



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:39 pm BST

PDB ID : 4NBU  
Title : Crystal structure of FabG from Bacillus sp  
Authors : Pereira, J.H.; Mcandrew, R.P.; Javidpour, P.; Beller, H.R.; Adams, P.D.  
Deposited on : 2013-10-23  
Resolution : 1.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

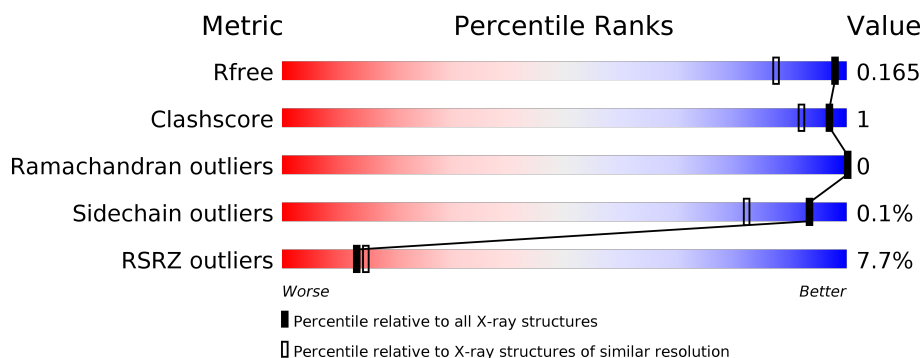
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.34 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	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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	250	<div> <div>8%</div> <div>96%</div> </div>
1	B	250	<div> <div>7%</div> <div>94%</div> </div>
1	C	250	<div> <div>7%</div> <div>94%</div> </div>
1	D	250	<div> <div>8%</div> <div>95%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8527 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 3-oxoacyl-(Acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	5	0
			1845	1164	323	347	11			
1	B	244	Total	C	N	O	S	0	4	0
			1861	1170	329	350	12			
1	C	242	Total	C	N	O	S	0	2	0
			1829	1152	321	345	11			
1	D	242	Total	C	N	O	S	0	1	0
			1824	1147	321	345	11			

There are 28 discrepancies between the modelled and reference sequences:

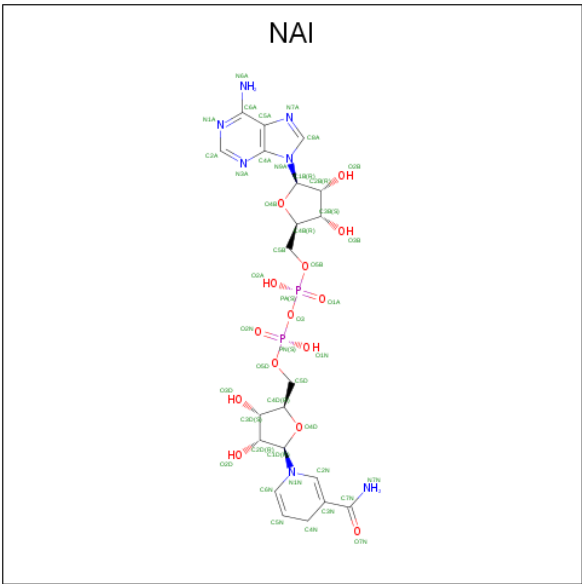
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A6CQL2
A	2	HIS	-	EXPRESSION TAG	UNP A6CQL2
A	3	HIS	-	EXPRESSION TAG	UNP A6CQL2
A	4	HIS	-	EXPRESSION TAG	UNP A6CQL2
A	5	HIS	-	EXPRESSION TAG	UNP A6CQL2
A	6	HIS	-	EXPRESSION TAG	UNP A6CQL2
A	7	HIS	-	EXPRESSION TAG	UNP A6CQL2
B	1	MET	-	EXPRESSION TAG	UNP A6CQL2
B	2	HIS	-	EXPRESSION TAG	UNP A6CQL2
B	3	HIS	-	EXPRESSION TAG	UNP A6CQL2
B	4	HIS	-	EXPRESSION TAG	UNP A6CQL2
B	5	HIS	-	EXPRESSION TAG	UNP A6CQL2
B	6	HIS	-	EXPRESSION TAG	UNP A6CQL2
B	7	HIS	-	EXPRESSION TAG	UNP A6CQL2
C	1	MET	-	EXPRESSION TAG	UNP A6CQL2
C	2	HIS	-	EXPRESSION TAG	UNP A6CQL2
C	3	HIS	-	EXPRESSION TAG	UNP A6CQL2
C	4	HIS	-	EXPRESSION TAG	UNP A6CQL2
C	5	HIS	-	EXPRESSION TAG	UNP A6CQL2
C	6	HIS	-	EXPRESSION TAG	UNP A6CQL2
C	7	HIS	-	EXPRESSION TAG	UNP A6CQL2

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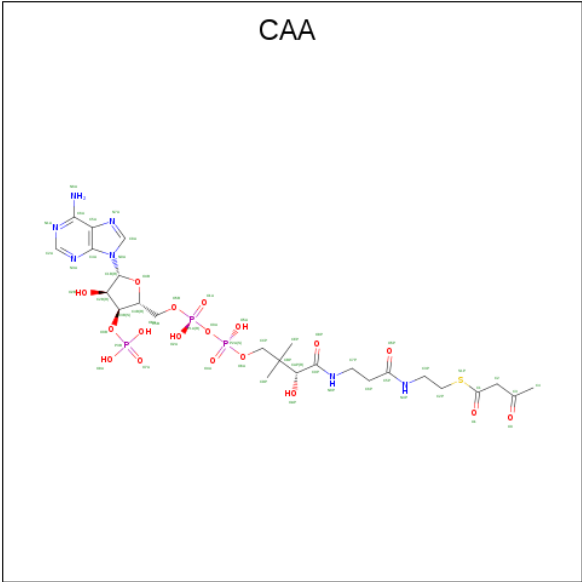
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	EXPRESSION TAG	UNP A6CQL2
D	2	HIS	-	EXPRESSION TAG	UNP A6CQL2
D	3	HIS	-	EXPRESSION TAG	UNP A6CQL2
D	4	HIS	-	EXPRESSION TAG	UNP A6CQL2
D	5	HIS	-	EXPRESSION TAG	UNP A6CQL2
D	6	HIS	-	EXPRESSION TAG	UNP A6CQL2
D	7	HIS	-	EXPRESSION TAG	UNP A6CQL2

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: C<sub>25</sub>H<sub>40</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	54	25	7	18	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	0
			213	213		
4	B	252	Total	O	0	0
			252	252		
4	C	230	Total	O	0	0
			230	230		
4	D	243	Total	O	0	0
			243	243		

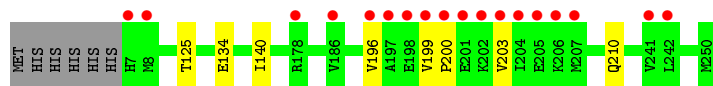
### 3 Residue-property plots [i](#)

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.

