



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:24 PM BST

PDB ID : 5XV0  
Title : Crystal structure of Rib7 mutant D33N from Methanosarcina mazei  
Authors : Yeh, T.M.; Chen, S.C.; Chang, T.H.; Huang, M.F.; Liaw, S.H.  
Deposited on : 2017-06-26  
Resolution : 1.95 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 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

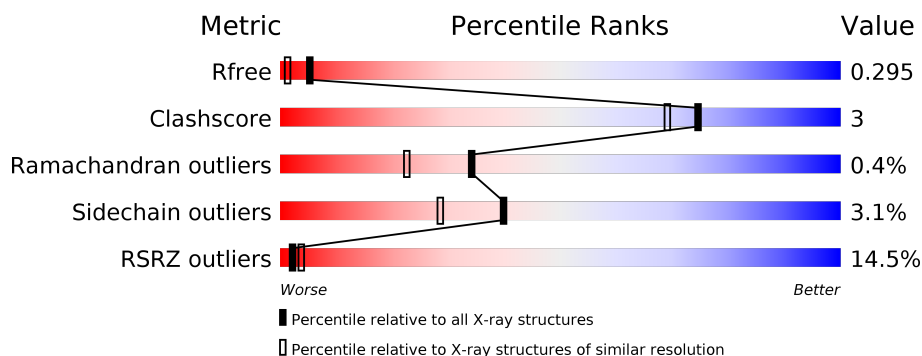
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	240	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	240	<div> <div>86%</div> <div>8%</div> <div>7%</div> </div>
1	C	240	<div> <div>40%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	D	240	<div> <div>39%</div> <div>77%</div> <div>15%</div> <div>7%</div> </div>
1	E	240	<div> <div>87%</div> <div>5%</div> <div>7%</div> </div>
1	F	240	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11390 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 Conserved protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1808	1136	321	343	8			
1	B	224	Total	C	N	O	S	0	0	0
			1698	1072	292	326	8			
1	C	224	Total	C	N	O	S	0	0	0
			1698	1072	292	326	8			
1	D	223	Total	C	N	O	S	0	0	0
			1690	1067	291	325	7			
1	E	223	Total	C	N	O	S	0	0	0
			1690	1067	291	325	7			
1	F	239	Total	C	N	O	S	0	0	0
			1819	1142	325	344	8			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q8PYN5
A	-10	ARG	-	expression tag	UNP Q8PYN5
A	-9	GLY	-	expression tag	UNP Q8PYN5
A	-8	SER	-	expression tag	UNP Q8PYN5
A	-7	HIS	-	expression tag	UNP Q8PYN5
A	-6	HIS	-	expression tag	UNP Q8PYN5
A	-5	HIS	-	expression tag	UNP Q8PYN5
A	-4	HIS	-	expression tag	UNP Q8PYN5
A	-3	HIS	-	expression tag	UNP Q8PYN5
A	-2	HIS	-	expression tag	UNP Q8PYN5
A	-1	GLY	-	expression tag	UNP Q8PYN5
A	0	SER	-	expression tag	UNP Q8PYN5
A	33	ASN	ASP	engineered mutation	UNP Q8PYN5
B	-11	MET	-	expression tag	UNP Q8PYN5
B	-10	ARG	-	expression tag	UNP Q8PYN5
B	-9	GLY	-	expression tag	UNP Q8PYN5
B	-8	SER	-	expression tag	UNP Q8PYN5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q8PYN5
B	-6	HIS	-	expression tag	UNP Q8PYN5
B	-5	HIS	-	expression tag	UNP Q8PYN5
B	-4	HIS	-	expression tag	UNP Q8PYN5
B	-3	HIS	-	expression tag	UNP Q8PYN5
B	-2	HIS	-	expression tag	UNP Q8PYN5
B	-1	GLY	-	expression tag	UNP Q8PYN5
B	0	SER	-	expression tag	UNP Q8PYN5
B	33	ASN	ASP	engineered mutation	UNP Q8PYN5
C	-11	MET	-	expression tag	UNP Q8PYN5
C	-10	ARG	-	expression tag	UNP Q8PYN5
C	-9	GLY	-	expression tag	UNP Q8PYN5
C	-8	SER	-	expression tag	UNP Q8PYN5
C	-7	HIS	-	expression tag	UNP Q8PYN5
C	-6	HIS	-	expression tag	UNP Q8PYN5
C	-5	HIS	-	expression tag	UNP Q8PYN5
C	-4	HIS	-	expression tag	UNP Q8PYN5
C	-3	HIS	-	expression tag	UNP Q8PYN5
C	-2	HIS	-	expression tag	UNP Q8PYN5
C	-1	GLY	-	expression tag	UNP Q8PYN5
C	0	SER	-	expression tag	UNP Q8PYN5
C	33	ASN	ASP	engineered mutation	UNP Q8PYN5
D	-11	MET	-	expression tag	UNP Q8PYN5
D	-10	ARG	-	expression tag	UNP Q8PYN5
D	-9	GLY	-	expression tag	UNP Q8PYN5
D	-8	SER	-	expression tag	UNP Q8PYN5
D	-7	HIS	-	expression tag	UNP Q8PYN5
D	-6	HIS	-	expression tag	UNP Q8PYN5
D	-5	HIS	-	expression tag	UNP Q8PYN5
D	-4	HIS	-	expression tag	UNP Q8PYN5
D	-3	HIS	-	expression tag	UNP Q8PYN5
D	-2	HIS	-	expression tag	UNP Q8PYN5
D	-1	GLY	-	expression tag	UNP Q8PYN5
D	0	SER	-	expression tag	UNP Q8PYN5
D	33	ASN	ASP	engineered mutation	UNP Q8PYN5
E	-11	MET	-	expression tag	UNP Q8PYN5
E	-10	ARG	-	expression tag	UNP Q8PYN5
E	-9	GLY	-	expression tag	UNP Q8PYN5
E	-8	SER	-	expression tag	UNP Q8PYN5
E	-7	HIS	-	expression tag	UNP Q8PYN5
E	-6	HIS	-	expression tag	UNP Q8PYN5
E	-5	HIS	-	expression tag	UNP Q8PYN5

*Continued on next page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q8PYN5
E	-3	HIS	-	expression tag	UNP Q8PYN5
E	-2	HIS	-	expression tag	UNP Q8PYN5
E	-1	GLY	-	expression tag	UNP Q8PYN5
E	0	SER	-	expression tag	UNP Q8PYN5
E	33	ASN	ASP	engineered mutation	UNP Q8PYN5
F	-11	MET	-	expression tag	UNP Q8PYN5
F	-10	ARG	-	expression tag	UNP Q8PYN5
F	-9	GLY	-	expression tag	UNP Q8PYN5
F	-8	SER	-	expression tag	UNP Q8PYN5
F	-7	HIS	-	expression tag	UNP Q8PYN5
F	-6	HIS	-	expression tag	UNP Q8PYN5
F	-5	HIS	-	expression tag	UNP Q8PYN5
F	-4	HIS	-	expression tag	UNP Q8PYN5
F	-3	HIS	-	expression tag	UNP Q8PYN5
F	-2	HIS	-	expression tag	UNP Q8PYN5
F	-1	GLY	-	expression tag	UNP Q8PYN5
F	0	SER	-	expression tag	UNP Q8PYN5
F	33	ASN	ASP	engineered mutation	UNP Q8PYN5

- # NAP
- 
- The chemical structure of Naproxen (NAP) is shown, featuring a naphthalene ring system. The structure includes a carboxylic acid group (-COOH) at the 2-position, a chiral center at the 1-position, and a 6-methoxy group (-OCH<sub>3</sub>). The stereochemistry is indicated by wedged and dashed bonds. The structure is labeled with various atoms and groups, including NH, N, O, C, and H, and is associated with the chemical formula C<sub>15</sub>H<sub>11</sub>NO<sub>4</sub>.

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

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

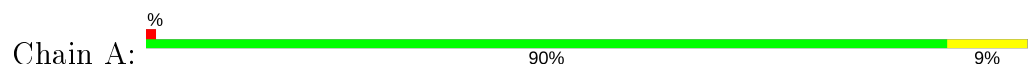
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total	O	0	0
			159	159		
3	B	141	Total	O	0	0
			141	141		
3	C	62	Total	O	0	0
			62	62		
3	D	55	Total	O	0	0
			55	55		
3	E	138	Total	O	0	0
			138	138		
3	F	144	Total	O	0	0
			144	144		

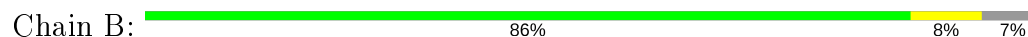
### 3 Residue-property plots [i](#)

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.

