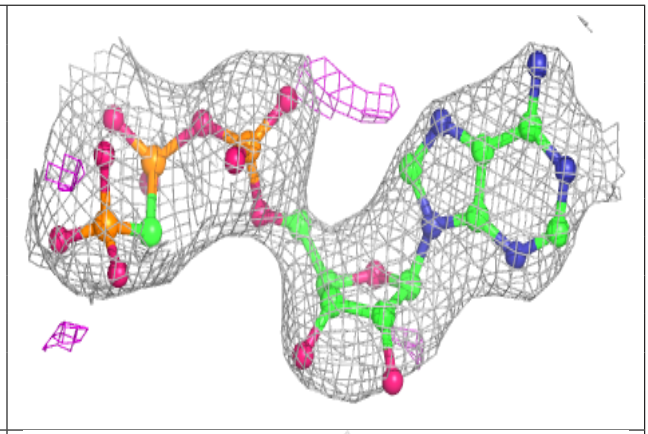
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

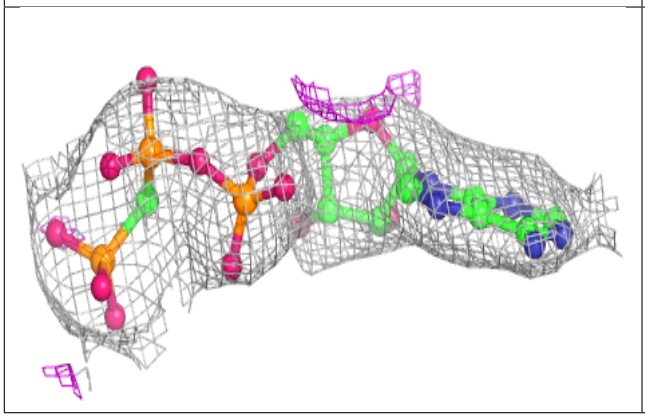
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	ACP	F	401	31/31	0.92	0.13	71,93,117,124	0
6	MG	D	502	1/1	0.94	0.13	69,69,69,69	0
10	MES	B	503	12/12	0.96	0.12	61,71,77,79	0
6	MG	C	502	1/1	0.97	0.13	36,36,36,36	0
5	GTP	D	501	32/32	0.97	0.11	48,58,77,87	0
7	CA	A	503	1/1	0.98	0.09	66,66,66,66	0
8	GOL	A	504	6/6	0.98	0.10	53,61,64,68	0
7	CA	C	503	1/1	0.99	0.03	49,49,49,49	0
5	GTP	C	501	32/32	0.99	0.14	31,33,38,38	0
9	GDP	B	501	28/28	0.99	0.14	30,36,40,44	0
5	GTP	A	501	32/32	0.99	0.12	34,38,43,45	0
6	MG	A	502	1/1	0.99	0.11	42,42,42,42	0
6	MG	B	502	1/1	1.00	0.16	37,37,37,37	0

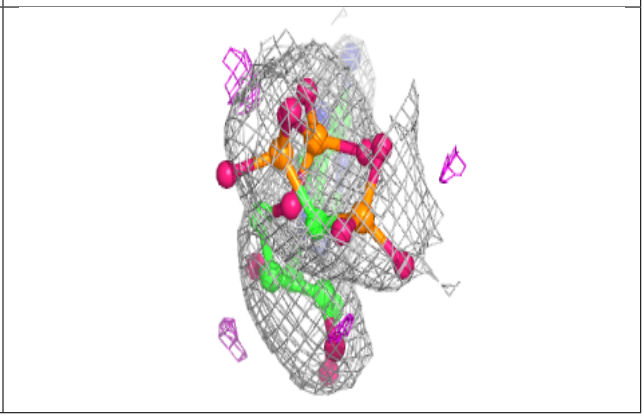
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

