



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2021 – 10:17 AM EDT

PDB ID : 6XER  
Title : Tubulin-RB3\_SLD in complex with colchicine  
Authors : White, S.W.; Yun, M.  
Deposited on : 2020-06-13  
Resolution : 2.50 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](mailto: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.

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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 : 2.23.1  
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) : 2.23.1

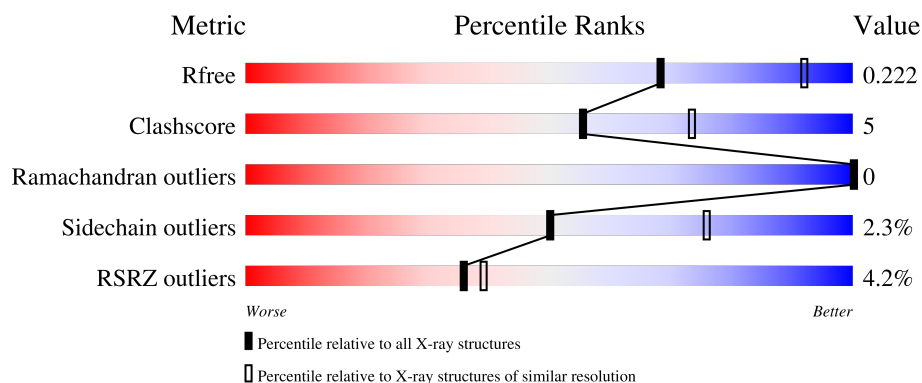
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	438	<div> <div>5%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	C	438	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
2	B	433	<div> <div>6%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	D	433	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
3	E	143	<div> <div>10%</div> <div>72%</div> <div>11%</div> <div>.</div> <div>16%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14606 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	426	Total	C	N	O	S	0	0	0
			3339	2116	567	634	22			
1	C	426	Total	C	N	O	S	0	0	0
			3335	2112	567	634	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	0	0
			3332	2091	569	645	27			
2	D	430	Total	C	N	O	S	0	0	0
			3379	2120	579	654	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			993	615	181	194	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

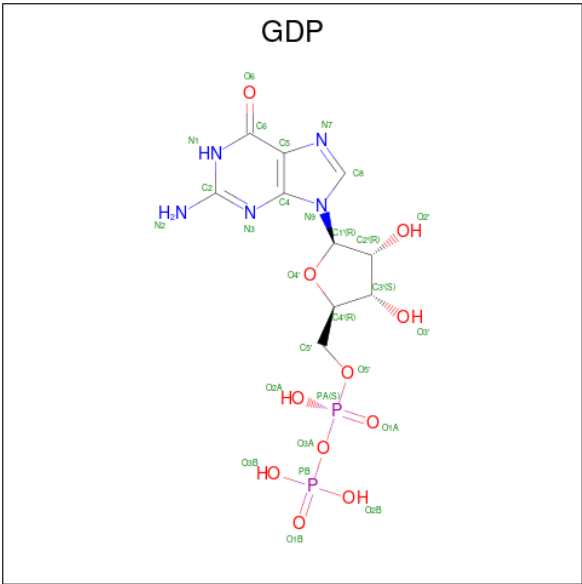
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



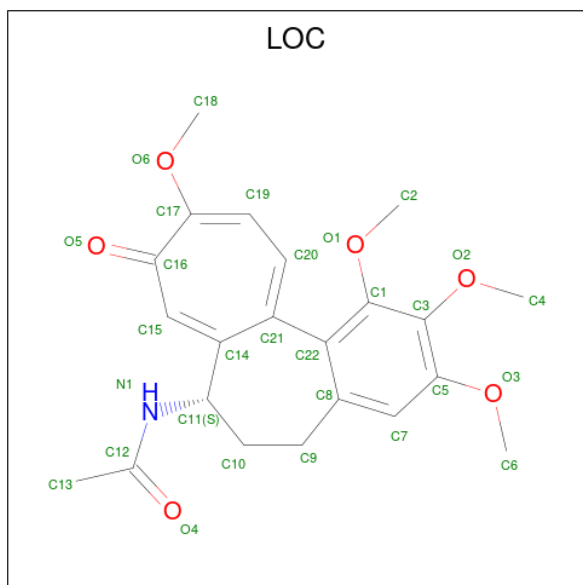
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	
			28	10	5	11	2	
								0
								0

- Molecule 8 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<sub>22</sub>H<sub>25</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

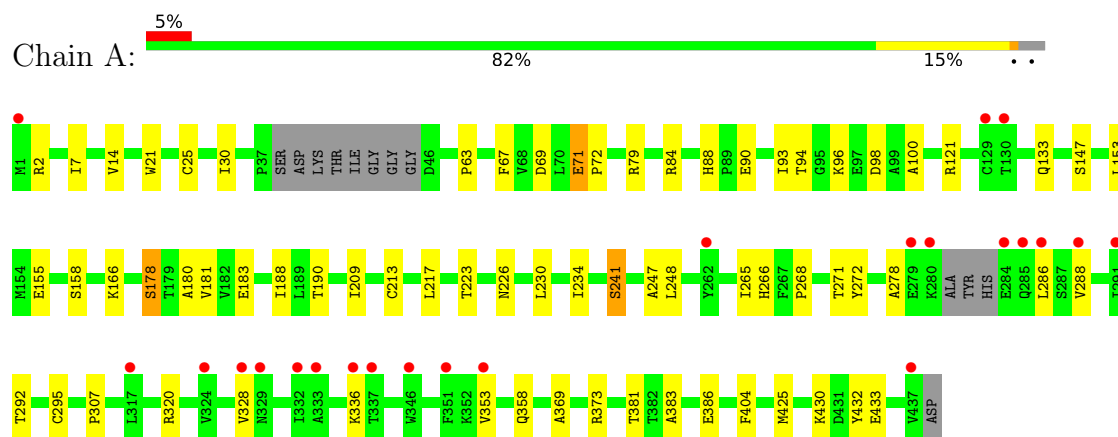
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O		
			9	9	0	0
9	B	3	Total	O		
			3	3	0	0
9	C	13	Total	O		
			13	13	0	0
9	D	3	Total	O		
			3	3	0	0
9	E	1	Total	O		
			1	1	0	0

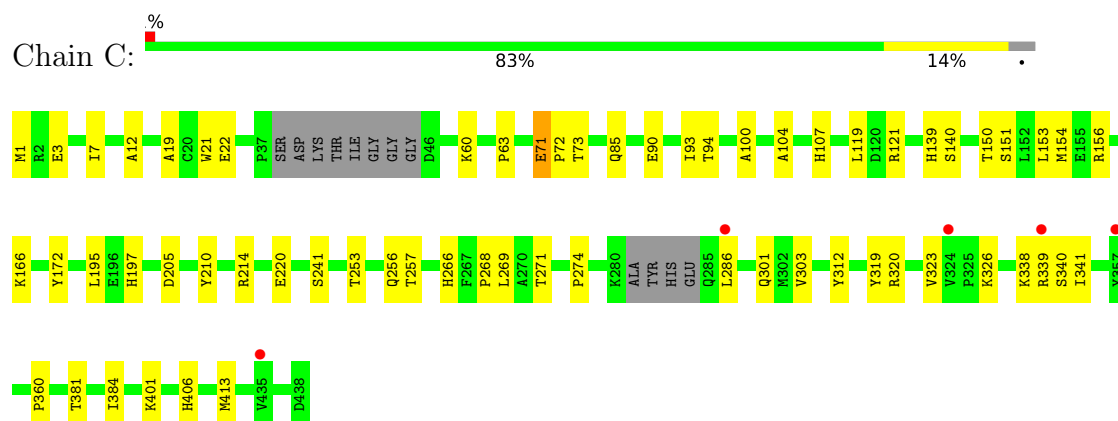
### 3 Residue-property plots [i](#)

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.