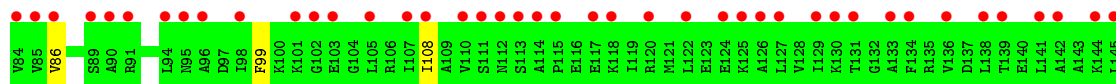
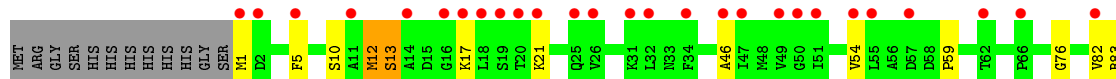
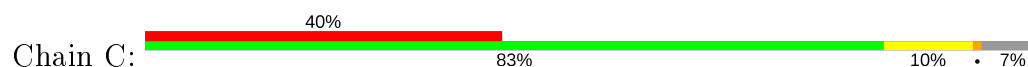
- Molecule 1: Conserved protein



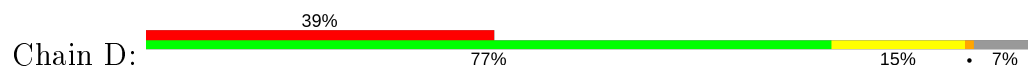
- Molecule 1: Conserved protein

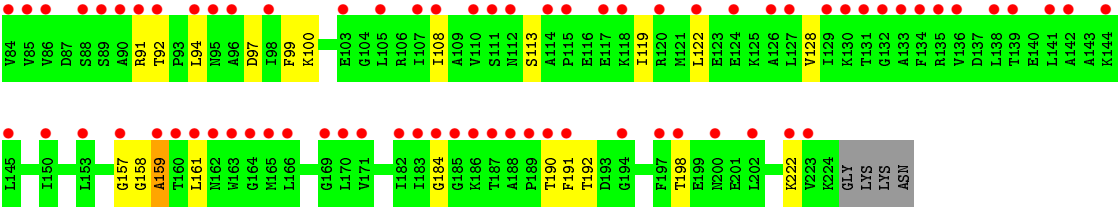


- Molecule 1: Conserved protein

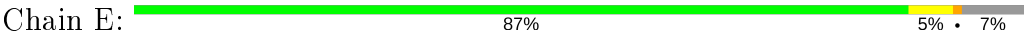


- Molecule 1: Conserved protein

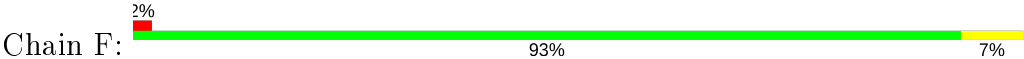




● Molecule 1: Conserved protein



● Molecule 1: Conserved protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.10Å 117.10Å 380.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.95 27.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.95) 99.8 (27.00-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.242 , 0.289 0.249 , 0.295	Depositor DCC
$R_{free}$ test set	6953 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.489 for -h-k,k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: 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	0.56	0/1834	0.75	1/2462 (0.0%)
1	B	0.52	0/1718	0.75	1/2308 (0.0%)
1	C	0.48	0/1718	0.69	1/2308 (0.0%)
1	D	0.49	0/1710	0.69	0/2298
1	E	0.53	1/1710 (0.1%)	0.74	0/2298
1	F	0.57	0/1845	0.74	1/2476 (0.0%)
All	All	0.53	1/10535 (0.0%)	0.73	4/14150 (0.0%)

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	B	0	1
1	E	0	1
1	F	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	158	GLY	N-CA	-5.39	1.38	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	MET	CG-SD-CE	6.21	110.14	100.20
1	F	68	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	68	ARG	NE-CZ-NH1	5.77	123.18	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ARG	NE-CZ-NH2	5.17	122.88	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	GLY	Peptide
1	E	157	GLY	Peptide
1	F	156	GLU	Peptide
1	F	157	GLY	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	1808	0	1861	16	0
1	B	1698	0	1768	11	0
1	C	1698	0	1768	14	0
1	D	1690	0	1756	17	0
1	E	1690	0	1756	11	0
1	F	1819	0	1874	7	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	3	0
2	F	48	0	25	2	0
3	A	159	0	0	11	1
3	B	141	0	0	0	0
3	C	62	0	0	3	0
3	D	55	0	0	2	0
3	E	138	0	0	0	0
3	F	144	0	0	3	0
All	All	11390	0	10933	70	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 (70) 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:F:132:GLY:N	3:F:401:HOH:O	1.93	1.00
1:A:41:ARG:N	3:A:401:HOH:O	1.92	1.00
1:A:38:ASP:C	3:A:401:HOH:O	2.14	0.84
1:A:37:MET:O	3:A:401:HOH:O	2.03	0.77
1:A:38:ASP:O	3:A:401:HOH:O	2.04	0.74
1:D:82:VAL:HG13	3:D:435:HOH:O	1.96	0.65
1:C:82:VAL:HG13	3:C:441:HOH:O	1.98	0.64
1:A:72:ARG:NH1	3:A:402:HOH:O	2.31	0.63
1:F:88:SER:OG	2:F:301:NAP:H8A	1.97	0.63
1:C:17:LYS:HA	1:C:190:THR:HA	1.82	0.62
1:A:88:SER:OG	2:A:301:NAP:H8A	2.00	0.61
1:E:41:ARG:HG2	1:E:154:MET:HE1	1.83	0.59
1:B:41:ARG:HG2	1:B:154:MET:HE1	1.83	0.59
1:A:32:LEU:HD12	1:A:214:GLU:HG3	1.84	0.59
1:B:5:PHE:CD1	1:C:76:GLY:HA3	2.39	0.58
1:D:76:GLY:HA3	1:E:5:PHE:CD1	2.39	0.57
1:A:48:MET:HE2	1:A:84:VAL:HG11	1.86	0.56
1:B:158:GLY:HA3	2:B:301:NAP:O2A	2.05	0.56
1:C:21:LYS:HE3	1:D:198:THR:HG23	1.88	0.56
1:E:176:THR:HG21	3:F:461:HOH:O	2.07	0.54
1:F:123:GLU:O	3:F:402:HOH:O	2.19	0.53
1:A:69:LYS:HG3	3:A:406:HOH:O	2.09	0.52
1:A:91:ARG:NE	3:A:407:HOH:O	2.41	0.52
1:E:29:SER:HB2	1:E:33:ASN:HB3	1.92	0.52
1:D:17:LYS:HE2	1:D:190:THR:HG22	1.92	0.52
1:B:29:SER:HB2	1:B:33:ASN:HB3	1.93	0.51
1:A:63:VAL:HG11	3:A:502:HOH:O	2.11	0.50
1:E:158:GLY:HA3	2:E:301:NAP:O2A	2.11	0.50
1:D:191:PHE:CD2	1:D:192:THR:HG23	2.46	0.50
1:C:155:VAL:HG13	3:C:412:HOH:O	2.11	0.49
1:D:10:SER:N	3:D:401:HOH:O	2.44	0.49
1:D:54:VAL:HA	1:D:59:PRO:HD2	1.94	0.48
1:B:158:GLY:HA3	2:B:301:NAP:PA	2.54	0.48
1:A:40:LEU:N	3:A:401:HOH:O	2.46	0.47
1:B:111:SER:HA	1:B:131:THR:O	2.13	0.47
1:D:119:ILE:HG23	1:D:128:VAL:HG11	1.95	0.47
1:E:111:SER:HA	1:E:131:THR:O	2.13	0.47
1:A:64:LYS:C	3:A:406:HOH:O	2.52	0.47
1:D:28:ILE:O	1:D:28:ILE:HG22	2.14	0.47
1:E:176:THR:HG22	1:E:176:THR:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:VAL:HG22	1:F:53:THR:HB	1.98	0.46
1:A:48:MET:HE2	1:A:141:LEU:HD21	1.98	0.46
1:C:99:PHE:HZ	1:C:108:ILE:HD11	1.81	0.46
1:B:18:LEU:HB3	2:B:301:NAP:H2N	1.98	0.46
1:B:76:GLY:HA3	1:C:5:PHE:CD1	2.51	0.45
1:E:18:LEU:HB3	2:E:301:NAP:H2N	1.98	0.45
1:F:88:SER:OG	2:F:301:NAP:C8A	2.65	0.45
1:D:54:VAL:HA	1:D:59:PRO:CD	2.46	0.45
1:C:197:PHE:HB3	1:C:201:GLU:HB2	2.00	0.44
1:C:46:ALA:O	1:C:153:LEU:HD12	2.17	0.44
1:D:99:PHE:HZ	1:D:108:ILE:HD11	1.81	0.44
1:E:158:GLY:HA3	2:E:301:NAP:PA	2.58	0.43
1:B:41:ARG:HA	1:B:154:MET:HE1	1.99	0.43
1:F:-2:HIS:CE1	1:F:152:SER:HB2	2.54	0.43
1:D:5:PHE:CD1	1:E:76:GLY:HA3	2.53	0.43
1:A:88:SER:OG	2:A:301:NAP:C8A	2.67	0.43
1:C:54:VAL:HA	1:C:59:PRO:HD2	2.01	0.42
3:A:403:HOH:O	1:B:20:THR:HG22	2.20	0.41
1:D:158:GLY:O	1:D:159:ALA:CB	2.68	0.41
1:D:38:ASP:OD2	1:D:68:ARG:NH1	2.53	0.41
1:F:107:ILE:HD11	1:F:148:MET:HE1	2.02	0.41
1:E:41:ARG:HA	1:E:154:MET:HE1	2.02	0.41
1:A:107:ILE:HD11	1:A:148:MET:HE1	2.03	0.40
1:C:13:SER:HA	3:C:402:HOH:O	2.19	0.40
1:D:94:LEU:HD23	1:D:122:LEU:HD23	2.03	0.40
1:C:86:VAL:HG21	1:C:161:LEU:HD11	2.03	0.40
1:D:15:ASP:OD2	1:D:184:GLY:N	2.50	0.40
1:C:46:ALA:HB2	1:C:82:VAL:HB	2.04	0.40
1:C:199:GLU:N	1:D:20:THR:HG21	2.36	0.40
1:B:119:ILE:HG23	1:B:128:VAL:HG11	2.03	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)
3:A:537:HOH:O	3:A:537:HOH:O[2_555]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/240 (98%)	233 (99%)	3 (1%)	0	100	100
1	B	222/240 (92%)	218 (98%)	4 (2%)	0	100	100
1	C	222/240 (92%)	206 (93%)	14 (6%)	2 (1%)	17	8
1	D	221/240 (92%)	203 (92%)	15 (7%)	3 (1%)	11	3
1	E	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
1	F	237/240 (99%)	232 (98%)	5 (2%)	0	100	100
All	All	1359/1440 (94%)	1308 (96%)	46 (3%)	5 (0%)	34	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113	SER
1	D	159	ALA
1	C	13	SER
1	C	214	GLU
1	D	157	GLY

