



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 12:09 pm BST

PDB ID : 4YJ3  
Title : Crystal structure of tubulin bound to compound 2  
Authors : McNamara, D.E.; Torres, J.Z.; Yeates, T.O.  
Deposited on : 2015-03-03  
Resolution : 3.75 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 : 2.11  
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

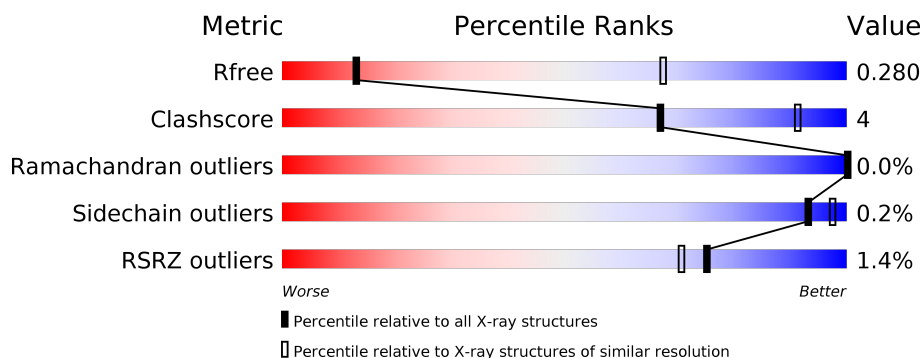
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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  $\geq 3$ , 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	451	<div> <div>7%</div> <div>89% 8%</div> </div>
1	C	451	<div> <div>85% 12%</div> </div>
2	B	445	<div> <div>82% 13% 5%</div> </div>
2	D	445	<div> <div>83% 11% 5%</div> </div>
3	E	143	<div> <div>79% 5% 15%</div> </div>
4	F	384	<div> <div>7%</div> <div>68% 5% 27%</div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17035 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	438	Total	C	N	O	S	0	2	0
			3432	2175	582	653	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-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3326	2092	567	640	27			
2	D	421	Total	C	N	O	S	0	1	0
			3313	2083	562	641	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
			1005	620	182	198	5			

There are 3 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	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	282	Total	C	N	O	S	0	0	0
			2310	1504	383	411	12			

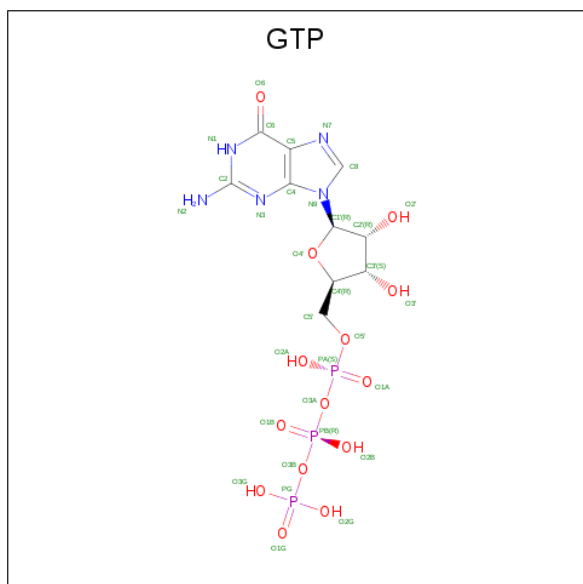
There are 6 discrepancies between the modelled and reference sequences:

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

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

- Molecule 6 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
6	A	1	Total C N O P 32 10 5 14 3	0	0

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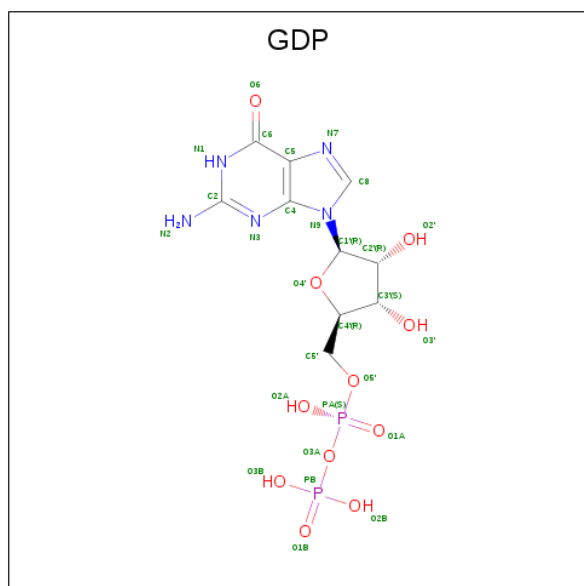
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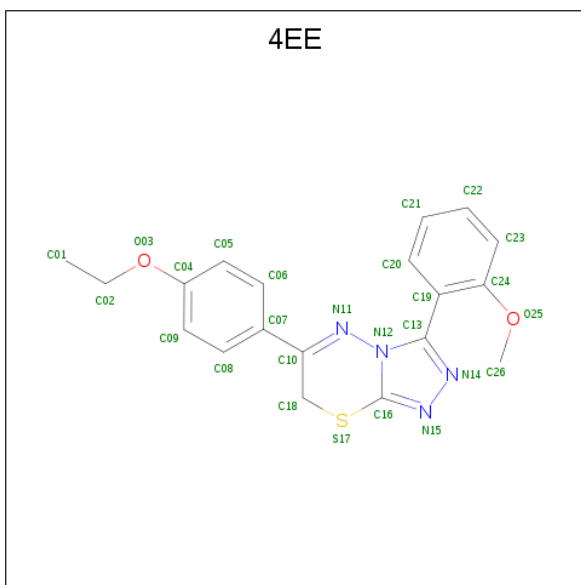
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

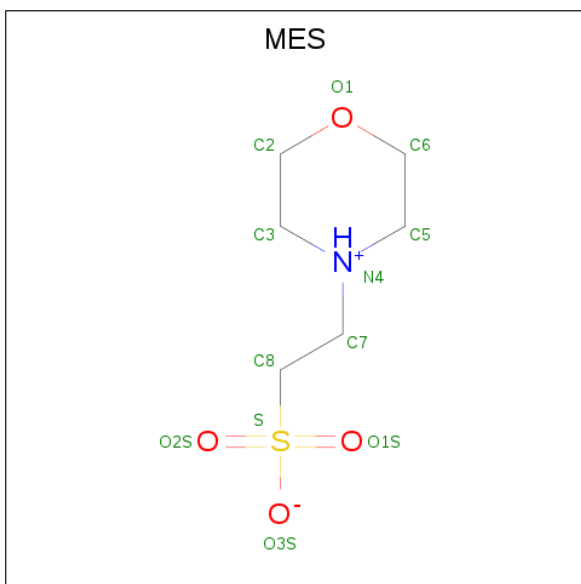
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).





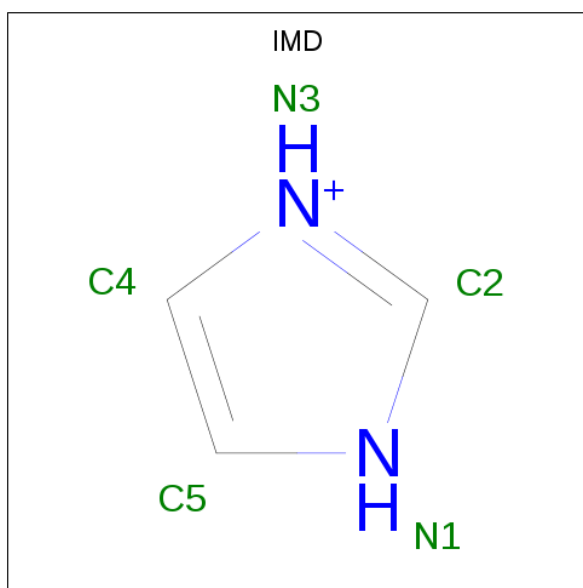
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			26	19	4	2	1		
9	D	1	Total	C	N	O	S	0	0
			26	19	4	2	1		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	N	0	0
			5	3	2		

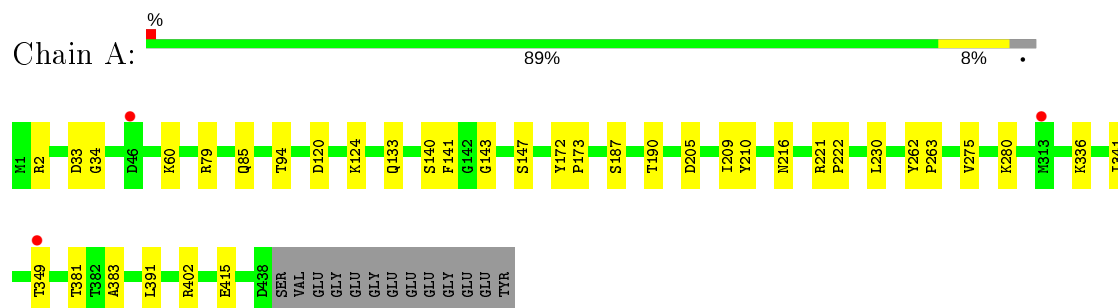
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	3	Total	O	0	0
			3	3		
12	B	4	Total	O	0	0
			4	4		
12	C	7	Total	O	0	0
			7	7		
12	D	2	Total	O	0	0
			2	2		