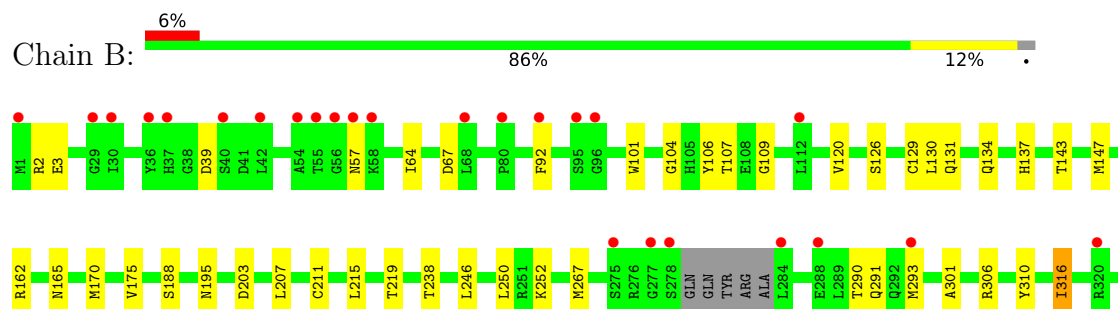
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

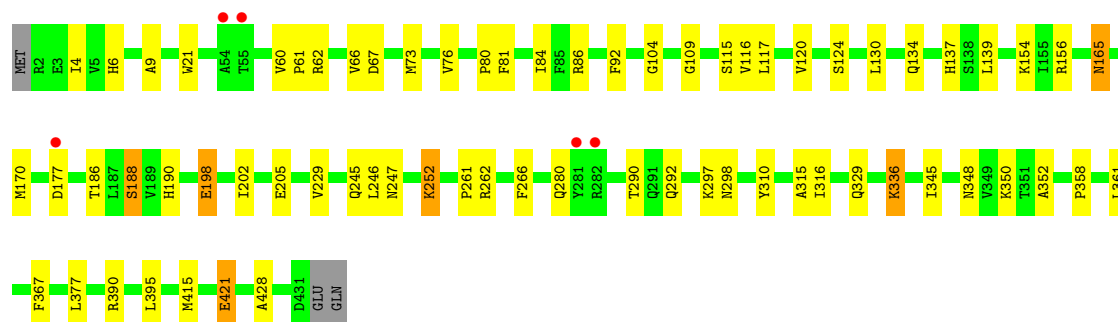
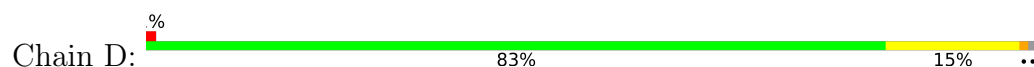


- Molecule 2: Tubulin beta chain

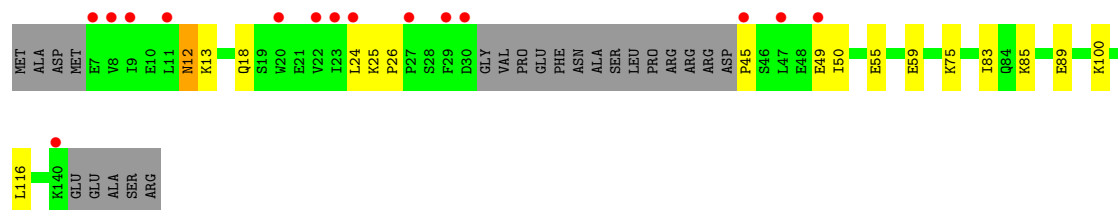




● Molecule 2: Tubulin beta chain



● Molecule 3: Stathmin-4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.72Å 127.03Å 254.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.34 – 2.50 48.07 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.34-2.50) 93.1 (48.07-2.48)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.168 , 0.223 0.168 , 0.222	Depositor DCC
$R_{free}$ test set	2000 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LOC, SO4, GDP, MG, GTP

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	0.39	0/3413	0.54	0/4631
1	C	0.42	0/3409	0.56	0/4626
2	B	0.40	0/3405	0.55	0/4611
2	D	0.43	0/3454	0.58	0/4679
3	E	0.35	0/1003	0.46	0/1332
All	All	0.41	0/14684	0.55	0/19879

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	3339	0	3259	43	0
1	C	3335	0	3248	36	0
2	B	3332	0	3209	32	0
2	D	3379	0	3249	38	0
3	E	993	0	1005	11	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	D	5	0	0	0	0
7	B	28	0	12	0	0
8	B	29	0	25	1	0
8	D	29	0	25	2	0
9	A	9	0	0	0	0
9	B	3	0	0	0	0
9	C	13	0	0	0	0
9	D	3	0	0	0	0
9	E	1	0	0	0	0
All	All	14606	0	14068	146	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 5.

