



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 03:14 PM JST

PDB ID : 4ZI7  
Title : CRYSTAL STRUCTURE OF TUBULIN-STATHMIN-TTL-HTI286 COMPLEX  
Authors : Wang, Y.; Zhang, R.  
Deposited on : 2015-04-27  
Resolution : 2.51 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>.

---

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

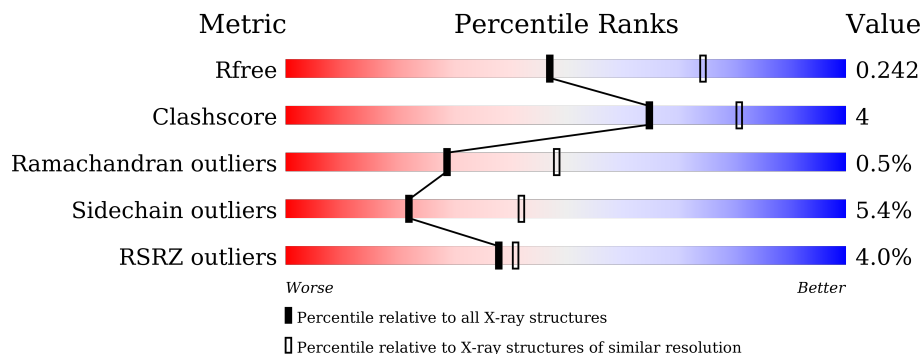
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	143	
4	F	384	

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 17939 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	439	Total	C	N	O	S	0	1	0
			3436	2173	584	656	23			
1	C	440	Total	C	N	O	S	0	2	0
			3452	2183	586	660	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	430	Total	C	N	O	S	0	1	0
			3387	2129	580	652	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	Total	C	N	O	S	0	1	0
			1024	631	186	202	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

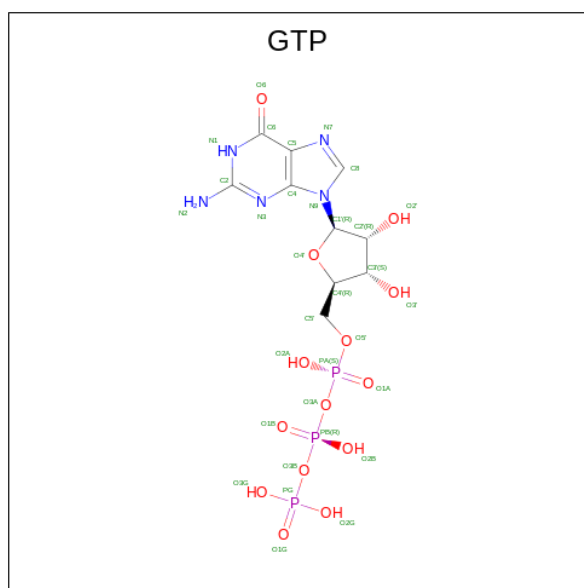
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	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		

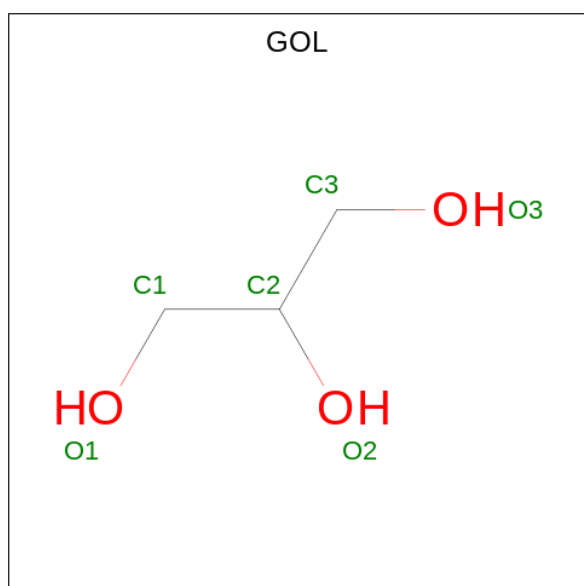
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		
6	D	1	Total	Mg	0	0
			1	1		

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

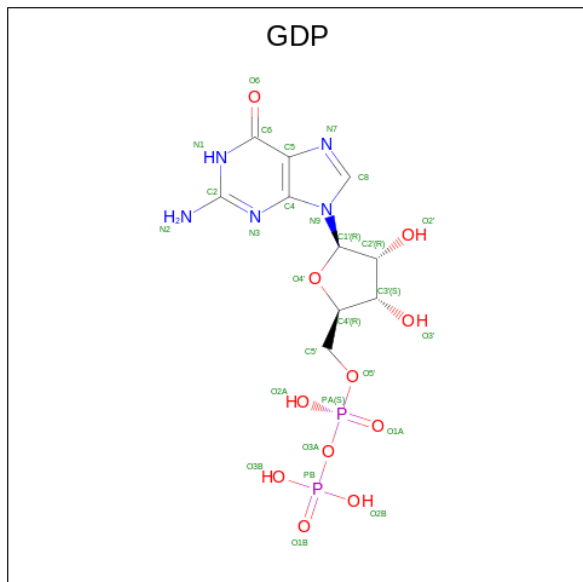
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	2	Total Ca 2 2	0	0

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



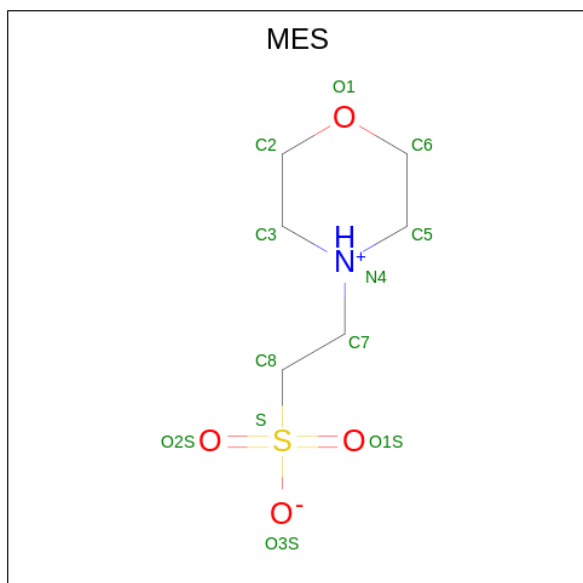
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



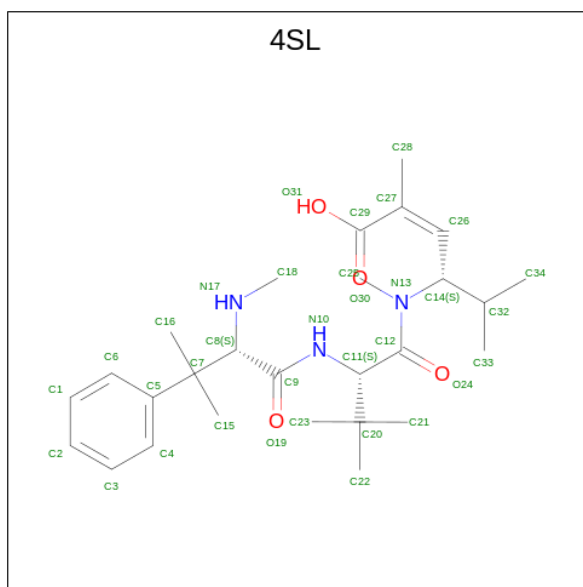
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



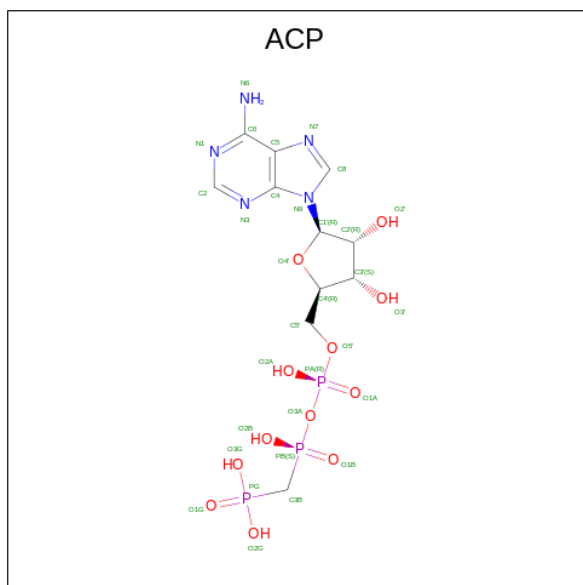
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
10	B	1	12	6	1	4	1	0	0
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is N,beta,beta-trimethyl-L-phenylalanyl-N-[(3S,4Z)-5-carboxy-2-methylhex-4-en-3-yl]-N,3-dimethyl-L-valinamide (three-letter code: 4SL) (formula: C<sub>27</sub>H<sub>43</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	B	1	34	27	3	4	0	0

- 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
			Total	C	N	O	P		
12	F	1	31	11	5	12	3	0	0

- Molecule 13 is water.

