



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 12:36 pm BST

PDB ID : 5CB4
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

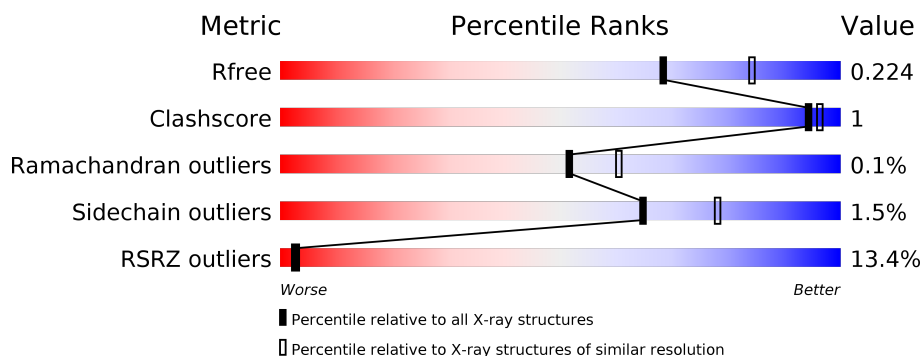
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	<div> <div>10%</div> <div>94%</div> <div>• •</div> </div>
1	C	450	<div> <div>3%</div> <div>95%</div> <div>• •</div> </div>
2	B	445	<div> <div>9%</div> <div>94%</div> <div>• •</div> </div>
2	D	445	<div> <div>18%</div> <div>89%</div> <div>5% • 5%</div> </div>
3	E	143	<div> <div>14%</div> <div>82%</div> <div>• 15%</div> </div>
4	F	384	<div> <div>24%</div> <div>82%</div> <div>5% 13%</div> </div>

2 Entry composition [i](#)

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 (three-letter code: 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		

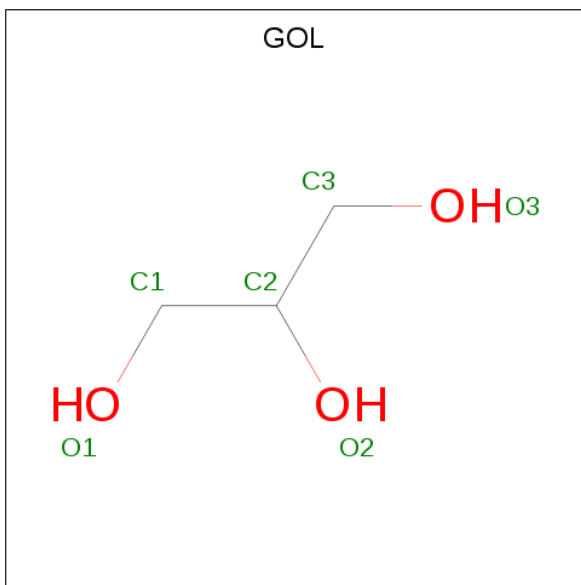
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

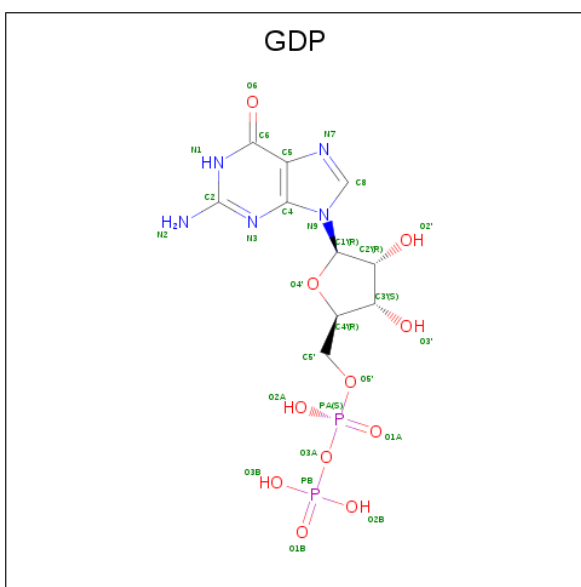
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



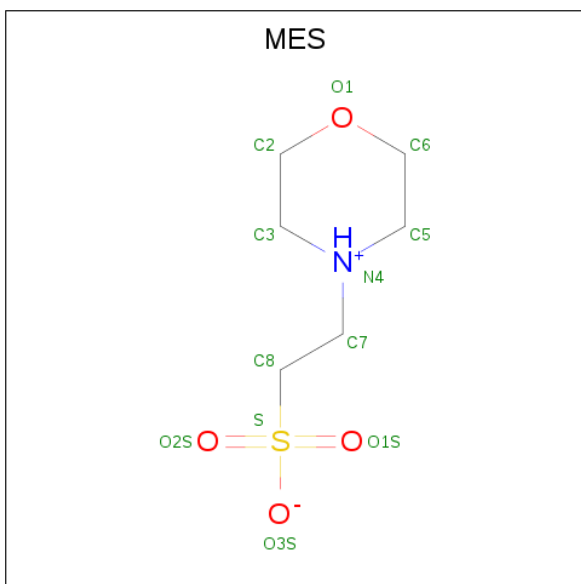
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

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



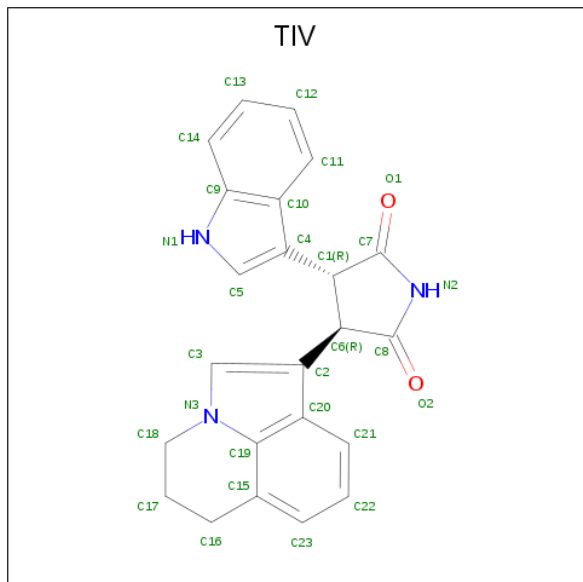
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
9	D	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



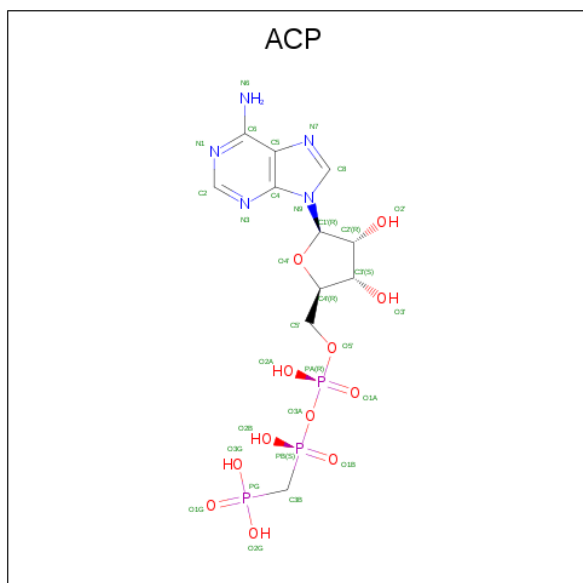
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- 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 (three-letter code: 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		

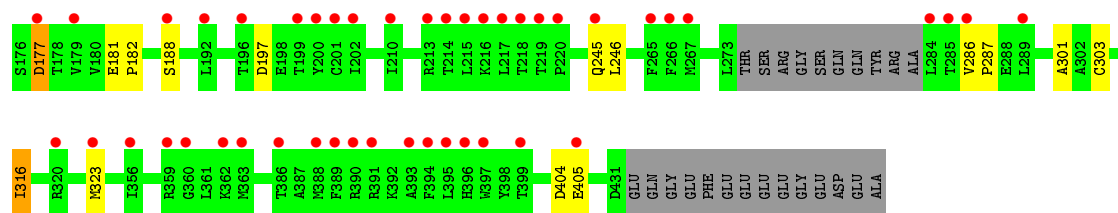
- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



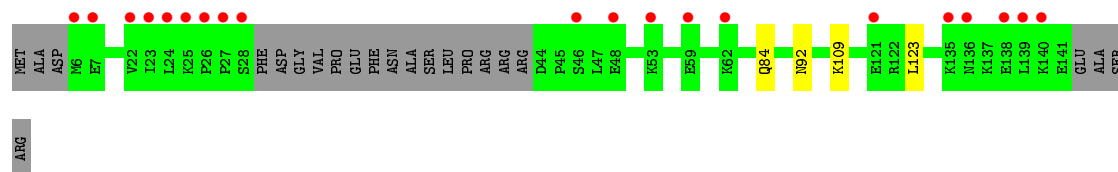
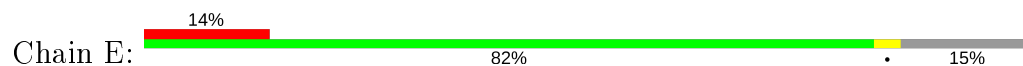
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			35	11	4	5	12	3		

- Molecule 13 is water.

