



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:45 pm BST

PDB ID : 5XIW
Title : Crystal structure of T2R-TTL-Colchicine complex
Authors : Wang, Y.; Yang, J.; Wang, T.; Chen, L.
Deposited on : 2017-04-27
Resolution : 2.90 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

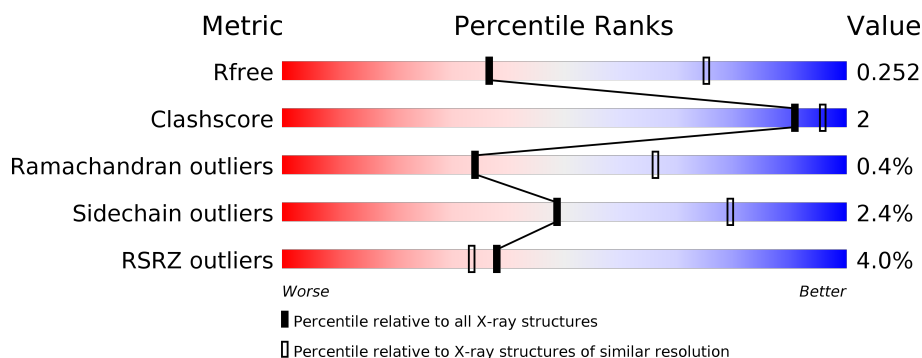
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	451	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	C	451	<div> <div>93%</div> <div>•</div> <div>•</div> </div>
2	B	445	<div> <div>3%</div> <div>87%</div> <div>8%</div> <div>•</div> <div>•</div> </div>
2	D	445	<div> <div>4%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
3	E	143	<div> <div>6%</div> <div>81%</div> <div>•</div> <div>•</div> <div>15%</div> </div>
4	F	384	<div> <div>11%</div> <div>81%</div> <div>5%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17509 atoms, of which 0 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	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	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

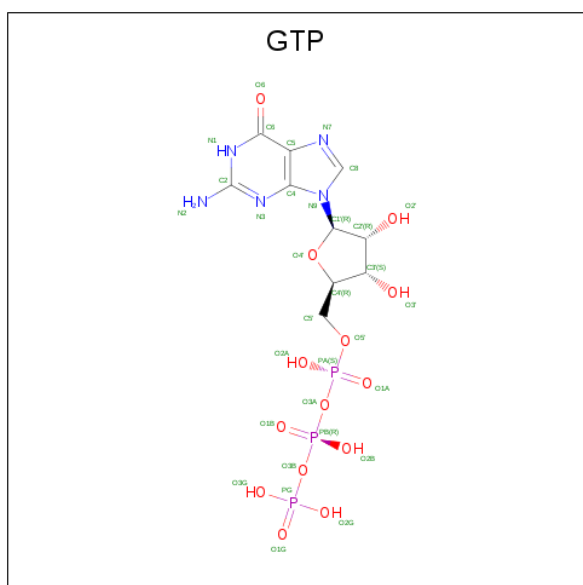
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	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	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	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		

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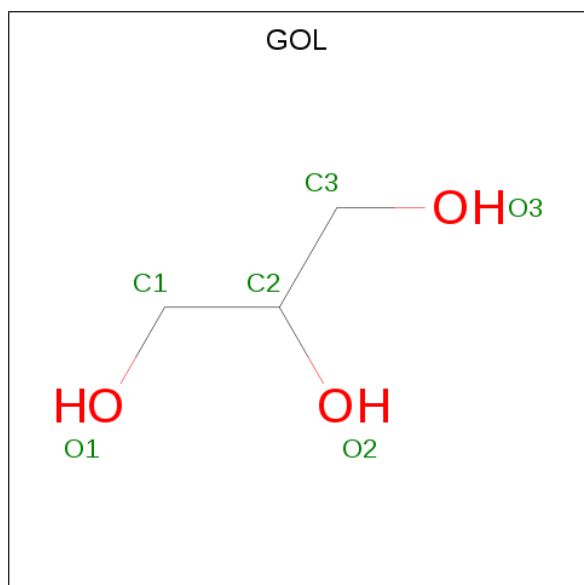
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

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

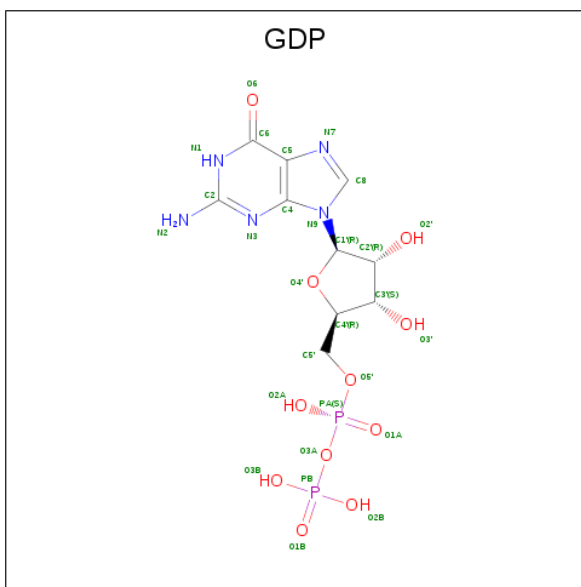
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



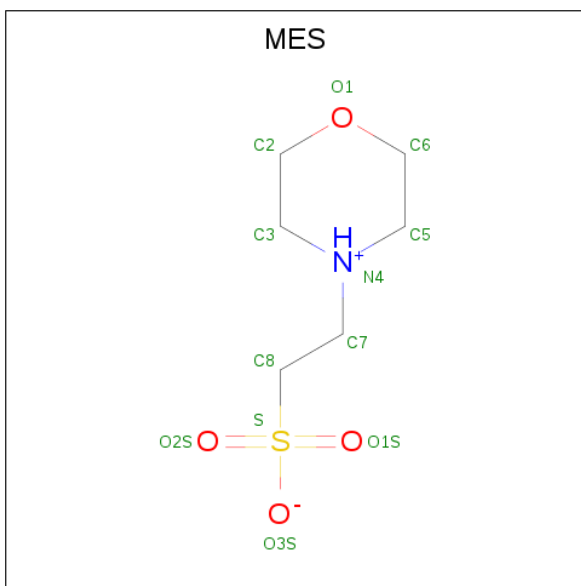
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



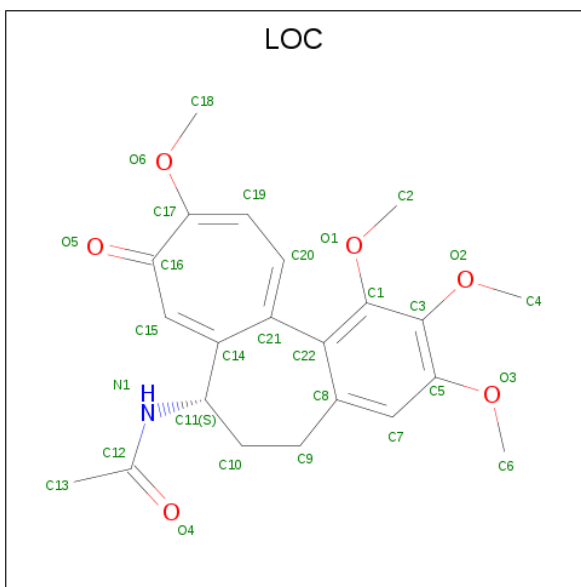
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	
			28	10	5	11	2	

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).

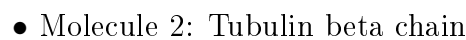


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			29	22	1	6		
11	D	1	Total	C	N	O	0	0
			29	22	1	6		


- Molecule 12 is water.

