



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 12:16 am BST

PDB ID : 3GGO  
Title : Crystal structure of prephenate dehydrogenase from *A. aeolicus* with HPP and NADH  
Authors : Sun, W.; Shahinas, D.; Christendat, D.  
Deposited on : 2009-03-01  
Resolution : 2.15 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

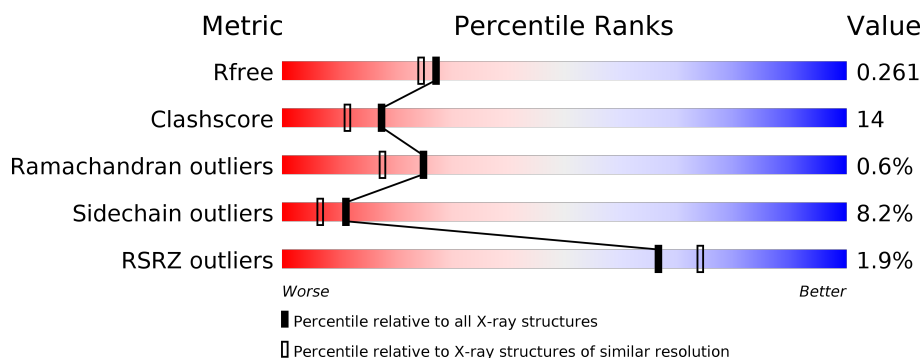
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	314	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 68%, yellow 19%, orange 2%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>68%</span> <span>19%</span> <span>• 9%</span> </div> </div>
1	B	314	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 68%, yellow 17%, orange 5%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>68%</span> <span>17%</span> <span>5%</span> <span>10%</span> </div> </div>
1	C	314	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 68%, yellow 19%, orange 2%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>68%</span> <span>19%</span> <span>• 11%</span> </div> </div>
1	D	314	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 66%, yellow 20%, orange 2%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>4%</span> <span>66%</span> <span>20%</span> <span>• 10%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9381 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 Prephenate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2252	1452	371	421	8			
1	B	282	Total	C	N	O	S	0	0	0
			2229	1437	367	417	8			
1	C	281	Total	C	N	O	S	0	0	0
			2215	1430	363	415	7			
1	D	282	Total	C	N	O	S	0	0	0
			2226	1435	367	416	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP O67636
A	-1	GLY	-	EXPRESSION TAG	UNP O67636
A	0	SER	-	EXPRESSION TAG	UNP O67636
A	1	SER	-	EXPRESSION TAG	UNP O67636
A	2	HIS	-	EXPRESSION TAG	UNP O67636
A	3	HIS	-	EXPRESSION TAG	UNP O67636
A	4	HIS	-	EXPRESSION TAG	UNP O67636
A	5	HIS	-	EXPRESSION TAG	UNP O67636
A	6	HIS	-	EXPRESSION TAG	UNP O67636
A	7	HIS	-	EXPRESSION TAG	UNP O67636
A	8	SER	-	EXPRESSION TAG	UNP O67636
A	9	SER	-	EXPRESSION TAG	UNP O67636
A	10	GLY	-	EXPRESSION TAG	UNP O67636
A	11	LEU	-	EXPRESSION TAG	UNP O67636
A	12	VAL	-	EXPRESSION TAG	UNP O67636
A	13	PRO	-	EXPRESSION TAG	UNP O67636
A	14	ARG	-	EXPRESSION TAG	UNP O67636
A	15	GLY	-	EXPRESSION TAG	UNP O67636
A	16	SER	-	EXPRESSION TAG	UNP O67636
A	17	HIS	-	EXPRESSION TAG	UNP O67636
A	18	MET	-	EXPRESSION TAG	UNP O67636

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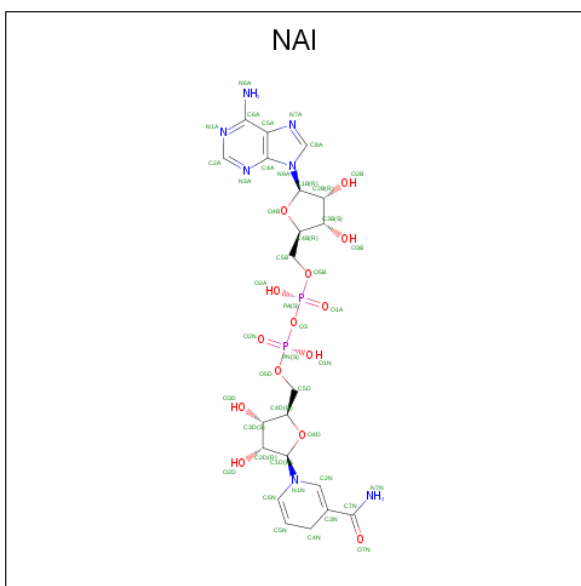
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP O67636
B	-1	GLY	-	EXPRESSION TAG	UNP O67636
B	0	SER	-	EXPRESSION TAG	UNP O67636
B	1	SER	-	EXPRESSION TAG	UNP O67636
B	2	HIS	-	EXPRESSION TAG	UNP O67636
B	3	HIS	-	EXPRESSION TAG	UNP O67636
B	4	HIS	-	EXPRESSION TAG	UNP O67636
B	5	HIS	-	EXPRESSION TAG	UNP O67636
B	6	HIS	-	EXPRESSION TAG	UNP O67636
B	7	HIS	-	EXPRESSION TAG	UNP O67636
B	8	SER	-	EXPRESSION TAG	UNP O67636
B	9	SER	-	EXPRESSION TAG	UNP O67636
B	10	GLY	-	EXPRESSION TAG	UNP O67636
B	11	LEU	-	EXPRESSION TAG	UNP O67636
B	12	VAL	-	EXPRESSION TAG	UNP O67636
B	13	PRO	-	EXPRESSION TAG	UNP O67636
B	14	ARG	-	EXPRESSION TAG	UNP O67636
B	15	GLY	-	EXPRESSION TAG	UNP O67636
B	16	SER	-	EXPRESSION TAG	UNP O67636
B	17	HIS	-	EXPRESSION TAG	UNP O67636
B	18	MET	-	EXPRESSION TAG	UNP O67636
C	-2	MET	-	EXPRESSION TAG	UNP O67636
C	-1	GLY	-	EXPRESSION TAG	UNP O67636
C	0	SER	-	EXPRESSION TAG	UNP O67636
C	1	SER	-	EXPRESSION TAG	UNP O67636
C	2	HIS	-	EXPRESSION TAG	UNP O67636
C	3	HIS	-	EXPRESSION TAG	UNP O67636
C	4	HIS	-	EXPRESSION TAG	UNP O67636
C	5	HIS	-	EXPRESSION TAG	UNP O67636
C	6	HIS	-	EXPRESSION TAG	UNP O67636
C	7	HIS	-	EXPRESSION TAG	UNP O67636
C	8	SER	-	EXPRESSION TAG	UNP O67636
C	9	SER	-	EXPRESSION TAG	UNP O67636
C	10	GLY	-	EXPRESSION TAG	UNP O67636
C	11	LEU	-	EXPRESSION TAG	UNP O67636
C	12	VAL	-	EXPRESSION TAG	UNP O67636
C	13	PRO	-	EXPRESSION TAG	UNP O67636
C	14	ARG	-	EXPRESSION TAG	UNP O67636
C	15	GLY	-	EXPRESSION TAG	UNP O67636
C	16	SER	-	EXPRESSION TAG	UNP O67636
C	17	HIS	-	EXPRESSION TAG	UNP O67636
C	18	MET	-	EXPRESSION TAG	UNP O67636

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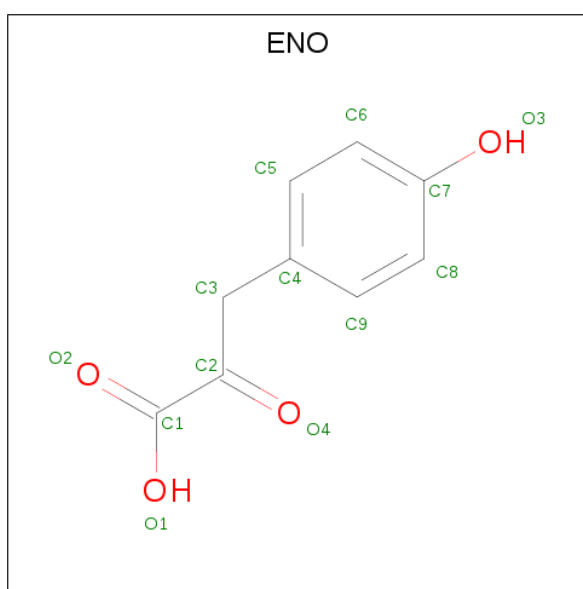
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	EXPRESSION TAG	UNP O67636
D	-1	GLY	-	EXPRESSION TAG	UNP O67636
D	0	SER	-	EXPRESSION TAG	UNP O67636
D	1	SER	-	EXPRESSION TAG	UNP O67636
D	2	HIS	-	EXPRESSION TAG	UNP O67636
D	3	HIS	-	EXPRESSION TAG	UNP O67636
D	4	HIS	-	EXPRESSION TAG	UNP O67636
D	5	HIS	-	EXPRESSION TAG	UNP O67636
D	6	HIS	-	EXPRESSION TAG	UNP O67636
D	7	HIS	-	EXPRESSION TAG	UNP O67636
D	8	SER	-	EXPRESSION TAG	UNP O67636
D	9	SER	-	EXPRESSION TAG	UNP O67636
D	10	GLY	-	EXPRESSION TAG	UNP O67636
D	11	LEU	-	EXPRESSION TAG	UNP O67636
D	12	VAL	-	EXPRESSION TAG	UNP O67636
D	13	PRO	-	EXPRESSION TAG	UNP O67636
D	14	ARG	-	EXPRESSION TAG	UNP O67636
D	15	GLY	-	EXPRESSION TAG	UNP O67636
D	16	SER	-	EXPRESSION TAG	UNP O67636
D	17	HIS	-	EXPRESSION TAG	UNP O67636
D	18	MET	-	EXPRESSION TAG	UNP O67636

