



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:58 am BST

PDB ID : 1WNB  
Title : Escherichia coli YdcW gene product is a medium-chain aldehyde dehydrogenase (complexed with nadh and betaine aldehyde)  
Authors : Gruez, A.; Roig-Zamboni, V.; Tegoni, M.; Cambillau, C.  
Deposited on : 2004-07-29  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

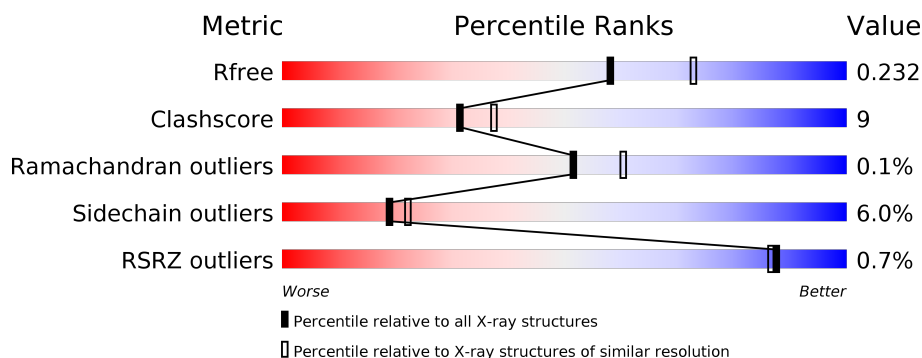
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	495	<div> <div>77%</div> <div>16%</div> <div>• •</div> </div>
1	B	495	<div> <div>77%</div> <div>16%</div> <div>• •</div> </div>
1	C	495	<div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	D	495	<div> <div>2%</div> <div>74%</div> <div>19%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BTL	B	5001	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15318 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 Putative betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	1	0
			3576	2263	616	679	18			
1	B	474	Total	C	N	O	S	9	1	0
			3576	2263	616	679	18			
1	C	474	Total	C	N	O	S	0	1	0
			3576	2263	616	679	18			
1	D	474	Total	C	N	O	S	4	1	0
			3576	2263	616	679	18			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	EXPRESSION TAG	UNP P77674
A	-19	TYR	-	EXPRESSION TAG	UNP P77674
A	-18	TYR	-	EXPRESSION TAG	UNP P77674
A	-17	HIS	-	EXPRESSION TAG	UNP P77674
A	-16	HIS	-	EXPRESSION TAG	UNP P77674
A	-15	HIS	-	EXPRESSION TAG	UNP P77674
A	-14	HIS	-	EXPRESSION TAG	UNP P77674
A	-13	HIS	-	EXPRESSION TAG	UNP P77674
A	-12	HIS	-	EXPRESSION TAG	UNP P77674
A	-11	LEU	-	EXPRESSION TAG	UNP P77674
A	-10	GLU	-	EXPRESSION TAG	UNP P77674
A	-9	SER	-	EXPRESSION TAG	UNP P77674
A	-8	THR	-	EXPRESSION TAG	UNP P77674
A	-7	SER	-	EXPRESSION TAG	UNP P77674
A	-6	LEU	-	EXPRESSION TAG	UNP P77674
A	-5	TYR	-	EXPRESSION TAG	UNP P77674
A	-4	LYS	-	EXPRESSION TAG	UNP P77674
A	-3	LYS	-	EXPRESSION TAG	UNP P77674
A	-2	ALA	-	EXPRESSION TAG	UNP P77674
A	-1	GLY	-	EXPRESSION TAG	UNP P77674
A	0	LEU	-	EXPRESSION TAG	UNP P77674

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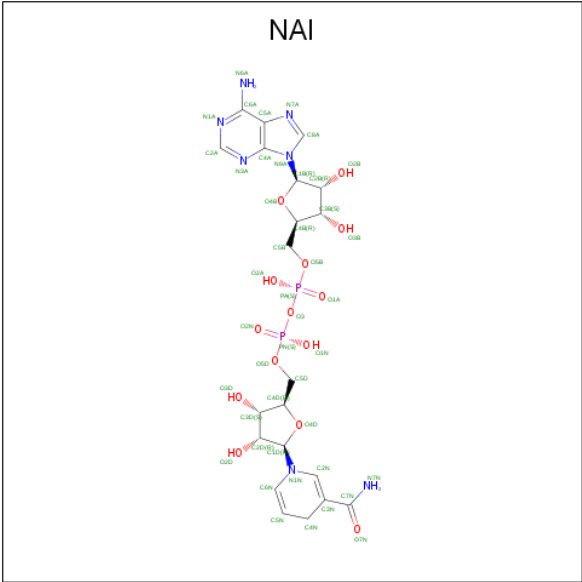
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	VAL	ILE	CONFLICT	UNP P77674
B	-20	SER	-	EXPRESSION TAG	UNP P77674
B	-19	TYR	-	EXPRESSION TAG	UNP P77674
B	-18	TYR	-	EXPRESSION TAG	UNP P77674
B	-17	HIS	-	EXPRESSION TAG	UNP P77674
B	-16	HIS	-	EXPRESSION TAG	UNP P77674
B	-15	HIS	-	EXPRESSION TAG	UNP P77674
B	-14	HIS	-	EXPRESSION TAG	UNP P77674
B	-13	HIS	-	EXPRESSION TAG	UNP P77674
B	-12	HIS	-	EXPRESSION TAG	UNP P77674
B	-11	LEU	-	EXPRESSION TAG	UNP P77674
B	-10	GLU	-	EXPRESSION TAG	UNP P77674
B	-9	SER	-	EXPRESSION TAG	UNP P77674
B	-8	THR	-	EXPRESSION TAG	UNP P77674
B	-7	SER	-	EXPRESSION TAG	UNP P77674
B	-6	LEU	-	EXPRESSION TAG	UNP P77674
B	-5	TYR	-	EXPRESSION TAG	UNP P77674
B	-4	LYS	-	EXPRESSION TAG	UNP P77674
B	-3	LYS	-	EXPRESSION TAG	UNP P77674
B	-2	ALA	-	EXPRESSION TAG	UNP P77674
B	-1	GLY	-	EXPRESSION TAG	UNP P77674
B	0	LEU	-	EXPRESSION TAG	UNP P77674
B	197	VAL	ILE	CONFLICT	UNP P77674
C	-20	SER	-	EXPRESSION TAG	UNP P77674
C	-19	TYR	-	EXPRESSION TAG	UNP P77674
C	-18	TYR	-	EXPRESSION TAG	UNP P77674
C	-17	HIS	-	EXPRESSION TAG	UNP P77674
C	-16	HIS	-	EXPRESSION TAG	UNP P77674
C	-15	HIS	-	EXPRESSION TAG	UNP P77674
C	-14	HIS	-	EXPRESSION TAG	UNP P77674
C	-13	HIS	-	EXPRESSION TAG	UNP P77674
C	-12	HIS	-	EXPRESSION TAG	UNP P77674
C	-11	LEU	-	EXPRESSION TAG	UNP P77674
C	-10	GLU	-	EXPRESSION TAG	UNP P77674
C	-9	SER	-	EXPRESSION TAG	UNP P77674
C	-8	THR	-	EXPRESSION TAG	UNP P77674
C	-7	SER	-	EXPRESSION TAG	UNP P77674
C	-6	LEU	-	EXPRESSION TAG	UNP P77674
C	-5	TYR	-	EXPRESSION TAG	UNP P77674
C	-4	LYS	-	EXPRESSION TAG	UNP P77674
C	-3	LYS	-	EXPRESSION TAG	UNP P77674
C	-2	ALA	-	EXPRESSION TAG	UNP P77674

