



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:55 am BST

PDB ID : 6TQ5  
Title : Alcohol dehydrogenase from *Candida magnoliae* DSMZ 70638 (ADHA): complex with NADP+  
Authors : Rovida, S.; Aalbers, F.S.; Fraaije, M.W.; Mattevi, A.  
Deposited on : 2019-12-16  
Resolution : 1.60 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



## 2 Entry composition [i](#)

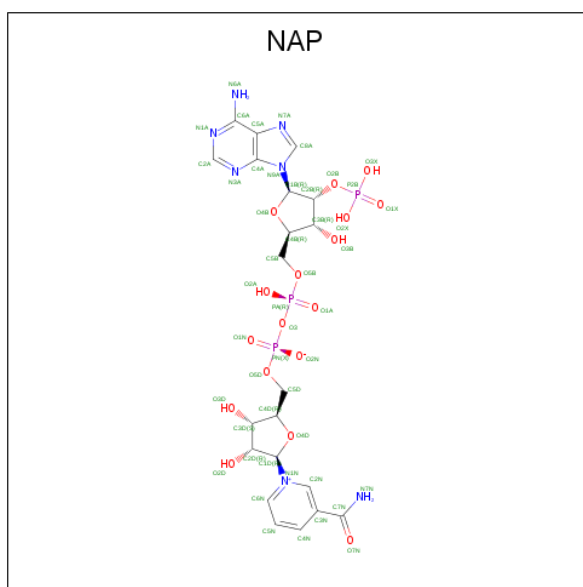
There are 5 unique types of molecules in this entry. The entry contains 7848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enzyme subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	Total	C	N	O	S	0	5	0
			1797	1133	307	349	8			
1	B	240	Total	C	N	O	S	0	4	0
			1781	1125	303	345	8			
1	C	240	Total	C	N	O	S	0	3	0
			1773	1118	301	346	8			
1	D	240	Total	C	N	O	S	0	0	0
			1761	1110	301	342	8			

- 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>) (labeled as "Ligand of Interest" by author).



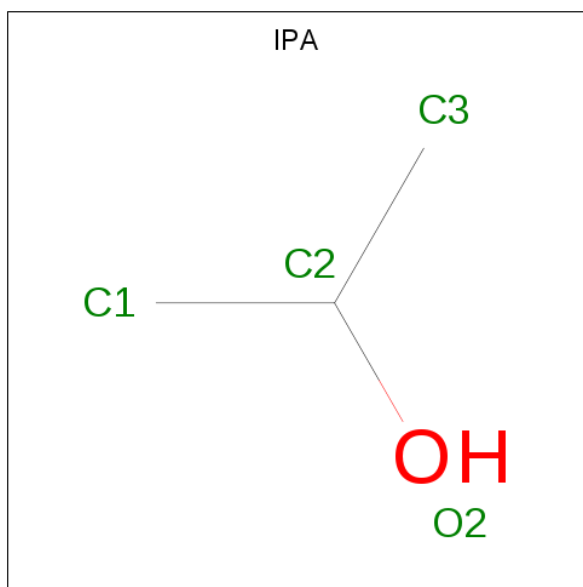
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		
2	B	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
2	D	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

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



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

- Molecule 4 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
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

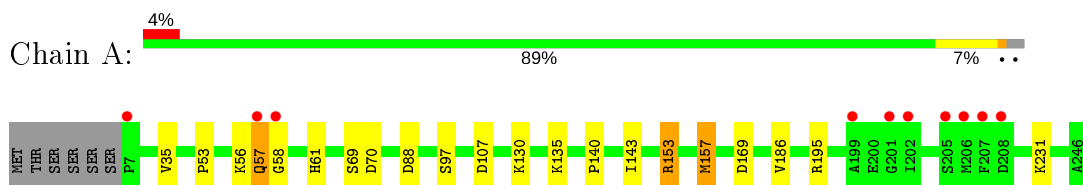
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	B	143	Total	O	0	0
			143	143		
5	C	140	Total	O	0	0
			140	140		
5	D	139	Total	O	0	0
			139	139		

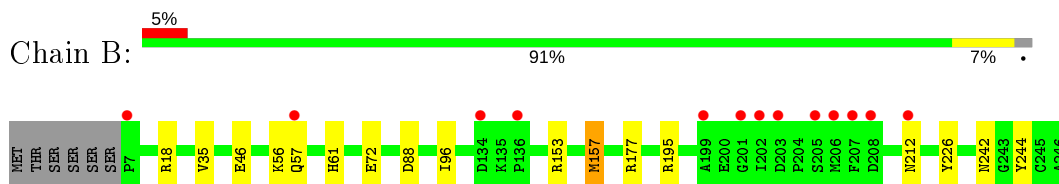
### 3 Residue-property plots [i](#)

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.

