



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 02:19 am GMT

PDB ID : 5OCM  
Title : Imine Reductase from *Streptosporangium roseum* in complex with NADP+ and 2,2,2-trifluoroacetophenone hydrate  
Authors : Sharma, M.; Nestl, B.; Grogan, G.  
Deposited on : 2017-07-03  
Resolution : 1.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

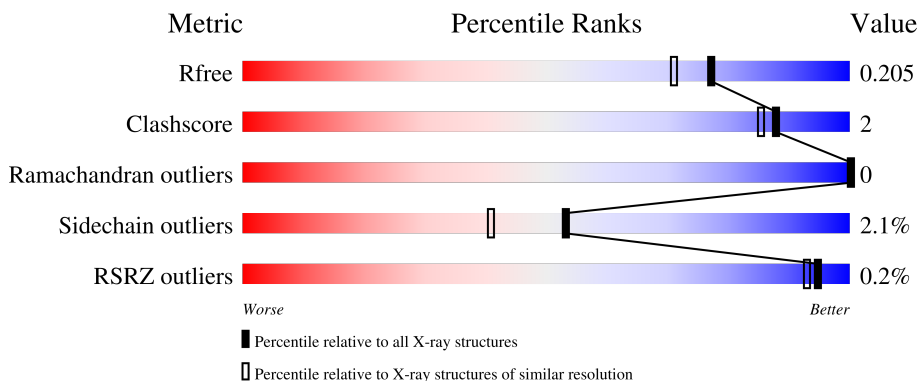
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	291	93% 6% .
1	B	291	91% 7% .
1	C	291	93% 6% .
1	D	291	92% 7%
1	E	291	92% 5% . .

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Mol	Chain	Length	Quality of chain
1	F	291	 92% 5% ..

## 2 Entry composition [i](#)

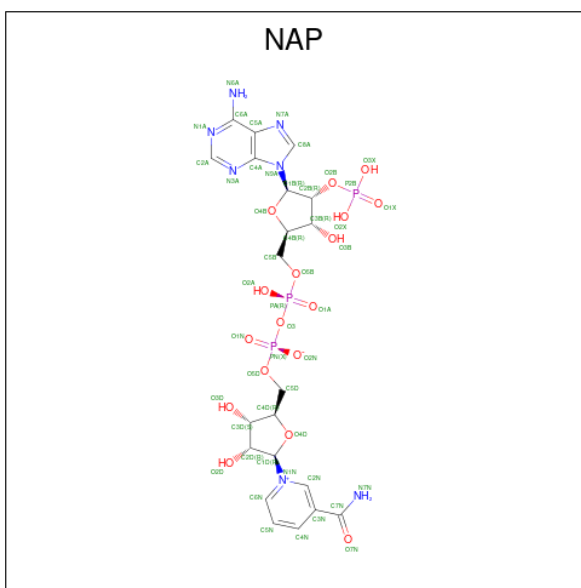
There are 5 unique types of molecules in this entry. The entry contains 13961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD\_Gly3P\_dh, NAD-dependent glycerol-3-phosphate dehydrogenase.

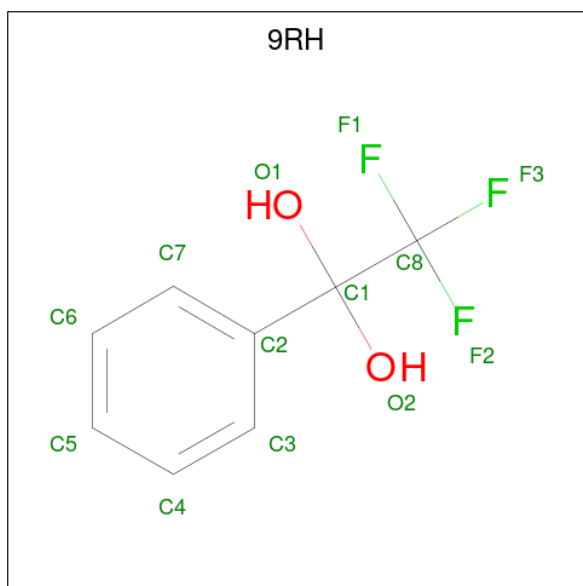
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	1	0
			2089	1316	360	408	5			
1	B	290	Total	C	N	O	S	0	1	0
			2074	1312	352	405	5			
1	C	288	Total	C	N	O	S	0	0	0
			2084	1314	359	406	5			
1	D	290	Total	C	N	O	S	0	0	0
			2083	1315	358	404	6			
1	E	286	Total	C	N	O	S	0	0	0
			2062	1301	351	405	5			
1	F	288	Total	C	N	O	S	0	0	0
			2057	1303	350	399	5			

- 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
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		
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		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2,2,2-trifluoromethyl acetophenone hydrate (three-letter code: 9RH) (formula:  $C_8H_7F_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			13	8	3	2		
3	B	1	Total	C	F	O	0	0
			13	8	3	2		
3	C	1	Total	C	F	O	0	0
			13	8	3	2		
3	D	1	Total	C	F	O	0	0
			13	8	3	2		
3	E	1	Total	C	F	O	0	0
			13	8	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	F	O	0	0
			13	8	3	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	3	Total	Mg	0	0
			3	3		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	188	Total	O	0	0
			188	188		
5	B	174	Total	O	0	0
			174	174		
5	C	201	Total	O	0	0
			201	201		
5	D	192	Total	O	0	0
			192	192		
5	E	213	Total	O	0	0
			213	213		
5	F	171	Total	O	0	0
			171	171		

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

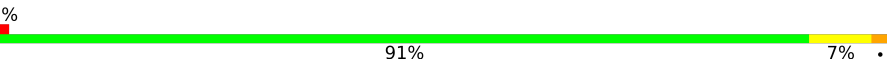
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NAD\_Gly3P\_dh, NAD-dependent glycerol-3-phosphate dehydrogenase

Chain A: 



- Molecule 1: NAD\_Gly3P\_dh, NAD-dependent glycerol-3-phosphate dehydrogenase

Chain B: 



- Molecule 1: NAD\_Gly3P\_dh, NAD-dependent glycerol-3-phosphate dehydrogenase

Chain C: 



- Molecule 1: NAD\_Gly3P\_dh, NAD-dependent glycerol-3-phosphate dehydrogenase

Chain D: 



- Molecule 1: NAD\_Gly3P\_dh, NAD-dependent glycerol-3-phosphate dehydrogenase

Chain E: 



- Molecule 1: NAD\_Gly3P\_dh, NAD-dependent glycerol-3-phosphate dehydrogenase

Chain F:  92% 5% \*\*





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.81Å 152.43Å 251.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.80 – 1.81 48.51 – 1.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (125.80-1.81) 100.0 (48.51-1.81)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.168 , 0.196 0.179 , 0.205	Depositor DCC
$R_{free}$ test set	8059 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtrriage
Anisotropy	0.449	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: MG, 9RH, NAP