All (146) 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:60:VAL:HG11	2:D:86:ARG:HG3	1.62	0.81
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.65	0.77
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.68	0.73
1:A:223:THR:HG23	1:A:226:ASN:H	1.56	0.70
2:B:170:MET:HG2	2:B:377:LEU:HD11	1.73	0.68
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.77	0.67
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.76	0.67
1:A:2:ARG:HB3	1:A:133:GLN:NE2	2.15	0.62
1:A:430:LYS:HA	1:A:433:GLU:HB2	1.83	0.61
2:D:73:MET:HA	2:D:76:VAL:HG12	1.83	0.60
2:D:350:LYS:HG3	8:D:502:LOC:C16	2.31	0.60
2:D:262:ARG:NE	2:D:421:GLU:OE2	2.34	0.58
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.86	0.57
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.87	0.56
3:E:85:LYS:O	3:E:89:GLU:HG2	2.05	0.56
2:B:336:LYS:HG2	2:B:337:ASN:OD1	2.06	0.56
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.71	0.55
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.89	0.55
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.89	0.54
2:B:397:TRP:NE1	1:C:257:THR:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HG2	1:C:73:THR:H	1.73	0.54
2:B:143:THR:HG23	2:B:147:MET:HE2	1.89	0.54
1:C:269:LEU:HD11	1:C:301:GLN:HB3	1.90	0.54
2:B:130:LEU:O	2:B:162:ARG:NH1	2.40	0.54
1:C:401:LYS:HE3	2:D:428:ALA:HB1	1.89	0.54
1:A:320:ARG:HG3	1:A:358:GLN:O	2.08	0.53
2:D:358:PRO:HG2	2:D:361:LEU:HD12	1.89	0.53
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.44	0.53
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.90	0.53
2:B:134:GLN:HA	2:B:165:ASN:O	2.09	0.53
1:A:69:ASP:O	1:A:94:THR:HA	2.09	0.52
2:D:139:LEU:HD22	2:D:188:SER:HB3	1.92	0.51
2:B:67:ASP:O	2:B:92:PHE:HA	2.11	0.51
1:A:181:VAL:HG11	1:A:404:PHE:CZ	2.46	0.51
2:B:195:ASN:HD21	3:E:75:LYS:NZ	2.09	0.51
2:D:292:GLN:HG2	2:D:298:ASN:OD1	2.12	0.50
1:A:213:CYS:HA	1:A:217:LEU:HD12	1.93	0.50
1:A:241:SER:HB3	1:A:248:LEU:O	2.12	0.50
1:A:266:HIS:O	1:A:268:PRO:HD3	2.11	0.50
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.94	0.50
1:C:104:ALA:HB2	1:C:413:MET:SD	2.51	0.50
1:C:274:PRO:HB3	1:C:286:LEU:HD12	1.94	0.50
2:D:124:SER:HB2	2:D:130:LEU:HD22	1.94	0.49
2:D:316:ILE:HD12	2:D:352:ALA:HB3	1.94	0.49
2:B:39:ASP:N	2:B:39:ASP:OD1	2.46	0.49
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.95	0.49
2:B:219:THR:HG21	1:C:326:LYS:O	2.12	0.49
1:A:178:SER:O	1:A:178:SER:OG	2.29	0.48
2:D:139:LEU:HD12	2:D:170:MET:SD	2.53	0.48
1:C:253:THR:O	1:C:257:THR:HG23	2.13	0.48
2:B:246:LEU:HD21	8:B:502:LOC:C12	2.43	0.48
1:A:180:ALA:O	1:A:183:GLU:HG3	2.14	0.48
1:C:72:PRO:HA	1:C:94:THR:HG21	1.95	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.48
1:A:88:HIS:HB3	1:A:90:GLU:OE1	2.13	0.48
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.49	0.48
2:D:336:LYS:HB3	2:D:336:LYS:HE2	1.68	0.48
2:B:131:GLN:OE1	2:B:250:LEU:N	2.40	0.47
2:B:64:ILE:HD13	2:B:120:VAL:HG22	1.94	0.47
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.96	0.47
2:B:238:THR:HB	2:B:316:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:O	1:A:292:THR:OG1	2.23	0.47
2:D:290:THR:HG21	2:D:329:GLN:HB2	1.97	0.47
1:A:158:SER:OG	1:A:166:LYS:NZ	2.48	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.96	0.46
1:C:338:LYS:HG3	1:C:340:SER:HB3	1.96	0.46
2:D:116:VAL:O	2:D:120:VAL:HG23	2.15	0.46
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.32	0.46
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.98	0.46
1:A:223:THR:HG22	1:A:226:ASN:OD1	2.16	0.46
2:B:310:TYR:CE1	2:B:367:PHE:HZ	2.33	0.46
1:A:234:ILE:HD12	1:A:272:TYR:HB2	1.97	0.46
1:A:247:ALA:HB1	3:E:12:ASN:HB3	1.98	0.46
1:C:60:LYS:NZ	1:C:85:GLN:O	2.44	0.45
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.99	0.45
3:E:55:GLU:O	3:E:59:GLU:HG2	2.17	0.45
2:D:9:ALA:HA	2:D:66:VAL:O	2.17	0.45
2:B:203:ASP:O	2:B:207:LEU:HG	2.17	0.45
1:C:312:TYR:CE2	1:C:341:ILE:HG23	2.52	0.45
1:C:107:HIS:HD2	1:C:151:SER:HB2	1.82	0.45
2:D:104:GLY:O	2:D:109:GLY:HA3	2.16	0.45
1:C:406:HIS:CD2	2:D:261:PRO:HD3	2.52	0.45
2:D:4:ILE:O	2:D:62:ARG:HD2	2.17	0.45
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.51	0.44
1:A:383:ALA:O	1:A:386:GLU:HG2	2.17	0.44
2:B:2:ARG:HG3	2:B:3:GLU:OE2	2.18	0.44
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.53	0.44
2:D:134:GLN:HA	2:D:165:ASN:O	2.17	0.44
3:E:13:LYS:HG3	3:E:18:GLN:HB3	1.99	0.44
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.98	0.44
1:A:234:ILE:HD12	1:A:272:TYR:CB	2.48	0.44
2:B:101:TRP:HE1	2:B:188:SER:HB3	1.83	0.44
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.98	0.44
2:B:211:CYS:HA	2:B:215:LEU:HD12	2.00	0.44
2:D:202:ILE:HG21	2:D:229:VAL:HG22	1.99	0.44
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.52	0.43
1:C:19:ALA:O	1:C:22:GLU:HG2	2.17	0.43
3:E:100:LYS:HD3	3:E:100:LYS:HA	1.72	0.43
2:B:104:GLY:O	2:B:109:GLY:HA3	2.18	0.43
1:C:266:HIS:O	1:C:268:PRO:HD3	2.18	0.43
2:B:316:ILE:HA	2:B:352:ALA:O	2.19	0.43
2:D:186:THR:HA	2:D:415:MET:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HD23	2:B:246:LEU:HA	1.87	0.43
2:B:290:THR:HG22	2:B:333:VAL:HG21	1.99	0.43
1:C:100:ALA:HA	2:D:252:LYS:HG3	2.00	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.01	0.42
2:B:357:PRO:HB2	2:B:361:LEU:O	2.19	0.42
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.54	0.42
2:D:67:ASP:O	2:D:92:PHE:HA	2.19	0.42
2:D:246:LEU:HA	2:D:246:LEU:HD23	1.65	0.42
1:A:180:ALA:H	1:A:183:GLU:HG3	1.84	0.42
2:D:198:GLU:HB3	2:D:266:PHE:CE2	2.54	0.42
2:B:306:ARG:HH11	2:B:337:ASN:HD21	1.67	0.42
1:A:79:ARG:O	1:A:84:ARG:HB2	2.20	0.42
2:B:397:TRP:CZ2	1:C:256:GLN:HB3	2.55	0.42
2:D:165:ASN:HD21	2:D:198:GLU:CD	2.23	0.42
1:A:234:ILE:HD13	1:A:234:ILE:N	2.35	0.42
1:A:307:PRO:HA	1:A:383:ALA:HB2	2.02	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.20	0.41
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.51	0.41
1:A:336:LYS:HD2	3:E:24:LEU:HD13	2.03	0.41
1:C:12:ALA:CB	1:C:140:SER:HB3	2.50	0.41
1:C:195:LEU:HD12	1:C:195:LEU:HA	1.73	0.41
1:A:96:LYS:HG3	2:B:129:CYS:HB2	2.02	0.41
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.03	0.41
2:B:106:TYR:O	3:E:83:ILE:HD11	2.20	0.41
1:C:214:ARG:HD2	1:C:220:GLU:O	2.21	0.41
1:C:320:ARG:HG3	1:C:360:PRO:HD3	2.02	0.41
2:D:297:LYS:HE2	2:D:297:LYS:HB2	1.71	0.41
3:E:25:LYS:HG2	3:E:26:PRO:O	2.21	0.41
1:A:155:GLU:HB3	3:E:50:ILE:HD13	2.02	0.41
1:A:271:THR:HG21	1:A:295:CYS:O	2.21	0.41
1:C:1:MET:N	1:C:3:GLU:OE2	2.48	0.40
1:C:210:TYR:O	1:C:214:ARG:HG3	2.21	0.40
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.03	0.40
2:D:80:PRO:O	2:D:81:PHE:HB2	2.21	0.40
2:D:395:LEU:HD23	2:D:395:LEU:HA	1.91	0.40
1:A:25:CYS:HB3	1:A:30:ILE:O	2.20	0.40
1:A:286:LEU:O	1:A:373:ARG:HD2	2.21	0.40
2:D:350:LYS:HG3	8:D:502:LOC:C17	2.52	0.40
1:A:100:ALA:HA	2:B:252:LYS:HG3	2.04	0.40
1:C:150:THR:O	1:C:154:MET:HG2	2.21	0.40
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:O	2:B:126:SER:OG	2.37	0.40
2:D:315:ALA:O	2:D:316:ILE:HD13	2.21	0.40
3:E:45:PRO:HB2	3:E:49:GLU:HB3	2.03	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	420/438 (96%)	405 (96%)	15 (4%)	0	100	100
1	C	420/438 (96%)	410 (98%)	10 (2%)	0	100	100
2	B	421/433 (97%)	407 (97%)	14 (3%)	0	100	100
2	D	428/433 (99%)	416 (97%)	12 (3%)	0	100	100
3	E	116/143 (81%)	113 (97%)	3 (3%)	0	100	100
All	All	1805/1885 (96%)	1751 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	361/369 (98%)	357 (99%)	4 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	360/369 (98%)	353 (98%)	7 (2%)	57 80
2	B	366/374 (98%)	360 (98%)	6 (2%)	62 84
2	D	370/374 (99%)	353 (95%)	17 (5%)	27 50
3	E	106/126 (84%)	104 (98%)	2 (2%)	57 80
All	All	1563/1612 (97%)	1527 (98%)	36 (2%)	50 76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	178	SER
1	A	241	SER
1	A	381	THR
2	B	57	ASN
2	B	107	THR
2	B	137	HIS
2	B	175	VAL
2	B	291	GLN
2	B	316	ILE
1	C	71	GLU
1	C	90	GLU
1	C	241	SER
1	C	271	THR
1	C	339	ARG
1	C	381	THR
1	C	384	ILE
2	D	84	ILE
2	D	115	SER
2	D	137	HIS
2	D	156	ARG
2	D	165	ASN
2	D	177	ASP
2	D	188	SER
2	D	190	HIS
2	D	198	GLU
2	D	205	GLU
2	D	245	GLN
2	D	247	ASN
2	D	252	LYS
2	D	280	GLN
2	D	336	LYS

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Mol	Chain	Res	Type
2	D	390	ARG
2	D	421	GLU
3	E	12	ASN
3	E	116	LEU

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

Mol	Chain	Res	Type
1	A	372	GLN
1	C	356	ASN
2	D	165	ASN
2	D	247	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 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	$\# Z  > 2$
4	GTP	D	501	-	26,34,34	1.00	1 (3%)	33,54,54	1.83	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	LOC	B	502	-	28,31,31	1.03	2 (7%)	28,44,44	0.71	0
6	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.13	0
8	LOC	D	502	-	28,31,31	0.98	2 (7%)	28,44,44	0.71	0
7	GDP	B	501	-	24,30,30	1.24	2 (8%)	31,47,47	1.96	8 (25%)
6	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.16	0
4	GTP	A	501	5	26,34,34	1.08	1 (3%)	33,54,54	1.91	7 (21%)
4	GTP	C	501	5	26,34,34	1.10	1 (3%)	33,54,54	1.98	10 (30%)
6	SO4	D	503	-	4,4,4	0.17	0	6,6,6	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LOC	B	502	-	-	0/10/25/25	0/3/3/3
4	GTP	D	501	-	-	7/18/38/38	0/3/3/3
8	LOC	D	502	-	-	0/10/25/25	0/3/3/3
7	GDP	B	501	-	-	4/12/32/32	0/3/3/3
4	GTP	A	501	5	-	6/18/38/38	0/3/3/3
4	GTP	C	501	5	-	5/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	GDP	C6-C5	4.25	1.48	1.41
8	B	502	LOC	C15-C16	4.24	1.48	1.39
8	D	502	LOC	C15-C16	3.87	1.47	1.39
4	A	501	GTP	C6-N1	3.76	1.39	1.33
4	C	501	GTP	C6-N1	3.53	1.39	1.33
4	D	501	GTP	C6-N1	2.88	1.38	1.33
7	B	501	GDP	C5-C4	2.71	1.48	1.40
8	B	502	LOC	C21-C22	-2.46	1.46	1.49
8	D	502	LOC	C21-C22	-2.38	1.46	1.49