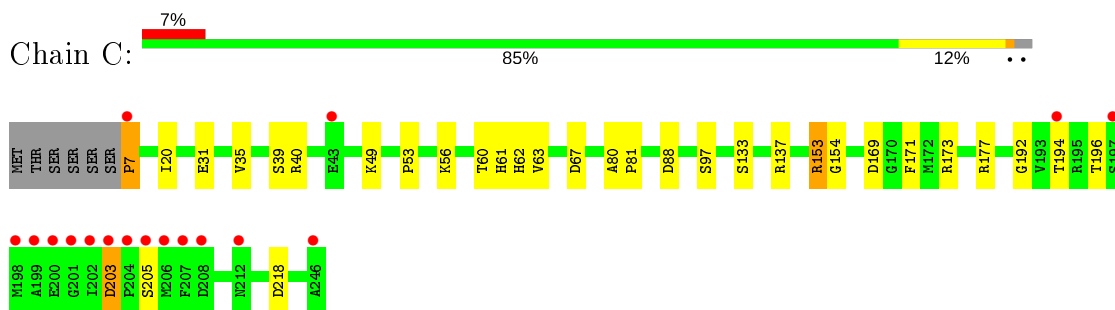
- Molecule 1: Enzyme subunit



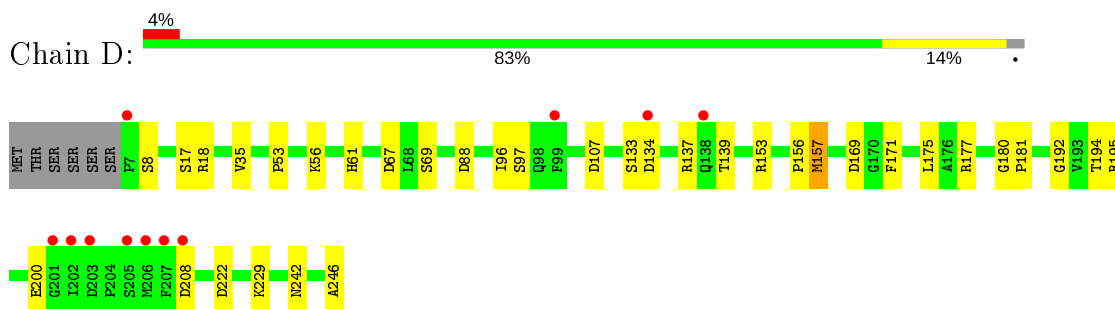
- Molecule 1: Enzyme subunit



- Molecule 1: Enzyme subunit



- Molecule 1: Enzyme subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.11Å 113.14Å 124.21Å 90.00° 94.04° 90.00°	Depositor
Resolution (Å)	83.55 – 1.60 45.54 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (83.55-1.60) 97.3 (45.54-1.60)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.141 , 0.197 0.146 , 0.195	Depositor DCC
$R_{free}$ test set	6542 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtrriage
Anisotropy	0.453	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.4	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	7848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: GOL, NAP, IPA

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	1.40	3/1830 (0.2%)	1.24	9/2487 (0.4%)
1	B	1.27	6/1823 (0.3%)	1.23	10/2477 (0.4%)
1	C	1.26	5/1815 (0.3%)	1.24	15/2468 (0.6%)
1	D	1.29	6/1794 (0.3%)	1.22	17/2439 (0.7%)
All	All	1.31	20/7262 (0.3%)	1.24	51/9871 (0.5%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	SER	CB-OG	-16.73	1.20	1.42
1	D	97	SER	CB-OG	-9.51	1.29	1.42
1	D	246	ALA	C-O	8.91	1.40	1.23
1	B	72	GLU	CD-OE1	8.69	1.35	1.25
1	A	157	MET	CB-CG	7.76	1.76	1.51
1	B	72	GLU	CD-OE2	7.37	1.33	1.25
1	B	88	ASP	CG-OD2	7.17	1.41	1.25
1	C	133	SER	CB-OG	-7.10	1.33	1.42
1	D	133	SER	CB-OG	-6.96	1.33	1.42
1	B	72	GLU	CG-CD	6.88	1.62	1.51
1	D	69	SER	CB-OG	-6.63	1.33	1.42
1	A	97	SER	CB-OG	-6.61	1.33	1.42
1	C	39	SER	CB-OG	-6.34	1.34	1.42
1	C	97	SER	CB-OG	-6.13	1.34	1.42
1	D	17	SER	CB-OG	5.30	1.49	1.42
1	C	7	PRO	N-CA	-5.27	1.38	1.47
1	D	88	ASP	CG-OD1	5.18	1.37	1.25
1	B	46	GLU	CG-CD	-5.11	1.44	1.51
1	B	226	TYR	CE2-CZ	-5.01	1.32	1.38
1	C	218	ASP	CG-OD1	5.00	1.36	1.25

All (51) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	ASP	CB-CG-OD1	-13.55	106.10	118.30
1	B	88	ASP	CB-CG-OD2	12.81	129.83	118.30
1	D	157	MET	CG-SD-CE	-9.66	84.74	100.20
1	A	153	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	B	18	ARG	NE-CZ-NH1	-9.59	115.51	120.30
1	A	157	MET	CG-SD-CE	9.09	114.73	100.20
1	D	246	ALA	CA-C-O	-8.96	101.28	120.10
1	D	88	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	C	169	ASP	CB-CG-OD1	8.34	125.81	118.30
1	C	218	ASP	CB-CG-OD2	-8.22	110.91	118.30
1	A	88	ASP	CB-CG-OD1	-8.18	110.94	118.30
1	B	18	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	B	177	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	169	ASP	CB-CG-OD1	7.92	125.43	118.30
1	C	88[A]	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	C	88[B]	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	C	137	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	C	153	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	D	222	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	C	171	PHE	CB-CG-CD2	-7.19	115.77	120.80
1	D	177	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	C	173	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	208	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	195	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	60	THR	CA-CB-CG2	-6.75	102.95	112.40
1	D	195	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	67	ASP	CB-CG-OD1	6.29	123.96	118.30
1	D	195	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	107	ASP	CB-CG-OD1	6.03	123.72	118.30
1	D	67	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	195	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	195	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	137	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	B	56	LYS	CA-CB-CG	5.54	125.59	113.40
1	C	40	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	70	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	D	137	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	56	LYS	CB-CA-C	-5.43	99.53	110.40
1	D	137	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	D	107	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	130	LYS	CD-CE-NZ	5.41	124.13	111.70
1	A	157	MET	CB-CG-SD	-5.36	96.31	112.40
1	B	157	MET	CG-SD-CE	-5.36	91.63	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	134	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	18	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	D	153	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	218	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	177	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	133	SER	CA-CB-OG	-5.09	97.45	111.20
1	D	229	LYS	CD-CE-NZ	-5.07	100.03	111.70
1	D	169	ASP	CB-CG-OD2	-5.05	113.75	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1797	0	1813	12	0
1	B	1781	0	1808	9	0
1	C	1773	0	1791	19	0
1	D	1761	0	1775	11	0
2	A	40	0	19	0	0
2	B	39	0	18	0	0
2	C	39	0	18	0	0
2	D	39	0	18	0	0
3	A	4	0	8	0	0
3	C	4	0	8	3	0
4	C	6	0	7	3	0
4	D	6	0	8	2	0
5	A	137	0	0	1	1
5	B	143	0	0	3	0
5	C	140	0	0	2	0
5	D	139	0	0	3	0
All	All	7848	0	7291	49	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 3.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:MET:CB	1:A:157:MET:CG	1.76	1.63
1:A:153:ARG:HD2	5:D:409:HOH:O	1.56	1.05
5:B:521:HOH:O	1:C:153:ARG:HD2	1.64	0.95
1:A:35:VAL:H	1:A:61:HIS:HD2	1.19	0.91
1:D:35:VAL:H	1:D:61:HIS:HD2	1.23	0.86
1:B:35:VAL:H	1:B:61:HIS:HD2	1.25	0.84
1:A:157:MET:SD	1:A:157:MET:CB	2.66	0.83
1:C:35:VAL:H	1:C:61:HIS:HD2	1.24	0.80
1:A:135:LYS:HE2	5:A:438:HOH:O	1.90	0.71
1:C:35:VAL:H	1:C:61:HIS:CD2	2.09	0.68
1:D:35:VAL:H	1:D:61:HIS:CD2	2.11	0.61
1:D:96:ILE:HD11	5:D:462:HOH:O	2.01	0.59
1:D:56:LYS:HE3	4:D:302:GOL:O2	2.04	0.58
1:C:62:HIS:HD1	4:C:303:GOL:C3	2.17	0.57
1:A:35:VAL:H	1:A:61:HIS:CD2	2.11	0.56
1:B:35:VAL:H	1:B:61:HIS:CD2	2.15	0.55
1:C:31:GLU:O	3:C:302:IPA:H32	2.09	0.53
1:C:49:LYS:HD3	1:C:63:VAL:HG13	1.91	0.53
1:C:192:GLY:O	1:C:194[A]:THR:HG23	2.08	0.53
1:C:31:GLU:O	3:C:302:IPA:C3	2.58	0.52
1:C:53:PRO:O	1:C:61:HIS:HE1	1.92	0.51
1:C:80:ALA:HB1	5:C:410:HOH:O	2.10	0.51
1:A:157:MET:CG	1:A:157:MET:CA	2.81	0.49
1:B:153:ARG:HG3	1:C:153:ARG:NH2	2.29	0.47
1:C:154:GLY:HA2	5:C:423:HOH:O	2.15	0.47
1:C:203:ASP:OD1	1:C:205:SER:OG	2.17	0.47
1:B:212:ASN:ND2	5:B:401:HOH:O	2.48	0.46
1:C:194[B]:THR:HG23	1:C:196:THR:HG23	1.97	0.46
1:B:96[B]:ILE:HA	1:B:96[B]:ILE:HD13	1.56	0.46
1:B:153:ARG:HG3	1:C:153:ARG:CZ	2.45	0.46
1:C:62:HIS:HD1	4:C:303:GOL:H31	1.82	0.45
1:A:157:MET:HB3	1:A:157:MET:CE	2.47	0.45
1:A:140:PRO:HD2	1:A:231[B]:LYS:HG2	1.99	0.44
1:C:56:LYS:HD2	3:C:302:IPA:H33	1.98	0.44
1:A:53:PRO:O	1:A:61:HIS:HE1	2.00	0.44
1:C:81:PRO:HB2	4:C:303:GOL:H31	1.99	0.43
1:D:171:PHE:CE2	1:D:175:LEU:HD11	2.53	0.43
1:D:192:GLY:O	1:D:194:THR:HG23	2.18	0.43
1:B:153:ARG:HD3	1:B:244:TYR:CZ	2.54	0.43
1:C:20:ILE:HD11	1:C:194[B]:THR:HG21	2.00	0.42
1:A:57:GLN:HG2	1:A:58:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PRO:O	1:D:61:HIS:HE1	2.03	0.42
1:B:96[B]:ILE:HG23	1:B:96[B]:ILE:HD12	1.70	0.42
1:D:139:THR:HG23	5:D:432:HOH:O	2.20	0.41
1:B:96[B]:ILE:HD13	5:B:434:HOH:O	2.20	0.41
1:D:180:GLY:N	1:D:181:PRO:CD	2.84	0.41
1:A:143:ILE:O	1:A:186:VAL:HA	2.21	0.40
1:D:156:PRO:C	1:D:157:MET:HG2	2.42	0.40
1:D:8:SER:HA	4:D:302:GOL:O3	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)
5:A:536:HOH:O	5:A:536:HOH:O[2_555]	0.68	1.52

