



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:06 am BST

PDB ID : 4TV8  
Title : Tubulin-Maytansine complex  
Authors : Prota, A.E.; Bargsten, K.; Diaz, J.F.; Marsh, M.; Cuevas, C.; Liniger, M.; Neuhaus, C.; Andreu, J.M.; Altmann, K.H.; Steinmetz, M.O.  
Deposited on : 2014-06-26  
Resolution : 2.10 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

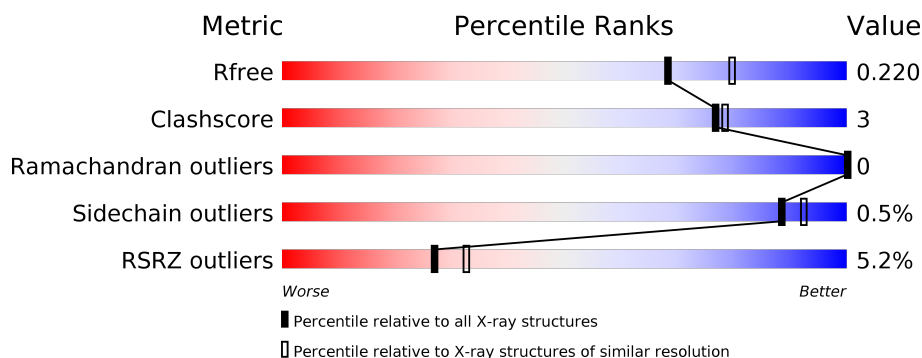
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>88%</span> <span>8%</span> </div> </div>
1	C	451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>88%</span> <span>9%</span> </div> </div>
2	B	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>89%</span> <span>7%</span> </div> </div>
2	D	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 94%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>87%</span> <span>8%</span> <span>5%</span> </div> </div>
3	E	143	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>77%</span> <span>8%</span> <span>15%</span> </div> </div>
4	F	384	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 21%, orange 1%, yellow 1%, green 77%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>80%</span> <span>7%</span> <span>13%</span> </div> </div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18278 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	436	Total	C	N	O	S	0	7	0
			3433	2175	580	654	24			
1	C	440	Total	C	N	O	S	0	11	0
			3483	2208	585	665	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	4	0
			3365	2116	572	650	27			
2	D	422	Total	C	N	O	S	0	3	0
			3326	2091	563	644	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			1006	621	182	198	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	335	Total	C	N	O	S	0	2	0
			2763	1776	473	500	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		

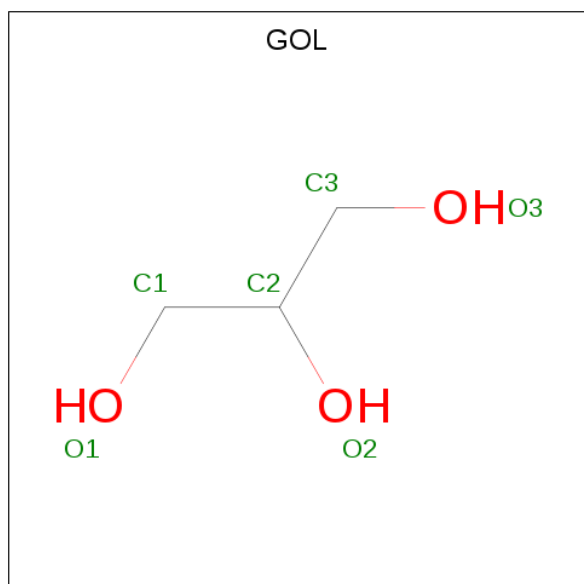
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

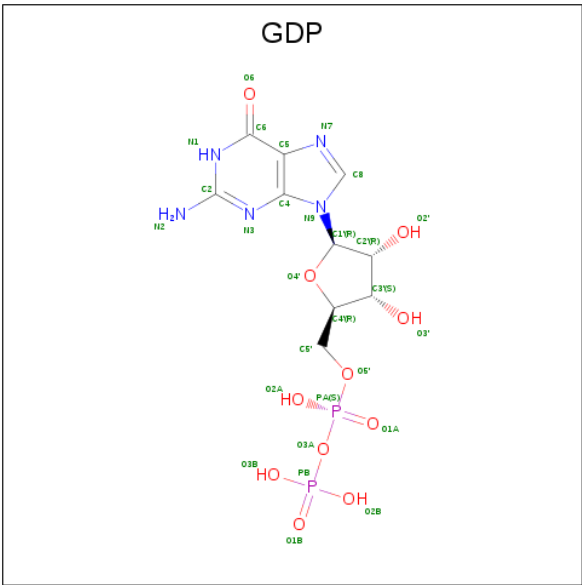
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



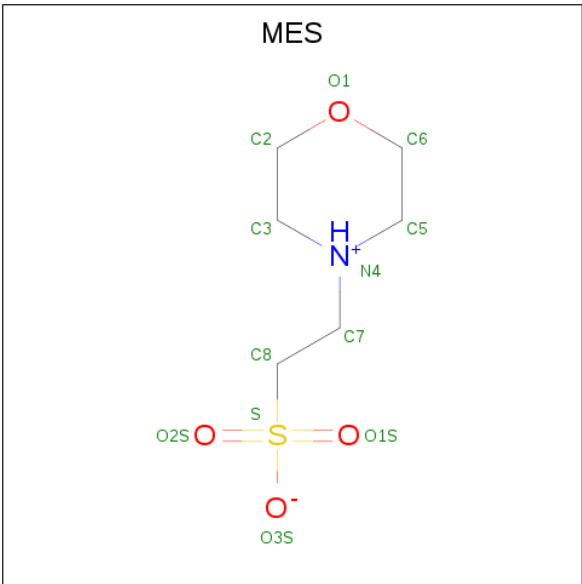
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 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>).



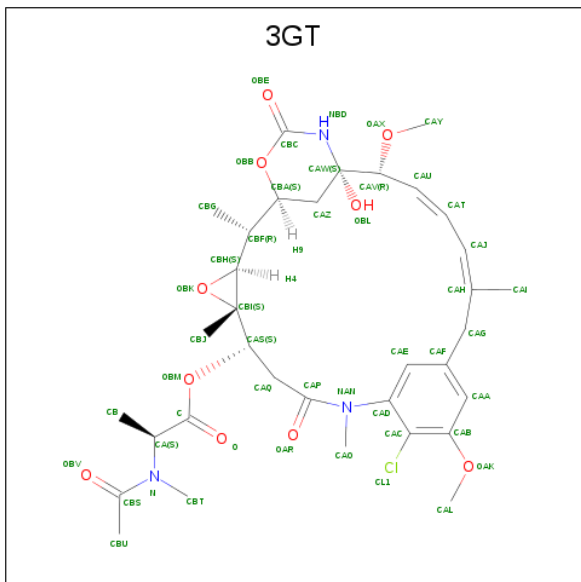
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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).



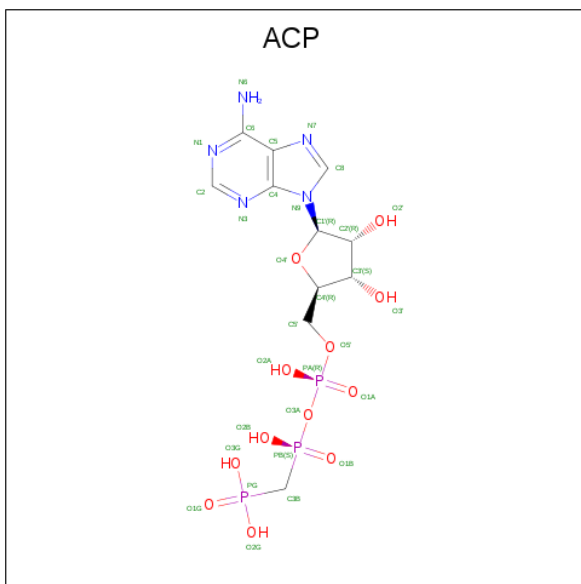
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3beta,4beta,5beta,10beta,11E,13E)-maytansine (three-letter code: 3GT) (formula: C<sub>34</sub>H<sub>46</sub>ClN<sub>3</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	Cl	N	O	0	0
			48	34	1	3	10		

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



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

- Molecule 13 is water.

