



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 08:00 PM BST

PDB ID : 7JFR
Title : Auristatin bound to tubulin
Authors : Moquist, P.N.; Waight, A.
Deposited on : 2020-07-17
Resolution : 2.35 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 : 2.14.4
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) : 2.14.4

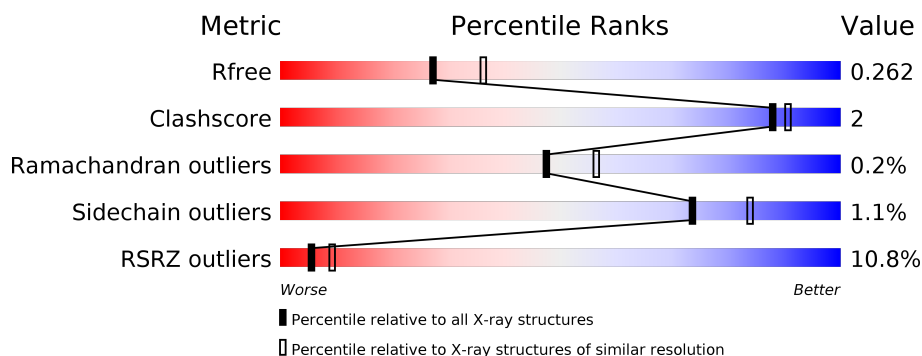
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	440	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>
1	C	440	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
2	B	445	<div> <div>2%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
2	D	445	<div> <div>10%</div> <div>91%</div> <div>5%</div> <div>5%</div> </div>
3	E	138	<div> <div>12%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
4	F	378	<div> <div>35%</div> <div>79%</div> <div>12%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	L	5	 A horizontal bar chart showing the quality of chain 5. The bar is divided into three segments: a green segment representing 60%, a yellow segment representing 20%, and an orange segment representing 20%. The percentages are labeled below the corresponding segments.

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 35292 atoms, of which 17339 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	439	Total	C	H	N	O	S	14	8	0
			6864	2203	3397	584	657	23			
1	C	440	Total	C	H	N	O	S	0	12	0
			6898	2212	3411	585	666	24			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	428	Total	C	H	N	O	S	39	14	0
			6762	2158	3336	580	659	29			
2	D	422	Total	C	H	N	O	S	0	4	0
			6533	2093	3205	563	645	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	6	0
			2108	644	1066	186	206	6			

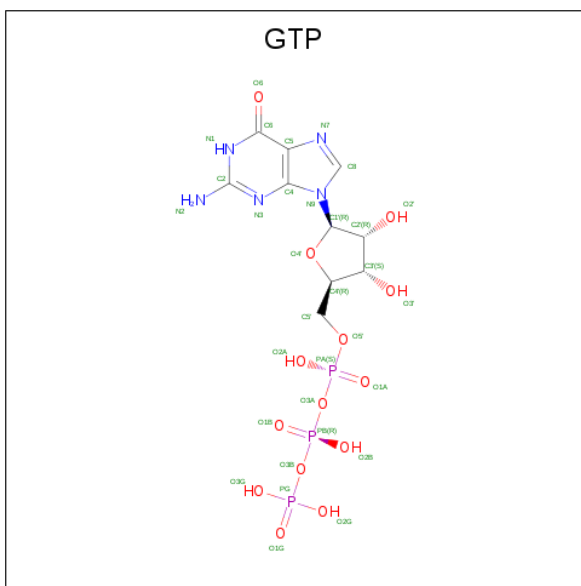
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	344	Total	C	H	N	O	S	0	2	0
			5605	1808	2787	479	517	14			

- Molecule 5 is a protein called Auristatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	5	Total	C	H	N	O	0	0	0
			147	49	85	5	8			

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

$$\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3).$$


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 41	C 10	H 9	N 5	O 14	P 3	0	0
6	C	1	Total 41	C 10	H 9	N 5	O 14	P 3	0	0

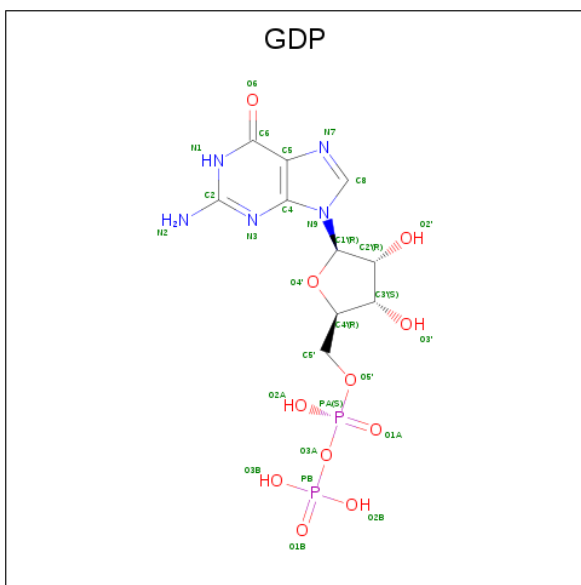
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Mg 2 2	0	0
7	A	1	Total Mg 1 1	0	0
7	C	2	Total Mg 2 2	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

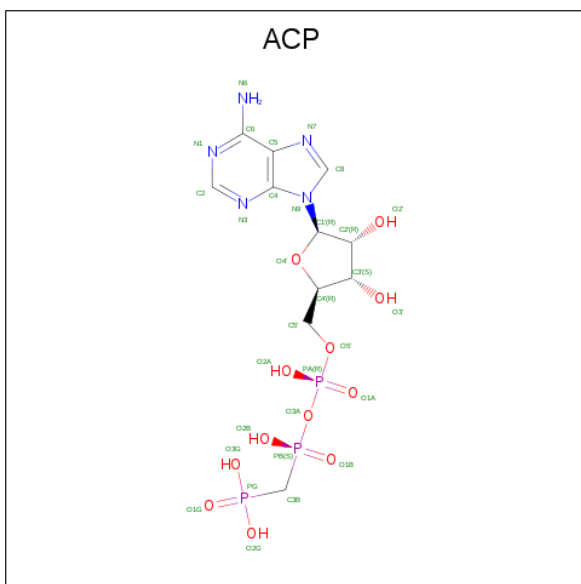
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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 PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

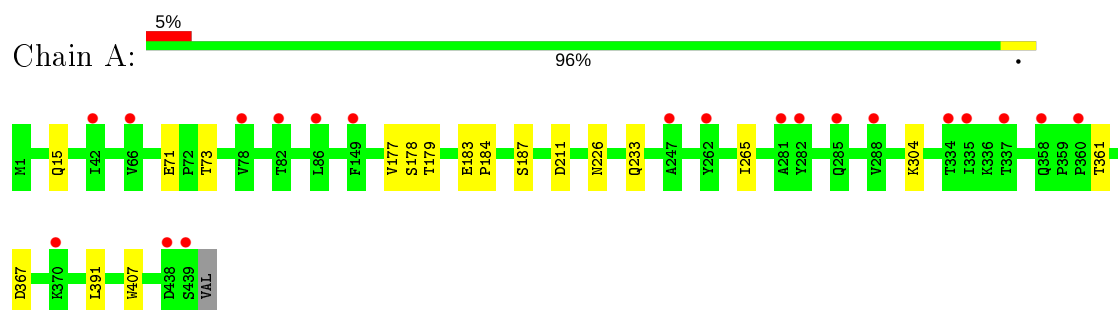
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	17	Total 17	O 17	0	0
11	B	53	Total 53	O 53	0	0
11	C	46	Total 46	O 46	0	0
11	D	20	Total 20	O 20	0	0
11	E	13	Total 13	O 13	0	0
11	F	17	Total 17	O 17	0	0