- 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 3-(4-HYDROXY-PHENYL)PYRUVIC ACID (three-letter code: ENO) (formula: C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	9	4		
3	C	1	Total	C	O	0	0
			13	9	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	71	Total	O	0	0
			71	71		
4	C	89	Total	O	0	0
			89	89		

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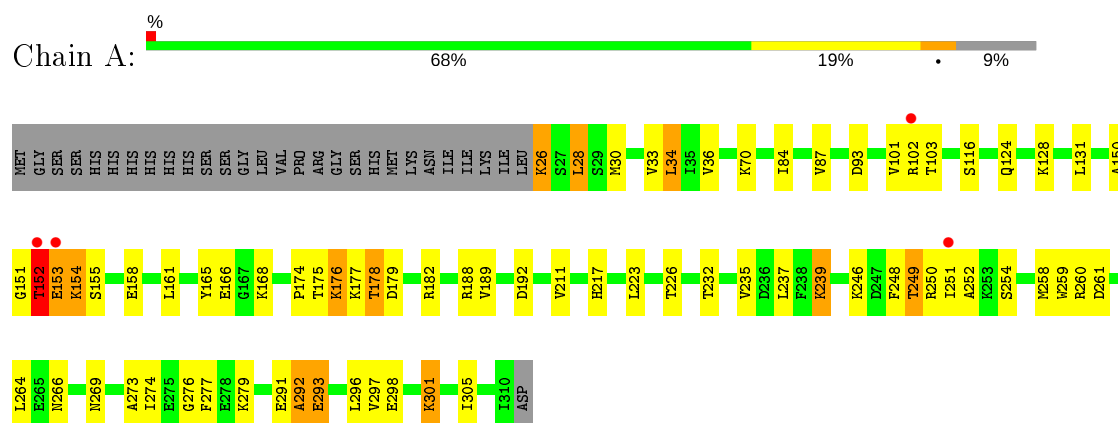
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	43	Total	O	0	0
			43	43		

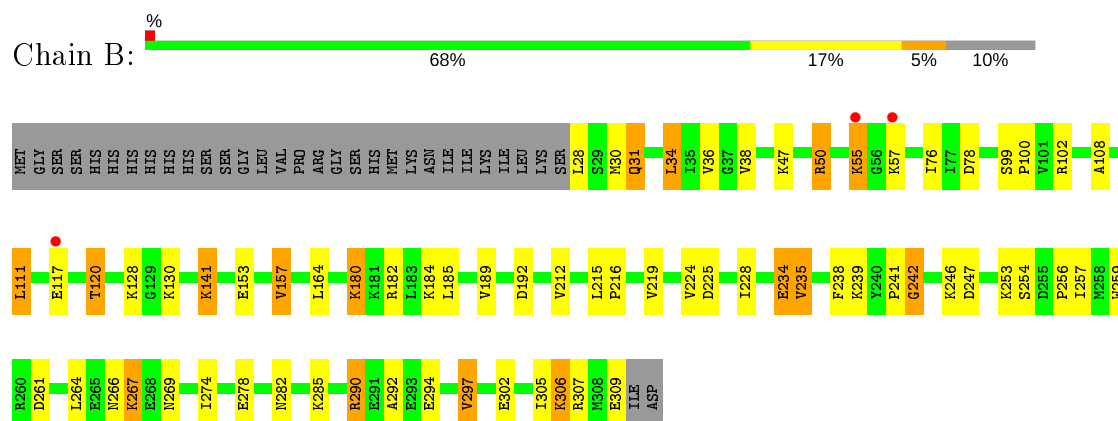
### 3 Residue-property plots

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.

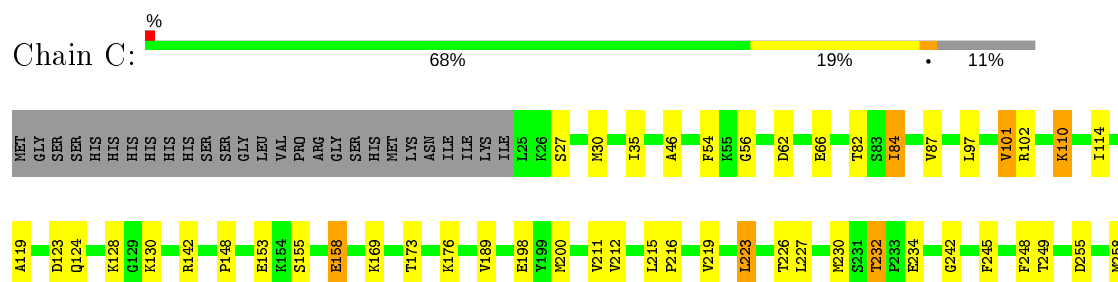
- Molecule 1: Prephenate dehydrogenase



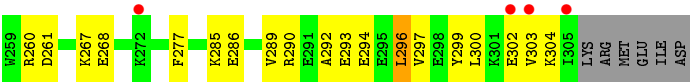
- Molecule 1: Prephenate dehydrogenase



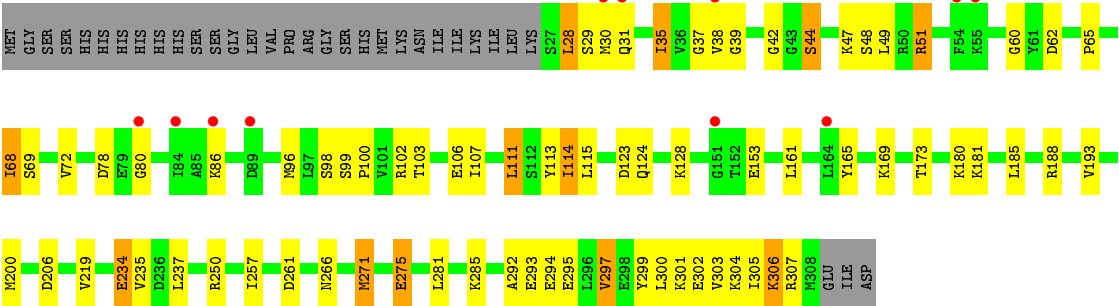
- Molecule 1: Prephenate dehydrogenase







● Molecule 1: Prephenate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.50 Å 92.48 Å 164.08 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.22 – 2.15 46.24 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.3 (46.22-2.15) 96.3 (46.24-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.16 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.218 , 0.262 0.216 , 0.261	Depositor DCC
$R_{free}$ test set	2030 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.3	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	0.95	EDS
Total number of atoms	9381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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: NAI, ENO

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	0.97	3/2295 (0.1%)	0.86	1/3087 (0.0%)
1	B	0.98	0/2272	0.85	1/3057 (0.0%)
1	C	0.96	0/2258	0.83	1/3040 (0.0%)
1	D	0.88	3/2269 (0.1%)	0.81	0/3053
All	All	0.95	6/9094 (0.1%)	0.84	3/12237 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	113	TYR	CG-CD2	9.51	1.51	1.39
1	D	113	TYR	CE2-CZ	7.88	1.48	1.38
1	A	70	LYS	CD-CE	7.79	1.70	1.51
1	D	113	TYR	CE1-CZ	7.07	1.47	1.38
1	A	165	TYR	CD2-CE2	6.20	1.48	1.39
1	A	165	TYR	CD1-CE1	5.17	1.47	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	LEU	CA-CB-CG	5.87	128.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	297	VAL	CB-CA-C	-5.03	101.84	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	242	GLY	Peptide
1	C	242	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2252	0	2307	82	0
1	B	2229	0	2278	67	0
1	C	2215	0	2266	69	0
1	D	2226	0	2277	72	0
2	A	44	0	27	3	0
2	B	44	0	27	1	0
2	C	44	0	27	5	0
2	D	44	0	27	4	0
3	B	13	0	7	0	0
3	C	13	0	6	0	0
4	A	54	0	0	1	0
4	B	71	0	0	1	0
4	C	89	0	0	6	0
4	D	43	0	0	2	0
All	All	9381	0	9249	251	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 14.

