



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:28 AM UTC

PDB ID : 7E4R / pdb_00007e4r
Title : Crystal structure of tubulin in complex with D-DM1-SMe
Authors : Wang, Y.; Li, W.
Deposited on : 2021-02-15
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

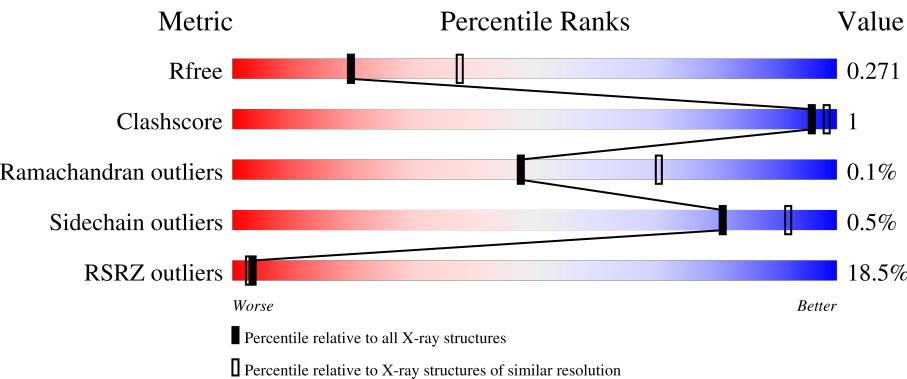
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	440	6% 97% ..
1	C	440	3% 99% .
2	B	431	12% 96% ..
2	D	431	30% 93% ..
3	E	138	21% 87% . 12%

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Mol	Chain	Length	Quality of chain
4	F	380	41% 82% 6% 12%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 34660 atoms, of which 16846 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6734	2163	3318	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6583	2110	3222	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2014	617	1014	181	197	5			

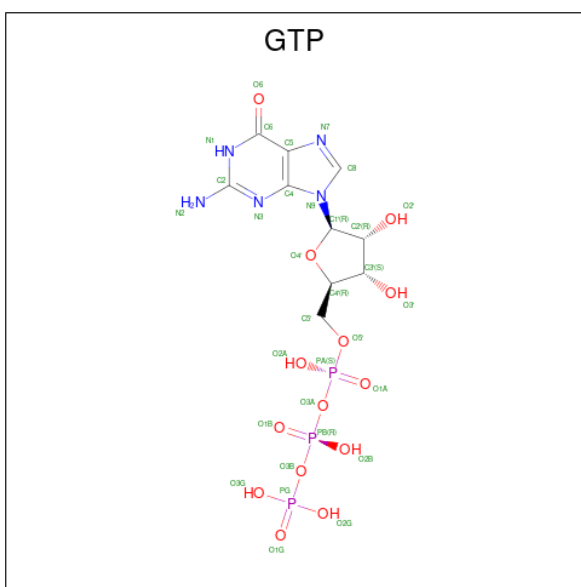
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	0	0
			5442	1761	2698	470	499	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

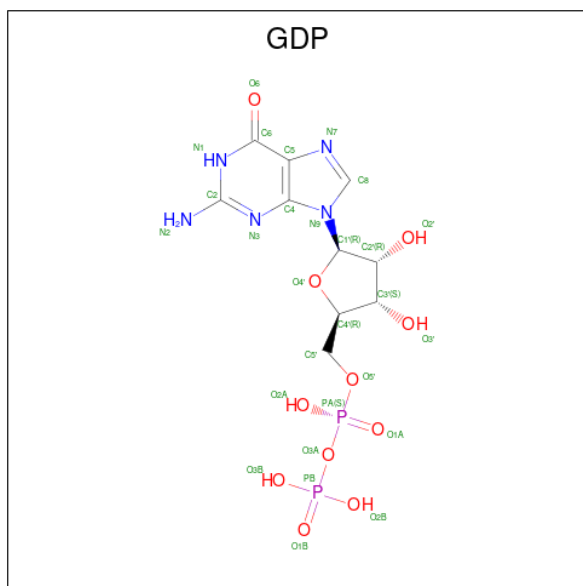
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

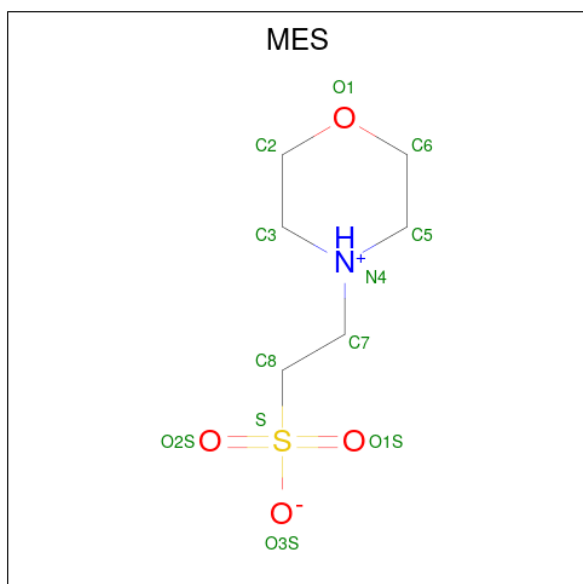
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca		
			1	1	0	0
7	C	1	Total	Ca		
			1	1	0	0

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



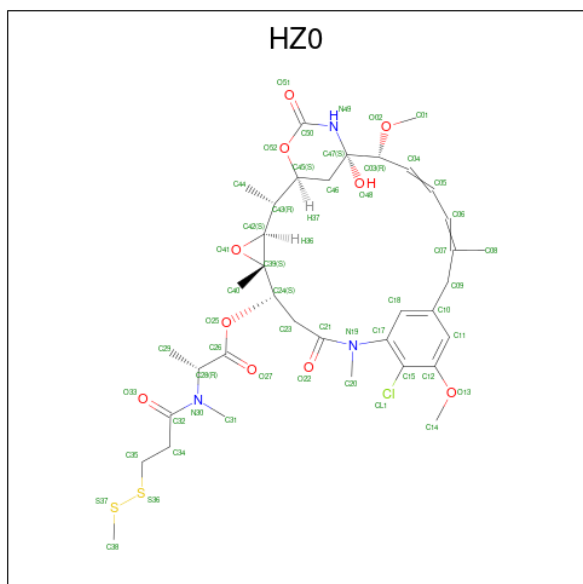
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

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



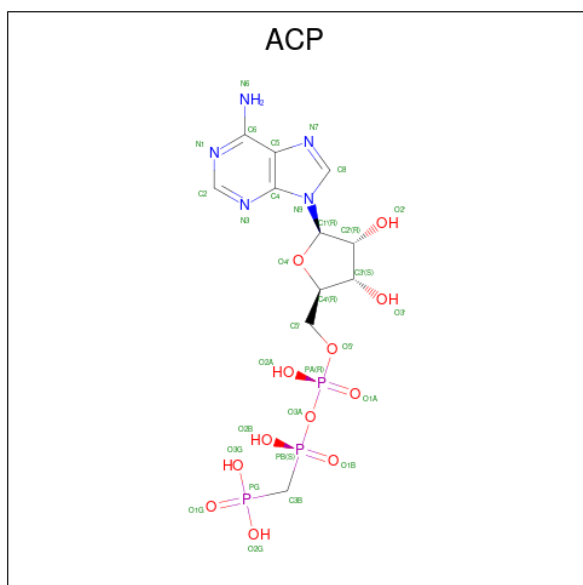
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 10 is (10E,12E)-86-chloro-14-hydroxy-85,14-dimethoxy-33,2,7,10-tetramethyl-12,6-dioxo-7-aza-1(6,4)-oxazinana-3(2,3)-oxirana-8(1,3)-benzenacyclotetradecaphane-10,12-dien-4-yl N-methyl-N-(3-(methylsulfinothioyl)propanoyl)-D-alaninate (CCD ID: HZ0) (formula: $C_{36}H_{50}ClN_3O_{10}S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	D	1	Total	C	Cl	H	N	O	S	0	0
			66	36	1	14	3	10	2		

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



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

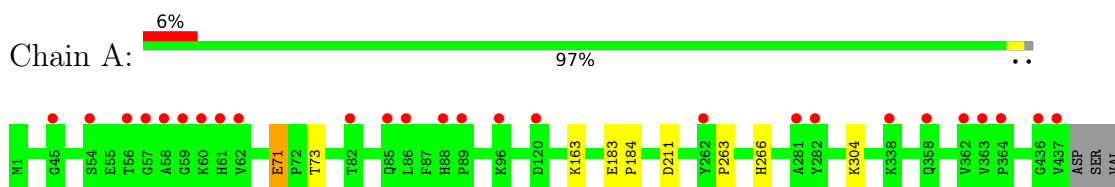
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	58	Total	O	0	0
			58	58		
12	B	68	Total	O	0	0
			68	68		
12	C	113	Total	O	0	0
			113	113		
12	D	31	Total	O	0	0
			31	31		
12	E	14	Total	O	0	0
			14	14		
12	F	38	Total	O	0	0
			38	38		

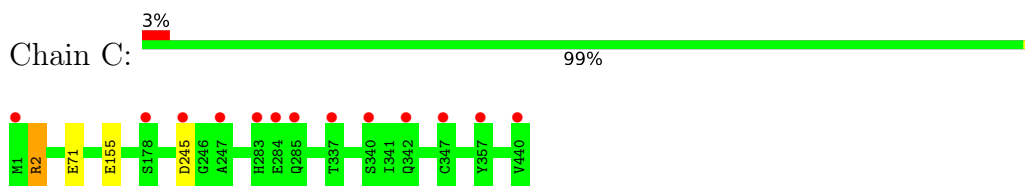
3 Residue-property plots [i](#)