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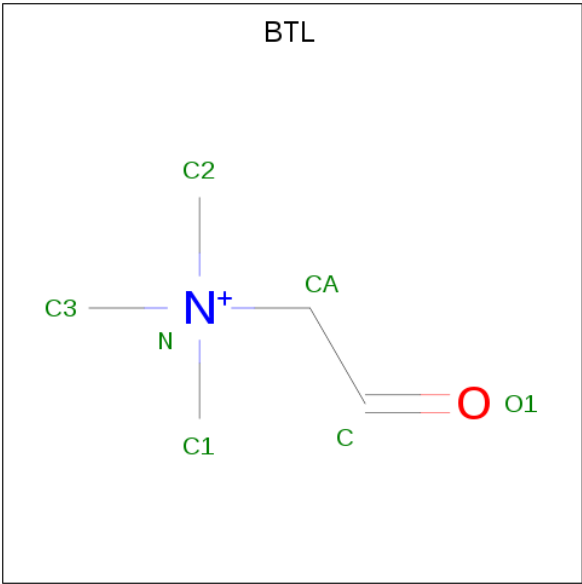
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P77674
C	0	LEU	-	EXPRESSION TAG	UNP P77674
C	197	VAL	ILE	CONFLICT	UNP P77674
D	-20	SER	-	EXPRESSION TAG	UNP P77674
D	-19	TYR	-	EXPRESSION TAG	UNP P77674
D	-18	TYR	-	EXPRESSION TAG	UNP P77674
D	-17	HIS	-	EXPRESSION TAG	UNP P77674
D	-16	HIS	-	EXPRESSION TAG	UNP P77674
D	-15	HIS	-	EXPRESSION TAG	UNP P77674
D	-14	HIS	-	EXPRESSION TAG	UNP P77674
D	-13	HIS	-	EXPRESSION TAG	UNP P77674
D	-12	HIS	-	EXPRESSION TAG	UNP P77674
D	-11	LEU	-	EXPRESSION TAG	UNP P77674
D	-10	GLU	-	EXPRESSION TAG	UNP P77674
D	-9	SER	-	EXPRESSION TAG	UNP P77674
D	-8	THR	-	EXPRESSION TAG	UNP P77674
D	-7	SER	-	EXPRESSION TAG	UNP P77674
D	-6	LEU	-	EXPRESSION TAG	UNP P77674
D	-5	TYR	-	EXPRESSION TAG	UNP P77674
D	-4	LYS	-	EXPRESSION TAG	UNP P77674
D	-3	LYS	-	EXPRESSION TAG	UNP P77674
D	-2	ALA	-	EXPRESSION TAG	UNP P77674
D	-1	GLY	-	EXPRESSION TAG	UNP P77674
D	0	LEU	-	EXPRESSION TAG	UNP P77674
D	197	VAL	ILE	CONFLICT	UNP P77674

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



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 BETAINE ALDEHYDE (three-letter code: BTL) (formula: C<sub>5</sub>H<sub>12</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 4 is water.

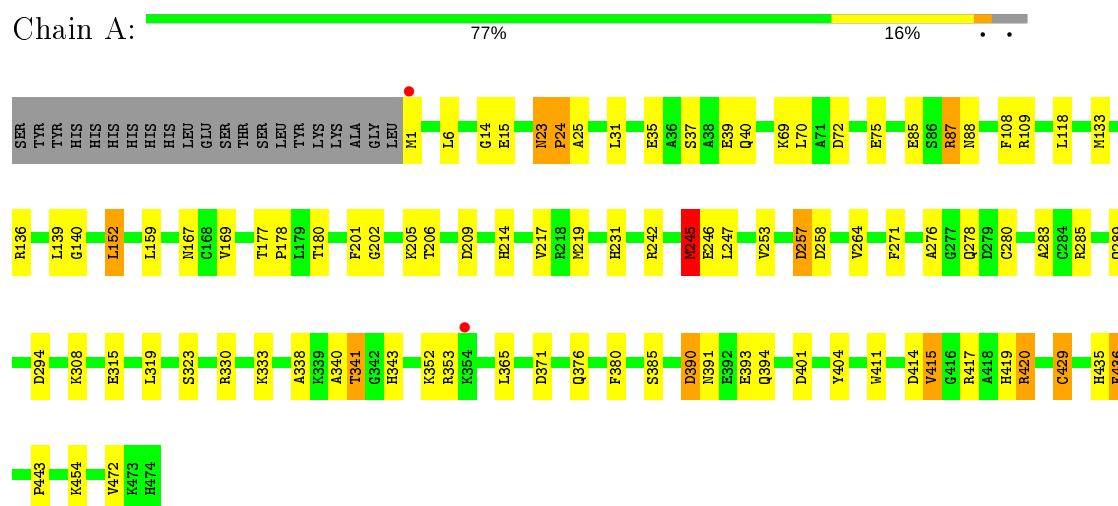
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		
4	B	216	Total	O	0	0
			216	216		
4	C	240	Total	O	0	0
			240	240		
4	D	176	Total	O	0	0
			176	176		