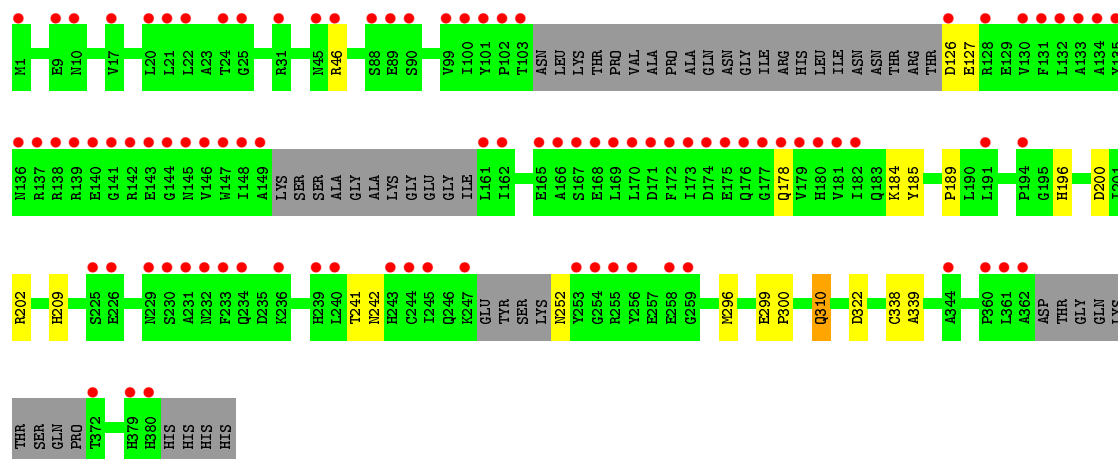
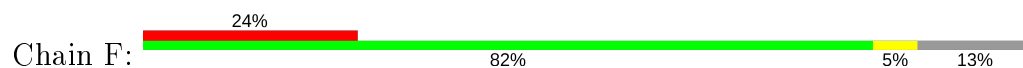
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	185	Total	O	0	0
			185	185		
13	B	164	Total	O	0	0
			164	164		
13	C	273	Total	O	0	0
			273	273		
13	D	92	Total	O	0	0
			92	92		
13	E	31	Total	O	0	0
			31	31		
13	F	84	Total	O	0	0
			84	84		



• 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 0.212 , 0.224	Depositor DCC
R_{free} test set	7564 reflections (4.90%)	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)	0.38 , 46.7	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	0.95	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: GDP, GOL, MG, TIV, GTP, ACP, MES, 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	0/3494	0.40	0/4743
1	C	0.23	0/3515	0.40	0/4772
2	B	0.23	0/3436	0.39	0/4654
2	D	0.23	0/3382	0.39	0/4581
3	E	0.22	0/1008	0.35	0/1337
4	F	0.22	0/2806	0.38	0/3791
All	All	0.23	0/17641	0.39	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	7	0
1	C	3437	3335	3348	6	0
2	B	3361	3228	3238	4	0
2	D	3309	3179	3189	12	0
3	E	1000	1014	1018	3	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	2	0
13	B	164	0	0	0	0
13	C	273	0	0	3	0
13	D	92	0	0	1	0
13	E	31	0	0	2	0
13	F	84	0	0	3	0
All	All	18326	16873	16952	43	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 (43) 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:196:HIS:NE2	13:F:502:HOH:O	2.30	0.65
2:B:145:SER:OG	2:B:188:SER:OG	2.16	0.62
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
3:E:109:LYS:NZ	13:E:202:HOH:O	2.43	0.51
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:A:253:THR:OG1	13:A:601:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:GLN:NE2	13:C:620:HOH:O	2.45	0.49
4:F:178:GLN:OE1	4:F:178:GLN:N	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
2:D:145:SER:HG	2:D:188:SER:HG	1.63	0.47
3:E:84:GLN:NE2	13:E:204:HOH:O	2.47	0.46
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.27	0.45
9:D:501:GDP:O3B	13:D:601:HOH:O	2.21	0.45
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.99	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:N	2:D:177:ASP:OD1	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:N	1:A:3:GLU:OE1	2.52	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%)	47	55
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%)	47	55
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%)	51	60

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%)	62	76
1	C	371/378 (98%)	364 (98%)	7 (2%)	57	71
2	B	369/383 (96%)	365 (99%)	4 (1%)	73	85
2	D	364/383 (95%)	357 (98%)	7 (2%)	57	71
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	88
4	F	301/342 (88%)	298 (99%)	3 (1%)	76	86
All	All	1882/1991 (94%)	1854 (98%)	28 (2%)	65	78

All (28) 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	137	HIS
2	B	190	HIS
2	B	245	GLN
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	41	ASP
2	D	137	HIS
2	D	177	ASP
2	D	245	GLN
2	D	246	LEU
2	D	316	ILE
2	D	323	MET
3	E	92	ASN
4	F	242	ASN
4	F	296	MET
4	F	310	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
8	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.29	0
12	ACP	F	401	-	27,33,33	1.75	6 (22%)	32,52,52	1.62	7 (21%)
11	TIV	B	504	-	32,33,33	2.48	7 (21%)	29,50,50	2.02	6 (20%)
9	GDP	D	501	-	24,30,30	1.10	2 (8%)	31,47,47	2.05	7 (22%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.82	6 (18%)
5	GTP	C	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.81	6 (18%)
9	GDP	B	501	6	24,30,30	1.10	2 (8%)	31,47,47	2.04	9 (29%)
10	MES	B	503	-	12,12,12	2.23	1 (8%)	14,16,16	2.55	5 (35%)
11	TIV	D	502	-	32,33,33	2.42	6 (18%)	29,50,50	1.98	6 (20%)

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
8	GOL	A	504	-	-	2/4/4/4	-
12	ACP	F	401	-	-	2/15/38/38	0/3/3/3
11	TIV	B	504	-	-	0/0/30/30	0/5/6/6
9	GDP	D	501	-	-	5/12/32/32	0/3/3/3
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	TIV	D	502	-	-	0/0/30/30	0/5/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.47	1.66	1.77
11	D	502	TIV	C4-C1	-7.16	1.46	1.52
11	D	502	TIV	C2-C6	-6.38	1.46	1.52
11	B	504	TIV	C4-C10	6.07	1.47	1.40
11	B	504	TIV	C2-C20	6.07	1.47	1.40
11	B	504	TIV	C4-C1	-5.82	1.47	1.52
11	B	504	TIV	C2-C6	-5.66	1.47	1.52
11	D	502	TIV	C4-C10	5.47	1.46	1.40
12	F	401	ACP	PB-O2B	-4.76	1.45	1.56
11	D	502	TIV	C2-C20	4.19	1.45	1.40
9	B	501	GDP	C6-C5	3.71	1.47	1.41
9	D	501	GDP	C6-C5	3.66	1.47	1.41
12	F	401	ACP	C2'-C1'	-3.43	1.48	1.53
11	D	502	TIV	C7-N2	3.33	1.41	1.37
11	D	502	TIV	C8-N2	3.28	1.41	1.37
5	A	501	GTP	C6-N1	3.19	1.38	1.33
5	C	501	GTP	C6-N1	3.08	1.38	1.33
11	B	504	TIV	C8-N2	3.08	1.41	1.37
11	B	504	TIV	C7-N2	2.90	1.41	1.37
12	F	401	ACP	C4-N3	-2.76	1.31	1.35
12	F	401	ACP	PB-O1B	2.72	1.58	1.51
12	F	401	ACP	PG-O2G	2.35	1.60	1.54
9	D	501	GDP	C5-C4	2.32	1.47	1.40
9	B	501	GDP	C5-C4	2.23	1.46	1.40
12	F	401	ACP	PG-O1G	-2.17	1.45	1.50
11	B	504	TIV	C5-N1	2.02	1.40	1.36