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	0.89	2/2131 (0.1%)	0.89	6/2913 (0.2%)
1	B	0.93	3/2116 (0.1%)	0.93	11/2894 (0.4%)
1	C	0.86	1/2123 (0.0%)	0.92	11/2900 (0.4%)
1	D	0.94	2/2122 (0.1%)	0.93	6/2900 (0.2%)
1	E	0.87	1/2100 (0.0%)	0.91	10/2870 (0.3%)
1	F	0.91	3/2096 (0.1%)	0.92	9/2866 (0.3%)
All	All	0.90	12/12688 (0.1%)	0.92	53/17343 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	SER	CB-OG	-11.38	1.27	1.42
1	A	16	GLN	CG-CD	-6.97	1.35	1.51
1	D	248	GLU	CD-OE1	-6.85	1.18	1.25
1	F	248	GLU	CD-OE1	-6.84	1.18	1.25
1	F	51	SER	CB-OG	-6.64	1.33	1.42
1	B	248	GLU	CD-OE2	-5.86	1.19	1.25
1	A	98	GLU	CD-OE2	-5.75	1.19	1.25
1	C	124	GLN	CD-NE2	5.73	1.47	1.32
1	B	124	GLN	CD-NE2	5.43	1.46	1.32
1	D	248	GLU	CD-OE2	-5.09	1.20	1.25
1	F	248	GLU	CD-OE2	-5.08	1.20	1.25
1	E	257	GLU	CD-OE2	-5.00	1.20	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	ARG	NE-CZ-NH2	9.59	125.10	120.30
1	D	87	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	D	3	ASP	CB-CG-OD2	-9.07	110.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	162	ASP	CB-CG-OD1	8.45	125.91	118.30
1	C	260	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	E	260	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	D	162	ASP	CB-CG-OD1	8.14	125.63	118.30
1	C	287	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	C	260	ARG	CG-CD-NE	-7.87	95.27	111.80
1	B	162	ASP	CB-CG-OD1	7.44	125.00	118.30
1	B	87	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	132	PHE	N-CA-CB	7.06	123.30	110.60
1	F	260	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	E	54	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	C	268	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	E	287	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	82	ASP	CB-CG-OD1	6.78	124.40	118.30
1	B	287	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	132	PHE	N-CA-CB	-6.58	98.77	110.60
1	B	132	PHE	N-CA-CB	-6.55	98.81	110.60
1	D	287	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	E	287	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	132	PHE	N-CA-CB	-6.25	99.35	110.60
1	E	260	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	260	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	132	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	A	132	PHE	N-CA-CB	-6.08	99.66	110.60
1	A	78	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	D	2	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	78	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	88	VAL	CG1-CB-CG2	5.90	120.34	110.90
1	E	132	PHE	N-CA-CB	-5.85	100.07	110.60
1	A	287	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	265	LEU	CA-CB-CG	5.76	128.54	115.30
1	F	87	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	287	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	260	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	78	ASP	CB-CG-OD1	5.64	123.37	118.30
1	F	88	VAL	CG1-CB-CG2	5.63	119.91	110.90
1	C	87	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	265	LEU	CB-CG-CD1	5.60	120.52	111.00
1	B	87	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	78	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	162	ASP	CB-CG-OD1	5.50	123.25	118.30
1	F	268	ARG	NE-CZ-NH1	5.43	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	E	162	ASP	CB-CG-OD1	5.09	122.88	118.30
1	E	268	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	F	78	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	87	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	C	162	ASP	CB-CG-OD1	5.04	122.84	118.30
1	F	3	ASP	CB-CG-OD1	5.03	122.83	118.30
1	F	268	ARG	CB-CG-CD	5.02	124.64	111.60

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	2089	0	2036	12	0
1	B	2074	0	2011	9	0
1	C	2084	0	2034	7	0
1	D	2083	0	2029	13	0
1	E	2062	0	2003	7	0
1	F	2057	0	2004	10	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
3	A	13	0	0	0	0
3	B	13	0	0	0	0
3	C	13	0	0	0	0
3	D	13	0	0	0	0
3	E	13	0	0	0	0
3	F	13	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	188	0	0	5	0
5	B	174	0	0	4	0
5	C	201	0	0	4	1
5	D	192	0	0	3	0
5	E	213	0	0	3	0
5	F	171	0	0	3	0
All	All	13961	0	12267	51	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 2.

All (51) 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:C:2:ARG:CZ	5:C:536:HOH:O	2.25	0.84
1:D:58:GLU:HG3	1:D:83:VAL:HG21	1.62	0.81
1:A:191:LEU:HD23	1:F:168:LEU:HD13	1.69	0.73
1:A:12:GLY:O	1:A:16:GLN:HG3	1.98	0.63
1:A:239:VAL:HG11	1:A:263:ARG:NH1	2.15	0.62
1:C:186:HIS:HD2	5:C:581:HOH:O	1.84	0.60
1:B:70:HIS:HE1	5:B:557:HOH:O	1.86	0.59
1:D:101:ARG:HD3	5:D:401:HOH:O	2.02	0.58
1:B:244:HIS:HD2	5:B:497:HOH:O	1.86	0.58
1:E:250:GLU:OE2	1:E:260:ARG:NH2	2.33	0.56
1:D:186:HIS:HD2	5:D:570:HOH:O	1.89	0.55
1:D:58:GLU:CG	1:D:83:VAL:HG21	2.34	0.55
1:E:244:HIS:HD2	5:E:586:HOH:O	1.90	0.55
1:C:244:HIS:HD2	5:C:506:HOH:O	1.90	0.54
1:D:58:GLU:CG	1:D:83:VAL:CG2	2.86	0.54
1:A:70:HIS:HD2	5:A:503:HOH:O	1.91	0.53
1:A:113:THR:HG23	5:A:406:HOH:O	2.10	0.51
1:E:186:HIS:HD2	5:E:593:HOH:O	1.94	0.50
1:F:186:HIS:HD2	5:F:553:HOH:O	1.95	0.50
1:B:186:HIS:HD2	5:B:561:HOH:O	1.94	0.50
1:D:244:HIS:HD2	5:D:490:HOH:O	1.94	0.49
1:F:244:HIS:HD2	5:F:478:HOH:O	1.96	0.49
5:A:499:HOH:O	1:F:244:HIS:HE1	1.96	0.48
1:D:58:GLU:HG2	1:D:83:VAL:HG23	1.96	0.48
1:D:58:GLU:HG2	1:D:83:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLU:OE2	1:D:260:ARG:NH2	2.39	0.47
1:C:54:ARG:HG3	1:C:83:VAL:HG21	1.96	0.47
1:B:244:HIS:HE1	5:C:518:HOH:O	1.99	0.46
1:D:65:VAL:HG21	1:D:77:LEU:HD21	1.98	0.45
1:B:257:GLU:OE1	1:C:268:ARG:NH2	2.49	0.45
1:E:54:ARG:NH1	1:E:58:GLU:OE1	2.50	0.44
1:A:257:GLU:OE1	1:F:268:ARG:NH2	2.50	0.44
1:C:70:HIS:CD2	1:C:74:ARG:HH11	2.36	0.44
1:A:186:HIS:HD2	5:A:575:HOH:O	2.00	0.43
1:B:88:VAL:HG11	1:B:145:HIS:CD2	2.54	0.43
1:D:183:SER:OG	1:E:176:ILE:HA	2.18	0.42
1:D:244:HIS:HE1	5:E:537:HOH:O	2.02	0.42
1:E:54:ARG:CZ	1:E:58:GLU:OE1	2.67	0.42
1:F:88:VAL:HG11	1:F:145:HIS:NE2	2.34	0.42
1:B:70:HIS:HD2	5:B:443:HOH:O	2.02	0.42
1:F:257:GLU:HG2	1:F:260:ARG:NH2	2.34	0.42
1:A:239:VAL:CG1	1:A:263:ARG:NH1	2.81	0.42
1:F:132:PHE:HB2	1:F:155:GLY:O	2.20	0.42
1:A:244:HIS:HD2	5:A:542:HOH:O	2.01	0.42
1:B:206:ASN:HD21	1:C:216:VAL:HB	1.85	0.41
1:A:176:ILE:HA	1:F:183:SER:OG	2.21	0.41
1:B:58:GLU:O	1:B:87:ARG:NH2	2.54	0.41
1:F:88:VAL:HG11	1:F:145:HIS:CD2	2.56	0.41
1:A:54:ARG:HG3	1:A:83:VAL:HG21	2.03	0.40
1:A:244:HIS:HE1	5:F:490:HOH:O	2.04	0.40
1:D:176:ILE:HA	1:E:183:SER:OG	2.22	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:C:571:HOH:O	5:C:571:HOH:O[3_655]	1.03	1.17

