wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 02:35 AM JST

PDB ID	:	5YZ3
Title	:	Crystal structure of T2R-TTL-28 complex
Authors	:	Yu, Y.; Chen, Q.
Deposited on	:	2017-12-12
Resolution	:	2.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

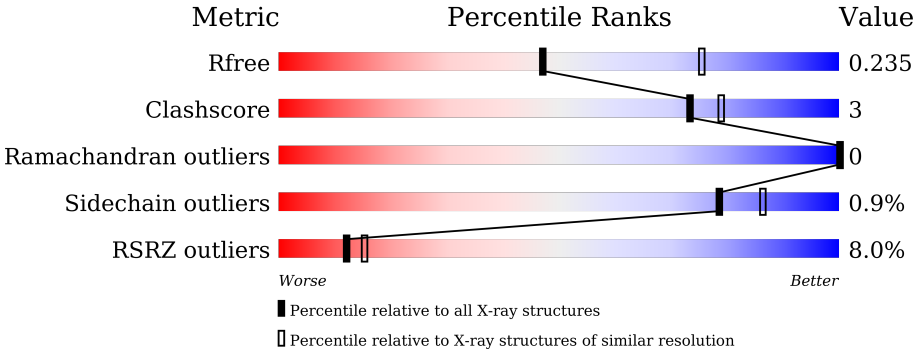
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	93% • •
1	C	450	.% 91% 7% •
2	B	445	4% 88% 8% •
2	D	445	9% 89% 5% 5%
3	E	143	8% 80% • • 15%
4	F	384	25% 80% 6% • 13%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 35117 atoms, of which 16904 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	H	N	O	S			
1	A	437	6743	2166	3321	582	651	23	0	1	0
1	C	440	6783	2178	3340	585	657	23	0	1	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	427	6615	2118	3239	578	653	27	0	2	0
2	D	421	6499	2083	3184	563	641	28	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	121	2014	617	1014	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

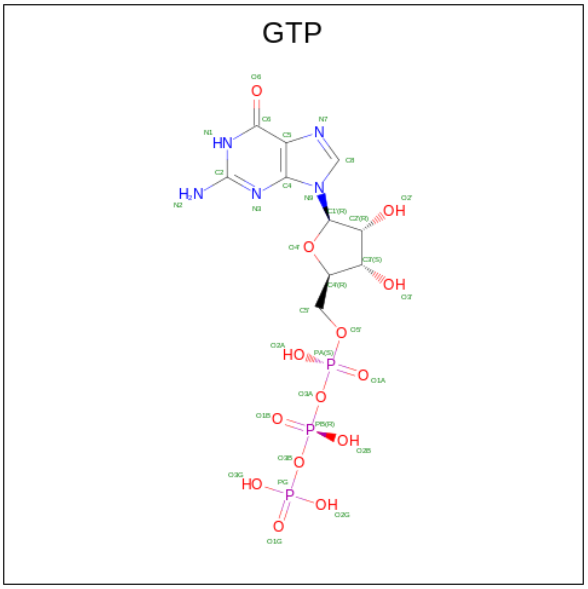
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	334	5465	1767	2710	474	500	14	0	1	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	H	N	O	P		
5	A	1	42	10	10	5	14	3	0	0
5	C	1	42	10	10	5	14	3	0	0
5	D	1	42	10	10	5	14	3	0	0

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

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

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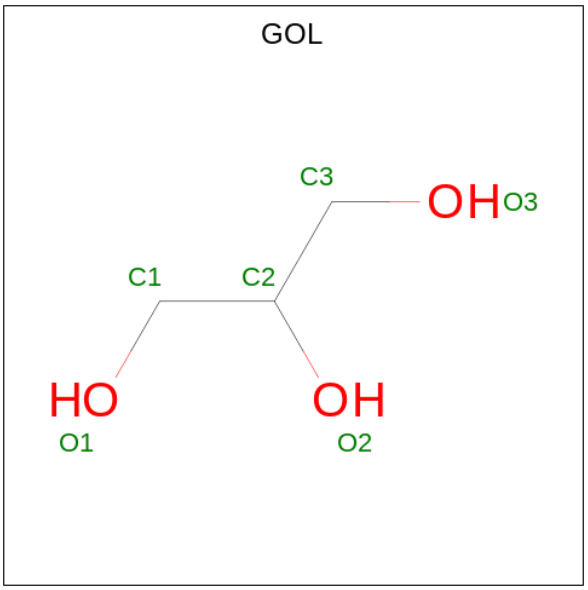
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	D	1	1	1	0	0

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

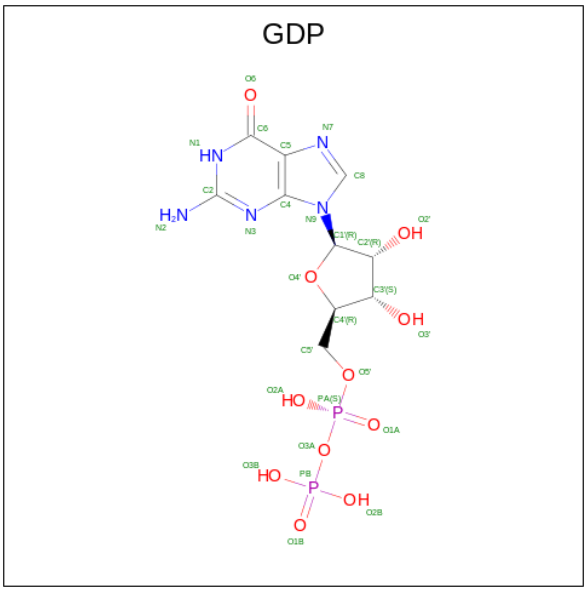
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0

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



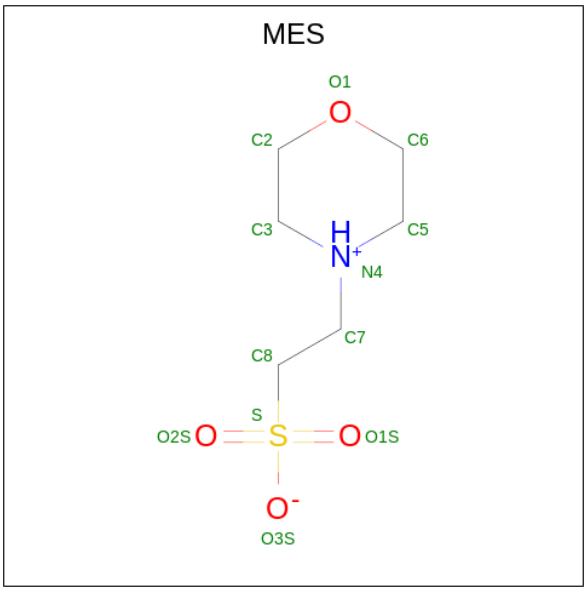
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	A	1	14	3	8	3	0	0

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



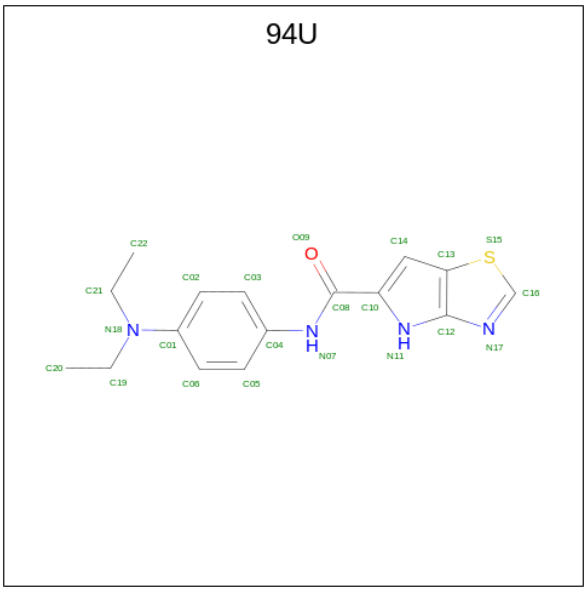
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
9	B	1	38	10	10	5	11	2	0	0

- 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	H	N	O	S		
10	B	1	24	6	12	1	4	1	0	0

- Molecule 11 is N-[4-(diethylamino)phenyl]-4H-pyrrolo[2,3-d][1,3]thiazole-5-carboxamide (three-letter code: 94U) (formula: $C_{16}H_{18}N_4OS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
11	B	1	40	16	18	4	1	1	0	0
			Total	C	H	N	O	S		
11	D	1	40	16	18	4	1	1	0	0