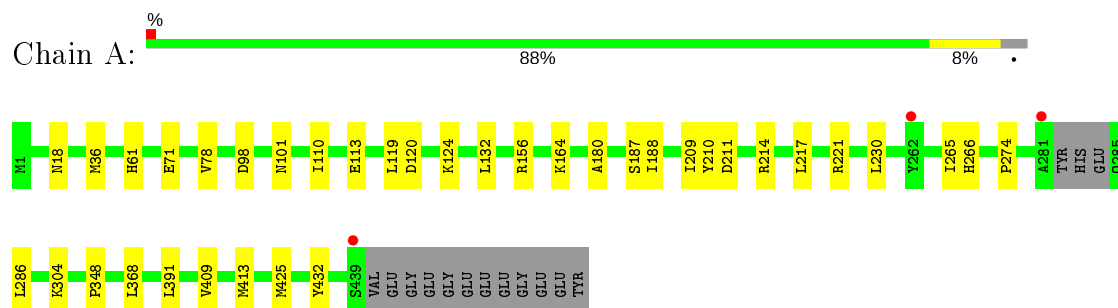
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	134	Total 134	O 134	0	0
13	B	113	Total 113	O 113	0	0
13	C	252	Total 252	O 252	0	0
13	D	97	Total 97	O 97	0	0
13	E	30	Total 30	O 30	0	0
13	F	45	Total 45	O 45	0	0



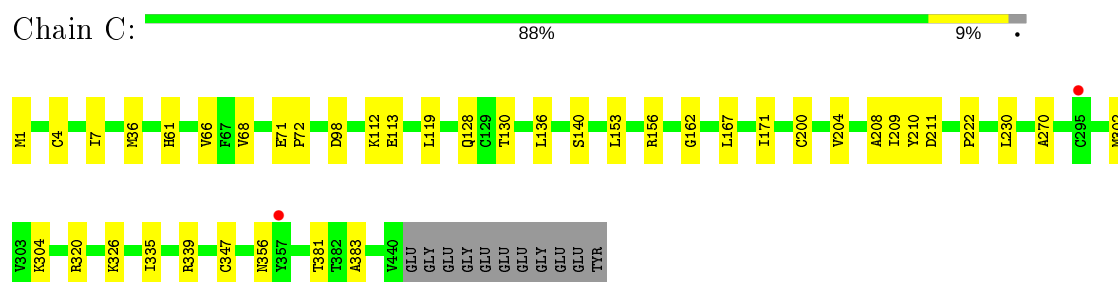
### 3 Residue-property plots [i](#)

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.

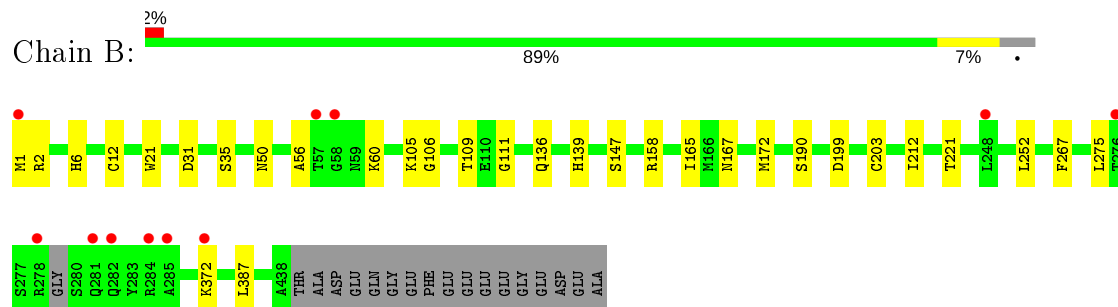
- Molecule 1: Tubulin alpha-1B chain



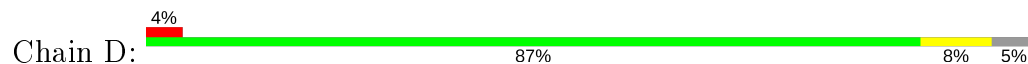
- Molecule 1: Tubulin alpha-1B chain

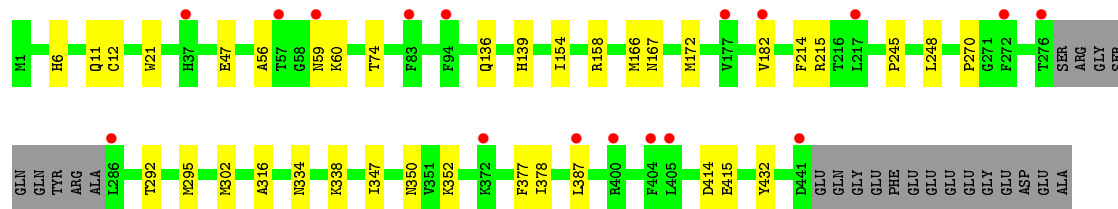


- Molecule 2: Tubulin beta-2B chain

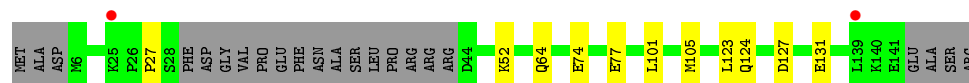
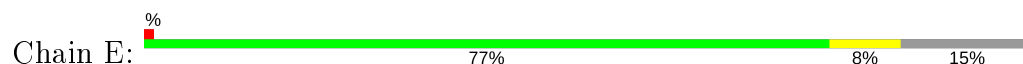


- Molecule 2: Tubulin beta-2B chain

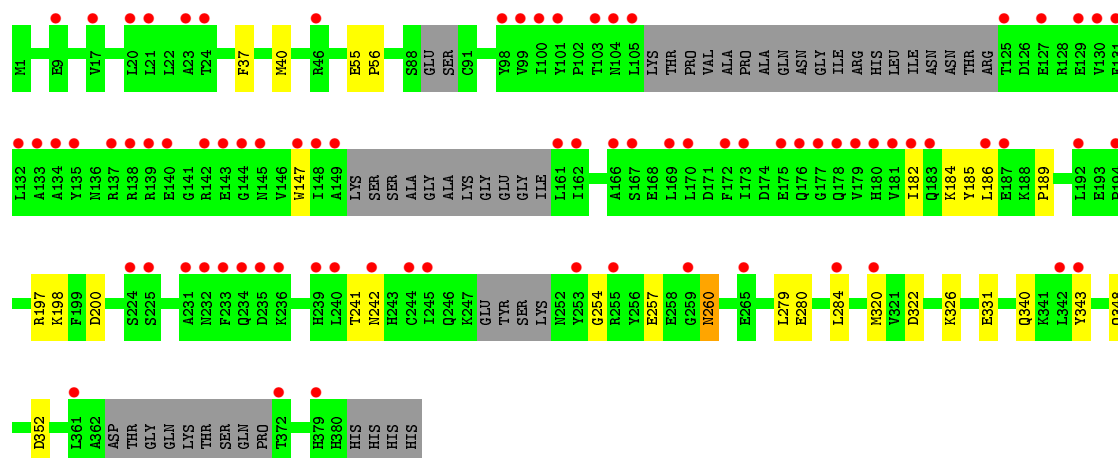
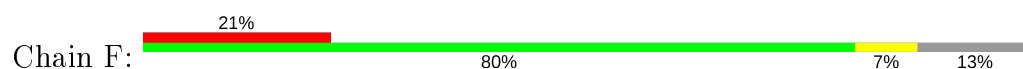




● Molecule 3: Stathmin-4



● 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, $\alpha$ , $\beta$ , $\gamma$	103.86Å 155.57Å 180.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.42 – 2.10 78.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.42-2.10) 99.8 (78.10-2.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.189 , 0.218 0.193 , 0.220	Depositor DCC
$R_{free}$ test set	8416 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, GOL, MG, CA, 3GT, GTP, ACP, 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	0.22	0/3527	0.39	0/4786
1	C	0.23	0/3594	0.40	0/4882
2	B	0.22	0/3451	0.38	0/4674
2	D	0.22	0/3408	0.38	0/4617
3	E	0.21	0/1017	0.32	0/1349
4	F	0.21	0/2830	0.37	0/3823
All	All	0.22	0/17827	0.38	0/24131

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	3433	0	3364	20	0
1	C	3483	0	3415	24	0
2	B	3365	0	3243	19	0
2	D	3326	0	3213	19	0
3	E	1006	0	1026	7	0
4	F	2763	0	2740	16	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	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	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
8	C	6	0	8	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	12	0	13	3	0
11	D	48	0	46	2	0
12	F	31	0	14	3	0
13	A	134	0	0	1	0
13	B	113	0	0	2	0
13	C	252	0	0	2	0
13	D	97	0	0	1	0
13	E	30	0	0	1	0
13	F	45	0	0	0	0
All	All	18278	0	17138	105	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 3.

