



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:09 am BST

PDB ID : 6DDS  
Title : Mycobacterium tuberculosis Dihydrofolate Reductase complexed with beta-NADPH and 4-[3-[3-[2,4-bis(azanyl)-6-ethyl-pyrimidin-5-yl]prop-2-ynyl]-5-methoxy-phenyl]benzoic acid  
Authors : Hajian, B.; Wright, D.; Scocchera, E.  
Deposited on : 2018-05-10  
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

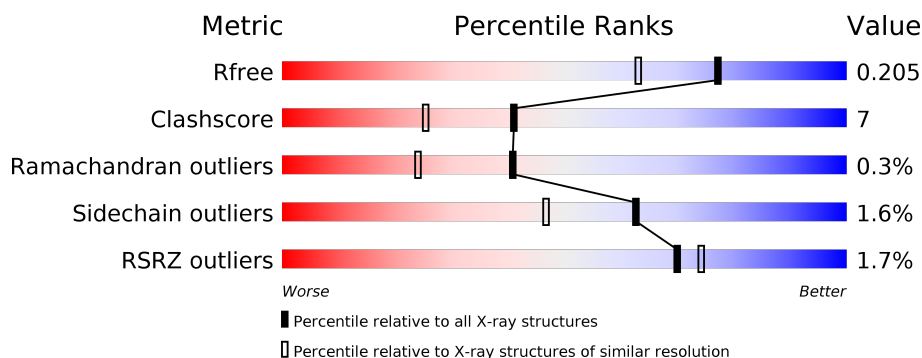
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	159	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	159	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	C	159	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
1	D	159	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>

## 2 Entry composition i

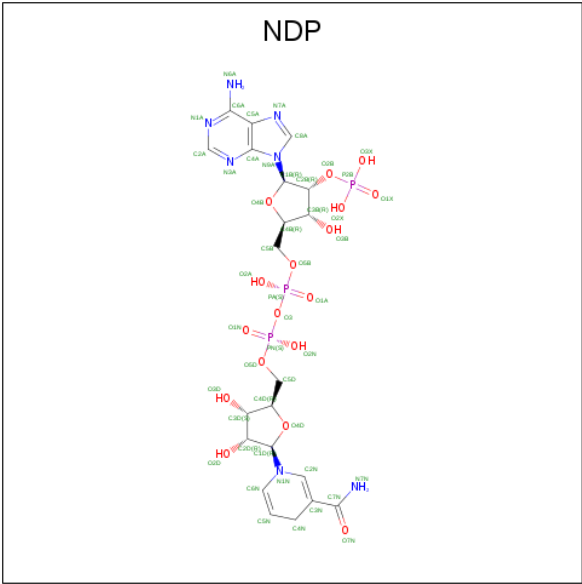
There are 7 unique types of molecules in this entry. The entry contains 5957 atoms, of which 43 are hydrogens and 0 are deuteriums.

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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	2	0
			1262	793	230	234	5			
1	B	159	Total	C	N	O	S	0	0	0
			1244	783	228	228	5			
1	C	159	Total	C	N	O	S	0	0	0
			1244	783	228	228	5			
1	D	159	Total	C	N	O	S	0	0	0
			1244	783	228	228	5			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



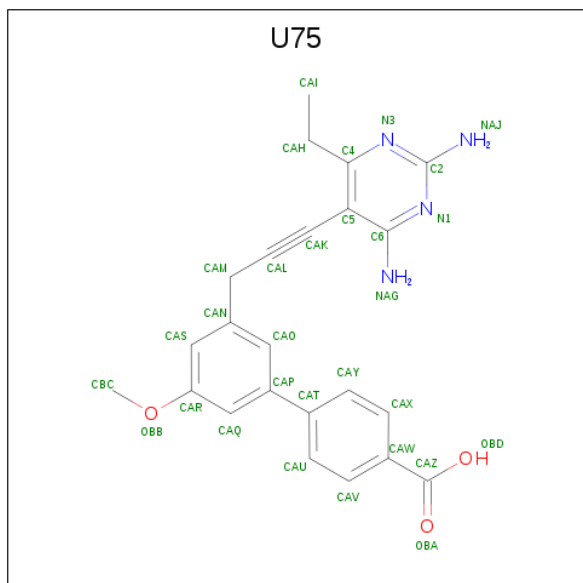
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 4-[3-[3-[2,4-bis(azanyl)-6-ethyl-pyrimidin-5-yl]prop-2-ynyl]-5-methoxy-phenyl] benzoic acid (three-letter code: U75) (formula:  $C_{23}H_{22}N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	23	4	3		
3	B	1	Total	C	N	O	0	0
			30	23	4	3		
3	C	1	Total	C	N	O	0	0
			30	23	4	3		
3	D	1	Total	C	N	O	0	0
			30	23	4	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 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
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	D	1	Total	C	H	O	0	0
			14	3	8	3		
6	D	1	Total	C	H	O	0	0
			14	3	8	3		

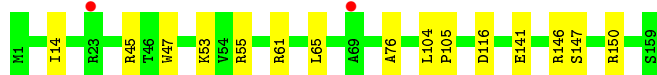
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	147	Total	O	0	0
			147	147		
7	B	140	Total	O	0	0
			140	140		
7	C	150	Total	O	0	0
			150	150		
7	D	136	Total	O	0	0
			136	136		

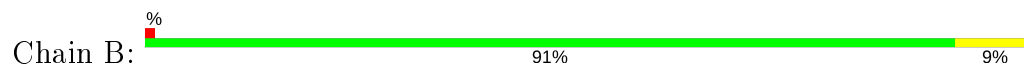
### 3 Residue-property plots [i](#)

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

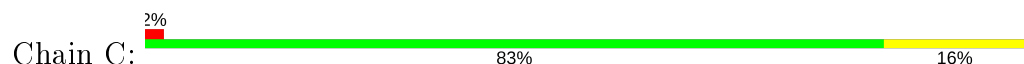
- Molecule 1: Dihydrofolate reductase



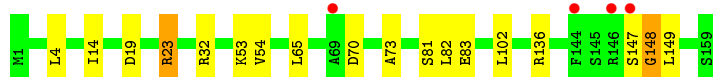
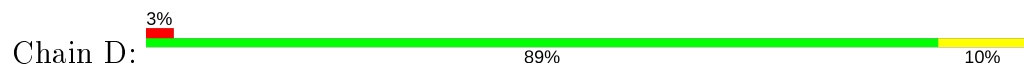
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.20Å 60.80Å 60.72Å 90.15° 89.94° 90.02°	Depositor
Resolution (Å)	27.00 – 1.72 27.00 – 1.72	Depositor EDS
% Data completeness (in resolution range)	77.8 (27.00-1.72) 77.2 (27.00-1.72)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.182 , 0.206 0.182 , 0.205	Depositor DCC
$R_{free}$ test set	2030 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage

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<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.



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Property	Value	Source
Estimated twinning fraction	0.456 for h,l,-k	Xtriage
	0.456 for h,-l,k	
	0.037 for k,-h,l	
	0.037 for -k,h,l	
	0.035 for l,k,-h	
	0.035 for -l,k,h	
	0.033 for l,-h,-k	
	0.033 for -k,-l,h	
	0.029 for -k,l,-h	
	0.029 for -l,-h,k	
	0.033 for k,-l,-h	
	0.033 for -l,h,-k	
	0.036 for l,h,k	
	0.036 for k,l,h	
	0.469 for h,-k,-l	
	0.065 for -h,-k,l	
	0.063 for -h,k,-l	
	0.035 for l,-k,h	
	0.033 for -l,-k,-h	
	0.036 for -k,-h,-l	
	0.056 for k,h,-l	
	0.055 for -h,-l,-k	
	0.052 for -h,l,k	
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5957	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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: GOL, ACT, NDP, U75, NA

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	0.36	0/1293	0.55	0/1756
1	B	0.37	0/1275	0.54	0/1732
1	C	0.37	0/1275	0.55	0/1732
1	D	0.36	0/1275	0.54	0/1732
All	All	0.36	0/5118	0.55	0/6952

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1262	0	1233	22	0
1	B	1244	0	1223	12	0
1	C	1244	0	1223	26	0
1	D	1244	0	1223	17	0
2	A	48	0	26	3	0
2	B	48	0	26	1	0
2	C	48	0	26	1	0
2	D	48	0	26	3	0
3	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	1	0
4	A	4	3	3	1	0
5	A	1	0	0	0	0
6	B	6	8	8	1	0
6	C	12	16	16	3	0
6	D	12	16	16	1	0
7	A	147	0	0	9	0
7	B	140	0	0	8	1
7	C	150	0	0	12	1
7	D	136	0	0	5	0
All	All	5914	43	5049	74	1

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 7.