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	TIV	C8-N2-C7	-6.00	109.55	113.92
11	B	504	TIV	C8-N2-C7	-5.86	109.66	113.92
5	A	501	GTP	N3-C2-N1	-5.54	119.83	127.22
5	C	501	GTP	N3-C2-N1	-5.47	119.92	127.22
10	B	503	MES	C7-N4-C5	5.16	124.43	111.23
11	B	504	TIV	C16-C15-C19	-5.01	112.00	119.48
9	D	501	GDP	C6-N1-C2	4.72	123.42	115.93
10	B	503	MES	C5-N4-C3	4.70	119.41	108.83
11	D	502	TIV	C16-C15-C19	-4.70	112.47	119.48
9	B	501	GDP	C6-N1-C2	4.68	123.37	115.93
9	B	501	GDP	C6-C5-C4	-4.58	116.42	120.80
5	A	501	GTP	C2-N3-C4	4.57	120.58	115.36
5	C	501	GTP	C2-N3-C4	4.38	120.36	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C2-N3-C4	4.35	120.33	115.36
9	D	501	GDP	C6-C5-C4	-4.28	116.71	120.80
9	B	501	GDP	C2-N3-C4	4.26	120.22	115.36
9	D	501	GDP	C5-C6-N1	-4.09	117.84	123.43
9	B	501	GDP	C5-C6-N1	-3.99	117.97	123.43
11	D	502	TIV	C23-C15-C19	-3.93	113.88	118.53
9	D	501	GDP	N3-C2-N1	-3.90	122.03	127.22
9	B	501	GDP	N3-C2-N1	-3.80	122.16	127.22
11	B	504	TIV	C23-C15-C19	-3.70	114.16	118.53
11	B	504	TIV	C6-C8-N2	3.69	110.29	107.90
10	B	503	MES	C6-C5-N4	-3.46	104.86	110.10
5	A	501	GTP	PB-O3B-PG	-3.34	121.35	132.83
5	A	501	GTP	PA-O3A-PB	-3.28	121.57	132.83
5	C	501	GTP	PA-O3A-PB	-3.28	121.57	132.83
12	F	401	ACP	C3'-C2'-C1'	3.19	105.78	100.98
12	F	401	ACP	O2'-C2'-C3'	-3.15	101.64	111.82
5	C	501	GTP	PB-O3B-PG	-3.12	122.13	132.83
12	F	401	ACP	N3-C2-N1	-3.03	123.95	128.68
9	B	501	GDP	PA-O3A-PB	-2.99	122.55	132.83
12	F	401	ACP	O3G-PG-O1G	-2.96	104.57	112.39
10	B	503	MES	O2S-S-C8	2.95	110.47	106.92
11	D	502	TIV	C4-C1-C6	-2.91	109.03	114.51
11	B	504	TIV	C21-C20-C2	2.91	140.48	134.68
9	D	501	GDP	PA-O3A-PB	-2.86	123.00	132.83
5	C	501	GTP	C5-C6-N1	-2.79	119.62	123.43
12	F	401	ACP	C4-C5-N7	-2.70	106.58	109.40
5	C	501	GTP	C6-N1-C2	2.69	120.21	115.93
5	A	501	GTP	C5-C6-N1	-2.68	119.76	123.43
12	F	401	ACP	O3G-PG-C3B	2.66	112.86	106.40
11	D	502	TIV	C21-C20-C2	2.65	139.97	134.68
5	A	501	GTP	C6-N1-C2	2.59	120.05	115.93
11	D	502	TIV	C6-C8-N2	2.52	109.53	107.90
10	B	503	MES	O1S-S-C8	2.42	109.83	106.92
12	F	401	ACP	PA-O3A-PB	-2.40	124.94	132.56
9	D	501	GDP	C3'-C2'-C1'	2.18	104.27	100.98
9	B	501	GDP	C1'-N9-C4	-2.15	122.86	126.64
11	B	504	TIV	C1-C7-N2	2.11	109.27	107.90
9	B	501	GDP	C4-C5-N7	-2.04	107.28	109.40
9	B	501	GDP	C3'-C2'-C1'	2.03	104.03	100.98

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	504	GOL	O1-C1-C2-O2
8	A	504	GOL	O1-C1-C2-C3
9	D	501	GDP	PA-O3A-PB-O2B
9	D	501	GDP	PA-O3A-PB-O3B
9	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
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-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
12	F	401	ACP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O1A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
12	F	401	ACP	PB-O3A-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A

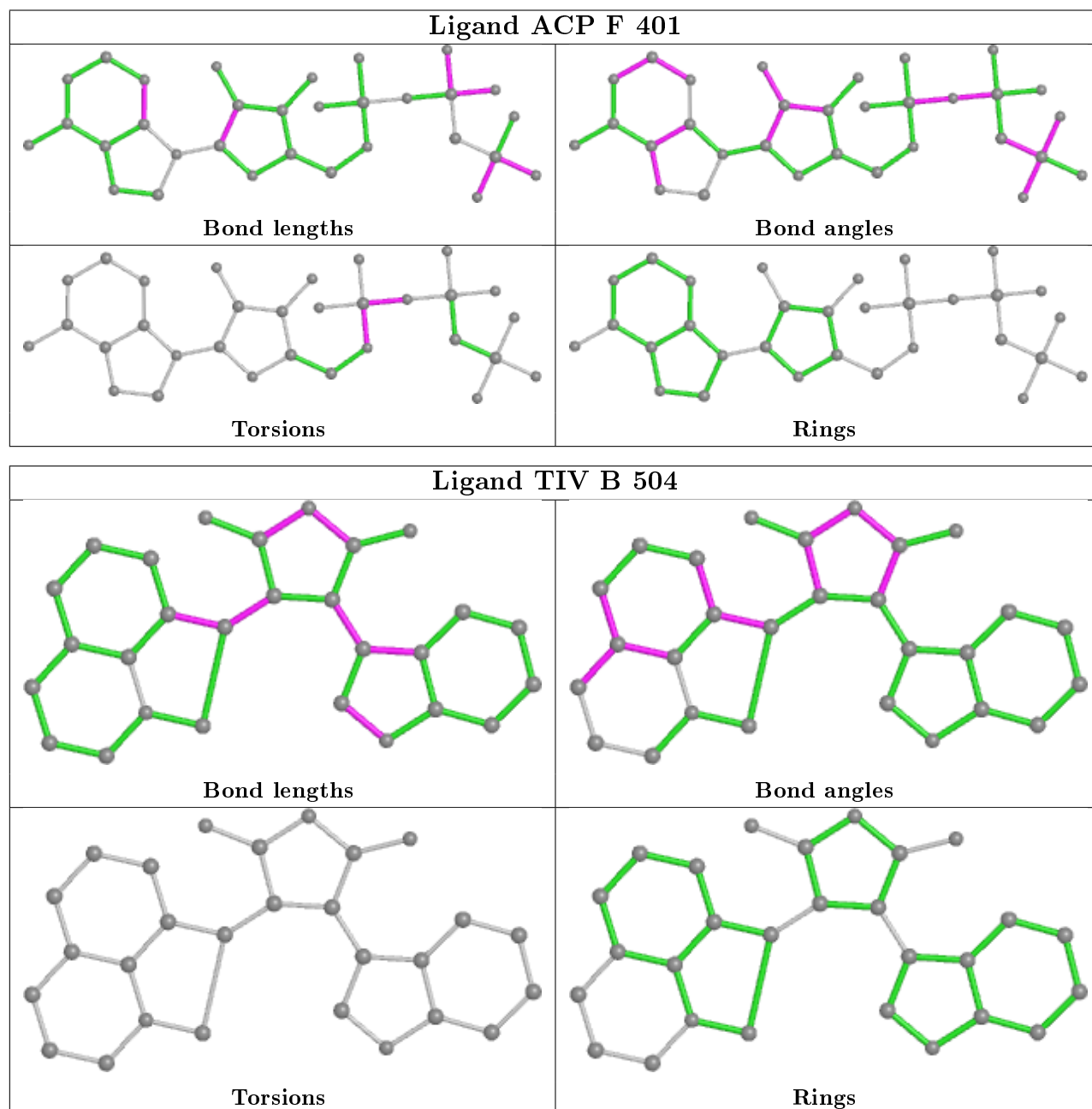
There are no ring outliers.

