



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 07:09 pm BST

PDB ID : 7YYX  
Title : Molecular snapshots of drug release from tubulin: 100 nanoseconds after photoactivation.  
Authors : Wranik, M.; Weinert, T.; Standfuss, J.  
Deposited on : 2022-02-18  
Resolution : 2.20 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 : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

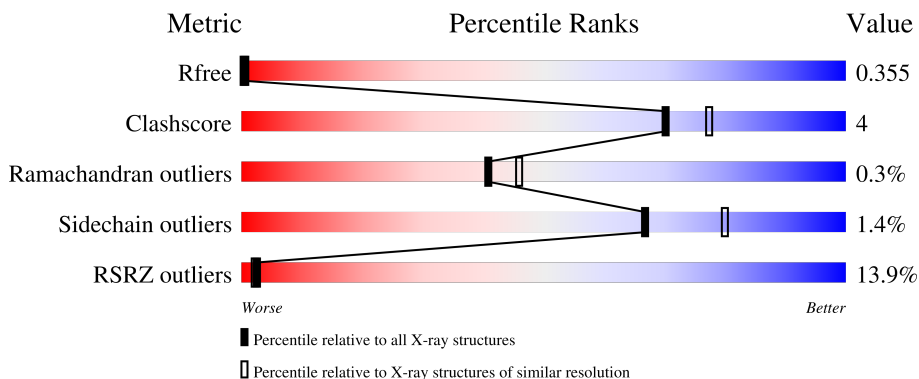
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

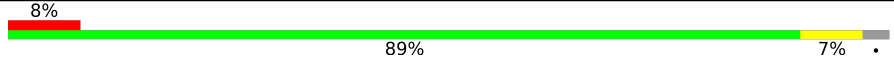


The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	
2	B	445	
3	F	169	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8211 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	3419	2166	580	650	23	4	3	0

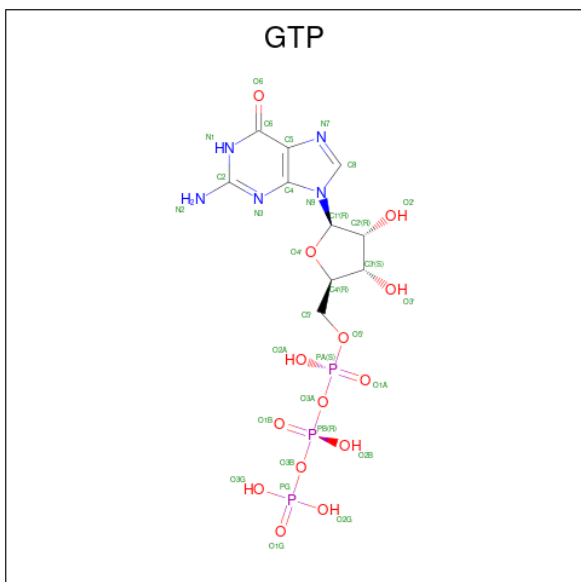
- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	3342	2100	569	646	27	0	2	0

- Molecule 3 is a protein called Designed Ankyrin Repeat Protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	155	1154	727	198	226	3	0	0	0

- Molecule 4 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
4	A	1	32	10	5	14	3	0	0

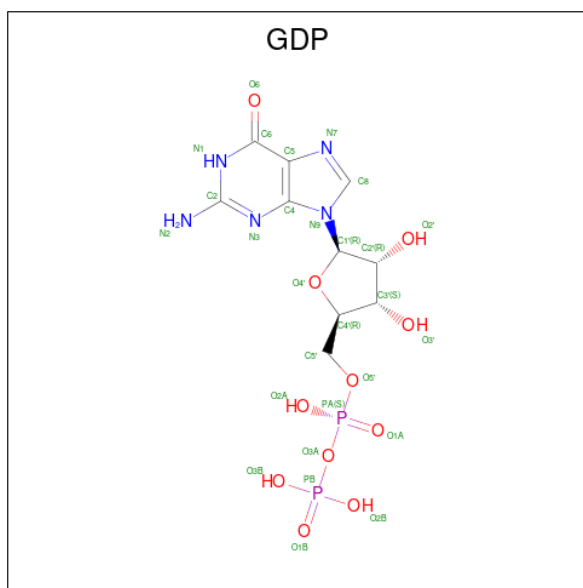
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