All (74) 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:D:23:ARG:HD3	1:D:23:ARG:H	1.29	0.96
1:B:136:ARG:NH1	7:B:301:HOH:O	2.02	0.92
1:C:147:SER:O	7:C:301:HOH:O	1.90	0.89
1:A:53:LYS:HD2	1:C:143:ARG:NH2	1.91	0.85
1:C:45:ARG:NH1	7:C:305:HOH:O	2.10	0.84
1:A:141:GLU:O	7:A:301:HOH:O	2.00	0.79
6:C:204:GOL:O1	7:C:302:HOH:O	2.02	0.77
7:A:311:HOH:O	1:C:140:GLY:HA3	1.85	0.77
1:B:133:GLU:OE1	7:B:302:HOH:O	2.03	0.75
1:B:67:ARG:NH2	1:C:146:ARG:O	2.21	0.74
1:A:61:ARG:NH1	7:A:305:HOH:O	2.21	0.73
1:C:147:SER:OG	7:C:303:HOH:O	2.06	0.73
1:C:23:ARG:HE	1:C:25:PRO:HG3	1.54	0.73
1:C:83:GLU:OE1	7:C:304:HOH:O	2.08	0.72
1:B:73:ALA:HA	6:B:203:GOL:H12	1.72	0.70
1:A:147:SER:OG	7:A:302:HOH:O	2.08	0.70
1:A:147:SER:O	7:A:303:HOH:O	2.09	0.70
1:B:84:GLU:O	7:B:303:HOH:O	2.10	0.69
1:D:23:ARG:HD3	1:D:23:ARG:N	2.05	0.68
1:D:32:ARG:NH2	3:D:202:U75:OBA	2.27	0.68
6:C:204:GOL:O3	7:C:306:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:HD22	7:C:307:HOH:O	1.97	0.64
1:D:147:SER:OG	7:D:301:HOH:O	2.16	0.62
1:B:61:ARG:NH1	7:B:306:HOH:O	2.33	0.61
1:A:53:LYS:HD2	1:C:143:ARG:HH22	1.65	0.60
1:C:61:ARG:NH1	7:D:303:HOH:O	2.35	0.59
1:A:53:LYS:HD2	1:C:143:ARG:HH21	1.66	0.59
1:C:159:SER:O	7:C:302:HOH:O	2.17	0.57
1:D:136:ARG:NE	7:D:305:HOH:O	2.36	0.55
1:A:53:LYS:HG2	7:A:410:HOH:O	2.05	0.55
7:B:330:HOH:O	1:C:150:ARG:HD3	2.07	0.54
1:D:82:LEU:HD22	1:D:102:LEU:HG	1.90	0.54
1:D:73:ALA:HA	6:D:203:GOL:H31	1.89	0.53
1:B:45:ARG:NH1	7:B:309:HOH:O	2.40	0.52
1:D:65:LEU:HG	2:D:201:NDP:C2A	2.39	0.52
1:A:55:ARG:HE	4:A:203:ACT:H2	1.75	0.51
1:A:116:ASP:OD2	1:A:150:ARG:HD3	2.11	0.50
1:C:68:GLN:HB3	1:C:71:PHE:HB2	1.93	0.49
1:A:14:ILE:O	2:A:201:NDP:H2N	2.13	0.49
1:D:23:ARG:NH2	1:D:149:LEU:HD11	2.27	0.49
1:B:104:LEU:HB3	1:B:105:PRO:HD3	1.93	0.49
1:D:23:ARG:CD	1:D:23:ARG:N	2.75	0.49
1:B:32:ARG:NE	7:B:312:HOH:O	2.46	0.48
1:D:14:ILE:O	2:D:201:NDP:H2N	2.14	0.48
1:A:53:LYS:NZ	7:A:311:HOH:O	2.38	0.47
1:D:81:SER:OG	1:D:83:GLU:HG2	2.14	0.47
1:A:116:ASP:HB3	1:A:150:ARG:HG2	1.97	0.47
1:C:28:GLN:NE2	7:C:308:HOH:O	2.35	0.47
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.97	0.46
1:C:14:ILE:O	2:C:201:NDP:H2N	2.16	0.46
1:D:65:LEU:HG	2:D:201:NDP:N3A	2.31	0.46
1:A:53:LYS:HE3	7:C:384:HOH:O	2.15	0.46
1:C:70:ASP:HA	1:D:83:GLU:OE1	2.16	0.46
1:C:136:ARG:NH2	1:C:159:SER:H	2.13	0.45
1:A:65:LEU:HG	2:A:201:NDP:N3A	2.32	0.45
7:A:311:HOH:O	1:C:153:LEU:HB2	2.18	0.44
1:C:116:ASP:HB3	1:C:150:ARG:HG2	2.00	0.44
1:B:14:ILE:O	2:B:201:NDP:H2N	2.19	0.43
1:A:53:LYS:HD3	7:C:446:HOH:O	2.19	0.43
1:C:104:LEU:HB3	1:C:105:PRO:HD3	2.00	0.43
1:C:47:TRP:CH2	1:C:76:ALA:HB2	2.53	0.43
1:B:136:ARG:HG3	1:B:136:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PRO:HD2	7:B:304:HOH:O	2.20	0.42
1:A:65:LEU:HG	2:A:201:NDP:C2A	2.48	0.42
1:A:47:TRP:CH2	1:A:76:ALA:HB2	2.55	0.42
1:A:116:ASP:HB3	1:A:150:ARG:CG	2.49	0.42
1:D:136:ARG:HG2	7:D:305:HOH:O	2.18	0.42
1:D:53:LYS:HG3	1:D:54:VAL:HG13	2.01	0.42
1:C:83:GLU:H	1:C:83:GLU:CD	2.23	0.42
1:C:108:THR:HG21	6:C:204:GOL:H12	2.02	0.41
1:A:47:TRP:CZ3	1:A:76:ALA:HB2	2.55	0.41
1:D:148:GLY:N	7:D:302:HOH:O	2.53	0.41
1:A:45:ARG:NH1	7:A:304:HOH:O	2.19	0.41
1:C:58:PRO:HG3	7:C:356:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:306:HOH:O	7:C:365:HOH:O[1_545]	2.11	0.09

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/159 (100%)	156 (98%)	3 (2%)	0	100	100
1	B	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	C	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	10
1	D	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	10
All	All	630/636 (99%)	613 (97%)	15 (2%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	148	GLY
1	C	148	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	129/127 (102%)	128 (99%)	1 (1%)	81	73
1	B	127/127 (100%)	125 (98%)	2 (2%)	62	47
1	C	127/127 (100%)	126 (99%)	1 (1%)	81	73
1	D	127/127 (100%)	123 (97%)	4 (3%)	40	19
All	All	510/508 (100%)	502 (98%)	8 (2%)	62	47

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	B	23	ARG
1	B	102	LEU
1	C	136	ARG
1	D	4	LEU
1	D	19	ASP
1	D	23	ARG
1	D	70	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\# Z  > 2$
2	NDP	C	201	-	45,52,52	2.04	7 (15%)	53,80,80	1.39	7 (13%)
3	U75	B	202	-	30,32,32	2.10	6 (20%)	37,44,44	1.78	11 (29%)
6	GOL	C	203	-	5,5,5	0.32	0	5,5,5	0.18	0
6	GOL	C	204	-	5,5,5	0.26	0	5,5,5	0.62	0
6	GOL	B	203	-	5,5,5	0.27	0	5,5,5	0.32	0
4	ACT	A	203	-	1,3,3	1.21	0	0,3,3	0.00	-
6	GOL	D	204	-	5,5,5	0.34	0	5,5,5	0.26	0
6	GOL	D	203	-	5,5,5	0.29	0	5,5,5	0.27	0
3	U75	A	202	-	30,32,32	2.07	5 (16%)	37,44,44	1.86	11 (29%)
3	U75	C	202	-	30,32,32	2.26	6 (20%)	37,44,44	1.67	9 (24%)
2	NDP	B	201	-	45,52,52	2.23	5 (11%)	53,80,80	1.40	8 (15%)
2	NDP	D	201	-	45,52,52	2.13	4 (8%)	53,80,80	1.38	6 (11%)
2	NDP	A	201	-	45,52,52	2.23	5 (11%)	53,80,80	1.39	6 (11%)
3	U75	D	202	-	30,32,32	2.11	6 (20%)	37,44,44	1.83	11 (29%)

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
2	NDP	C	201	-	-	5/30/77/77	0/5/5/5
3	U75	B	202	-	-	0/13/18/18	0/3/3/3
6	GOL	C	203	-	-	3/4/4/4	-
6	GOL	C	204	-	-	2/4/4/4	-
6	GOL	B	203	-	-	2/4/4/4	-
6	GOL	D	204	-	-	2/4/4/4	-
6	GOL	D	203	-	-	2/4/4/4	-
3	U75	A	202	-	-	2/13/18/18	0/3/3/3
3	U75	C	202	-	-	0/13/18/18	0/3/3/3
2	NDP	B	201	-	-	3/30/77/77	0/5/5/5
2	NDP	D	201	-	-	3/30/77/77	0/5/5/5
2	NDP	A	201	-	-	3/30/77/77	0/5/5/5
3	U75	D	202	-	-	0/13/18/18	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	NDP	P2B-O2B	12.55	1.83	1.59
2	B	201	NDP	P2B-O2B	12.53	1.83	1.59
2	D	201	NDP	P2B-O2B	11.69	1.81	1.59
2	C	201	NDP	P2B-O2B	10.64	1.79	1.59
3	C	202	U75	CAW-CAZ	-7.57	1.40	1.47
3	A	202	U75	CAW-CAZ	-7.44	1.40	1.47
3	B	202	U75	CAW-CAZ	-7.28	1.40	1.47
3	D	202	U75	CAW-CAZ	-7.04	1.40	1.47
3	C	202	U75	CAH-C4	-6.47	1.40	1.51
3	B	202	U75	CAH-C4	-6.41	1.40	1.51
3	D	202	U75	CAH-C4	-6.34	1.40	1.51
3	A	202	U75	CAH-C4	-6.06	1.40	1.51
3	C	202	U75	CAM-CAL	4.98	1.51	1.47
2	D	201	NDP	PN-O5D	3.68	1.74	1.59
2	B	201	NDP	PN-O5D	3.55	1.73	1.59
2	C	201	NDP	PN-O5D	3.54	1.73	1.59
3	B	202	U75	CAT-CAP	-3.40	1.40	1.49
2	A	201	NDP	PN-O5D	3.35	1.72	1.59
3	A	202	U75	CAT-CAP	-3.29	1.40	1.49
3	C	202	U75	CAT-CAP	-3.24	1.41	1.49
3	D	202	U75	CAT-CAP	-3.17	1.41	1.49
2	C	201	NDP	O2B-C2B	-3.02	1.33	1.44
3	A	202	U75	CAM-CAN	-2.97	1.41	1.51
2	D	201	NDP	O2B-C2B	-2.94	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	202	U75	CAM-CAN	-2.93	1.41	1.51
3	D	202	U75	C5-C6	-2.92	1.38	1.42
2	A	201	NDP	O2B-C2B	-2.89	1.33	1.44
3	C	202	U75	CAM-CAN	-2.80	1.42	1.51
3	B	202	U75	CAM-CAN	-2.75	1.42	1.51
2	B	201	NDP	O2B-C2B	-2.72	1.34	1.44
3	B	202	U75	CAM-CAL	2.62	1.49	1.47
2	C	201	NDP	C7N-N7N	2.52	1.40	1.33
3	A	202	U75	C5-C6	-2.48	1.39	1.42
2	B	201	NDP	C2A-N1A	2.46	1.38	1.33
2	A	201	NDP	C2A-N1A	2.37	1.38	1.33
2	D	201	NDP	C2A-N1A	2.26	1.38	1.33
3	B	202	U75	C5-C6	-2.23	1.39	1.42
2	B	201	NDP	C4A-N3A	2.15	1.38	1.35
2	C	201	NDP	C2A-N1A	2.11	1.37	1.33
3	C	202	U75	C5-C6	-2.06	1.39	1.42
2	A	201	NDP	C7N-N7N	2.05	1.38	1.33
2	C	201	NDP	O4B-C1B	2.04	1.43	1.41
2	C	201	NDP	C4A-N3A	2.02	1.38	1.35
3	D	202	U75	CAK-CAL	2.01	1.22	1.19