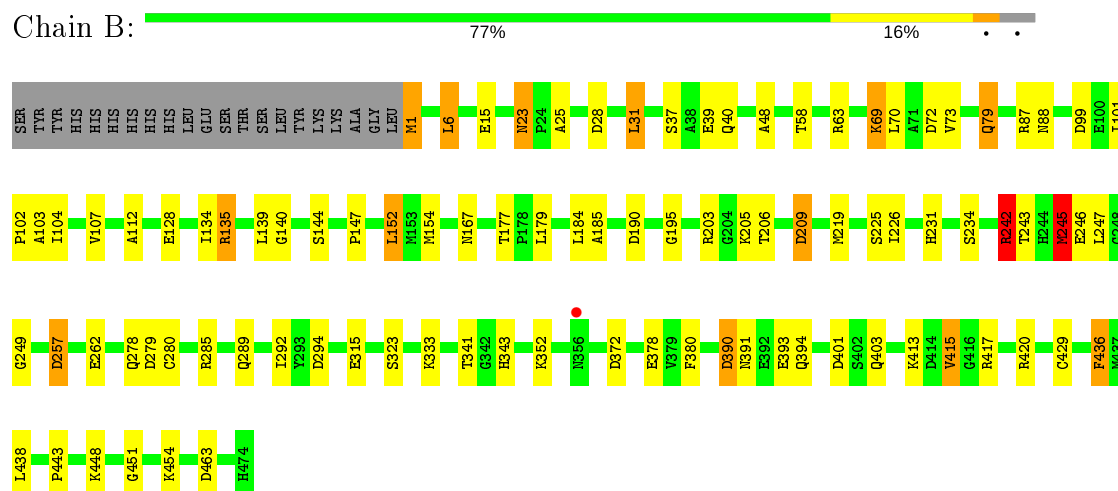
### 3 Residue-property plots

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.

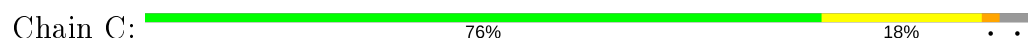
- Molecule 1: Putative betaine aldehyde dehydrogenase

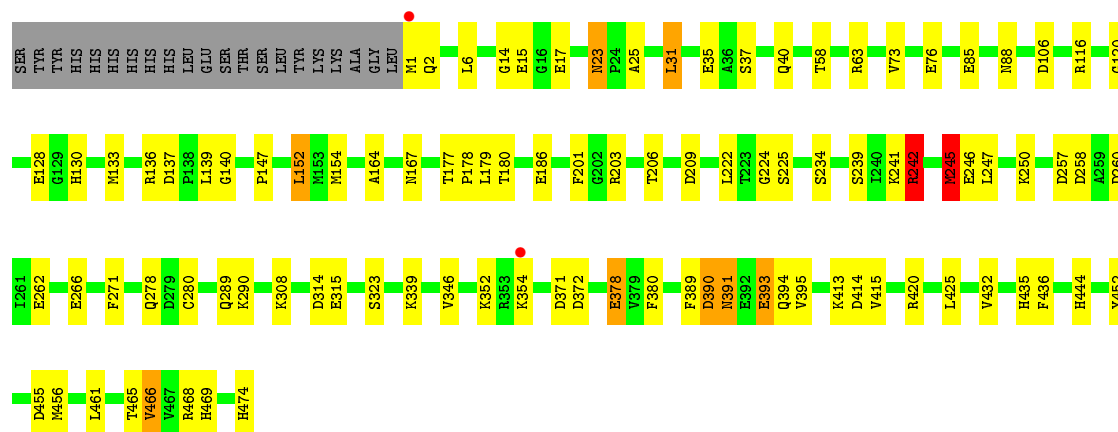


- Molecule 1: Putative betaine aldehyde dehydrogenase

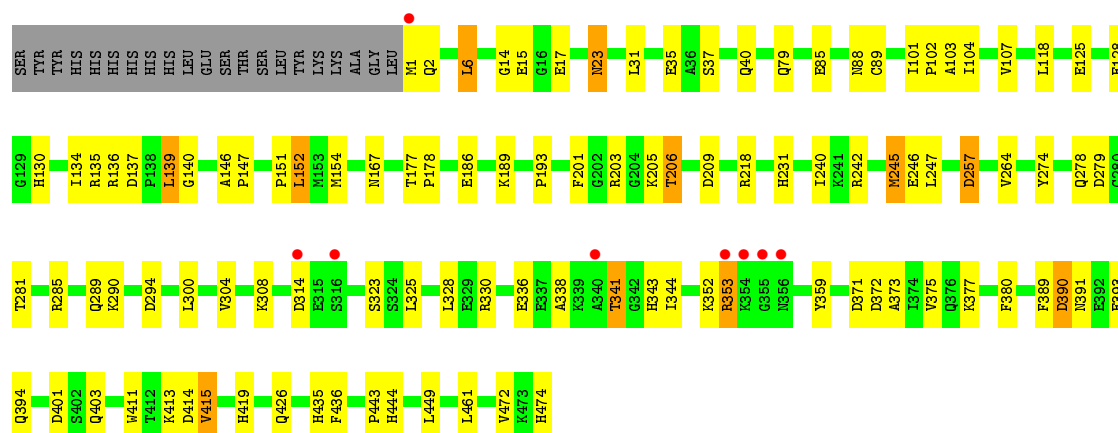
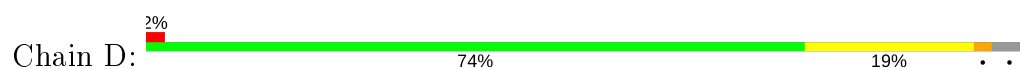


