



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 11:53 AM JST

PDB ID : 5YLJ  
Title : Crystal structure of T2R-TTL-Millepachine complex  
Authors : Yang, J.H.; Chen, L.J.  
Deposited on : 2017-10-17  
Resolution : 2.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

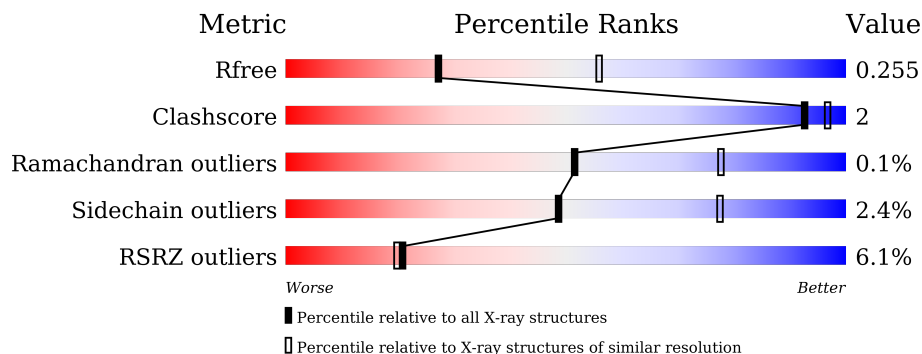
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	451	
1	C	451	
2	B	445	
2	D	445	
3	E	143	
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
11	8X0	D	503	-	-	-	X

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 17533 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
			Total	C	N	O	S			
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

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

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

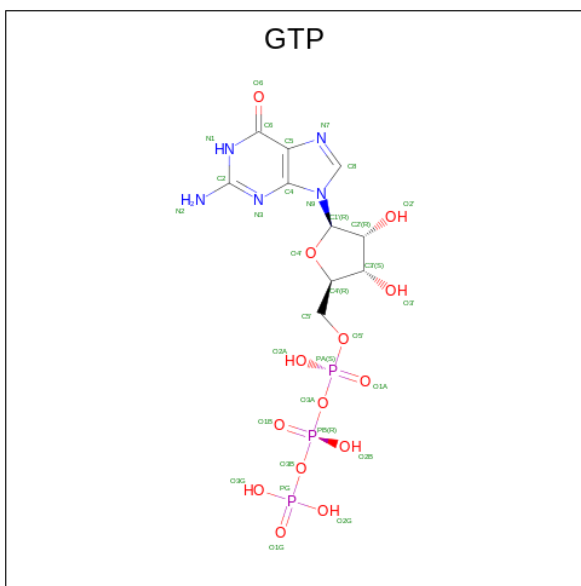
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

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

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

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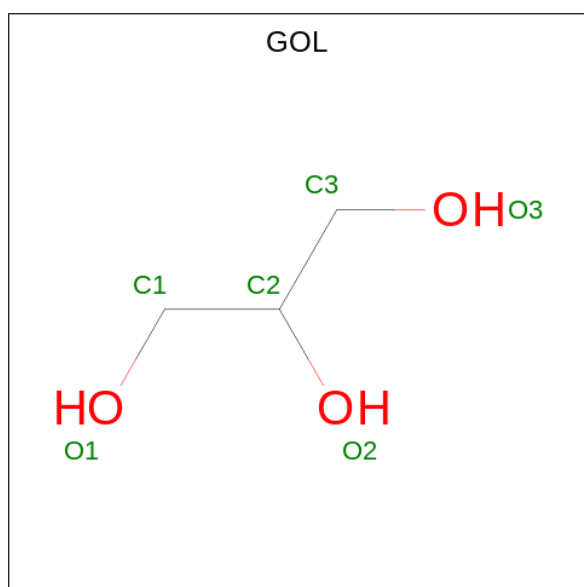
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

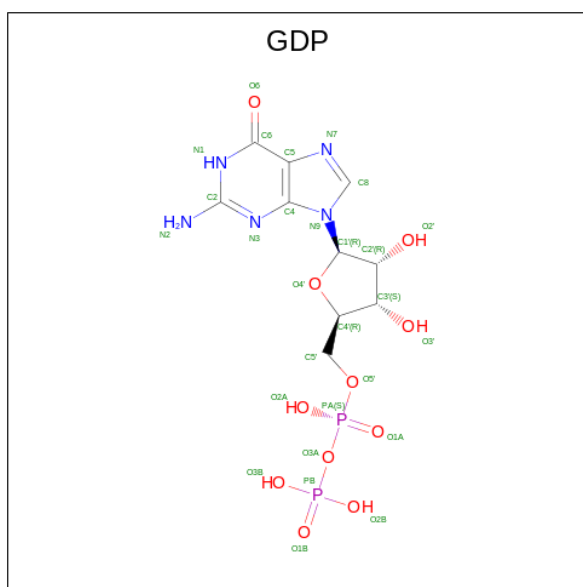
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



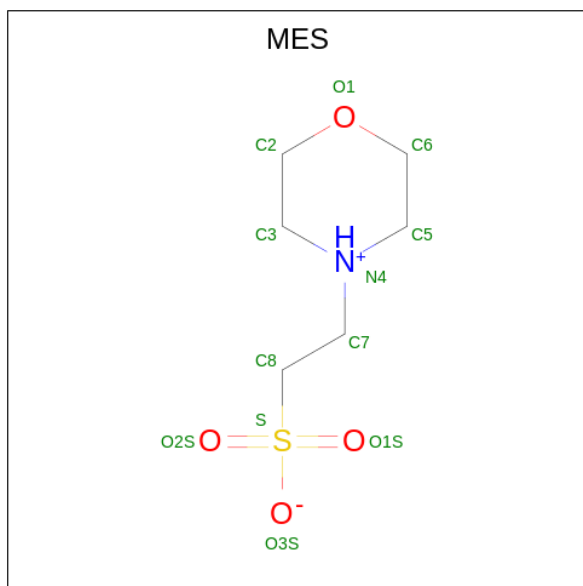
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- 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>).



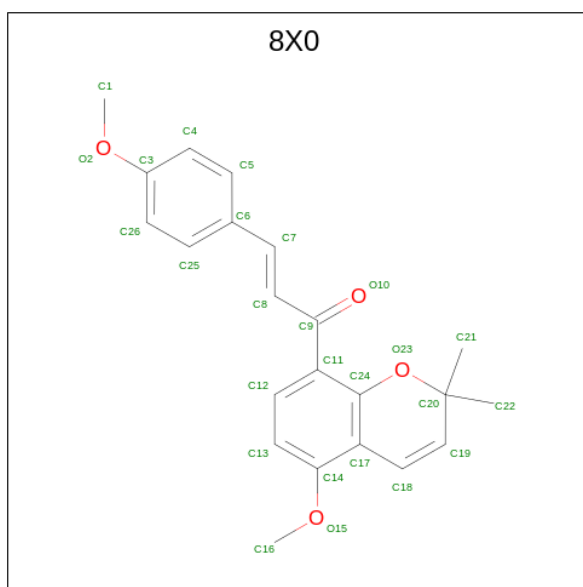
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0

- 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).



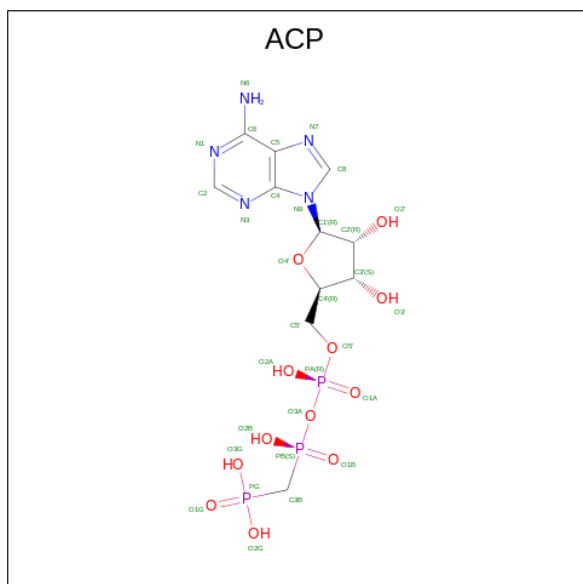
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is (E)-1-(5-methoxy-2,2-dimethyl-chromen-8-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (three-letter code: 8X0) (formula: C<sub>22</sub>H<sub>22</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	C O	0	0
			26	22 4		
11	D	1	Total	C O	0	0
			26	22 4		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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



