



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:06 AM BST

PDB ID : 6A3G  
Title : Levoglucosan dehydrogenase, complex with NADH  
Authors : Sugiura, M.; Yamada, C.; Arakawa, T.; Fushinobu, S.  
Deposited on : 2018-06-15  
Resolution : 1.90 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 : 2.13.1  
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

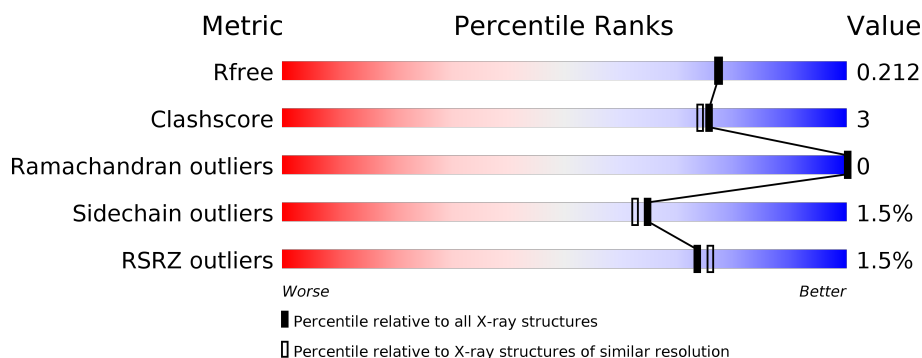
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	410	<div> <div> <div></div> <div>83%</div> <div>7%</div> <div>9%</div> </div> </div>
1	B	410	<div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	C	410	<div> <div> <div></div> <div>86%</div> <div>6%</div> <div>9%</div> </div> </div>
1	D	410	<div> <div> <div></div> <div>86%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12385 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 dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2865	1823	497	535	10			
1	B	372	Total	C	N	O	S	0	0	0
			2864	1823	497	535	9			
1	C	374	Total	C	N	O	S	0	0	0
			2876	1829	499	539	9			
1	D	371	Total	C	N	O	S	0	0	0
			2855	1818	495	533	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP F0M433
A	-18	GLY	-	expression tag	UNP F0M433
A	-17	SER	-	expression tag	UNP F0M433
A	-16	SER	-	expression tag	UNP F0M433
A	-15	HIS	-	expression tag	UNP F0M433
A	-14	HIS	-	expression tag	UNP F0M433
A	-13	HIS	-	expression tag	UNP F0M433
A	-12	HIS	-	expression tag	UNP F0M433
A	-11	HIS	-	expression tag	UNP F0M433
A	-10	HIS	-	expression tag	UNP F0M433
A	-9	SER	-	expression tag	UNP F0M433
A	-8	SER	-	expression tag	UNP F0M433
A	-7	GLY	-	expression tag	UNP F0M433
A	-6	LEU	-	expression tag	UNP F0M433
A	-5	VAL	-	expression tag	UNP F0M433
A	-4	PRO	-	expression tag	UNP F0M433
A	-3	ARG	-	expression tag	UNP F0M433
A	-2	GLY	-	expression tag	UNP F0M433
A	-1	SER	-	expression tag	UNP F0M433
A	0	HIS	-	expression tag	UNP F0M433
B	-19	MET	-	expression tag	UNP F0M433

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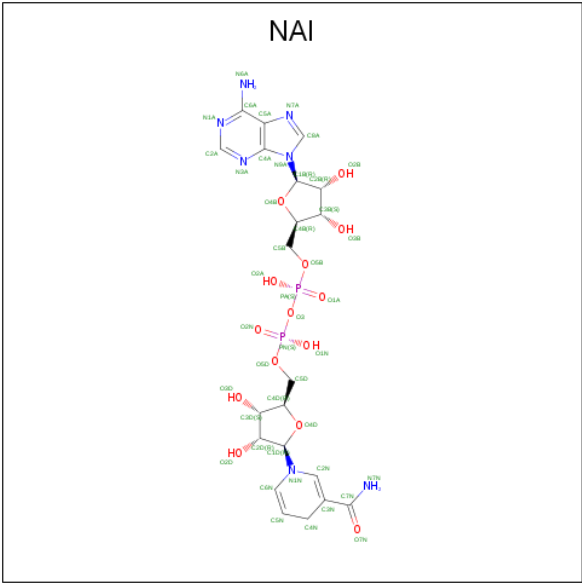
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP F0M433
B	-17	SER	-	expression tag	UNP F0M433
B	-16	SER	-	expression tag	UNP F0M433
B	-15	HIS	-	expression tag	UNP F0M433
B	-14	HIS	-	expression tag	UNP F0M433
B	-13	HIS	-	expression tag	UNP F0M433
B	-12	HIS	-	expression tag	UNP F0M433
B	-11	HIS	-	expression tag	UNP F0M433
B	-10	HIS	-	expression tag	UNP F0M433
B	-9	SER	-	expression tag	UNP F0M433
B	-8	SER	-	expression tag	UNP F0M433
B	-7	GLY	-	expression tag	UNP F0M433
B	-6	LEU	-	expression tag	UNP F0M433
B	-5	VAL	-	expression tag	UNP F0M433
B	-4	PRO	-	expression tag	UNP F0M433
B	-3	ARG	-	expression tag	UNP F0M433
B	-2	GLY	-	expression tag	UNP F0M433
B	-1	SER	-	expression tag	UNP F0M433
B	0	HIS	-	expression tag	UNP F0M433
C	-19	MET	-	expression tag	UNP F0M433
C	-18	GLY	-	expression tag	UNP F0M433
C	-17	SER	-	expression tag	UNP F0M433
C	-16	SER	-	expression tag	UNP F0M433
C	-15	HIS	-	expression tag	UNP F0M433
C	-14	HIS	-	expression tag	UNP F0M433
C	-13	HIS	-	expression tag	UNP F0M433
C	-12	HIS	-	expression tag	UNP F0M433
C	-11	HIS	-	expression tag	UNP F0M433
C	-10	HIS	-	expression tag	UNP F0M433
C	-9	SER	-	expression tag	UNP F0M433
C	-8	SER	-	expression tag	UNP F0M433
C	-7	GLY	-	expression tag	UNP F0M433
C	-6	LEU	-	expression tag	UNP F0M433
C	-5	VAL	-	expression tag	UNP F0M433
C	-4	PRO	-	expression tag	UNP F0M433
C	-3	ARG	-	expression tag	UNP F0M433
C	-2	GLY	-	expression tag	UNP F0M433
C	-1	SER	-	expression tag	UNP F0M433
C	0	HIS	-	expression tag	UNP F0M433
D	-19	MET	-	expression tag	UNP F0M433
D	-18	GLY	-	expression tag	UNP F0M433
D	-17	SER	-	expression tag	UNP F0M433

