



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:50 pm BST

PDB ID : 5XLT
Title : The crystal structure of tubulin in complex with 4'-demethylepipodophyllotoxin
Authors : Yu, Y.; Chen, Q.
Deposited on : 2017-05-11
Resolution : 2.81 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

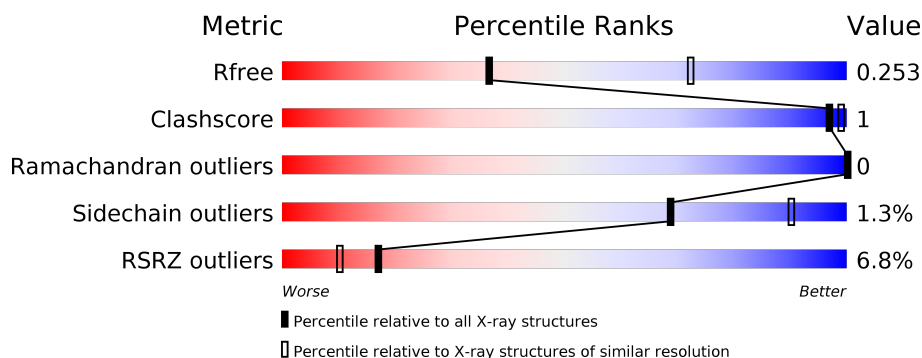
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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>0%</div> <div>95%</div> <div>• •</div> </div>
1	C	450	<div> <div>96%</div> <div>• •</div> </div>
2	B	445	<div> <div>2%</div> <div>92%</div> <div>• •</div> </div>
2	D	445	<div> <div>8%</div> <div>90%</div> <div>• 5%</div> </div>
3	E	143	<div> <div>6%</div> <div>83%</div> <div>• 15%</div> </div>
4	F	384	<div> <div>23%</div> <div>83%</div> <div>• 13%</div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 34508 atoms, of which 16893 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6734	2163	3318	581	650	22			
1	C	440	Total	C	H	N	O	S	0	1	0
			6789	2180	3344	585	657	23			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	1	0
			6604	2115	3235	577	650	27			
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 Tubulin tyrosine ligase.

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

There are 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		

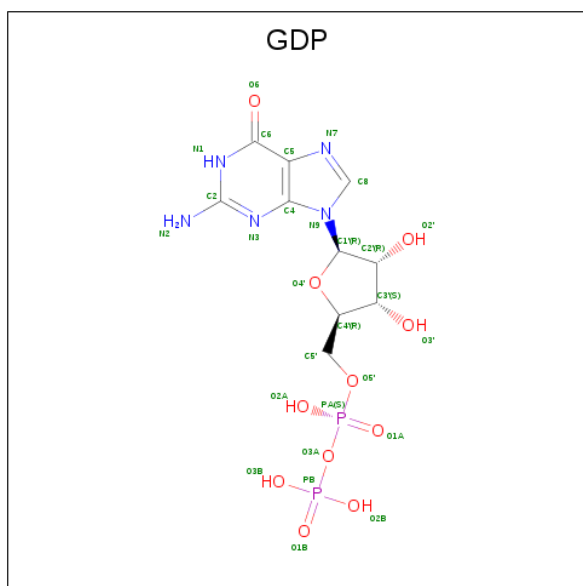
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	D	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).

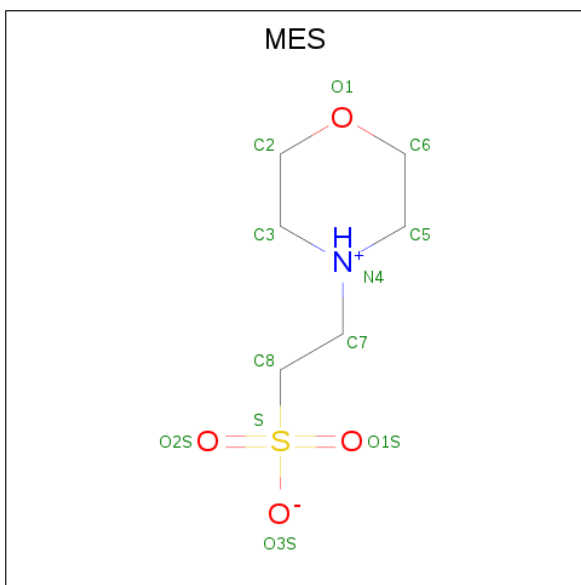
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



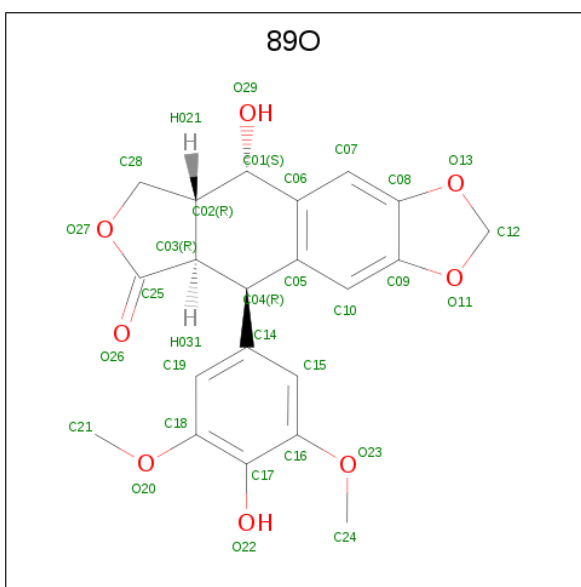
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
8	D	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		
9	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 10 is (5S,5aR,8aR,9R)-9-(3,5-dimethoxy-4-oxidanyl-phenyl)-5-oxidanyl-5a,6,8a,9-tetrahydro-5H-[2]benzofuro[6,5-f][1,3]benzodioxol-8-one (three-letter code: 89O) (formula: C₂₁H₂₀O₈).



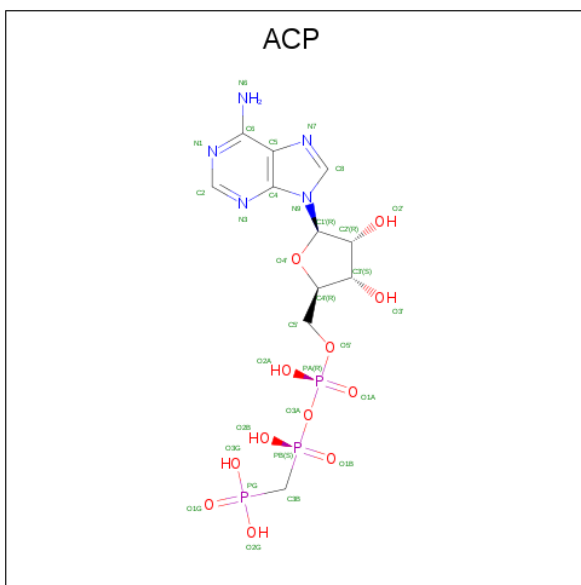
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			49	21	20	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	H	O	0	0
			49	21	20	8		

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

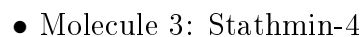


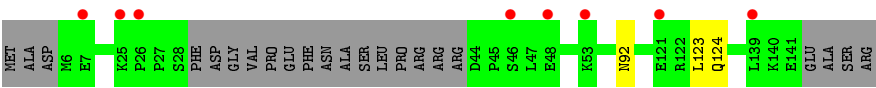
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

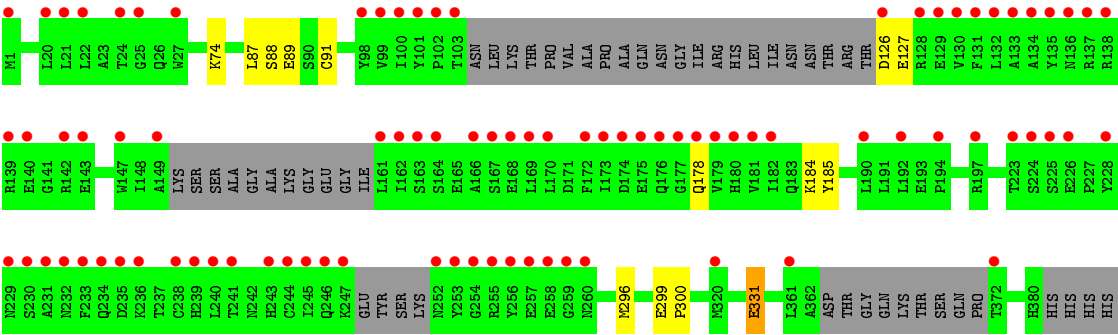
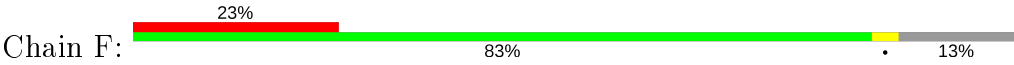
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	25	Total	O	0	0
			25	25		
12	B	16	Total	O	0	0
			16	16		
12	C	37	Total	O	0	0
			37	37		
12	D	9	Total	O	0	0
			9	9		
12	E	2	Total	O	0	0
			2	2		
12	F	4	Total	O	0	0
			4	4		