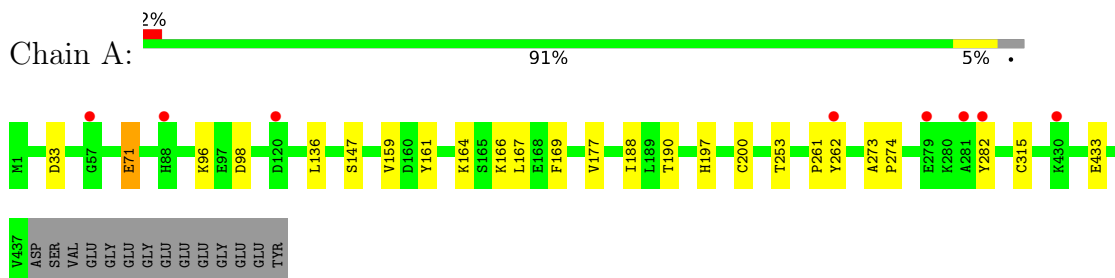
- Molecule 13 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
13	A	4	Total O 4 4	0	0
13	B	11	Total O 11 11	0	0
13	C	7	Total O 7 7	0	0
13	D	5	Total O 5 5	0	0

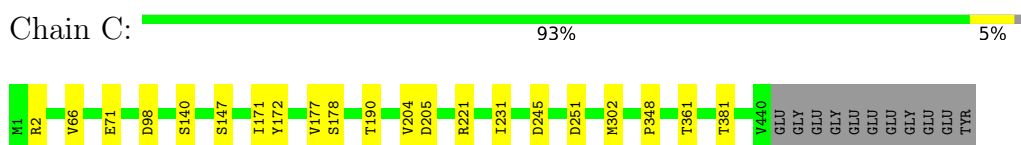
### 3 Residue-property plots [i](#)

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.

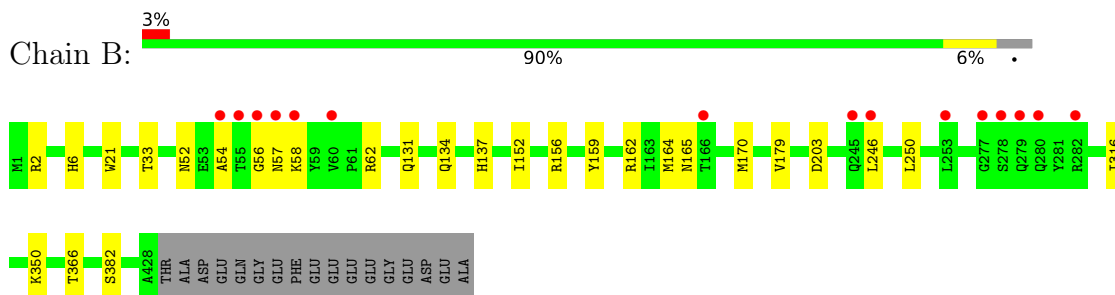
- Molecule 1: Tubulin alpha-1B chain



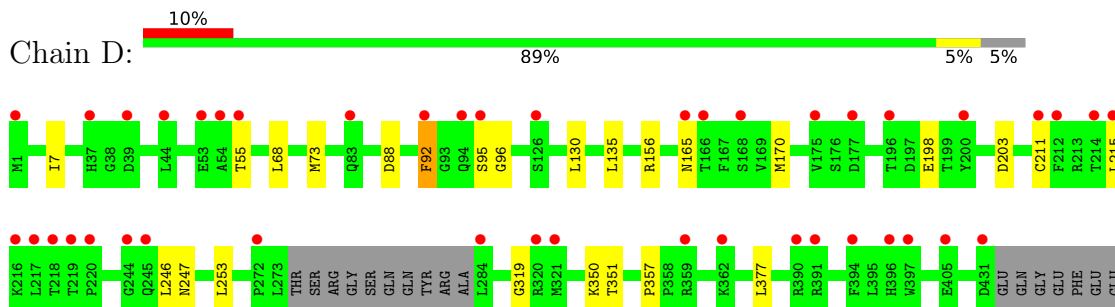
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain

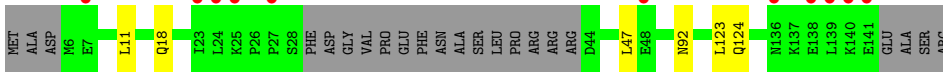
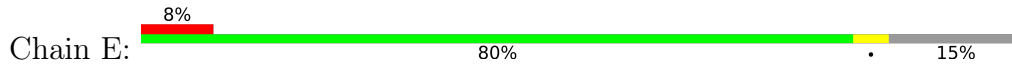


- Molecule 2: Tubulin beta chain

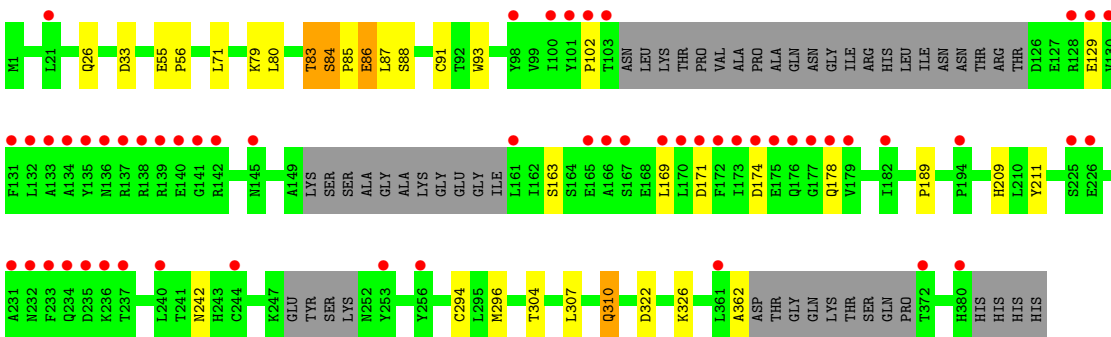
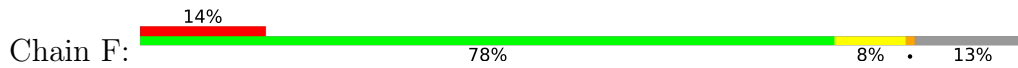


GLU  
GLU  
GLY  
GLY  
ASP  
GLU  
ALA

• 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, $\alpha$ , $\beta$ , $\gamma$	105.23Å 157.37Å 182.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.90 – 2.70 41.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.90-2.70) 99.7 (41.90-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.216 , 0.255 0.216 , 0.255	Depositor DCC
$R_{free}$ test set	4187 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: GTP, MES, ACP, GDP, MG, CA, 8X0, GOL

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	0.40	0/3494	0.58	0/4743
1	C	0.44	0/3515	0.62	0/4772
2	B	0.40	0/3444	0.57	0/4664
2	D	0.41	0/3382	0.58	0/4581
3	E	0.36	0/1008	0.57	0/1337
4	F	0.45	0/2806	0.60	0/3791
All	All	0.42	0/17649	0.59	0/23888