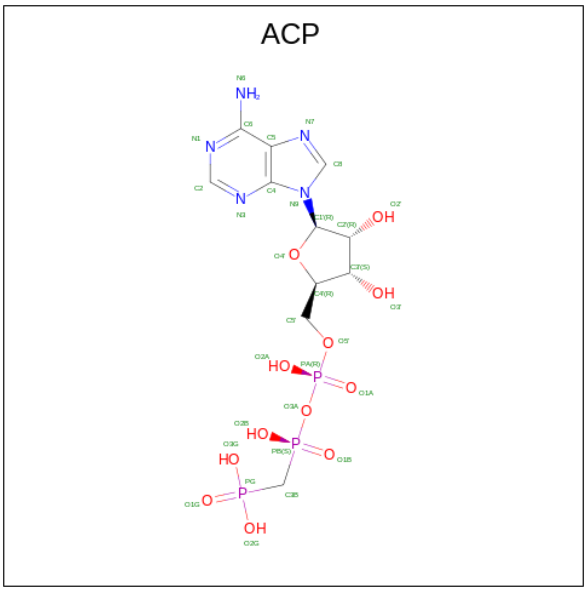
- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
12	B	1	1	1	0	0

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
13	D	1	1	1	0	0

- Molecule 14 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		
14	F	1	31	11	5	12	3	0	0

- Molecule 15 is water.

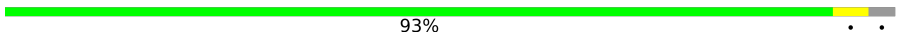
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	151	151	151	0	0
15	B	127	127	127	0	0
15	C	243	243	243	0	0
15	D	75	75	75	0	0
15	E	27	27	27	0	0
15	F	54	54	54	0	0

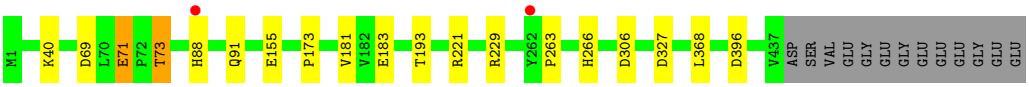
3 Residue-property plots (i)

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

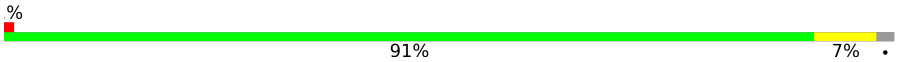
Chain A:

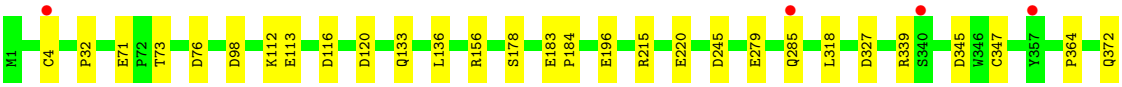




• Molecule 1: Tubulin alpha-1B chain

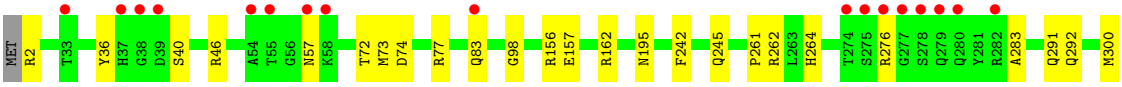
Chain C:

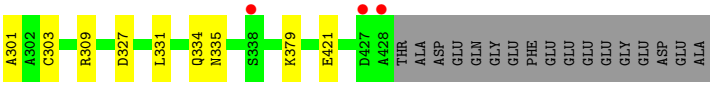




• Molecule 2: Tubulin beta-2B chain

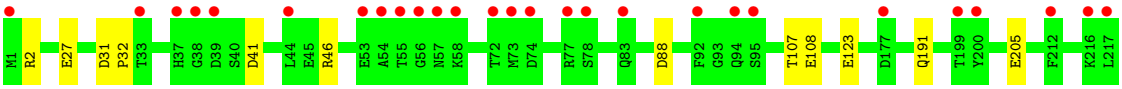
Chain B:

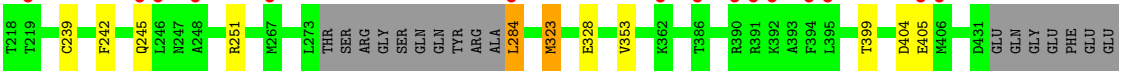


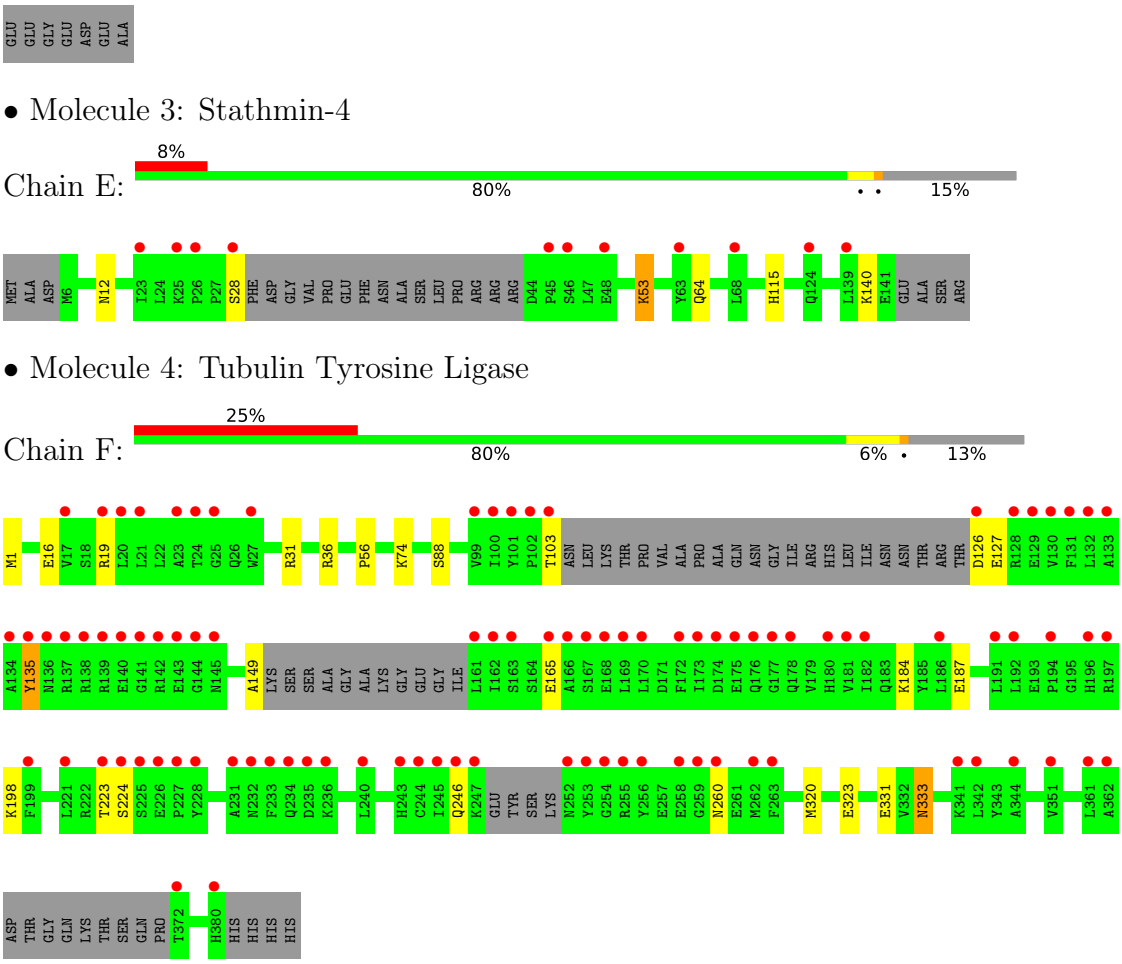


• Molecule 2: Tubulin beta-2B chain

Chain D:






GLU GLU GLY GLU ASP GLU ALA
• Molecule 3: Stathmin-4
Chain E:
8%
80%
15%
MET ALA ASP M6 N12 I23 L24 K25 P26 P27 S28 PHE ASP GLY VAL PRO GLU PHE ASN ALA SER LEU PRO ARG ARG ARG D44 P45 S46 L47 E48 K53 Y63 Q64 L68 H115 Q124 L139 K140 E141 GLU ALA SER ARG
• Molecule 4: Tubulin Tyrosine Ligase
Chain F:
25%
80%
6%
13%
M1 E16 V17 S18 R19 L20 L21 L22 A23 T24 G25 Q26 W27 R31 R36 P56 K74 S88 V99 I100 Y101 P102 T103 ASN LEU LYS THR PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG THR D126 E127 R128 E129 V130 F131 L132 A133
A134 Y135 N136 R137 R138 R139 E140 G141 R142 E143 G144 N145 A149 LYS SER SER ALA GLY ALA LYS GLY GLU GLY ILE L161 I162 S163 S164 E165 A166 S167 E168 L169 L170 D171 F172 I173 D174 E175 Q176 G177 Q178 V179 H180 V181 I182 Q183 K184 Y185 L186 E187 L191 L192 E193 P194 G195 H196 R197
K198 F199 L221 R222 T223 S224 S225 E226 P227 Y228 A231 N232 F233 Q234 D235 K236 L240 H243 C244 I245 Q246 K247 GLU TYR SER LYS N252 Y253 G254 R255 Y256 E257 E258 G259 N260 E261 M262 F263 M320 E323 E331 V332 N333 K341 L342 Y343 A344 V351 L361 A362
ASP THR GLY GLN LYS THR SER GLN PRO T372 H380 HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.89Å 157.50Å 180.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 2.54 49.62 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.62-2.54) 92.1 (49.62-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.210 , 0.234 0.212 , 0.235	Depositor DCC
R_{free} test set	1500 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.4	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	0.92	EDS
Total number of atoms	35117	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: NA, GDP, MG, 94U, ACP, CL, MES, GTP, GOL, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.23	0/3500	0.38	0/4751
1	C	0.24	0/3521	0.38	0/4780
2	B	0.23	0/3451	0.38	0/4674
2	D	0.24	0/3388	0.38	0/4589
3	E	0.23	0/1008	0.34	0/1337
4	F	0.23	0/2817	0.40	1/3805 (0.0%)
All	All	0.24	0/17685	0.38	1/23936 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	88	SER	C-N-CA	7.20	139.70	121.70

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	3422	3321	3334	16	0
1	C	3443	3340	3352	27	0
2	B	3376	3239	3247	24	0
2	D	3315	3184	3193	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1000	1014	1018	6	0
4	F	2755	2710	2721	21	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	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	8	8	0	0
9	B	28	10	12	0	0
10	B	12	12	12	0	0
11	B	22	18	0	0	0
11	D	22	18	0	0	0
12	B	1	0	0	0	0
13	D	1	0	0	1	0
14	F	31	0	14	7	0
15	A	151	0	0	11	2
15	B	127	0	0	14	0
15	C	243	0	0	21	2
15	D	75	0	0	12	0
15	E	27	0	0	4	0
15	F	54	0	0	6	0
All	All	18213	16904	16947	114	2

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 3.

The worst 5 of 114 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:331:GLU:CD	14:F:401:ACP:H3B2	1.73	1.08
4:F:331:GLU:OE2	14:F:401:ACP:H3B2	1.53	1.07
1:A:40:LYS:NZ	15:A:602:HOH:O	1.92	1.02
1:C:339:ARG:O	15:C:601:HOH:O	1.81	0.98
4:F:331:GLU:OE2	14:F:401:ACP:C3B	2.11	0.98

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:641:HOH:O	15:C:731:HOH:O[3_545]	1.84	0.36
15:A:691:HOH:O	15:C:772:HOH:O[3_545]	2.19	0.01

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	436/450 (97%)	421 (97%)	15 (3%)	0	100	100
1	C	439/450 (98%)	430 (98%)	9 (2%)	0	100	100
2	B	427/445 (96%)	412 (96%)	15 (4%)	0	100	100
2	D	418/445 (94%)	404 (97%)	14 (3%)	0	100	100
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	325/384 (85%)	318 (98%)	7 (2%)	0	100	100
All	All	2162/2317 (93%)	2100 (97%)	62 (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	369/378 (98%)	366 (99%)	3 (1%)	81	88
1	C	372/378 (98%)	371 (100%)	1 (0%)	92	96
2	B	371/383 (97%)	368 (99%)	3 (1%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	365/383 (95%)	362 (99%)	3 (1%)	81	88
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	86
4	F	302/342 (88%)	297 (98%)	5 (2%)	60	75
All	All	1888/1991 (95%)	1872 (99%)	16 (1%)	78	88

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	320	MET
4	F	135	TYR
2	D	284	LEU
4	F	31	ARG
2	D	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	333	ASN
4	F	260	ASN
3	E	71	HIS
3	E	12	ASN
4	F	246	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 17 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
10	MES	B	503	-	12,12,12	2.20	1 (8%)	14,16,16	2.45	5 (35%)
8	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.20	0
5	GTP	C	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.40	5 (15%)
5	GTP	D	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.54	6 (18%)
9	GDP	B	501	6	24,30,30	0.96	1 (4%)	30,47,47	1.07	3 (10%)
5	GTP	A	501	6	26,34,34	1.18	2 (7%)	32,54,54	1.38	6 (18%)
11	94U	D	502	-	20,24,24	2.16	9 (45%)	20,33,33	1.76	3 (15%)
14	ACP	F	401	-	27,33,33	2.02	6 (22%)	32,52,52	1.55	6 (18%)
11	94U	B	504	-	20,24,24	1.94	7 (35%)	20,33,33	1.67	3 (15%)

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
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3
11	94U	D	502	-	-	4/13/16/16	0/3/3/3
14	ACP	F	401	-	-	5/15/38/38	0/3/3/3
11	94U	B	504	-	-	8/13/16/16	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.43	1.66	1.77
14	F	401	ACP	PB-O2B	-4.80	1.45	1.56
14	F	401	ACP	PG-O1G	4.66	1.60	1.50
5	A	501	GTP	C5-C6	-4.25	1.38	1.47
5	C	501	GTP	C5-C6	-4.14	1.39	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	503	MES	C5-N4-C3	5.44	121.07	108.83
11	D	502	94U	C10-C08-N07	5.04	126.26	114.04
11	B	504	94U	C10-C08-N07	4.79	125.67	114.04
10	B	503	MES	C7-N4-C5	4.28	122.19	111.23
5	D	501	GTP	PB-O3B-PG	-3.54	120.68	132.83

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A

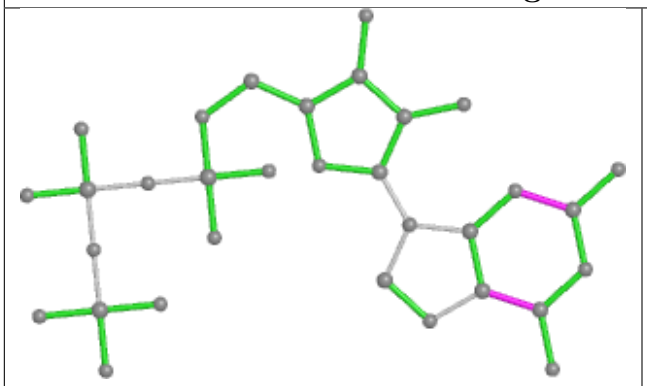
There are no ring outliers.

1 monomer is involved in 7 short contacts:

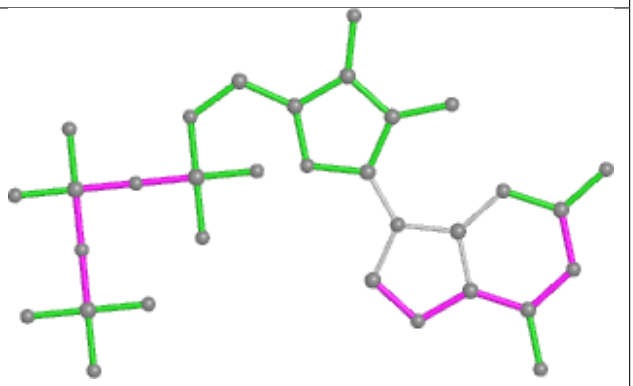
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	401	ACP	7	0

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.