- Molecule 1: Tubulin alpha-1B chain





● Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.47Å 156.93Å 180.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.81 49.65 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.86-2.81) 96.5 (49.65-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.206 , 0.249 0.211 , 0.253	Depositor DCC
R_{free} test set	1043 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.3	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	0.93	EDS
Total number of atoms	34508	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, CA, GTP, ACP, MES, 89O

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	0.22	0/3494	0.37	0/4743
1	C	0.22	0/3523	0.37	0/4782
2	B	0.22	0/3444	0.37	0/4664
2	D	0.22	0/3382	0.36	0/4581
3	E	0.21	0/1008	0.31	0/1337
4	F	0.21	0/2806	0.35	0/3791
All	All	0.22	0/17657	0.36	0/23898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3318	3330	3	0
1	C	3445	3344	3356	2	0
2	B	3369	3235	3246	9	0
2	D	3309	3179	3189	10	0
3	E	1000	1014	1018	1	0
4	F	2744	2698	2709	7	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
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
8	D	28	10	12	0	0
9	B	24	25	25	1	0
10	B	29	20	0	1	0
10	D	29	20	0	2	0
11	F	31	0	14	1	0
12	A	25	0	0	0	0
12	B	16	0	0	1	0
12	C	37	0	0	0	0
12	D	9	0	0	1	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17615	16893	16935	32	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 (32) 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)
10:B:505:89O:O27	10:B:505:89O:C25	1.65	1.32
10:D:502:89O:O27	10:D:502:89O:C25	1.65	1.28
1:A:221:ARG:NH2	2:B:327:ASP:OD2	2.35	0.60
2:D:404:ASP:OD1	2:D:405:GLU:N	2.36	0.58
4:F:178:GLN:OE1	4:F:178:GLN:N	2.38	0.57
4:F:126:ASP:OD1	4:F:127:GLU:N	2.39	0.55
2:B:296:SER:N	9:B:504:MES:O3S	2.39	0.54
2:B:309:ARG:NH1	12:B:604:HOH:O	2.39	0.54
1:C:245:ASP:N	1:C:245:ASP:OD1	2.41	0.53
2:B:234:SER:O	2:B:241:ARG:NH2	2.41	0.53
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.42	0.51
2:B:261:PRO:O	2:B:264:HIS:ND1	2.41	0.50
2:D:256:ASN:ND2	10:D:502:89O:O29	2.45	0.49
2:D:165:ASN:ND2	12:D:603:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.36	0.46
2:D:301:ALA:O	2:D:303:CYS:N	2.50	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.32	0.45
4:F:184:LYS:NZ	4:F:185:TYR:O	2.47	0.44
2:D:137:HIS:ND1	2:D:144:GLY:O	2.32	0.44
2:B:145:SER:HG	2:B:188:SER:HG	1.64	0.44
2:D:177:ASP:OD1	2:D:177:ASP:N	2.51	0.43
2:B:301:ALA:O	2:B:303:CYS:N	2.48	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.81	0.43
2:B:145:SER:OG	2:B:188:SER:OG	2.32	0.43
2:B:262:ARG:NE	2:B:421:GLU:OE2	2.52	0.42
4:F:331:GLU:OE2	11:F:401:ACP:H3B2	2.18	0.42
4:F:299:GLU:N	4:F:300:PRO:HD2	2.35	0.42
4:F:87:LEU:O	4:F:88:SER:OG	2.28	0.41
1:C:183:GLU:N	1:C:184:PRO:CD	2.84	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.03	0.40
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.03	0.40
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.02	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%)	419 (96%)	16 (4%)	0	100	100
1	C	439/450 (98%)	430 (98%)	9 (2%)	0	100	100
2	B	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	324/384 (84%)	314 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2158/2317 (93%)	2100 (97%)	58 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	364 (99%)	4 (1%)	73	91
1	C	372/378 (98%)	367 (99%)	5 (1%)	69	90
2	B	370/383 (97%)	367 (99%)	3 (1%)	81	94
2	D	364/383 (95%)	358 (98%)	6 (2%)	62	87
3	E	109/127 (86%)	107 (98%)	2 (2%)	59	85
4	F	301/342 (88%)	297 (99%)	4 (1%)	69	90
All	All	1884/1991 (95%)	1860 (99%)	24 (1%)	69	90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ASP
1	A	256	GLN
1	A	279	GLU
1	A	420	GLU
2	B	137	HIS
2	B	190	HIS
2	B	245	GLN
1	C	2	ARG
1	C	177	VAL
1	C	178	SER
1	C	245	ASP
1	C	251	ASP
2	D	41	ASP
2	D	137	HIS

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Mol	Chain	Res	Type
2	D	177	ASP
2	D	245	GLN
2	D	323	MET
2	D	390	ARG
3	E	92	ASN
3	E	124	GLN
4	F	89	GLU
4	F	91	CYS
4	F	296	MET
4	F	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	165	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 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
11	ACP	F	401	-	27,33,33	2.79	12 (44%)	32,52,52	4.13	11 (34%)
10	89O	D	502	-	33,33,33	5.42	19 (57%)	50,50,50	3.63	18 (36%)
9	MES	B	503	-	12,12,12	2.32	1 (8%)	14,16,16	2.43	6 (42%)
10	89O	B	505	-	33,33,33	5.36	18 (54%)	50,50,50	3.60	16 (32%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.76	7 (21%)
8	GDP	B	501	6	24,30,30	1.12	2 (8%)	31,47,47	1.98	8 (25%)
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.79	7 (21%)
8	GDP	D	501	6	24,30,30	1.15	2 (8%)	31,47,47	1.97	8 (25%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.37	3 (21%)