## 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	243/246 (99%)	235 (97%)	8 (3%)	0	100	100
1	B	242/246 (98%)	237 (98%)	5 (2%)	0	100	100
1	C	241/246 (98%)	234 (97%)	7 (3%)	0	100	100
1	D	238/246 (97%)	231 (97%)	7 (3%)	0	100	100
All	All	964/984 (98%)	937 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	194/195 (100%)	192 (99%)	2 (1%)	76	61
1	B	193/195 (99%)	190 (98%)	3 (2%)	62	41
1	C	192/195 (98%)	190 (99%)	2 (1%)	76	61
1	D	189/195 (97%)	187 (99%)	2 (1%)	73	57
All	All	768/780 (98%)	759 (99%)	9 (1%)	71	54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	57	GLN
1	B	57	GLN
1	B	157	MET
1	B	242	ASN
1	C	7	PRO
1	C	203	ASP
1	D	200	GLU
1	D	242	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	142	HIS
1	A	232	ASN
1	A	242	ASN
1	B	61	HIS
1	B	142	HIS
1	B	212	ASN
1	B	232	ASN
1	B	242	ASN
1	C	57	GLN

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Mol	Chain	Res	Type
1	C	61	HIS
1	C	142	HIS
1	C	212	ASN
1	C	232	ASN
1	C	242	ASN
1	D	57	GLN
1	D	61	HIS
1	D	65	GLN
1	D	212	ASN
1	D	232	ASN
1	D	242	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	A	301	-	36,43,52	1.06	2 (5%)	44,67,80	1.74	7 (15%)
4	GOL	D	302	-	5,5,5	0.49	0	5,5,5	1.74	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IPA	A	302	-	3,3,3	0.95	0	3,3,3	1.16	0
4	GOL	C	303	-	5,5,5	1.92	2 (40%)	5,5,5	2.67	2 (40%)
2	NAP	D	301	-	36,42,52	1.42	5 (13%)	43,65,80	1.94	11 (25%)
2	NAP	B	301	-	36,42,52	1.64	6 (16%)	43,65,80	2.04	12 (27%)
2	NAP	C	301	-	36,42,52	1.26	5 (13%)	43,65,80	1.51	7 (16%)
3	IPA	C	302	-	3,3,3	0.83	0	3,3,3	1.85	1 (33%)

