



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:01 AM BST

PDB ID : 5LDQ  
Title : Crystal structure of E.coli LigT complexed with NADP+  
Authors : Myllykoski, M.; Kursula, P.  
Deposited on : 2016-06-27  
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.13.1  
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) : 2.13.1

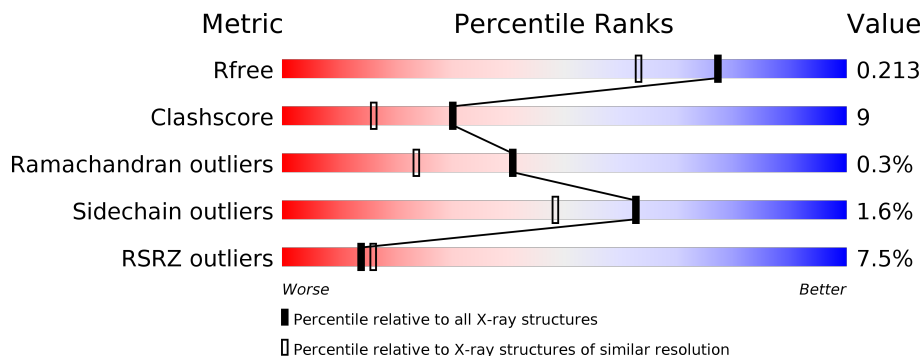
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	177	 6% 80% 18% ...
1	B	177	 5% 79% 16% • 5%
1	C	177	 11% 81% 17% ••
1	D	177	 8% 85% 12% ••

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7048 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.

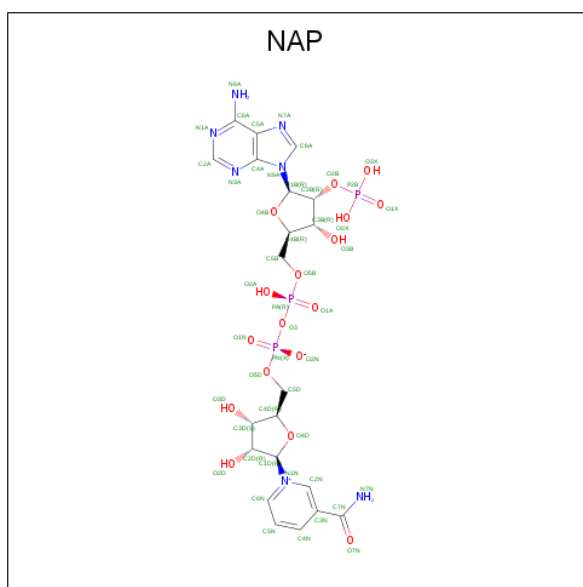
- Molecule 1 is a protein called RNA 2',3'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1542	983	292	263	4	0	15	0
1	B	169	1483	945	283	252	3	0	13	0
1	C	175	1537	979	294	260	4	0	14	0
1	D	172	1497	956	281	255	5	0	13	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A140NFI1
B	0	GLY	-	expression tag	UNP A0A140NFI1
C	0	GLY	-	expression tag	UNP A0A140NFI1
D	0	GLY	-	expression tag	UNP A0A140NFI1

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	96	42	14	34	6	0	1
2	A	1	31	10	5	13	3	0	0
2	B	1	48	21	7	17	3	0	0
2	C	1	96	42	14	34	6	0	1
2	D	1	27	10	5	10	2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total 1 Cl	0	0
3	A	1	Total 1 Cl	0	0
3	C	1	Total 1 Cl	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).




- Molecule 6 is water.

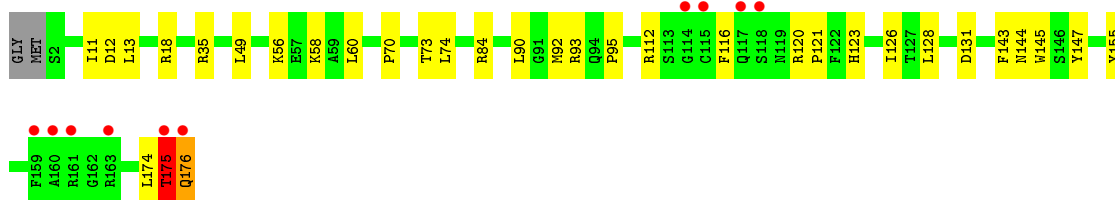
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	198	Total 198	O 198	0	0
6	B	170	Total 170	O 170	0	0
6	C	135	Total 135	O 135	0	0
6	D	135	Total 135	O 135	0	0

### 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.

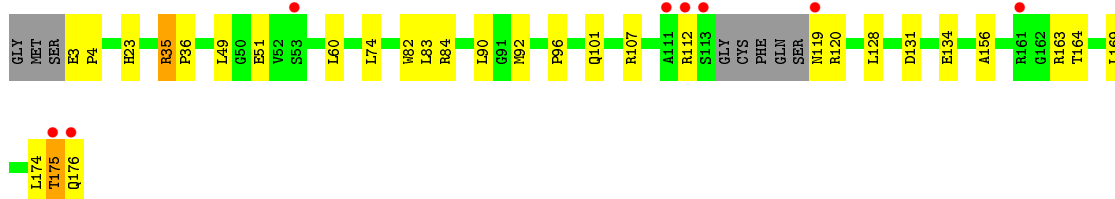
- Molecule 1: RNA 2',3'-cyclic phosphodiesterase

Chain A: 




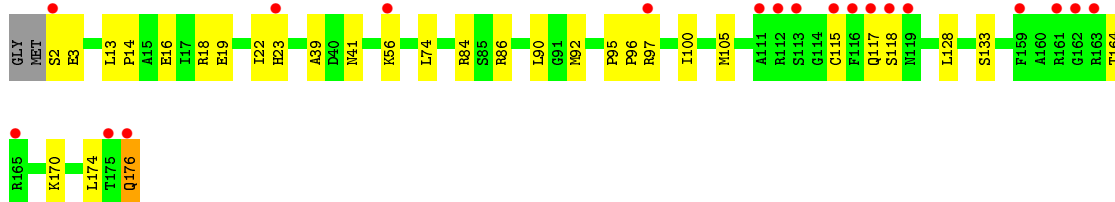
- Molecule 1: RNA 2',3'-cyclic phosphodiesterase

Chain B: 




- Molecule 1: RNA 2',3'-cyclic phosphodiesterase

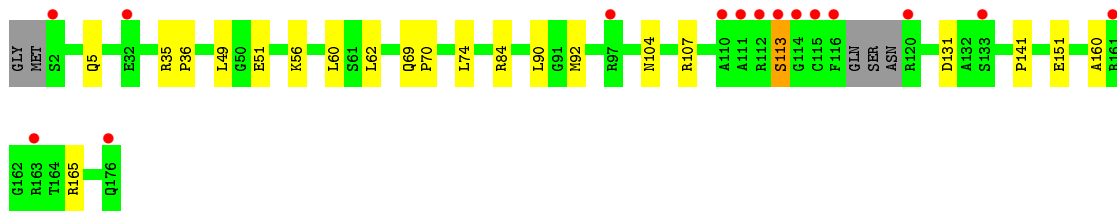
Chain C: 



- Molecule 1: RNA 2',3'-cyclic phosphodiesterase

Chain D: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.74Å 91.62Å 120.61Å 90.00° 102.31° 90.00°	Depositor
Resolution (Å)	117.83 – 1.70 117.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (117.83-1.70) 99.8 (117.84-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.183 , 0.213 0.183 , 0.213	Depositor DCC
$R_{free}$ test set	2000 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtrriage
Anisotropy	0.685	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: PO4, CL, NAP, IPE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/1583	0.55	0/2144
1	B	0.37	0/1522	0.55	0/2061
1	C	0.34	0/1578	0.54	0/2136
1	D	0.35	0/1538	0.56	0/2083
All	All	0.37	0/6221	0.55	0/8424

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175[B]	THR	Peptide

### 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	1542	0	1546	41	0
1	B	1483	0	1488	31	0
1	C	1537	0	1544	26	0
1	D	1497	0	1492	17	0
2	A	127	0	61	6	0
2	B	48	0	25	1	0
2	C	96	0	49	3	0
2	D	27	0	11	1	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
4	A	16	0	22	4	0
4	B	16	0	22	5	0
4	C	13	0	17	6	0
5	D	5	0	0	0	0
6	A	198	0	0	16	2
6	B	170	0	0	10	2
6	C	135	0	0	6	0
6	D	135	0	0	6	0
All	All	7048	0	6277	118	2

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 9.