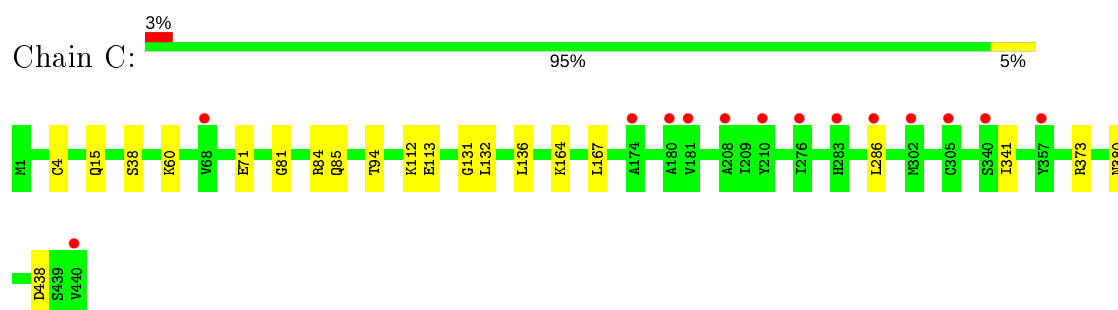
3 Residue-property plots [i](#)

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

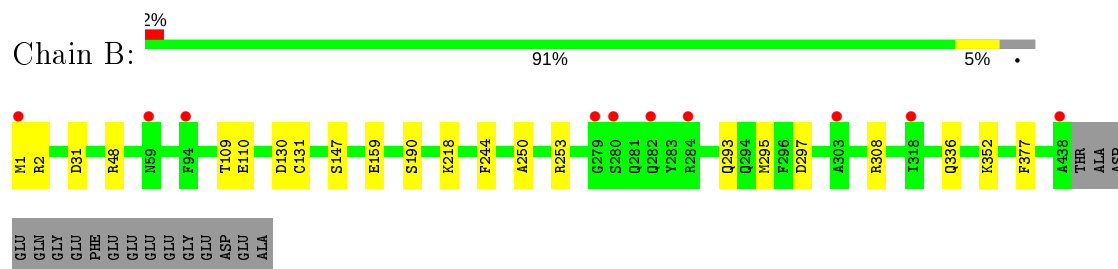
- Molecule 1: Tubulin alpha-1B chain



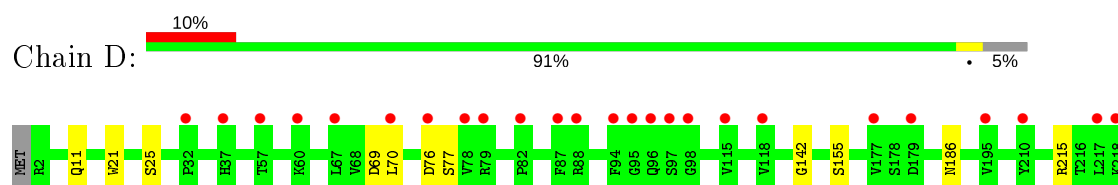
- Molecule 1: Tubulin alpha-1B chain

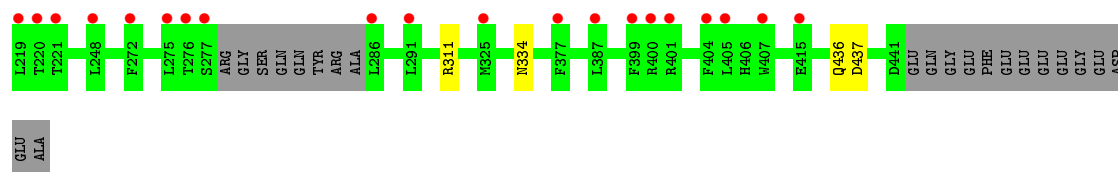


- Molecule 2: Tubulin beta-2B chain

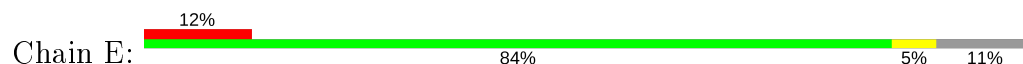


- Molecule 2: Tubulin beta-2B chain

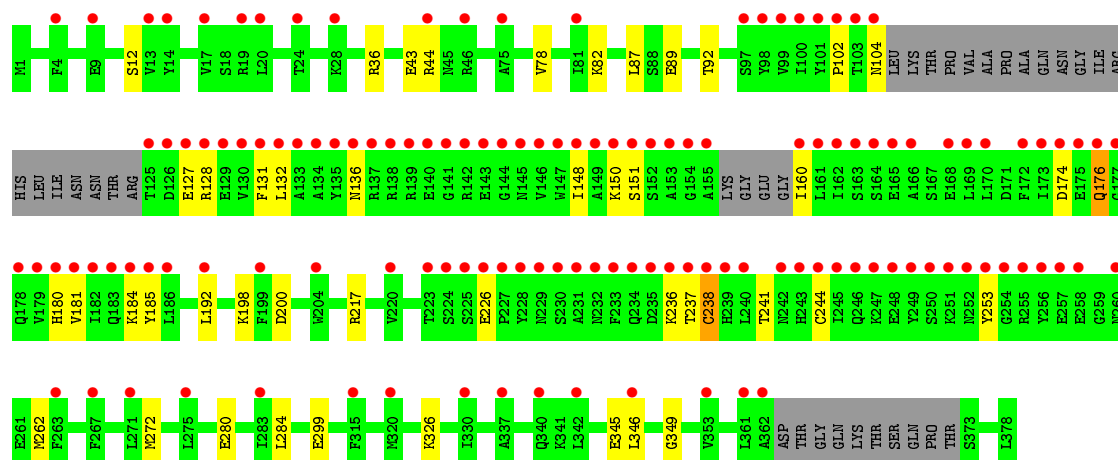
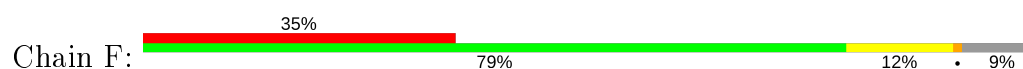




- Molecule 3: Stathmin-4



- Molecule 4: Uncharacterized protein



- Molecule 5: Auristatin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.49Å 155.15Å 181.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.74 – 2.35 62.74 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.9 (62.74-2.35) 96.9 (62.74-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.226 , 0.256 0.233 , 0.262	Depositor DCC
R_{free} test set	1954 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35292	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, MG, 3FB, CA, GTP, ACP, 3WU, 3WT, V9M

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	0/3570	0.41	0/4847
1	C	0.25	0/3601	0.41	0/4892
2	B	0.25	0/3550	0.40	0/4807
2	D	0.24	0/3413	0.39	0/4624
3	E	0.23	0/1068	0.35	0/1418
4	F	0.24	0/2886	0.42	0/3899
5	L	1.55	0/6	1.53	0/7
All	All	0.24	0/18094	0.40	0/24494

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	3467	3397	3410	9	0
1	C	3487	3411	3424	12	0
2	B	3426	3336	3336	14	0
2	D	3328	3205	3215	11	0
3	E	1042	1066	1070	4	0
4	F	2818	2787	2796	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	62	85	54	2	0
6	A	32	9	12	1	0
6	C	32	9	12	1	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
8	A	1	0	0	0	0
9	B	28	10	12	0	0
9	D	28	10	12	1	0
10	F	31	14	14	2	0
11	A	17	0	0	1	0
11	B	53	0	0	5	0
11	C	46	0	0	4	0
11	D	20	0	0	5	0
11	E	13	0	0	1	0
11	F	17	0	0	4	0
All	All	17953	17339	17367	71	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 2.