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3331	8	0
1	C	3437	0	3348	6	0
2	B	3369	0	3250	12	0
2	D	3309	0	3189	10	0
3	E	1000	0	1018	3	0
4	F	2744	0	2709	16	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	1	0
11	B	26	0	0	0	0
11	D	26	0	0	1	0
12	F	31	0	14	1	0
13	A	4	0	0	0	0
13	B	11	0	0	0	0
13	C	7	0	0	0	0
13	D	5	0	0	0	0
All	All	17533	0	16928	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:86:GLU:N	4:F:86:GLU:OE2	1.87	1.06
4:F:79:LYS:O	4:F:83:THR:OG1	1.89	0.89
2:B:131:GLN:HE21	2:B:250:LEU:H	1.39	0.69
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.80	0.63
2:B:56:GLY:O	2:B:57:ASN:HB2	1.99	0.61
4:F:86:GLU:H	4:F:86:GLU:CD	2.01	0.60
4:F:87:LEU:O	4:F:88:SER:HB3	2.01	0.59
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.83	0.59
4:F:80:LEU:O	4:F:84:SER:HB2	2.04	0.58
2:B:156:ARG:HG3	10:B:503:MES:H62	1.87	0.57
2:B:54:ALA:HB3	2:B:58:LYS:O	2.06	0.55
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.89	0.54
2:B:52:ASN:OD1	2:B:62:ARG:NH2	2.40	0.54
2:D:350:LYS:HG3	11:D:503:8X0:C4	2.37	0.54
4:F:102:PRO:HB3	4:F:174:ASP:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HE2	1:A:197:HIS:O	2.11	0.51
2:B:159:TYR:HB3	2:B:162:ARG:HG3	1.93	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.49
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.93	0.49
2:B:152:ILE:HG23	2:B:164:MET:HG2	1.94	0.49
4:F:85:PRO:HD2	4:F:86:GLU:OE2	2.13	0.48
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.95	0.48
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.95	0.48
2:D:198:GLU:OE2	2:D:253:LEU:HD23	2.13	0.47
4:F:242:ASN:HD21	12:F:401:ACP:H5'2	1.79	0.47
2:B:134:GLN:HA	2:B:165:ASN:O	2.15	0.46
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.97	0.46
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.09	0.46
4:F:189:PRO:HA	4:F:322:ASP:HA	1.98	0.46
1:A:136:LEU:HD22	1:A:169:PHE:HE2	1.81	0.45
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.45
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.98	0.45
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.99	0.44
2:D:73:MET:HG3	2:D:92:PHE:HB3	2.00	0.44
2:D:170:MET:HB2	2:D:203:ASP:HA	1.99	0.44
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.83	0.44
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.00	0.44
2:B:170:MET:HB2	2:B:203:ASP:HA	2.01	0.43
2:D:68:LEU:HB3	2:D:96:GLY:H	1.83	0.43
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.01	0.43
4:F:26:GLN:HE22	4:F:362:ALA:H	1.66	0.42
4:F:163:SER:HB3	4:F:169:LEU:HG	2.01	0.42
1:A:273:ALA:HA	1:A:274:PRO:HA	1.84	0.42
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.02	0.42
1:C:147:SER:HB2	1:C:190:THR:OG1	2.19	0.42
4:F:55:GLU:HA	4:F:56:PRO:HD2	1.96	0.42
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.02	0.41
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.41
2:B:316:ILE:HG23	2:B:366:THR:HB	2.02	0.41
1:A:159:VAL:HG11	3:E:47:LEU:HB2	2.03	0.41
2:D:7:ILE:O	2:D:135:LEU:HA	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	425 (98%)	8 (2%)	2 (0%)	29	54
1	C	438/451 (97%)	430 (98%)	8 (2%)	0	100	100
2	B	426/445 (96%)	417 (98%)	9 (2%)	0	100	100
2	D	417/445 (94%)	405 (97%)	11 (3%)	1 (0%)	47	73
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	314 (97%)	10 (3%)	0	100	100
All	All	2157/2319 (93%)	2106 (98%)	48 (2%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
2	D	95	SER
1	A	261	PRO

### 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	368/379 (97%)	359 (98%)	9 (2%)	49	77
1	C	371/379 (98%)	361 (97%)	10 (3%)	44	74
2	B	370/383 (97%)	364 (98%)	6 (2%)	62	85
2	D	364/383 (95%)	356 (98%)	8 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	109/127 (86%)	107 (98%)	2 (2%)	59	83
4	F	301/342 (88%)	290 (96%)	11 (4%)	34	63
All	All	1883/1993 (94%)	1837 (98%)	46 (2%)	49	77

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

Mol	Chain	Res	Type
1	A	33	ASP
1	A	71	GLU
1	A	96	LYS
1	A	177	VAL
1	A	188	ILE
1	A	253	THR
1	A	262	TYR
1	A	315	CYS
1	A	433	GLU
2	B	2	ARG
2	B	33	THR
2	B	137	HIS
2	B	246	LEU
2	B	350	LYS
2	B	382	SER
1	C	2	ARG
1	C	66	VAL
1	C	177	VAL
1	C	178	SER
1	C	221	ARG
1	C	245	ASP
1	C	251	ASP
1	C	302	MET
1	C	361	THR
1	C	381	THR
2	D	55	THR
2	D	88	ASP
2	D	92	PHE
2	D	130	LEU
2	D	165	ASN
2	D	246	LEU
2	D	247	ASN
2	D	351	THR
3	E	92	ASN

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Mol	Chain	Res	Type
3	E	124	GLN
4	F	33	ASP
4	F	83	THR
4	F	84	SER
4	F	86	GLU
4	F	129	GLU
4	F	171	ASP
4	F	178	GLN
4	F	211	TYR
4	F	296	MET
4	F	310	GLN
4	F	326	LYS

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

Mol	Chain	Res	Type
1	A	88	HIS
1	A	176	GLN
1	A	329	ASN
2	B	131	GLN
2	B	375	GLN
2	D	99	ASN
3	E	18	GLN
4	F	26	GLN
4	F	260	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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	A	501	6	26,34,34	0.87	0	32,54,54	1.18	4 (12%)
10	MES	B	503	-	12,12,12	2.09	1 (8%)	14,16,16	6.78	5 (35%)
8	GOL	A	504	-	5,5,5	0.22	0	5,5,5	0.30	0
11	8X0	D	503	-	28,28,28	3.50	15 (53%)	39,40,40	1.69	11 (28%)
5	GTP	C	501	6	26,34,34	0.87	0	32,54,54	1.11	3 (9%)
11	8X0	B	504	-	28,28,28	3.52	14 (50%)	39,40,40	1.42	7 (17%)
5	GTP	D	501	6	26,34,34	0.95	2 (7%)	32,54,54	1.22	4 (12%)
12	ACP	F	401	-	27,33,33	1.80	7 (25%)	32,52,52	1.34	4 (12%)
9	GDP	B	501	6	24,30,30	0.94	0	30,47,47	1.13	3 (10%)

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	A	501	6	-	6/18/38/38	0/3/3/3
10	MES	B	503	-	-	3/6/14/14	0/1/1/1
8	GOL	A	504	-	-	2/4/4/4	-
11	8X0	D	503	-	-	6/13/24/24	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
11	8X0	B	504	-	-	7/13/24/24	0/3/3/3
5	GTP	D	501	6	-	8/18/38/38	0/3/3/3
12	ACP	F	401	-	-	1/15/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	8X0	C18-C19	10.78	1.47	1.33
11	D	503	8X0	C18-C19	10.47	1.47	1.33
11	D	503	8X0	O23-C24	10.15	1.53	1.37
11	B	504	8X0	O23-C24	9.71	1.52	1.37
10	B	503	MES	C8-S	-6.61	1.68	1.77
12	F	401	ACP	PG-O1G	5.36	1.61	1.50
11	B	504	8X0	C8-C9	4.74	1.55	1.47
11	B	504	8X0	C5-C4	4.48	1.46	1.38
11	D	503	8X0	C5-C4	4.43	1.46	1.38
11	D	503	8X0	C8-C9	4.08	1.54	1.47
11	B	504	8X0	C6-C7	3.88	1.58	1.47
11	D	503	8X0	C6-C7	3.75	1.58	1.47
11	D	503	8X0	C26-C3	3.38	1.45	1.38
12	F	401	ACP	PB-O3A	3.37	1.62	1.58
11	B	504	8X0	C26-C3	3.29	1.45	1.38
11	D	503	8X0	O15-C14	3.20	1.42	1.37
11	D	503	8X0	C17-C14	3.20	1.46	1.41
11	B	504	8X0	C8-C7	3.19	1.41	1.33
11	B	504	8X0	C17-C14	3.09	1.46	1.41
11	B	504	8X0	O15-C14	3.08	1.42	1.37
11	D	503	8X0	C11-C24	2.96	1.46	1.40
11	D	503	8X0	C8-C7	2.93	1.40	1.33
12	F	401	ACP	PG-O3G	2.89	1.61	1.54
12	F	401	ACP	PG-O2G	-2.82	1.48	1.54
12	F	401	ACP	C5-C4	2.72	1.48	1.40
11	B	504	8X0	C20-C19	2.69	1.55	1.50
11	B	504	8X0	C11-C24	2.54	1.45	1.40
11	B	504	8X0	C25-C6	2.33	1.44	1.39
11	D	503	8X0	C20-C19	2.29	1.54	1.50
12	F	401	ACP	C2-N3	2.21	1.35	1.32
12	F	401	ACP	PB-O2B	2.15	1.61	1.56
5	D	501	GTP	C6-N1	-2.12	1.34	1.37
11	D	503	8X0	O23-C20	2.07	1.51	1.47
11	D	503	8X0	C13-C12	2.06	1.42	1.38
11	B	504	8X0	C13-C12	2.06	1.42	1.38
11	D	503	8X0	O2-C3	2.03	1.41	1.37
11	D	503	8X0	C25-C6	2.03	1.43	1.39
11	B	504	8X0	O2-C3	2.01	1.41	1.37
5	D	501	GTP	C5-C4	2.01	1.48	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O3S-S-C8	-13.70	83.61	105.77
10	B	503	MES	O3S-S-O2S	-11.33	83.59	111.27
10	B	503	MES	O3S-S-O1S	-10.82	84.83	111.27
10	B	503	MES	O2S-S-C8	10.09	119.07	106.92
10	B	503	MES	O1S-S-C8	9.90	118.84	106.92
11	D	503	8X0	C22-C20-C21	-4.66	98.04	111.29
11	D	503	8X0	C7-C8-C9	-4.03	115.07	121.64
11	B	504	8X0	C22-C20-C21	-3.90	100.20	111.29
12	F	401	ACP	N3-C2-N1	-3.56	123.11	128.68
12	F	401	ACP	C3'-C2'-C1'	3.38	106.07	100.98
11	B	504	8X0	C16-O15-C14	-3.24	112.64	117.53
5	D	501	GTP	PA-O3A-PB	-3.07	122.29	132.83
11	B	504	8X0	O15-C14-C13	-2.92	119.36	124.37
11	D	503	8X0	O23-C20-C21	2.92	112.01	105.98
11	D	503	8X0	O15-C14-C13	-2.85	119.49	124.37
11	B	504	8X0	O15-C14-C17	2.79	120.66	115.26
12	F	401	ACP	C4-C5-N7	-2.64	106.65	109.40
11	D	503	8X0	O15-C14-C17	2.63	120.35	115.26
11	B	504	8X0	C7-C8-C9	-2.55	117.47	121.64
5	C	501	GTP	C8-N7-C5	2.50	107.75	102.99
11	D	503	8X0	C25-C6-C5	2.42	121.22	117.64
5	A	501	GTP	PA-O3A-PB	-2.41	124.56	132.83
9	B	501	GDP	PA-O3A-PB	-2.37	124.69	132.83
5	D	501	GTP	PB-O3B-PG	-2.35	124.75	132.83
5	A	501	GTP	C8-N7-C5	2.35	107.47	102.99
11	D	503	8X0	C16-O15-C14	-2.34	114.00	117.53
9	B	501	GDP	C5-C6-N1	2.30	118.01	113.95
5	D	501	GTP	C8-N7-C5	2.30	107.37	102.99
5	A	501	GTP	C5-C6-N1	2.29	117.99	113.95
5	C	501	GTP	C5-C6-N1	2.28	117.98	113.95
5	C	501	GTP	PA-O3A-PB	-2.27	125.02	132.83
9	B	501	GDP	C8-N7-C5	2.26	107.30	102.99
5	D	501	GTP	C5-C6-N1	2.24	117.91	113.95
12	F	401	ACP	PB-O3A-PA	-2.22	125.51	132.56
11	B	504	8X0	C22-C20-C19	2.20	115.52	111.45
5	A	501	GTP	O6-C6-C5	-2.20	120.08	124.37
11	D	503	8X0	C20-C19-C18	-2.17	118.53	121.49
11	B	504	8X0	C25-C6-C5	2.15	120.83	117.64
11	D	503	8X0	C4-C5-C6	-2.08	118.53	121.25
11	D	503	8X0	C11-C9-C8	-2.04	117.17	120.10
11	D	503	8X0	C24-C17-C18	2.02	120.00	117.86

