



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:06 AM UTC

PDB ID : 7JFR / pdb_00007jfr
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 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

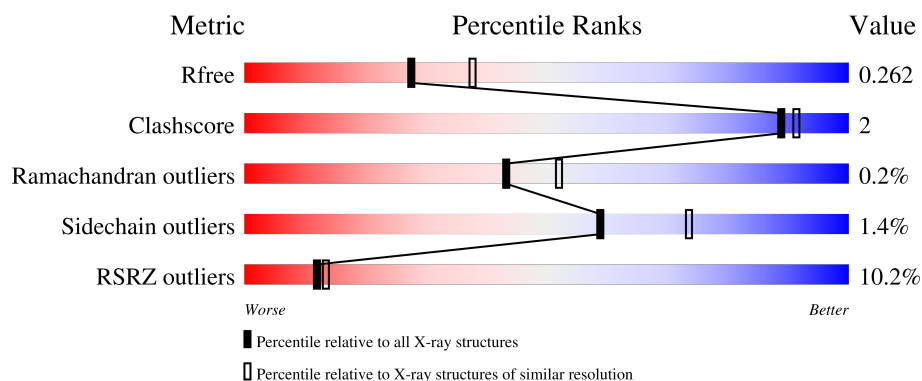
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	10% 95% 5%
1	C	440	5% 95% 5%
2	B	445	3% 92% • •
2	D	445	9% 91% • 5%
3	E	138	14% 84% 5% 11%

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Mol	Chain	Length	Quality of chain
4	F	378	21% 79% 11% 9%
5	L	5	60% 20% 20%

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			

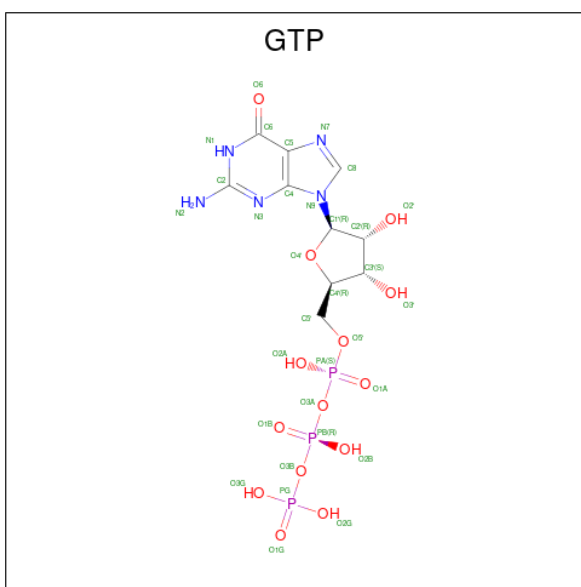
- Molecule 4 is a protein called Uncharacterized protein.

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 (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

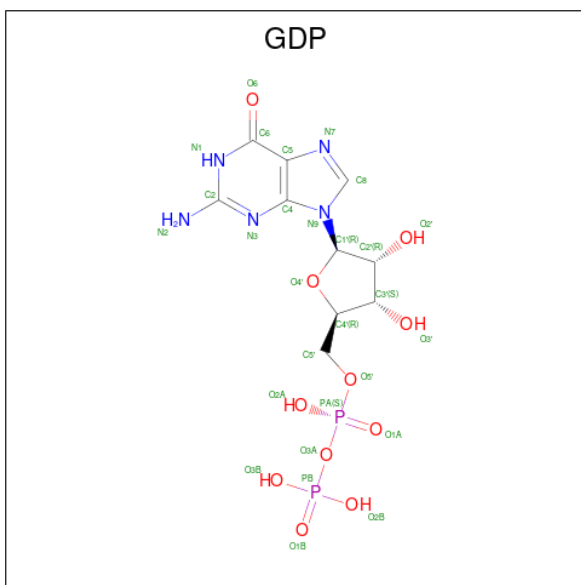
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

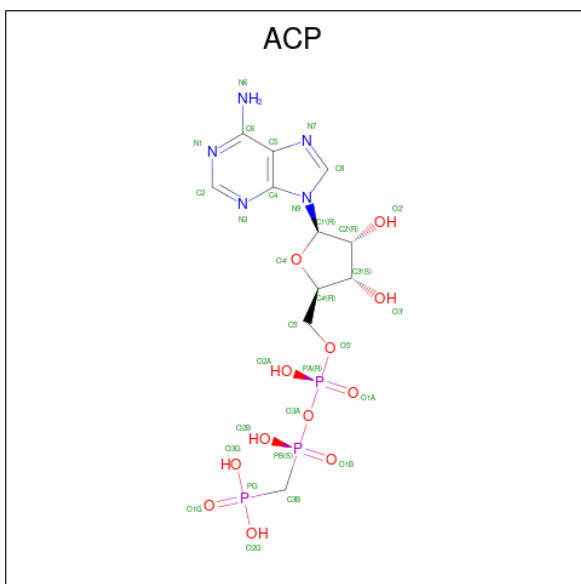
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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 (CCD ID: 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		

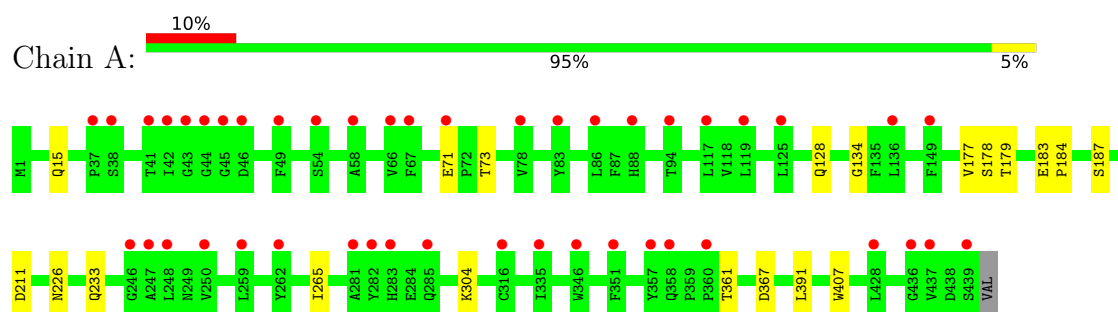
- Molecule 11 is water.