- Molecule 1: Putative betaine aldehyde dehydrogenase





● Molecule 1: Putative betaine aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.28Å 168.90Å 85.48Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	18.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.6 (18.00-2.20) 69.9 (20.00-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.182 , 0.239 0.179 , 0.232	Depositor DCC
$R_{free}$ test set	6660 reflections (8.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BTL, 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	0.96	0/3655	1.00	15/4963 (0.3%)
1	B	0.99	1/3655 (0.0%)	1.01	20/4963 (0.4%)
1	C	1.03	2/3655 (0.1%)	1.04	18/4963 (0.4%)
1	D	0.97	3/3655 (0.1%)	1.00	15/4963 (0.3%)
All	All	0.99	6/14620 (0.0%)	1.01	68/19852 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	PRO	N-CD	-9.41	1.34	1.47
1	B	112	ALA	CA-CB	5.88	1.64	1.52
1	D	137	ASP	C-N	5.78	1.45	1.34
1	C	378	GLU	CD-OE2	5.41	1.31	1.25
1	C	466	VAL	CB-CG1	-5.33	1.41	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	MET	CG-SD-CE	13.05	121.08	100.20
1	A	390	ASP	CB-CG-OD2	12.81	129.82	118.30
1	C	136	ARG	NE-CZ-NH1	-12.45	114.07	120.30
1	D	390	ASP	CB-CG-OD2	11.26	128.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ARG	NE-CZ-NH2	11.17	125.88	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	ARG	Sidechain

## 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	3576	0	3559	62	0
1	B	3576	0	3559	58	0
1	C	3576	0	3559	76	0
1	D	3576	0	3559	63	0
2	A	44	0	27	10	0
2	B	44	0	27	3	0
2	C	44	0	27	7	0
2	D	44	0	27	2	0
3	B	7	0	12	6	0
4	A	199	0	0	10	0
4	B	216	0	0	5	0
4	C	240	0	0	13	0
4	D	176	0	0	6	0
All	All	15318	0	14356	260	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 9.

The worst 5 of 260 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280[B]:CYS:SG	2:B:2001:NAI:N7N	2.28	1.06
2:A:1001:NAI:H51N	2:A:1001:NAI:H6N	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HB3	1:C:245:MET:HE2	1.06	1.04
1:C:222:LEU:HB3	1:C:245:MET:CE	1.91	1.00
1:B:139:LEU:H	1:B:167:ASN:HD21	1.17	0.93

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	473/495 (96%)	458 (97%)	15 (3%)	0	100	100
1	B	473/495 (96%)	459 (97%)	14 (3%)	0	100	100
1	C	473/495 (96%)	462 (98%)	11 (2%)	0	100	100
1	D	473/495 (96%)	457 (97%)	15 (3%)	1 (0%)	47	55
All	All	1892/1980 (96%)	1836 (97%)	55 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	189	LYS

### 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	372/390 (95%)	349 (94%)	23 (6%)	18	21
1	B	372/390 (95%)	346 (93%)	26 (7%)	15	16
1	C	372/390 (95%)	352 (95%)	20 (5%)	22	26
1	D	372/390 (95%)	352 (95%)	20 (5%)	22	26
All	All	1488/1560 (95%)	1399 (94%)	89 (6%)	19	22

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	315	GLU
1	C	6	LEU
1	D	308	LYS
1	B	333	LYS
1	B	403	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	403	GLN
1	C	77	ASN
1	D	289	GLN
1	B	444	HIS
1	C	3	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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
2	NAI	C	3001	-	42,48,48	1.96	7 (16%)	47,73,73	1.89	13 (27%)
2	NAI	A	1001	-	42,48,48	1.99	6 (14%)	47,73,73	2.32	17 (36%)
2	NAI	D	4001	-	42,48,48	2.06	7 (16%)	47,73,73	1.79	8 (17%)
3	BTL	B	5001	-	6,6,6	1.06	0	4,8,8	2.80	2 (50%)
2	NAI	B	2001	-	42,48,48	1.97	8 (19%)	47,73,73	1.75	7 (14%)

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	NAI	C	3001	-	-	11/25/72/72	0/5/5/5
2	NAI	A	1001	-	-	11/25/72/72	0/5/5/5
2	NAI	D	4001	-	-	11/25/72/72	0/5/5/5
3	BTL	B	5001	-	-	1/3/4/4	-
2	NAI	B	2001	-	-	9/25/72/72	0/5/5/5

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4001	NAI	O7N-C7N	8.19	1.43	1.24
2	C	3001	NAI	O7N-C7N	7.49	1.42	1.24
2	B	2001	NAI	O7N-C7N	6.56	1.40	1.24
2	A	1001	NAI	O7N-C7N	6.46	1.39	1.24
2	A	1001	NAI	C4N-C3N	-5.86	1.38	1.49

The worst 5 of 47 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	4001	NAI	PN-O3-PA	-7.34	107.65	132.83
2	B	2001	NAI	N3A-C2A-N1A	-6.98	117.77	128.68
2	C	3001	NAI	O4D-C1D-N1N	6.40	120.56	108.06
2	A	1001	NAI	C1D-N1N-C2N	5.77	130.72	121.11
2	A	1001	NAI	C3N-C2N-N1N	-5.61	115.09	123.10