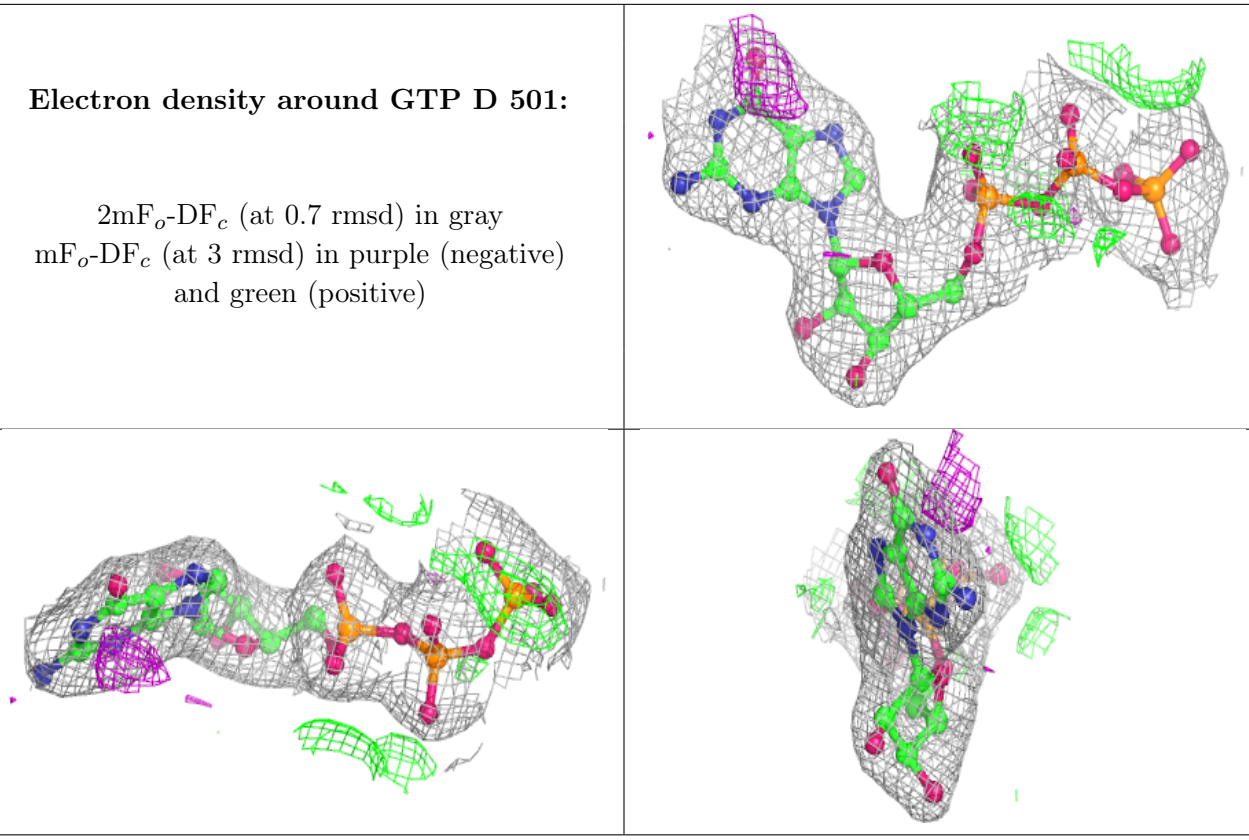






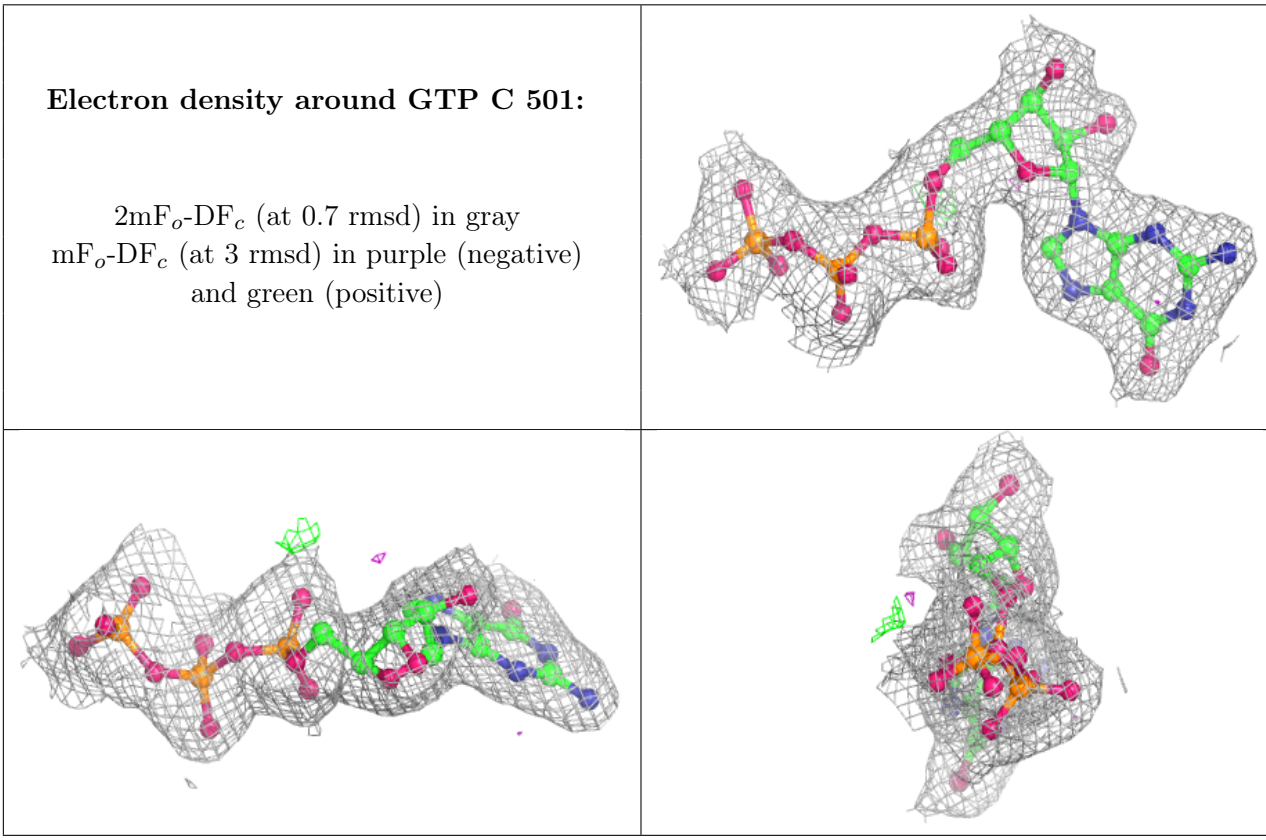
Electron density around GTP D 501:

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



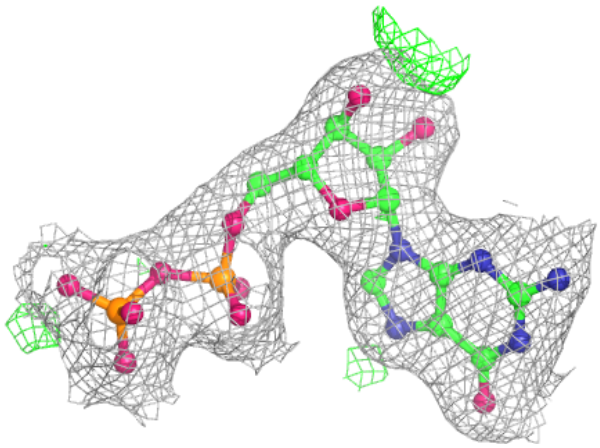
Electron density around GTP C 501:

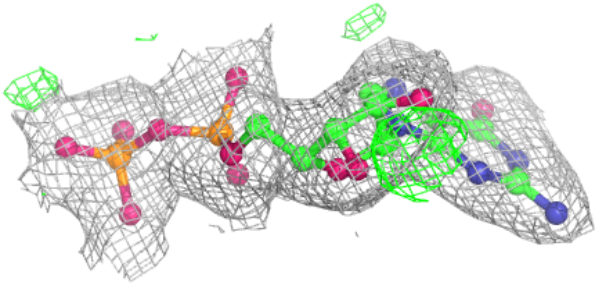
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

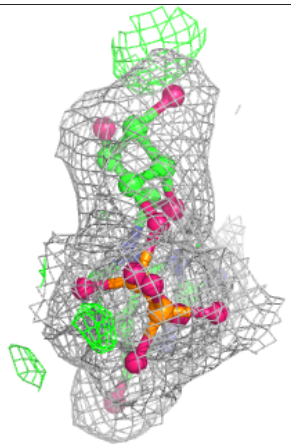


Electron density around GDP B 501:

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

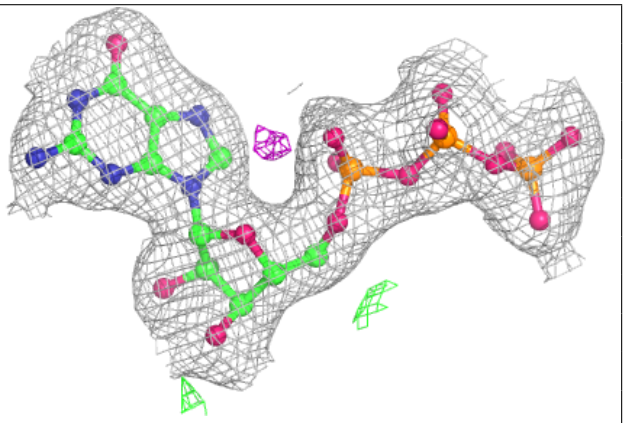


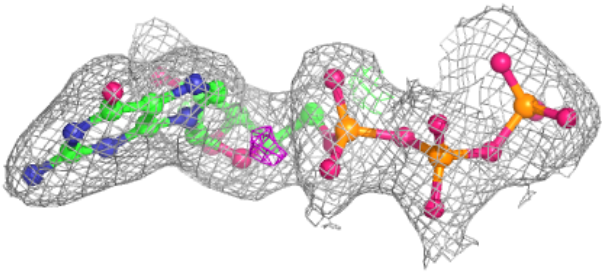


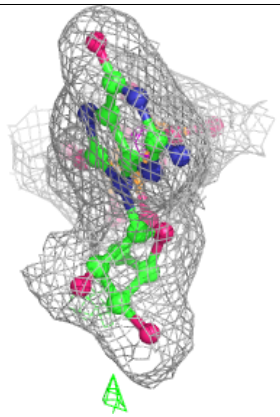


Electron density around GTP A 501:

$2mF_o$-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.