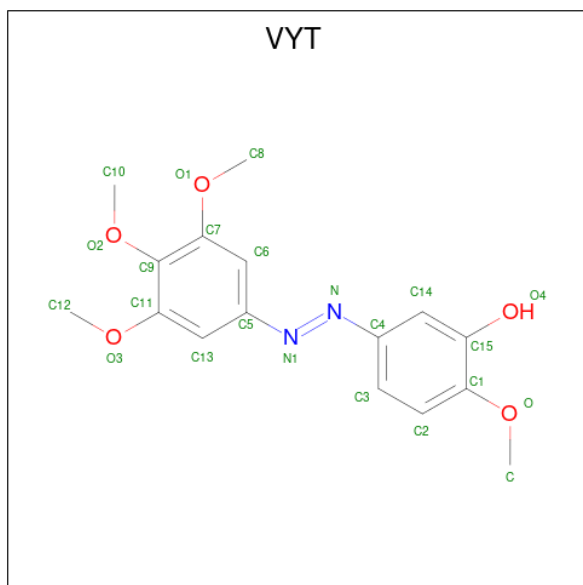
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	1	1	1	0	0

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



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

- Molecule 8 is Azo-Combretastatin A4 (trans) (three-letter code: VYT) (formula: C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	23	16	2	5	0	0

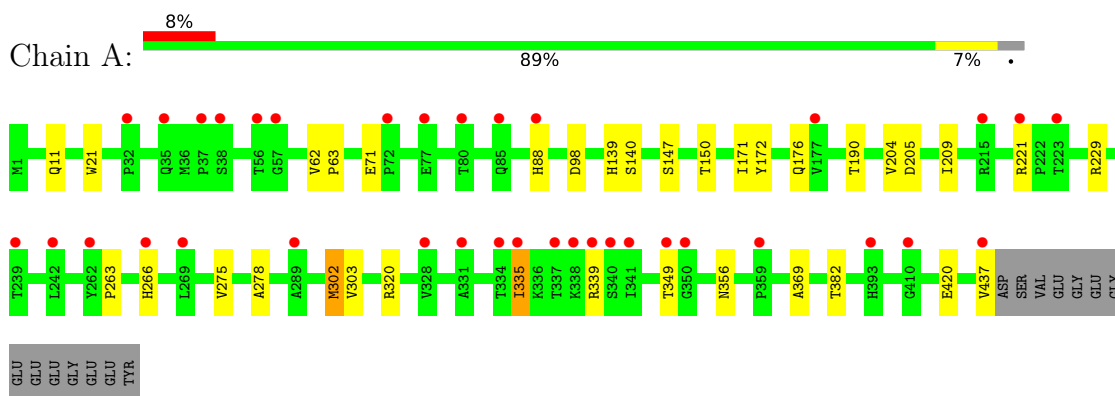
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	99	Total	O	0	0
			99	99		
9	B	68	Total	O	0	0
			68	68		
9	F	44	Total	O	0	0
			44	44		

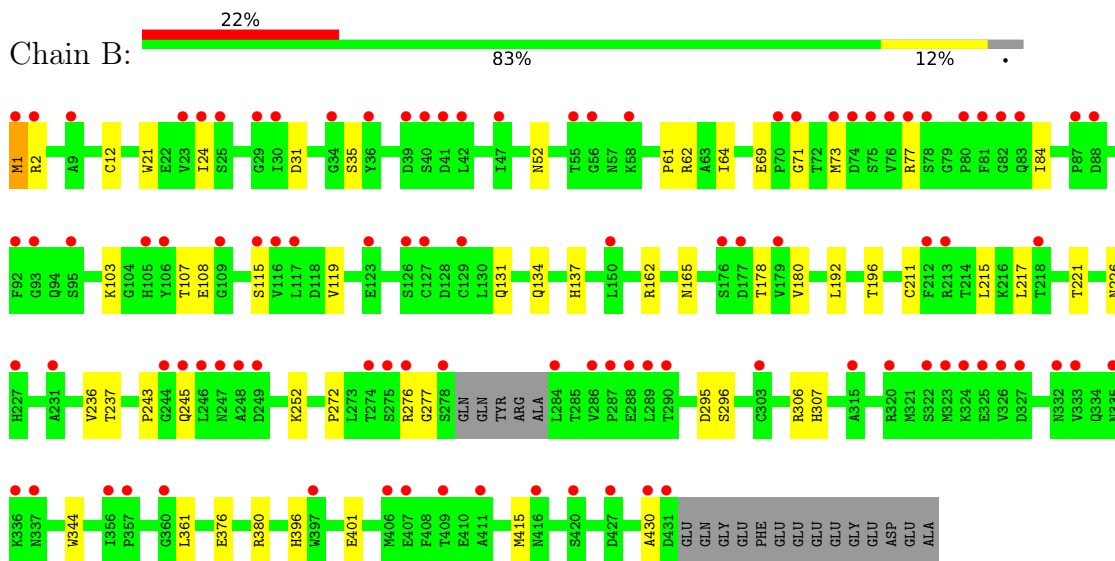
### 3 Residue-property plots [i](#)

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.