All (118) 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:B:175[A]:THR:OG1	6:B:301:HOH:O	1.84	0.96
1:A:147:TYR:OH	6:A:301:HOH:O	1.96	0.83
1:C:97:ARG:NH1	6:C:302:HOH:O	2.11	0.83
2:A:201[B]:NAP:H6N	2:A:201[B]:NAP:H51N	1.63	0.80
1:D:104:ASN:OD1	6:D:301:HOH:O	2.00	0.79
1:C:18[B]:ARG:HH12	4:C:203:1PE:H131	1.45	0.79
1:A:116:PHE:O	6:A:302:HOH:O	1.98	0.78
1:A:56:LYS:NZ	6:A:303:HOH:O	2.08	0.77
1:A:95:PRO:HG2	4:A:204:1PE:H131	1.67	0.76
1:C:90:LEU:HG	1:C:128:LEU:HD11	1.67	0.76
1:B:131[B]:ASP:OD1	6:B:302:HOH:O	2.04	0.76
1:A:70:PRO:HA	1:A:175[B]:THR:HA	1.69	0.74
2:D:201:NAP:O2X	6:D:302:HOH:O	2.06	0.74
1:B:90[A]:LEU:HG	1:B:128:LEU:HD11	1.70	0.73
1:B:83:LEU:H	4:B:203:1PE:H151	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLU:OE1	6:D:303:HOH:O	2.08	0.70
1:C:174[B]:LEU:O	6:C:301:HOH:O	2.09	0.69
1:C:176[B]:GLN:HG2	6:C:418:HOH:O	1.92	0.69
1:A:90[A]:LEU:HG	1:A:128:LEU:HD11	1.74	0.69
1:A:176[B]:GLN:OXT	6:A:304:HOH:O	2.09	0.69
1:B:107[A]:ARG:NH2	1:B:120:ARG:O	2.27	0.68
1:C:95:PRO:HB2	1:C:100[A]:ILE:HD11	1.76	0.67
1:C:16[A]:GLU:OE1	6:C:303:HOH:O	2.12	0.66
1:B:119:ASN:ND2	6:B:307:HOH:O	2.29	0.66
1:A:147:TYR:CE2	6:A:305:HOH:O	2.48	0.65
1:A:147:TYR:OH	6:A:305:HOH:O	2.13	0.65
1:B:51:GLU:OE1	6:B:304:HOH:O	2.15	0.64
1:A:131[B]:ASP:OD1	6:A:306:HOH:O	2.15	0.64
1:A:74:LEU:HD22	1:A:92[B]:MET:SD	2.39	0.63
1:C:14:PRO:HA	4:C:203:1PE:H251	1.79	0.63
1:B:83:LEU:N	4:B:203:1PE:H151	2.13	0.62
2:A:202:NAP:H8A	2:A:202:NAP:O2A	1.99	0.62
1:A:143:PHE:HD2	4:C:203:1PE:H132	1.64	0.62
1:A:90[B]:LEU:HD13	1:A:128:LEU:HD11	1.81	0.62
1:A:175[B]:THR:HG23	6:A:310:HOH:O	2.01	0.61
1:A:84:ARG:NH2	1:B:134:GLU:OE1	2.34	0.60
1:A:123:HIS:ND1	4:A:204:1PE:H161	2.17	0.60
1:A:93:ARG:HH12	1:C:170[A]:LYS:HE3	1.67	0.60
1:D:74:LEU:HD22	1:D:92[B]:MET:SD	2.42	0.59
1:B:74:LEU:HD22	1:B:92[B]:MET:SD	2.43	0.59
1:B:112:ARG:NE	6:B:303:HOH:O	2.05	0.59
1:A:176[B]:GLN:HG3	6:A:304:HOH:O	2.02	0.59
1:D:84:ARG:HG2	1:D:84:ARG:HH11	1.68	0.58
1:A:120:ARG:HD3	2:A:202:NAP:O3X	2.06	0.56
1:B:83:LEU:H	4:B:203:1PE:H261	1.70	0.55
1:B:107[B]:ARG:NH2	6:B:312:HOH:O	2.35	0.55
1:A:174[B]:LEU:O	1:A:176[B]:GLN:N	2.40	0.55
1:B:35[B]:ARG:HH22	1:B:163:ARG:HH11	1.55	0.54
1:D:131[B]:ASP:OD1	6:D:304:HOH:O	2.19	0.54
1:A:147:TYR:HE2	6:A:305:HOH:O	1.88	0.54
1:A:176[B]:GLN:C	6:A:304:HOH:O	2.46	0.53
1:A:116:PHE:HB2	1:B:35[B]:ARG:HD3	1.90	0.53
4:A:204:1PE:H252	6:A:327:HOH:O	2.10	0.52
3:A:203:CL:CL	6:A:471:HOH:O	2.56	0.52
1:C:164:THR:HG21	2:C:201[B]:NAP:O2N	2.10	0.51
1:C:18[B]:ARG:HD2	1:C:39:ALA:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174[B]:LEU:O	1:B:176[B]:GLN:N	2.42	0.51
1:A:12:ASP:OD2	1:A:155:TYR:OH	2.24	0.51
1:C:41:ASN:ND2	3:C:202:CL:CL	2.74	0.51
1:D:160:ALA:HB3	1:D:165:ARG:HG3	1.91	0.51
1:A:144:ASN:ND2	4:C:203:1PE:OH6	2.41	0.49
1:A:84:ARG:HB2	2:A:202:NAP:O2A	2.12	0.49
1:C:13[B]:LEU:O	1:C:18[B]:ARG:NH2	2.46	0.49
1:C:74:LEU:HD22	1:C:92[B]:MET:SD	2.53	0.48
2:A:202:NAP:H8A	2:A:202:NAP:O5B	2.13	0.48
1:B:23[A]:HIS:HD2	6:B:442:HOH:O	1.95	0.47
1:C:16[A]:GLU:CD	6:C:305:HOH:O	2.52	0.47
1:C:56:LYS:HD2	1:C:115:CYS:SG	2.54	0.47
1:A:35[A]:ARG:NH2	1:B:84:ARG:HE	2.13	0.47
1:B:176[B]:GLN:OE1	6:B:305:HOH:O	2.20	0.47
1:A:143:PHE:CD2	4:C:203:1PE:H132	2.48	0.47
1:A:112[A]:ARG:NH2	6:A:307:HOH:O	2.19	0.47
1:B:35[B]:ARG:HH22	1:B:163:ARG:NH1	2.13	0.47
1:B:82:TRP:CE3	4:B:203:1PE:H222	2.50	0.47
1:A:11[B]:ILE:HG22	6:A:301:HOH:O	2.14	0.47
2:A:202:NAP:PA	2:A:202:NAP:H8A	2.55	0.46
1:B:156:ALA:HB2	1:B:169:LEU:HD11	1.98	0.46
2:C:201[A]:NAP:H2D	2:C:201[A]:NAP:H6N	1.77	0.46
1:D:60:LEU:HD21	1:D:113:SER:CB	2.46	0.45
1:B:3:GLU:HG3	1:B:4:PRO:HD2	1.98	0.45
1:C:19:GLU:OE2	1:C:23[A]:HIS:NE2	2.50	0.45
1:B:83:LEU:H	4:B:203:1PE:C26	2.30	0.45
1:D:49:LEU:HD13	1:D:60:LEU:HD13	1.98	0.45
1:A:13:LEU:HD21	1:A:126:ILE:HD13	2.00	0.44
1:D:56:LYS:HA	1:D:56:LYS:HD2	1.64	0.44
1:A:58:LYS:HB2	1:A:58:LYS:HE3	1.72	0.44
1:D:35:ARG:NH1	6:D:308:HOH:O	2.44	0.44
1:C:95:PRO:HB2	1:C:100[A]:ILE:CD1	2.46	0.44
1:D:69:GLN:HA	1:D:70:PRO:HD3	1.88	0.44
1:C:84[A]:ARG:HB2	6:C:367:HOH:O	2.17	0.44
1:D:90[A]:LEU:HD21	1:D:141:PRO:HB3	1.99	0.44
1:A:13:LEU:O	1:A:18:ARG:HD3	2.18	0.44
1:C:92[A]:MET:SD	1:C:96:PRO:HD3	2.58	0.43
1:A:147:TYR:CZ	6:A:305:HOH:O	2.65	0.43
1:A:90[B]:LEU:HD21	1:A:145:TRP:CZ3	2.53	0.43
1:D:69:GLN:NE2	6:D:313:HOH:O	2.52	0.43
1:B:164:THR:HG21	2:B:201:NAP:O1N	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD13	1:B:60:LEU:HD13	2.00	0.43
1:A:120:ARG:HA	1:A:121:PRO:HD3	1.83	0.43
1:A:95:PRO:CD	4:A:204:1PE:H242	2.50	0.42
1:B:92[A]:MET:SD	1:B:96:PRO:HD3	2.59	0.42
1:B:92[B]:MET:HE3	6:B:356:HOH:O	2.19	0.42
1:D:60:LEU:HD21	1:D:113:SER:HB2	2.02	0.42
1:A:49:LEU:HD13	1:A:60:LEU:HD13	2.01	0.42
1:C:86[B]:ARG:HG2	1:C:133:SER:HA	2.02	0.42
1:C:22:ILE:HG21	1:C:39:ALA:HB2	2.02	0.41
1:A:35[B]:ARG:HH21	1:B:84:ARG:NH2	2.19	0.41
1:C:18[B]:ARG:HH12	4:C:203:1PE:H242	1.85	0.41
1:A:56:LYS:HE3	1:A:56:LYS:HB2	1.93	0.41
2:C:201[B]:NAP:O3X	2:C:201[B]:NAP:O2D	2.36	0.41
1:A:73:THR:HG21	1:C:176[B]:GLN:HG3	2.02	0.41
1:D:5:GLN:O	1:D:51:GLU:HA	2.21	0.41
1:B:101:GLN:HG3	6:B:427:HOH:O	2.21	0.41
1:B:35[A]:ARG:HA	1:B:36:PRO:HD3	1.87	0.41
1:D:90[B]:LEU:HD11	1:D:141:PRO:HB3	2.03	0.41
1:C:18[A]:ARG:NH1	1:C:39:ALA:O	2.42	0.40
1:C:2:SER:HB3	1:C:3:GLU:H	1.60	0.40
1:D:35:ARG:HA	1:D:36:PRO:HD3	1.91	0.40

All (2) 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)
6:A:339:HOH:O	6:B:425:HOH:O[4_556]	1.88	0.32
6:A:464:HOH:O	6:B:456:HOH:O[4_556]	1.97	0.23

## 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	187/177 (106%)	181 (97%)	4 (2%)	2 (1%)	14	3
1	B	177/177 (100%)	175 (99%)	0	2 (1%)	14	3
1	C	186/177 (105%)	184 (99%)	2 (1%)	0	100	100
1	D	181/177 (102%)	179 (99%)	2 (1%)	0	100	100
All	All	731/708 (103%)	719 (98%)	8 (1%)	4 (0%)	41	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175[A]	THR
1	A	175[B]	THR
1	B	175[A]	THR
1	B	175[B]	THR

### 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	160/146 (110%)	158 (99%)	2 (1%)	69	56
1	B	153/146 (105%)	151 (99%)	2 (1%)	69	56
1	C	159/146 (109%)	154 (97%)	5 (3%)	40	21
1	D	155/146 (106%)	151 (97%)	4 (3%)	46	28
All	All	627/584 (107%)	614 (98%)	13 (2%)	62	36