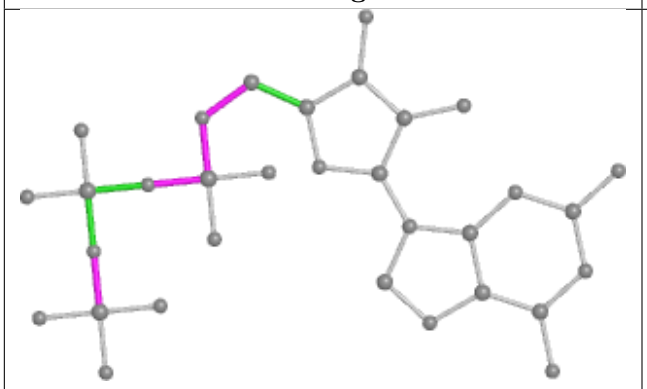
Ligand GTP C 501



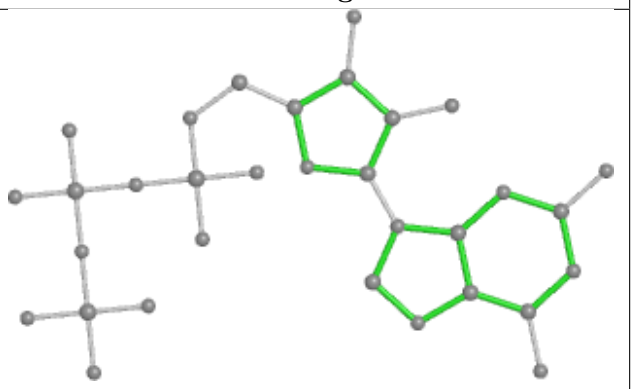
Bond lengths



Bond angles

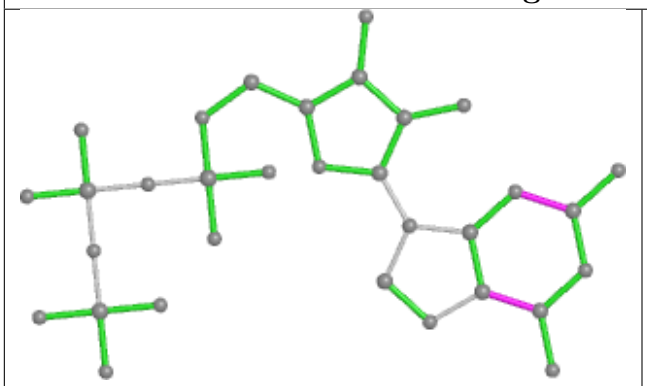


Torsions

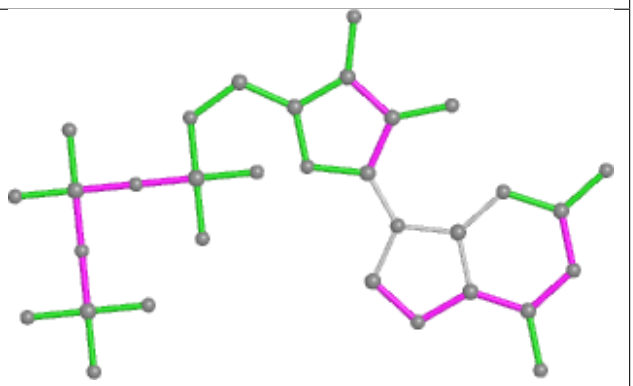


Rings

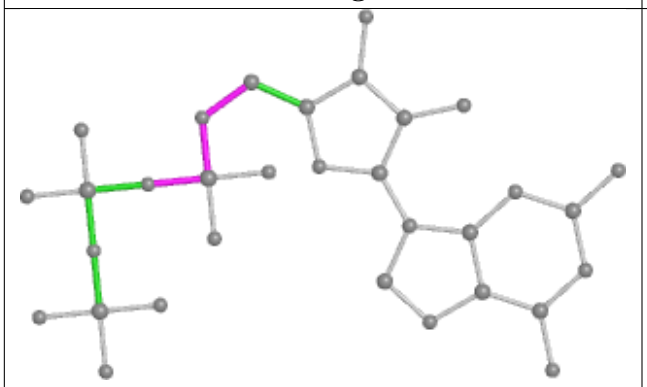
Ligand GTP D 501



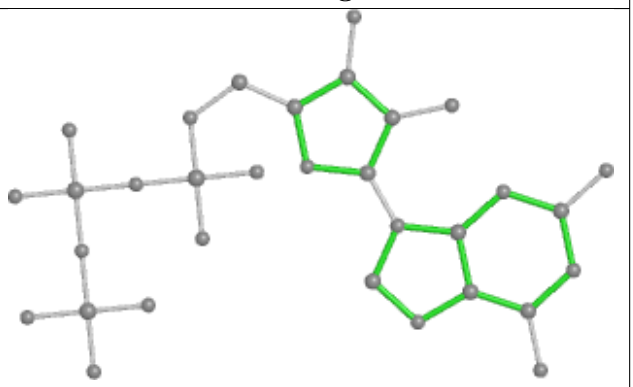
Bond lengths



Bond angles

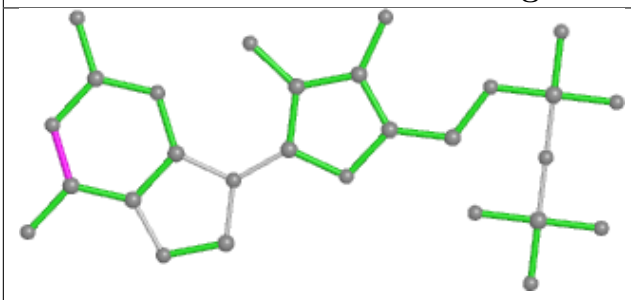


Torsions

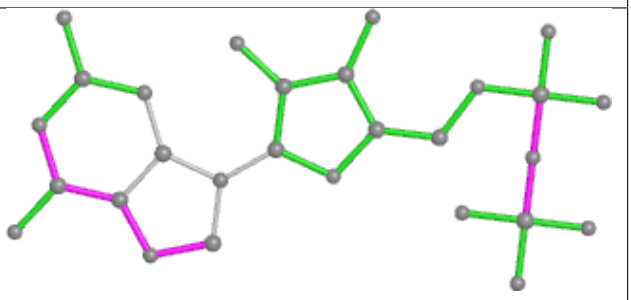


Rings

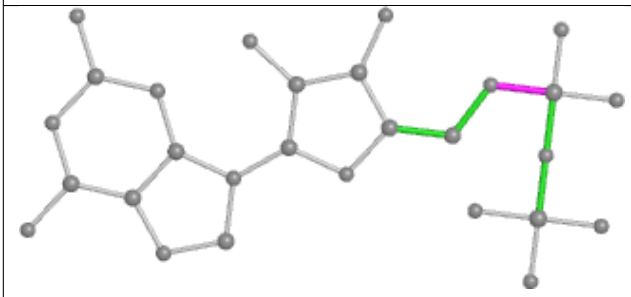
Ligand GDP B 501



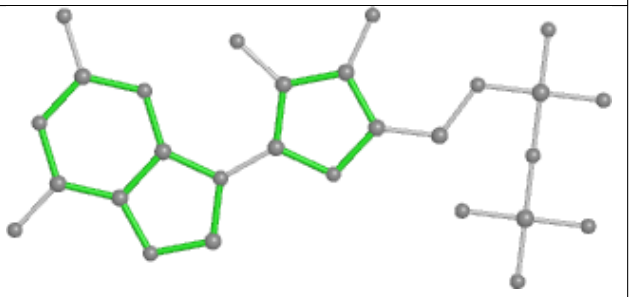
Bond lengths



Bond angles

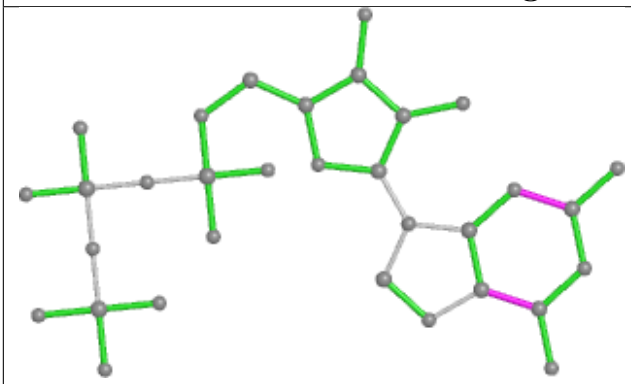


Torsions

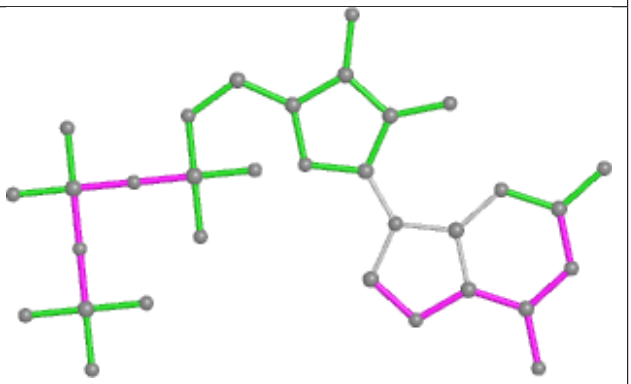


Rings

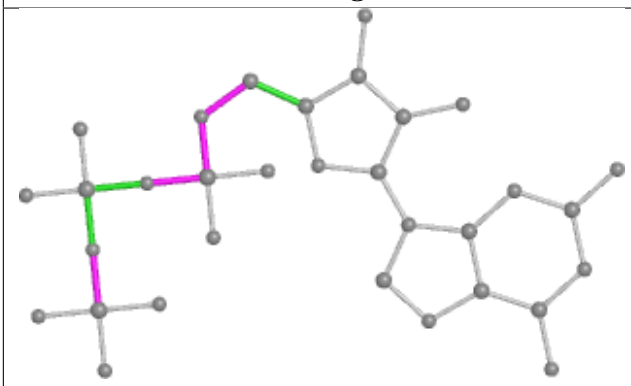
Ligand GTP A 501



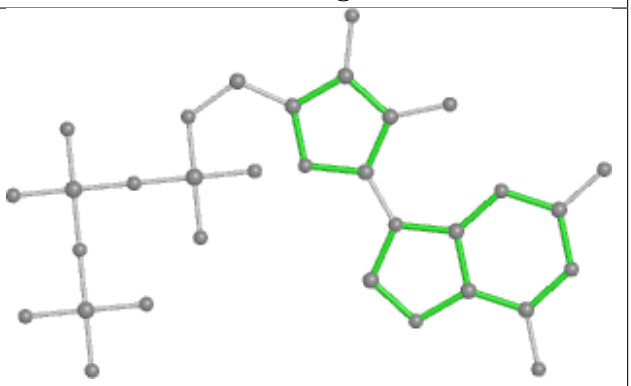
Bond lengths



Bond angles