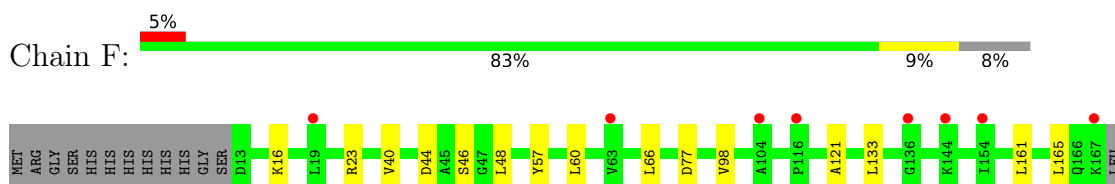
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Designed Ankyrin Repeat Protein (DARPIN) D1



ASIN

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.53Å 92.58Å 83.99Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	9.49 – 2.20 9.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (9.49-2.20) 92.3 (9.49-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.74 (at 2.21Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.311 , 0.355 0.311 , 0.355	Depositor DCC
$R_{free}$ test set	1815 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, VYT, GDP, MG, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/3506	0.46	0/4762
2	B	0.24	0/3421	0.46	0/4633
3	F	0.23	0/1170	0.40	0/1590
All	All	0.24	0/8097	0.45	0/10985

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

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	3419	0	3329	19	0
2	B	3342	0	3217	30	0
3	F	1154	0	1156	9	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	B	28	0	12	2	0
8	B	23	0	0	0	0
9	A	99	0	0	4	0
9	B	68	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	44	0	0	1	0
All	All	8211	0	7726	56	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 (56) 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)
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.75	0.69
1:A:229:ARG:NH2	9:A:604:HOH:O	2.31	0.62
1:A:98:ASP:OD2	2:B:252:LYS:NZ	2.28	0.61
2:B:52:ASN:OD1	2:B:62:ARG:NH2	2.36	0.58
1:A:221:ARG:NH2	9:A:609:HOH:O	2.37	0.57
2:B:103:LYS:NZ	2:B:401:GLU:OE2	2.38	0.55
2:B:31:ASP:OD1	2:B:35:SER:N	2.41	0.54
1:A:11:GLN:NE2	9:A:614:HOH:O	2.40	0.54
3:F:23:ARG:NH2	9:F:206:HOH:O	2.39	0.53
2:B:245:GLN:NE2	9:B:614:HOH:O	2.35	0.51
1:A:147:SER:HB2	1:A:190:THR:HB	1.92	0.51
2:B:115:SER:O	9:B:601:HOH:O	2.20	0.51
2:B:211:CYS:HB3	2:B:217:LEU:HD12	1.94	0.50
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.93	0.50
1:A:263:PRO:O	1:A:266:HIS:ND1	2.41	0.50
2:B:344:TRP:HB3	2:B:430:ALA:HB2	1.94	0.49
2:B:69:GLU:HG2	2:B:71:GLY:H	1.78	0.49
2:B:307:HIS:ND1	2:B:376:GLU:OE2	2.40	0.49
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.48	0.48
2:B:12:CYS:HB2	7:B:501:GDP:C8	2.49	0.48
2:B:1:MET:HE1	2:B:162:ARG:HH12	1.79	0.47
2:B:178:THR:HG22	2:B:180:VAL:HG22	1.97	0.47
2:B:61:PRO:HD3	2:B:84:ILE:HG13	1.97	0.46
3:F:44:ASP:OD2	3:F:48:LEU:HB2	2.16	0.46
2:B:134:GLN:HA	2:B:165:ASN:O	2.15	0.45
2:B:73:MET:HG2	2:B:77:ARG:HE	1.80	0.45
2:B:226:ASN:OD1	7:B:501:GDP:N1	2.37	0.45
1:A:320:ARG:HA	1:A:356:ASN:O	2.17	0.45
2:B:211:CYS:HA	2:B:215:LEU:HB2	1.98	0.45
2:B:192:LEU:O	2:B:196:THR:OG1	2.34	0.45
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.51	0.45
3:F:16:LYS:HA	3:F:16:LYS:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:N	9:A:613:HOH:O	2.39	0.44
3:F:133:LEU:HD11	3:F:165:LEU:HD23	2.00	0.44
1:A:382:THR:HB	1:A:437:VAL:HB	2.00	0.44
2:B:396:HIS:NE2	3:F:57:TYR:OH	2.40	0.44
1:A:171:ILE:HD13	1:A:204:VAL:HB	1.99	0.44
2:B:380:ARG:NH1	9:B:607:HOH:O	2.31	0.43
2:B:107:THR:OG1	2:B:108:GLU:N	2.50	0.43
2:B:1:MET:HE1	2:B:162:ARG:NH1	2.34	0.43
3:F:40:VAL:HG13	3:F:66:LEU:HD22	2.01	0.42
3:F:60:LEU:HD11	3:F:98:VAL:HG21	2.00	0.42
1:A:205:ASP:HB2	1:A:303:VAL:HA	2.01	0.42
2:B:236:VAL:HG23	2:B:237:THR:HG23	1.99	0.42
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.02	0.42
2:B:1:MET:HG3	2:B:131:GLN:HB3	2.00	0.42
1:A:140:SER:HA	1:A:171:ILE:HB	2.02	0.42
2:B:272:PRO:HD2	2:B:361:LEU:HD13	2.02	0.41
2:B:295:ASP:OD1	2:B:296:SER:N	2.54	0.41
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.55	0.41
3:F:46:SER:O	3:F:77:ASP:HB2	2.21	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.41
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.55	0.41
2:B:64:ILE:HD13	2:B:119:VAL:HG13	2.03	0.41
1:A:209:ILE:HD11	1:A:302[B]:MET:HG3	2.02	0.41
1:A:335:ILE:HG23	1:A:339:ARG:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	438/451 (97%)	422 (96%)	15 (3%)	1 (0%)	47 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	424/445 (95%)	412 (97%)	10 (2%)	2 (0%)	29	31
3	F	153/169 (90%)	150 (98%)	3 (2%)	0	100	100
All	All	1015/1065 (95%)	984 (97%)	28 (3%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	B	277	GLY
1	A	335	ILE