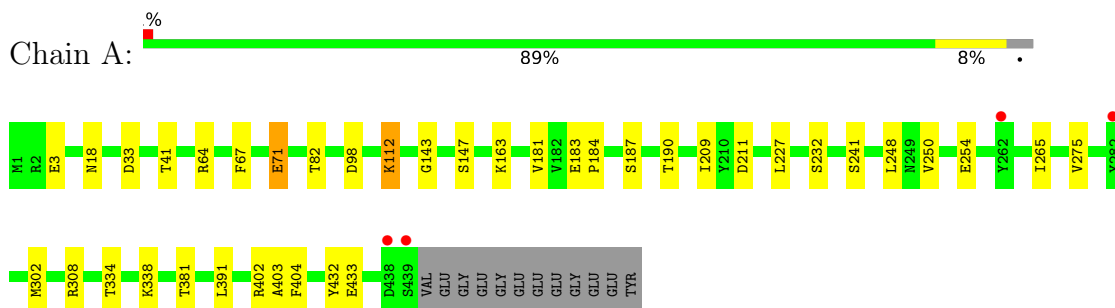
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	51	Total	O	0	0
			51	51		
13	B	47	Total	O	0	0
			47	47		
13	C	86	Total	O	0	0
			86	86		
13	D	13	Total	O	0	0
			13	13		
13	E	2	Total	O	0	0
			2	2		
13	F	16	Total	O	0	0
			16	16		



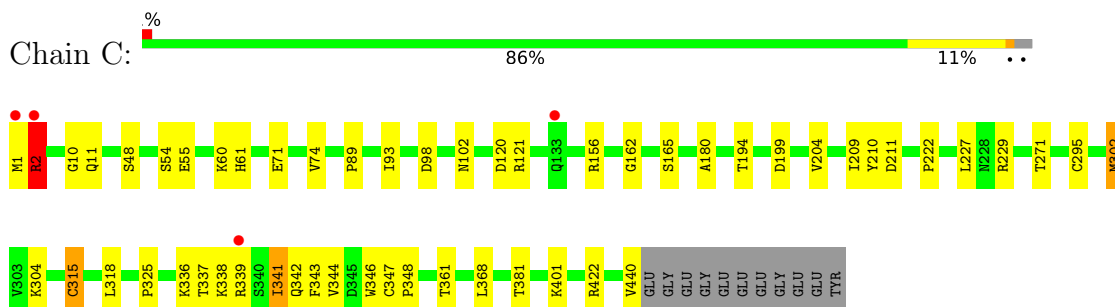
### 3 Residue-property plots [i](#)

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

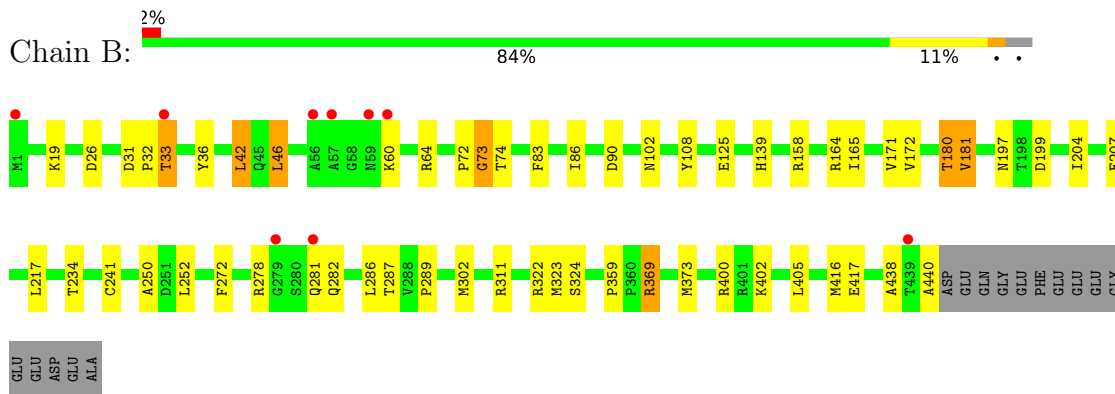
- Molecule 1: Tubulin alpha-1B chain



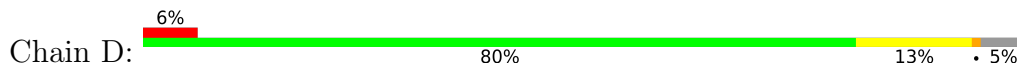
- Molecule 1: Tubulin alpha-1B chain

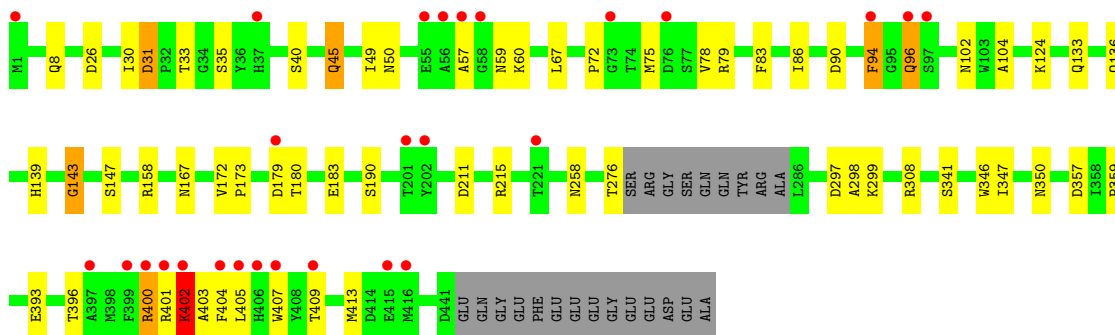


- Molecule 2: Tubulin beta chain

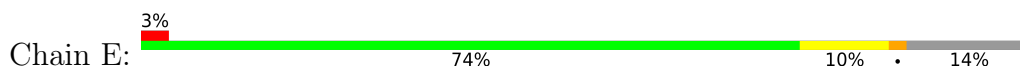


- Molecule 2: Tubulin beta chain

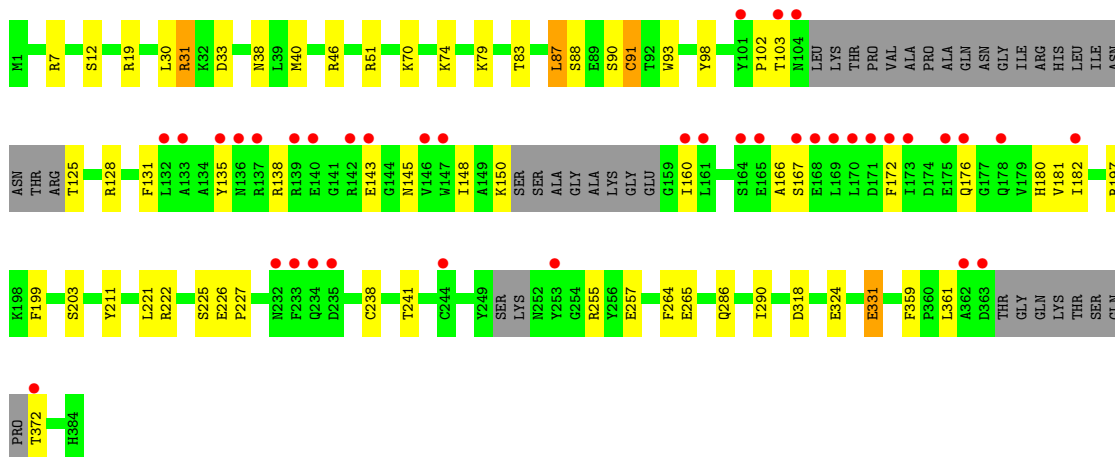
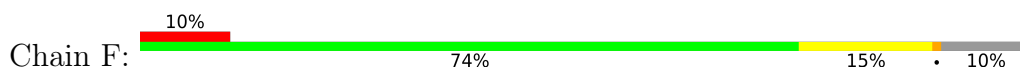




• Molecule 3: Stathmin-4



• 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, $\alpha$ , $\beta$ , $\gamma$	105.37Å 157.34Å 181.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.51 45.59 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.51) 99.6 (45.59-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.183 , 0.239 0.191 , 0.242	Depositor DCC
$R_{free}$ test set	5193 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: CA, 4SL, GTP, MES, GOL, MG, GDP, ACP

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	0.77	0/3514	0.85	2/4770 (0.0%)
1	C	0.86	1/3530 (0.0%)	0.91	5/4794 (0.1%)
2	B	0.83	1/3463 (0.0%)	0.86	3/4692 (0.1%)
2	D	0.71	1/3384 (0.0%)	0.81	3/4586 (0.1%)
3	E	0.76	0/1033	0.84	1/1371 (0.1%)
4	F	0.61	0/2916	0.76	1/3940 (0.0%)
All	All	0.77	3/17840 (0.0%)	0.84	15/24153 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	207	GLU	CD-OE2	6.45	1.32	1.25
2	D	173	PRO	N-CD	5.34	1.55	1.47
1	C	315	CYS	CB-SG	-5.08	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	MET	CB-CG-SD	-6.09	94.12	112.40
2	B	311	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	156	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	D	359	PRO	C-N-CD	5.79	140.56	128.40
2	B	359	PRO	C-N-CD	5.76	140.51	128.40
1	C	422	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	C	211	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	308	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	B	172	VAL	C-N-CD	5.41	139.77	128.40
1	A	402	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	229	ARG	NE-CZ-NH1	-5.25	117.68	120.30
3	E	76	ARG	NE-CZ-NH1	5.23	122.91	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	51	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	D	158	ARG	NE-CZ-NH2	5.05	122.82	120.30
2	D	172	VAL	C-N-CD	5.04	138.97	128.40