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O1A
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O1A
10	B	503	MES	N4-C7-C8-S
10	B	503	MES	C7-C8-S-O2S
10	B	503	MES	C7-C8-S-O3S
11	D	503	8X0	C7-C8-C9-O10
11	D	503	8X0	C7-C8-C9-C11
11	B	504	8X0	C13-C14-O15-C16
11	D	503	8X0	C13-C14-O15-C16
11	B	504	8X0	C4-C3-O2-C1
11	B	504	8X0	C17-C14-O15-C16
11	D	503	8X0	C17-C14-O15-C16
11	B	504	8X0	C26-C3-O2-C1
11	B	504	8X0	C7-C8-C9-C11
11	B	504	8X0	C7-C8-C9-O10
8	A	504	GOL	O1-C1-C2-O2
11	D	503	8X0	C24-C11-C9-O10
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
5	D	501	GTP	PB-O3A-PA-O2A
11	D	503	8X0	C24-C11-C9-C8
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
11	B	504	8X0	C24-C11-C9-O10
5	D	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G

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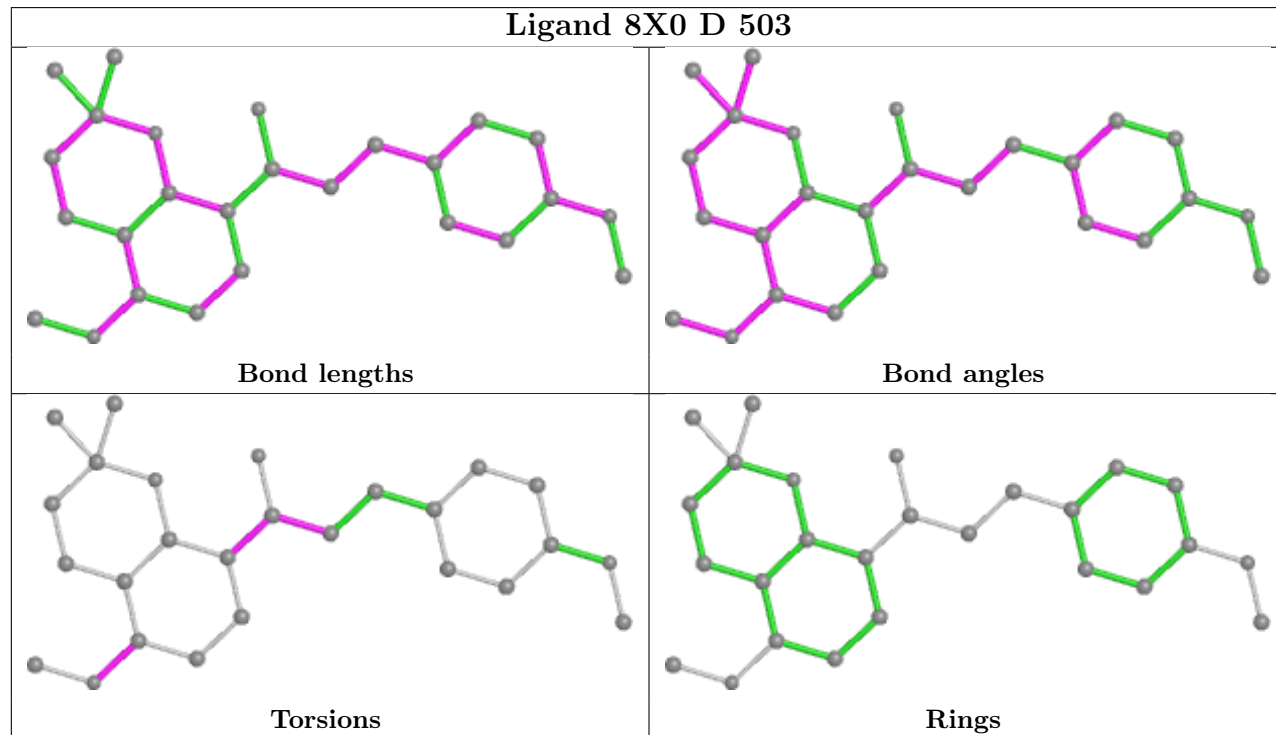
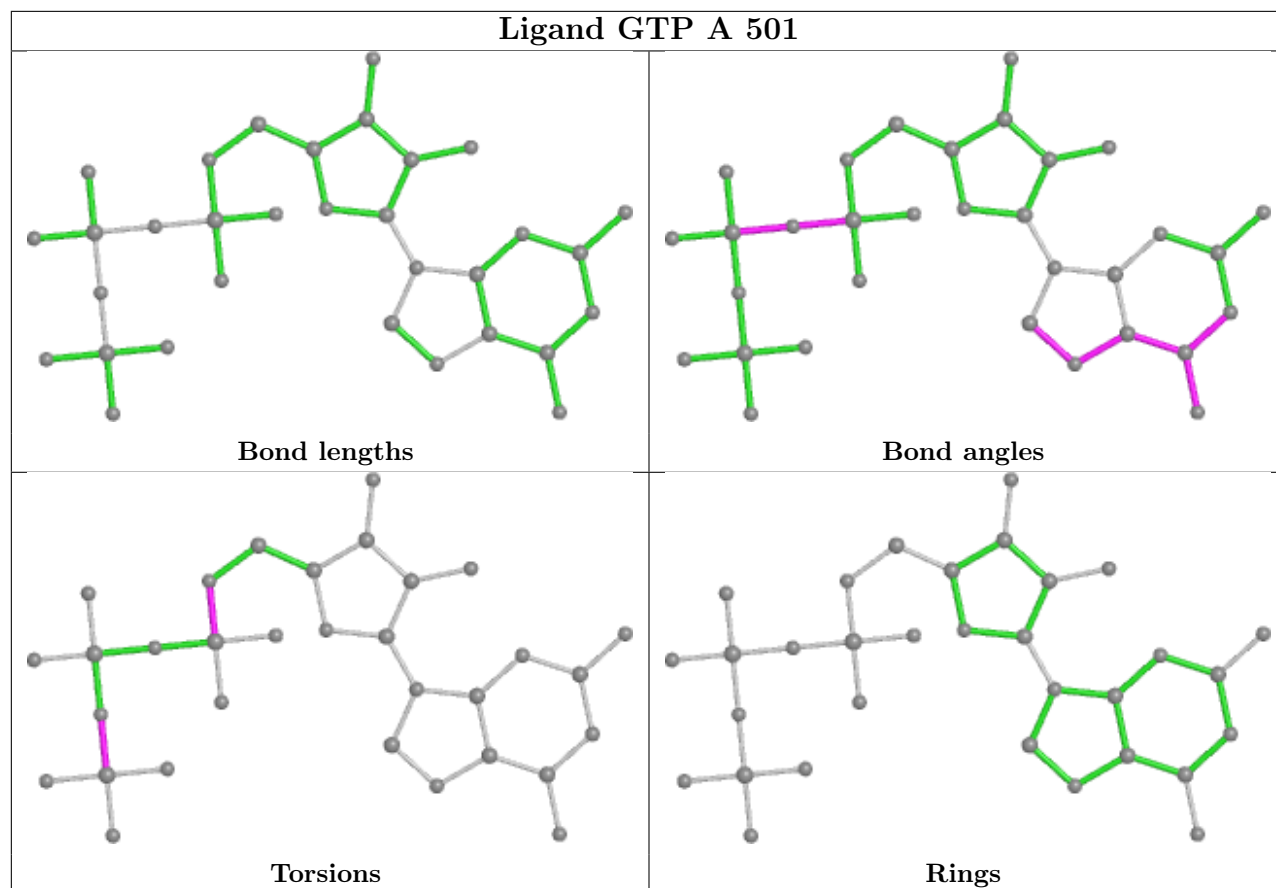
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