## 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	289/291 (99%)	282 (98%)	7 (2%)	0	100	100
1	B	289/291 (99%)	283 (98%)	6 (2%)	0	100	100
1	C	286/291 (98%)	279 (98%)	7 (2%)	0	100	100
1	D	288/291 (99%)	282 (98%)	6 (2%)	0	100	100
1	E	284/291 (98%)	278 (98%)	6 (2%)	0	100	100
1	F	286/291 (98%)	281 (98%)	5 (2%)	0	100	100
All	All	1722/1746 (99%)	1685 (98%)	37 (2%)	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	201/207 (97%)	199 (99%)	2 (1%)	76	70
1	B	197/207 (95%)	189 (96%)	8 (4%)	30	15
1	C	201/207 (97%)	199 (99%)	2 (1%)	76	70
1	D	199/207 (96%)	196 (98%)	3 (2%)	65	55
1	E	197/207 (95%)	192 (98%)	5 (2%)	47	33
1	F	195/207 (94%)	190 (97%)	5 (3%)	46	32
All	All	1190/1242 (96%)	1165 (98%)	25 (2%)	53	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	157	THR
1	B	51	SER
1	B	78	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	113	THR
1	B	136	SER
1	B	157	THR
1	B	263	ARG
1	B	265	LEU
1	B	270	LEU
1	C	157	THR
1	C	263	ARG
1	D	1	MET
1	D	157	THR
1	D	263	ARG
1	E	51	SER
1	E	78	ASP
1	E	157	THR
1	E	263	ARG
1	E	265	LEU
1	F	113	THR
1	F	132	PHE
1	F	157	THR
1	F	168	LEU
1	F	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	16	GLN
1	A	70	HIS
1	A	186	HIS
1	A	206	ASN
1	A	225	GLN
1	A	244	HIS
1	B	16	GLN
1	B	70	HIS
1	B	186	HIS
1	B	206	ASN
1	B	225	GLN
1	B	244	HIS
1	B	274	GLN
1	C	16	GLN
1	C	45	GLN
1	C	186	HIS
1	C	206	ASN

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Mol	Chain	Res	Type
1	C	225	GLN
1	C	244	HIS
1	D	186	HIS
1	D	206	ASN
1	D	225	GLN
1	D	244	HIS
1	E	186	HIS
1	E	206	ASN
1	E	225	GLN
1	E	244	HIS
1	E	247	HIS
1	F	186	HIS
1	F	206	ASN
1	F	225	GLN
1	F	244	HIS
1	F	274	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 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	D	301	-	45,52,52	1.40	4 (8%)	56,80,80	1.57	11 (19%)
3	9RH	C	302	-	12,13,13	0.70	0	16,20,20	1.16	2 (12%)
2	NAP	A	301	-	45,52,52	1.13	3 (6%)	56,80,80	1.45	10 (17%)
3	9RH	D	302	-	12,13,13	0.71	0	16,20,20	1.56	2 (12%)
2	NAP	C	301	-	45,52,52	1.44	8 (17%)	56,80,80	1.64	10 (17%)
3	9RH	A	302	-	12,13,13	1.15	1 (8%)	16,20,20	0.70	0
3	9RH	E	302	-	12,13,13	0.81	1 (8%)	16,20,20	1.24	2 (12%)
3	9RH	B	302	-	12,13,13	0.95	1 (8%)	16,20,20	1.86	4 (25%)
2	NAP	E	301	-	45,52,52	1.37	7 (15%)	56,80,80	1.69	13 (23%)
3	9RH	F	302	-	12,13,13	0.38	0	16,20,20	1.15	1 (6%)
2	NAP	B	301	-	45,52,52	1.21	4 (8%)	56,80,80	1.56	5 (8%)
2	NAP	F	301	-	45,52,52	1.32	3 (6%)	56,80,80	1.43	10 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	301	-	-	3/31/67/67	0/5/5/5
3	9RH	C	302	-	-	0/15/15/15	0/1/1/1
2	NAP	A	301	-	-	4/31/67/67	0/5/5/5
3	9RH	D	302	-	-	0/15/15/15	0/1/1/1
2	NAP	C	301	-	-	4/31/67/67	0/5/5/5
3	9RH	A	302	-	-	0/15/15/15	0/1/1/1
3	9RH	E	302	-	-	0/15/15/15	0/1/1/1
3	9RH	B	302	-	-	0/15/15/15	0/1/1/1
2	NAP	E	301	-	-	4/31/67/67	0/5/5/5
3	9RH	F	302	-	-	0/15/15/15	0/1/1/1
2	NAP	B	301	-	-	6/31/67/67	0/5/5/5
2	NAP	F	301	-	-	5/31/67/67	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAP	O4B-C1B	4.20	1.46	1.41
2	D	301	NAP	O4B-C1B	4.05	1.46	1.41
2	D	301	NAP	C2A-N3A	3.89	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	C2N-N1N	3.69	1.39	1.35
2	F	301	NAP	O4D-C1D	3.68	1.46	1.41
2	C	301	NAP	C2A-N3A	3.66	1.38	1.32
2	E	301	NAP	O4B-C1B	3.64	1.46	1.41
2	E	301	NAP	C2N-N1N	3.57	1.39	1.35
3	A	302	9RH	O1-C1	3.56	1.45	1.39
2	F	301	NAP	C2A-N3A	3.28	1.37	1.32
2	A	301	NAP	O4B-C1B	3.19	1.45	1.41
2	B	301	NAP	O4B-C1B	3.16	1.45	1.41
2	B	301	NAP	C2A-N3A	3.09	1.37	1.32
2	C	301	NAP	O4B-C4B	-3.01	1.38	1.45
2	B	301	NAP	O4D-C1D	2.90	1.45	1.41
2	C	301	NAP	C5A-C4A	2.87	1.48	1.40
2	C	301	NAP	O4B-C1B	2.80	1.45	1.41
2	E	301	NAP	C5A-C4A	2.55	1.47	1.40
2	C	301	NAP	P2B-O2B	2.50	1.64	1.59
2	E	301	NAP	O7N-C7N	-2.46	1.19	1.24
2	D	301	NAP	C8A-N7A	-2.41	1.30	1.34
2	B	301	NAP	C5A-N7A	-2.40	1.31	1.39
2	E	301	NAP	C2A-N3A	2.37	1.35	1.32
2	E	301	NAP	P2B-O3X	-2.36	1.45	1.54
3	E	302	9RH	O1-C1	2.33	1.43	1.39
2	C	301	NAP	C4A-N3A	-2.29	1.32	1.35
2	A	301	NAP	C2N-N1N	-2.24	1.32	1.35
2	E	301	NAP	C8A-N7A	2.20	1.38	1.34
3	B	302	9RH	O1-C1	2.18	1.43	1.39
2	C	301	NAP	P2B-O3X	-2.15	1.46	1.54
2	C	301	NAP	C8A-N7A	-2.12	1.30	1.34
2	A	301	NAP	O4D-C4D	2.05	1.49	1.45

