Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 04:08 PM JST

PDB ID	:	4U0M
Title	:	Structure of the Vibrio cholerae di-nucleotide cyclase (DncV) mutant D193N in complex with ATP, GTP and 5MTHFGLU2
Authors	:	Zhu, D.; Xiang, Y.
Deposited on	:	2014-07-12
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 ⓘ 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:

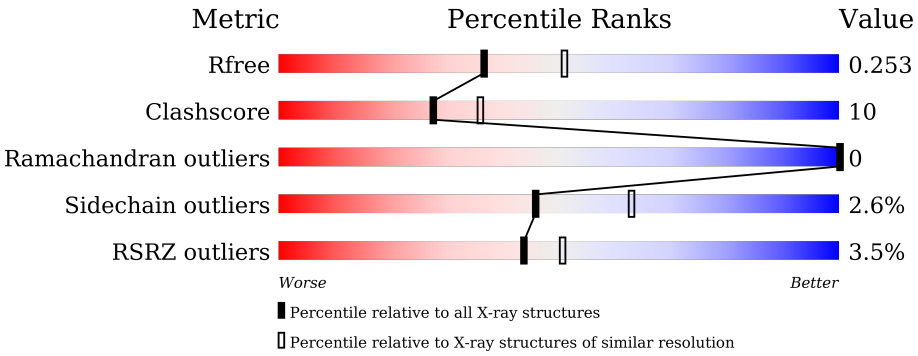
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

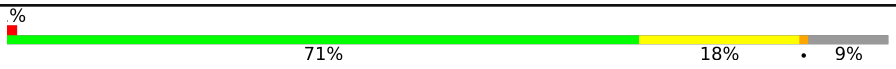
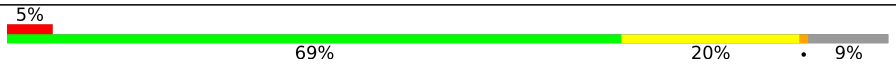
The reported resolution of this entry is 2.30 Å.

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	427	
1	B	427	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6834 atoms, of which 29 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.

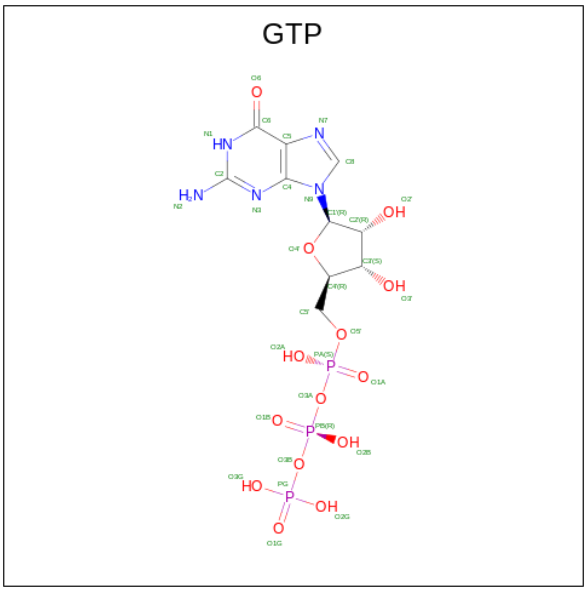
- Molecule 1 is a protein called Cyclic AMP-GMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	1	0
			3114	1966	541	591	16			
1	B	388	Total	C	N	O	S	0	0	0
			3113	1965	539	593	16			

There are 18 discrepancies between the modelled and reference sequences:

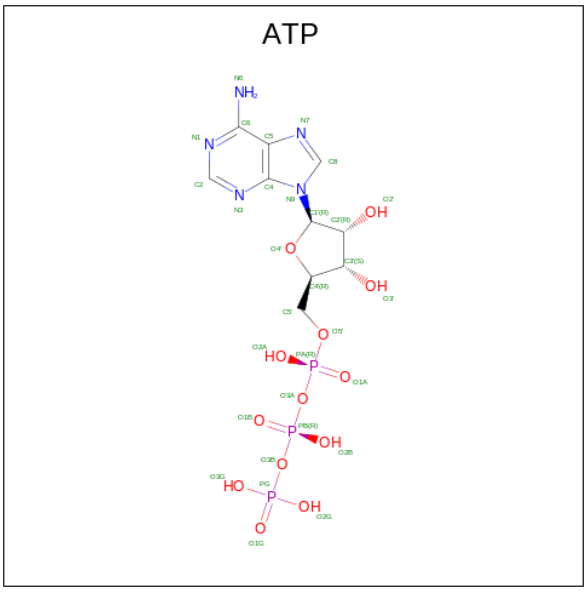
Chain	Residue	Modelled	Actual	Comment	Reference
A	193	ASN	ASP	engineered mutation	UNP Q9KVG7
A	420	LEU	-	expression tag	UNP Q9KVG7
A	421	GLU	-	expression tag	UNP Q9KVG7
A	422	HIS	-	expression tag	UNP Q9KVG7
A	423	HIS	-	expression tag	UNP Q9KVG7
A	424	HIS	-	expression tag	UNP Q9KVG7
A	425	HIS	-	expression tag	UNP Q9KVG7
A	426	HIS	-	expression tag	UNP Q9KVG7
A	427	HIS	-	expression tag	UNP Q9KVG7
B	193	ASN	ASP	engineered mutation	UNP Q9KVG7
B	420	LEU	-	expression tag	UNP Q9KVG7
B	421	GLU	-	expression tag	UNP Q9KVG7
B	422	HIS	-	expression tag	UNP Q9KVG7
B	423	HIS	-	expression tag	UNP Q9KVG7
B	424	HIS	-	expression tag	UNP Q9KVG7
B	425	HIS	-	expression tag	UNP Q9KVG7
B	426	HIS	-	expression tag	UNP Q9KVG7
B	427	HIS	-	expression tag	UNP Q9KVG7

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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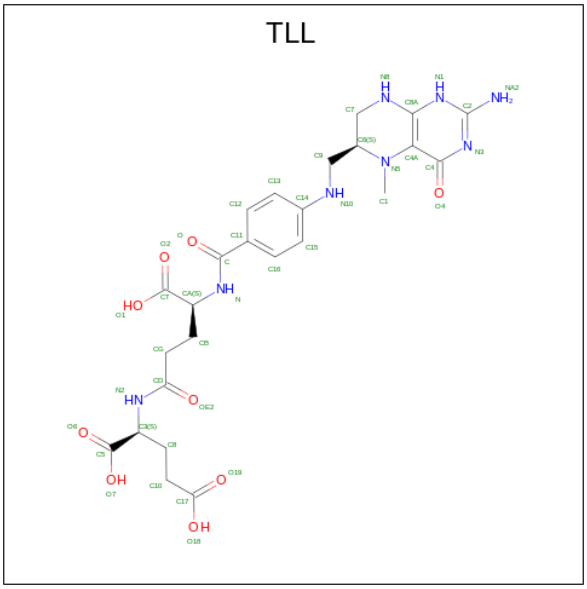
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	1
			62	20	10	26	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is N-[4-({[(6S)-2-amino-5-methyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-gamma-glutamyl-L-glutamic acid (three-letter code: TLL) (formula: $C_{25}H_{32}N_8O_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			71	25	29	8	9		

- Molecule 6 is water.