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP F0M433
D	-15	HIS	-	expression tag	UNP F0M433
D	-14	HIS	-	expression tag	UNP F0M433
D	-13	HIS	-	expression tag	UNP F0M433
D	-12	HIS	-	expression tag	UNP F0M433
D	-11	HIS	-	expression tag	UNP F0M433
D	-10	HIS	-	expression tag	UNP F0M433
D	-9	SER	-	expression tag	UNP F0M433
D	-8	SER	-	expression tag	UNP F0M433
D	-7	GLY	-	expression tag	UNP F0M433
D	-6	LEU	-	expression tag	UNP F0M433
D	-5	VAL	-	expression tag	UNP F0M433
D	-4	PRO	-	expression tag	UNP F0M433
D	-3	ARG	-	expression tag	UNP F0M433
D	-2	GLY	-	expression tag	UNP F0M433
D	-1	SER	-	expression tag	UNP F0M433
D	0	HIS	-	expression tag	UNP F0M433

- 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 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

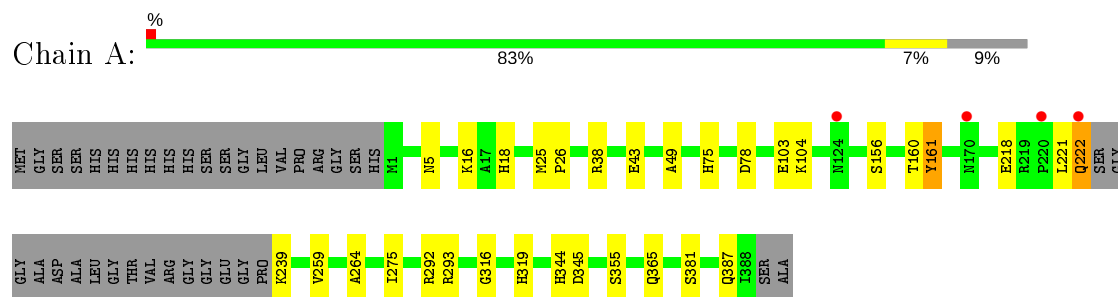
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total	O	0	0
			188	188		
3	B	187	Total	O	0	0
			187	187		
3	C	168	Total	O	0	0
			168	168		
3	D	206	Total	O	0	0
			206	206		

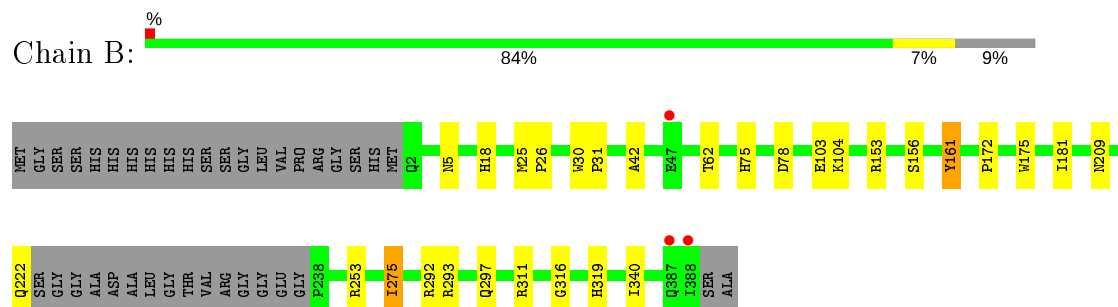
### 3 Residue-property plots

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.

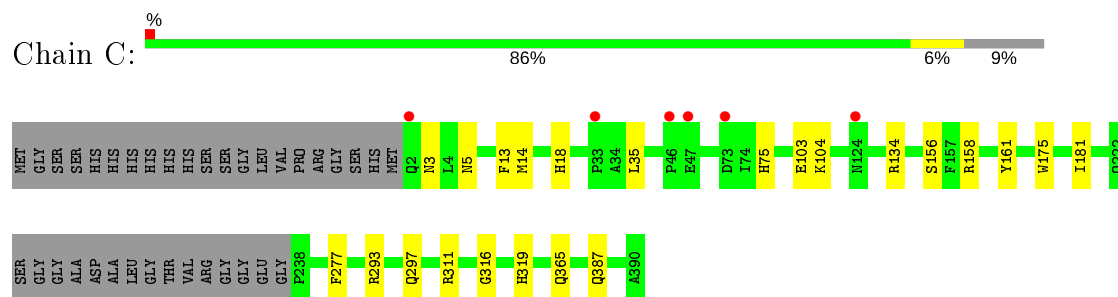
- Molecule 1: Putative dehydrogenase



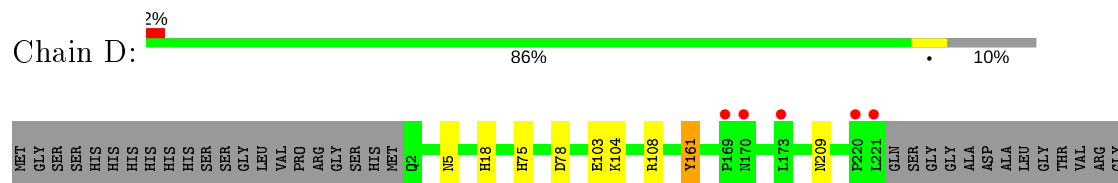
- Molecule 1: Putative dehydrogenase

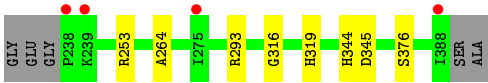


- Molecule 1: Putative dehydrogenase



- Molecule 1: Putative dehydrogenase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.74Å 93.79Å 100.99Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	36.53 – 1.90 36.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.53-1.90) 98.6 (36.51-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.169 , 0.204 0.179 , 0.212	Depositor DCC
$R_{free}$ test set	5652 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: 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	0.58	0/2937	0.71	0/3991
1	B	0.55	0/2937	0.70	1/3992 (0.0%)
1	C	0.56	0/2949	0.70	0/4007
1	D	0.57	0/2928	0.68	0/3980
All	All	0.57	0/11751	0.70	1/15970 (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	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	NE-CZ-NH2	-5.25	117.67	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	38	ARG	Sidechain
1	B	293	ARG	Sidechain
1	C	293	ARG	Sidechain
1	D	108	ARG	Sidechain
1	D	293	ARG	Sidechain