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	A	301	-	-	5/23/59/67	0/4/4/5
4	GOL	D	302	-	-	2/4/4/4	-
4	GOL	C	303	-	-	1/4/4/4	-
2	NAP	D	301	-	-	5/23/56/67	0/4/4/5
2	NAP	B	301	-	-	4/23/56/67	0/4/4/5
2	NAP	C	301	-	-	5/23/56/67	0/4/4/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C2A-N3A	4.75	1.39	1.32
2	B	301	NAP	P2B-O2B	4.60	1.68	1.59
2	D	301	NAP	P2B-O2B	4.53	1.67	1.59
2	D	301	NAP	O4D-C1D	3.88	1.52	1.43
2	C	301	NAP	P2B-O2B	3.78	1.66	1.59
2	A	301	NAP	C2A-N3A	3.51	1.37	1.32
2	B	301	NAP	O4D-C1D	3.21	1.50	1.43
4	C	303	GOL	O1-C1	2.94	1.54	1.42
2	B	301	NAP	O4D-C4D	2.79	1.49	1.44
2	D	301	NAP	C2A-N3A	2.61	1.36	1.32
2	C	301	NAP	C4A-N3A	2.58	1.39	1.35
2	B	301	NAP	C4A-N3A	-2.48	1.32	1.35
2	D	301	NAP	C6A-C5A	2.31	1.51	1.43
2	D	301	NAP	C1D-C2D	2.27	1.55	1.51
2	A	301	NAP	P2B-O2B	2.24	1.63	1.59
2	C	301	NAP	O4B-C1B	2.23	1.44	1.41
4	C	303	GOL	O3-C3	-2.20	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	PN-O1N	2.15	1.58	1.50
2	C	301	NAP	O4D-C1D	2.08	1.48	1.43
2	B	301	NAP	C5A-C4A	2.07	1.46	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	O4D-C1D-C2D	-8.88	88.81	105.99
2	B	301	NAP	O4D-C1D-C2D	-6.75	92.92	105.99
2	B	301	NAP	N3A-C2A-N1A	-5.86	119.52	128.68
2	A	301	NAP	O4B-C4B-C3B	5.11	115.22	105.11
4	C	303	GOL	O2-C2-C3	-4.78	88.08	109.12
2	C	301	NAP	O4D-C1D-C2D	-4.52	97.25	105.99
2	C	301	NAP	O5D-C5D-C4D	-3.96	95.38	108.99
2	A	301	NAP	O2D-C2D-C1D	3.73	122.47	110.02
2	B	301	NAP	C2A-N1A-C6A	3.22	124.25	118.75
2	A	301	NAP	O2A-PA-O1A	3.16	127.85	112.24
2	A	301	NAP	C4A-C5A-N7A	-3.12	106.15	109.40
2	A	301	NAP	O4D-C4D-C3D	-2.91	99.36	105.11
4	D	302	GOL	O1-C1-C2	-2.88	96.39	110.20
2	B	301	NAP	O2B-P2B-O1X	-2.81	98.53	109.39
2	D	301	NAP	O4D-C4D-C3D	-2.79	102.23	104.70
4	C	303	GOL	O2-C2-C1	2.61	120.61	109.12
2	B	301	NAP	PN-O3-PA	-2.60	123.90	132.83
2	C	301	NAP	O4B-C4B-C3B	2.57	110.21	105.11
2	A	301	NAP	O5B-PA-O1A	-2.52	99.23	109.07
2	B	301	NAP	O2N-PN-O1N	2.45	124.34	112.24
3	C	302	IPA	O2-C2-C1	2.41	126.44	110.36
2	B	301	NAP	O4D-C4D-C3D	-2.40	102.58	104.70
2	D	301	NAP	O2D-C2D-C3D	2.39	115.79	111.27
2	C	301	NAP	C4A-C5A-N7A	-2.37	106.93	109.40
2	C	301	NAP	O2N-PN-O1N	2.37	123.95	112.24
2	D	301	NAP	C3B-C2B-C1B	-2.36	98.45	102.89
2	D	301	NAP	O2N-PN-O5D	2.32	118.54	107.75
2	C	301	NAP	N3A-C2A-N1A	-2.26	125.15	128.68
2	C	301	NAP	PN-O3-PA	-2.22	125.21	132.83
2	D	301	NAP	O2B-P2B-O1X	-2.21	100.86	109.39
2	A	301	NAP	C4D-O4D-C1D	2.21	113.24	108.49
2	D	301	NAP	N3A-C2A-N1A	-2.17	125.28	128.68
2	B	301	NAP	C1B-N9A-C4A	-2.16	122.85	126.64
2	B	301	NAP	O5D-C5D-C4D	-2.15	101.59	108.99
2	B	301	NAP	N6A-C6A-N1A	2.15	123.03	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	O3X-P2B-O2X	2.12	115.75	107.64
2	B	301	NAP	C4A-C5A-N7A	2.11	111.59	109.40
2	D	301	NAP	C1B-N9A-C4A	-2.09	122.97	126.64
2	D	301	NAP	O2A-PA-O1A	2.08	122.54	112.24
2	B	301	NAP	O2X-P2B-O1X	2.04	118.67	110.68
2	D	301	NAP	O3X-P2B-O2B	-2.02	96.95	105.99

There are no chirality outliers.

All (22) torsion outliers are listed below:

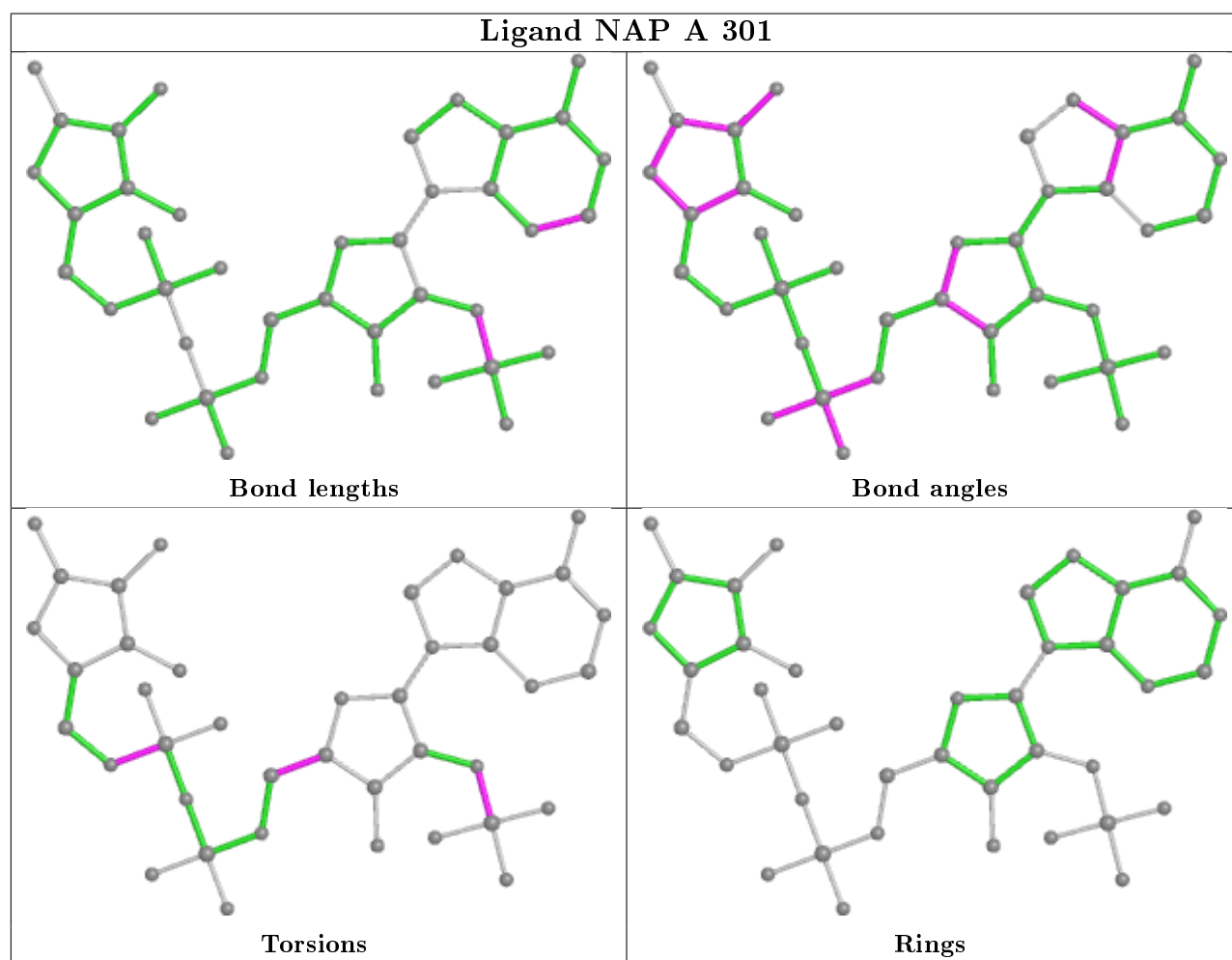
Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5D-O5D-PN-O2N
4	D	302	GOL	O1-C1-C2-C3
2	D	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C2B-O2B-P2B-O3X
2	C	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O2N
4	D	302	GOL	O1-C1-C2-O2
4	C	303	GOL	O1-C1-C2-O2
2	A	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C5D-O5D-PN-O1N
2	D	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O2N
2	A	301	NAP	C2B-O2B-P2B-O2X
2	D	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	O4B-C4B-C5B-O5B

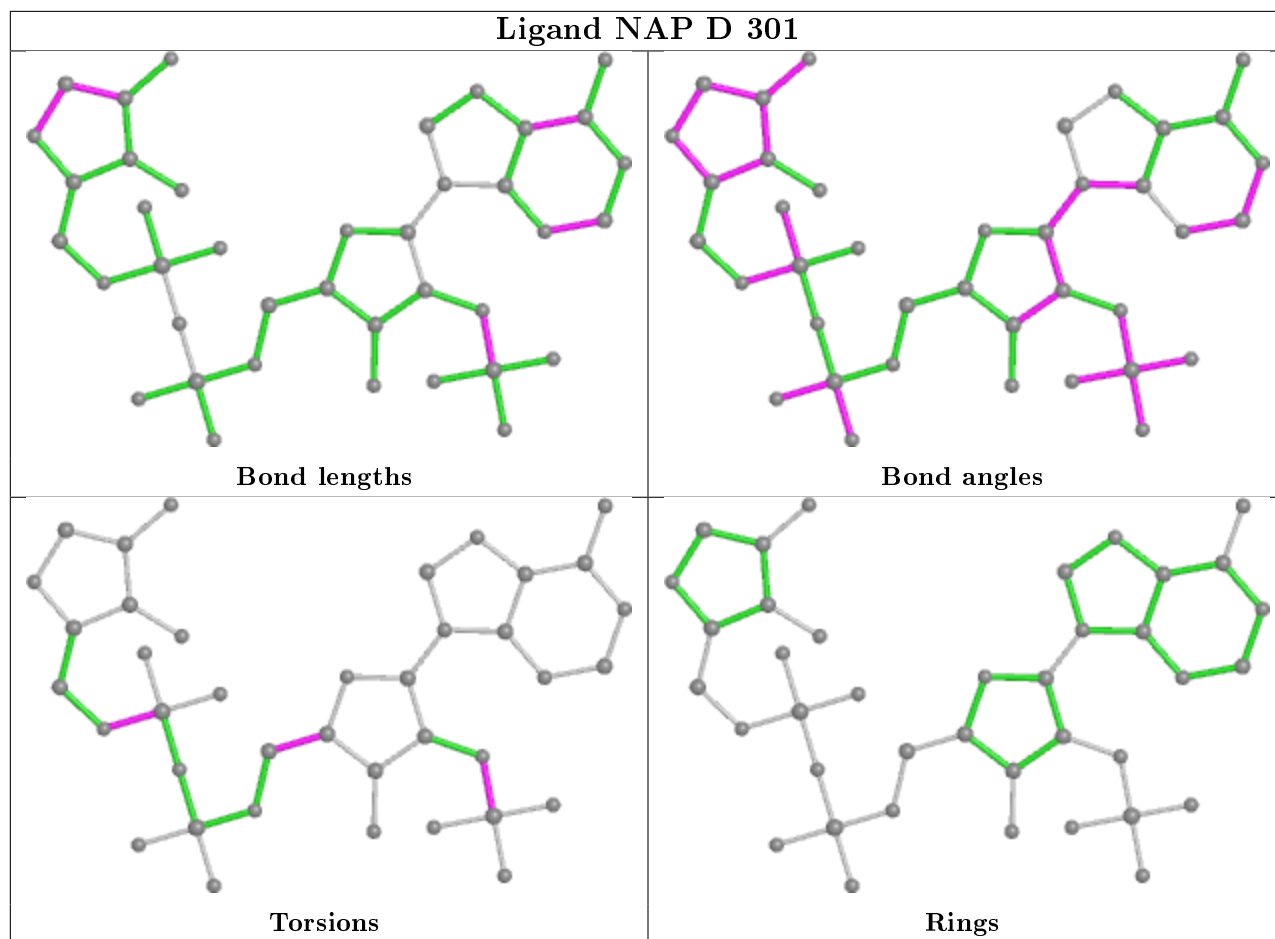
There are no ring outliers.