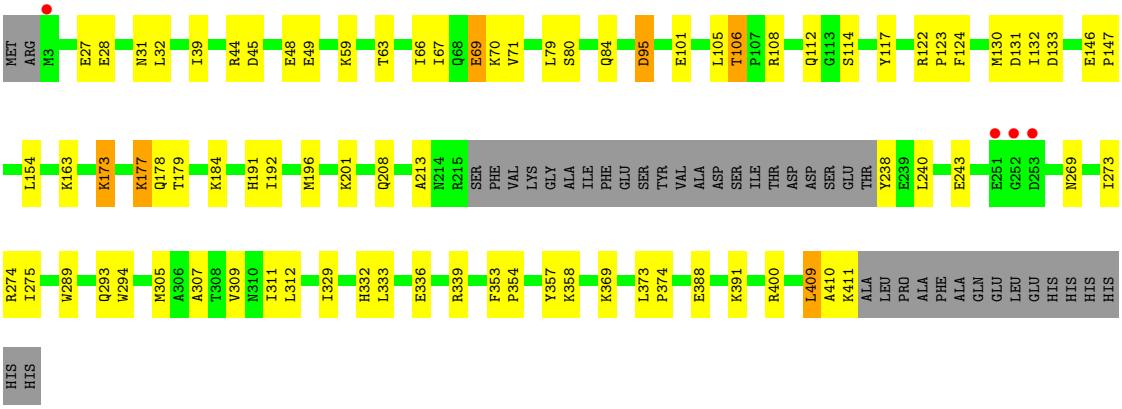
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total	O	0	0
			191	191		
6	B	186	Total	O	0	0
			186	186		

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.

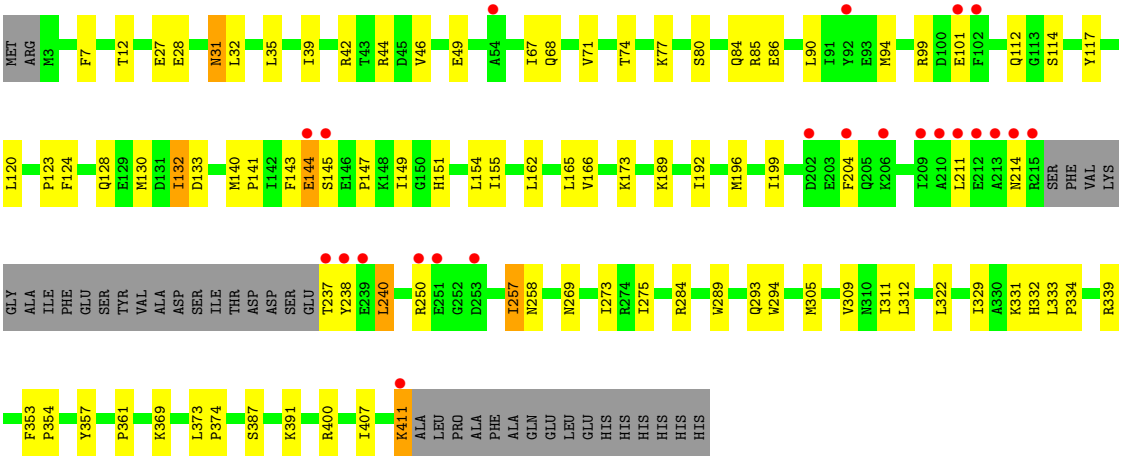
• Molecule 1: Cyclic AMP-GMP synthase

Chain A:



• Molecule 1: Cyclic AMP-GMP synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.90Å 59.86Å 104.19Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	42.57 – 2.30 45.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.57-2.30) 95.0 (45.38-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.199 , 0.253 0.199 , 0.253	Depositor DCC
R_{free} test set	1920 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.0	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	0.94	EDS
Total number of atoms	6834	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GTP, TLL, MG

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	0.20	0/3178	0.35	0/4281
1	B	0.21	0/3174	0.36	0/4277
All	All	0.20	0/6352	0.36	0/8558

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

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	3114	0	3113	59	0
1	B	3113	0	3107	67	0
2	A	32	0	12	0	0
2	B	32	0	12	1	0
3	A	31	0	12	1	0
3	B	62	0	24	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	42	29	29	3	0
6	A	191	0	0	3	0
6	B	186	0	0	7	0
All	All	6805	29	6309	127	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 10.