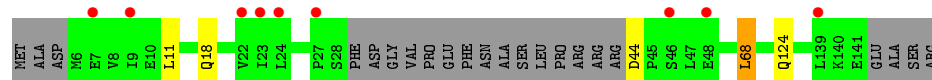
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	7	Total	O	0	0
			7	7		
12	B	10	Total	O	0	0
			10	10		
12	C	9	Total	O	0	0
			9	9		
12	D	2	Total	O	0	0
			2	2		

- Molecule 1: Tubulin alpha-1B chain




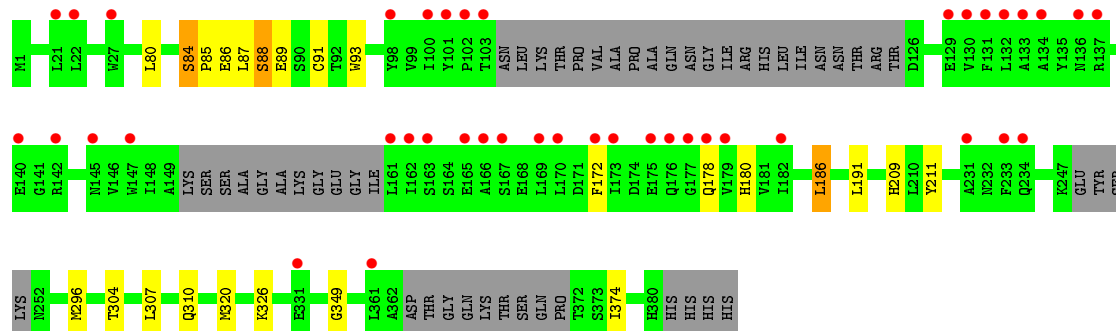
- Molecule 3: Stathmin-4

Chain E: 



- Molecule 4: Tubulin tyrosine ligase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.49Å 159.15Å 181.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.72 – 2.90 37.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (119.72-2.90) 99.8 (37.40-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.204 , 0.253 0.203 , 0.252	Depositor DCC
R_{free} test set	3404 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.4	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	0.94	EDS
Total number of atoms	17509	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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, LOC, MG, GOL, CA, GTP, MES

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	0.41	0/3494	0.59	0/4743
1	C	0.42	0/3515	0.62	0/4772
2	B	0.41	0/3444	0.59	0/4664
2	D	0.40	0/3382	0.59	1/4581 (0.0%)
3	E	0.35	0/1008	0.56	0/1337
4	F	0.46	0/2806	0.62	0/3791
All	All	0.42	0/17649	0.60	1/23888 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	130	LEU	CA-CB-CG	5.48	127.91	115.30

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	0	3331	10	0
1	C	3437	0	3349	6	0
2	B	3369	0	3250	24	0
2	D	3309	0	3189	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1000	0	1018	2	0
4	F	2744	0	2709	10	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	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	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	2	0
11	B	29	0	25	2	0
11	D	29	0	25	3	0
12	A	7	0	0	0	0
12	B	10	0	0	0	0
12	C	9	0	0	0	0
12	D	2	0	0	0	0
All	All	17509	0	16965	60	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 (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:86:GLU:OE2	4:F:86:GLU:N	1.88	1.06
4:F:80:LEU:O	4:F:84:SER:OG	1.76	1.01
2:B:316:ILE:HD11	11:B:504:LOC:H4	1.60	0.84
2:B:190:HIS:HD2	2:B:411:ALA:HA	1.55	0.70
4:F:87:LEU:O	4:F:88:SER:OG	2.07	0.69
2:B:134:GLN:HA	2:B:165:ASN:O	1.97	0.65
2:B:156:ARG:HG3	10:B:503:MES:H62	1.84	0.59
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.86	0.57
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.87	0.57
2:B:245:GLN:H	2:B:245:GLN:HE21	1.55	0.54
2:B:316:ILE:HD11	11:B:504:LOC:C4	2.36	0.54
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.89	0.53
2:D:131:GLN:NE2	2:D:250:LEU:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.52
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.91	0.52
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.92	0.51
1:C:209:ILE:HD11	1:C:302:MET:HG3	1.91	0.51
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.93	0.50
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.92	0.49
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.94	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.95	0.49
2:B:159:TYR:HB3	2:B:162:ARG:HG3	1.95	0.49
4:F:209:HIS:HB2	4:F:310:GLN:CG	2.43	0.48
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.96	0.47
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.80	0.46
1:C:100:ALA:HA	2:D:252:LYS:HG3	1.98	0.46
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.45
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.97	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.45
4:F:85:PRO:HD2	4:F:86:GLU:OE2	2.16	0.45
1:A:166:LYS:HE2	1:A:197:HIS:O	2.16	0.45
2:B:1:MET:HB3	2:B:131:GLN:HG3	1.98	0.45
2:D:252:LYS:HB3	11:D:503:LOC:H9A	1.99	0.44
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.10	0.44
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.98	0.44
1:A:179:THR:O	2:B:350:LYS:HD3	2.18	0.44
2:B:67:ASP:HA	2:B:143:THR:HG21	2.00	0.43
2:B:135:LEU:HB3	2:B:166:THR:HG22	2.00	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.43
1:C:72:PRO:HA	1:C:94:THR:HG21	1.99	0.43
2:B:280:GLN:HE22	2:B:284:LEU:HD13	1.83	0.43
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.42
1:A:210:TYR:HE2	1:A:214:ARG:HH11	1.67	0.42
2:B:55:THR:C	2:B:57:ASN:N	2.72	0.42
2:B:152:ILE:HG23	2:B:164:MET:HG2	2.01	0.42
2:B:274:THR:HB	2:B:279:GLN:HG2	2.02	0.42
2:D:131:GLN:HE22	2:D:250:LEU:H	1.68	0.42
2:D:240:LEU:HG	11:D:503:LOC:H6	2.01	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.19	0.42
2:B:156:ARG:NH2	3:E:68:LEU:HD11	2.35	0.41
2:B:170:MET:HB2	2:B:203:ASP:HA	2.03	0.41
2:B:55:THR:C	2:B:57:ASN:H	2.22	0.41
2:D:67:ASP:HA	2:D:143:THR:HG21	2.02	0.41
2:D:304:ASP:HA	2:D:305:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:ASP:OD1	10:B:503:MES:H32	2.21	0.41
4:F:209:HIS:HB2	4:F:310:GLN:HG3	2.02	0.41
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.03	0.41
2:D:253:LEU:HD12	11:D:503:LOC:H20	2.02	0.41
1:C:228:ASN:HA	1:C:231:ILE:HD12	2.04	0.40
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	435/451 (96%)	423 (97%)	9 (2%)	3 (1%)	22	54
1	C	438/451 (97%)	429 (98%)	8 (2%)	1 (0%)	47	78
2	B	426/445 (96%)	413 (97%)	12 (3%)	1 (0%)	47	78
2	D	417/445 (94%)	402 (96%)	13 (3%)	2 (0%)	29	61
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	310 (96%)	13 (4%)	1 (0%)	41	71
All	All	2157/2319 (93%)	2092 (97%)	57 (3%)	8 (0%)	34	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	178	SER
1	A	178	SER
1	A	282	TYR
2	D	95	SER
1	A	261	PRO
4	F	88	SER

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Mol	Chain	Res	Type
2	B	55	THR
2	D	219	THR

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	368/379 (97%)	360 (98%)	8 (2%)	52	81
1	C	371/379 (98%)	362 (98%)	9 (2%)	49	79
2	B	370/383 (97%)	363 (98%)	7 (2%)	57	84
2	D	364/383 (95%)	355 (98%)	9 (2%)	47	78
3	E	109/127 (86%)	106 (97%)	3 (3%)	43	76
4	F	301/342 (88%)	291 (97%)	10 (3%)	38	72
All	All	1883/1993 (94%)	1837 (98%)	46 (2%)	49	79

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	250	VAL
1	A	251	ASP
1	A	253	THR
1	A	262	TYR
1	A	315	CYS
1	A	433	GLU
2	B	39	ASP
2	B	48	ASN
2	B	137	HIS
2	B	245	GLN
2	B	284	LEU
2	B	327	ASP
2	B	350	LYS
1	C	2	ARG