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	GTP	N3-C2-N1	-6.03	119.18	127.22
4	A	501	GTP	N3-C2-N1	-5.61	119.74	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	GDP	C2-N3-C4	4.72	120.75	115.36
4	A	501	GTP	C2-N3-C4	4.67	120.69	115.36
4	C	501	GTP	C2-N3-C4	4.50	120.50	115.36
4	D	501	GTP	N3-C2-N1	-4.43	121.31	127.22
4	D	501	GTP	PB-O3B-PG	-4.36	117.87	132.83
7	B	501	GDP	C6-C5-C4	-4.29	116.71	120.80
7	B	501	GDP	C6-N1-C2	3.98	122.25	115.93
7	B	501	GDP	C5-C6-N1	-3.90	118.09	123.43
4	A	501	GTP	PB-O3B-PG	-3.83	119.70	132.83
4	D	501	GTP	C2-N3-C4	3.59	119.45	115.36
4	D	501	GTP	C5-C6-N1	-3.42	118.75	123.43
4	C	501	GTP	PA-O3A-PB	-3.15	122.02	132.83
7	B	501	GDP	N3-C2-N1	-3.09	123.10	127.22
4	C	501	GTP	C6-C5-C4	-3.03	117.91	120.80
4	C	501	GTP	C6-N1-C2	2.95	120.62	115.93
4	C	501	GTP	C5-C6-N1	-2.85	119.54	123.43
7	B	501	GDP	O4'-C1'-C2'	-2.82	102.81	106.93
4	A	501	GTP	PA-O3A-PB	-2.77	123.31	132.83
4	D	501	GTP	C4-C5-N7	-2.77	106.52	109.40
7	B	501	GDP	PA-O3A-PB	-2.73	123.47	132.83
4	C	501	GTP	N2-C2-N1	2.70	121.46	117.25
4	A	501	GTP	C6-C5-C4	-2.65	118.27	120.80
4	D	501	GTP	C6-N1-C2	2.54	119.96	115.93
4	A	501	GTP	C6-N1-C2	2.54	119.96	115.93
4	C	501	GTP	O3G-PG-O3B	2.51	113.04	104.64
4	D	501	GTP	O3'-C3'-C4'	-2.34	104.27	111.05
4	A	501	GTP	C5-C6-N1	-2.33	120.25	123.43
7	B	501	GDP	C4-C5-N7	-2.32	106.98	109.40
4	C	501	GTP	C5'-C4'-C3'	-2.18	107.02	115.18
4	C	501	GTP	C1'-N9-C4	-2.10	122.94	126.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A

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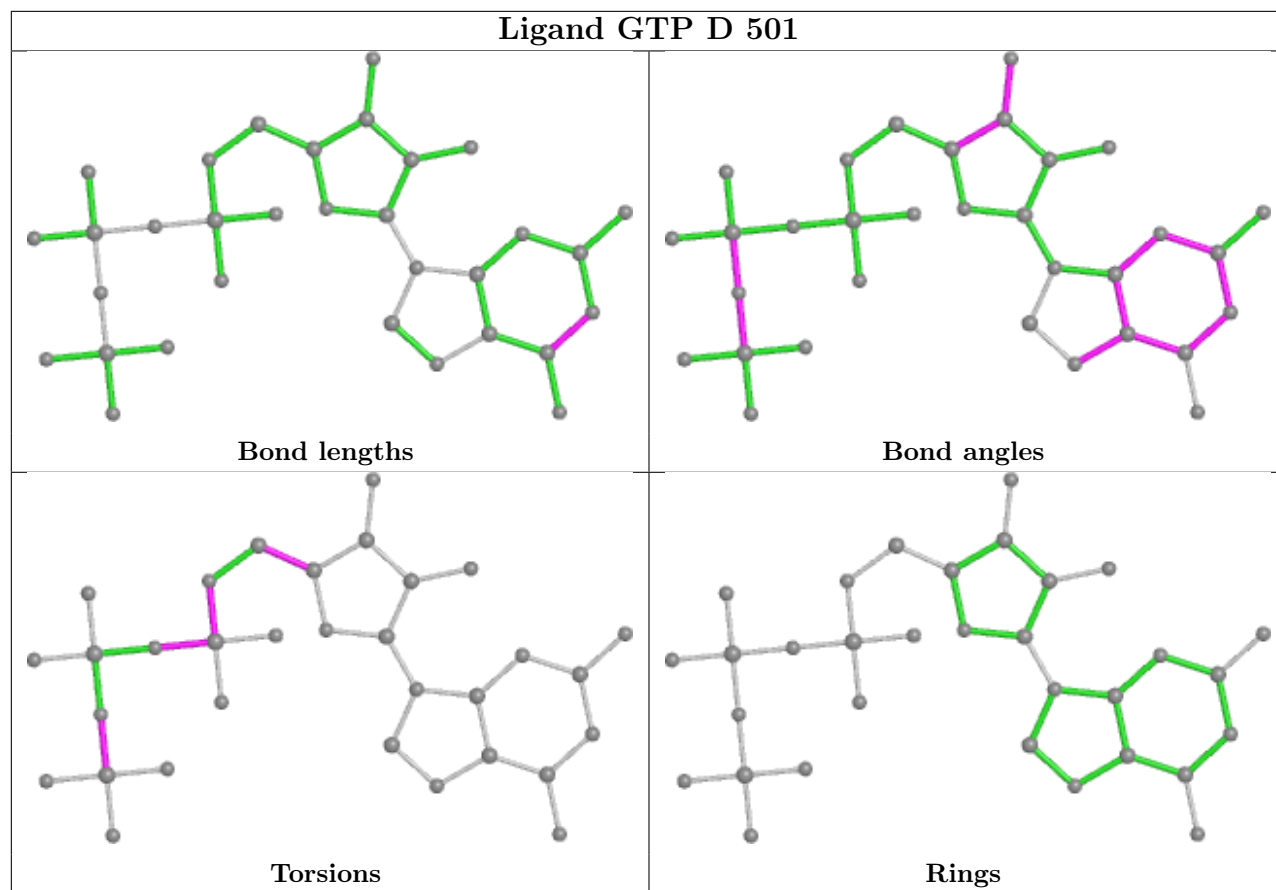
Mol	Chain	Res	Type	Atoms
4	D	501	GTP	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O1G
4	D	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	C5'-O5'-PA-O3A
7	B	501	GDP	PB-O3A-PA-O2A
4	A	501	GTP	C4'-C5'-O5'-PA
4	C	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O3A
4	D	501	GTP	PB-O3A-PA-O1A
4	D	501	GTP	C3'-C4'-C5'-O5'