All (71) 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:D:437:ASP:OD1	11:D:601:HOH:O	1.83	0.96
2:B:1:MET:N	2:B:131:CYS:SG	2.49	0.86
2:B:308:ARG:NE	11:B:602:HOH:O	2.09	0.83
2:B:159:GLU:OE1	11:B:601:HOH:O	1.97	0.80
1:C:94:THR:OG1	11:C:601:HOH:O	1.91	0.80
1:C:38:SER:OG	11:C:602:HOH:O	2.05	0.75
1:C:60:LYS:NZ	1:C:85:GLN:O	2.16	0.75
4:F:160:ILE:N	11:F:501:HOH:O	2.20	0.72
2:B:218:LYS:NZ	11:B:604:HOH:O	2.24	0.69
1:C:132:LEU:O	1:C:164:LYS:NZ	2.26	0.69
1:A:407:TRP:O	11:A:601:HOH:O	2.12	0.68
2:B:253:ARG:NH2	11:B:606:HOH:O	2.27	0.68
1:C:438:ASP:OD1	11:C:603:HOH:O	2.12	0.68
4:F:36:ARG:NH1	11:F:503:HOH:O	2.26	0.68
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.23	0.67
4:F:184:LYS:O	10:F:401:ACP:N6	2.29	0.65
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:102:PRO:O	4:F:104:ASN:ND2	2.29	0.64
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.33	0.61
1:A:178:SER:OG	2:B:352:LYS:NZ	2.35	0.59
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.36	0.58
2:D:334:ASN:ND2	11:D:605:HOH:O	2.36	0.58
3:E:48:GLU:OE2	11:E:201:HOH:O	2.17	0.58
4:F:236:LYS:O	4:F:238:CYS:N	2.36	0.58
2:D:76:ASP:N	11:D:602:HOH:O	2.36	0.58
2:B:297:ASP:OD1	11:B:603:HOH:O	2.18	0.56
2:B:2:ARG:NH2	2:B:130:ASP:OD2	2.39	0.56
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.54	0.55
4:F:150:LYS:NZ	10:F:401:ACP:O1A	2.40	0.54
2:B:48:ARG:NH2	2:B:250:ALA:O	2.43	0.51
4:F:217:ARG:NH2	4:F:345:GLU:OE2	2.42	0.51
1:C:15:GLN:NE2	6:C:501:GTP:O6	2.44	0.50
1:C:81:GLY:O	1:C:84:ARG:NH2	2.43	0.50
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.43	0.50
4:F:176:GLN:HG3	4:F:180:HIS:HE2	1.78	0.49
2:D:215:ARG:NH1	11:D:610:HOH:O	2.45	0.49
1:A:233:GLN:NE2	1:A:361:THR:O	2.43	0.49
2:D:142:GLY:O	2:D:186:ASN:ND2	2.44	0.48
1:C:380:ASN:OD1	11:C:604:HOH:O	2.20	0.48
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.46	0.48
2:B:48:ARG:NH1	2:B:244:PHE:O	2.45	0.47
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.97	0.46
2:B:336:GLN:OE1	4:F:36:ARG:NH2	2.48	0.46
1:C:286:LEU:O	1:C:373:ARG:NH1	2.46	0.45
4:F:151:SER:HG	4:F:180:HIS:CG	2.32	0.45
2:D:11:GLN:N	9:D:501:GDP:O2B	2.47	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.45
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.99	0.45
4:F:43:GLU:OE2	4:F:43:GLU:N	2.48	0.45
5:L:3:3WT:H30	5:L:3:3WT:H51	1.99	0.45
2:D:311:ARG:NH1	2:D:436:GLN:O	2.50	0.44
4:F:12:SER:N	11:F:508:HOH:O	2.44	0.44
2:B:295[B]:MET:CG	2:B:377:PHE:HB2	2.48	0.44
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.44	0.44
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.43
2:B:109:THR:OG1	2:B:110:GLU:N	2.51	0.42
2:D:77:SER:N	11:D:602:HOH:O	2.29	0.42
4:F:346:LEU:O	4:F:349:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:NE2	6:A:501:GTP:O6	2.52	0.42
2:D:21:TRP:O	2:D:25:SER:OG	2.29	0.42
4:F:280:GLU:HA	4:F:284:LEU:HB2	2.02	0.42
2:D:155[A]:SER:HB2	3:E:126:LYS:HZ1	1.84	0.41
2:D:69:ASP:OD1	2:D:70:LEU:N	2.51	0.41
5:L:3:3WT:H51	5:L:3:3WT:C26	2.50	0.41
4:F:192:LEU:HD11	4:F:262:MET:CE	2.51	0.41
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.61	0.41
4:F:92:THR:O	4:F:326:LYS:NZ	2.54	0.40
4:F:44:ARG:NH1	11:F:509:HOH:O	2.47	0.40
3:E:44:ASP:HB3	3:E:45:PRO:HD3	2.01	0.40
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.35	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	445/440 (101%)	428 (96%)	16 (4%)	1 (0%)	47	56
1	C	450/440 (102%)	436 (97%)	12 (3%)	2 (0%)	34	38
2	B	440/445 (99%)	428 (97%)	12 (3%)	0	100	100
2	D	422/445 (95%)	407 (96%)	15 (4%)	0	100	100
3	E	125/138 (91%)	125 (100%)	0	0	100	100
4	F	338/378 (89%)	319 (94%)	18 (5%)	1 (0%)	41	47
All	All	2220/2286 (97%)	2143 (96%)	73 (3%)	4 (0%)	47	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	237	THR

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Mol	Chain	Res	Type
1	C	341	ILE
1	A	177	VAL
1	C	131	GLY

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	378/371 (102%)	376 (100%)	2 (0%)	88	94
1	C	383/371 (103%)	382 (100%)	1 (0%)	92	96
2	B	384/383 (100%)	382 (100%)	2 (0%)	88	94
2	D	369/383 (96%)	369 (100%)	0	100	100
3	E	116/123 (94%)	113 (97%)	3 (3%)	46	56
4	F	310/336 (92%)	297 (96%)	13 (4%)	30	36
5	L	1/1 (100%)	1 (100%)	0	100	100
All	All	1941/1968 (99%)	1920 (99%)	21 (1%)	73	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	THR
1	A	265	ILE
2	B	31	ASP
2	B	293	GLN
1	C	71	GLU
3	E	46	SER
3	E	90[A]	ASN
3	E	90[B]	ASN
4	F	87	LEU
4	F	89	GLU
4	F	131	PHE
4	F	132	LEU
4	F	136	ASN
4	F	148	ILE

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Mol	Chain	Res	Type
4	F	176	GLN
4	F	226	GLU
4	F	238	CYS
4	F	244	CYS
4	F	253	TYR
4	F	272	MET
4	F	299	GLU

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

Mol	Chain	Res	Type
2	B	139	HIS
2	B	192	HIS
4	F	104	ASN
4	F	243	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	3WT	L	3	5	11,12,13	0.92	1 (9%)	8,14,16	2.53	1 (12%)
5	3WU	L	4	5	12,12,13	1.30	1 (8%)	9,15,17	1.37	1 (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	3WT	L	3	5	-	3/17/17/18	-
5	3WU	L	4	5	-	0/11/19/21	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	4	3WU	C3-C2	-2.42	1.49	1.53
5	L	3	3WT	C26-C27	2.22	1.55	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	3	3WT	C25-N3-C19	6.80	124.29	114.38
5	L	4	3WU	C3-C2-N1	2.61	107.96	103.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	3	3WT	C20-C19-N3-C25
5	L	3	3WT	O5-C20-C26-C27
5	L	3	3WT	C19-C20-C26-C27

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	3	3WT	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	B	501	-	24,30,30	1.05	2 (8%)	31,47,47	1.89	7 (22%)
6	GTP	A	501	7	26,34,34	0.97	1 (3%)	33,54,54	1.64	6 (18%)
10	ACP	F	401	-	27,33,33	1.44	6 (22%)	32,52,52	1.32	5 (15%)
6	GTP	C	501	7	26,34,34	0.96	1 (3%)	33,54,54	1.70	7 (21%)
9	GDP	D	501	-	24,30,30	1.14	2 (8%)	31,47,47	1.89	9 (29%)