### 5.3.2 Protein sidechains

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	193/195 (99%)	188 (97%)	5 (3%)	46	36
1	B	182/195 (93%)	179 (98%)	3 (2%)	62	58
1	C	182/195 (93%)	175 (96%)	7 (4%)	33	21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	181/195 (93%)	169 (93%)	12 (7%)	16	6
1	E	181/195 (93%)	178 (98%)	3 (2%)	60	55
1	F	194/195 (100%)	190 (98%)	4 (2%)	53	46
All	All	1113/1170 (95%)	1079 (97%)	34 (3%)	40	28

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	31	LYS
1	A	37	MET
1	A	94	LEU
1	A	222	LYS
1	B	21	LYS
1	B	77	LYS
1	B	176	THR
1	C	1	MET
1	C	10	SER
1	C	12	MET
1	C	83	ARG
1	C	181	LEU
1	C	199	GLU
1	C	222	LYS
1	D	2	ASP
1	D	15	ASP
1	D	19	SER
1	D	22	GLU
1	D	29	SER
1	D	83	ARG
1	D	91	ARG
1	D	92	THR
1	D	97	ASP
1	D	100	LYS
1	D	161	LEU
1	D	222	LYS
1	E	95	ASN
1	E	97	ASP
1	E	176	THR
1	F	-8	SER
1	F	21	LYS
1	F	31	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	120	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	25	GLN
1	E	95	ASN
1	F	-4	HIS
1	F	112	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	B	301	-	45,52,52	1.06	4 (8%)	56,80,80	1.36	6 (10%)
2	NAP	F	301	-	45,52,52	1.15	4 (8%)	56,80,80	1.24	5 (8%)
2	NAP	D	301	-	45,52,52	1.02	4 (8%)	56,80,80	1.18	6 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	A	301	-	45,52,52	1.13	4 (8%)	56,80,80	1.28	8 (14%)
2	NAP	E	301	-	45,52,52	1.04	4 (8%)	56,80,80	1.25	6 (10%)
2	NAP	C	301	-	45,52,52	1.01	3 (6%)	56,80,80	1.19	6 (10%)

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	B	301	-	-	3/31/67/67	0/5/5/5
2	NAP	F	301	-	-	9/31/67/67	0/5/5/5
2	NAP	D	301	-	-	6/31/67/67	0/5/5/5
2	NAP	A	301	-	-	14/31/67/67	0/5/5/5
2	NAP	E	301	-	-	3/31/67/67	0/5/5/5
2	NAP	C	301	-	-	14/31/67/67	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAP	C2A-N3A	2.95	1.36	1.32
2	A	301	NAP	C5A-C4A	2.88	1.48	1.40
2	A	301	NAP	C2A-N3A	2.85	1.36	1.32
2	D	301	NAP	C5A-C4A	2.82	1.48	1.40
2	F	301	NAP	C5A-C4A	2.77	1.48	1.40
2	C	301	NAP	C5A-C4A	2.74	1.48	1.40
2	D	301	NAP	O4B-C1B	2.72	1.44	1.41
2	A	301	NAP	O4B-C1B	2.68	1.44	1.41
2	F	301	NAP	O4B-C1B	2.65	1.44	1.41
2	C	301	NAP	C2A-N3A	2.63	1.36	1.32
2	D	301	NAP	C2A-N3A	2.63	1.36	1.32
2	F	301	NAP	O4D-C1D	2.49	1.44	1.41
2	B	301	NAP	O4D-C1D	2.43	1.44	1.41
2	B	301	NAP	C5A-C4A	2.42	1.47	1.40
2	E	301	NAP	C5A-C4A	2.32	1.47	1.40
2	B	301	NAP	C4A-N3A	2.27	1.38	1.35
2	B	301	NAP	P2B-O2B	2.25	1.63	1.59
2	E	301	NAP	P2B-O2B	2.23	1.63	1.59
2	C	301	NAP	O4B-C1B	2.19	1.44	1.41
2	E	301	NAP	O4D-C1D	2.15	1.44	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	P2B-O2B	2.13	1.63	1.59
2	E	301	NAP	C4A-N3A	2.11	1.38	1.35
2	A	301	NAP	O4D-C1D	2.07	1.44	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	N3A-C2A-N1A	-3.60	123.05	128.68
2	B	301	NAP	C6N-N1N-C2N	-3.59	118.70	121.97
2	A	301	NAP	N3A-C2A-N1A	-3.57	123.10	128.68
2	F	301	NAP	N3A-C2A-N1A	-3.52	123.17	128.68
2	B	301	NAP	C3N-C7N-N7N	3.42	121.85	117.75
2	E	301	NAP	C6N-N1N-C2N	-3.31	118.95	121.97
2	E	301	NAP	N3A-C2A-N1A	-3.27	123.57	128.68
2	C	301	NAP	N3A-C2A-N1A	-3.23	123.63	128.68
2	D	301	NAP	N3A-C2A-N1A	-3.15	123.76	128.68
2	C	301	NAP	C3N-C7N-N7N	3.12	121.49	117.75
2	E	301	NAP	C3N-C2N-N1N	3.02	123.38	120.43
2	B	301	NAP	C3N-C2N-N1N	3.00	123.36	120.43
2	E	301	NAP	C3N-C7N-N7N	2.94	121.28	117.75
2	C	301	NAP	O7N-C7N-N7N	-2.84	118.54	122.58
2	A	301	NAP	C4A-C5A-N7A	-2.76	106.52	109.40
2	D	301	NAP	C3D-C2D-C1D	2.65	104.97	100.98
2	D	301	NAP	C1B-N9A-C4A	2.62	131.25	126.64
2	F	301	NAP	C3N-C2N-N1N	2.59	122.96	120.43
2	C	301	NAP	C4A-C5A-N7A	-2.53	106.76	109.40
2	D	301	NAP	C3N-C7N-N7N	2.49	120.74	117.75
2	A	301	NAP	O5D-C5D-C4D	2.49	117.56	108.99
2	D	301	NAP	C4A-C5A-N7A	-2.49	106.80	109.40
2	C	301	NAP	C1B-N9A-C4A	2.46	130.97	126.64
2	F	301	NAP	O2A-PA-O1A	2.45	124.35	112.24
2	A	301	NAP	C3N-C2N-N1N	2.44	122.81	120.43
2	F	301	NAP	C6N-N1N-C2N	-2.38	119.81	121.97
2	F	301	NAP	C3N-C7N-N7N	2.33	120.55	117.75
2	B	301	NAP	O2A-PA-O1A	2.28	123.53	112.24
2	A	301	NAP	C3N-C7N-N7N	2.21	120.41	117.75
2	B	301	NAP	O2N-PN-O1N	2.17	122.95	112.24
2	A	301	NAP	O2A-PA-O1A	2.14	122.81	112.24
2	A	301	NAP	C6N-N1N-C2N	-2.12	120.04	121.97
2	C	301	NAP	N6A-C6A-N1A	2.11	122.95	118.57
2	D	301	NAP	N6A-C6A-N1A	2.06	122.86	118.57
2	A	301	NAP	O4D-C4D-C5D	2.05	116.12	109.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	NAP	N6A-C6A-N1A	2.04	122.81	118.57
2	E	301	NAP	O2A-PA-O1A	2.01	122.16	112.24

