



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 09:09 am BST

PDB ID : 5ZI5
Title : Crystal structure of Legionella pneumophila aminopeptidase A
Authors : Marapaka, A.K.; Addlagatta, A.
Deposited on : 2018-03-14
Resolution : 2.60 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

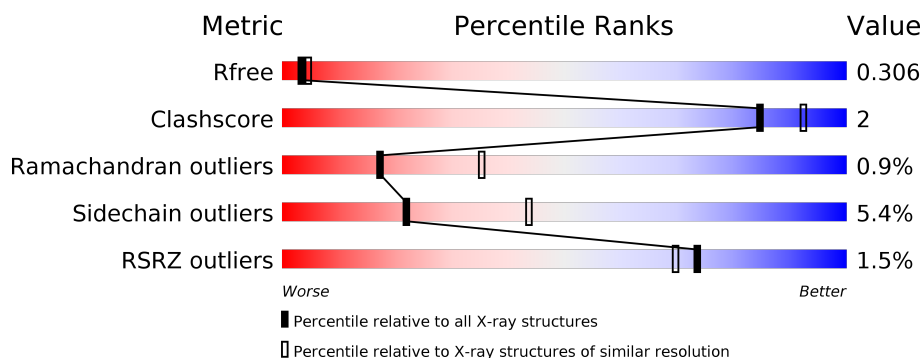
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 ≥ 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	921	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	921	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13662 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	0	0
			6815	4370	1113	1306	26			
1	B	850	Total	C	N	O	S	0	0	0
			6815	4370	1113	1306	26			