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

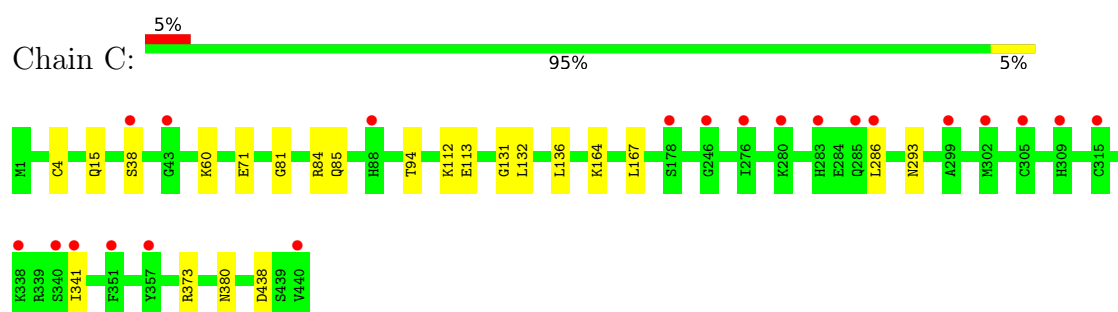
3 Residue-property plots [i](#)

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.

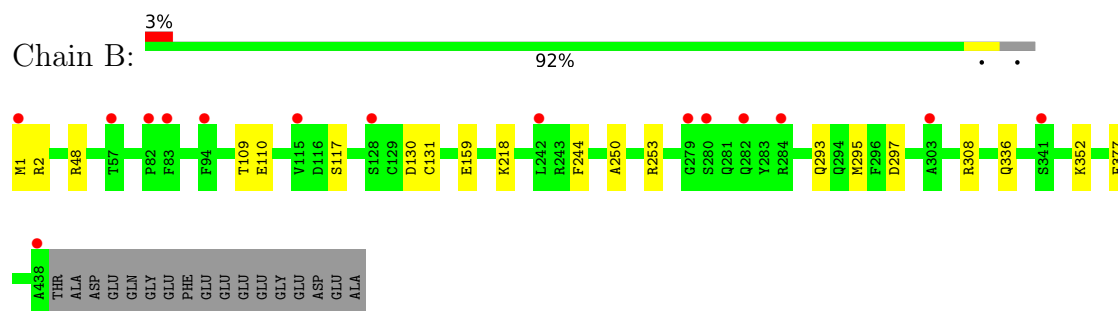
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

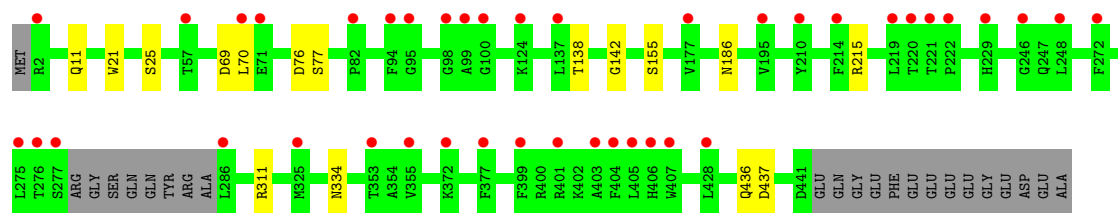


- Molecule 2: Tubulin beta-2B chain

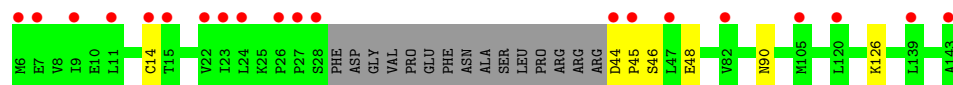
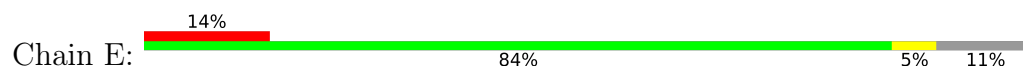


- Molecule 2: Tubulin beta-2B chain

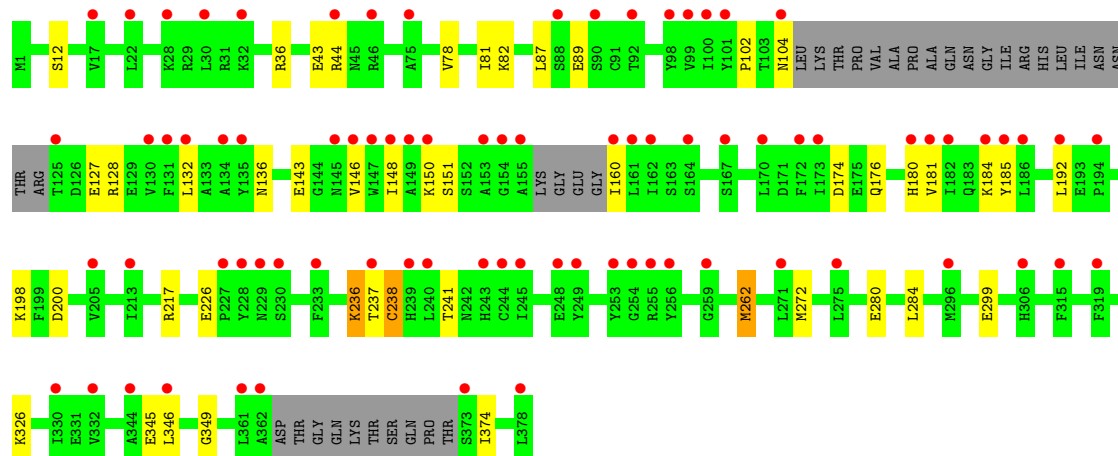
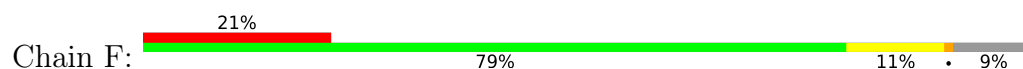