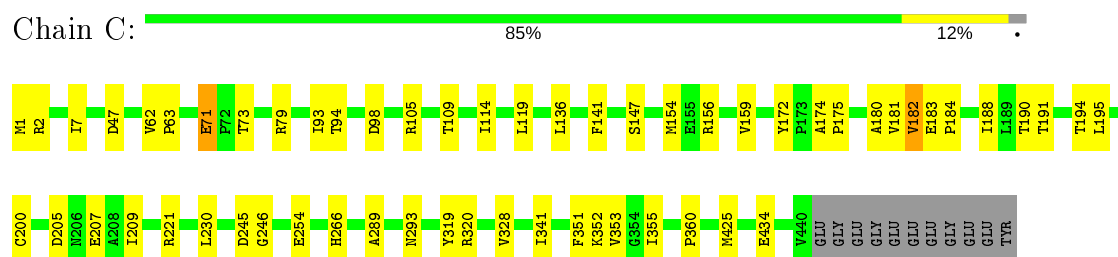
### 3 Residue-property plots [i](#)

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

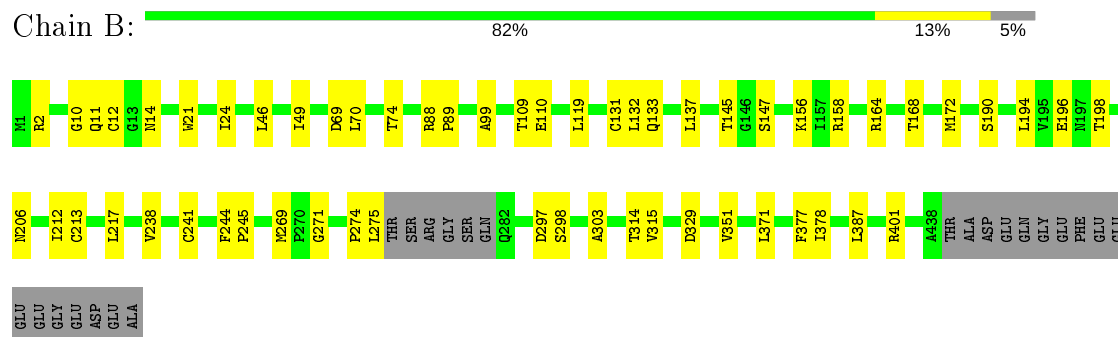
- Molecule 1: Tubulin alpha-1B chain



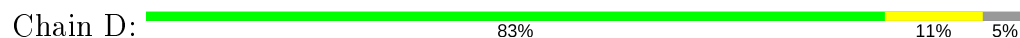
- Molecule 1: Tubulin alpha-1B chain



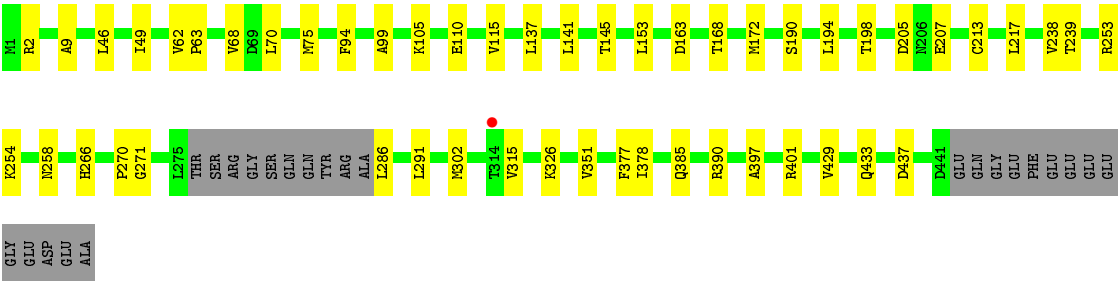
- Molecule 2: Tubulin beta-2B chain



- Molecule 2: Tubulin beta-2B chain



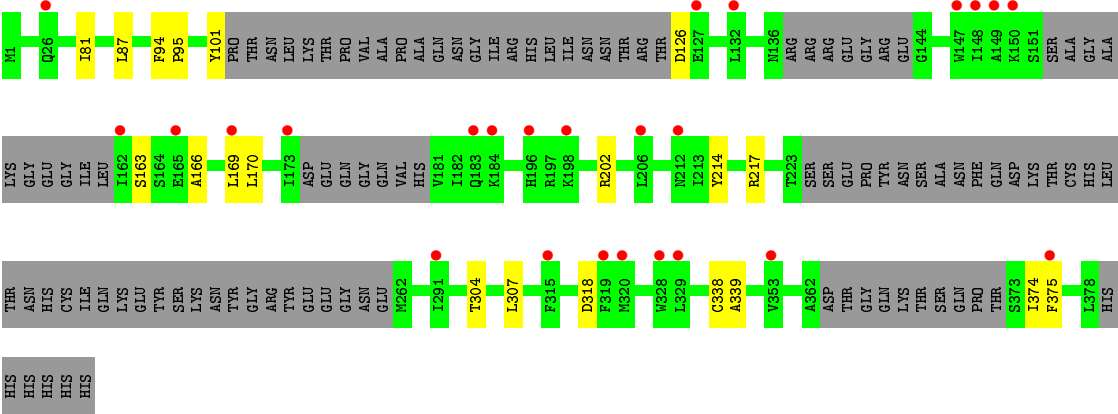




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.20Å 157.69Å 181.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.07 – 3.75 91.07 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.07-3.75) 99.2 (91.07-3.75)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 3.78Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.239 , 0.279 0.241 , 0.280	Depositor DCC
$R_{free}$ test set	3149 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	17035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: GDP, MG, IMD, CA, 4EE, 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	0.21	0/3516	0.35	0/4774
1	C	0.22	0/3515	0.36	0/4772
2	B	0.21	0/3400	0.35	0/4604
2	D	0.21	0/3389	0.35	0/4592
3	E	0.19	0/1014	0.29	0/1347
4	F	0.21	0/2359	0.34	0/3184
All	All	0.21	0/17193	0.35	0/23273

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	3432	0	3352	20	0
1	C	3437	0	3348	39	0
2	B	3326	0	3208	34	0
2	D	3313	0	3196	29	0
3	E	1005	0	1018	5	0
4	F	2310	0	2325	10	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	32	0	12	2	0
6	C	32	0	12	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	2	0
8	D	28	0	12	1	0
9	B	26	0	18	3	0
9	D	26	0	18	2	0
10	B	12	0	12	0	0
11	C	5	0	5	0	0
12	A	3	0	0	0	0
12	B	4	0	0	1	0
12	C	7	0	0	2	0
12	D	2	0	0	0	0
All	All	17035	0	16548	131	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 4.