All (105) 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:B:147[A]:SER:HG	2:B:190:SER:HG	1.32	0.77
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.67	0.76
1:C:381:THR:HG22	1:C:383:ALA:H	1.53	0.74
1:A:18:ASN:HD21	1:A:78:VAL:HG13	1.60	0.66
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.76	0.65
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.80	0.62
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.83	0.61
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.83	0.60
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.82	0.60
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.34	0.59
2:B:221:THR:HG21	1:C:326:LYS:HA	1.84	0.59
3:E:64:GLN:NE2	13:E:222:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:NH1	13:B:658:HOH:O	2.38	0.57
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.37	0.57
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.30	0.56
2:B:158:ARG:CZ	10:B:505:MES:H21	2.35	0.56
2:D:432:TYR:OH	13:D:686:HOH:O	2.16	0.56
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.56
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.55
1:A:71:GLU:O	13:A:609:HOH:O	2.18	0.54
4:F:348:GLN:NE2	4:F:352:ASP:OD2	2.41	0.53
1:C:128:GLN:NE2	13:C:602:HOH:O	2.40	0.53
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.89	0.53
1:C:162:GLY:N	13:C:601:HOH:O	2.42	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.53
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.43	0.53
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.28	0.52
2:B:31:ASP:OD1	2:B:35:SER:N	2.40	0.52
2:B:372:LYS:NZ	13:B:601:HOH:O	2.41	0.52
2:B:1:MET:SD	2:B:50:ASN:ND2	2.83	0.52
1:C:320:ARG:HA	1:C:356:ASN:O	2.10	0.52
12:F:401:ACP:O2G	12:F:401:ACP:O1B	2.29	0.51
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.92	0.51
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.92	0.51
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.93	0.50
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.93	0.50
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.50
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.94	0.50
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.94	0.50
1:C:140:SER:HA	1:C:171:ILE:HB	1.94	0.50
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.44	0.50
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.93	0.49
4:F:241:THR:OG1	12:F:401:ACP:O3'	2.22	0.49
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.47	0.49
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.93	0.49
4:F:184:LYS:NZ	4:F:185:TYR:O	2.45	0.49
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.40	0.48
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.96	0.48
4:F:189:PRO:HA	4:F:322:ASP:HA	1.95	0.48
11:D:502:3GT:H42	11:D:502:3GT:H20	1.96	0.47
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.55	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.79	0.47
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.96	0.47
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.98	0.46
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.46
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.15	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.45
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.98	0.45
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.52	0.45
2:D:214:PHE:HD2	2:D:215:ARG:HG3	1.81	0.45
4:F:331:GLU:OE2	12:F:401:ACP:O2G	2.35	0.44
2:B:199:ASP:OD2	10:B:505:MES:H52	2.17	0.44
1:A:132:LEU:O	1:A:164:LYS:NZ	2.44	0.44
3:E:127:ASP:O	3:E:131:GLU:HG2	2.18	0.44
1:C:1:MET:HB3	1:C:130:THR:OG1	2.17	0.44
1:A:110:ILE:O	1:A:113:GLU:HG2	2.17	0.44
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.43
2:D:414:ASP:OD1	2:D:415:GLU:N	2.51	0.43
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.00	0.43
2:B:199:ASP:OD1	10:B:505:MES:H32	2.18	0.43
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.99	0.43
2:D:292:THR:O	2:D:295:MET:HG2	2.18	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.99	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.43
11:D:502:3GT:H5	11:D:502:3GT:H3	1.56	0.43
3:E:52:LYS:HE3	3:E:52:LYS:HB2	1.84	0.43
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.01	0.43
2:D:136:GLN:HA	2:D:167:ASN:O	2.17	0.43
1:C:204:VAL:HG22	1:C:302:MET:HE3	2.01	0.42
1:C:208:ALA:HB2	1:C:304:LYS:HG2	2.02	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.42
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.01	0.42
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.35	0.41
4:F:254:GLY:H	4:F:260:ASN:ND2	2.19	0.41
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.02	0.41
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
3:E:74:GLU:O	3:E:77:GLU:HG2	2.20	0.41
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.56	0.41
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.21	0.41
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.41
4:F:37:PHE:CE1	4:F:40:MET:HB2	2.55	0.41
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.52	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
3:E:101:LEU:O	3:E:105:MET:HG2	2.21	0.40
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.40
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	2.04	0.40
4:F:55:GLU:HA	4:F:56:PRO:HD2	1.97	0.40
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.20	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	439/451 (97%)	432 (98%)	7 (2%)	0	100	100
1	C	449/451 (100%)	441 (98%)	8 (2%)	0	100	100
2	B	427/445 (96%)	420 (98%)	7 (2%)	0	100	100
2	D	421/445 (95%)	412 (98%)	9 (2%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	325/384 (85%)	315 (97%)	10 (3%)	0	100	100
All	All	2179/2319 (94%)	2138 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/379 (99%)	373 (100%)	1 (0%)	92	95
1	C	382/379 (101%)	380 (100%)	2 (0%)	88	92
2	B	370/383 (97%)	369 (100%)	1 (0%)	92	95
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	86
3	E	110/127 (87%)	109 (99%)	1 (1%)	78	84
4	F	304/342 (89%)	301 (99%)	3 (1%)	76	82
All	All	1908/1993 (96%)	1897 (99%)	11 (1%)	88	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	139	HIS
1	C	347[A]	CYS
1	C	347[B]	CYS
2	D	59	ASN
2	D	139	HIS
2	D	182	VAL
3	E	124	GLN
4	F	242	ASN
4	F	260	ASN
4	F	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	301	GLN
4	F	260	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 17 ligands modelled in this entry, 8 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
5	GTP	C	501	6	26,34,34	1.16	2 (7%)	33,54,54	1.98	8 (24%)
9	GDP	B	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.92	7 (22%)
9	GDP	D	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.98	8 (25%)
12	ACP	F	401	-	27,33,33	1.44	5 (18%)	32,52,52	1.43	4 (12%)
10	MES	B	505	-	12,12,12	2.23	1 (8%)	14,16,16	1.44	2 (14%)
8	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.27	0
8	GOL	C	503	-	5,5,5	0.37	0	5,5,5	0.28	0
11	3GT	D	502	-	49,51,51	1.67	8 (16%)	57,77,77	1.76	11 (19%)
5	GTP	A	501	6	26,34,34	1.17	2 (7%)	33,54,54	1.99	8 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3
12	ACP	F	401	-	-	8/15/38/38	0/3/3/3
10	MES	B	505	-	-	3/6/14/14	0/1/1/1
8	GOL	A	504	-	-	2/4/4/4	-
8	GOL	C	503	-	-	2/4/4/4	-
11	3GT	D	502	-	-	10/57/84/84	0/2/4/4
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-7.52	1.66	1.77
11	D	502	3GT	OBB-CBC	6.73	1.45	1.35
11	D	502	3GT	OBM-C	5.19	1.46	1.34
11	D	502	3GT	CBI-CBH	4.41	1.52	1.47
5	C	501	GTP	C6-C5	4.21	1.48	1.41
9	D	501	GDP	C6-C5	4.21	1.48	1.41
5	A	501	GTP	C6-C5	4.18	1.48	1.41
9	B	501	GDP	C6-C5	4.15	1.48	1.41
12	F	401	ACP	PB-O3A	3.18	1.61	1.58
11	D	502	3GT	CAC-CL1	3.09	1.79	1.72
12	F	401	ACP	PG-O3G	3.07	1.61	1.54
12	F	401	ACP	PG-O2G	2.92	1.61	1.54
11	D	502	3GT	CAD-NAN	-2.67	1.40	1.44
11	D	502	3GT	OBK-CBI	-2.59	1.42	1.45
12	F	401	ACP	C5-C4	2.47	1.47	1.40
5	A	501	GTP	C5-C4	2.44	1.47	1.40
9	D	501	GDP	C5-C4	2.44	1.47	1.40
9	B	501	GDP	C5-C4	2.42	1.47	1.40
5	C	501	GTP	C5-C4	2.42	1.47	1.40
12	F	401	ACP	PB-O2B	2.31	1.61	1.56
11	D	502	3GT	OBB-CBA	-2.29	1.43	1.46
11	D	502	3GT	CAD-CAC	-2.09	1.38	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	3GT	CBI-OBK-CBH	6.04	64.42	60.79
9	B	501	GDP	C2-N3-C4	4.91	120.97	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	4.86	120.91	115.36
5	A	501	GTP	C2-N3-C4	4.82	120.87	115.36
9	D	501	GDP	C2-N3-C4	4.82	120.86	115.36
5	C	501	GTP	C6-N1-C2	4.36	122.86	115.93
11	D	502	3GT	OBM-C-CA	4.31	120.15	110.80
5	A	501	GTP	C6-N1-C2	4.30	122.77	115.93
5	C	501	GTP	C6-C5-C4	-4.16	116.83	120.80
9	D	501	GDP	C6-N1-C2	4.15	122.52	115.93
5	A	501	GTP	C5-C6-N1	-4.14	117.77	123.43
9	B	501	GDP	C6-C5-C4	-4.13	116.86	120.80
5	C	501	GTP	C5-C6-N1	-4.12	117.80	123.43
9	D	501	GDP	C5-C6-N1	-4.05	117.89	123.43
9	B	501	GDP	C6-N1-C2	4.04	122.35	115.93
5	A	501	GTP	C6-C5-C4	-4.02	116.96	120.80
9	D	501	GDP	C6-C5-C4	-3.96	117.02	120.80
12	F	401	ACP	PA-O3A-PB	-3.87	120.28	132.56
9	B	501	GDP	C5-C6-N1	-3.81	118.22	123.43
5	C	501	GTP	N3-C2-N1	-3.60	122.42	127.22
11	D	502	3GT	OAK-CAB-CAC	3.53	119.71	115.53
5	A	501	GTP	N3-C2-N1	-3.53	122.52	127.22
11	D	502	3GT	CBA-OBH-CBC	-3.50	112.11	121.06
11	D	502	3GT	OBK-CBH-CBI	-3.38	57.43	59.83
9	B	501	GDP	N3-C2-N1	-3.37	122.73	127.22
9	D	501	GDP	N3-C2-N1	-3.33	122.79	127.22
12	F	401	ACP	C3'-C2'-C1'	3.32	105.97	100.98
12	F	401	ACP	N3-C2-N1	-3.12	123.81	128.68
5	C	501	GTP	PA-O3A-PB	-3.01	122.49	132.83
5	A	501	GTP	PA-O3A-PB	-2.99	122.58	132.83
11	D	502	3GT	CAS-OBH-C	-2.91	113.00	118.18
5	A	501	GTP	C4-C5-N7	-2.80	106.49	109.40
9	D	501	GDP	C4-C5-N7	-2.76	106.52	109.40
9	D	501	GDP	PA-O3A-PB	-2.74	123.41	132.83
5	C	501	GTP	C4-C5-N7	-2.74	106.54	109.40
9	B	501	GDP	C4-C5-N7	-2.69	106.59	109.40
12	F	401	ACP	C4-C5-N7	-2.66	106.62	109.40
10	B	505	MES	O3S-S-C8	2.62	110.00	105.77
9	B	501	GDP	PA-O3A-PB	-2.61	123.86	132.83
11	D	502	3GT	CAO-NAN-CAP	2.55	123.35	119.15
5	A	501	GTP	PB-O3B-PG	-2.51	124.21	132.83
10	B	505	MES	O2S-S-C8	2.44	109.85	106.92
11	D	502	3GT	CAE-CAD-CAC	-2.39	119.48	122.53
11	D	502	3GT	OAK-CAB-CAA	-2.38	120.03	124.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	3GT	CBJ-CBI-CAS	2.32	120.93	114.51
11	D	502	3GT	OBM-C-O	-2.30	119.65	123.94
9	D	501	GDP	C3'-C2'-C1'	2.27	104.39	100.98
5	C	501	GTP	PB-O3B-PG	-2.18	125.33	132.83