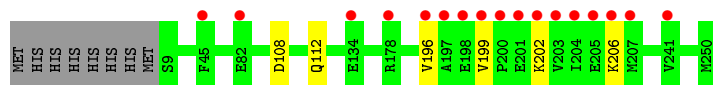
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



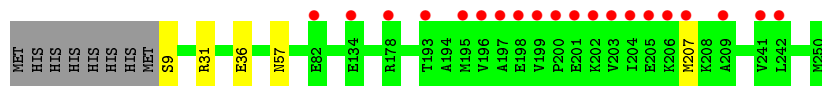
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.41Å 68.77Å 70.00Å 67.85° 88.65° 62.64°	Depositor
Resolution (Å)	23.32 – 1.34 38.48 – 1.34	Depositor EDS
% Data completeness (in resolution range)	93.7 (23.32-1.34) 88.6 (38.48-1.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 1.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1405)	Depositor
R, $R_{free}$	0.156 , 0.164 0.157 , 0.165	Depositor DCC
$R_{free}$ test set	2006 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: CAA, NAI

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	0.31	0/1886	0.52	0/2547
1	B	0.32	0/1900	0.51	0/2564
1	C	0.32	0/1861	0.51	0/2513
1	D	0.30	0/1853	0.51	0/2502
All	All	0.32	0/7500	0.51	0/10126

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1845	0	1886	2	0
1	B	1861	0	1891	4	0
1	C	1829	0	1861	4	0
1	D	1824	0	1850	3	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	0	0
3	B	54	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	213	0	0	0	0
4	B	252	0	0	0	0
4	C	230	0	0	0	0
4	D	243	0	0	0	0
All	All	8527	0	7632	13	0

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 1.

All (13) 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:108:ASP:OD2	1:C:112:GLN:NE2	2.37	0.57
1:A:108:ASP:OD2	1:A:112:GLN:NE2	2.36	0.56
1:A:210:GLN:HE22	1:B:210:GLN:HE22	1.54	0.54
1:C:108:ASP:CG	1:C:112:GLN:HE21	2.20	0.45
1:C:202:LYS:O	1:C:206:LYS:HD3	2.17	0.45
1:D:207:MET:HB2	1:D:207:MET:HE2	1.85	0.44
1:B:196:VAL:O	1:B:199:VAL:HG22	2.18	0.43
1:D:31:ARG:NH1	1:D:57:ASN:OD1	2.52	0.42
1:C:196:VAL:O	1:C:199:VAL:HG22	2.21	0.41
1:B:200:PRO:O	1:B:203:VAL:HG12	2.20	0.41
1:D:9:SER:HB3	1:D:36:GLU:O	2.20	0.41
1:B:125:THR:HG23	1:B:140:ILE:HD13	2.02	0.41
3:B:302:CAA:O1	3:B:302:CAA:H31	2.19	0.40

There are no symmetry-related clashes.

## 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	245/250 (98%)	240 (98%)	5 (2%)	0	100	100
1	B	246/250 (98%)	239 (97%)	7 (3%)	0	100	100
1	C	242/250 (97%)	237 (98%)	5 (2%)	0	100	100
1	D	241/250 (96%)	236 (98%)	5 (2%)	0	100	100
All	All	974/1000 (97%)	952 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	195/198 (98%)	195 (100%)	0	100	100
1	B	196/198 (99%)	195 (100%)	1 (0%)	88	71
1	C	192/198 (97%)	192 (100%)	0	100	100
1	D	191/198 (96%)	191 (100%)	0	100	100
All	All	774/792 (98%)	773 (100%)	1 (0%)	93	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	B	7	HIS
1	C	210	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 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	$\# Z  > 2$
3	CAA	B	302	-	47,56,56	1.94	10 (21%)	60,83,83	1.58	10 (16%)
2	NAI	D	301	-	42,48,48	1.40	8 (19%)	47,73,73	1.32	6 (12%)
2	NAI	C	301	-	42,48,48	1.45	8 (19%)	47,73,73	1.31	5 (10%)
2	NAI	B	301	-	42,48,48	1.39	6 (14%)	47,73,73	1.29	6 (12%)
2	NAI	A	301	-	42,48,48	1.45	8 (19%)	47,73,73	1.25	3 (6%)