All (127) 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:A:39:ILE:HD12	1:A:192:ILE:HD13	1.34	1.07
1:A:178:GLN:HG3	1:A:179:THR:HG23	1.59	0.83
1:B:132:ILE:HD13	1:B:132:ILE:H	1.55	0.72
1:B:140:MET:HB2	1:B:141:PRO:HD2	1.74	0.69
1:A:240:LEU:H	5:A:504:TLL:HN1	1.41	0.69
1:B:311:ILE:HD12	1:B:332:HIS:HB3	1.75	0.68
1:B:411:LYS:HZ2	1:B:411:LYS:HB3	1.57	0.68
1:A:32:LEU:HD22	1:A:132:ILE:HD11	1.76	0.68
1:A:294:TRP:CZ2	1:A:369:LYS:HG3	2.29	0.67
1:B:211:LEU:HD22	1:B:238:TYR:CE1	2.30	0.67
1:A:44[B]:ARG:HH22	5:A:504:TLL:CT	2.09	0.66
1:B:77:LYS:NZ	6:B:601:HOH:O	2.29	0.65
1:B:39:ILE:HG13	1:B:192:ILE:HD13	1.79	0.63
1:B:99:ARG:NH2	6:B:703:HOH:O	2.32	0.61
1:A:177:LYS:HE3	1:A:177:LYS:HA	1.81	0.61
1:B:257:ILE:HD13	1:B:258:ASN:N	2.15	0.60
1:B:331:LYS:HE3	1:B:332:HIS:CE1	2.37	0.59
1:B:294:TRP:CZ2	1:B:369:LYS:HD2	2.38	0.59
1:B:112:GLN:O	1:B:133:ASP:HB2	2.04	0.58
1:B:123:PRO:HD3	1:B:130:MET:HG3	1.86	0.58
1:B:149:ILE:H	1:B:149:ILE:HD12	1.69	0.57
1:A:213:ALA:HA	1:B:339:ARG:HD3	1.85	0.57
1:B:411:LYS:H	1:B:411:LYS:HZ3	1.53	0.57
1:A:173:LYS:HG2	1:A:184:LYS:HB3	1.88	0.56
1:B:143:PHE:CD1	1:B:147:PRO:HB3	2.41	0.56
3:B:502[A]:ATP:N6	6:B:739:HOH:O	2.40	0.55
1:B:411:LYS:H	1:B:411:LYS:NZ	2.05	0.55
1:A:63:THR:OG1	1:A:66:ILE:HG12	2.06	0.54
1:B:211:LEU:HD12	1:B:214:ASN:ND2	2.23	0.53
1:B:101:GLU:HB3	1:B:149:ILE:HD11	1.91	0.53
1:B:149:ILE:HD12	1:B:149:ILE:N	2.24	0.52
3:B:502[A]:ATP:N3	6:B:776:HOH:O	2.34	0.52
1:B:27:GLU:O	1:B:31:ASN:HB2	2.10	0.52
1:B:204:PHE:HE1	1:B:237:THR:HA	1.75	0.52
1:B:373:LEU:N	1:B:374:PRO:HD2	2.25	0.52
1:B:80:SER:O	1:B:84:GLN:HG3	2.10	0.52
1:A:133:ASP:OD1	3:A:502:ATP:O3'	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HB3	1:A:132:ILE:CD1	2.41	0.51
1:A:373:LEU:N	1:A:374:PRO:HD2	2.25	0.51
1:B:269:ASN:O	1:B:273:ILE:HG12	2.11	0.51
1:A:79:LEU:HD23	1:A:163:LYS:HD2	1.92	0.51
1:B:144:GLU:O	1:B:145:SER:HB3	2.11	0.50
1:A:112:GLN:O	1:A:133:ASP:HB2	2.12	0.50
1:B:250:ARG:NH2	6:B:733:HOH:O	2.44	0.49
1:A:131:ASP:HB3	1:A:191:HIS:CE1	2.47	0.49
1:B:132:ILE:HG12	1:B:192:ILE:HG13	1.93	0.49
1:A:124:PHE:HB2	1:A:400:ARG:NH2	2.26	0.49
1:B:35:LEU:O	1:B:39:ILE:HG12	2.12	0.49
1:A:274:ARG:NH2	6:A:665:HOH:O	2.39	0.49
1:A:311:ILE:HD12	1:A:332:HIS:CB	2.42	0.49
1:B:68:GLN:NE2	1:B:85:ARG:HG2	2.28	0.48
1:A:63:THR:O	1:A:67:ILE:HG12	2.14	0.48
1:B:154:LEU:HB3	1:B:196:MET:SD	2.53	0.48
1:A:28:GLU:OE2	1:A:122:ARG:NH1	2.42	0.48
1:A:80:SER:O	1:A:84:GLN:HG3	2.13	0.48
1:B:329:ILE:O	1:B:333:LEU:HG	2.14	0.48
1:B:42:ARG:HG2	1:B:165:LEU:HG	1.96	0.47
1:B:67:ILE:O	1:B:71:VAL:HG23	2.14	0.47
1:B:7:PHE:CD1	1:B:407:ILE:HD12	2.49	0.47
1:A:409:LEU:HD13	1:A:410:ALA:N	2.30	0.47
1:A:388:GLU:HA	1:A:391:LYS:HE3	1.96	0.47
1:A:39:ILE:CD1	1:A:192:ILE:HG21	2.45	0.47
1:A:275:ILE:HD13	1:A:312:LEU:HB2	1.96	0.47
1:A:101:GLU:OE1	1:A:201:LYS:NZ	2.47	0.47
1:A:311:ILE:HD12	1:A:332:HIS:HB3	1.95	0.47
1:A:357:TYR:CE2	1:A:358:LYS:HG3	2.49	0.47
1:B:311:ILE:CD1	1:B:332:HIS:HB3	2.45	0.47
1:A:32:LEU:HB3	1:A:132:ILE:HD11	1.97	0.46
1:B:123:PRO:HD3	1:B:130:MET:CG	2.44	0.46
1:A:95:ASP:N	1:A:95:ASP:OD1	2.46	0.46
1:A:123:PRO:HD3	1:A:130:MET:CG	2.45	0.46
1:B:12:THR:CG2	1:B:322:LEU:HD12	2.45	0.46
1:B:331:LYS:HE3	1:B:332:HIS:HE1	1.80	0.46
1:B:42:ARG:O	1:B:46:VAL:HG23	2.15	0.46
1:A:289:TRP:O	1:A:293:GLN:HG2	2.16	0.46
1:A:329:ILE:O	1:A:333:LEU:HG	2.16	0.46
1:A:388:GLU:HG3	1:A:391:LYS:NZ	2.31	0.46
1:A:45:ASP:O	1:A:49:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:HG3	1:B:361:PRO:HG2	1.98	0.46
1:A:339:ARG:HG3	6:A:610:HOH:O	2.16	0.45
1:B:387:SER:O	1:B:391:LYS:HG3	2.16	0.45
2:B:501:GTP:H5'	3:B:502[B]:ATP:O2'	2.14	0.45
1:A:311:ILE:HD11	1:A:336:GLU:CG	2.46	0.45
1:A:32:LEU:CD2	1:A:132:ILE:HD11	2.45	0.45
1:B:28:GLU:O	1:B:32:LEU:HG	2.16	0.45
1:A:357:TYR:CD2	1:A:358:LYS:HG3	2.51	0.45
1:A:131:ASP:HB3	1:A:191:HIS:NE2	2.32	0.45
1:A:44[B]:ARG:NH2	5:A:504:TLL:O2	2.50	0.45
1:A:67:ILE:O	1:A:71:VAL:HG23	2.16	0.45
1:B:237:THR:HG22	1:B:240:LEU:HD11	1.98	0.45
1:B:143:PHE:CG	1:B:147:PRO:HB3	2.52	0.45
1:A:269:ASN:O	1:A:273:ILE:HG12	2.17	0.45
1:A:69:GLU:HG3	1:A:70:LYS:N	2.32	0.45
1:B:132:ILE:HD13	1:B:132:ILE:N	2.28	0.44
1:B:353:PHE:HA	1:B:354:PRO:HD3	1.84	0.44
1:B:162:LEU:O	1:B:166:VAL:HG23	2.17	0.44
1:B:289:TRP:O	1:B:293:GLN:HG2	2.16	0.44
1:B:151:HIS:O	1:B:155:ILE:HG12	2.18	0.44
3:B:502[B]:ATP:N6	6:B:739:HOH:O	2.41	0.44
1:A:154:LEU:HB3	1:A:196:MET:SD	2.58	0.44
1:B:44:ARG:NH1	6:B:693:HOH:O	2.31	0.44
1:A:39:ILE:HD11	1:A:192:ILE:HG21	1.98	0.44
1:B:305:MET:O	1:B:309:VAL:HG23	2.18	0.43
1:B:124:PHE:HB2	1:B:400:ARG:NH2	2.34	0.43
1:A:146:GLU:CD	1:A:147:PRO:HD2	2.39	0.43
1:A:305:MET:O	1:A:309:VAL:HG23	2.19	0.43
1:B:240:LEU:HD12	1:B:240:LEU:N	2.33	0.43
1:B:275:ILE:HD13	1:B:312:LEU:HB2	2.00	0.43
1:B:120:LEU:O	1:B:284:ARG:NH1	2.48	0.42
1:B:94:MET:O	1:B:99:ARG:NH2	2.53	0.42
1:B:128:GLN:O	1:B:189:LYS:HE2	2.19	0.42
1:B:240:LEU:HD12	1:B:240:LEU:H	1.83	0.42
1:A:388:GLU:HA	1:A:391:LYS:CE	2.50	0.42
1:B:199:ILE:HB	1:B:240:LEU:HD22	2.02	0.42
1:B:32:LEU:HD22	1:B:132:ILE:HD12	2.02	0.42
1:B:49:GLU:OE1	1:B:74:THR:HB	2.18	0.42
1:A:131:ASP:HA	1:A:191:HIS:O	2.19	0.41
1:A:27:GLU:O	1:A:31:ASN:HB2	2.20	0.41
1:A:114:SER:HA	1:A:117:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HG2	1:B:357:TYR:HB3	2.01	0.41
1:A:339:ARG:NH1	6:A:734:HOH:O	2.46	0.41
1:A:106:THR:OG1	1:A:108:ARG:HD3	2.21	0.41
1:A:307:ALA:O	1:A:311:ILE:HG12	2.21	0.41
1:A:353:PHE:HA	1:A:354:PRO:HD3	1.82	0.41
1:B:114:SER:HA	1:B:117:TYR:CE1	2.56	0.41
1:B:333:LEU:HB2	1:B:334:PRO:HD3	2.03	0.40
1:B:86:GLU:O	1:B:90:LEU:HG	2.20	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	384/427 (90%)	375 (98%)	9 (2%)	0	100	100
1	B	384/427 (90%)	371 (97%)	13 (3%)	0	100	100
All	All	768/854 (90%)	746 (97%)	22 (3%)	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	342/375 (91%)	331 (97%)	11 (3%)	39	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	342/375 (91%)	335 (98%)	7 (2%)	55 72
All	All	684/750 (91%)	666 (97%)	18 (3%)	46 63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	69	GLU
1	A	95	ASP
1	A	105	LEU
1	A	106	THR
1	A	173	LYS
1	A	177	LYS
1	A	238	TYR
1	A	243	GLU
1	A	409	LEU
1	A	411	LYS
1	B	31	ASN
1	B	132	ILE
1	B	144	GLU
1	B	173	LYS
1	B	240	LEU
1	B	257	ILE
1	B	411	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	B	116	GLN
1	B	125	GLN
1	B	208	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	ATP	B	502[A]	-	26,33,33	0.93	1 (3%)	31,52,52	1.53	5 (16%)
2	GTP	B	501	4	26,34,34	0.92	1 (3%)	32,54,54	1.46	5 (15%)
5	TLL	A	504	-	41,44,44	3.83	11 (26%)	50,61,61	1.26	7 (14%)
2	GTP	A	501	4	26,34,34	0.92	1 (3%)	32,54,54	1.44	5 (15%)
3	ATP	B	502[B]	-	26,33,33	0.93	1 (3%)	31,52,52	1.49	5 (16%)
3	ATP	A	502	-	26,33,33	0.94	1 (3%)	31,52,52	1.60	5 (16%)