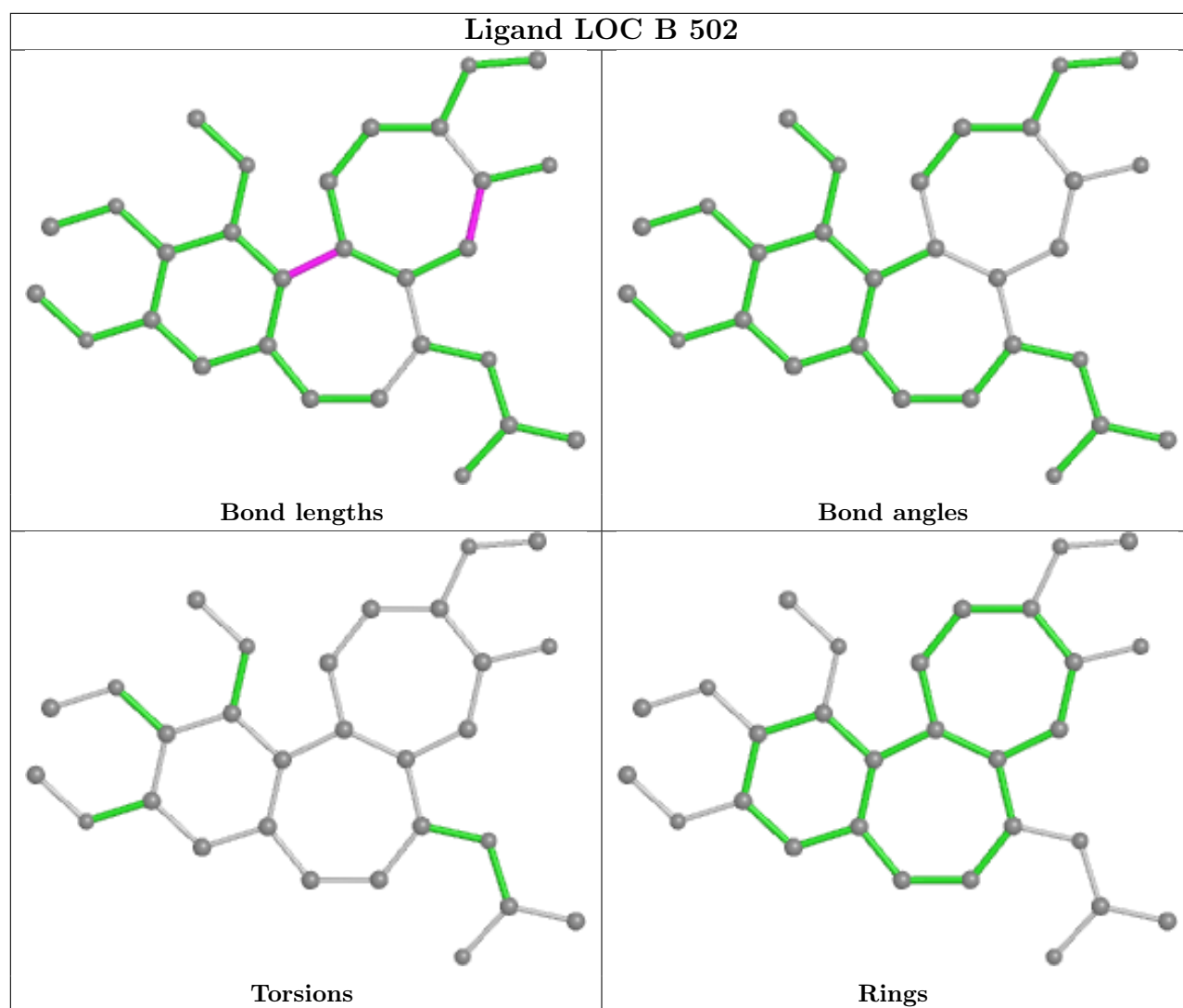
There are no ring outliers.

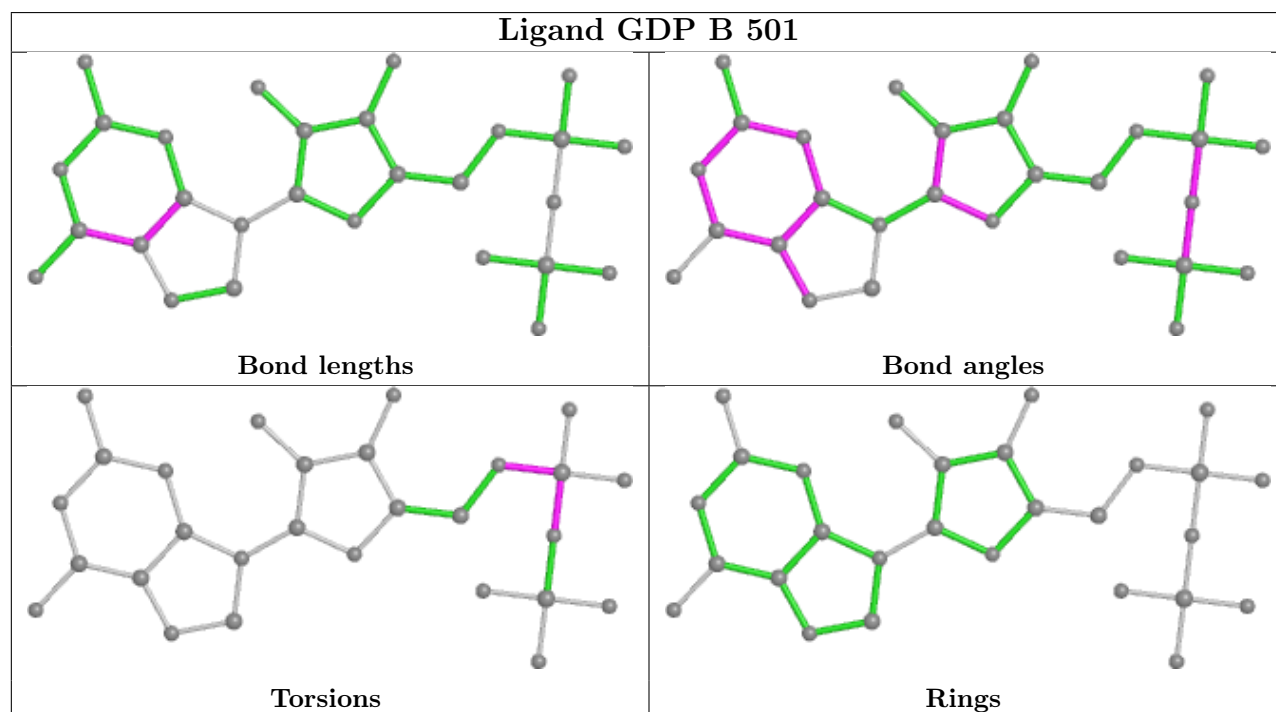
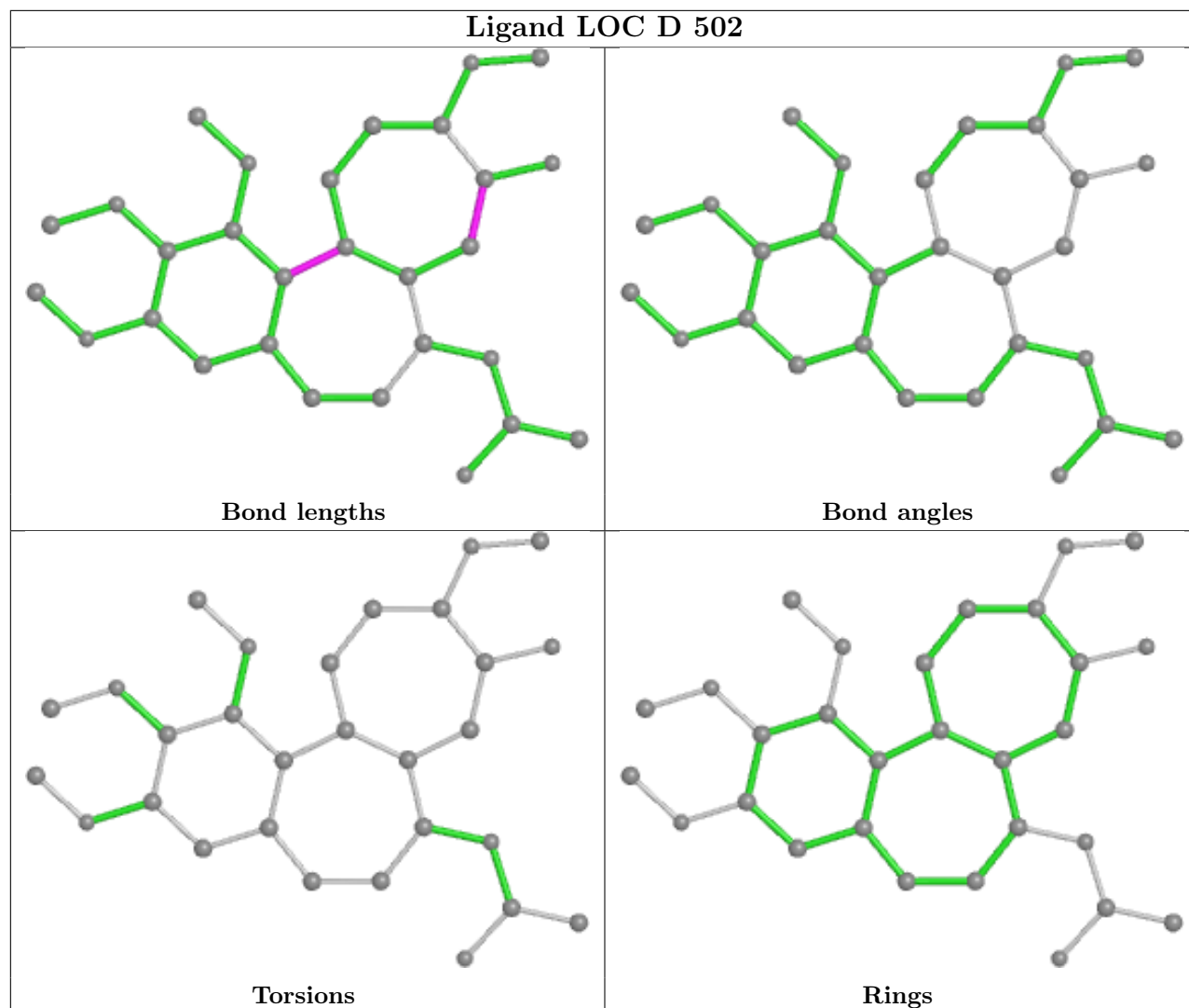
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	502	LOC	1	0
8	D	502	LOC	2	0