All (251) 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:251:ILE:CG2	1:C:248:PHE:CZ	2.11	1.32
1:A:251:ILE:HG22	1:C:248:PHE:CZ	1.68	1.25
1:B:50:ARG:HG3	1:B:50:ARG:HH11	1.12	1.10
1:B:234:GLU:HG3	1:B:235:VAL:HG12	1.31	1.09
1:A:251:ILE:HG23	1:C:248:PHE:HZ	1.24	1.02
1:A:217:HIS:CD2	1:A:251:ILE:HG12	1.96	0.99
1:A:251:ILE:HG13	1:A:254:SER:OG	1.60	0.99
1:A:251:ILE:CG2	1:C:248:PHE:HZ	1.59	0.99
1:A:30:MET:CE	1:A:189:VAL:HG21	1.94	0.98
1:B:239:LYS:O	1:D:169:LYS:NZ	1.99	0.96
1:B:234:GLU:CG	1:B:235:VAL:HG12	1.94	0.96
1:C:303:VAL:HG23	1:C:304:LYS:HD3	1.51	0.91
1:C:232:THR:HG23	1:C:234:GLU:H	1.35	0.90
1:B:256:PRO:HG2	1:D:301:LYS:HG2	1.52	0.89
1:B:50:ARG:NH1	1:B:50:ARG:HG3	1.86	0.88
1:D:96:MET:HE2	1:D:124:GLN:HG3	1.56	0.88
1:A:175:THR:H	1:A:178:THR:HG23	1.39	0.87
1:D:96:MET:CE	1:D:124:GLN:HG3	2.04	0.87
1:C:35:ILE:HD13	1:C:46:ALA:HB2	1.55	0.87
1:A:292:ALA:O	1:A:293:GLU:HB2	1.72	0.87
1:A:239:LYS:HB2	1:A:239:LYS:NZ	1.93	0.83
1:B:120:THR:HB	1:B:182:ARG:HD3	1.60	0.81
1:A:102:ARG:HG2	1:A:261:ASP:OD2	1.80	0.81
1:A:30:MET:HE1	1:A:189:VAL:HG21	1.61	0.80
1:A:239:LYS:HZ3	1:A:239:LYS:HB2	1.43	0.80
1:D:271:MET:O	1:D:275:GLU:HG2	1.84	0.78
1:A:30:MET:HE3	1:A:189:VAL:CG2	2.14	0.77
1:B:234:GLU:HG3	1:B:235:VAL:CG1	2.14	0.76
1:D:48:SER:HB3	1:D:193:VAL:HG13	1.68	0.76
1:A:217:HIS:NE2	1:A:251:ILE:HG12	2.00	0.76
1:B:50:ARG:CG	1:B:50:ARG:HH11	1.95	0.76
1:C:84:ILE:HG21	1:C:110:LYS:HD3	1.67	0.76
1:A:175:THR:H	1:A:178:THR:CG2	1.98	0.76
1:A:292:ALA:O	1:A:293:GLU:CB	2.34	0.75
1:C:30:MET:HE1	1:C:189:VAL:HG21	1.68	0.75
1:A:30:MET:HE3	1:A:189:VAL:HG21	1.67	0.75
1:A:251:ILE:CG2	1:C:248:PHE:CE2	2.70	0.74
1:A:211:VAL:HG22	1:C:230:MET:HE3	1.70	0.73
1:A:293:GLU:OE2	1:C:102:ARG:NH2	2.22	0.72
1:D:96:MET:HE3	1:D:123:ASP:CA	2.19	0.72
1:A:251:ILE:CG1	1:A:254:SER:OG	2.38	0.71
1:C:215:LEU:HB3	1:C:216:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:O	1:C:303:VAL:HG22	1.91	0.70
1:A:251:ILE:HG23	1:C:248:PHE:CZ	2.05	0.70
1:D:102:ARG:HG3	1:D:261:ASP:OD2	1.90	0.69
1:D:193:VAL:HG12	1:D:193:VAL:O	1.93	0.69
1:D:96:MET:HE3	1:D:123:ASP:C	2.14	0.68
1:B:306:LYS:HD2	1:B:307:ARG:H	1.57	0.68
1:D:28:LEU:HD12	1:D:28:LEU:H	1.59	0.68
1:B:31:GLN:HE22	1:B:57:LYS:HE3	1.59	0.67
1:A:174:PRO:HA	1:A:178:THR:HG21	1.75	0.66
1:B:224:VAL:HB	1:D:303:VAL:HG13	1.77	0.66
1:D:65:PRO:HA	1:D:68:ILE:HG23	1.77	0.66
1:C:30:MET:CE	1:C:189:VAL:HG21	2.27	0.65
1:A:239:LYS:CB	1:A:239:LYS:NZ	2.54	0.65
1:B:290:ARG:HD3	1:B:292:ALA:HB2	1.78	0.65
1:B:99:SER:HB2	1:B:100:PRO:HD2	1.80	0.64
1:D:96:MET:HE1	1:D:124:GLN:HG3	1.79	0.64
1:B:34:LEU:HD13	1:B:36:VAL:HG23	1.79	0.64
1:C:258:MET:HE1	2:C:4372:NAI:O1N	1.98	0.63
1:B:306:LYS:O	1:B:309:GLU:HG2	1.99	0.63
1:C:35:ILE:CD1	1:C:46:ALA:HB2	2.26	0.62
1:D:99:SER:HB2	1:D:100:PRO:HD2	1.80	0.62
1:A:151:GLY:O	1:A:152:THR:O	2.17	0.62
1:B:30:MET:HE1	1:B:189:VAL:HG22	1.81	0.62
1:D:103:THR:O	1:D:107:ILE:HG12	2.00	0.62
1:C:223:LEU:HD22	1:C:249:THR:CG2	2.29	0.62
1:B:306:LYS:N	1:B:306:LYS:HD2	2.15	0.61
1:B:102:ARG:NH2	1:D:293:GLU:HG2	2.14	0.61
1:C:223:LEU:HD22	1:C:249:THR:HG21	1.82	0.61
1:D:35:ILE:HD11	1:D:42:GLY:HA3	1.83	0.61
1:D:107:ILE:HG22	1:D:111:LEU:HD22	1.81	0.60
1:D:111:LEU:HA	1:D:114:ILE:HD11	1.81	0.60
1:A:34:LEU:HD13	1:A:36:VAL:HG23	1.83	0.60
1:D:44:SER:HB2	1:D:161:LEU:H	1.67	0.60
1:B:274:ILE:HG21	1:D:285:LYS:HD2	1.83	0.60
1:C:299:TYR:O	1:C:302:GLU:HB2	2.01	0.60
1:A:251:ILE:HG22	1:C:248:PHE:CE1	2.34	0.59
1:C:232:THR:CG2	1:C:234:GLU:H	2.10	0.59
1:B:102:ARG:HH22	1:D:293:GLU:HG2	1.67	0.59
1:D:180:LYS:NZ	4:D:1172:HOH:O	2.28	0.59
1:A:153:GLU:HG3	1:A:251:ILE:HD12	1.83	0.59
2:B:3372:NAI:O1N	4:B:1003:HOH:O	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ILE:H	1:D:257:ILE:HD12	1.68	0.59
1:C:258:MET:HE1	2:C:4372:NAI:H71N	1.67	0.58
1:B:282:ASN:HA	1:B:285:LYS:HD3	1.84	0.58
1:A:252:ALA:O	1:C:303:VAL:HG21	2.04	0.58
1:D:96:MET:CE	1:D:123:ASP:C	2.71	0.58
1:A:217:HIS:HD2	1:A:251:ILE:HG12	1.63	0.58
1:A:258:MET:HE1	2:A:2372:NAI:H2N	1.83	0.58
1:B:294:GLU:CD	1:B:294:GLU:H	2.07	0.58
1:B:215:LEU:HB3	1:B:216:PRO:HD3	1.85	0.58
1:A:251:ILE:HG21	1:C:248:PHE:CE2	2.38	0.58
1:D:35:ILE:HD11	1:D:37:GLY:O	2.04	0.58
1:A:232:THR:OG1	1:A:235:VAL:HG12	2.04	0.57
1:A:273:ALA:HA	1:C:230:MET:CE	2.34	0.57
1:A:291:GLU:OE1	1:C:267:LYS:HE3	2.04	0.57
1:A:217:HIS:NE2	1:A:251:ILE:CD1	2.68	0.57
1:B:256:PRO:CG	1:D:301:LYS:HG2	2.30	0.57
1:B:302:GLU:O	1:B:305:ILE:HG12	2.05	0.56
1:B:257:ILE:HD13	1:D:297:VAL:HG21	1.87	0.56
1:B:306:LYS:NZ	1:B:306:LYS:H	2.03	0.56
1:A:217:HIS:NE2	1:A:251:ILE:CG1	2.67	0.56
1:A:178:THR:HG22	4:A:1199:HOH:O	2.06	0.56
1:B:47:LYS:HE3	1:B:76:ILE:CD1	2.35	0.56
1:A:151:GLY:O	1:A:152:THR:C	2.44	0.56
1:C:258:MET:CE	4:C:1005:HOH:O	2.54	0.56
1:A:150:ALA:HA	1:A:168:LYS:HE2	1.87	0.56
1:D:69:SER:HA	1:D:72:VAL:HG12	1.87	0.55
1:A:274:ILE:HG21	1:C:285:LYS:HD2	1.88	0.55
1:D:292:ALA:HB1	1:D:295:GLU:HG3	1.88	0.55
1:D:96:MET:HE3	1:D:123:ASP:HA	1.86	0.55
1:A:226:THR:OG1	1:C:277:PHE:HA	2.06	0.55
1:C:299:TYR:HD2	1:C:300:LEU:HD23	1.72	0.54
1:A:239:LYS:HG2	1:A:239:LYS:O	2.08	0.54
2:C:4372:NAI:O1N	4:C:1005:HOH:O	2.18	0.54
1:B:55:LYS:H	1:B:55:LYS:HE3	1.72	0.54
1:C:285:LYS:O	1:C:289:VAL:HG12	2.07	0.54
1:D:173:THR:HA	1:D:200:MET:O	2.08	0.54
1:C:293:GLU:HB2	4:C:1154:HOH:O	2.07	0.53
1:B:31:GLN:HE21	1:B:31:GLN:C	2.11	0.53
1:A:239:LYS:CB	1:A:239:LYS:HZ3	2.16	0.53
1:A:26:LYS:HA	1:A:26:LYS:HE3	1.89	0.53
1:B:266:ASN:HD21	1:B:269:ASN:HD22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HG3	1:A:103:THR:N	2.23	0.53
1:B:180:LYS:O	1:B:184:LYS:HG3	2.08	0.53
1:C:119:ALA:O	1:C:142:ARG:HG2	2.08	0.53
1:C:258:MET:HE1	4:C:1005:HOH:O	2.09	0.53
1:A:188:ARG:HD3	1:A:192:ASP:OD2	2.09	0.52