All (131) 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:217:ARG:HE	4:F:374:ILE:HA	1.59	0.67
1:A:140:SER:OG	6:A:502:GTP:O2A	2.14	0.66
1:C:181:VAL:HG13	1:C:182:VAL:HG13	1.79	0.64
1:C:221:ARG:HE	2:D:326:LYS:HA	1.61	0.64
1:C:180:ALA:HA	9:D:503:4EE:H13	1.80	0.63
1:C:200:CYS:HA	1:C:266:HIS:HB2	1.82	0.62
1:C:289:ALA:O	1:C:293:ASN:ND2	2.33	0.61
2:B:269:MET:HE3	2:B:303:ALA:HB3	1.83	0.61
1:C:181:VAL:HG22	1:C:182:VAL:H	1.67	0.60
2:D:198:THR:OG1	2:D:266:HIS:NE2	2.34	0.59
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.65	0.59
1:A:221:ARG:HH21	2:B:329:ASP:HB3	1.69	0.58
2:B:10:GLY:O	2:B:14:ASN:ND2	2.30	0.57
2:B:158:ARG:NH1	2:B:196:GLU:O	2.38	0.57
2:D:378:ILE:HD12	9:D:503:4EE:H3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:VAL:HB	2:B:351:VAL:HG22	1.85	0.56
2:D:254:LYS:O	2:D:258:ASN:ND2	2.37	0.56
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.88	0.56
1:C:47:ASP:OD2	12:C:601:HOH:O	2.17	0.56
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.88	0.56
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.88	0.55
2:D:207:GLU:OE1	2:D:390:ARG:NH1	2.39	0.55
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.89	0.55
1:C:181:VAL:O	1:C:182:VAL:HG22	2.06	0.55
2:D:194:LEU:O	2:D:198:THR:OG1	2.24	0.54
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.89	0.54
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.90	0.54
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.90	0.54
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.88	0.54
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.72	0.53
1:C:180:ALA:O	1:C:183:GLU:HG2	2.09	0.53
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.91	0.52
1:A:381:THR:HG22	1:A:383:ALA:H	1.73	0.52
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.89	0.52
2:D:46:LEU:HA	2:D:49:ILE:HB	1.91	0.52
4:F:101:TYR:HD2	4:F:126:ASP:HB3	1.73	0.52
1:C:98:ASP:OD2	2:D:2:ARG:NH2	2.43	0.52
2:B:2:ARG:NH2	2:B:131:CYS:SG	2.78	0.51
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.91	0.51
2:D:397:ALA:O	2:D:401:ARG:NH1	2.43	0.51
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.93	0.51
2:D:286:LEU:HD21	2:D:291:LEU:HD13	1.94	0.50
1:A:141:PHE:HB2	1:A:173:PRO:HD3	1.94	0.50
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.76	0.50
2:D:238:VAL:HG23	2:D:239:THR:HG23	1.93	0.49
2:B:69:ASP:HA	2:B:145:THR:HG21	1.95	0.49
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.95	0.49
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.94	0.49
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.95	0.49
1:C:1:MET:HG3	1:C:2:ARG:HG2	1.94	0.49
2:B:314:THR:HB	9:B:503:4EE:H8	1.96	0.48
2:B:401:ARG:NH2	1:C:434:GLU:O	2.46	0.48
1:C:79:ARG:HH12	1:C:94:THR:HG21	1.77	0.48
4:F:338:CYS:SG	4:F:339:ALA:N	2.86	0.48
2:D:145:THR:N	8:D:501:GDP:O2B	2.46	0.48
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:502:GTP:O1G	12:C:602:HOH:O	2.20	0.48
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.96	0.47
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.95	0.47
1:C:245:ASP:OD1	1:C:246:GLY:N	2.46	0.47
2:B:46:LEU:HA	2:B:49:ILE:HB	1.97	0.47
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.97	0.46
1:C:7:ILE:N	1:C:136:LEU:O	2.42	0.46
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.97	0.46
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.97	0.46
2:D:270:PRO:HB2	2:D:302:MET:HB2	1.96	0.46
1:C:180:ALA:HB1	2:D:258:ASN:OD1	2.15	0.46
2:D:271:GLY:O	2:D:377:PHE:N	2.41	0.46
4:F:202:ARG:NE	4:F:318:ASP:OD1	2.38	0.46
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.98	0.46
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.96	0.46
1:C:147:SER:HB2	1:C:190:THR:HB	1.98	0.46
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.97	0.45
1:C:159:VAL:HA	3:E:94:ILE:HG23	1.99	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.45
2:B:297:ASP:OD1	2:B:298:SER:N	2.49	0.45
1:C:79:ARG:HH22	1:C:94:THR:HG23	1.82	0.45
1:A:147:SER:HB2	1:A:190:THR:HB	1.98	0.45
1:A:143:GLY:N	6:A:502:GTP:H5'	2.32	0.45
2:B:241:CYS:SG	9:B:503:4EE:H7	2.57	0.45
2:B:238:VAL:HG22	2:B:378:ILE:HD11	1.98	0.44
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.99	0.44
2:B:274:PRO:HD2	2:B:371:LEU:HD13	1.99	0.44
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.49	0.44
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.99	0.44
4:F:166:ALA:O	4:F:170:LEU:HG	2.18	0.44
2:B:109:THR:OG1	2:B:110:GLU:N	2.49	0.44
2:D:172:MET:HB2	2:D:205:ASP:HA	1.99	0.44
2:B:11:GLN:NE2	12:B:601:HOH:O	2.50	0.44
2:D:163:ASP:O	2:D:253:ARG:NH2	2.34	0.44
2:B:194:LEU:O	2:B:198:THR:OG1	2.24	0.43
2:B:11:GLN:HA	2:B:74:THR:HG21	2.00	0.43
2:B:206:ASN:ND2	8:B:501:GDP:O2'	2.51	0.43
2:D:75:MET:SD	2:D:94:PHE:HB3	2.58	0.43
1:A:402:ARG:NE	1:A:415:GLU:OE1	2.49	0.43
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.54	0.43
2:D:141:LEU:HD22	2:D:190:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.89	0.43
1:C:183:GLU:HB2	1:C:184:PRO:HD3	2.00	0.43
4:F:81:ILE:HG23	4:F:87:LEU:HB3	2.00	0.43
2:B:378:ILE:HD12	9:B:503:4EE:H3	2.01	0.42
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.01	0.42
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.92	0.42
1:A:33:ASP:HA	1:A:85:GLN:HB2	2.02	0.42
1:C:174:ALA:HA	1:C:175:PRO:HD3	1.91	0.42
1:C:183:GLU:OE1	6:C:502:GTP:O3'	2.36	0.42
1:C:154:MET:HG3	1:C:194:THR:HG23	2.01	0.42
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.84	0.42
1:C:191:THR:O	1:C:195:LEU:HB2	2.20	0.42
2:D:62:VAL:HA	2:D:63:PRO:HD3	1.93	0.42
3:E:8:VAL:HG13	3:E:20:TRP:CD1	2.54	0.42
2:D:433:GLN:NE2	2:D:437:ASP:OD2	2.52	0.42
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.55	0.41
2:B:137:LEU:HB3	2:B:168:THR:HG22	2.02	0.41
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.02	0.41
2:D:105:LYS:O	2:D:110:GLU:N	2.53	0.41
2:B:132:LEU:O	2:B:164:ARG:NH1	2.46	0.41
1:A:349:THR:HB	3:E:25:LYS:HB3	2.02	0.41
1:C:62:VAL:HA	1:C:63:PRO:HD3	1.93	0.41
2:D:9:ALA:HA	2:D:68:VAL:O	2.21	0.41
1:C:105:ARG:HA	1:C:109:THR:HB	2.02	0.41
2:B:271:GLY:HA3	2:B:377:PHE:HB3	2.03	0.41
2:B:244:PHE:HA	2:B:245:PRO:HD3	1.92	0.41
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.02	0.40
3:E:14:CYS:O	3:E:17:GLY:N	2.53	0.40
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.04	0.40
2:B:88:ARG:HA	2:B:89:PRO:HD3	1.88	0.40
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.36	0.40
2:B:147:SER:OG	2:B:190:SER:OG	2.26	0.40
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.55	0.40
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.24	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	438/451 (97%)	424 (97%)	14 (3%)	0	100	100
1	C	438/451 (97%)	421 (96%)	16 (4%)	1 (0%)	47	78
2	B	418/445 (94%)	400 (96%)	18 (4%)	0	100	100
2	D	418/445 (94%)	398 (95%)	20 (5%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	268/384 (70%)	254 (95%)	14 (5%)	0	100	100
All	All	2097/2319 (90%)	2014 (96%)	82 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	182	VAL

### 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	371/379 (98%)	370 (100%)	1 (0%)	92	96
1	C	371/379 (98%)	369 (100%)	2 (0%)	88	94
2	B	365/383 (95%)	365 (100%)	0	100	100
2	D	365/383 (95%)	365 (100%)	0	100	100
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	88
4	F	254/342 (74%)	254 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1835/1993 (92%)	1831 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	LYS
1	C	71	GLU
1	C	141	PHE
3	E	14	CYS

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

Mol	Chain	Res	Type
1	A	133	GLN

### 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, 7 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
8	GDP	D	501	5	24,30,30	1.19	2 (8%)	31,47,47	1.98	8 (25%)
8	GDP	B	501	5	24,30,30	1.17	2 (8%)	31,47,47	1.96	8 (25%)
9	4EE	D	503	-	26,29,29	2.86	8 (30%)	28,40,40	3.32	11 (39%)
6	GTP	A	502	5	26,34,34	0.98	1 (3%)	33,54,54	1.81	7 (21%)
10	MES	B	505	-	12,12,12	2.25	1 (8%)	14,16,16	1.97	6 (42%)
6	GTP	C	502	5	26,34,34	0.96	1 (3%)	33,54,54	1.77	7 (21%)
11	IMD	C	504	-	3,5,5	0.40	0	4,5,5	0.64	0
9	4EE	B	503	-	26,29,29	2.87	8 (30%)	28,40,40	3.33	13 (46%)