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
3	ATP	B	502[A]	-	-	3/18/38/38	0/3/3/3
2	GTP	B	501	4	-	5/18/38/38	0/3/3/3
5	TLL	A	504	-	-	5/35/48/48	0/3/3/3
2	GTP	A	501	4	-	9/18/38/38	0/3/3/3
3	ATP	B	502[B]	-	-	4/18/38/38	0/3/3/3
3	ATP	A	502	-	-	4/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	TLL	C8A-N8	10.80	1.42	1.32
5	A	504	TLL	O4-C4	10.20	1.40	1.23
5	A	504	TLL	C12-C13	8.26	1.53	1.38
5	A	504	TLL	C15-C14	7.99	1.52	1.39
5	A	504	TLL	C16-C11	7.90	1.52	1.39
5	A	504	TLL	C4-N3	7.51	1.51	1.38
5	A	504	TLL	C-N	5.19	1.45	1.34
5	A	504	TLL	CD-N2	5.00	1.44	1.34
5	A	504	TLL	C2-NA2	4.03	1.43	1.34
5	A	504	TLL	C7-N8	-3.28	1.43	1.46
3	B	502[B]	ATP	C5-C4	2.55	1.47	1.40
3	A	502	ATP	C5-C4	2.53	1.47	1.40
3	B	502[A]	ATP	C5-C4	2.52	1.47	1.40
5	A	504	TLL	C4A-N5	2.43	1.44	1.36
2	B	501	GTP	C6-N1	-2.35	1.34	1.37
2	A	501	GTP	C6-N1	-2.31	1.34	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	GTP	PA-O3A-PB	-4.57	117.13	132.83
3	A	502	ATP	PA-O3A-PB	-3.58	120.53	132.83
2	A	501	GTP	PA-O3A-PB	-3.53	120.72	132.83
3	A	502	ATP	C3'-C2'-C1'	3.51	106.26	100.98
3	A	502	ATP	PB-O3B-PG	-3.50	120.81	132.83
3	B	502[B]	ATP	PB-O3B-PG	-3.36	121.30	132.83
3	B	502[A]	ATP	C3'-C2'-C1'	3.29	105.93	100.98
5	A	504	TLL	N1-C2-N3	-3.26	117.24	123.32
2	A	501	GTP	C3'-C2'-C1'	3.24	105.85	100.98
3	B	502[A]	ATP	N3-C2-N1	-3.18	123.70	128.68
3	B	502[B]	ATP	N3-C2-N1	-3.17	123.72	128.68
2	A	501	GTP	PB-O3B-PG	-3.14	122.03	132.83
3	A	502	ATP	N3-C2-N1	-3.13	123.78	128.68
2	B	501	GTP	C3'-C2'-C1'	3.12	105.67	100.98
3	B	502[A]	ATP	PB-O3B-PG	-3.04	122.40	132.83
3	B	502[A]	ATP	PA-O3A-PB	-2.99	122.57	132.83
3	B	502[B]	ATP	PA-O3A-PB	-2.86	123.02	132.83
3	B	502[B]	ATP	C3'-C2'-C1'	2.84	105.25	100.98
5	A	504	TLL	N1-C8A-N8	2.78	122.69	117.38
3	B	502[A]	ATP	C4-C5-N7	-2.61	106.68	109.40
3	B	502[B]	ATP	C4-C5-N7	-2.59	106.70	109.40
3	A	502	ATP	C4-C5-N7	-2.58	106.72	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	504	TLL	CG-CD-N2	2.55	120.26	115.83
2	B	501	GTP	PB-O3B-PG	-2.38	124.67	132.83
2	B	501	GTP	C8-N7-C5	2.37	107.51	102.99
2	A	501	GTP	C8-N7-C5	2.32	107.42	102.99
2	B	501	GTP	C5-C6-N1	2.29	117.99	113.95
2	A	501	GTP	C5-C6-N1	2.28	117.98	113.95
5	A	504	TLL	NA2-C2-N1	2.26	121.52	116.71
5	A	504	TLL	O7-C5-O6	-2.09	119.33	124.09
5	A	504	TLL	O1-CT-CA	2.03	120.15	113.40
5	A	504	TLL	O7-C5-C3	2.02	120.10	113.40

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GTP	C5'-O5'-PA-O1A
2	A	501	GTP	C5'-O5'-PA-O2A
3	A	502	ATP	C5'-O5'-PA-O2A
3	A	502	ATP	C5'-O5'-PA-O3A
3	B	502[A]	ATP	PB-O3B-PG-O2G
3	B	502[B]	ATP	C5'-O5'-PA-O1A
5	A	504	TLL	N2-C3-C8-C10
5	A	504	TLL	C5-C3-C8-C10
3	B	502[B]	ATP	O4'-C4'-C5'-O5'
2	B	501	GTP	PB-O3B-PG-O1G
2	A	501	GTP	PB-O3A-PA-O1A
3	A	502	ATP	PB-O3A-PA-O5'
2	B	501	GTP	PB-O3B-PG-O3G
3	B	502[B]	ATP	C5'-O5'-PA-O3A
2	A	501	GTP	PG-O3B-PB-O2B
2	B	501	GTP	PB-O3A-PA-O2A
2	A	501	GTP	PB-O3A-PA-O2A
5	A	504	TLL	C6-C9-N10-C14
2	A	501	GTP	PA-O3A-PB-O1B
2	B	501	GTP	PB-O3A-PA-O1A
5	A	504	TLL	N-CA-CB-CG
3	B	502[A]	ATP	PB-O3B-PG-O3G
5	A	504	TLL	C8-C3-C5-O7
2	A	501	GTP	C5'-O5'-PA-O3A
2	A	501	GTP	PG-O3B-PB-O1B
2	A	501	GTP	PA-O3A-PB-O2B
2	B	501	GTP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	B	502[B]	ATP	PA-O3A-PB-O2B
3	A	502	ATP	C3'-C4'-C5'-O5'
3	B	502[A]	ATP	PB-O3B-PG-O1G

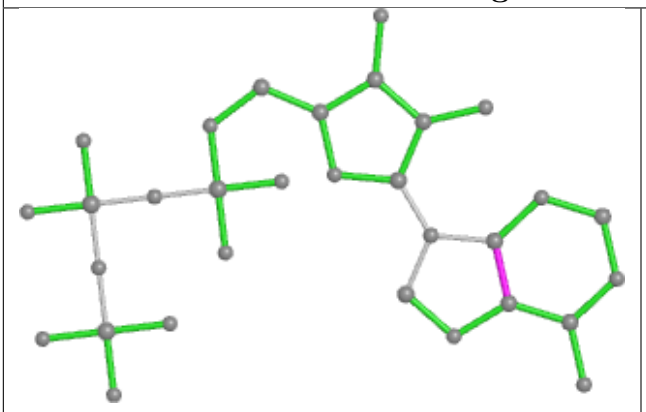
There are no ring outliers.

5 monomers are involved in 8 short contacts:

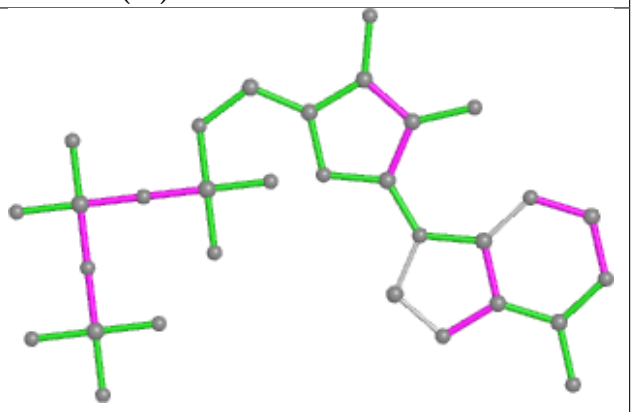
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502[A]	ATP	2	0
2	B	501	GTP	1	0
5	A	504	TLL	3	0
3	B	502[B]	ATP	2	0
3	A	502	ATP	1	0

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 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.