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
11	ACP	F	401	-	-	5/15/38/38	0/3/3/3
10	89O	D	502	-	-	4/8/43/43	0/5/5/5
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
10	89O	B	505	-	-	4/8/43/43	0/5/5/5
5	GTP	A	501	6	-	10/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	89O	O27-C25	13.81	1.65	1.35
10	B	505	89O	O27-C25	13.67	1.65	1.35
10	D	502	89O	C06-C05	12.08	1.61	1.40
10	B	505	89O	C05-C04	12.06	1.68	1.51
10	B	505	89O	C06-C05	12.05	1.61	1.40
10	D	502	89O	C05-C04	11.83	1.68	1.51
10	B	505	89O	C10-C09	10.72	1.58	1.38
10	D	502	89O	C10-C09	10.72	1.58	1.38
10	D	502	89O	C06-C01	10.18	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	89O	C07-C08	10.07	1.57	1.38
10	B	505	89O	C07-C08	9.82	1.56	1.38
10	B	505	89O	C06-C01	9.46	1.66	1.51
9	B	503	MES	C8-S	-7.79	1.66	1.77
9	B	504	MES	C8-S	-7.52	1.66	1.77
11	F	401	ACP	O4'-C1'	6.65	1.50	1.41
11	F	401	ACP	PB-O1B	5.83	1.65	1.51
11	F	401	ACP	PG-O1G	5.63	1.62	1.50
11	F	401	ACP	C2-N3	4.87	1.39	1.32
10	B	505	89O	C18-C17	4.46	1.46	1.40
10	D	502	89O	C18-C17	4.38	1.46	1.40
10	B	505	89O	C03-C02	4.31	1.63	1.54
10	D	502	89O	C03-C02	4.27	1.63	1.54
10	D	502	89O	C16-C17	4.15	1.45	1.40
10	B	505	89O	C16-C17	4.12	1.45	1.40
8	D	501	GDP	C6-C5	4.07	1.48	1.41
8	B	501	GDP	C6-C5	3.98	1.48	1.41
11	F	401	ACP	PB-O3A	3.98	1.62	1.58
10	D	502	89O	C14-C04	3.62	1.57	1.52
10	B	505	89O	O20-C18	3.61	1.42	1.37
10	B	505	89O	C14-C04	3.61	1.57	1.52
10	B	505	89O	C03-C25	-3.50	1.46	1.51
10	B	505	89O	C19-C18	3.36	1.44	1.38
10	D	502	89O	O20-C18	3.35	1.42	1.37
10	D	502	89O	O13-C08	3.28	1.43	1.38
10	D	502	89O	C19-C18	3.27	1.44	1.38
11	F	401	ACP	C2-N1	3.27	1.40	1.33
10	D	502	89O	O11-C09	3.24	1.43	1.38
10	D	502	89O	C03-C25	-3.17	1.47	1.51
10	D	502	89O	C15-C16	3.13	1.44	1.38
10	B	505	89O	O11-C09	3.13	1.42	1.38
11	F	401	ACP	PG-O2G	3.12	1.62	1.54
10	B	505	89O	C15-C16	3.10	1.44	1.38
10	B	505	89O	O13-C08	3.08	1.42	1.38
5	C	501	GTP	C6-N1	3.06	1.38	1.33
5	A	501	GTP	C6-N1	3.03	1.38	1.33
10	B	505	89O	O23-C16	2.98	1.41	1.37
10	D	502	89O	O23-C16	2.95	1.41	1.37
11	F	401	ACP	C5-C4	-2.77	1.33	1.40
11	F	401	ACP	PG-O3G	-2.64	1.48	1.54
10	D	502	89O	C02-C01	2.62	1.56	1.52
11	F	401	ACP	C6-C5	-2.54	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C5-C4	2.40	1.47	1.40
10	D	502	89O	C19-C14	2.40	1.42	1.39
10	B	505	89O	C19-C14	2.38	1.42	1.39
11	F	401	ACP	PB-O2B	-2.35	1.50	1.56
8	B	501	GDP	C5-C4	2.31	1.47	1.40
11	F	401	ACP	C2'-C3'	-2.01	1.47	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	89O	O27-C25-O26	17.48	139.55	121.42
10	B	505	89O	O27-C25-O26	17.38	139.44	121.42
11	F	401	ACP	O4'-C4'-C3'	-13.98	77.44	105.11
11	F	401	ACP	O4'-C1'-C2'	-13.11	87.77	106.93
10	D	502	89O	O27-C25-C03	-9.16	96.40	109.52
10	B	505	89O	O27-C25-C03	-8.92	96.75	109.52
11	F	401	ACP	N3-C2-N1	-6.88	117.93	128.68
10	B	505	89O	C28-O27-C25	6.38	116.10	110.28
11	F	401	ACP	C2'-C3'-C4'	-6.13	90.73	102.64
10	B	505	89O	C02-C03-C25	5.91	110.98	103.07
10	D	502	89O	C02-C03-C25	5.69	110.68	103.07
5	A	501	GTP	N3-C2-N1	-5.33	120.11	127.22
5	C	501	GTP	N3-C2-N1	-5.32	120.12	127.22
10	D	502	89O	C28-O27-C25	5.30	115.12	110.28
11	F	401	ACP	C1'-N9-C4	-5.27	117.38	126.64
10	D	502	89O	O20-C18-C17	4.86	119.45	114.54
9	B	503	MES	C7-N4-C5	4.81	123.52	111.23
9	B	503	MES	C5-N4-C3	4.77	119.56	108.83
8	B	501	GDP	C6-C5-C4	-4.61	116.40	120.80
10	B	505	89O	O20-C18-C17	4.54	119.12	114.54
8	B	501	GDP	C6-N1-C2	4.46	123.02	115.93
8	B	501	GDP	C2-N3-C4	4.46	120.45	115.36
8	D	501	GDP	C2-N3-C4	4.43	120.42	115.36
8	D	501	GDP	C6-N1-C2	4.37	122.87	115.93
10	B	505	89O	O26-C25-C03	-4.36	123.77	129.38
10	B	505	89O	C18-C19-C14	4.31	126.72	119.83
10	D	502	89O	C18-C19-C14	4.23	126.59	119.83
8	D	501	GDP	C6-C5-C4	-4.18	116.80	120.80
10	D	502	89O	O26-C25-C03	-4.18	124.01	129.38
5	C	501	GTP	C2-N3-C4	4.17	120.11	115.36
10	D	502	89O	C03-C02-C01	4.11	116.47	109.67
5	A	501	GTP	C2-N3-C4	4.08	120.02	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C6-N1	-3.97	118.01	123.43
10	B	505	89O	C06-C05-C04	3.90	124.71	114.40
8	B	501	GDP	C5-C6-N1	-3.89	118.11	123.43
10	D	502	89O	O23-C16-C17	3.88	118.45	114.54
10	D	502	89O	C06-C05-C04	3.74	124.29	114.40
8	B	501	GDP	N3-C2-N1	-3.63	122.38	127.22
10	D	502	89O	C19-C14-C15	-3.48	113.13	118.08
10	D	502	89O	O11-C09-C10	3.43	132.44	127.85
10	B	505	89O	O23-C16-C17	3.43	118.00	114.54
8	D	501	GDP	N3-C2-N1	-3.41	122.68	127.22
10	B	505	89O	C19-C18-C17	-3.40	117.25	120.60
10	B	505	89O	O11-C09-C10	3.39	132.39	127.85
10	D	502	89O	C16-C15-C14	3.38	125.23	119.83
9	B	503	MES	C6-C5-N4	-3.36	105.01	110.10
10	B	505	89O	C19-C14-C15	-3.23	113.48	118.08
5	C	501	GTP	PB-O3B-PG	-3.21	121.83	132.83
5	C	501	GTP	PA-O3A-PB	-3.20	121.86	132.83
10	B	505	89O	C03-C02-C01	3.18	114.94	109.67
5	A	501	GTP	PB-O3B-PG	-3.14	122.04	132.83
5	A	501	GTP	PA-O3A-PB	-3.11	122.16	132.83
11	F	401	ACP	O2B-PB-C3B	3.11	119.29	106.58
8	D	501	GDP	PA-O3A-PB	-3.06	122.32	132.83
10	B	505	89O	C16-C15-C14	3.05	124.70	119.83
5	C	501	GTP	C5-C6-N1	-2.97	119.37	123.43
5	A	501	GTP	C5-C6-N1	-2.97	119.37	123.43
10	D	502	89O	C19-C18-C17	-2.91	117.73	120.60
11	F	401	ACP	O3G-PG-C3B	2.85	113.32	106.40
8	B	501	GDP	PA-O3A-PB	-2.82	123.17	132.83
11	F	401	ACP	O5'-C5'-C4'	2.74	118.41	108.99
11	F	401	ACP	O2G-PG-O1G	-2.70	105.25	112.39
10	D	502	89O	C10-C09-C08	-2.69	118.60	122.02
5	A	501	GTP	C6-N1-C2	2.65	120.14	115.93
10	B	505	89O	C10-C09-C08	-2.62	118.70	122.02
5	C	501	GTP	C6-N1-C2	2.60	120.06	115.93
8	D	501	GDP	C3'-C2'-C1'	2.52	104.77	100.98
11	F	401	ACP	O1B-PB-C3B	2.50	115.68	109.07
11	F	401	ACP	C5-C6-N6	-2.47	116.59	120.35
5	C	501	GTP	C3'-C2'-C1'	2.41	104.61	100.98
8	B	501	GDP	C3'-C2'-C1'	2.33	104.48	100.98
8	D	501	GDP	C4-C5-N7	-2.32	106.98	109.40
9	B	503	MES	O1S-S-C8	2.30	109.69	106.92
8	B	501	GDP	C4-C5-N7	-2.29	107.01	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	O2S-S-C8	2.28	109.66	106.92
9	B	503	MES	O2S-S-C8	2.25	109.63	106.92
10	D	502	89O	O27-C28-C02	-2.24	101.44	104.71
9	B	504	MES	C7-N4-C5	2.20	116.86	111.23
9	B	504	MES	O3S-S-C8	2.19	109.31	105.77
9	B	503	MES	C7-N4-C3	2.16	116.75	111.23
10	D	502	89O	C02-C03-C04	2.12	117.21	113.21
10	B	505	89O	C02-C03-C04	2.08	117.14	113.21
10	D	502	89O	C14-C04-C05	2.02	115.91	112.86
5	A	501	GTP	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	503	MES	C8-C7-N4-C5
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
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	504	MES	C7-C8-S-O1S
10	D	502	89O	C17-C18-O20-C21
10	D	502	89O	C19-C18-O20-C21
10	B	505	89O	C15-C16-O23-C24
10	D	502	89O	C17-C16-O23-C24
10	B	505	89O	C17-C16-O23-C24
10	D	502	89O	C15-C16-O23-C24
9	B	504	MES	C7-C8-S-O3S
10	B	505	89O	C17-C18-O20-C21
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C3'-C4'-C5'-O5'
11	F	401	ACP	C4'-C5'-O5'-PA
8	B	501	GDP	C5'-O5'-PA-O1A

