



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:55 AM UTC

PDB ID : 5CA1 / pdb\_00005ca1  
Title : Crystal structure of T2R-TTL-Nocodazole complex  
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.  
Deposited on : 2015-06-29  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

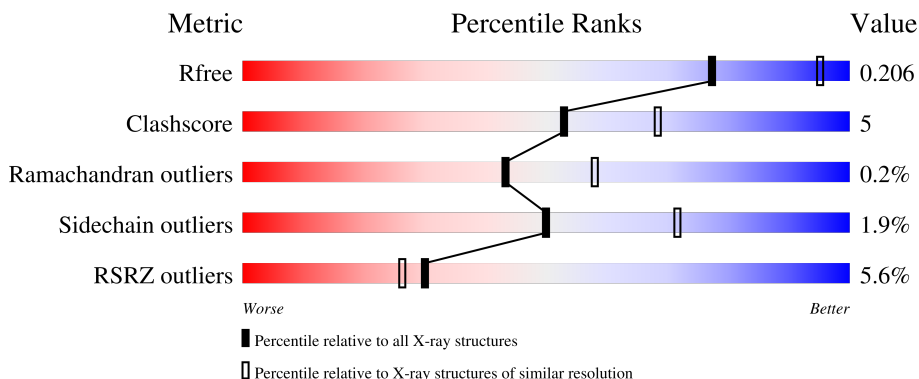
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.



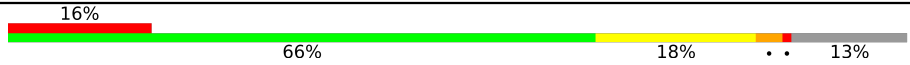
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	450	
1	C	450	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '16%', a large green segment labeled '66%', a yellow segment labeled '18%', and a small grey segment on the far right labeled '13%'. There are two small black dots between the yellow and grey segments.</p>

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 17872 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.

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-2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
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 Uncharacterized protein.

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 (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			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 (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

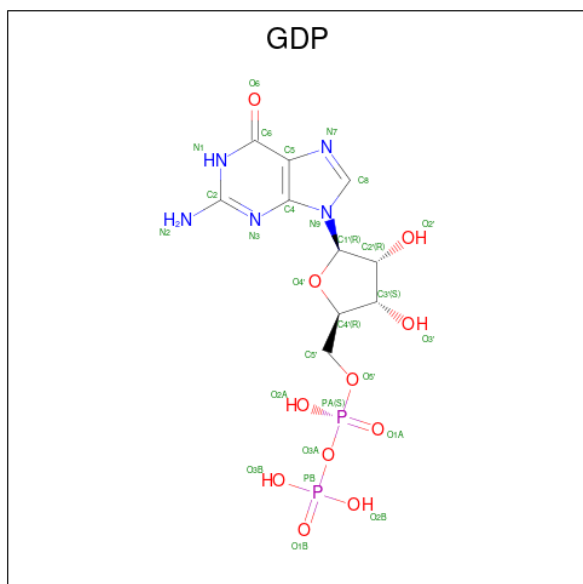
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



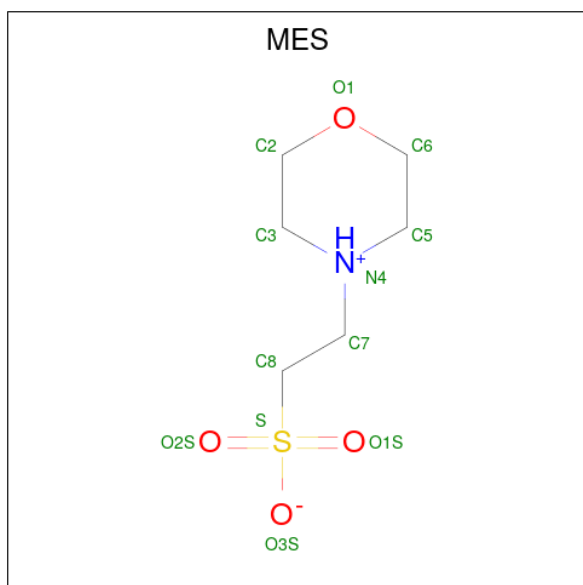
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



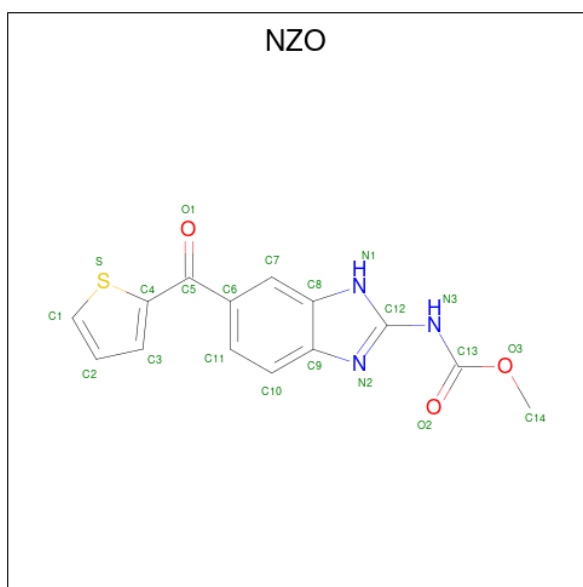
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0
9	D	1	28	10	5	11	2	0	0

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



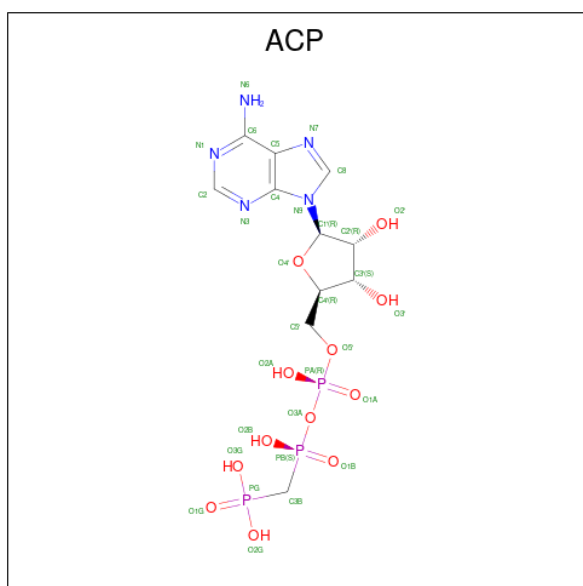
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0
10	D	1	12	6	1	4	1	0	0

- Molecule 11 is nocodazole (CCD ID: NZO) (formula: C<sub>14</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
11	B	1	21	14	3	3	1	0	0
11	D	1	21	14	3	3	1	0	0