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	GDP	D	501	5	-	2/12/32/32	0/3/3/3
8	GDP	B	501	5	-	4/12/32/32	0/3/3/3
9	4EE	D	503	-	-	7/13/22/22	0/3/4/4
6	GTP	A	502	5	-	5/18/38/38	0/3/3/3
10	MES	B	505	-	-	1/6/14/14	0/1/1/1
6	GTP	C	502	5	-	8/18/38/38	0/3/3/3
11	IMD	C	504	-	-	-	0/1/1/1
9	4EE	B	503	-	-	9/13/22/22	0/3/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	4EE	C13-N12	9.82	1.50	1.36
9	D	503	4EE	C13-N12	9.75	1.50	1.36
10	B	505	MES	C8-S	-7.50	1.66	1.77
9	B	503	4EE	C07-C10	6.54	1.60	1.47
9	D	503	4EE	C07-C10	6.53	1.60	1.47
8	D	501	GDP	C6-C5	4.18	1.48	1.41
9	B	503	4EE	C10-N11	4.14	1.36	1.29
8	B	501	GDP	C6-C5	4.09	1.48	1.41
9	D	503	4EE	C10-N11	4.07	1.36	1.29
9	B	503	4EE	C19-C24	3.37	1.47	1.40
9	D	503	4EE	C19-C24	3.35	1.47	1.40
9	D	503	4EE	C08-C07	3.09	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	4EE	C16-N12	3.08	1.42	1.37
6	A	502	GTP	C6-N1	3.06	1.38	1.33
9	B	503	4EE	C08-C07	3.01	1.44	1.39
6	C	502	GTP	C6-N1	3.00	1.38	1.33
9	D	503	4EE	C16-N12	2.98	1.42	1.37
9	D	503	4EE	C18-S17	2.65	1.87	1.80
9	B	503	4EE	C18-S17	2.62	1.87	1.80
8	D	501	GDP	C5-C4	2.47	1.47	1.40
8	B	501	GDP	C5-C4	2.45	1.47	1.40
9	B	503	4EE	C05-C04	2.31	1.43	1.38
9	D	503	4EE	C05-C04	2.31	1.43	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	4EE	C06-C07-C10	7.79	130.31	120.84
9	B	503	4EE	C06-C07-C10	7.52	129.98	120.84
9	D	503	4EE	C08-C07-C06	-7.14	108.42	118.59
9	B	503	4EE	C08-C07-C06	-7.13	108.43	118.59
9	B	503	4EE	C05-C06-C07	6.97	128.88	120.78
9	D	503	4EE	C05-C06-C07	6.97	128.88	120.78
9	B	503	4EE	C09-C04-C05	-5.29	112.03	120.18
6	C	502	GTP	N3-C2-N1	-5.27	120.19	127.22
6	A	502	GTP	N3-C2-N1	-5.27	120.19	127.22
9	D	503	4EE	C09-C04-C05	-5.22	112.14	120.18
8	D	501	GDP	C2-N3-C4	4.89	120.94	115.36
8	B	501	GDP	C2-N3-C4	4.88	120.92	115.36
9	D	503	4EE	C10-N11-N12	4.84	125.78	116.55
9	B	503	4EE	C10-N11-N12	4.77	125.64	116.55
6	A	502	GTP	C2-N3-C4	4.26	120.22	115.36
6	C	502	GTP	C2-N3-C4	4.25	120.21	115.36
9	B	503	4EE	C21-C20-C19	4.24	127.49	120.33
9	D	503	4EE	C21-C20-C19	4.17	127.37	120.33
10	B	505	MES	C5-N4-C3	4.06	117.96	108.83
8	D	501	GDP	C6-N1-C2	4.04	122.35	115.93
8	B	501	GDP	C6-N1-C2	4.03	122.34	115.93
8	B	501	GDP	C5-C6-N1	-4.00	117.96	123.43
8	D	501	GDP	C5-C6-N1	-3.99	117.98	123.43
9	D	503	4EE	C09-C08-C07	3.70	125.08	120.78
9	B	503	4EE	C20-C19-C24	-3.69	112.08	117.39
8	D	501	GDP	C6-C5-C4	-3.68	117.28	120.80
9	B	503	4EE	C09-C08-C07	3.68	125.06	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C6-C5-C4	-3.66	117.31	120.80
9	D	503	4EE	C20-C19-C24	-3.54	112.30	117.39
6	A	502	GTP	PA-O3A-PB	-3.53	120.73	132.83
9	B	503	4EE	C08-C09-C04	3.40	123.90	119.73
8	D	501	GDP	C3'-C2'-C1'	3.29	105.93	100.98
6	C	502	GTP	PA-O3A-PB	-3.29	121.55	132.83
8	D	501	GDP	N3-C2-N1	-3.28	122.84	127.22
8	B	501	GDP	N3-C2-N1	-3.27	122.86	127.22
9	D	503	4EE	C08-C09-C04	3.26	123.72	119.73
6	A	502	GTP	PB-O3B-PG	-3.22	121.79	132.83
8	D	501	GDP	PA-O3A-PB	-3.18	121.93	132.83
8	B	501	GDP	C3'-C2'-C1'	3.12	105.68	100.98
6	A	502	GTP	C3'-C2'-C1'	2.99	105.48	100.98
6	C	502	GTP	C5-C6-N1	-2.88	119.49	123.43
6	C	502	GTP	C3'-C2'-C1'	2.88	105.31	100.98
8	B	501	GDP	PA-O3A-PB	-2.87	122.97	132.83
6	A	502	GTP	C5-C6-N1	-2.82	119.58	123.43
10	B	505	MES	C6-C5-N4	-2.79	105.88	110.10
9	B	503	4EE	C22-C23-C24	2.74	124.74	119.71
9	D	503	4EE	C22-C23-C24	2.70	124.68	119.71
8	D	501	GDP	C4-C5-N7	-2.61	106.68	109.40
9	B	503	4EE	C18-C10-C07	-2.58	117.11	120.18
6	C	502	GTP	PB-O3B-PG	-2.57	124.02	132.83
8	B	501	GDP	C4-C5-N7	-2.54	106.75	109.40
6	C	502	GTP	C6-N1-C2	2.52	119.92	115.93
6	A	502	GTP	C6-N1-C2	2.48	119.87	115.93
10	B	505	MES	O3S-S-C8	2.47	109.77	105.77
9	B	503	4EE	O03-C02-C01	2.36	116.29	108.21
9	D	503	4EE	O03-C02-C01	2.34	116.22	108.21
10	B	505	MES	O1S-S-C8	2.23	109.60	106.92
10	B	505	MES	C7-N4-C5	2.14	116.70	111.23
10	B	505	MES	C7-N4-C3	2.12	116.67	111.23
9	B	503	4EE	C10-C18-S17	2.08	114.84	111.71

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	PA-O3A-PB-O3B
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	C	502	GTP	PB-O3A-PA-O5'
6	C	502	GTP	C5'-O5'-PA-O1A
6	C	502	GTP	C5'-O5'-PA-O2A
9	B	503	4EE	C06-C07-C10-C18
9	B	503	4EE	C08-C07-C10-C18
9	B	503	4EE	C23-C24-O25-C26
9	D	503	4EE	C23-C24-O25-C26
9	B	503	4EE	C19-C24-O25-C26
9	D	503	4EE	C19-C24-O25-C26
9	D	503	4EE	C05-C04-O03-C02
9	D	503	4EE	C09-C04-O03-C02
6	C	502	GTP	C3'-C4'-C5'-O5'
6	A	502	GTP	PB-O3B-PG-O1G
6	C	502	GTP	PA-O3A-PB-O1B
9	B	503	4EE	C01-C02-O03-C04
6	A	502	GTP	O4'-C4'-C5'-O5'
9	D	503	4EE	C01-C02-O03-C04
6	C	502	GTP	C5'-O5'-PA-O3A
6	C	502	GTP	O4'-C4'-C5'-O5'
9	D	503	4EE	C06-C07-C10-C18
8	D	501	GDP	C5'-O5'-PA-O2A
6	C	502	GTP	C4'-C5'-O5'-PA
6	A	502	GTP	C4'-C5'-O5'-PA
9	B	503	4EE	C06-C07-C10-N11
10	B	505	MES	C8-C7-N4-C3
9	D	503	4EE	C08-C07-C10-C18
9	B	503	4EE	C08-C07-C10-N11
6	A	502	GTP	C3'-C4'-C5'-O5'
8	B	501	GDP	PA-O3A-PB-O1B
9	B	503	4EE	C05-C04-O03-C02
6	A	502	GTP	C5'-O5'-PA-O1A
9	B	503	4EE	C09-C04-O03-C02

There are no ring outliers.