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	3436	0	3344	16	0
1	C	3452	0	3359	29	0
2	B	3387	0	3266	36	0
2	D	3311	0	3192	31	0
3	E	1024	0	1035	9	0
4	F	2849	0	2796	25	0
5	A	32	0	12	1	0
5	C	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	B	1	0	0	0	0
7	C	2	0	0	0	0
8	A	24	0	32	1	0
8	B	6	0	8	0	0
8	C	12	0	16	3	0
8	F	6	0	8	0	0
9	B	28	0	12	2	0
9	D	28	0	12	3	0
10	B	24	0	26	2	0
11	B	34	0	0	0	0
12	F	31	0	14	2	0
13	A	51	0	0	0	0
13	B	47	0	0	4	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	86	0	0	2	0
13	D	13	0	0	2	0
13	E	2	0	0	0	0
13	F	16	0	0	0	0
All	All	17939	0	17144	144	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 (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:SER:O	2:D:45:GLN:HG3	1.60	1.02
2:D:33:THR:OG1	2:D:60:LYS:NZ	2.05	0.90
2:D:40:SER:O	2:D:45:GLN:CG	2.20	0.89
1:C:336:LYS:HE2	13:C:676:HOH:O	1.71	0.88
2:B:26:ASP:OD1	2:B:369:ARG:NH1	2.09	0.85
2:D:33:THR:CB	2:D:60:LYS:NZ	2.40	0.85
2:B:36:TYR:CE1	2:B:46:LEU:HD21	2.12	0.84
9:B:501:GDP:O3B	13:B:601:HOH:O	1.96	0.82
3:E:124:GLN:HE21	3:E:124:GLN:HA	1.44	0.82
9:D:501:GDP:O3B	13:D:601:HOH:O	1.99	0.80
2:D:33:THR:HB	2:D:60:LYS:NZ	1.98	0.79
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.16	0.77
2:B:36:TYR:CE1	2:B:46:LEU:CD2	2.68	0.75
2:D:33:THR:HB	2:D:60:LYS:HZ2	1.56	0.70
2:B:26:ASP:CG	2:B:369:ARG:NH1	2.46	0.69
9:D:501:GDP:O3B	13:D:602:HOH:O	2.12	0.67
2:D:401:ARG:O	2:D:403:ALA:N	2.28	0.65
3:E:124:GLN:HE21	3:E:124:GLN:CA	2.10	0.64
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.80	0.63
2:B:83:PHE:O	2:B:86:ILE:HG22	1.99	0.63
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.33	0.63
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.81	0.63
2:B:199:ASP:OD2	10:B:504:MES:H52	1.99	0.63
2:B:36:TYR:CZ	2:B:46:LEU:CD2	2.83	0.62
2:D:136:GLN:HA	2:D:167:ASN:O	2.00	0.62
2:B:36:TYR:CZ	2:B:46:LEU:HD21	2.35	0.61
2:B:26:ASP:OD2	2:B:369:ARG:NH1	2.33	0.61
4:F:88:SER:HG	4:F:90:SER:HG	1.28	0.61
2:D:297:ASP:OD1	2:D:298:ALA:N	2.34	0.61

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:131:GLU:HA	3:E:131:GLU:OE2	2.01	0.60
2:B:26:ASP:CG	2:B:369:ARG:HH11	2.05	0.60
1:C:204:VAL:HG22	1:C:302:MET:CE	2.31	0.59
2:B:72:PRO:O	2:B:73:GLY:C	2.41	0.59
1:C:1:MET:O	1:C:2:ARG:HB2	2.04	0.58
1:C:165:SER:HA	1:C:199:ASP:OD2	2.05	0.57
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.88	0.56
2:B:33:THR:O	2:B:60:LYS:HE3	2.07	0.54
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.90	0.54
2:B:164:ARG:HD2	13:B:641:HOH:O	2.06	0.54
4:F:87:LEU:O	4:F:88:SER:OG	2.26	0.54
9:B:501:GDP:O1A	13:B:602:HOH:O	2.19	0.54
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.43	0.53
2:D:33:THR:CB	2:D:60:LYS:HZ1	2.20	0.53
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.26	0.53
1:C:339:ARG:O	1:C:339:ARG:HG3	2.08	0.53
1:C:346:TRP:CZ3	1:C:347[A]:CYS:SG	3.01	0.53
2:D:40:SER:O	2:D:45:GLN:HG2	2.07	0.53
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.45	0.52
2:B:241:CYS:O	2:B:250:ALA:HA	2.10	0.52
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.92	0.52
1:A:147:SER:HB2	1:A:190:THR:HB	1.92	0.51
1:C:194:THR:O	1:C:194:THR:HG22	2.10	0.51
4:F:331:GLU:OE2	12:F:401:ACP:O1B	2.28	0.51
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.94	0.50
3:E:124:GLN:CA	3:E:124:GLN:NE2	2.73	0.50
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.45	0.50
1:C:271:THR:HG21	1:C:295:CYS:O	2.11	0.50
2:D:31:ASP:OD1	2:D:31:ASP:C	2.49	0.50
2:D:83:PHE:O	2:D:86:ILE:HG22	2.12	0.49
1:A:183:GLU:N	1:A:184:PRO:CD	2.74	0.49
2:B:440:ALA:HB3	4:F:31:ARG:HH22	1.78	0.49
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.47	0.49
8:C:506:GOL:HO3	8:C:506:GOL:HO1	1.54	0.48
4:F:128:ARG:O	4:F:131:PHE:HB3	2.13	0.48
1:C:304:LYS:HE3	8:C:505:GOL:H31	1.96	0.48
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.96	0.48
2:D:33:THR:CB	2:D:60:LYS:HZ2	2.17	0.48
4:F:222:ARG:O	4:F:241:THR:HB	2.13	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.48
1:C:204:VAL:HG13	1:C:302:MET:HE2	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.96	0.47
4:F:88:SER:OG	4:F:90:SER:OG	2.11	0.47
1:C:194:THR:O	1:C:194:THR:CG2	2.62	0.47
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.15	0.47
2:D:211:ASP:O	2:D:215:ARG:HB2	2.14	0.47
4:F:98:TYR:HB2	4:F:182:ILE:HG22	1.97	0.47
1:A:241:SER:HB2	1:A:248:LEU:O	2.15	0.47
4:F:19:ARG:HB3	4:F:19:ARG:NH1	2.29	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.47
1:A:209:ILE:HD11	1:A:302:MET:SD	2.55	0.46
1:A:403:ALA:O	1:A:404:PHE:HB2	2.15	0.46
2:B:181:VAL:HG23	1:C:348:PRO:CG	2.45	0.46
2:B:36:TYR:CE1	2:B:46:LEU:HD22	2.51	0.46
2:B:19:LYS:HB2	2:B:19:LYS:HE2	1.70	0.46
3:E:131:GLU:OE2	3:E:131:GLU:CA	2.63	0.46
2:D:393:GLU:O	2:D:396:THR:HG22	2.16	0.46
1:C:304:LYS:HG3	8:C:505:GOL:H12	1.97	0.46
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.46
4:F:172:PHE:O	4:F:176:GLN:HG2	2.17	0.45
4:F:264:PHE:O	4:F:265:GLU:C	2.53	0.45
2:B:234:THR:HG1	2:B:272[B]:PHE:HD2	1.64	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.45
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.17	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.45
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.16	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.45
2:D:72:PRO:HG3	2:D:96:GLN:HA	1.99	0.45
1:C:341:ILE:HD11	1:C:343:PHE:CE1	2.52	0.45
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.99	0.45
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.17	0.44
3:E:137:LYS:O	3:E:137:LYS:HG2	2.16	0.44
1:A:433:GLU:OE2	4:F:46:ARG:NH1	2.49	0.44
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.99	0.44
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.99	0.44
2:B:180:THR:HB	13:C:619:HOH:O	2.18	0.44
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.22	0.43
2:B:286:LEU:HD12	2:B:286:LEU:N	2.33	0.43
2:D:67:LEU:CD2	2:D:78:VAL:HG11	2.48	0.43
1:C:11:GLN:HG3	1:C:74:VAL:HG21	2.01	0.43
4:F:286:GLN:O	4:F:290:ILE:HG13	2.17	0.43
4:F:74:LYS:HB3	4:F:181:VAL:HG21	2.00	0.43