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

Mol	Chain	Res	Type
1	A	176[A]	GLN
1	A	176[B]	GLN
1	B	35[A]	ARG
1	B	35[B]	ARG
1	C	105	MET
1	C	117	GLN
1	C	118	SER

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Mol	Chain	Res	Type
1	C	176[A]	GLN
1	C	176[B]	GLN
1	D	62	LEU
1	D	107[A]	ARG
1	D	107[B]	ARG
1	D	113	SER

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

Mol	Chain	Res	Type
1	A	69	GLN
1	A	101	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	NAP	C	201[B]	-	45,52,52	0.88	2 (4%)	56,80,80	1.33	6 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	A	201[A]	-	45,52,52	0.84	1 (2%)	56,80,80	1.25	6 (10%)
4	1PE	C	203	-	12,12,15	0.38	0	11,11,14	0.63	0
2	NAP	A	201[B]	-	45,52,52	0.87	1 (2%)	56,80,80	1.29	5 (8%)
2	NAP	C	201[A]	-	45,52,52	0.85	1 (2%)	56,80,80	1.26	8 (14%)
5	PO4	D	202	-	4,4,4	1.01	0	6,6,6	0.61	0
2	NAP	B	201	-	45,52,52	0.88	1 (2%)	56,80,80	1.15	6 (10%)
4	1PE	B	203	-	15,15,15	0.52	0	14,14,14	0.57	0
2	NAP	D	201	-	25,29,52	1.01	2 (8%)	31,45,80	1.39	5 (16%)
4	1PE	A	204	-	15,15,15	0.50	0	14,14,14	0.40	0
2	NAP	A	202	-	27,33,52	1.08	3 (11%)	35,52,80	1.42	4 (11%)

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	NAP	C	201[B]	-	-	9/31/67/67	0/5/5/5
2	NAP	A	201[A]	-	-	9/31/67/67	0/5/5/5
4	1PE	C	203	-	-	5/10/10/13	-
2	NAP	A	201[B]	-	-	12/31/67/67	0/5/5/5
2	NAP	C	201[A]	-	-	16/31/67/67	0/5/5/5
4	1PE	B	203	-	-	2/13/13/13	-
2	NAP	B	201	-	-	4/31/67/67	0/5/5/5
2	NAP	D	201	-	-	4/11/31/67	0/3/3/5
4	1PE	A	204	-	-	9/13/13/13	-
2	NAP	A	202	-	-	6/17/37/67	0/3/3/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	NAP	C5A-C4A	2.75	1.48	1.40
2	A	202	NAP	C5A-C4A	2.74	1.48	1.40
2	C	201[B]	NAP	C5A-C4A	2.57	1.47	1.40
2	C	201[A]	NAP	C5A-C4A	2.49	1.47	1.40
2	A	201[B]	NAP	C5A-C4A	2.47	1.47	1.40
2	A	201[A]	NAP	C5A-C4A	2.45	1.47	1.40
2	D	201	NAP	C5A-C4A	2.35	1.47	1.40
2	C	201[B]	NAP	O4D-C1D	2.24	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	NAP	O4B-C1B	2.10	1.44	1.41
2	A	202	NAP	C2A-N3A	2.08	1.35	1.32
2	A	202	NAP	O4B-C1B	2.00	1.43	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	NAP	PA-O3-PN	-4.24	118.26	132.83
2	C	201[B]	NAP	C2D-C3D-C4D	-4.13	94.62	102.64
2	D	201	NAP	N3A-C2A-N1A	-3.66	122.95	128.68
2	C	201[B]	NAP	O4D-C4D-C5D	3.53	120.98	109.37
2	C	201[A]	NAP	N3A-C2A-N1A	-3.39	123.38	128.68
2	B	201	NAP	N3A-C2A-N1A	-3.34	123.46	128.68
2	A	201[B]	NAP	N3A-C2A-N1A	-3.34	123.46	128.68
2	A	201[B]	NAP	PN-O3-PA	-3.34	121.38	132.83
2	A	201[A]	NAP	C4A-C5A-N7A	-3.31	105.95	109.40
2	A	201[A]	NAP	N3A-C2A-N1A	-3.30	123.51	128.68
2	A	202	NAP	N3A-C2A-N1A	-3.28	123.55	128.68
2	C	201[B]	NAP	N3A-C2A-N1A	-3.20	123.68	128.68
2	A	201[B]	NAP	C4A-C5A-N7A	-3.19	106.07	109.40
2	C	201[A]	NAP	PN-O3-PA	-3.16	121.97	132.83
2	A	202	NAP	C4A-C5A-N7A	-3.04	106.23	109.40
2	B	201	NAP	PN-O3-PA	-3.02	122.45	132.83
2	A	201[A]	NAP	PN-O3-PA	-2.99	122.55	132.83
2	A	201[A]	NAP	C3D-C2D-C1D	2.89	105.33	100.98
2	C	201[B]	NAP	PN-O3-PA	-2.85	123.06	132.83
2	C	201[B]	NAP	C4A-C5A-N7A	-2.75	106.53	109.40
2	C	201[A]	NAP	C3D-C2D-C1D	2.66	104.98	100.98
2	B	201	NAP	C4A-C5A-N7A	-2.66	106.63	109.40
2	D	201	NAP	C4A-C5A-N7A	-2.64	106.65	109.40
2	C	201[A]	NAP	C4A-C5A-N7A	-2.61	106.67	109.40
2	D	201	NAP	C1B-N9A-C4A	-2.37	122.48	126.64
2	B	201	NAP	C3D-C2D-C1D	2.33	104.49	100.98
2	C	201[B]	NAP	C3D-C2D-C1D	2.32	104.47	100.98
2	C	201[A]	NAP	O3X-P2B-O2X	2.25	116.24	107.64
2	C	201[A]	NAP	C1B-N9A-C4A	-2.25	122.69	126.64
2	D	201	NAP	C2A-N1A-C6A	2.20	122.52	118.75
2	C	201[A]	NAP	C2A-N1A-C6A	2.19	122.50	118.75
2	B	201	NAP	C2A-N1A-C6A	2.17	122.46	118.75
2	A	201[B]	NAP	C1B-N9A-C4A	-2.13	122.90	126.64
2	A	202	NAP	O2N-PN-O1N	2.13	119.02	110.68
2	A	201[A]	NAP	C2B-C3B-C4B	2.10	106.55	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201[B]	NAP	C2B-C3B-C4B	2.08	106.52	101.99
2	D	201	NAP	O2A-PA-O1A	2.08	118.83	110.68
2	B	201	NAP	O2B-P2B-O1X	-2.06	101.44	109.39
2	A	201[A]	NAP	C1B-N9A-C4A	-2.04	123.06	126.64
2	C	201[A]	NAP	C2B-C3B-C4B	2.02	106.38	101.99

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201[B]	NAP	C4D-C5D-O5D-PN
2	C	201[B]	NAP	C2N-C3N-C7N-N7N
2	A	201[A]	NAP	C2B-O2B-P2B-O2X
2	A	201[A]	NAP	C5D-O5D-PN-O3
2	A	201[B]	NAP	C2B-O2B-P2B-O2X
2	A	201[B]	NAP	C5D-O5D-PN-O2N
2	A	201[B]	NAP	O4D-C1D-N1N-C6N
2	C	201[A]	NAP	C2B-O2B-P2B-O2X
2	C	201[A]	NAP	C5D-O5D-PN-O1N
2	C	201[A]	NAP	O4D-C1D-N1N-C2N
2	C	201[A]	NAP	O4D-C1D-N1N-C6N
2	C	201[A]	NAP	C2D-C1D-N1N-C2N
2	C	201[A]	NAP	C2N-C3N-C7N-O7N
2	C	201[A]	NAP	C2N-C3N-C7N-N7N
2	D	201	NAP	C2B-O2B-P2B-O3X
2	A	202	NAP	C5B-O5B-PA-O1A
2	A	202	NAP	C5B-O5B-PA-O2A
2	A	202	NAP	O4B-C4B-C5B-O5B
2	C	201[A]	NAP	C4N-C3N-C7N-N7N
2	C	201[B]	NAP	C4N-C3N-C7N-N7N
2	C	201[A]	NAP	C4N-C3N-C7N-O7N
2	C	201[B]	NAP	C4N-C3N-C7N-O7N
2	C	201[B]	NAP	C2N-C3N-C7N-O7N
2	C	201[B]	NAP	O4D-C4D-C5D-O5D
2	A	201[B]	NAP	O4D-C4D-C5D-O5D
2	A	202	NAP	C3B-C4B-C5B-O5B
4	A	204	1PE	OH7-C16-C26-OH6
4	A	204	1PE	OH4-C13-C23-OH3
2	A	201[A]	NAP	C1B-C2B-O2B-P2B
2	A	201[B]	NAP	C1B-C2B-O2B-P2B
2	D	201	NAP	C1B-C2B-O2B-P2B
2	A	201[A]	NAP	C3B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
2	A	201[B]	NAP	C3B-C2B-O2B-P2B
2	C	201[A]	NAP	C3B-C2B-O2B-P2B
2	D	201	NAP	C3B-C2B-O2B-P2B
4	A	204	1PE	OH5-C14-C24-OH4
2	C	201[A]	NAP	C1B-C2B-O2B-P2B
4	C	203	1PE	OH5-C14-C24-OH4
2	A	201[A]	NAP	O4D-C4D-C5D-O5D
2	A	201[B]	NAP	C3D-C4D-C5D-O5D
4	C	203	1PE	OH4-C13-C23-OH3
2	B	201	NAP	C4N-C3N-C7N-N7N
2	A	201[A]	NAP	C3D-C4D-C5D-O5D
2	B	201	NAP	C4N-C3N-C7N-O7N
2	C	201[B]	NAP	PN-O3-PA-O5B
2	A	201[B]	NAP	PA-O3-PN-O5D
2	C	201[A]	NAP	PA-O3-PN-O5D
2	A	201[A]	NAP	C2B-O2B-P2B-O1X
2	A	201[B]	NAP	C2B-O2B-P2B-O1X
2	C	201[A]	NAP	C2B-O2B-P2B-O1X
4	C	203	1PE	C13-C23-OH3-C22
4	A	204	1PE	C16-C26-OH6-C15
4	A	204	1PE	C15-C25-OH5-C14
4	B	203	1PE	C14-C24-OH4-C13
2	A	201[B]	NAP	C5D-O5D-PN-O3
2	C	201[A]	NAP	C5D-O5D-PN-O3
2	A	201[A]	NAP	C5D-O5D-PN-O1N
2	A	201[B]	NAP	C5D-O5D-PN-O1N
4	C	203	1PE	C15-C25-OH5-C14
2	B	201	NAP	C2N-C3N-C7N-N7N
4	A	204	1PE	C14-C24-OH4-C13
2	C	201[A]	NAP	PA-O3-PN-O1N
4	A	204	1PE	C25-C15-OH6-C26
2	B	201	NAP	C2N-C3N-C7N-O7N
2	C	201[B]	NAP	C3D-C4D-C5D-O5D
4	A	204	1PE	C23-C13-OH4-C24
4	A	204	1PE	C13-C23-OH3-C22
2	A	202	NAP	C2B-O2B-P2B-O1X
4	B	203	1PE	C13-C23-OH3-C22
2	C	201[A]	NAP	C2D-C1D-N1N-C6N
2	D	201	NAP	C2B-O2B-P2B-O2X
2	A	202	NAP	C5B-O5B-PA-O3
2	C	201[B]	NAP	PA-O3-PN-O2N
2	A	201[A]	NAP	PN-O3-PA-O2A