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	B	501	-	-	4/12/32/32	0/3/3/3
6	GTP	A	501	7	-	8/18/38/38	0/3/3/3
10	ACP	F	401	-	-	8/15/38/38	0/3/3/3
6	GTP	C	501	7	-	9/18/38/38	0/3/3/3
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	C6-C5	3.94	1.48	1.41
10	F	401	ACP	PB-O3A	3.57	1.62	1.58
9	B	501	GDP	C6-C5	3.43	1.47	1.41
6	A	501	GTP	C6-N1	2.99	1.38	1.33
6	C	501	GTP	C6-N1	2.96	1.38	1.33
10	F	401	ACP	PG-O3G	2.56	1.60	1.54
10	F	401	ACP	C5-C4	2.47	1.47	1.40
10	F	401	ACP	PG-O2G	2.46	1.60	1.54
9	D	501	GDP	C5-C4	2.32	1.47	1.40
9	B	501	GDP	C5-C4	2.22	1.46	1.40
10	F	401	ACP	PB-O2B	2.17	1.61	1.56
10	F	401	ACP	C2'-C1'	-2.01	1.50	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	501	GTP	N3-C2-N1	-5.25	120.22	127.22
6	A	501	GTP	N3-C2-N1	-5.01	120.54	127.22
9	D	501	GDP	C2-N3-C4	4.58	120.58	115.36
9	B	501	GDP	C6-N1-C2	4.55	123.16	115.93
9	B	501	GDP	C6-C5-C4	-4.33	116.66	120.80
9	B	501	GDP	C5-C6-N1	-4.18	117.72	123.43
6	A	501	GTP	C2-N3-C4	4.16	120.11	115.36
9	D	501	GDP	C6-N1-C2	4.12	122.48	115.93
6	C	501	GTP	C2-N3-C4	4.03	119.96	115.36
9	D	501	GDP	C6-C5-C4	-3.99	116.99	120.80
9	D	501	GDP	C5-C6-N1	-3.98	117.99	123.43
9	B	501	GDP	C2-N3-C4	3.97	119.89	115.36
9	B	501	GDP	N3-C2-N1	-3.46	122.60	127.22
9	D	501	GDP	N3-C2-N1	-3.27	122.86	127.22
10	F	401	ACP	N3-C2-N1	-3.05	123.91	128.68
6	C	501	GTP	PA-O3A-PB	-2.96	122.65	132.83
6	C	501	GTP	PB-O3B-PG	-2.89	122.90	132.83
6	A	501	GTP	PB-O3B-PG	-2.80	123.20	132.83
6	A	501	GTP	C5-C6-N1	-2.79	119.62	123.43
6	A	501	GTP	PA-O3A-PB	-2.74	123.42	132.83
10	F	401	ACP	C3'-C2'-C1'	2.63	104.94	100.98
6	C	501	GTP	C5-C6-N1	-2.63	119.84	123.43
9	B	501	GDP	PA-O3A-PB	-2.58	123.96	132.83
6	C	501	GTP	C6-N1-C2	2.47	119.86	115.93
9	D	501	GDP	C4-C5-N7	-2.44	106.85	109.40
9	D	501	GDP	PA-O3A-PB	-2.40	124.59	132.83
6	A	501	GTP	C6-N1-C2	2.34	119.65	115.93
9	D	501	GDP	C3'-C2'-C1'	2.24	104.36	100.98
10	F	401	ACP	PA-O3A-PB	-2.24	125.46	132.56
9	B	501	GDP	C4-C5-N7	-2.10	107.21	109.40
6	C	501	GTP	C3'-C2'-C1'	2.09	104.12	100.98
10	F	401	ACP	C2-N1-C6	2.04	122.25	118.75
10	F	401	ACP	O4'-C1'-C2'	-2.04	103.95	106.93
9	D	501	GDP	O2B-PB-O3A	2.02	111.41	104.64

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	401	ACP	PB-C3B-PG-O1G
10	F	401	ACP	PB-C3B-PG-O2G
10	F	401	ACP	PB-C3B-PG-O3G
10	F	401	ACP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	F	401	ACP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
6	A	501	GTP	C5'-O5'-PA-O1A
6	C	501	GTP	C5'-O5'-PA-O1A
6	C	501	GTP	C5'-O5'-PA-O2A
6	A	501	GTP	PB-O3B-PG-O1G
6	C	501	GTP	PB-O3B-PG-O1G
6	A	501	GTP	C5'-O5'-PA-O3A
6	A	501	GTP	C5'-O5'-PA-O2A
10	F	401	ACP	PB-O3A-PA-O1A
10	F	401	ACP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
6	A	501	GTP	PB-O3A-PA-O2A
6	C	501	GTP	PB-O3A-PA-O2A
6	C	501	GTP	C4'-C5'-O5'-PA
6	C	501	GTP	PB-O3A-PA-O1A
9	D	501	GDP	PA-O3A-PB-O3B
6	A	501	GTP	PB-O3B-PG-O2G
6	A	501	GTP	PB-O3B-PG-O3G
6	C	501	GTP	PB-O3B-PG-O2G
6	C	501	GTP	PB-O3B-PG-O3G
10	F	401	ACP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
6	C	501	GTP	C5'-O5'-PA-O3A
6	A	501	GTP	PB-O3A-PA-O1A

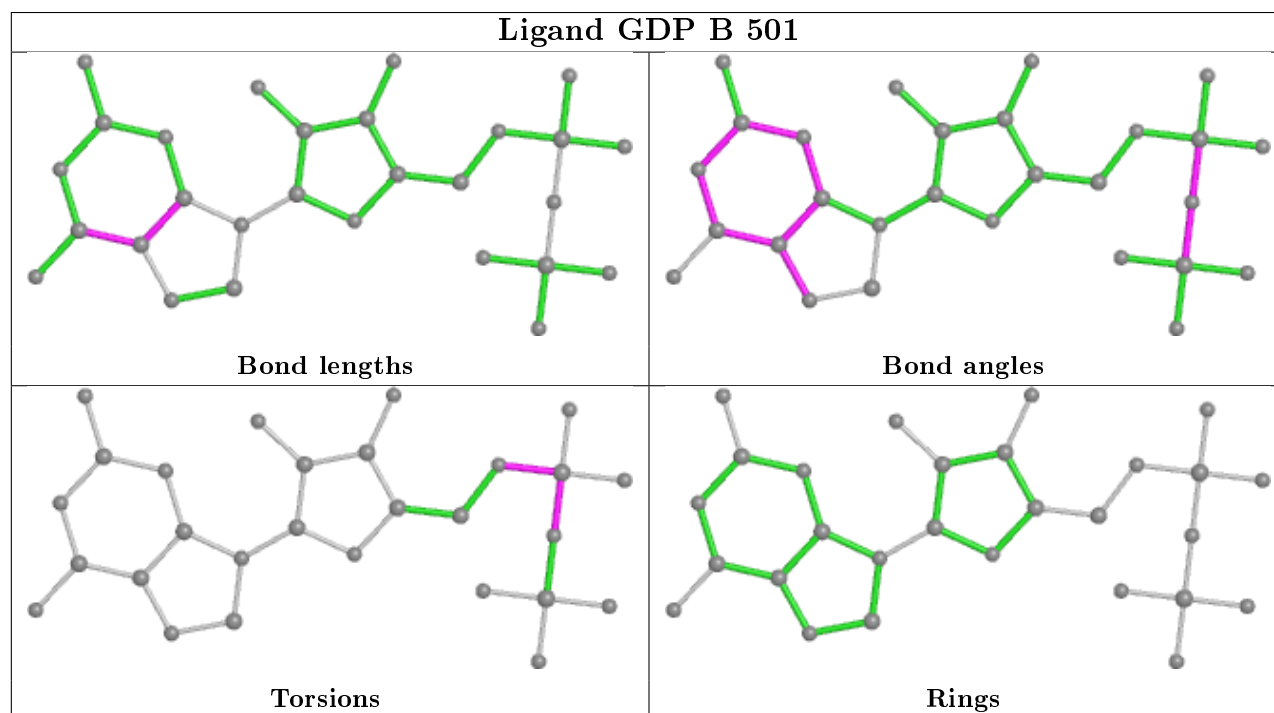
There are no ring outliers.