### 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%)	362 (98%)	6 (2%)	62	76
2	B	366/383 (96%)	359 (98%)	7 (2%)	57	71
3	F	120/132 (91%)	120 (100%)	0	100	100
All	All	854/894 (96%)	841 (98%)	13 (2%)	67	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	176	GLN
1	A	302[A]	MET
1	A	302[B]	MET
1	A	349	THR
1	A	420	GLU
2	B	1	MET
2	B	2	ARG
2	B	137	HIS
2	B	221	THR
2	B	276	ARG

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Mol	Chain	Res	Type
2	B	306	ARG
2	B	415	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	37	HIS
2	B	165	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	VYT	B	502	-	24,24,24	0.41	0	32,32,32	1.01	0
4	GTP	A	501	5	26,34,34	1.14	2 (7%)	32,54,54	1.48	7 (21%)
7	GDP	B	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.27	4 (13%)

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	VYT	B	502	-	-	2/13/13/13	0/2/2/2
4	GTP	A	501	5	-	7/18/38/38	0/3/3/3
7	GDP	B	501	-	-	4/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	C5-C6	-4.05	1.39	1.47
7	B	501	GDP	C6-N1	-2.40	1.34	1.37
4	A	501	GTP	C2-N3	2.18	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	PB-O3B-PG	-3.18	121.92	132.83
4	A	501	GTP	C5-C6-N1	3.14	119.49	113.95
4	A	501	GTP	C8-N7-C5	3.00	108.70	102.99
7	B	501	GDP	PA-O3A-PB	-2.99	122.56	132.83
4	A	501	GTP	C2-N1-C6	-2.78	119.99	125.10
4	A	501	GTP	PA-O3A-PB	-2.74	123.41	132.83
7	B	501	GDP	C3'-C2'-C1'	2.74	105.10	100.98
7	B	501	GDP	C8-N7-C5	2.33	107.43	102.99
7	B	501	GDP	C5-C6-N1	2.32	118.05	113.95
4	A	501	GTP	C3'-C2'-C1'	2.17	104.24	100.98
4	A	501	GTP	O6-C6-C5	-2.15	120.16	124.37

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
8	B	502	VYT	C15-C1-O-C
4	A	501	GTP	PB-O3B-PG-O1G
4	A	501	GTP	C5'-O5'-PA-O3A