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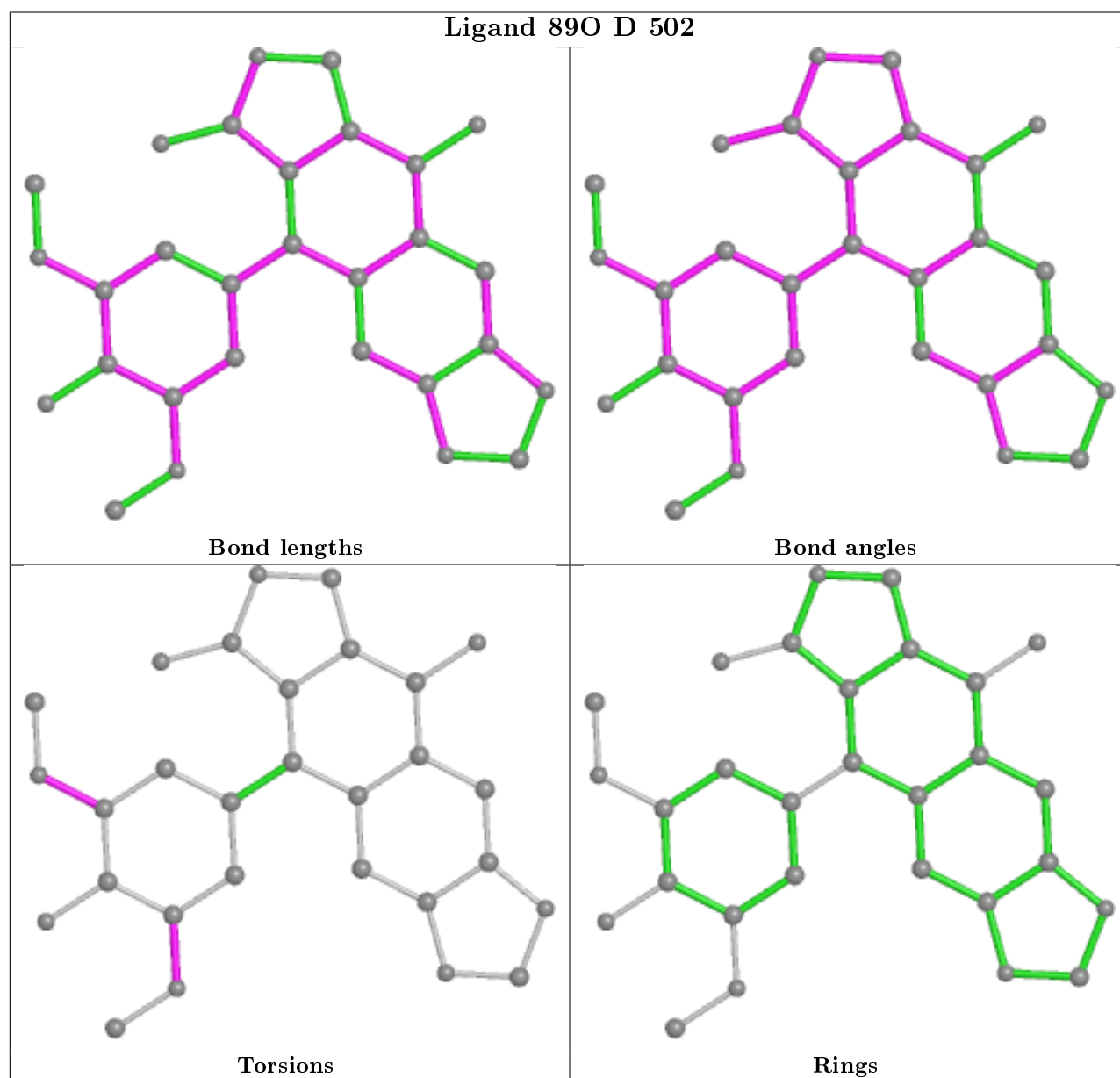
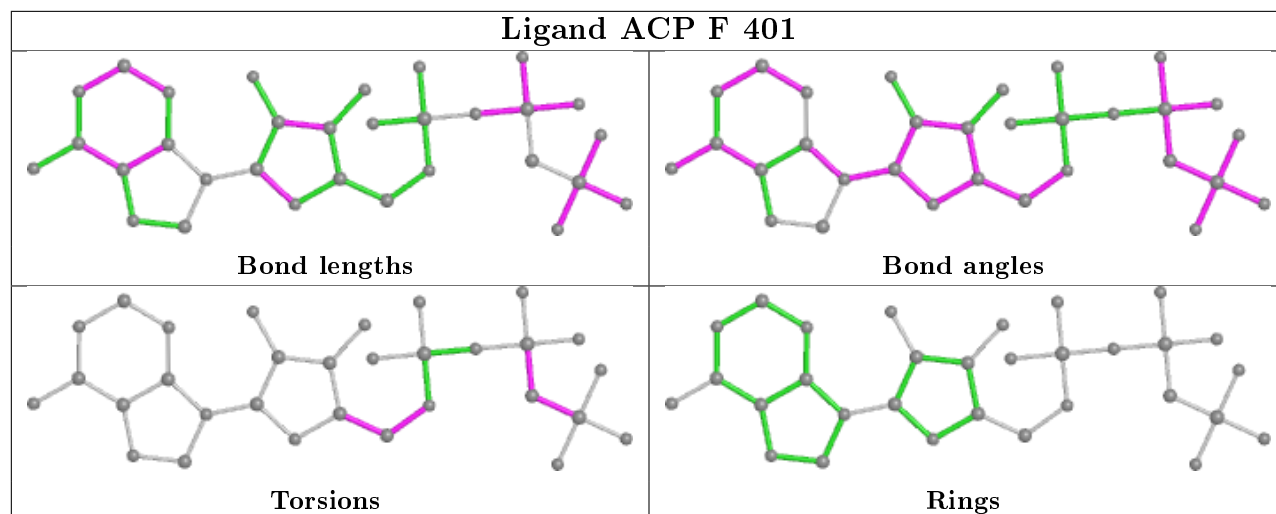
Mol	Chain	Res	Type	Atoms
9	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	C3'-C4'-C5'-O5'
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O2B
5	C	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	505	89O	C19-C18-O20-C21
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A

There are no ring outliers.

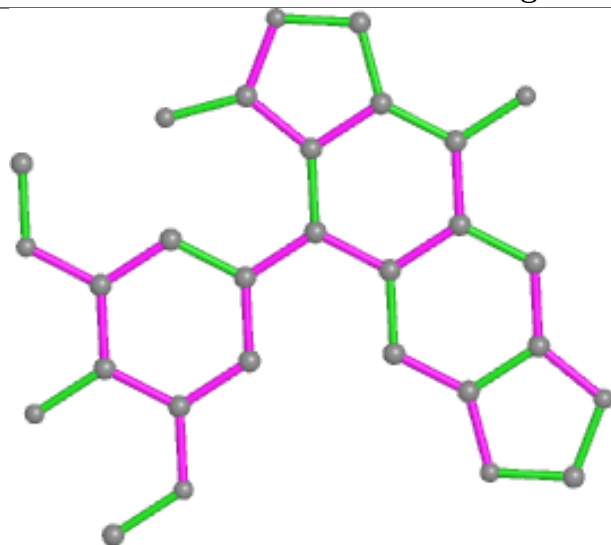
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	1	0
10	D	502	89O	2	0
10	B	505	89O	1	0
9	B	504	MES	1	0