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

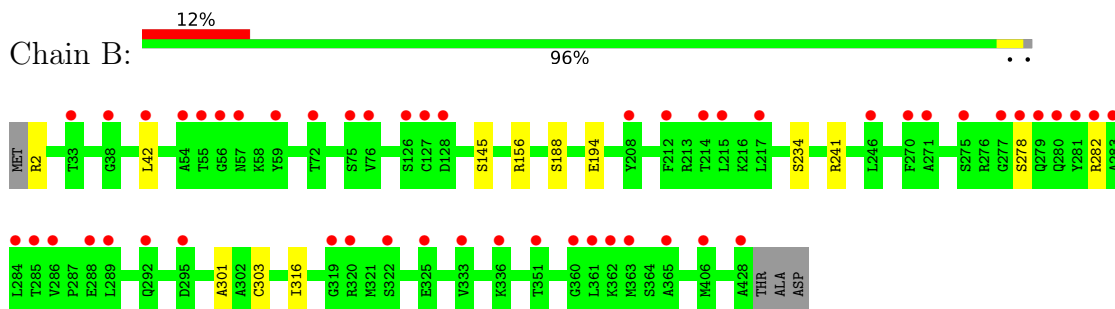
- Molecule 1: Tubulin alpha-1B chain



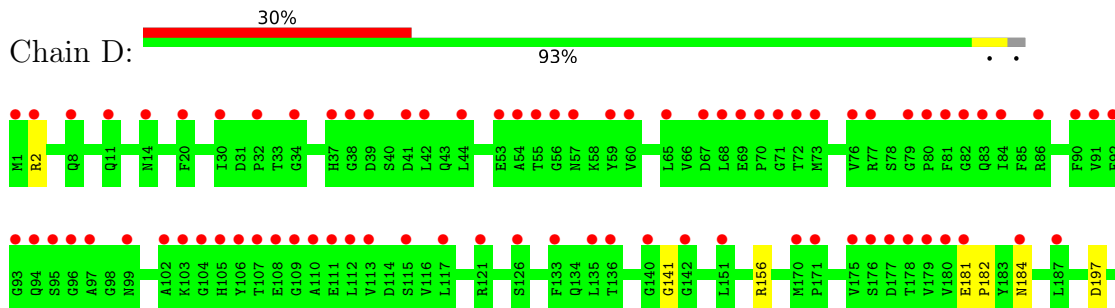
- Molecule 1: Tubulin alpha-1B chain

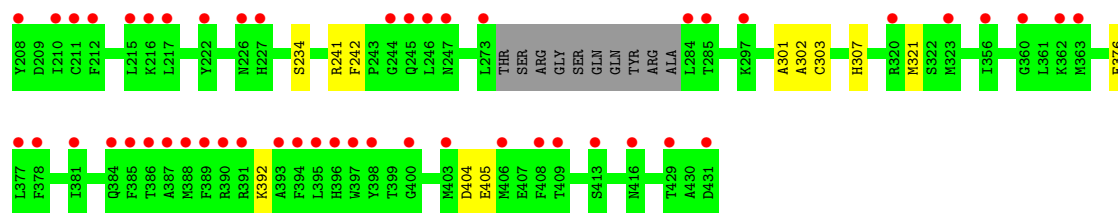


- Molecule 2: Tubulin beta-2B chain

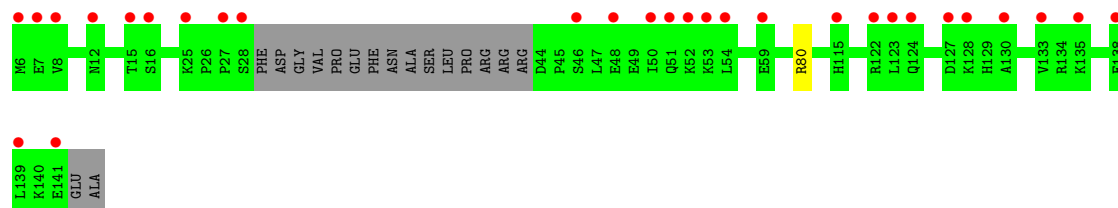
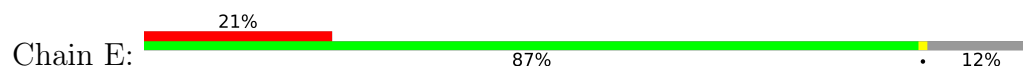


- Molecule 2: Tubulin beta-2B chain

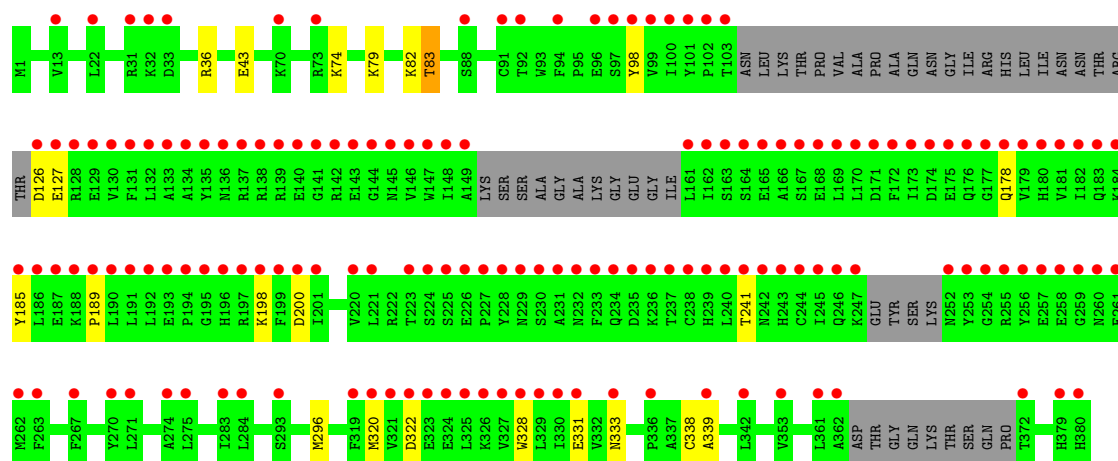
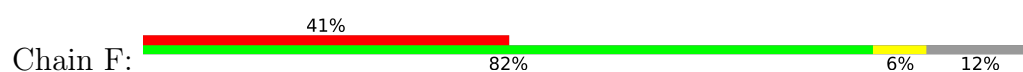




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.98Å 157.23Å 182.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 2.60 45.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.45-2.60) 97.8 (45.45-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.224 , 0.265 0.229 , 0.271	Depositor DCC
R_{free} test set	1465 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34660	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HZ0, GTP, GDP, ACP, MES, CA, 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	0.30	0/3494	0.62	0/4743
1	C	0.29	0/3515	0.61	0/4772
2	B	0.29	0/3436	0.60	0/4654
2	D	0.28	0/3382	0.59	0/4581
3	E	0.27	0/1008	0.57	0/1337
4	F	0.25	0/2806	0.57	0/3791
All	All	0.28	0/17641	0.60	0/23878

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3318	3330	5	0
1	C	3437	3335	3348	2	0
2	B	3361	3222	3238	6	0
2	D	3309	3179	3189	9	0
3	E	1000	1014	1018	1	0
4	F	2744	2698	2709	13	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	B	28	10	12	0	0
9	B	12	12	12	1	0
10	D	52	14	0	1	0
11	F	31	14	14	1	0
12	A	58	0	0	1	0
12	B	68	0	0	3	0
12	C	113	0	0	1	0
12	D	31	0	0	2	0
12	E	14	0	0	1	0
12	F	38	0	0	1	0
All	All	17814	16846	16906	38	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (38) 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)
2:B:2:ARG:N	12:B:603:HOH:O	2.28	0.66
4:F:79:LYS:O	4:F:83:THR:OG1	2.15	0.65
4:F:333:ASN:ND2	11:F:401:ACP:O1G	2.33	0.62
9:B:503:MES:O2S	12:B:601:HOH:O	2.15	0.62
1:C:155:GLU:OE1	12:C:601:HOH:O	2.17	0.59
1:A:163:LYS:NZ	12:A:601:HOH:O	2.35	0.59
2:D:404:ASP:OD1	2:D:405:GLU:N	2.35	0.59
4:F:178:GLN:N	4:F:178:GLN:OE1	2.37	0.58
3:E:80:ARG:NH1	12:E:203:HOH:O	2.36	0.58
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.18	0.56
4:F:126:ASP:OD1	4:F:127:GLU:N	2.38	0.55
4:F:338:CYS:SG	4:F:339:ALA:N	2.80	0.55
2:D:2:ARG:NH1	12:D:611:HOH:O	2.41	0.53
4:F:36:ARG:NH2	12:F:506:HOH:O	2.43	0.51
2:B:282:ARG:NH2	12:B:611:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:SER:HG	2:B:188:SER:HG	1.59	0.51
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.45	0.50
2:D:301:ALA:O	2:D:303:CYS:N	2.45	0.49
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.35	0.48
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.38	0.48
1:A:71:GLU:OE1	1:A:73:THR:N	2.48	0.47
1:A:263:PRO:O	1:A:266:HIS:ND1	2.38	0.46
2:B:156:ARG:NH1	2:B:194:GLU:O	2.48	0.46
2:D:307:HIS:ND1	2:D:376:GLU:OE1	2.40	0.46
2:B:301:ALA:O	2:B:303:CYS:N	2.50	0.45
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.44	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.33	0.44
2:D:234:SER:O	2:D:241:ARG:NH2	2.51	0.44
2:D:141:GLY:O	2:D:184:ASN:ND2	2.51	0.43
2:B:234:SER:O	2:B:241:ARG:NH2	2.49	0.43
10:D:502:HZ0:C29	10:D:502:HZ0:C34	2.97	0.42
2:D:242:PHE:O	12:D:601:HOH:O	2.21	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
1:C:2:ARG:HA	1:C:2:ARG:HE	1.84	0.41
4:F:82:LYS:HZ2	4:F:98:TYR:HA	1.86	0.41
4:F:189:PRO:HA	4:F:322:ASP:HA	2.02	0.41
4:F:320:MET:O	4:F:328:TRP:N	2.47	0.41
4:F:43:GLU:OE2	4:F:43:GLU:N	2.52	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	435/440 (99%)	421 (97%)	14 (3%)	0	100	100
1	C	438/440 (100%)	429 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	425/431 (99%)	412 (97%)	12 (3%)	1 (0%)	43	66
2	D	417/431 (97%)	403 (97%)	13 (3%)	1 (0%)	43	66
3	E	117/138 (85%)	116 (99%)	1 (1%)	0	100	100
4	F	324/380 (85%)	310 (96%)	14 (4%)	0	100	100
All	All	2156/2260 (95%)	2091 (97%)	63 (3%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	302	ALA
2	B	278	SER