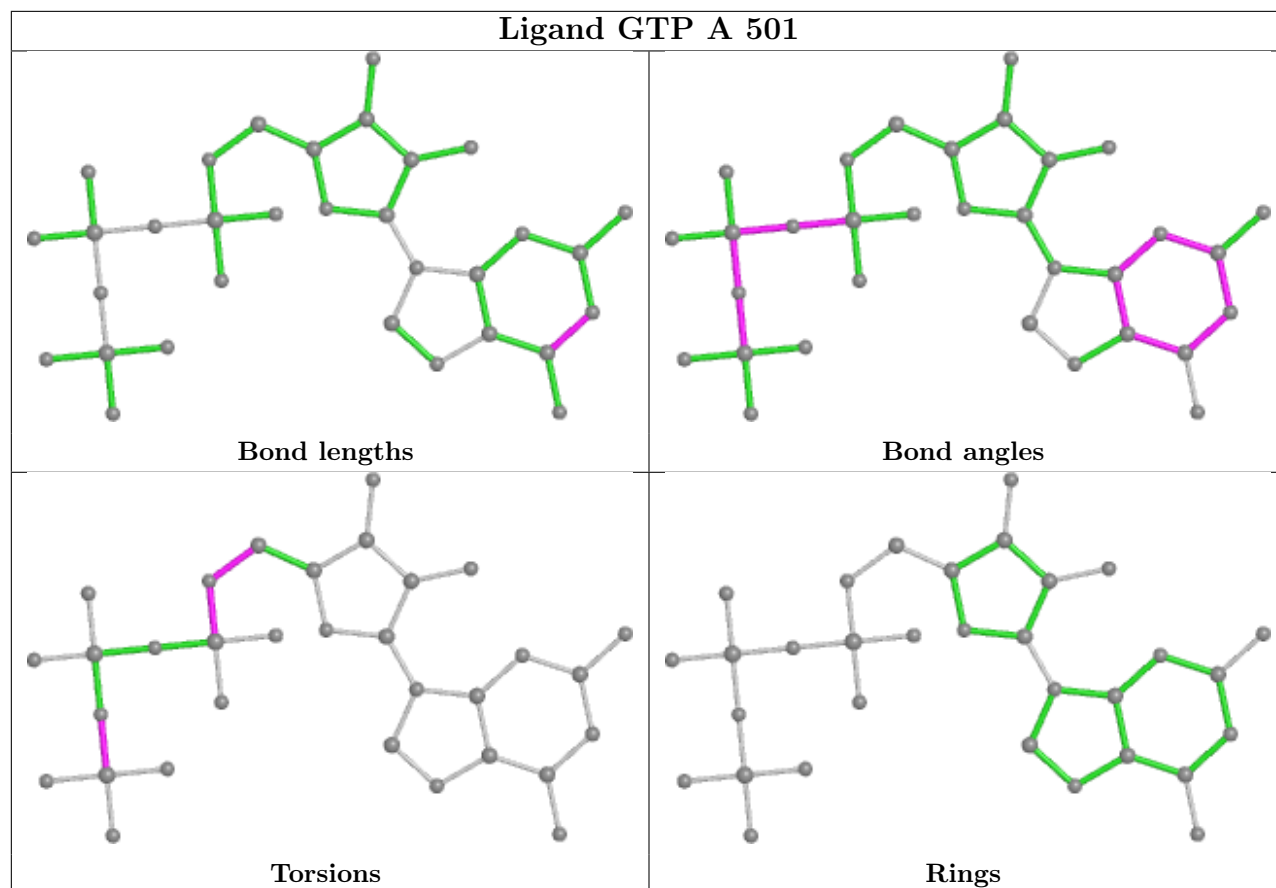
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