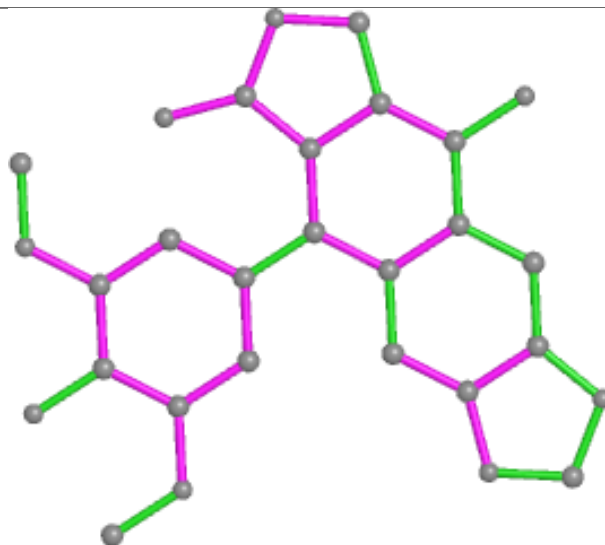
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



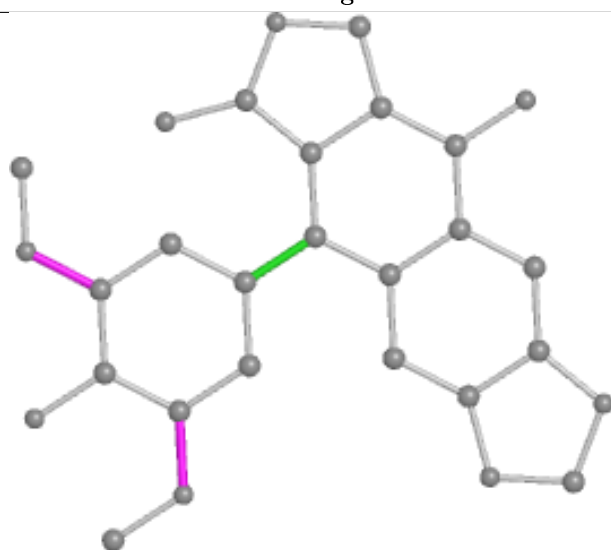
Ligand 89O B 505



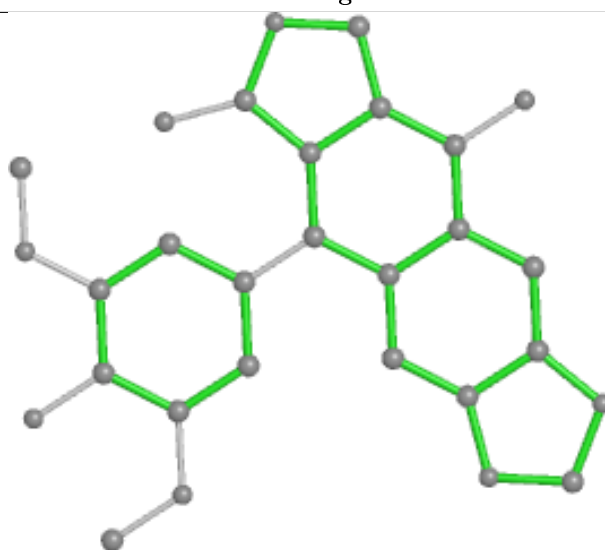
Bond lengths



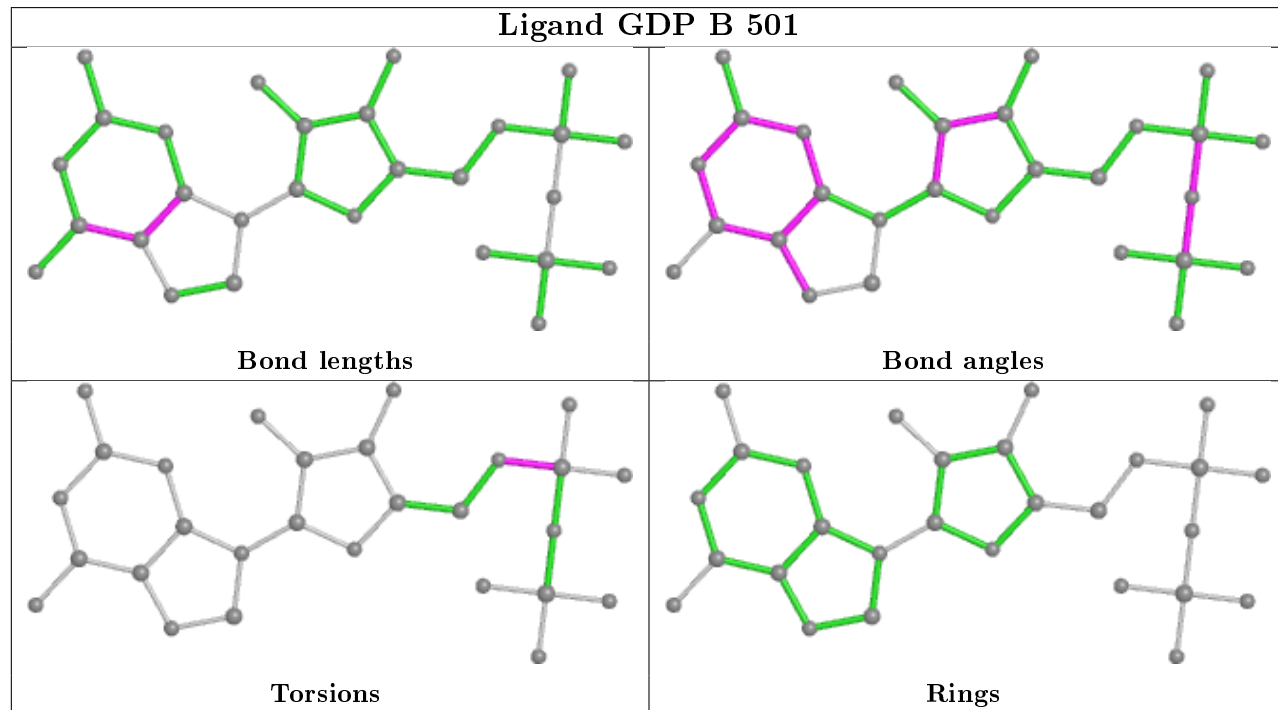
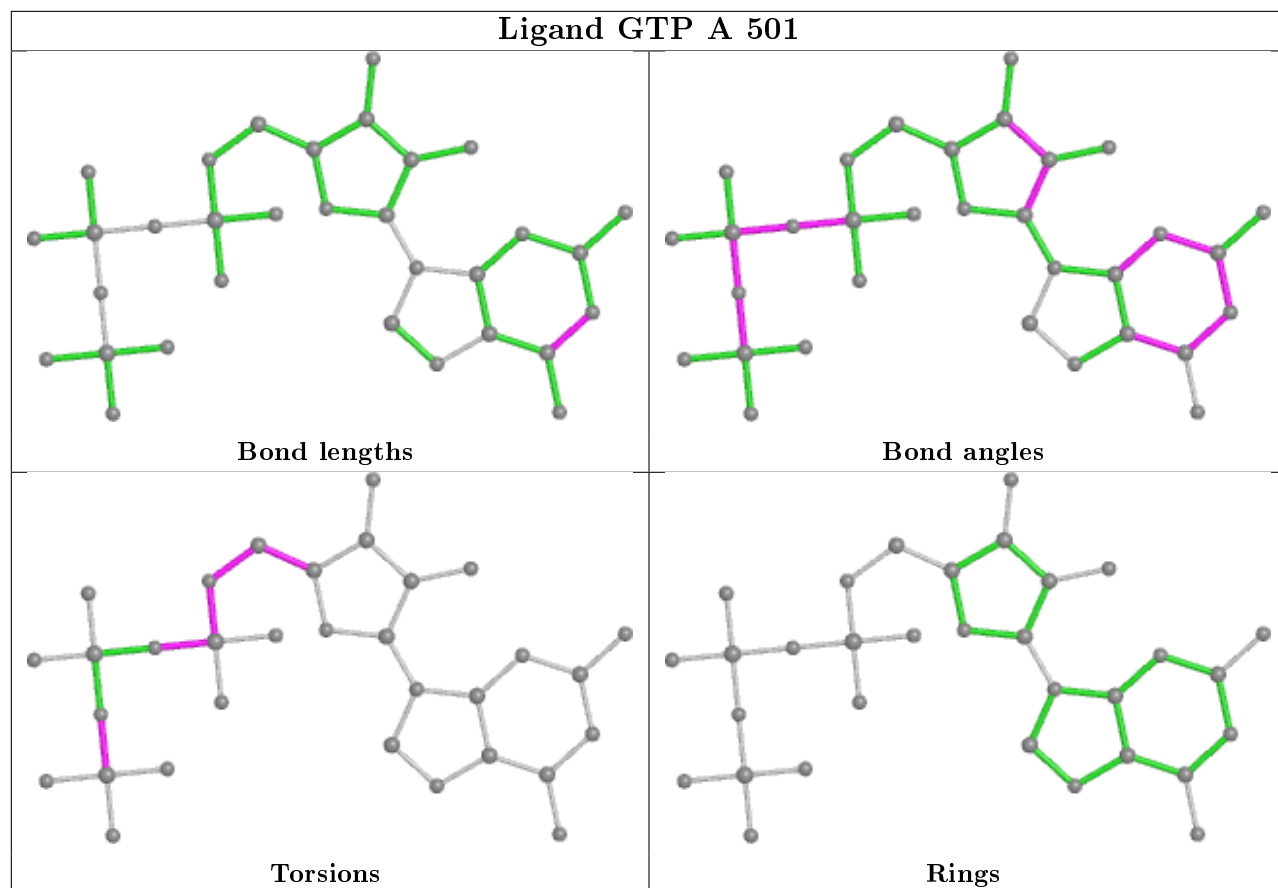
Bond angles