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
3	CAA	B	302	-	-	17/50/71/71	0/3/3/3
2	NAI	D	301	-	-	6/25/72/72	0/5/5/5
2	NAI	C	301	-	-	6/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	B	301	-	-	6/25/72/72	0/5/5/5
2	NAI	A	301	-	-	7/25/72/72	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	CAA	O4B-C1B	6.24	1.49	1.41
3	B	302	CAA	C9P-N8P	5.89	1.46	1.33
3	B	302	CAA	C5P-N4P	4.99	1.44	1.33
3	B	302	CAA	C2B-C1B	-4.06	1.47	1.53
2	C	301	NAI	C7N-N7N	3.49	1.42	1.33
2	C	301	NAI	C2B-C1B	-3.44	1.48	1.53
2	D	301	NAI	C7N-N7N	3.38	1.42	1.33
2	A	301	NAI	C7N-N7N	3.37	1.42	1.33
2	B	301	NAI	C7N-N7N	3.30	1.42	1.33
2	A	301	NAI	C2B-C1B	-3.20	1.48	1.53
2	B	301	NAI	C2B-C1B	-3.14	1.49	1.53
3	B	302	CAA	OAP-CAP	-2.82	1.37	1.42
3	B	302	CAA	O4B-C4B	2.76	1.51	1.45
2	D	301	NAI	C2B-C1B	-2.76	1.49	1.53
2	A	301	NAI	C2A-N3A	2.74	1.36	1.32
2	B	301	NAI	C2A-N3A	2.65	1.36	1.32
2	A	301	NAI	C6A-N6A	2.63	1.43	1.34
2	D	301	NAI	C6A-N6A	2.63	1.43	1.34
2	D	301	NAI	C2A-N3A	2.62	1.36	1.32
2	C	301	NAI	C2A-N3A	2.61	1.36	1.32
2	C	301	NAI	C5D-C4D	2.60	1.59	1.51
2	B	301	NAI	C5D-C4D	2.45	1.59	1.51
2	A	301	NAI	C5D-C4D	2.44	1.59	1.51
2	C	301	NAI	C6A-N6A	2.43	1.42	1.34
2	B	301	NAI	C6A-N6A	2.42	1.42	1.34
2	D	301	NAI	C5D-C4D	2.36	1.58	1.51
3	B	302	CAA	C6A-N6A	2.30	1.42	1.34
2	A	301	NAI	C2D-C3D	-2.28	1.47	1.53
2	C	301	NAI	O3D-C3D	-2.26	1.37	1.43
2	A	301	NAI	O4B-C4B	-2.26	1.39	1.45
2	C	301	NAI	C2D-C3D	-2.26	1.47	1.53
2	A	301	NAI	O3D-C3D	-2.25	1.37	1.43
2	B	301	NAI	C2D-C3D	-2.19	1.47	1.53
2	D	301	NAI	C2D-C3D	-2.19	1.47	1.53
3	B	302	CAA	C2B-C3B	-2.18	1.48	1.52
2	D	301	NAI	O3D-C3D	-2.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAI	O4B-C4B	-2.12	1.40	1.45
3	B	302	CAA	C5A-C4A	2.12	1.46	1.40
3	B	302	CAA	C3B-C4B	-2.08	1.47	1.52
2	D	301	NAI	O4B-C4B	-2.08	1.40	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAI	N3A-C2A-N1A	-5.31	120.38	128.68
2	D	301	NAI	N3A-C2A-N1A	-5.19	120.57	128.68
3	B	302	CAA	C4A-C5A-N7A	-5.08	104.10	109.40
2	B	301	NAI	N3A-C2A-N1A	-4.93	120.97	128.68
2	C	301	NAI	N3A-C2A-N1A	-4.69	121.35	128.68
3	B	302	CAA	C1B-N9A-C4A	-4.26	119.15	126.64
3	B	302	CAA	N3A-C2A-N1A	-4.12	122.23	128.68
3	B	302	CAA	C2P-S1P-C1	3.55	112.92	101.87
3	B	302	CAA	C2-C1-S1P	3.32	117.83	113.69
2	B	301	NAI	C1D-N1N-C2N	-2.73	116.57	121.11
2	C	301	NAI	C1D-N1N-C2N	-2.65	116.69	121.11
3	B	302	CAA	CAP-C9P-N8P	2.65	121.85	116.58
2	D	301	NAI	C4A-C5A-N7A	-2.60	106.69	109.40
2	C	301	NAI	C3N-C7N-N7N	2.47	122.05	117.67
3	B	302	CAA	P2A-O3A-P1A	-2.44	124.44	132.83
3	B	302	CAA	C3B-C2B-C1B	2.38	105.17	99.89
2	D	301	NAI	C3N-C7N-N7N	2.37	121.88	117.67
2	A	301	NAI	C3N-C7N-N7N	2.36	121.86	117.67
2	B	301	NAI	C3N-C2N-N1N	-2.29	119.83	123.10
2	C	301	NAI	C4D-O4D-C1D	-2.28	104.43	109.47
2	C	301	NAI	C4A-C5A-N7A	-2.28	107.02	109.40
2	B	301	NAI	C3N-C7N-N7N	2.27	121.69	117.67
2	D	301	NAI	O4B-C4B-C3B	2.25	109.57	105.11
2	D	301	NAI	C3N-C2N-N1N	-2.22	119.92	123.10
2	D	301	NAI	C1D-N1N-C2N	-2.22	117.41	121.11
3	B	302	CAA	O1-C1-C2	-2.15	119.62	123.35
2	A	301	NAI	O4B-C4B-C3B	2.07	109.21	105.11
2	B	301	NAI	C4D-O4D-C1D	-2.04	104.98	109.47
3	B	302	CAA	C6P-C5P-N4P	2.03	119.84	116.42
2	B	301	NAI	C2D-C1D-N1N	2.01	118.33	113.30

There are no chirality outliers.

All (42) torsion outliers are listed below:

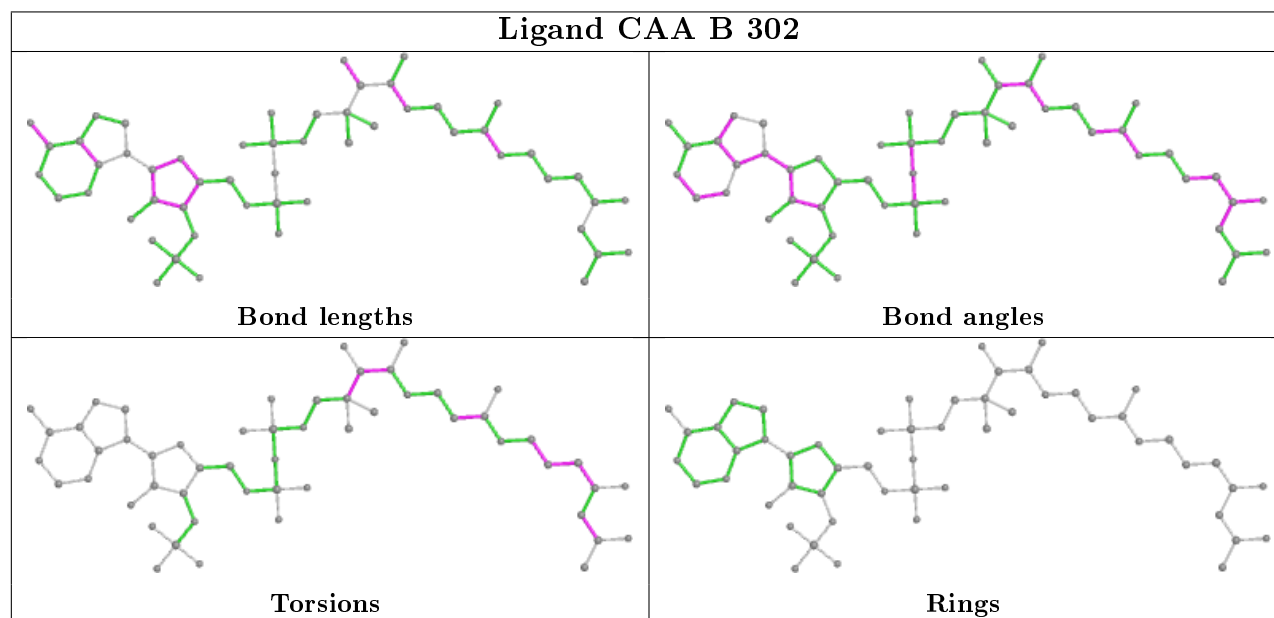
Mol	Chain	Res	Type	Atoms
3	B	302	CAA	OAP-CAP-CBP-CCP
3	B	302	CAA	C9P-CAP-CBP-CCP
3	B	302	CAA	OAP-CAP-CBP-CEP
3	B	302	CAA	C9P-CAP-CBP-CEP
3	B	302	CAA	O9P-C9P-CAP-CBP
3	B	302	CAA	N8P-C9P-CAP-CBP
3	B	302	CAA	N8P-C9P-CAP-OAP
3	B	302	CAA	S1P-C2P-C3P-N4P
3	B	302	CAA	C3P-C2P-S1P-C1
3	B	302	CAA	O1-C1-S1P-C2P
3	B	302	CAA	C2-C1-S1P-C2P
3	B	302	CAA	C1-C2-C3-O3
3	B	302	CAA	C1-C2-C3-C4
2	D	301	NAI	C5D-O5D-PN-O1N
2	D	301	NAI	C5D-O5D-PN-O2N
2	C	301	NAI	C5D-O5D-PN-O3
2	C	301	NAI	C5D-O5D-PN-O1N
2	C	301	NAI	C5D-O5D-PN-O2N
2	B	301	NAI	C5D-O5D-PN-O1N
2	B	301	NAI	C5D-O5D-PN-O2N
2	A	301	NAI	C5D-O5D-PN-O1N
2	A	301	NAI	C5D-O5D-PN-O2N
3	B	302	CAA	OAP-CAP-CBP-CDP
2	C	301	NAI	PN-O3-PA-O5B
2	B	301	NAI	PN-O3-PA-O5B
2	A	301	NAI	PN-O3-PA-O5B
3	B	302	CAA	C9P-CAP-CBP-CDP
2	B	301	NAI	C5D-O5D-PN-O3
2	A	301	NAI	C5D-O5D-PN-O3
2	D	301	NAI	O4D-C1D-N1N-C6N
2	B	301	NAI	O4D-C1D-N1N-C6N
2	C	301	NAI	O4D-C1D-N1N-C6N
2	A	301	NAI	O4D-C1D-N1N-C6N
3	B	302	CAA	O5P-C5P-C6P-C7P
2	D	301	NAI	PA-O3-PN-O2N
3	B	302	CAA	N4P-C5P-C6P-C7P
2	D	301	NAI	C5D-O5D-PN-O3
2	A	301	NAI	PA-O3-PN-O1N
2	D	301	NAI	O4B-C4B-C5B-O5B
2	C	301	NAI	O4B-C4B-C5B-O5B
2	B	301	NAI	O4B-C4B-C5B-O5B
2	A	301	NAI	O4B-C4B-C5B-O5B

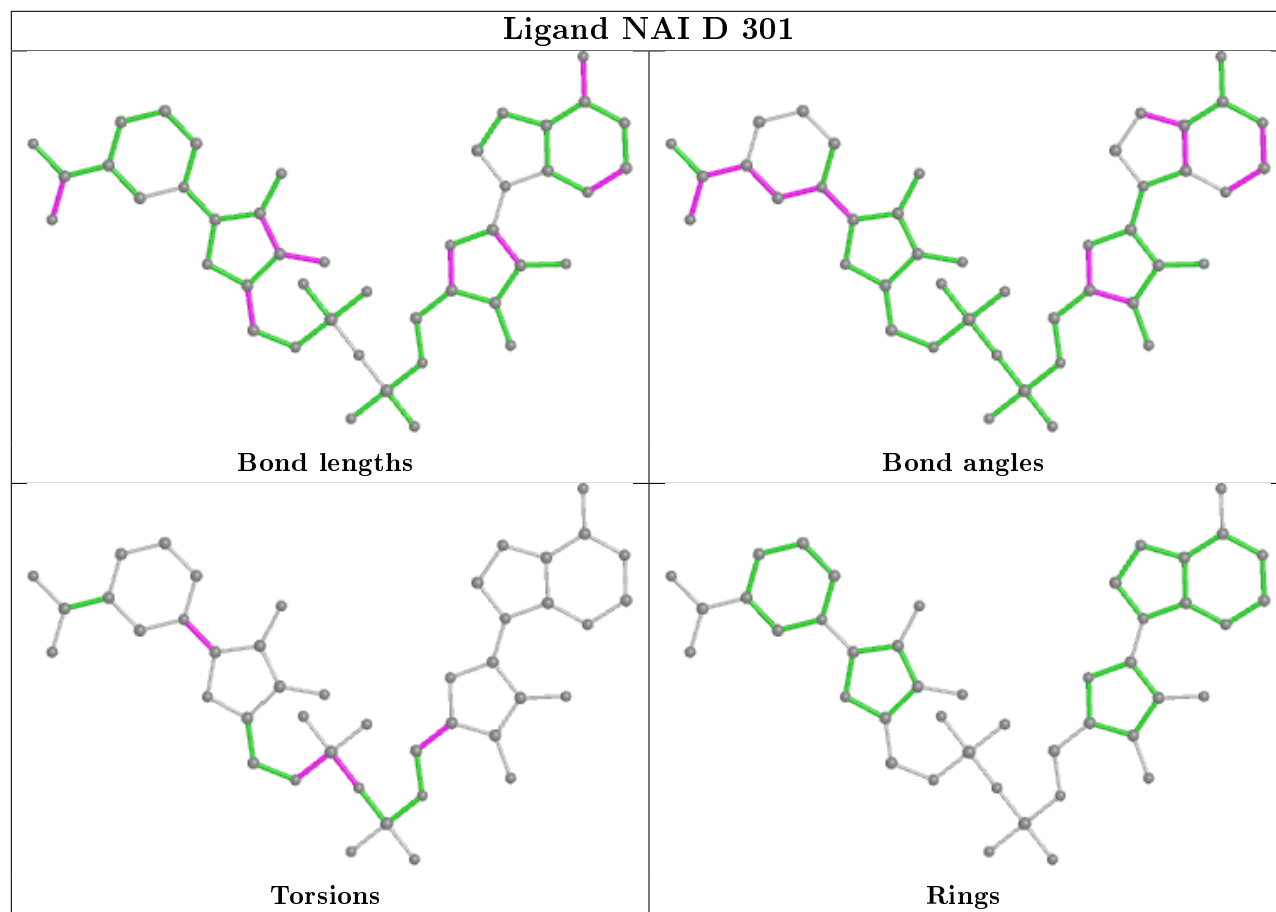
There are no ring outliers.