5.3.2 Protein sidechains ⓘ

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	368/371 (99%)	367 (100%)	1 (0%)	86	94
1	C	371/371 (100%)	368 (99%)	3 (1%)	73	88
2	B	369/372 (99%)	367 (100%)	2 (0%)	81	92
2	D	364/372 (98%)	362 (100%)	2 (0%)	81	92
3	E	109/123 (89%)	109 (100%)	0	100	100
4	F	301/338 (89%)	299 (99%)	2 (1%)	76	89
All	All	1882/1947 (97%)	1872 (100%)	10 (0%)	81	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
2	B	42	LEU
2	B	316	ILE
1	C	2	ARG
1	C	71	GLU

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Mol	Chain	Res	Type
1	C	245	ASP
2	D	321	MET
2	D	392	LYS
4	F	83	THR
4	F	296	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	258	ASN
1	A	300	ASN
1	A	393	HIS
2	B	8	GLN
2	B	134	GLN
2	B	298	ASN
2	B	375	GLN
2	B	423	GLN
2	B	426	GLN
1	C	293	ASN
2	D	8	GLN
2	D	37	HIS
2	D	48	ASN
2	D	134	GLN
2	D	165	ASN
2	D	334	GLN
3	E	18	GLN
4	F	180	HIS
4	F	269	GLN
4	F	306	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
10	HZ0	D	502	-	53,55,55	2.26	13 (24%)	61,81,81	4.49	29 (47%)
5	GTP	A	501	6	33,34,34	0.98	1 (3%)	50,54,54	1.58	8 (16%)
5	GTP	D	501	6	33,34,34	0.85	1 (3%)	50,54,54	1.55	9 (18%)
9	MES	B	503	-	12,12,12	2.37	1 (8%)	15,16,16	2.24	5 (33%)
11	ACP	F	401	-	31,33,33	4.21	10 (32%)	47,52,52	1.65	10 (21%)
8	GDP	B	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.76	5 (11%)

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	-	9/22/38/38	0/3/3/3
10	HZ0	D	502	-	-	21/62/89/89	0/2/4/4
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
5	GTP	D	501	6	-	7/22/38/38	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	ACP	F	401	-	-	3/19/38/38	0/3/3/3
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	20.03	1.80	1.58
9	B	503	MES	C8-S	-7.97	1.66	1.77
10	D	502	HZ0	C32-N30	7.62	1.47	1.35
11	F	401	ACP	PA-O5'	7.54	1.88	1.59
10	D	502	HZ0	C21-N19	5.55	1.46	1.35
10	D	502	HZ0	O52-C45	-5.55	1.38	1.46
10	D	502	HZ0	O25-C26	4.31	1.44	1.34
10	D	502	HZ0	O25-C24	-4.14	1.39	1.46
11	F	401	ACP	C5'-C4'	3.92	1.63	1.51
10	D	502	HZ0	O41-C39	3.71	1.50	1.46
10	D	502	HZ0	C05-C06	3.68	1.54	1.43
10	D	502	HZ0	O13-C12	3.34	1.42	1.37
10	D	502	HZ0	C09-C07	3.20	1.55	1.52
11	F	401	ACP	O5'-C5'	-3.04	1.33	1.44
8	B	501	GDP	C5-C4	3.00	1.47	1.38
11	F	401	ACP	C8-N7	2.86	1.37	1.31
11	F	401	ACP	C2-N1	2.80	1.38	1.33
11	F	401	ACP	PA-O3A	-2.77	1.56	1.59
10	D	502	HZ0	C50-N49	2.71	1.40	1.34
10	D	502	HZ0	C09-C10	2.67	1.55	1.51
8	B	501	GDP	C6-N1	-2.67	1.33	1.38
11	F	401	ACP	C8-N9	2.62	1.42	1.37
10	D	502	HZ0	C46-C45	2.56	1.57	1.52
11	F	401	ACP	C4-N3	2.49	1.39	1.34
10	D	502	HZ0	C17-N19	2.34	1.47	1.44
11	F	401	ACP	C5-C4	2.28	1.43	1.39
5	C	501	GTP	PA-O3A	2.26	1.61	1.59
5	A	501	GTP	C2-N3	2.16	1.38	1.33
5	C	501	GTP	C2-N3	2.14	1.38	1.33
5	D	501	GTP	C2-N3	2.06	1.38	1.33

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	HZ0	O41-C39-C40	-20.95	84.63	114.12
10	D	502	HZ0	C40-C39-C24	-10.63	86.76	114.62
10	D	502	HZ0	O48-C47-N49	-9.74	86.33	110.45
10	D	502	HZ0	O41-C39-C24	8.88	132.43	114.62
10	D	502	HZ0	O41-C42-C43	-8.47	107.26	117.41
10	D	502	HZ0	O48-C47-C46	-7.99	87.76	109.98
10	D	502	HZ0	C05-C06-C07	-5.91	119.38	127.69
10	D	502	HZ0	O13-C12-C15	5.88	121.89	115.44
8	B	501	GDP	C5-C4-N3	-5.83	119.12	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	HZ0	C24-O25-C26	-5.74	108.18	118.20
9	B	503	MES	C5-N4-C3	5.72	121.16	108.84
10	D	502	HZ0	O25-C24-C39	5.23	117.29	105.48
10	D	502	HZ0	C18-C17-C15	-5.14	116.31	122.54
5	A	501	GTP	C5-C4-N3	-5.05	120.35	128.39
5	D	501	GTP	C5-C4-N3	-5.02	120.40	128.39
5	C	501	GTP	C5-C4-N3	-4.96	120.49	128.39
11	F	401	ACP	O2A-PA-O3A	4.91	120.54	107.27
8	B	501	GDP	C2-N3-C4	4.90	120.74	112.30
10	D	502	HZ0	C40-C39-C42	4.84	131.76	121.17
5	C	501	GTP	C2-N3-C4	4.61	120.23	112.30
5	A	501	GTP	C2-N3-C4	4.59	120.20	112.30
5	D	501	GTP	C2-N3-C4	4.47	119.99	112.30
8	B	501	GDP	N9-C4-N3	4.45	134.85	125.95
10	D	502	HZ0	O25-C26-C28	4.42	119.85	110.82
11	F	401	ACP	O1B-PB-C3B	3.99	119.57	109.05
11	F	401	ACP	O5'-PA-O1A	-3.86	93.64	108.94
10	D	502	HZ0	C08-C07-C09	3.75	118.67	115.53
10	D	502	HZ0	C34-C32-N30	3.68	125.39	119.14
9	B	503	MES	C7-N4-C5	3.68	121.05	111.24
10	D	502	HZ0	O25-C26-O27	-3.53	117.58	123.95
8	B	501	GDP	C6-C5-N7	3.37	136.43	130.29
5	A	501	GTP	N9-C4-N3	3.26	132.47	125.95
10	D	502	HZ0	C31-N30-C32	-3.21	115.01	122.16
5	C	501	GTP	N9-C4-N3	3.15	132.26	125.95
10	D	502	HZ0	C20-N19-C17	3.14	121.15	116.74
5	D	501	GTP	N9-C4-N3	3.04	132.03	125.95
5	D	501	GTP	C2-N1-C6	-3.02	119.62	125.11
10	D	502	HZ0	O13-C12-C11	-3.02	118.87	124.08
11	F	401	ACP	PB-O3A-PA	-2.97	122.67	132.37
5	A	501	GTP	C2-N1-C6	-2.86	119.92	125.11
10	D	502	HZ0	C17-C18-C10	2.84	124.71	120.28
5	C	501	GTP	C2-N1-C6	-2.78	120.07	125.11
10	D	502	HZ0	C29-C28-N30	2.72	116.65	112.02
5	C	501	GTP	N9-C8-N7	-2.67	108.45	113.40
10	D	502	HZ0	O33-C32-N30	-2.67	117.45	121.92
5	A	501	GTP	N9-C8-N7	-2.66	108.46	113.40
9	B	503	MES	C6-C5-N4	-2.65	106.09	110.12
10	D	502	HZ0	C44-C43-C45	-2.60	107.60	111.39
5	C	501	GTP	C8-N7-C5	2.57	108.84	104.26
11	F	401	ACP	O2A-PA-O5'	-2.56	95.96	107.57
5	D	501	GTP	N9-C8-N7	-2.56	108.66	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	HZ0	O41-C42-C39	2.55	61.54	59.82
5	A	501	GTP	C8-N7-C5	2.54	108.79	104.26
5	D	501	GTP	C8-N7-C5	2.53	108.76	104.26
10	D	502	HZ0	C45-C43-C42	2.52	117.67	111.19
11	F	401	ACP	C5-C4-N3	-2.47	123.32	126.72
8	B	501	GDP	C4-C5-N7	-2.46	106.77	110.67
10	D	502	HZ0	C14-O13-C12	-2.46	113.91	117.51
5	A	501	GTP	C5-C6-N1	2.45	119.49	113.25
5	C	501	GTP	C5-C6-N1	2.45	119.49	113.25
10	D	502	HZ0	O25-C24-C23	2.45	109.82	105.09
5	D	501	GTP	C5-C6-N1	2.39	119.33	113.25
5	C	501	GTP	O6-C6-C5	-2.37	120.28	126.53
5	A	501	GTP	O6-C6-C5	-2.37	120.29	126.53
11	F	401	ACP	O1G-PG-C3B	-2.30	106.36	111.37
10	D	502	HZ0	O41-C39-C42	-2.17	58.00	59.38
5	D	501	GTP	O6-C6-C5	-2.16	120.82	126.53
10	D	502	HZ0	C44-C43-C42	-2.14	107.73	112.42
11	F	401	ACP	O2B-PB-C3B	2.09	115.40	106.73
5	D	501	GTP	O2B-PB-O3A	2.08	112.90	107.27
11	F	401	ACP	O2B-PB-O1B	2.04	116.59	109.95
9	B	503	MES	O2S-S-C8	2.04	109.81	106.73
11	F	401	ACP	O3'-C3'-C4'	2.03	116.91	111.08
9	B	503	MES	C7-N4-C3	2.01	116.59	111.24