6 monomers are involved in 12 short contacts:

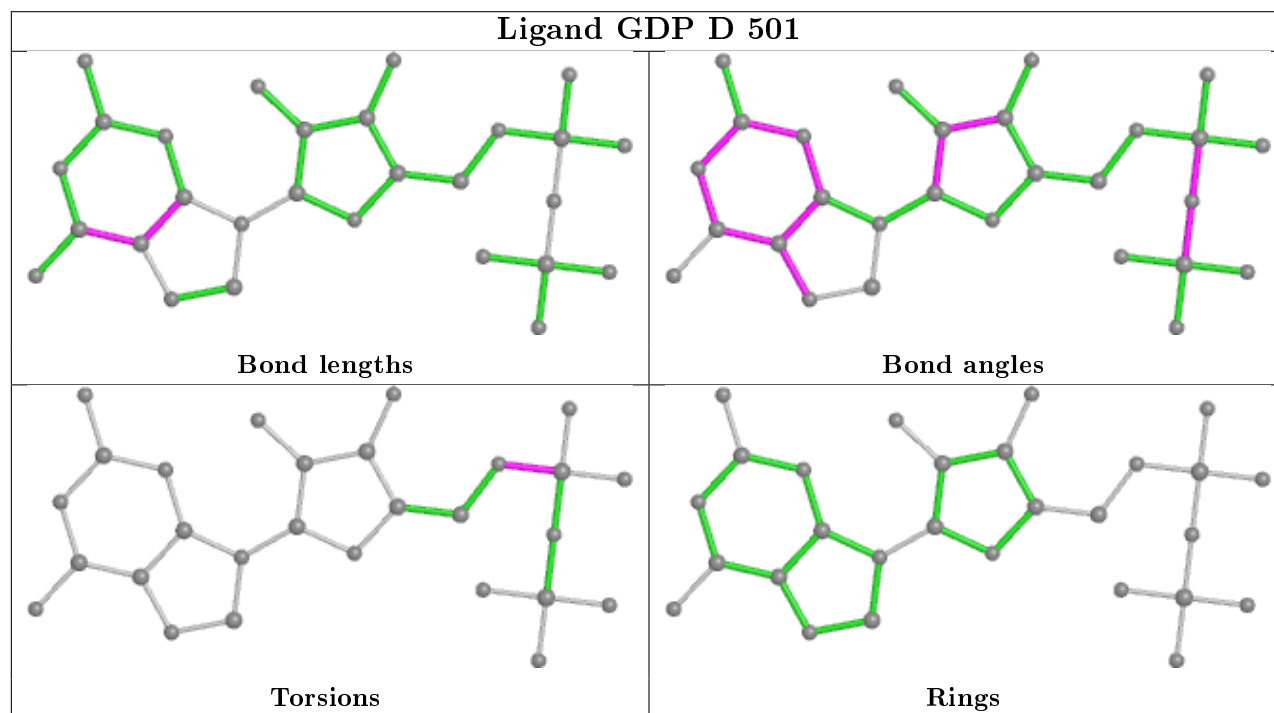
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
8	B	501	GDP	2	0
9	D	503	4EE	2	0
6	A	502	GTP	2	0
6	C	502	GTP	2	0