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O2G
12	F	401	ACP	PB-C3B-PG-O3G
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
8	A	504	GOL	O1-C1-C2-C3
8	C	503	GOL	O1-C1-C2-C3
11	D	502	3GT	CAU-CAV-OAX-CAY
11	D	502	3GT	CAC-CAB-OAK-CAL
10	B	505	MES	C7-C8-S-O1S
10	B	505	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	C3'-C4'-C5'-O5'
11	D	502	3GT	CAA-CAB-OAK-CAL
11	D	502	3GT	C-CA-N-CBT
11	D	502	3GT	C-CA-N-CBS
8	C	503	GOL	O1-C1-C2-O2
11	D	502	3GT	CB-CA-N-CBT
8	A	504	GOL	O1-C1-C2-O2
11	D	502	3GT	CB-CA-N-CBS
9	D	501	GDP	C5'-O5'-PA-O3A
10	B	505	MES	C7-C8-S-O2S
11	D	502	3GT	CAZ-CBA-CBF-CBG

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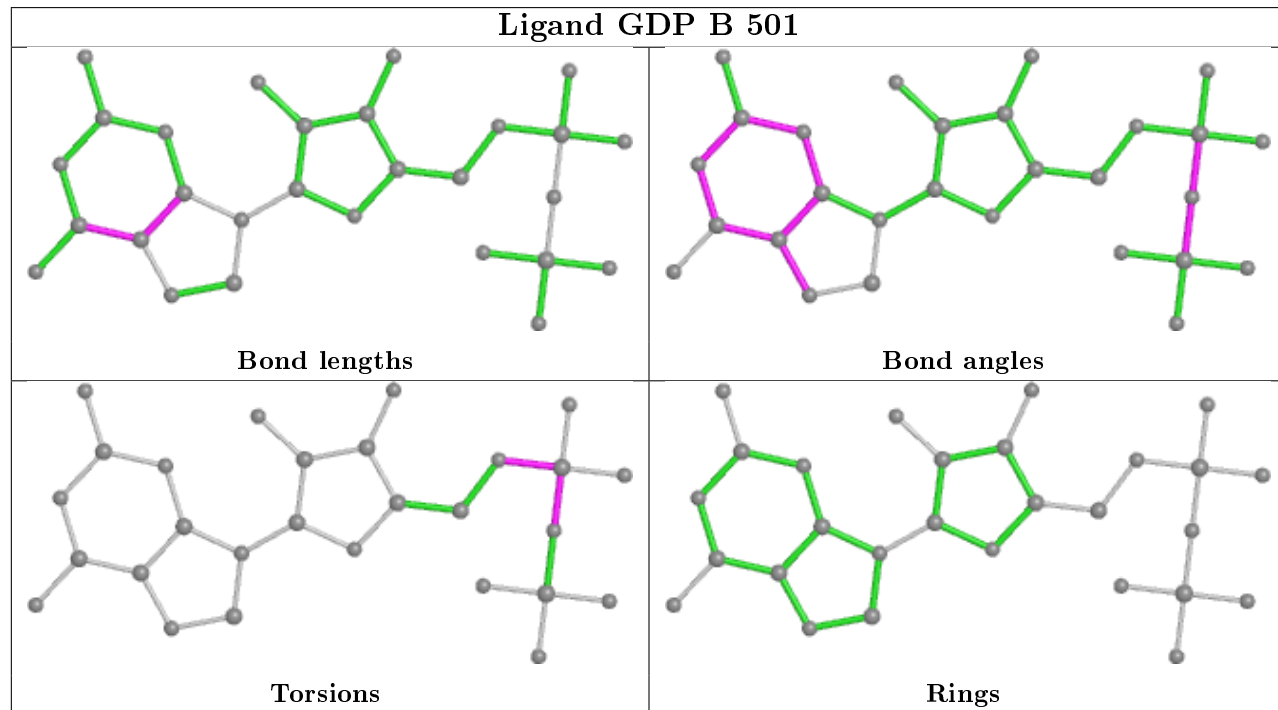
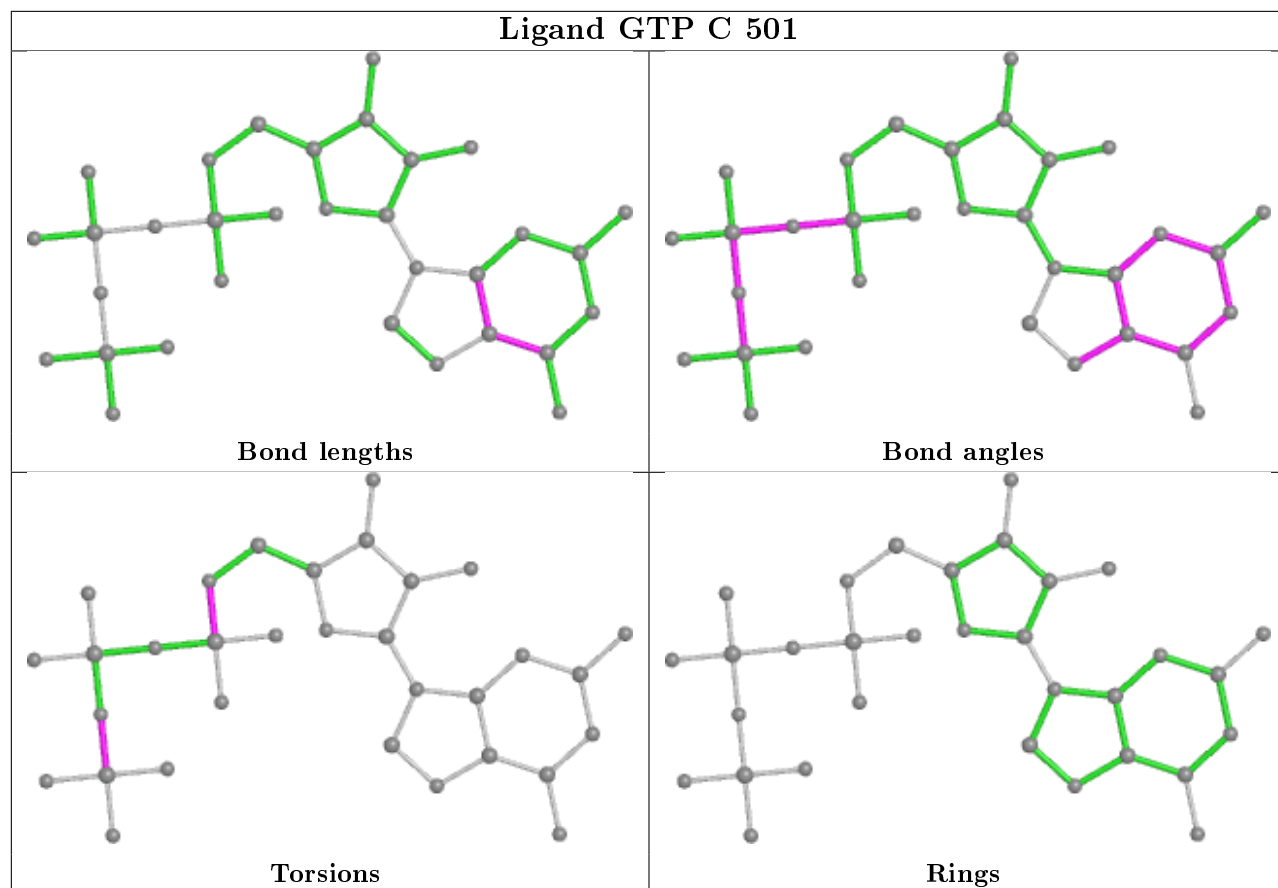
Mol	Chain	Res	Type	Atoms
11	D	502	3GT	O-C-CA-N
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	PB-O3A-PA-O1A
11	D	502	3GT	CBG-CBF-CBH-CBI

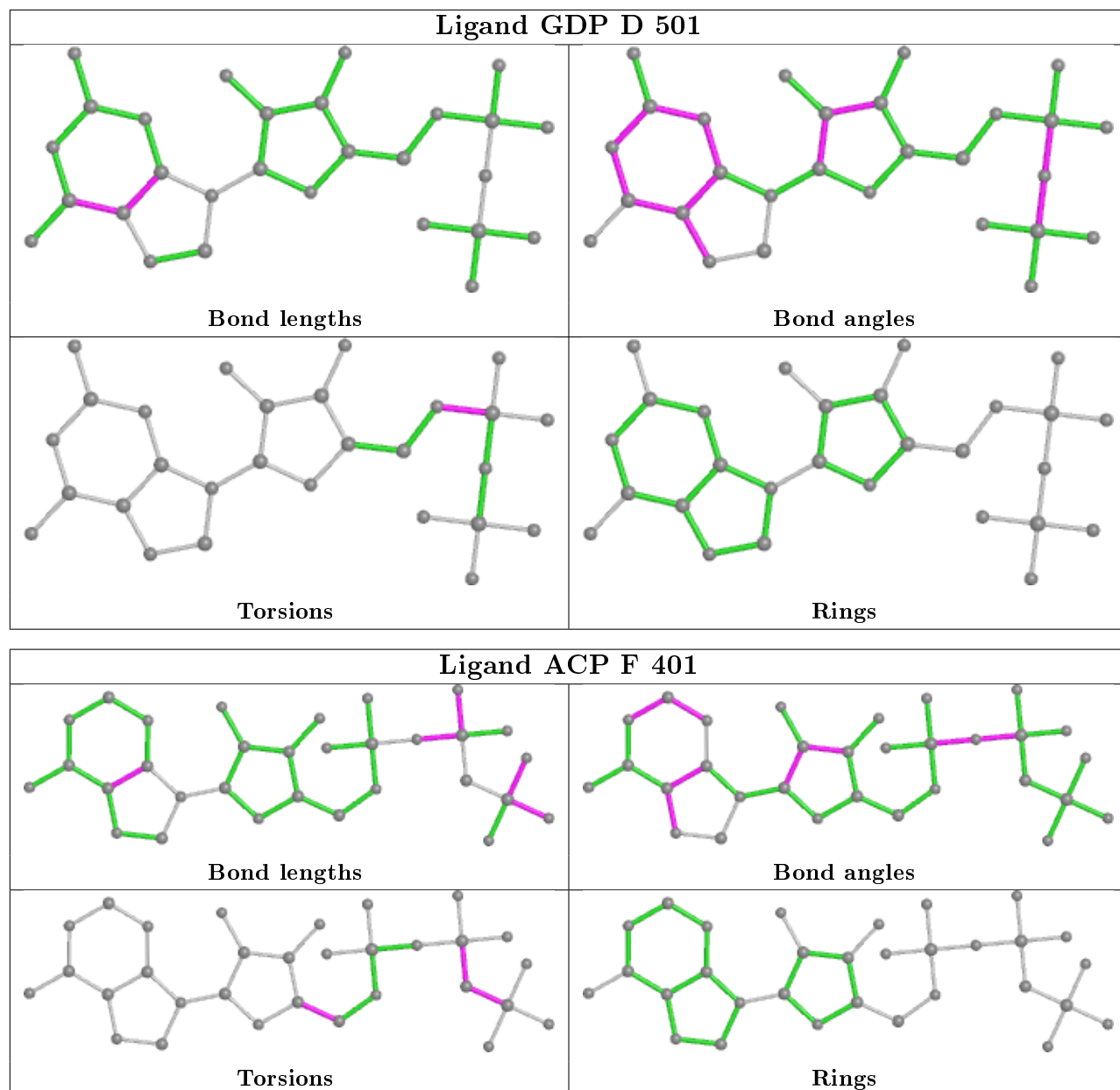
There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
9	B	501	GDP	1	0
9	D	501	GDP	1	0
12	F	401	ACP	3	0
10	B	505	MES	3	0
11	D	502	3GT	2	0
5	A	501	GTP	1	0

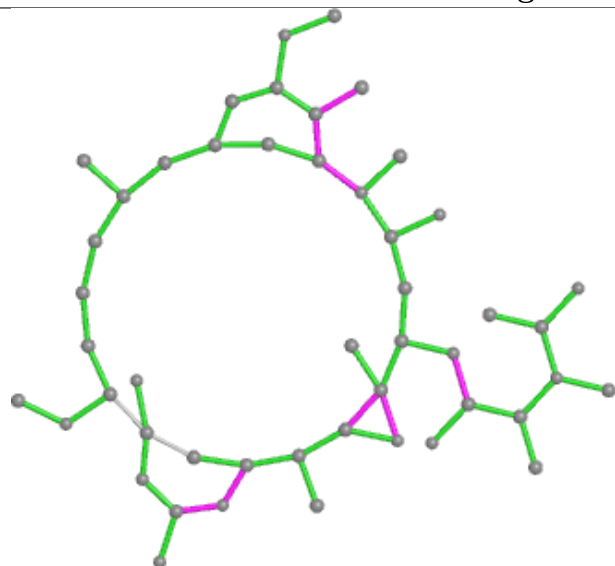
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