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAP	O4D-C1D-N1N-C6N
2	F	301	NAP	C2B-O2B-P2B-O2X
2	F	301	NAP	O4D-C1D-N1N-C2N
2	F	301	NAP	O4D-C1D-N1N-C6N
2	D	301	NAP	C5B-O5B-PA-O2A
2	D	301	NAP	C3B-C4B-C5B-O5B
2	A	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C5D-O5D-PN-O2N
2	A	301	NAP	O4D-C4D-C5D-O5D
2	A	301	NAP	C3D-C4D-C5D-O5D
2	E	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	C5B-O5B-PA-O2A
2	C	301	NAP	C5B-O5B-PA-O3
2	C	301	NAP	C2B-O2B-P2B-O1X
2	C	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	C3B-C4B-C5B-O5B
2	C	301	NAP	O4D-C4D-C5D-O5D
2	C	301	NAP	C3D-C4D-C5D-O5D
2	A	301	NAP	C3B-C4B-C5B-O5B
2	F	301	NAP	C1B-C2B-O2B-P2B
2	A	301	NAP	C1B-C2B-O2B-P2B
2	A	301	NAP	C3B-C2B-O2B-P2B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	C3B-C2B-O2B-P2B
2	A	301	NAP	PN-O3-PA-O1A
2	A	301	NAP	O4B-C4B-C5B-O5B
2	E	301	NAP	C1B-C2B-O2B-P2B
2	C	301	NAP	C1B-C2B-O2B-P2B
2	D	301	NAP	C5B-O5B-PA-O3
2	A	301	NAP	C5B-O5B-PA-O3
2	A	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C5B-O5B-PA-O1A
2	A	301	NAP	C5B-O5B-PA-O2A

*Continued on next page...*

*Continued from previous page...*

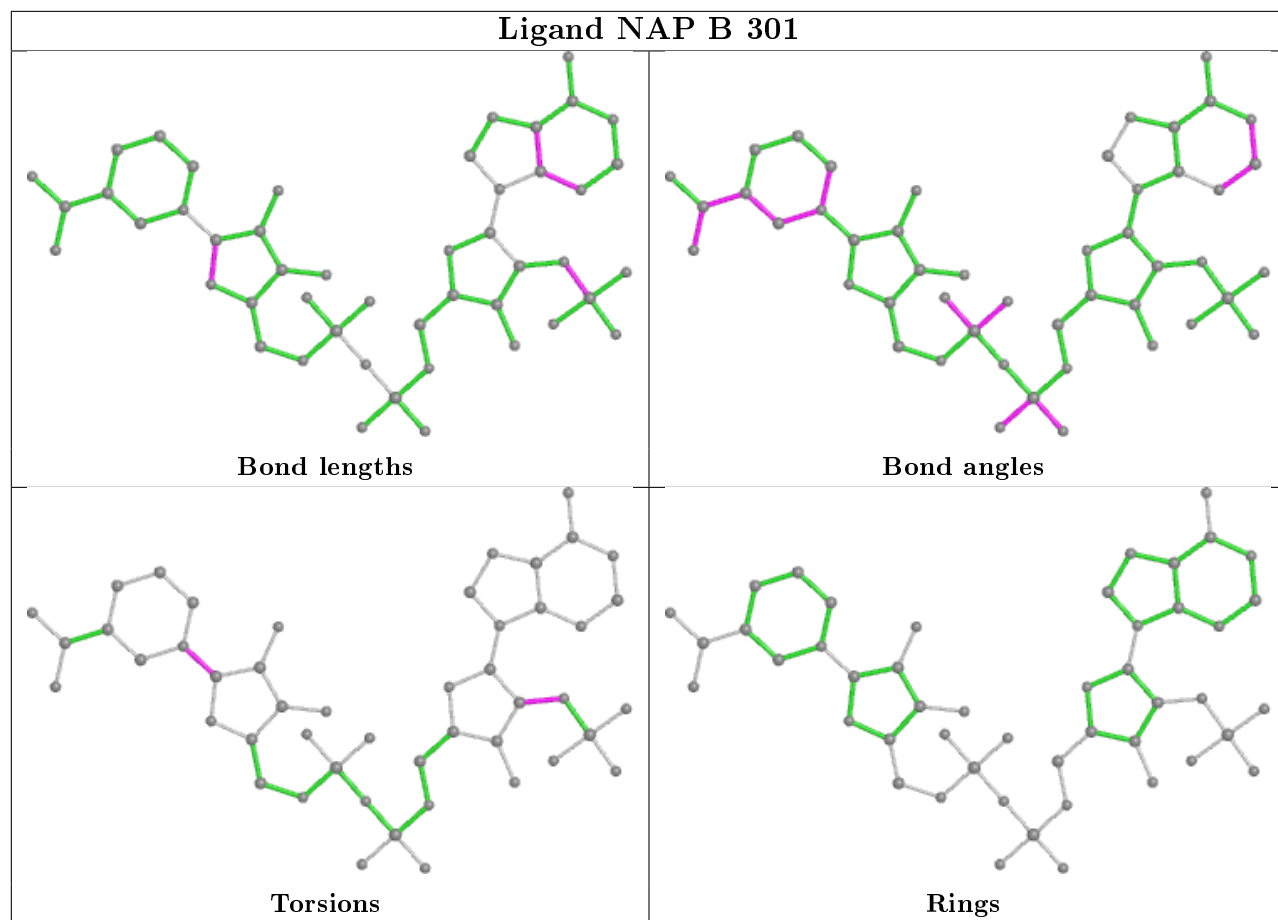
Mol	Chain	Res	Type	Atoms
2	C	301	NAP	C5B-O5B-PA-O1A
2	C	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C1B-C2B-O2B-P2B
2	F	301	NAP	C3B-C4B-C5B-O5B
2	F	301	NAP	PN-O3-PA-O2A
2	D	301	NAP	PN-O3-PA-O2A
2	A	301	NAP	PN-O3-PA-O2A
2	C	301	NAP	PN-O3-PA-O2A
2	F	301	NAP	C3D-C4D-C5D-O5D
2	C	301	NAP	C2B-O2B-P2B-O3X
2	F	301	NAP	PN-O3-PA-O1A
2	B	301	NAP	C3B-C2B-O2B-P2B
2	E	301	NAP	C3B-C2B-O2B-P2B
2	C	301	NAP	C3B-C2B-O2B-P2B

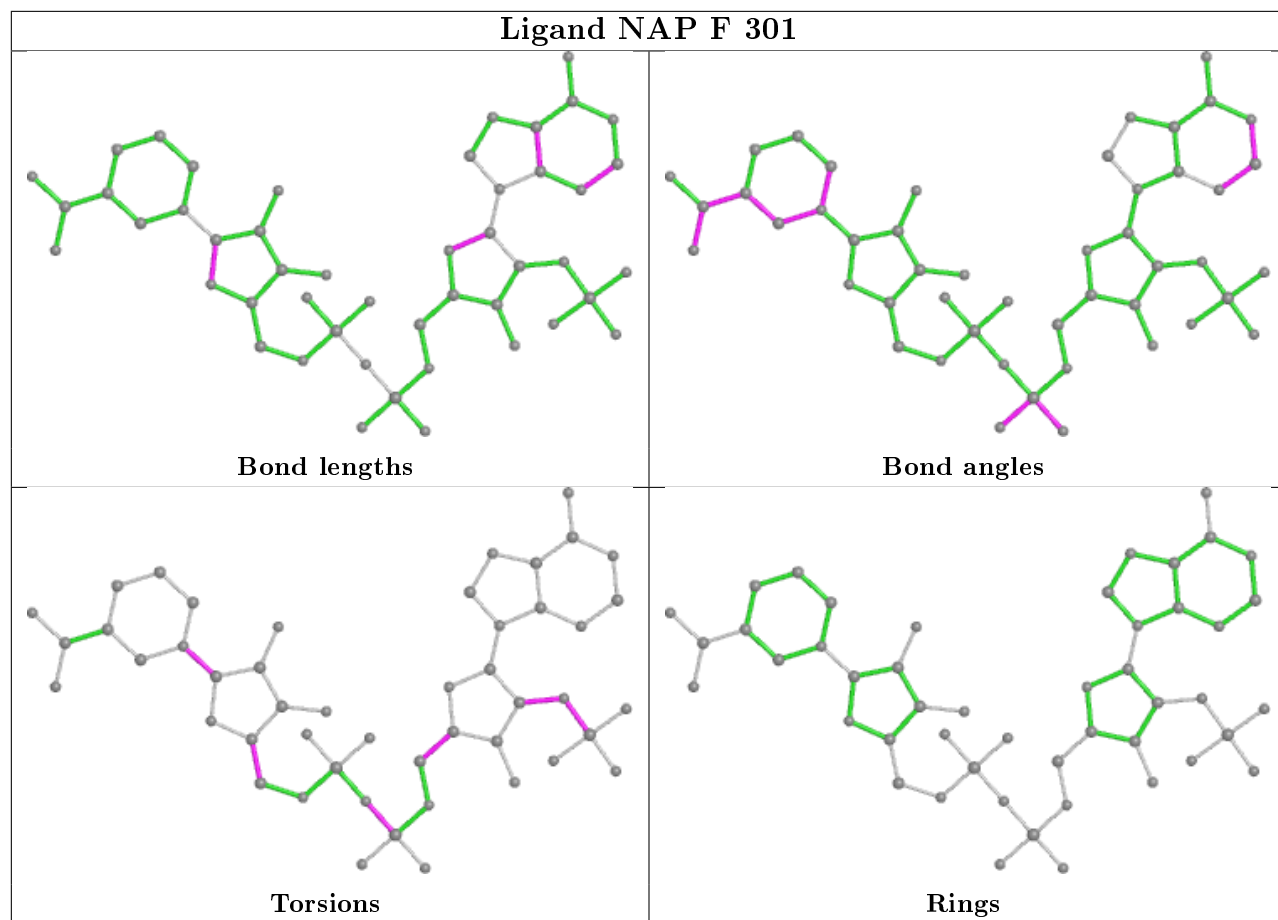
There are no ring outliers.