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C3N-C7N-N7N	6.26	125.26	117.75
3	B	302	9RH	O1-C1-C8	-5.61	96.39	107.60
2	E	301	NAP	C3N-C7N-N7N	5.40	124.23	117.75
2	B	301	NAP	O7N-C7N-C3N	-5.25	113.34	119.63
3	D	302	9RH	O1-C1-C8	-5.20	97.21	107.60
2	D	301	NAP	N3A-C2A-N1A	-5.07	120.76	128.68
2	C	301	NAP	O7N-C7N-C3N	-4.54	114.20	119.63
2	C	301	NAP	C3N-C7N-N7N	4.32	122.93	117.75
2	E	301	NAP	N3A-C2A-N1A	-4.06	122.33	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	9RH	O1-C1-C8	-3.84	99.92	107.60
2	A	301	NAP	O7N-C7N-C3N	-3.75	115.14	119.63
2	A	301	NAP	N3A-C2A-N1A	-3.62	123.01	128.68
2	C	301	NAP	C1B-N9A-C4A	-3.56	120.39	126.64
2	C	301	NAP	O2B-P2B-O1X	-3.53	95.75	109.39
2	D	301	NAP	C6N-N1N-C2N	-3.50	118.79	121.97
2	D	301	NAP	C2N-C3N-C4N	3.46	122.18	118.26
2	D	301	NAP	C3N-C7N-N7N	3.37	121.79	117.75
2	F	301	NAP	N3A-C2A-N1A	-3.24	123.62	128.68
3	F	302	9RH	O1-C1-C8	-3.22	101.17	107.60
2	A	301	NAP	C1B-N9A-C4A	-3.21	121.00	126.64
2	C	301	NAP	N3A-C2A-N1A	-3.14	123.76	128.68
3	C	302	9RH	O1-C1-C8	-3.06	101.48	107.60
3	B	302	9RH	C8-C1-C2	2.94	112.19	109.53
2	F	301	NAP	C1B-N9A-C4A	-2.87	121.59	126.64
2	E	301	NAP	C2A-N1A-C6A	2.86	123.64	118.75
2	D	301	NAP	C2A-N1A-C6A	2.85	123.63	118.75
2	D	301	NAP	PN-O3-PA	-2.82	123.13	132.83
2	F	301	NAP	O7N-C7N-C3N	-2.82	116.25	119.63
2	B	301	NAP	N3A-C2A-N1A	-2.79	124.31	128.68
2	C	301	NAP	O3X-P2B-O2X	2.76	118.20	107.64
2	A	301	NAP	O4D-C4D-C3D	2.73	110.51	105.11
2	A	301	NAP	O2N-PN-O1N	2.70	125.57	112.24
2	E	301	NAP	O7N-C7N-C3N	-2.69	116.41	119.63
2	E	301	NAP	PN-O3-PA	-2.66	123.69	132.83
2	E	301	NAP	O2N-PN-O1N	2.65	125.36	112.24
2	B	301	NAP	C1B-N9A-C4A	-2.65	121.98	126.64
2	D	301	NAP	O7N-C7N-C3N	-2.64	116.47	119.63
2	D	301	NAP	O3X-P2B-O1X	2.64	121.00	110.68
2	C	301	NAP	C5A-C6A-N6A	-2.61	116.39	120.35
2	F	301	NAP	N6A-C6A-N1A	2.60	123.98	118.57
2	E	301	NAP	C6N-N1N-C2N	-2.60	119.61	121.97
2	A	301	NAP	PN-O3-PA	-2.54	124.11	132.83
2	C	301	NAP	N6A-C6A-N1A	2.53	123.82	118.57
3	C	302	9RH	C8-C1-C2	2.52	111.81	109.53
2	A	301	NAP	C3N-C7N-N7N	2.52	120.78	117.75
2	F	301	NAP	C5A-C6A-N6A	-2.51	116.54	120.35
2	E	301	NAP	C5N-C4N-C3N	-2.46	117.43	120.34
3	B	302	9RH	O1-C1-C2	2.45	114.91	108.75
2	E	301	NAP	O2A-PA-O1A	2.42	124.19	112.24
2	F	301	NAP	C3N-C2N-N1N	2.39	122.76	120.43
2	E	301	NAP	C3B-C2B-C1B	-2.39	98.41	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	NAP	C1B-N9A-C4A	-2.34	122.53	126.64
2	F	301	NAP	C3B-C2B-C1B	-2.34	98.50	102.89
2	E	301	NAP	O7N-C7N-N7N	-2.33	119.27	122.58
2	C	301	NAP	C5N-C4N-C3N	-2.32	117.60	120.34
2	E	301	NAP	O4B-C1B-C2B	-2.28	102.63	106.59
2	A	301	NAP	C5N-C4N-C3N	-2.23	117.70	120.34
2	C	301	NAP	C3B-C2B-C1B	-2.23	98.70	102.89
2	F	301	NAP	C4A-C5A-N7A	-2.21	107.09	109.40
2	D	301	NAP	O4B-C1B-C2B	-2.20	102.77	106.59
3	D	302	9RH	O1-C1-C2	2.19	114.27	108.75
2	B	301	NAP	C2N-N1N-C1D	-2.18	114.28	119.14
2	F	301	NAP	O2D-C2D-C1D	2.12	118.69	110.85
2	F	301	NAP	C5N-C6N-N1N	-2.10	117.39	120.40
2	A	301	NAP	O3X-P2B-O1X	2.09	118.85	110.68
3	B	302	9RH	O2-C1-C2	2.08	113.99	108.75
3	E	302	9RH	C8-C1-C2	2.08	111.41	109.53
2	D	301	NAP	C4N-C3N-C7N	-2.07	115.49	121.04
2	A	301	NAP	C2A-N1A-C6A	2.07	122.30	118.75
2	D	301	NAP	C5N-C6N-N1N	2.04	123.32	120.40

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	O4D-C1D-N1N-C6N
2	B	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	C2B-O2B-P2B-O1X
2	C	301	NAP	C2B-O2B-P2B-O3X
2	C	301	NAP	O4D-C1D-N1N-C2N
2	D	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	O4D-C1D-N1N-C6N
2	F	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	C2B-O2B-P2B-O3X
2	B	301	NAP	C2D-C1D-N1N-C6N
2	E	301	NAP	C2D-C1D-N1N-C6N