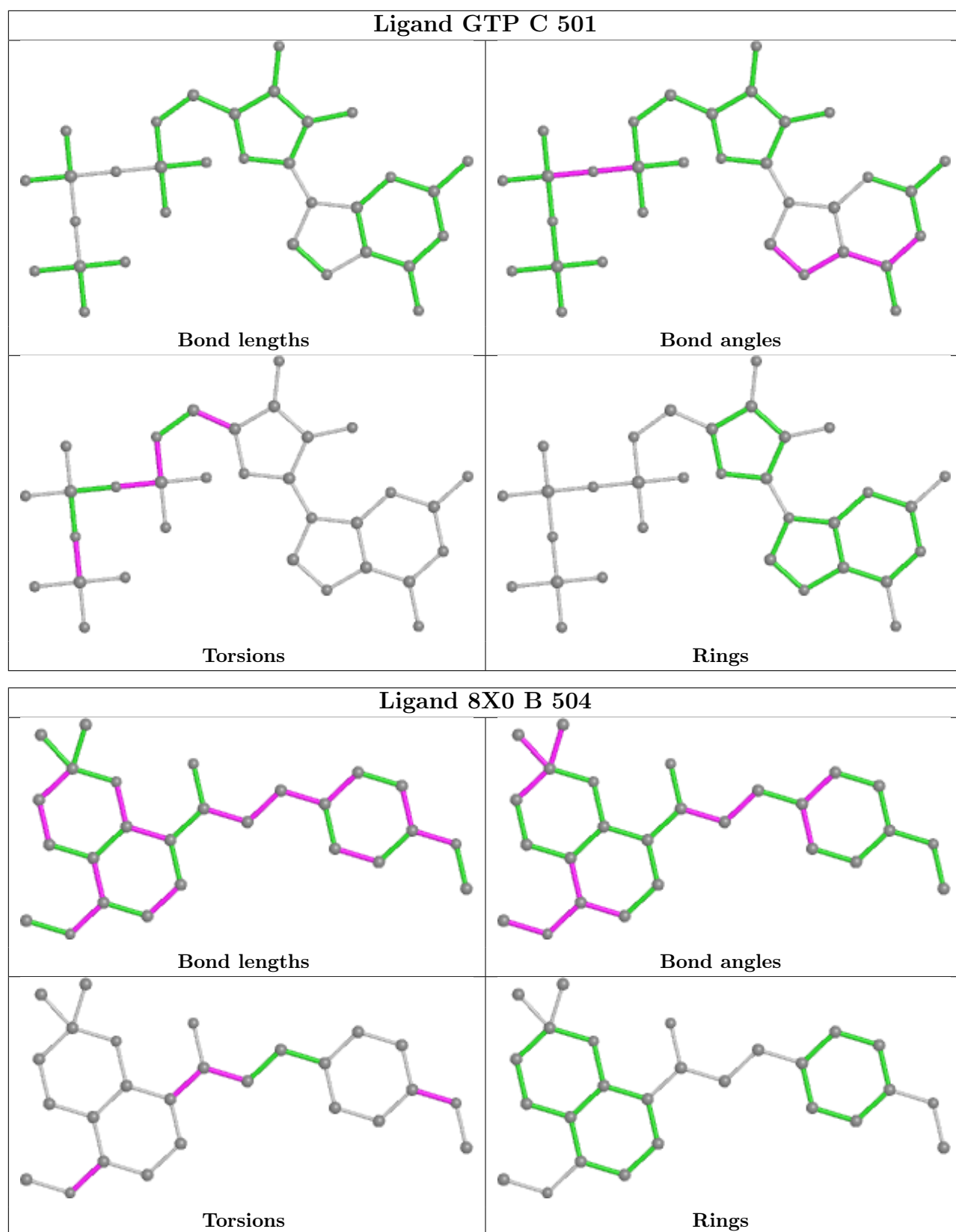
3 monomers are involved in 3 short contacts:

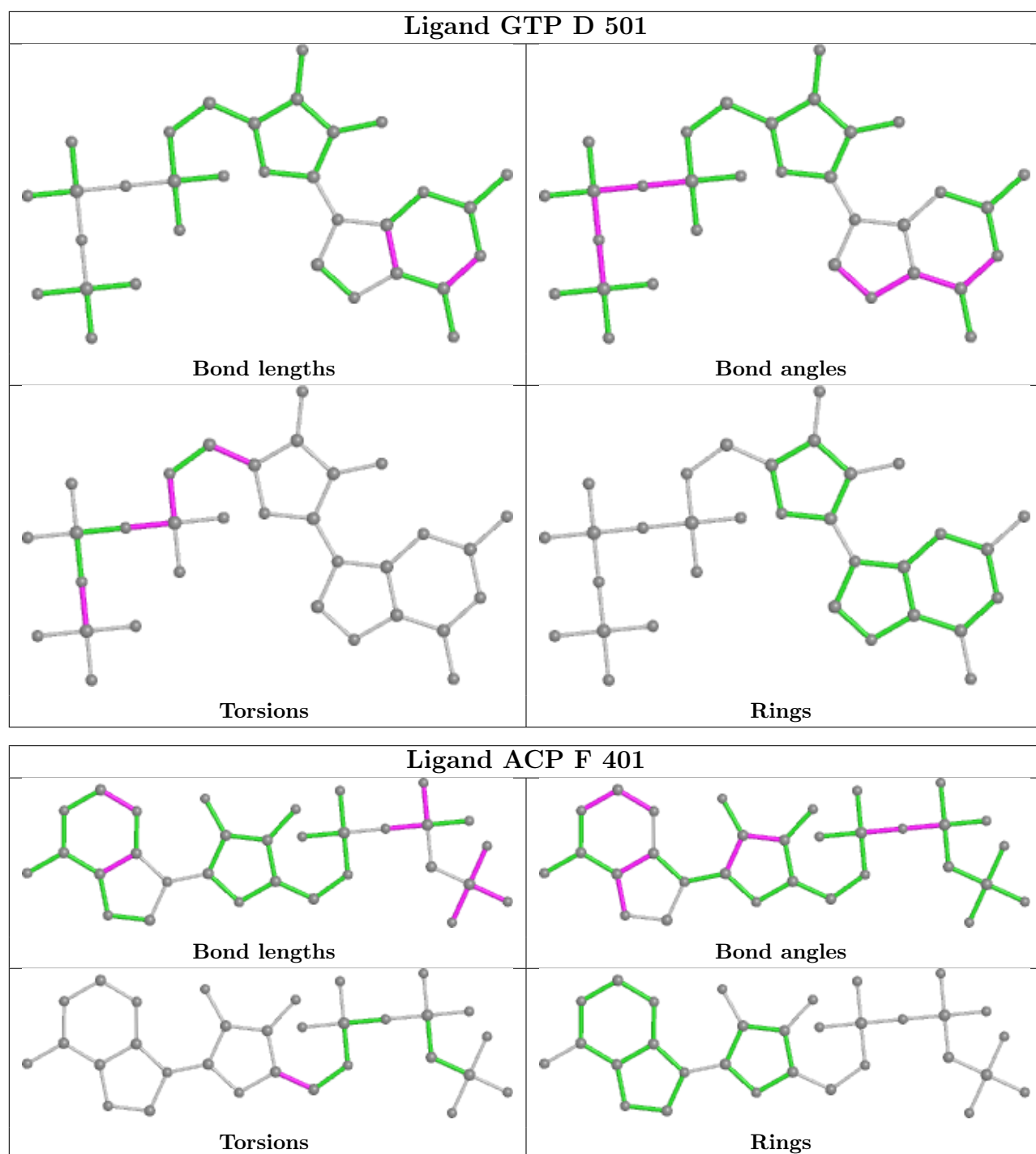
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	1	0
11	D	503	8X0	1	0
12	F	401	ACP	1	0