## 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	2865	0	2787	22	0
1	B	2864	0	2783	20	0
1	C	2876	0	2793	14	0
1	D	2855	0	2775	16	0
2	A	44	0	27	2	0
2	B	44	0	27	1	0
2	C	44	0	27	3	0
2	D	44	0	27	1	0
3	A	188	0	0	3	0
3	B	187	0	0	2	0
3	C	168	0	0	2	0
3	D	206	0	0	3	0
All	All	12385	0	11246	70	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 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:A:221:LEU:O	1:A:222:GLN:HG3	1.53	1.09
1:D:5:ASN:H	1:D:75:HIS:HD2	1.22	0.87
1:B:5:ASN:H	1:B:75:HIS:HD2	1.26	0.83
1:A:5:ASN:H	1:A:75:HIS:HD2	1.32	0.75
1:D:5:ASN:H	1:D:75:HIS:CD2	2.07	0.72
1:C:3:ASN:HD22	1:C:35:LEU:HB2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:HIS:HE1	1:C:103:GLU:OE2	1.78	0.65
2:C:401:NAI:N7A	3:C:501:HOH:O	2.30	0.65
1:A:316:GLY:H	1:A:319:HIS:HD2	1.46	0.63
1:B:18:HIS:HD2	1:B:78:ASP:OD2	1.82	0.63
1:B:316:GLY:H	1:B:319:HIS:HD2	1.46	0.63
1:B:161:TYR:CE2	1:B:275:ILE:HG12	2.34	0.62
1:A:18:HIS:HD2	1:A:78:ASP:OD2	1.83	0.62
1:B:18:HIS:HE1	1:B:103:GLU:OE2	1.82	0.61
1:A:103:GLU:OE1	2:A:401:NAI:H2N	2.00	0.61
1:C:5:ASN:H	1:C:75:HIS:HD2	1.48	0.61
1:D:18:HIS:HD2	1:D:78:ASP:OD2	1.83	0.60
1:B:175:TRP:HB2	1:B:181:ILE:HG21	1.82	0.60
1:B:316:GLY:H	1:B:319:HIS:CD2	2.21	0.58
1:A:344:HIS:HD2	1:A:345:ASP:OD1	1.85	0.58
1:C:297:GLN:NE2	3:C:502:HOH:O	2.34	0.58
1:A:18:HIS:HE1	1:A:103:GLU:OE2	1.87	0.57
1:A:221:LEU:O	1:A:222:GLN:CG	2.43	0.56
1:A:5:ASN:H	1:A:75:HIS:CD2	2.20	0.56
1:B:297:GLN:NE2	3:B:502:HOH:O	2.38	0.56
1:B:5:ASN:H	1:B:75:HIS:CD2	2.16	0.56
1:A:316:GLY:H	1:A:319:HIS:CD2	2.24	0.56
1:B:103:GLU:OE1	2:B:401:NAI:H2N	2.05	0.55
1:D:316:GLY:H	1:D:319:HIS:HD2	1.55	0.55
1:D:344:HIS:HD2	1:D:345:ASP:OD1	1.90	0.54
1:D:18:HIS:HE1	1:D:103:GLU:OE2	1.90	0.53
1:A:16:LYS:NZ	3:A:501:HOH:O	2.27	0.53
1:D:316:GLY:H	1:D:319:HIS:CD2	2.28	0.52
1:D:103:GLU:OE1	2:D:401:NAI:H2N	2.08	0.51
2:A:401:NAI:C3N	3:A:552:HOH:O	2.61	0.49
1:D:344:HIS:HE1	3:D:688:HOH:O	1.96	0.48
1:A:292:ARG:CZ	1:B:292:ARG:HD3	2.43	0.48
1:B:30:TRP:CD2	1:B:31:PRO:HA	2.48	0.48
1:A:160:THR:O	1:A:275:ILE:HA	2.15	0.47
1:C:18:HIS:CE1	1:C:103:GLU:OE2	2.64	0.46
1:C:103:GLU:OE1	2:C:401:NAI:H2N	2.15	0.46
1:B:209:ASN:HD21	1:D:209:ASN:HD21	1.64	0.46
1:B:25:MET:HB3	1:B:26:PRO:HD3	1.98	0.46
1:D:209:ASN:HA	1:D:376:SER:OG	2.17	0.45
1:C:316:GLY:H	1:C:319:HIS:HD2	1.63	0.45
1:C:175:TRP:HB2	1:C:181:ILE:HG21	1.99	0.45
1:C:316:GLY:H	1:C:319:HIS:CD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLN:HE22	1:A:387:GLN:HA	1.81	0.45
1:C:3:ASN:ND2	1:C:35:LEU:HB2	2.31	0.44
1:A:156:SER:HA	1:A:259:VAL:O	2.17	0.44
1:A:319:HIS:HE1	3:D:628:HOH:O	2.00	0.44
1:B:209:ASN:HD21	1:D:209:ASN:ND2	2.14	0.44
1:C:158:ARG:O	1:C:277:PHE:HA	2.18	0.44
1:B:311:ARG:HG2	1:C:311:ARG:HG2	1.99	0.44
1:A:18:HIS:CD2	1:A:78:ASP:OD2	2.68	0.43
1:D:253:ARG:NE	3:D:501:HOH:O	2.31	0.43
1:D:18:HIS:CD2	1:D:78:ASP:OD2	2.69	0.43
1:A:43:GLU:HB2	1:A:49:ALA:HA	2.02	0.42
1:B:153:ARG:NH1	3:B:506:HOH:O	2.45	0.42
1:B:42:ALA:HA	1:B:62:THR:O	2.20	0.42
1:C:14:MET:CE	2:C:401:NAI:H4N	2.50	0.42
1:A:25:MET:HB3	1:A:26:PRO:HD3	2.00	0.42
1:B:172:PRO:HB3	1:B:222:GLN:HB2	2.01	0.42
1:A:355:SER:HB2	3:A:672:HOH:O	2.20	0.41
1:A:161:TYR:O	1:A:264:ALA:HA	2.21	0.41
1:A:316:GLY:N	1:A:319:HIS:HD2	2.17	0.41
1:B:25:MET:HA	1:B:340:ILE:HG23	2.03	0.41
1:D:316:GLY:N	1:D:319:HIS:HD2	2.18	0.41
1:D:161:TYR:O	1:D:264:ALA:HA	2.21	0.40
1:C:365:GLN:HE22	1:C:387:GLN:HA	1.85	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	368/410 (90%)	361 (98%)	7 (2%)	0	100	100
1	B	368/410 (90%)	361 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	370/410 (90%)	360 (97%)	10 (3%)	0	100	100
1	D	367/410 (90%)	360 (98%)	7 (2%)	0	100	100
All	All	1473/1640 (90%)	1442 (98%)	31 (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	290/316 (92%)	284 (98%)	6 (2%)	53	48
1	B	290/316 (92%)	286 (99%)	4 (1%)	67	65
1	C	291/316 (92%)	286 (98%)	5 (2%)	60	57
1	D	289/316 (92%)	287 (99%)	2 (1%)	84	84
All	All	1160/1264 (92%)	1143 (98%)	17 (2%)	65	62