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
10	D	502	HZ0	C23-C24-C39-C42
10	D	502	HZ0	O25-C26-C28-N30

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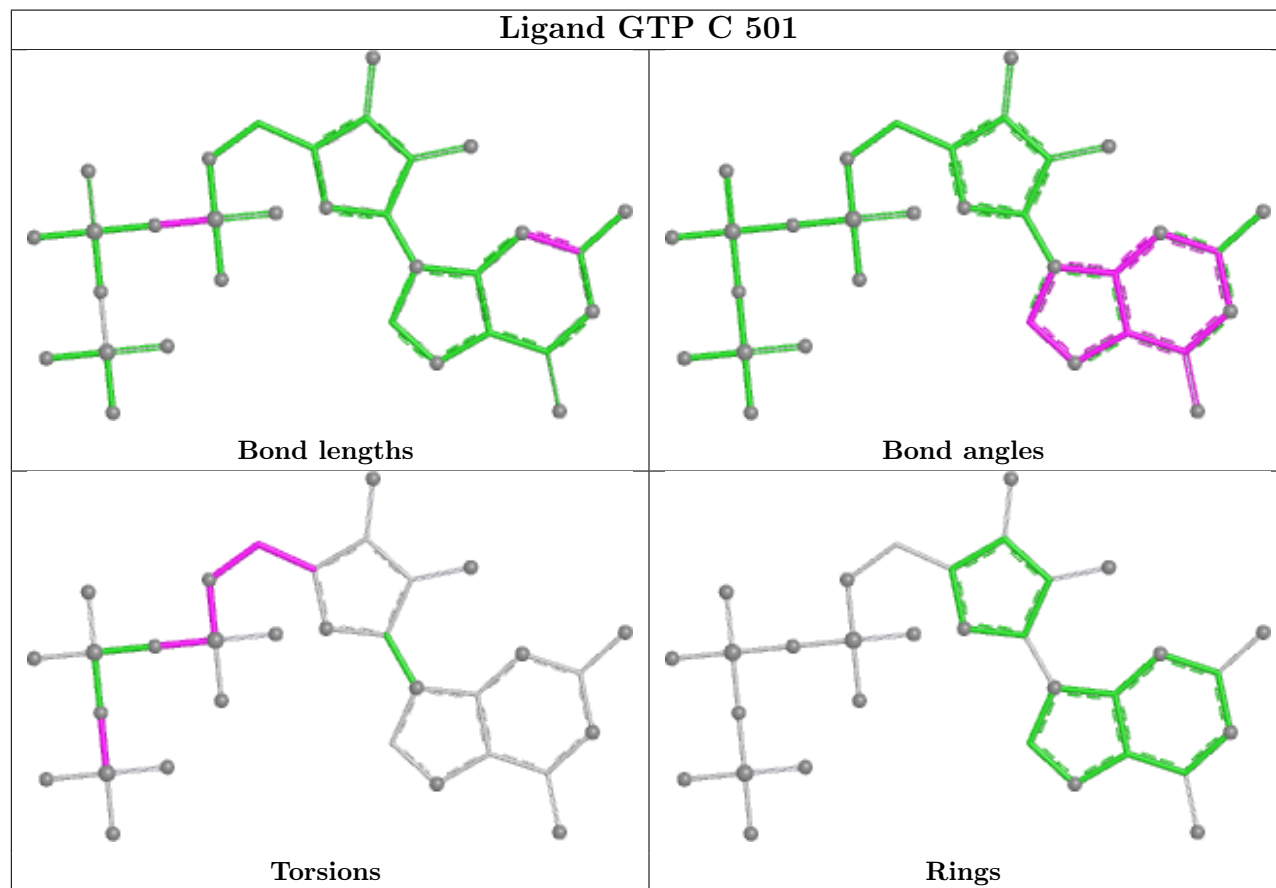
Mol	Chain	Res	Type	Atoms
10	D	502	HZ0	O27-C26-C28-N30
10	D	502	HZ0	C29-C28-N30-C31
10	D	502	HZ0	C29-C28-N30-C32
10	D	502	HZ0	C04-C03-O02-C01
10	D	502	HZ0	O02-C03-C47-C46
10	D	502	HZ0	C03-C04-C05-C06
10	D	502	HZ0	C05-C06-C07-C08
10	D	502	HZ0	C05-C06-C07-C09
10	D	502	HZ0	C15-C12-O13-C14
10	D	502	HZ0	C32-C34-C35-S36
10	D	502	HZ0	C44-C43-C45-C46
10	D	502	HZ0	C04-C05-C06-C07
10	D	502	HZ0	O27-C26-O25-C24
10	D	502	HZ0	C28-C26-O25-C24
10	D	502	HZ0	C11-C12-O13-C14
5	A	501	GTP	C3'-C4'-C5'-O5'
10	D	502	HZ0	C44-C43-C45-O52
5	A	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
11	F	401	ACP	PG-C3B-PB-O2B
10	D	502	HZ0	O25-C26-C28-C29
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
10	D	502	HZ0	O33-C32-C34-C35
11	F	401	ACP	PB-O3A-PA-O2A
10	D	502	HZ0	N30-C32-C34-C35
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	PB-O3B-PG-O2G
8	B	501	GDP	PA-O3A-PB-O3B
5	D	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	D	501	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

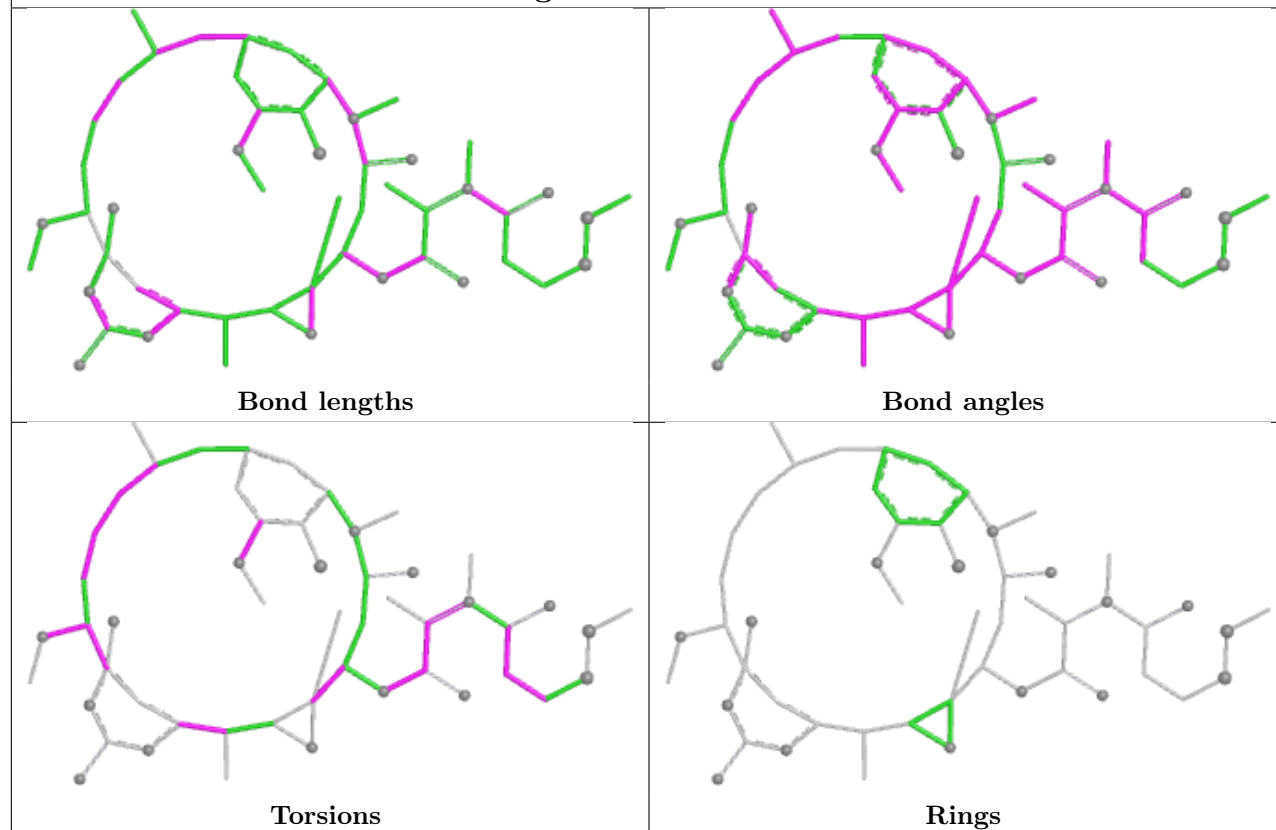
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	HZ0	1	0
9	B	503	MES	1	0
11	F	401	ACP	1	0