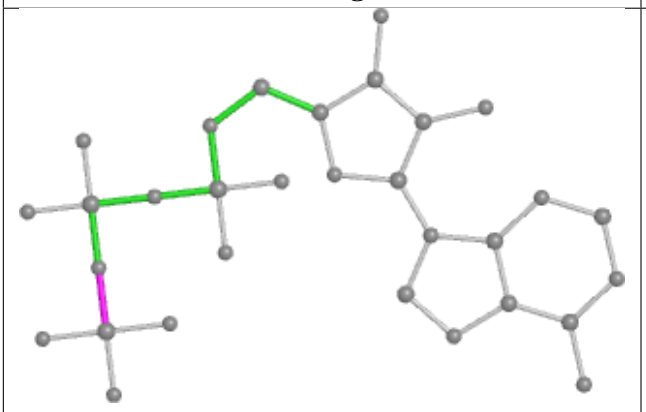
Ligand ATP B 502 (A)



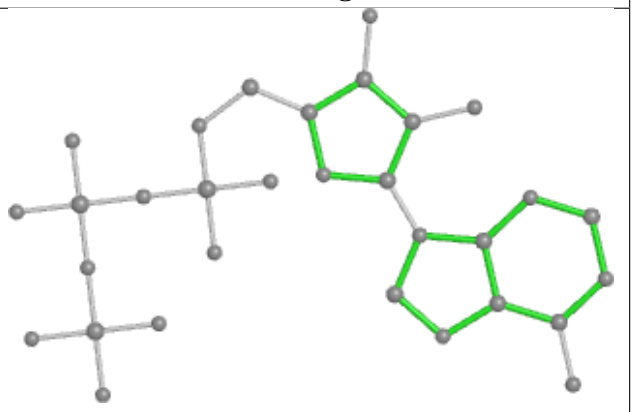
Bond lengths



Bond angles

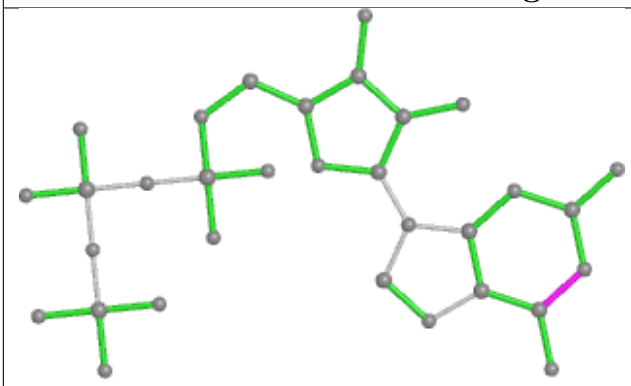


Torsions

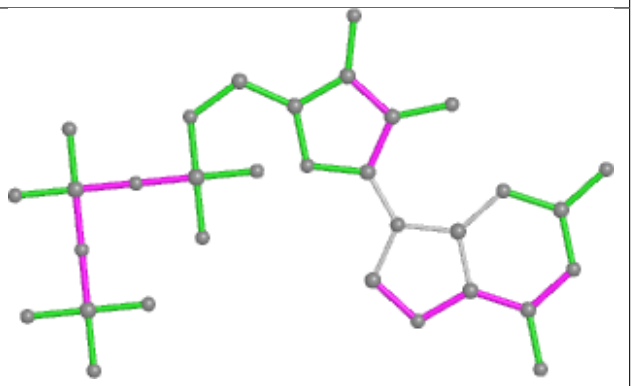


Rings

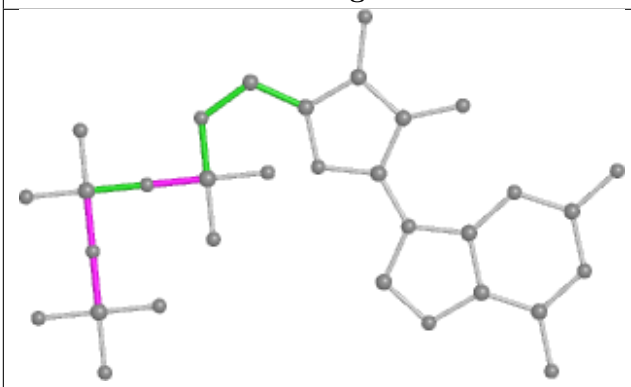
Ligand GTP B 501



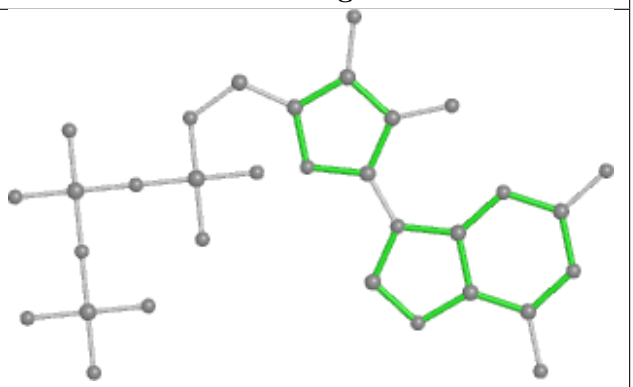
Bond lengths



Bond angles

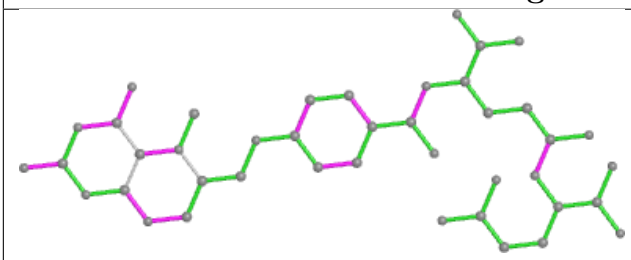


Torsions

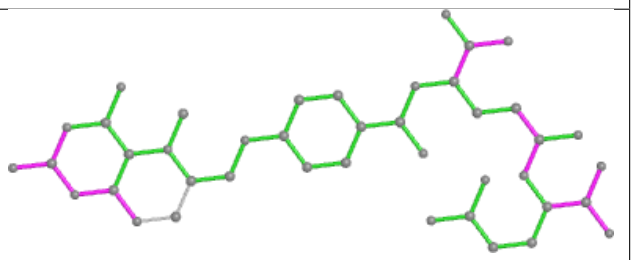


Rings

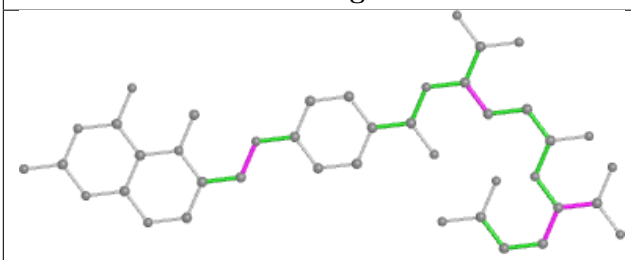
