



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:24 AM UTC

PDB ID : 5CB4 / pdb_00005cb4
Title : Crystal structure of T2R-TTL-Tivantinib complex
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on : 2015-06-30
Resolution : 2.19 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

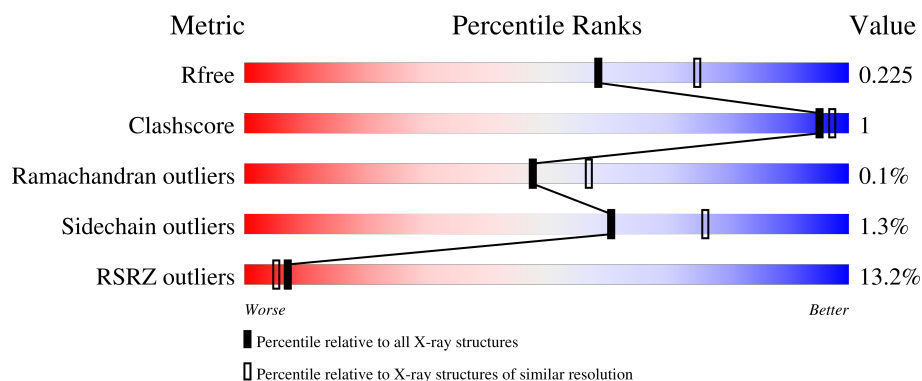
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	450	5% 94% • •
1	C	450	2% 95% • •
2	B	445	5% 94% • •
2	D	445	19% 89% 5% 5%
3	E	143	14% 82% • 15%

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Mol	Chain	Length	Quality of chain
4	F	384	33% 82% 5% 13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 35199 atoms, of which 16873 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6733	2163	3317	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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6589	2110	3228	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			

There are 2 discrepancies between the modelled and reference sequences:

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

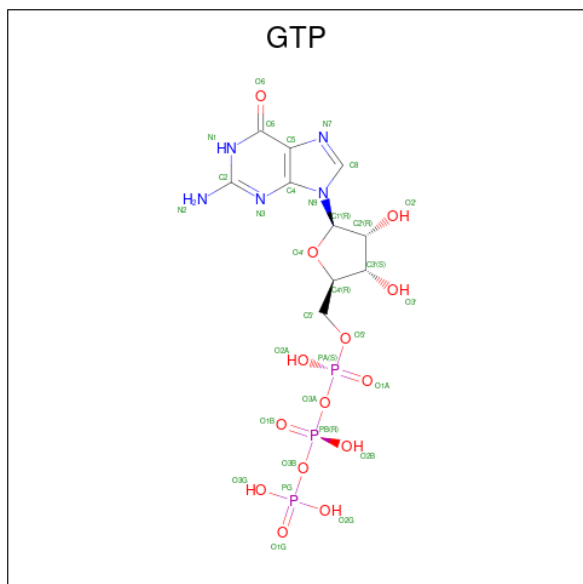
- Molecule 4 is a protein called Uncharacterized protein.

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

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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

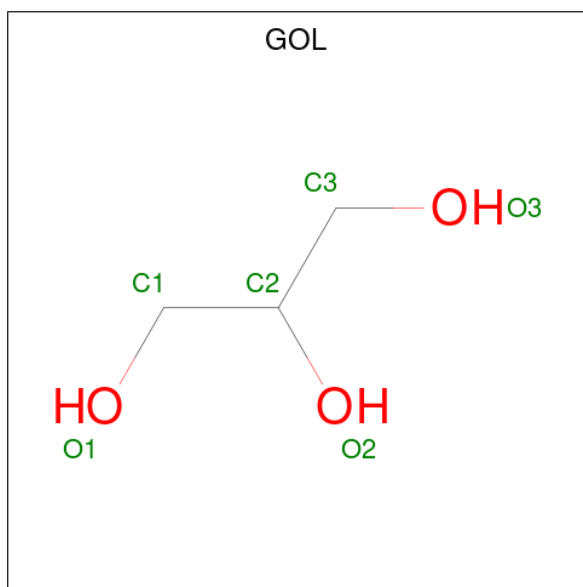
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

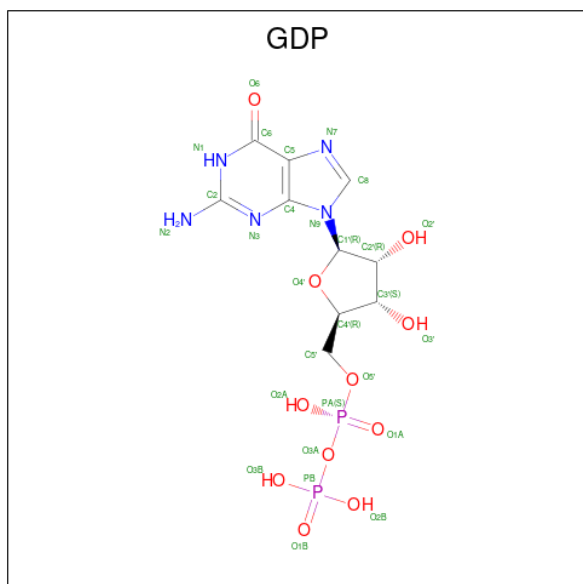
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



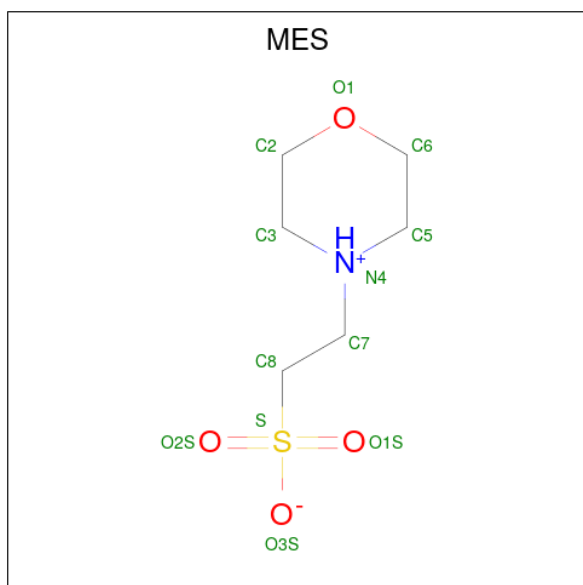
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

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



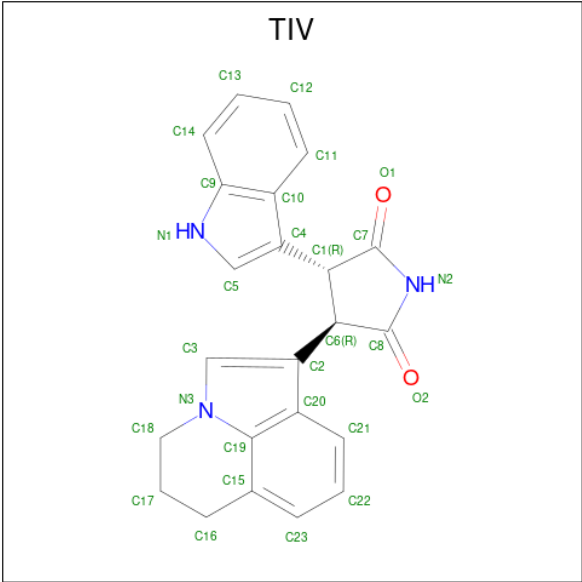
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	
9	D	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



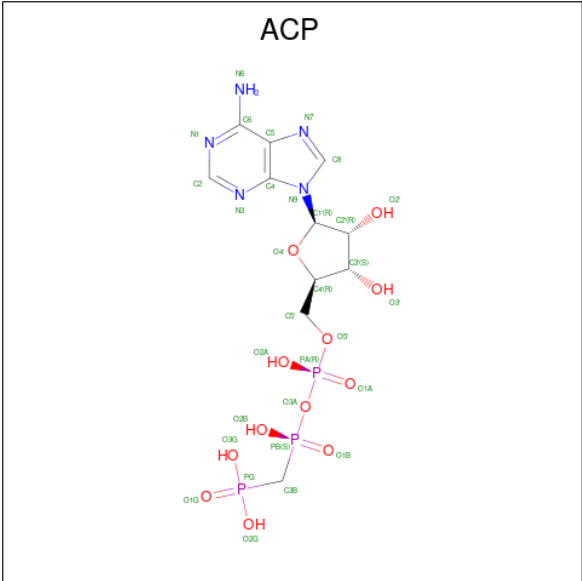
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			24	6	12	1	4	1	

- Molecule 11 is (3R,4R)-3-(5,6-dihydro-4H-pyrrolo[3,2,1-ij]quinolin-1-yl)-4-(1H-indol-3-yl)pyrrolidine-2,5-dione (CCD ID: TIV) (formula: C₂₃H₁₉N₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	0	0
			47	23	19	3	2		
11	D	1	Total	C	H	N	O	0	0
			47	23	19	3	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	0	0
			35	11	4	5	12		

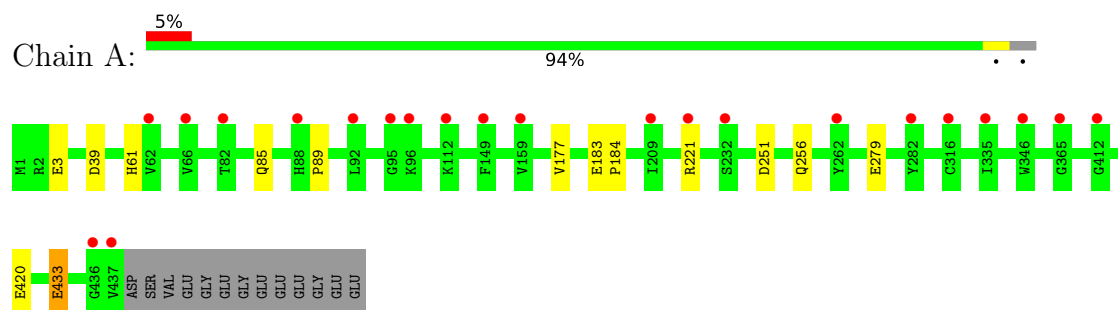
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	185	Total 185	O 185	0	0
13	B	164	Total 164	O 164	0	0
13	C	273	Total 273	O 273	0	0
13	D	92	Total 92	O 92	0	0
13	E	31	Total 31	O 31	0	0
13	F	84	Total 84	O 84	0	0

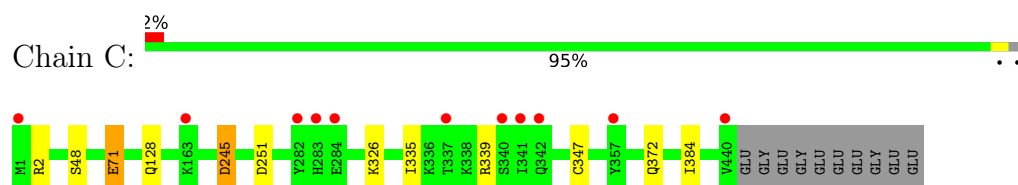
3 Residue-property plots [i](#)

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.