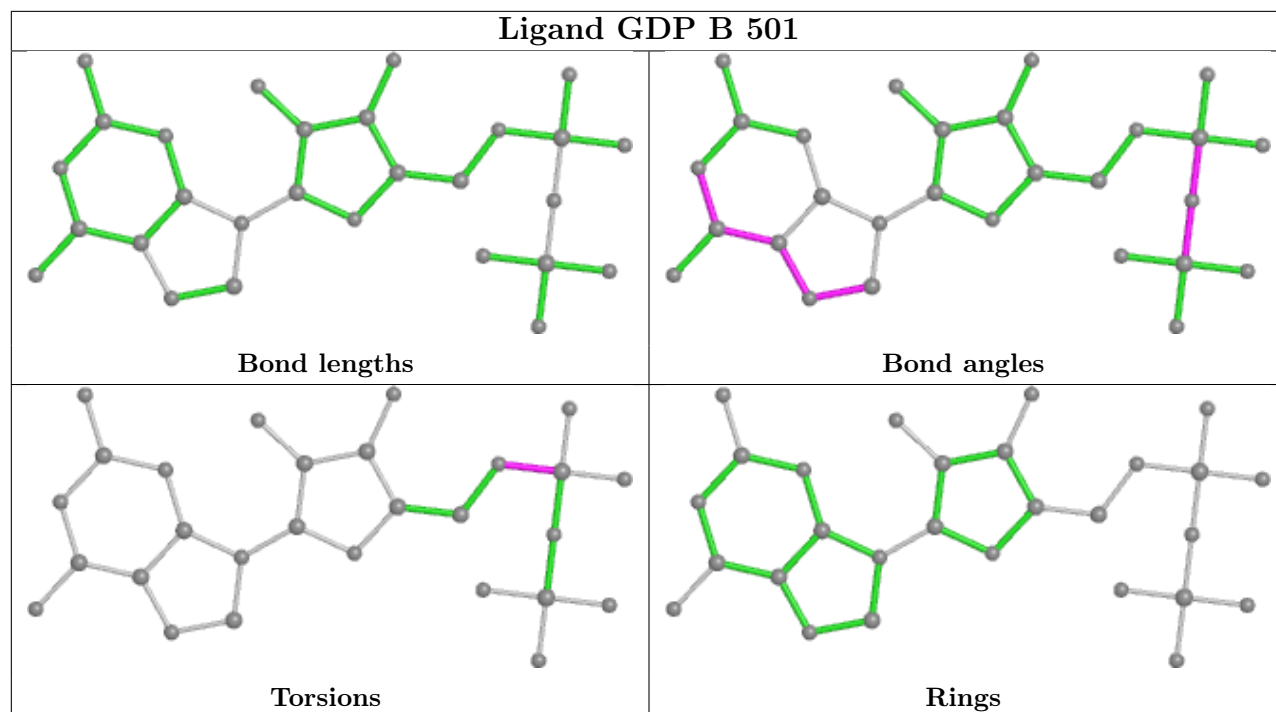
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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	437/451 (96%)	0.17	8 (1%) 68 70	35, 58, 82, 105	0
1	C	440/451 (97%)	-0.19	0 100 100	30, 48, 72, 94	0
2	B	428/445 (96%)	0.16	15 (3%) 44 44	35, 55, 85, 129	0
2	D	421/445 (94%)	0.60	43 (10%) 6 5	45, 79, 114, 136	0
3	E	121/143 (84%)	0.47	11 (9%) 9 7	47, 70, 105, 121	0
4	F	334/384 (86%)	0.73	55 (16%) 1 1	48, 83, 147, 159	0
All	All	2181/2319 (94%)	0.28	132 (6%) 21 20	30, 63, 114, 159	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	7.6
4	F	161	LEU	6.5
2	B	57	ASN	6.5
4	F	133	ALA	6.4
4	F	130	VAL	5.7
4	F	132	LEU	5.7
4	F	100	ILE	5.5
4	F	233	PHE	5.5
4	F	234	GLN	5.2
4	F	176	GLN	5.0
2	D	216	LYS	5.0
4	F	169	LEU	4.9
4	F	244	CYS	4.9
4	F	372	THR	4.9
2	D	245	GLN	4.7
4	F	166	ALA	4.7
2	B	55	THR	4.4
4	F	175	GLU	4.4
4	F	101	TYR	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	136	ASN	4.3
4	F	140	GLU	4.2
4	F	142	ARG	4.1
3	E	25	LYS	4.0
4	F	137	ARG	4.0
4	F	236	LYS	4.0
2	D	218	THR	3.9
3	E	139	LEU	3.9
2	D	1	MET	3.9
2	D	391	ARG	3.9
4	F	170	LEU	3.9
4	F	129	GLU	3.7
4	F	177	GLY	3.7
4	F	131	PHE	3.7
2	B	278	SER	3.7
2	D	175	VAL	3.7
2	B	279	GLN	3.7
4	F	134	ALA	3.7
2	D	390	ARG	3.6
4	F	167	SER	3.6
4	F	178	GLN	3.6
4	F	172	PHE	3.5
2	D	219	THR	3.5
4	F	103	THR	3.5
2	D	37	HIS	3.4
3	E	140	LYS	3.4
3	E	27	PRO	3.3
2	B	277	GLY	3.3
3	E	24	LEU	3.3
4	F	231	ALA	3.2
2	D	396	HIS	3.1
3	E	23	ILE	3.1
4	F	361	LEU	3.0
2	D	217	LEU	3.0
2	D	53	GLU	3.0
2	D	215	LEU	2.9
4	F	232	ASN	2.9
2	D	211	CYS	2.9
2	D	220	PRO	2.9
2	D	55	THR	2.9
3	E	7	GLU	2.8
2	B	56	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	262	TYR	2.8
2	D	126	SER	2.8
4	F	174	ASP	2.7
2	B	58	LYS	2.7
2	D	214	THR	2.7
2	B	54	ALA	2.7
1	A	57	GLY	2.7
4	F	98	TYR	2.7
2	D	244	GLY	2.7
1	A	282	TYR	2.6
1	A	88	HIS	2.6
4	F	182	ILE	2.6
3	E	138	GLU	2.6
2	D	394	PHE	2.6
2	D	94	GLN	2.5
4	F	240	LEU	2.5
2	D	166	THR	2.5
4	F	226	GLU	2.5
3	E	136	ASN	2.5
2	B	282	ARG	2.5
1	A	279	GLU	2.5
2	B	253	LEU	2.5
4	F	141	GLY	2.4
2	D	95	SER	2.4
2	D	44	LEU	2.4
4	F	194	PRO	2.4
4	F	237	THR	2.4
2	D	397	TRP	2.4
2	D	212	PHE	2.4
4	F	225	SER	2.4
2	D	321	MET	2.3
1	A	281	ALA	2.3
2	D	431	ASP	2.3
4	F	138	ARG	2.3
2	D	177	ASP	2.3
2	D	359	ARG	2.3
2	D	405	GLU	2.3
4	F	128	ARG	2.3
4	F	165	GLU	2.3
2	B	280	GLN	2.3
4	F	171	ASP	2.3
3	E	48	GLU	2.3

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
2	D	92	PHE	2.3
2	B	60	VAL	2.3
2	D	39	ASP	2.3
2	D	168	SER	2.2
4	F	179	VAL	2.2
3	E	141	GLU	2.2
4	F	139	ARG	2.2
4	F	380	HIS	2.2
2	D	196	THR	2.2
4	F	256	TYR	2.2
2	D	320	ARG	2.2
2	B	245	GLN	2.2
2	B	246	LEU	2.2
4	F	253	TYR	2.1
2	B	166	THR	2.1
2	D	362	LYS	2.1
4	F	135	TYR	2.1
1	A	430	LYS	2.1
4	F	145	ASN	2.1
2	D	165	ASN	2.1
2	D	284	LEU	2.1
2	D	83	GLN	2.1
2	D	54	ALA	2.1
4	F	235	ASP	2.1
2	D	200	TYR	2.0
4	F	102	PRO	2.0
4	F	21	LEU	2.0
1	A	120	ASP	2.0
2	D	272	PRO	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

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.