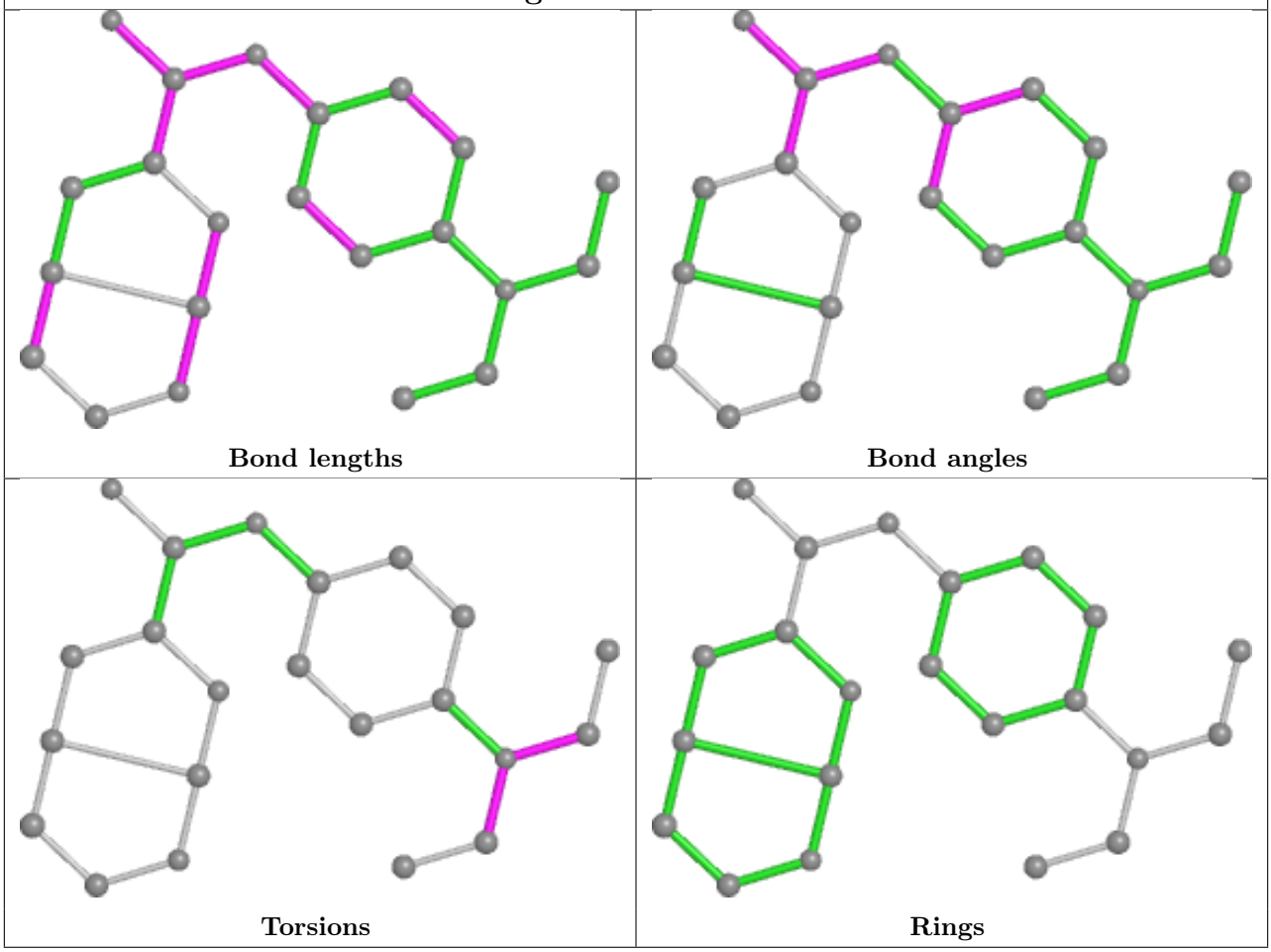


Torsions

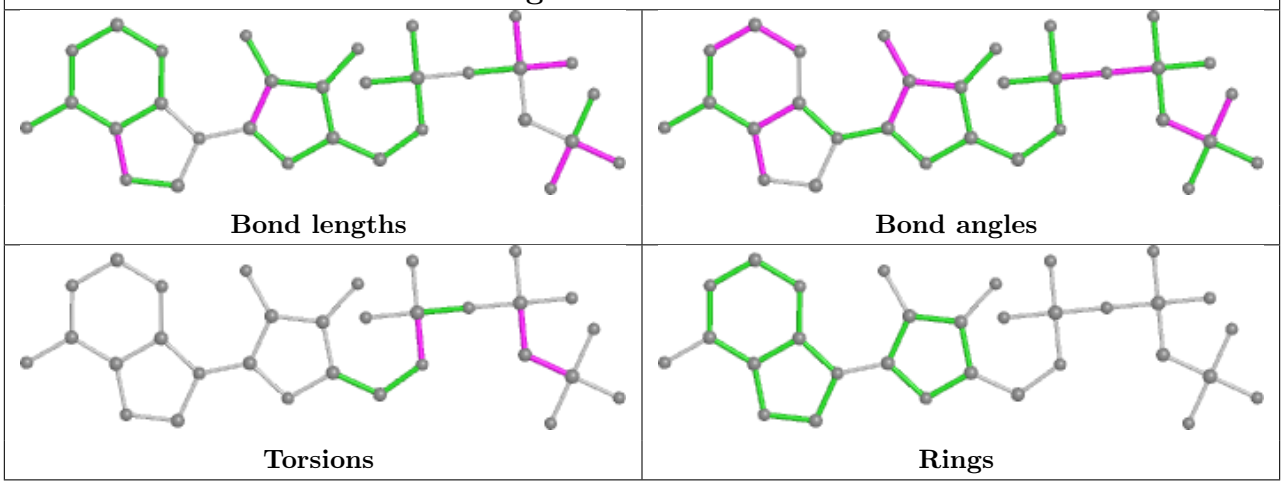


Rings

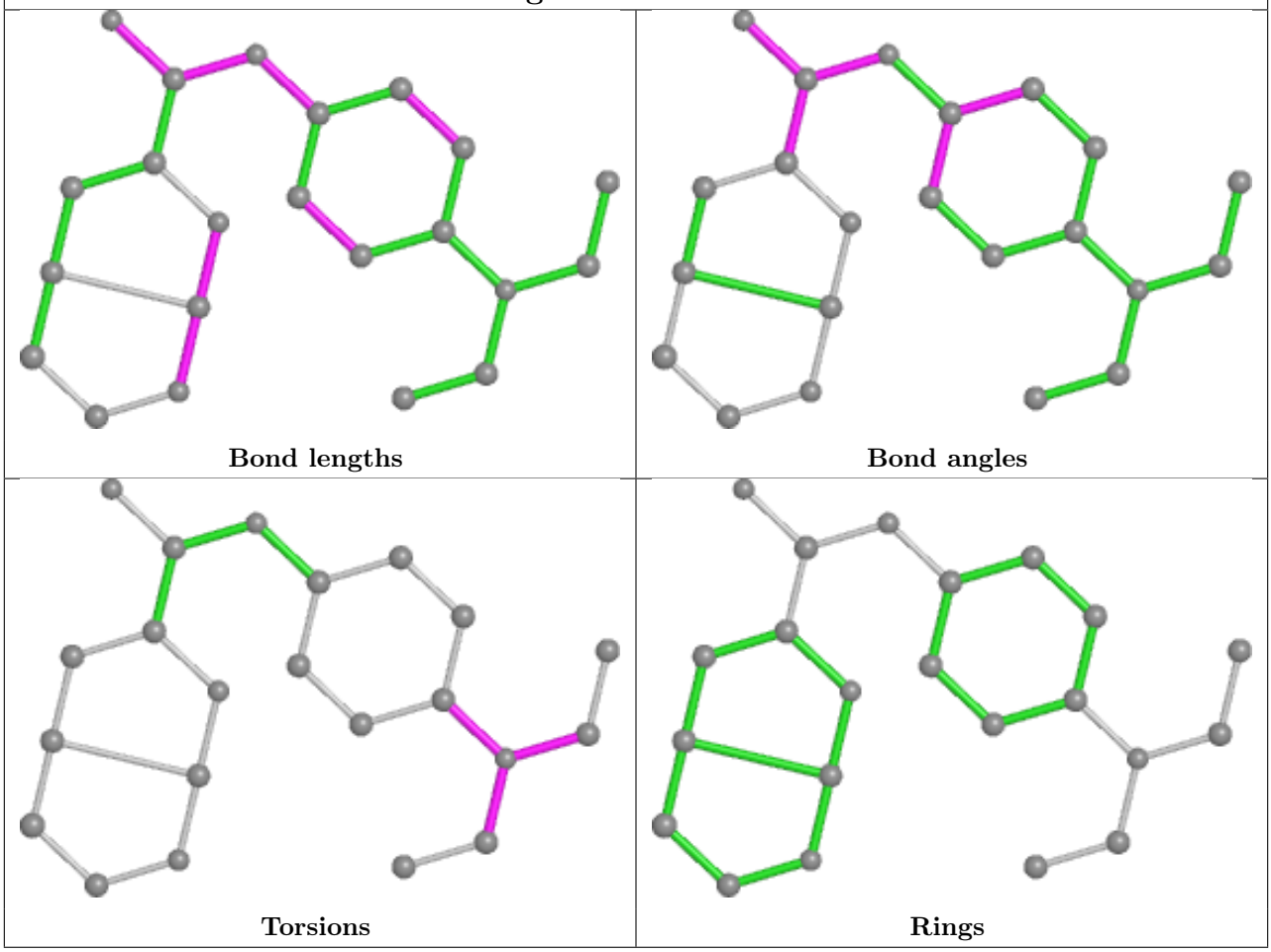
Ligand 94U D 502



Ligand ACP F 401



Ligand 94U B 504



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%)	0.16	2 (0%)	91	94	23, 37, 64, 82	0
1	C	440/450 (97%)	-0.08	4 (0%)	84	88	17, 29, 51, 72	0
2	B	427/445 (95%)	0.28	20 (4%)	31	38	19, 37, 75, 115	0
2	D	421/445 (94%)	0.71	42 (9%)	7	9	27, 54, 85, 111	0
3	E	121/143 (84%)	0.60	11 (9%)	9	11	26, 51, 85, 103	0
4	F	334/384 (86%)	1.38	95 (28%)	0	0	32, 64, 126, 150	0
All	All	2180/2317 (94%)	0.45	174 (7%)	12	15	17, 42, 89, 150	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	136	ASN	11.6
4	F	142	ARG	10.6
2	B	279	GLN	9.3
2	B	280	GLN	7.7
4	F	101	TYR	6.2

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)