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	202	U75	C2-N3-C4	4.92	120.34	116.24
3	D	202	U75	C2-N1-C6	4.83	122.32	116.99
3	B	202	U75	C2-N3-C4	4.77	120.22	116.24
3	C	202	U75	C2-N3-C4	4.68	120.14	116.24
3	A	202	U75	C2-N3-C4	4.65	120.11	116.24
3	A	202	U75	C2-N1-C6	4.54	122.00	116.99
2	A	201	NDP	PN-O3-PA	-3.91	119.42	132.83
3	C	202	U75	C2-N1-C6	3.88	121.28	116.99
2	D	201	NDP	PN-O3-PA	-3.87	119.56	132.83
3	B	202	U75	C2-N1-C6	3.80	121.19	116.99
2	C	201	NDP	PN-O3-PA	-3.74	119.99	132.83
2	B	201	NDP	PN-O3-PA	-3.67	120.25	132.83
3	D	202	U75	N3-C2-N1	-3.49	119.95	125.42
3	A	202	U75	CBC-OBB-CAR	-3.41	110.10	117.51
3	A	202	U75	CAH-C4-C5	-3.26	120.34	122.66
3	A	202	U75	N3-C2-N1	-3.25	120.32	125.42
2	A	201	NDP	O2B-P2B-O1X	-3.09	97.47	109.39
3	B	202	U75	CAH-C4-C5	-3.04	120.50	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	NDP	O2B-P2B-O1X	-3.04	97.67	109.39
3	D	202	U75	NAG-C6-N1	3.03	121.31	117.03
3	C	202	U75	CAN-CAM-CAL	-3.01	107.68	113.65
2	D	201	NDP	O2B-P2B-O1X	-3.00	97.83	109.39
3	A	202	U75	CAN-CAM-CAL	-2.94	107.81	113.65
2	C	201	NDP	O2B-P2B-O1X	-2.94	98.03	109.39
3	B	202	U75	CAN-CAM-CAL	-2.93	107.84	113.65
3	B	202	U75	NAG-C6-N1	2.92	121.17	117.03
3	B	202	U75	C6-C5-CAK	2.90	123.59	118.57
3	B	202	U75	N3-C2-N1	-2.88	120.90	125.42
3	D	202	U75	C6-C5-CAK	2.78	123.38	118.57
3	B	202	U75	CAI-CAH-C4	-2.77	108.04	114.88
3	C	202	U75	N3-C2-N1	-2.77	121.08	125.42
3	C	202	U75	CBC-OBB-CAR	-2.76	111.52	117.51
3	A	202	U75	NAG-C6-N1	2.74	120.91	117.03
3	D	202	U75	CAH-C4-C5	-2.74	120.71	122.66
3	A	202	U75	C6-C5-CAK	2.73	123.30	118.57
3	D	202	U75	CAN-CAM-CAL	-2.71	108.28	113.65
2	D	201	NDP	O3X-P2B-O2X	2.65	117.75	107.64
2	A	201	NDP	O3X-P2B-O2X	2.64	117.71	107.64
2	C	201	NDP	O3X-P2B-O2X	2.61	117.63	107.64
3	B	202	U75	CBC-OBB-CAR	-2.58	111.92	117.51
2	B	201	NDP	C3N-C2N-N1N	-2.56	119.44	123.10
2	B	201	NDP	O3X-P2B-O2X	2.56	117.42	107.64
3	C	202	U75	C6-C5-CAK	2.54	122.97	118.57
3	C	202	U75	CAH-C4-C5	-2.53	120.85	122.66
3	C	202	U75	NAG-C6-N1	2.53	120.60	117.03
3	D	202	U75	CAI-CAH-C4	-2.49	108.74	114.88
3	A	202	U75	NAJ-C2-N3	2.46	121.08	117.25
3	A	202	U75	CAI-CAH-C4	-2.40	108.96	114.88
3	D	202	U75	NAJ-C2-N3	2.23	120.73	117.25
2	A	201	NDP	C2A-N1A-C6A	-2.23	114.94	118.75
3	B	202	U75	C5-C6-NAG	-2.23	119.05	121.62
3	C	202	U75	NAJ-C2-N3	2.20	120.68	117.25
2	A	201	NDP	C3N-C2N-N1N	-2.20	119.95	123.10
2	C	201	NDP	PA-O5B-C5B	-2.19	108.82	121.68
2	A	201	NDP	PA-O5B-C5B	-2.16	109.00	121.68
2	B	201	NDP	C3B-C2B-C1B	-2.16	98.83	102.89
2	B	201	NDP	PA-O5B-C5B	-2.16	109.03	121.68
2	C	201	NDP	C3B-C2B-C1B	-2.14	98.86	102.89
3	A	202	U75	CAM-CAN-CAS	-2.14	117.65	120.76
2	D	201	NDP	PA-O5B-C5B	-2.13	109.19	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	NDP	C3N-C2N-N1N	-2.12	120.06	123.10
2	C	201	NDP	PN-O5D-C5D	-2.12	109.24	121.68
2	B	201	NDP	C2A-N1A-C6A	-2.11	115.15	118.75
2	D	201	NDP	PN-O5D-C5D	-2.10	109.39	121.68
2	D	201	NDP	C3B-C2B-C1B	-2.07	99.00	102.89
3	B	202	U75	CAM-CAN-CAS	-2.04	117.78	120.76
2	B	201	NDP	PN-O5D-C5D	-2.04	109.71	121.68
3	D	202	U75	C5-C6-NAG	-2.03	119.28	121.62
3	D	202	U75	CBC-OBB-CAR	-2.00	113.17	117.51

There are no chirality outliers.

All (27) torsion outliers are listed below:

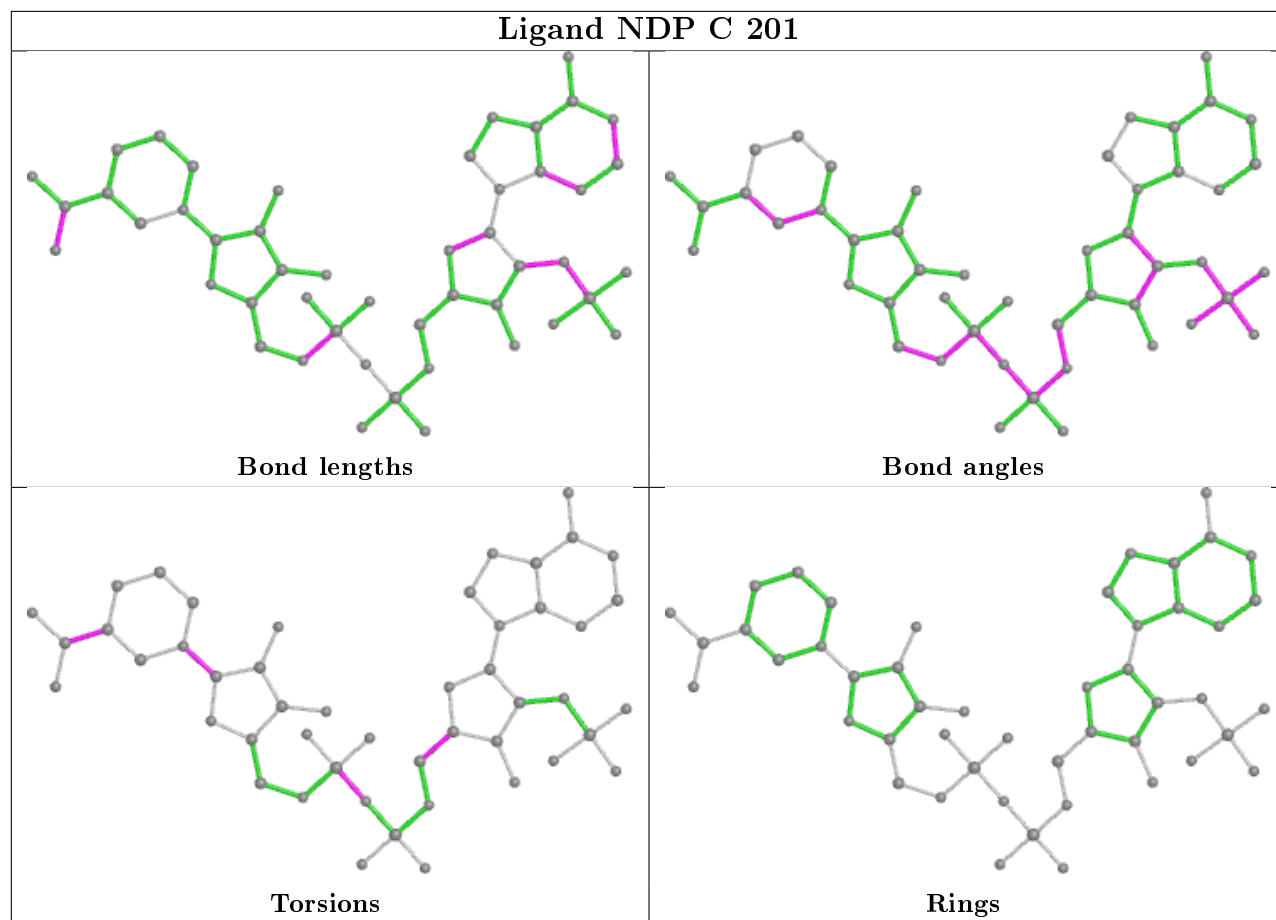
Mol	Chain	Res	Type	Atoms
2	C	201	NDP	PA-O3-PN-O5D
6	C	203	GOL	C1-C2-C3-O3
6	D	204	GOL	O1-C1-C2-O2
6	D	204	GOL	O1-C1-C2-C3
2	B	201	NDP	PA-O3-PN-O5D
2	A	201	NDP	PA-O3-PN-O5D
6	B	203	GOL	O2-C2-C3-O3
6	D	203	GOL	O1-C1-C2-O2
6	C	204	GOL	C1-C2-C3-O3
6	B	203	GOL	C1-C2-C3-O3
6	D	203	GOL	O1-C1-C2-C3
6	C	203	GOL	O2-C2-C3-O3
2	D	201	NDP	PA-O3-PN-O5D
6	C	204	GOL	O2-C2-C3-O3
2	D	201	NDP	O4D-C1D-N1N-C2N
2	A	201	NDP	O4D-C1D-N1N-C2N
2	C	201	NDP	O4D-C1D-N1N-C2N
2	C	201	NDP	C3B-C4B-C5B-O5B
2	B	201	NDP	O4D-C1D-N1N-C2N
2	B	201	NDP	C2D-C1D-N1N-C2N
2	A	201	NDP	C2D-C1D-N1N-C2N
3	A	202	U75	CAQ-CAR-OBB-CBC
2	C	201	NDP	C2D-C1D-N1N-C2N
2	D	201	NDP	C2D-C1D-N1N-C2N
3	A	202	U75	CAS-CAR-OBB-CBC
2	C	201	NDP	C2N-C3N-C7N-N7N
6	C	203	GOL	O1-C1-C2-O2

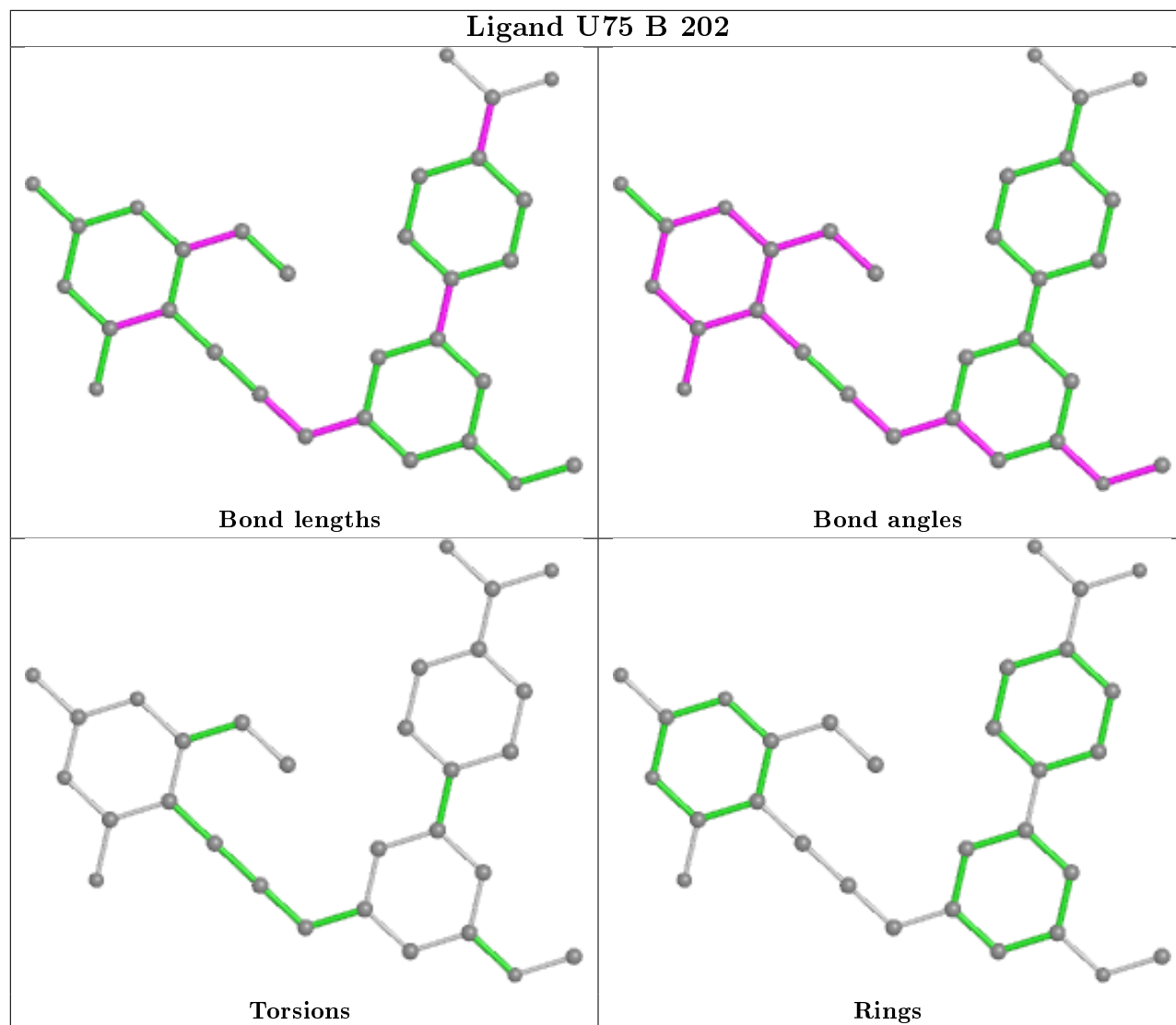
There are no ring outliers.

9 monomers are involved in 15 short contacts:

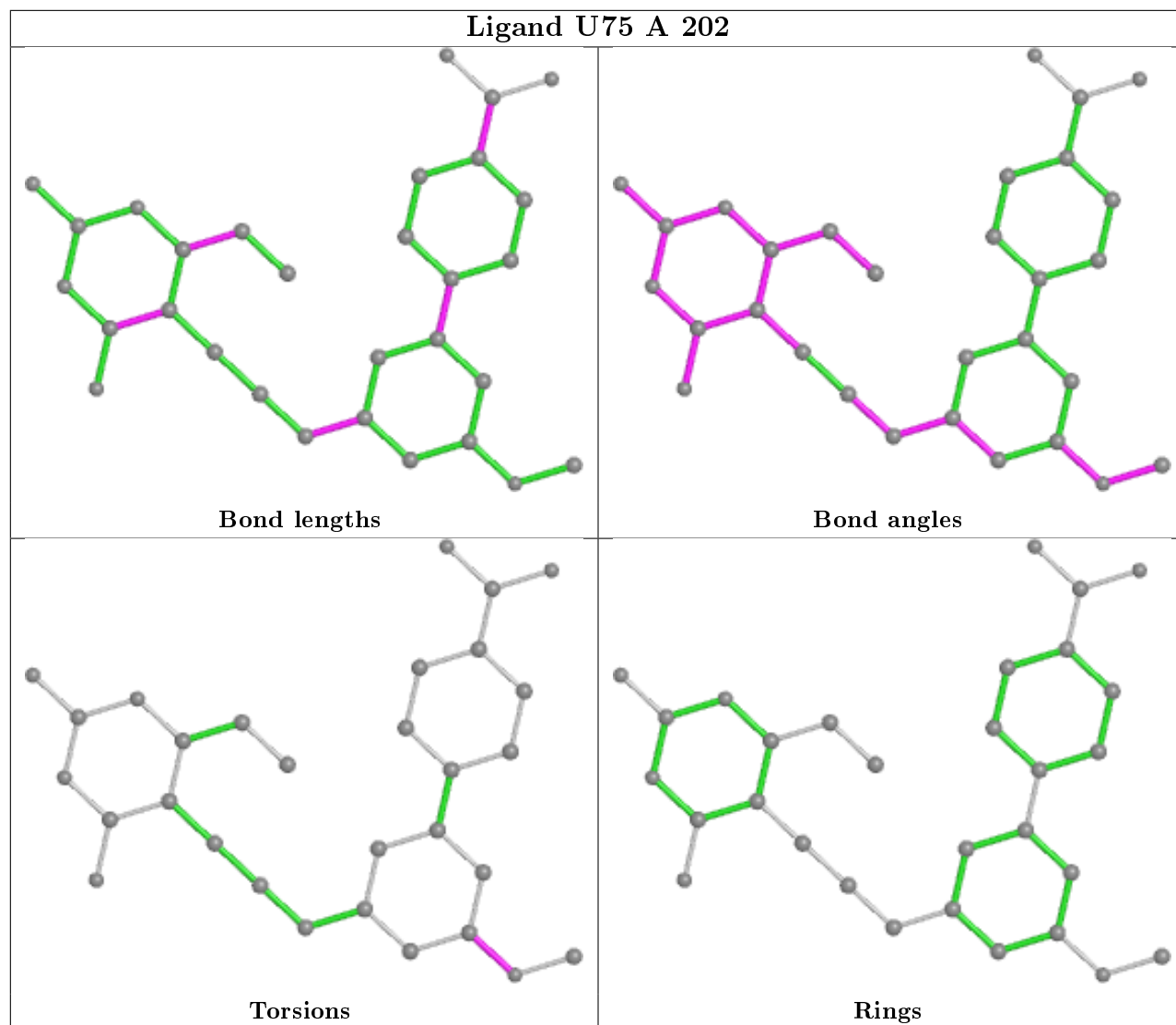
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	NDP	1	0
6	C	204	GOL	3	0
6	B	203	GOL	1	0
4	A	203	ACT	1	0
6	D	203	GOL	1	0
2	B	201	NDP	1	0
2	D	201	NDP	3	0
2	A	201	NDP	3	0
3	D	202	U75	1	0