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



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

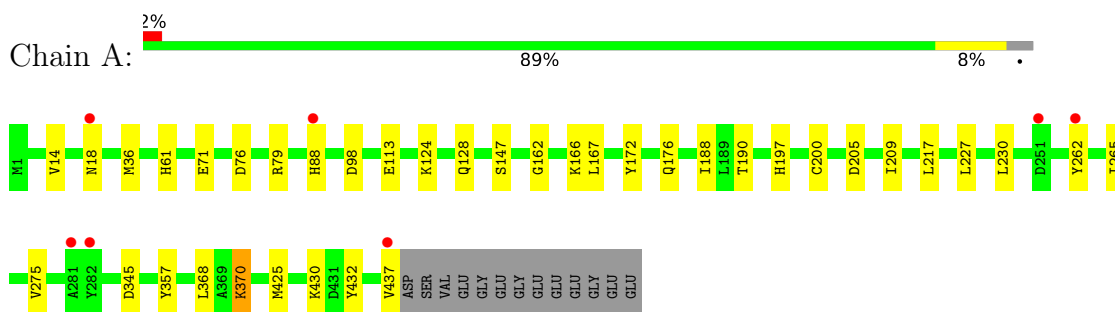
- Molecule 13 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
13	A	101	Total 101	O 101	0	0
13	B	74	Total 74	O 74	0	0
13	C	131	Total 131	O 131	0	0
13	D	33	Total 33	O 33	0	0
13	E	13	Total 13	O 13	0	0
13	F	25	Total 25	O 25	0	0

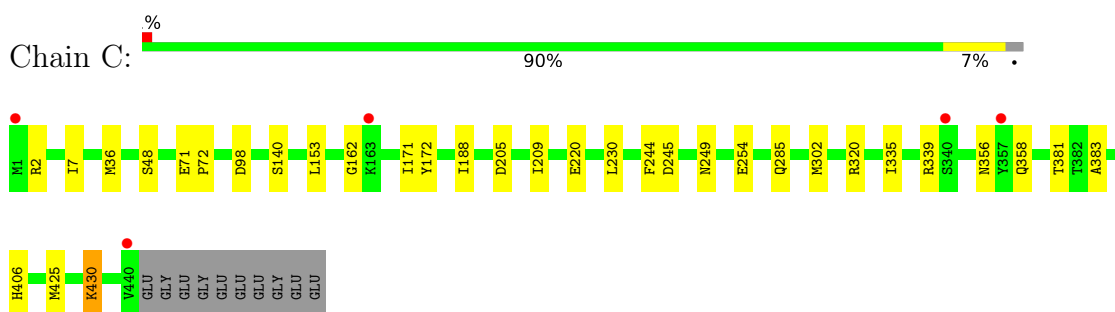
### 3 Residue-property plots [i](#)

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.

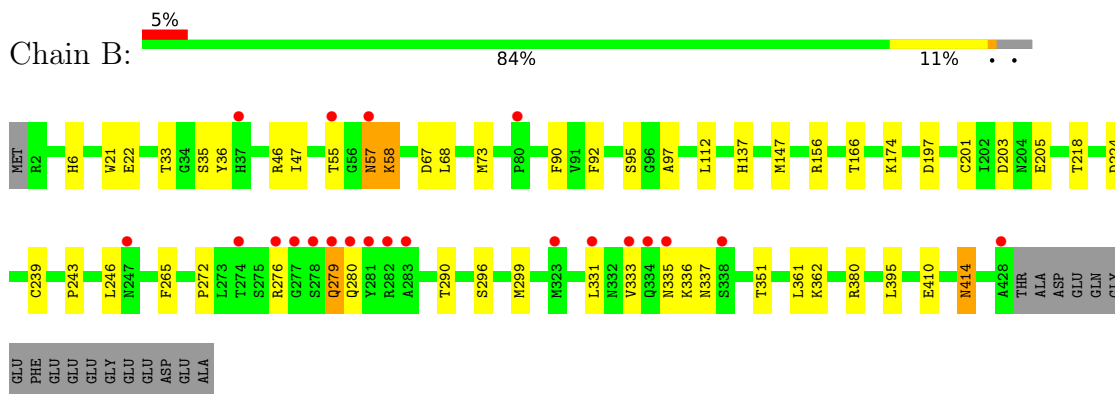
- Molecule 1: Tubulin alpha



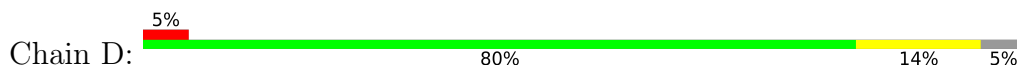
- Molecule 1: Tubulin alpha



- Molecule 2: Tubulin beta-2 chain



- Molecule 2: Tubulin beta-2 chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.44Å 158.36Å 180.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.52 – 2.40 41.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.52-2.40) 99.7 (41.52-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.192 , 0.225 0.198 , 0.206	Depositor DCC
$R_{free}$ test set	5924 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.8	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	17872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, GDP, ACP, GTP, MG, MES, GOL, NZO

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	0.31	0/3494	0.74	5/4743 (0.1%)
1	C	0.32	0/3515	0.72	2/4772 (0.0%)
2	B	0.33	0/3436	0.73	2/4654 (0.0%)
2	D	0.31	0/3382	0.74	1/4581 (0.0%)
3	E	0.31	0/1008	0.68	0/1337
4	F	0.37	0/2806	0.86	7/3791 (0.2%)
All	All	0.33	0/17641	0.75	17/23878 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	3

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	143	GLU	N-CA-C	7.45	121.62	109.85
4	F	172	PHE	N-CA-C	-7.34	102.89	111.03
4	F	138	ARG	N-CA-C	-7.20	101.82	113.19
4	F	139	ARG	N-CA-C	-6.83	102.43	111.24
1	A	262	TYR	CA-C-N	6.03	125.51	119.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	138	ARG	Peptide
4	F	142	ARG	Peptide
4	F	242	ASN	Peptide

## 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	3330	20	0
1	C	3437	0	3348	19	0
2	B	3361	0	3238	30	0
2	D	3309	0	3189	39	0
3	E	1000	0	1018	11	0
4	F	2744	0	2709	60	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
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
9	D	28	0	12	2	0
10	B	12	0	12	2	0
10	D	12	0	12	3	0
11	B	21	0	11	1	0
11	D	21	0	11	2	0
12	F	31	0	14	5	0
13	A	101	0	0	0	0
13	B	74	0	0	1	0
13	C	131	0	0	0	0
13	D	33	0	0	0	0
13	E	13	0	0	0	0
13	F	25	0	0	3	0
All	All	17872	0	16948	173	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 5.