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

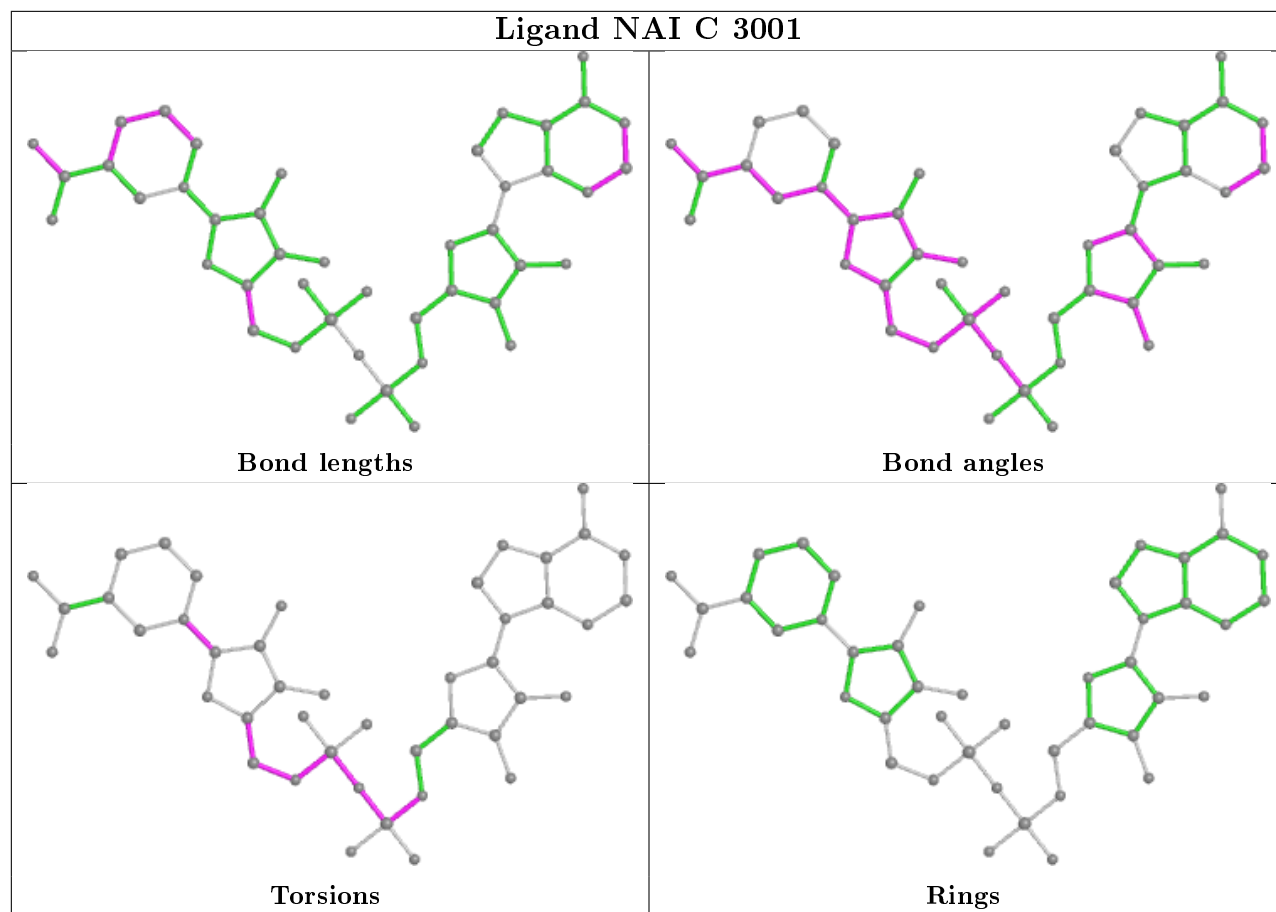
Mol	Chain	Res	Type	Atoms
2	A	1001	NAI	C5B-O5B-PA-O3
2	A	1001	NAI	PA-O3-PN-O5D
2	A	1001	NAI	C5D-O5D-PN-O3
2	D	4001	NAI	C5D-O5D-PN-O3
2	D	4001	NAI	C5D-O5D-PN-O2N

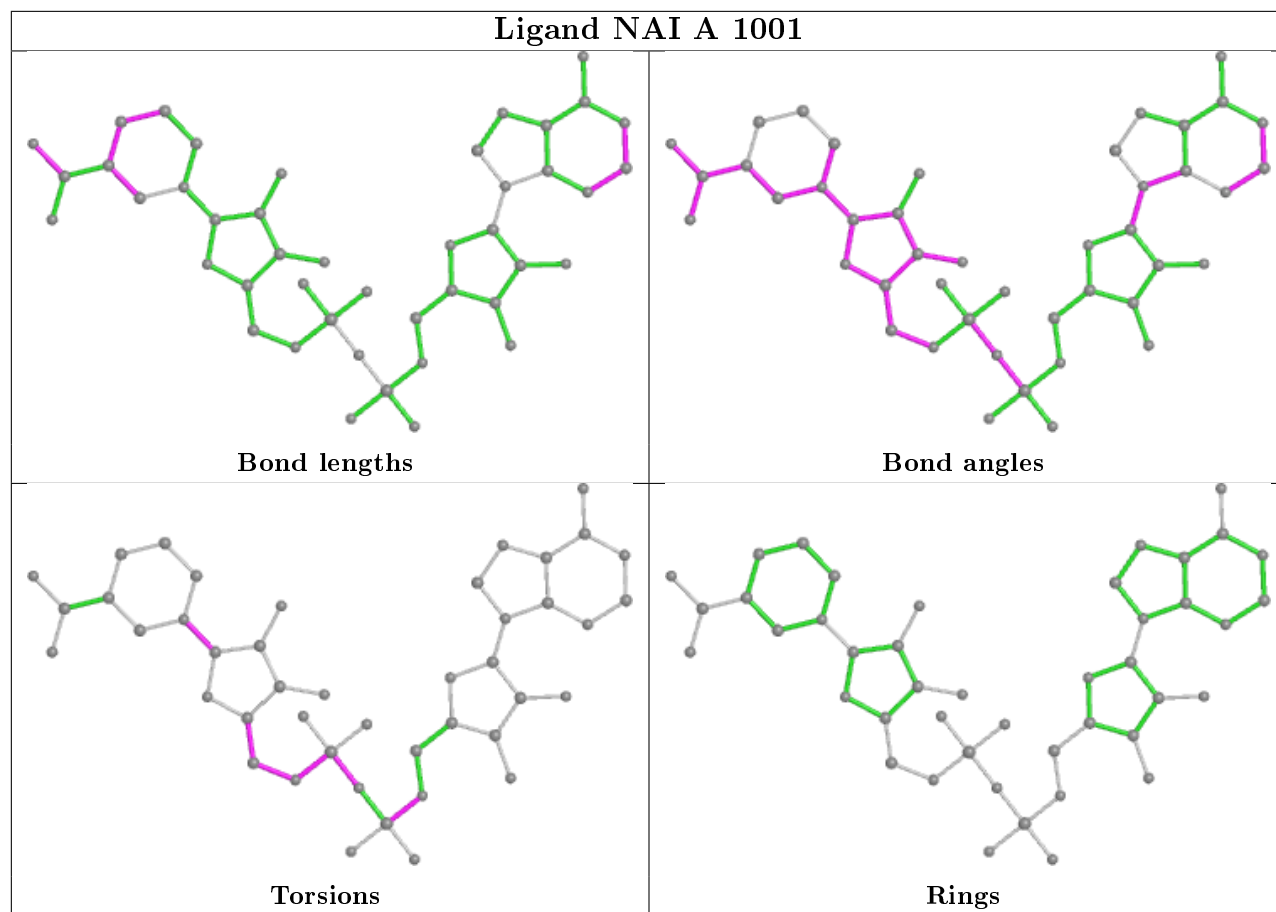
There are no ring outliers.