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:O	8:A:505:GOL:H12	2.18	0.43
2:B:42:LEU:HD12	2:B:42:LEU:HA	1.81	0.43
2:B:369:ARG:CZ	2:B:369:ARG:HB2	2.48	0.42
1:C:102:ASN:C	1:C:102:ASN:OD1	2.58	0.42
2:D:102:ASN:OD1	2:D:102:ASN:C	2.58	0.42
2:B:74:THR:HB	13:B:607:HOH:O	2.20	0.42
4:F:79:LYS:O	4:F:83:THR:OG1	2.32	0.42
2:B:287:THR:HB	2:B:289:PRO:HD2	2.01	0.42
2:B:323:MET:HB3	2:B:373:MET:HE1	2.01	0.42
2:B:272[B]:PHE:CD2	2:B:302:MET:HE3	2.55	0.42
1:C:10:GLY:O	1:C:11:GLN:C	2.58	0.42
4:F:150:LYS:N	4:F:181:VAL:O	2.50	0.42
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.20	0.42
1:A:112:LYS:HG3	3:E:54:LEU:HD13	2.02	0.42
1:C:55:GLU:HA	1:C:60:LYS:O	2.19	0.42
1:C:1:MET:O	1:C:2:ARG:CB	2.67	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.51	0.41
4:F:138:ARG:HB2	4:F:145:ASN:ND2	2.35	0.41
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.56	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.50	0.41
2:B:158:ARG:NH1	2:B:197:ASN:OD1	2.52	0.41
2:D:400:ARG:HG3	2:D:401:ARG:N	2.36	0.41
2:B:102:ASN:OD1	2:B:102:ASN:C	2.60	0.40
2:D:104:ALA:HB2	2:D:413:MET:SD	2.61	0.40
2:D:147:SER:HB2	2:D:190:SER:OG	2.21	0.40
1:C:54:SER:O	1:C:61:HIS:HA	2.21	0.40
2:D:402:LYS:O	2:D:405:LEU:HB2	2.20	0.40
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.15	0.40
1:A:67:PHE:CD1	1:A:67:PHE:N	2.90	0.40
3:E:76:ARG:O	3:E:80:ARG:HG3	2.21	0.40
2:D:180:THR:HB	2:D:183:GLU:HG3	2.04	0.40
2:B:199:ASP:OD1	10:B:504:MES:H32	2.22	0.40
2:D:57:ALA:C	2:D:59:ASN:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/451 (97%)	422 (96%)	16 (4%)	0	100	100
1	C	440/451 (98%)	431 (98%)	8 (2%)	1 (0%)	47	68
2	B	429/445 (96%)	418 (97%)	9 (2%)	2 (0%)	29	48
2	D	418/445 (94%)	396 (95%)	19 (4%)	3 (1%)	22	39
3	E	120/143 (84%)	114 (95%)	5 (4%)	1 (1%)	19	35
4	F	336/384 (88%)	304 (90%)	29 (9%)	3 (1%)	17	31
All	All	2181/2319 (94%)	2085 (96%)	86 (4%)	10 (0%)	29	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	GLY
2	D	402	LYS
3	E	27	PRO
1	C	2	ARG
2	D	404	PHE
4	F	102	PRO
4	F	91	CYS
4	F	227	PRO
2	B	438	ALA
2	D	143	GLY

### 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	371/379 (98%)	358 (96%)	13 (4%)	36	62
1	C	373/379 (98%)	358 (96%)	15 (4%)	31	56
2	B	370/381 (97%)	352 (95%)	18 (5%)	25	47
2	D	363/381 (95%)	338 (93%)	25 (7%)	15	30
3	E	111/127 (87%)	100 (90%)	11 (10%)	8	15
4	F	312/342 (91%)	291 (93%)	21 (7%)	16	31
All	All	1900/1989 (96%)	1797 (95%)	103 (5%)	22	42

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	33	ASP
1	A	41	THR
1	A	71	GLU
1	A	82	THR
1	A	112	LYS
1	A	163	LYS
1	A	181	VAL
1	A	211	ASP
1	A	232	SER
1	A	334	THR
1	A	338	LYS
1	A	381	THR
2	B	33	THR
2	B	42	LEU
2	B	46	LEU
2	B	90	ASP
2	B	139	HIS
2	B	180	THR
2	B	181	VAL
2	B	217	LEU
2	B	278	ARG
2	B	281	GLN
2	B	282	GLN
2	B	322	ARG
2	B	324	SER
2	B	369	ARG
2	B	400	ARG
2	B	402	LYS
2	B	405	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	416	MET
1	C	2	ARG
1	C	48	SER
1	C	89	PRO
1	C	120	ASP
1	C	315	CYS
1	C	318	LEU
1	C	325	PRO
1	C	337	THR
1	C	338	LYS
1	C	341	ILE
1	C	342	GLN
1	C	361	THR
1	C	368	LEU
1	C	381	THR
1	C	440	VAL
2	D	8	GLN
2	D	26	ASP
2	D	30	ILE
2	D	31	ASP
2	D	35	SER
2	D	45	GLN
2	D	49	ILE
2	D	50	ASN
2	D	79	ARG
2	D	90	ASP
2	D	94	PHE
2	D	96	GLN
2	D	124	LYS
2	D	133	GLN
2	D	139	HIS
2	D	179	ASP
2	D	276	THR
2	D	299	LYS
2	D	308	ARG
2	D	341	SER
2	D	357	ASP
2	D	400	ARG
2	D	402	LYS
2	D	407	TRP
2	D	409	THR
3	E	25	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	E	44	ASP
3	E	53	LYS
3	E	77	GLU
3	E	92	ASN
3	E	95	LYS
3	E	124	GLN
3	E	125	GLU
3	E	127	ASP
3	E	131	GLU
3	E	140	LYS
4	F	12	SER
4	F	30	LEU
4	F	31	ARG
4	F	33	ASP
4	F	70	LYS
4	F	87	LEU
4	F	103	THR
4	F	125	THR
4	F	143	GLU
4	F	167	SER
4	F	180	HIS
4	F	203	SER
4	F	211	TYR
4	F	225	SER
4	F	226	GLU
4	F	238	CYS
4	F	255	ARG
4	F	324	GLU
4	F	331	GLU
4	F	361	LEU
4	F	372	THR

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

Mol	Chain	Res	Type
3	E	124	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	GOL	B	506	-	5,5,5	0.48	0	5,5,5	0.40	0
8	GOL	A	504	-	5,5,5	0.40	0	5,5,5	0.08	0
5	GTP	A	501	6	26,34,34	1.27	3 (11%)	32,54,54	1.36	6 (18%)
5	GTP	C	502	6	26,34,34	1.15	2 (7%)	32,54,54	1.37	5 (15%)
8	GOL	C	506	-	5,5,5	0.38	0	5,5,5	0.50	0
9	GDP	D	501	6	24,30,30	0.91	1 (4%)	30,47,47	1.49	7 (23%)
11	4SL	B	507	-	31,34,34	3.28	6 (19%)	40,50,50	1.37	8 (20%)
8	GOL	A	505	-	5,5,5	0.40	0	5,5,5	0.99	0
8	GOL	C	505	-	5,5,5	0.77	0	5,5,5	0.84	0
8	GOL	F	402	-	5,5,5	0.78	0	5,5,5	0.47	0
10	MES	B	504	-	12,12,12	2.00	2 (16%)	14,16,16	6.37	10 (71%)
9	GDP	B	501	6	24,30,30	1.39	4 (16%)	30,47,47	1.40	4 (13%)
8	GOL	A	506	-	5,5,5	0.55	0	5,5,5	0.22	0
10	MES	B	505	-	12,12,12	2.30	1 (8%)	14,16,16	1.74	3 (21%)
12	ACP	F	401	-	27,33,33	2.02	7 (25%)	32,52,52	1.29	5 (15%)
8	GOL	A	507	-	5,5,5	0.75	0	5,5,5	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	506	-	-	3/4/4/4	-
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
5	GTP	C	502	6	-	6/18/38/38	0/3/3/3
8	GOL	C	506	-	-	2/4/4/4	-
9	GDP	D	501	6	-	4/12/32/32	0/3/3/3
11	4SL	B	507	-	-	7/52/52/52	0/1/1/1
8	GOL	A	505	-	-	0/4/4/4	-
8	GOL	C	505	-	-	2/4/4/4	-
8	GOL	F	402	-	-	2/4/4/4	-
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
8	GOL	A	506	-	-	2/4/4/4	-
10	MES	B	505	-	-	5/6/14/14	0/1/1/1
12	ACP	F	401	-	-	3/15/38/38	0/3/3/3
8	GOL	A	507	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	4SL	C26-C27	14.19	1.52	1.33
11	B	507	4SL	C7-C5	-8.32	1.39	1.54
10	B	505	MES	C8-S	-7.31	1.67	1.77
12	F	401	ACP	PG-O1G	5.79	1.62	1.50
10	B	504	MES	C8-S	-5.64	1.69	1.77
12	F	401	ACP	PB-O3A	4.96	1.63	1.58
11	B	507	4SL	C29-C27	-4.48	1.38	1.49
5	A	501	GTP	C6-N1	-3.45	1.32	1.37
9	B	501	GDP	O4'-C1'	3.31	1.45	1.41
9	B	501	GDP	C2'-C1'	-3.24	1.48	1.53
5	C	502	GTP	C6-N1	-3.17	1.33	1.37
12	F	401	ACP	PG-O3G	3.09	1.62	1.54
11	B	507	4SL	C11-C12	2.98	1.58	1.53
10	B	504	MES	O2S-S	2.95	1.53	1.45
12	F	401	ACP	C5-C4	2.95	1.48	1.40
11	B	507	4SL	C32-C14	2.75	1.57	1.54
5	A	501	GTP	C2'-C1'	-2.62	1.49	1.53
9	B	501	GDP	C6-N1	-2.58	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PG-O2G	-2.49	1.49	1.54
12	F	401	ACP	PB-O2B	2.43	1.62	1.56
9	B	501	GDP	C2-N1	-2.33	1.31	1.37
5	C	502	GTP	O6-C6	2.20	1.27	1.23
12	F	401	ACP	C2-N3	2.16	1.35	1.32
5	A	501	GTP	C2-N1	-2.12	1.32	1.37
11	B	507	4SL	O30-C29	2.08	1.28	1.22
9	D	501	GDP	C8-N7	2.05	1.38	1.35