The worst 5 of 173 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:GLU:O	2:B:414:ASN:ND2	2.00	0.93
4:F:180:HIS:O	13:F:501:HOH:O	1.92	0.87
2:B:35:SER:OG	2:B:58:LYS:NZ	2.16	0.78
4:F:138:ARG:HE	4:F:143:GLU:HB2	1.46	0.78
4:F:136:ASN:O	4:F:140:GLU:N	2.13	0.78

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	435/450 (97%)	425 (98%)	10 (2%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	413 (97%)	11 (3%)	1 (0%)	43	58
2	D	417/445 (94%)	399 (96%)	18 (4%)	0	100	100
3	E	117/143 (82%)	114 (97%)	3 (3%)	0	100	100
4	F	324/384 (84%)	308 (95%)	13 (4%)	3 (1%)	14	22
All	All	2156/2317 (93%)	2086 (97%)	66 (3%)	4 (0%)	43	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	ASN
4	F	236	LYS
4	F	142	ARG
4	F	140	GLU

### 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	368/378 (97%)	364 (99%)	4 (1%)	65 82
1	C	371/378 (98%)	367 (99%)	4 (1%)	65 82
2	B	369/383 (96%)	361 (98%)	8 (2%)	45 67
2	D	364/383 (95%)	358 (98%)	6 (2%)	55 76
3	E	109/127 (86%)	105 (96%)	4 (4%)	30 51
4	F	301/342 (88%)	291 (97%)	10 (3%)	33 55
All	All	1882/1991 (94%)	1846 (98%)	36 (2%)	50 71

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	89	GLU
4	F	243	HIS
4	F	140	GLU
4	F	234	GLN
1	C	254	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	293	ASN
4	F	176	GLN
2	D	426	GLN
4	F	232	ASN
2	B	137	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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
9	GDP	B	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.75	8 (17%)
10	MES	B	503	-	12,12,12	2.21	1 (8%)	15,16,16	1.91	5 (33%)
11	NZO	D	503	-	23,23,23	1.48	3 (13%)	32,32,32	2.47	10 (31%)
5	GTP	A	501	6	33,34,34	0.99	3 (9%)	50,54,54	1.52	8 (16%)
10	MES	D	502	-	12,12,12	2.33	1 (8%)	15,16,16	1.94	2 (13%)
12	ACP	F	401	-	31,33,33	1.89	7 (22%)	47,52,52	1.98	11 (23%)
8	GOL	A	504	-	5,5,5	0.39	0	5,5,5	0.24	0
11	NZO	B	504	-	23,23,23	1.45	3 (13%)	32,32,32	2.51	10 (31%)
5	GTP	C	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.49	8 (16%)
9	GDP	D	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	8 (17%)

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
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
10	MES	B	503	-	-	5/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NZO	D	503	-	-	4/14/14/14	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
10	MES	D	502	-	-	3/6/14/14	0/1/1/1
12	ACP	F	401	-	-	4/19/38/38	0/3/3/3
8	GOL	A	504	-	-	4/4/4/4	-
11	NZO	B	504	-	-	2/14/14/14	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
9	GDP	D	501	-	-	5/16/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	MES	C8-S	-7.82	1.66	1.77
10	B	503	MES	C8-S	-7.32	1.67	1.77
12	F	401	ACP	PG-O3G	-4.36	1.45	1.55
12	F	401	ACP	PG-O1G	4.04	1.58	1.50
12	F	401	ACP	C5-N7	-3.84	1.32	1.39

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	NZO	O3-C13-N3	8.51	118.94	109.15
11	D	503	NZO	O3-C13-N3	7.74	118.06	109.15
12	F	401	ACP	C5-C4-N3	-6.14	118.27	126.72
9	D	501	GDP	C5-C4-N3	-5.98	118.87	128.39
9	B	501	GDP	C5-C4-N3	-5.82	119.14	128.39

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

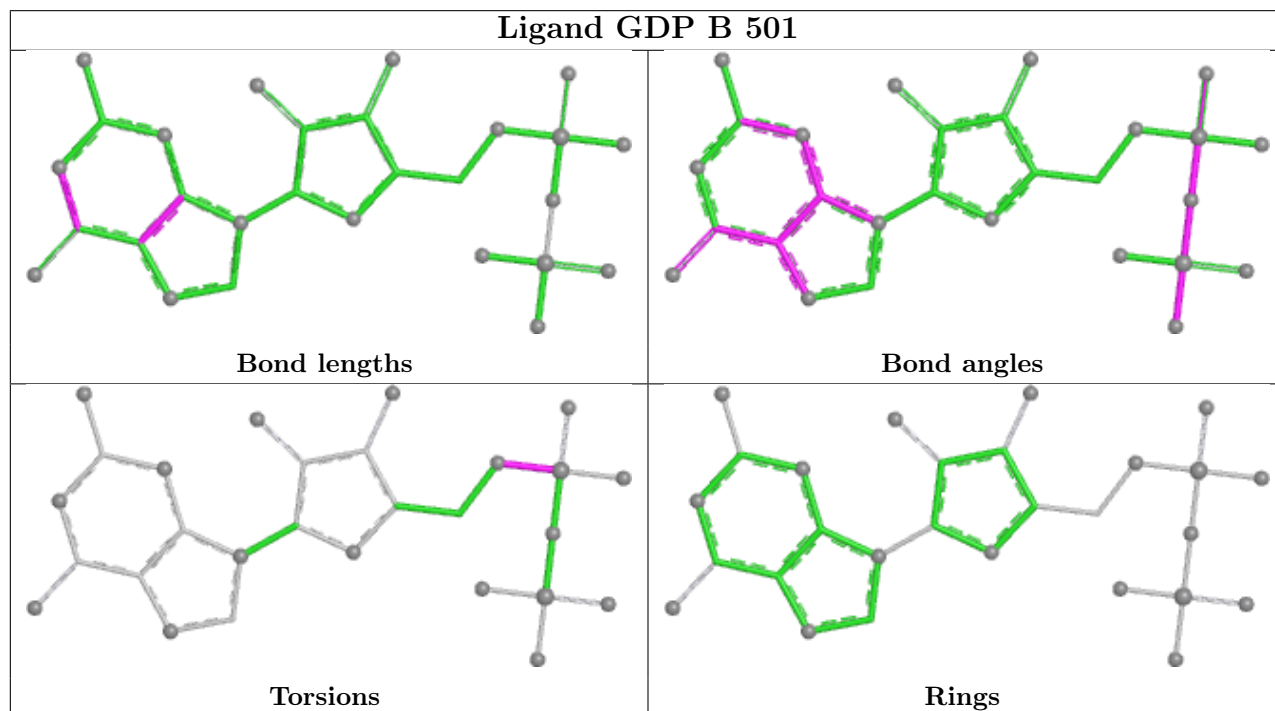
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G