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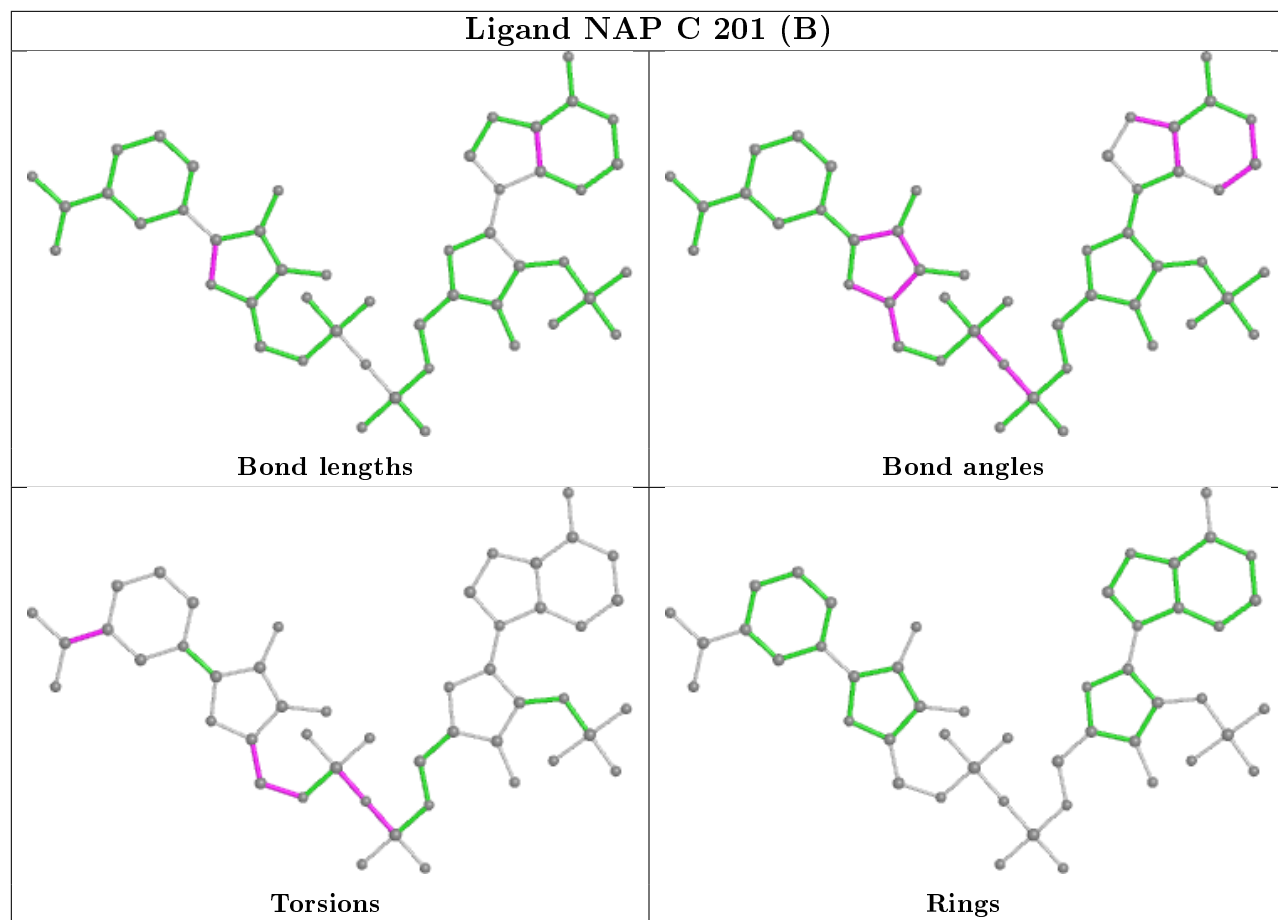
Mol	Chain	Res	Type	Atoms
2	A	201[B]	NAP	PN-O3-PA-O2A
4	C	203	1PE	OH2-C12-C22-OH3

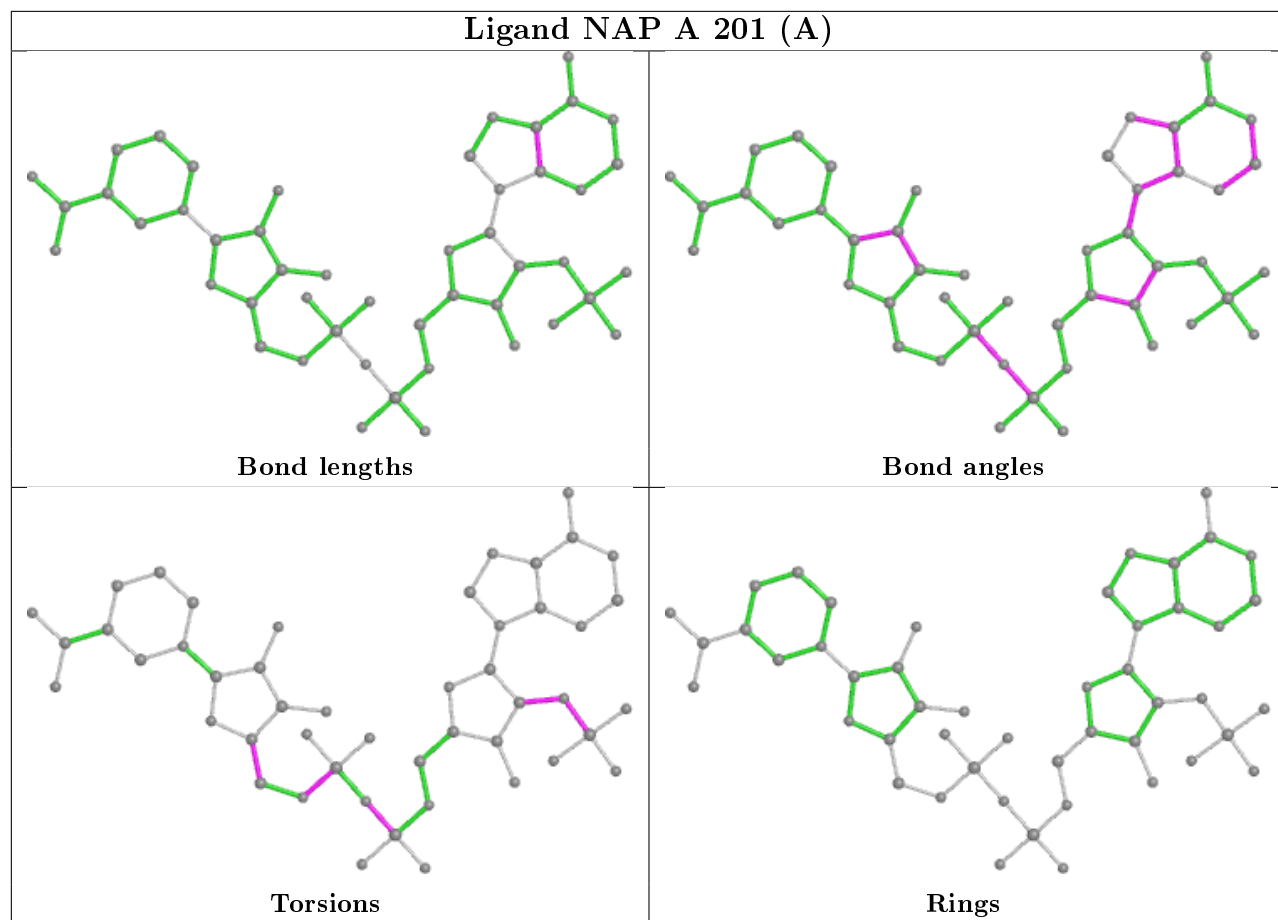
There are no ring outliers.