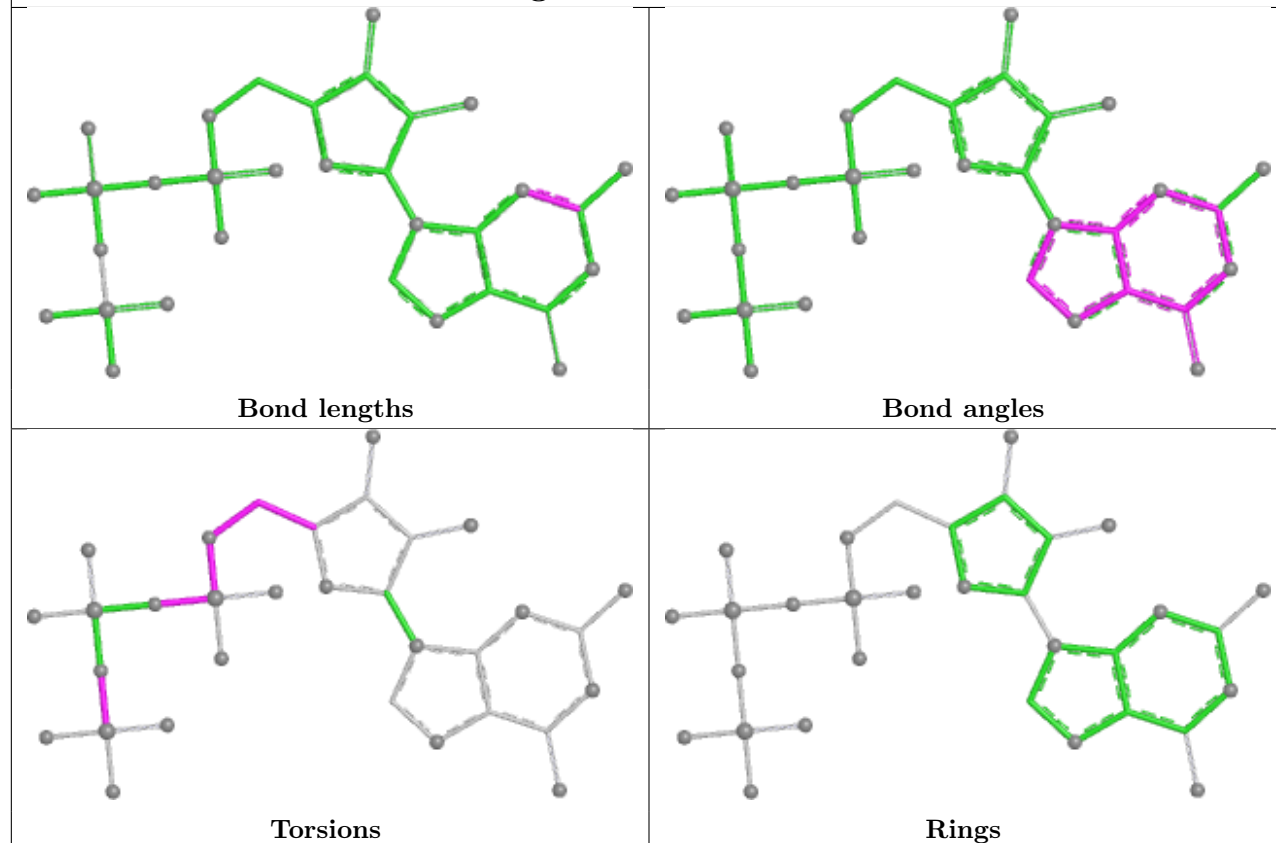
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

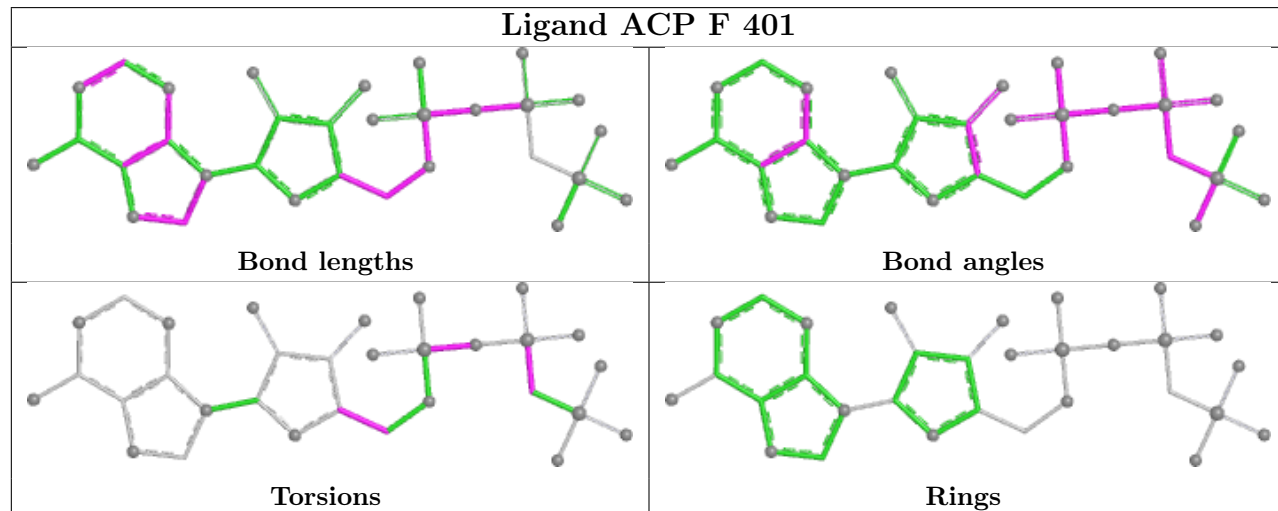
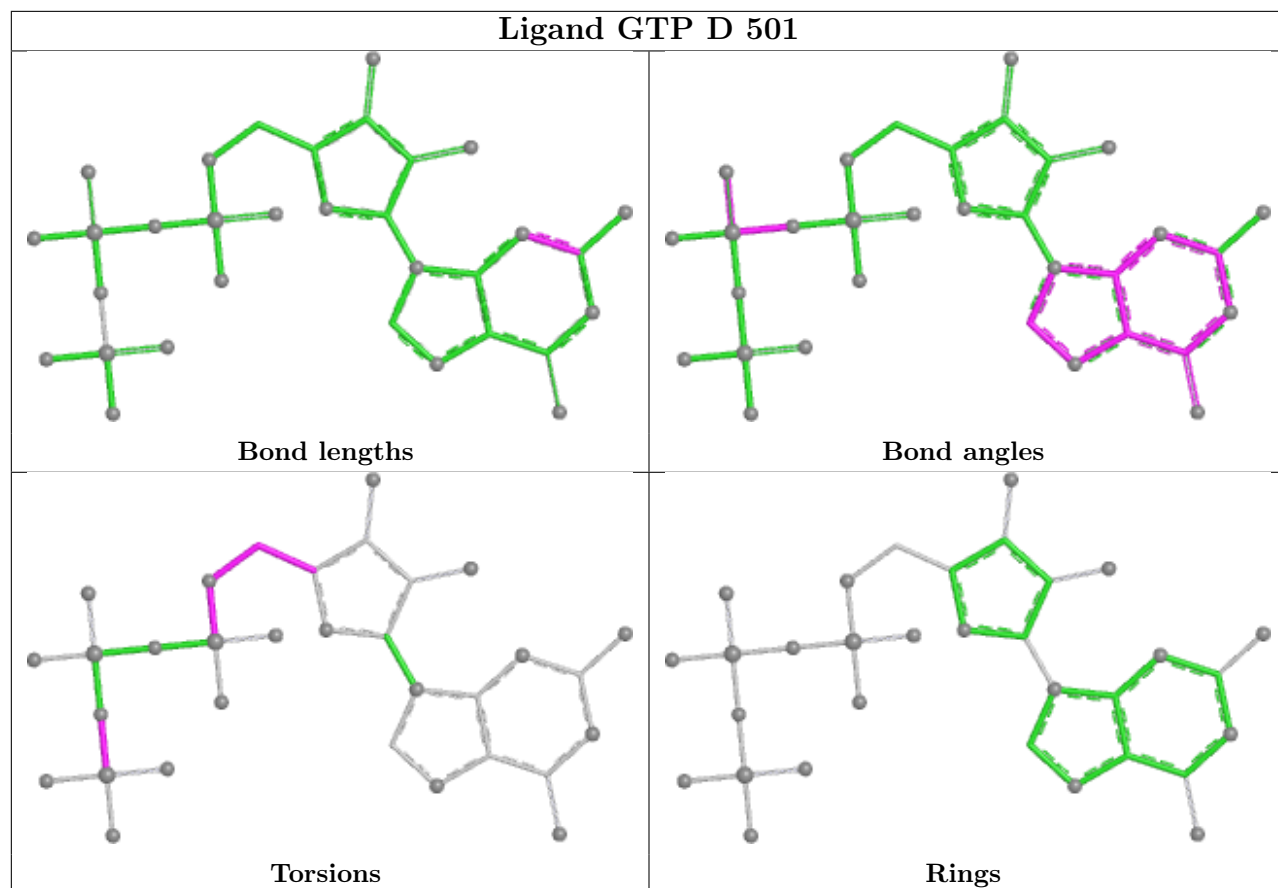