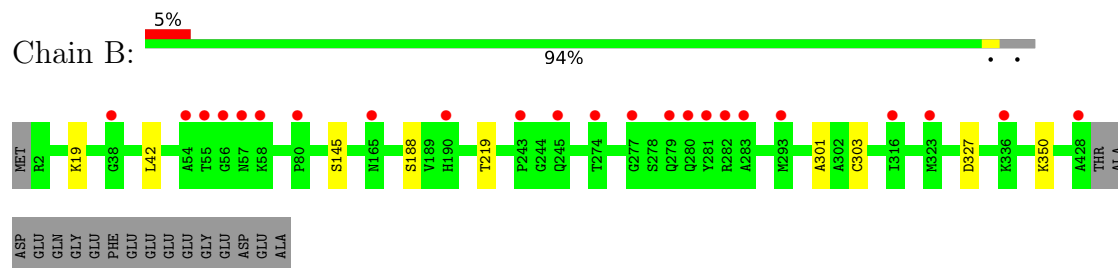
• Molecule 1: Tubulin alpha



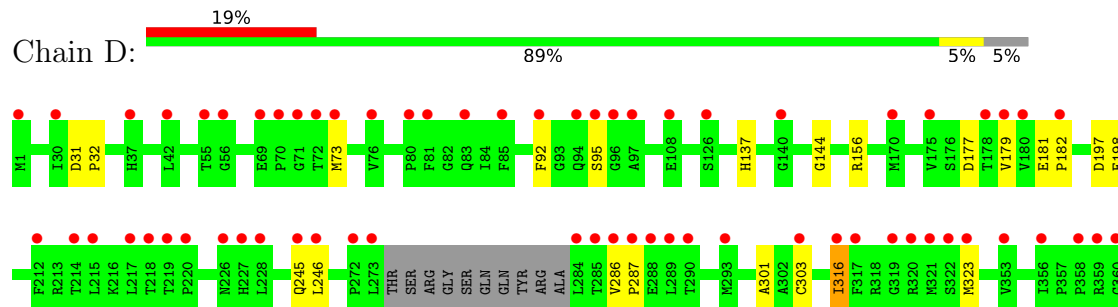
• Molecule 1: Tubulin alpha

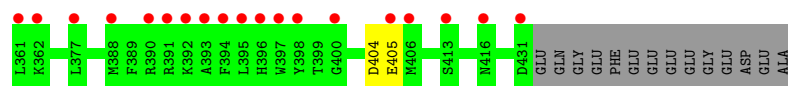


• Molecule 2: Tubulin beta

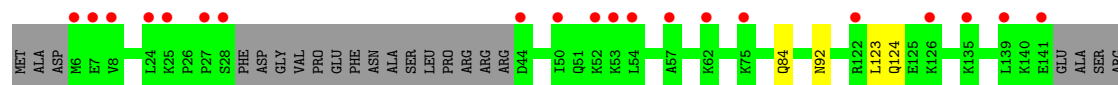
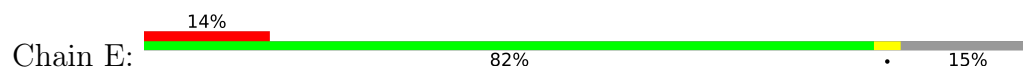


• Molecule 2: Tubulin beta

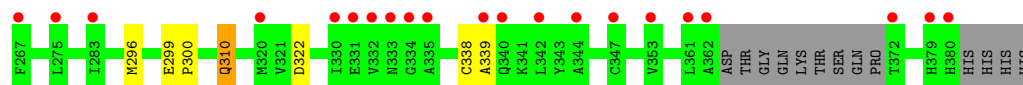
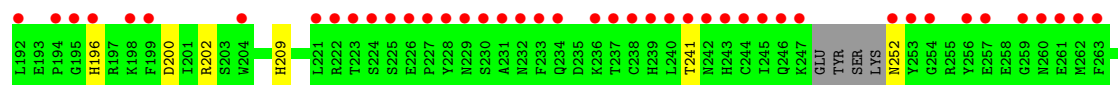
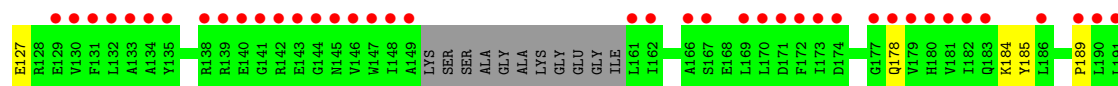
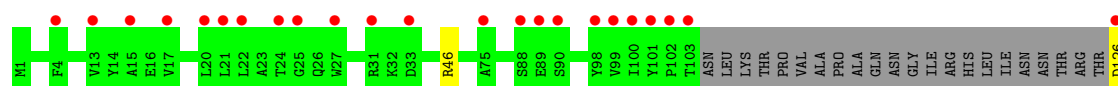
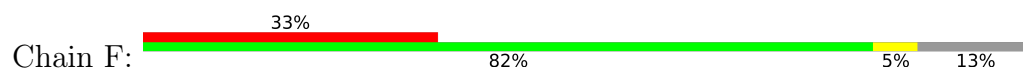




● Molecule 3: Stathmin-4



● Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.06Å 158.44Å 181.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.82 – 2.19 39.82 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.82-2.19) 99.3 (39.82-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.207 , 0.232 0.214 , 0.225	Depositor DCC
R_{free} test set	7564 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.1	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	0.95	EDS
Total number of atoms	35199	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: MG, ACP, GOL, CA, GTP, TIV, MES, GDP

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	0.31	0/3494	0.63	0/4743
1	C	0.30	0/3515	0.62	0/4772
2	B	0.30	0/3436	0.60	0/4654
2	D	0.30	0/3382	0.61	0/4581
3	E	0.28	0/1008	0.58	0/1337
4	F	0.27	0/2806	0.58	0/3791
All	All	0.30	0/17641	0.61	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	3317	3330	6	0
1	C	3437	3335	3348	6	0
2	B	3361	3228	3238	5	0
2	D	3309	3179	3189	11	0
3	E	1000	1014	1018	2	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
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	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
9	D	28	10	12	1	0
10	B	12	12	12	0	0
11	B	28	19	19	0	0
11	D	28	19	19	1	0
12	F	31	4	14	2	0
13	A	185	0	0	1	0
13	B	164	0	0	1	0
13	C	273	0	0	3	0
13	D	92	0	0	1	0
13	E	31	0	0	1	0
13	F	84	0	0	3	0
All	All	18326	16873	16952	41	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 (41) 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:145:SER:HG	2:B:188:SER:HG	1.32	0.75
4:F:196:HIS:NE2	13:F:502:HOH:O	2.30	0.65
1:A:221:ARG:NH2	2:B:327:ASP:OD2	2.34	0.61
4:F:126:ASP:N	13:F:510:HOH:O	2.34	0.59
4:F:252:ASN:N	13:F:508:HOH:O	2.35	0.58
2:D:404:ASP:OD1	2:D:405:GLU:N	2.36	0.58
1:C:128:GLN:NE2	13:C:615:HOH:O	2.39	0.55
4:F:184:LYS:NZ	4:F:185:TYR:O	2.41	0.52
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.44	0.51
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.27	0.50
1:C:245:ASP:N	1:C:245:ASP:OD1	2.44	0.50
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.94	0.50
4:F:126:ASP:OD1	4:F:127:GLU:N	2.45	0.49
1:C:372:GLN:NE2	13:C:620:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:178:GLN:N	4:F:178:GLN:OE1	2.46	0.49
1:A:433:GLU:OE2	4:F:46:ARG:NH2	2.46	0.49
1:A:85:GLN:NE2	13:A:621:HOH:O	2.45	0.48
3:E:84:GLN:NE2	13:E:204:HOH:O	2.47	0.46
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.99	0.45
9:D:501:GDP:O3B	13:D:601:HOH:O	2.21	0.45
1:C:71:GLU:O	13:C:601:HOH:O	2.21	0.44
2:B:301:ALA:O	2:B:303:CYS:N	2.47	0.44
4:F:202:ARG:NH2	12:F:401:ACP:O3G	2.51	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.92	0.43
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.00	0.43
12:F:401:ACP:H3B2	12:F:401:ACP:O2A	2.19	0.43
2:D:177:ASP:OD1	2:D:177:ASP:N	2.51	0.43
2:B:219:THR:HG21	1:C:326:LYS:HA	2.01	0.42
2:D:301:ALA:O	2:D:303:CYS:N	2.52	0.42
4:F:189:PRO:HA	4:F:322:ASP:HA	2.00	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.42
2:D:181:GLU:N	2:D:182:PRO:HD2	2.35	0.42
2:D:137:HIS:ND1	2:D:144:GLY:O	2.41	0.41
1:A:3:GLU:OE1	1:A:3:GLU:N	2.52	0.41
2:B:350:LYS:NZ	13:B:627:HOH:O	2.54	0.41
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.03	0.40
2:D:316:ILE:HG13	11:D:502:TIV:H11	2.02	0.40
4:F:299:GLU:N	4:F:300:PRO:HD2	2.37	0.40
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.03	0.40
1:A:183:GLU:N	1:A:184:PRO:CD	2.85	0.40
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	422 (97%)	12 (3%)	1 (0%)	43	51
1	C	438/450 (97%)	430 (98%)	8 (2%)	0	100	100
2	B	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	D	417/445 (94%)	407 (98%)	9 (2%)	1 (0%)	43	51
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	324/384 (84%)	312 (96%)	12 (4%)	0	100	100
All	All	2156/2317 (93%)	2100 (97%)	54 (2%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	95	SER
1	A	89	PRO