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O3S-S-O1S	-12.76	80.09	111.27
10	B	504	MES	O3S-S-O2S	-11.39	83.45	111.27
10	B	504	MES	O2S-S-C8	9.71	118.61	106.92
10	B	504	MES	O1S-S-C8	8.75	117.45	106.92
10	B	504	MES	O3S-S-C8	-7.57	93.52	105.77
10	B	505	MES	O1S-S-C8	4.02	111.75	106.92
10	B	504	MES	C6-C5-N4	3.73	115.75	110.10
11	B	507	4SL	O30-C29-C27	-3.47	112.96	122.11
9	B	501	GDP	C5-C6-N1	3.46	120.06	113.95
5	C	502	GTP	PA-O3A-PB	-3.40	121.16	132.83
10	B	504	MES	C2-C3-N4	3.34	115.16	110.10
12	F	401	ACP	N3-C2-N1	-3.33	123.48	128.68
9	B	501	GDP	O6-C6-C5	-3.09	118.34	124.37
5	C	502	GTP	PB-O3B-PG	-3.08	122.25	132.83
9	D	501	GDP	C5-C6-N1	2.97	119.20	113.95
9	D	501	GDP	C8-N7-C5	2.92	108.56	102.99
9	D	501	GDP	O3B-PB-O1B	2.87	121.93	110.68
10	B	505	MES	C2-C3-N4	-2.86	105.77	110.10
12	F	401	ACP	O2G-PG-C3B	2.83	113.25	106.40
5	A	501	GTP	C5-C6-N1	2.79	118.87	113.95
5	C	502	GTP	C8-N7-C5	2.76	108.26	102.99
9	B	501	GDP	O3B-PB-O2B	2.75	118.13	107.64
10	B	504	MES	C5-N4-C3	2.74	115.00	108.83
9	B	501	GDP	PA-O3A-PB	-2.67	123.66	132.83
10	B	504	MES	C6-O1-C2	2.63	118.68	109.89
5	A	501	GTP	O6-C6-C5	-2.62	119.26	124.37
11	B	507	4SL	C16-C7-C15	2.56	110.56	107.43
5	A	501	GTP	C8-N7-C5	2.56	107.86	102.99
5	A	501	GTP	O4'-C1'-C2'	2.51	110.59	106.93
5	C	502	GTP	O3'-C3'-C4'	-2.43	104.03	111.05

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	PA-O3A-PB	-2.42	124.53	132.83
10	B	504	MES	O2S-S-O1S	2.37	122.16	113.95
11	B	507	4SL	C32-C14-N13	-2.37	108.23	112.83
5	A	501	GTP	PA-O3A-PB	-2.36	124.72	132.83
11	B	507	4SL	C28-C27-C29	-2.34	112.05	115.69
12	F	401	ACP	C2-N1-C6	2.32	122.72	118.75
5	C	502	GTP	O2'-C2'-C3'	2.28	119.20	111.82
9	D	501	GDP	C2'-C3'-C4'	2.25	107.01	102.64
11	B	507	4SL	C7-C8-C9	-2.19	110.79	112.80
5	A	501	GTP	O3G-PG-O3B	-2.18	97.32	104.64
10	B	505	MES	C7-N4-C3	-2.18	105.66	111.23
11	B	507	4SL	C26-C27-C29	2.17	122.40	119.51
11	B	507	4SL	C4-C5-C7	-2.16	117.62	121.39
9	D	501	GDP	C2-N1-C6	-2.14	121.16	125.10
12	F	401	ACP	C3'-C2'-C1'	2.11	104.15	100.98
9	D	501	GDP	O6-C6-C5	-2.09	120.29	124.37
11	B	507	4SL	O31-C29-O30	2.09	128.38	123.61
12	F	401	ACP	C4-C5-N7	-2.01	107.31	109.40

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O1A
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O1S
10	B	505	MES	C7-C8-S-O2S
11	B	507	4SL	C26-C14-C32-C34
11	B	507	4SL	C26-C14-C32-C33
11	B	507	4SL	N13-C14-C32-C34
11	B	507	4SL	C26-C14-N13-C12
11	B	507	4SL	C26-C14-N13-C25
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
8	A	504	GOL	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	B	505	MES	C7-C8-S-O3S
8	A	506	GOL	O1-C1-C2-C3
8	A	507	GOL	C1-C2-C3-O3
8	B	506	GOL	O1-C1-C2-C3
8	C	505	GOL	O1-C1-C2-C3
8	C	506	GOL	C1-C2-C3-O3
8	A	506	GOL	O1-C1-C2-O2
8	B	506	GOL	O1-C1-C2-O2
10	B	504	MES	N4-C7-C8-S
10	B	505	MES	C8-C7-N4-C3
8	F	402	GOL	O2-C2-C3-O3
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C3'-C4'-C5'-O5'
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O2S
11	B	507	4SL	N13-C14-C32-C33
8	C	505	GOL	O1-C1-C2-O2
11	B	507	4SL	C32-C14-N13-C25
5	C	502	GTP	PB-O3B-PG-O1G
5	C	502	GTP	PB-O3B-PG-O2G
5	C	502	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
8	A	507	GOL	O1-C1-C2-O2
8	C	506	GOL	O2-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	PB-O3A-PA-O1A
8	B	506	GOL	C1-C2-C3-O3
8	F	402	GOL	C1-C2-C3-O3
10	B	505	MES	C7-C8-S-O1S
10	B	505	MES	C8-C7-N4-C5

There are no ring outliers.

8 monomers are involved in 14 short contacts:

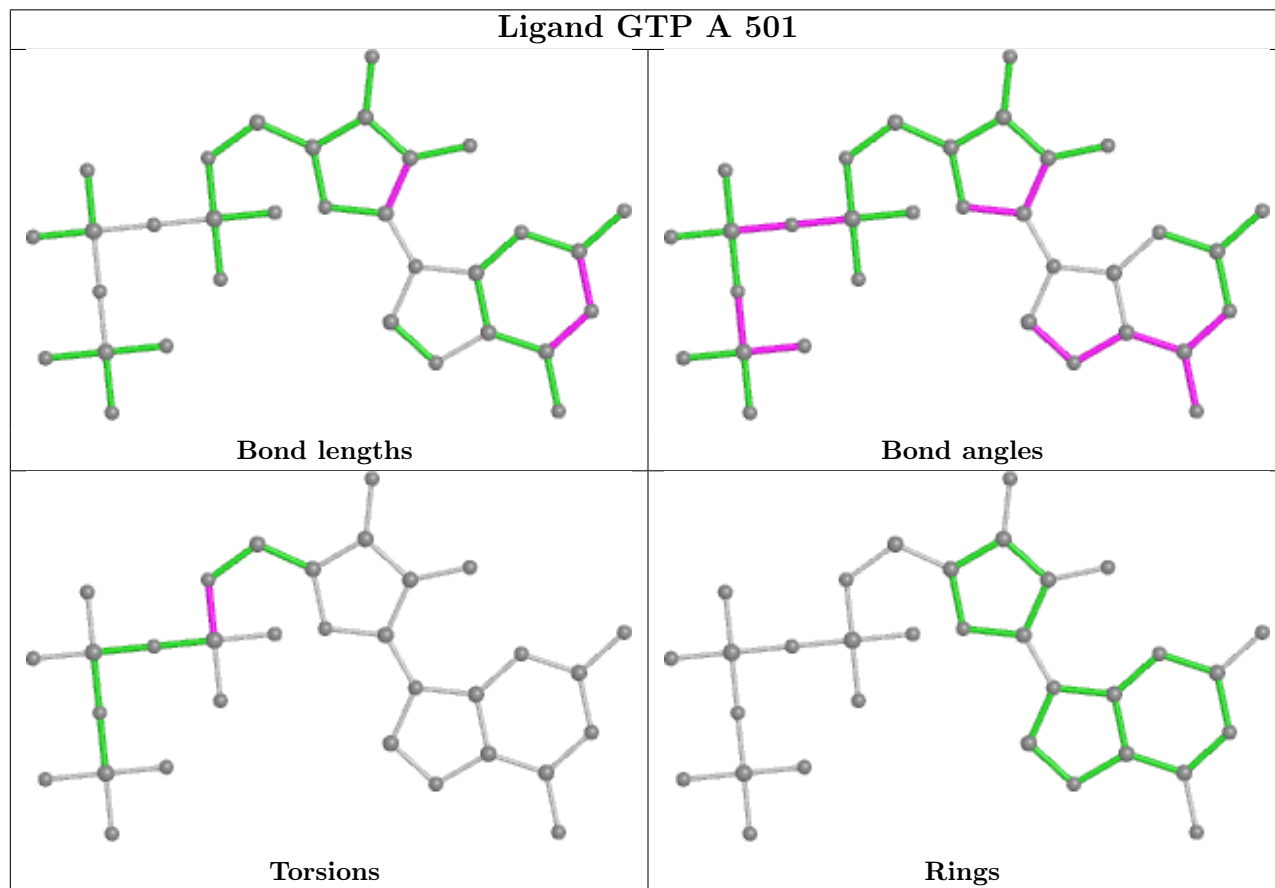
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	C	506	GOL	1	0
9	D	501	GDP	3	0
8	A	505	GOL	1	0
8	C	505	GOL	2	0