1:C:87:VAL:HG23	1:C:114:ILE:HG21	1.91	0.52
1:D:28:LEU:N	1:D:28:LEU:HD12	2.22	0.52
1:A:273:ALA:HA	1:C:230:MET:HE3	1.90	0.52
1:D:153:GLU:HG2	2:D:1372:NAI:O7N	2.10	0.52
1:C:232:THR:HG23	1:C:234:GLU:N	2.13	0.52
1:C:124:GLN:HE21	1:C:148:PRO:HG3	1.75	0.52
1:B:234:GLU:HG2	1:B:235:VAL:HG12	1.85	0.52
1:D:111:LEU:HA	1:D:114:ILE:CD1	2.40	0.52
1:B:120:THR:CB	1:B:182:ARG:HD3	2.38	0.51
1:B:99:SER:HB2	1:B:100:PRO:CD	2.40	0.51
1:B:102:ARG:HH22	1:D:293:GLU:CD	2.14	0.51
1:A:260:ARG:HG2	1:C:296:LEU:HD13	1.93	0.51
1:B:120:THR:HG22	1:B:182:ARG:HH11	1.76	0.51
1:B:189:VAL:O	1:B:192:ASP:HB2	2.10	0.51
1:B:102:ARG:NH2	1:D:293:GLU:OE2	2.34	0.50
1:D:29:SER:OG	1:D:30:MET:N	2.43	0.50
1:B:102:ARG:HH22	1:D:293:GLU:CG	2.23	0.50
1:B:253:LYS:HD2	1:D:307:ARG:HG3	1.92	0.50
1:A:152:THR:HG22	1:A:154:LYS:HE2	1.93	0.50
2:C:4372:NAI:N7N	4:C:1005:HOH:O	2.35	0.50
1:D:193:VAL:CG1	1:D:193:VAL:O	2.59	0.50
1:C:101:VAL:HG12	1:C:261:ASP:HB3	1.94	0.49
1:B:212:VAL:CG1	1:D:237:LEU:HB3	2.42	0.49
1:D:35:ILE:CD1	1:D:42:GLY:HA3	2.42	0.49
1:C:66:GLU:HA	1:C:66:GLU:OE2	2.13	0.49
1:D:48:SER:HB3	1:D:193:VAL:CG1	2.41	0.49
1:A:211:VAL:CG1	1:C:230:MET:HE2	2.43	0.48
1:C:155:SER:OG	1:C:255:ASP:HB2	2.12	0.48
1:B:55:LYS:H	1:B:55:LYS:CE	2.26	0.48
1:C:158:GLU:CD	1:C:158:GLU:H	2.16	0.48
1:A:152:THR:CG2	1:A:154:LYS:HE2	2.44	0.48
1:B:290:ARG:HG2	1:B:290:ARG:O	2.13	0.48
1:D:111:LEU:HD12	1:D:114:ILE:HD11	1.95	0.48
1:A:101:VAL:HG13	1:A:131:LEU:HD22	1.96	0.48
1:A:84:ILE:O	1:A:87:VAL:HB	2.13	0.48
1:B:239:LYS:O	1:B:241:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LYS:H	1:B:306:LYS:HZ2	1.61	0.48
1:A:153:GLU:CG	1:A:251:ILE:HD12	2.44	0.48
1:A:260:ARG:HG3	1:C:297:VAL:HG23	1.96	0.48
1:D:124:GLN:O	2:D:1372:NAI:H6N	2.14	0.47
1:D:96:MET:HE1	1:D:124:GLN:CG	2.43	0.47
1:A:153:GLU:OE2	1:A:251:ILE:HD12	2.14	0.47
1:B:234:GLU:HG3	1:B:235:VAL:N	2.30	0.47
1:A:254:SER:HB3	1:A:259:TRP:CD1	2.49	0.47
1:C:62:ASP:O	1:C:82:THR:HA	2.15	0.47
1:A:232:THR:OG1	1:A:235:VAL:CG1	2.62	0.46
1:C:176:LYS:HG3	1:C:176:LYS:O	2.16	0.46
1:A:211:VAL:HG13	1:C:230:MET:HE2	1.97	0.46
1:D:301:LYS:O	1:D:305:ILE:HG13	2.15	0.46
1:D:38:VAL:HG13	1:D:38:VAL:O	2.16	0.46
1:A:277:PHE:HA	1:C:226:THR:OG1	2.16	0.46
1:D:234:GLU:O	1:D:235:VAL:HG12	2.15	0.46
1:B:28:LEU:HD12	1:B:28:LEU:C	2.36	0.46
1:D:28:LEU:CD1	1:D:28:LEU:H	2.26	0.46
1:A:176:LYS:HD3	1:A:176:LYS:H	1.81	0.46
1:A:296:LEU:HD23	1:C:260:ARG:HG2	1.98	0.46
1:A:102:ARG:CG	1:A:261:ASP:OD2	2.58	0.45
1:B:141:LYS:H	1:B:141:LYS:NZ	2.14	0.45
1:C:30:MET:CE	1:C:189:VAL:CG2	2.93	0.45
1:A:179:ASP:C	1:A:179:ASP:OD2	2.55	0.45
1:A:276:GLY:O	1:A:279:LYS:HB3	2.17	0.45
1:D:60:GLY:O	1:D:80:GLY:HA2	2.16	0.45
1:D:38:VAL:HG12	1:D:62:ASP:OD1	2.17	0.45
1:A:124:GLN:O	2:A:2372:NAI:H6N	2.17	0.45
1:C:169:LYS:HD3	1:C:198:GLU:OE1	2.17	0.44
1:B:278:GLU:OE2	1:D:285:LYS:NZ	2.49	0.44
1:C:54:PHE:CZ	1:C:56:GLY:HA3	2.51	0.44
1:D:35:ILE:HD13	1:D:42:GLY:CA	2.47	0.44
1:A:266:ASN:HD21	1:A:269:ASN:HD22	1.65	0.44
1:B:239:LYS:C	1:B:241:PRO:HD3	2.37	0.44
1:B:31:GLN:NE2	1:B:31:GLN:C	2.71	0.44
1:A:248:PHE:C	1:A:250:ARG:H	2.19	0.44
1:B:120:THR:HB	1:B:182:ARG:CD	2.39	0.44
1:A:34:LEU:HD13	1:A:36:VAL:CG2	2.48	0.44
1:D:165:TYR:CD2	1:D:193:VAL:HG11	2.52	0.43
1:A:237:LEU:HB3	1:C:212:VAL:CG1	2.47	0.43
1:A:28:LEU:CD1	1:A:30:MET:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:O	1:B:267:LYS:HB3	2.18	0.43
1:D:306:LYS:HA	1:D:306:LYS:HD2	1.74	0.43
1:B:30:MET:HE1	1:B:189:VAL:CG2	2.48	0.43
1:A:274:ILE:CG2	1:C:285:LYS:HD2	2.48	0.43
1:D:188:ARG:HD2	1:D:188:ARG:C	2.39	0.43
1:A:246:LYS:O	1:A:249:THR:HG22	2.19	0.43
1:C:258:MET:HE3	4:C:1005:HOH:O	2.17	0.43
1:D:111:LEU:HG	1:D:115:LEU:HD11	2.00	0.43
1:D:39:GLY:HA3	2:D:1372:NAI:O5B	2.18	0.43
1:A:217:HIS:NE2	1:A:251:ILE:HD13	2.34	0.43
1:B:30:MET:HE2	1:B:185:LEU:HD11	2.00	0.43
1:B:100:PRO:HB2	1:B:261:ASP:OD2	2.20	0.42
1:D:257:ILE:HD12	1:D:257:ILE:N	2.32	0.42
1:B:253:LYS:O	1:D:304:LYS:HE2	2.20	0.42
1:A:28:LEU:HD12	1:A:30:MET:O	2.19	0.42
1:B:254:SER:HB3	1:B:259:TRP:CD1	2.55	0.42
1:D:302:GLU:O	1:D:306:LYS:HB2	2.20	0.42
1:C:97:LEU:HB2	1:C:123:ASP:CB	2.50	0.42
1:C:258:MET:CE	2:C:4372:NAI:H71N	2.33	0.42
1:B:38:VAL:HG12	1:B:157:VAL:HG11	2.02	0.42
1:A:211:VAL:HG22	1:C:230:MET:CE	2.46	0.41
1:C:173:THR:HA	1:C:200:MET:O	2.20	0.41
1:C:30:MET:HE3	1:C:189:VAL:CG2	2.50	0.41
1:D:35:ILE:CD1	1:D:42:GLY:CA	2.98	0.41
1:A:102:ARG:HE	1:A:103:THR:HG23	1.86	0.41
1:B:238:PHE:CD2	1:D:306:LYS:HE2	2.55	0.41
1:B:225:ASP:HA	1:B:228:ILE:HD12	2.01	0.41
1:B:241:PRO:O	1:B:242:GLY:C	2.58	0.41
1:C:87:VAL:CG2	1:C:114:ILE:HG21	2.50	0.41
1:C:227:LEU:HD22	1:C:245:PHE:CE1	2.55	0.41
1:C:286:GLU:O	1:C:290:ARG:HG2	2.21	0.41
1:B:108:ALA:HA	1:B:111:LEU:HB2	2.02	0.41
1:B:306:LYS:HD2	1:B:307:ARG:N	2.30	0.41
1:D:250:ARG:HG2	1:D:250:ARG:O	2.21	0.41
1:D:124:GLN:NE2	1:D:165:TYR:OH	2.54	0.41
1:B:219:VAL:HG11	1:D:219:VAL:HG13	2.02	0.41
1:D:47:LYS:O	1:D:51:ARG:HB2	2.21	0.41
1:A:264:LEU:HD21	1:C:296:LEU:HD12	2.03	0.41
1:C:292:ALA:O	1:C:293:GLU:C	2.59	0.40
1:A:301:LYS:O	1:A:305:ILE:HG13	2.21	0.40
2:D:1372:NAI:H3D	4:D:1054:HOH:O	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LEU:HB2	1:C:123:ASP:HB3	2.04	0.40
1:D:307:ARG:O	1:D:307:ARG:HD2	2.21	0.40
1:A:103:THR:HG21	2:A:2372:NAI:N6A	2.36	0.40
1:D:206:ASP:HB3	1:D:266:ASN:OD1	2.22	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	283/314 (90%)	264 (93%)	14 (5%)	5 (2%)	8	3
1	B	280/314 (89%)	264 (94%)	15 (5%)	1 (0%)	34	29
1	C	279/314 (89%)	268 (96%)	11 (4%)	0	100	100
1	D	280/314 (89%)	266 (95%)	13 (5%)	1 (0%)	34	29
All	All	1122/1256 (89%)	1062 (95%)	53 (5%)	7 (1%)	25	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	292	ALA
1	A	293	GLU
1	D	78	ASP
1	A	152	THR
1	A	153	GLU
1	B	141	LYS