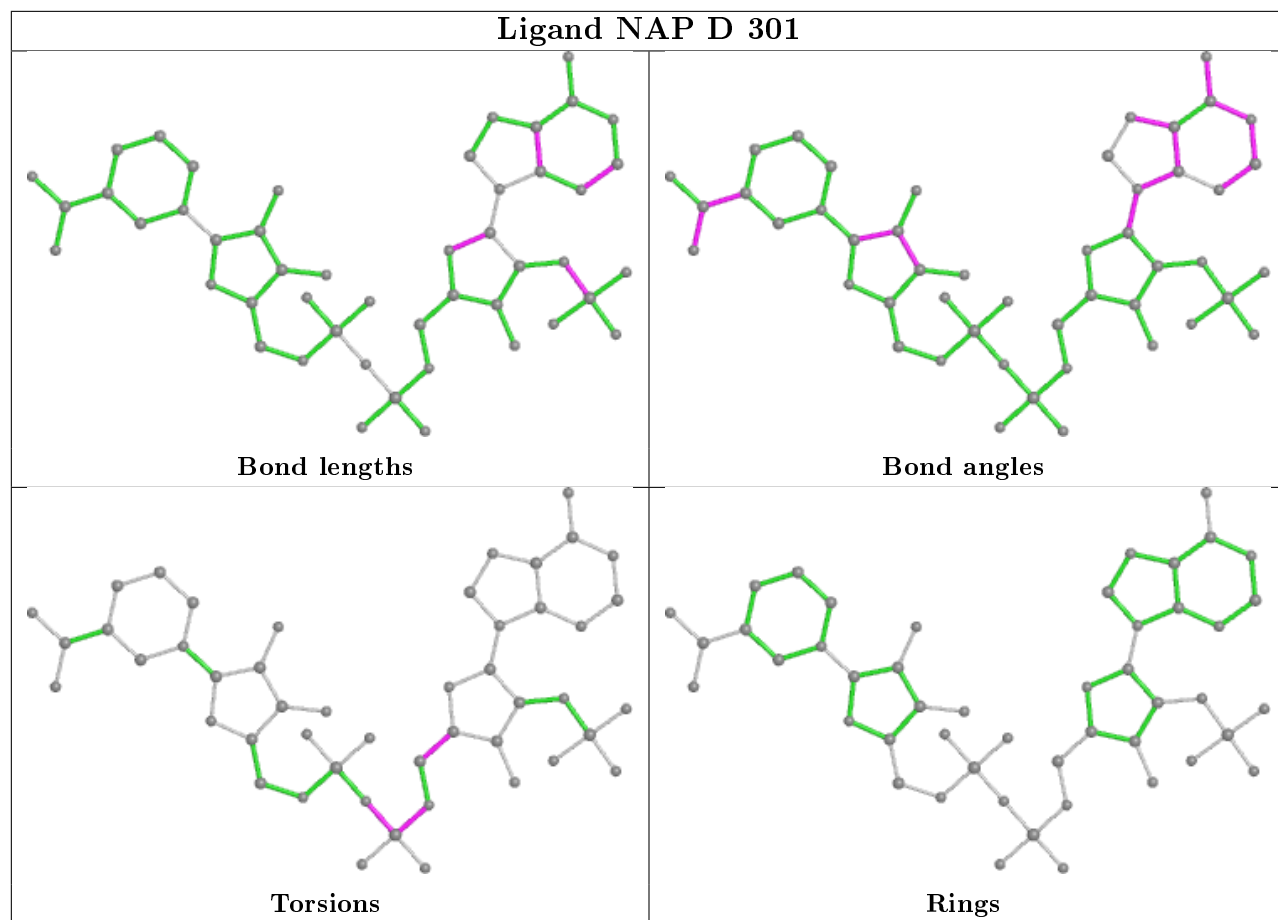
4 monomers are involved in 10 short contacts:

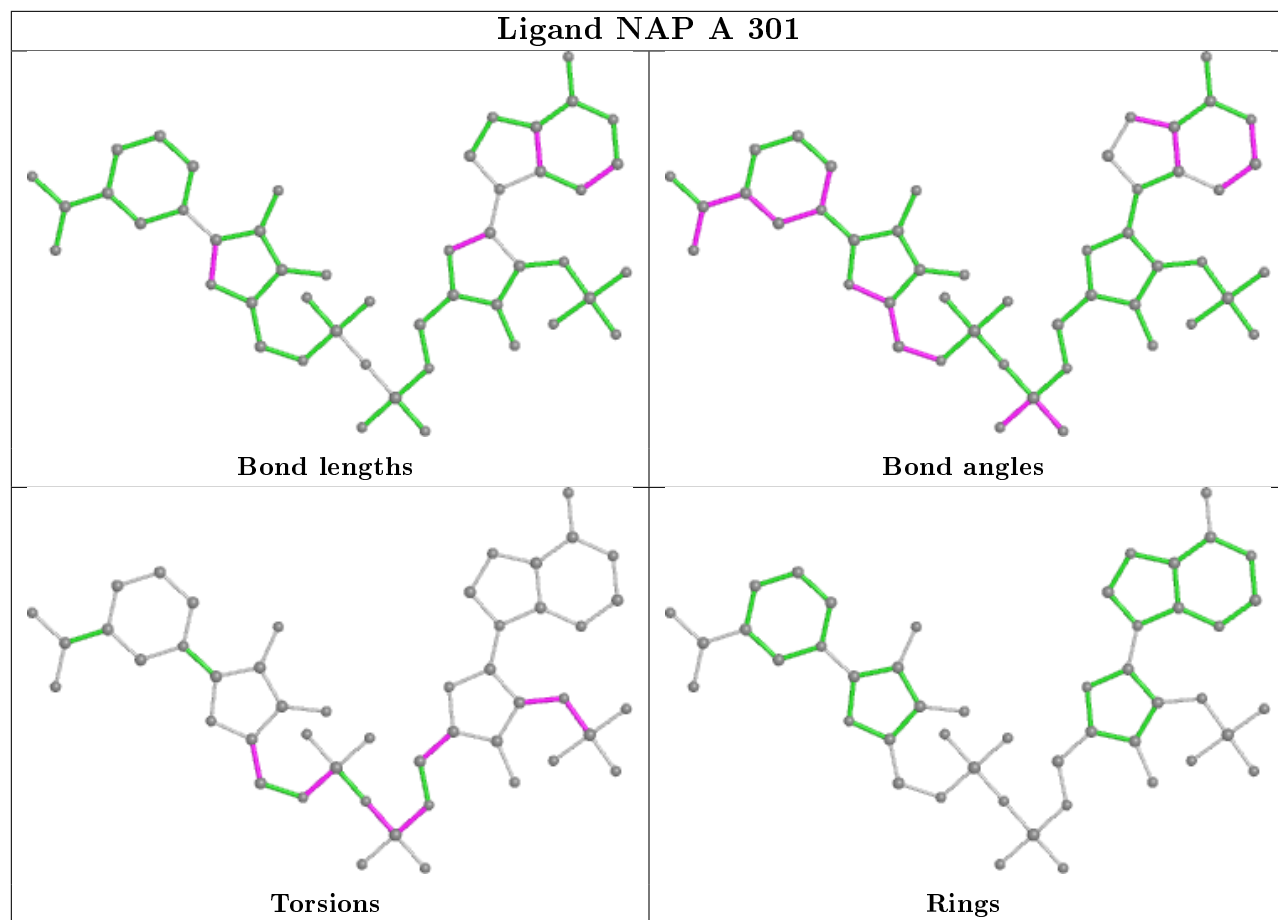
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	3	0
2	F	301	NAP	2	0
2	A	301	NAP	2	0
2	E	301	NAP	3	0

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.