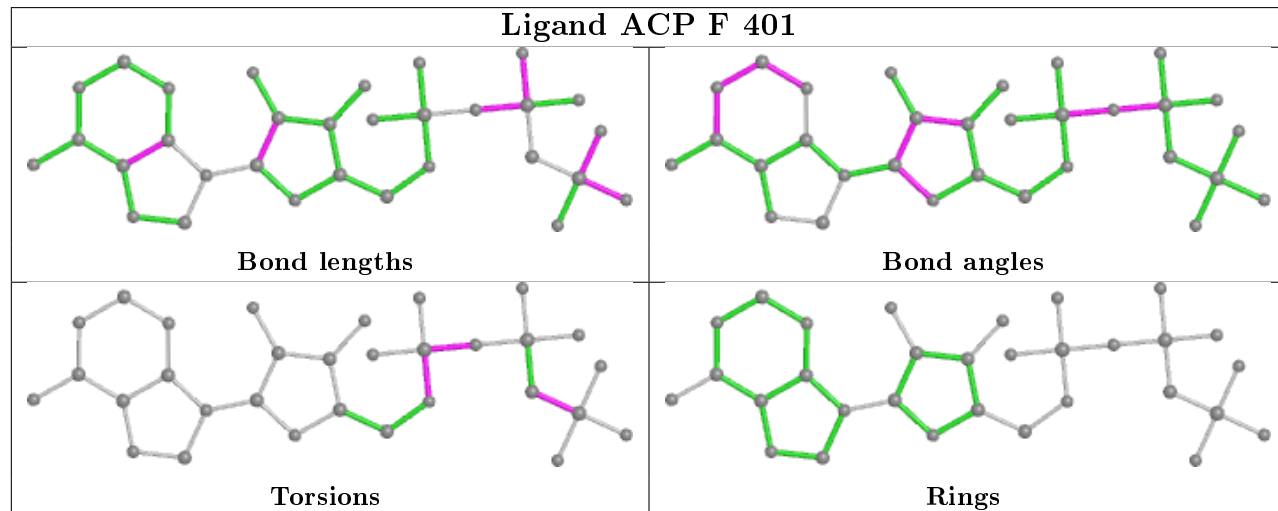
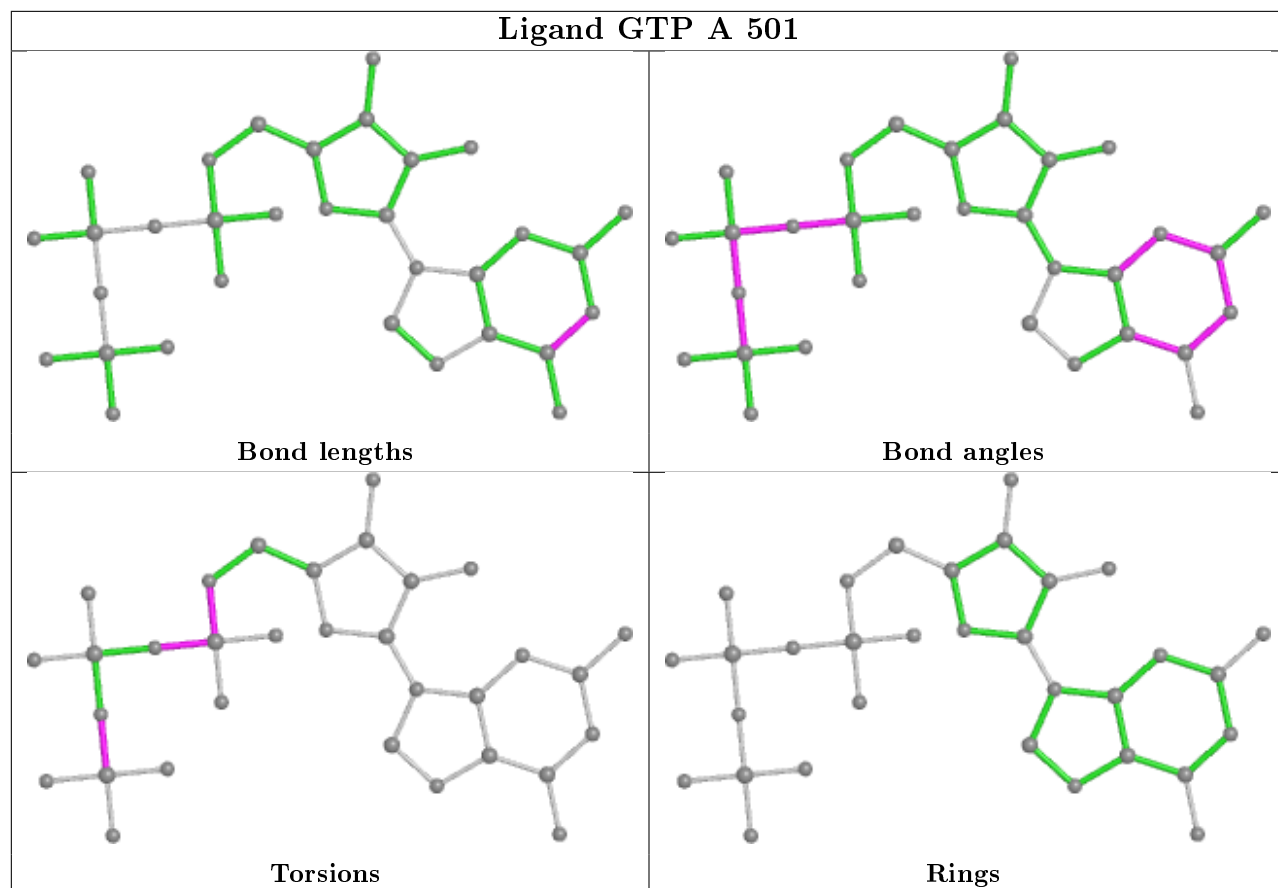
4 monomers are involved in 5 short contacts:

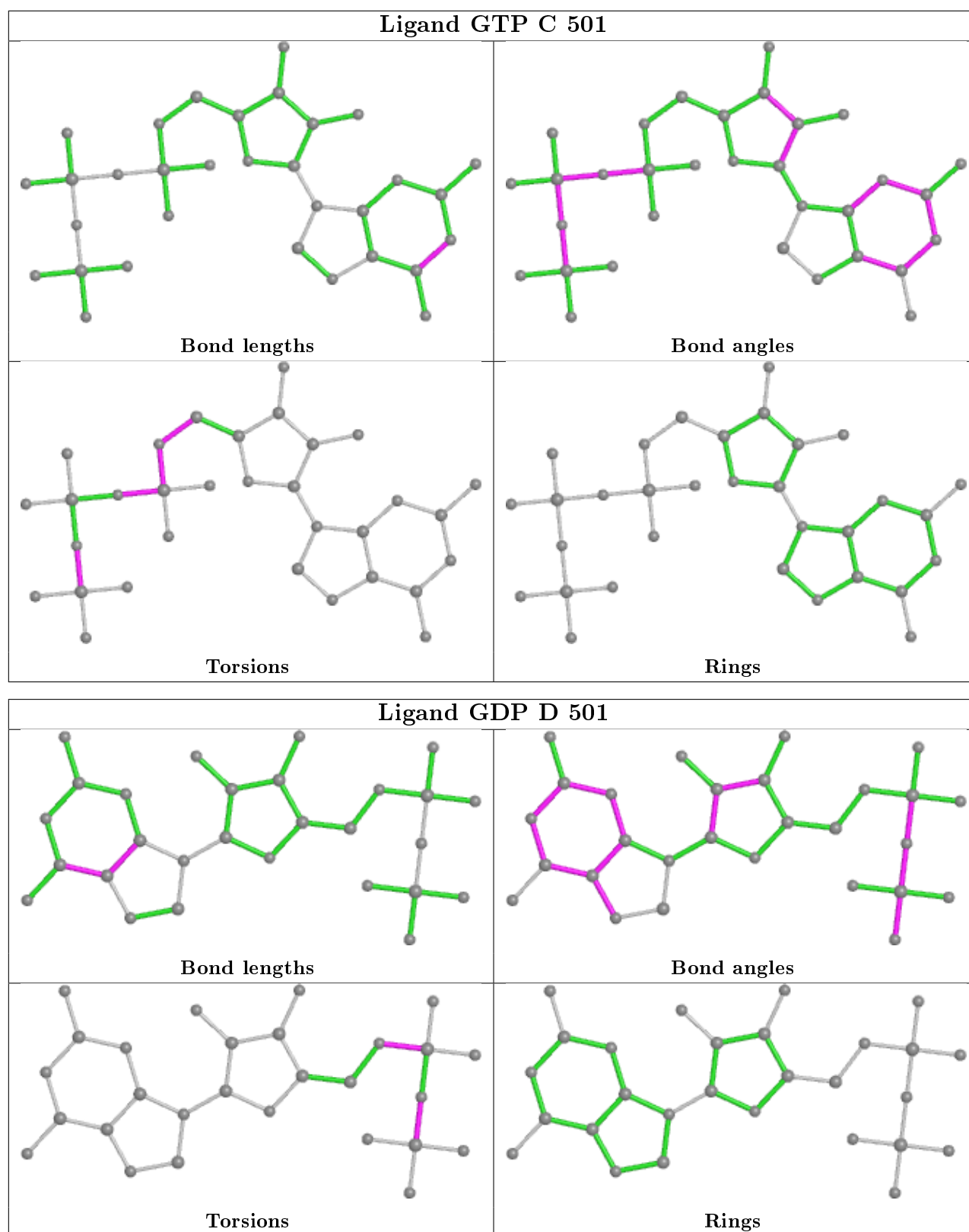
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	GTP	1	0
10	F	401	ACP	2	0
6	C	501	GTP	1	0
9	D	501	GDP	1	0

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

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	439/440 (99%)	0.66	20 (4%) 32 45	45, 66, 105, 160	0
1	C	440/440 (100%)	0.55	14 (3%) 47 59	36, 53, 80, 115	0
2	B	428/445 (96%)	0.53	10 (2%) 60 70	42, 59, 87, 123	1 (0%)
2	D	422/445 (94%)	0.80	45 (10%) 6 9	48, 72, 99, 123	2 (0%)
3	E	123/138 (89%)	0.94	17 (13%) 2 4	50, 76, 113, 147	0
4	F	344/378 (91%)	2.04	132 (38%) 0 0	57, 94, 170, 275	0
5	L	1/5 (20%)	1.04	0 100 100	49, 49, 49, 49	0
All	All	2197/2291 (95%)	0.87	238 (10%) 5 9	36, 67, 127, 275	3 (0%)

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	11.1
4	F	177	GLY	9.6
4	F	233	PHE	9.5
4	F	173	ILE	9.2
4	F	253	TYR	8.7
4	F	150	LYS	8.7
4	F	161	LEU	8.7
4	F	240	LEU	8.7
4	F	245	ILE	8.1
4	F	251	LYS	8.0
4	F	249	TYR	7.5
4	F	99	VAL	6.9
4	F	234	GLN	6.9
4	F	147	TRP	6.8
4	F	128	ARG	6.6
4	F	235	ASP	6.6
4	F	139	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
4	F	225	SER	6.3
4	F	228	TYR	6.2
4	F	176	GLN	6.2
4	F	142	ARG	6.1
4	F	178	GLN	6.1
4	F	137	ARG	6.0
3	E	15[A]	THR	5.9
4	F	248	GLU	5.9
4	F	160	ILE	5.8
4	F	102	PRO	5.7
1	A	438	ASP	5.7
4	F	255	ARG	5.7
4	F	182	ILE	5.6
4	F	149	ALA	5.5
4	F	132	LEU	5.4
4	F	238	CYS	5.4
4	F	239	HIS	5.3
4	F	101	TYR	5.3
4	F	172	PHE	5.3
4	F	104	ASN	5.2
4	F	229	ASN	5.2
4	F	103	THR	5.2
4	F	138	ARG	5.1
4	F	136	ASN	5.0
1	A	282	TYR	5.0
4	F	170	LEU	4.9
2	D	405	LEU	4.9
4	F	131	PHE	4.9
2	D	57	THR	4.9
4	F	140	GLU	4.8
4	F	250	SER	4.8
4	F	230	SER	4.7
4	F	134	ALA	4.7
4	F	330	ILE	4.6
4	F	143	GLU	4.6
4	F	146	VAL	4.5
4	F	130	VAL	4.4
2	B	279	GLY	4.4
4	F	151	SER	4.4
4	F	227	PRO	4.3
4	F	166	ALA	4.3
4	F	169	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	284	ARG	4.2
4	F	256	TYR	4.2
4	F	236	LYS	4.2
4	F	17	VAL	4.2
4	F	179	VAL	4.1
1	C	305	CYS	4.1
2	D	177	VAL	4.1
1	A	335	ILE	4.1
4	F	100	ILE	4.1
4	F	362	ALA	4.0
4	F	242	ASN	4.0
4	F	162	ILE	4.0
4	F	237	THR	4.0
4	F	126	ASP	4.0
2	D	218	LYS	3.9
4	F	163	SER	3.9
1	C	340	SER	3.9
4	F	145	ASN	3.8
4	F	141	GLY	3.8
2	D	404	PHE	3.8
4	F	148	ILE	3.8
2	D	407	TRP	3.8
3	E	142	GLU	3.8
4	F	243	HIS	3.7
2	D	82	PRO	3.7
4	F	46	ARG	3.6
4	F	361	LEU	3.6
4	F	20	LEU	3.6
4	F	180	HIS	3.6
2	D	220	THR	3.6
4	F	186	LEU	3.6
4	F	154	GLY	3.5
4	F	168	GLU	3.5
2	D	275	LEU	3.5
2	D	401	ARG	3.5
1	C	440	VAL	3.5
4	F	155	ALA	3.5
4	F	153	ALA	3.4
4	F	135	TYR	3.4
1	A	86	LEU	3.4
4	F	232	ASN	3.4
3	E	14	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	220[A]	VAL	3.3
2	D	221	THR	3.3
4	F	125	THR	3.3
2	D	286	LEU	3.3
1	A	281	ALA	3.3
4	F	224	SER	3.3
4	F	75	ALA	3.2
2	D	94	PHE	3.2
2	B	282	GLN	3.2
4	F	183	GLN	3.2
4	F	144	GLY	3.2
1	A	66[A]	VAL	3.2
4	F	231	ALA	3.2
1	A	262	TYR	3.1
4	F	127	GLU	3.1
3	E	54	LEU	3.1
4	F	174	ASP	3.1
2	D	400	ARG	3.0
4	F	181	VAL	3.0
4	F	342	LEU	3.0
4	F	320	MET	3.0
1	A	439	SER	2.9
3	E	48	GLU	2.9
3	E	130	ALA	2.9
1	C	357	TYR	2.9
4	F	258	GLU	2.9
1	A	78	VAL	2.9
1	A	82	THR	2.9
2	B	280	SER	2.9
2	D	97	SER	2.8
4	F	192	LEU	2.8
2	D	277	SER	2.8
4	F	246	GLN	2.8
4	F	28	LYS	2.8
4	F	260	ASN	2.8
4	F	98	TYR	2.8
2	D	32	PRO	2.8
4	F	24	THR	2.8
4	F	346	LEU	2.7
4	F	165	GLU	2.7
4	F	254	GLY	2.7
4	F	199	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	47	LEU	2.7
4	F	247	LYS	2.7
2	D	95	GLY	2.7
4	F	152	SER	2.7
2	D	179	ASP	2.7
2	D	67	LEU	2.7
4	F	257	GLU	2.6
2	D	415	GLU	2.6
2	D	37	HIS	2.6
2	D	276	THR	2.6
4	F	133	ALA	2.6
4	F	175	GLU	2.6
2	D	76	ASP	2.6
4	F	97	SER	2.5
1	A	288	VAL	2.5
4	F	337	ALA	2.5
1	A	285	GLN	2.5
1	C	283	HIS	2.5
2	D	78	VAL	2.5
4	F	9	GLU	2.5
2	B	303	ALA	2.5
3	E	11	LEU	2.5
4	F	223	THR	2.5
1	C	302	MET	2.4
3	E	133	VAL	2.4
4	F	129	GLU	2.4
1	C	210	TYR	2.4
2	D	88	ARG	2.4
1	C	180	ALA	2.4
2	D	399	PHE	2.4
4	F	204	TRP	2.4
4	F	226	GLU	2.4
3	E	23	ILE	2.4
2	D	195	VAL	2.4
2	D	98	GLY	2.4
2	D	87	PHE	2.4
2	D	115	VAL	2.4
2	D	217	LEU	2.4
1	A	247	ALA	2.3
1	A	337	THR	2.3
4	F	263	PHE	2.3
3	E	26	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	14	TYR	2.3
4	F	164	SER	2.3
3	E	141	GLU	2.3
4	F	283	ILE	2.3
2	D	219	LEU	2.3
2	D	291	LEU	2.3
2	D	79	ARG	2.3
1	C	276	ILE	2.3
3	E	46	SER	2.3
2	D	60	LYS	2.3
2	D	387	LEU	2.2
2	B	94	PHE	2.2
1	A	360	PRO	2.2
2	B	318	ILE	2.2
2	D	70	LEU	2.2
2	D	248	LEU	2.2
1	A	42	ILE	2.2
4	F	81	ILE	2.2
4	F	340	GLN	2.2
2	D	210	TYR	2.2
2	D	272	PHE	2.2
3	E	28	SER	2.2
4	F	315	PHE	2.2
1	C	208	ALA	2.2
2	B	438	ALA	2.2
1	C	286	LEU	2.2
1	A	334	THR	2.2
4	F	184	LYS	2.2
2	D	377	PHE	2.2
4	F	4	PHE	2.2
4	F	275	LEU	2.1
2	B	1	MET	2.1
2	D	325	MET	2.1
4	F	44	ARG	2.1
4	F	252	ASN	2.1
3	E	68	LEU	2.1
4	F	353	VAL	2.1
1	A	370	LYS	2.1
4	F	271	LEU	2.1
1	C	174	ALA	2.1
3	E	82	VAL	2.1
4	F	13	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	59	ASN	2.1
4	F	185	TYR	2.1
1	C	68[A]	VAL	2.0
1	C	181[A]	VAL	2.0
2	D	118	VAL	2.0
1	A	149	PHE	2.0
4	F	19	ARG	2.0
3	E	140	LYS	2.0
1	A	358	GLN	2.0
2	D	96	GLN	2.0
4	F	267	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
5	3WT	L	3	13/14	0.96	0.18	45,61,73,73	0
5	3WU	L	4	12/13	0.96	0.13	43,53,69,69	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CA	A	503	1/1	0.68	0.09	115,115,115,115	0
7	MG	B	503	1/1	0.77	0.26	72,72,72,72	0
7	MG	A	502	1/1	0.78	0.25	56,56,56,56	0
7	MG	C	502	1/1	0.81	0.37	48,48,48,48	0
10	ACP	F	401	31/31	0.82	0.21	104,133,172,179	0