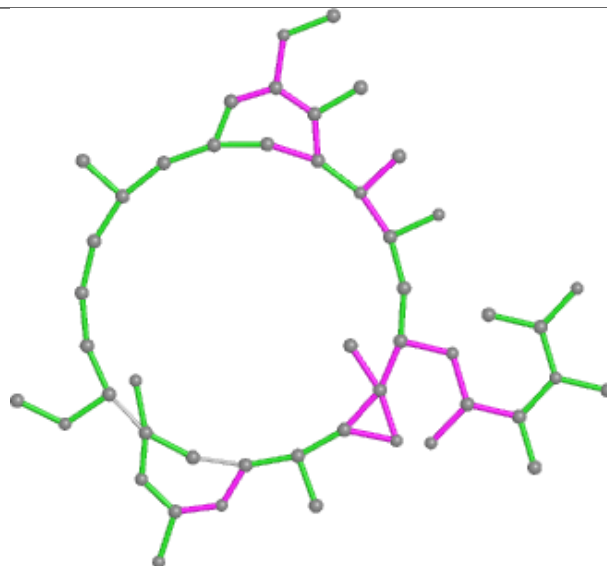




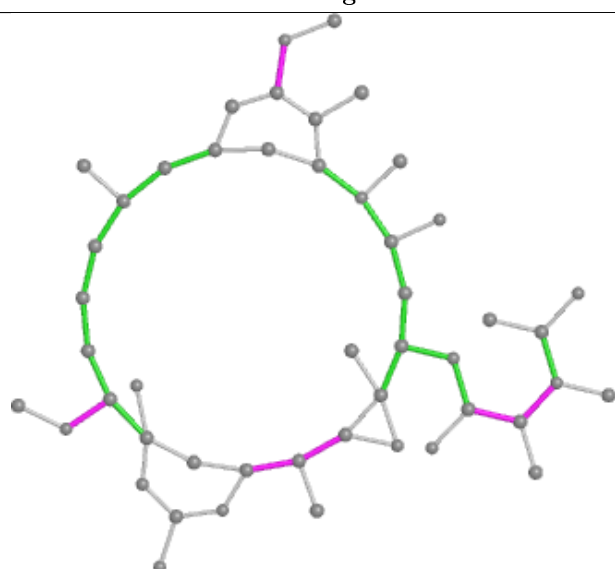
## Ligand 3GT D 502



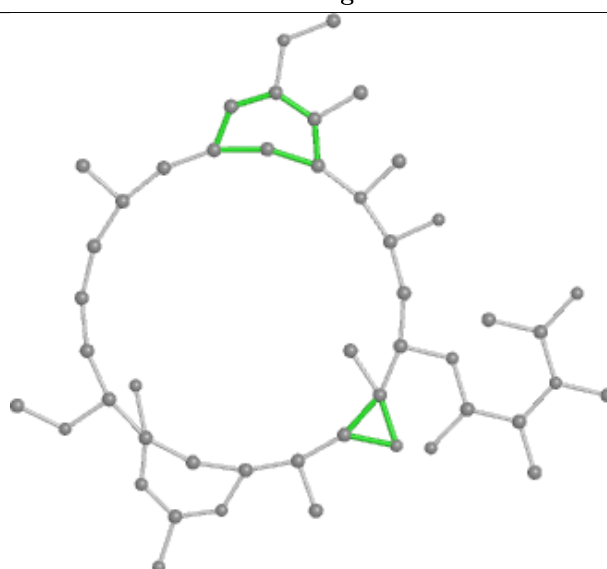
Bond lengths



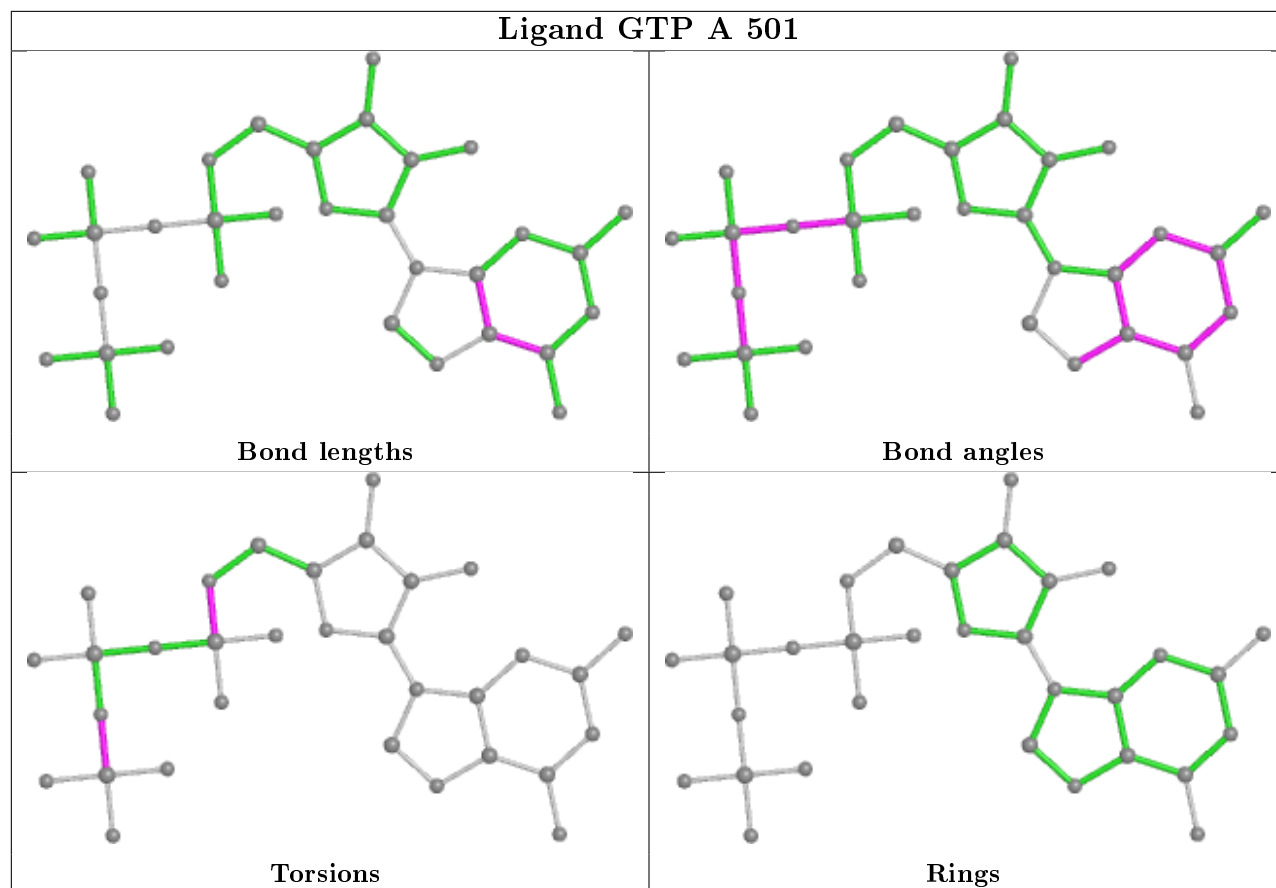
Bond angles



Torsions



Rings



## 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	436/451 (96%)	0.06	3 (0%) 87 89	42, 60, 95, 133	0
1	C	440/451 (97%)	0.21	2 (0%) 91 92	36, 48, 76, 111	0
2	B	427/445 (95%)	0.25	11 (2%) 56 61	36, 56, 96, 139	2 (0%)
2	D	422/445 (94%)	0.19	17 (4%) 38 44	43, 67, 100, 139	3 (0%)
3	E	121/143 (84%)	0.34	2 (1%) 70 74	49, 73, 111, 128	0
4	F	335/384 (87%)	1.14	79 (23%) 0 0	51, 85, 161, 181	0
All	All	2181/2319 (94%)	0.33	114 (5%) 27 32	36, 62, 113, 181	5 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	8.1
4	F	182	ILE	7.1
4	F	233	PHE	7.1
4	F	100	ILE	6.8
4	F	105	LEU	5.8
4	F	134	ALA	5.6
4	F	103	THR	5.6
4	F	161	LEU	5.5
4	F	132	LEU	5.5
4	F	234	GLN	5.4
4	F	232	ASN	5.0
4	F	125	THR	4.9
4	F	99	VAL	4.8
4	F	181	VAL	4.8
4	F	138	ARG	4.8
4	F	133	ALA	4.7
4	F	244	CYS	4.7
4	F	130	VAL	4.5
4	F	172	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	282	GLN	4.4
4	F	131	PHE	4.2
4	F	231	ALA	4.1
4	F	177	GLY	4.0
4	F	372	THR	3.9
4	F	253	TYR	3.9
4	F	166	ALA	3.9
4	F	167	SER	3.9
4	F	147	TRP	3.9
4	F	101	TYR	3.9
4	F	98	TYR	3.8
4	F	236	LYS	3.8
4	F	142	ARG	3.7
4	F	178	GLN	3.7
4	F	143	GLU	3.7
4	F	104	ASN	3.7
4	F	145	ASN	3.6
2	B	1	MET	3.6
3	E	139	LEU	3.6
2	D	276	THR	3.6
4	F	179	VAL	3.5
4	F	162	ILE	3.5
2	B	57	THR	3.5
4	F	135	TYR	3.4
4	F	240	LEU	3.4
2	B	281	GLN	3.3
1	A	262	TYR	3.3
4	F	129	GLU	3.3
4	F	235	ASP	3.2
2	B	58	GLY	3.1
4	F	139	ARG	3.1
2	D	405	LEU	3.1
4	F	169	LEU	3.1
4	F	186	LEU	3.1
2	B	276	THR	3.1
2	B	248	LEU	3.0
2	B	278	ARG	3.0
2	B	285	ALA	3.0
2	B	284	ARG	2.9
1	A	439	SER	2.9
4	F	144	GLY	2.9
1	C	357	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	259	GLY	2.8
2	D	404	PHE	2.8
4	F	224	SER	2.8
4	F	225	SER	2.8
4	F	183	GLN	2.8
4	F	24	THR	2.7
4	F	148	ILE	2.7
4	F	239	HIS	2.7
4	F	245	ILE	2.7
2	D	57	THR	2.7
2	D	217	LEU	2.6