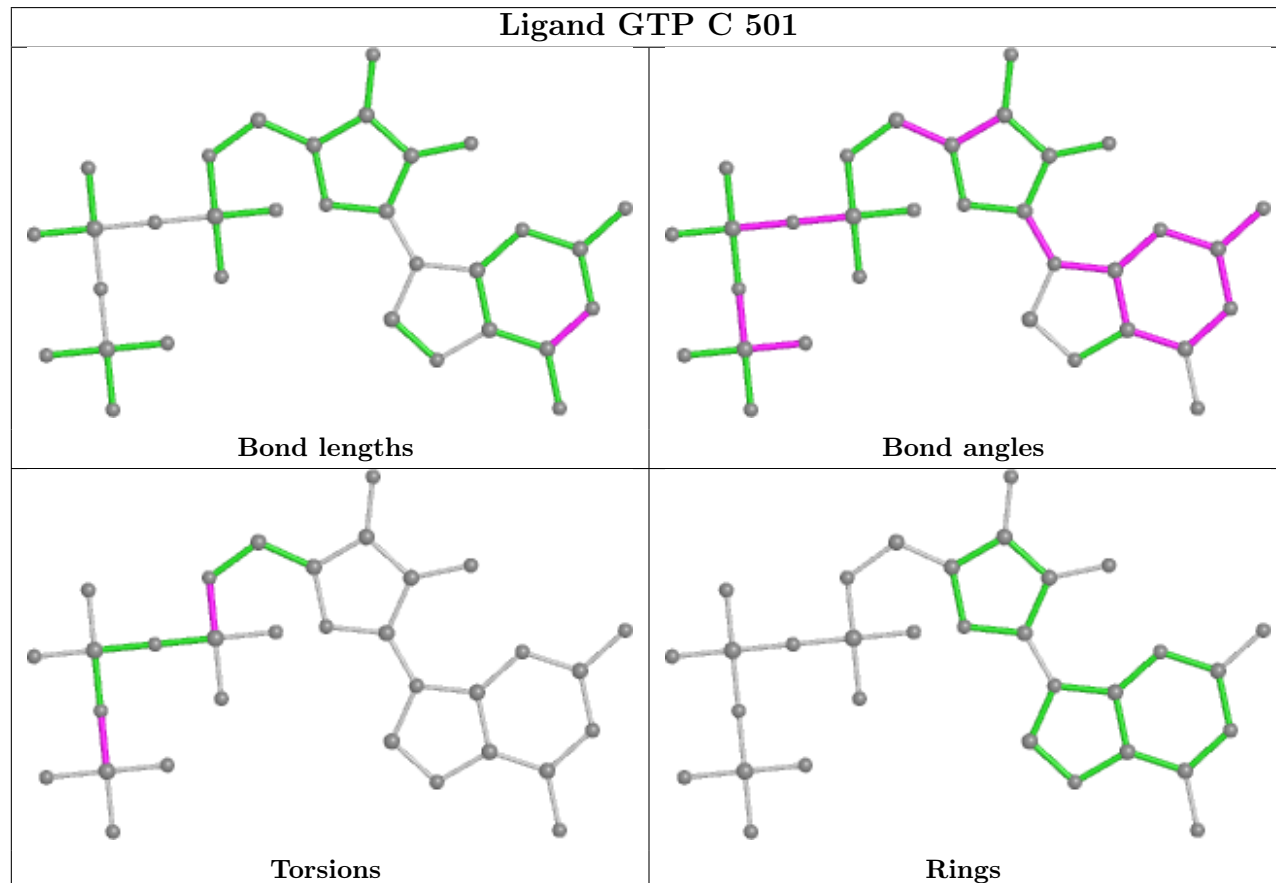




## Ligand GTP A 501



## Ligand GTP C 501





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	426/438 (97%)	0.11	23 (5%) 25 27	49, 78, 118, 163	0
1	C	426/438 (97%)	-0.01	5 (1%) 79 80	45, 71, 102, 139	0
2	B	425/433 (98%)	0.37	28 (6%) 18 19	51, 73, 116, 142	0
2	D	430/433 (99%)	0.08	5 (1%) 79 80	46, 66, 107, 130	0
3	E	120/143 (83%)	0.62	15 (12%) 3 3	72, 90, 121, 142	0
All	All	1827/1885 (96%)	0.17	76 (4%) 36 39	45, 74, 113, 163	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	8	VAL	4.5
1	A	1	MET	4.5
2	D	282	ARG	4.2
1	A	337	THR	4.1
2	B	36	TYR	4.1
2	B	361	LEU	4.1
2	B	363	MET	4.0
1	A	351	PHE	4.0
1	A	336	LYS	3.8
2	B	55	THR	3.8
3	E	7	GLU	3.5
2	B	80	PRO	3.4
1	A	280	LYS	3.3
3	E	9	ILE	3.3
3	E	140	LYS	3.2
1	A	437	VAL	3.2
2	D	281	TYR	3.1
3	E	23	ILE	3.1
2	B	95	SER	3.1
2	D	55	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	54	ALA	3.0
2	B	1	MET	3.0
2	B	56	GLY	2.9
1	A	284	GLU	2.9
2	B	284	LEU	2.9
1	A	130	THR	2.9
1	A	129	CYS	2.9
1	A	324	VAL	2.8
2	B	37	HIS	2.8
2	B	320	ARG	2.8
2	B	288	GLU	2.8
1	A	332	ILE	2.8
3	E	29	PHE	2.8
1	A	291	ILE	2.8
1	A	346	TRP	2.7
2	B	58	LYS	2.7
2	B	277	GLY	2.7
2	B	360	GLY	2.7
3	E	27	PRO	2.7
2	B	278	SER	2.7
3	E	24	LEU	2.7
2	B	42	LEU	2.6
2	B	68	LEU	2.6
2	B	57	ASN	2.6
1	C	324	VAL	2.6
3	E	30	ASP	2.6
1	A	333	ALA	2.6
2	B	30	ILE	2.6
2	B	293	MET	2.6
2	D	54	ALA	2.5
1	A	317	LEU	2.5
1	A	329	ASN	2.5
1	A	286	LEU	2.5
2	B	96	GLY	2.4
3	E	20	TRP	2.4
2	B	92	PHE	2.4
3	E	49	GLU	2.4
1	C	435	VAL	2.4
1	C	357	TYR	2.4
1	A	328	VAL	2.4
1	A	285	GLN	2.4
1	A	353	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.3
2	B	40	SER	2.3
3	E	22	VAL	2.3
2	B	112	LEU	2.3
1	A	288	VAL	2.2
3	E	45	PRO	2.2
2	B	275	SER	2.2
2	B	29	GLY	2.1
2	D	177	ASP	2.1
1	C	339	ARG	2.1
3	E	11	LEU	2.1
1	C	286	LEU	2.1
1	A	279	GLU	2.0
3	E	47	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

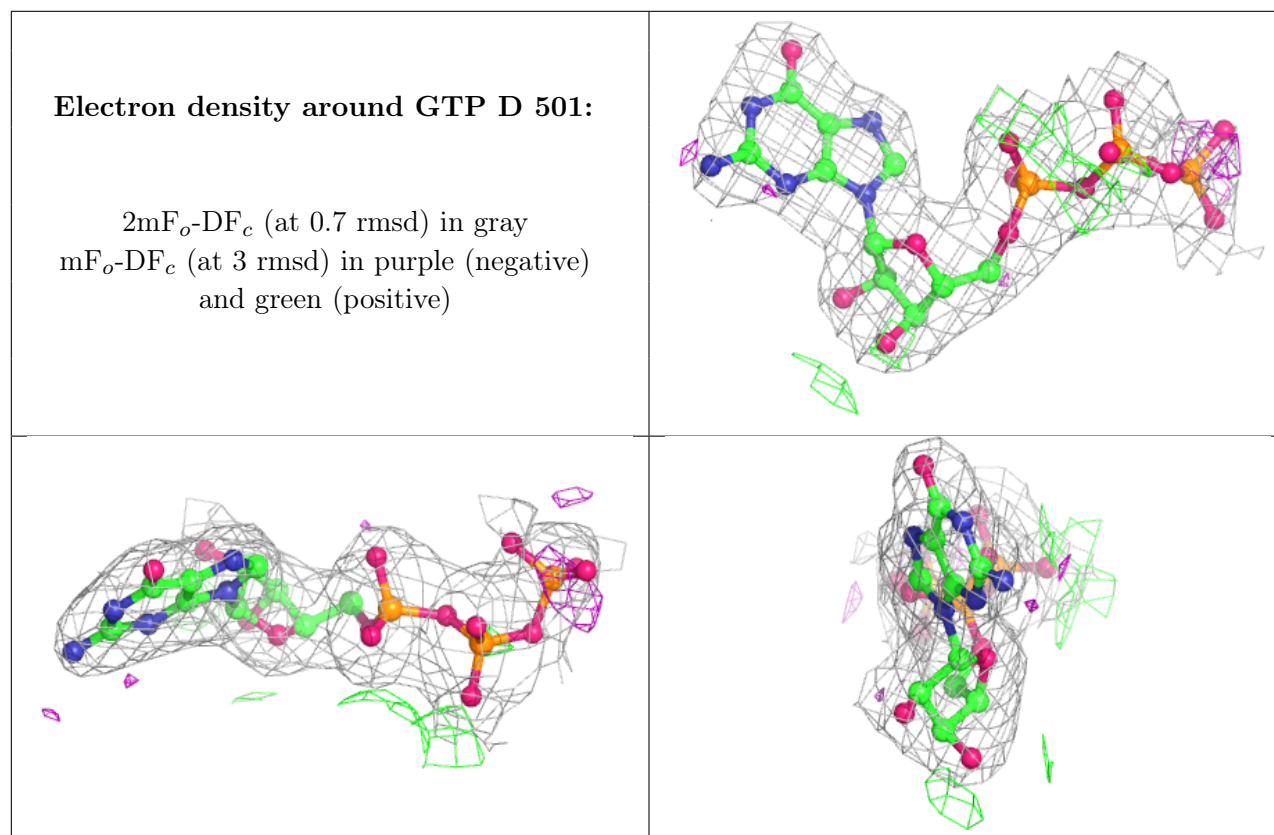
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	D	503	5/5	0.88	0.14	132,136,138,156	0
6	SO4	B	503	5/5	0.92	0.10	133,133,134,134	0
5	MG	C	502	1/1	0.92	0.16	53,53,53,53	0
5	MG	A	502	1/1	0.94	0.18	56,56,56,56	0
6	SO4	A	503	5/5	0.95	0.23	136,138,138,141	0
4	GTP	D	501	32/32	0.97	0.14	48,56,133,138	0
7	GDP	B	501	28/28	0.97	0.20	54,62,72,76	0
8	LOC	B	502	29/29	0.97	0.17	49,58,68,74	0
4	GTP	A	501	32/32	0.98	0.20	45,56,70,77	0

*Continued on next page...*

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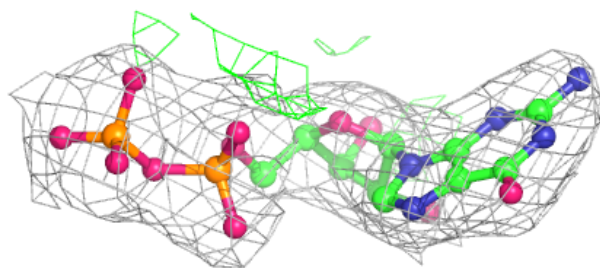
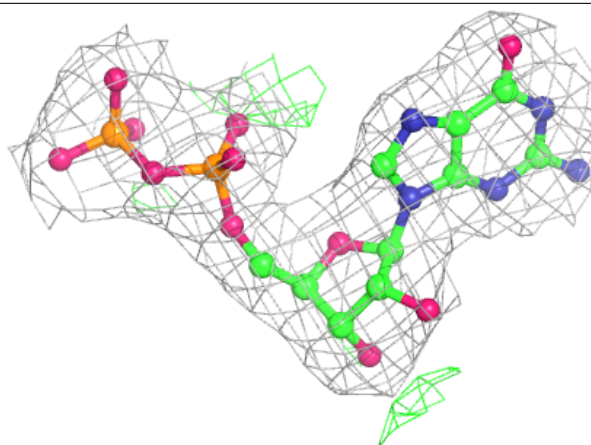
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GTP	C	501	32/32	0.98	0.21	43,55,63,64	0
8	LOC	D	502	29/29	0.98	0.23	46,55,63,66	0

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.