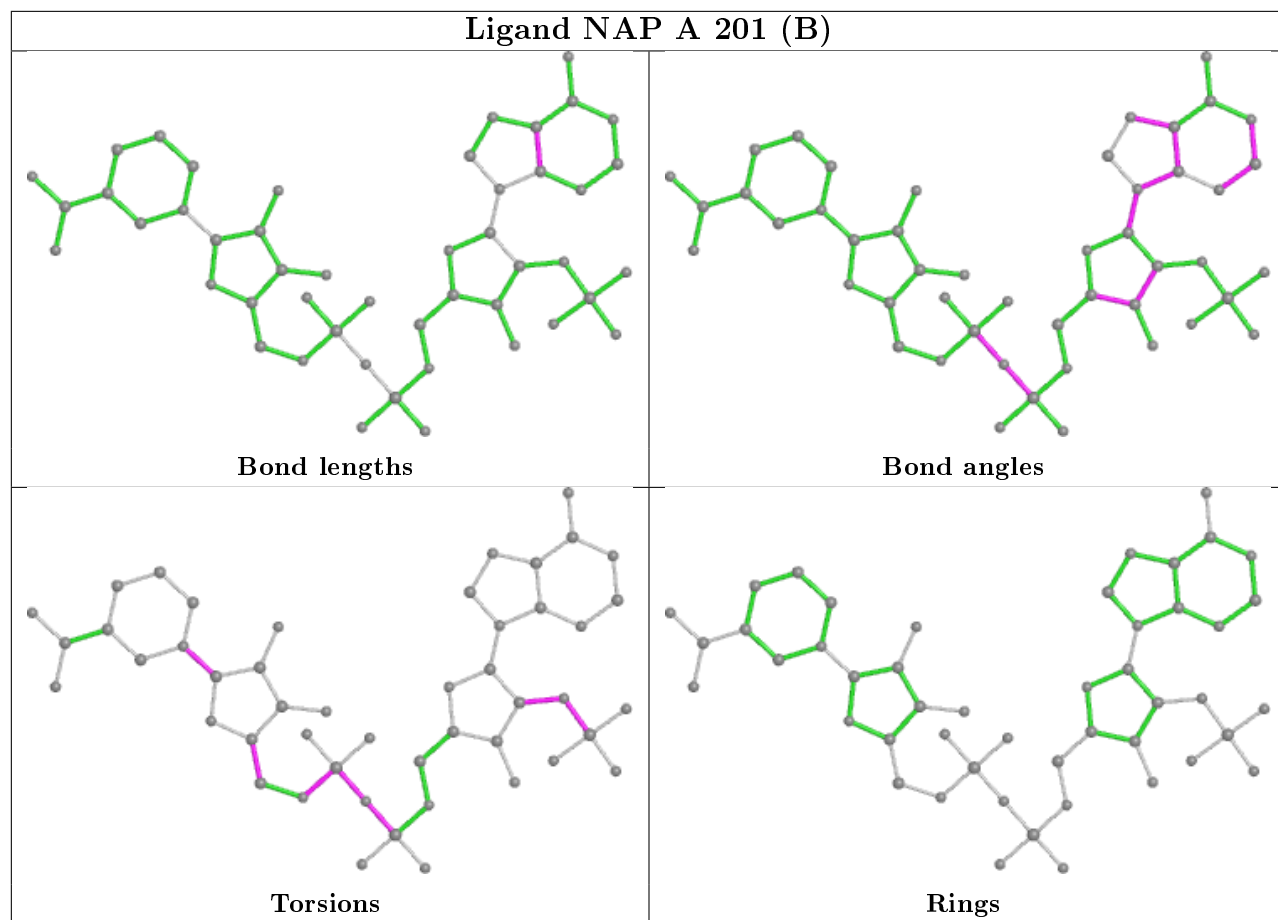
9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201[B]	NAP	2	0
4	C	203	1PE	6	0
2	A	201[B]	NAP	1	0
2	C	201[A]	NAP	1	0
2	B	201	NAP	1	0
4	B	203	1PE	5	0
2	D	201	NAP	1	0
4	A	204	1PE	4	0
2	A	202	NAP	5	0

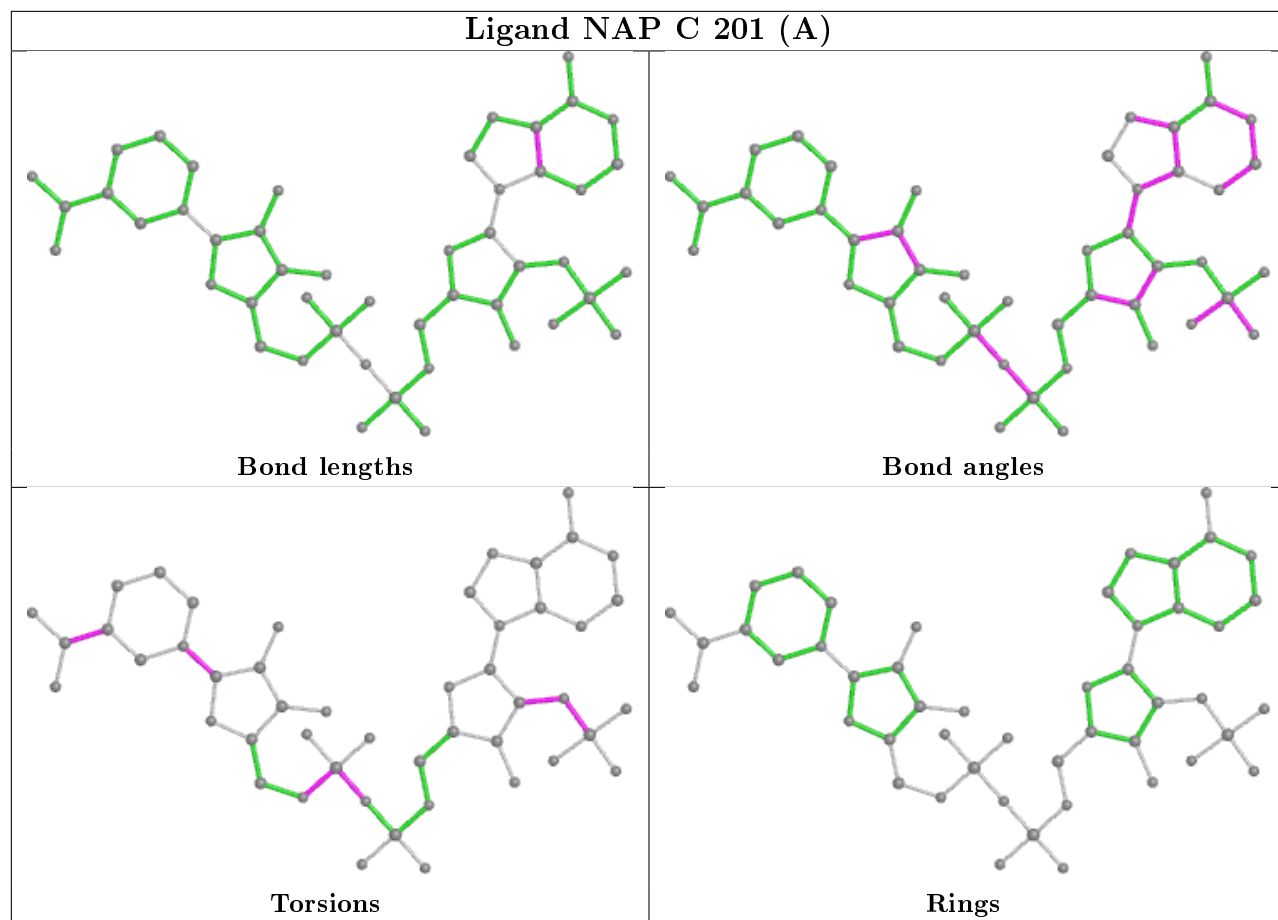
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