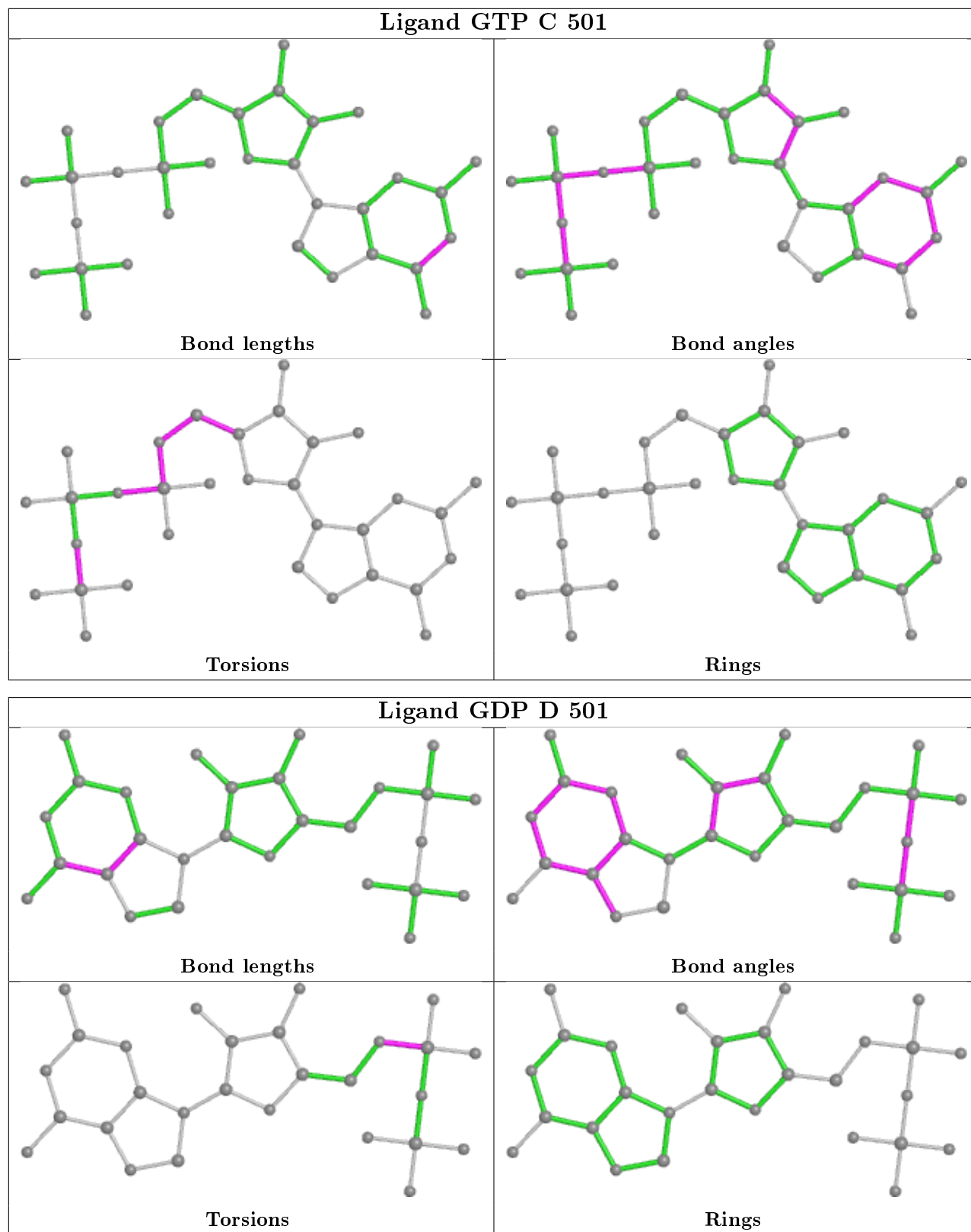


Torsions



Rings





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	437/450 (97%)	0.14	4 (0%) 84 80	23, 43, 76, 101	0
1	C	440/450 (97%)	-0.17	2 (0%) 91 88	17, 32, 60, 79	0
2	B	427/445 (95%)	0.10	10 (2%) 60 50	20, 41, 75, 132	0
2	D	421/445 (94%)	0.51	36 (8%) 10 5	28, 60, 95, 117	0
3	E	121/143 (84%)	0.45	8 (6%) 18 11	29, 59, 94, 105	0
4	F	334/384 (86%)	1.24	89 (26%) 0 0	33, 70, 134, 151	0
All	All	2180/2317 (94%)	0.33	149 (6%) 17 10	17, 48, 99, 151	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	177	GLY	7.5
4	F	173	ILE	7.1
4	F	231	ALA	6.8
4	F	233	PHE	6.3
4	F	170	LEU	6.1
4	F	103	THR	5.7
4	F	100	ILE	5.6
4	F	161	LEU	5.5
4	F	130	VAL	5.2
4	F	178	GLN	4.8
4	F	136	ASN	4.7
4	F	234	GLN	4.7
4	F	232	ASN	4.6
4	F	101	TYR	4.6
2	B	56	GLY	4.5
4	F	182	ILE	4.5
2	B	57	ASN	4.4
4	F	169	LEU	4.4
4	F	102	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
4	F	176	GLN	4.3
4	F	245	ILE	4.3
4	F	138	ARG	4.3
4	F	133	ALA	4.2
4	F	239	HIS	4.2
2	D	177	ASP	4.2
4	F	235	ASP	4.2
4	F	99	VAL	4.1
2	B	55	THR	4.1
4	F	240	LEU	4.1
2	D	55	THR	4.0
2	D	245	GLN	4.0
4	F	256	TYR	3.9
4	F	236	LYS	3.9
4	F	22	LEU	3.8
4	F	253	TYR	3.7
4	F	162	ILE	3.7
4	F	179	VAL	3.7
4	F	224	SER	3.7
4	F	132	LEU	3.7
2	B	279	GLN	3.7
4	F	254	GLY	3.5
4	F	163	SER	3.5
2	D	394	PHE	3.5
2	D	81	PHE	3.4
1	A	57	GLY	3.4
4	F	180	HIS	3.4
4	F	246	GLN	3.4
4	F	361	LEU	3.4
4	F	167	SER	3.4
4	F	259	GLY	3.4
4	F	243	HIS	3.4
1	A	178	SER	3.3
2	D	390	ARG	3.3
4	F	230	SER	3.3
4	F	228	TYR	3.3
4	F	244	CYS	3.3
2	B	280	GLN	3.3
2	D	180	VAL	3.2
4	F	194	PRO	3.2
2	D	175	VAL	3.2
2	D	78	SER	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	164	SER	3.1
4	F	131	PHE	3.1
2	B	37	HIS	3.1
2	D	73	MET	3.0
4	F	174	ASP	3.0
4	F	129	GLU	3.0
2	D	395	LEU	3.0
4	F	225	SER	3.0
2	D	37	HIS	3.0
4	F	223	THR	2.9
4	F	241	THR	2.9
4	F	247	LYS	2.9
4	F	137	ARG	2.9
4	F	252	ASN	2.9
3	E	46	SER	2.9
4	F	147	TRP	2.9
2	D	389	PHE	2.9
2	D	80	PRO	2.9
4	F	255	ARG	2.9
2	D	94	GLN	2.9
4	F	175	GLU	2.9
2	D	115	SER	2.8
4	F	172	PHE	2.8
4	F	166	ALA	2.8
2	D	172	SER	2.8
4	F	126	ASP	2.7
4	F	320	MET	2.7
4	F	181	VAL	2.7
4	F	149	ALA	2.7
4	F	1	MET	2.7
4	F	192	LEU	2.7
4	F	27	TRP	2.6
4	F	197	ARG	2.7
2	D	1	MET	2.6
2	D	77	ARG	2.6
2	D	391	ARG	2.6
2	B	59	TYR	2.6
3	E	139	LEU	2.6
4	F	140	GLU	2.6
2	D	70	PRO	2.6
2	D	92	PHE	2.5
4	F	128	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	388	MET	2.5
3	E	121	GLU	2.5
1	A	88	HIS	2.5
2	D	83	GLN	2.5
4	F	257	GLU	2.5
4	F	143	GLU	2.4
2	D	74	ASP	2.4
2	D	33	THR	2.4
4	F	226	GLU	2.4
4	F	168	GLU	2.4
2	D	403	MET	2.4
4	F	258	GLU	2.3
4	F	260	ASN	2.3
2	D	218	THR	2.3
2	B	35	SER	2.3
4	F	229	ASN	2.3
4	F	21	LEU	2.3
4	F	139	ARG	2.2
2	D	396	HIS	2.2
4	F	135	TYR	2.2
3	E	25	LYS	2.2
3	E	26	PRO	2.2
4	F	372	THR	2.2
1	C	253	THR	2.2
4	F	142	ARG	2.2
4	F	134	ALA	2.2
3	E	7	GLU	2.2
4	F	20	LEU	2.2
2	D	323	MET	2.2
2	D	362	LYS	2.2
2	D	34	GLY	2.1
3	E	48	GLU	2.1
4	F	238	CYS	2.1
2	B	58	LYS	2.1
3	E	53	LYS	2.1
4	F	25	GLY	2.1
2	D	397	TRP	2.1
2	B	427	ASP	2.1
4	F	24	THR	2.1
1	C	340	SER	2.1
2	D	39	ASP	2.0
4	F	190	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	405	GLU	2.0
1	A	362	VAL	2.0
4	F	98	TYR	2.0
2	D	100	ASN	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](#)