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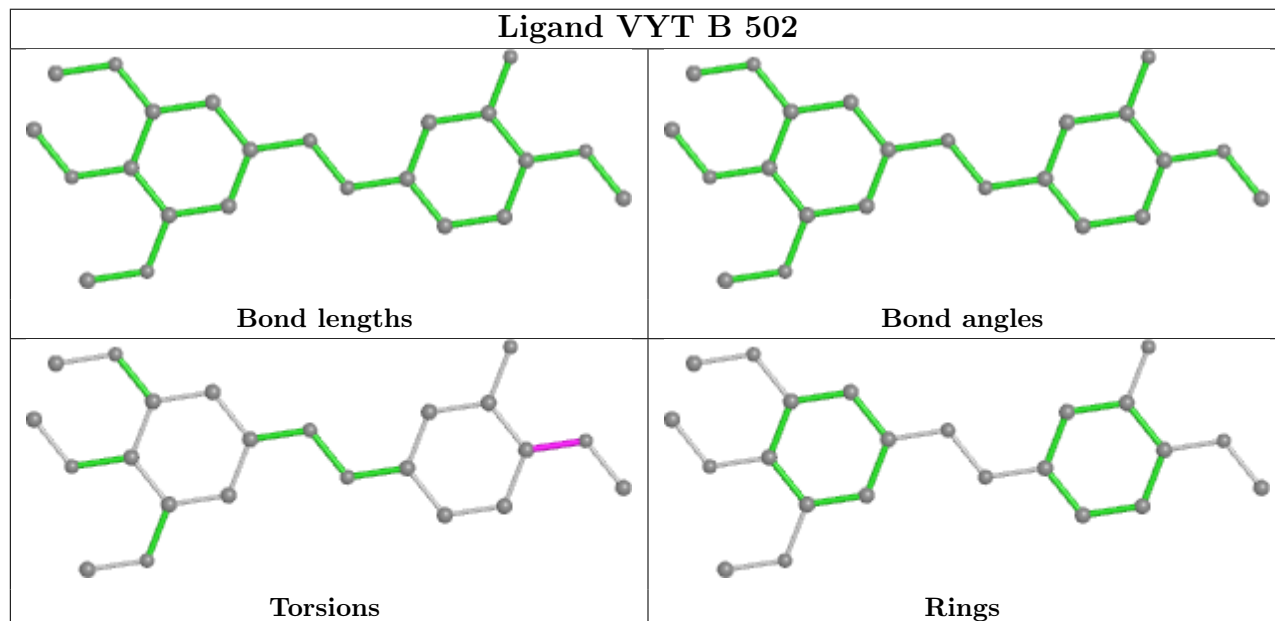
Mol	Chain	Res	Type	Atoms
8	B	502	VYT	C2-C1-O-C
4	A	501	GTP	C4'-C5'-O5'-PA
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3B-PG-O3G
7	B	501	GDP	C5'-O5'-PA-O3A
7	B	501	GDP	PB-O3A-PA-O2A

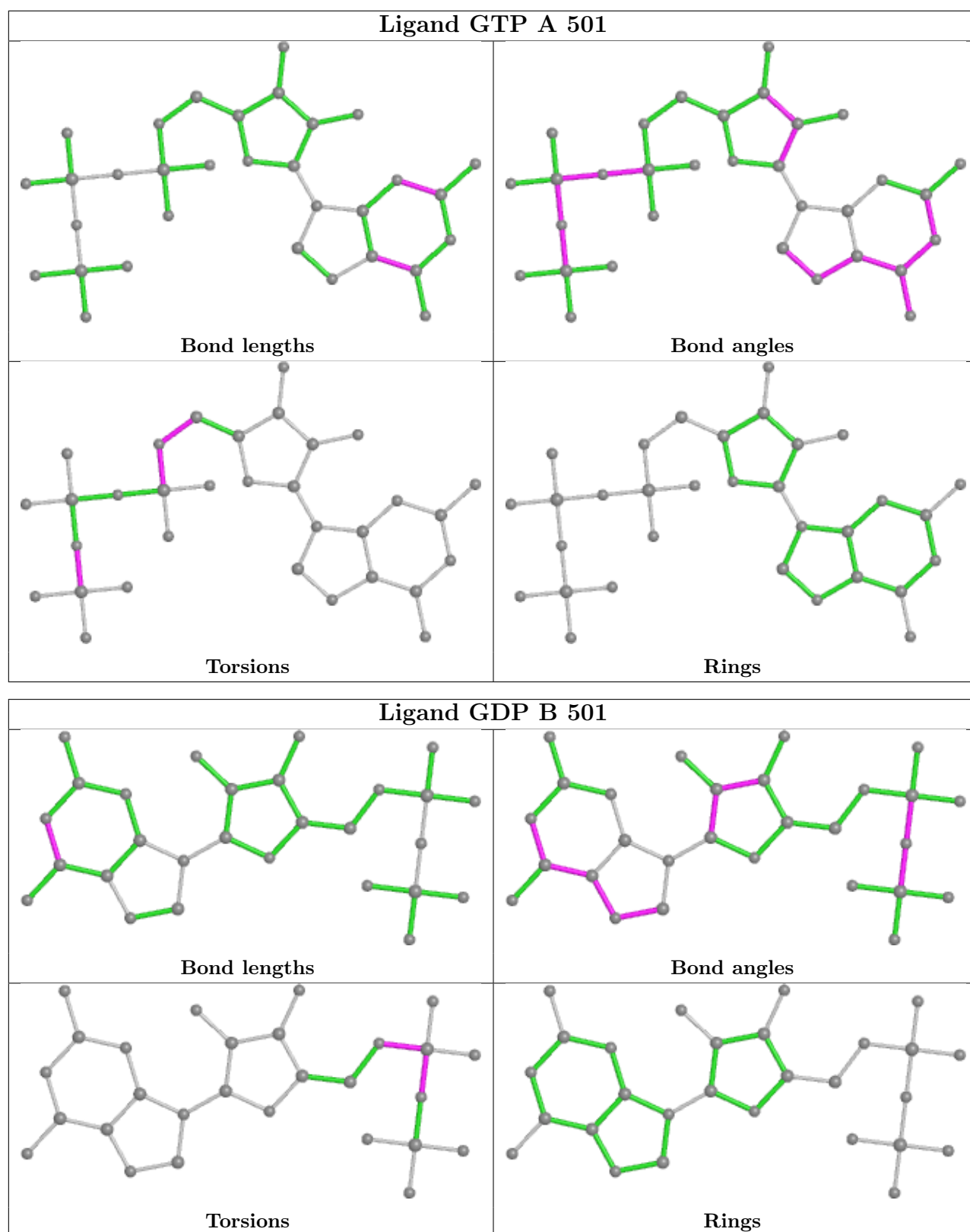
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	GDP	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