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	161	TYR
1	A	218	GLU
1	A	222	GLN
1	A	239	LYS
1	A	381	SER
1	B	104	LYS
1	B	156	SER
1	B	161	TYR
1	B	275	ILE
1	C	13	PHE
1	C	104	LYS
1	C	134	ARG
1	C	156	SER

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Mol	Chain	Res	Type
1	C	161	TYR
1	D	104	LYS
1	D	161	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	75	HIS
1	A	222	GLN
1	A	267	ASN
1	A	319	HIS
1	A	344	HIS
1	A	365	GLN
1	B	18	HIS
1	B	75	HIS
1	B	124	ASN
1	B	209	ASN
1	B	267	ASN
1	B	297	GLN
1	B	319	HIS
1	B	365	GLN
1	C	3	ASN
1	C	18	HIS
1	C	75	HIS
1	C	222	GLN
1	C	267	ASN
1	C	319	HIS
1	C	365	GLN
1	C	387	GLN
1	D	18	HIS
1	D	75	HIS
1	D	267	ASN
1	D	319	HIS
1	D	344	HIS
1	D	365	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	A	401	-	42,48,48	1.31	6 (14%)	47,73,73	1.24	4 (8%)
2	NAI	B	401	-	42,48,48	1.42	7 (16%)	47,73,73	1.37	6 (12%)
2	NAI	C	401	-	42,48,48	1.49	7 (16%)	47,73,73	1.28	7 (14%)
2	NAI	D	401	-	42,48,48	1.29	4 (9%)	47,73,73	1.30	5 (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	NAI	A	401	-	-	5/25/72/72	0/5/5/5
2	NAI	B	401	-	-	4/25/72/72	0/5/5/5
2	NAI	C	401	-	-	6/25/72/72	0/5/5/5
2	NAI	D	401	-	-	5/25/72/72	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAI	C6N-C5N	4.62	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C4N-C3N	-4.33	1.41	1.49
2	B	401	NAI	C6N-C5N	4.33	1.41	1.33
2	A	401	NAI	C4N-C3N	-3.89	1.42	1.49
2	D	401	NAI	C6N-C5N	3.76	1.40	1.33
2	D	401	NAI	C4N-C3N	-3.64	1.42	1.49
2	C	401	NAI	C4N-C3N	-3.64	1.42	1.49
2	A	401	NAI	C6N-C5N	3.64	1.39	1.33
2	C	401	NAI	C7N-C3N	3.58	1.56	1.48
2	A	401	NAI	C2N-C3N	3.00	1.43	1.34
2	D	401	NAI	C4N-C5N	-2.76	1.41	1.48
2	C	401	NAI	C2N-C3N	2.71	1.42	1.34
2	D	401	NAI	C2A-N3A	2.61	1.36	1.32
2	C	401	NAI	C4N-C5N	-2.50	1.42	1.48
2	A	401	NAI	C4N-C5N	-2.50	1.42	1.48
2	B	401	NAI	C2N-C3N	2.49	1.41	1.34
2	B	401	NAI	C7N-C3N	2.37	1.53	1.48
2	C	401	NAI	C2A-N3A	2.35	1.35	1.32
2	B	401	NAI	C2A-N3A	2.34	1.35	1.32
2	B	401	NAI	C4N-C5N	-2.34	1.42	1.48
2	A	401	NAI	C2A-N3A	2.23	1.35	1.32
2	A	401	NAI	C7N-C3N	2.22	1.53	1.48
2	C	401	NAI	C5A-C4A	2.13	1.46	1.40
2	B	401	NAI	C5A-C4A	2.06	1.46	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAI	N3A-C2A-N1A	-4.07	122.31	128.68
2	C	401	NAI	N3A-C2A-N1A	-3.70	122.89	128.68
2	A	401	NAI	N3A-C2A-N1A	-3.60	123.05	128.68
2	D	401	NAI	N3A-C2A-N1A	-3.26	123.58	128.68
2	A	401	NAI	PN-O3-PA	-3.25	121.68	132.83
2	C	401	NAI	O2A-PA-O1A	3.09	127.53	112.24
2	D	401	NAI	C4A-C5A-N7A	-3.07	106.20	109.40
2	D	401	NAI	C1B-N9A-C4A	-3.04	121.31	126.64
2	B	401	NAI	O2A-PA-O1A	2.85	126.31	112.24
2	D	401	NAI	PN-O3-PA	-2.82	123.15	132.83
2	B	401	NAI	O4B-C1B-C2B	-2.60	103.12	106.93
2	A	401	NAI	C4A-C5A-N7A	-2.58	106.70	109.40
2	B	401	NAI	PN-O3-PA	-2.49	124.29	132.83
2	B	401	NAI	C2D-C3D-C4D	2.47	107.44	102.64
2	A	401	NAI	C1B-N9A-C4A	-2.35	122.52	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAI	C2D-C1D-N1N	2.31	119.08	113.30
2	C	401	NAI	C4A-C5A-N7A	-2.30	107.00	109.40
2	C	401	NAI	O7N-C7N-N7N	-2.27	117.58	122.88
2	C	401	NAI	PN-O3-PA	-2.18	125.34	132.83
2	D	401	NAI	O4B-C4B-C3B	2.11	109.29	105.11
2	B	401	NAI	C4A-C5A-N7A	-2.10	107.21	109.40
2	C	401	NAI	C1B-N9A-C4A	-2.02	123.09	126.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