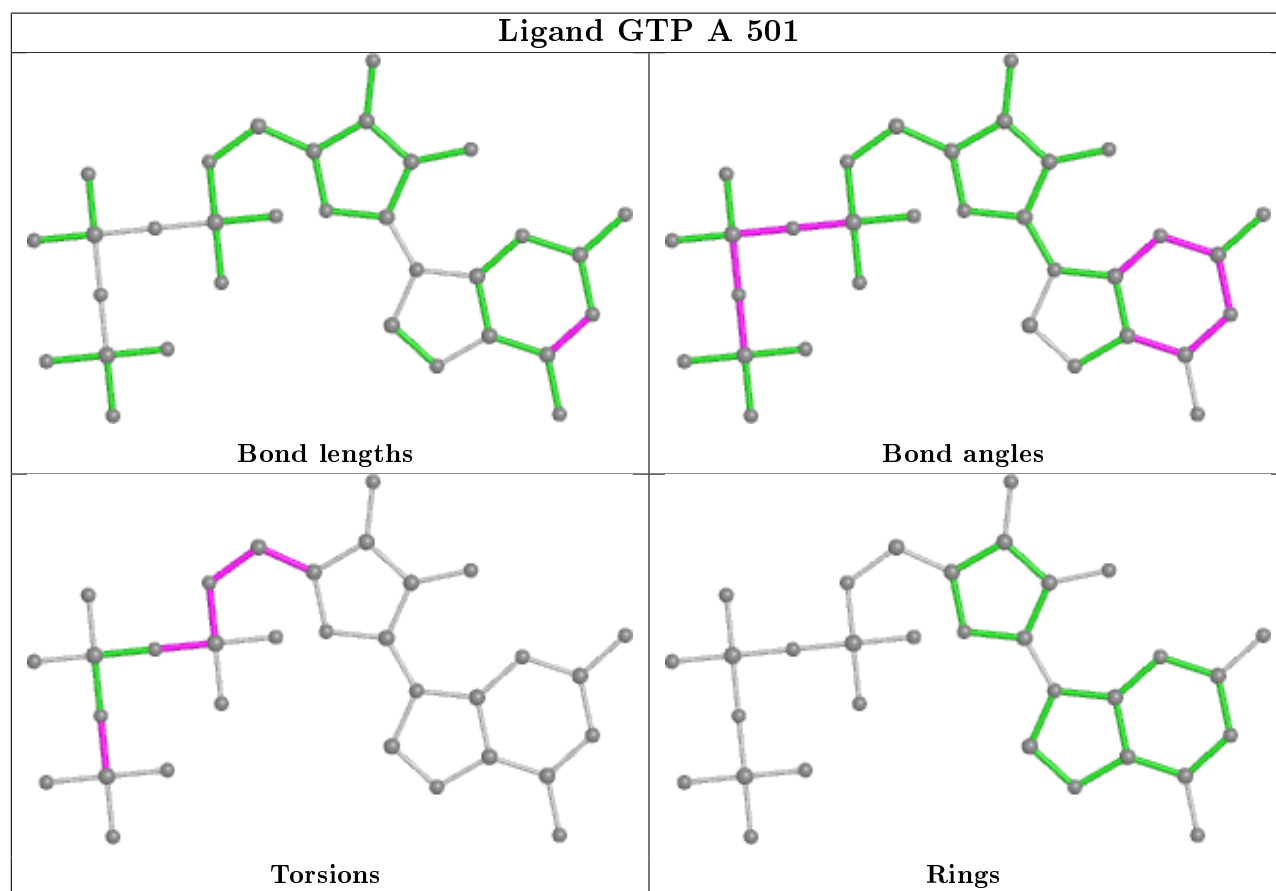
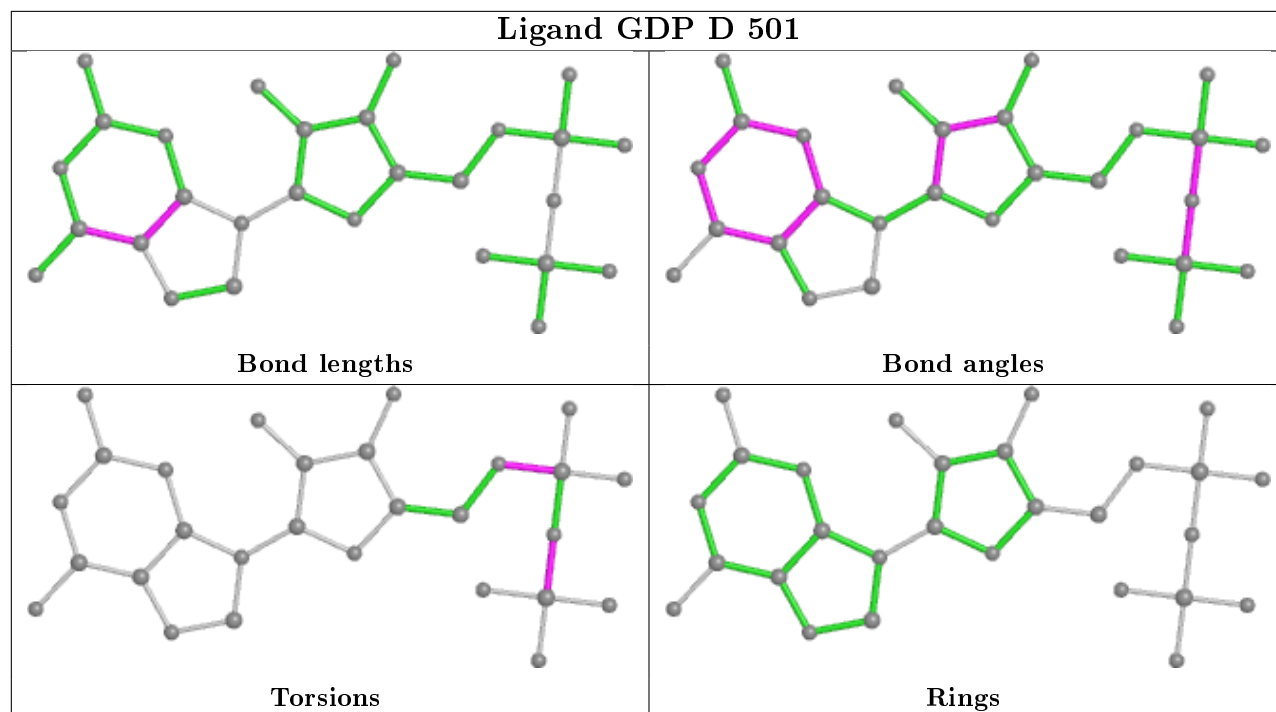
3 monomers are involved in 4 short contacts:

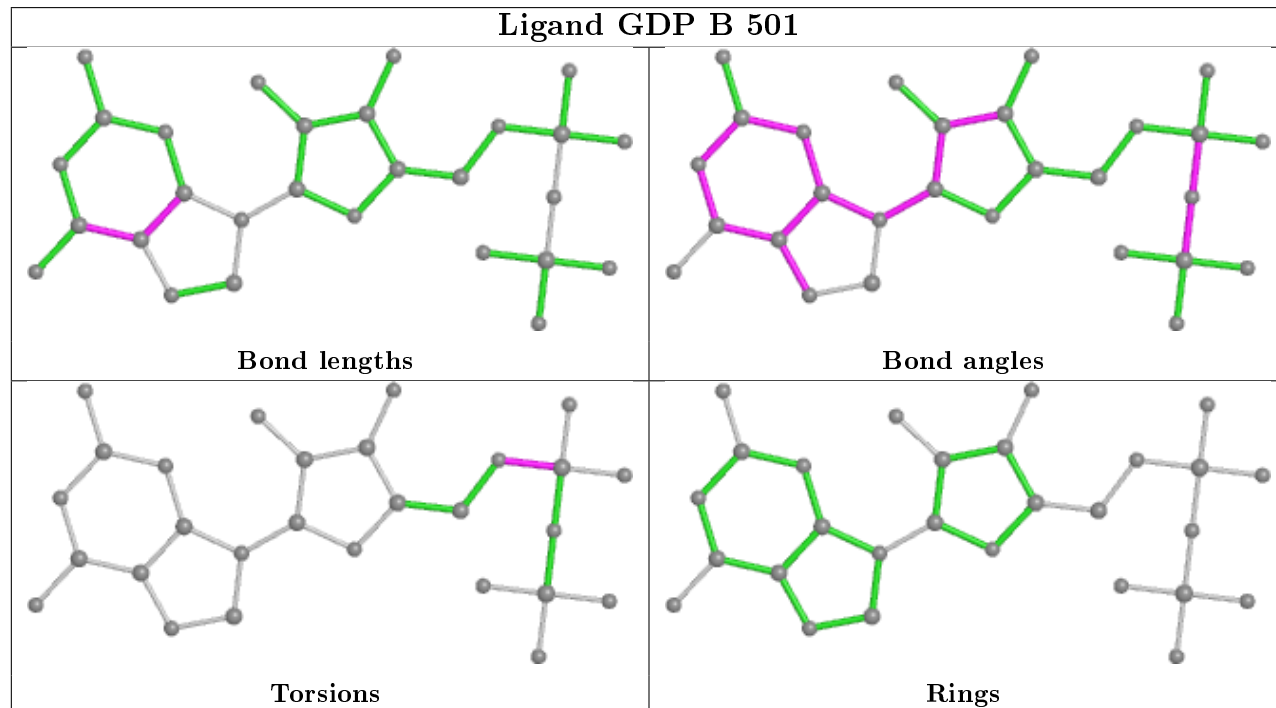
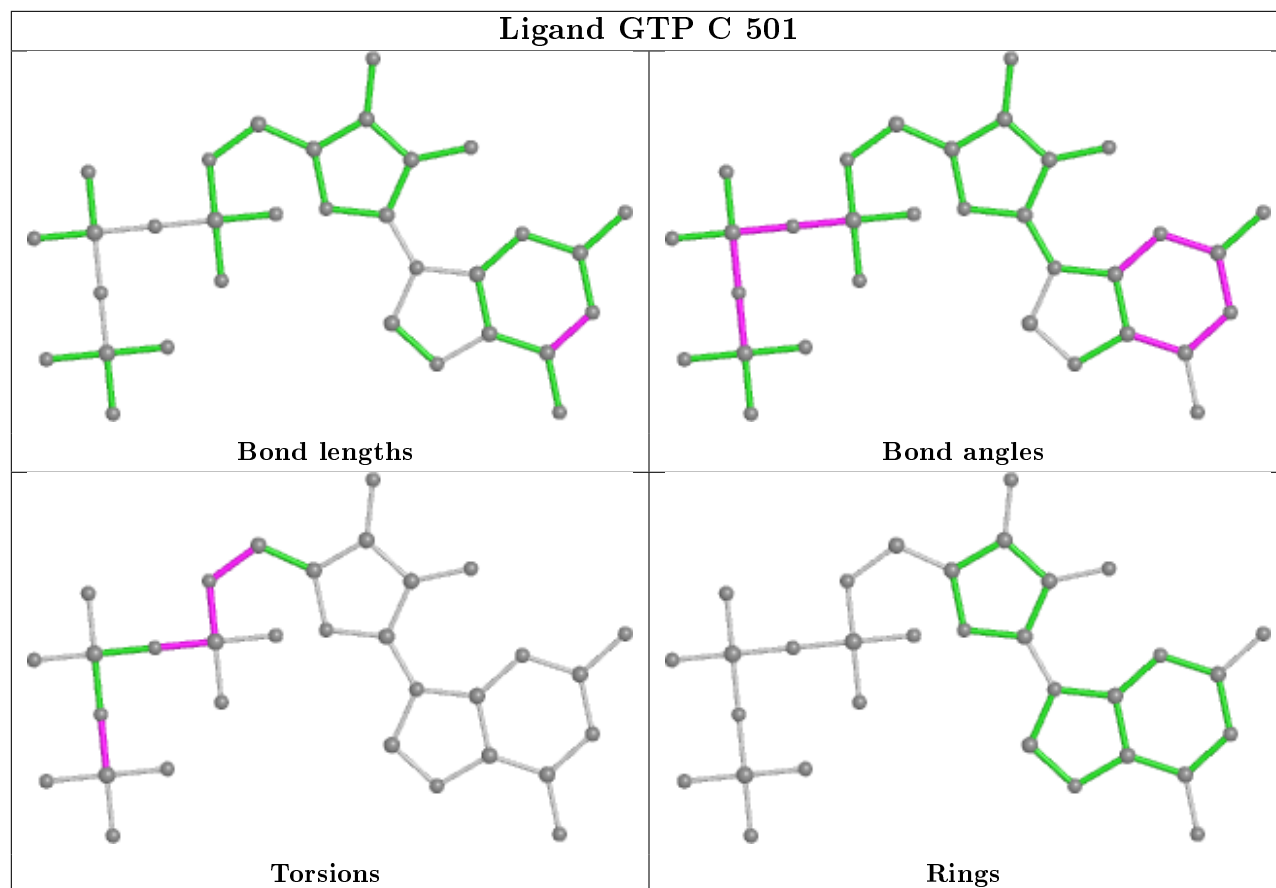
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	2	0
9	D	501	GDP	1	0
11	D	502	TIV	1	0