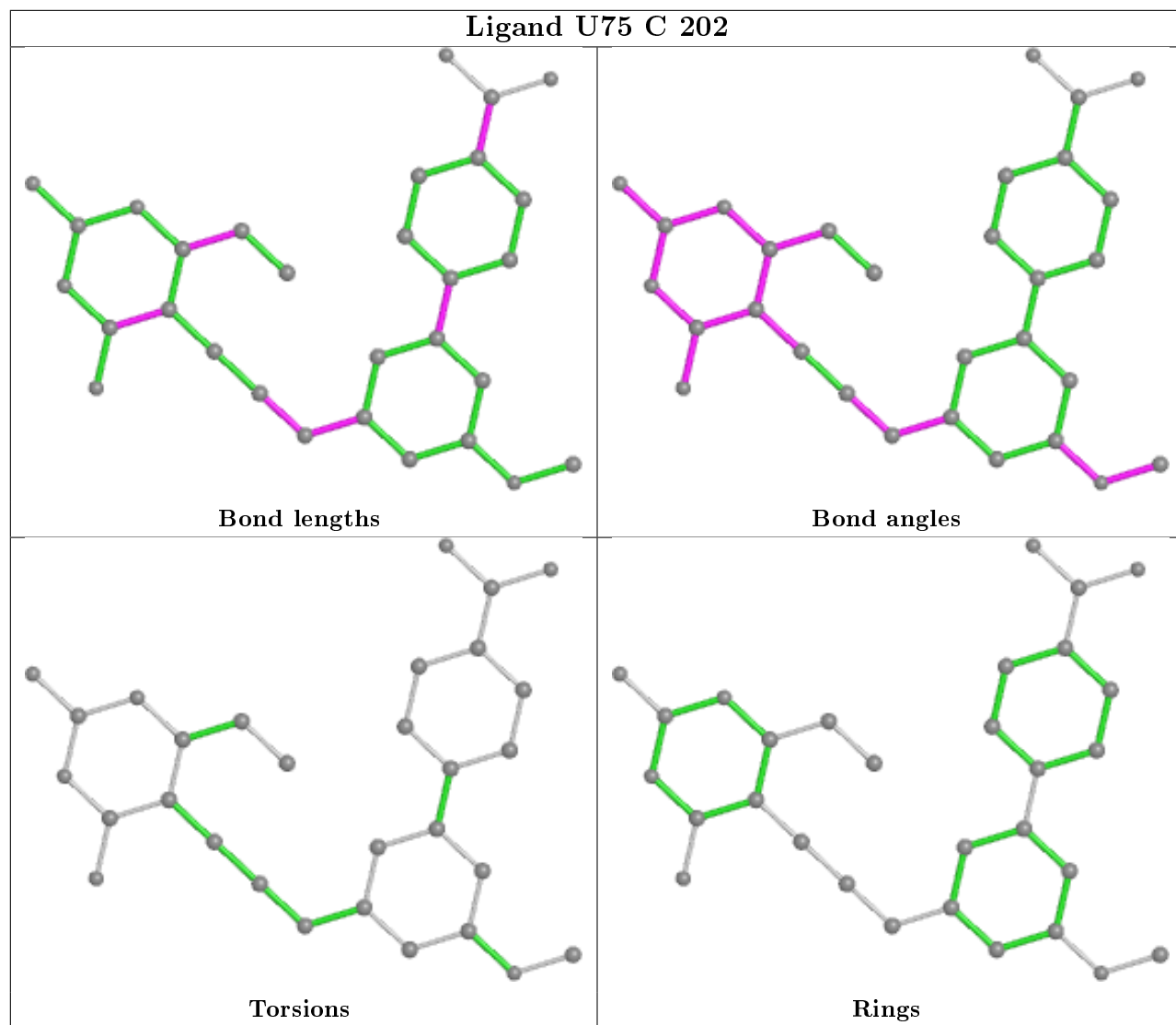
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