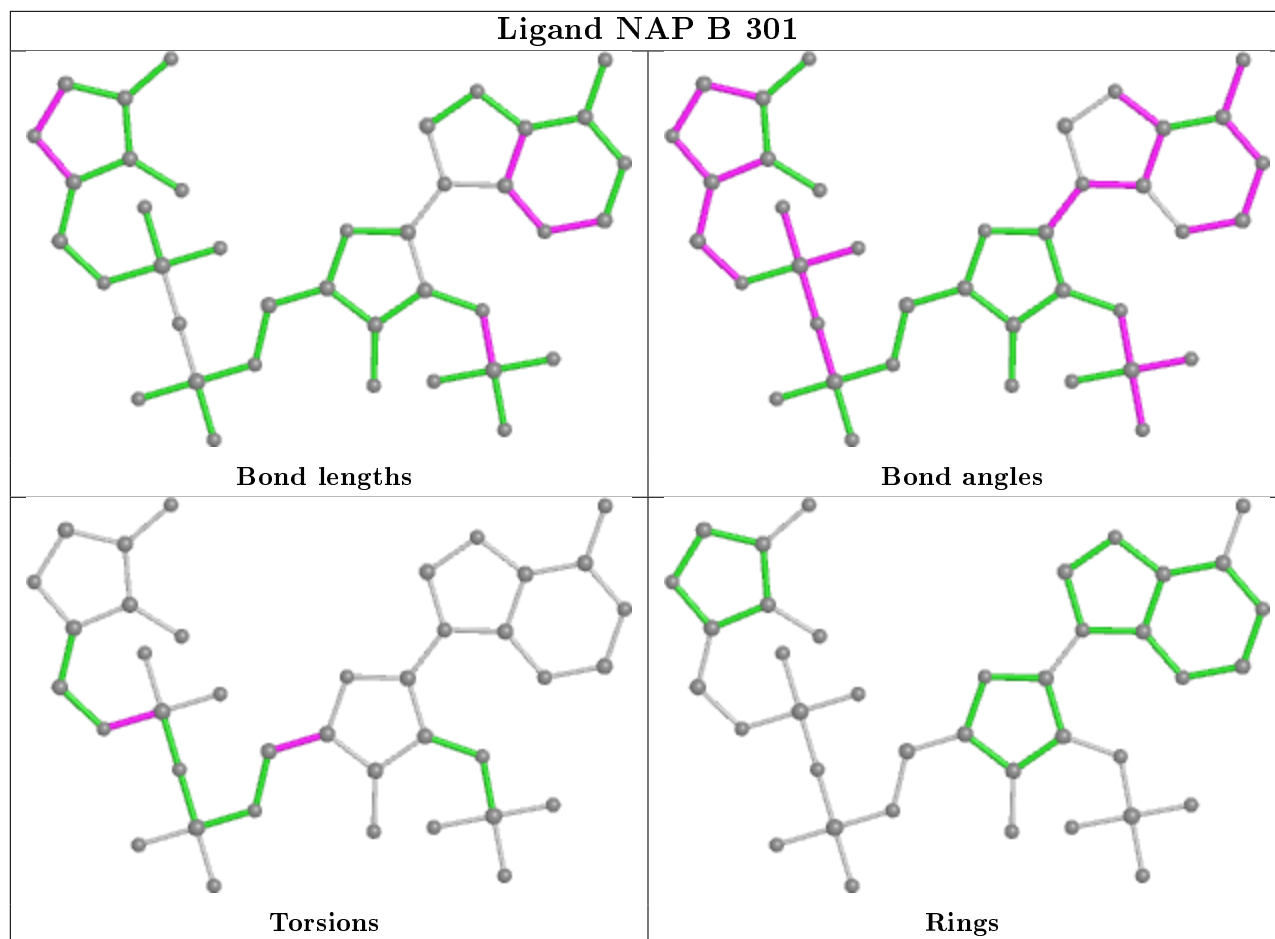
3 monomers are involved in 8 short contacts:

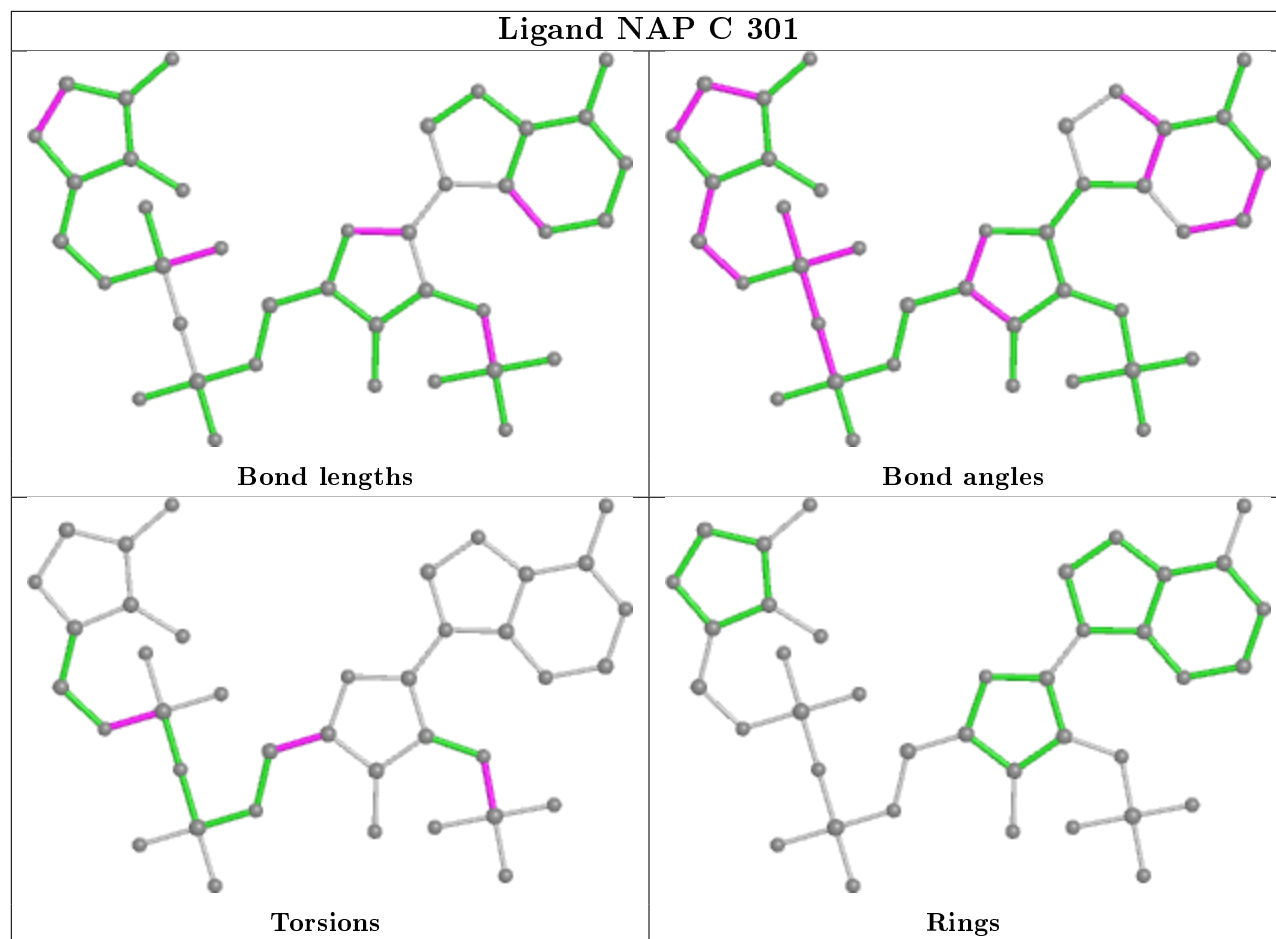
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	GOL	2	0
4	C	303	GOL	3	0
3	C	302	IPA	3	0