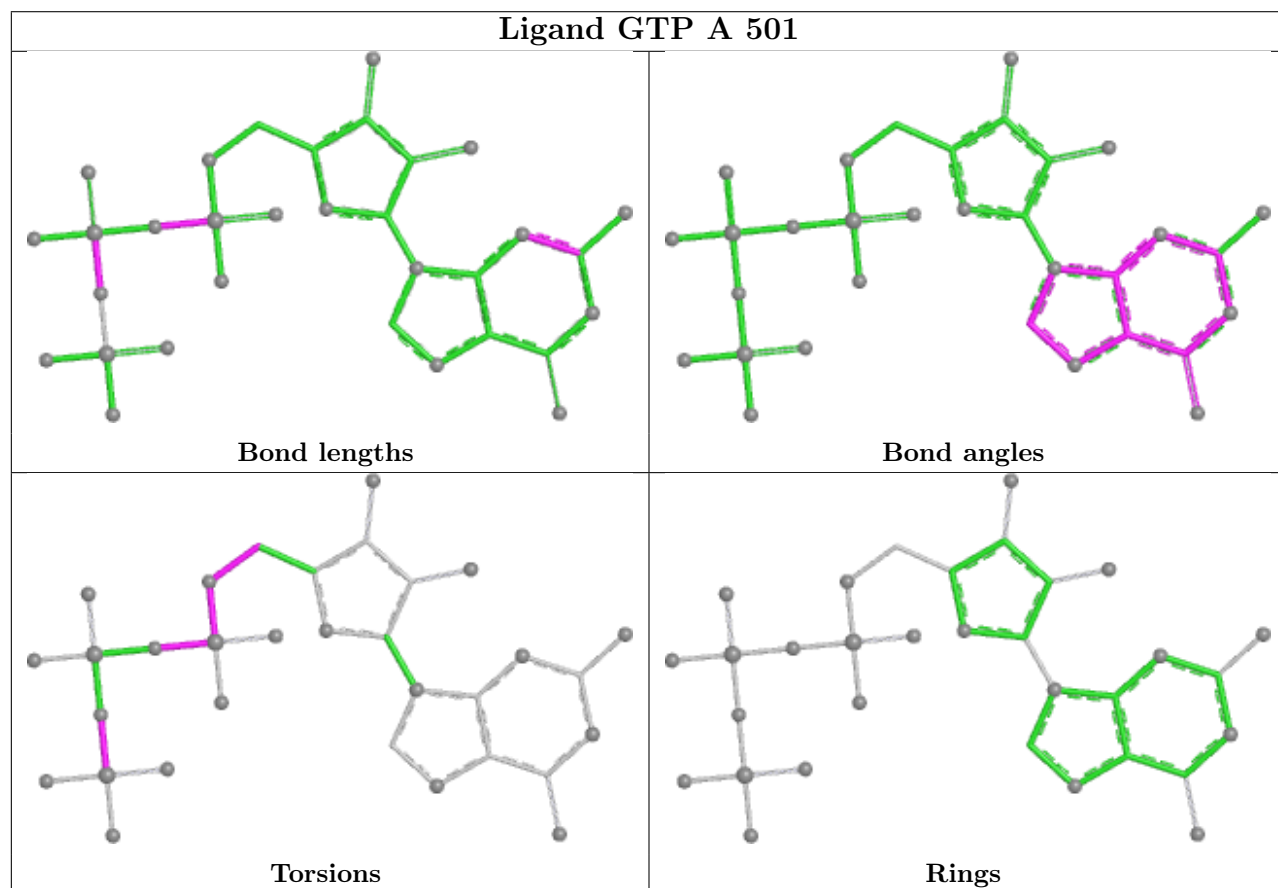
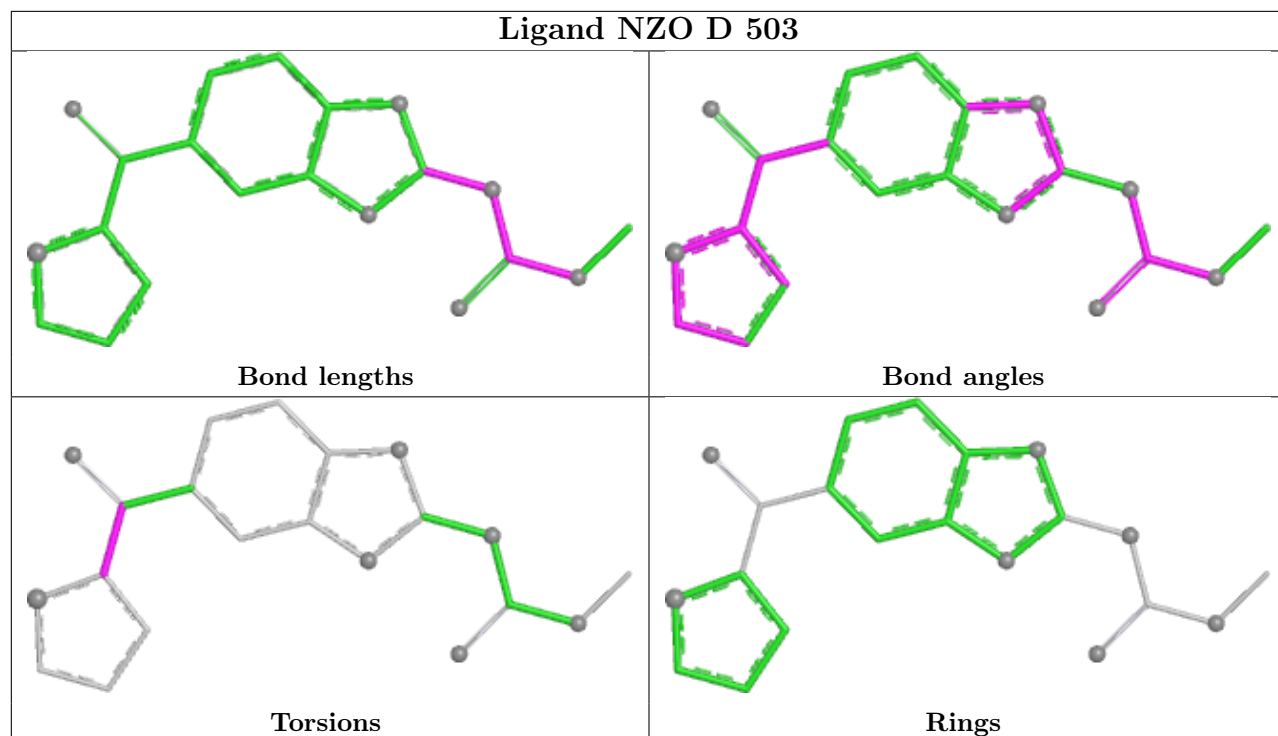
There are no ring outliers.