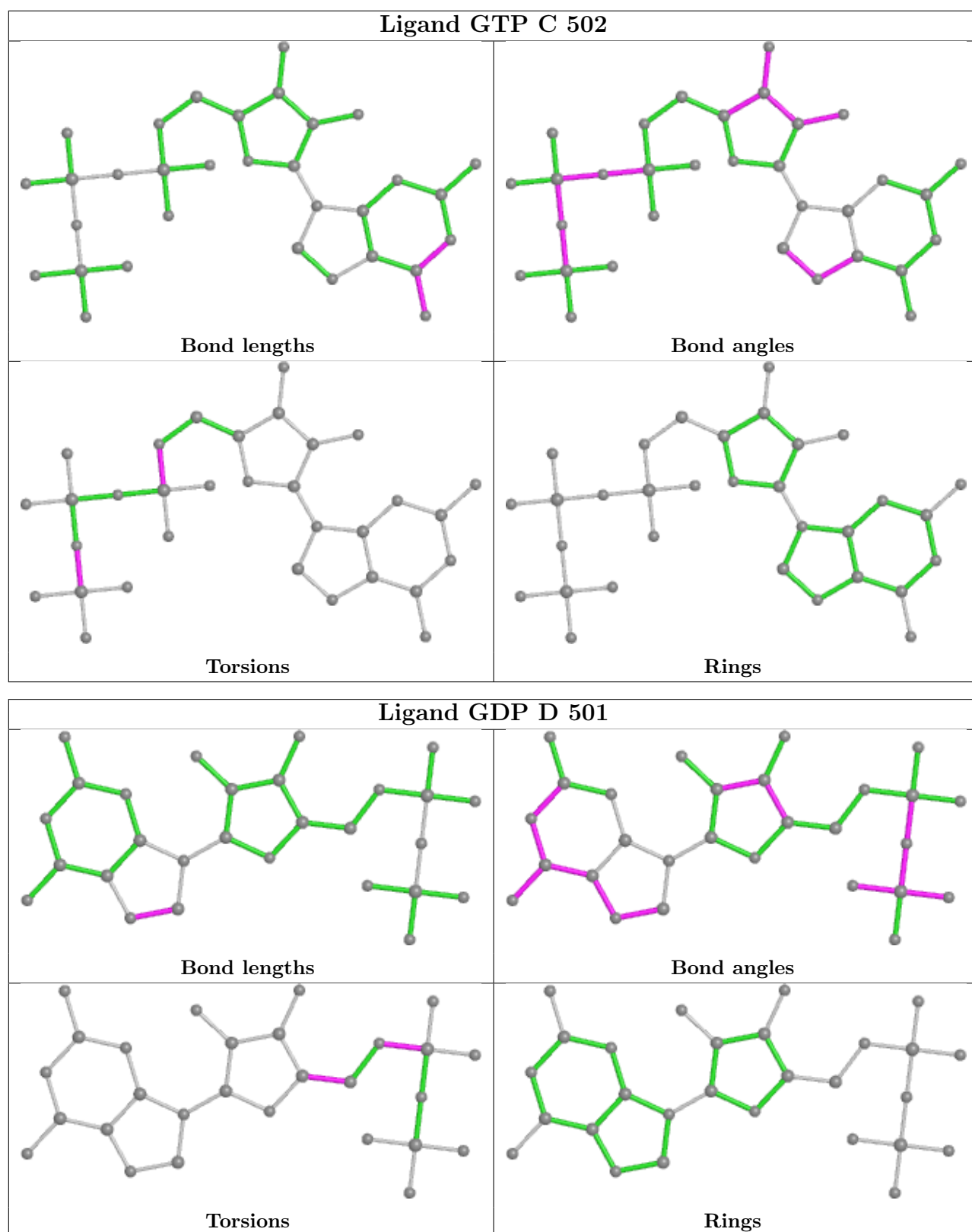
*Continued on next page...*

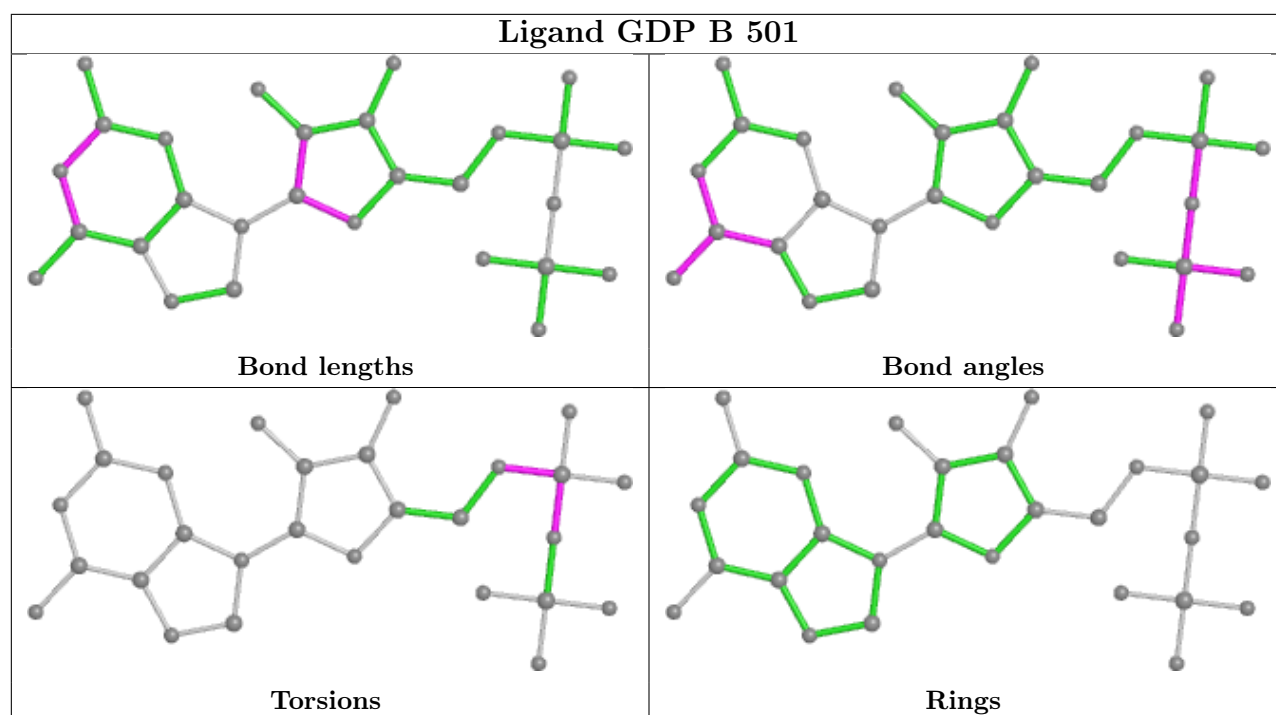
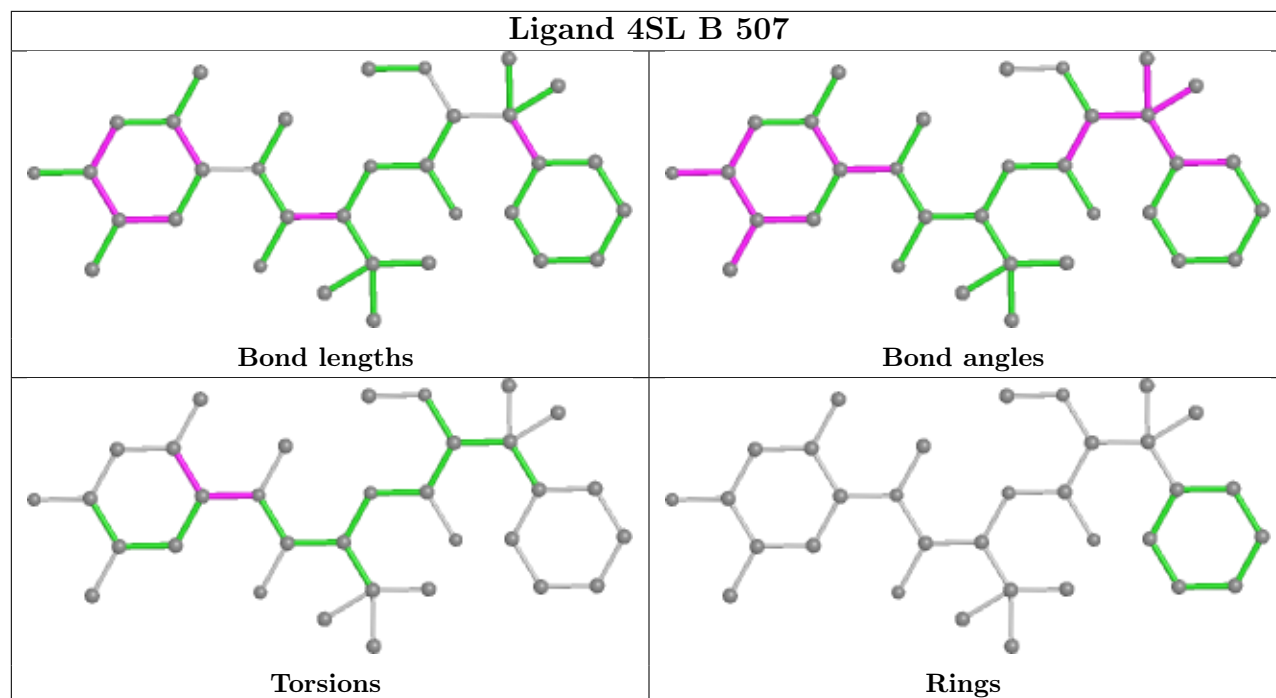
Continued from previous page...