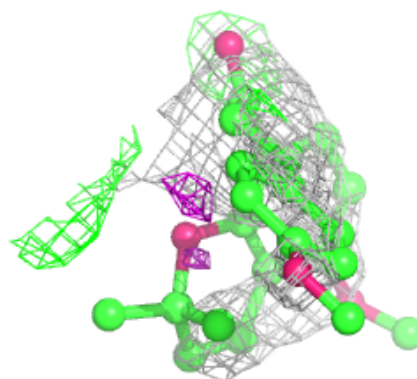
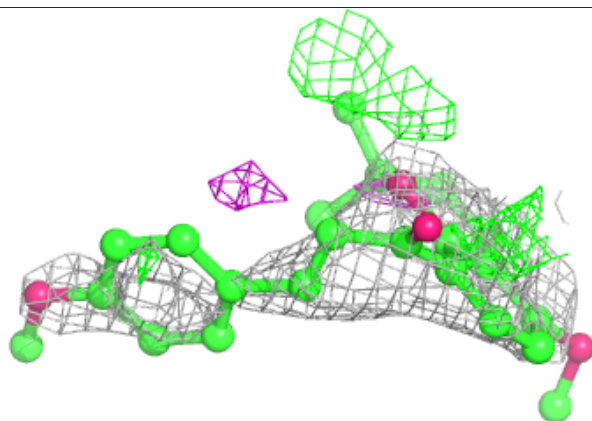
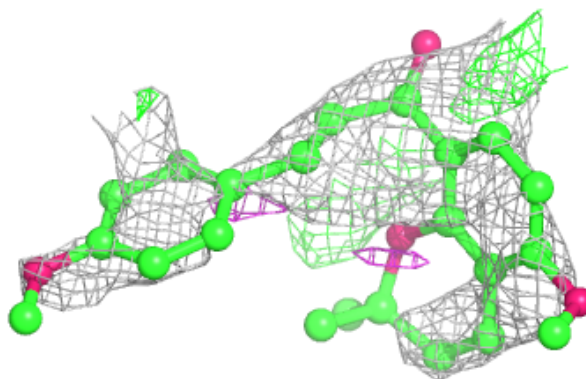
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	8X0	D	503	26/26	0.77	0.42	108,125,137,139	0
7	CA	C	503	1/1	0.83	0.14	64,64,64,64	0
12	ACP	F	401	31/31	0.86	0.20	104,110,133,139	0
10	MES	B	503	12/12	0.88	0.26	85,93,98,100	0
11	8X0	B	504	26/26	0.89	0.33	75,81,86,87	0
5	GTP	D	501	32/32	0.93	0.15	67,73,88,92	0
8	GOL	A	504	6/6	0.93	0.24	73,74,75,76	0
7	CA	A	503	1/1	0.95	0.08	70,70,70,70	0
6	MG	D	502	1/1	0.96	0.05	83,83,83,83	0
6	MG	A	502	1/1	0.97	0.16	34,34,34,34	0
6	MG	B	502	1/1	0.97	0.13	43,43,43,43	0
6	MG	C	502	1/1	0.98	0.16	40,40,40,40	0
9	GDP	B	501	28/28	0.98	0.15	36,41,43,44	0
5	GTP	A	501	32/32	0.98	0.23	37,41,42,44	0
5	GTP	C	501	32/32	0.99	0.16	35,39,40,40	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.

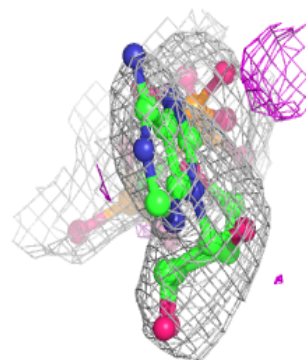
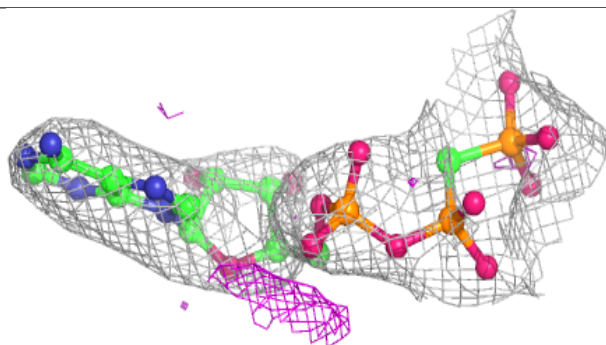
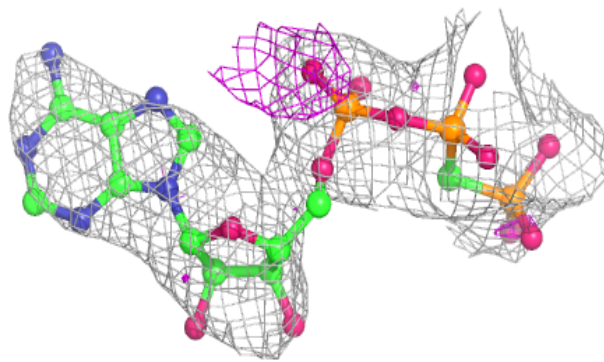


**Electron density around 8X0 D 503:**

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

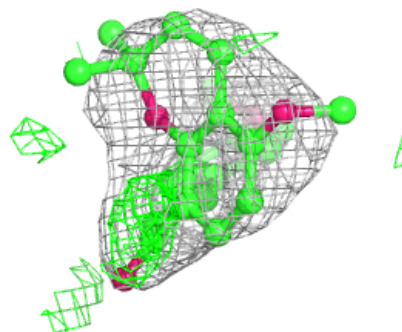
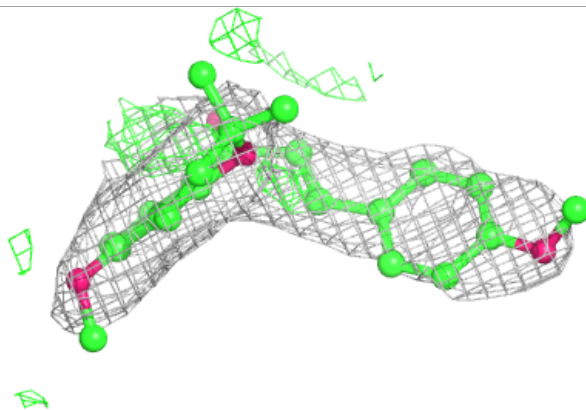
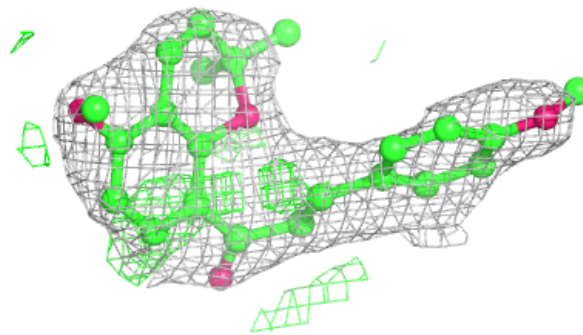
**Electron density around ACP F 401:**