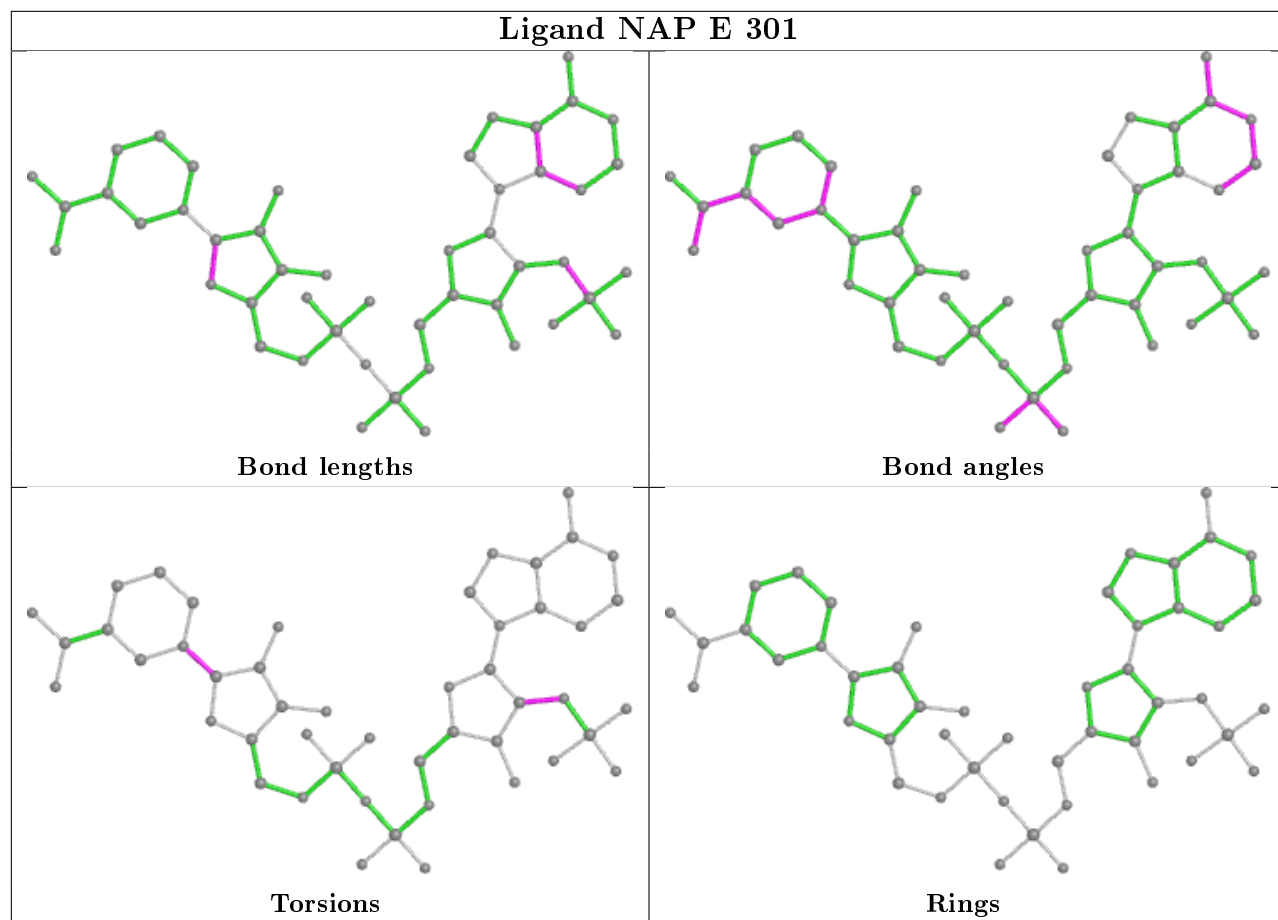


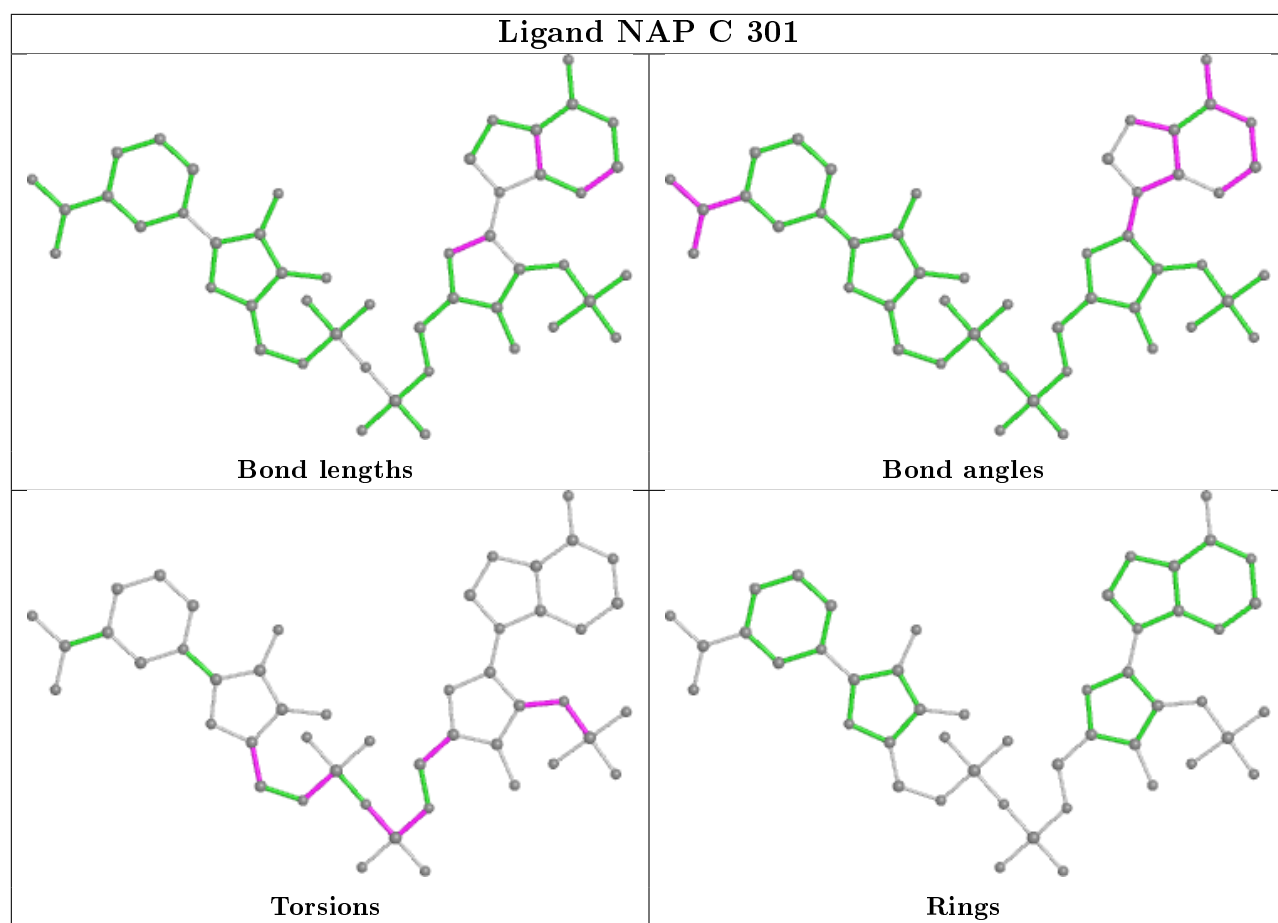












## 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	238/240 (99%)	-0.02	3 (1%) 77 83	20, 28, 49, 72	0
1	B	224/240 (93%)	-0.02	0 100 100	20, 32, 47, 84	0
1	C	224/240 (93%)	2.16	97 (43%) 0 0	37, 65, 101, 112	0
1	D	223/240 (92%)	2.06	94 (42%) 0 0	37, 63, 99, 118	0
1	E	223/240 (92%)	-0.02	0 100 100	20, 32, 48, 56	0
1	F	239/240 (99%)	0.00	5 (2%) 63 72	21, 28, 48, 91	0
All	All	1371/1440 (95%)	0.68	199 (14%) 2 4	20, 37, 86, 118	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	GLY	11.0
1	C	157	GLY	10.4
1	C	134	PHE	10.0
1	D	134	PHE	8.3
1	C	122	LEU	8.1
1	C	131	THR	8.1
1	D	185	GLY	7.9
1	D	94	LEU	7.5
1	C	90	ALA	6.8
1	D	21	LYS	6.8
1	C	118	LYS	6.8
1	C	138	LEU	6.8
1	C	197	PHE	6.7
1	D	138	LEU	6.6
1	C	111	SER	6.6
1	C	51	ILE	6.3
1	D	122	LEU	6.2
1	C	34	PHE	6.2
1	C	21	LYS	6.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	90	ALA	6.2
1	D	129	ILE	6.1
1	C	127	LEU	6.0
1	C	112	ASN	6.0
1	D	19	SER	5.5
1	C	183	ILE	5.2
1	D	144	LYS	5.2
1	D	197	PHE	5.2
1	D	118	LYS	5.2
1	C	200	ASN	5.1
1	C	145	LEU	4.9
1	C	129	ILE	4.8
1	C	170	LEU	4.8
1	D	47	ILE	4.8
1	C	94	LEU	4.7
1	D	161	LEU	4.6
1	D	34	PHE	4.5
1	D	200	ASN	4.5
1	C	130	LYS	4.5
1	D	51	ILE	4.5
1	C	133	ALA	4.4
1	D	130	LYS	4.4
1	D	131	THR	4.4
1	C	2	ASP	4.4
1	C	11	ALA	4.3
1	C	120	ARG	4.2
1	D	120	ARG	4.2
1	D	170	LEU	4.2
1	D	186	LYS	4.2
1	C	114	ALA	4.2
1	D	166	LEU	4.1
1	D	183	ILE	4.1
1	C	19	SER	4.0
1	C	144	LYS	4.0
1	C	110	VAL	4.0
1	D	111	SER	4.0
1	D	91	ARG	4.0
1	D	114	ALA	3.9
1	C	47	ILE	3.8
1	C	187	THR	3.8
1	D	115	PRO	3.8
1	D	194	GLY	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.7
1	F	-2	HIS	3.7
1	D	163	TRP	3.7
1	D	145	LEU	3.7
1	D	110	VAL	3.6
1	C	202	LEU	3.6
1	C	85	VAL	3.6
1	C	142	ALA	3.6
1	D	84	VAL	3.6
1	F	228	ASN	3.5
1	D	127	LEU	3.5
1	C	26	VAL	3.5
1	D	117	GLU	3.5
1	C	20	THR	3.5
1	C	89	SER	3.5
1	D	150	ILE	3.5
1	C	82	VAL	3.5
1	D	95	ASN	3.5
1	C	168	ALA	3.5
1	C	185	GLY	3.5
1	C	108	ILE	3.4
1	A	-2	HIS	3.4
1	C	95	ASN	3.4
1	C	49	VAL	3.4
1	D	55	LEU	3.4
1	D	96	ALA	3.4
1	C	55	LEU	3.4
1	D	46	ALA	3.3
1	C	161	LEU	3.3
1	D	112	ASN	3.3
1	D	89	SER	3.2
1	C	171	VAL	3.2
1	D	86	VAL	3.2
1	D	184	GLY	3.2
1	C	84	VAL	3.2
1	D	107	ILE	3.2
1	C	125	LYS	3.2
1	C	25	GLN	3.2
1	C	126	ALA	3.1
1	D	136	VAL	3.1