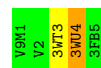
● Molecule 3: Stathmin-4



● 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 0.235 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (1.62%)	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)	0.37 , 40.6	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V9M, 3WU, CA, 3FB, 3WT, ACP, MG, GTP, 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	0/3570	0.65	1/4847 (0.0%)
1	C	0.32	0/3601	0.65	0/4892
2	B	0.31	0/3550	0.61	0/4807
2	D	0.31	0/3413	0.61	0/4624
3	E	0.29	0/1068	0.63	0/1418
4	F	0.30	0/2886	0.65	0/3899
5	L	1.50	0/6	1.49	0/7
All	All	0.31	0/18094	0.63	1/24494 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	L	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	GLY	N-CA-C	5.11	117.09	110.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	4	3WU	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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	13	0
2	D	3328	3205	3215	11	0
3	E	1042	1066	1070	4	0
4	F	2818	2787	2796	22	0
5	L	62	85	33	0	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	17346	68	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 (68) 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
1:C:94:THR:OG1	11:C:601:HOH:O	1.91	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:F:151:SER:HG	4:F:180:HIS:HD1	1.47	0.59
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
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
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
4:F:151:SER:HG	4:F:180:HIS:CG	2.30	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:F:236:LYS:C	4:F:238:CYS:H	2.24	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
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
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: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%)	43	52
1	C	450/440 (102%)	436 (97%)	12 (3%)	2 (0%)	30	34
2	B	440/445 (99%)	428 (97%)	12 (3%)	0	100	100
2	D	422/445 (95%)	407 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	125/138 (91%)	125 (100%)	0	0	100	100
4	F	338/378 (89%)	319 (94%)	18 (5%)	1 (0%)	36	43
5	L	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2221/2291 (97%)	2144 (96%)	73 (3%)	4 (0%)	43	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	237	THR
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%)	375 (99%)	3 (1%)	73	84
1	C	383/371 (103%)	380 (99%)	3 (1%)	73	84
2	B	384/383 (100%)	382 (100%)	2 (0%)	81	89
2	D	369/383 (96%)	368 (100%)	1 (0%)	86	92
3	E	116/123 (94%)	113 (97%)	3 (3%)	40	54
4	F	310/336 (92%)	293 (94%)	17 (6%)	19	24
5	L	1/1 (100%)	1 (100%)	0	100	100
All	All	1941/1968 (99%)	1912 (98%)	29 (2%)	59	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	179	THR
1	A	265	ILE

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Mol	Chain	Res	Type
2	B	117	SER
2	B	293	GLN
1	C	71	GLU
1	C	293[A]	ASN
1	C	293[B]	ASN
2	D	138	THR
3	E	46	SER
3	E	90[A]	ASN
3	E	90[B]	ASN
4	F	81	ILE
4	F	87	LEU
4	F	89	GLU
4	F	132	LEU
4	F	136	ASN
4	F	143	GLU
4	F	146	VAL
4	F	148	ILE
4	F	176	GLN
4	F	226	GLU
4	F	236	LYS
4	F	238	CYS
4	F	262	MET
4	F	272	MET
4	F	299	GLU
4	F	326	LYS
4	F	374	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	101	ASN
1	A	293	ASN
1	A	300	ASN
1	A	309	HIS
1	A	358	GLN
2	B	136	GLN
2	B	192	HIS
1	C	61	HIS
1	C	283	HIS
1	C	356	ASN
1	C	372	GLN

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Mol	Chain	Res	Type
2	D	37	HIS
2	D	107	HIS
2	D	136	GLN
2	D	229	HIS
2	D	294	GLN
2	D	300	ASN
2	D	331	GLN
2	D	349	ASN
2	D	424	ASN
3	E	12	ASN
3	E	92	ASN
4	F	104	ASN
4	F	183	GLN
4	F	243	HIS
4	F	246	GLN
4	F	260	ASN

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	0.90	1 (9%)	9,14,16	2.70	1 (11%)
5	3WU	L	4	5	12,12,13	1.24	1 (8%)	9,15,17	1.40	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	-	0/12/19/21	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-CA	-2.18	1.49	1.53
5	L	3	3WT	C26-C	2.13	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	3	3WT	C25-N-CA	7.80	124.29	114.23
5	L	4	3WU	C3-CA-N	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-CA-N-C25
5	L	3	3WT	O5-C20-C26-C
5	L	3	3WT	CA-C20-C26-C