### 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	249/275 (90%)	228 (92%)	21 (8%)	11	6
1	B	246/275 (90%)	224 (91%)	22 (9%)	9	5
1	C	245/275 (89%)	231 (94%)	14 (6%)	20	16
1	D	246/275 (90%)	222 (90%)	24 (10%)	8	4
All	All	986/1100 (90%)	905 (92%)	81 (8%)	11	7

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	28	LEU
1	A	33	VAL
1	A	34	LEU
1	A	93	ASP
1	A	116	SER
1	A	128	LYS
1	A	152	THR
1	A	155	SER
1	A	158	GLU
1	A	161	LEU
1	A	166	GLU
1	A	176	LYS
1	A	177	LYS
1	A	178	THR
1	A	223	LEU
1	A	239	LYS
1	A	249	THR
1	A	297	VAL
1	A	298	GLU
1	A	301	LYS
1	B	31	GLN
1	B	34	LEU
1	B	50	ARG

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Mol	Chain	Res	Type
1	B	55	LYS
1	B	78	ASP
1	B	111	LEU
1	B	117	GLU
1	B	120	THR
1	B	128	LYS
1	B	130	LYS
1	B	153	GLU
1	B	157	VAL
1	B	164	LEU
1	B	180	LYS
1	B	234	GLU
1	B	235	VAL
1	B	246	LYS
1	B	247	ASP
1	B	267	LYS
1	B	290	ARG
1	B	297	VAL
1	B	306	LYS
1	C	27	SER
1	C	84	ILE
1	C	101	VAL
1	C	110	LYS
1	C	128	LYS
1	C	130	LYS
1	C	153	GLU
1	C	158	GLU
1	C	211	VAL
1	C	219	VAL
1	C	232	THR
1	C	268	GLU
1	C	294	GLU
1	C	296	LEU
1	D	28	LEU
1	D	31	GLN
1	D	35	ILE
1	D	44	SER
1	D	49	LEU
1	D	51	ARG
1	D	68	ILE
1	D	86	LYS
1	D	98	SER

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Mol	Chain	Res	Type
1	D	106	GLU
1	D	111	LEU
1	D	114	ILE
1	D	128	LYS
1	D	181	LYS
1	D	185	LEU
1	D	234	GLU
1	D	271	MET
1	D	275	GLU
1	D	281	LEU
1	D	294	GLU
1	D	297	VAL
1	D	299	TYR
1	D	300	LEU
1	D	306	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	266	ASN
1	A	269	ASN
1	B	31	GLN
1	B	266	ASN
1	C	124	GLN
1	C	266	ASN
1	C	269	ASN
1	D	124	GLN
1	D	282	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ENO	B	3168	-	10,13,13	0.89	0	12,17,17	1.10	1 (8%)
2	NAI	D	1372	-	42,48,48	1.44	5 (11%)	47,73,73	1.39	6 (12%)
3	ENO	C	3167	-	10,13,13	2.11	5 (50%)	12,17,17	1.65	5 (41%)
2	NAI	A	2372	-	42,48,48	1.46	6 (14%)	47,73,73	1.45	6 (12%)
2	NAI	C	4372	-	42,48,48	1.46	8 (19%)	47,73,73	1.53	9 (19%)
2	NAI	B	3372	-	42,48,48	1.49	4 (9%)	47,73,73	1.71	10 (21%)

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	ENO	B	3168	-	-	0/4/8/8	0/1/1/1
2	NAI	D	1372	-	-	5/25/72/72	0/5/5/5
3	ENO	C	3167	-	-	0/4/8/8	0/1/1/1
2	NAI	A	2372	-	-	3/25/72/72	0/5/5/5
2	NAI	C	4372	-	-	6/25/72/72	0/5/5/5
2	NAI	B	3372	-	-	6/25/72/72	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2372	NAI	C6N-C5N	5.03	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3372	NAI	C4N-C3N	-4.37	1.41	1.49
2	D	1372	NAI	C6N-C5N	4.22	1.40	1.33
2	D	1372	NAI	C4N-C3N	-4.13	1.41	1.49
2	C	4372	NAI	C4N-C5N	-3.89	1.38	1.48
2	C	4372	NAI	C4N-C3N	-3.87	1.42	1.49
2	B	3372	NAI	C4N-C5N	-3.77	1.39	1.48
2	B	3372	NAI	C6N-C5N	3.61	1.39	1.33
2	A	2372	NAI	C2N-C3N	3.56	1.44	1.34
2	D	1372	NAI	C4N-C5N	-3.29	1.40	1.48
2	C	4372	NAI	C6N-C5N	3.23	1.39	1.33
3	C	3167	ENO	C8-C9	3.20	1.44	1.38
2	A	2372	NAI	C4N-C3N	-3.19	1.43	1.49
2	A	2372	NAI	C4N-C5N	-2.97	1.41	1.48
3	C	3167	ENO	C5-C4	2.92	1.45	1.38
2	D	1372	NAI	C5A-C4A	2.85	1.48	1.40
3	C	3167	ENO	C9-C4	2.58	1.44	1.38
2	C	4372	NAI	PA-O2A	-2.51	1.43	1.55
2	D	1372	NAI	C2A-N3A	2.40	1.36	1.32
2	A	2372	NAI	C7N-C3N	2.40	1.53	1.48
2	C	4372	NAI	C2B-C1B	-2.37	1.50	1.53
2	C	4372	NAI	O4B-C4B	-2.30	1.39	1.45
3	C	3167	ENO	C5-C6	2.28	1.42	1.38
2	C	4372	NAI	C5A-C4A	2.25	1.46	1.40
2	C	4372	NAI	C8A-N7A	2.11	1.38	1.34
3	C	3167	ENO	C8-C7	2.10	1.42	1.38
2	A	2372	NAI	C2A-N3A	2.06	1.35	1.32
2	B	3372	NAI	C2N-C3N	2.02	1.40	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2372	NAI	N3A-C2A-N1A	-4.66	121.40	128.68
2	C	4372	NAI	PN-O3-PA	-4.30	118.08	132.83
2	B	3372	NAI	N3A-C2A-N1A	-4.23	122.07	128.68
2	B	3372	NAI	PN-O3-PA	-4.11	118.74	132.83
2	C	4372	NAI	O4B-C1B-C2B	-3.97	101.12	106.93
2	D	1372	NAI	PN-O3-PA	-3.41	121.11	132.83
2	D	1372	NAI	N3A-C2A-N1A	-3.40	123.37	128.68
2	B	3372	NAI	C3N-C2N-N1N	-3.38	118.28	123.10
2	C	4372	NAI	N3A-C2A-N1A	-3.24	123.61	128.68
2	B	3372	NAI	O2A-PA-O1A	3.19	128.03	112.24
2	C	4372	NAI	C3N-C2N-N1N	-3.19	118.55	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3372	NAI	C4A-C5A-N7A	-3.15	106.11	109.40
2	B	3372	NAI	C2A-N1A-C6A	3.09	124.05	118.75
2	C	4372	NAI	C2A-N1A-C6A	3.06	123.99	118.75
2	B	3372	NAI	C1B-N9A-C4A	-3.06	121.27	126.64
2	A	2372	NAI	O1N-PN-O2N	2.75	125.82	112.24
3	C	3167	ENO	C9-C8-C7	-2.72	116.89	119.88
2	B	3372	NAI	C1D-N1N-C6N	-2.71	115.00	120.83
2	C	4372	NAI	O2A-PA-O1A	2.69	125.54	112.24
3	C	3167	ENO	O4-C2-C3	2.67	124.96	120.75
2	C	4372	NAI	N6A-C6A-N1A	2.51	123.79	118.57
2	D	1372	NAI	N6A-C6A-N1A	2.44	123.64	118.57
2	B	3372	NAI	C2D-C1D-N1N	2.41	119.35	113.30
2	A	2372	NAI	C2A-N1A-C6A	2.37	122.80	118.75
2	D	1372	NAI	O2A-PA-O1A	2.33	123.75	112.24
2	D	1372	NAI	C2A-N1A-C6A	2.29	122.66	118.75
2	B	3372	NAI	C2B-C3B-C4B	2.28	107.08	102.64
2	C	4372	NAI	C1D-N1N-C6N	-2.26	115.96	120.83
3	B	3168	ENO	C5-C6-C7	2.20	122.29	119.88
3	C	3167	ENO	C6-C5-C4	-2.20	118.00	121.03
2	A	2372	NAI	N6A-C6A-N1A	2.20	123.13	118.57
3	C	3167	ENO	C3-C4-C9	-2.19	117.75	120.89
2	D	1372	NAI	O4B-C1B-C2B	-2.17	103.75	106.93
2	A	2372	NAI	C3N-C2N-N1N	-2.14	120.05	123.10
3	C	3167	ENO	C6-C7-C8	2.12	123.34	119.77
2	C	4372	NAI	C5A-C6A-N1A	-2.08	115.63	120.35
2	A	2372	NAI	PN-O3-PA	-2.05	125.79	132.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1372	NAI	C2N-C3N-C7N-N7N
2	D	1372	NAI	O4B-C4B-C5B-O5B
2	D	1372	NAI	C3B-C4B-C5B-O5B
2	B	3372	NAI	C2D-C1D-N1N-C6N
2	C	4372	NAI	C2D-C1D-N1N-C6N
2	B	3372	NAI	O4D-C1D-N1N-C6N
2	C	4372	NAI	O4D-C1D-N1N-C6N
2	A	2372	NAI	O4D-C1D-N1N-C6N
2	D	1372	NAI	O4D-C1D-N1N-C6N
2	B	3372	NAI	C2D-C1D-N1N-C2N
2	B	3372	NAI	O4B-C4B-C5B-O5B