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	368/378 (97%)	362 (98%)	6 (2%)	55	71
1	C	371/378 (98%)	364 (98%)	7 (2%)	50	66
2	B	369/383 (96%)	367 (100%)	2 (0%)	81	90
2	D	364/383 (95%)	358 (98%)	6 (2%)	55	71
3	E	109/127 (86%)	107 (98%)	2 (2%)	51	68
4	F	301/342 (88%)	299 (99%)	2 (1%)	76	87
All	All	1882/1991 (94%)	1857 (99%)	25 (1%)	61	76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	A	251	ASP
1	A	256	GLN

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Mol	Chain	Res	Type
1	A	279	GLU
1	A	420	GLU
1	A	433	GLU
2	B	19	LYS
2	B	42	LEU
1	C	2	ARG
1	C	48	SER
1	C	71	GLU
1	C	245	ASP
1	C	251	ASP
1	C	347	CYS
1	C	384	ILE
2	D	179	VAL
2	D	198	GLU
2	D	245	GLN
2	D	246	LEU
2	D	316	ILE
2	D	323	MET
3	E	92	ASN
3	E	124	GLN
4	F	296	MET
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	342	GLN
2	B	8	GLN
2	B	14	ASN
2	B	134	GLN
2	B	227	HIS
2	B	298	ASN
2	B	347	ASN
2	B	375	GLN
2	B	426	GLN
1	C	85	GLN
1	C	293	ASN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	11	GLN

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Mol	Chain	Res	Type
2	D	426	GLN
3	E	92	ASN
4	F	269	GLN
4	F	379	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 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
9	GDP	D	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.70	6 (13%)
8	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.32	0
5	GTP	A	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.55	8 (16%)
11	TIV	B	504	-	33,33,33	1.90	12 (36%)	43,50,50	2.45	20 (46%)
10	MES	B	503	-	12,12,12	2.28	1 (8%)	15,16,16	2.38	5 (33%)
9	GDP	B	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.70	7 (15%)
11	TIV	D	502	-	33,33,33	1.76	8 (24%)	43,50,50	2.37	18 (41%)
5	GTP	C	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.53	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ACP	F	401	-	31,33,33	1.84	9 (29%)	47,52,52	1.88	12 (25%)

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
9	GDP	D	501	-	-	5/16/32/32	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
11	TIV	B	504	-	-	0/8/30/30	0/6/6/6
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
11	TIV	D	502	-	-	0/8/30/30	0/6/6/6
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
12	ACP	F	401	-	-	2/19/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.63	1.66	1.77
12	F	401	ACP	PB-O2B	-4.58	1.45	1.56
11	D	502	TIV	C1-C4	-4.52	1.46	1.51
11	B	504	TIV	C9-N1	4.38	1.44	1.37
11	D	502	TIV	C6-C2	-3.84	1.46	1.51
12	F	401	ACP	C5-C4	3.52	1.45	1.39
12	F	401	ACP	C5-N7	-3.49	1.32	1.39
11	D	502	TIV	C9-N1	3.47	1.43	1.37
11	B	504	TIV	C1-C4	-3.36	1.47	1.51
11	B	504	TIV	C6-C2	-3.21	1.47	1.51
12	F	401	ACP	C4-N9	-3.20	1.31	1.37
11	D	502	TIV	C7-N2	3.20	1.41	1.37
11	D	502	TIV	C8-N2	3.15	1.41	1.37
9	D	501	GDP	C5-C4	3.03	1.47	1.38
11	B	504	TIV	C8-N2	2.95	1.41	1.37
9	B	501	GDP	C5-C4	2.94	1.46	1.38
9	B	501	GDP	C6-N1	-2.79	1.33	1.38
12	F	401	ACP	PB-O1B	2.78	1.58	1.51
11	B	504	TIV	C7-N2	2.77	1.41	1.37
11	B	504	TIV	C14-C9	2.73	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	C6-N1	-2.65	1.33	1.38
11	B	504	TIV	C22-C23	2.46	1.43	1.38
12	F	401	ACP	PG-O2G	2.39	1.60	1.55
11	B	504	TIV	C3-C2	2.37	1.39	1.36
11	B	504	TIV	C19-N3	2.26	1.41	1.39
12	F	401	ACP	PG-O1G	-2.24	1.45	1.50
11	B	504	TIV	C5-N1	2.23	1.40	1.37
11	B	504	TIV	C11-C10	2.23	1.43	1.39
12	F	401	ACP	C5-C6	2.19	1.47	1.41
5	A	501	GTP	C2-N3	2.17	1.38	1.33
5	C	501	GTP	C2-N3	2.17	1.38	1.33
9	B	501	GDP	C4-N9	-2.14	1.32	1.38
11	D	502	TIV	C3-C2	2.14	1.39	1.36
11	D	502	TIV	C11-C10	2.10	1.43	1.39
12	F	401	ACP	C8-N9	-2.08	1.34	1.37
9	D	501	GDP	C5-N7	-2.08	1.34	1.39
5	C	501	GTP	PA-O3A	2.05	1.61	1.59
11	D	502	TIV	C22-C23	2.04	1.42	1.38
11	B	504	TIV	C20-C19	2.04	1.44	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	TIV	C8-N2-C7	-6.15	109.55	113.87
11	B	504	TIV	C8-N2-C7	-6.00	109.66	113.87
12	F	401	ACP	C5-C4-N3	-5.86	118.64	126.72
9	D	501	GDP	C5-C4-N3	-5.48	119.67	128.39
9	B	501	GDP	C5-C4-N3	-5.36	119.86	128.39
11	B	504	TIV	C16-C15-C23	5.28	132.08	121.05
11	D	502	TIV	C16-C15-C23	5.17	131.84	121.05
5	A	501	GTP	C5-C4-N3	-5.01	120.41	128.39
5	C	501	GTP	C5-C4-N3	-5.00	120.44	128.39
10	B	503	MES	C7-N4-C5	4.95	124.43	111.24
10	B	503	MES	C5-N4-C3	4.91	119.41	108.84
5	A	501	GTP	C2-N3-C4	4.81	120.58	112.30
5	C	501	GTP	C2-N3-C4	4.68	120.36	112.30
9	D	501	GDP	C2-N3-C4	4.66	120.33	112.30
11	B	504	TIV	C18-N3-C19	4.66	125.99	120.19
9	B	501	GDP	C2-N3-C4	4.60	120.22	112.30
9	D	501	GDP	N9-C4-N3	4.50	134.94	125.95
9	B	501	GDP	N9-C4-N3	4.46	134.86	125.95
11	B	504	TIV	C16-C15-C19	-4.46	112.00	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	TIV	C18-N3-C19	4.42	125.69	120.19
11	D	502	TIV	C16-C15-C19	-4.18	112.47	119.47
12	F	401	ACP	N3-C4-N9	4.16	134.24	127.17
11	B	504	TIV	C21-C20-C2	3.99	140.48	133.68
11	D	502	TIV	C10-C4-C5	3.97	109.28	106.25
11	B	504	TIV	C10-C4-C5	3.93	109.26	106.25
12	F	401	ACP	C2-N3-C4	3.79	121.09	111.83
11	D	502	TIV	C21-C20-C2	3.69	139.97	133.68
11	B	504	TIV	C6-C8-N2	3.68	110.29	107.69
11	B	504	TIV	C19-N3-C3	3.54	110.31	108.19
11	D	502	TIV	C19-N3-C3	3.50	110.29	108.19
12	F	401	ACP	C4-C5-N7	-3.50	106.58	110.58
10	B	503	MES	C6-C5-N4	-3.46	104.86	110.12
9	B	501	GDP	C6-C5-N7	3.30	136.30	130.29
5	A	501	GTP	N9-C4-N3	3.18	132.30	125.95
12	F	401	ACP	O2'-C2'-C3'	-3.17	101.64	111.82
5	C	501	GTP	N9-C4-N3	3.16	132.28	125.95
9	D	501	GDP	C6-C5-N7	3.11	135.94	130.29
12	F	401	ACP	N3-C2-N1	-3.06	123.95	128.58
12	F	401	ACP	O3G-PG-O1G	-3.02	104.57	112.39
11	D	502	TIV	C1-C6-C8	-2.91	102.30	104.30
11	D	502	TIV	C23-C15-C19	-2.86	113.88	117.88
11	D	502	TIV	C4-C5-N1	-2.85	108.00	110.31
5	A	501	GTP	C2-N1-C6	-2.79	120.05	125.11
11	B	504	TIV	C4-C5-N1	-2.75	108.08	110.31
11	D	502	TIV	C20-C2-C6	2.74	132.03	127.46
5	C	501	GTP	C2-N1-C6	-2.70	120.21	125.11
5	A	501	GTP	N9-C8-N7	-2.69	108.42	113.40
12	F	401	ACP	O3G-PG-C3B	2.66	112.86	106.40
11	B	504	TIV	C23-C15-C19	-2.66	114.16	117.88
11	B	504	TIV	C20-C2-C6	2.66	131.89	127.46
11	B	504	TIV	C1-C4-C5	-2.63	121.15	126.25
11	B	504	TIV	C1-C6-C8	-2.63	102.50	104.30
5	C	501	GTP	N9-C8-N7	-2.62	108.53	113.40
11	D	502	TIV	C6-C8-N2	2.60	109.53	107.69
5	A	501	GTP	C5-C6-N1	2.56	119.76	113.25
5	A	501	GTP	C8-N7-C5	2.51	108.74	104.26
5	C	501	GTP	C5-C6-N1	2.50	119.62	113.25
5	C	501	GTP	C8-N7-C5	2.49	108.70	104.26
11	D	502	TIV	C2-C3-N3	-2.48	108.19	110.64
10	B	503	MES	O2S-S-C8	2.47	110.47	106.73
5	A	501	GTP	O6-C6-C5	-2.47	120.01	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O6-C6-C5	-2.47	120.02	126.53
11	D	502	TIV	C1-C4-C5	-2.43	121.54	126.25
11	B	504	TIV	C2-C3-N3	-2.39	108.28	110.64
11	B	504	TIV	C20-C2-C3	2.38	108.75	106.41
11	D	502	TIV	C20-C2-C3	2.33	108.70	106.41
12	F	401	ACP	C5-N7-C8	2.31	107.08	103.45
9	B	501	GDP	C8-N9-C4	2.30	110.34	106.03
12	F	401	ACP	C3'-C2'-C1'	2.28	105.78	101.46
11	D	502	TIV	C17-C16-C15	2.28	117.87	112.43
12	F	401	ACP	PB-O3A-PA	-2.28	124.94	132.37
11	B	504	TIV	C17-C16-C15	2.27	117.84	112.43
11	B	504	TIV	C17-C18-N3	2.26	111.71	109.73
11	B	504	TIV	C1-C7-N2	2.23	109.27	107.69
11	D	502	TIV	C23-C22-C21	2.19	123.06	120.24
9	B	501	GDP	C4-C5-N7	-2.14	107.28	110.67
11	B	504	TIV	C23-C22-C21	2.14	122.99	120.24
11	D	502	TIV	C17-C18-N3	2.12	111.58	109.73
11	B	504	TIV	C21-C20-C19	-2.10	114.38	119.41
9	D	501	GDP	C4-C5-N7	-2.09	107.35	110.67
9	B	501	GDP	O6-C6-C5	-2.06	121.08	126.53
10	B	503	MES	O1S-S-C8	2.05	109.83	106.73
12	F	401	ACP	C6-C5-N7	2.03	136.00	132.09
9	D	501	GDP	C8-N9-C4	2.02	109.81	106.03