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
10	ACP	F	401	-	31,33,33	1.72	9 (29%)	47,52,52	1.88	12 (25%)
6	GTP	C	501	7	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
9	GDP	B	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.62	6 (13%)
9	GDP	D	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.73	7 (15%)
6	GTP	A	501	7	33,34,34	1.03	3 (9%)	50,54,54	1.55	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ACP	F	401	-	-	8/19/38/38	0/3/3/3
6	GTP	C	501	7	-	9/22/38/38	0/3/3/3
9	GDP	B	501	-	-	5/16/32/32	0/3/3/3
9	GDP	D	501	-	-	4/16/32/32	0/3/3/3
6	GTP	A	501	7	-	8/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	ACP	C5-C4	4.69	1.47	1.39
10	F	401	ACP	PB-O3A	3.55	1.62	1.58
9	D	501	GDP	C5-C4	3.04	1.47	1.38
9	B	501	GDP	C6-N1	-2.95	1.33	1.38
9	B	501	GDP	C5-C4	2.94	1.46	1.38
10	F	401	ACP	PG-O3G	2.60	1.60	1.55
9	D	501	GDP	C6-N1	-2.53	1.34	1.38
10	F	401	ACP	C5-N7	-2.52	1.34	1.39
10	F	401	ACP	PA-O3A	2.51	1.62	1.59
10	F	401	ACP	PG-O2G	2.50	1.60	1.55
9	D	501	GDP	PA-O3A	2.47	1.62	1.59
6	A	501	GTP	PB-O3A	2.45	1.62	1.59
10	F	401	ACP	C5-C6	2.41	1.47	1.41
6	C	501	GTP	C2-N3	2.29	1.38	1.33
6	A	501	GTP	C2-N3	2.20	1.38	1.33
9	B	501	GDP	C5-N7	-2.16	1.34	1.39
10	F	401	ACP	C4-N9	-2.16	1.33	1.37
6	A	501	GTP	PA-O3A	2.14	1.61	1.59
9	B	501	GDP	C4-N9	-2.12	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	ACP	PB-O2B	2.08	1.61	1.56
9	D	501	GDP	C5-N7	-2.08	1.34	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C5-C4-N3	-5.84	119.10	128.39
10	F	401	ACP	C5-C4-N3	-5.41	119.27	126.72
9	B	501	GDP	C5-C4-N3	-5.29	119.96	128.39
6	A	501	GTP	C5-C4-N3	-5.13	120.22	128.39
6	C	501	GTP	C5-C4-N3	-4.93	120.54	128.39
9	D	501	GDP	C2-N3-C4	4.81	120.58	112.30
10	F	401	ACP	N3-C4-N9	4.71	135.18	127.17
9	D	501	GDP	N9-C4-N3	4.56	135.07	125.95
6	A	501	GTP	C2-N3-C4	4.54	120.11	112.30
6	C	501	GTP	C2-N3-C4	4.45	119.96	112.30
9	B	501	GDP	C2-N3-C4	4.41	119.89	112.30
9	B	501	GDP	N9-C4-N3	4.25	134.45	125.95
10	F	401	ACP	O4'-C1'-N9	4.14	116.04	108.09
10	F	401	ACP	C2-N3-C4	3.44	120.23	111.83
6	C	501	GTP	N9-C4-N3	3.41	132.76	125.95
6	A	501	GTP	N9-C4-N3	3.32	132.58	125.95
9	D	501	GDP	C6-C5-N7	3.22	136.16	130.29
9	B	501	GDP	C6-C5-N7	3.21	136.12	130.29
10	F	401	ACP	N3-C2-N1	-3.09	123.91	128.58
6	A	501	GTP	C2-N1-C6	-3.01	119.65	125.11
6	C	501	GTP	C2-N1-C6	-2.90	119.86	125.11
6	C	501	GTP	N9-C8-N7	-2.82	108.17	113.40
10	F	401	ACP	C2'-C1'-N9	-2.77	106.41	113.30
6	A	501	GTP	N9-C8-N7	-2.60	108.58	113.40
6	C	501	GTP	O6-C6-C5	-2.59	119.69	126.53
6	C	501	GTP	C8-N7-C5	2.59	108.88	104.26
6	C	501	GTP	C5-C6-N1	2.59	119.84	113.25
6	A	501	GTP	C5-C6-N1	2.50	119.62	113.25
6	A	501	GTP	C8-N7-C5	2.48	108.68	104.26
10	F	401	ACP	C4-N9-C8	2.42	108.28	105.74
9	D	501	GDP	C4-C5-N7	-2.41	106.85	110.67
6	A	501	GTP	O6-C6-C5	-2.40	120.19	126.53
10	F	401	ACP	C4-C5-N7	-2.37	107.88	110.58
10	F	401	ACP	C4'-O4'-C1'	-2.35	104.28	109.47
9	B	501	GDP	C4-C5-N7	-2.18	107.21	110.67
10	F	401	ACP	C2-N1-C6	2.14	122.25	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	401	ACP	PB-O3A-PA	-2.12	125.46	132.37
9	B	501	GDP	O2A-PA-O3A	2.11	112.98	107.27
9	D	501	GDP	O6-C6-C5	-2.05	121.12	126.53
6	C	501	GTP	O2A-PA-O3A	2.05	112.82	107.27
10	F	401	ACP	O4'-C4'-C5'	2.04	115.88	109.33
9	D	501	GDP	O2B-PB-O3A	2.02	111.41	104.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

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

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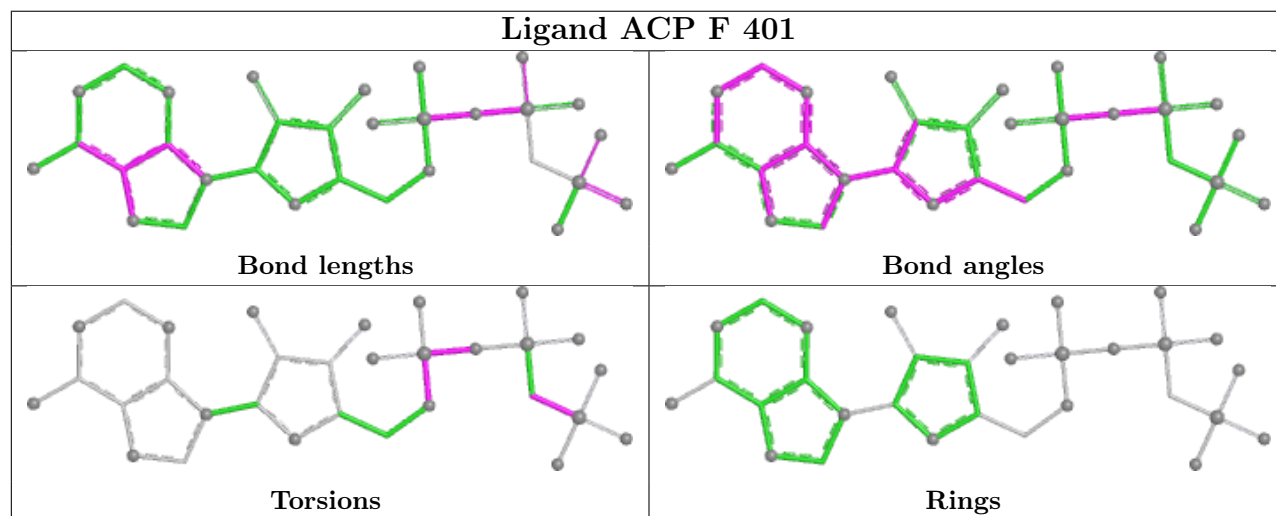
Mol	Chain	Res	Type	Atoms
9	D	501	GDP	PA-O3A-PB-O3B
6	A	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A