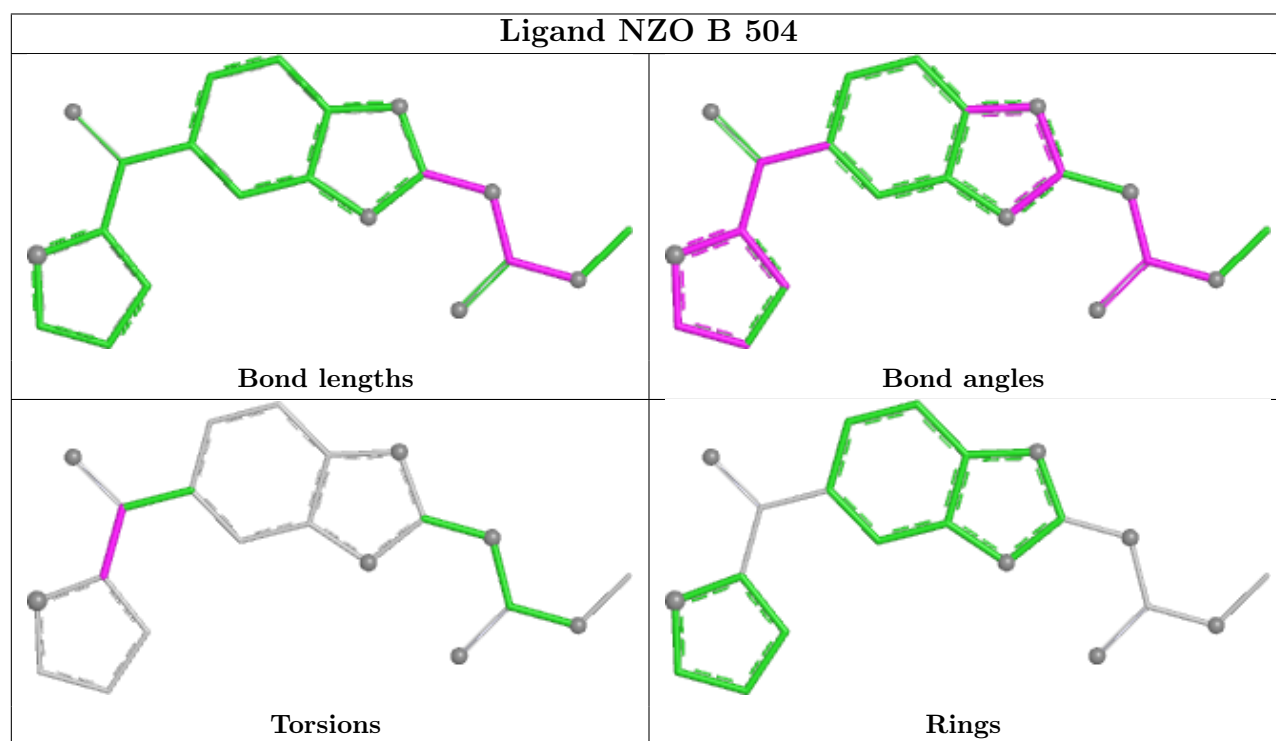
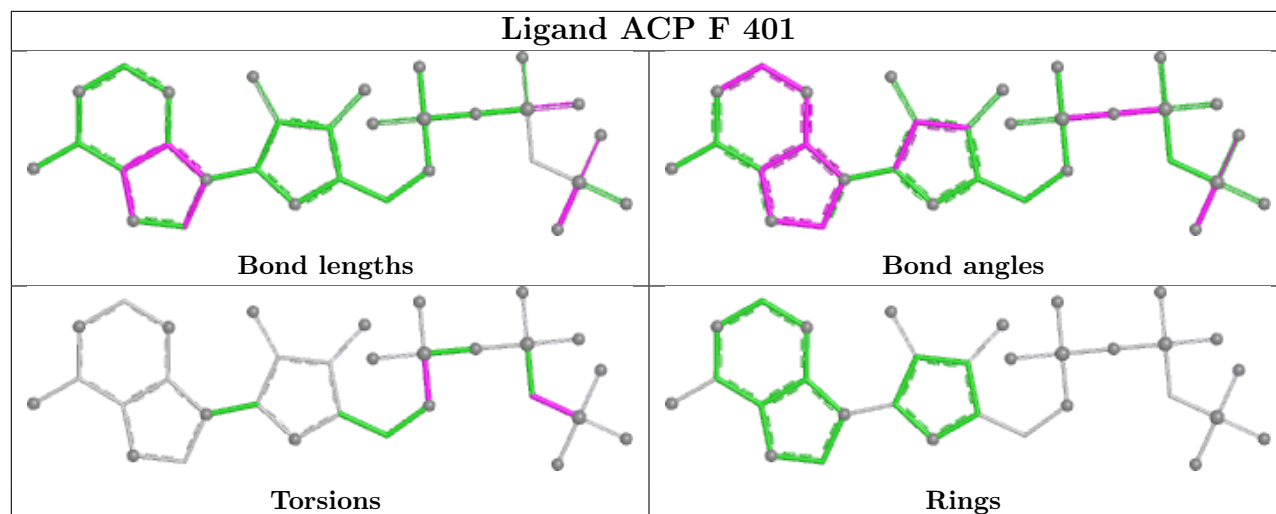
7 monomers are involved in 16 short contacts:

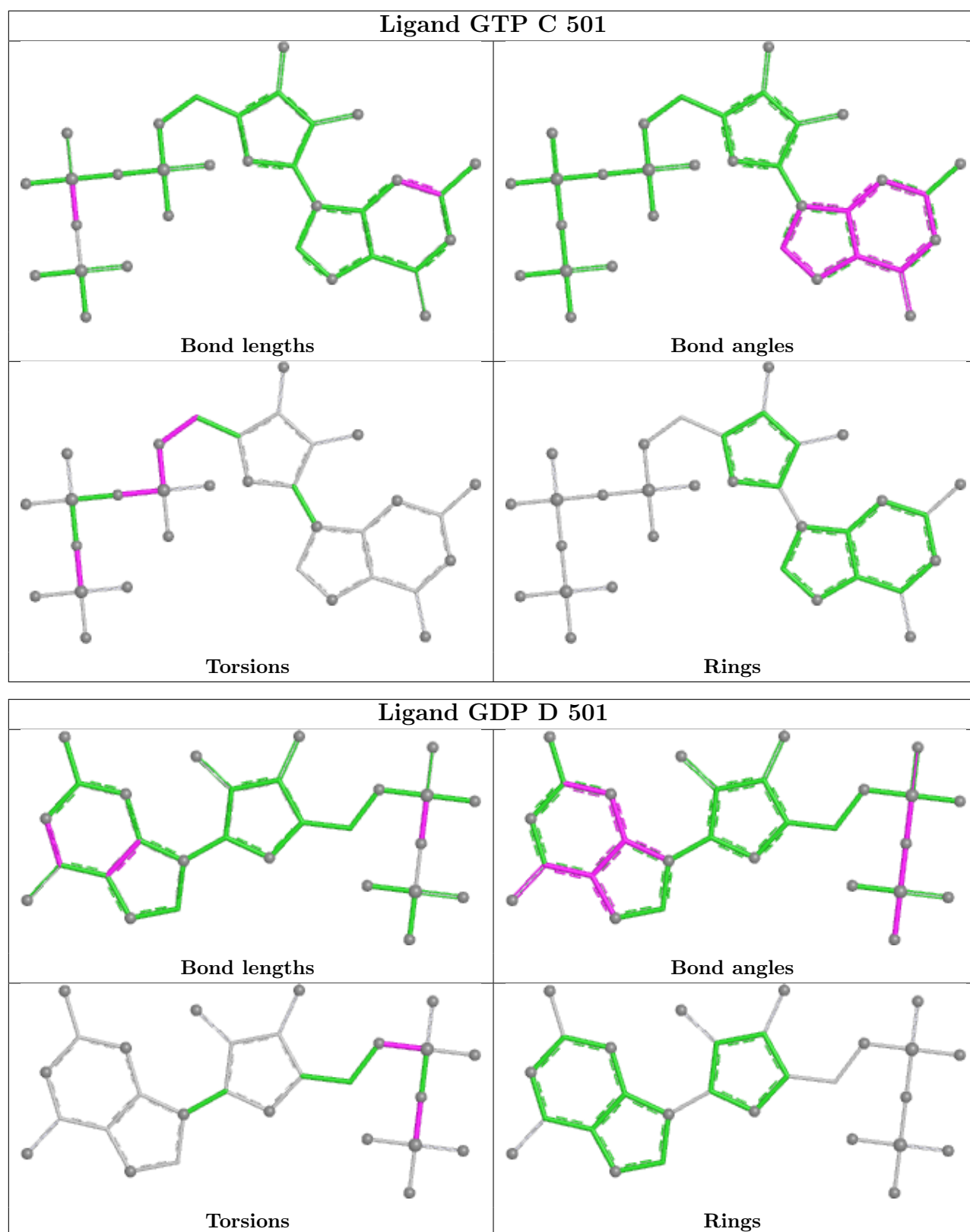
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	2	0
11	D	503	NZO	2	0
5	A	501	GTP	1	0
10	D	502	MES	3	0
12	F	401	ACP	5	0
11	B	504	NZO	1	0
9	D	501	GDP	2	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	437/450 (97%)	-0.08	7 (1%) 70 66	24, 39, 62, 87	0
1	C	440/450 (97%)	-0.40	5 (1%) 78 74	19, 31, 53, 69	0
2	B	427/445 (95%)	-0.02	21 (4%) 35 31	22, 38, 69, 103	0
2	D	421/445 (94%)	0.34	21 (4%) 34 30	26, 48, 78, 101	0
3	E	121/143 (84%)	0.56	7 (5%) 29 25	29, 53, 83, 94	0
4	F	334/384 (86%)	0.93	60 (17%) 3 3	32, 59, 116, 135	0
All	All	2180/2317 (94%)	0.14	121 (5%) 30 26	19, 42, 82, 135	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	5.4
2	B	335	ASN	4.9
4	F	103	THR	4.6
2	B	331	LEU	4.4
4	F	372	THR	4.4

### 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 oligosaccharides in this entry.

## 6.4 Ligands

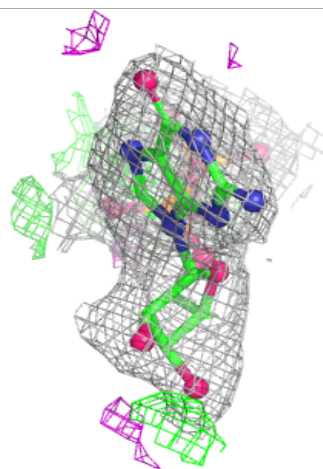
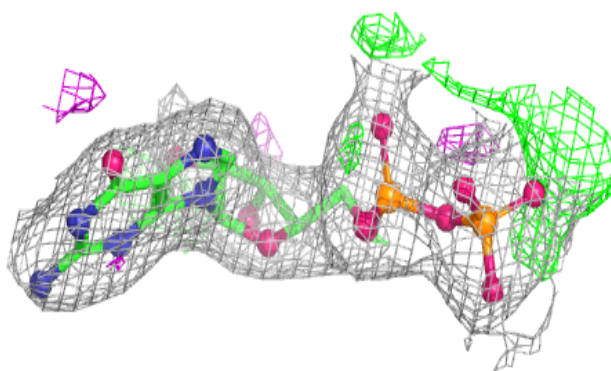
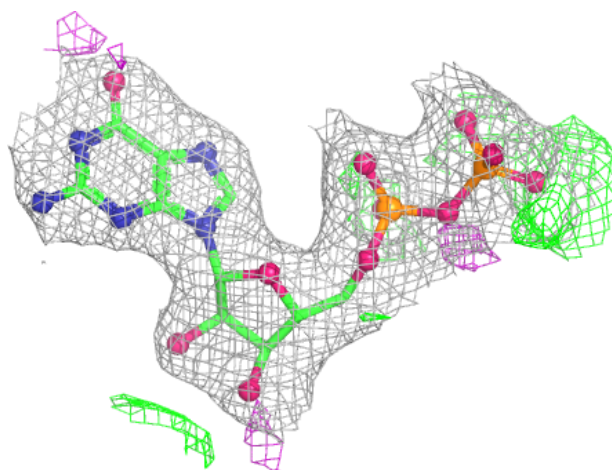
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
8	GOL	A	504	6/6	0.86	0.14	45,54,59,59	0
10	MES	D	502	12/12	0.86	0.17	50,58,63,66	0
9	GDP	D	501	28/28	0.90	0.10	37,43,57,63	0
12	ACP	F	401	31/31	0.90	0.11	73,81,94,97	0
11	NZO	D	503	21/21	0.93	0.09	25,40,50,69	0
10	MES	B	503	12/12	0.93	0.10	32,43,51,53	0
7	CA	A	503	1/1	0.94	0.05	54,54,54,54	0
11	NZO	B	504	21/21	0.96	0.07	14,29,35,50	0
7	CA	C	503	1/1	0.97	0.04	45,45,45,45	0
6	MG	B	502	1/1	0.97	0.09	26,26,26,26	0
5	GTP	A	501	32/32	0.98	0.05	21,29,33,36	0
5	GTP	C	501	32/32	0.98	0.05	19,24,30,30	0
9	GDP	B	501	28/28	0.98	0.05	23,29,31,40	0
6	MG	A	502	1/1	0.99	0.03	28,28,28,28	0
6	MG	C	502	1/1	1.00	0.04	24,24,24,24	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.