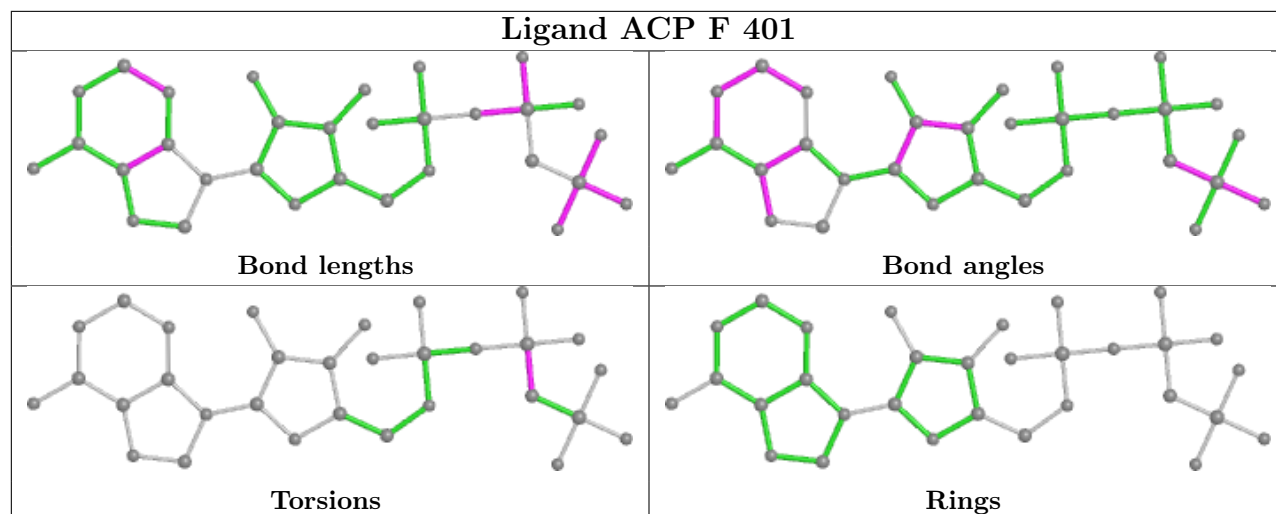
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	2	0
9	B	501	GDP	2	0
12	F	401	ACP	2	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	439/451 (97%)	-0.22	4 (0%) 84 86	28, 46, 78, 114	0
1	C	440/451 (97%)	-0.29	4 (0%) 84 86	26, 42, 66, 111	0
2	B	430/445 (96%)	-0.13	9 (2%) 63 66	27, 43, 78, 117	0
2	D	422/445 (94%)	0.24	27 (6%) 19 20	33, 59, 94, 117	0
3	E	123/143 (86%)	0.12	5 (4%) 37 40	38, 61, 98, 127	0
4	F	346/384 (90%)	0.31	38 (10%) 5 5	33, 67, 127, 148	0
All	All	2200/2319 (94%)	-0.02	87 (3%) 38 41	26, 51, 96, 148	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	372	THR	4.9
4	F	139	ARG	4.8
3	E	143	ALA	4.7
2	B	279	GLY	4.6
4	F	135	TYR	4.5
2	B	1	MET	4.3
4	F	169	LEU	4.3
4	F	235	ASP	4.3
4	F	234	GLN	4.1
4	F	104	ASN	4.1
4	F	363	ASP	4.1
2	D	57	ALA	4.0
2	D	97	SER	3.9
4	F	233	PHE	3.6
4	F	101	TYR	3.6
4	F	176	GLN	3.5
4	F	132	LEU	3.4
2	D	400	ARG	3.3
4	F	178	GLN	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	1	MET	3.3
2	B	56	ALA	3.3
4	F	168	GLU	3.3
4	F	182	ILE	3.2
3	E	142	GLU	3.2
4	F	244	CYS	3.2
4	F	232	ASN	3.1
2	D	94	PHE	3.1
4	F	160	ILE	3.1
4	F	172	PHE	3.1
4	F	161	LEU	3.1
4	F	170	LEU	3.1
4	F	140	GLU	3.0
2	B	59	ASN	3.0
4	F	164	SER	2.9
2	D	401	ARG	2.9
2	D	73	GLY	2.9
4	F	171	ASP	2.8
4	F	103	THR	2.8
4	F	133	ALA	2.8
2	D	56	ALA	2.7
4	F	362	ALA	2.7
2	D	405	LEU	2.7
2	D	76	ASP	2.7
2	D	402	LYS	2.7
2	D	58	GLY	2.6
1	C	339	ARG	2.6
2	B	57	ALA	2.5
2	B	281	GLN	2.5
2	D	407	TRP	2.5
2	B	33	THR	2.5
4	F	175	GLU	2.5
2	D	415	GLU	2.5
1	C	2	ARG	2.4
4	F	253	TYR	2.4
2	D	399	PHE	2.4
3	E	28	SER	2.4
2	D	96	GLN	2.4
2	D	406	HIS	2.4
2	D	37	HIS	2.3
2	D	179	ASP	2.3
2	D	201	THR	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	146	VAL	2.3
4	F	147	TRP	2.3
4	F	165	GLU	2.3
1	A	282	TYR	2.3
1	A	438	ASP	2.3
2	D	221	THR	2.3
1	A	262	TYR	2.3
2	D	404	PHE	2.2
4	F	142	ARG	2.2
4	F	136	ASN	2.2
2	D	1	MET	2.2
3	E	138	GLU	2.2
2	D	202	TYR	2.2
2	D	416	MET	2.2
4	F	143	GLU	2.2
2	D	397	ALA	2.1
2	D	409	THR	2.1
4	F	137	ARG	2.1
1	C	133	GLN	2.1
4	F	167	SER	2.1
2	D	55	GLU	2.1
1	A	439	SER	2.1
2	B	439	THR	2.1
3	E	25	LYS	2.1
2	B	60	LYS	2.0
4	F	173	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

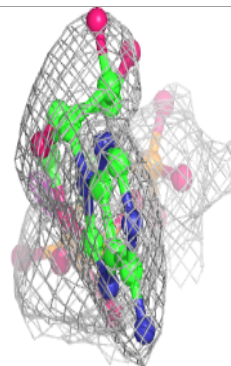
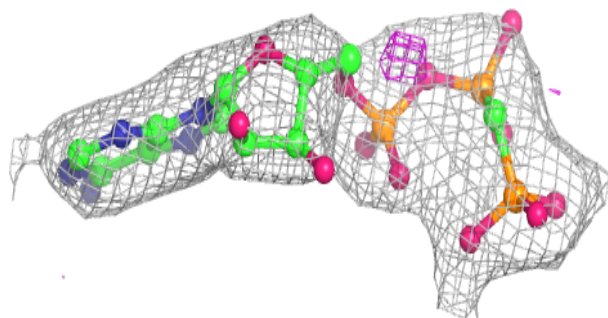
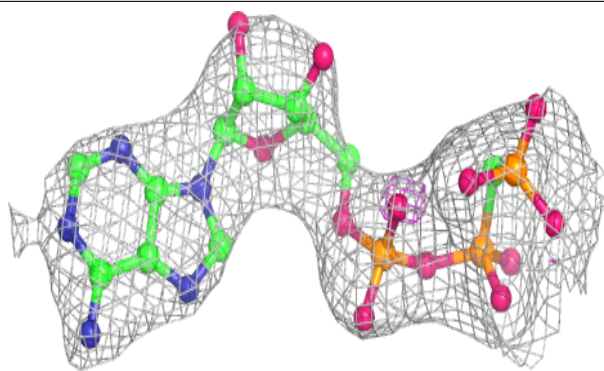
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	GOL	B	506	6/6	0.77	0.31	82,87,88,94	0
7	CA	C	501	1/1	0.78	0.07	96,96,96,96	0
8	GOL	F	402	6/6	0.82	0.16	63,81,85,86	0
8	GOL	C	505	6/6	0.86	0.30	54,69,71,76	0
8	GOL	A	507	6/6	0.86	0.22	50,61,66,71	0
8	GOL	A	506	6/6	0.88	0.26	65,72,84,89	0
8	GOL	A	504	6/6	0.90	0.13	89,98,101,104	0
6	MG	B	502	1/1	0.91	0.35	57,57,57,57	0
12	ACP	F	401	31/31	0.92	0.17	77,88,105,117	0
7	CA	B	503	1/1	0.93	0.13	89,89,89,89	0
11	4SL	B	507	34/34	0.95	0.14	32,40,45,49	0
10	MES	B	504	12/12	0.95	0.12	55,68,82,83	0
8	GOL	A	505	6/6	0.96	0.23	62,66,74,84	0
8	GOL	C	506	6/6	0.96	0.15	47,51,56,62	0
6	MG	D	502	1/1	0.96	0.06	72,72,72,72	0
7	CA	A	503	1/1	0.97	0.03	62,62,62,62	0
10	MES	B	505	12/12	0.97	0.15	51,62,64,66	0
6	MG	C	503	1/1	0.98	0.14	37,37,37,37	0
9	GDP	D	501	28/28	0.98	0.10	40,49,60,66	0
5	GTP	C	502	32/32	0.98	0.15	27,30,34,36	0
5	GTP	A	501	32/32	0.99	0.16	26,31,33,37	0
6	MG	A	502	1/1	0.99	0.09	35,35,35,35	0
9	GDP	B	501	28/28	0.99	0.17	26,32,34,38	0
7	CA	C	504	1/1	0.99	0.03	48,48,48,48	0