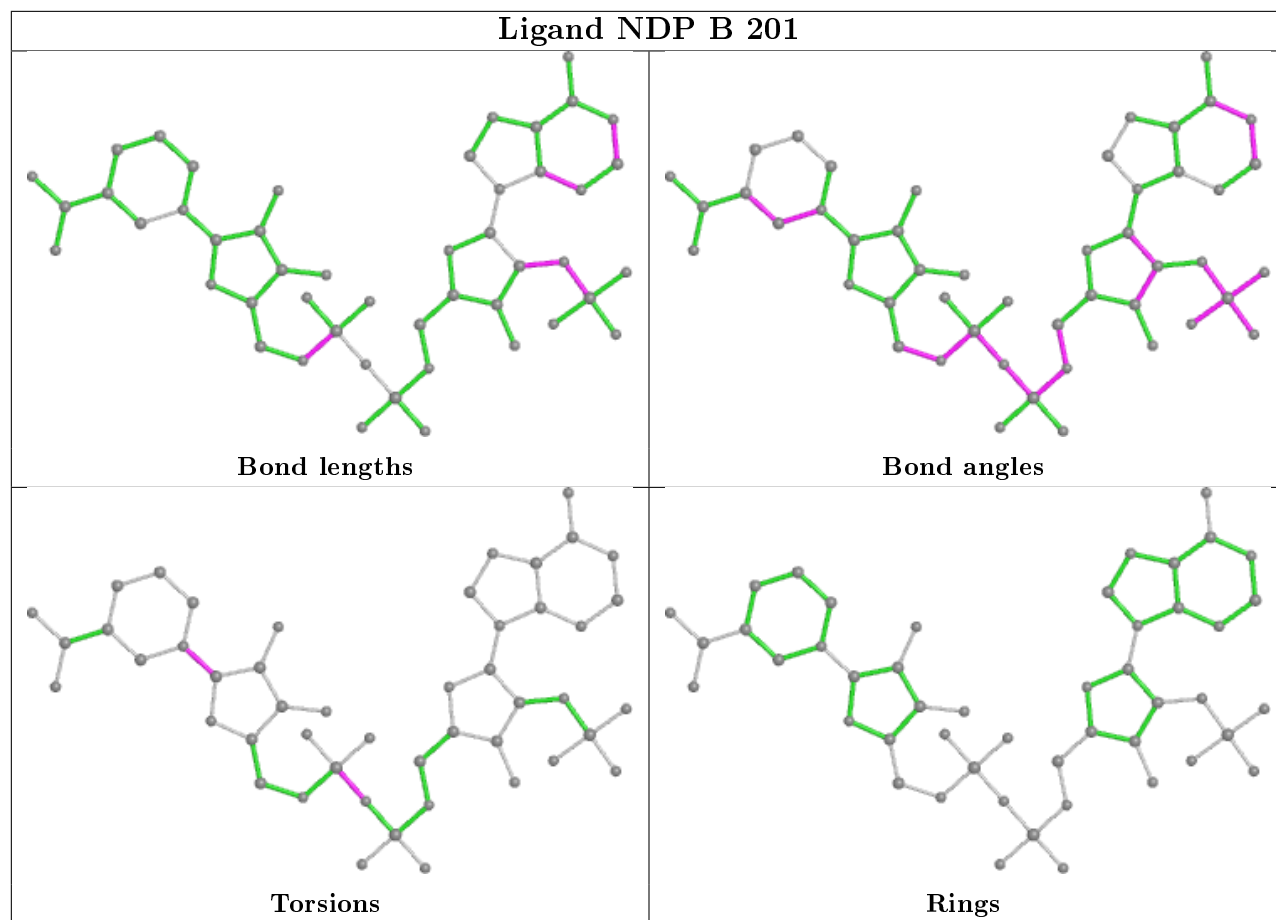


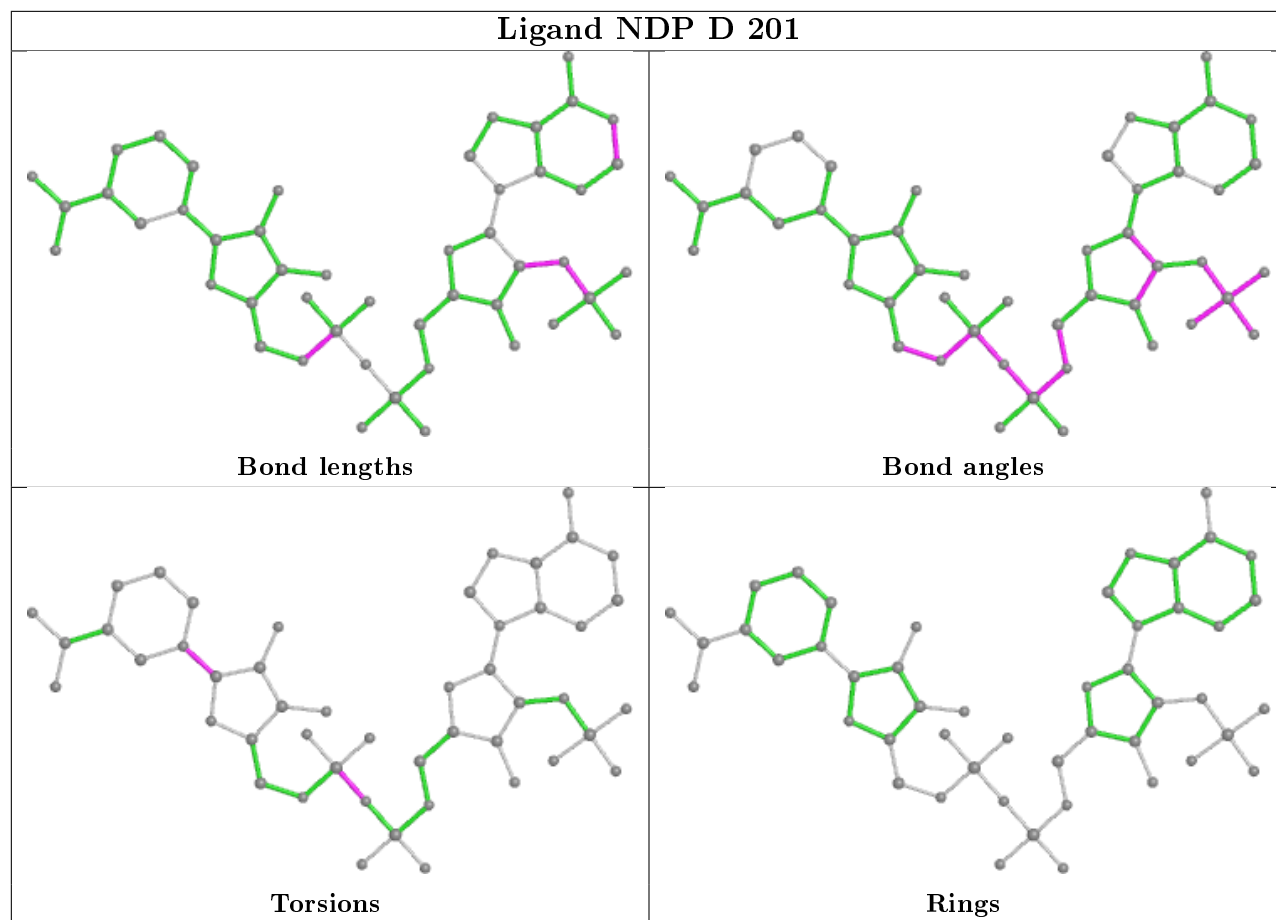
## Ligand U75 A 202

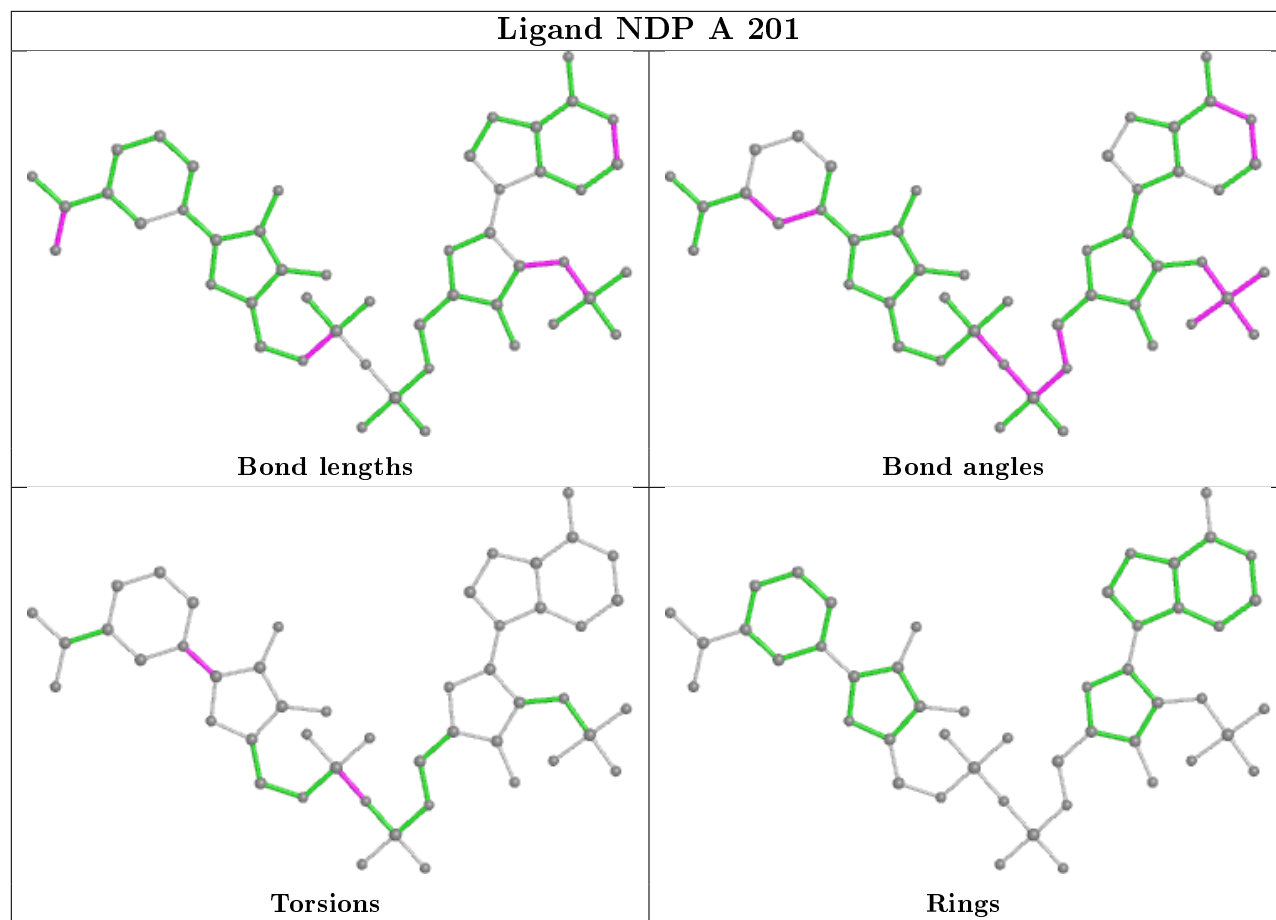


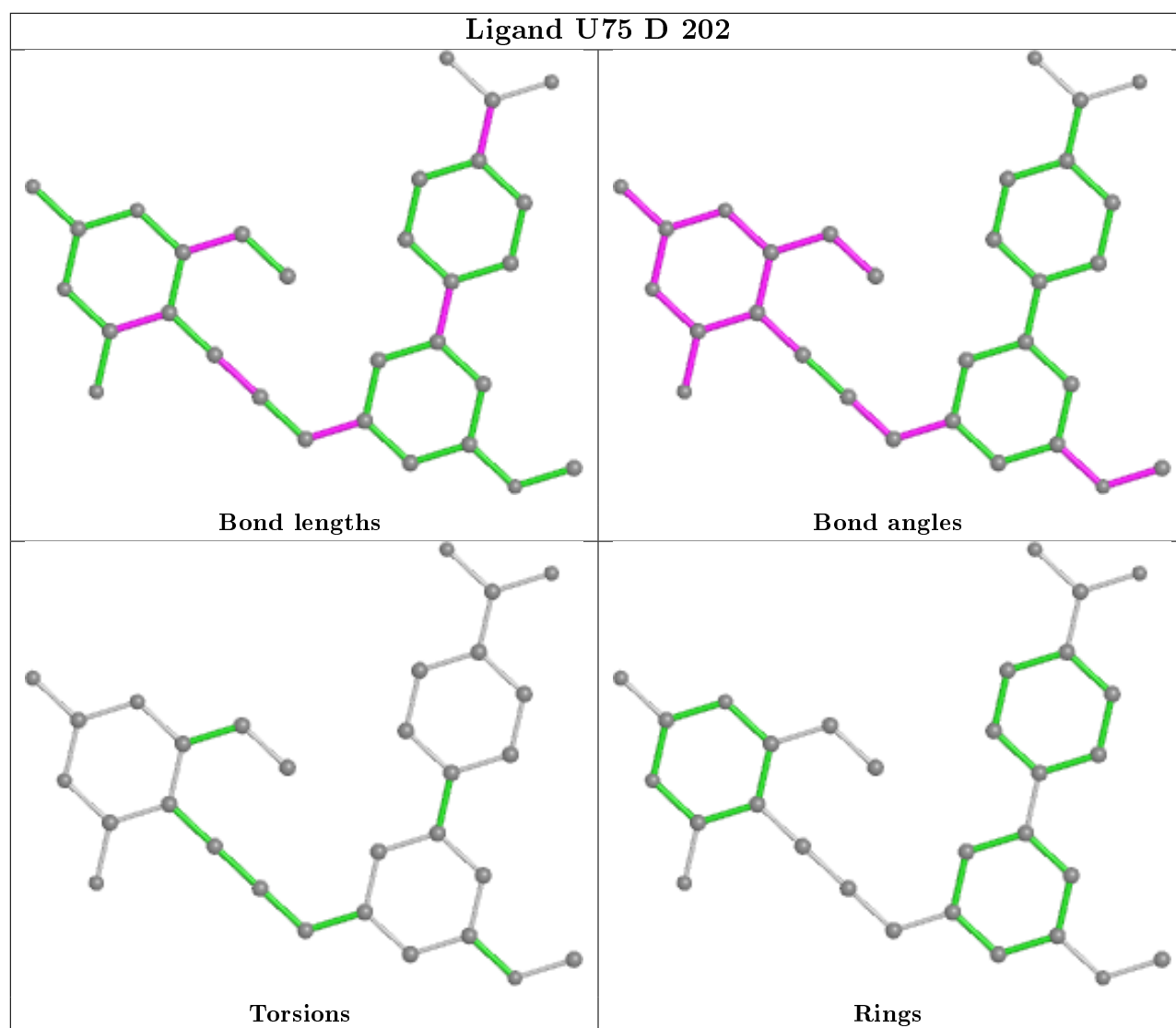












## 5.7 Other polymers [i](#)

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 [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	159/159 (100%)	0.11	2 (1%) 77 81	18, 26, 42, 60	0
1	B	159/159 (100%)	0.09	2 (1%) 77 81	19, 26, 40, 53	0
1	C	159/159 (100%)	0.12	3 (1%) 66 70	19, 26, 41, 57	0
1	D	159/159 (100%)	0.14	4 (2%) 57 61	18, 26, 43, 56	0
All	All	636/636 (100%)	0.12	11 (1%) 70 74	18, 26, 42, 60	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	ARG	4.1
1	C	149	LEU	3.1
1	A	23	ARG	3.0
1	C	69	ALA	2.9
1	D	69	ALA	2.9
1	B	52	ALA	2.7
1	C	23	ARG	2.4
1	A	69	ALA	2.4
1	B	147	SER	2.3
1	D	147	SER	2.3
1	D	144	PHE	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

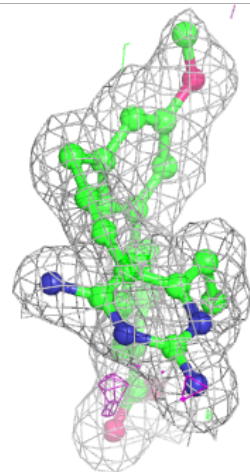
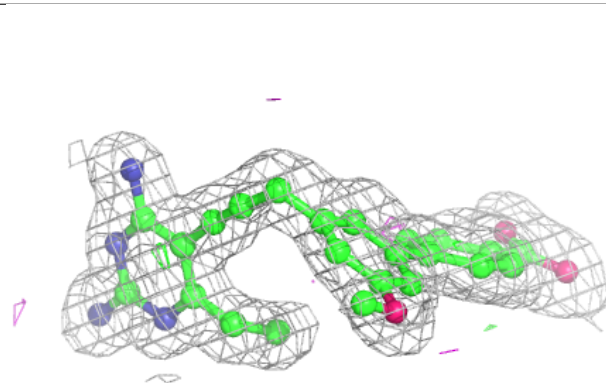
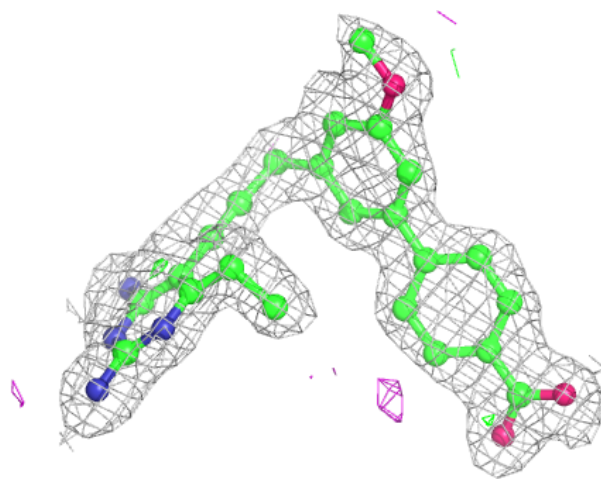
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	GOL	D	203	6/6	0.61	0.23	42,52,62,65	0