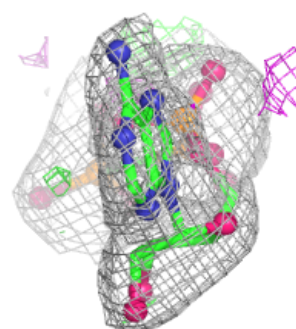
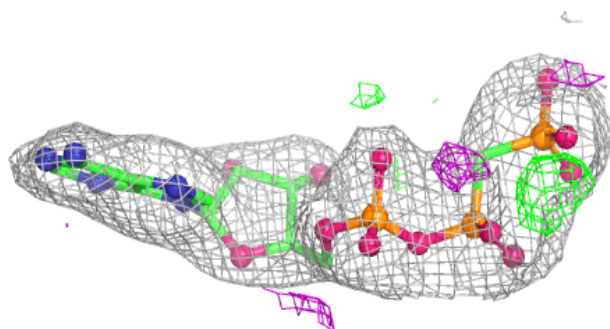
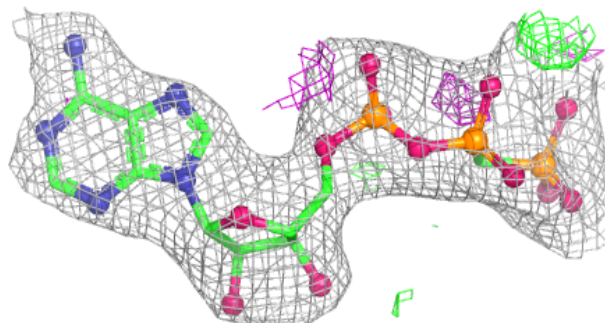
**Electron density around GDP D 501:**

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

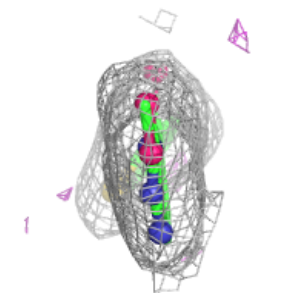
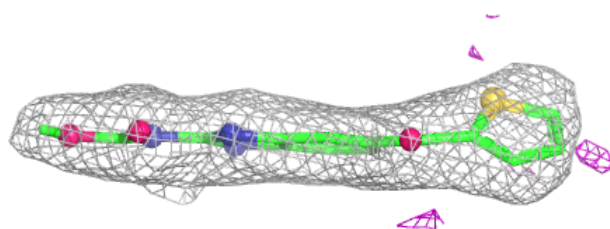
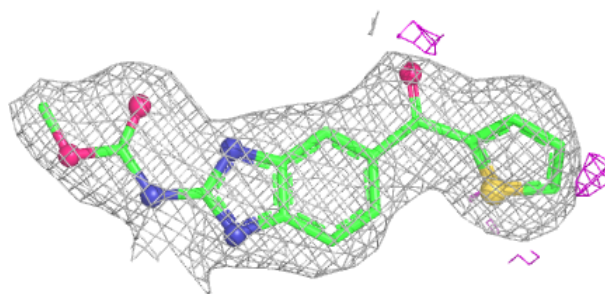