1 monomer is involved in 1 short contact:

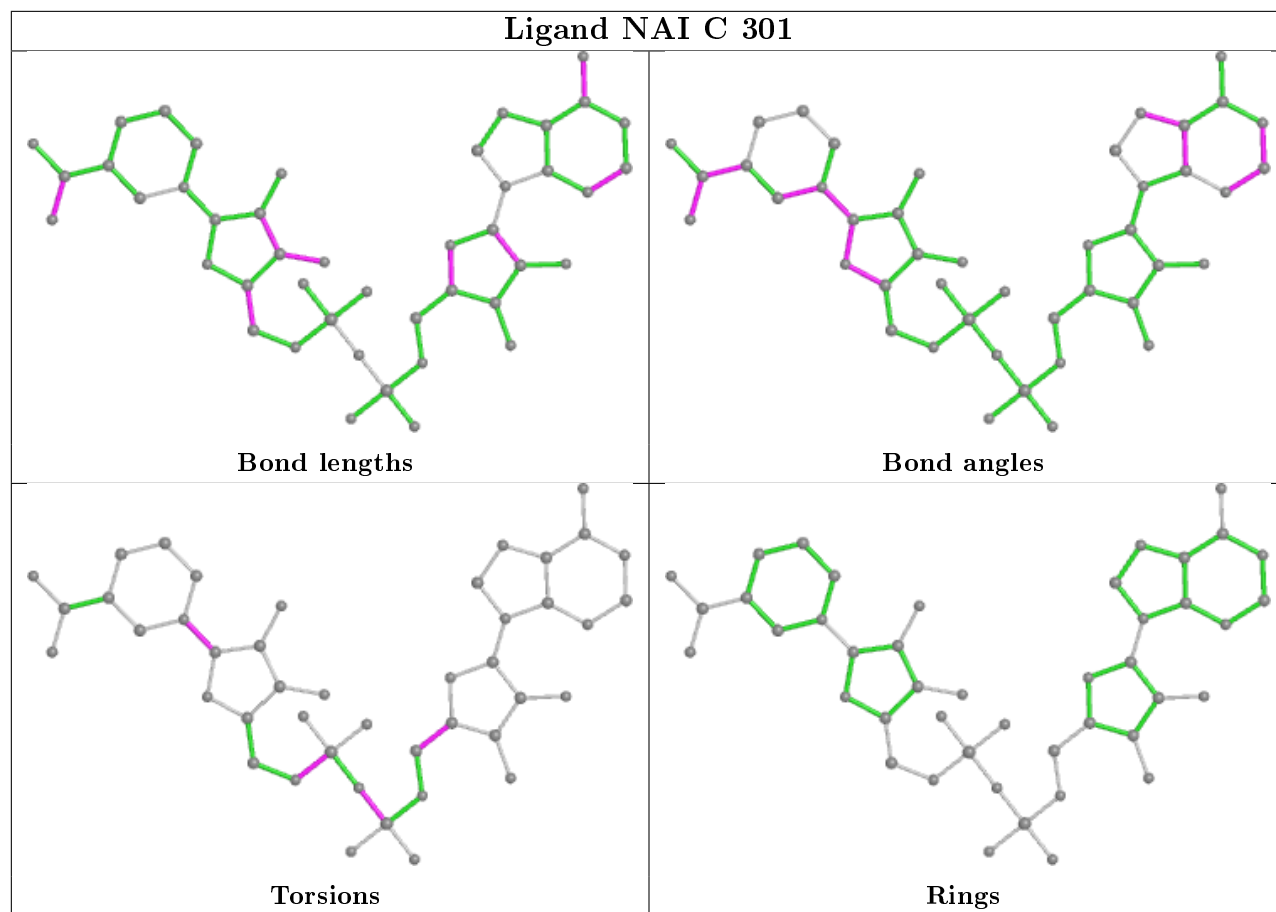
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	CAA	1	0