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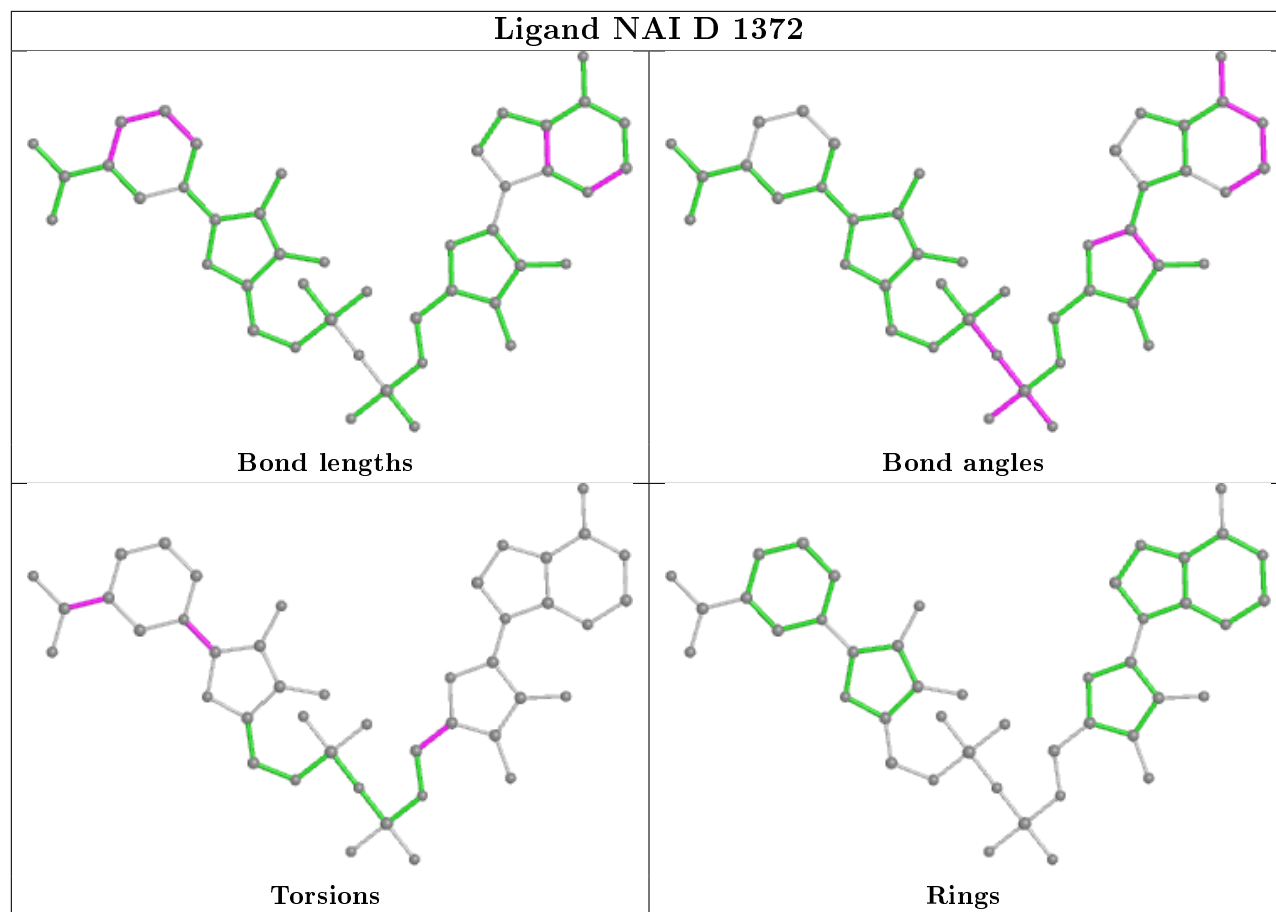
Mol	Chain	Res	Type	Atoms
2	B	3372	NAI	C3B-C4B-C5B-O5B
2	A	2372	NAI	C2D-C1D-N1N-C6N
2	C	4372	NAI	C2D-C1D-N1N-C2N
2	C	4372	NAI	O4D-C1D-N1N-C2N
2	B	3372	NAI	O4D-C1D-N1N-C2N
2	D	1372	NAI	C2D-C1D-N1N-C6N
2	C	4372	NAI	C2N-C3N-C7N-N7N
2	A	2372	NAI	O4B-C4B-C5B-O5B
2	C	4372	NAI	O4B-C4B-C5B-O5B