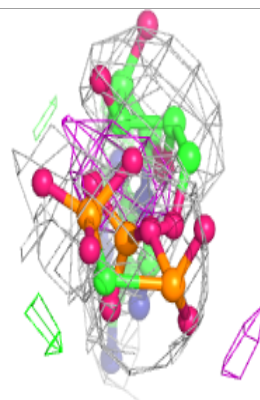
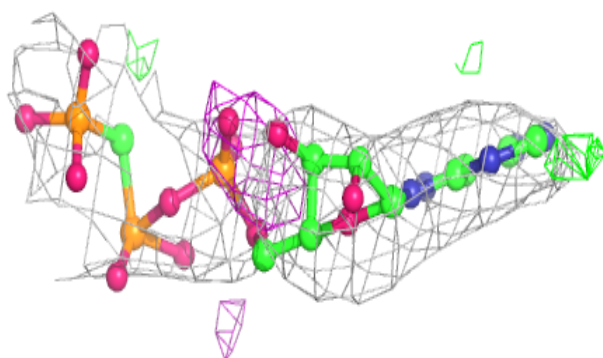
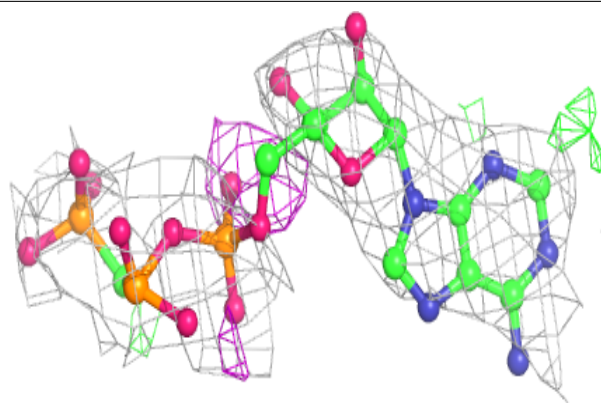
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACP	F	401	31/31	0.76	0.30	87,104,134,140	0
6	MG	D	503	1/1	0.77	0.12	53,53,53,53	0
10	89O	B	505	29/29	0.92	0.28	26,44,62,67	0
8	GDP	D	501	28/28	0.92	0.20	42,61,78,82	0
10	89O	D	502	29/29	0.92	0.28	37,55,69,73	0
9	MES	B	504	12/12	0.93	0.29	59,72,80,83	0
7	CA	A	503	1/1	0.95	0.08	86,86,86,86	0
9	MES	B	503	12/12	0.95	0.19	27,46,67,75	0
6	MG	A	502	1/1	0.96	0.23	22,22,22,22	0
8	GDP	B	501	28/28	0.97	0.23	14,26,36,49	0
5	GTP	C	501	32/32	0.98	0.18	12,24,39,50	0
5	GTP	A	501	32/32	0.98	0.23	18,29,39,45	0
6	MG	B	502	1/1	0.98	0.37	30,30,30,30	0
7	CA	C	503	1/1	0.98	0.09	42,42,42,42	0
6	MG	C	502	1/1	0.99	0.23	22,22,22,22	0

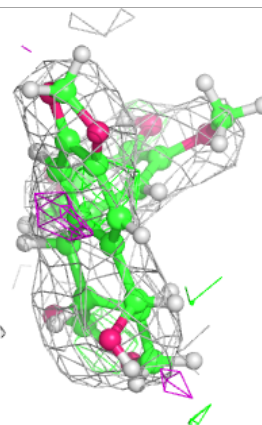
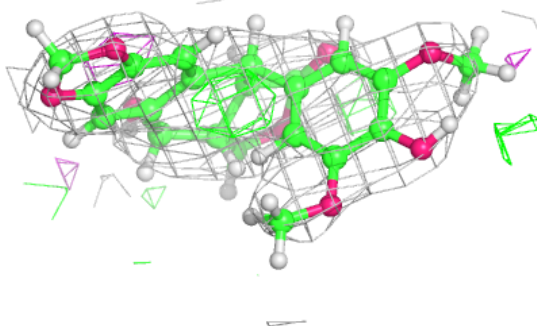
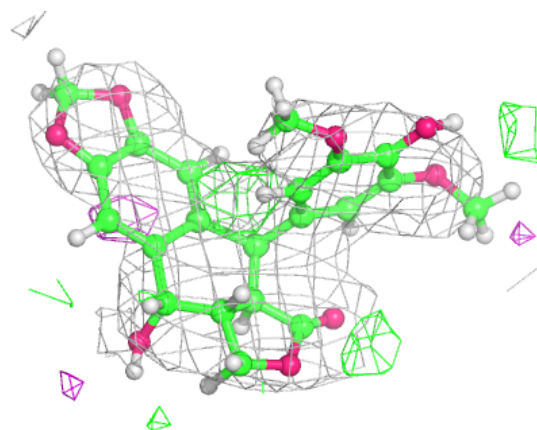
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

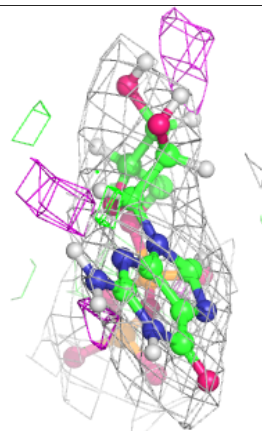
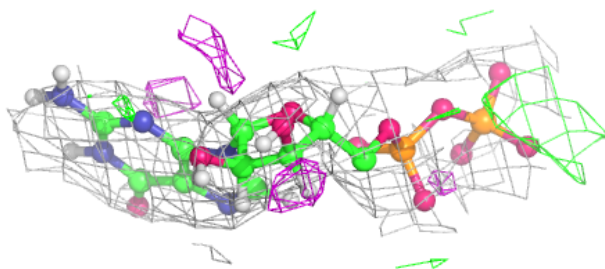
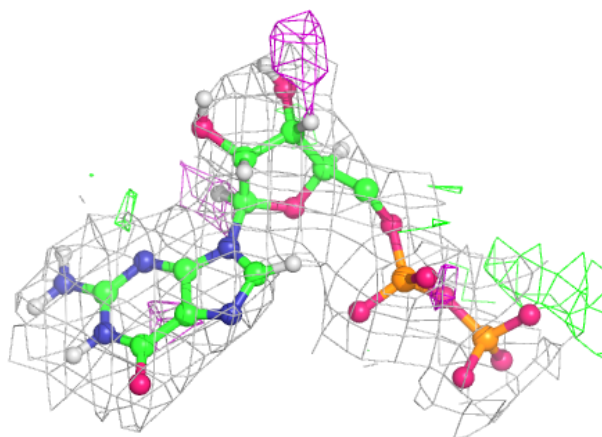
**Electron density around 89O B 505:**