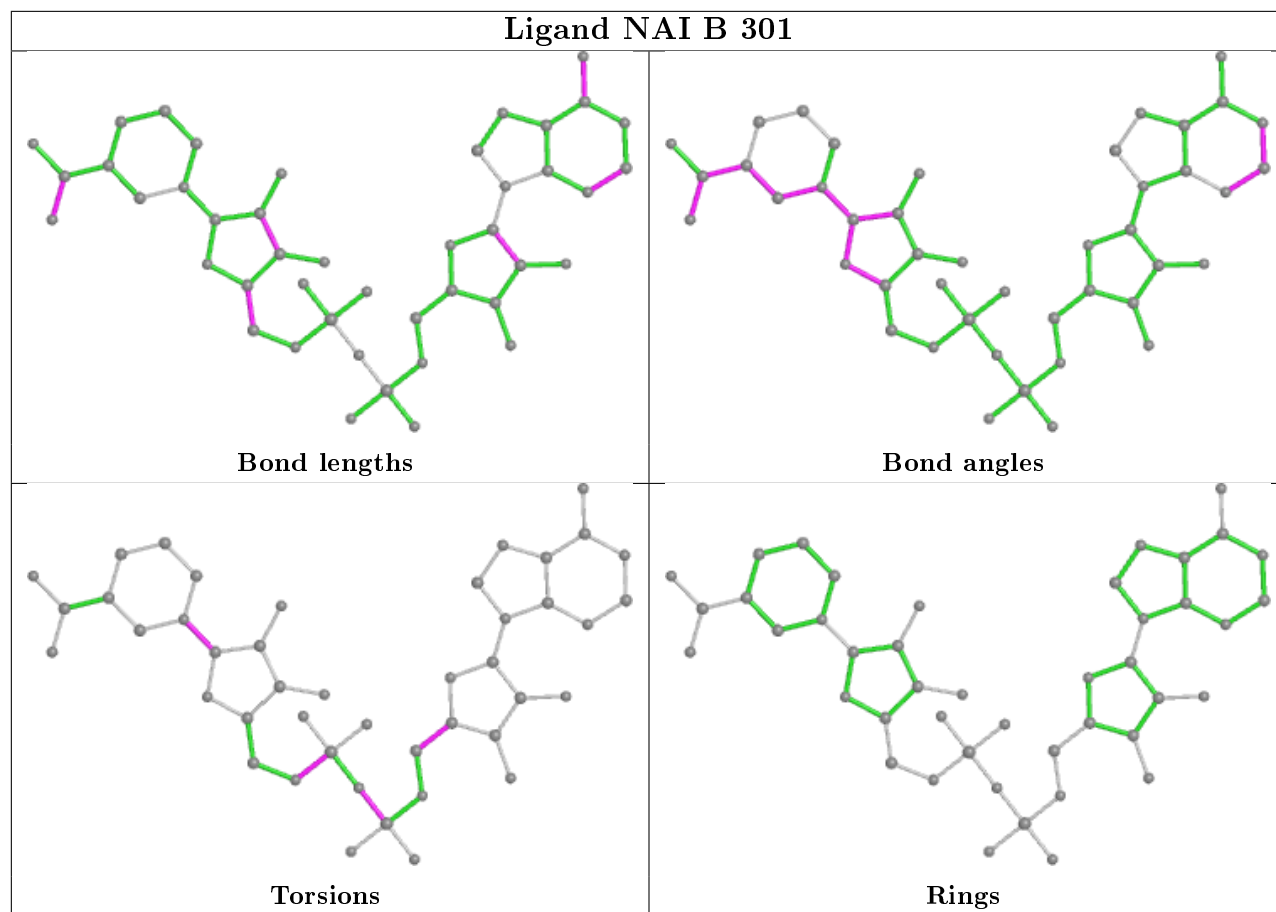
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