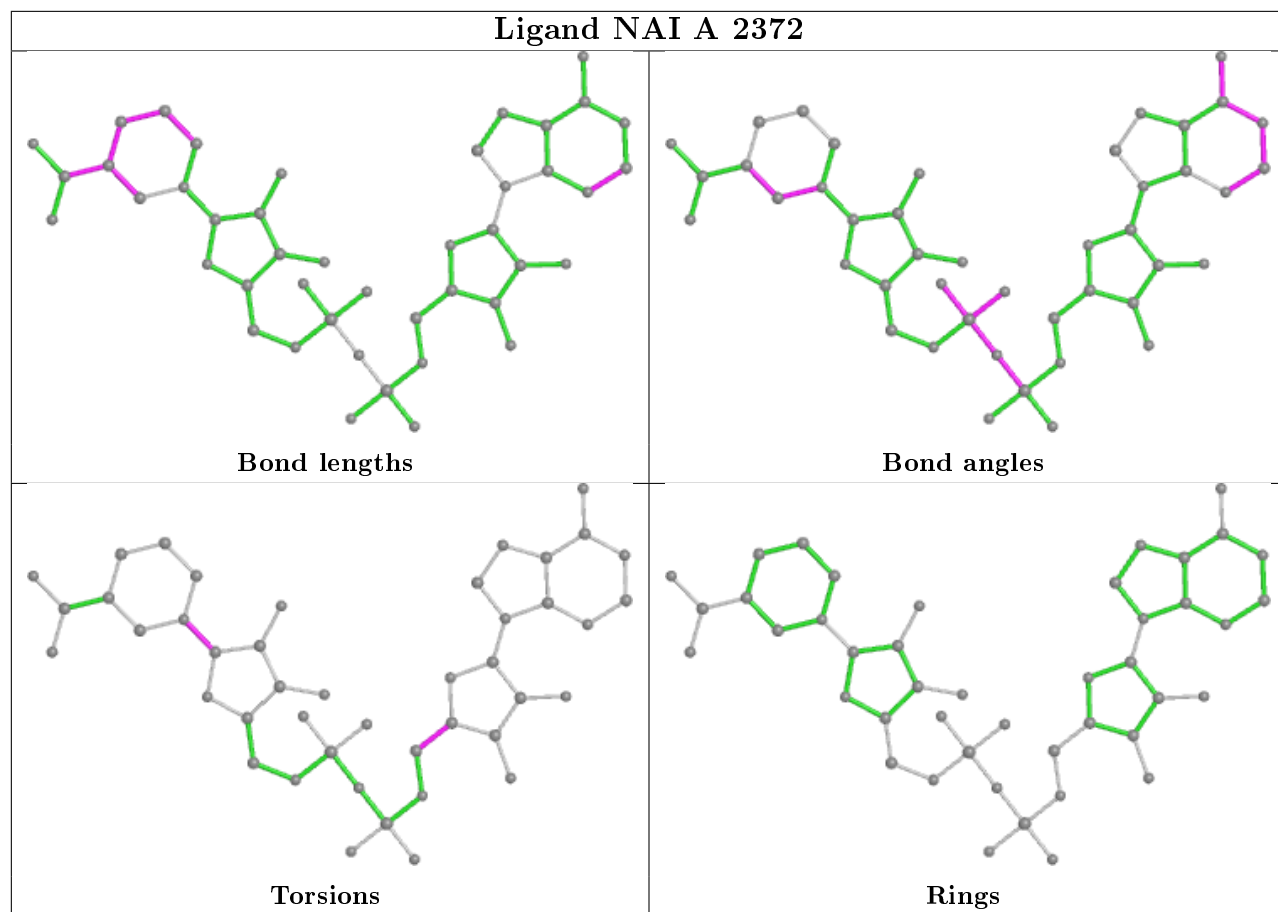
There are no ring outliers.

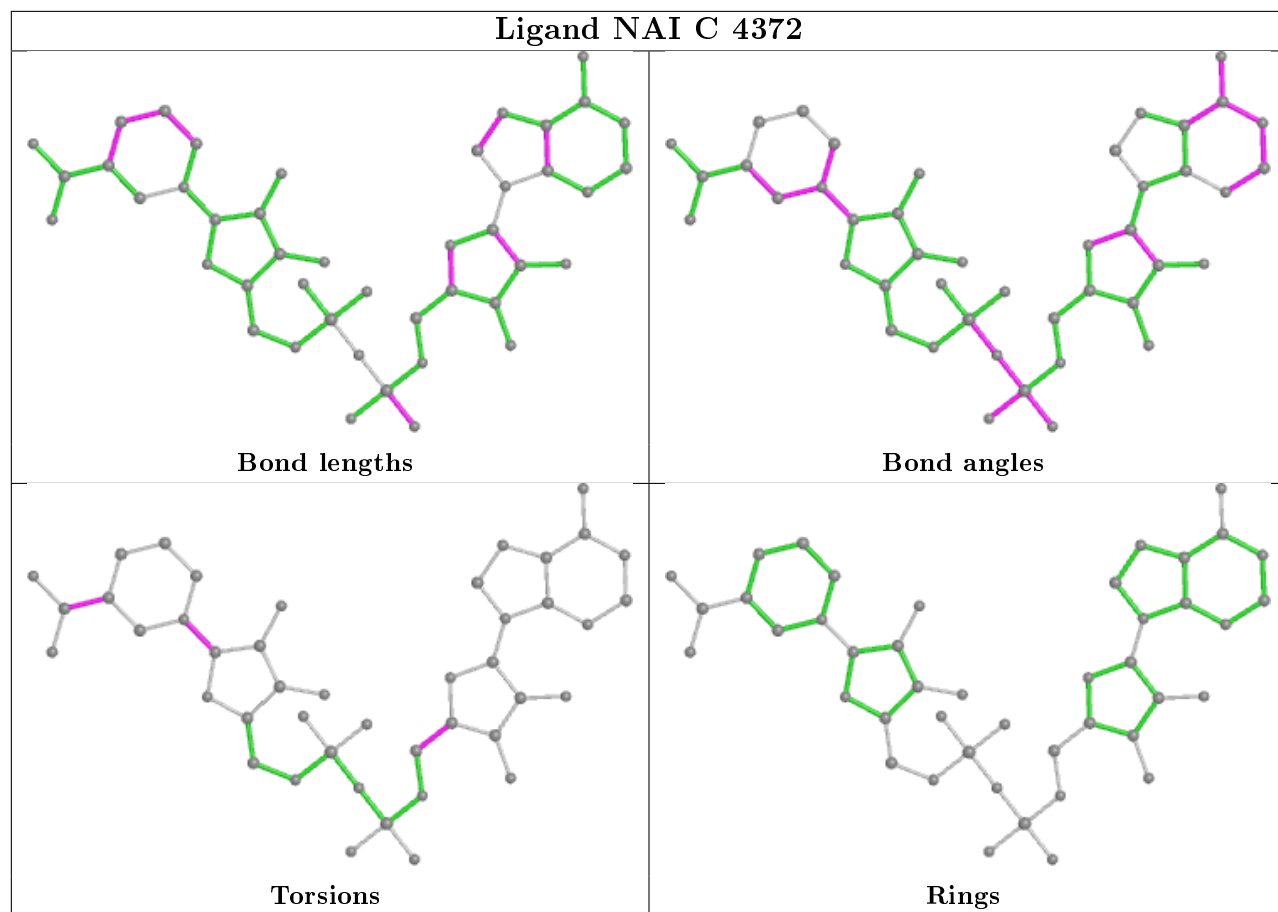
4 monomers are involved in 13 short contacts:

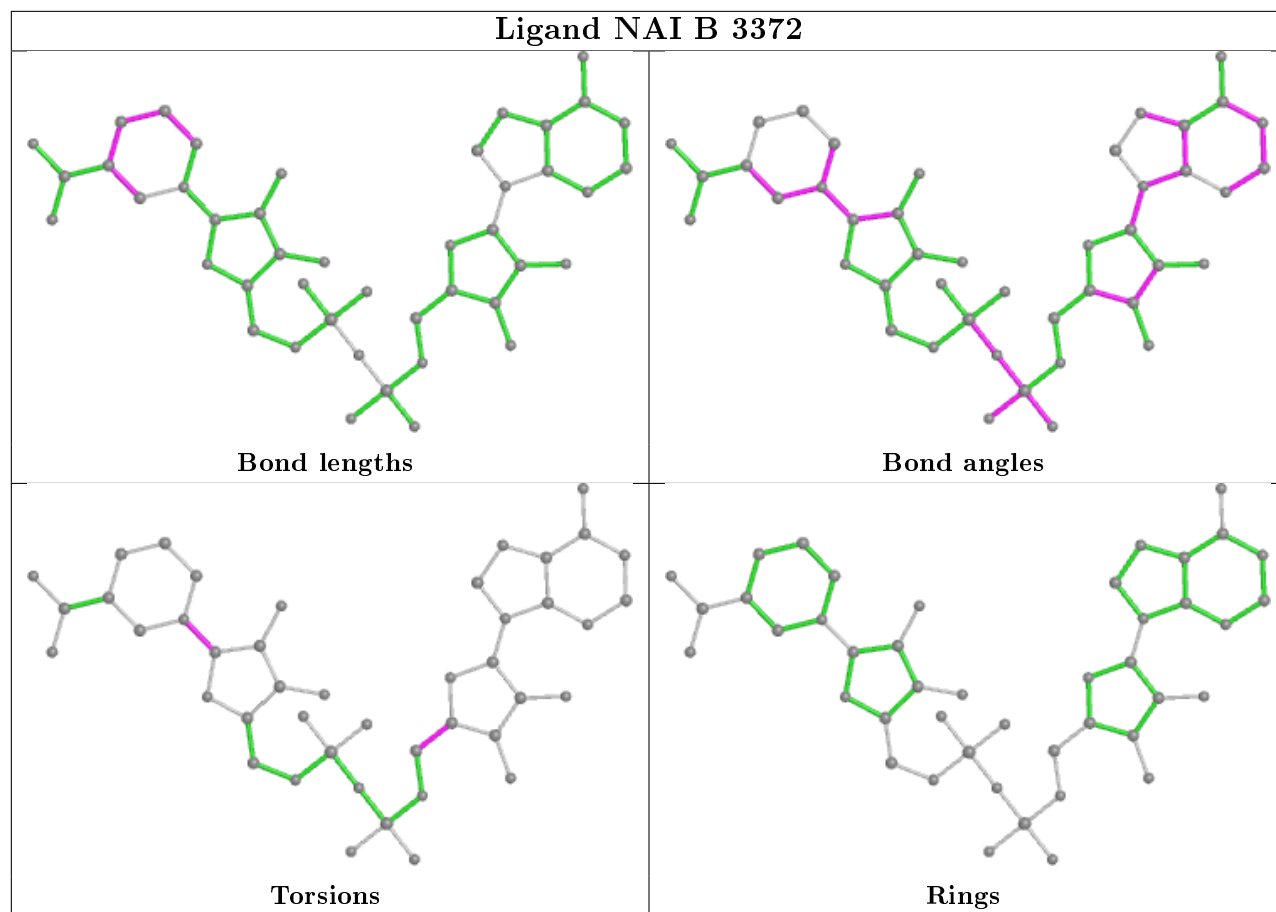
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1372	NAI	4	0
2	A	2372	NAI	3	0
2	C	4372	NAI	5	0
2	B	3372	NAI	1	0

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.