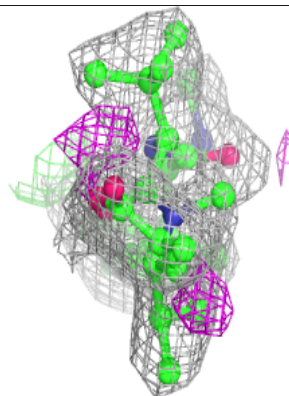
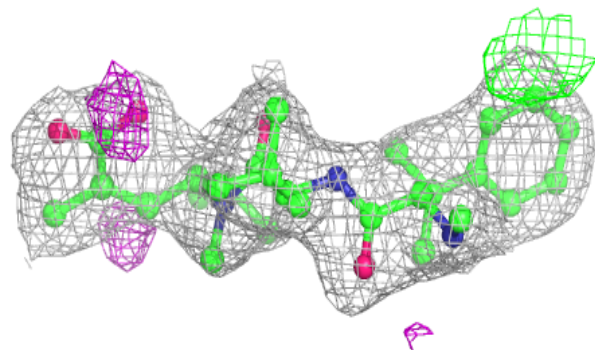
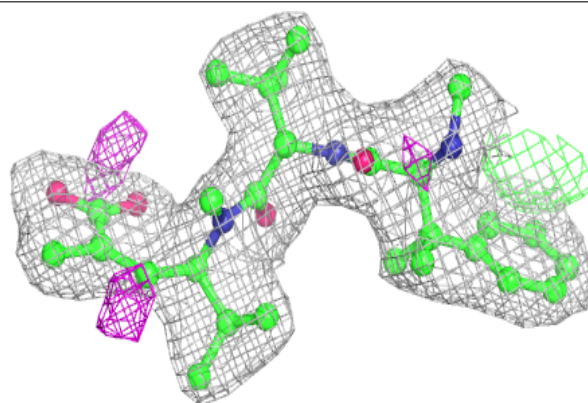
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACP F 401:**

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

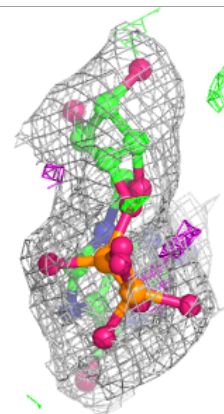
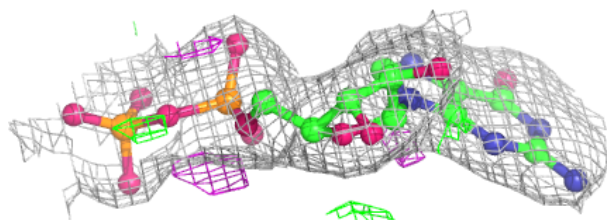
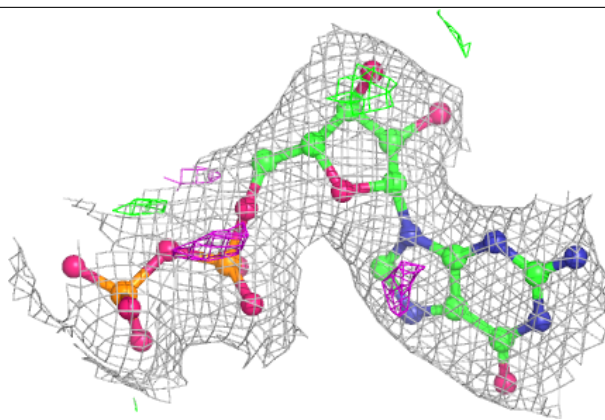
**Electron density around 4SL B 507:**

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

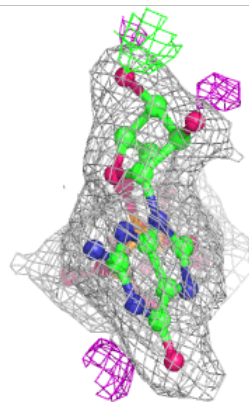
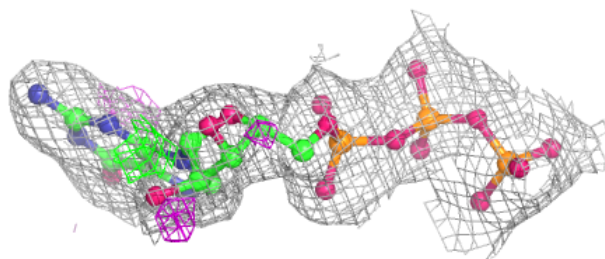
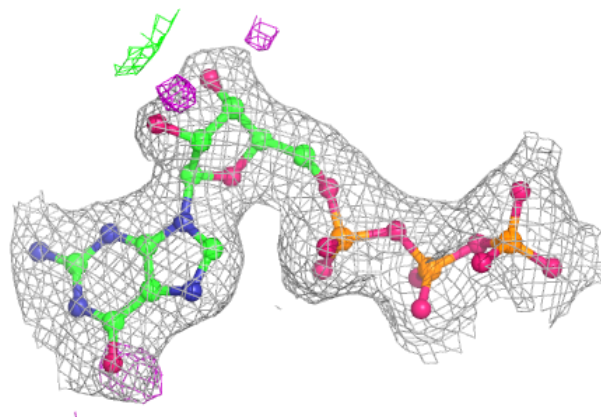


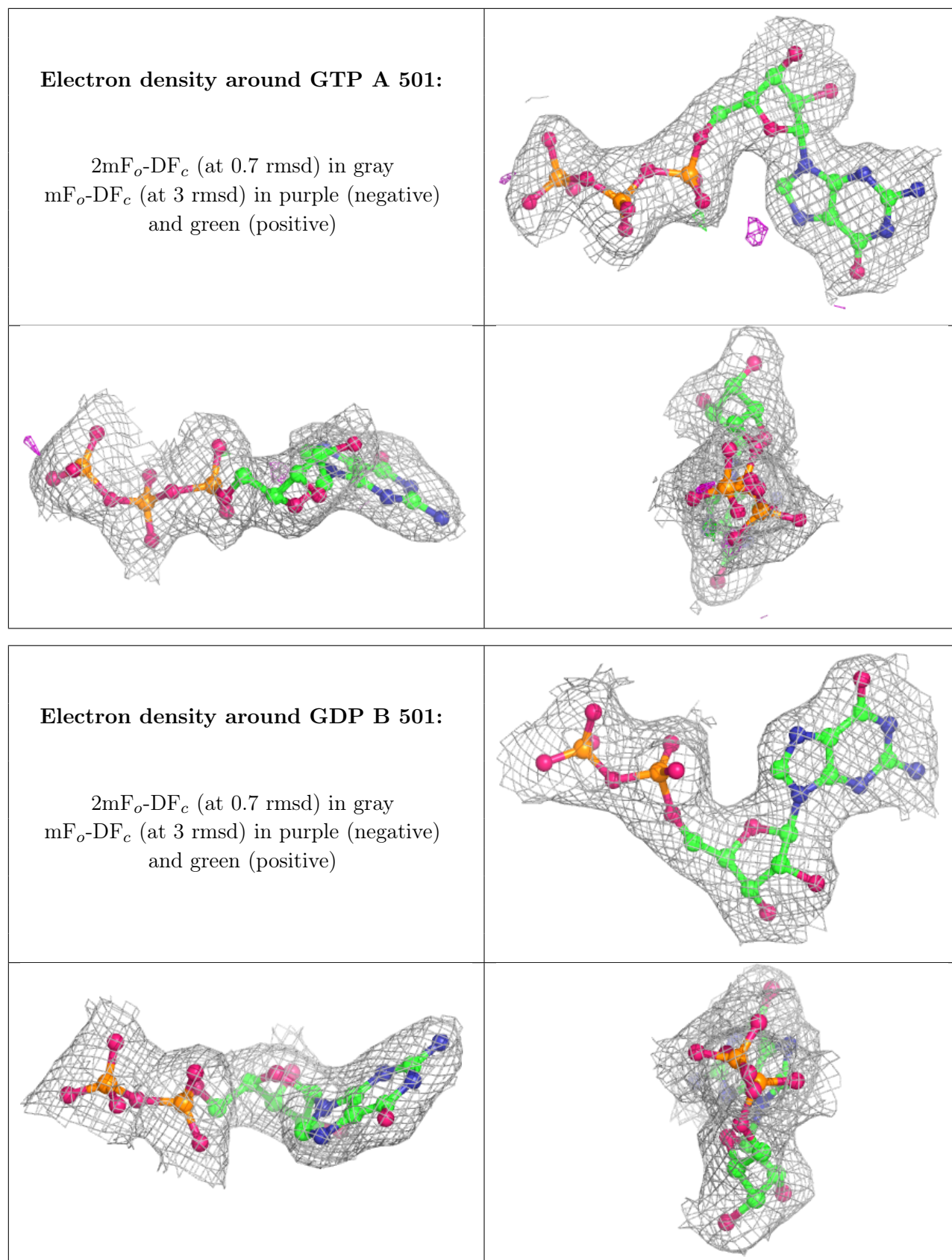
**Electron density around GDP D 501:**

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

**Electron density around GTP C 502:**

$2mF_o-DF_c$  (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.