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Mol	Chain	Res	Type
1	C	178	SER
1	C	190	THR
1	C	221	ARG
1	C	251	ASP
1	C	302	MET
1	C	361	THR
1	C	381	THR
1	C	430	LYS
2	D	2	ARG
2	D	41	ASP
2	D	42	LEU
2	D	55	THR
2	D	137	HIS
2	D	165	ASN
2	D	178	THR
2	D	246	LEU
2	D	323	MET
3	E	44	ASP
3	E	68	LEU
3	E	124	GLN
4	F	84	SER
4	F	89	GLU
4	F	172	PHE
4	F	178	GLN
4	F	180	HIS
4	F	186	LEU
4	F	191	LEU
4	F	211	TYR
4	F	296	MET
4	F	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	245	GLN
2	B	280	GLN
2	B	375	GLN
1	C	293	ASN
1	C	372	GLN
2	D	131	GLN
2	D	347	ASN
3	E	18	GLN

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Mol	Chain	Res	Type
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	LOC	B	504	-	28,31,31	3.03	17 (60%)	28,44,44	2.61	4 (14%)
5	GTP	A	501	6	26,34,34	1.25	2 (7%)	33,54,54	1.96	7 (21%)
9	GDP	B	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.96	7 (22%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	33,54,54	1.86	7 (21%)
11	LOC	D	503	-	28,31,31	3.05	16 (57%)	28,44,44	2.68	5 (17%)
8	GOL	A	504	-	5,5,5	0.27	0	5,5,5	0.33	0
5	GTP	D	501	-	26,34,34	1.22	2 (7%)	33,54,54	2.01	8 (24%)
10	MES	B	503	-	12,12,12	2.12	1 (8%)	14,16,16	7.25	6 (42%)

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	LOC	B	504	-	-	2/10/25/25	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
11	LOC	D	503	-	-	2/10/25/25	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	D	501	-	-	3/18/38/38	0/3/3/3
10	MES	B	503	-	-	4/6/14/14	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-6.74	1.67	1.77
11	B	504	LOC	C11-N1	-5.93	1.38	1.46
11	D	503	LOC	C11-N1	-5.77	1.39	1.46
11	D	503	LOC	C7-C8	5.60	1.49	1.39
11	B	504	LOC	C7-C8	5.29	1.48	1.39
11	B	504	LOC	O3-C5	4.67	1.44	1.37
11	D	503	LOC	O3-C5	4.67	1.44	1.37
11	D	503	LOC	O6-C17	4.64	1.44	1.37
11	B	504	LOC	O6-C17	4.58	1.44	1.37
5	A	501	GTP	C6-C5	4.57	1.49	1.41
11	D	503	LOC	O1-C1	4.46	1.46	1.38
5	D	501	GTP	C6-C5	4.42	1.49	1.41
11	B	504	LOC	O1-C1	4.23	1.46	1.38
11	D	503	LOC	C12-N1	4.21	1.48	1.34
11	B	504	LOC	C15-C16	4.21	1.47	1.39
11	B	504	LOC	C12-N1	4.18	1.48	1.34
11	D	503	LOC	C15-C16	4.17	1.47	1.39
9	B	501	GDP	C6-C5	4.13	1.48	1.41
5	C	501	GTP	C6-C5	3.99	1.48	1.41
11	D	503	LOC	C1-C3	3.68	1.47	1.39
11	B	504	LOC	C21-C22	-3.64	1.44	1.49
11	B	504	LOC	C1-C3	3.43	1.46	1.39
11	D	503	LOC	O2-C3	3.35	1.44	1.38
11	D	503	LOC	C22-C1	3.23	1.48	1.40
11	D	503	LOC	C21-C22	-3.21	1.45	1.49
11	B	504	LOC	O2-C3	3.09	1.44	1.38
11	B	504	LOC	C22-C8	-3.08	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	LOC	O4-C12	-3.03	1.16	1.23
11	D	503	LOC	O4-C12	-2.90	1.16	1.23
11	B	504	LOC	C22-C1	2.89	1.47	1.40
11	B	504	LOC	C15-C14	2.83	1.49	1.39
11	D	503	LOC	C15-C14	2.81	1.49	1.39
11	D	503	LOC	C22-C8	-2.71	1.36	1.40
5	D	501	GTP	C5-C4	2.68	1.48	1.40
5	A	501	GTP	C5-C4	2.56	1.47	1.40
11	B	504	LOC	C21-C14	-2.55	1.29	1.40
11	D	503	LOC	C21-C14	-2.54	1.29	1.40
5	C	501	GTP	C5-C4	2.53	1.47	1.40
9	B	501	GDP	C5-C4	2.51	1.47	1.40
11	D	503	LOC	C7-C5	2.14	1.42	1.38
11	B	504	LOC	C19-C17	2.12	1.43	1.39
11	B	504	LOC	C7-C5	2.04	1.42	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O2S-S-C8	-18.86	84.21	106.92
10	B	503	MES	O3S-S-O2S	-11.22	83.87	111.27
10	B	503	MES	O1S-S-C8	9.63	118.52	106.92
11	D	503	LOC	C21-C22-C8	9.24	130.51	120.50
11	B	504	LOC	C21-C22-C8	8.95	130.20	120.50
11	D	503	LOC	C21-C22-C1	-8.86	108.97	121.07
11	B	504	LOC	C21-C22-C1	-8.63	109.28	121.07
10	B	503	MES	O3S-S-C8	8.50	119.51	105.77
10	B	503	MES	O2S-S-O1S	-8.47	84.63	113.95
5	A	501	GTP	C2-N3-C4	4.89	120.94	115.36
5	D	501	GTP	C2-N3-C4	4.68	120.70	115.36
9	B	501	GDP	C2-N3-C4	4.64	120.66	115.36
9	B	501	GDP	C6-C5-C4	-4.49	116.51	120.80
9	B	501	GDP	C6-N1-C2	4.48	123.05	115.93
5	C	501	GTP	C2-N3-C4	4.45	120.44	115.36
5	A	501	GTP	C6-C5-C4	-4.37	116.62	120.80
5	D	501	GTP	C6-N1-C2	4.37	122.87	115.93
5	A	501	GTP	C6-N1-C2	4.28	122.72	115.93
5	D	501	GTP	C5-C6-N1	-4.23	117.65	123.43
5	C	501	GTP	C6-N1-C2	4.16	122.55	115.93
5	A	501	GTP	C5-C6-N1	-4.06	117.88	123.43
5	C	501	GTP	C6-C5-C4	-4.03	116.95	120.80
5	C	501	GTP	C5-C6-N1	-3.97	118.00	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C5-C6-N1	-3.91	118.08	123.43
9	B	501	GDP	N3-C2-N1	-3.83	122.12	127.22
5	D	501	GTP	C6-C5-C4	-3.82	117.15	120.80
5	A	501	GTP	N3-C2-N1	-3.60	122.42	127.22
5	D	501	GTP	N3-C2-N1	-3.51	122.54	127.22
5	C	501	GTP	N3-C2-N1	-3.40	122.69	127.22
10	B	503	MES	O3S-S-O1S	3.16	118.99	111.27
5	D	501	GTP	PB-O3B-PG	-2.97	122.63	132.83
5	A	501	GTP	C4-C5-N7	-2.87	106.41	109.40
5	D	501	GTP	PA-O3A-PB	-2.78	123.27	132.83
5	D	501	GTP	C4-C5-N7	-2.70	106.58	109.40
5	C	501	GTP	PA-O3A-PB	-2.70	123.55	132.83
11	B	504	LOC	O1-C1-C22	2.70	124.22	119.08
11	D	503	LOC	O1-C1-C22	2.62	124.07	119.08
11	D	503	LOC	O3-C5-C3	2.41	119.40	115.16
5	A	501	GTP	PA-O3A-PB	-2.32	124.88	132.83
9	B	501	GDP	C4-C5-N7	-2.27	107.03	109.40
11	B	504	LOC	O3-C5-C3	2.25	119.11	115.16
5	C	501	GTP	C4-C5-N7	-2.20	107.11	109.40
11	D	503	LOC	O3-C5-C7	-2.20	120.34	124.12
9	B	501	GDP	PA-O3A-PB	-2.09	125.66	132.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	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
5	D	501	GTP	C5'-O5'-PA-O2A
10	B	503	MES	N4-C7-C8-S
11	D	503	LOC	C3-C5-O3-C6
11	D	503	LOC	C7-C5-O3-C6
10	B	503	MES	C7-C8-S-O3S
8	A	504	GOL	C1-C2-C3-O3
8	A	504	GOL	O2-C2-C3-O3
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A