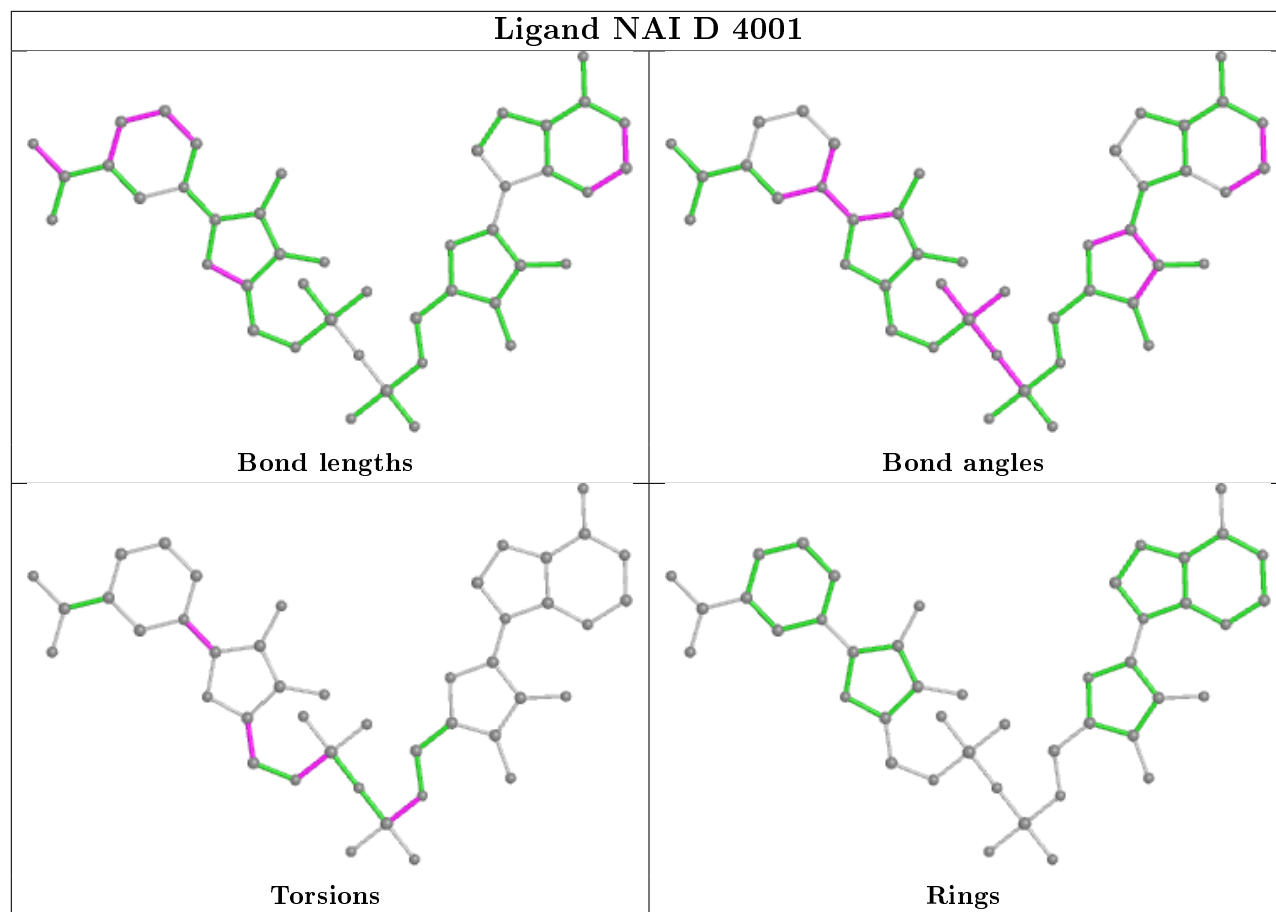
5 monomers are involved in 28 short contacts:

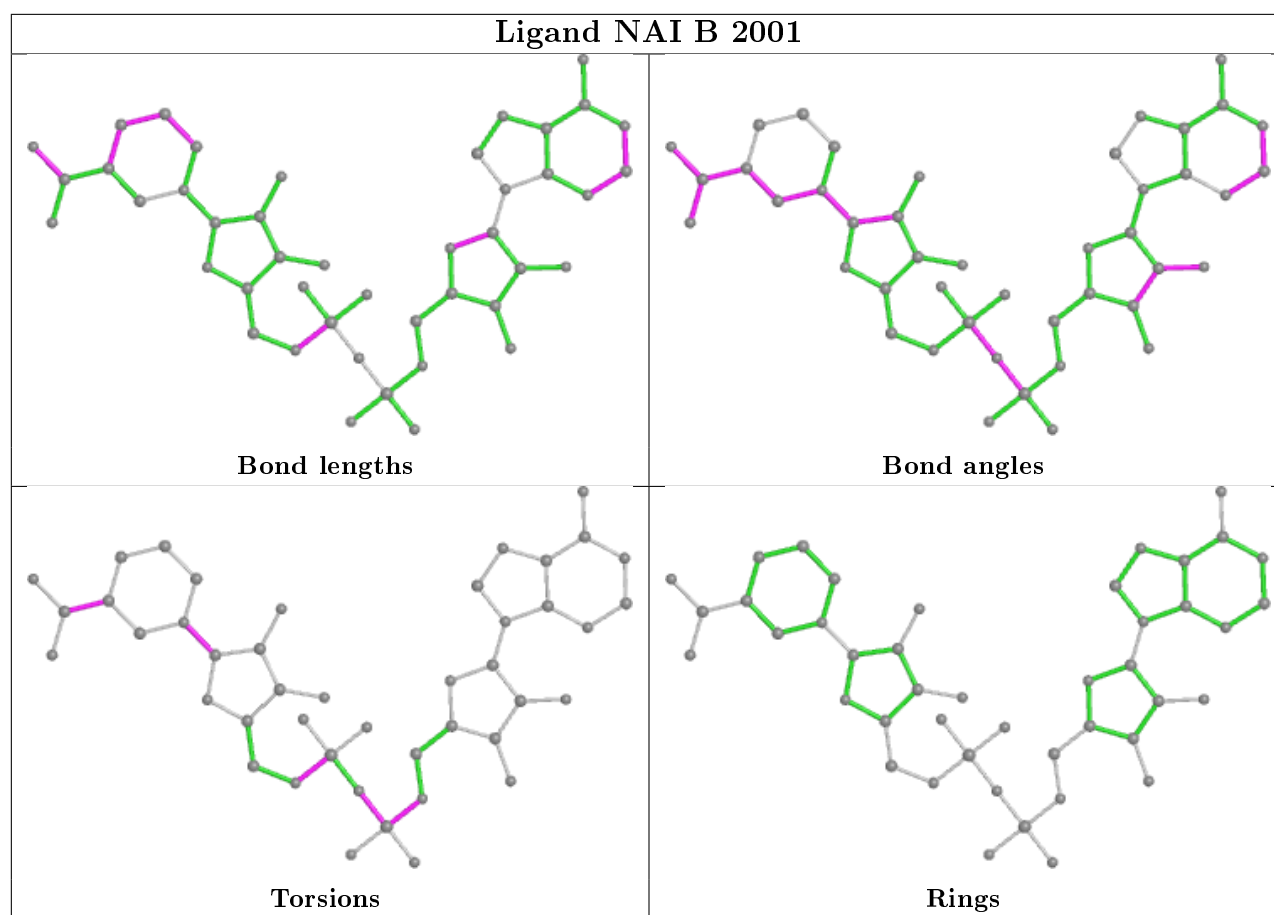
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3001	NAI	7	0
2	A	1001	NAI	10	0
2	D	4001	NAI	2	0
3	B	5001	BTL	6	0
2	B	2001	NAI	3	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	474/495 (95%)	-0.63	2 (0%) 92 91	7, 13, 18, 24	12 (2%)
1	B	474/495 (95%)	-0.66	1 (0%) 95 94	7, 12, 18, 23	11 (2%)
1	C	474/495 (95%)	-0.72	2 (0%) 92 91	7, 12, 18, 25	8 (1%)
1	D	474/495 (95%)	-0.55	8 (1%) 70 68	7, 13, 18, 26	10 (2%)
All	All	1896/1980 (95%)	-0.64	13 (0%) 87 86	7, 12, 18, 26	41 (2%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	340	ALA	3.5
1	D	354	LYS	3.2
1	A	1	MET	2.8
1	C	1	MET	2.6
1	C	354	LYS	2.6

### 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](#)

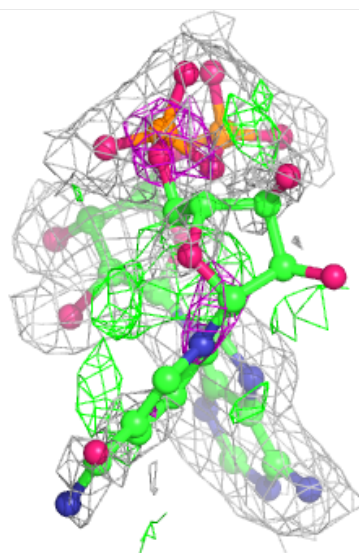
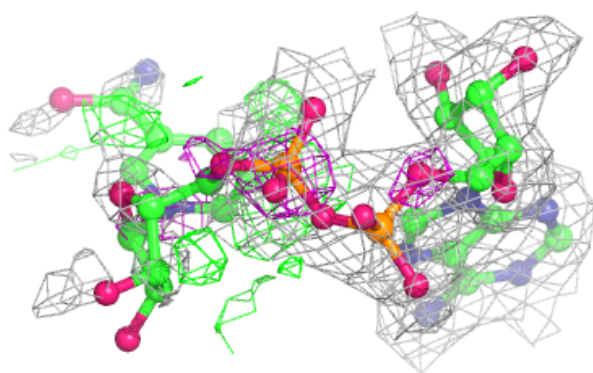
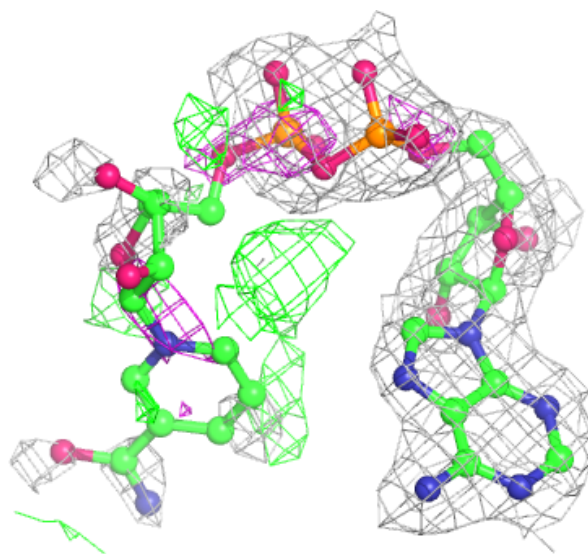
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	BTL	B	5001	7/7	0.91	0.17	31,32,34,34	0
2	NAI	D	4001	44/44	0.93	0.22	19,25,32,39	18
2	NAI	C	3001	44/44	0.93	0.15	18,22,31,39	17
2	NAI	B	2001	44/44	0.93	0.17	18,24,29,36	17
2	NAI	A	1001	44/44	0.94	0.14	21,24,29,32	21

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.