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%)	0.80	36 (8%) 11 10	20, 29, 45, 65	0
2	B	426/445 (95%)	1.28	97 (22%) 0 0	23, 37, 59, 68	0
3	F	155/169 (91%)	0.77	8 (5%) 27 26	21, 30, 43, 56	0
All	All	1018/1065 (95%)	0.99	141 (13%) 2 2	20, 32, 55, 68	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	73	MET	6.5
2	B	1	MET	5.9
1	A	437	VAL	5.8
2	B	244	GLY	5.6
2	B	332	ASN	5.4
2	B	177	ASP	5.2
3	F	167	LYS	5.0
2	B	431	ASP	4.9
2	B	71	GLY	4.7
2	B	55	THR	4.7
1	A	339	ARG	4.6
2	B	245	GLN	4.5
2	B	93	GLY	4.4
1	A	37	PRO	4.4
3	F	154	ILE	4.4
1	A	334	THR	4.3
2	B	409	THR	4.2
1	A	335	ILE	4.2
2	B	218	THR	4.1
2	B	246	LEU	4.1
2	B	326	VAL	4.0
2	B	333	VAL	4.0
2	B	82	GLY	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	80	PRO	3.9
2	B	95	SER	3.8
2	B	41	ASP	3.7
2	B	39	ASP	3.7
2	B	287	PRO	3.6
1	A	350	GLY	3.6
2	B	212	PHE	3.5
2	B	36	TYR	3.5
2	B	34	GLY	3.4
2	B	286	VAL	3.4
2	B	420	SER	3.4
2	B	427	ASP	3.3
2	B	56	GLY	3.3
2	B	360	GLY	3.3
2	B	70	PRO	3.3
2	B	42	LEU	3.3
1	A	341	ILE	3.2
2	B	231	ALA	3.2
2	B	92	PHE	3.1
2	B	324	LYS	3.1
1	A	269	LEU	3.1
2	B	249	ASP	3.1
2	B	81	PHE	3.1
1	A	85	GLN	3.1
2	B	87	PRO	3.1
2	B	278	SER	3.1
2	B	274	THR	3.1
2	B	322	SER	3.0
1	A	340	SER	3.0
1	A	331	ALA	3.0
2	B	323	MET	2.9
2	B	416	ASN	2.9
1	A	80	THR	2.9
1	A	88	HIS	2.9
1	A	337	THR	2.9
2	B	357	PRO	2.9
2	B	288	GLU	2.9
2	B	325	GLU	2.9
2	B	406	MET	2.9
2	B	289	LEU	2.9
1	A	410	GLY	2.8
2	B	126	SER	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	83	GLN	2.8
2	B	179	VAL	2.8
2	B	24	ILE	2.8
2	B	397	TRP	2.8
2	B	75	SER	2.7
2	B	9	ALA	2.7
2	B	411	ALA	2.7
1	A	177	VAL	2.7
2	B	29	GLY	2.7
2	B	77	ARG	2.6
2	B	336	LYS	2.6
2	B	290	THR	2.6
2	B	327	ASP	2.6
2	B	227	HIS	2.6
2	B	127	CYS	2.6
2	B	58	LYS	2.6
1	A	32	PRO	2.6
2	B	117	LEU	2.6
2	B	88	ASP	2.6
1	A	338	LYS	2.6
2	B	213	ARG	2.5
2	B	276	ARG	2.5
2	B	47	ILE	2.5
3	F	116	PRO	2.5
1	A	393	HIS	2.5
2	B	284	LEU	2.5
3	F	63	VAL	2.5
3	F	136	GLY	2.4
3	F	19	LEU	2.4
2	B	40	SER	2.4
2	B	78	SER	2.4
2	B	248	ALA	2.4
1	A	349	THR	2.4
1	A	262	TYR	2.4
1	A	239	THR	2.4
1	A	242	LEU	2.4
1	A	289	ALA	2.4
2	B	116	VAL	2.4
2	B	74	ASP	2.3
3	F	144	LYS	2.3
1	A	38	SER	2.3
2	B	129	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	123	GLU	2.3
1	A	359	PRO	2.3
2	B	106	TYR	2.2
3	F	104	ALA	2.2
2	B	247	ASN	2.2
2	B	356	ILE	2.2
1	A	328	VAL	2.2
2	B	23	VAL	2.2
1	A	56	THR	2.2
1	A	72	PRO	2.2
2	B	25	SER	2.2
1	A	266	HIS	2.1
2	B	2	ARG	2.1
2	B	176	SER	2.1
1	A	35	GLN	2.1
1	A	223	THR	2.1
2	B	430	ALA	2.1
1	A	57	GLY	2.1
2	B	275	SER	2.1
1	A	221	ARG	2.1
2	B	337	ASN	2.1
2	B	407	GLU	2.1
2	B	335	ASN	2.1
2	B	76	VAL	2.1
2	B	303	CYS	2.1
1	A	77	GLU	2.0
2	B	150	LEU	2.0
2	B	320	ARG	2.0
2	B	315	ALA	2.0
2	B	30	ILE	2.0
2	B	105	HIS	2.0
2	B	109	GLY	2.0
1	A	215	ARG	2.0
2	B	115	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates [i](#)