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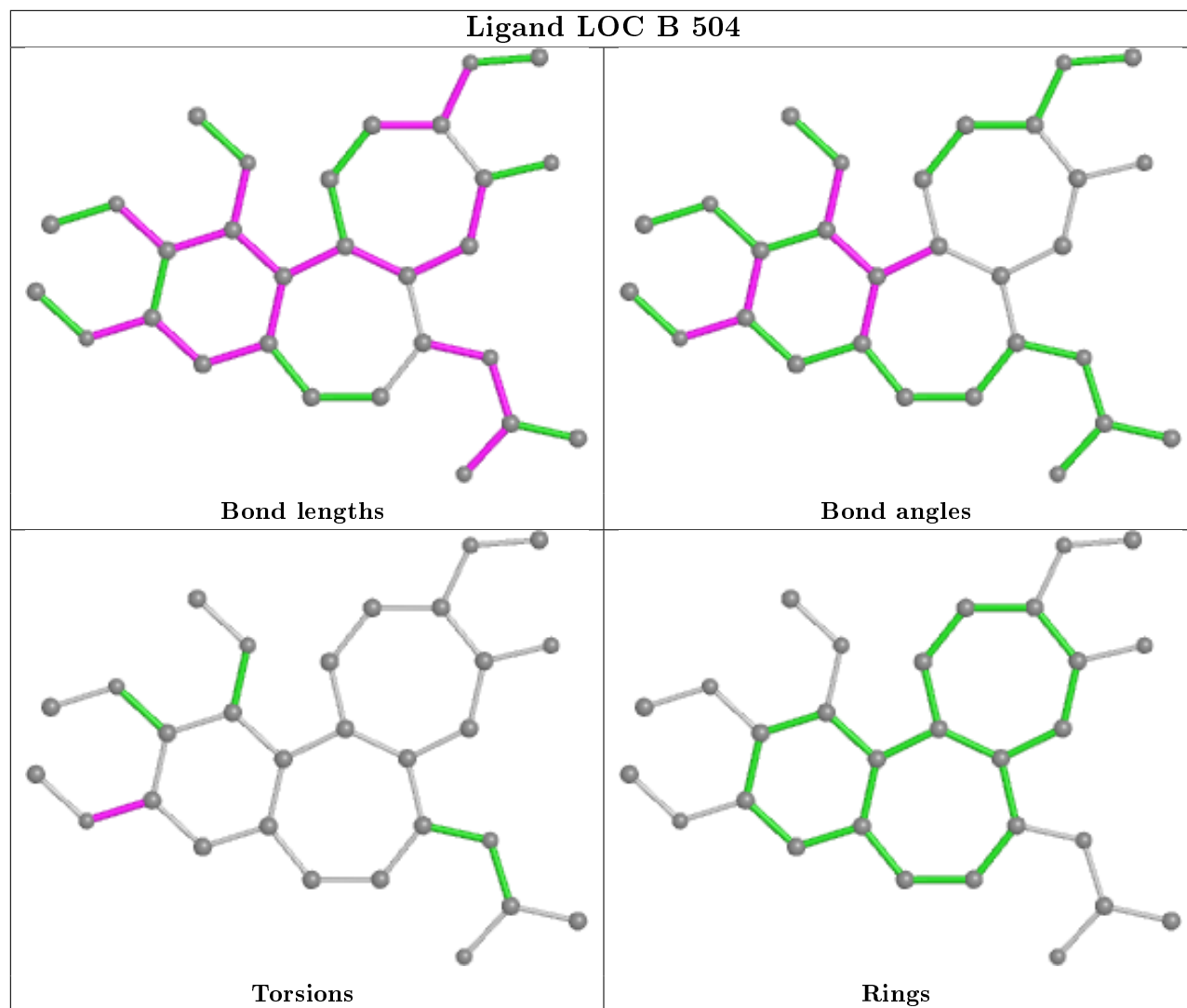
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O1A
10	B	503	MES	C7-C8-S-O1S
11	B	504	LOC	C3-C5-O3-C6
10	B	503	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
11	B	504	LOC	C7-C5-O3-C6
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A

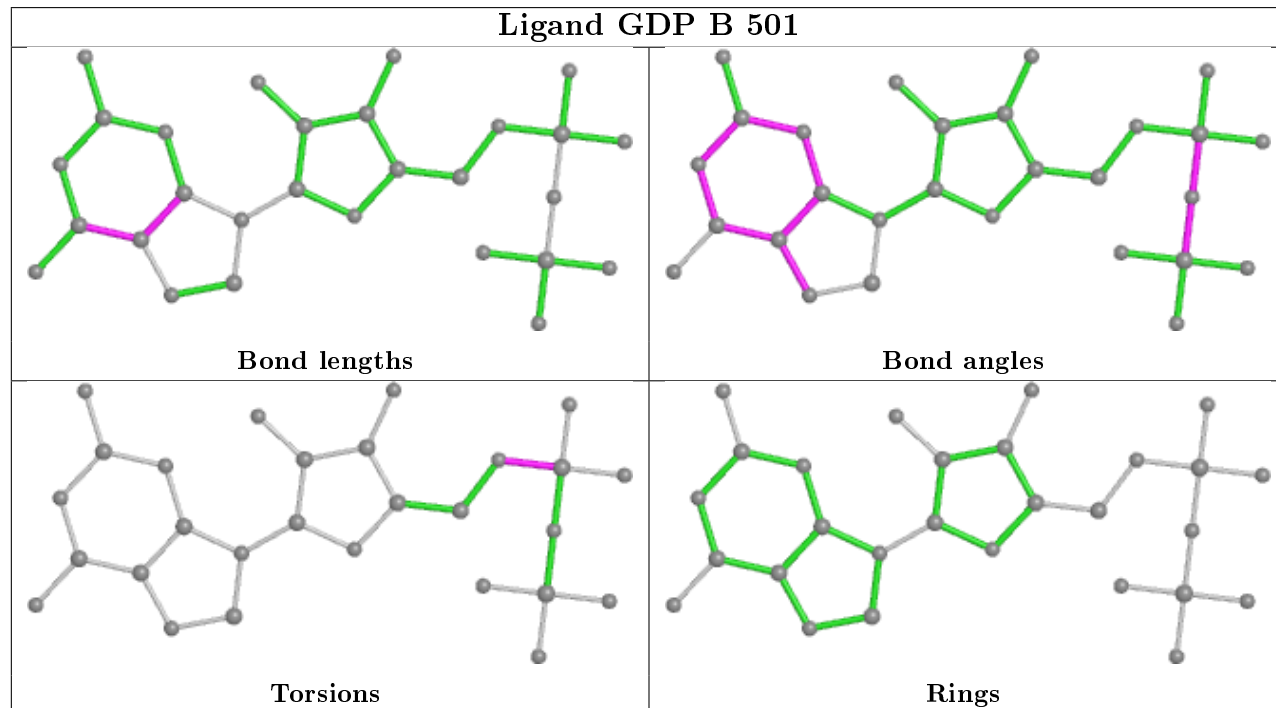
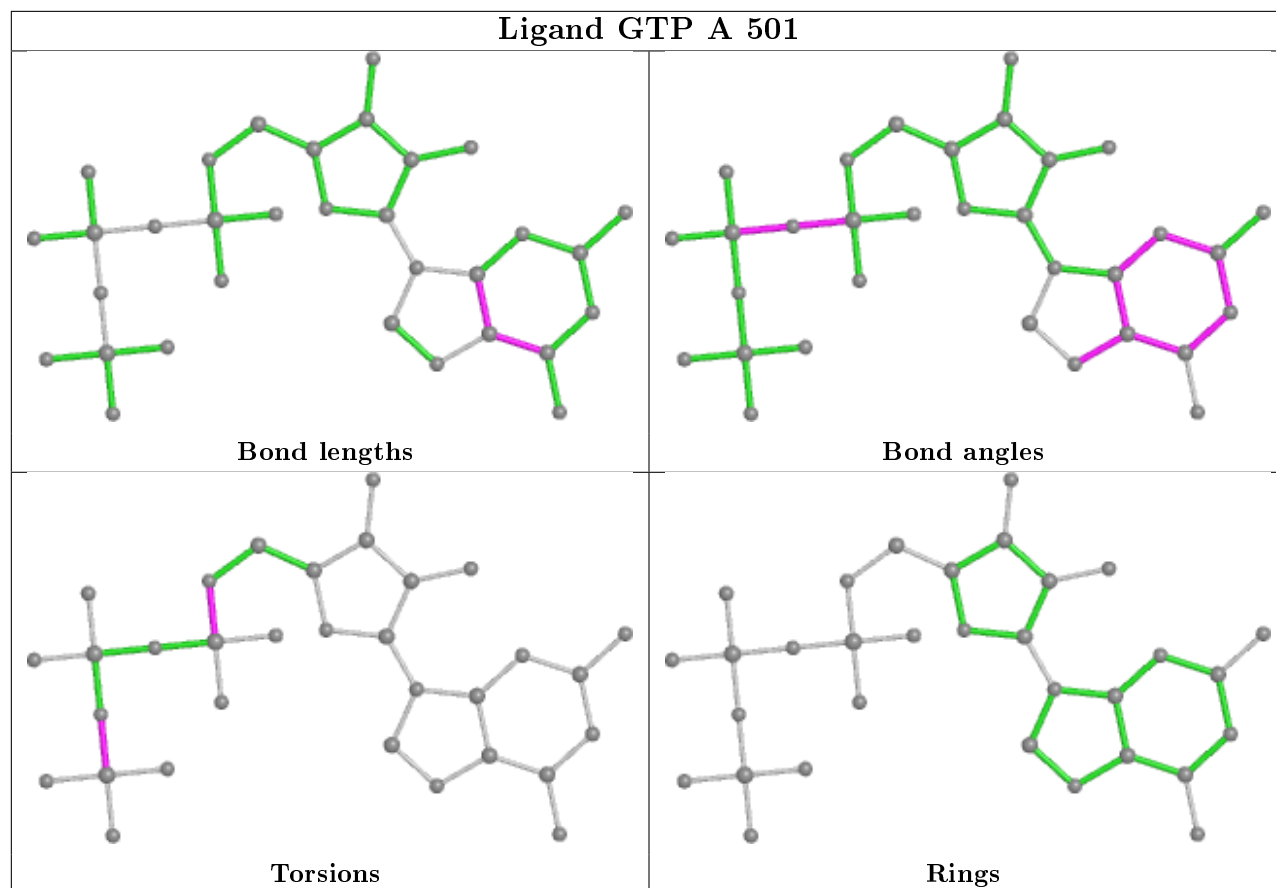
There are no ring outliers.