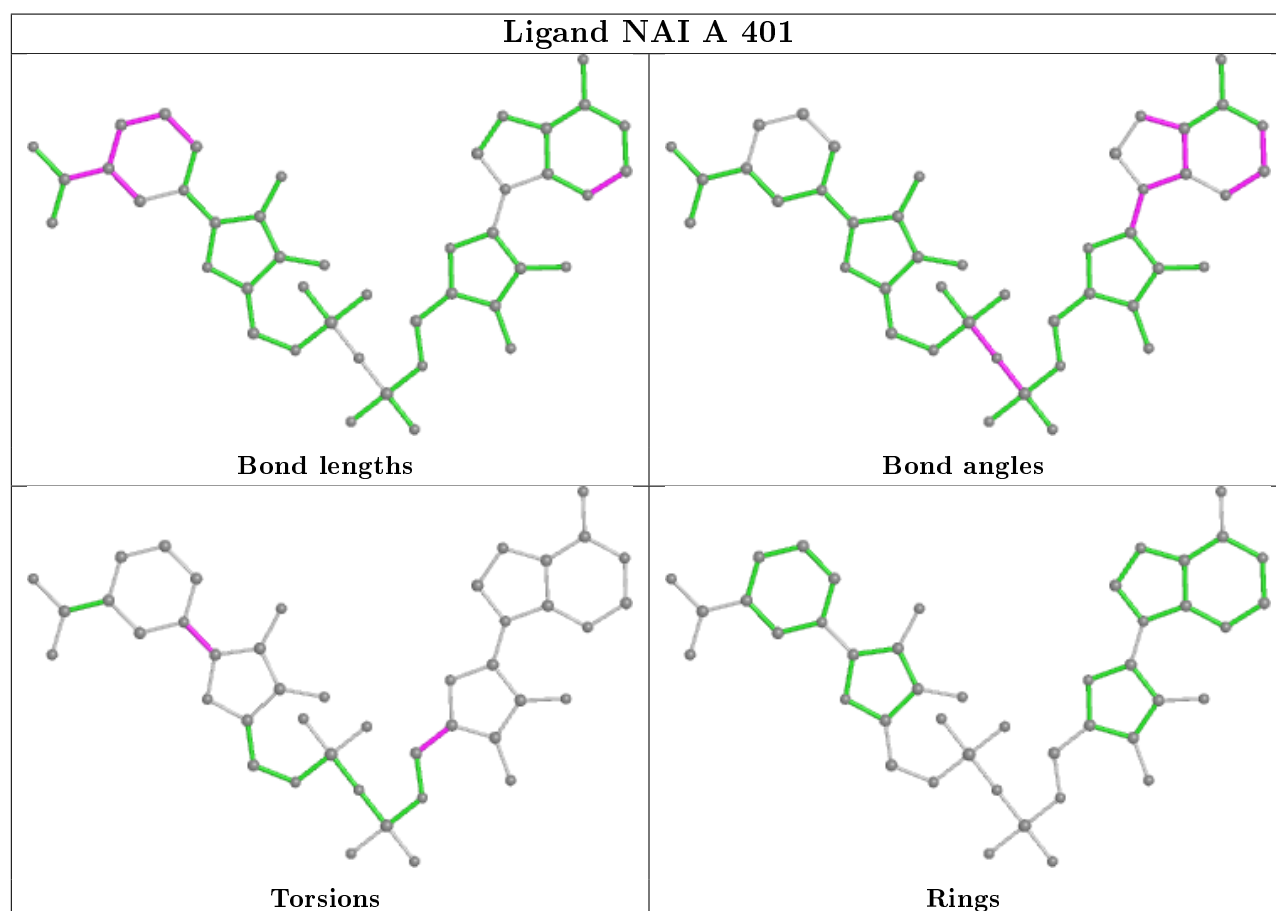
Mol	Chain	Res	Type	Atoms
2	B	401	NAI	C2D-C1D-N1N-C2N
2	A	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	C	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	O4B-C4B-C5B-O5B
2	C	401	NAI	PN-O3-PA-O2A
2	C	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	O4D-C1D-N1N-C6N

There are no ring outliers.