4	F	20	LEU	2.6
2	D	400	ARG	2.6
4	F	140	GLU	2.6
2	D	59	ASN	2.5
4	F	284[A]	LEU	2.5
2	D	94	PHE	2.5
4	F	149	ALA	2.4
4	F	170	LEU	2.4
4	F	180	HIS	2.4
4	F	361	LEU	2.4
4	F	255	ARG	2.4
4	F	176	GLN	2.4
4	F	320	MET	2.4
2	D	286	LEU	2.3
4	F	23	ALA	2.3
4	F	175	GLU	2.3
2	D	37	HIS	2.3
2	D	182	VAL	2.3
4	F	137	ARG	2.3
4	F	46	ARG	2.3
4	F	9	GLU	2.3
1	A	281	ALA	2.2
4	F	127	GLU	2.2
3	E	25	LYS	2.2
4	F	342	LEU	2.2
2	D	272	PHE	2.2
2	B	372	LYS	2.2
2	D	372	LYS	2.2
1	C	295[A]	CYS	2.2
2	D	83	PHE	2.2
4	F	17	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	387	LEU	2.1
4	F	265	GLU	2.1
4	F	194	PRO	2.1
2	D	177	VAL	2.1
4	F	187	GLU	2.1
4	F	379	HIS	2.1
4	F	343	TYR	2.1
4	F	192	LEU	2.0
2	D	441	ASP	2.0
4	F	242	ASN	2.0
4	F	21	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 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
7	CA	B	504	1/1	0.68	0.30	115,115,115,115	0
8	GOL	A	504	6/6	0.77	0.14	86,87,90,92	0
12	ACP	F	401	31/31	0.80	0.14	87,97,167,172	0
6	MG	D	503	1/1	0.86	0.09	62,62,62,62	0
7	CA	A	503	1/1	0.89	0.12	85,85,85,85	0
11	3GT	D	502	48/48	0.90	0.20	80,89,105,188	0
7	CA	B	503	1/1	0.94	0.08	101,101,101,101	0
8	GOL	C	503	6/6	0.94	0.21	77,79,82,82	0
9	GDP	D	501	28/28	0.94	0.13	56,64,74,85	0
10	MES	B	505	12/12	0.95	0.14	57,65,77,82	0
6	MG	B	502	1/1	0.96	0.26	39,39,39,39	0
6	MG	C	502	1/1	0.96	0.13	41,41,41,41	0

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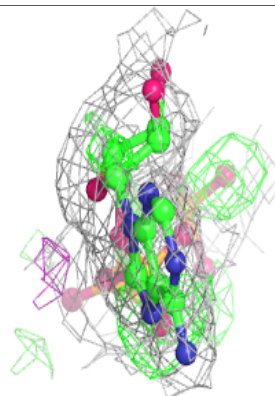
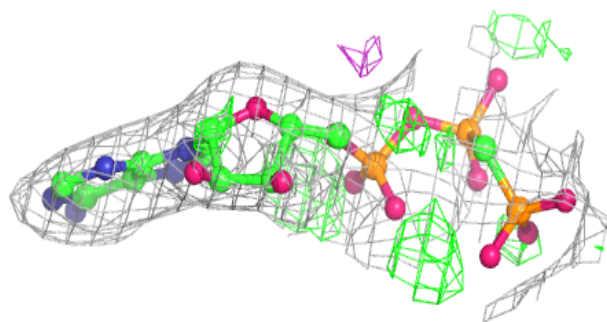
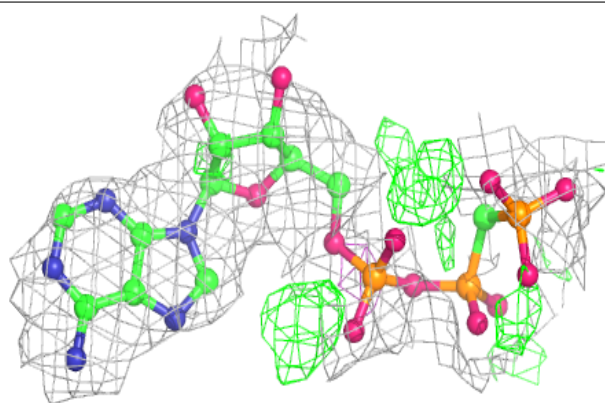
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	A	502	1/1	0.97	0.09	44,44,44,44	0
9	GDP	B	501	28/28	0.98	0.16	32,43,47,50	0
5	GTP	C	501	32/32	0.98	0.13	30,37,41,46	0
5	GTP	A	501	32/32	0.98	0.13	37,44,49,74	0
7	CA	C	504	1/1	0.99	0.12	67,67,67,67	0

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

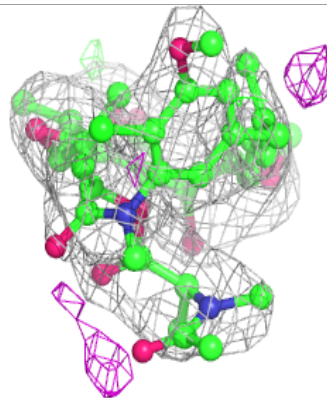
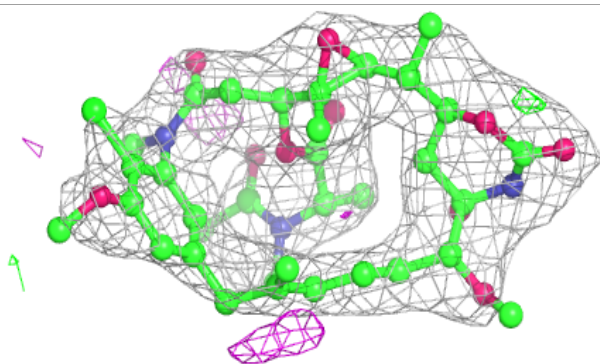
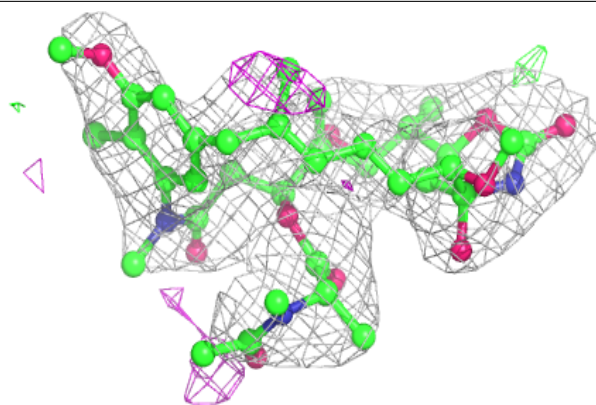
**Electron density around ACP F 401:**