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	240/246 (97%)	0.36	10 (4%) 36 33	9, 13, 32, 53	0
1	B	240/246 (97%)	0.38	13 (5%) 25 23	10, 16, 35, 52	0
1	C	240/246 (97%)	0.50	17 (7%) 16 14	9, 15, 42, 83	0
1	D	240/246 (97%)	0.41	11 (4%) 32 29	10, 16, 38, 54	0
All	All	960/984 (97%)	0.41	51 (5%) 26 24	9, 15, 36, 83	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	GLY	7.8
1	C	197	SER	7.8
1	C	202	ILE	6.8
1	D	7	PRO	5.3
1	D	206	MET	5.1
1	C	199	ALA	5.1
1	A	206	MET	5.0
1	C	200	GLU	4.9
1	B	206	MET	4.6
1	B	208	ASP	4.6
1	C	206	MET	4.6
1	C	205	SER	4.5
1	C	207	PHE	4.4
1	B	202	ILE	4.4
1	A	208	ASP	4.3
1	D	138	GLN	4.1
1	C	198	MET	4.1
1	A	7	PRO	4.0
1	B	7	PRO	4.0
1	A	207	PHE	3.9
1	D	134	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	207	PHE	3.7
1	D	208	ASP	3.6
1	A	202	ILE	3.5
1	C	203	ASP	3.5
1	C	204	PRO	3.4
1	D	207	PHE	3.3
1	A	199	ALA	3.2
1	D	202	ILE	3.1
1	B	203	ASP	3.1
1	B	205	SER	3.1
1	D	205	SER	3.1
1	B	134	ASP	3.0
1	D	99	PHE	2.9
1	C	43	GLU	2.9
1	B	57	GLN	2.9
1	C	208	ASP	2.8
1	B	201	GLY	2.6
1	B	136	PRO	2.5
1	A	201	GLY	2.4
1	A	58	GLY	2.4
1	D	201	GLY	2.3
1	B	199	ALA	2.3
1	B	212	ASN	2.3
1	C	246	ALA	2.3
1	C	212	ASN	2.1
1	A	205	SER	2.1
1	C	194[A]	THR	2.1
1	D	203	ASP	2.1
1	C	7	PRO	2.0
1	A	57	GLN	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](#)

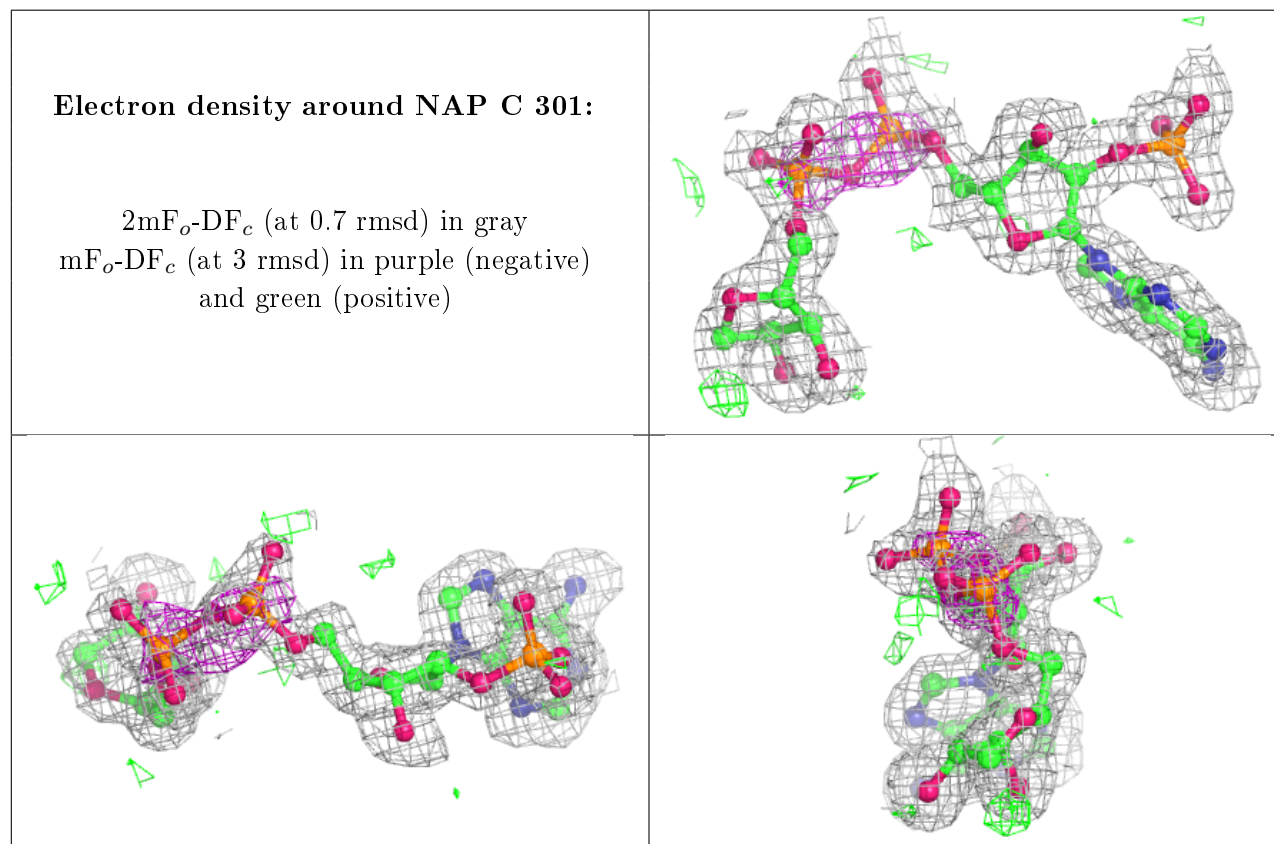
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IPA	C	302	4/4	0.73	0.13	27,29,29,36	0
4	GOL	D	302	6/6	0.81	0.18	27,37,46,51	0
2	NAP	C	301	39/48	0.87	0.16	17,24,41,44	0
4	GOL	C	303	6/6	0.90	0.18	26,27,34,48	0
2	NAP	B	301	39/48	0.94	0.11	16,18,23,25	0
3	IPA	A	302	4/4	0.95	0.14	29,29,31,38	0
2	NAP	A	301	40/48	0.95	0.09	10,15,20,34	0
2	NAP	D	301	39/48	0.95	0.09	14,19,25,27	0