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

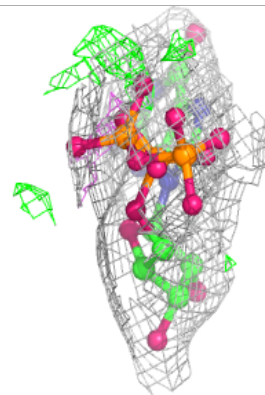
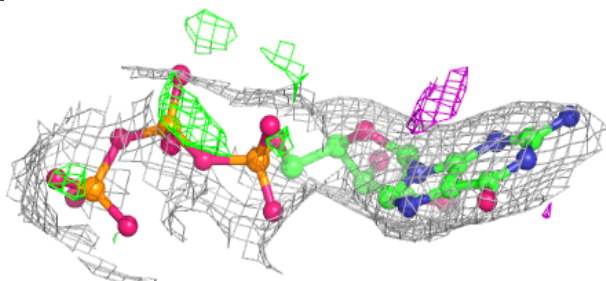
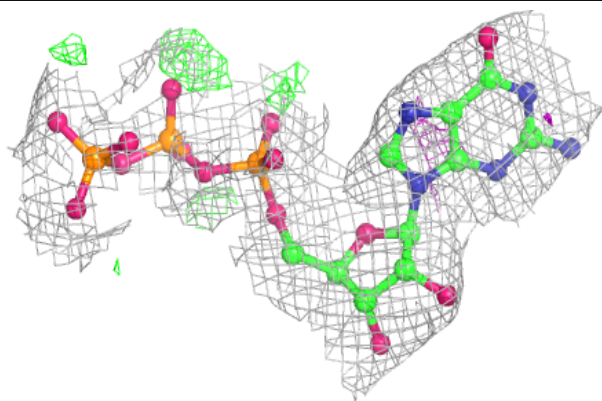


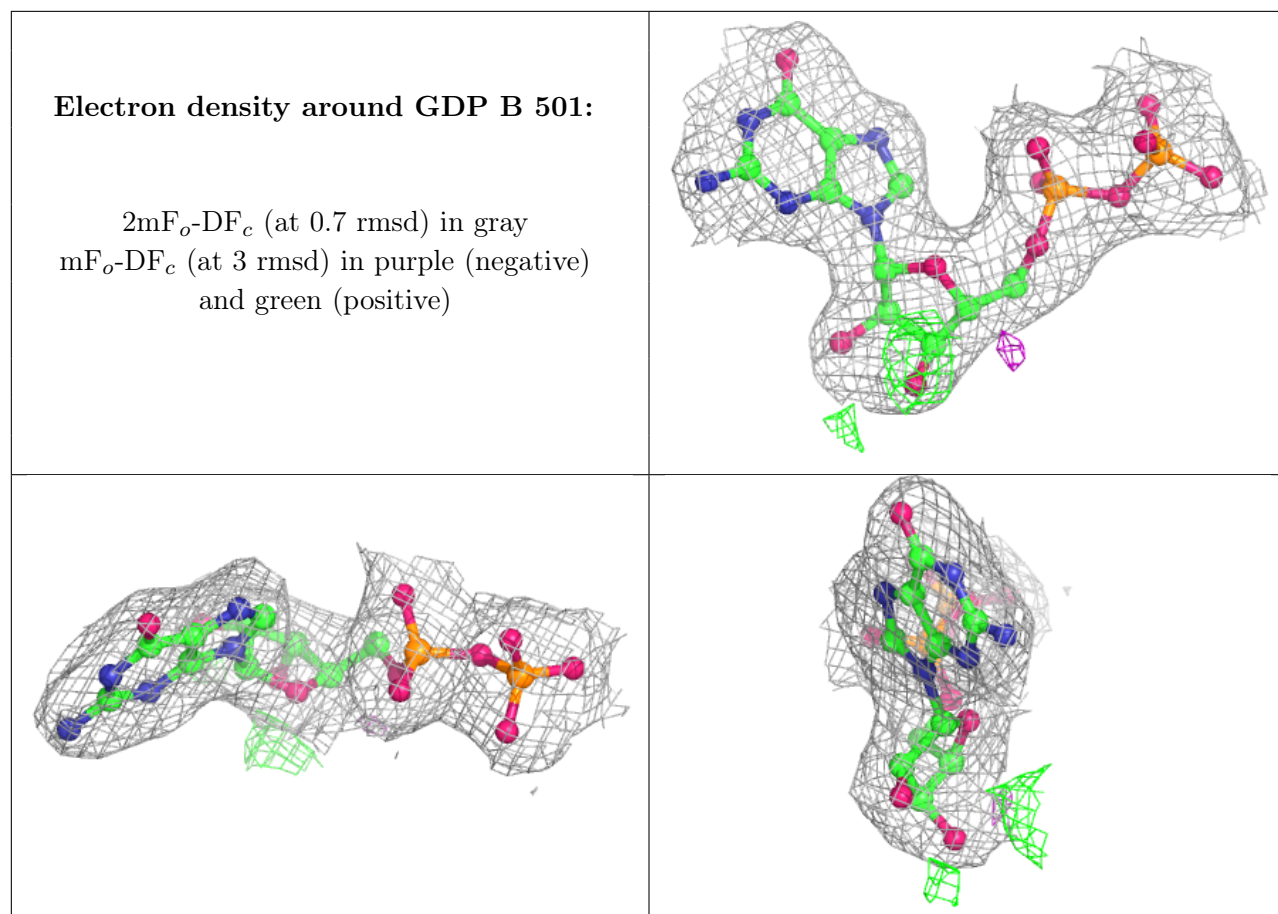
**Electron density around 8X0 B 504:**

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

**Electron density around GTP D 501:**

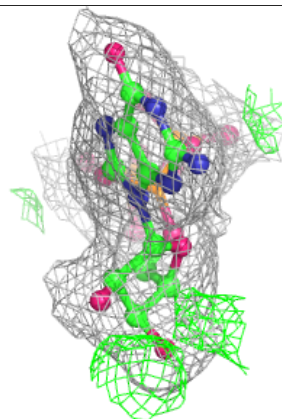
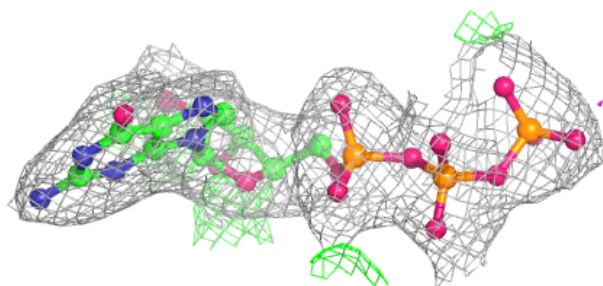
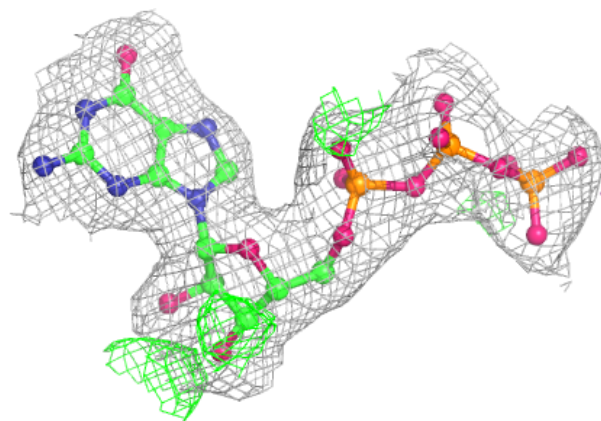
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



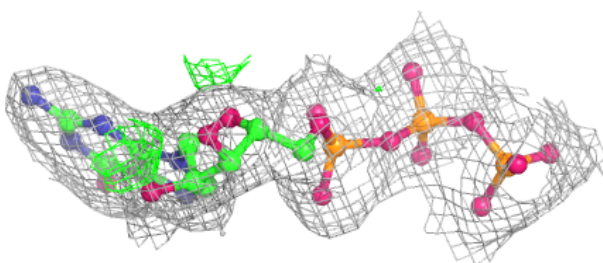
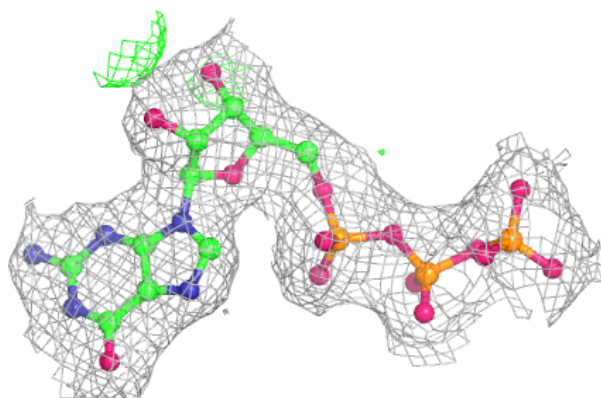


**Electron density around GTP A 501:**

$2mF_o-DF_c$  (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.