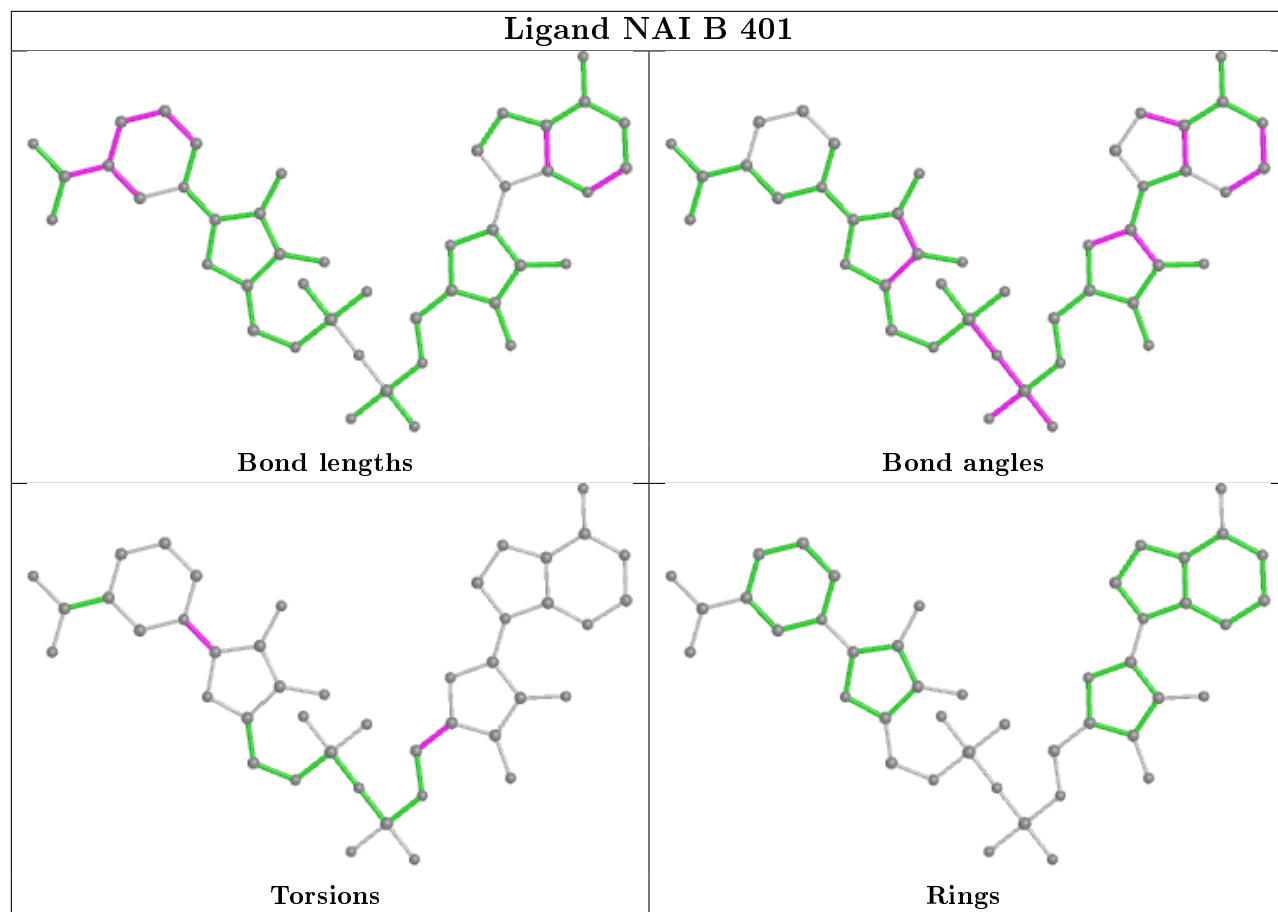
4 monomers are involved in 7 short contacts:

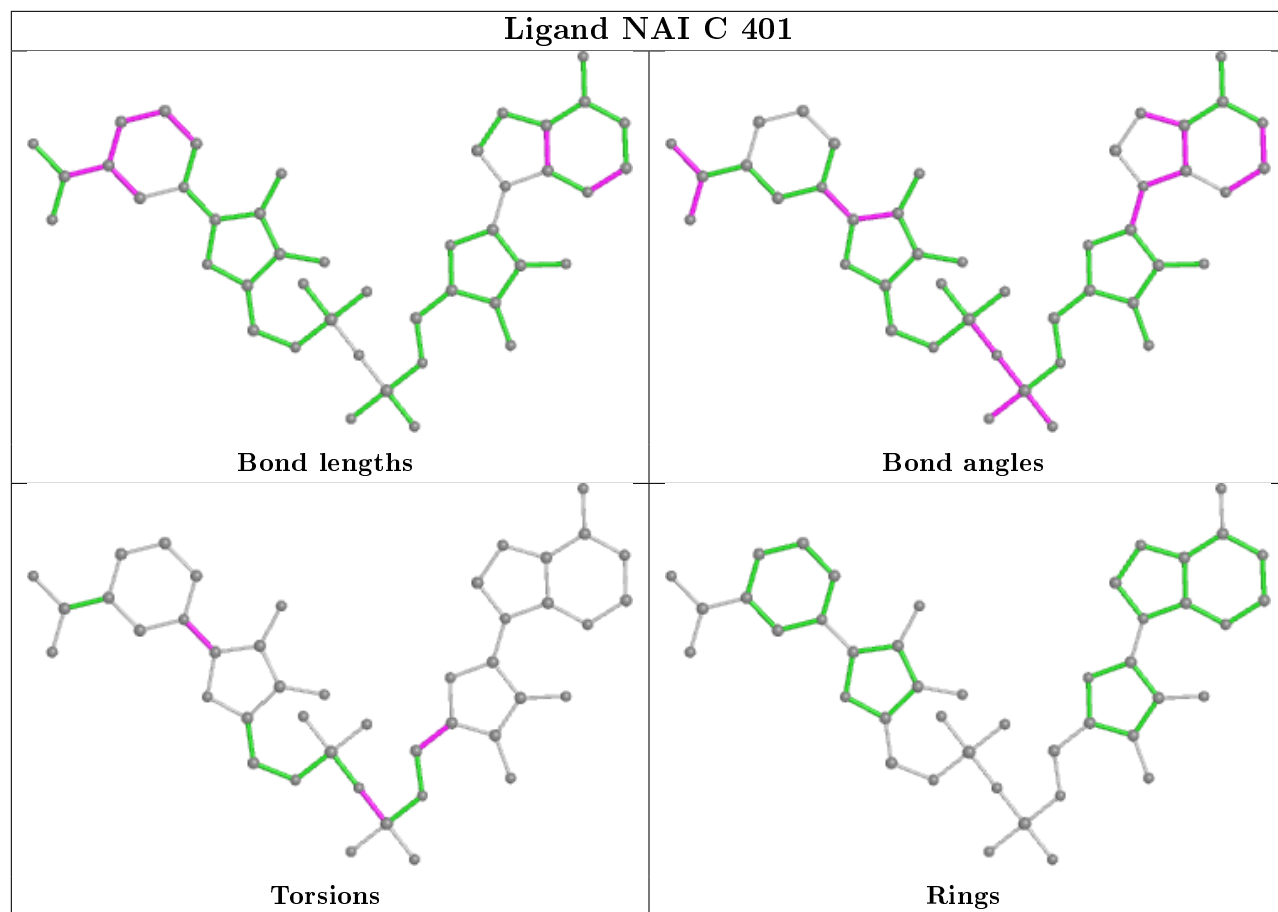
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAI	2	0
2	B	401	NAI	1	0
2	C	401	NAI	3	0
2	D	401	NAI	1	0