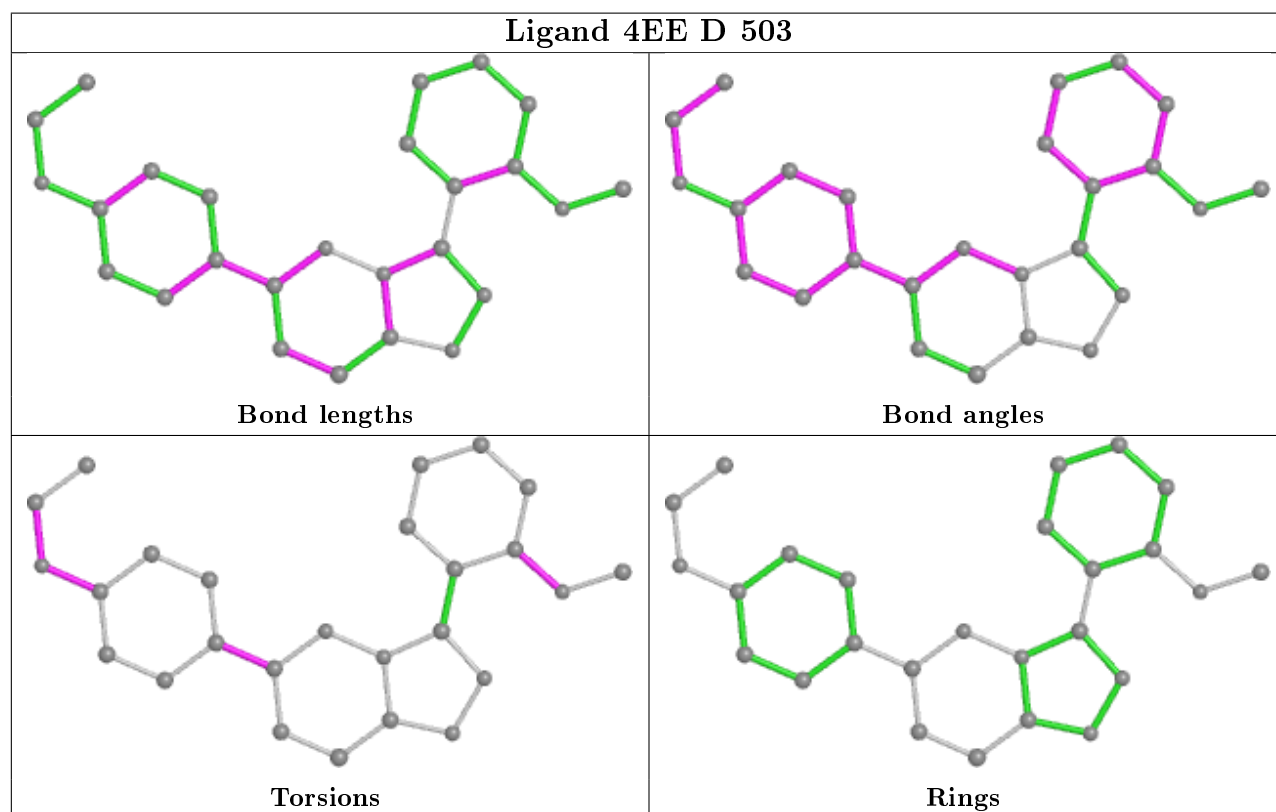
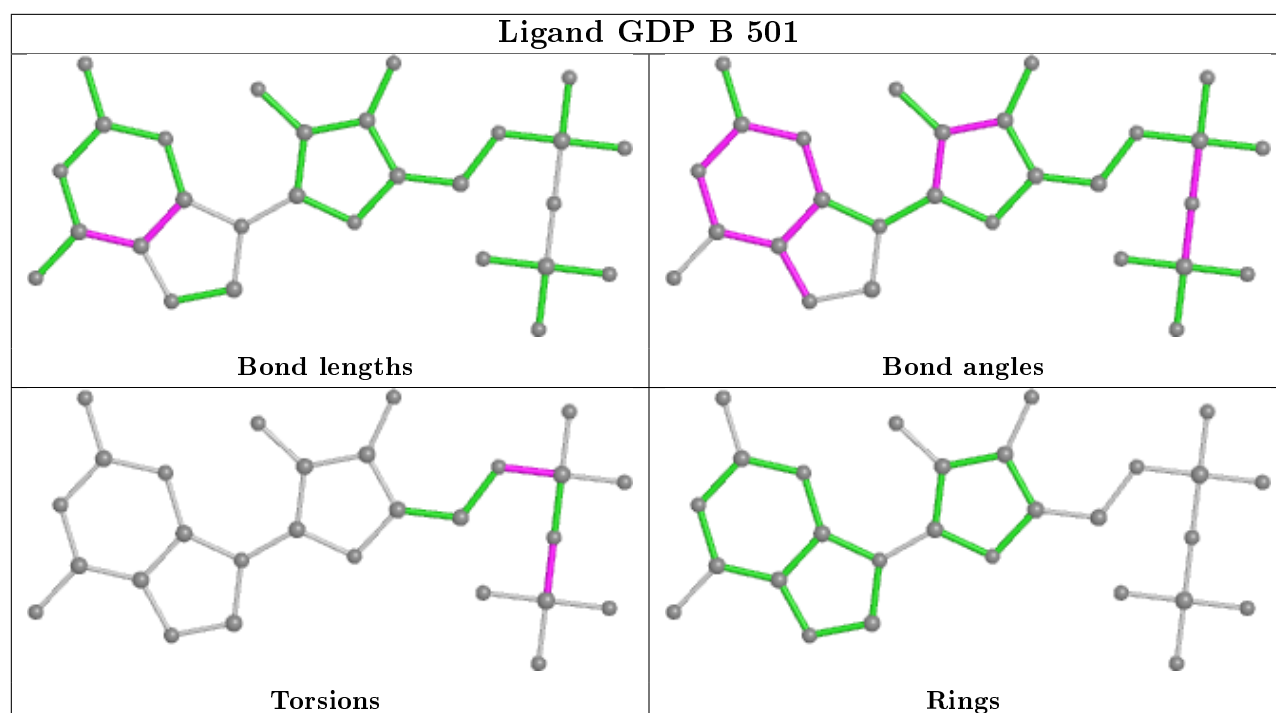
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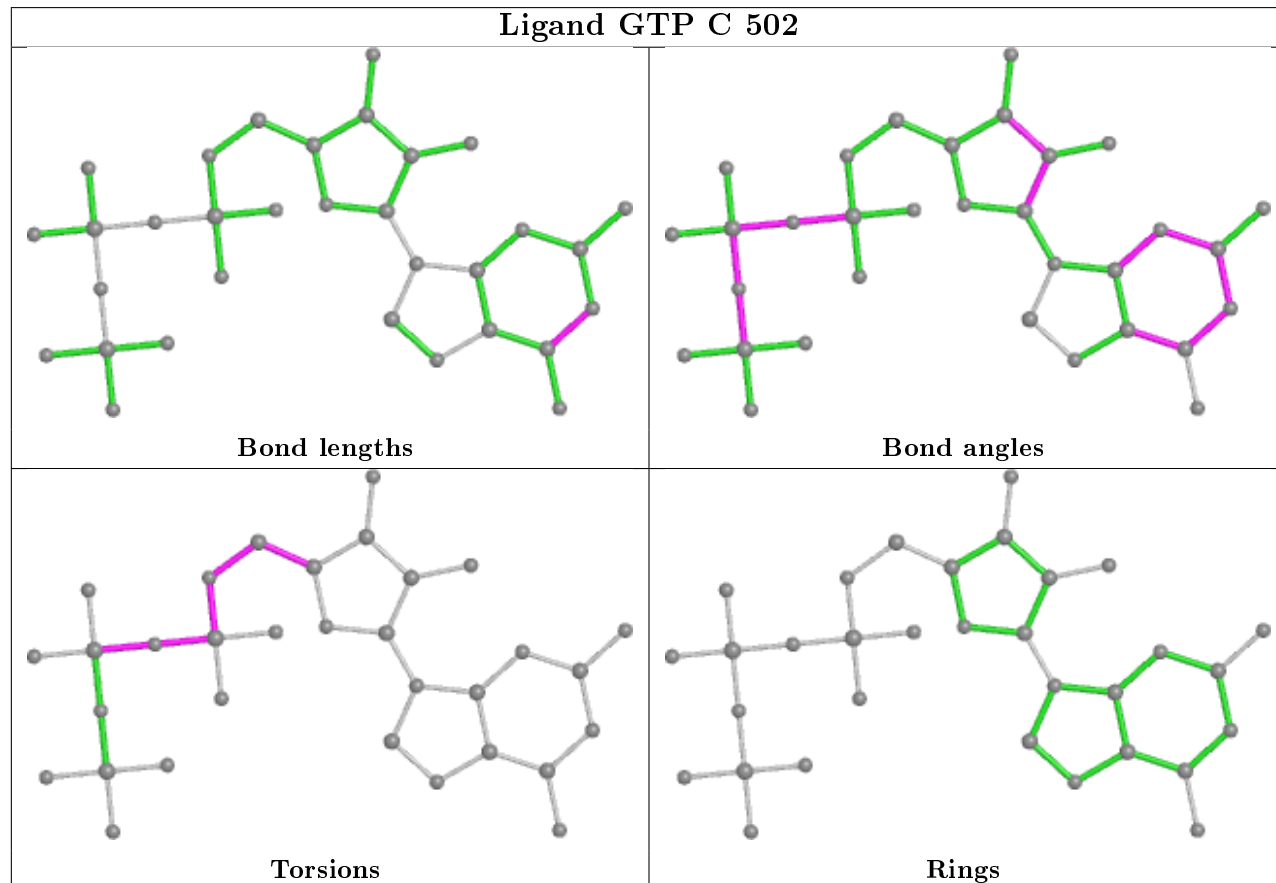
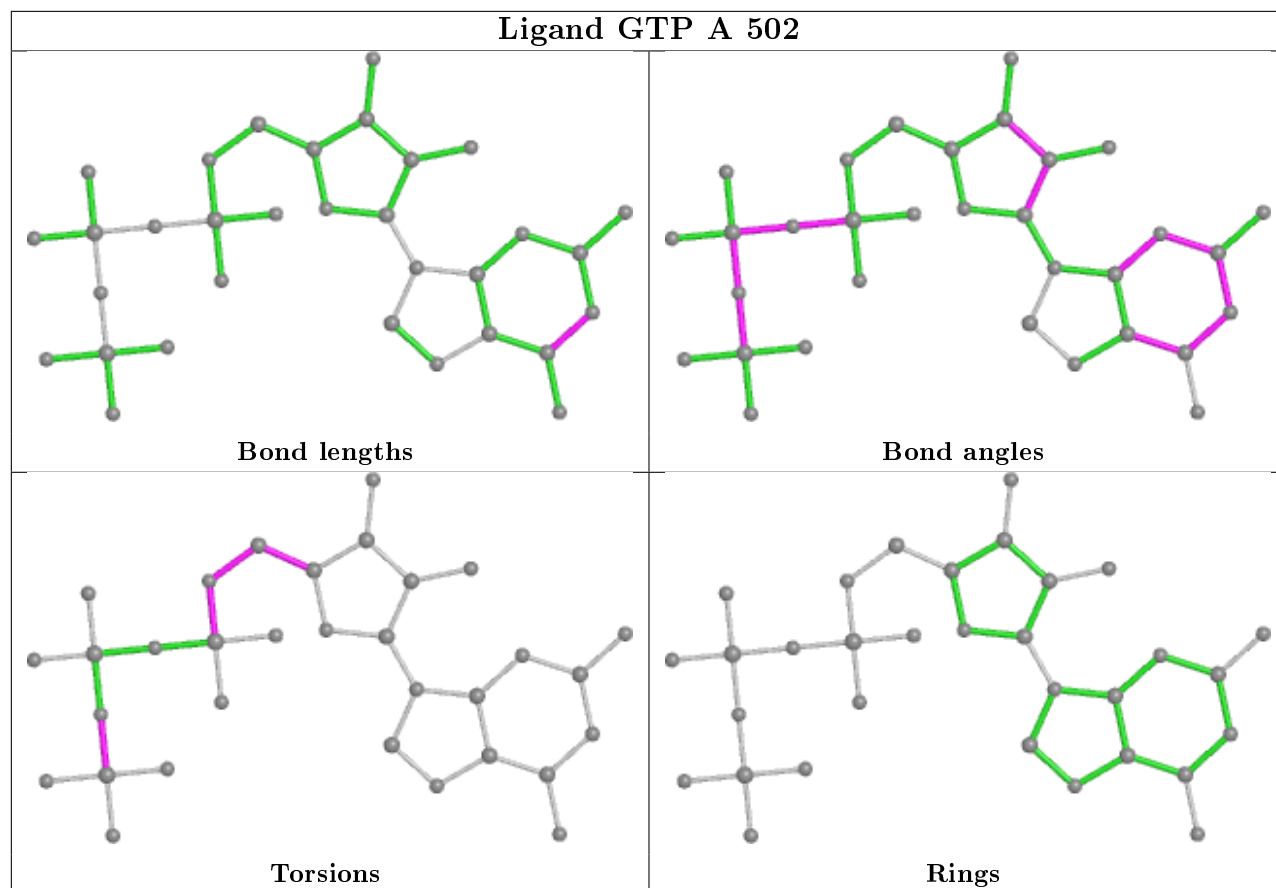
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	4EE	3	0