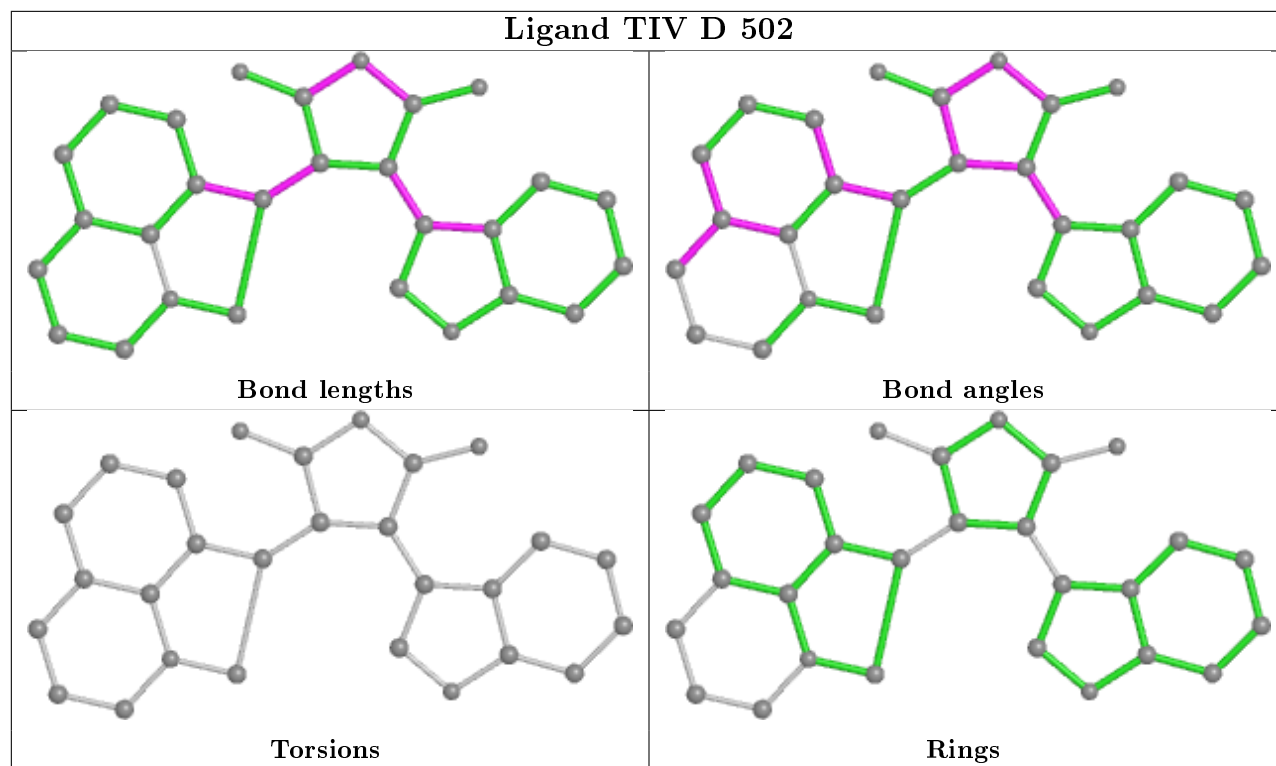
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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%)	0.71	47 (10%) 5 5	26, 42, 66, 96	0
1	C	440/450 (97%)	0.18	12 (2%) 54 52	20, 34, 54, 70	0
2	B	427/445 (95%)	0.56	41 (9%) 8 6	24, 42, 71, 121	0
2	D	421/445 (94%)	1.01	80 (19%) 1 1	27, 54, 88, 108	0
3	E	121/143 (84%)	0.83	20 (16%) 1 1	32, 56, 84, 98	0
4	F	334/384 (86%)	1.48	92 (27%) 0 0	33, 64, 119, 142	0
All	All	2180/2317 (94%)	0.75	292 (13%) 3 2	20, 46, 89, 142	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	11.8
4	F	161	LEU	9.3
4	F	138	ARG	8.7
4	F	169	LEU	8.6
2	D	55	THR	7.4
2	B	279	GLN	7.2
4	F	177	GLY	7.2
1	A	282	TYR	7.1
4	F	175	GLU	7.0
3	E	139	LEU	6.9
2	D	390	ARG	6.9
2	D	285	THR	6.8
4	F	236	LYS	6.7
4	F	103	THR	6.7
4	F	139	ARG	6.5
2	D	394	PHE	6.5
4	F	231	ALA	6.5
2	B	56	GLY	6.5
4	F	143	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
2	B	55	THR	6.4
2	D	284	LEU	6.3
4	F	176	GLN	6.2
4	F	102	PRO	6.1
4	F	178	GLN	6.1
2	D	219	THR	6.1
4	F	142	ARG	6.0
2	B	57	ASN	6.0
4	F	101	TYR	6.0
4	F	132	LEU	5.9
4	F	130	VAL	5.9
4	F	372	THR	5.9
2	D	397	TRP	5.8
4	F	253	TYR	5.7
4	F	134	ALA	5.5
4	F	234	GLN	5.4
4	F	88	SER	5.4
4	F	225	SER	5.4
2	D	391	ARG	5.3
4	F	149	ALA	5.3
4	F	137	ARG	5.2
4	F	131	PHE	5.0
4	F	232	ASN	4.9
1	A	281	ALA	4.9
4	F	362	ALA	4.9
4	F	135	TYR	4.8
4	F	361	LEU	4.8
4	F	182	ILE	4.7
4	F	20	LEU	4.6
2	B	428	ALA	4.6
4	F	194	PRO	4.6
2	D	245	GLN	4.6
4	F	170	LEU	4.6
2	D	167	PHE	4.6
4	F	247	LYS	4.5
4	F	144	GLY	4.4
4	F	172	PHE	4.3
2	D	395	LEU	4.3
1	A	346	TRP	4.2
4	F	24	THR	4.2
4	F	100	ILE	4.2
3	E	140	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	94	GLN	4.2
2	D	168	SER	4.2
2	D	359	ARG	4.2
4	F	244	CYS	4.2
4	F	233	PHE	4.1
4	F	180	HIS	4.1
4	F	167	SER	4.1
3	E	27	PRO	4.1
4	F	25	GLY	4.1
2	D	54	ALA	4.1
2	D	135	LEU	4.1
1	A	365	GLY	4.0
2	D	166	THR	4.0
3	E	7	GLU	4.0
4	F	128	ARG	4.0
2	D	137	HIS	4.0
4	F	240	LEU	4.0
2	D	360	GLY	4.0
1	A	235	VAL	3.9
4	F	99	VAL	3.9
1	A	201	ALA	3.9
2	B	58	LYS	3.9
1	A	262	TYR	3.9
4	F	140	GLU	3.8
2	D	286	VAL	3.8
2	D	136	THR	3.8
2	B	280	GLN	3.8
1	A	202	PHE	3.8
1	C	440	VAL	3.7
2	D	56	GLY	3.7
4	F	22	LEU	3.6
2	D	125	GLU	3.6
2	D	356	ILE	3.6
4	F	21	LEU	3.6
4	F	90	SER	3.6
2	D	1	MET	3.6
2	D	362	LYS	3.5
4	F	1	MET	3.5
2	D	405	GLU	3.5
2	D	177	ASP	3.5
4	F	166	ALA	3.4
4	F	145	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	3.4
2	D	200	TYR	3.4
2	D	388	MET	3.4
1	C	200	CYS	3.4
1	A	238	ILE	3.4
1	A	171	ILE	3.4
2	D	217	LEU	3.4
1	A	200	CYS	3.4
3	E	6	MET	3.3
2	D	7	ILE	3.3
2	D	37	HIS	3.3
4	F	46	ARG	3.3
2	D	30	ILE	3.3
1	A	20	CYS	3.3
3	E	24	LEU	3.3
4	F	146	VAL	3.3
2	D	126	SER	3.3
4	F	17	VAL	3.3
3	E	26	PRO	3.2
2	B	142	GLY	3.2
4	F	179	VAL	3.2
2	D	320	ARG	3.2
1	A	203	MET	3.2
2	B	166	THR	3.2
1	A	163	LYS	3.2
1	A	58	ALA	3.2
4	F	181	VAL	3.2
4	F	133	ALA	3.1
2	B	54	ALA	3.1
4	F	136	ASN	3.0
4	F	162	ILE	3.0
3	E	25	LYS	3.0
2	B	38	GLY	3.0
4	F	254	GLY	3.0
2	D	199	THR	3.0
2	D	81	PHE	2.9
1	A	234	ILE	2.9
2	D	216	LYS	2.9
2	D	323	MET	2.9
1	A	416	GLY	2.9
2	B	282	ARG	2.9
1	A	172	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	277	GLY	2.9
3	E	135	LYS	2.9
2	D	95	SER	2.9
2	D	179	VAL	2.8
3	E	46	SER	2.8
1	A	88	HIS	2.8
4	F	226	GLU	2.8
2	B	41	ASP	2.8
4	F	174	ASP	2.8
1	A	170	SER	2.8
1	C	340	SER	2.8
4	F	344	ALA	2.8
2	B	37	HIS	2.8
4	F	171	ASP	2.7
4	F	141	GLY	2.7
1	A	430	LYS	2.7
1	C	201	ALA	2.7
3	E	136	ASN	2.7
1	A	348	PRO	2.7
4	F	239	HIS	2.7
2	B	320	ARG	2.7
4	F	256	TYR	2.7
4	F	126	ASP	2.7
4	F	168	GLU	2.7
2	D	165	ASN	2.7
2	D	192	LEU	2.7
2	B	72	THR	2.7
4	F	9	GLU	2.7
2	D	175	VAL	2.7
2	D	201	CYS	2.7
2	D	396	HIS	2.7
2	B	266	PHE	2.7
2	D	220	PRO	2.7
2	D	218	THR	2.7
1	A	141	PHE	2.6
2	B	167	PHE	2.6
3	E	121	GLU	2.6
2	B	362	LYS	2.6
2	D	289	LEU	2.6
1	A	237	SER	2.6
3	E	28	SER	2.6
4	F	255	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	138	GLU	2.6
2	B	276	ARG	2.6
1	A	167	LEU	2.6
4	F	229	ASN	2.6
2	B	200	TYR	2.6
2	D	9	ALA	2.6
1	A	136	LEU	2.6
2	B	427	ASP	2.6
4	F	89	GLU	2.6
2	D	149	THR	2.6
2	D	266	PHE	2.6
2	D	57	ASN	2.5
2	D	92	PHE	2.5
1	A	236	SER	2.5
4	F	380	HIS	2.5
2	D	53	GLU	2.5
2	D	202	ILE	2.5
2	D	145	SER	2.5
3	E	48	GLU	2.5
2	B	139	LEU	2.5
2	B	283	ALA	2.5
2	B	201	CYS	2.5
2	D	169	VAL	2.5
4	F	379	HIS	2.5
2	D	399	THR	2.5
1	A	137	VAL	2.5
2	D	59	TYR	2.5
3	E	53	LYS	2.4
2	D	393	ALA	2.4
1	C	202	PHE	2.4
4	F	258	GLU	2.4
2	D	58	LYS	2.4
4	F	360	PRO	2.4
2	D	265	PHE	2.4
2	B	278	SER	2.4
2	D	13	GLY	2.4
1	A	209	ILE	2.4
2	D	214	THR	2.4
2	D	215	LEU	2.4
2	B	275	SER	2.4
4	F	31	ARG	2.4
2	D	389	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	245	ILE	2.4
2	D	363	MET	2.3
1	A	42	ILE	2.3
4	F	165	GLU	2.3
2	B	83	GLN	2.3
2	D	138	SER	2.3
2	B	33	THR	2.3
2	B	199	THR	2.3
1	A	138	PHE	2.3
2	B	125	GLU	2.3
4	F	147	TRP	2.3
2	B	219	THR	2.3
1	A	142	GLY	2.3
2	D	134	GLN	2.3
4	F	10	ASN	2.3
1	C	190	THR	2.2
2	B	274	THR	2.2
1	A	139	HIS	2.2
1	A	180	ALA	2.2
1	A	303	VAL	2.2
2	B	165	ASN	2.2
1	A	17	GLY	2.2
1	A	173	PRO	2.2
2	D	210	ILE	2.2
1	C	266	HIS	2.2
1	C	270	ALA	2.2
2	B	265	PHE	2.2
2	D	146	GLY	2.2
2	D	188	SER	2.2
1	C	341	ILE	2.2
2	D	196	THR	2.2
2	D	213	ARG	2.2
2	B	39	ASP	2.2
4	F	243	HIS	2.2
1	C	260	VAL	2.1
1	A	270	ALA	2.1
1	C	167	LEU	2.1
4	F	191	LEU	2.1
1	A	204	VAL	2.1
1	A	24	TYR	2.1
2	B	36	TYR	2.1
1	A	240	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	62	LYS	2.1
4	F	45	ASN	2.1
2	D	39	ASP	2.1
1	A	434	GLU	2.1
1	A	231	ILE	2.1
4	F	259	GLY	2.1
1	A	239	THR	2.1
1	A	140	SER	2.1
3	E	23	ILE	2.1
2	B	253	LEU	2.1
4	F	230	SER	2.1
3	E	59	GLU	2.1
1	C	357	TYR	2.1
2	D	267	MET	2.0
4	F	148	ILE	2.0
2	D	386	THR	2.0
2	D	10	GLY	2.0
2	B	322	SER	2.0
1	A	56	THR	2.0
2	B	202	ILE	2.0
3	E	22	VAL	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 carbohydrates 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(\AA^2)	Q<0.9
11	TIV	D	502	28/28	0.88	0.19	28,48,63,70	0
12	ACP	F	401	31/31	0.90	0.17	70,84,103,107	0