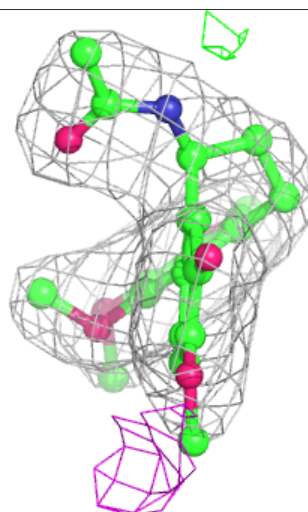
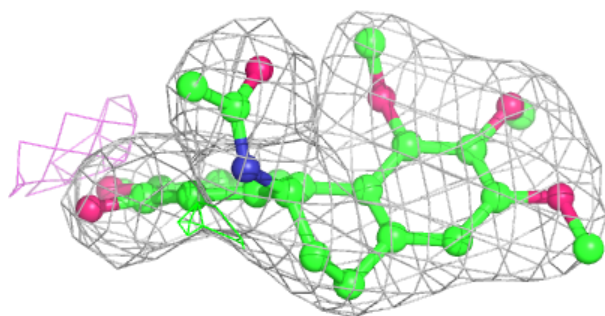
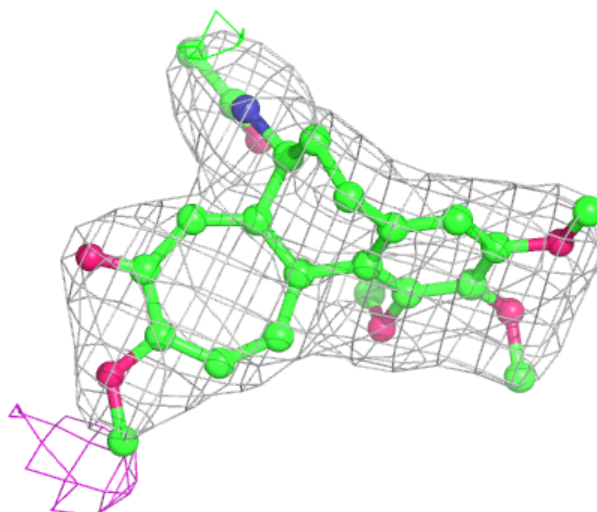
**Electron density around GDP B 501:**

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



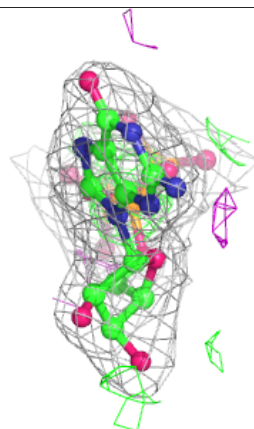
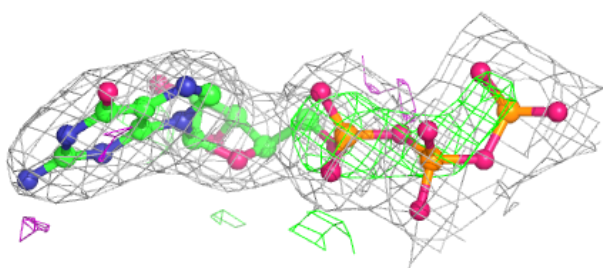
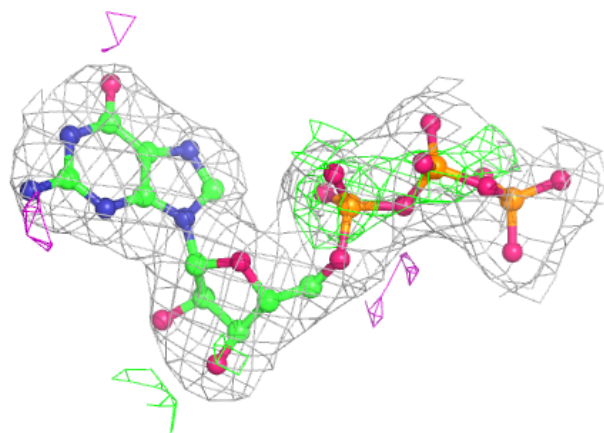
**Electron density around LOC B 502:**

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

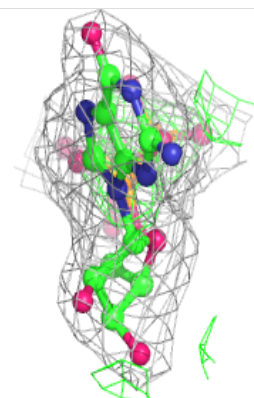
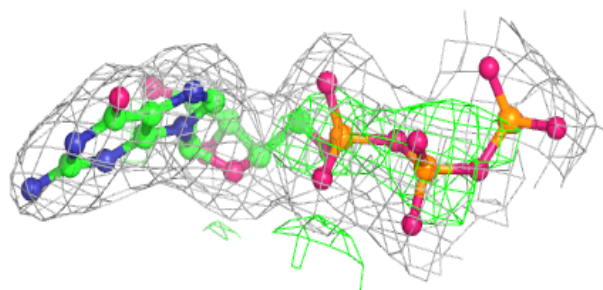
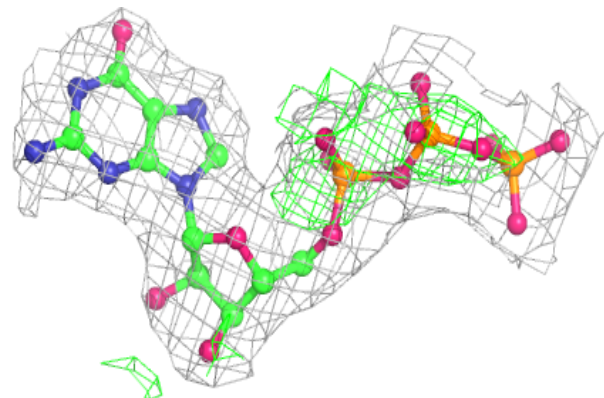


**Electron density around GTP A 501:**

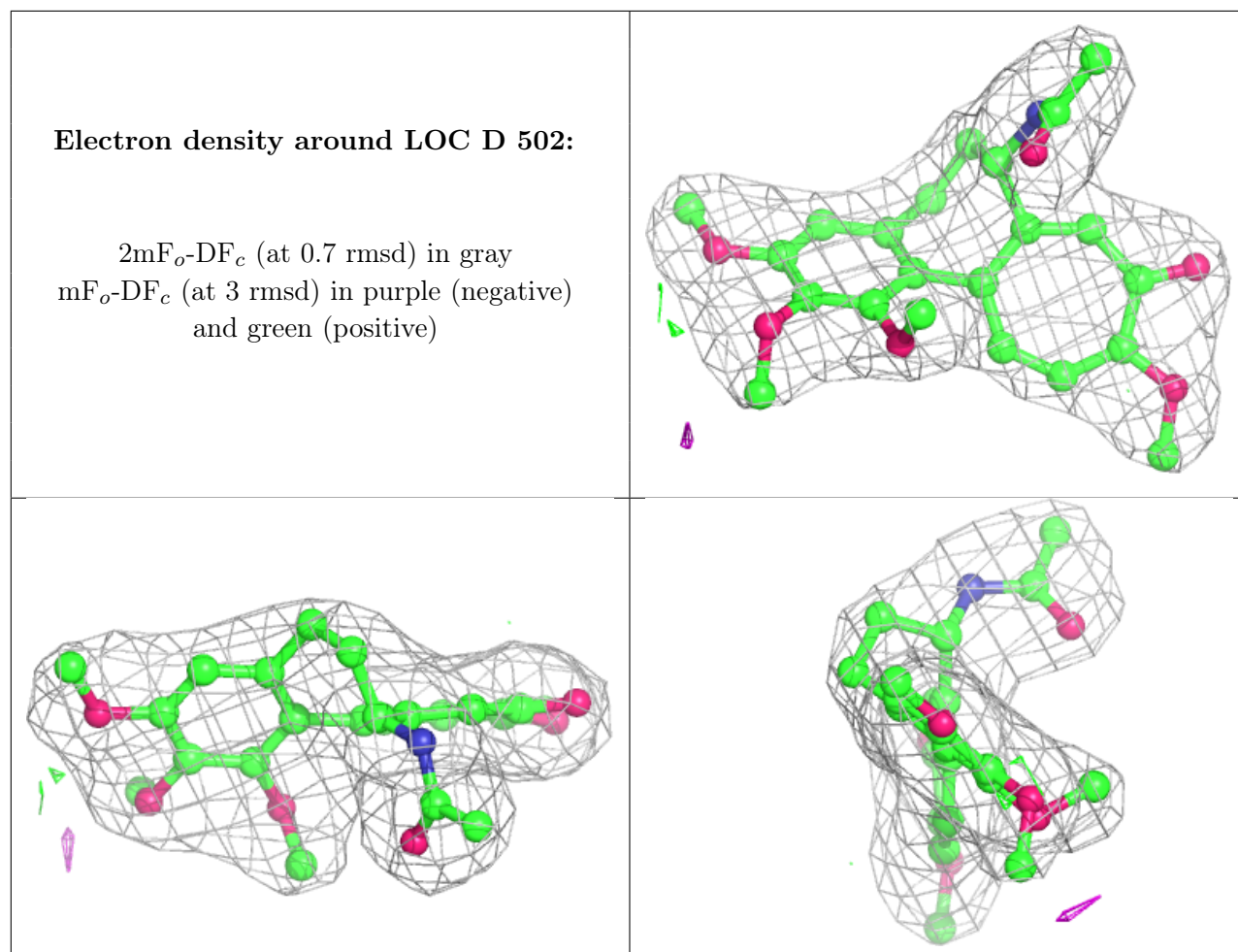
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GTP C 501:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.