1	D	171	VAL	3.1
1	D	188	ALA	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	85	VAL	3.1
1	C	105	LEU	3.1
1	C	117	GLU	3.1
1	C	31	LYS	3.1
1	D	165	MET	3.1
1	C	166	LEU	3.1
1	C	182	ILE	3.0
1	D	198	THR	3.0
1	D	108	ILE	3.0
1	C	57	ASP	3.0
1	D	141	LEU	3.0
1	C	107	ILE	2.9
1	D	20	THR	2.9
1	C	163	TRP	2.9
1	C	86	VAL	2.9
1	C	195	GLU	2.9
1	D	142	ALA	2.9
1	C	141	LEU	2.9
1	D	182	ILE	2.9
1	C	66	PRO	2.8
1	C	188	ALA	2.8
1	C	198	THR	2.8
1	D	92	THR	2.8
1	C	136	VAL	2.8
1	D	26	VAL	2.8
1	D	133	ALA	2.7
1	F	34	PHE	2.7
1	C	115	PRO	2.7
1	D	49	VAL	2.7
1	D	126	ALA	2.7
1	C	102	GLY	2.7
1	D	187	THR	2.7
1	D	191	PHE	2.7
1	C	113	SER	2.7
1	C	101	LYS	2.7
1	C	174	VAL	2.7
1	D	159	ALA	2.6
1	C	223	VAL	2.6
1	D	82	VAL	2.6
1	A	34	PHE	2.6
1	A	-1	GLY	2.6
1	C	191	PHE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	165	MET	2.6
1	C	181	LEU	2.5
1	D	103	GLU	2.5
1	C	16	GLY	2.5
1	C	46	ALA	2.5
1	D	50	GLY	2.5
1	D	18	LEU	2.5
1	D	105	LEU	2.5
1	D	28	ILE	2.4
1	D	202	LEU	2.4
1	D	17	LYS	2.4
1	D	139	THR	2.4
1	D	16	GLY	2.4
1	C	17	LYS	2.4
1	C	150	ILE	2.4
1	D	164	GLY	2.4
1	C	91	ARG	2.4
1	C	169	GLY	2.4
1	C	98	ILE	2.4
1	C	32	LEU	2.3
1	D	135	ARG	2.3
1	C	50	GLY	2.3
1	F	-1	GLY	2.3
1	C	186	LYS	2.3
1	D	160	THR	2.3
1	D	169	GLY	2.3
1	D	23	ARG	2.3
1	C	124	GLU	2.2
1	C	96	ALA	2.2
1	D	190	THR	2.2
1	F	-10	ARG	2.2
1	D	66	PRO	2.2
1	C	62	THR	2.2
1	C	222	LYS	2.2
1	D	153	LEU	2.2
1	D	124	GLU	2.2
1	D	5	PHE	2.2
1	C	54	VAL	2.2
1	D	98	ILE	2.1
1	C	18	LEU	2.1
1	D	189	PRO	2.1
1	D	222	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	132	GLY	2.1
1	C	103	GLU	2.1
1	D	56	ALA	2.1
1	C	14	ALA	2.1
1	D	162	ASN	2.0
1	C	5	PHE	2.0
1	D	223	VAL	2.0
1	C	192	THR	2.0
1	D	88	SER	2.0
1	C	205	LEU	2.0
1	D	6	ILE	2.0
1	C	139	THR	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 [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.

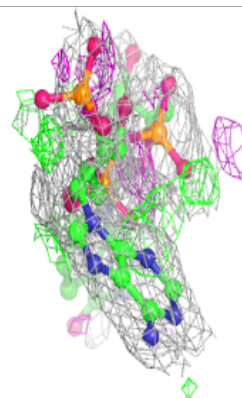
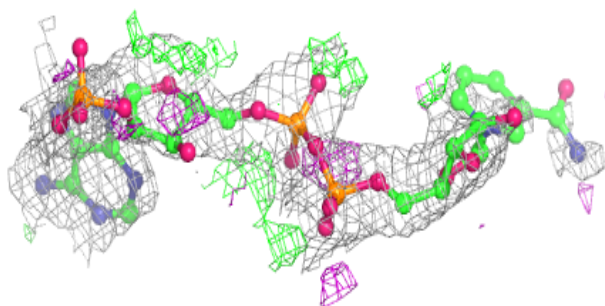
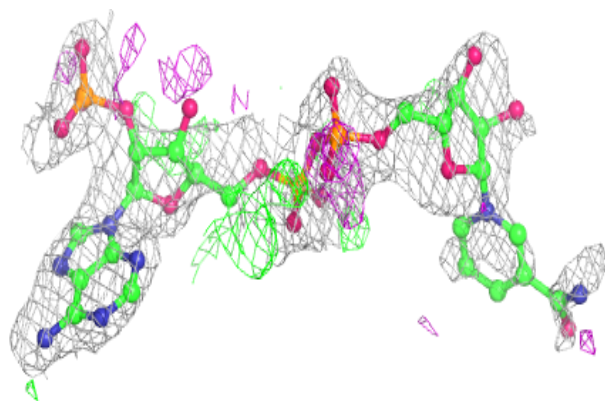
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	C	301	48/48	0.80	0.24	58,81,100,108	0
2	NAP	D	301	48/48	0.81	0.21	59,77,97,104	0
2	NAP	A	301	48/48	0.82	0.30	25,52,71,72	0
2	NAP	F	301	48/48	0.83	0.27	25,50,63,65	0
2	NAP	E	301	48/48	0.98	0.11	20,25,38,46	0
2	NAP	B	301	48/48	0.98	0.10	20,25,37,43	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.