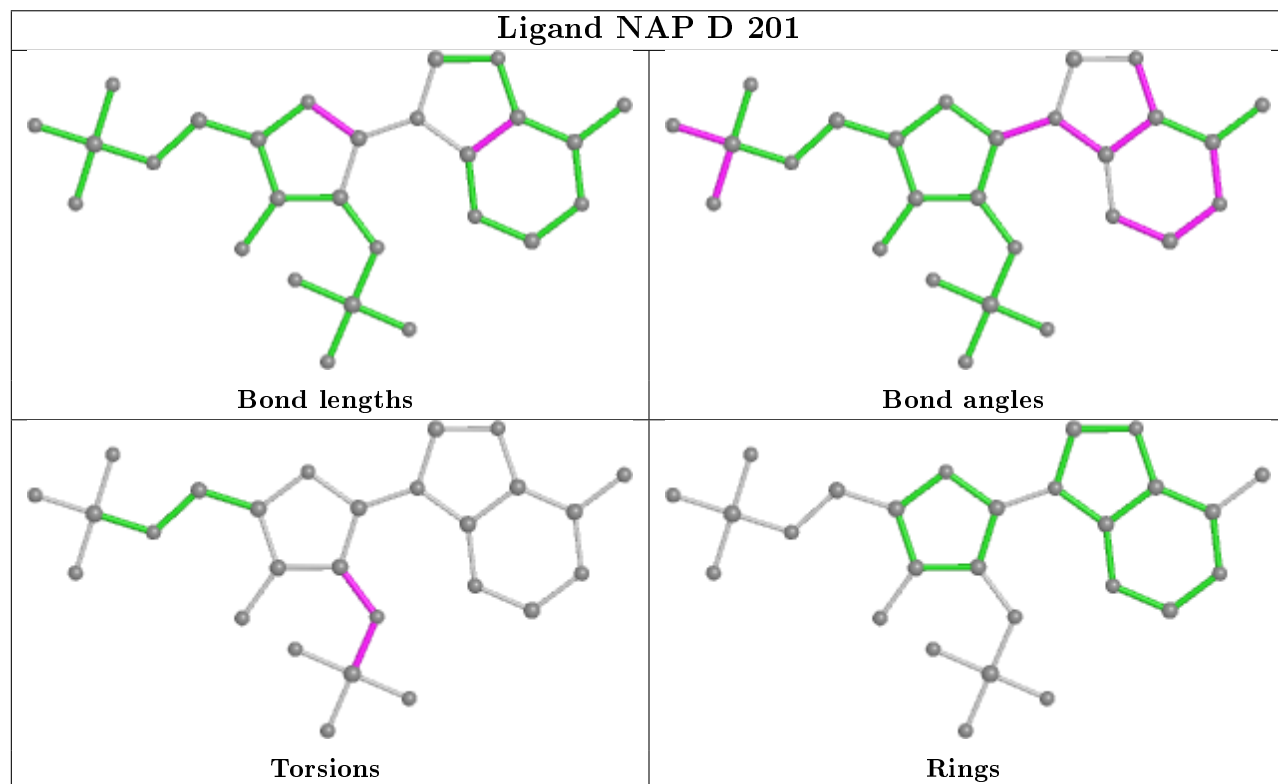
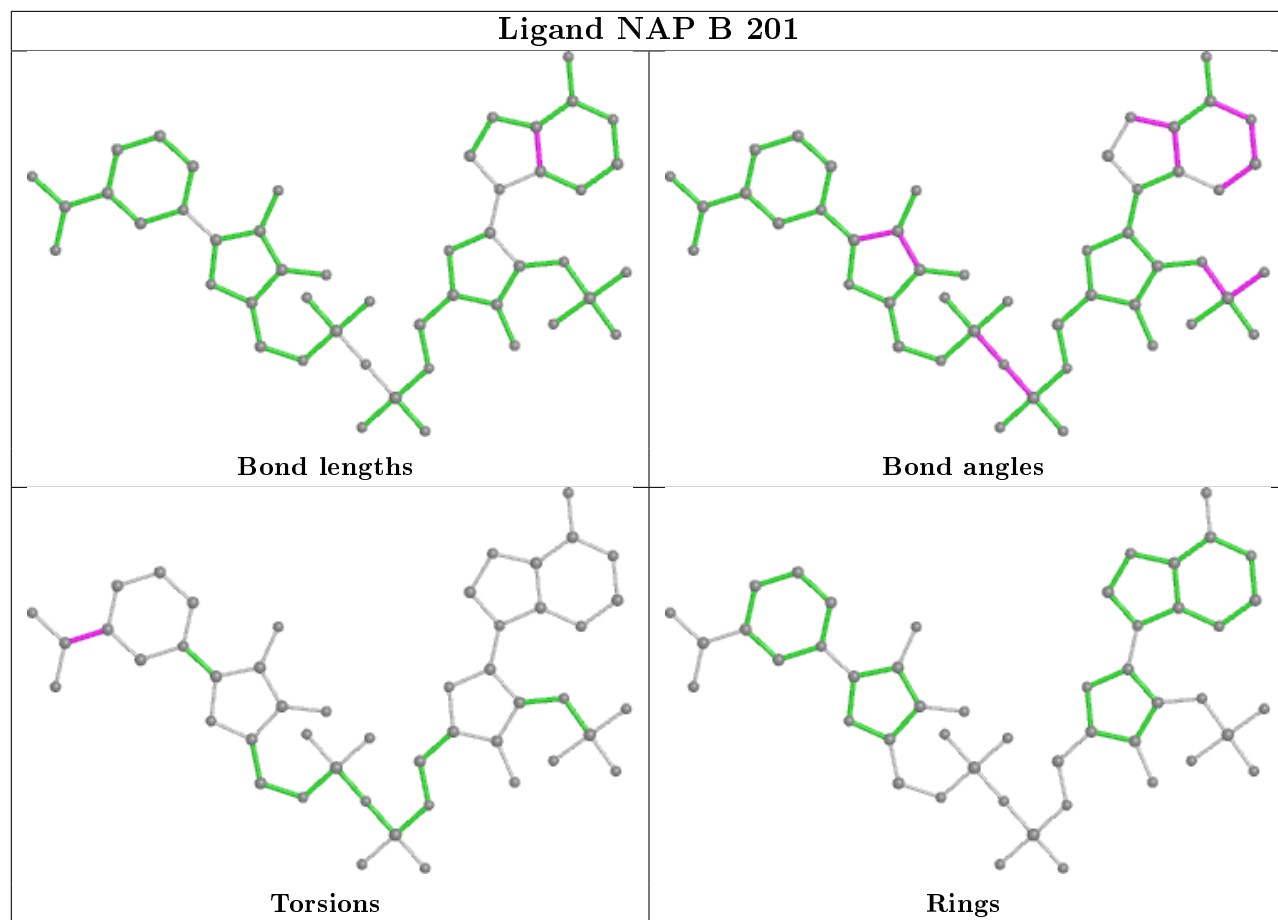


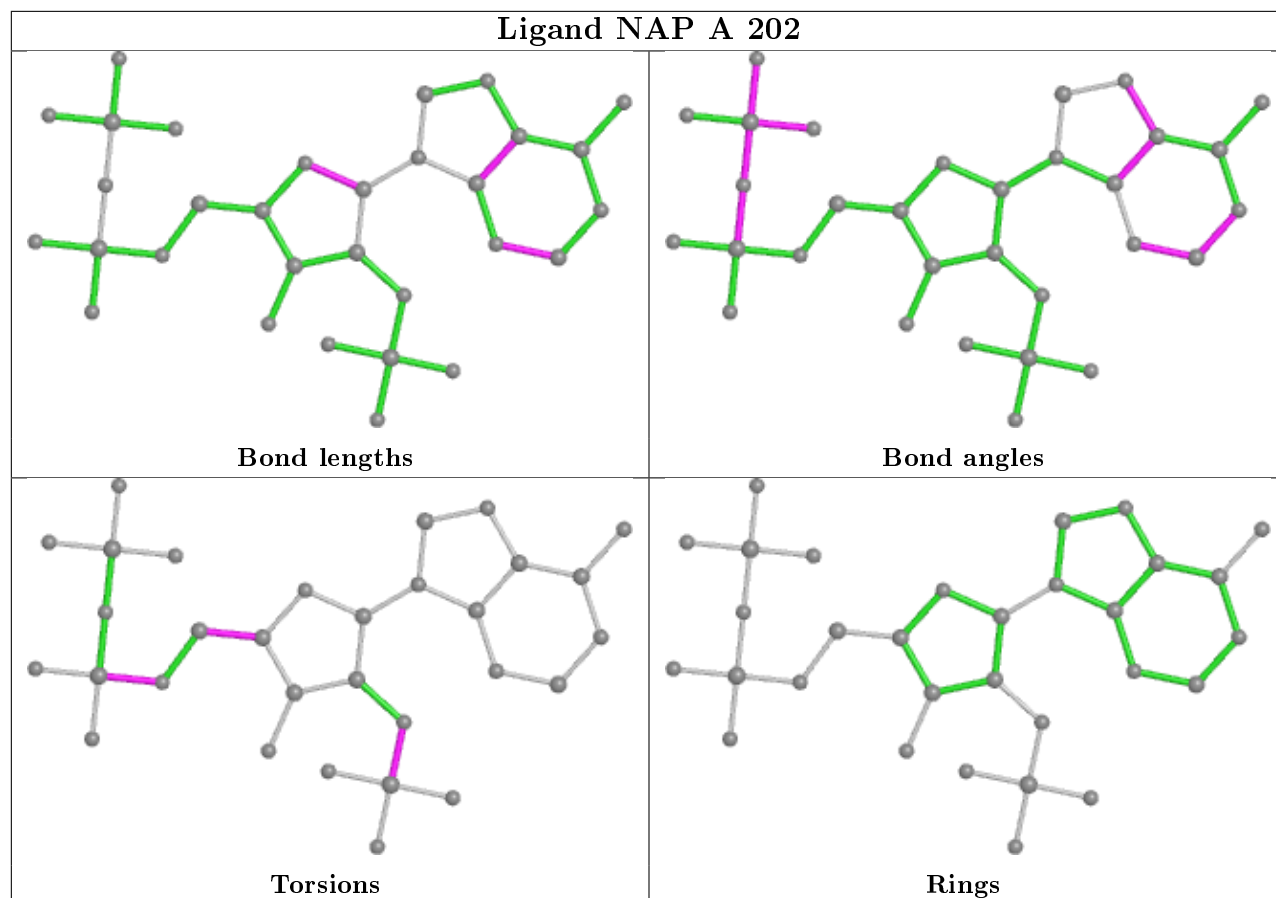












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	175/177 (98%)	0.37	10 (5%) 23 26	15, 27, 73, 87	0
1	B	169/177 (95%)	0.31	8 (4%) 31 35	15, 29, 64, 105	0
1	C	175/177 (98%)	0.55	19 (10%) 5 6	20, 37, 89, 102	0
1	D	172/177 (97%)	0.53	15 (8%) 10 11	21, 37, 81, 136	0
All	All	691/708 (97%)	0.44	52 (7%) 14 16	15, 32, 78, 136	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	115	CYS	7.4
1	D	116	PHE	6.8
1	C	162	GLY	6.0
1	D	113	SER	5.9
1	D	112	ARG	5.8
1	C	161	ARG	5.1
1	D	120	ARG	5.0
1	D	161	ARG	4.9
1	D	114	GLY	4.6
1	A	160	ALA	4.1
1	B	119	ASN	4.0
1	C	111	ALA	3.9
1	D	97	ARG	3.9
1	C	2	SER	3.9
1	C	163	ARG	3.8
1	C	116	PHE	3.8
1	C	159	PHE	3.7
1	C	117	GLN	3.6
1	C	119	ASN	3.1
1	A	175[A]	THR	3.1
1	B	176[A]	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	115	CYS	3.0
1	A	176[A]	GLN	3.0
1	D	111	ALA	3.0
1	A	117	GLN	3.0
1	B	175[A]	THR	2.9
1	A	118	SER	2.9
1	C	176[A]	GLN	2.9
1	C	23[A]	HIS	2.9
1	D	163	ARG	2.8
1	A	161	ARG	2.8
1	D	176	GLN	2.8
1	C	112	ARG	2.7
1	D	2	SER	2.5
1	D	133	SER	2.5
1	C	175[A]	THR	2.5
1	D	32	GLU	2.5
1	A	114	GLY	2.4
1	A	115	CYS	2.3
1	B	112	ARG	2.3
1	C	97	ARG	2.3
1	D	110	ALA	2.3
1	B	161	ARG	2.3
1	A	159	PHE	2.2
1	A	163	ARG	2.2
1	C	118	SER	2.2
1	B	111	ALA	2.2
1	B	113	SER	2.1
1	C	165	ARG	2.1
1	B	53	SER	2.1
1	C	56	LYS	2.0
1	C	113	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