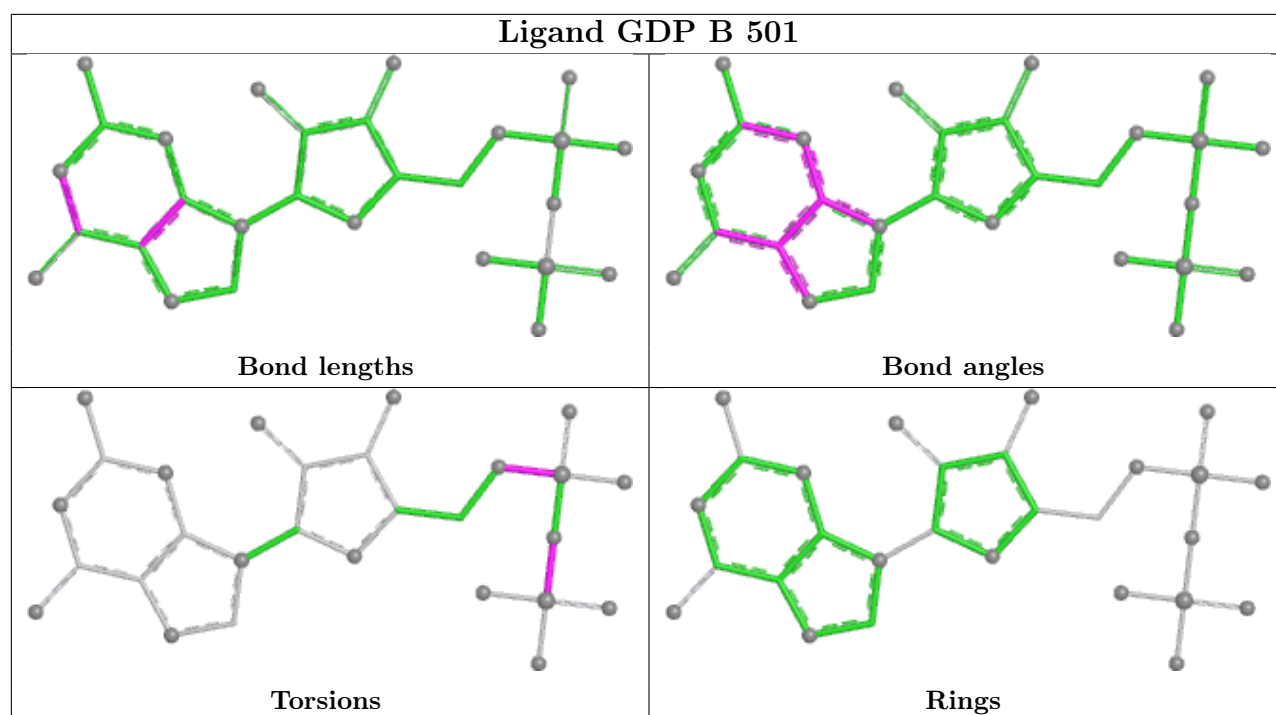
Ligand HZ0 D 502



Ligand GTP A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	437/440 (99%)	0.48	26 (5%)	28 23	23, 44, 78, 98	0
1	C	440/440 (100%)	-0.00	13 (2%)	52 47	17, 34, 65, 89	0
2	B	427/431 (99%)	0.65	51 (11%)	9 7	21, 44, 81, 138	0
2	D	421/431 (97%)	1.47	131 (31%)	1 1	32, 64, 102, 137	0
3	E	121/138 (87%)	1.18	29 (23%)	2 1	33, 61, 101, 112	0
4	F	334/380 (87%)	1.96	154 (46%)	0 0	35, 74, 150, 167	0
All	All	2180/2260 (96%)	0.87	404 (18%)	3 3	17, 51, 112, 167	0