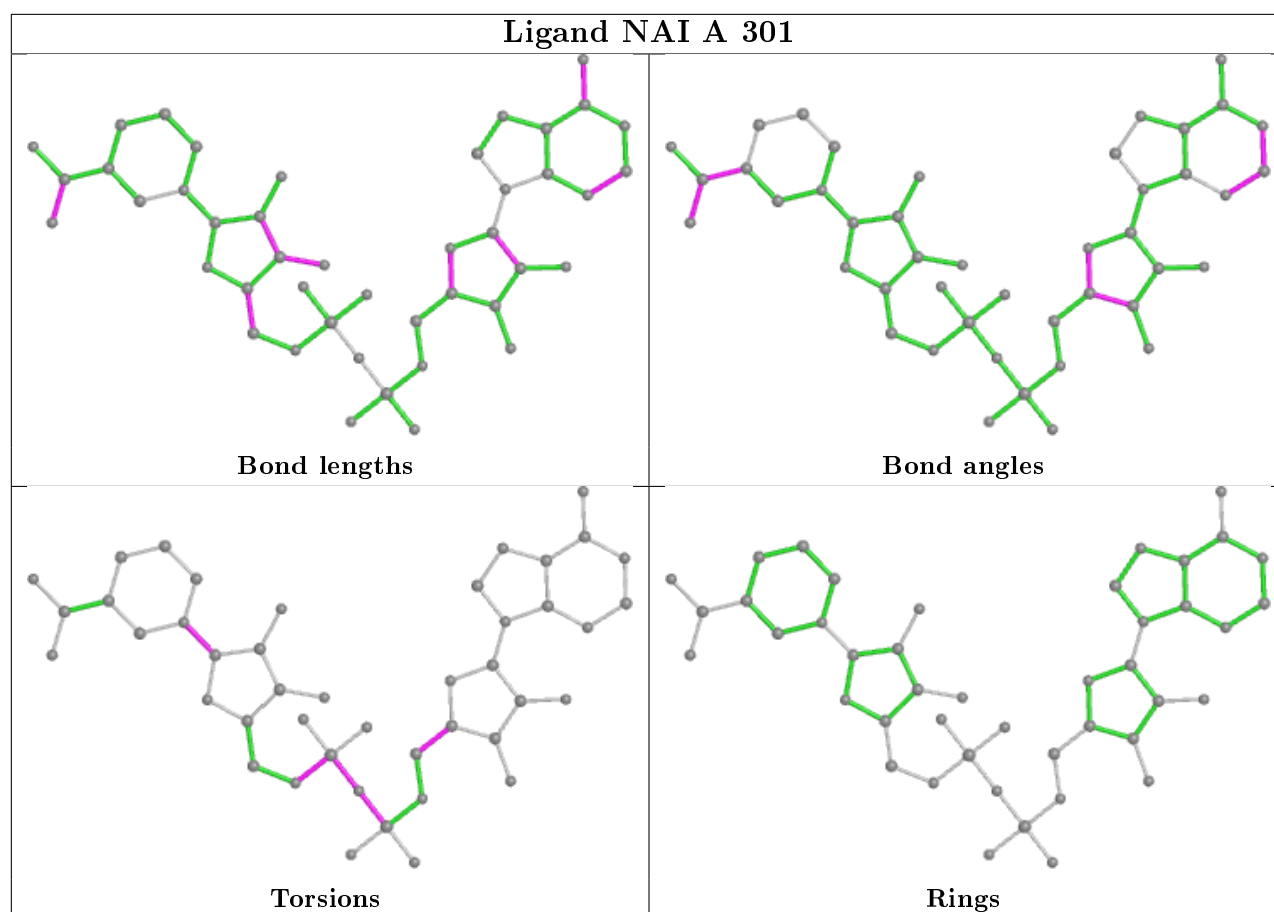












## 5.7 Other polymers [i](#)

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	242/250 (96%)	0.54	20 (8%)	11 12	10, 18, 37, 62	0
1	B	244/250 (97%)	0.53	18 (7%)	14 16	9, 15, 37, 69	0
1	C	242/250 (96%)	0.58	17 (7%)	16 18	10, 17, 39, 66	0
1	D	242/250 (96%)	0.65	20 (8%)	11 12	10, 16, 40, 67	0
All	All	970/1000 (97%)	0.57	75 (7%)	13 15	9, 17, 40, 69	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	199	VAL	12.4
1	B	204	ILE	10.9
1	D	204	ILE	10.8
1	B	199	VAL	8.7
1	B	200	PRO	8.5
1	D	200	PRO	8.4
1	D	197	ALA	8.4
1	B	201	GLU	8.0
1	C	202	LYS	7.9
1	B	202	LYS	7.9
1	C	203	VAL	7.6
1	D	203	VAL	7.6
1	C	199	VAL	6.9
1	C	197	ALA	6.7
1	A	199	VAL	6.6
1	A	198	GLU	6.5
1	D	196	VAL	6.5
1	D	202	LYS	6.5
1	A	204	ILE	6.3
1	A	200	PRO	6.2
1	B	205	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	198	GLU	6.1
1	C	204	ILE	5.9
1	A	197	ALA	5.9
1	B	203	VAL	5.7
1	C	198	GLU	5.6
1	C	200	PRO	5.5
1	A	203	VAL	5.4
1	D	201	GLU	5.4
1	B	198	GLU	5.0
1	B	206	LYS	5.0
1	C	201	GLU	5.0
1	D	205	GLU	4.9
1	B	207	MET	4.9
1	C	196	VAL	4.8
1	A	202	LYS	4.8
1	D	178	ARG	4.8
1	A	201	GLU	4.6
1	C	178	ARG	4.0
1	C	82	GLU	3.6
1	C	205	GLU	3.6
1	C	241	VAL	3.5
1	D	241	VAL	3.5
1	D	195	MET	3.5
1	A	206	LYS	3.3
1	A	196	VAL	3.3
1	A	34	MET	3.3
1	B	7	HIS	3.2
1	A	178	ARG	3.1
1	D	206	LYS	3.1
1	C	134	GLU	3.0
1	A	241	VAL	3.0
1	C	45	PHE	2.9
1	C	206	LYS	2.9
1	D	207	MET	2.9
1	B	196	VAL	2.9
1	D	82	GLU	2.8
1	A	84	PHE	2.8
1	B	178	ARG	2.7
1	D	193	THR	2.7
1	C	207	MET	2.7
1	D	209	ALA	2.7
1	A	82	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	8	MET	2.6
1	A	83	ARG	2.5
1	B	197	ALA	2.5
1	A	205	GLU	2.5
1	A	55	GLU	2.4
1	B	242	LEU	2.4
1	A	242	LEU	2.3
1	D	134	GLU	2.3
1	B	241	VAL	2.2
1	B	186	VAL	2.1
1	D	242	LEU	2.1
1	A	237	VAL	2.1

## 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](#)

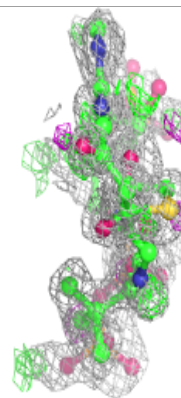
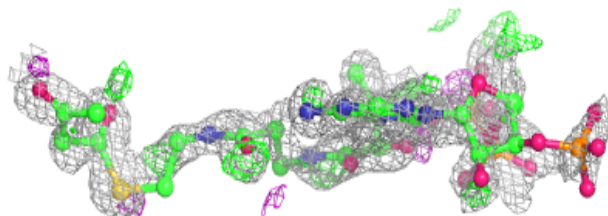
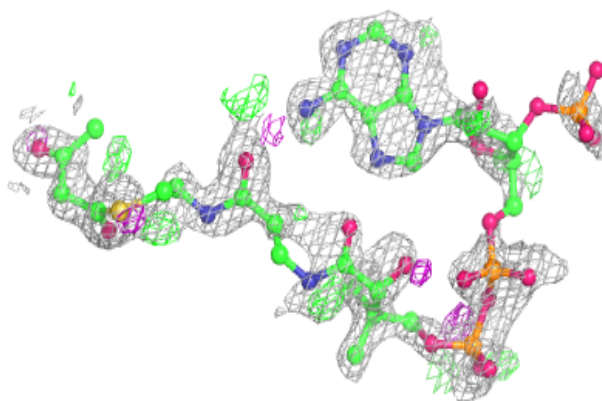
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	CAA	B	302	54/54	0.77	0.24	19,42,97,98	54
2	NAI	D	301	44/44	0.97	0.07	11,14,19,27	0
2	NAI	C	301	44/44	0.97	0.07	11,14,18,23	0
2	NAI	B	301	44/44	0.97	0.07	10,13,16,21	0
2	NAI	A	301	44/44	0.97	0.07	11,14,18,26	0