There are no chirality outliers.

All (31) 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	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-O2
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A

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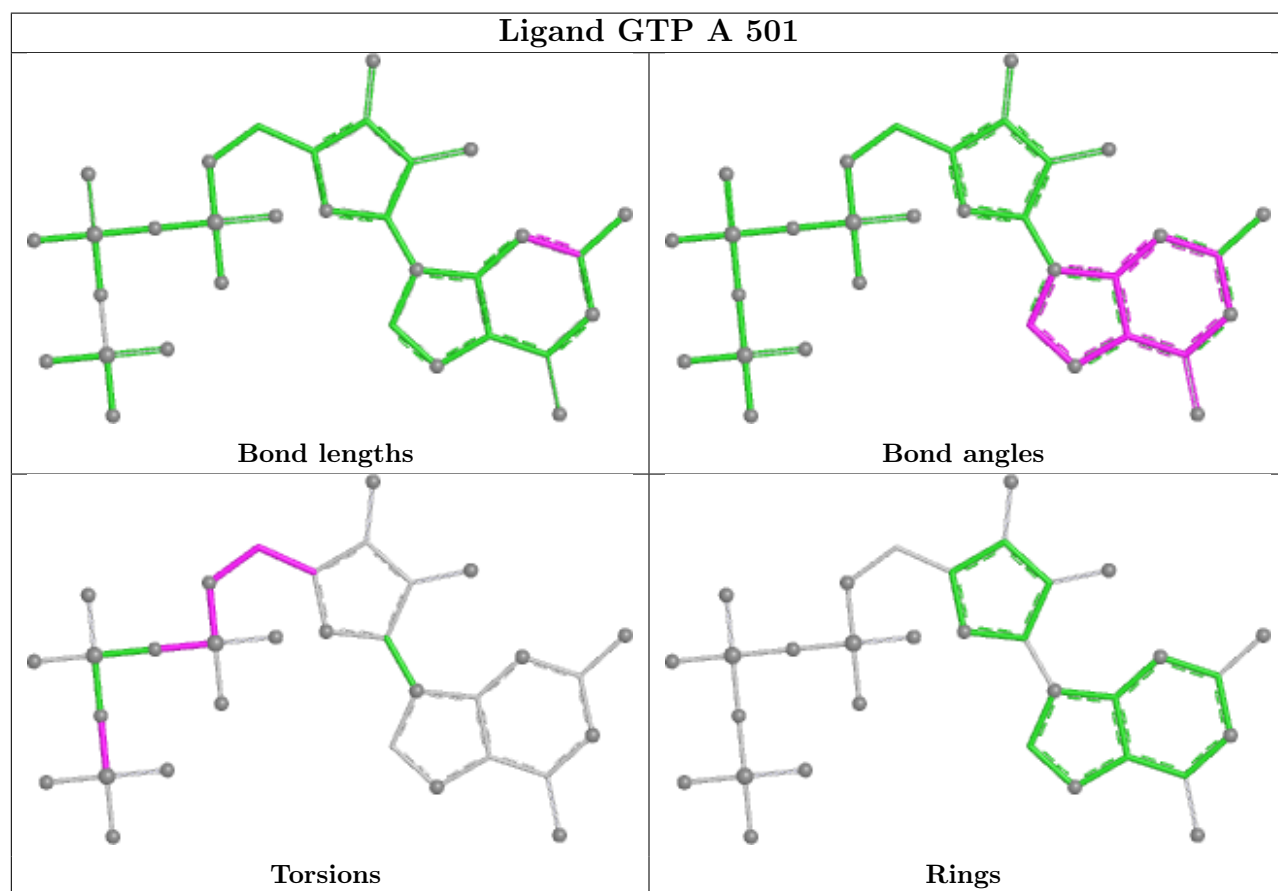
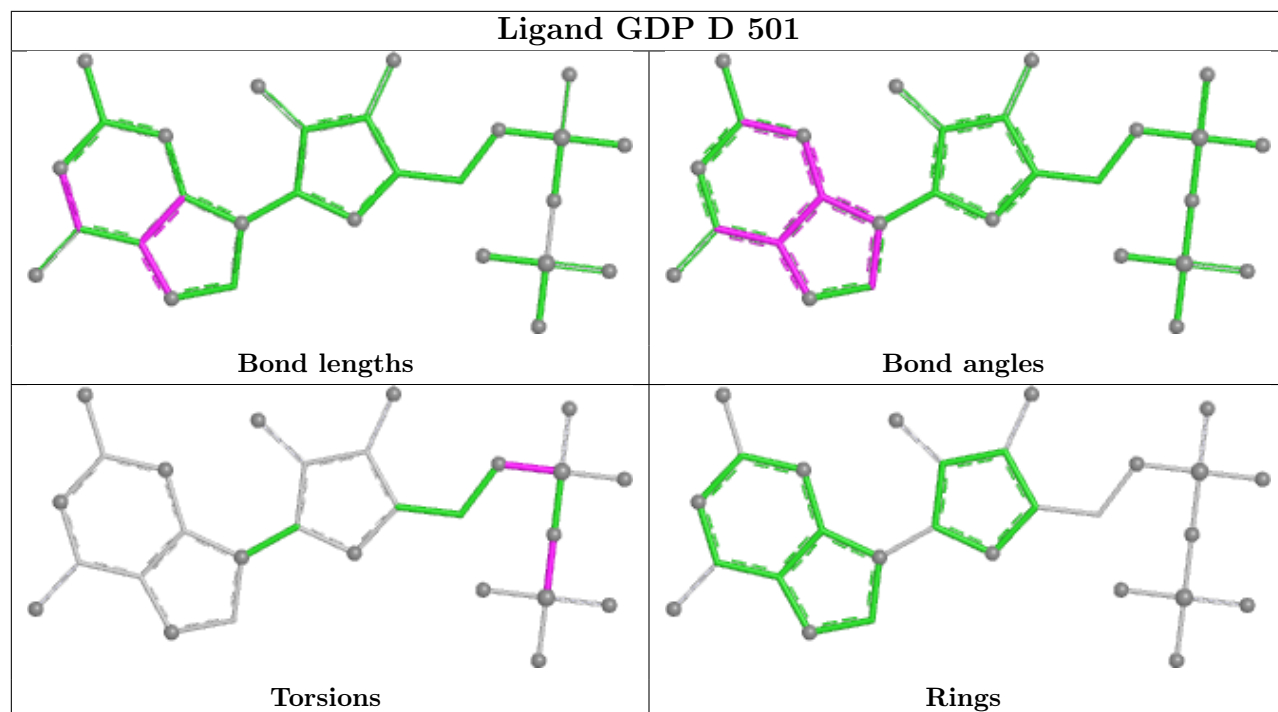
Mol	Chain	Res	Type	Atoms
9	D	501	GDP	PA-O3A-PB-O2B
9	D	501	GDP	PA-O3A-PB-O3B
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
5	C	501	GTP	PB-O3A-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
12	F	401	ACP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