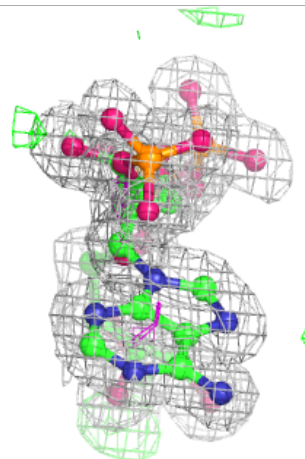
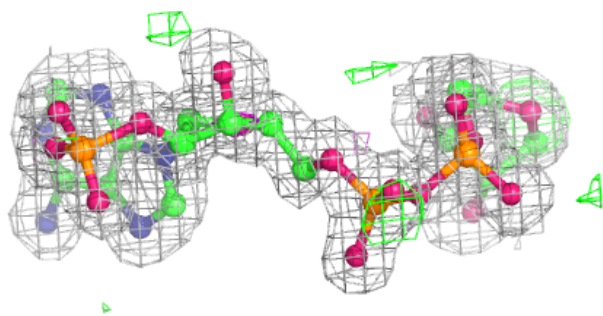
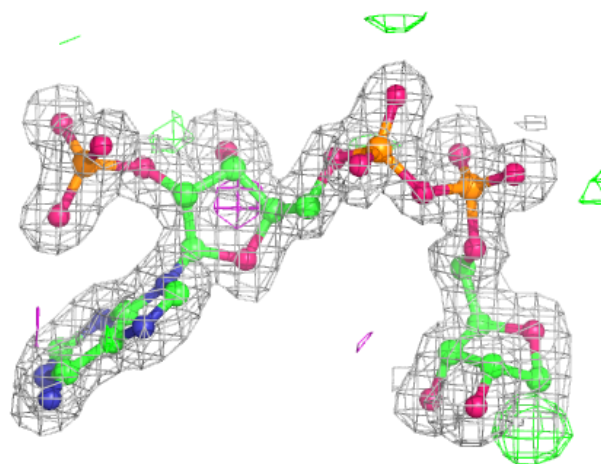
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





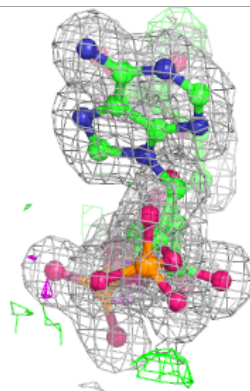
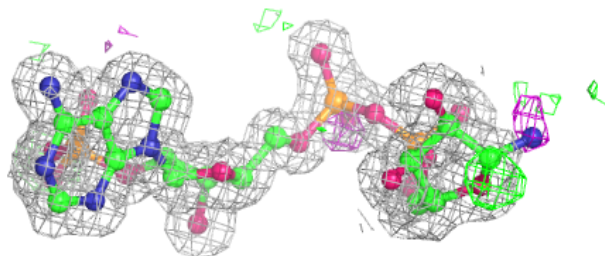
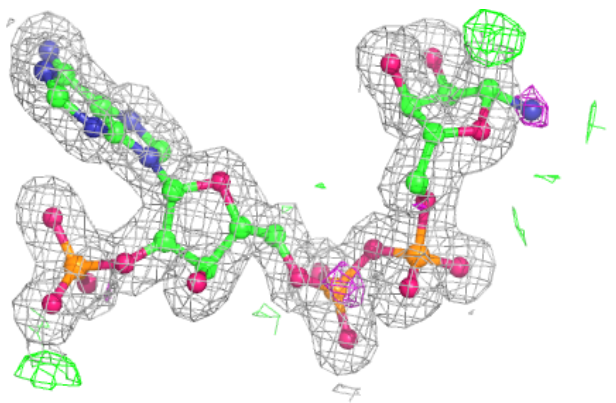
**Electron density around NAP B 301:**

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

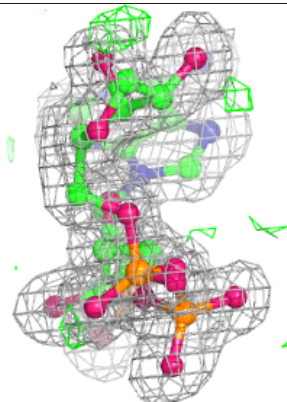
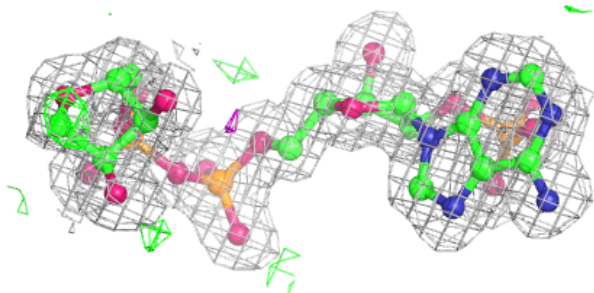
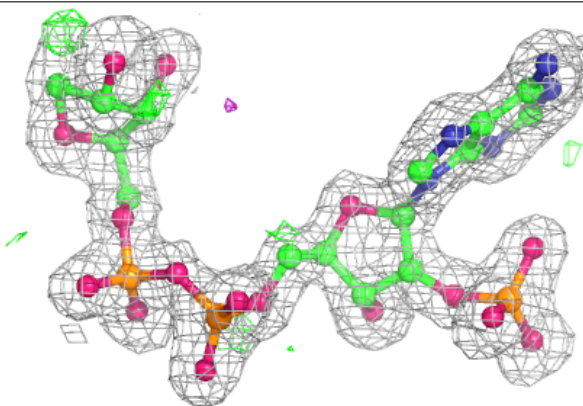


**Electron density around NAP A 301:**

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

**Electron density around NAP D 301:**

$2mF_o-DF_c$  (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.