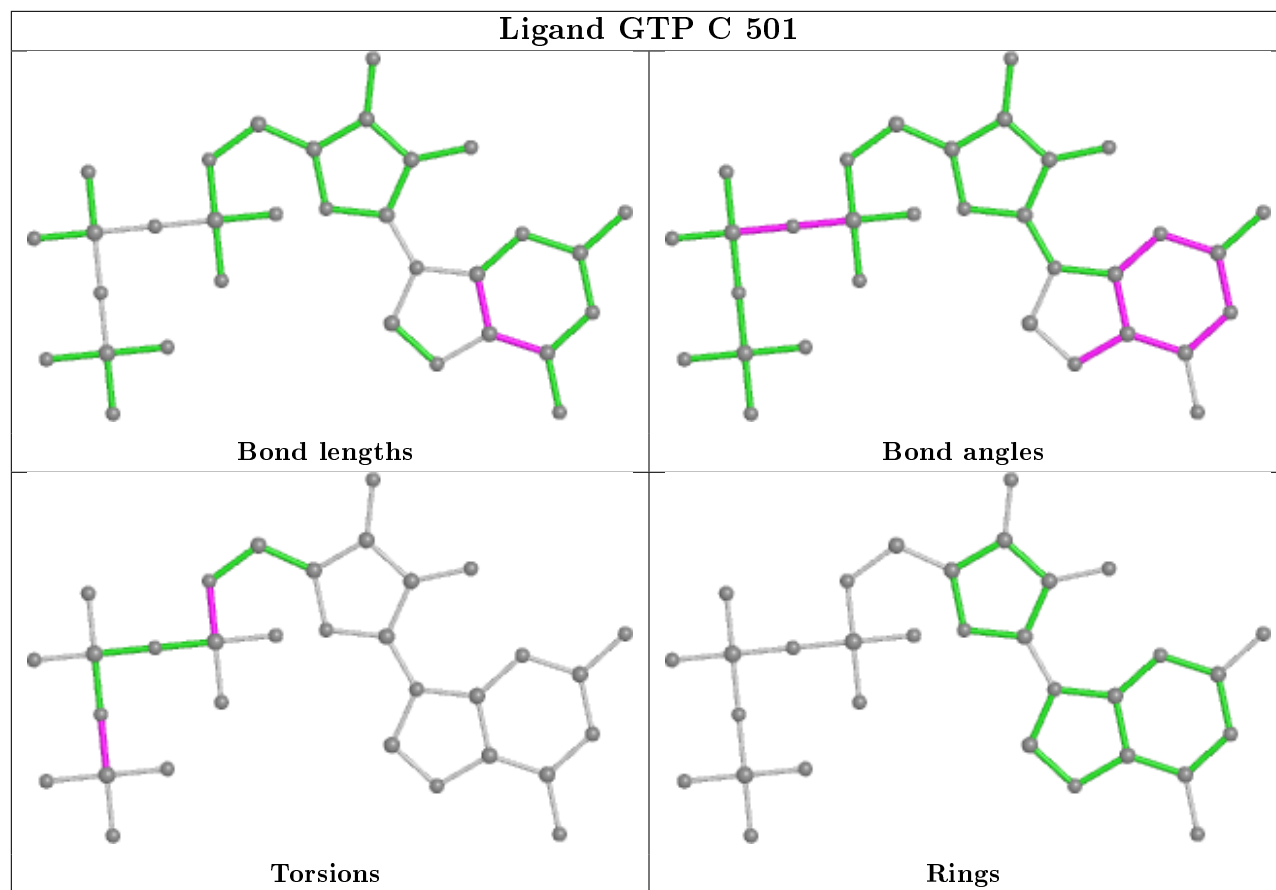
3 monomers are involved in 7 short contacts:

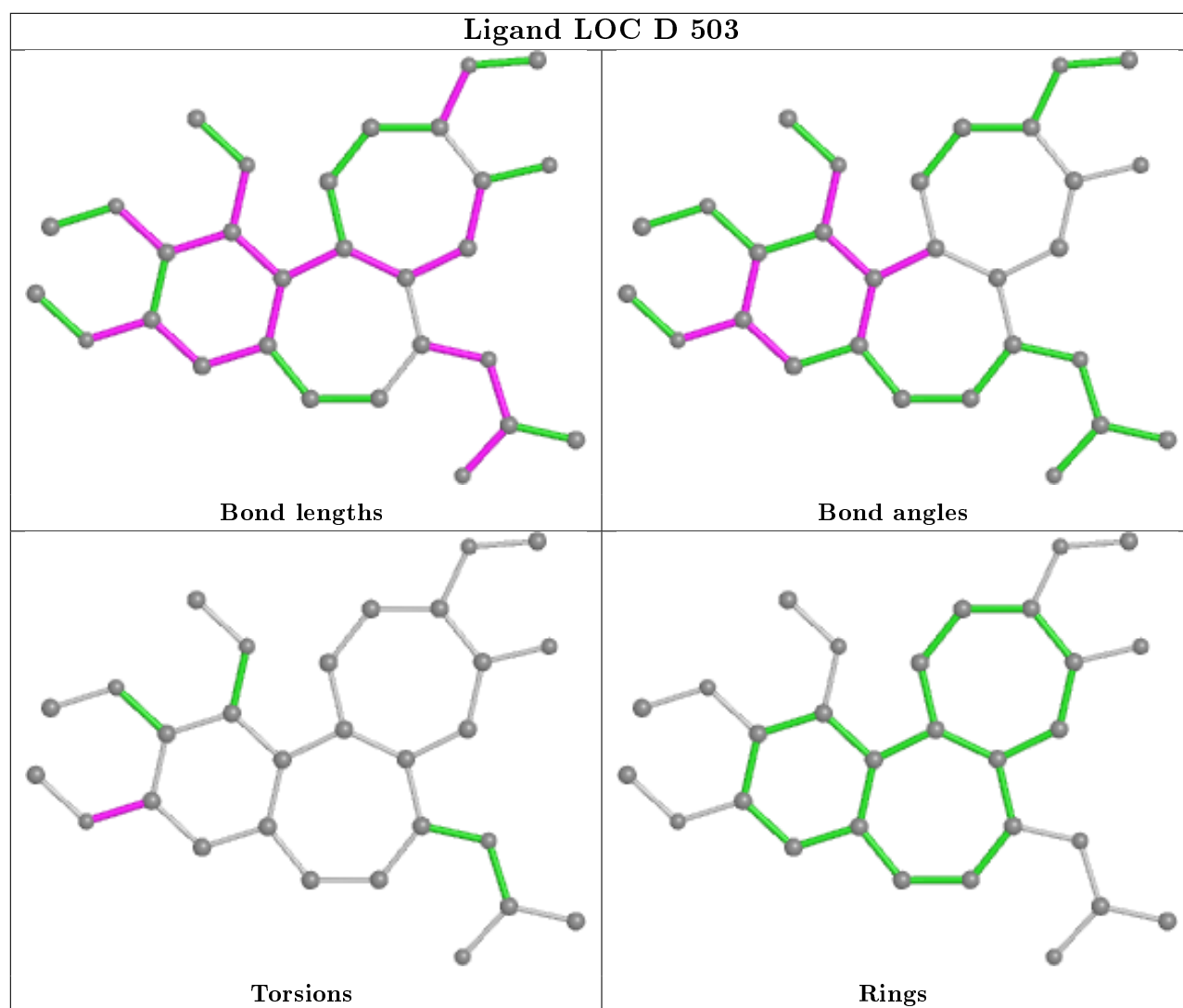
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	504	LOC	2	0
11	D	503	LOC	3	0
10	B	503	MES	2	0

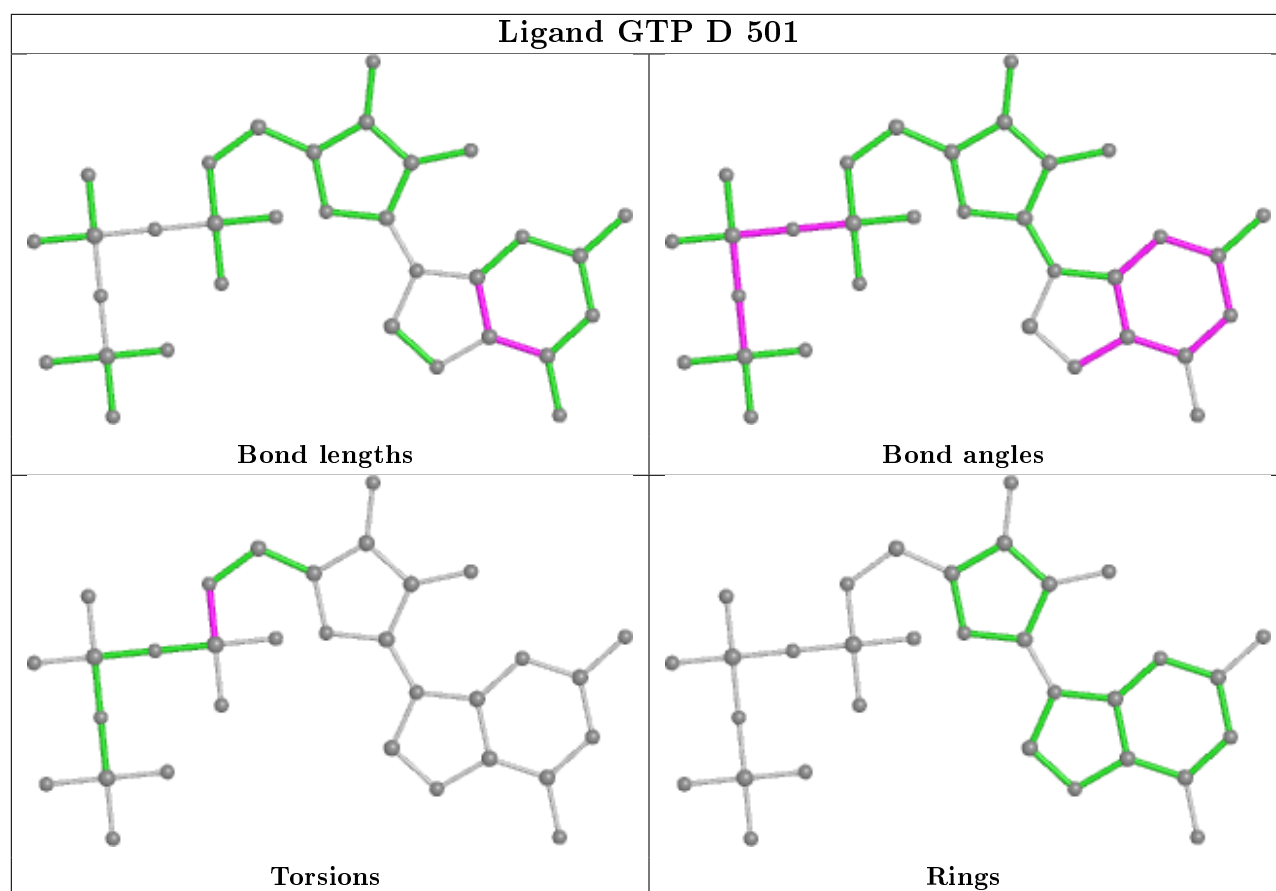
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	-0.09	3 (0%)	87 87	57, 74, 101, 131	0
1	C	440/451 (97%)	-0.29	2 (0%)	91 91	49, 66, 93, 108	0
2	B	428/445 (96%)	-0.01	13 (3%)	50 45	52, 75, 113, 164	0
2	D	421/445 (94%)	0.24	20 (4%)	30 27	60, 93, 132, 149	0
3	E	121/143 (84%)	0.37	9 (7%)	14 11	59, 93, 125, 138	0
4	F	334/384 (86%)	0.48	41 (12%)	4 3	65, 101, 161, 183	0
All	All	2181/2319 (94%)	0.06	88 (4%)	38 33	49, 80, 131, 183	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	5.3
4	F	233	PHE	4.9
4	F	161	LEU	4.7
4	F	132	LEU	4.4
2	B	278	SER	4.4
4	F	177	GLY	4.3
4	F	178	GLN	4.3
4	F	176	GLN	4.1
2	D	1	MET	4.0
4	F	173	ILE	4.0
4	F	167	SER	4.0
4	F	182	ILE	3.9
4	F	134	ALA	3.9
2	D	390	ARG	3.8
2	D	405	GLU	3.7
2	B	277	GLY	3.7
4	F	136	ASN	3.6
4	F	234	GLN	3.6
4	F	147	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	140	GLU	3.5
4	F	169	LEU	3.5
4	F	98	TYR	3.5
2	B	276	ARG	3.3
4	F	231	ALA	3.3
4	F	137	ARG	3.3
4	F	331	GLU	3.3
4	F	131	PHE	3.3
4	F	163	SER	3.2
3	E	27	PRO	3.2
4	F	102	PRO	3.2
2	D	391	ARG	3.2
4	F	142	ARG	3.2
2	D	218	THR	3.2
4	F	133	ALA	3.2
2	B	279	GLN	3.2
4	F	100	ILE	3.1
2	D	37	HIS	3.1
2	D	219	THR	3.1
1	C	340	SER	3.1
4	F	165	GLU	3.1
4	F	162	ILE	3.0
2	B	280	GLN	2.9
4	F	166	ALA	2.9
2	D	94	GLN	2.9
2	B	274	THR	2.9
4	F	21	LEU	2.8
4	F	361	LEU	2.8
2	D	166	THR	2.8
4	F	101	TYR	2.7
1	A	282	TYR	2.7
2	D	359	ARG	2.6
2	B	275	SER	2.6
2	B	55	THR	2.5
4	F	103	THR	2.5
2	D	408	PHE	2.5
2	B	57	ASN	2.5
4	F	172	PHE	2.5
2	D	165	ASN	2.5
2	D	389	PHE	2.5
2	B	428	ALA	2.4
3	E	139	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	168	SER	2.4
2	D	284	LEU	2.4
4	F	27	TRP	2.4
1	C	357	TYR	2.4
4	F	145	ASN	2.3
3	E	48	GLU	2.3
4	F	175	GLU	2.3
3	E	7	GLU	2.3
3	E	23	ILE	2.3
3	E	24	LEU	2.3
2	D	199	THR	2.3
4	F	170	LEU	2.2
1	A	348	PRO	2.2
1	A	237	SER	2.2
2	B	1	MET	2.2
2	B	243	PRO	2.2
4	F	179	VAL	2.2
4	F	22	LEU	2.2
2	D	331	LEU	2.2
3	E	22	VAL	2.1
3	E	46	SER	2.1
2	D	216	LYS	2.1
2	D	317	PHE	2.1
2	B	282	ARG	2.1
2	D	392	LYS	2.0
3	E	9	ILE	2.0
4	F	129	GLU	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.