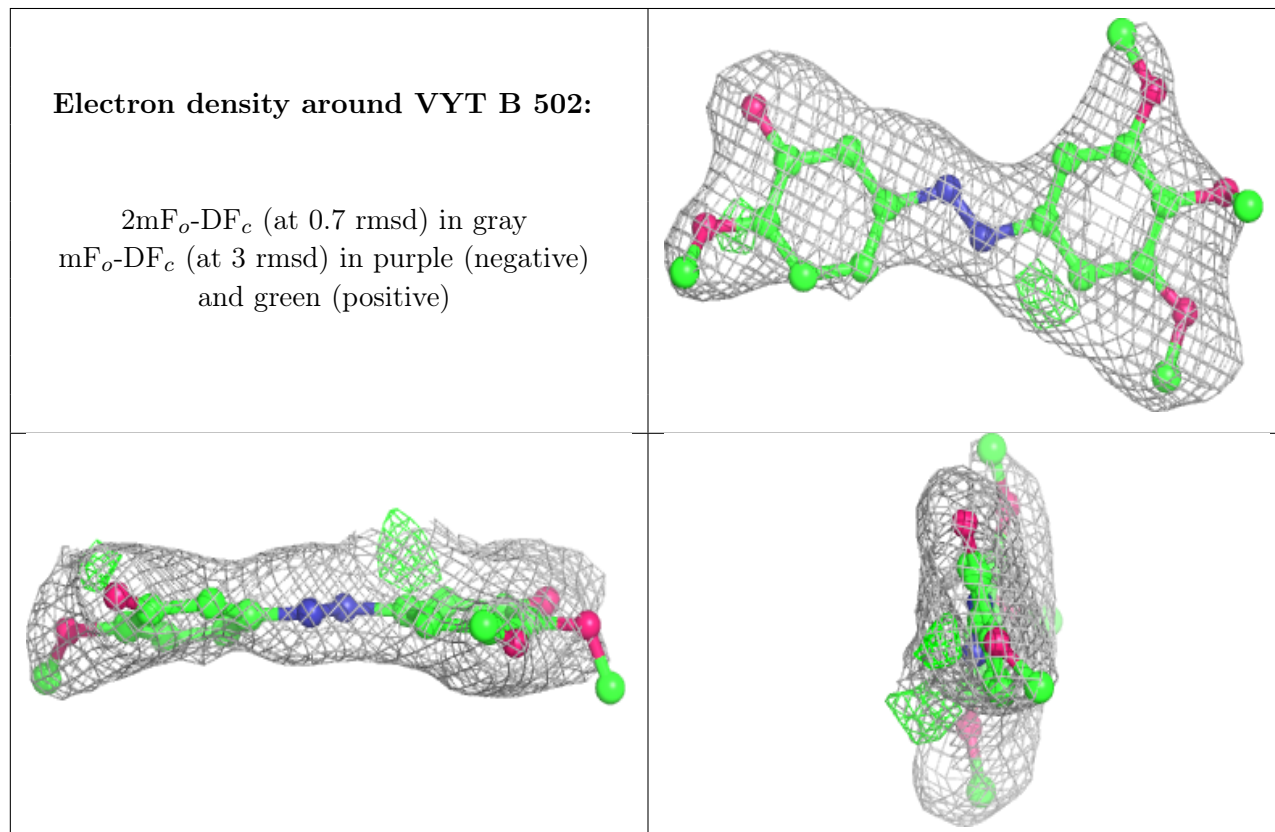
There are no monosaccharides in this entry.