Ligand TLL A 504



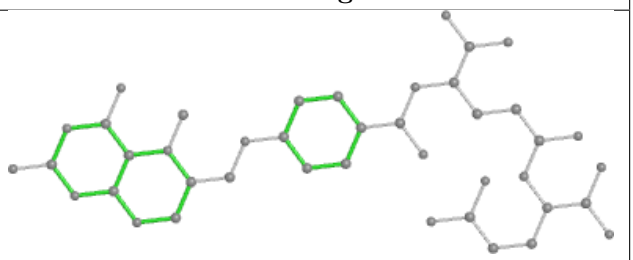
Bond lengths



Bond angles

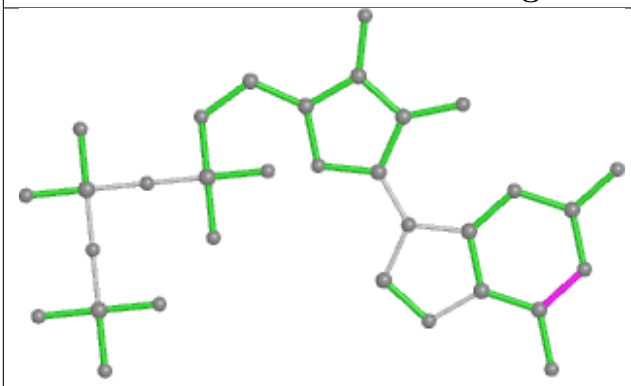


Torsions

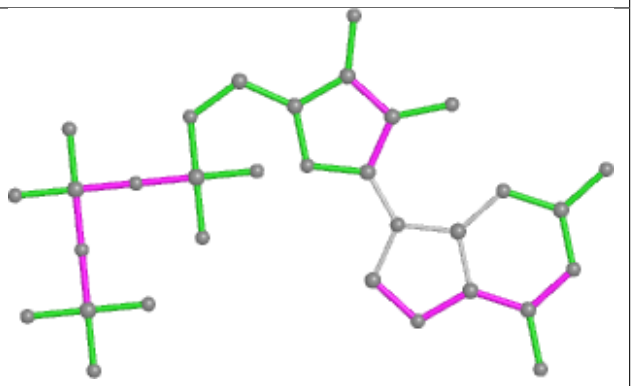


Rings

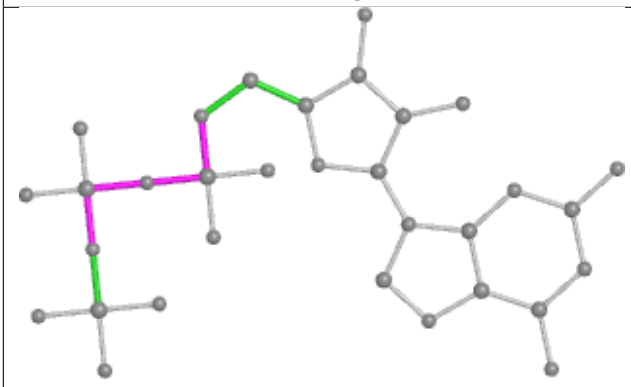
Ligand GTP A 501



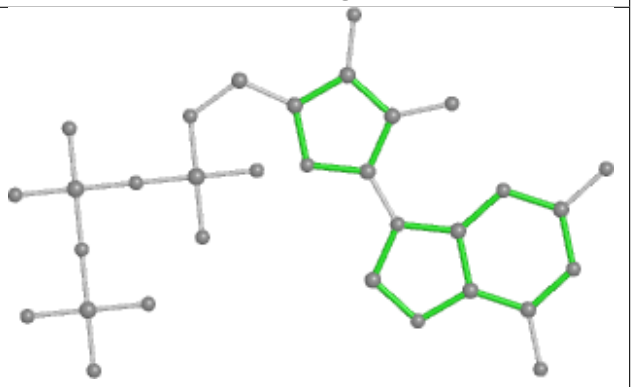
Bond lengths



Bond angles

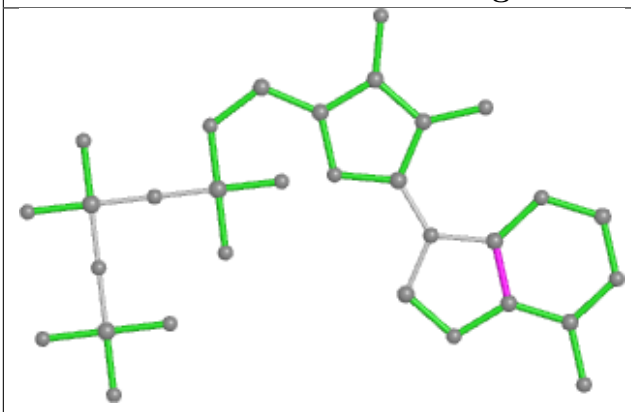


Torsions

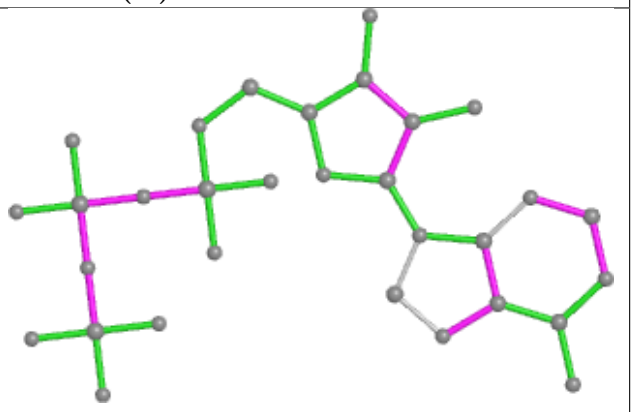


Rings

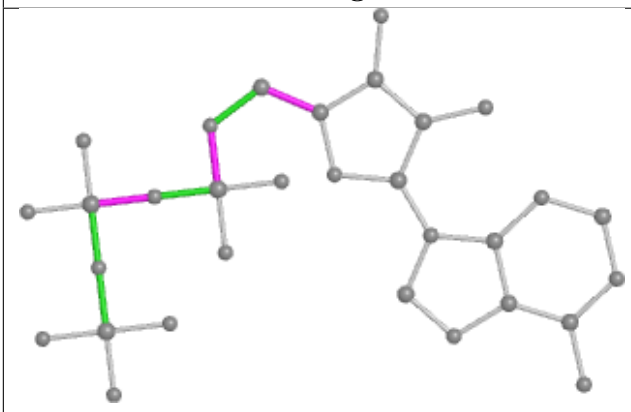
Ligand ATP B 502 (B)