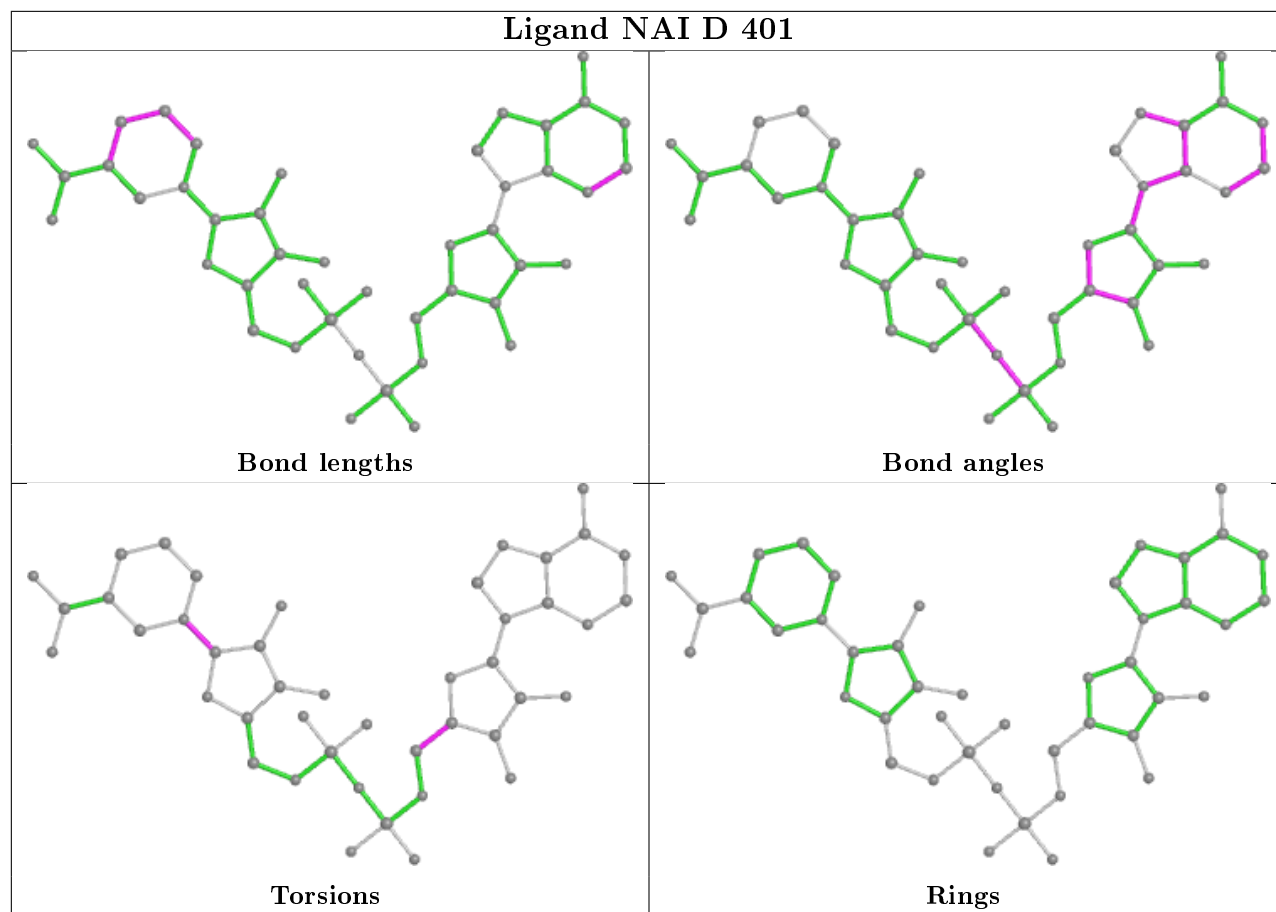
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand NAI B 401







## 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	372/410 (90%)	-0.24	4 (1%) 80 82	15, 21, 34, 60	0
1	B	372/410 (90%)	-0.29	3 (0%) 86 87	16, 23, 36, 55	0
1	C	374/410 (91%)	-0.18	6 (1%) 72 74	15, 23, 40, 65	0
1	D	371/410 (90%)	-0.22	9 (2%) 59 62	16, 22, 34, 54	0
All	All	1489/1640 (90%)	-0.23	22 (1%) 73 76	15, 22, 37, 65	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	PRO	3.9
1	B	388	ILE	3.7
1	D	388	ILE	3.4
1	C	2	GLN	3.2
1	A	222	GLN	3.1
1	D	221	LEU	3.0
1	C	73	ASP	3.0
1	D	220	PRO	2.9
1	A	170	ASN	2.6
1	C	46	PRO	2.6
1	D	275	ILE	2.4
1	C	124	ASN	2.4
1	C	47	GLU	2.3
1	B	47	GLU	2.2
1	D	169	PRO	2.2
1	D	239	LYS	2.2
1	D	170	ASN	2.1
1	C	33	PRO	2.1
1	B	387	GLN	2.1
1	D	173	LEU	2.1
1	A	124	ASN	2.1
1	A	220	PRO	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.