4	ACT	A	203	4/4	0.67	0.20	35,43,47,50	0
6	GOL	B	203	6/6	0.69	0.20	38,55,65,71	0
6	GOL	D	204	6/6	0.82	0.13	42,53,64,77	0
6	GOL	C	203	6/6	0.82	0.13	44,54,60,65	0
6	GOL	C	204	6/6	0.83	0.20	33,43,53,58	0
3	U75	D	202	30/30	0.92	0.11	16,26,31,35	0
3	U75	C	202	30/30	0.93	0.10	16,25,32,34	0
3	U75	B	202	30/30	0.94	0.09	16,26,30,35	0
3	U75	A	202	30/30	0.94	0.08	16,25,31,33	0
2	NDP	B	201	48/48	0.95	0.10	20,25,34,37	0
2	NDP	D	201	48/48	0.96	0.09	19,26,33,38	0
5	NA	A	204	1/1	0.96	0.07	38,38,38,38	0
2	NDP	A	201	48/48	0.96	0.09	19,24,31,36	0
2	NDP	C	201	48/48	0.96	0.09	21,26,34,38	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.

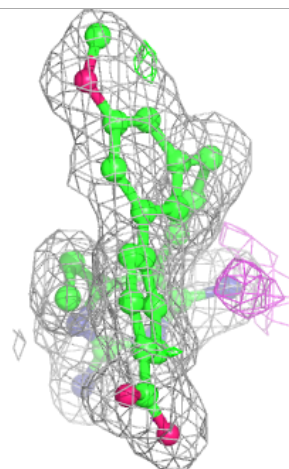
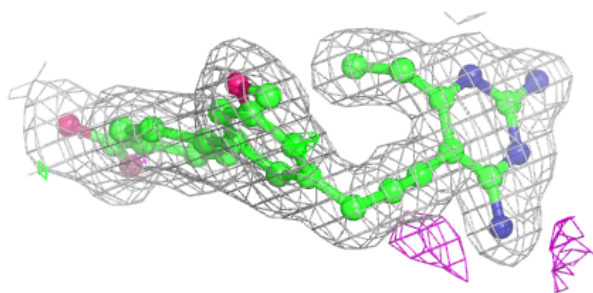
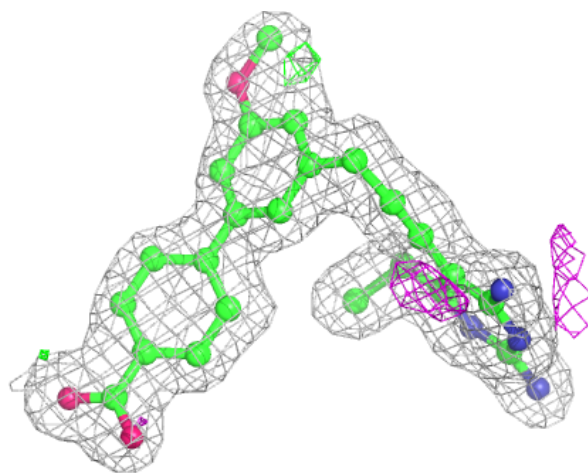
**Electron density around U75 D 202:**

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



**Electron density around U75 C 202:**

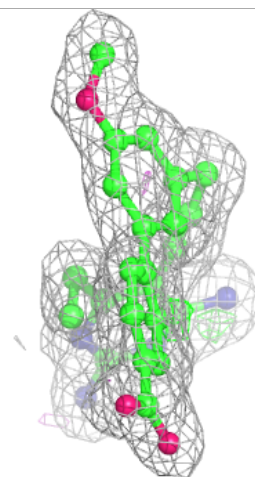
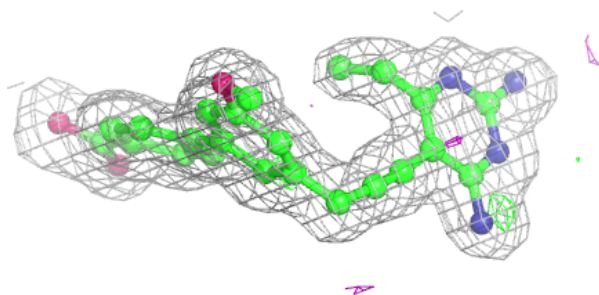
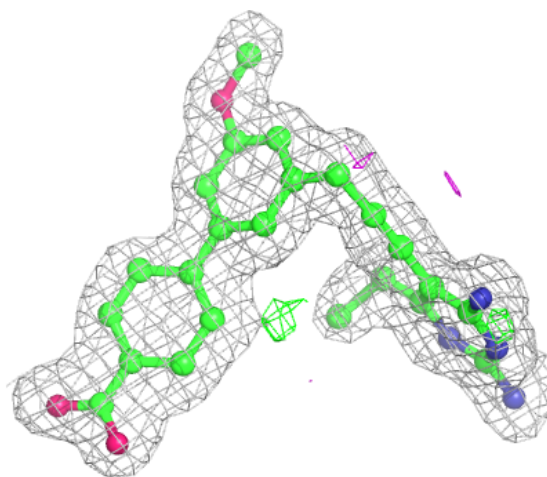
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