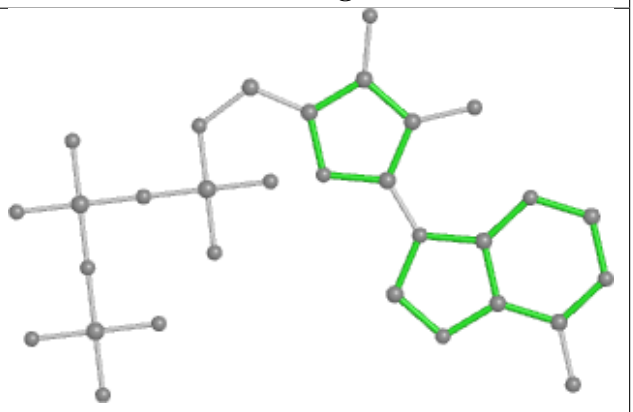
Bond lengths



Bond angles

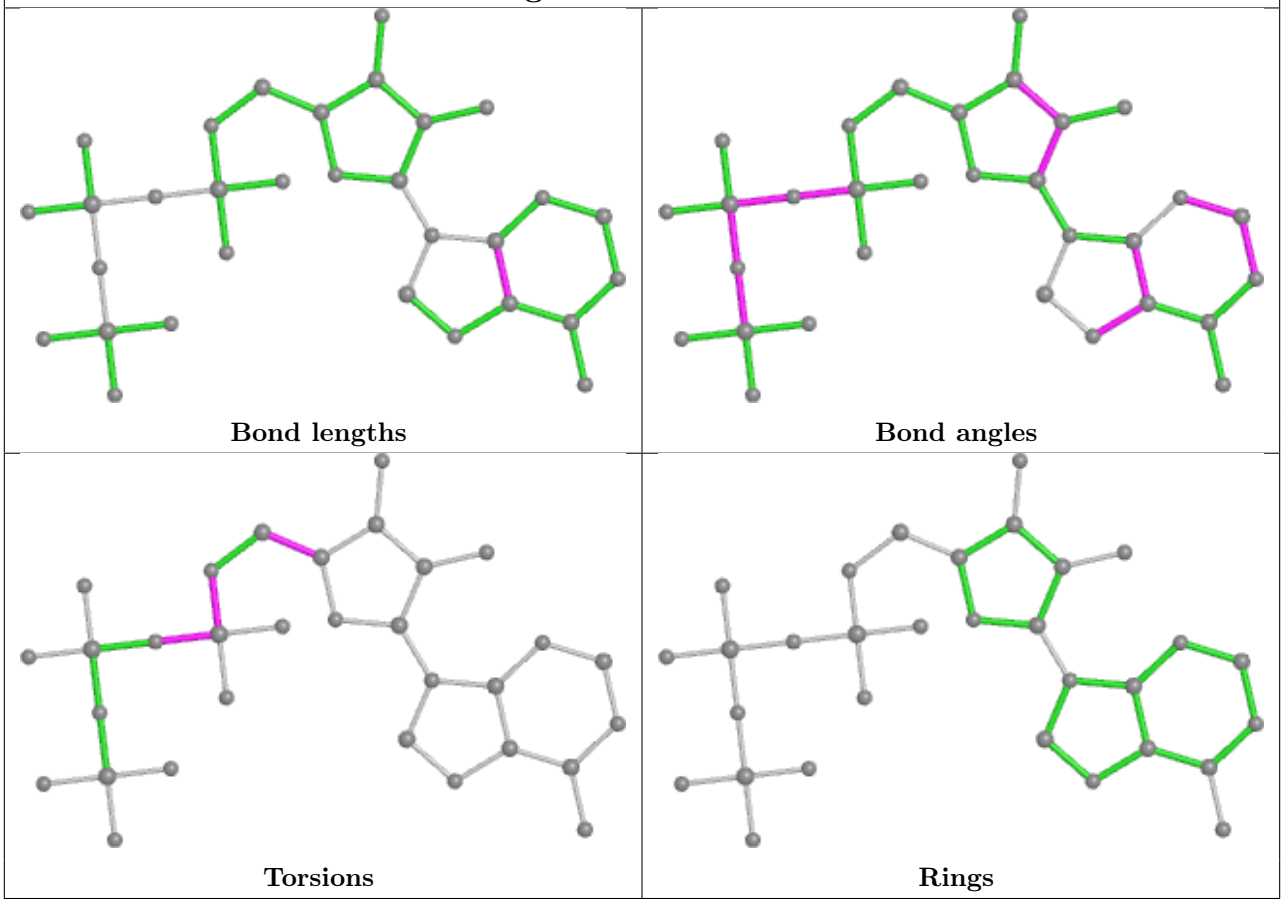


Torsions



Rings

Ligand ATP A 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	387/427 (90%)	-0.13	4 (1%) 82 86	15, 29, 62, 88	0
1	B	388/427 (90%)	0.22	23 (5%) 22 28	15, 33, 85, 104	0
All	All	775/854 (90%)	0.04	27 (3%) 44 51	15, 31, 78, 104	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	GLU	7.2
1	B	215	ARG	7.0
1	B	213	ALA	6.9
1	B	211	LEU	6.0
1	B	238	TYR	5.8
1	B	210	ALA	5.1
1	A	252	GLY	5.0
1	B	411	LYS	4.5
1	B	209	ILE	4.5
1	B	237	THR	4.0
1	B	239	GLU	3.1
1	B	251	GLU	3.1
1	B	92	TYR	3.0
1	A	3	MET	2.9
1	B	204	PHE	2.7
1	B	250	ARG	2.7
1	B	144	GLU	2.7
1	B	145	SER	2.5
1	B	214	ASN	2.5
1	A	253	ASP	2.5
1	B	253	ASP	2.4
1	B	206	LYS	2.3
1	B	202	ASP	2.3
1	B	101	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	102	PHE	2.2
1	A	251	GLU	2.0
1	B	54	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

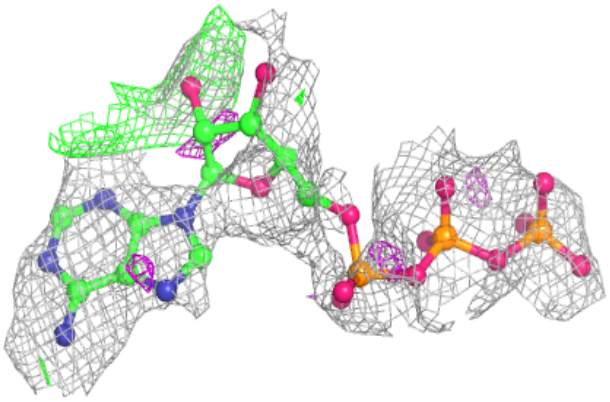
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

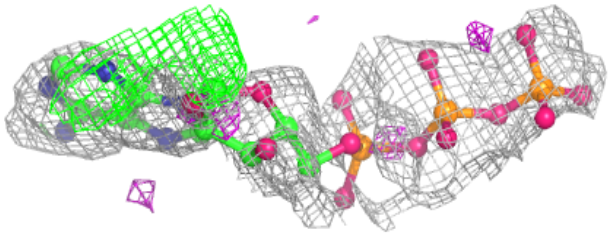
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ATP	A	502	31/31	0.62	0.28	64,96,146,148	0
4	MG	B	503	1/1	0.86	0.11	18,18,18,18	0
3	ATP	B	502[B]	31/31	0.87	0.17	27,49,60,63	31
3	ATP	B	502[A]	31/31	0.87	0.17	43,49,59,61	31
4	MG	A	503	1/1	0.89	0.09	14,14,14,14	0
5	TLL	A	504	42/42	0.91	0.19	17,32,106,118	0
2	GTP	B	501	32/32	0.96	0.13	16,27,37,50	0
2	GTP	A	501	32/32	0.97	0.11	14,22,32,45	0

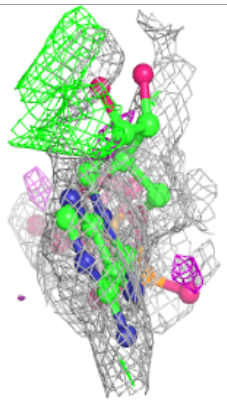
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 502:

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

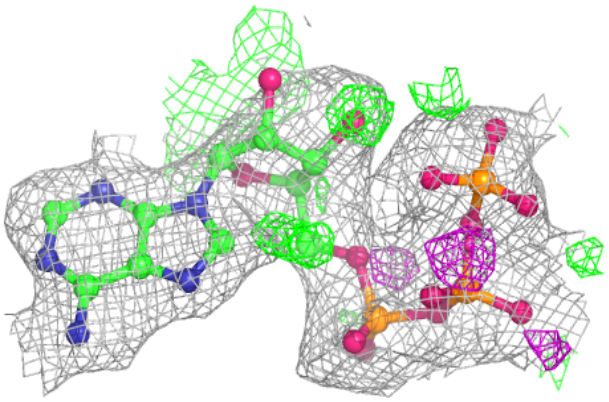


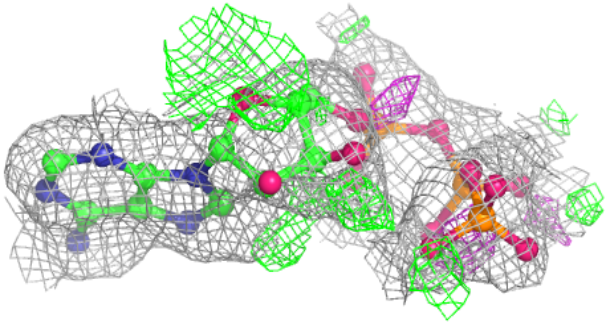


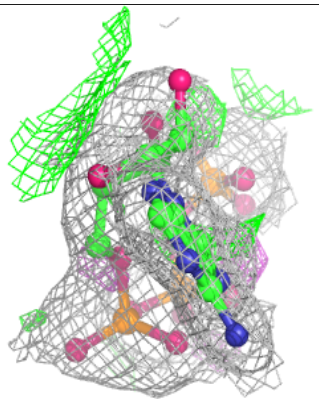


Electron density around ATP B 502 (B):