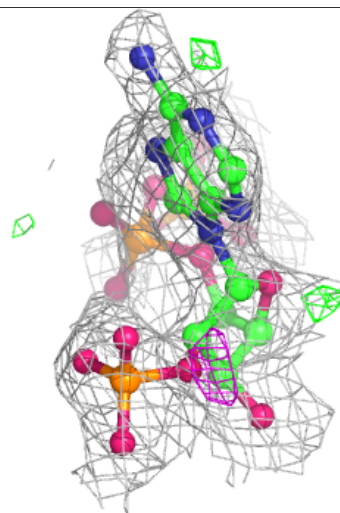
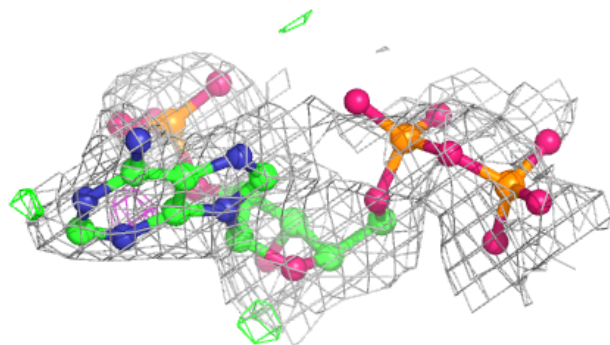
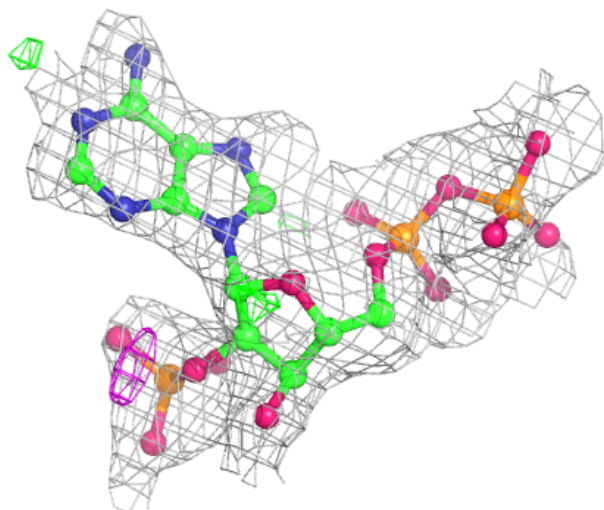
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	1PE	B	203	16/16	0.64	0.23	46,72,81,85	0
4	1PE	A	204	16/16	0.67	0.34	56,75,77,78	0
2	NAP	A	202	31/48	0.76	0.19	37,96,164,166	0
2	NAP	C	201[A]	48/48	0.84	0.23	32,67,103,105	48
2	NAP	C	201[B]	48/48	0.84	0.23	32,67,104,105	48
2	NAP	D	201	27/48	0.89	0.14	27,34,54,63	0
2	NAP	A	201[B]	48/48	0.90	0.18	25,37,70,73	48
2	NAP	A	201[A]	48/48	0.90	0.18	26,37,70,71	48
4	1PE	C	203	13/16	0.91	0.23	35,63,68,70	0
5	PO4	D	202	5/5	0.92	0.17	43,49,56,57	0
3	CL	B	202	1/1	0.95	0.11	38,38,38,38	0
3	CL	C	202	1/1	0.96	0.16	63,63,63,63	0
2	NAP	B	201	48/48	0.96	0.09	20,32,41,44	0
3	CL	A	203	1/1	0.99	0.10	33,33,33,33	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.

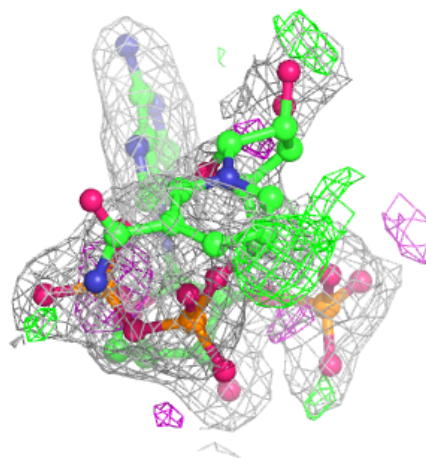
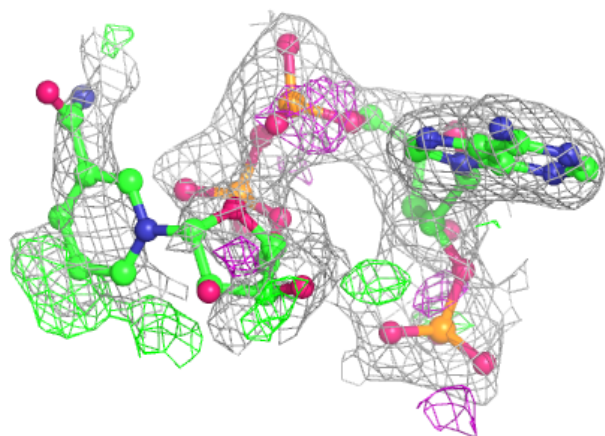
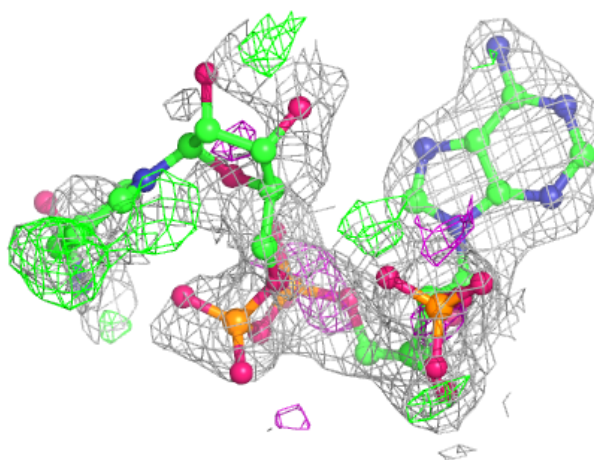
**Electron density around NAP A 202:**

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



**Electron density around NAP C 201 (A):**

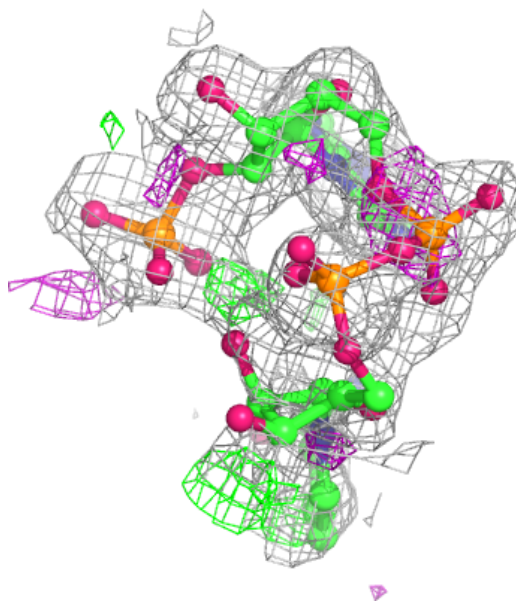
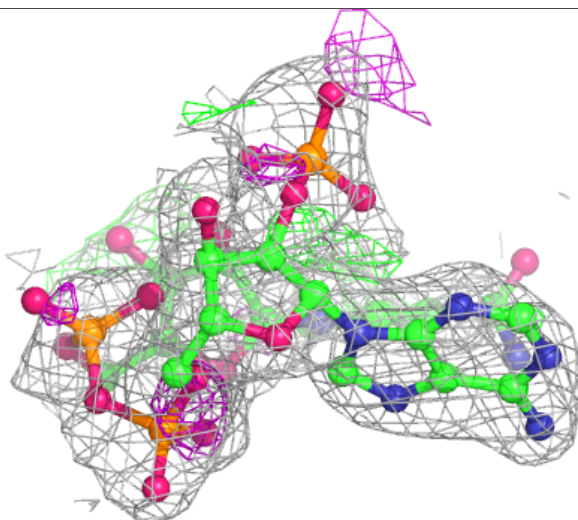
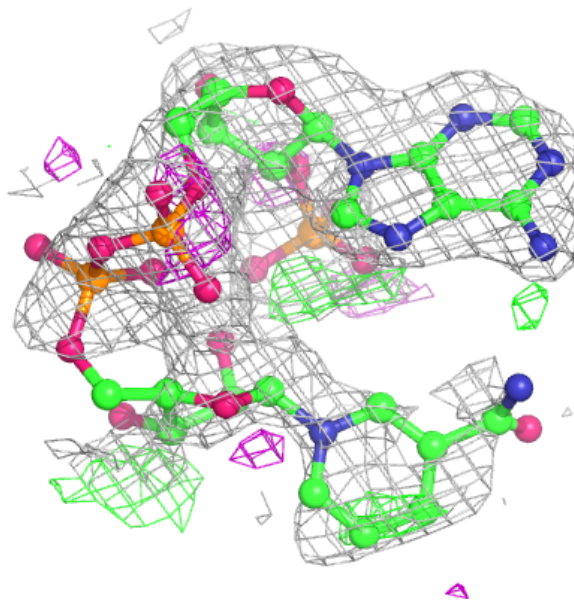
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