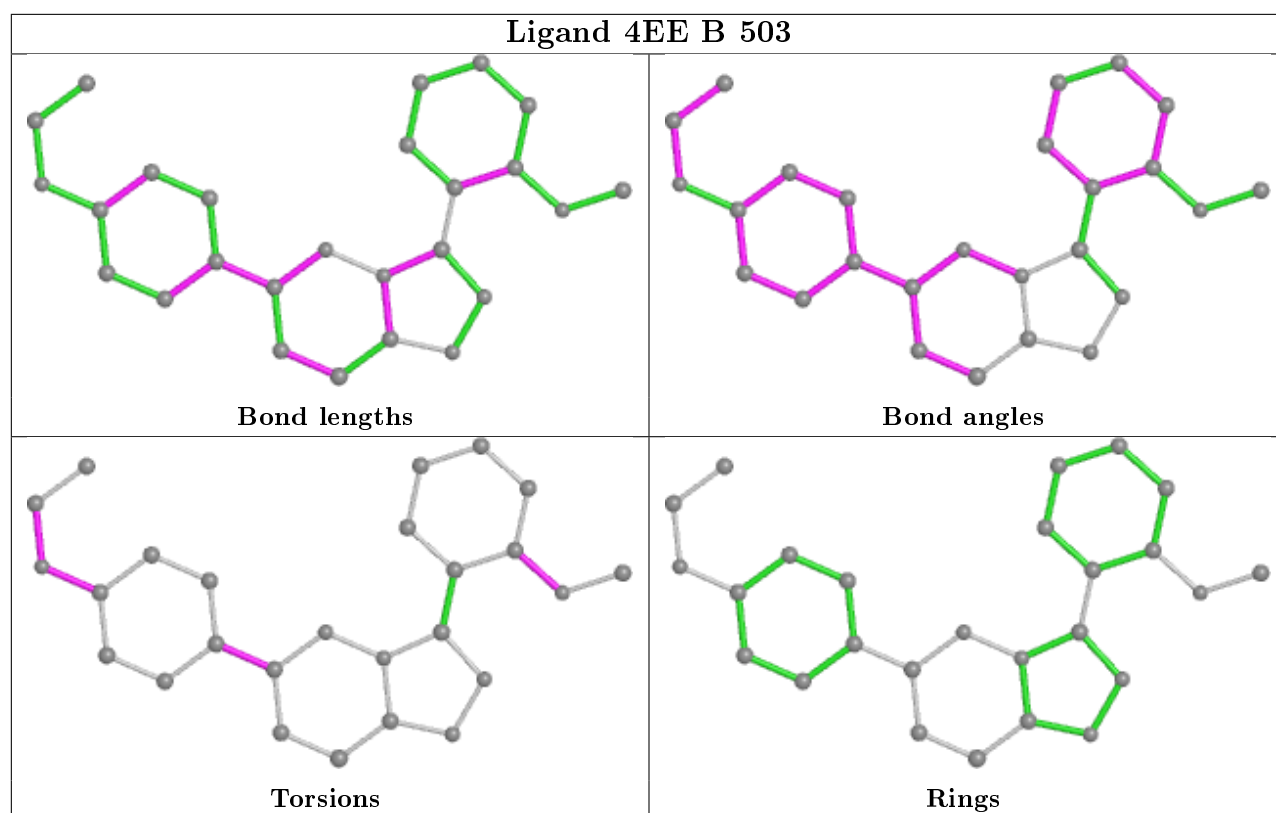
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	438/451 (97%)	0.20	3 (0%) 87 86	77, 101, 132, 156	0
1	C	440/451 (97%)	-0.11	0 100 100	51, 75, 96, 107	0
2	B	422/445 (94%)	-0.10	0 100 100	57, 83, 111, 133	0
2	D	421/445 (94%)	0.18	1 (0%) 95 95	78, 110, 132, 171	0
3	E	121/143 (84%)	0.02	0 100 100	81, 113, 144, 150	0
4	F	282/384 (73%)	0.85	25 (8%) 9 8	87, 125, 176, 193	0
All	All	2124/2319 (91%)	0.15	29 (1%) 75 71	51, 97, 141, 193	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	3.8
4	F	319	PHE	3.2
4	F	183	GLN	3.2
4	F	162	ILE	2.9
1	A	349	THR	2.9
4	F	132	LEU	2.7
4	F	169	LEU	2.7
4	F	173	ILE	2.6
4	F	165	GLU	2.6
4	F	320	MET	2.4
4	F	329	LEU	2.4
4	F	206	LEU	2.4
4	F	375	PHE	2.4
4	F	353	VAL	2.4
1	A	46	ASP	2.3
4	F	147	TRP	2.3
4	F	127	GLU	2.3
4	F	150	LYS	2.3
4	F	184	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	196	HIS	2.2
4	F	148	ILE	2.2
4	F	26	GLN	2.2
4	F	198	LYS	2.1
4	F	328	TRP	2.1
1	A	313	MET	2.1
4	F	315	PHE	2.1
2	D	314	THR	2.0
4	F	291	ILE	2.0
4	F	212	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, 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
11	IMD	C	504	5/5	0.80	0.37	72,72,72,72	0
7	CA	A	503	1/1	0.81	0.10	122,122,122,122	0
7	CA	B	504	1/1	0.82	0.31	71,71,71,71	0
5	MG	A	501	1/1	0.89	0.13	133,133,133,133	0
9	4EE	D	503	26/26	0.89	0.59	85,85,85,85	0
8	GDP	D	501	28/28	0.90	0.20	114,114,114,114	0
9	4EE	B	503	26/26	0.91	0.36	76,76,76,76	0
7	CA	C	503	1/1	0.91	0.09	109,109,109,109	0
10	MES	B	505	12/12	0.91	0.18	96,96,96,96	0
6	GTP	A	502	32/32	0.93	0.21	83,83,83,83	0
5	MG	D	502	1/1	0.95	0.08	114,114,114,114	0
5	MG	B	502	1/1	0.95	0.14	65,65,65,65	0
8	GDP	B	501	28/28	0.95	0.23	67,67,67,67	0

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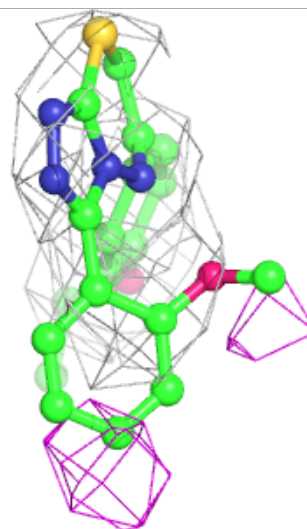
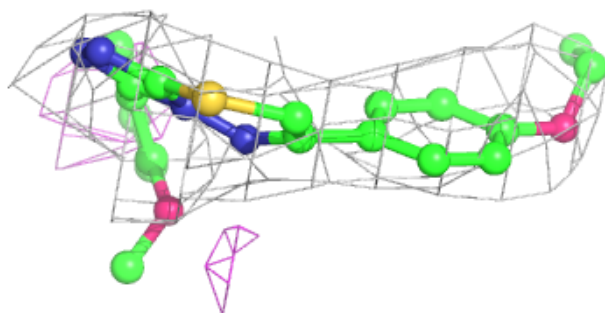
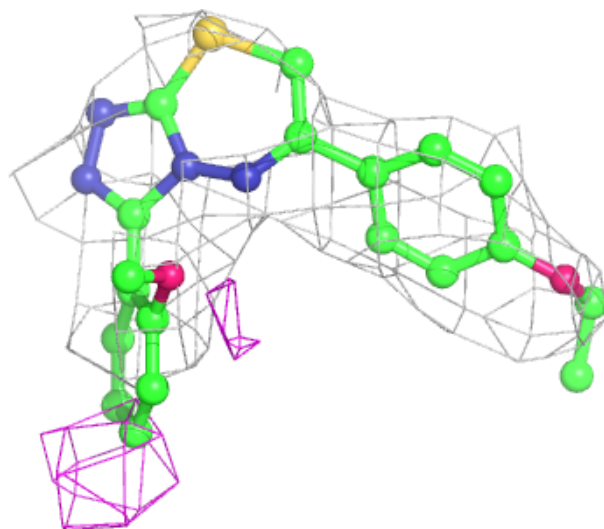
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GTP	C	502	32/32	0.96	0.21	70,70,70,70	0
5	MG	C	501	1/1	0.97	0.14	66,66,66,66	0

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.

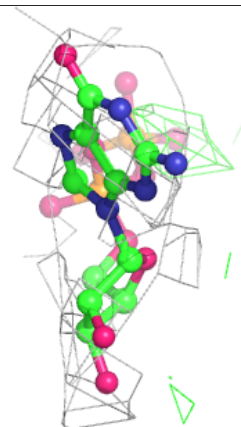
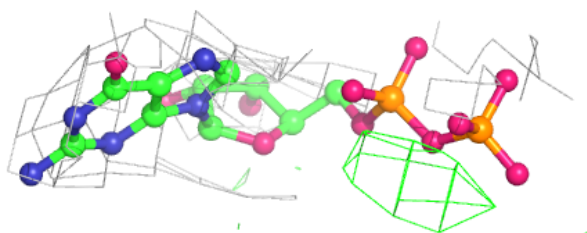
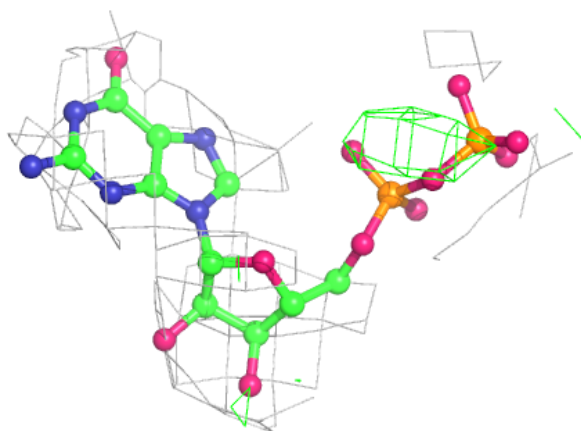
**Electron density around 4EE D 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