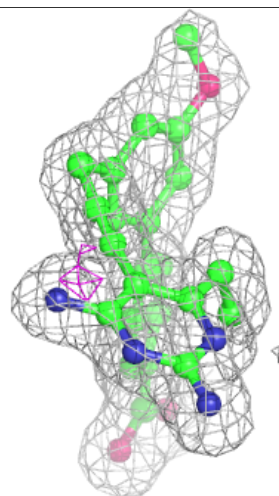
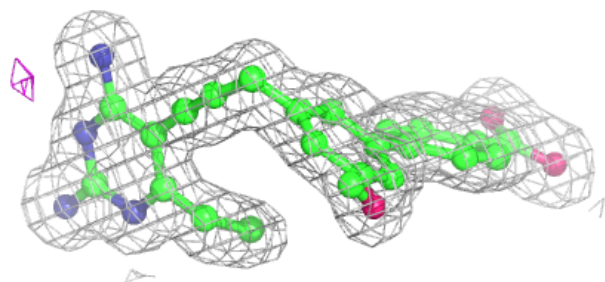
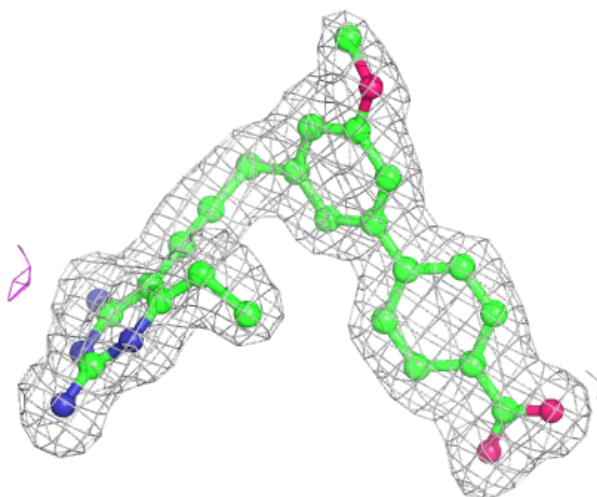
**Electron density around U75 B 202:**

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



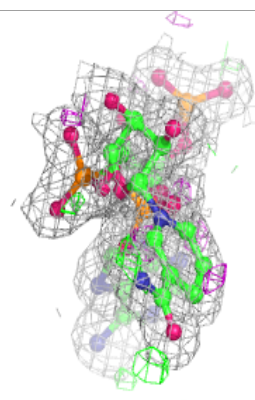
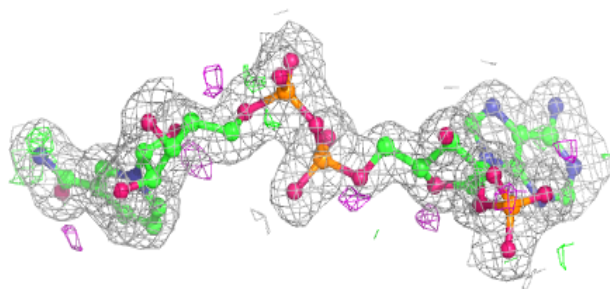
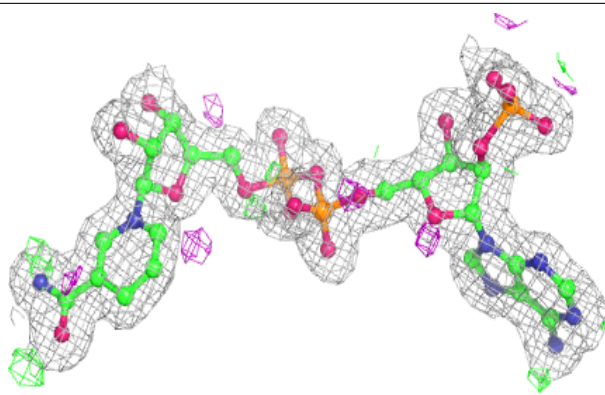
**Electron density around U75 A 202:**

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

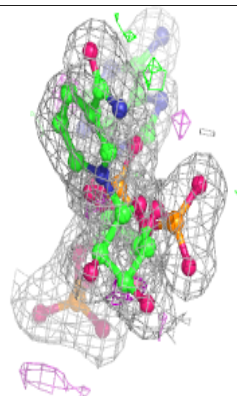
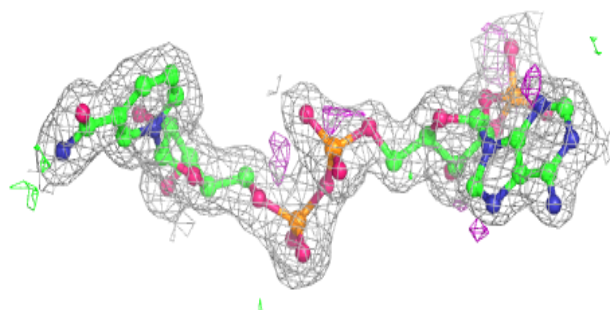
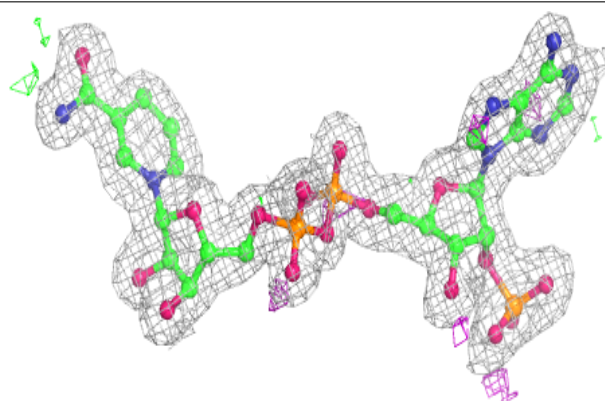


**Electron density around NDP B 201:**

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

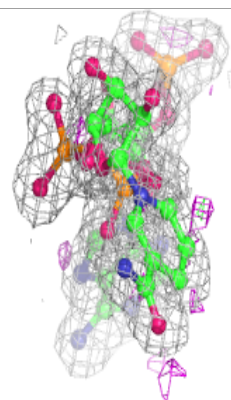
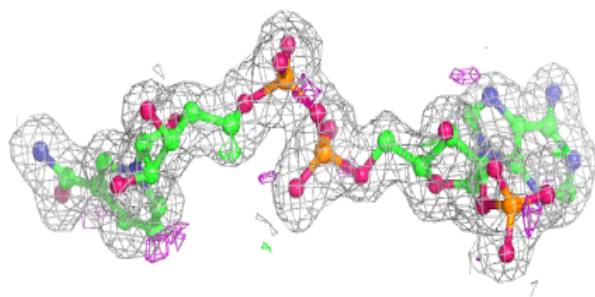
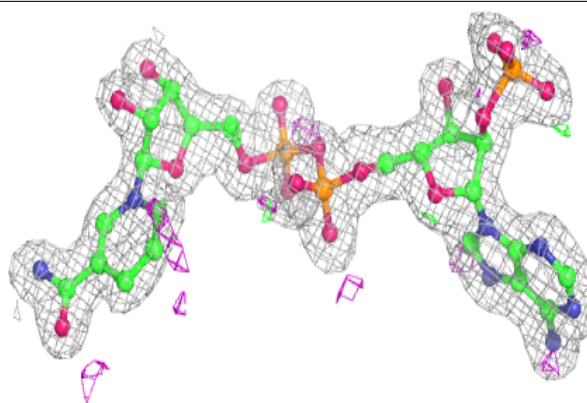
**Electron density around NDP D 201:**

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

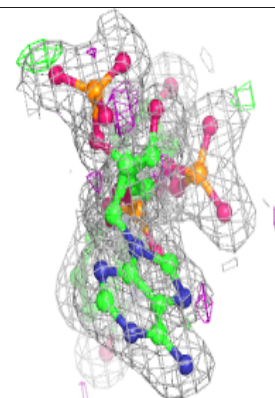
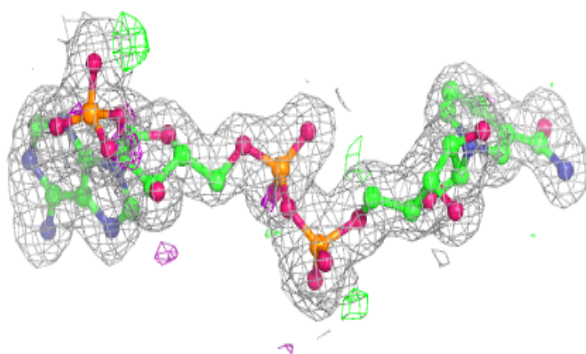
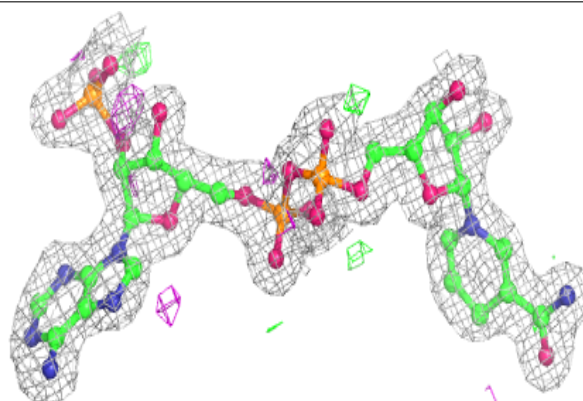


**Electron density around NDP A 201:**

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

**Electron density around NDP C 201:**

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



## 6.5 Other polymers

There are no such residues in this entry.