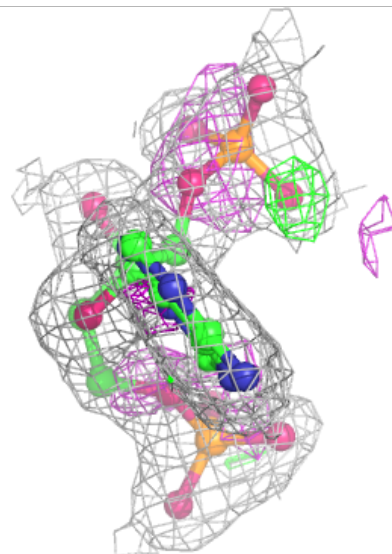
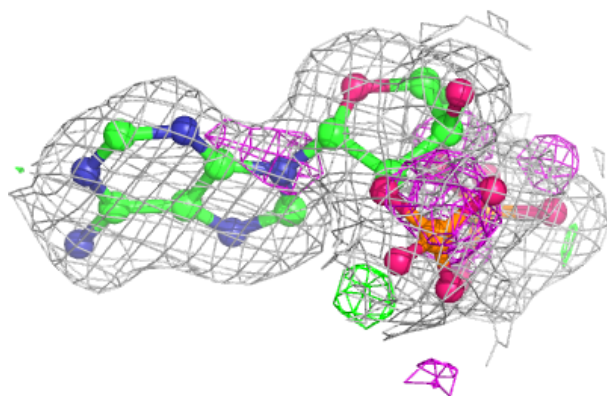
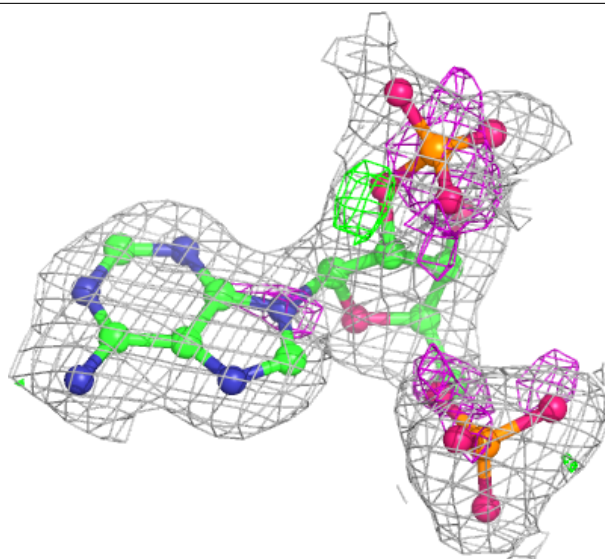
**Electron density around NAP C 201 (B):**

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



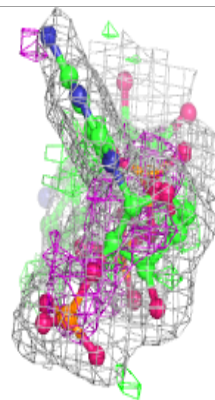
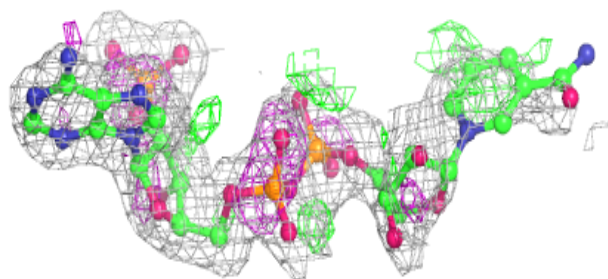
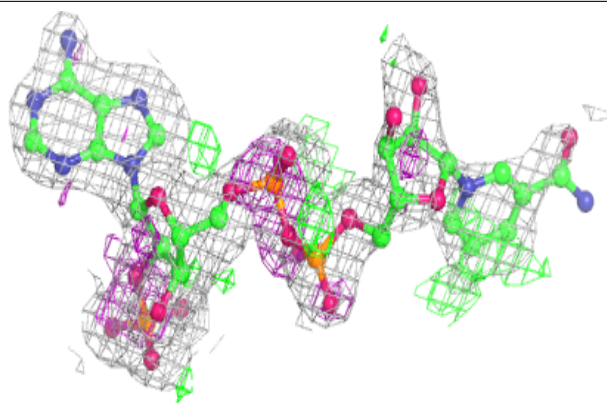
**Electron density around NAP D 201:**

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

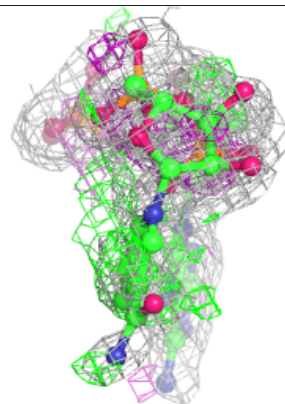
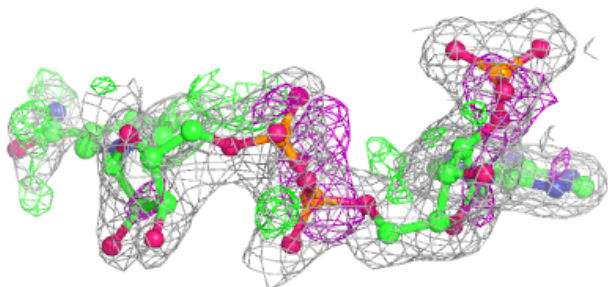
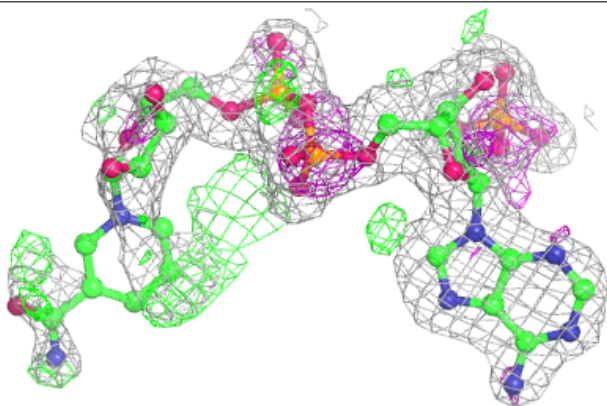


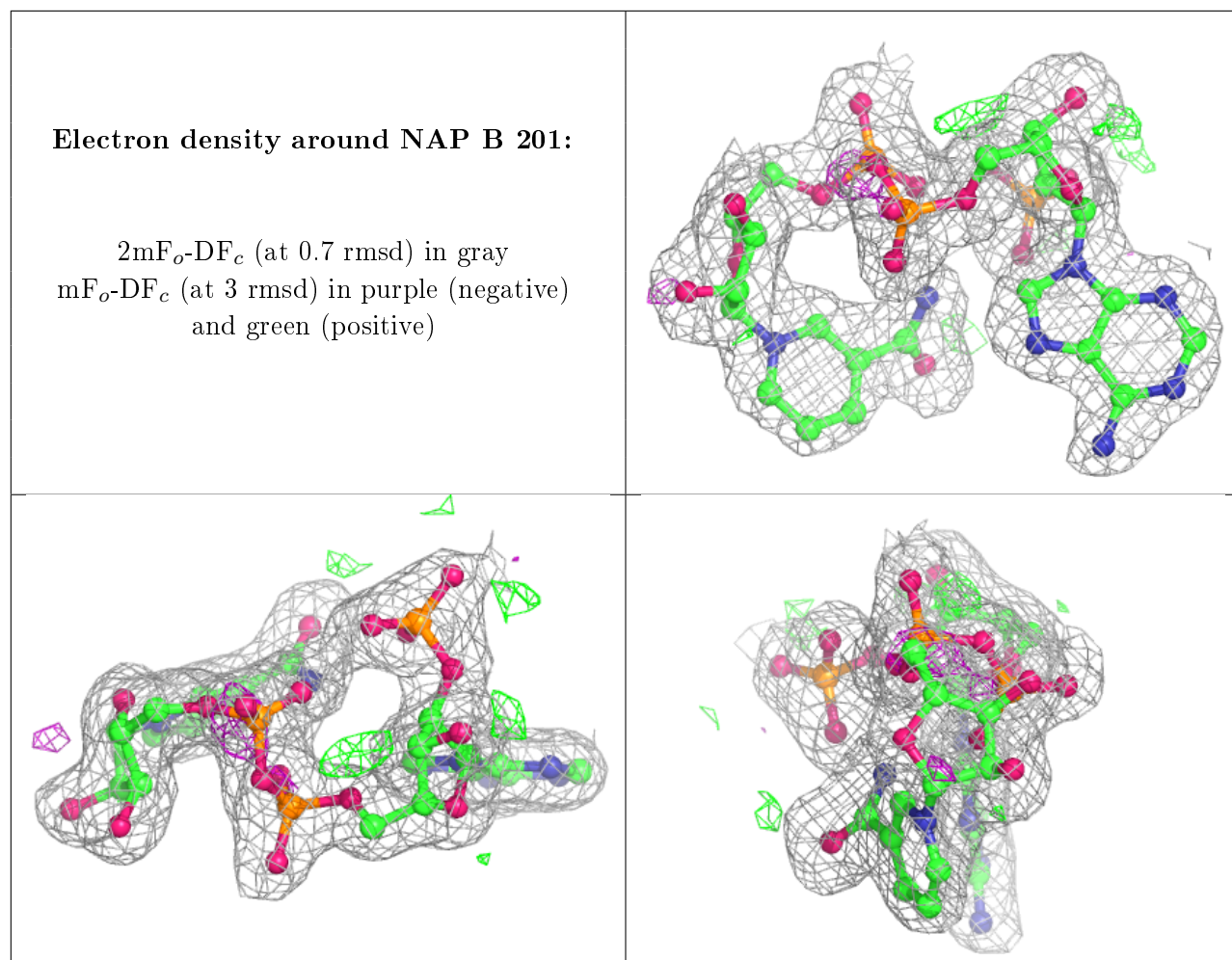
**Electron density around NAP A 201 (B):**

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

**Electron density around NAP A 201 (A):**

$2mF_o-DF_c$  (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.