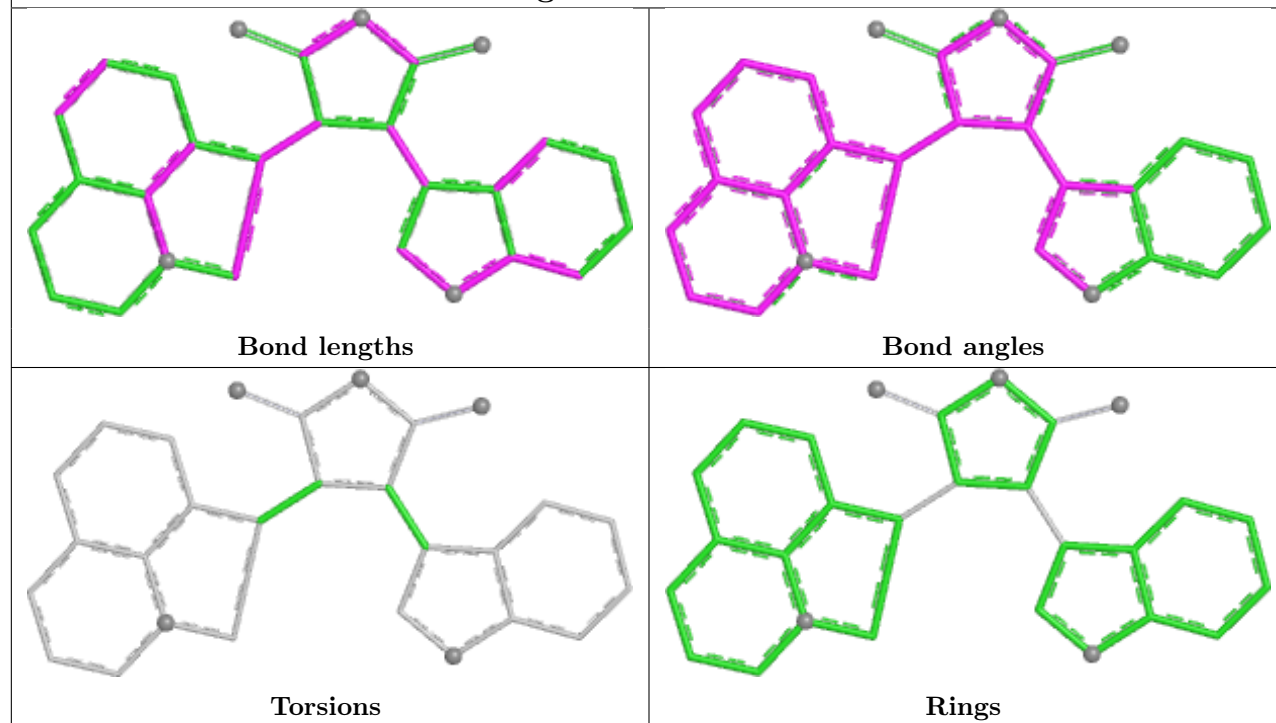
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
11	D	502	TIV	1	0
12	F	401	ACP	2	0

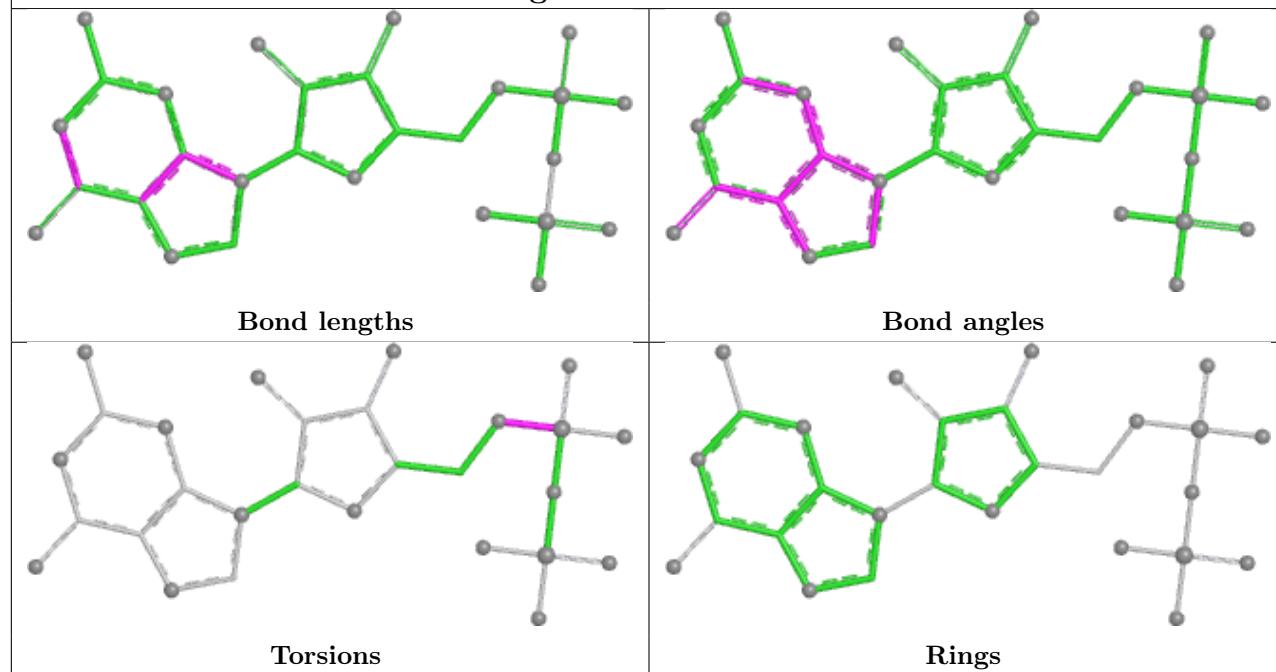
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