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



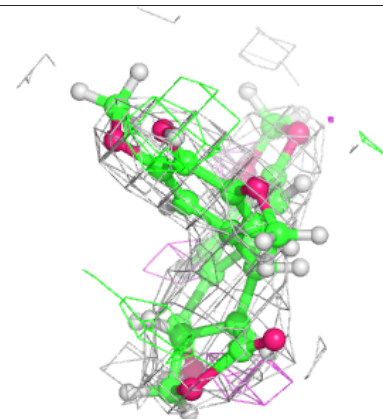
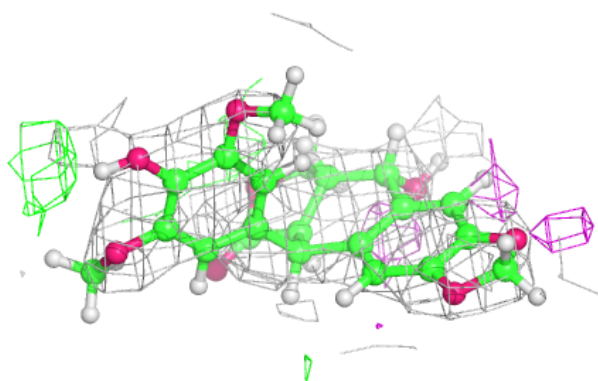
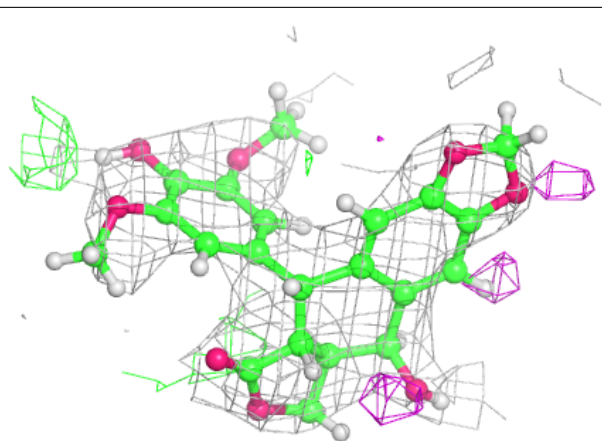
Electron density around GDP D 501:

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



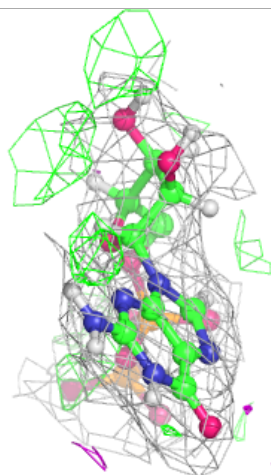
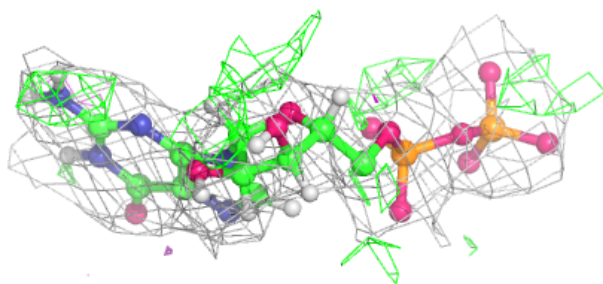
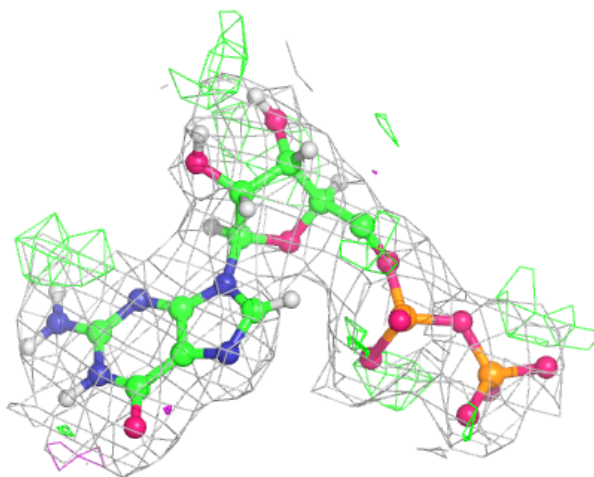
Electron density around 89O D 502:

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



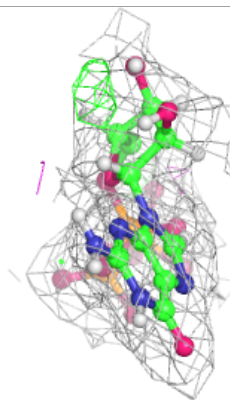
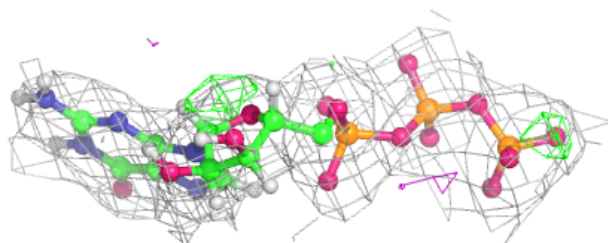
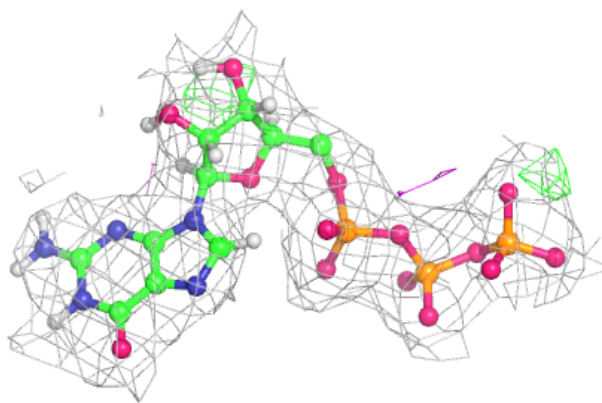
Electron density around GDP B 501:

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

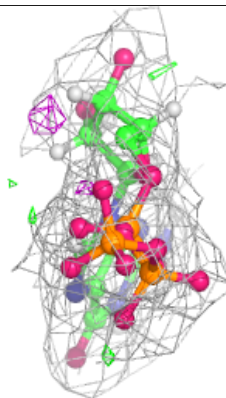
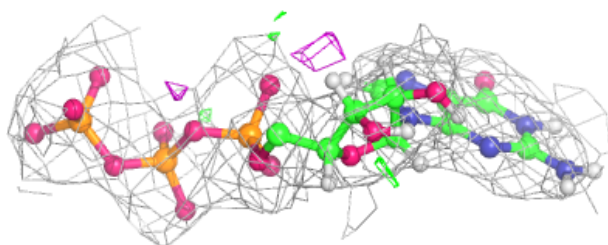
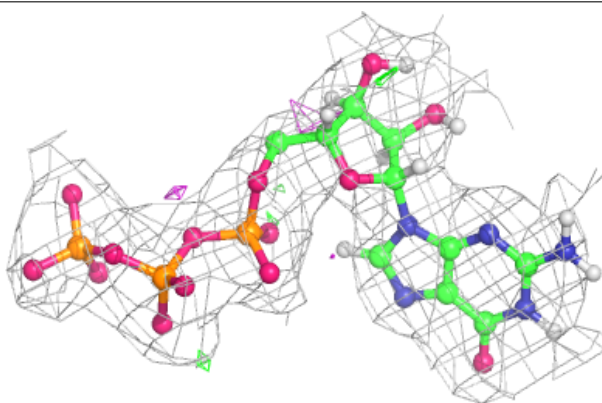


Electron density around GTP C 501:

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

**Electron density around GTP A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.