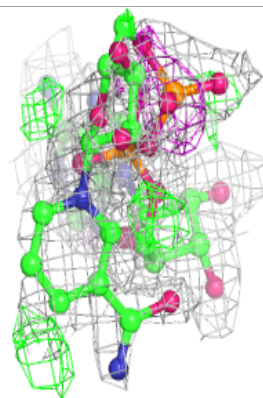
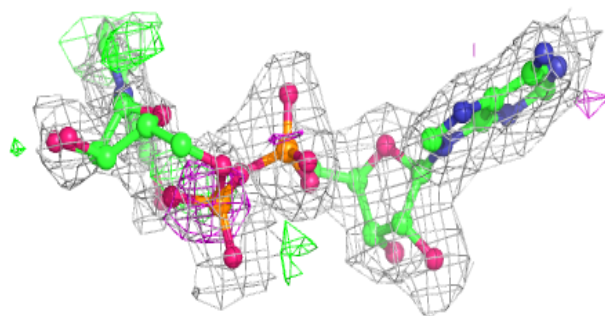
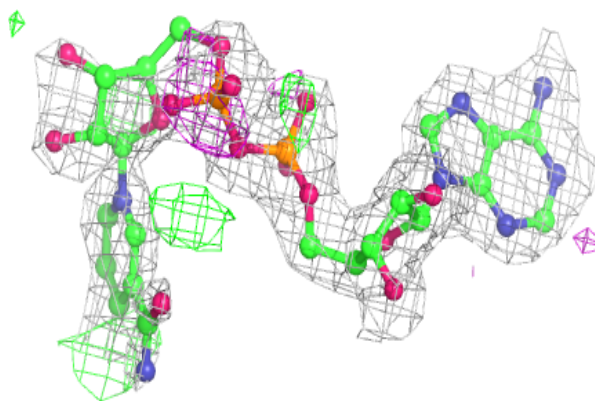
**Electron density around NAI D 4001:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

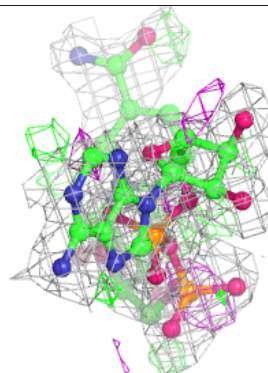
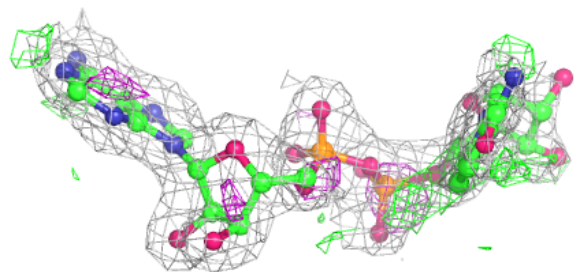
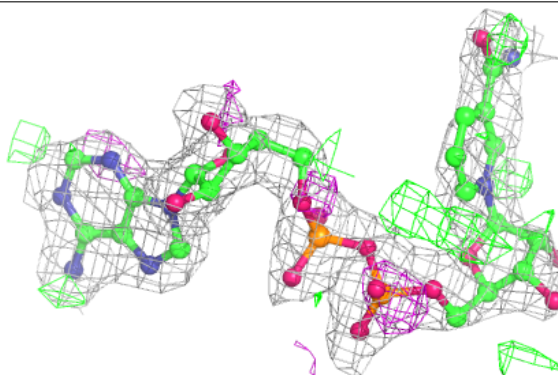


**Electron density around NAI C 3001:**

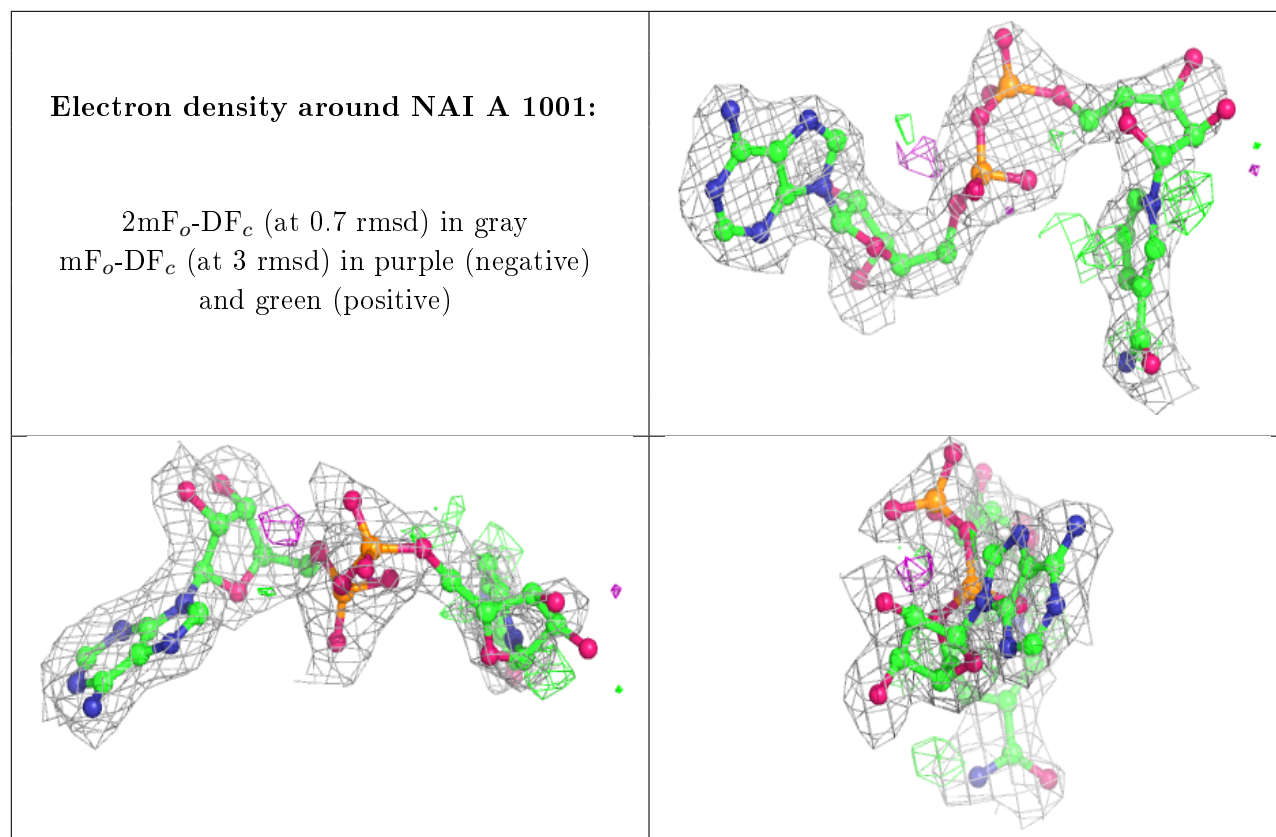
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAI B 2001:**

$2mF_o-DF_c$  (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.