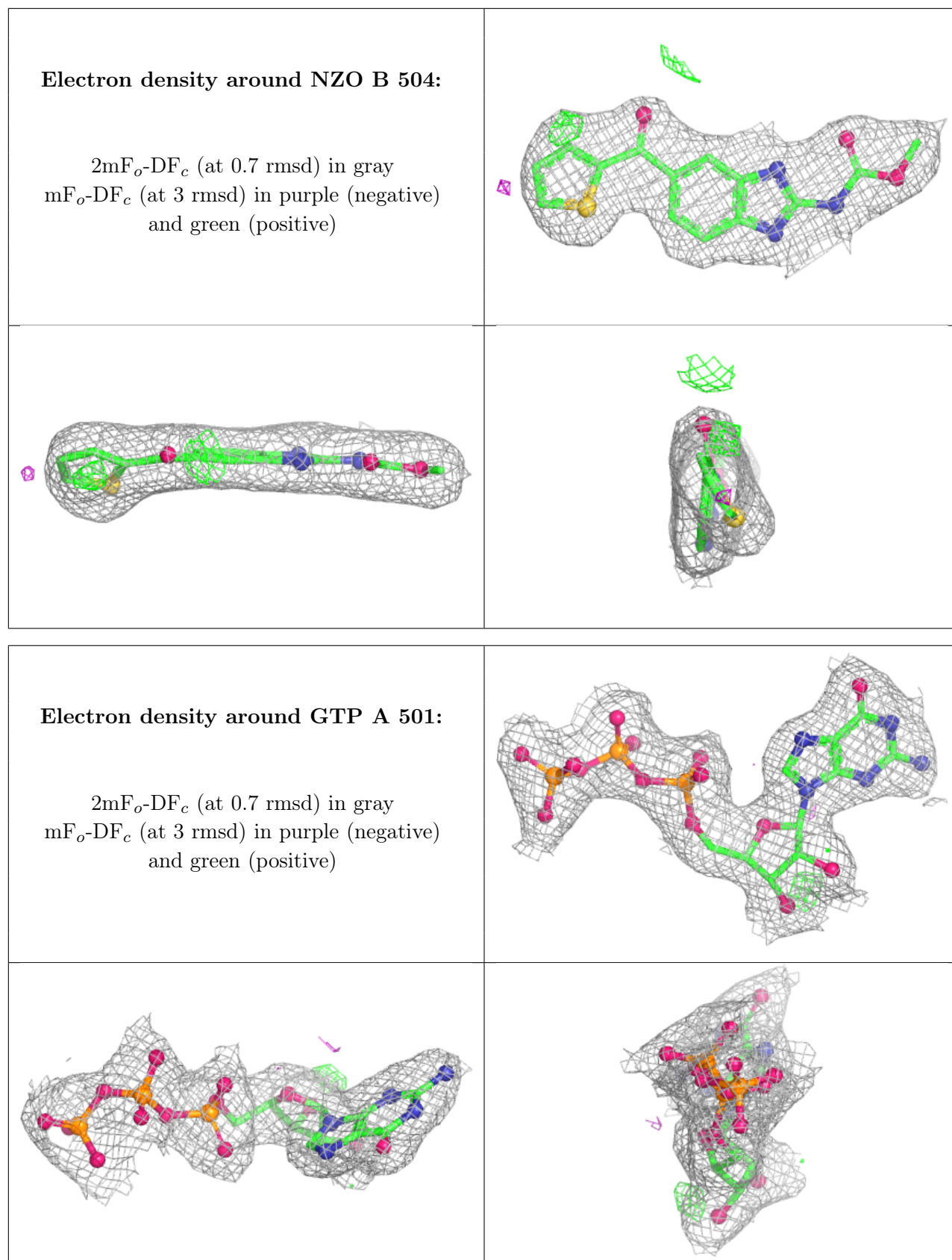
**Electron density around ACP F 401:**

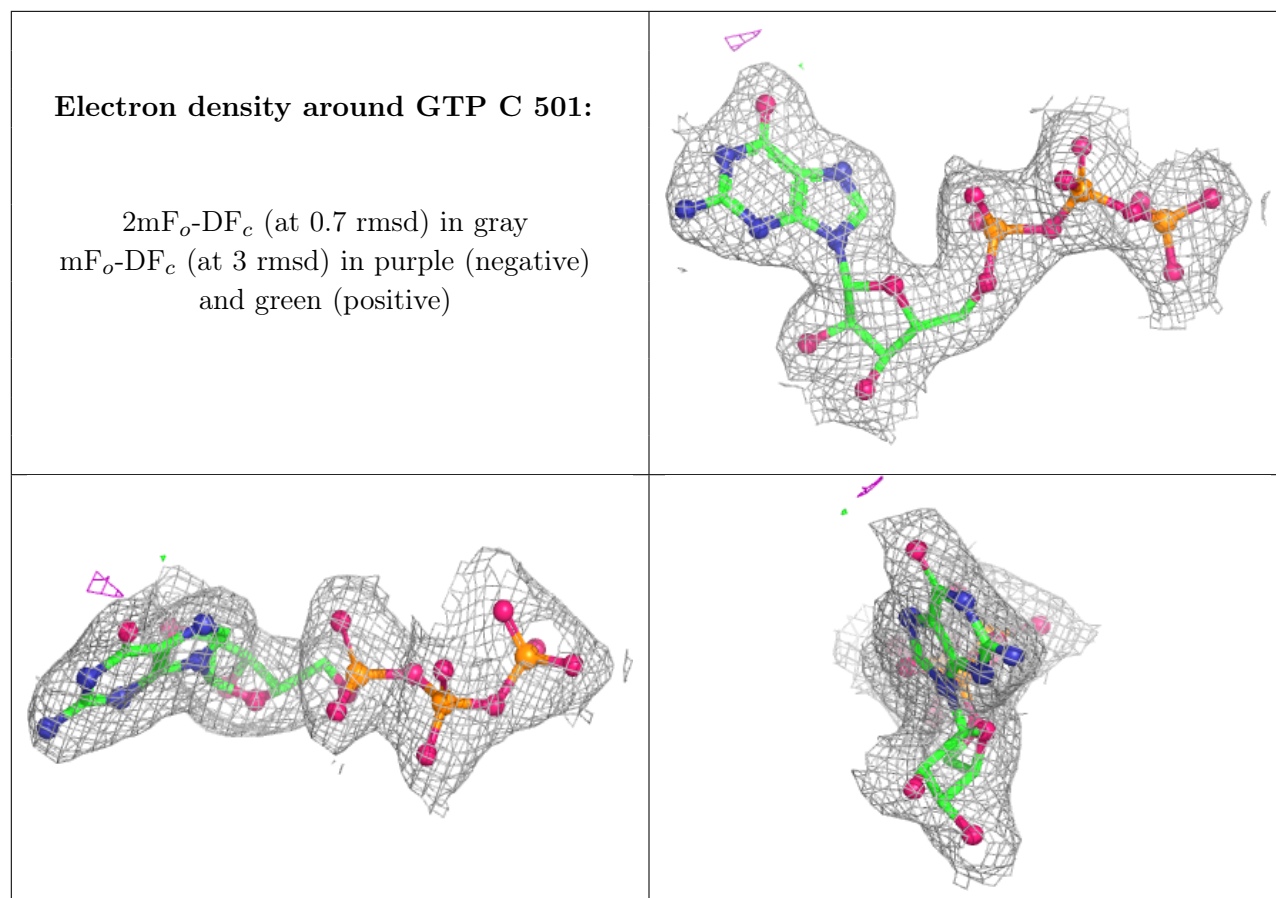
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

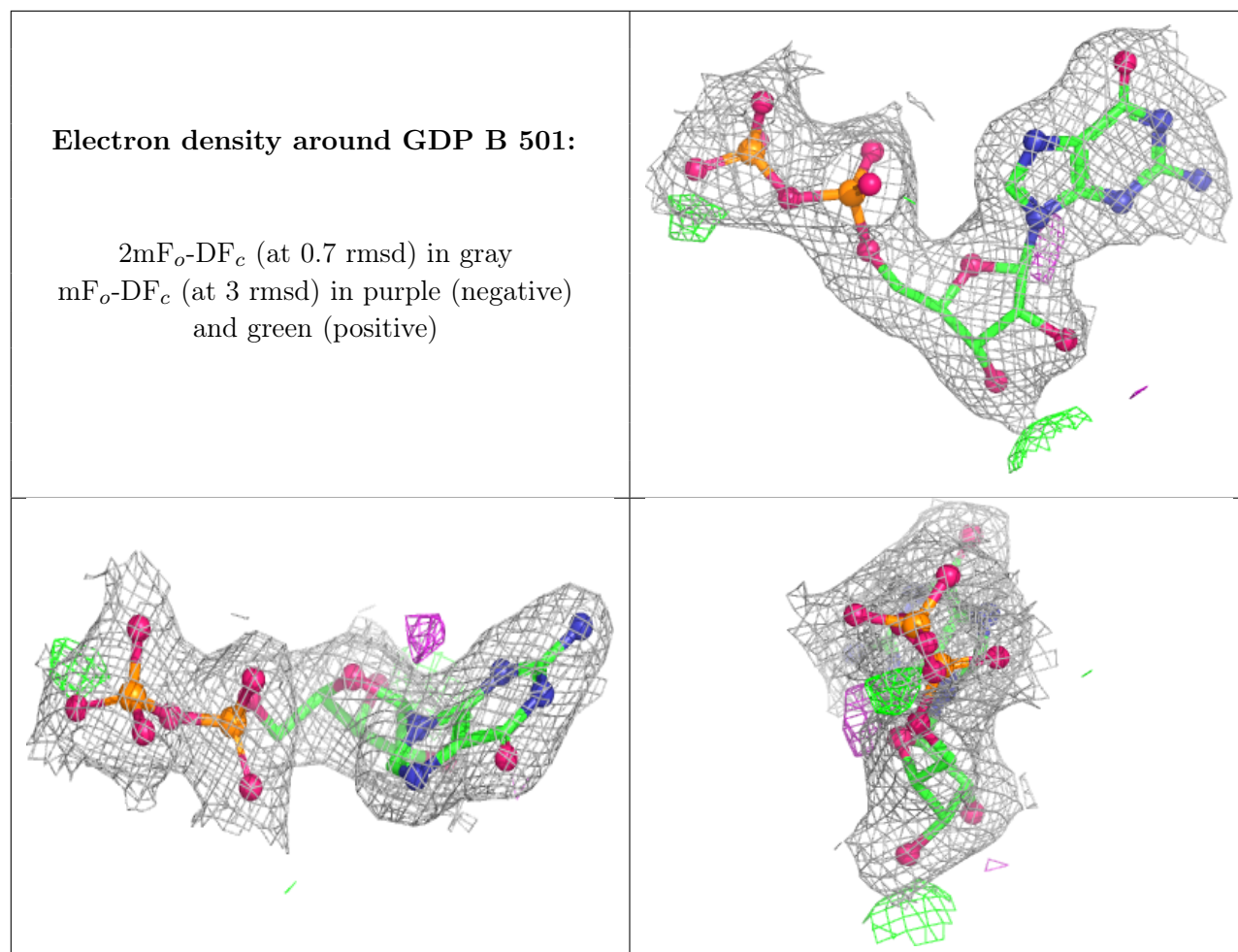
**Electron density around NZO D 503:**

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









## 6.5 Other polymers [i](#)

There are no such residues in this entry.