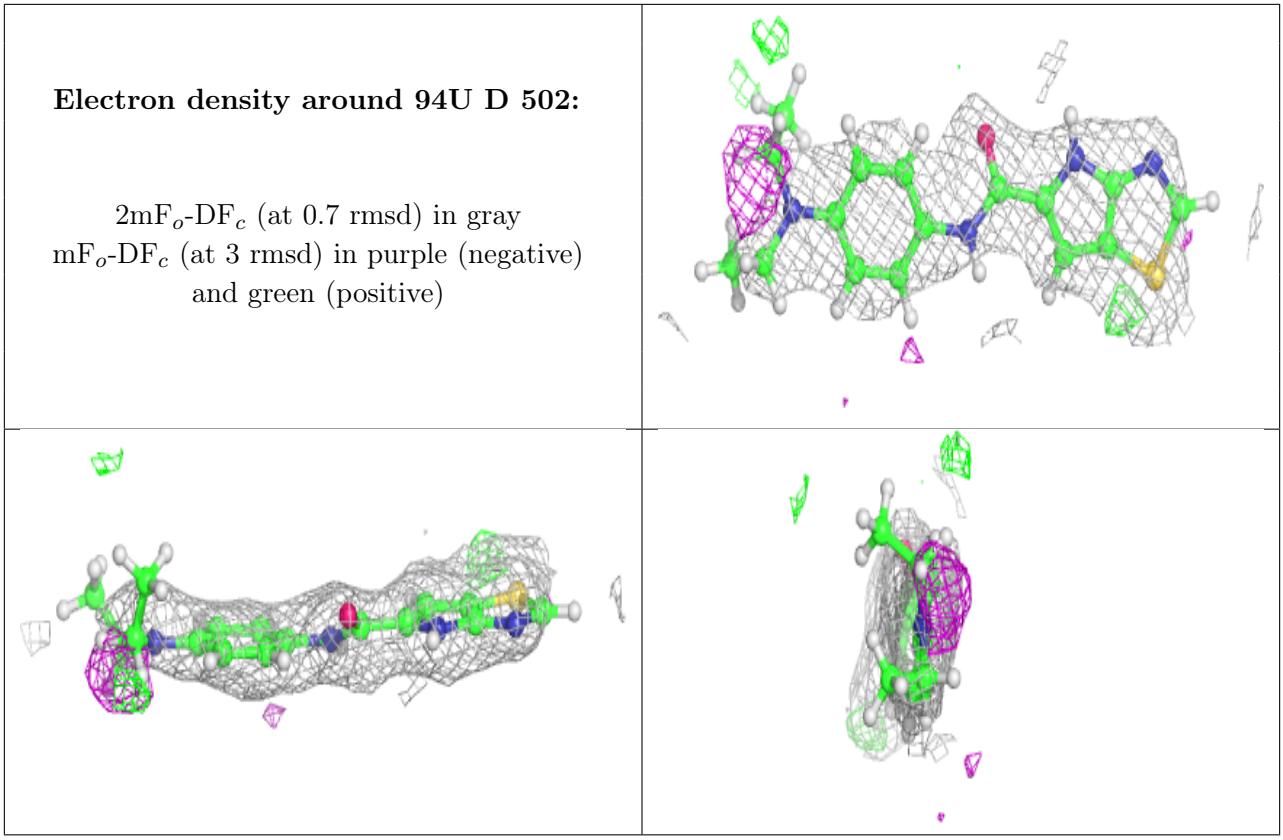
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	NA	B	505	1/1	0.78	0.18	55,55,55,55	0
13	CL	D	504	1/1	0.79	0.26	43,43,43,43	0
6	MG	D	503	1/1	0.88	0.06	57,57,57,57	0
11	94U	D	502	22/22	0.89	0.28	39,50,63,73	0
14	ACP	F	401	31/31	0.91	0.20	48,59,85,98	0
11	94U	B	504	22/22	0.93	0.22	28,36,54,54	0
8	GOL	A	504	6/6	0.94	0.17	42,55,58,67	0
6	MG	A	502	1/1	0.94	0.22	21,21,21,21	0
6	MG	B	502	1/1	0.95	0.18	27,27,27,27	0
5	GTP	D	501	32/32	0.95	0.14	40,50,61,65	0
10	MES	B	503	12/12	0.96	0.16	28,35,47,48	0
7	CA	A	503	1/1	0.96	0.06	50,50,50,50	0
9	GDP	B	501	28/28	0.97	0.23	21,26,36,40	0
7	CA	C	503	1/1	0.98	0.07	37,37,37,37	0
5	GTP	C	501	32/32	0.98	0.17	14,22,28,33	0
5	GTP	A	501	32/32	0.98	0.22	18,27,34,40	0
6	MG	C	502	1/1	0.99	0.21	22,22,22,22	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.