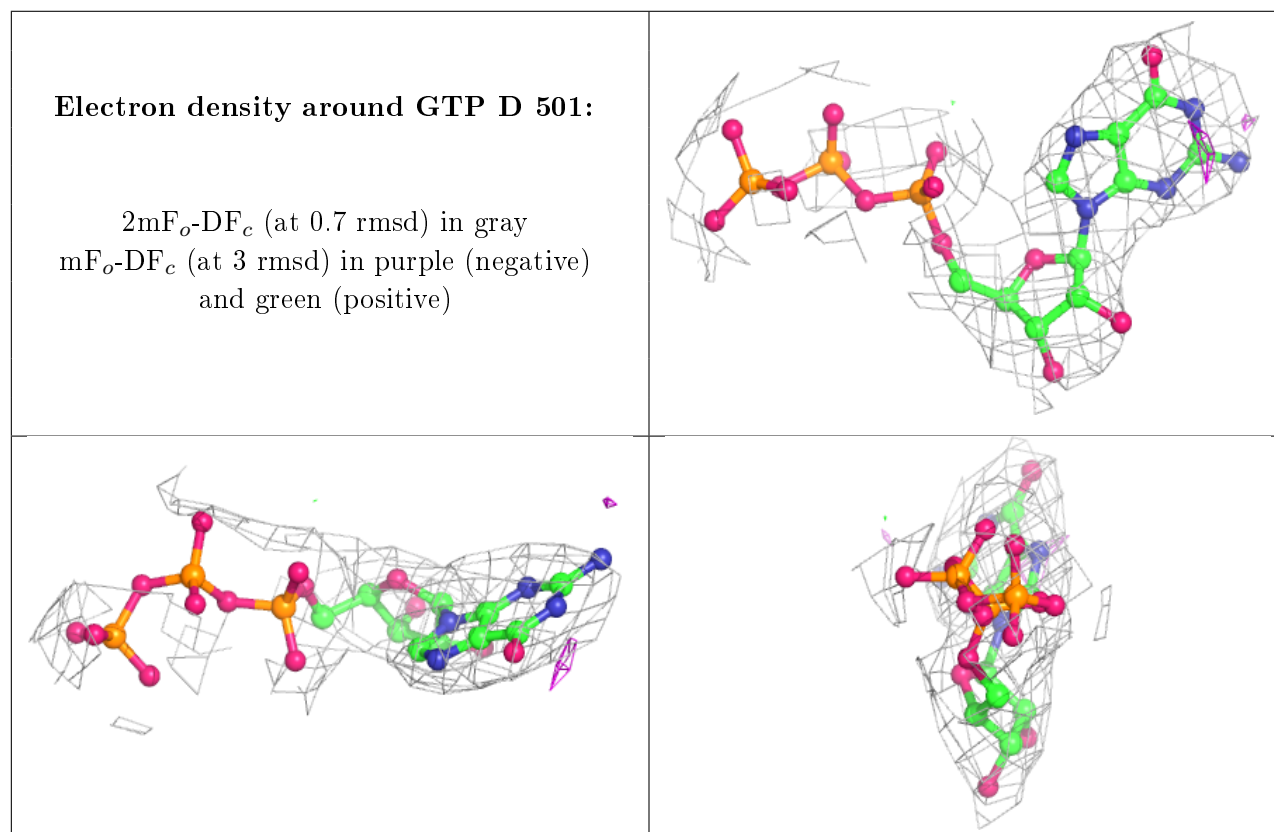
6.4 Ligands [i](#)

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.

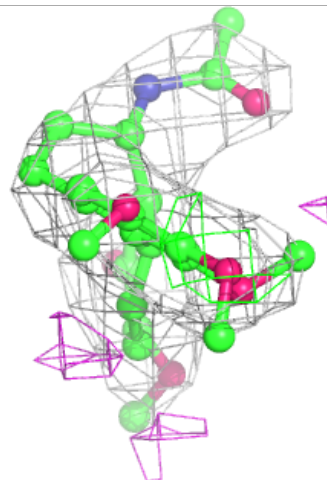
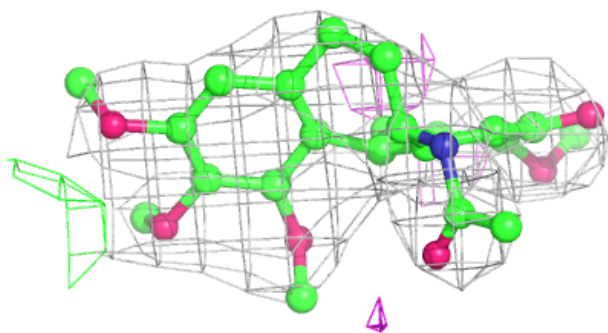
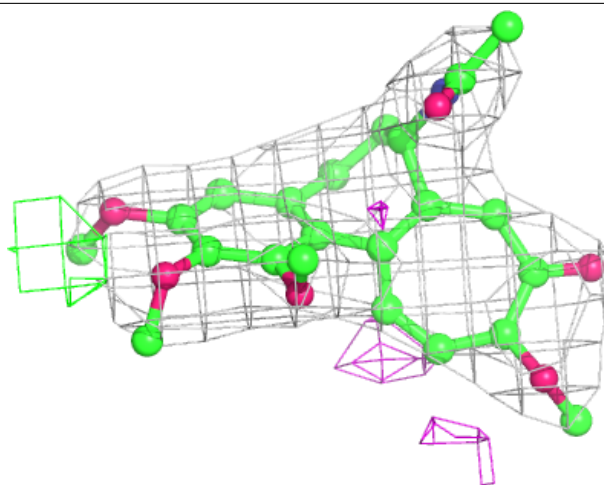
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.83	0.28	130,130,130,130	0
8	GOL	A	504	6/6	0.90	0.36	88,94,96,99	0
10	MES	B	503	12/12	0.92	0.25	102,110,125,128	0
7	CA	A	503	1/1	0.93	0.12	101,101,101,101	0
5	GTP	D	501	32/32	0.94	0.16	72,89,118,120	0
11	LOC	D	503	29/29	0.96	0.19	69,75,80,84	0
6	MG	A	502	1/1	0.96	0.22	69,69,69,69	0
9	GDP	B	501	28/28	0.97	0.20	59,63,68,70	0
11	LOC	B	504	29/29	0.97	0.20	55,60,63,65	0
7	CA	C	503	1/1	0.97	0.07	84,84,84,84	0
5	GTP	C	501	32/32	0.98	0.21	54,56,63,64	0
5	GTP	A	501	32/32	0.98	0.17	58,65,68,69	0
6	MG	B	502	1/1	0.98	0.15	55,55,55,55	0
6	MG	C	502	1/1	0.99	0.21	56,56,56,56	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.