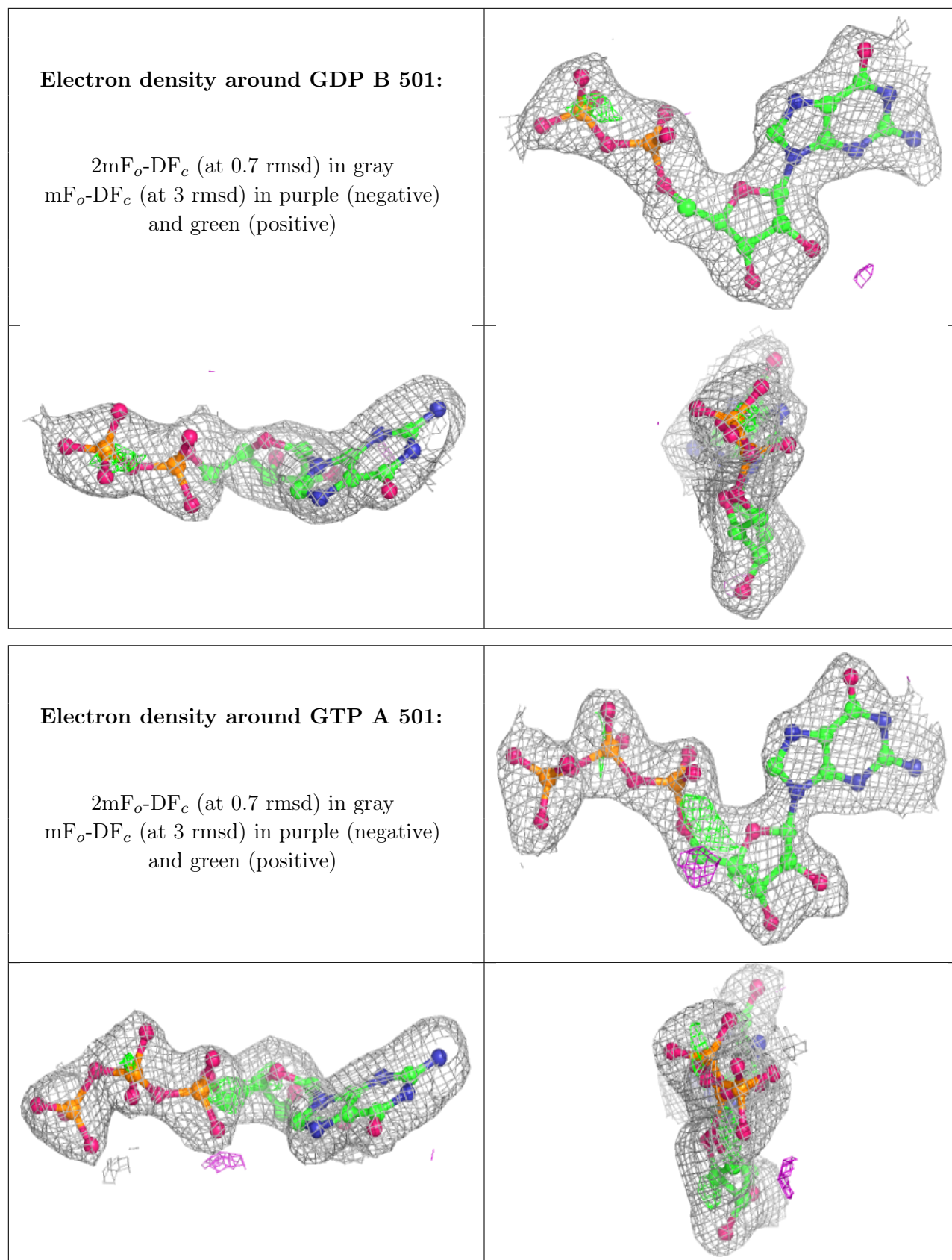
### 6.4 Ligands [i](#)

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	VYT	B	502	23/23	0.85	0.18	28,35,48,52	0
5	MG	A	502	1/1	0.87	0.35	31,31,31,31	0
6	CA	A	503	1/1	0.92	0.05	38,38,38,38	0
7	GDP	B	501	28/28	0.93	0.15	26,33,37,40	0
4	GTP	A	501	32/32	0.93	0.15	19,22,25,26	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.