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

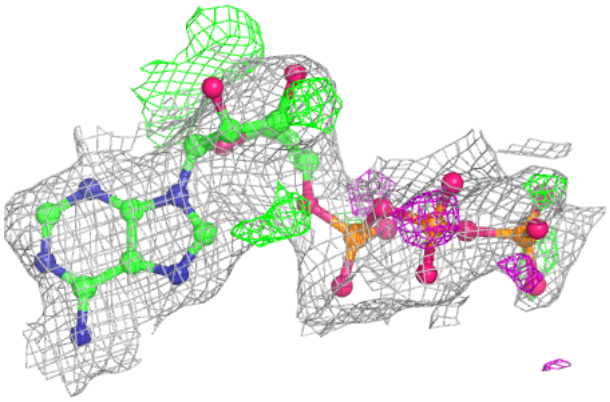


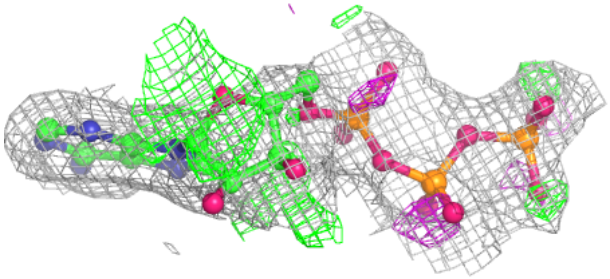


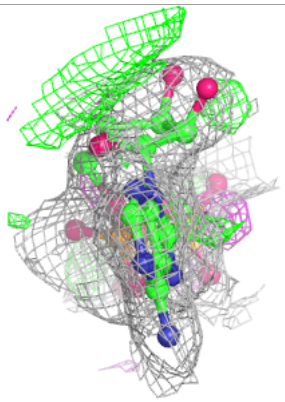


Electron density around ATP B 502 (A):

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

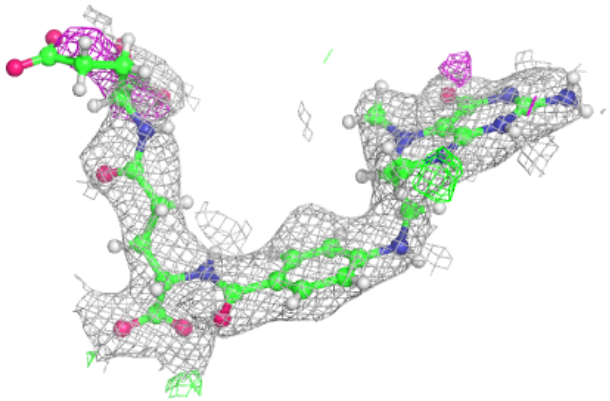


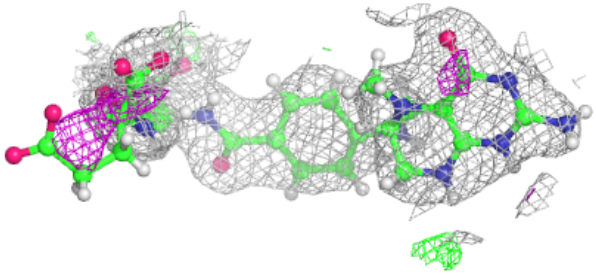


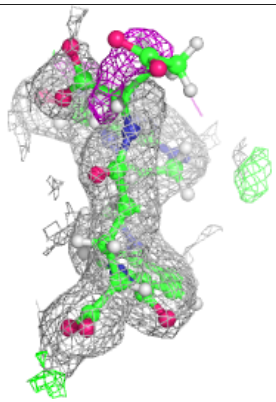


Electron density around TLL A 504:

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

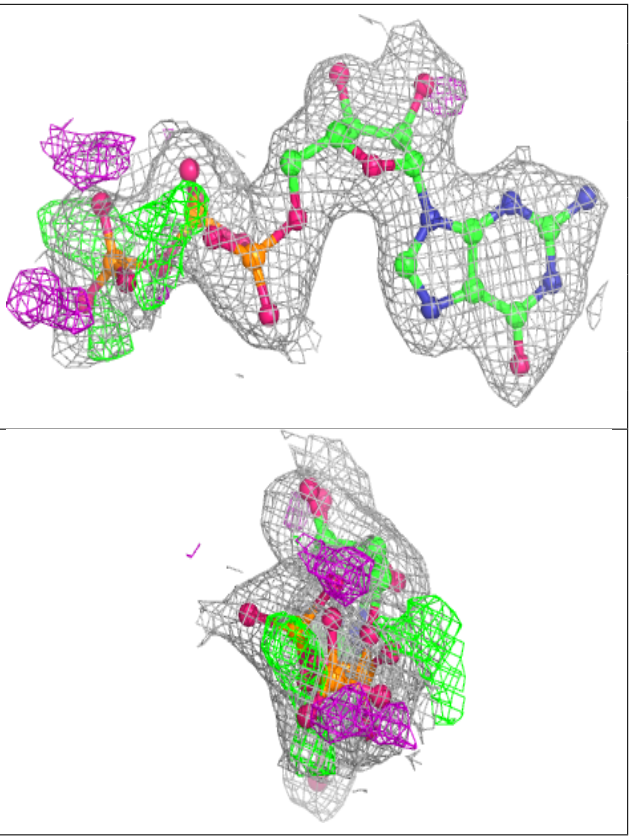


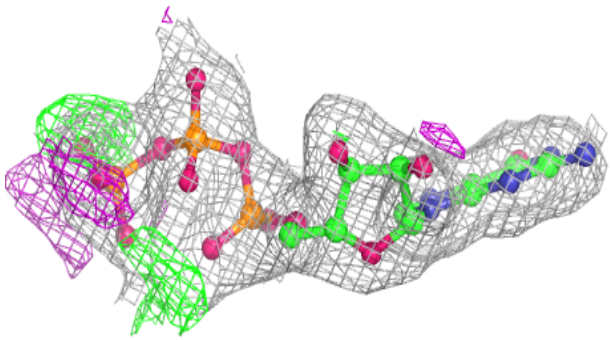




Electron density around GTP B 501:

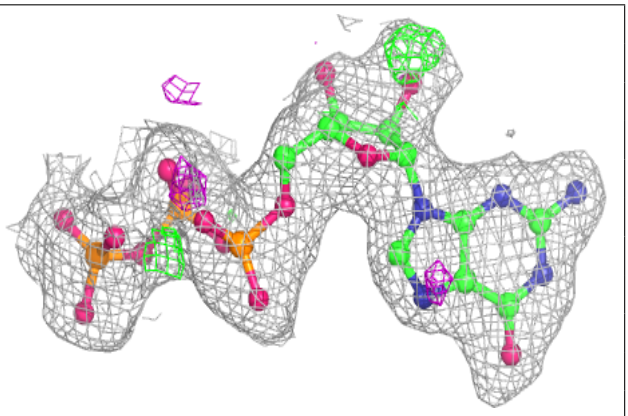
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

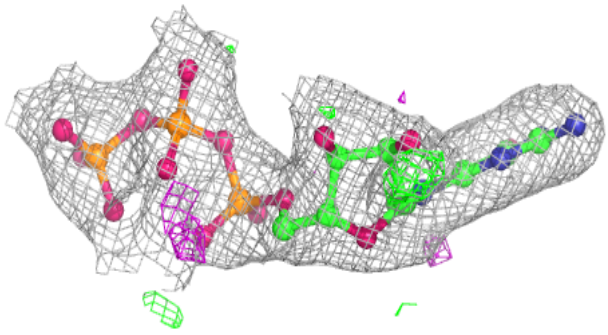


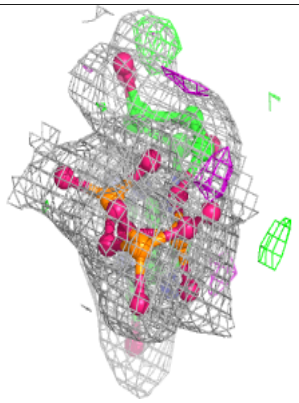


Electron density around GTP A 501:

$2mF_o$-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.