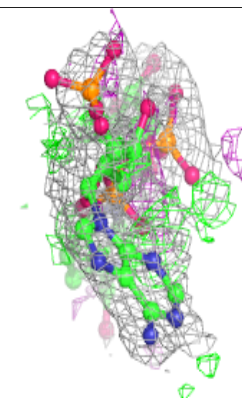
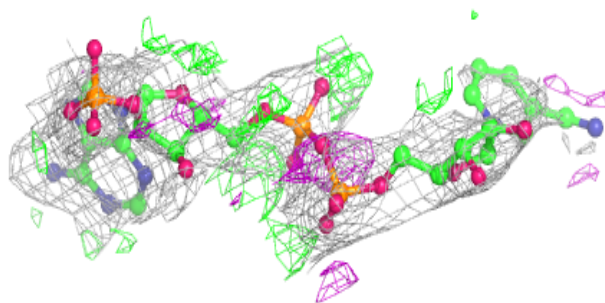
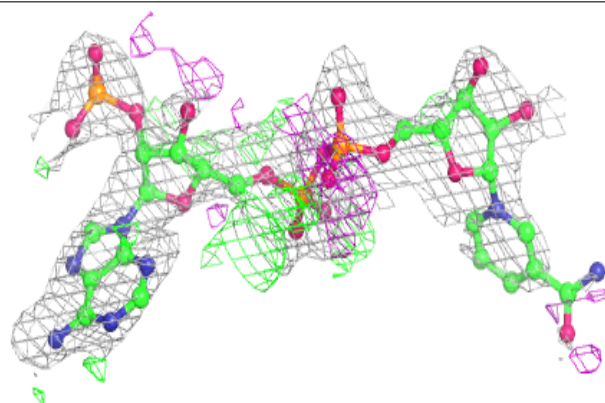


**Electron density around NAP C 301:**

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

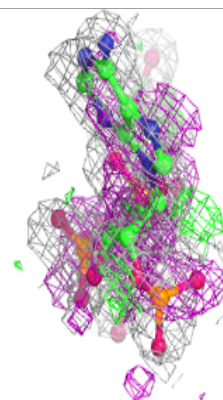
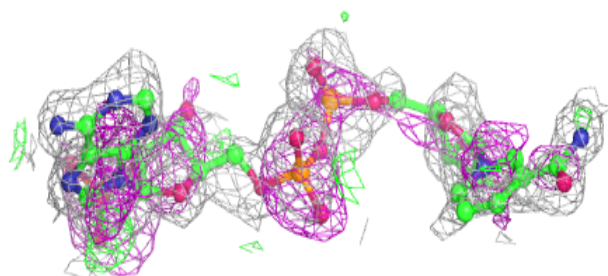
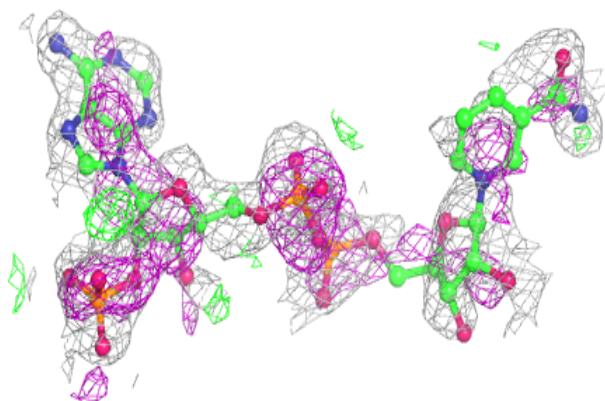
**Electron density around NAP D 301:**

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

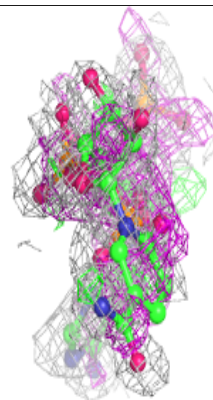
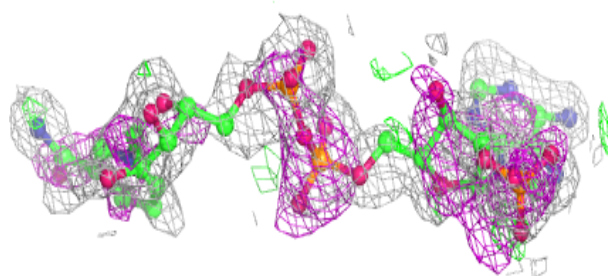
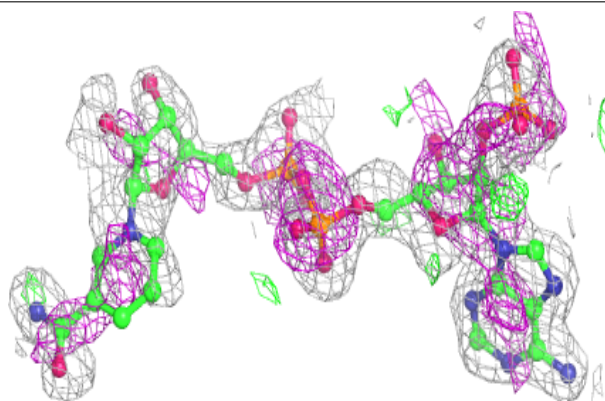


**Electron density around NAP A 301:**

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

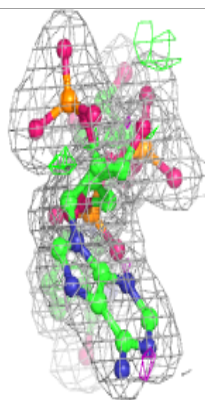
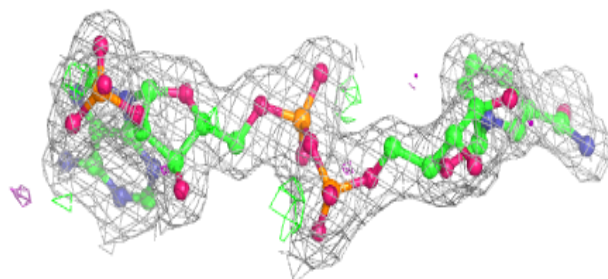
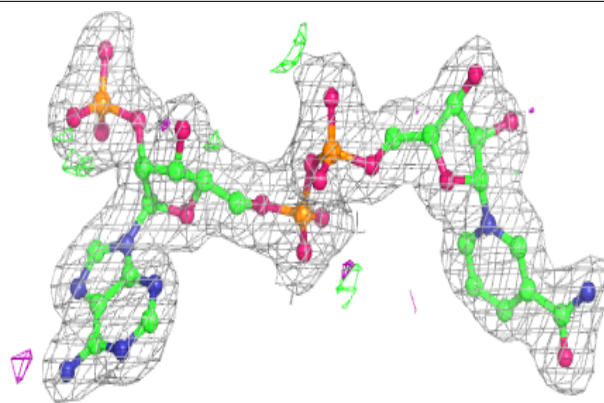
**Electron density around NAP F 301:**

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

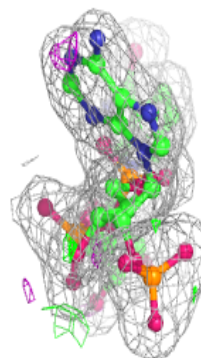
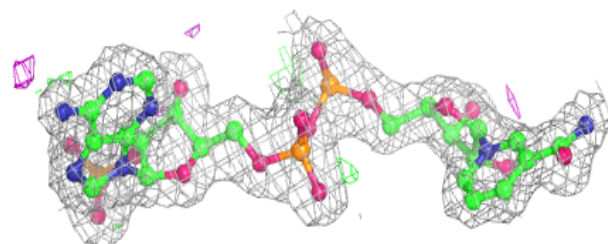
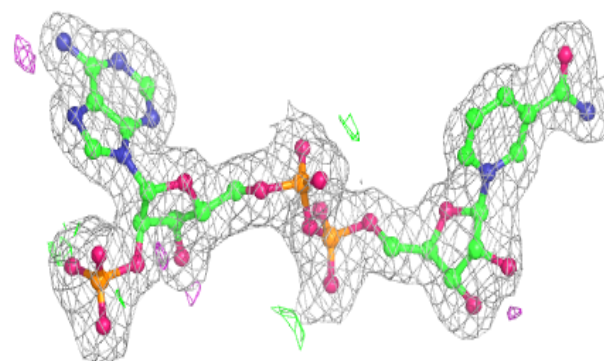


**Electron density around NAP E 301:**

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

**Electron density around NAP 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)



## 6.5 Other polymers

There are no such residues in this entry.