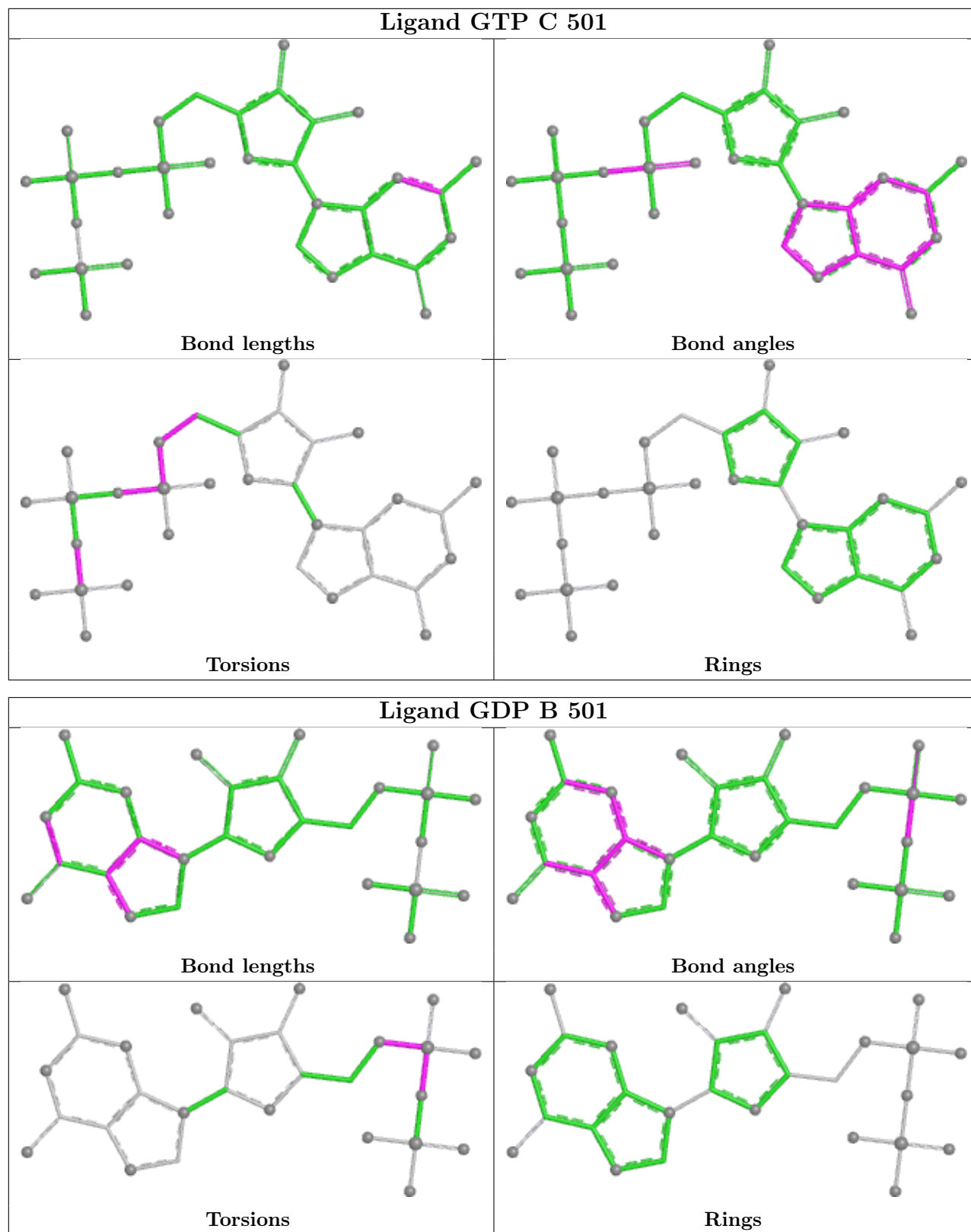
There are no ring outliers.