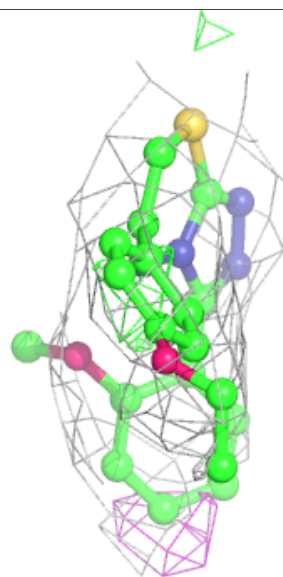
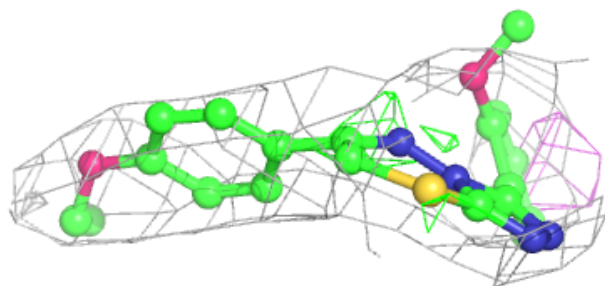
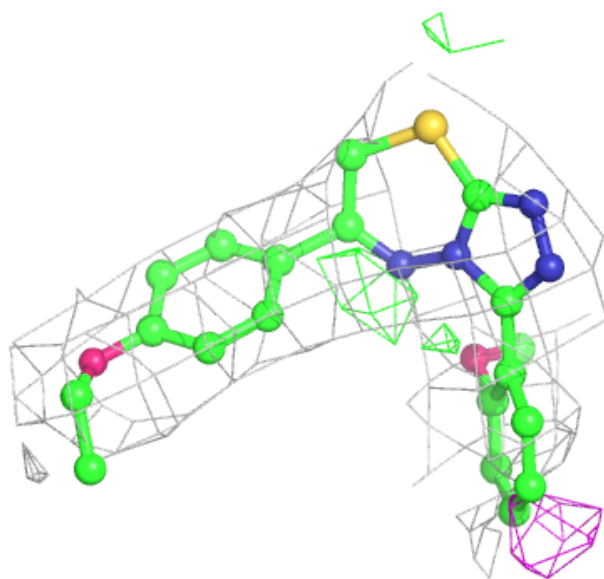
**Electron density around GDP D 501:**

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



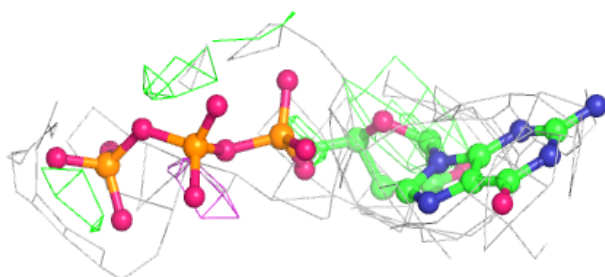
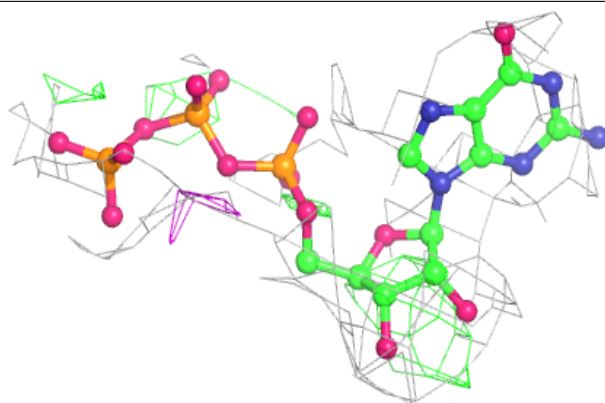
**Electron density around 4EE B 503:**

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

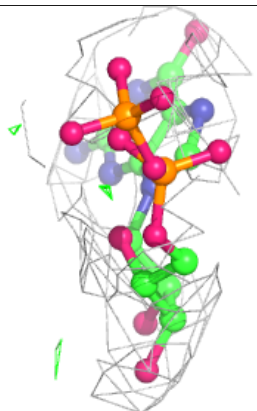
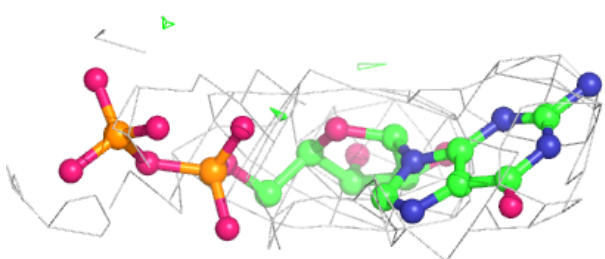
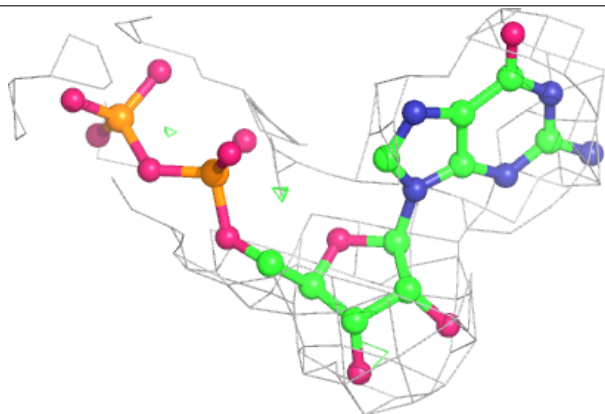


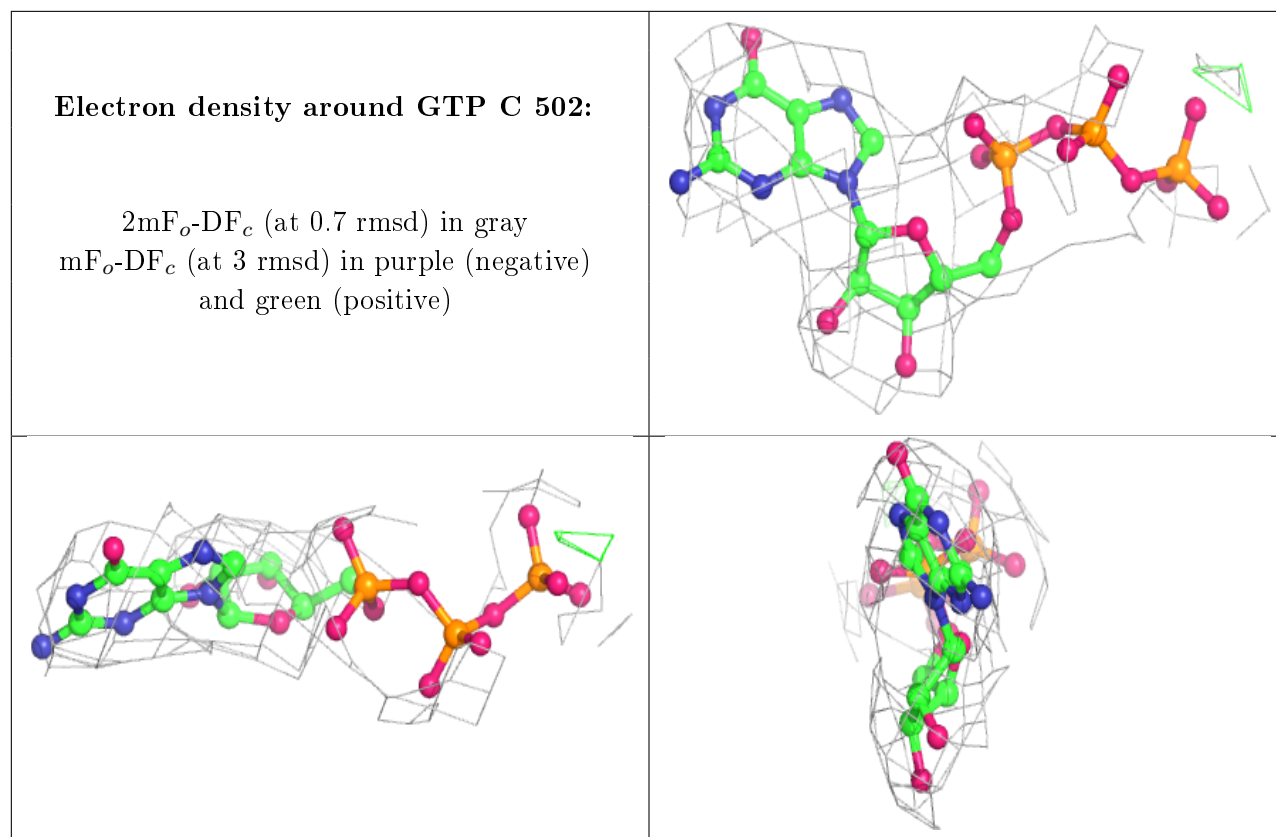
**Electron density around GTP A 502:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.