## 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	285/314 (90%)	0.14	4 (1%) 75 80	25, 36, 47, 66	0
1	B	282/314 (89%)	0.12	3 (1%) 80 85	26, 38, 46, 55	0
1	C	281/314 (89%)	0.04	4 (1%) 75 80	29, 36, 51, 66	0
1	D	282/314 (89%)	0.32	11 (3%) 39 48	28, 39, 52, 57	0
All	All	1130/1256 (89%)	0.15	22 (1%) 66 74	25, 37, 50, 66	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	ILE	7.2
1	C	305	ILE	5.1
1	A	152	THR	3.4
1	D	31	GLN	3.4
1	D	86	LYS	3.3
1	D	151	GLY	3.0
1	D	54	PHE	3.0
1	D	80	GLY	2.9
1	D	38	VAL	2.9
1	A	153	GLU	2.8
1	D	55	LYS	2.8
1	B	55	LYS	2.7
1	D	84	ILE	2.6
1	D	164	LEU	2.6
1	A	102	ARG	2.5
1	C	303	VAL	2.5
1	B	117	GLU	2.3
1	C	302	GLU	2.2
1	B	57	LYS	2.2
1	D	30	MET	2.2
1	D	89	ASP	2.2
1	C	272	LYS	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.

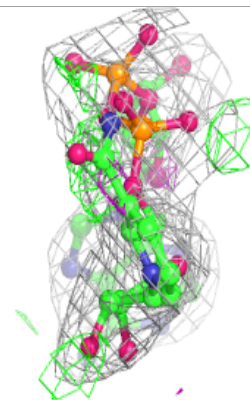
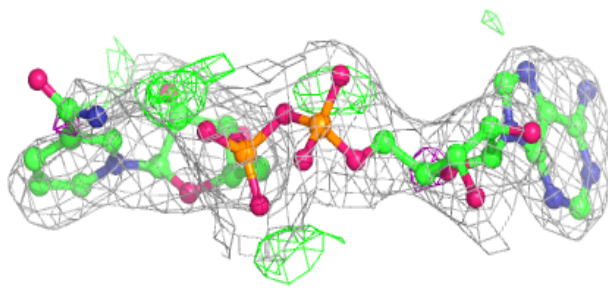
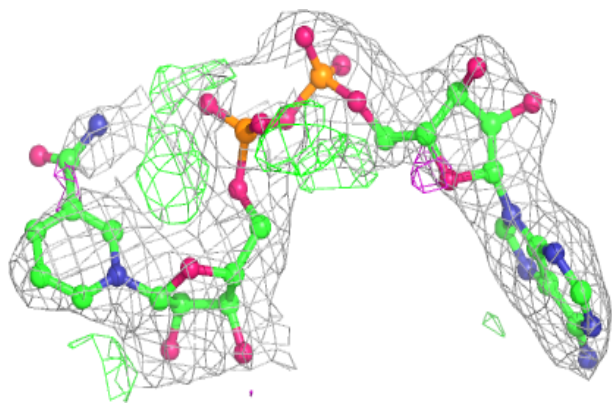
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAI	D	1372	44/44	0.90	0.14	64,74,87,90	0
3	ENO	C	3167	13/13	0.93	0.13	38,43,46,47	0
2	NAI	A	2372	44/44	0.95	0.10	48,54,64,65	0
3	ENO	B	3168	13/13	0.96	0.10	32,37,43,46	0
2	NAI	B	3372	44/44	0.96	0.11	32,39,47,57	0
2	NAI	C	4372	44/44	0.97	0.11	35,40,48,53	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.

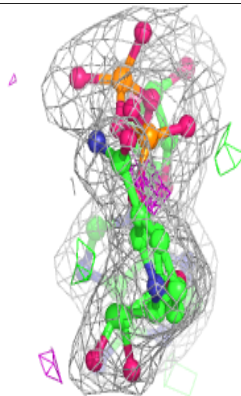
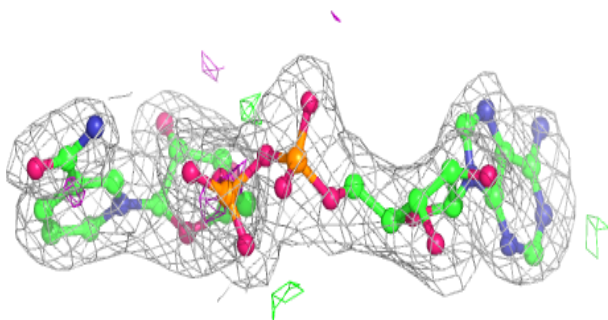
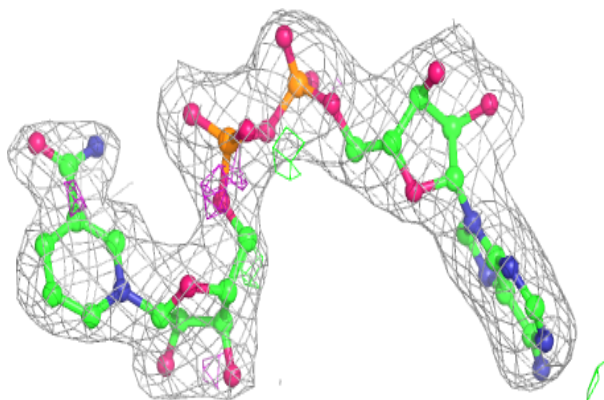


**Electron density around NAI D 1372:**

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

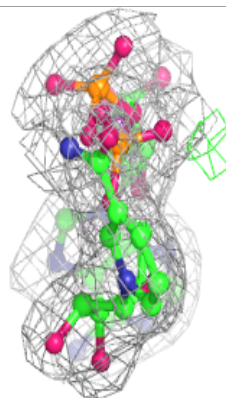
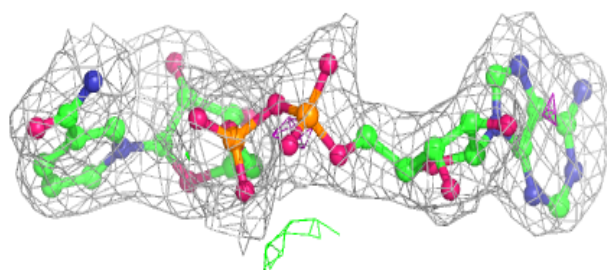
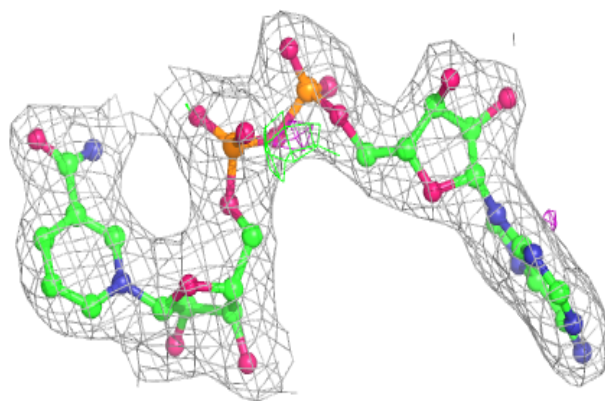
**Electron density around NAI A 2372:**

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

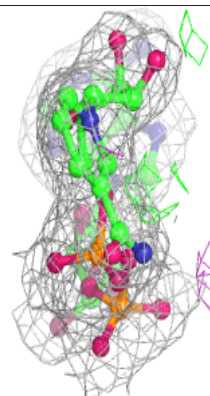
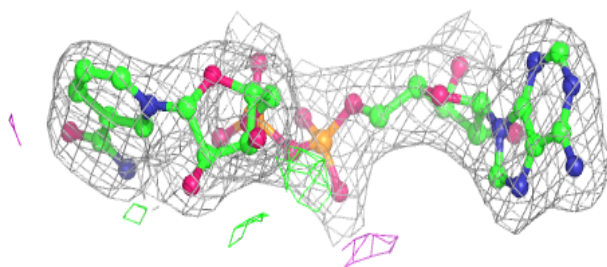
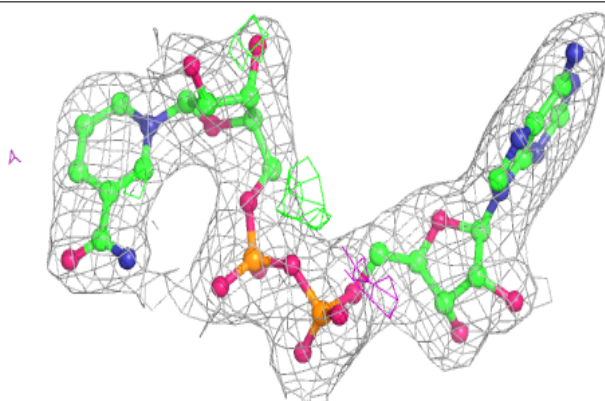


**Electron density around NAI B 3372:**

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

**Electron density around NAI C 4372:**

$2mF_o-DF_c$  (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.