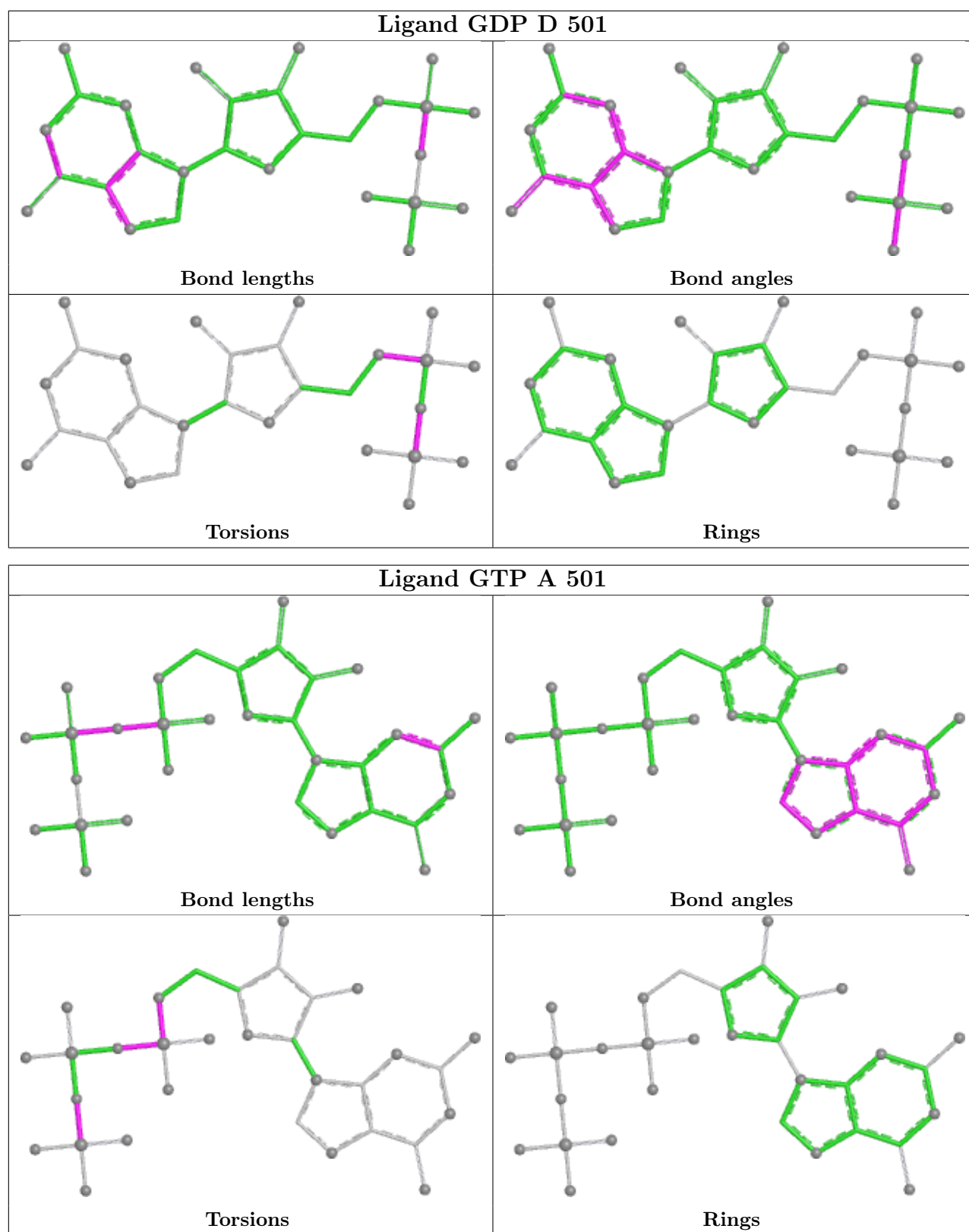
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	401	ACP	2	0
6	C	501	GTP	1	0
9	D	501	GDP	1	0
6	A	501	GTP	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%)	0.95	45 (10%) 12 13	32, 72, 113, 169	8 (1%)
1	C	440/440 (100%)	0.39	21 (4%) 35 41	30, 57, 86, 131	12 (2%)
2	B	428/445 (96%)	0.55	15 (3%) 47 53	30, 64, 95, 134	14 (3%)
2	D	422/445 (94%)	0.96	41 (9%) 13 15	37, 78, 107, 134	6 (1%)
3	E	123/138 (89%)	1.21	20 (16%) 4 5	31, 83, 122, 161	6 (4%)
4	F	344/378 (91%)	1.49	81 (23%) 2 1	57, 102, 185, 341	2 (0%)
5	L	1/5 (20%)	0.61	0 100 100	53, 53, 53, 53	0
All	All	2197/2291 (95%)	0.86	223 (10%) 12 13	30, 73, 138, 341	48 (2%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	15[A]	THR	7.6
4	F	155	ALA	7.1
4	F	150	LYS	5.4
3	E	143	ALA	5.2
1	C	305	CYS	5.1
2	D	277	SER	4.8
2	D	404	PHE	4.7
4	F	254	GLY	4.6
4	F	160	ILE	4.6
4	F	181	VAL	4.5
2	D	286	LEU	4.5
2	D	407	TRP	4.5
4	F	146	VAL	4.4
4	F	148	ILE	4.4
4	F	240	LEU	4.4
1	A	335	ILE	4.4
4	F	253	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
4	F	330	ILE	4.3
4	F	149	ALA	4.2
3	E	14	CYS	4.2
1	A	246	GLY	4.1
4	F	153	ALA	4.1
1	C	440	VAL	4.1
1	A	43	GLY	3.9
1	C	283	HIS	3.9
1	A	247	ALA	3.9
1	A	281	ALA	3.8
4	F	362	ALA	3.7
2	D	248	LEU	3.7
2	B	438	ALA	3.7
4	F	154	GLY	3.6
2	D	275	LEU	3.6
4	F	228	TYR	3.6
3	E	44	ASP	3.6
4	F	125	THR	3.6
1	A	439	SER	3.6
4	F	245	ILE	3.6
1	A	42	ILE	3.5
1	A	45	GLY	3.5
4	F	255	ARG	3.5
4	F	233	PHE	3.4
1	A	41	THR	3.4
4	F	296	MET	3.4
4	F	147	TRP	3.4
4	F	161	LEU	3.4
4	F	131	PHE	3.4
2	D	220	THR	3.3
3	E	11	LEU	3.3
2	D	276	THR	3.3
3	E	139	LEU	3.3
3	E	24	LEU	3.2
4	F	98	TYR	3.2
1	A	436	GLY	3.2
3	E	6	MET	3.2
4	F	186	LEU	3.2
1	C	341	ILE	3.2
4	F	192	LEU	3.1
4	F	182	ILE	3.1
2	D	71	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	3.1
4	F	134	ALA	3.1
1	A	437	VAL	3.1
2	D	195	VAL	3.1
1	A	149	PHE	3.1
1	A	250	VAL	3.1
4	F	194	PRO	3.1
2	B	1	MET	3.1
2	B	303	ALA	3.0
2	D	406	HIS	3.0
2	D	403	ALA	3.0
3	E	23	ILE	3.0
2	B	279	GLY	3.0
2	D	272	PHE	3.0
1	C	286	LEU	2.9
4	F	173	ILE	2.9
1	C	280	LYS	2.9
3	E	9	ILE	2.9
4	F	237	THR	2.9
2	D	177	VAL	2.9
4	F	92	THR	2.9
1	A	71	GLU	2.8
2	D	405	LEU	2.8
4	F	99	VAL	2.8
2	B	280	SER	2.8
1	A	282	TYR	2.8
4	F	378	LEU	2.8
1	A	86	LEU	2.8
2	D	214	PHE	2.8
2	D	221	THR	2.7
1	A	119	LEU	2.7
2	D	70	LEU	2.7
2	B	115	VAL	2.7
4	F	306	HIS	2.7
2	B	282	GLN	2.7
4	F	271	LEU	2.7
4	F	249	TYR	2.7
4	F	88	SER	2.7
2	D	82	PRO	2.7
2	D	222	PRO	2.7
4	F	180	HIS	2.6
4	F	145	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	37	PRO	2.6
4	F	162	ILE	2.6
1	C	357	TYR	2.6
1	C	43	GLY	2.6
2	D	57	THR	2.6
4	F	130	VAL	2.6
4	F	332	VAL	2.6
2	D	100	GLY	2.6
1	C	309	HIS	2.6
2	D	94	PHE	2.6
1	A	262	TYR	2.6
1	A	67	PHE	2.5
2	B	57	THR	2.5
2	D	246	GLY	2.5
4	F	17	VAL	2.5
4	F	229	ASN	2.5
2	D	98	GLY	2.5
1	A	283	HIS	2.5
1	C	351	PHE	2.5
4	F	319	PHE	2.5
1	A	66[A]	VAL	2.5
4	F	184	LYS	2.5
2	B	128	SER	2.5
4	F	205	VAL	2.5
3	E	26	PRO	2.5
3	E	22	VAL	2.4
4	F	172	PHE	2.4
1	A	88	HIS	2.4
1	C	285	GLN	2.4
2	B	94	PHE	2.4
1	A	360	PRO	2.4
1	A	351	PHE	2.4
2	D	355	VAL	2.4
4	F	213	ILE	2.4
1	A	83	TYR	2.4
1	A	358	GLN	2.4
4	F	167	SER	2.4
2	D	399	PHE	2.4
1	A	46	ASP	2.3
4	F	256	TYR	2.3
4	F	28	LYS	2.3
4	F	344	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	340	SER	2.3
3	E	105[A]	MET	2.3
1	A	49	PHE	2.3
2	B	83	PHE	2.3
4	F	100	ILE	2.3
4	F	239	HIS	2.3
1	A	44	GLY	2.3
4	F	230	SER	2.3
1	A	316	CYS	2.3
4	F	75	ALA	2.3
1	A	94	THR	2.3
1	A	428	LEU	2.3
4	F	132	LEU	2.3
4	F	275	LEU	2.3
4	F	104	ASN	2.3
3	E	7	GLU	2.3
1	C	338	LYS	2.3
1	A	78	VAL	2.3
2	B	242	LEU	2.2
4	F	170	LEU	2.2
4	F	315	PHE	2.2
1	A	58	ALA	2.2
1	C	88	HIS	2.2
4	F	248	GLU	2.2
2	B	284	ARG	2.2
3	E	45	PRO	2.2
1	A	38	SER	2.2
1	A	357	TYR	2.2
2	D	210	TYR	2.2
1	A	346	TRP	2.2
3	E	47	LEU	2.2
1	C	302	MET	2.2
3	E	28	SER	2.2
4	F	101	TYR	2.2
4	F	135	TYR	2.2
1	A	125	LEU	2.2
2	D	325	MET	2.2
3	E	27	PRO	2.2
4	F	227	PRO	2.2
2	B	341	SER	2.2
1	A	248	LEU	2.1
2	D	377	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	259	GLY	2.1
4	F	164	SER	2.1
4	F	373	SER	2.1
4	F	185	TYR	2.1
1	A	136[A]	LEU	2.1
1	A	259	LEU	2.1
2	D	428	LEU	2.1
2	D	95	GLY	2.1
2	D	124	LYS	2.1
2	D	372	LYS	2.1
4	F	346	LEU	2.1
4	F	361	LEU	2.1
1	A	285	GLN	2.1
2	D	2	ARG	2.1
4	F	44	ARG	2.1
1	C	178	SER	2.1
2	D	99	ALA	2.1
3	E	120	LEU	2.1
4	F	243	HIS	2.1
3	E	82	VAL	2.1
1	C	246	GLY	2.1
1	C	38	SER	2.0
4	F	90	SER	2.0
1	A	117	LEU	2.0
2	D	219	LEU	2.0
2	B	82	PRO	2.0
4	F	32	LYS	2.0
1	A	54	SER	2.0
2	D	353	THR	2.0
1	C	299	ALA	2.0
1	C	315	CYS	2.0
2	D	229	HIS	2.0
2	D	137	LEU	2.0
4	F	22	LEU	2.0
4	F	30	LEU	2.0
1	C	276	ILE	2.0
2	D	401	ARG	2.0
4	F	46	ARG	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	0.94	0.10	45,61,73,73	0
5	3WU	L	4	12/13	0.95	0.07	43,53,69,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