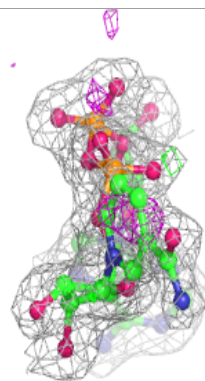
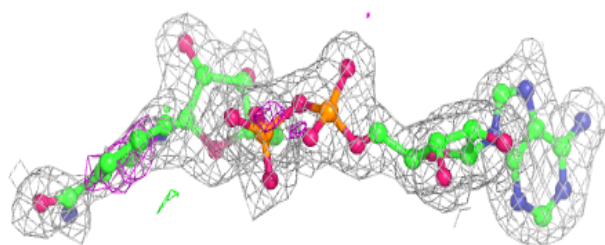
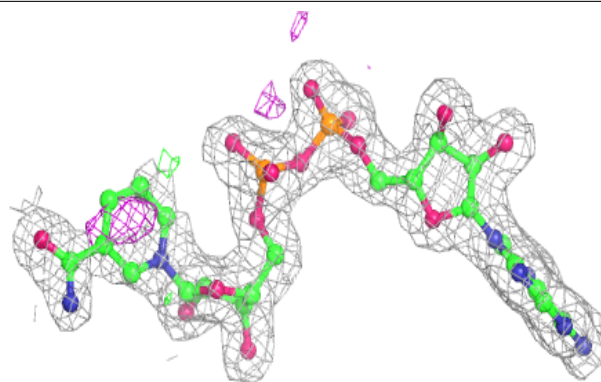
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAI	C	401	44/44	0.95	0.09	21,26,37,39	0
2	NAI	D	401	44/44	0.95	0.09	19,24,28,31	0
2	NAI	B	401	44/44	0.96	0.08	20,25,28,31	0
2	NAI	A	401	44/44	0.97	0.11	16,22,30,36	0

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.

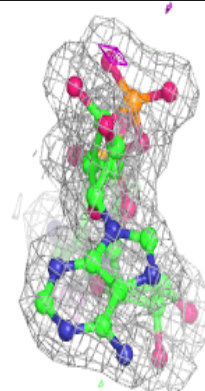
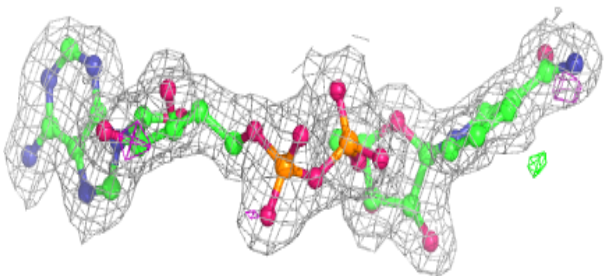
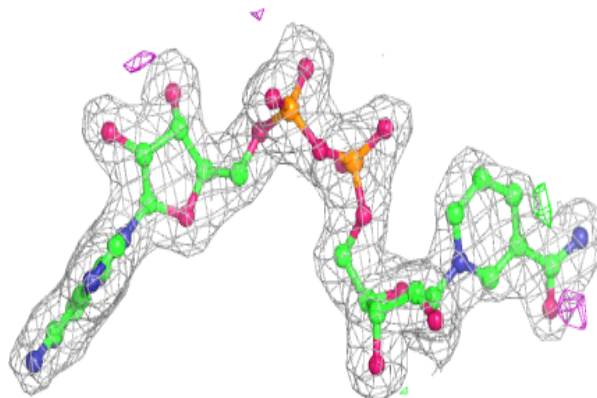


**Electron density around NAI C 401:**

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

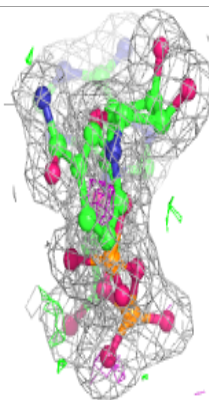
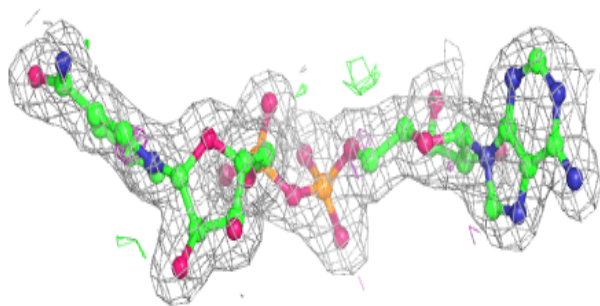
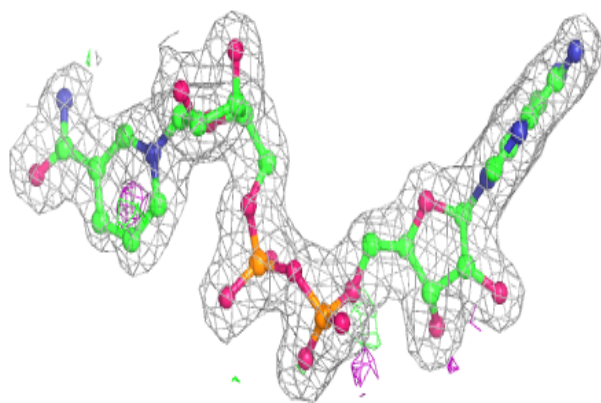
**Electron density around NAI D 401:**

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

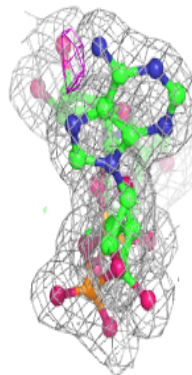
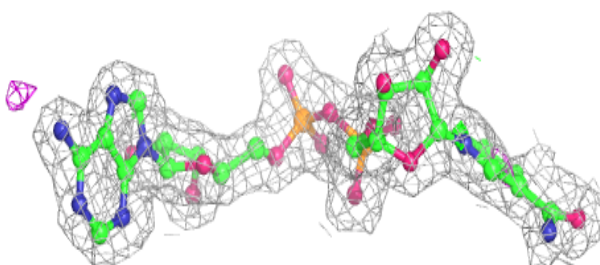
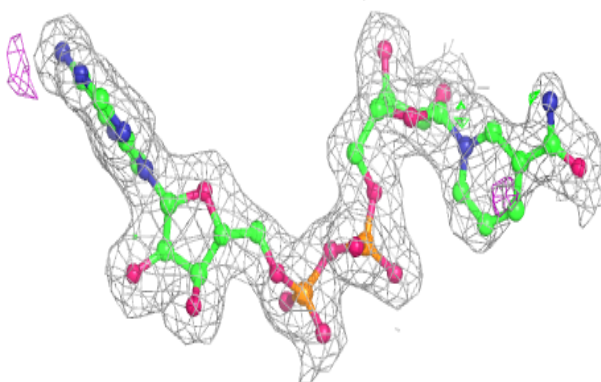


**Electron density around NAI B 401:**

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

**Electron density around NAI A 401:**

$2mF_o-DF_c$  (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.