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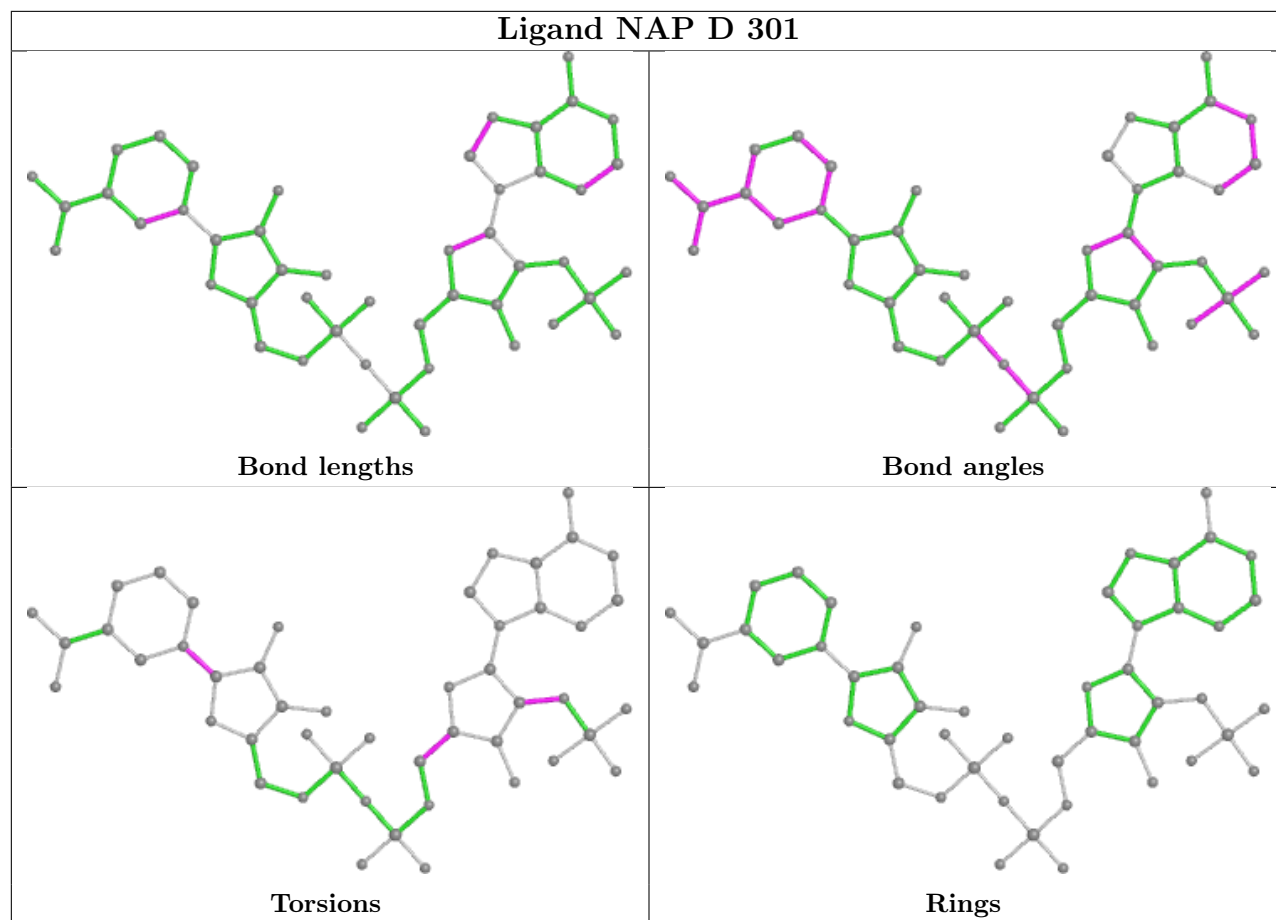
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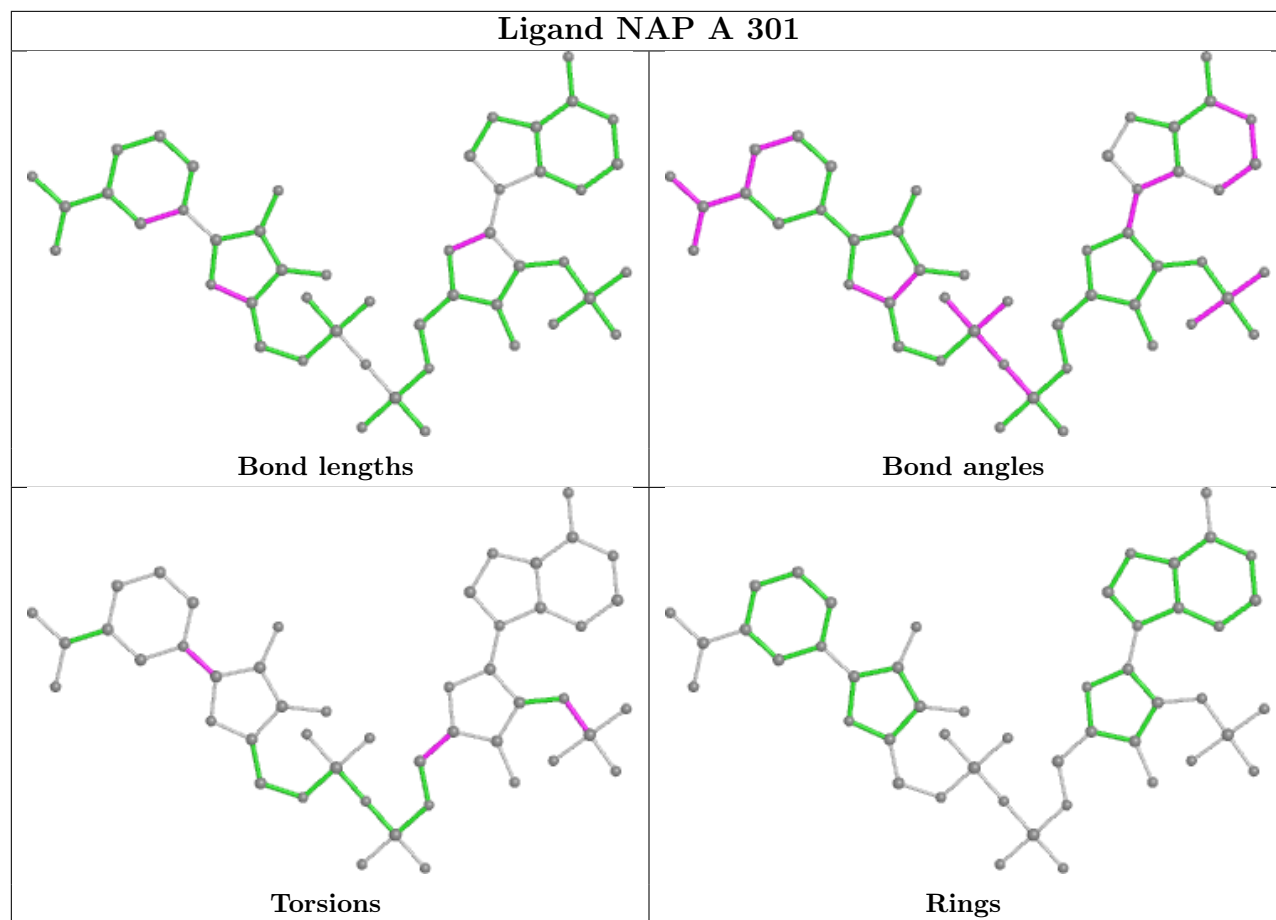
Mol	Chain	Res	Type	Atoms
2	F	301	NAP	C2B-O2B-P2B-O2X
2	F	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	E	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C3B-C2B-O2B-P2B

There are no ring outliers.

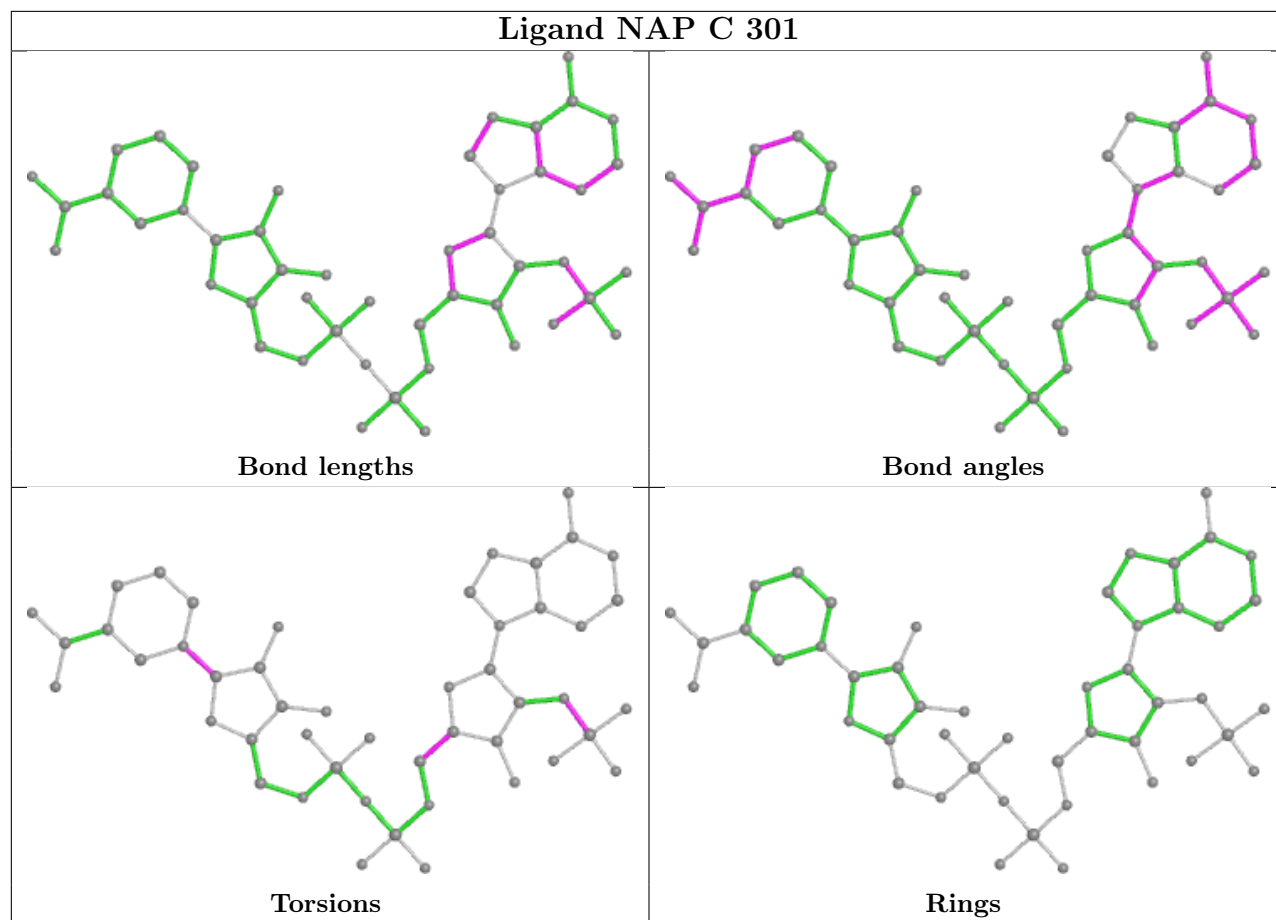
No monomer is involved in short contacts.