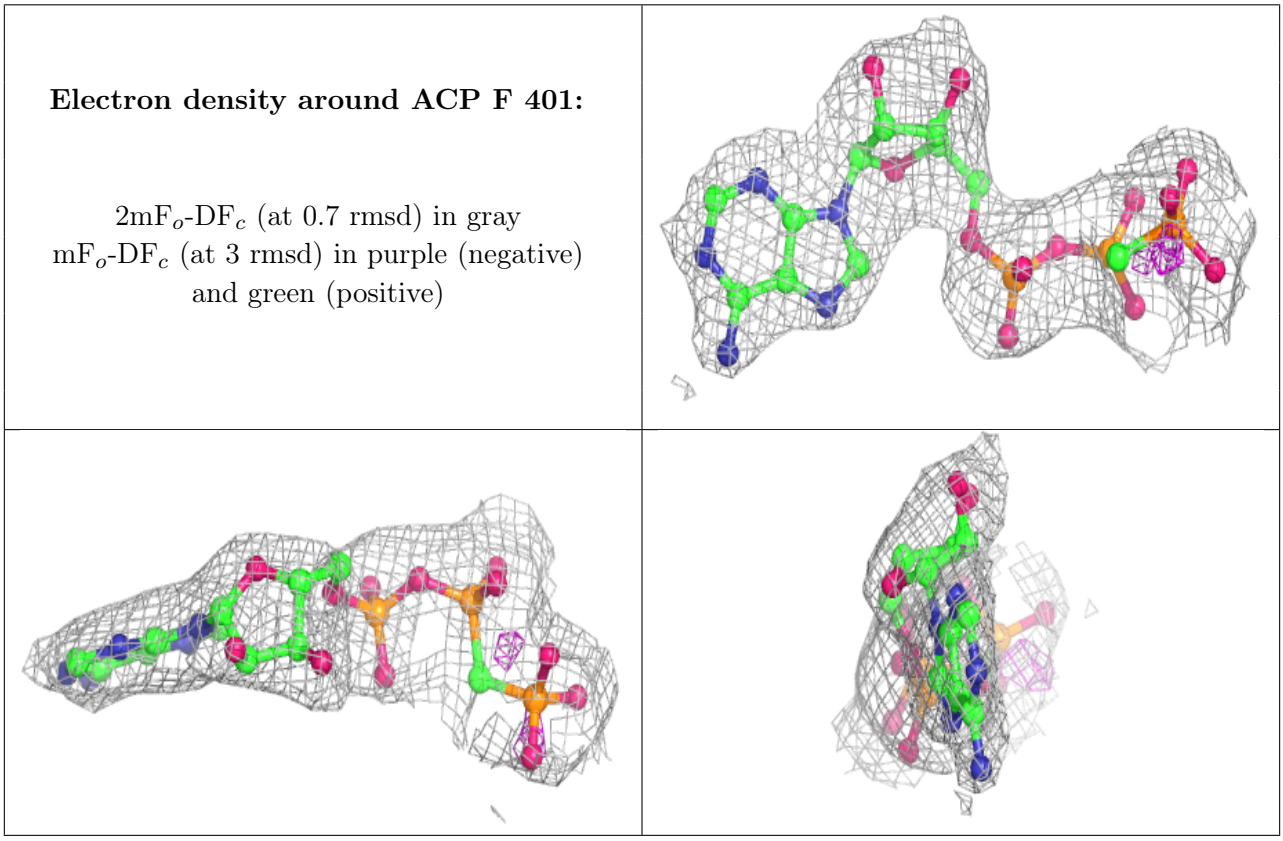
Electron density around 94U D 502:

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



Electron density around 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 94U B 504:

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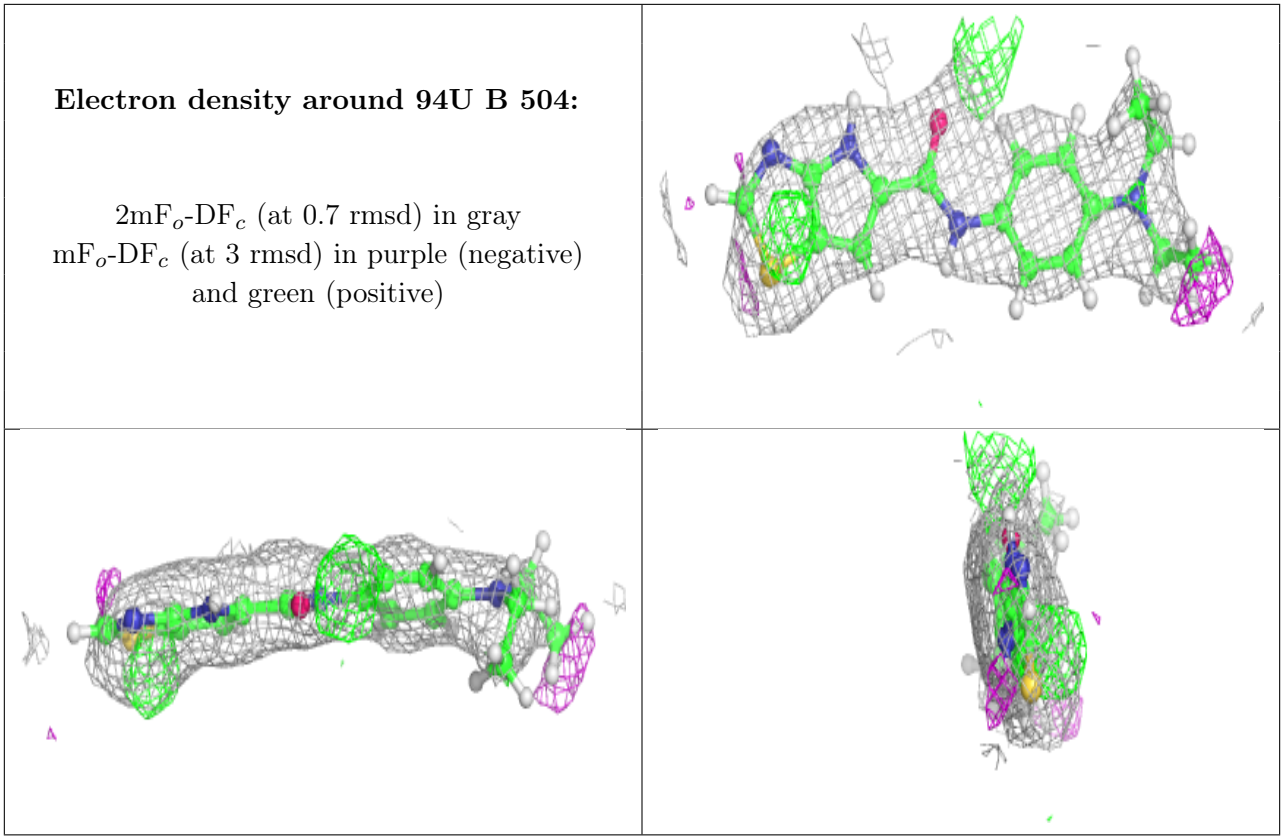
and green (positive)



Electron density around GTP D 501:

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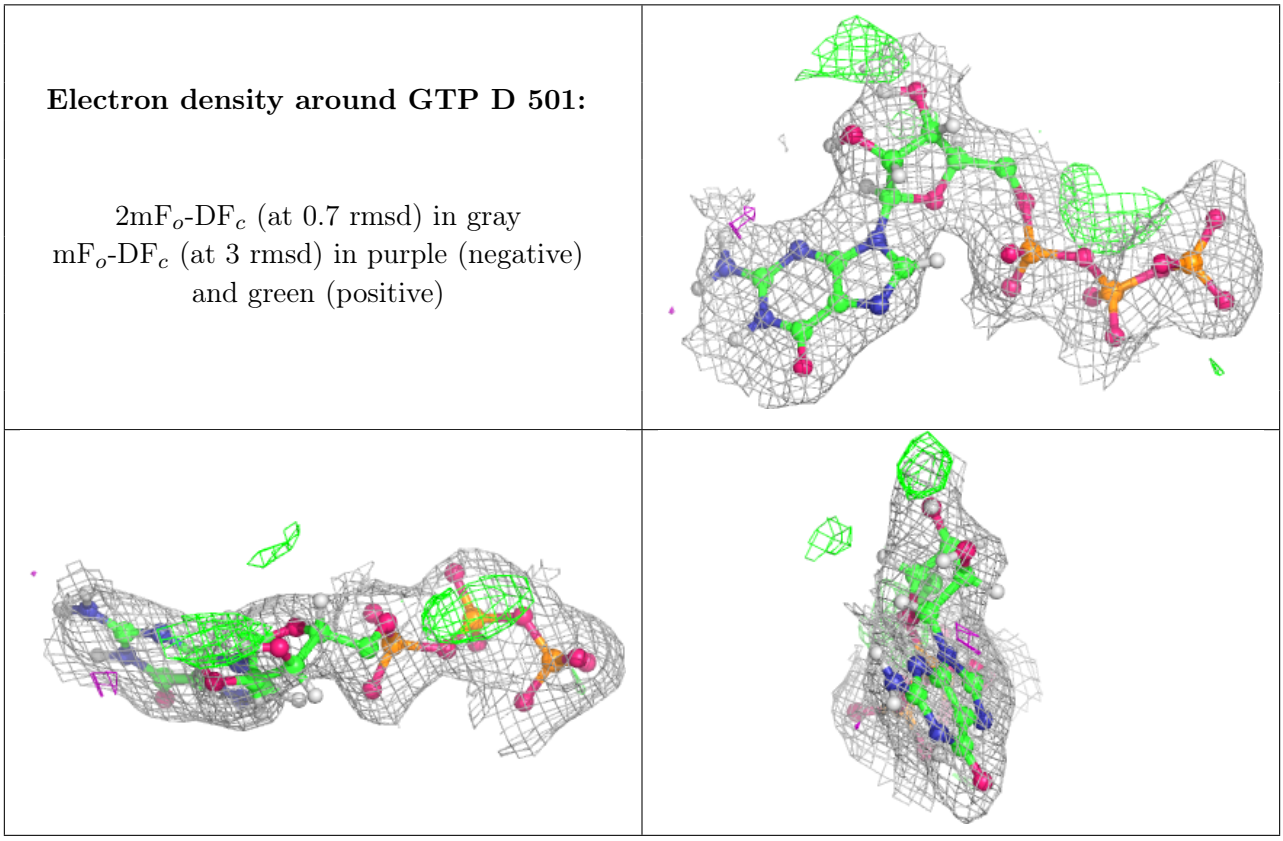
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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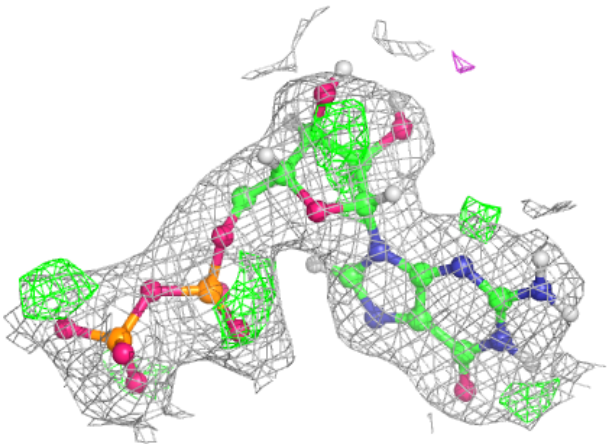
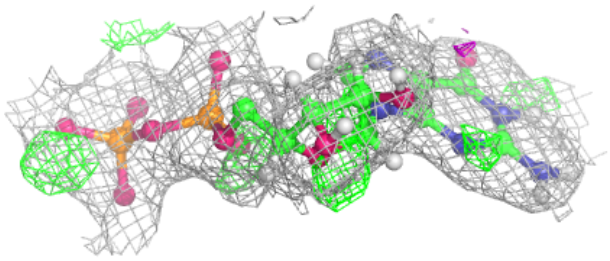
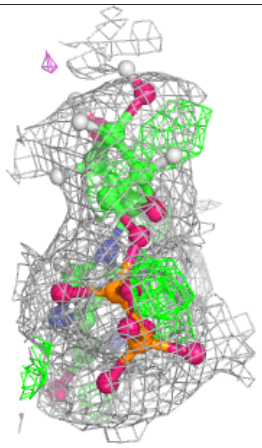
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

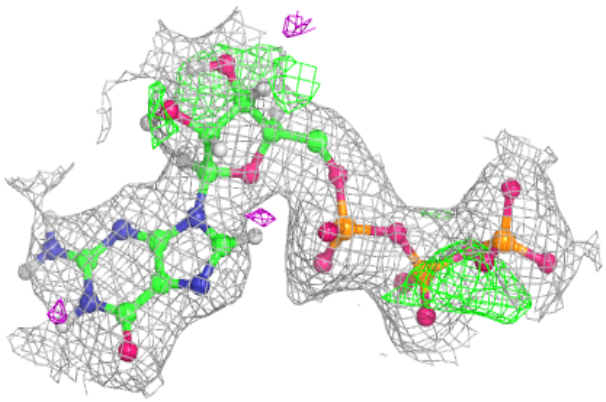


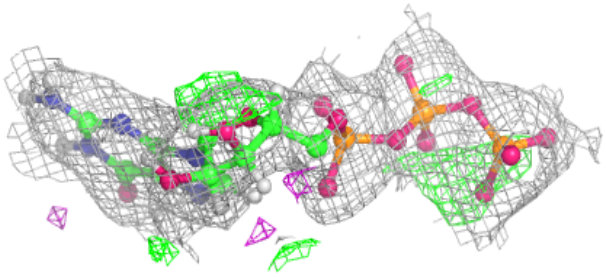


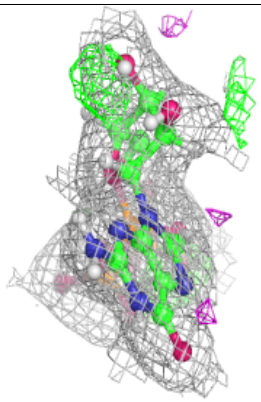


Electron density around GTP C 501:

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

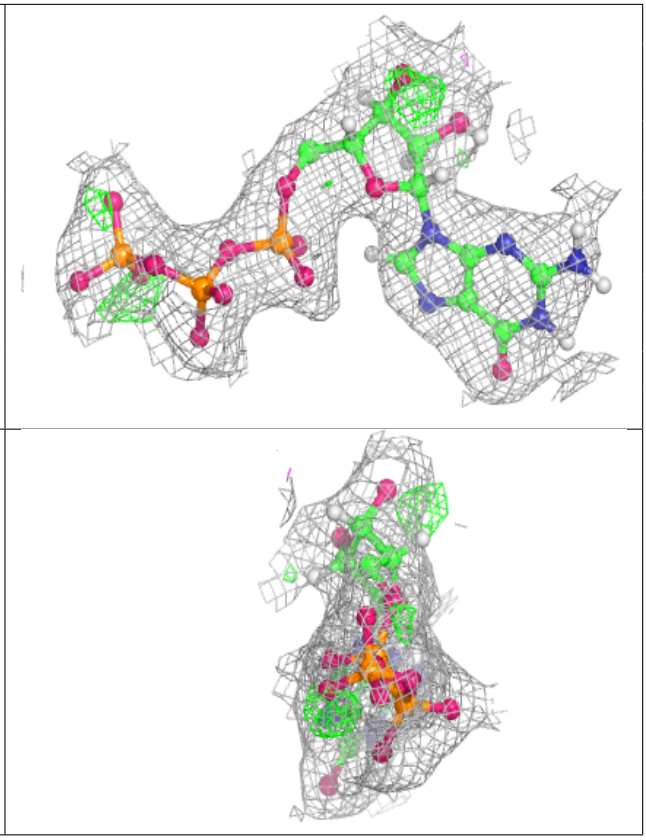






Electron density around GTP A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.