All (404) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	7.3
2	D	92	PHE	6.1
4	F	186	LEU	5.8
4	F	103	THR	5.5
4	F	149	ALA	5.4
4	F	131	PHE	5.4
2	D	180	VAL	5.4
4	F	196	HIS	5.3
4	F	182	ILE	5.3
2	D	55	THR	5.2
4	F	148	ILE	5.1
4	F	184	LYS	5.1
4	F	320	MET	5.0
2	D	112	LEU	5.0
4	F	162	ILE	4.9
4	F	237	THR	4.9
4	F	191	LEU	4.9
4	F	161	LEU	4.8
4	F	100	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	4.7
4	F	133	ALA	4.7
2	D	69	GLU	4.7
4	F	181	VAL	4.7
4	F	233	PHE	4.7
2	D	93	GLY	4.6
4	F	192	LEU	4.5
4	F	223	THR	4.5
4	F	236	LYS	4.5
2	D	170	MET	4.5
4	F	240	LEU	4.5
4	F	130	VAL	4.5
2	D	108	GLU	4.4
2	B	55	THR	4.4
2	D	245	GLN	4.4
4	F	147	TRP	4.4
4	F	231	ALA	4.4
2	D	362	LYS	4.4
4	F	173	ILE	4.3
4	F	146	VAL	4.3
4	F	228	TYR	4.3
2	D	246	LEU	4.3
4	F	144	GLY	4.2
4	F	170	LEU	4.2
4	F	135	TYR	4.2
4	F	185	TYR	4.2
4	F	180	HIS	4.2
4	F	243	HIS	4.2
4	F	132	LEU	4.2
4	F	172	PHE	4.2
2	D	176	SER	4.1
2	D	72	THR	4.1
4	F	199	PHE	4.1
2	B	280	GLN	4.1
4	F	245	ILE	4.1
4	F	244	CYS	4.0
4	F	98	TYR	4.0
4	F	253	TYR	4.0
4	F	247	LYS	3.9
4	F	254	GLY	3.9
2	D	96	GLY	3.9
4	F	177	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
4	F	230	SER	3.9
2	D	83	GLN	3.9
4	F	256	TYR	3.9
2	D	356	ILE	3.9
3	E	133	VAL	3.9
4	F	241	THR	3.9
4	F	232	ASN	3.8
2	D	179	VAL	3.8
2	D	73	MET	3.8
1	A	88	HIS	3.8
1	C	440	VAL	3.7
4	F	167	SER	3.7
1	C	340	SER	3.7
2	B	54	ALA	3.7
3	E	53	LYS	3.7
4	F	379	HIS	3.7
2	D	431	ASP	3.7
2	D	70	PRO	3.6
2	D	94	GLN	3.6
2	D	284	LEU	3.6
4	F	195	GLY	3.6
2	D	95	SER	3.6
3	E	139	LEU	3.6
2	D	106	TYR	3.5
4	F	189	PRO	3.5
2	D	175	VAL	3.5
4	F	372	THR	3.5
2	D	107	THR	3.5
4	F	99	VAL	3.5
4	F	225	SER	3.5
1	C	357	TYR	3.4
2	D	54	ALA	3.4
4	F	163	SER	3.4
4	F	319	PHE	3.4
2	D	67	ASP	3.4
2	D	121	ARG	3.4
4	F	102	PRO	3.4
2	D	211	CYS	3.3
2	B	246	LEU	3.3
4	F	190	LEU	3.3
4	F	142	ARG	3.3
4	F	201	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	362	LYS	3.3
4	F	188	LYS	3.3
2	B	281	TYR	3.3
2	B	284	LEU	3.3
4	F	138	ARG	3.3
2	D	178	THR	3.3
2	D	30	ILE	3.3
2	D	320	ARG	3.3
2	D	97	ALA	3.3
2	D	387	ALA	3.3
2	B	275	SER	3.2
4	F	139	ARG	3.2
1	C	337	THR	3.2
2	B	319	GLY	3.2
4	F	380	HIS	3.2
2	B	336	LYS	3.2
2	B	56	GLY	3.2
4	F	362	ALA	3.2
2	D	11	GLN	3.2
4	F	327	VAL	3.2
4	F	183	GLN	3.2
1	A	61	HIS	3.1
2	D	37	HIS	3.1
2	D	396	HIS	3.1
1	A	262	TYR	3.1
2	D	82	GLY	3.1
4	F	92	THR	3.1
4	F	255	ARG	3.1
4	F	193	GLU	3.1
2	D	388	MET	3.1
4	F	171	ASP	3.1
4	F	271	LEU	3.1
4	F	136	ASN	3.1
2	D	244	GLY	3.1
2	B	286	VAL	3.1
2	D	391	ARG	3.1
1	A	56	THR	3.1
4	F	330	ILE	3.1
3	E	130	ALA	3.1
3	E	6	MET	3.1
4	F	226	GLU	3.1
4	F	321	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	283	HIS	3.0
2	D	42	LEU	3.0
4	F	221	LEU	3.0
4	F	263	PHE	3.0
4	F	101	TYR	3.0
2	B	322	SER	3.0
2	B	57	ASN	3.0
4	F	229	ASN	3.0
4	F	246	GLN	3.0
2	D	1	MET	3.0
4	F	234	GLN	3.0
1	C	284	GLU	3.0
2	B	33	THR	3.0
2	D	363	MET	3.0
4	F	257	GLU	3.0
2	D	110	ALA	3.0
2	B	212	PHE	2.9
2	D	115	SER	2.9
4	F	164	SER	2.9
4	F	259	GLY	2.9
4	F	331	GLU	2.9
2	B	128	ASP	2.9
4	F	267	PHE	2.9
4	F	165	GLU	2.9
4	F	323	GLU	2.9
2	D	217	LEU	2.9
4	F	328	TRP	2.9
1	C	178	SER	2.8
2	B	42	LEU	2.8
4	F	22	LEU	2.8
2	D	323	MET	2.8
2	D	389	PHE	2.8
4	F	270	TYR	2.8
2	D	416	ASN	2.8
4	F	333	ASN	2.8
4	F	238	CYS	2.8
4	F	274	ALA	2.8
2	D	187	LEU	2.8
1	A	437	VAL	2.8
2	D	395	LEU	2.8
2	D	103	LYS	2.8
4	F	258	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	394	PHE	2.8
2	D	109	GLY	2.8
2	D	210	ILE	2.8
2	D	91	VAL	2.8
4	F	361	LEU	2.8
2	D	390	ARG	2.8
4	F	137	ARG	2.8
4	F	88	SER	2.7
2	D	76	VAL	2.7
4	F	325	LEU	2.7
1	A	338	LYS	2.7
1	A	85	GLN	2.7
2	B	277	GLY	2.7
1	A	54	SER	2.7
2	D	126	SER	2.7
4	F	179	VAL	2.7
4	F	126	ASP	2.7
4	F	200	ASP	2.7
1	A	282	TYR	2.7
1	C	1	MET	2.7
2	D	117	LEU	2.7
2	D	216	LYS	2.7
4	F	70	LYS	2.7
4	F	284	LEU	2.7
1	C	247	ALA	2.7
2	B	285	THR	2.7
2	B	292	GLN	2.7
4	F	239	HIS	2.7
2	B	295	ASP	2.7
4	F	336	PRO	2.7
2	B	282	ARG	2.7
2	D	377	LEU	2.7
4	F	275	LEU	2.7
2	D	222	TYR	2.7
3	E	124	GLN	2.7
1	A	60	LYS	2.6
4	F	94	PHE	2.6
4	F	31	ARG	2.6
4	F	242	ASN	2.6
4	F	97	SER	2.6
2	D	151	LEU	2.6
3	E	48	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	141	GLU	2.6
4	F	143	GLU	2.6
3	E	28	SER	2.6
2	B	283	ALA	2.6
2	B	428	ALA	2.6
4	F	198	LYS	2.6
4	F	227	PRO	2.6
4	F	91	CYS	2.6
4	F	129	GLU	2.6
4	F	324	GLU	2.6
2	B	333	VAL	2.6
4	F	197	ARG	2.6
2	B	76	VAL	2.6
1	A	58	ALA	2.6
4	F	224	SER	2.6
2	B	214	THR	2.6
2	D	32	PRO	2.5
4	F	187	GLU	2.5
4	F	261	GLU	2.5
4	F	252	ASN	2.5
2	D	177	ASP	2.5
2	D	381	ILE	2.5
2	B	217	LEU	2.5
2	D	102	ALA	2.5
2	D	403	MET	2.5
4	F	262	MET	2.5
3	E	59	GLU	2.5
1	C	342	GLN	2.5
3	E	8	VAL	2.5
4	F	145	ASN	2.5
2	B	320	ARG	2.5
2	D	406	MET	2.5
2	B	59	TYR	2.5
4	F	235	ASP	2.5
2	D	384	GLN	2.5
4	F	178	GLN	2.5
2	D	184	ASN	2.5
1	A	57	GLY	2.4
2	B	215	LEU	2.4
2	D	81	PHE	2.4
4	F	128	ARG	2.4
2	D	80	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	96	LYS	2.4
3	E	52	LYS	2.4
4	F	141	GLY	2.4
2	D	398	TYR	2.4
4	F	73	ARG	2.4
2	D	397	TRP	2.4
2	D	409	THR	2.4
3	E	15	THR	2.4
1	A	364	PRO	2.4
2	B	360	GLY	2.4
2	D	142	GLY	2.4
3	E	51	GLN	2.4
2	B	271	ALA	2.4
4	F	134	ALA	2.4
2	D	285	THR	2.4
1	A	436	GLY	2.4
2	D	360	GLY	2.4
1	C	285	GLN	2.4
2	B	279	GLN	2.4
4	F	13	VAL	2.4
2	D	226	ASN	2.4
3	E	115	HIS	2.3
1	C	347	CYS	2.3
4	F	326	LYS	2.3
4	F	96	GLU	2.3
2	D	413	SER	2.3
4	F	329	LEU	2.3
2	D	41	ASP	2.3
4	F	33	ASP	2.3
2	B	363	MET	2.3
2	D	393	ALA	2.3
2	D	400	GLY	2.3
2	D	84	ILE	2.3
4	F	283	ILE	2.3
3	E	135	LYS	2.3
2	B	127	CYS	2.3
4	F	127	GLU	2.3
1	A	45	GLY	2.3
2	B	278	SER	2.3
4	F	293	SER	2.3
1	A	86	LEU	2.3
2	D	65	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	68	LEU	2.3
2	D	53	GLU	2.3
2	D	90	PHE	2.3
1	A	281	ALA	2.2
2	B	208	TYR	2.3
2	D	208	TYR	2.3
1	A	358	GLN	2.2
2	D	44	LEU	2.2
2	D	135	LEU	2.2
4	F	32	LYS	2.2
2	D	378	PHE	2.2
2	D	60	VAL	2.2
3	E	27	PRO	2.2
4	F	260	ASN	2.2
2	B	72	THR	2.2
2	D	8	GLN	2.2
2	D	105	HIS	2.2
4	F	176	GLN	2.2
2	D	297	LYS	2.2
2	B	288	GLU	2.2
3	E	122	ARG	2.2
2	D	385	PHE	2.2
4	F	194	PRO	2.2
3	E	25	LYS	2.2
2	B	406	MET	2.2
3	E	16	SER	2.2
4	F	168	GLU	2.2
2	D	2	ARG	2.2
4	F	353	VAL	2.2
2	D	247	ASN	2.2
2	D	386	THR	2.2
2	B	289	LEU	2.2
2	D	38	GLY	2.2
2	D	56	GLY	2.2
2	D	59	TYR	2.2
2	D	71	GLY	2.2
3	E	46	SER	2.2
2	D	77	ARG	2.2
2	D	171	PRO	2.2
2	D	20	PHE	2.2
2	D	212	PHE	2.2
3	E	128	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	62	VAL	2.1
1	A	362	VAL	2.1
4	F	220	VAL	2.1
2	B	365	ALA	2.1
2	D	34	GLY	2.1
2	D	273	LEU	2.1
1	A	120	ASP	2.1
4	F	174	ASP	2.1
4	F	322	ASP	2.1
2	D	408	PHE	2.1
2	D	113	VAL	2.1
4	F	339	ALA	2.1
1	A	82	THR	2.1
3	E	54	LEU	2.1
3	E	123	LEU	2.1
4	F	342	LEU	2.1
2	B	75	SER	2.1
1	A	59	GLY	2.1
2	B	361	LEU	2.1
2	B	351	THR	2.1
3	E	138	GLU	2.1
4	F	140	GLU	2.1
4	F	175	GLU	2.1
2	D	39	ASP	2.1
2	D	227	HIS	2.1
2	D	57	ASN	2.1
2	D	215	LEU	2.1
2	B	38	GLY	2.1
2	D	79	GLY	2.1
2	D	136	THR	2.1
2	D	429	THR	2.1
3	E	127	ASP	2.1
2	D	133	PHE	2.0
2	D	14	ASN	2.0
3	E	12	ASN	2.0
2	B	325	GLU	2.0
2	D	104	GLY	2.0
2	D	111	GLU	2.0
3	E	7	GLU	2.0
1	A	89	PRO	2.0
2	B	126	SER	2.0
1	A	363	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	270	PHE	2.0
2	D	86	ARG	2.0
2	D	181	GLU	2.0
2	D	99	ASN	2.0
2	D	140	GLY	2.0
3	E	50	ILE	2.0
1	C	245	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

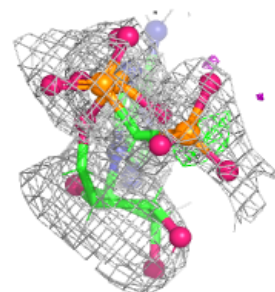
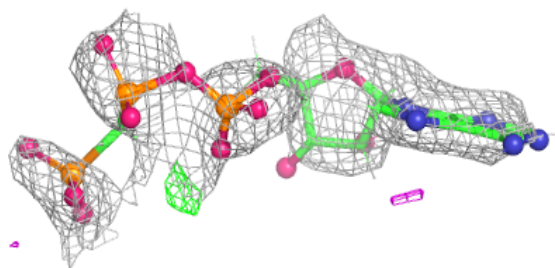
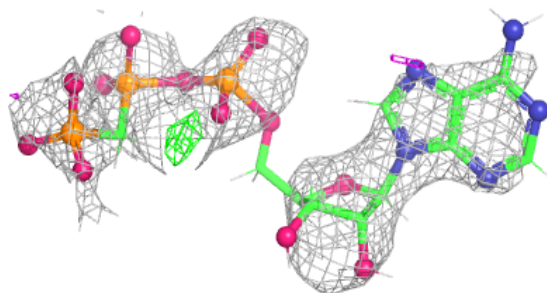
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ACP	F	401	31/31	0.72	0.18	97,127,164,171	0
6	MG	D	503	1/1	0.74	0.30	73,73,73,73	0
10	HZ0	D	502	52/52	0.80	0.28	81,104,153,186	0
5	GTP	D	501	32/32	0.86	0.19	46,68,105,129	0
9	MES	B	503	12/12	0.93	0.12	35,49,71,72	0
7	CA	A	503	1/1	0.94	0.09	67,67,67,67	0
6	MG	B	502	1/1	0.94	0.13	40,40,40,40	0
8	GDP	B	501	28/28	0.95	0.10	17,33,50,60	0
5	GTP	A	501	32/32	0.96	0.08	18,33,45,54	0
5	GTP	C	501	32/32	0.97	0.06	19,24,35,39	0
7	CA	C	503	1/1	0.98	0.03	42,42,42,42	0
6	MG	C	502	1/1	1.00	0.03	22,22,22,22	0
6	MG	A	502	1/1	1.00	0.04	21,21,21,21	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.