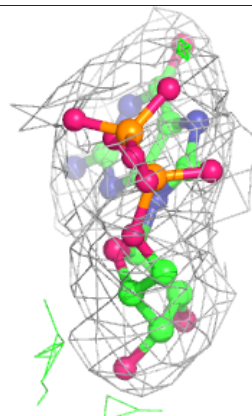
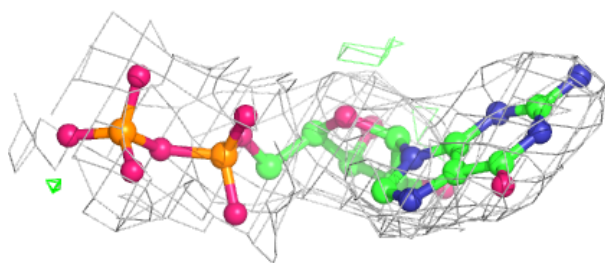
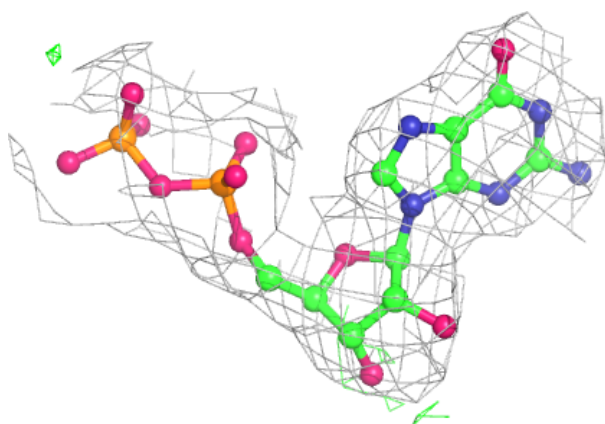
Electron density around LOC D 503:

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



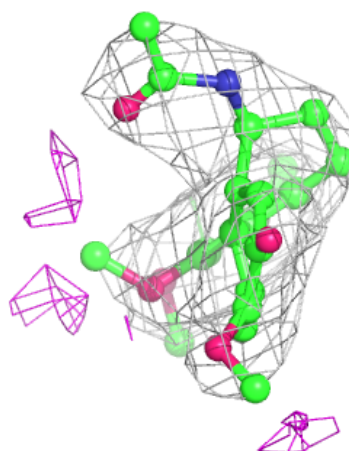
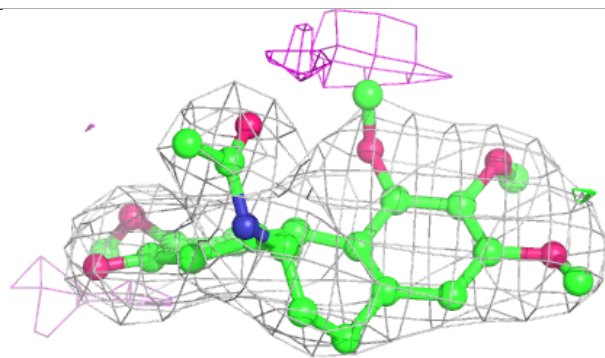
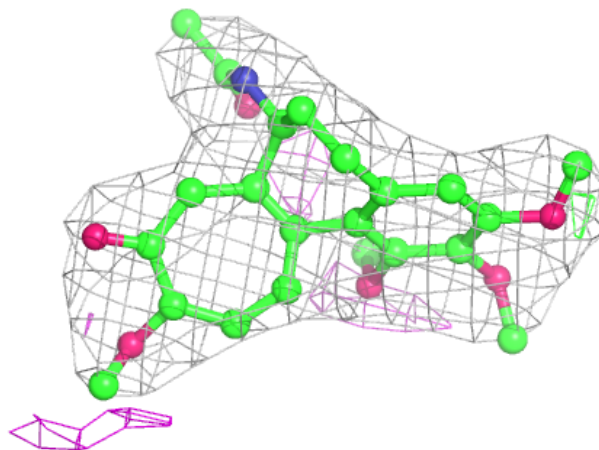
Electron density around GDP B 501:

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



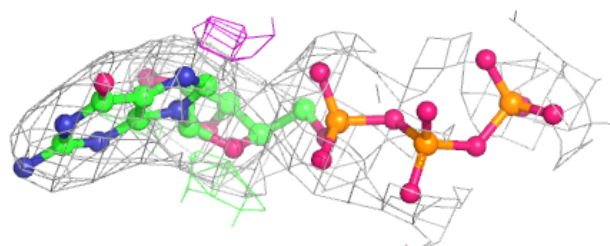
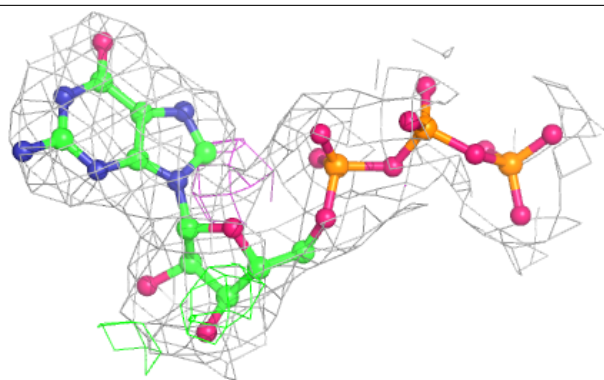
Electron density around LOC B 504:

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

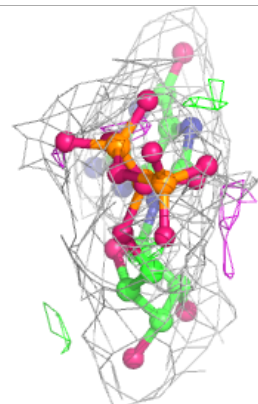
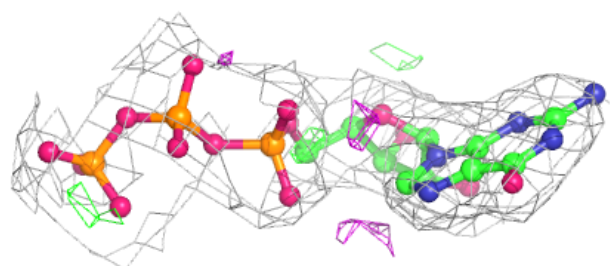
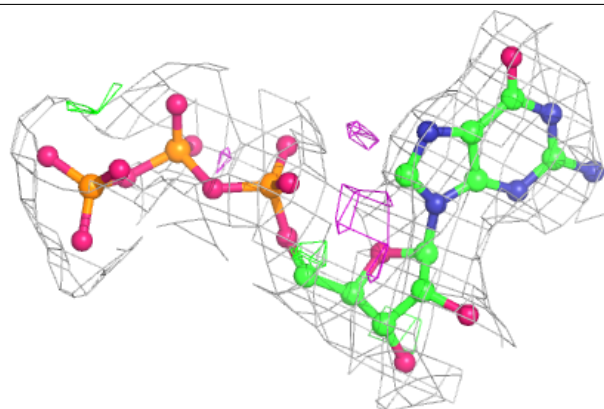


Electron density around GTP C 501:

$2mF_o - DF_c$ (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.