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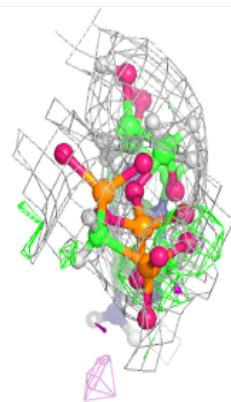
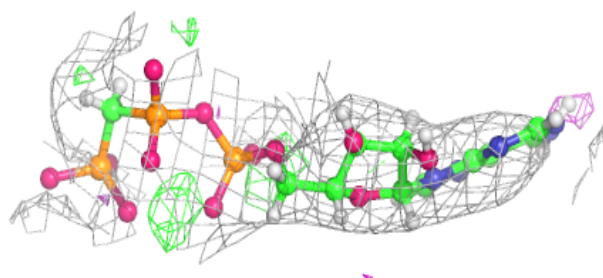
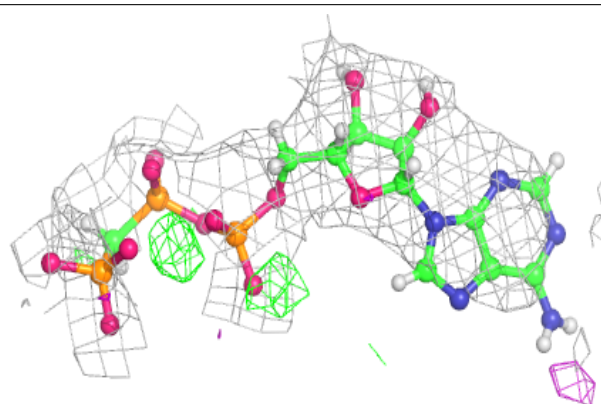
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	C	503	1/1	0.94	0.14	82,82,82,82	0
7	MG	B	502	1/1	0.94	0.17	76,76,76,76	0
9	GDP	D	501	28/28	0.95	0.16	61,75,98,118	0
6	GTP	A	501	32/32	0.96	0.20	45,55,75,84	0
9	GDP	B	501	28/28	0.98	0.19	40,49,72,81	0
6	GTP	C	501	32/32	0.98	0.23	38,47,61,80	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.

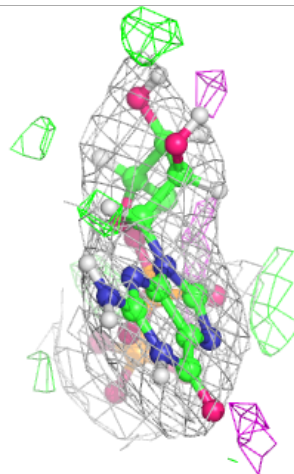
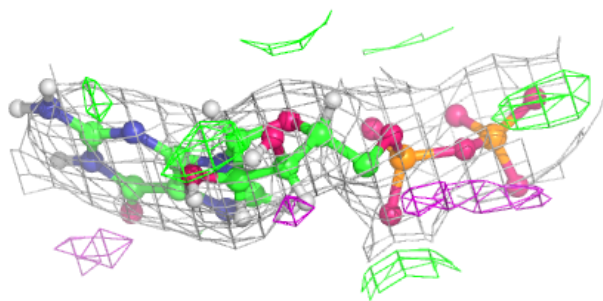
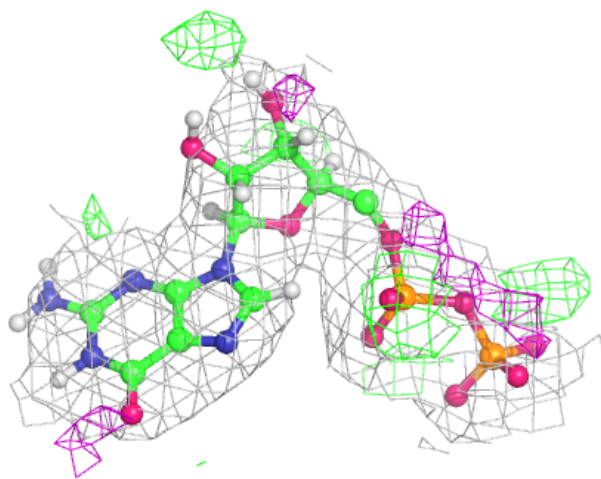
Electron density around ACP F 401:

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



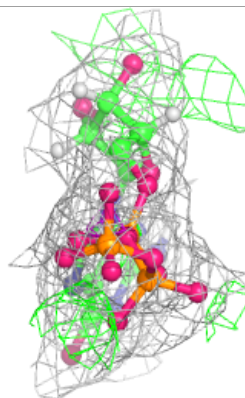
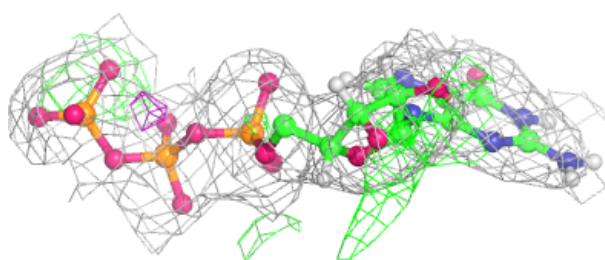
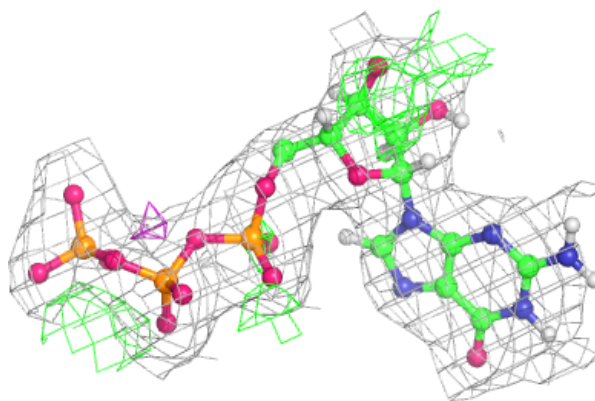
Electron density around GDP D 501:

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

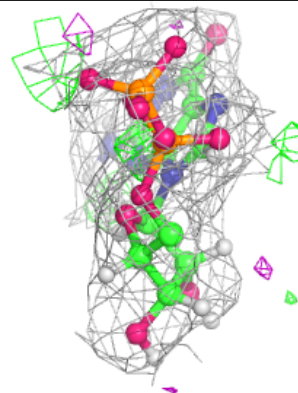
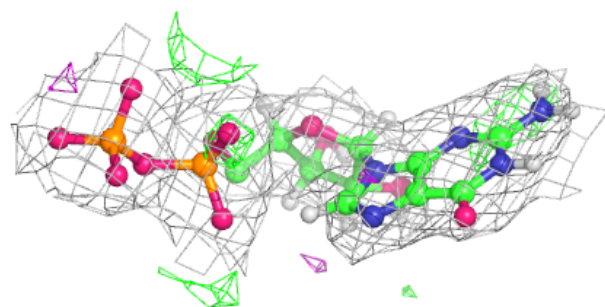
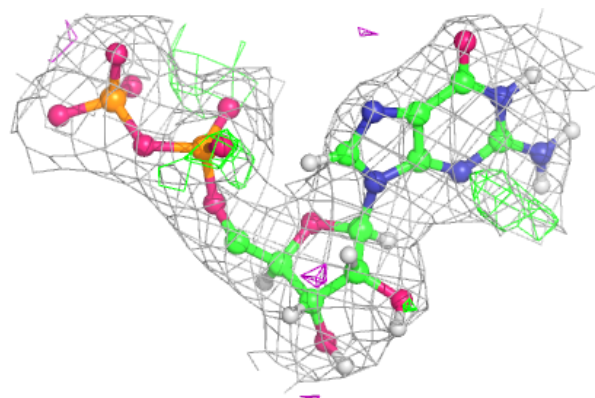


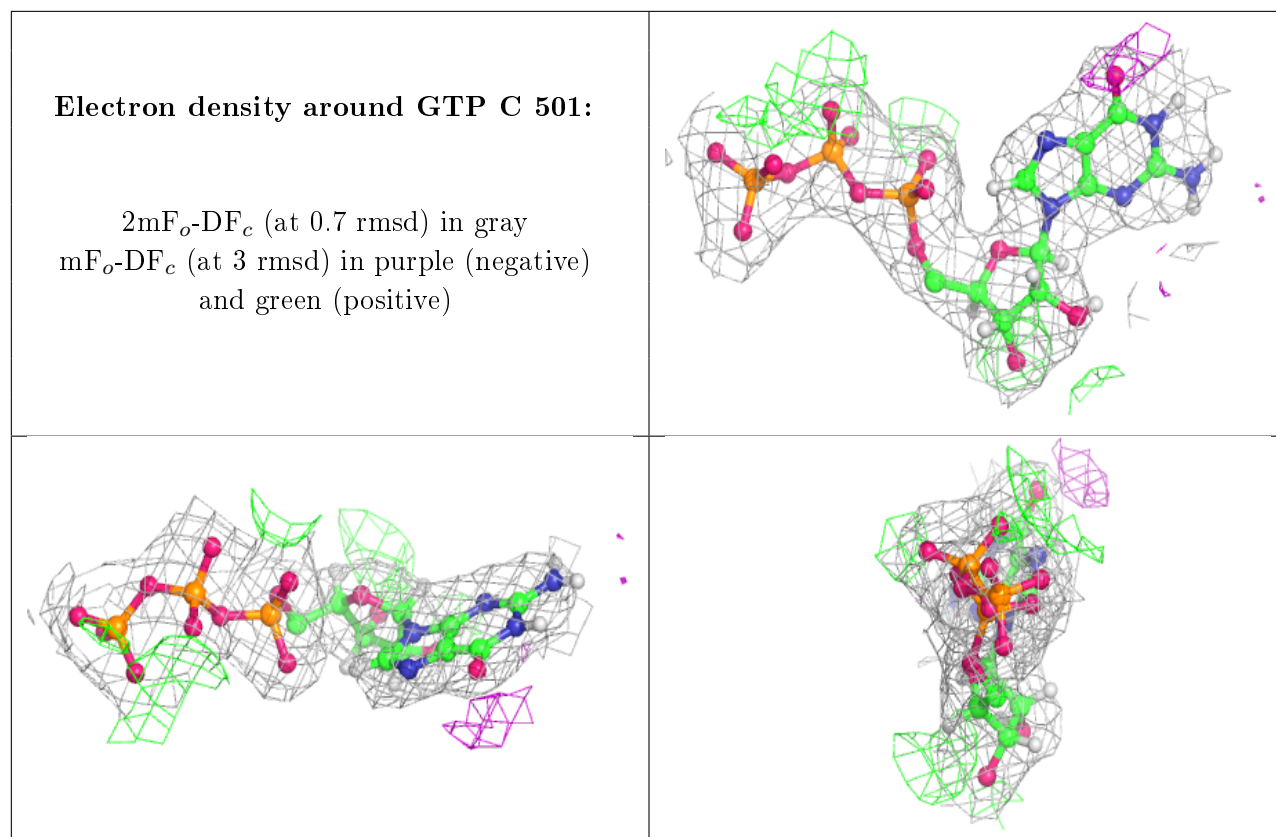
Electron density around GTP A 501:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.