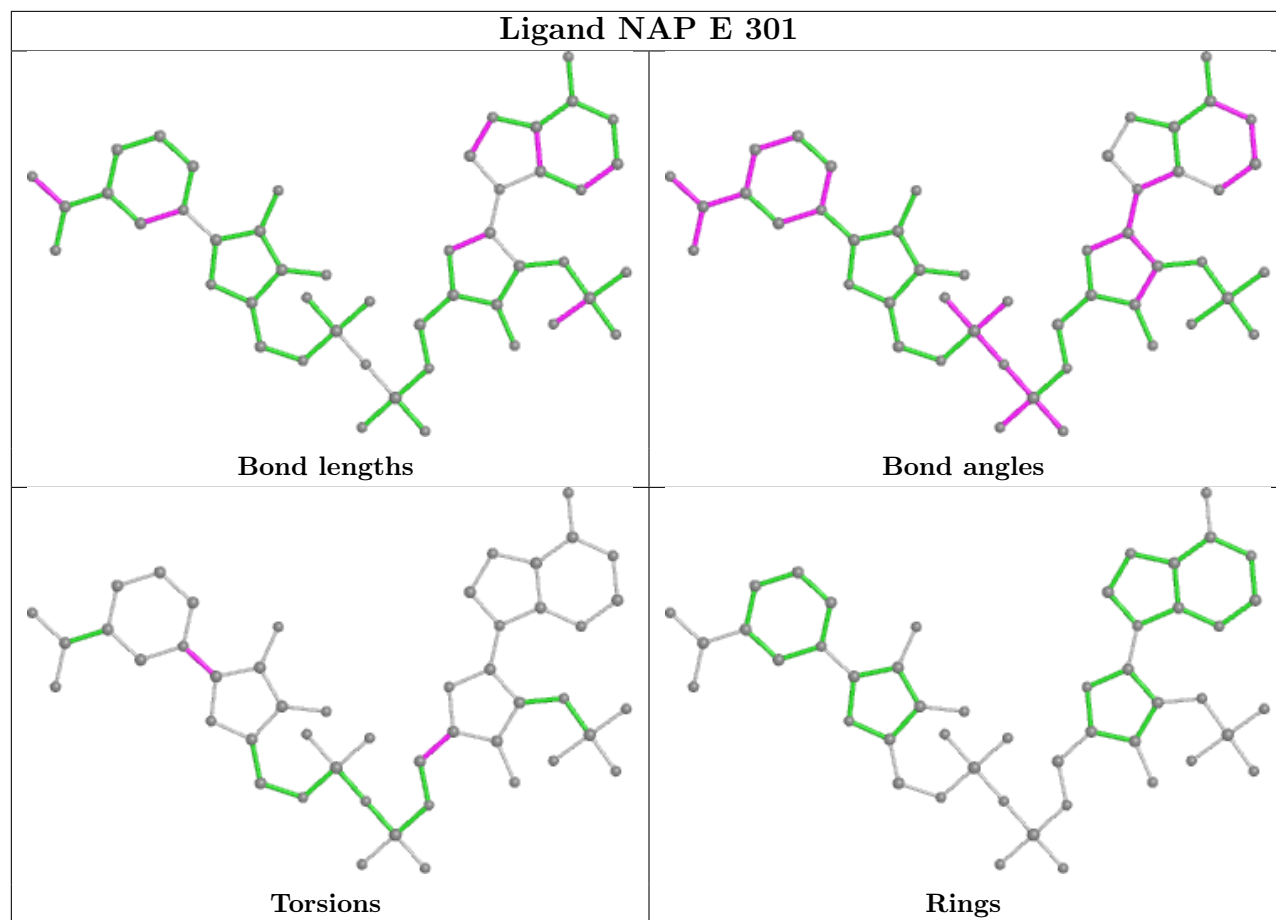
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