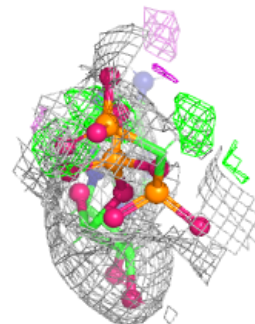
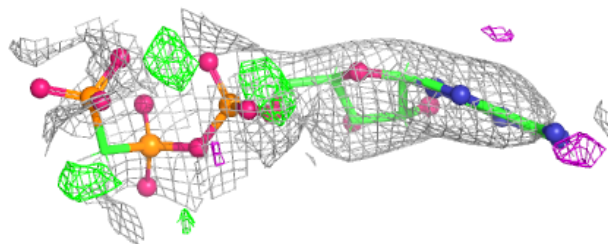
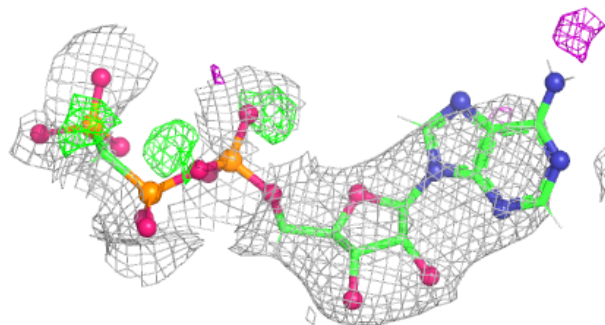
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	B	502	1/1	0.75	0.23	76,76,76,76	0
7	MG	B	503	1/1	0.75	0.24	72,72,72,72	0
7	MG	C	502	1/1	0.80	0.29	48,48,48,48	0
10	ACP	F	401	31/31	0.82	0.16	104,133,172,179	0
7	MG	A	502	1/1	0.83	0.16	56,56,56,56	0
9	GDP	D	501	28/28	0.90	0.14	61,75,98,118	0
7	MG	C	503	1/1	0.93	0.13	82,82,82,82	0
8	CA	A	503	1/1	0.93	0.10	115,115,115,115	0
6	GTP	A	501	32/32	0.95	0.10	45,55,75,84	0
6	GTP	C	501	32/32	0.97	0.07	38,47,61,80	0
9	GDP	B	501	28/28	0.97	0.09	40,49,72,81	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.

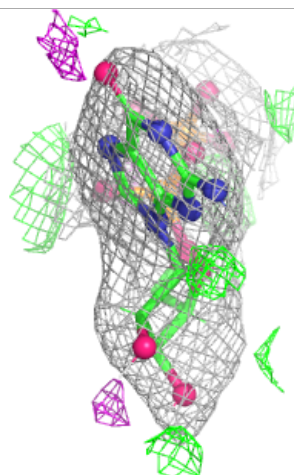
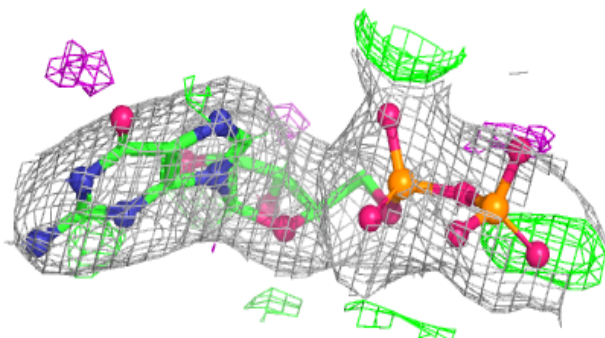
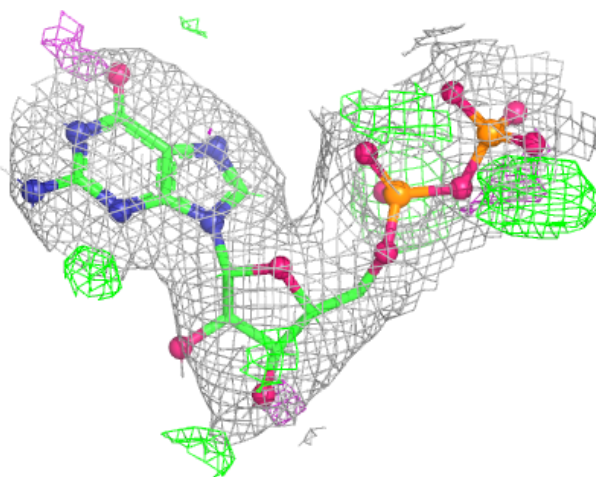
Electron density around ACP F 401:

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



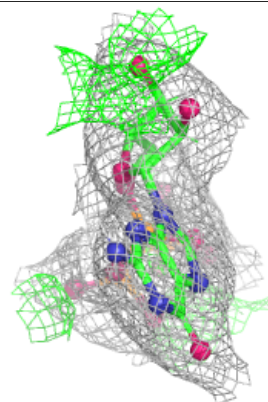
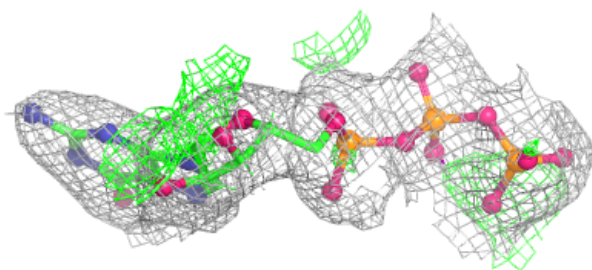
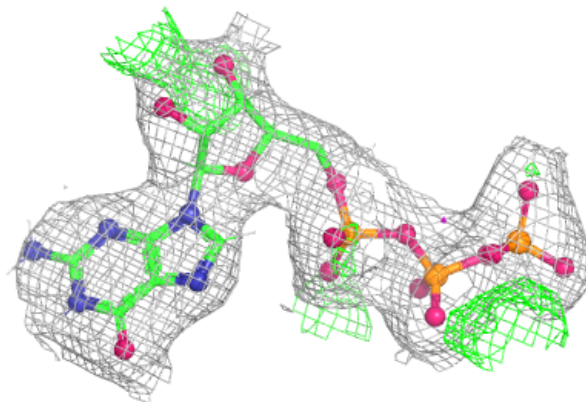
Electron density around GDP D 501:

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

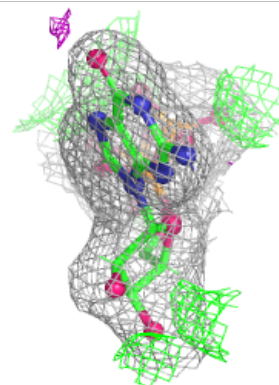
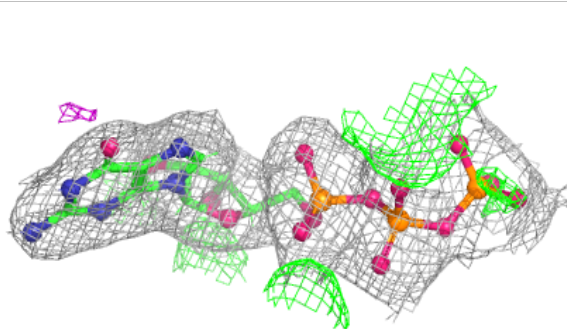
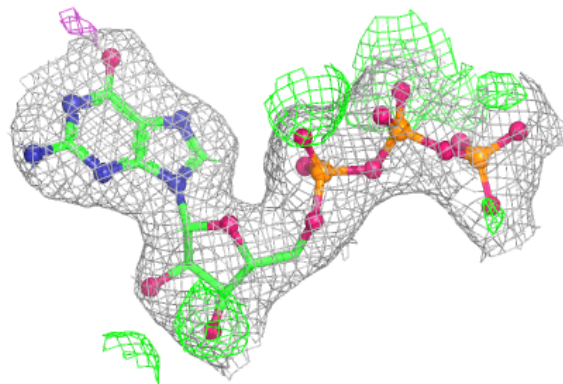


Electron density around GTP A 501:

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

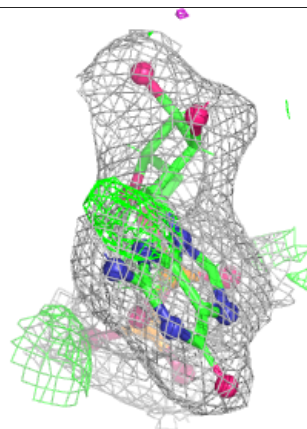
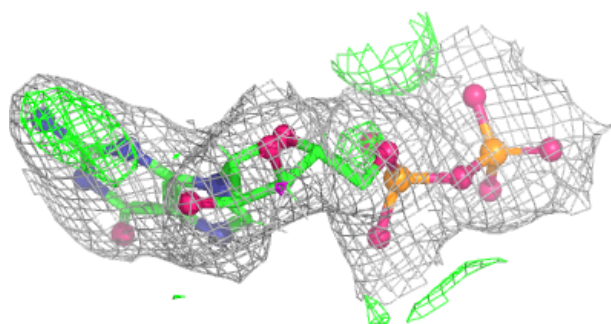
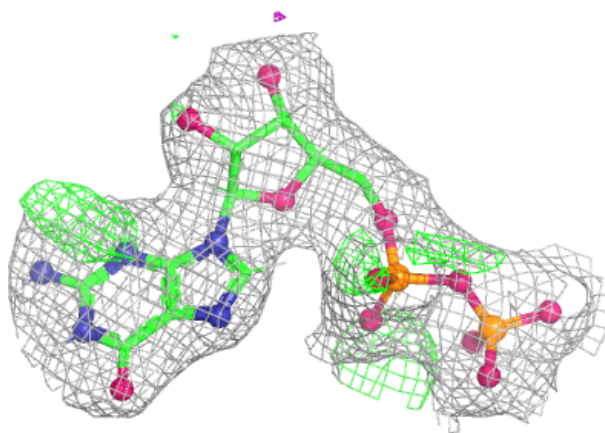
**Electron density around GTP C 501:**

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



Electron density around 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.