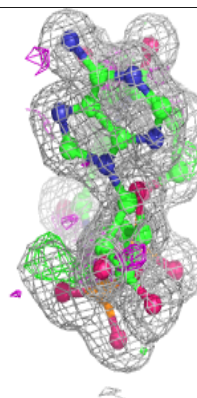
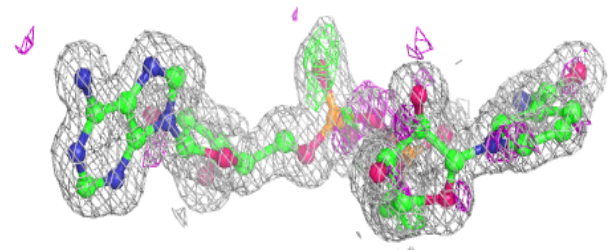
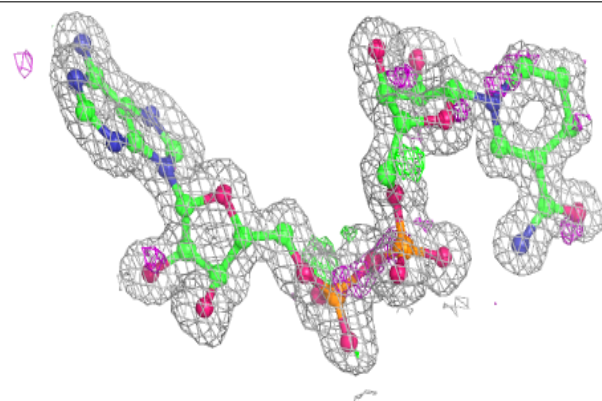
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CAA B 302:**

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

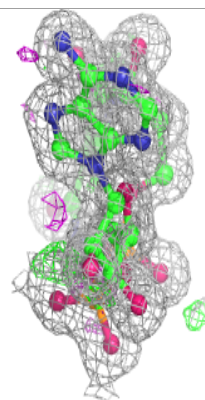
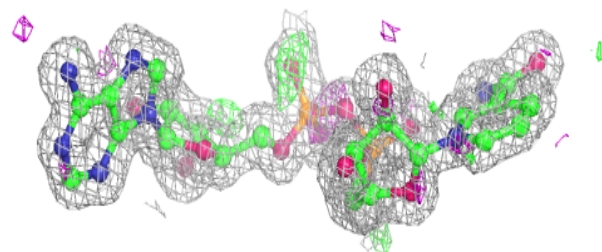
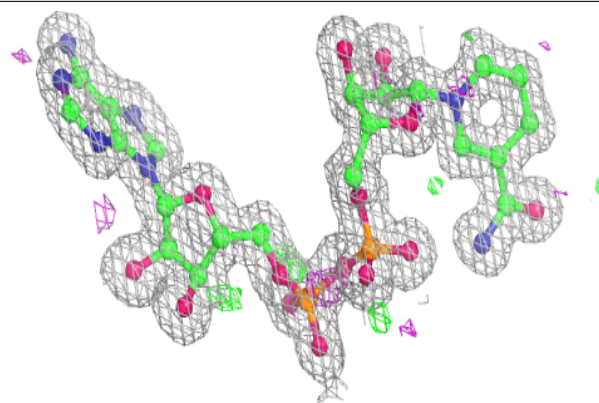
**Electron density around NAI D 301:**

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

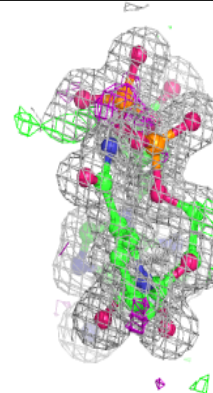
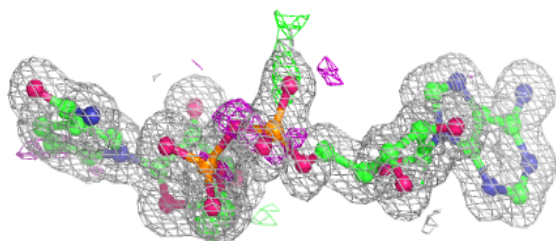
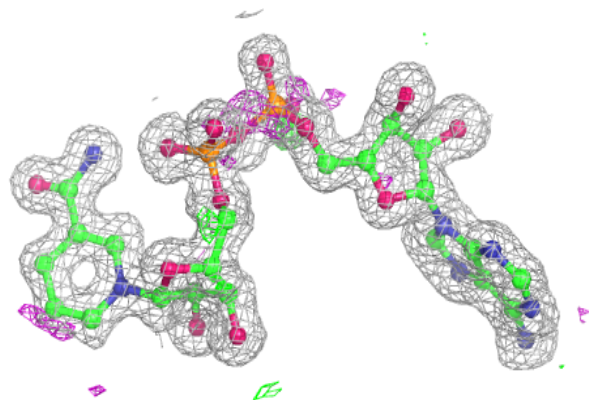


**Electron density around NAI C 301:**

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

**Electron density around NAI B 301:**

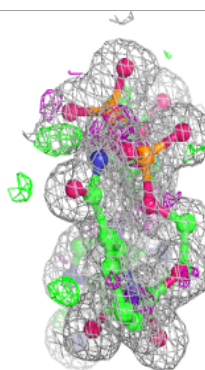
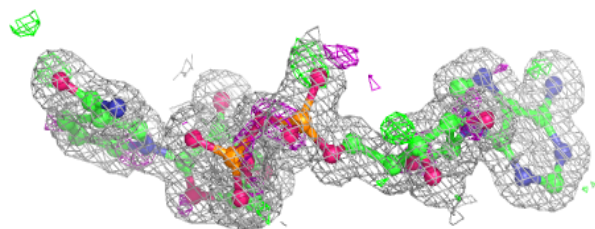
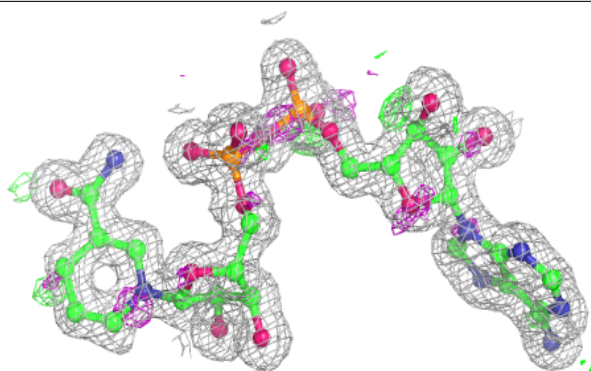
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around NAI 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.