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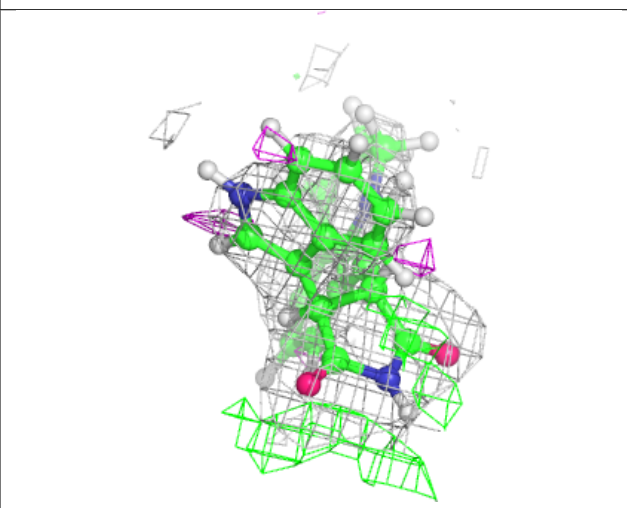
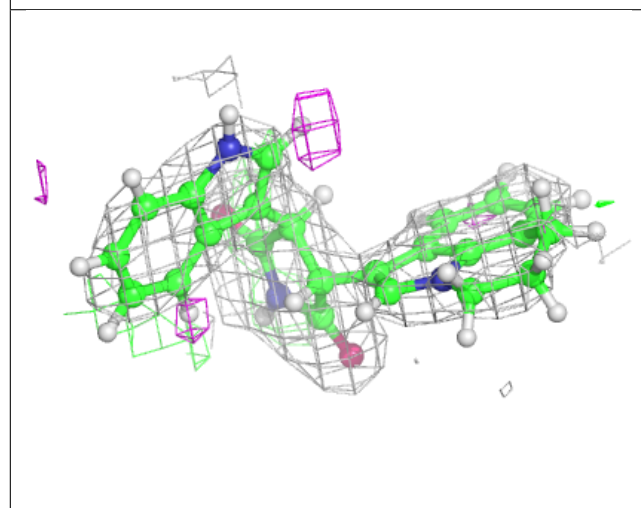
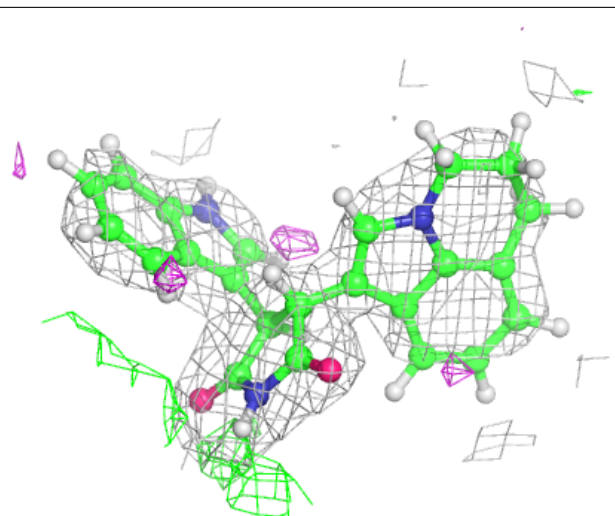
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	A	503	1/1	0.90	0.08	56,56,56,56	0
6	MG	A	502	1/1	0.90	0.21	35,35,35,35	0
8	GOL	A	504	6/6	0.92	0.15	39,56,65,78	0
9	GDP	D	501	28/28	0.94	0.16	42,54,73,87	0
10	MES	B	503	12/12	0.95	0.14	44,56,63,72	0
9	GDP	B	501	28/28	0.95	0.20	25,32,41,49	0
7	CA	C	503	1/1	0.97	0.04	44,44,44,44	0
11	TIV	B	504	28/28	0.97	0.19	23,35,44,53	0
5	GTP	A	501	32/32	0.97	0.19	23,32,41,52	0
5	GTP	C	501	32/32	0.97	0.18	20,29,38,44	0
6	MG	C	502	1/1	0.98	0.17	26,26,26,26	0
6	MG	B	502	1/1	0.99	0.22	28,28,28,28	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.

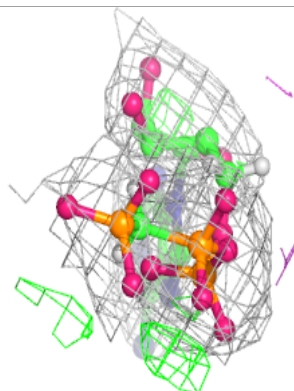
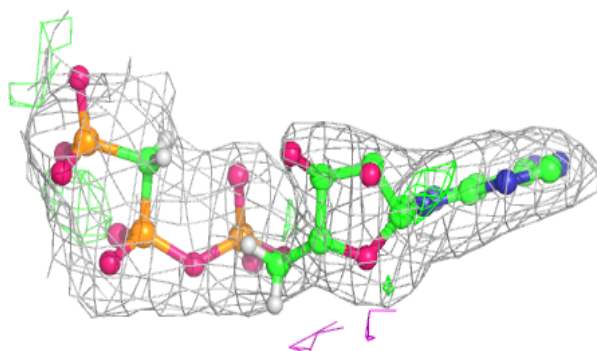
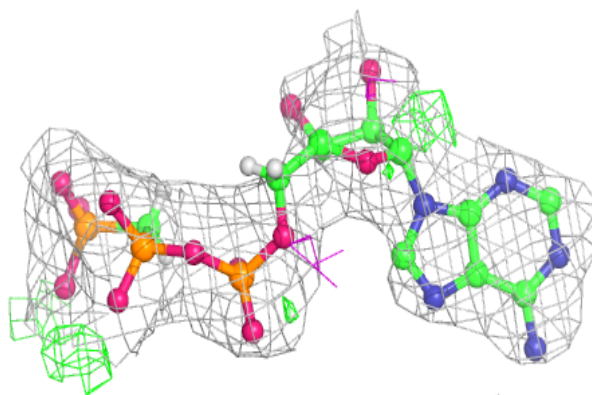
Electron density around TIV D 502:

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

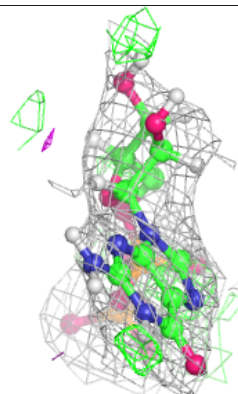
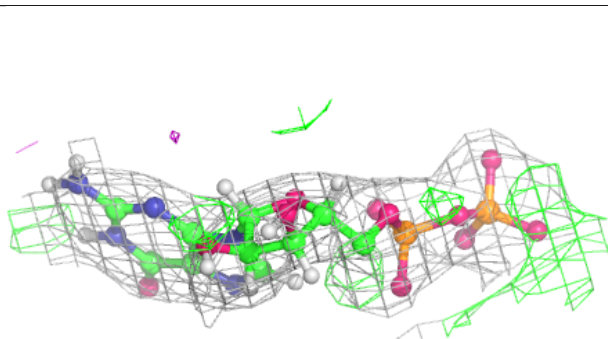
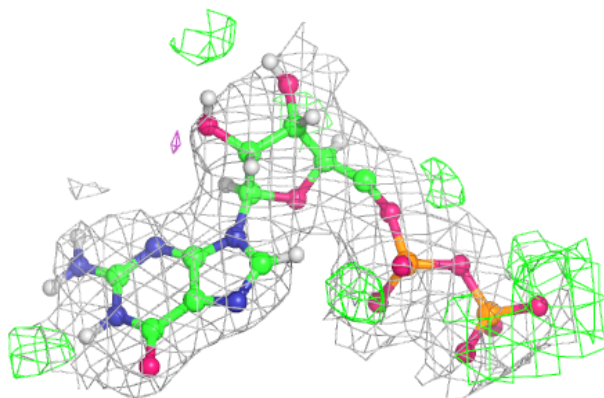


Electron density around ACP F 401:

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

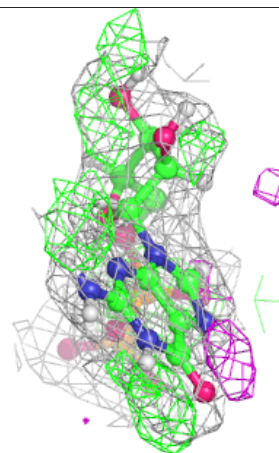
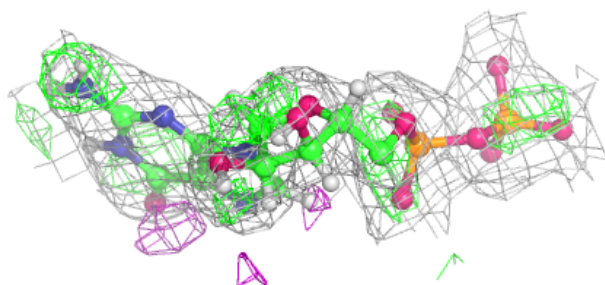
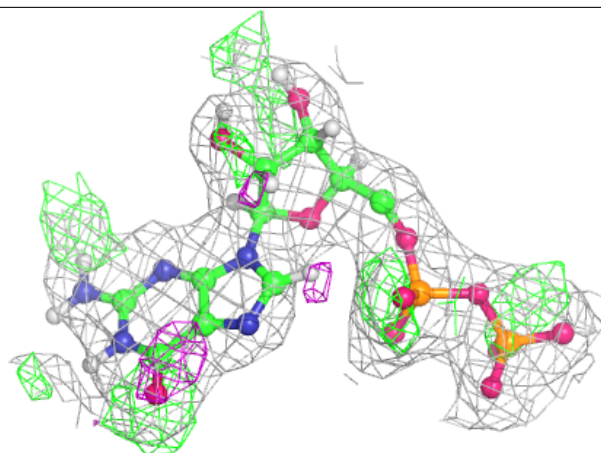
**Electron density around GDP D 501:**

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

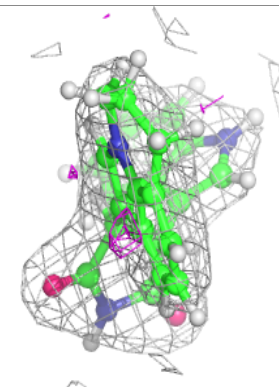
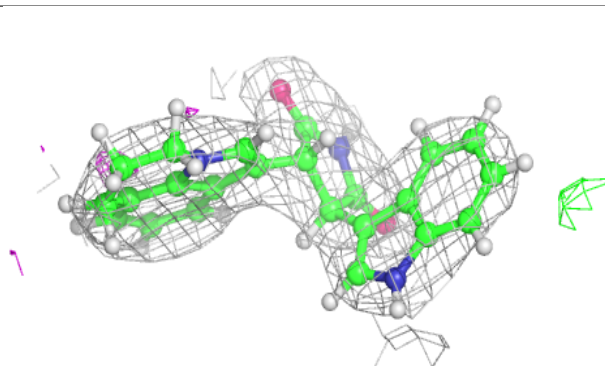
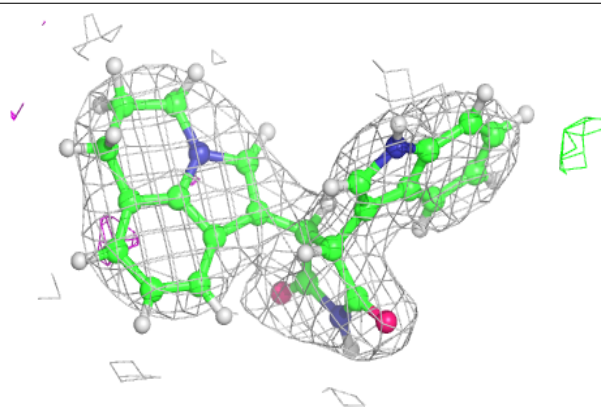


Electron density around GDP B 501:

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

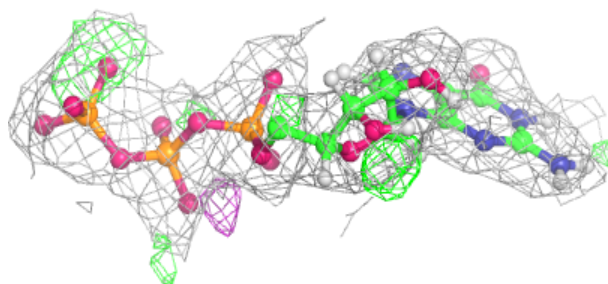
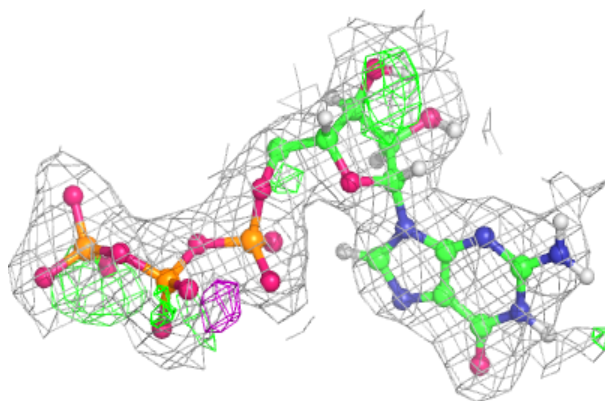
**Electron density around TIV B 504:**

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

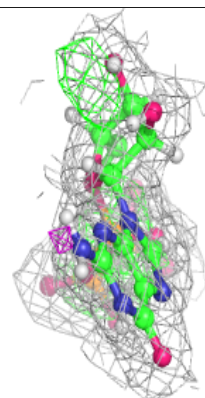
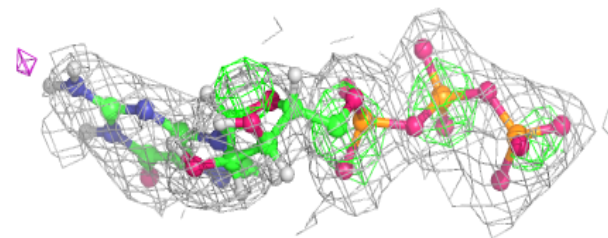
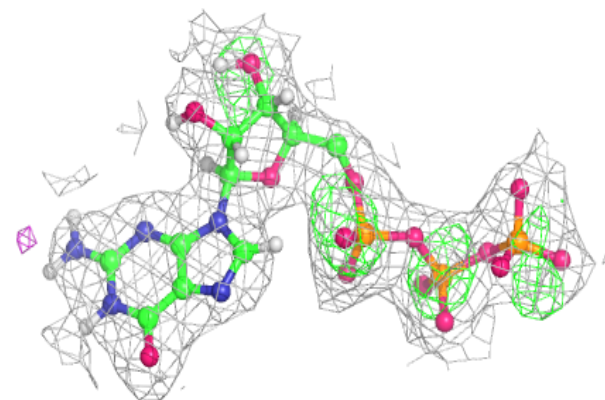


Electron density around GTP A 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.