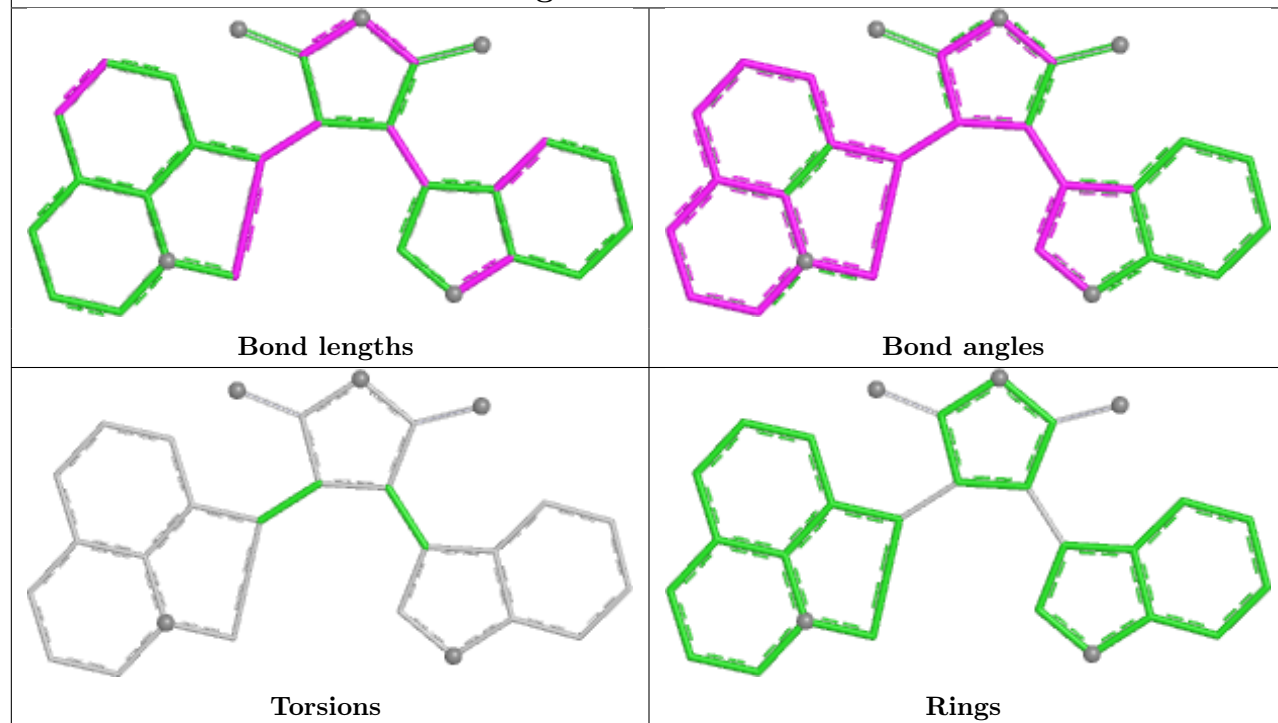
Ligand TIV B 504



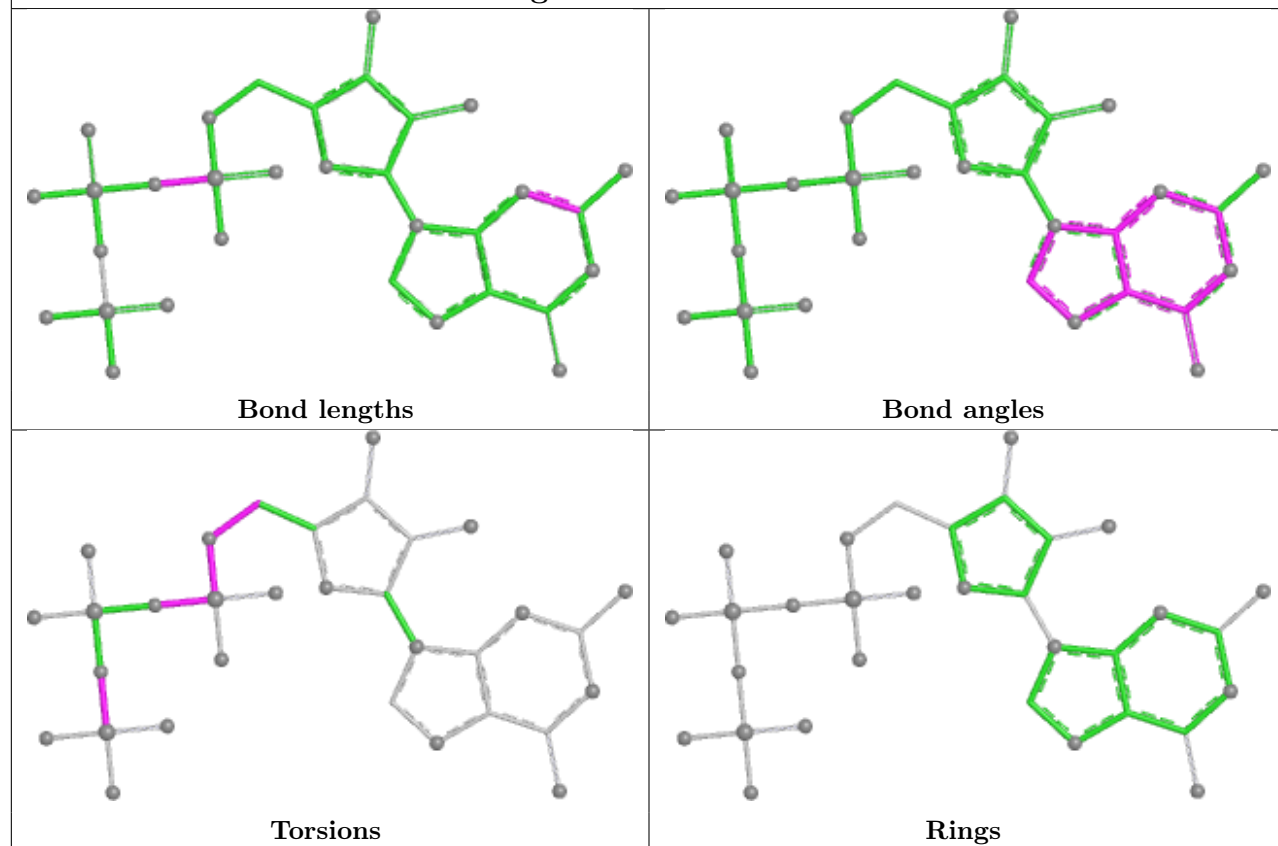
Ligand GDP B 501

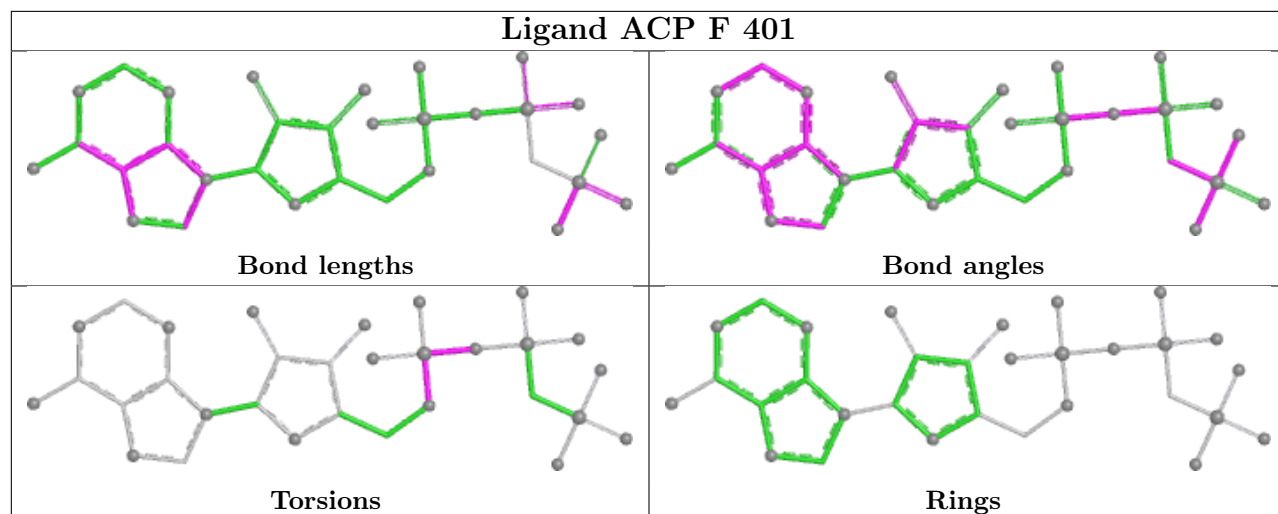


Ligand TIV D 502



Ligand GTP C 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	437/450 (97%)	0.62	22 (5%) 34 31	29, 47, 71, 105	0
1	C	440/450 (97%)	0.05	11 (2%) 58 55	23, 37, 62, 80	0
2	B	427/445 (95%)	0.47	23 (5%) 31 28	26, 46, 78, 136	0
2	D	421/445 (94%)	1.15	84 (19%) 3 2	29, 59, 96, 121	0
3	E	121/143 (84%)	1.11	20 (16%) 4 3	36, 60, 94, 109	0
4	F	334/384 (86%)	1.77	127 (38%) 1 0	35, 69, 130, 152	0
All	All	2180/2317 (94%)	0.78	287 (13%) 7 5	23, 50, 97, 152	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	9.2
4	F	161	LEU	7.2
2	D	397	TRP	5.9
2	D	285	THR	5.8
4	F	240	LEU	5.4
4	F	103	THR	5.3
4	F	173	ILE	5.3
2	D	286	VAL	5.3
2	D	394	PHE	5.3
2	B	428	ALA	5.3
2	B	55	THR	5.2
2	D	284	LEU	5.1
4	F	362	ALA	5.0
4	F	231	ALA	4.8
4	F	181	VAL	4.8
4	F	182	ILE	4.8
1	A	437	VAL	4.7
4	F	263	PHE	4.6
1	C	440	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
4	F	239	HIS	4.5
4	F	88	SER	4.4
4	F	233	PHE	4.4
4	F	162	ILE	4.4
2	D	55	THR	4.3
2	B	56	GLY	4.2
3	E	6	MET	4.2
4	F	169	LEU	4.2
4	F	146	VAL	4.1
4	F	180	HIS	4.1
3	E	141	GLU	4.1
4	F	253	TYR	4.1
2	D	71	GLY	4.0
2	D	72	THR	4.0
4	F	144	GLY	4.0
4	F	179	VAL	4.0
4	F	148	ILE	4.0
2	D	81	PHE	3.9
2	D	92	PHE	3.9
4	F	186	LEU	3.9
4	F	90	SER	3.8
2	D	388	MET	3.8
4	F	172	PHE	3.8
1	A	282	TYR	3.8
4	F	361	LEU	3.8
2	D	319	GLY	3.8
2	D	323	MET	3.8
4	F	236	LYS	3.7
2	D	245	GLN	3.7
2	B	280	GLN	3.7
4	F	245	ILE	3.7
4	F	166	ALA	3.7
2	D	356	ILE	3.7
2	B	283	ALA	3.7
2	D	30	ILE	3.6
4	F	100	ILE	3.6
4	F	254	GLY	3.6
2	D	289	LEU	3.6
4	F	232	ASN	3.5
4	F	194	PRO	3.5
4	F	335	ALA	3.5
4	F	372	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	97	ALA	3.5
4	F	147	TRP	3.4
2	D	217	LEU	3.4
3	E	7	GLU	3.4
2	D	179	VAL	3.4
4	F	132	LEU	3.4
2	B	54	ALA	3.4
1	A	316	CYS	3.4
4	F	98	TYR	3.4
4	F	225	SER	3.4
1	A	88	HIS	3.3
4	F	99	VAL	3.3
2	D	94	GLN	3.3
4	F	252	ASN	3.3
4	F	228	TYR	3.3
2	D	395	LEU	3.3
2	B	279	GLN	3.3
4	F	177	GLY	3.2
2	D	391	ARG	3.2
4	F	191	LEU	3.2
2	B	282	ARG	3.2
2	D	362	LYS	3.2
2	D	80	PRO	3.2
4	F	75	ALA	3.1
2	D	273	LEU	3.1
4	F	330	ILE	3.1
2	D	390	ARG	3.1
2	B	281	TYR	3.1
4	F	226	GLU	3.1
4	F	331	GLU	3.1
1	A	92	LEU	3.1
2	B	336	LYS	3.1
4	F	25	GLY	3.1
2	D	358	PRO	3.1
2	D	1	MET	3.0
2	D	360	GLY	3.0
4	F	143	GLU	3.0
4	F	227	PRO	3.0
2	D	393	ALA	3.0
4	F	238	CYS	3.0
2	D	219	THR	3.0
1	C	357	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	133	ALA	3.0
4	F	17	VAL	3.0
4	F	229	ASN	3.0
4	F	247	LYS	3.0
4	F	131	PHE	3.0
4	F	199	PHE	3.0
1	C	340	SER	2.9
4	F	230	SER	2.9
4	F	20	LEU	2.9
3	E	8	VAL	2.9
4	F	130	VAL	2.9
4	F	237	THR	2.9
2	D	70	PRO	2.9
4	F	15	ALA	2.9
4	F	22	LEU	2.9
1	C	1	MET	2.9
4	F	257	GLU	2.9
3	E	25	LYS	2.8
2	B	57	ASN	2.8
4	F	256	TYR	2.8
4	F	339	ALA	2.8
4	F	344	ALA	2.8
2	D	431	ASP	2.8
4	F	13	VAL	2.8
1	A	95	GLY	2.8
1	A	436	GLY	2.8
2	D	377	LEU	2.8
4	F	102	PRO	2.8
1	C	341	ILE	2.8
2	D	73	MET	2.7
4	F	243	HIS	2.7
2	D	69	GLU	2.7
2	D	405	GLU	2.7
2	D	272	PRO	2.7
4	F	138	ARG	2.7
2	D	180	VAL	2.7
3	E	28	SER	2.7
3	E	24	LEU	2.7
4	F	24	THR	2.7
1	C	163	LYS	2.7
2	D	170	MET	2.6
4	F	21	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	167	SER	2.6
4	F	174	ASP	2.6
4	F	198	LYS	2.6
2	D	396	HIS	2.6
4	F	170	LEU	2.6