2mF<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 3GT D 502:**

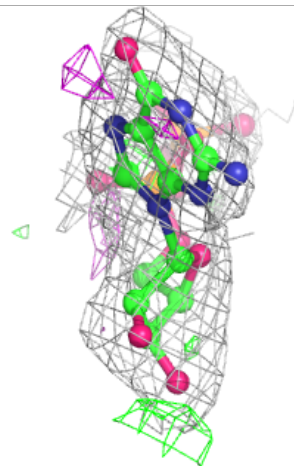
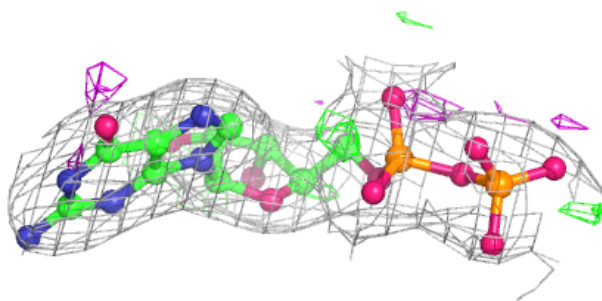
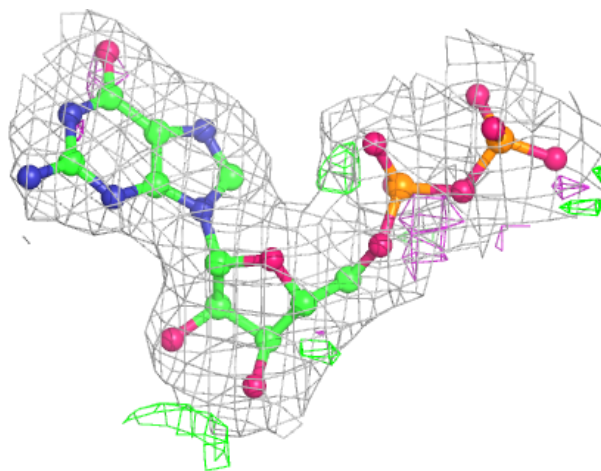
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





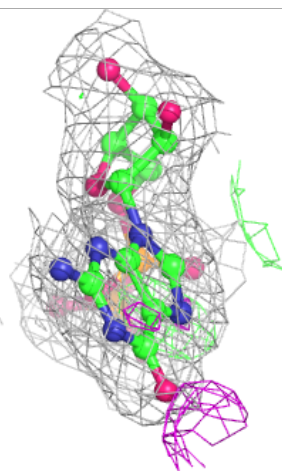
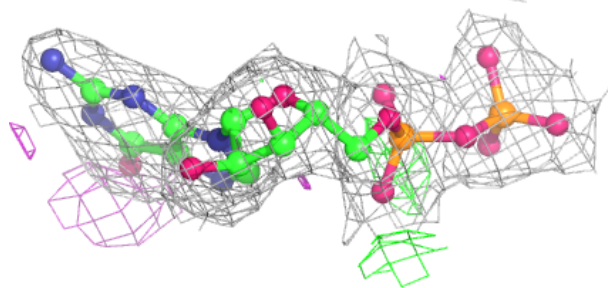
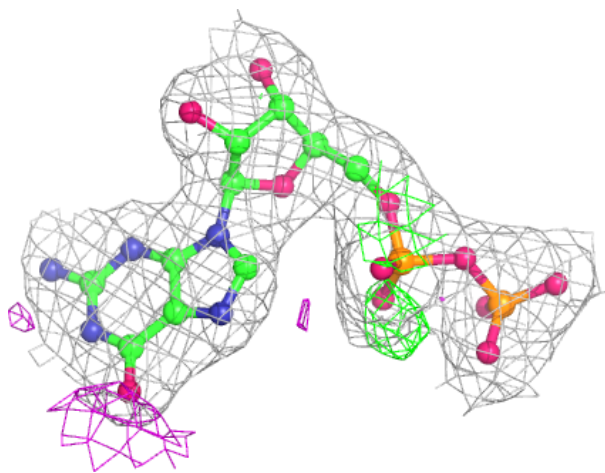
**Electron density around GDP D 501:**

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



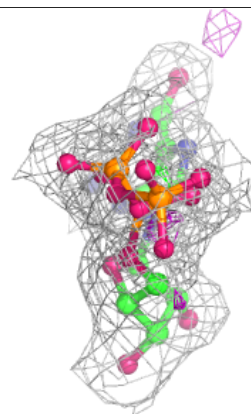
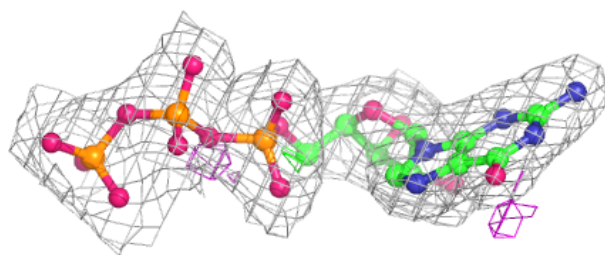
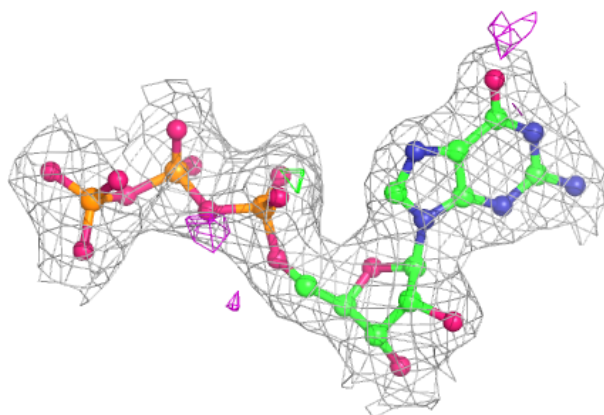
**Electron density around GDP B 501:**

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

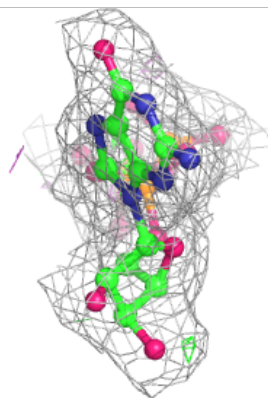
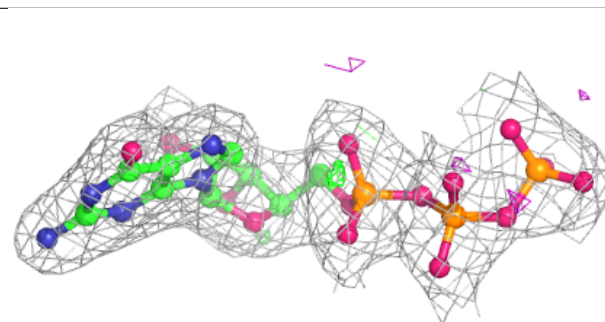
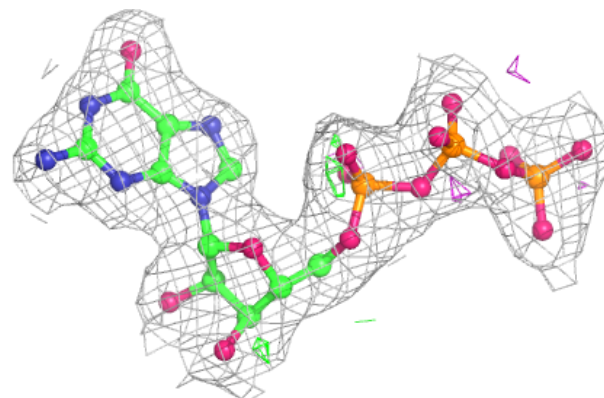


**Electron density around GTP C 501:**

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

**Electron density around GTP A 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.