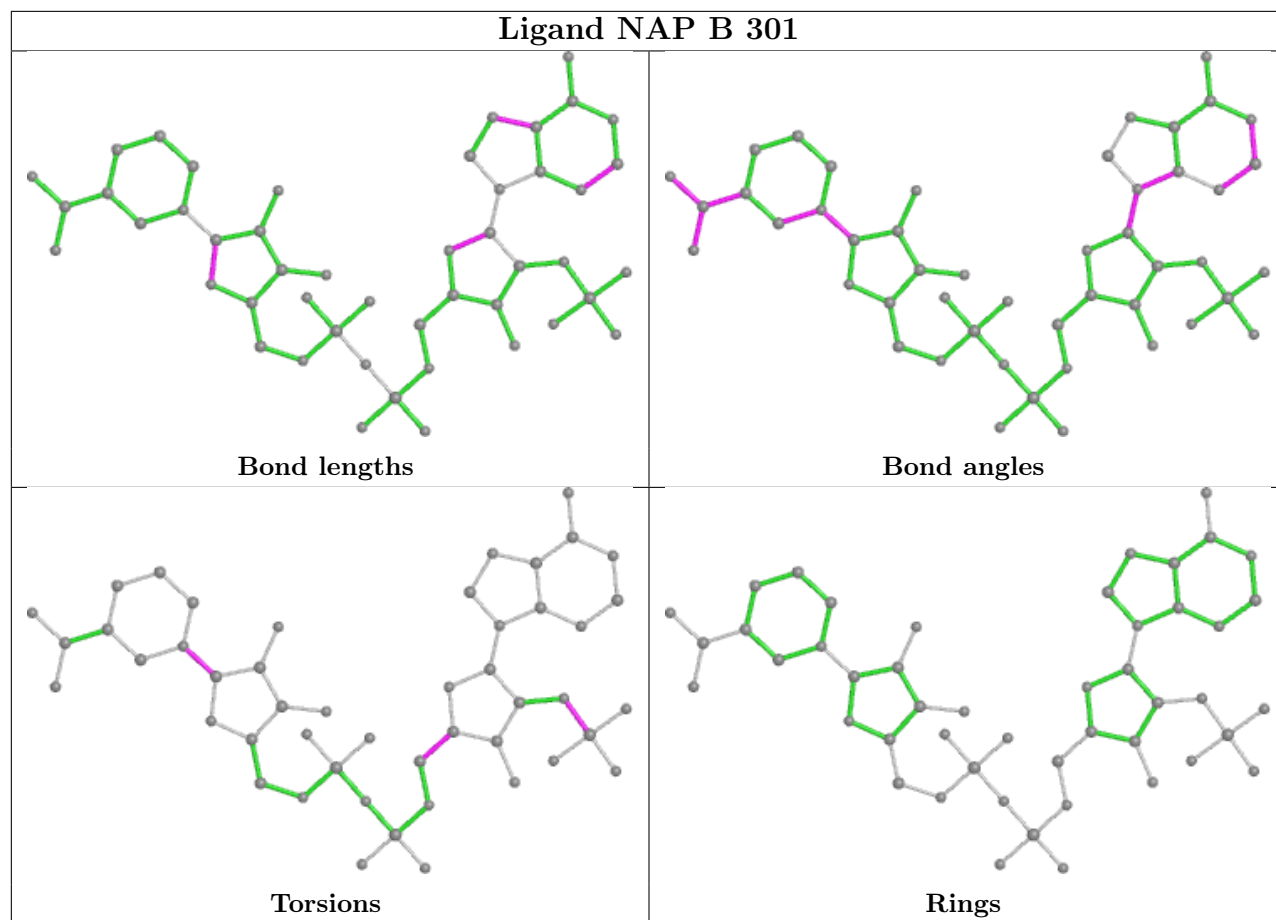


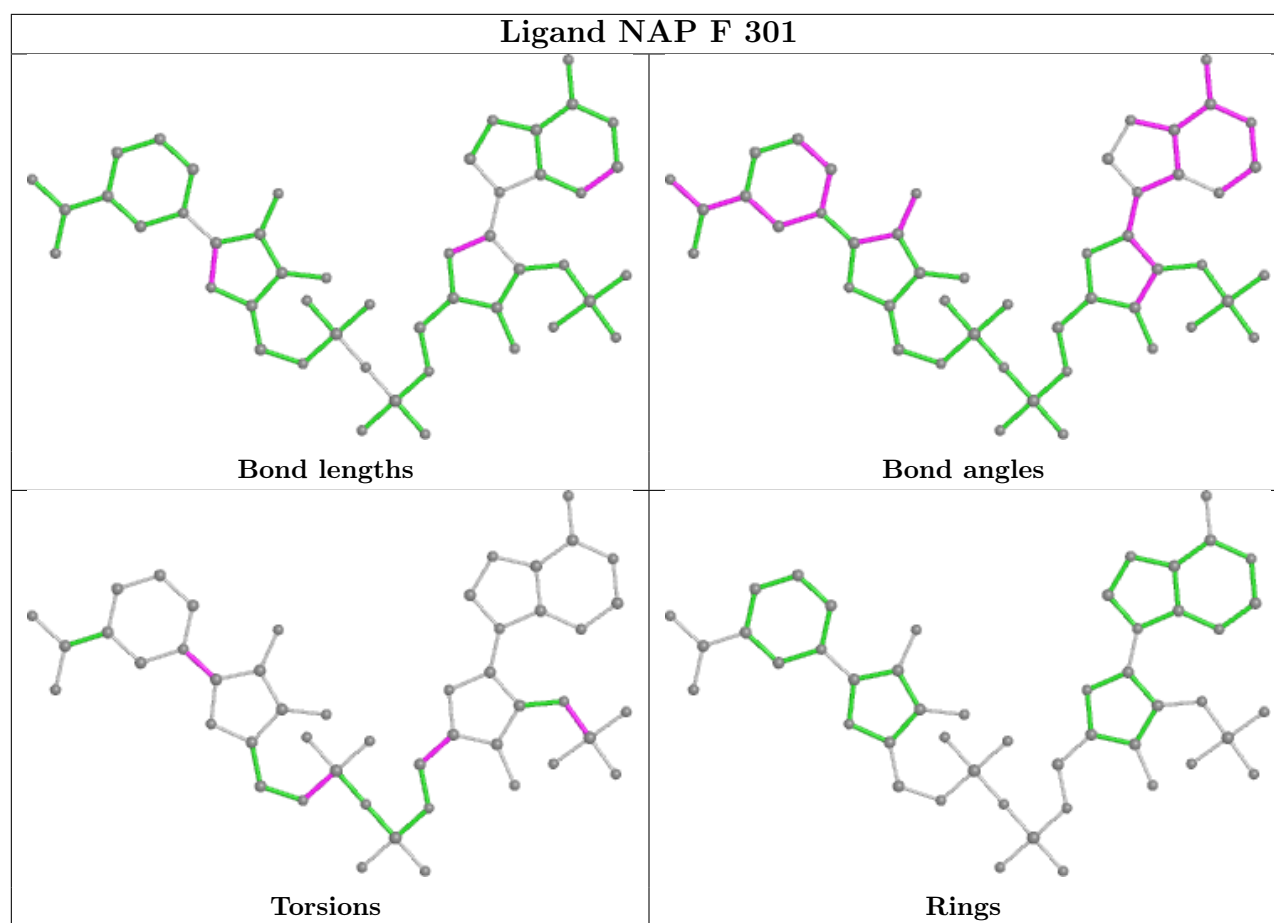












## 5.7 Other polymers [i](#)

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	290/291 (99%)	-0.44	0 <b>100</b>   <b>100</b>	12, 17, 28, 47	0
1	B	290/291 (99%)	-0.27	3 (1%) <b>82</b>   <b>80</b>	12, 20, 32, 52	0
1	C	288/291 (98%)	-0.44	0 <b>100</b>   <b>100</b>	12, 17, 28, 49	0
1	D	290/291 (99%)	-0.34	1 (0%) <b>94</b>   <b>92</b>	11, 19, 35, 51	0
1	E	286/291 (98%)	-0.46	0 <b>100</b>   <b>100</b>	12, 16, 27, 42	0
1	F	288/291 (98%)	-0.34	0 <b>100</b>   <b>100</b>	12, 20, 33, 45	0
All	All	1732/1746 (99%)	-0.38	4 (0%) <b>95</b>   <b>93</b>	11, 18, 31, 52	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.1
1	D	1	MET	2.5
1	B	290	SER	2.3
1	B	51	SER	2.3

### 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.

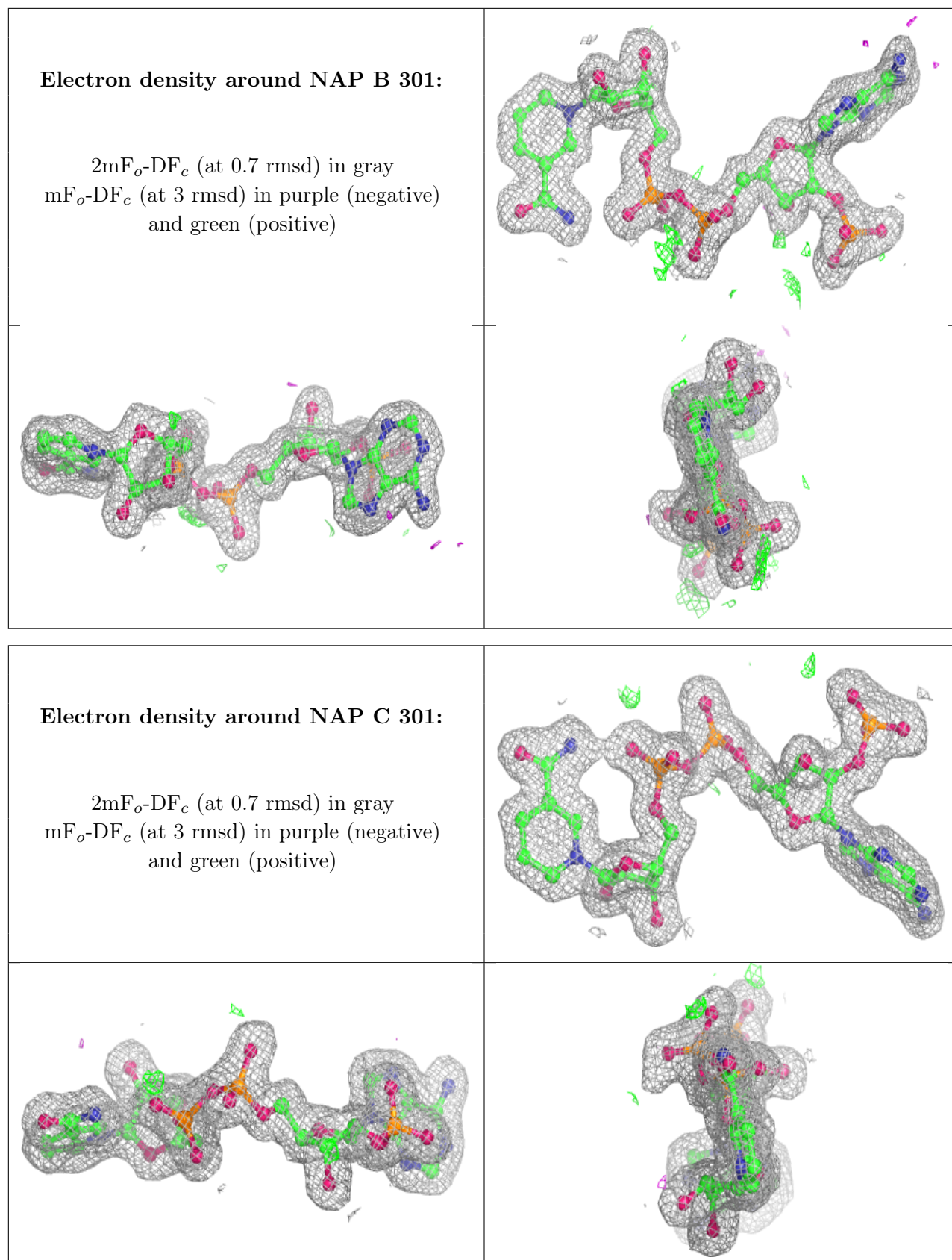
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