3	E	122	ARG	2.6
2	D	353	VAL	2.6
4	F	134	ALA	2.6
1	A	209	ILE	2.6
1	A	262	TYR	2.6
2	D	406	MET	2.6
4	F	379	HIS	2.6
4	F	333	ASN	2.6
3	E	44	ASP	2.6
2	D	83	GLN	2.5
2	D	96	GLY	2.5
4	F	135	TYR	2.5
4	F	260	ASN	2.5
2	D	95	SER	2.5
1	A	66	VAL	2.5
2	D	175	VAL	2.5
4	F	142	ARG	2.5
4	F	89	GLU	2.5
2	D	42	LEU	2.5
2	D	398	TYR	2.5
4	F	101	TYR	2.5
2	D	287	PRO	2.5
2	D	215	LEU	2.5
2	D	361	LEU	2.5
2	B	58	LYS	2.5
2	B	190	HIS	2.5
4	F	223	THR	2.4
4	F	320	MET	2.4
2	D	392	LYS	2.4
4	F	221	LEU	2.4
2	D	227	HIS	2.4
4	F	31	ARG	2.4
1	A	159	VAL	2.4
4	F	27	TRP	2.4
3	E	53	LYS	2.4
3	E	75	LYS	2.4
3	E	139	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	342	LEU	2.4
4	F	259	GLY	2.4
4	F	267	PHE	2.4
2	D	218	THR	2.4
3	E	52	LYS	2.4
4	F	241	THR	2.4
4	F	380	HIS	2.4
4	F	129	GLU	2.4
2	D	416	ASN	2.4
1	A	112	LYS	2.4
4	F	178	GLN	2.3
4	F	195	GLY	2.3
4	F	171	ASP	2.3
1	A	96	LYS	2.3
4	F	262	MET	2.3
4	F	244	CYS	2.3
1	A	365	GLY	2.3
2	D	140	GLY	2.3
2	D	320	ARG	2.3
2	D	359	ARG	2.3
2	B	323	MET	2.3
2	D	126	SER	2.3
1	C	284	GLU	2.3
3	E	27	PRO	2.3
2	D	226	ASN	2.3
2	D	228	LEU	2.3
2	D	37	HIS	2.3
2	D	85	PHE	2.3
2	D	212	PHE	2.3
1	C	337	THR	2.3
2	B	277	GLY	2.3
3	E	126	LYS	2.3
3	E	135	LYS	2.3
2	D	246	LEU	2.3
2	D	108	GLU	2.2
4	F	196	HIS	2.2
4	F	4	PHE	2.2
1	A	62	VAL	2.2
2	D	220	PRO	2.2
2	D	321	MET	2.2
4	F	246	GLN	2.2
2	D	317	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	189	PRO	2.2
2	B	38	GLY	2.2
2	D	56	GLY	2.2
4	F	347	CYS	2.2
4	F	190	LEU	2.2
4	F	275	LEU	2.2
1	C	342	GLN	2.2
1	C	282	TYR	2.2
1	A	232	SER	2.2
2	D	413	SER	2.2
1	A	221	ARG	2.2
4	F	222	ARG	2.2
4	F	145	ASN	2.2
4	F	242	ASN	2.2
2	B	80	PRO	2.2
2	D	182	PRO	2.2
2	D	214	THR	2.2
4	F	183	GLN	2.2
1	A	346	TRP	2.2
4	F	204	TRP	2.2
2	B	274	THR	2.2
4	F	353	VAL	2.1
4	F	141	GLY	2.1
2	D	288	GLU	2.1
4	F	140	GLU	2.1
4	F	261	GLU	2.1
1	A	82	THR	2.1
2	B	245	GLN	2.1
2	D	76	VAL	2.1
2	D	293	MET	2.1
2	D	178	THR	2.1
4	F	340	GLN	2.1
1	A	335	ILE	2.1
2	B	316	ILE	2.1
2	D	316	ILE	2.1
4	F	139	ARG	2.1
4	F	224	SER	2.1
2	B	165	ASN	2.1
4	F	126	ASP	2.1
3	E	50	ILE	2.1
4	F	283	ILE	2.1
1	A	149	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	332	VAL	2.1
2	D	322	SER	2.1
2	B	293	MET	2.0
4	F	234	GLN	2.0
2	D	290	THR	2.0
1	A	412	GLY	2.0
3	E	57	ALA	2.0
3	E	54	LEU	2.0
4	F	192	LEU	2.0
4	F	33	ASP	2.0
2	D	303	CYS	2.0
1	C	283	HIS	2.0
3	E	62	LYS	2.0
2	B	243	PRO	2.0
2	D	400	GLY	2.0
4	F	334	GLY	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
8	GOL	A	504	6/6	0.85	0.14	39,56,65,78	0
9	GDP	D	501	28/28	0.87	0.13	42,54,73,87	0
11	TIV	D	502	28/28	0.87	0.12	28,48,63,70	0
12	ACP	F	401	31/31	0.87	0.13	70,84,103,107	0
10	MES	B	503	12/12	0.91	0.12	44,56,63,72	0
9	GDP	B	501	28/28	0.94	0.10	25,32,41,49	0
5	GTP	C	501	32/32	0.95	0.09	20,29,38,44	0

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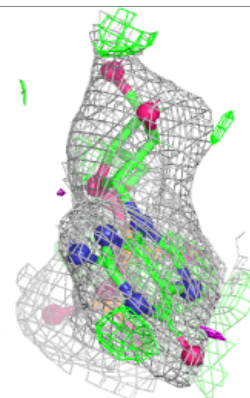
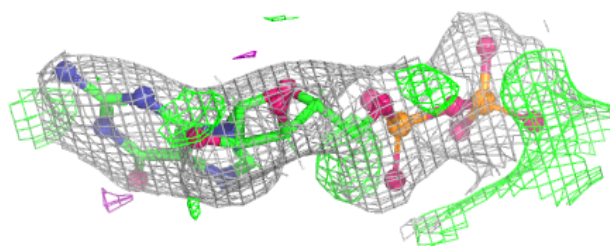
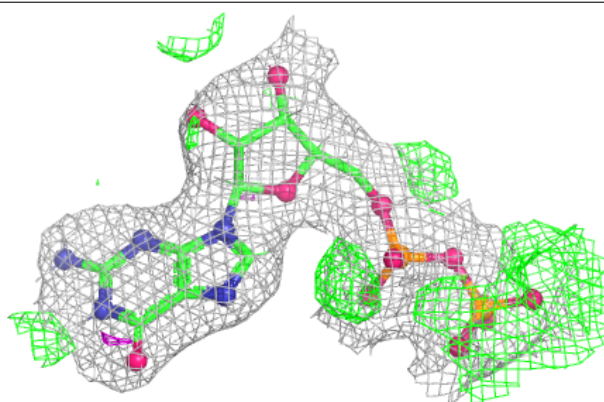
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	502	1/1	0.95	0.10	35,35,35,35	0
11	TIV	B	504	28/28	0.96	0.07	23,35,44,53	0
5	GTP	A	501	32/32	0.96	0.07	23,32,41,52	0
7	CA	A	503	1/1	0.96	0.06	56,56,56,56	0
7	CA	C	503	1/1	0.98	0.03	44,44,44,44	0
6	MG	B	502	1/1	0.98	0.10	28,28,28,28	0
6	MG	C	502	1/1	0.99	0.07	26,26,26,26	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.