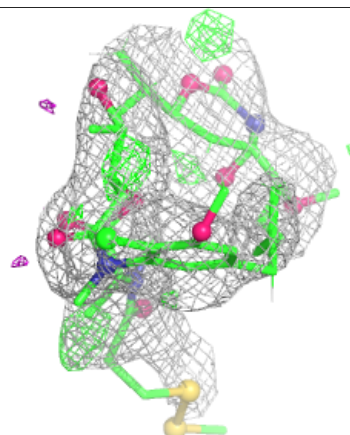
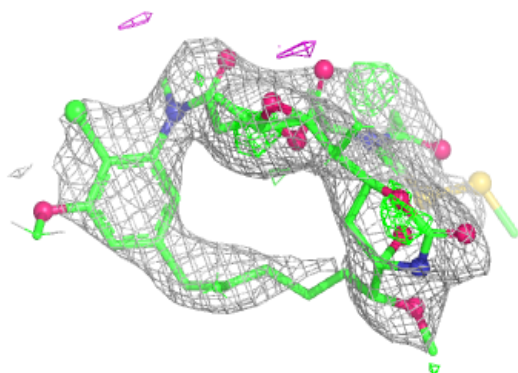
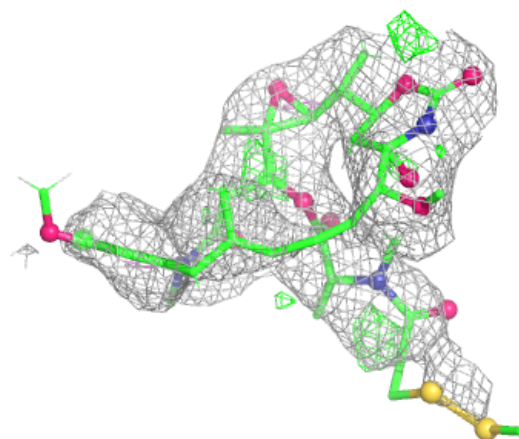
Electron density around ACP F 401:

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

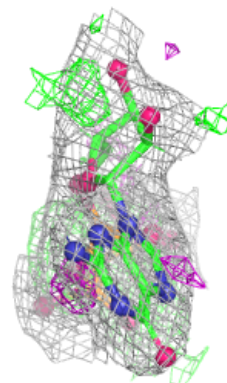
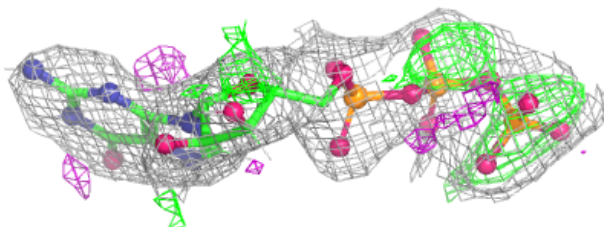
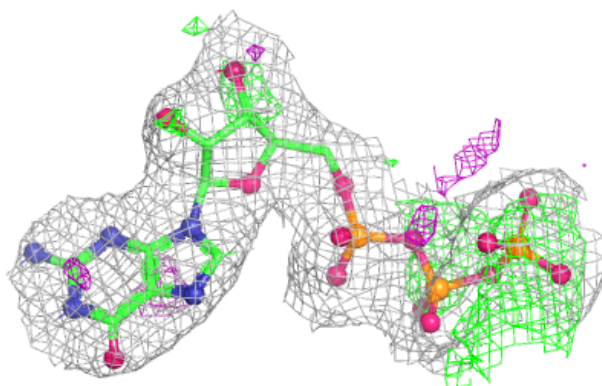


Electron density around HZ0 D 502:

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

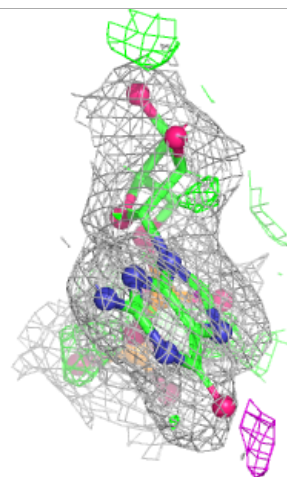
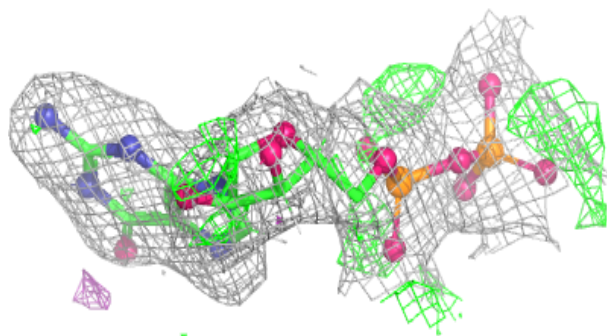
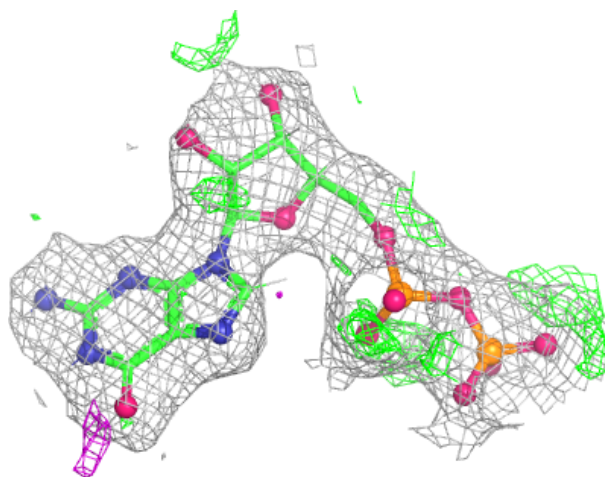
**Electron density around GTP D 501:**

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



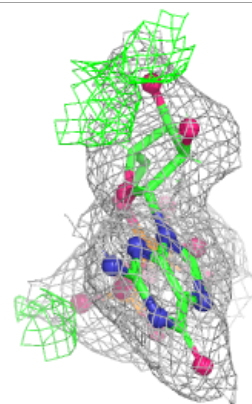
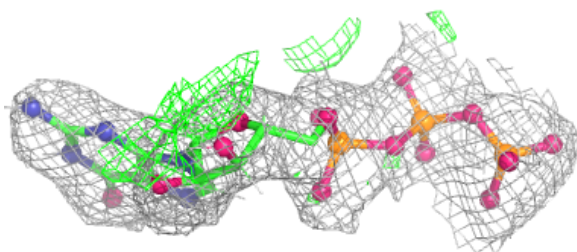
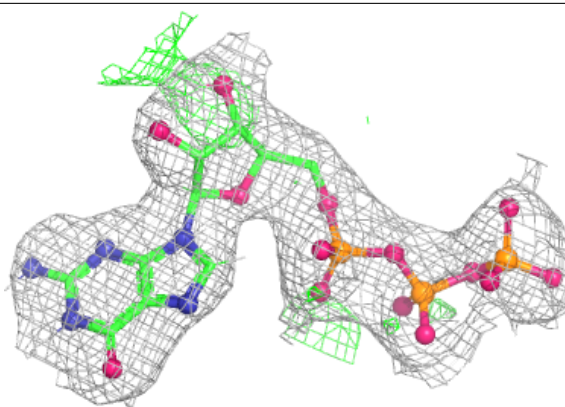
Electron density around GDP B 501:

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

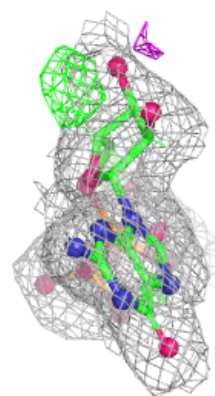
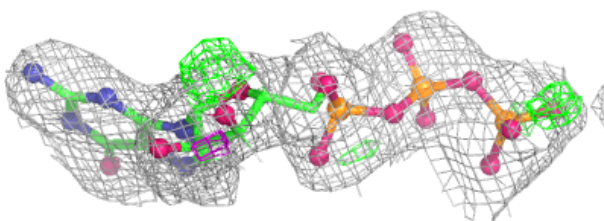
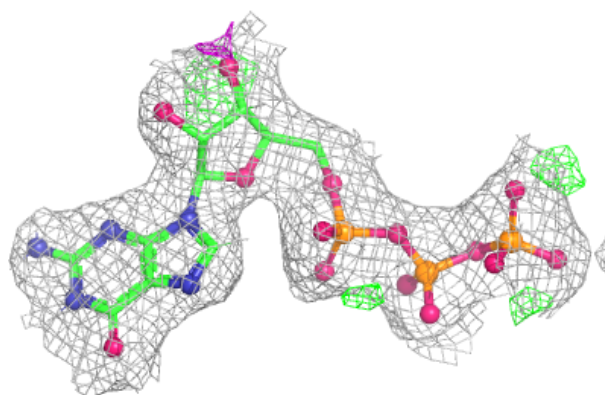


Electron density around GTP A 501:

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

**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)



6.5 Other polymers ⓘ

There are no such residues in this entry.