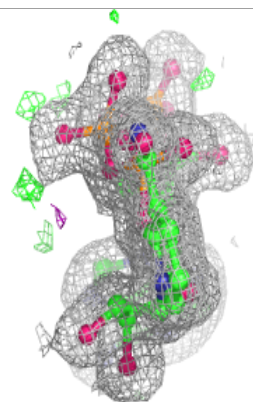
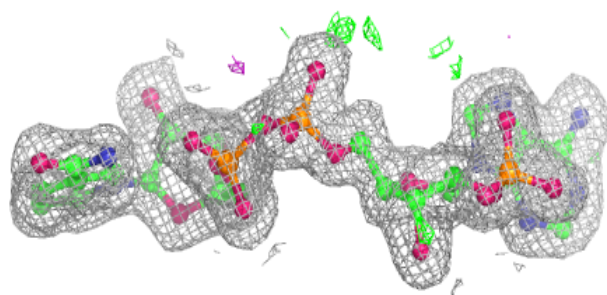
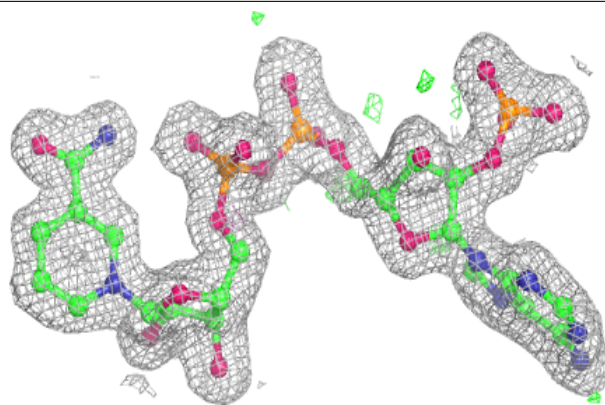
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	D	305	1/1	0.63	0.12	40,40,40,40	0
4	MG	D	304	1/1	0.84	0.36	46,46,46,46	0
4	MG	A	303	1/1	0.87	0.22	39,39,39,39	0
4	MG	C	303	1/1	0.89	0.18	34,34,34,34	0
3	9RH	A	302	13/13	0.93	0.10	19,22,26,26	0
3	9RH	D	302	13/13	0.94	0.10	18,21,25,26	0
3	9RH	F	302	13/13	0.94	0.10	18,20,26,26	0
3	9RH	E	302	13/13	0.95	0.10	18,20,24,28	0
3	9RH	B	302	13/13	0.95	0.10	18,20,24,27	0
4	MG	F	303	1/1	0.95	0.16	43,43,43,43	0
3	9RH	C	302	13/13	0.96	0.08	18,20,22,24	0
4	MG	E	303	1/1	0.97	0.19	32,32,32,32	0
4	MG	D	303	1/1	0.97	0.20	41,41,41,41	0
2	NAP	B	301	48/48	0.98	0.08	13,17,22,23	0
2	NAP	C	301	48/48	0.98	0.07	13,15,18,19	0
2	NAP	D	301	48/48	0.98	0.07	14,15,19,21	0
2	NAP	E	301	48/48	0.98	0.07	12,15,17,18	0
2	NAP	F	301	48/48	0.98	0.07	14,17,21,23	0
2	NAP	A	301	48/48	0.98	0.07	12,15,18,20	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.

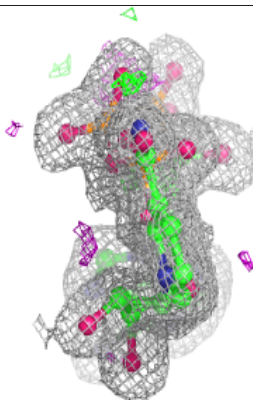
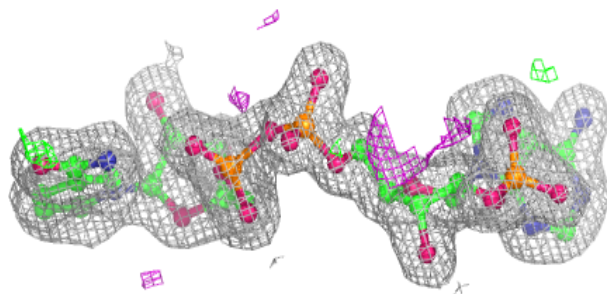
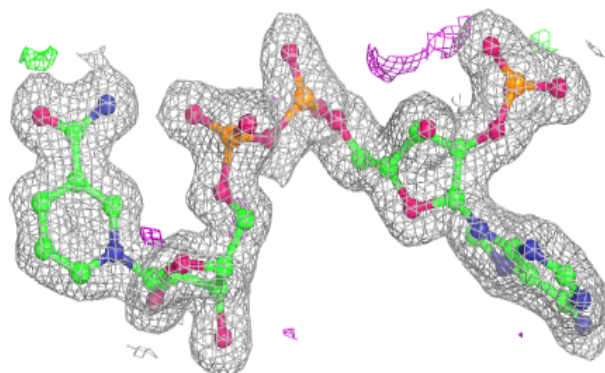


**Electron density around NAP D 301:**

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

**Electron density around NAP E 301:**

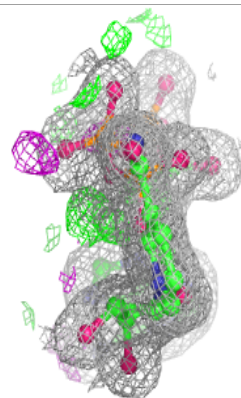
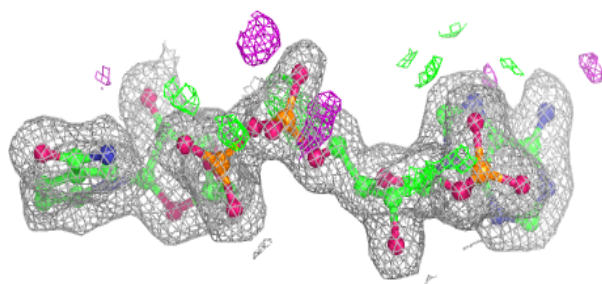
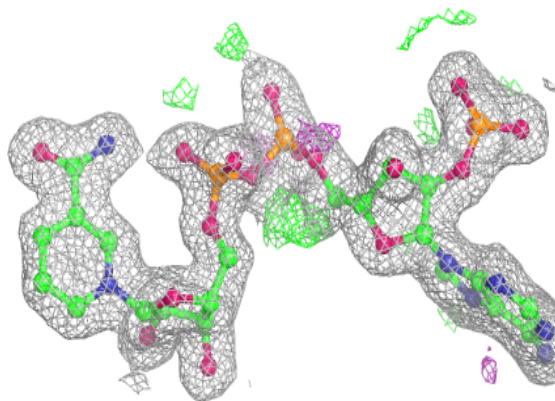
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



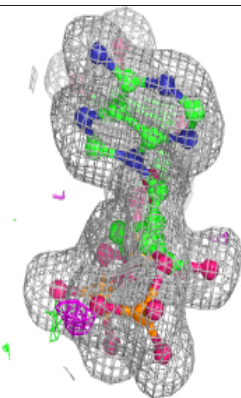
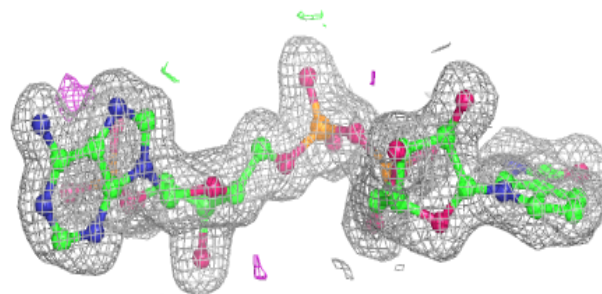
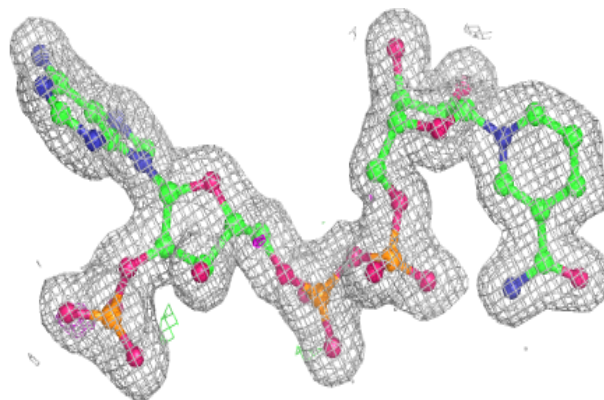


**Electron density around NAP F 301:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.