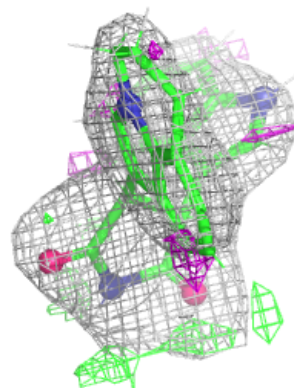
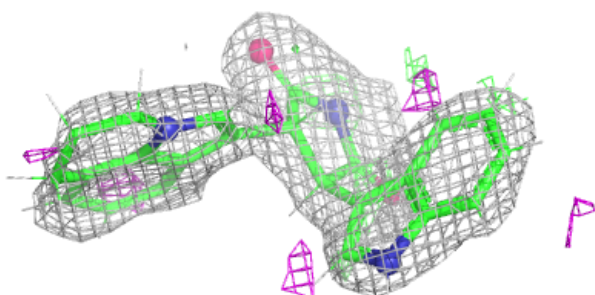
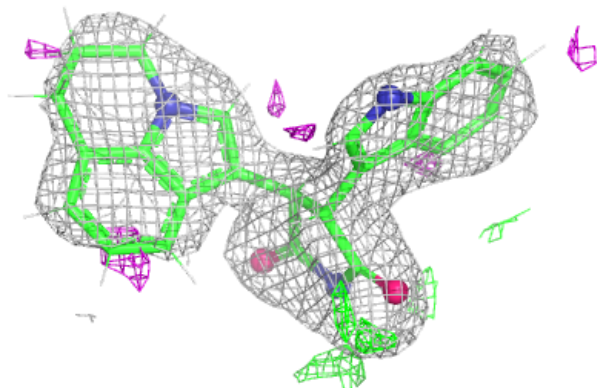
Electron density around GDP D 501:

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

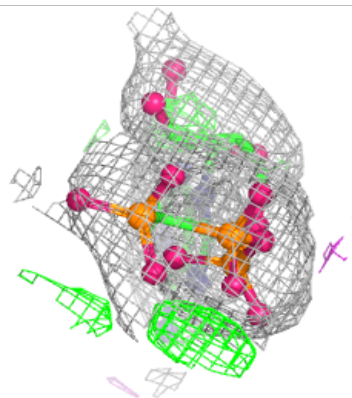
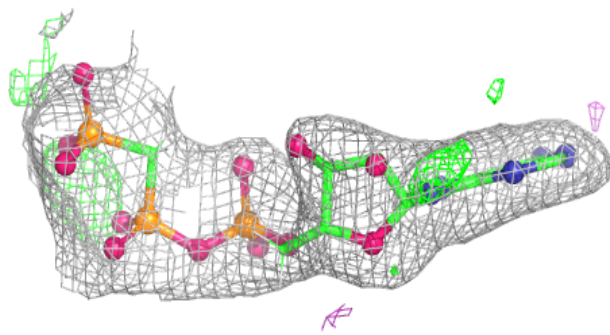
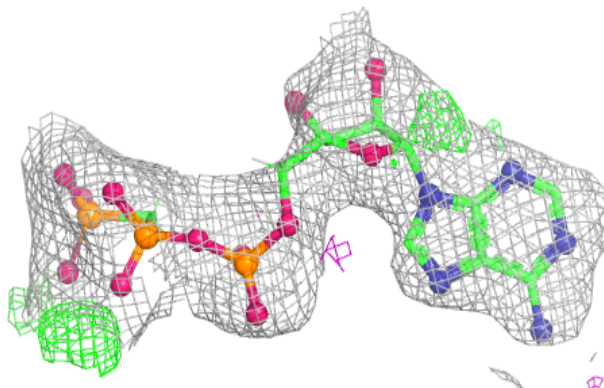


Electron density around TIV D 502:

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

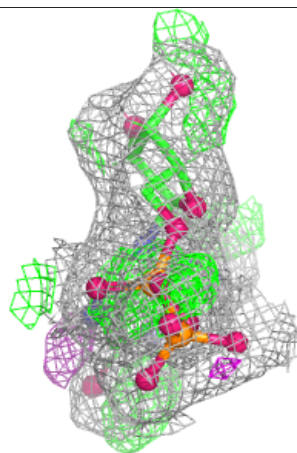
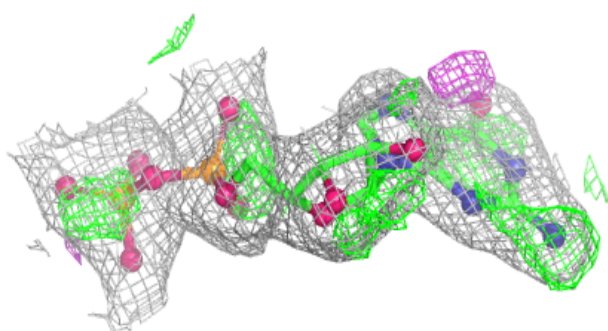
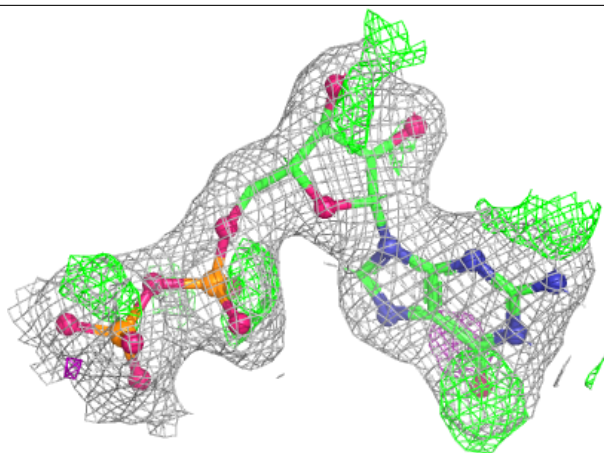
**Electron density around ACP F 401:**

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

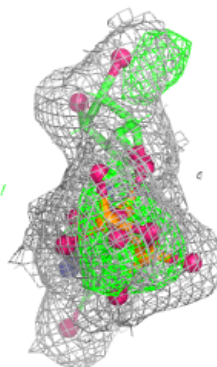
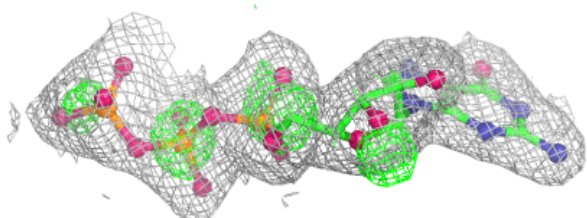
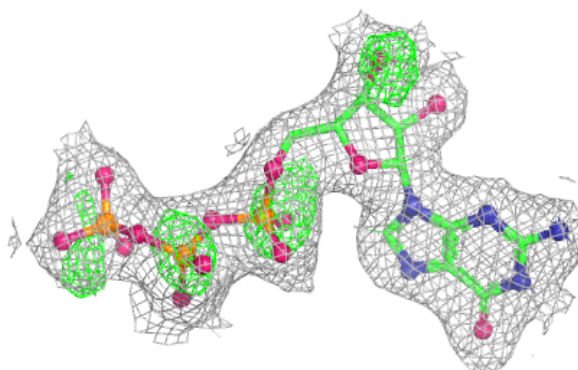


Electron density around GDP B 501:

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

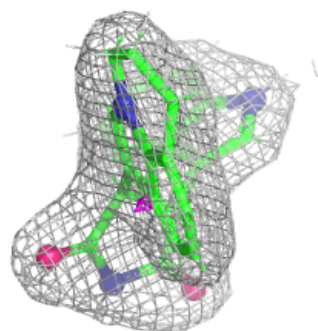
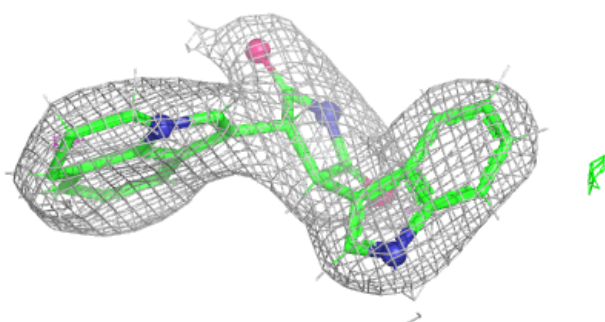
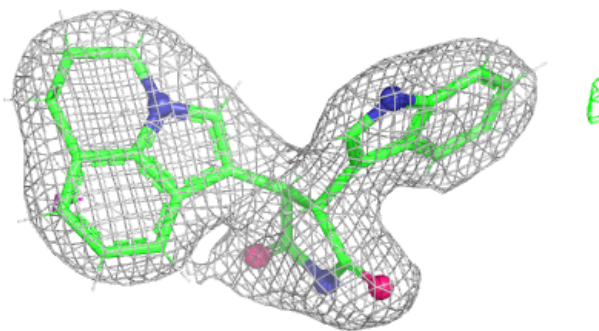
**Electron density around GTP C 501:**

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

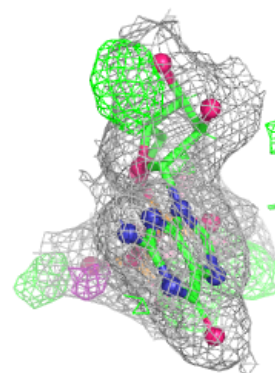
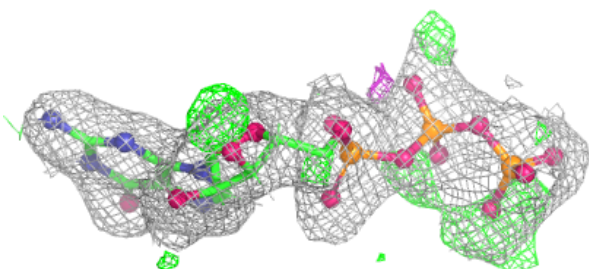
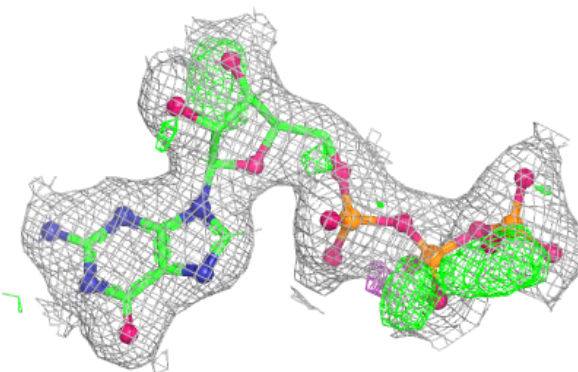


Electron density around TIV B 504:

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

**Electron density around GTP A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.