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q5ZVE3
A	-19	GLY	-	expression tag	UNP Q5ZVE3
A	-18	SER	-	expression tag	UNP Q5ZVE3
A	-17	SER	-	expression tag	UNP Q5ZVE3
A	-16	HIS	-	expression tag	UNP Q5ZVE3
A	-15	HIS	-	expression tag	UNP Q5ZVE3
A	-14	HIS	-	expression tag	UNP Q5ZVE3
A	-13	HIS	-	expression tag	UNP Q5ZVE3
A	-12	HIS	-	expression tag	UNP Q5ZVE3
A	-11	HIS	-	expression tag	UNP Q5ZVE3
A	-10	SER	-	expression tag	UNP Q5ZVE3
A	-9	SER	-	expression tag	UNP Q5ZVE3
A	-8	GLY	-	expression tag	UNP Q5ZVE3
A	-7	LEU	-	expression tag	UNP Q5ZVE3
A	-6	VAL	-	expression tag	UNP Q5ZVE3
A	-5	PRO	-	expression tag	UNP Q5ZVE3
A	-4	ARG	-	expression tag	UNP Q5ZVE3
A	-3	GLY	-	expression tag	UNP Q5ZVE3
A	-2	SER	-	expression tag	UNP Q5ZVE3
A	-1	HIS	-	expression tag	UNP Q5ZVE3
A	0	MET	-	expression tag	UNP Q5ZVE3
A	1	MET	-	expression tag	UNP Q5ZVE3
A	2	VAL	-	expression tag	UNP Q5ZVE3
A	3	LYS	-	expression tag	UNP Q5ZVE3
A	4	GLN	-	expression tag	UNP Q5ZVE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP Q5ZVE3
A	6	VAL	-	expression tag	UNP Q5ZVE3
A	7	PHE	-	expression tag	UNP Q5ZVE3
A	8	MET	-	expression tag	UNP Q5ZVE3
A	9	LYS	-	expression tag	UNP Q5ZVE3
A	10	THR	-	expression tag	UNP Q5ZVE3
A	11	ASP	-	expression tag	UNP Q5ZVE3
A	12	GLN	-	expression tag	UNP Q5ZVE3
A	863	LYS	-	expression tag	UNP Q5ZVE3
A	864	GLU	-	expression tag	UNP Q5ZVE3
A	865	ASP	-	expression tag	UNP Q5ZVE3
A	866	LEU	-	expression tag	UNP Q5ZVE3
A	867	PRO	-	expression tag	UNP Q5ZVE3
A	868	LEU	-	expression tag	UNP Q5ZVE3
A	869	PRO	-	expression tag	UNP Q5ZVE3
A	870	ILE	-	expression tag	UNP Q5ZVE3
A	871	HIS	-	expression tag	UNP Q5ZVE3
A	872	LEU	-	expression tag	UNP Q5ZVE3
A	873	THR	-	expression tag	UNP Q5ZVE3
A	874	PHE	-	expression tag	UNP Q5ZVE3
A	875	HIS	-	expression tag	UNP Q5ZVE3
A	876	GLY	-	expression tag	UNP Q5ZVE3
A	877	GLY	-	expression tag	UNP Q5ZVE3
A	878	SER	-	expression tag	UNP Q5ZVE3
A	879	THR	-	expression tag	UNP Q5ZVE3
A	880	MET	-	expression tag	UNP Q5ZVE3
A	881	GLN	-	expression tag	UNP Q5ZVE3
A	882	ASP	-	expression tag	UNP Q5ZVE3
A	883	ARG	-	expression tag	UNP Q5ZVE3
A	884	THR	-	expression tag	UNP Q5ZVE3
A	885	ALA	-	expression tag	UNP Q5ZVE3
A	886	GLN	-	expression tag	UNP Q5ZVE3
A	887	LEU	-	expression tag	UNP Q5ZVE3
A	888	ILE	-	expression tag	UNP Q5ZVE3
A	889	ALA	-	expression tag	UNP Q5ZVE3
A	890	ASP	-	expression tag	UNP Q5ZVE3
A	891	GLY	-	expression tag	UNP Q5ZVE3
A	892	ASN	-	expression tag	UNP Q5ZVE3
A	893	LYS	-	expression tag	UNP Q5ZVE3
A	894	GLU	-	expression tag	UNP Q5ZVE3
A	895	ASN	-	expression tag	UNP Q5ZVE3
A	896	ALA	-	expression tag	UNP Q5ZVE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	897	TYR	-	expression tag	UNP Q5ZVE3
A	898	GLN	-	expression tag	UNP Q5ZVE3
A	899	LEU	-	expression tag	UNP Q5ZVE3
A	900	HIS	-	expression tag	UNP Q5ZVE3
B	-20	MET	-	initiating methionine	UNP Q5ZVE3
B	-19	GLY	-	expression tag	UNP Q5ZVE3
B	-18	SER	-	expression tag	UNP Q5ZVE3
B	-17	SER	-	expression tag	UNP Q5ZVE3
B	-16	HIS	-	expression tag	UNP Q5ZVE3
B	-15	HIS	-	expression tag	UNP Q5ZVE3
B	-14	HIS	-	expression tag	UNP Q5ZVE3
B	-13	HIS	-	expression tag	UNP Q5ZVE3
B	-12	HIS	-	expression tag	UNP Q5ZVE3
B	-11	HIS	-	expression tag	UNP Q5ZVE3
B	-10	SER	-	expression tag	UNP Q5ZVE3
B	-9	SER	-	expression tag	UNP Q5ZVE3
B	-8	GLY	-	expression tag	UNP Q5ZVE3
B	-7	LEU	-	expression tag	UNP Q5ZVE3
B	-6	VAL	-	expression tag	UNP Q5ZVE3
B	-5	PRO	-	expression tag	UNP Q5ZVE3
B	-4	ARG	-	expression tag	UNP Q5ZVE3
B	-3	GLY	-	expression tag	UNP Q5ZVE3
B	-2	SER	-	expression tag	UNP Q5ZVE3
B	-1	HIS	-	expression tag	UNP Q5ZVE3
B	0	MET	-	expression tag	UNP Q5ZVE3
B	1	MET	-	expression tag	UNP Q5ZVE3
B	2	VAL	-	expression tag	UNP Q5ZVE3
B	3	LYS	-	expression tag	UNP Q5ZVE3
B	4	GLN	-	expression tag	UNP Q5ZVE3
B	5	GLY	-	expression tag	UNP Q5ZVE3
B	6	VAL	-	expression tag	UNP Q5ZVE3
B	7	PHE	-	expression tag	UNP Q5ZVE3
B	8	MET	-	expression tag	UNP Q5ZVE3
B	9	LYS	-	expression tag	UNP Q5ZVE3
B	10	THR	-	expression tag	UNP Q5ZVE3
B	11	ASP	-	expression tag	UNP Q5ZVE3
B	12	GLN	-	expression tag	UNP Q5ZVE3
B	863	LYS	-	expression tag	UNP Q5ZVE3
B	864	GLU	-	expression tag	UNP Q5ZVE3
B	865	ASP	-	expression tag	UNP Q5ZVE3
B	866	LEU	-	expression tag	UNP Q5ZVE3
B	867	PRO	-	expression tag	UNP Q5ZVE3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	868	LEU	-	expression tag	UNP Q5ZVE3
B	869	PRO	-	expression tag	UNP Q5ZVE3
B	870	ILE	-	expression tag	UNP Q5ZVE3
B	871	HIS	-	expression tag	UNP Q5ZVE3
B	872	LEU	-	expression tag	UNP Q5ZVE3
B	873	THR	-	expression tag	UNP Q5ZVE3
B	874	PHE	-	expression tag	UNP Q5ZVE3
B	875	HIS	-	expression tag	UNP Q5ZVE3
B	876	GLY	-	expression tag	UNP Q5ZVE3
B	877	GLY	-	expression tag	UNP Q5ZVE3
B	878	SER	-	expression tag	UNP Q5ZVE3
B	879	THR	-	expression tag	UNP Q5ZVE3
B	880	MET	-	expression tag	UNP Q5ZVE3
B	881	GLN	-	expression tag	UNP Q5ZVE3
B	882	ASP	-	expression tag	UNP Q5ZVE3
B	883	ARG	-	expression tag	UNP Q5ZVE3
B	884	THR	-	expression tag	UNP Q5ZVE3
B	885	ALA	-	expression tag	UNP Q5ZVE3
B	886	GLN	-	expression tag	UNP Q5ZVE3
B	887	LEU	-	expression tag	UNP Q5ZVE3
B	888	ILE	-	expression tag	UNP Q5ZVE3
B	889	ALA	-	expression tag	UNP Q5ZVE3
B	890	ASP	-	expression tag	UNP Q5ZVE3
B	891	GLY	-	expression tag	UNP Q5ZVE3
B	892	ASN	-	expression tag	UNP Q5ZVE3
B	893	LYS	-	expression tag	UNP Q5ZVE3
B	894	GLU	-	expression tag	UNP Q5ZVE3
B	895	ASN	-	expression tag	UNP Q5ZVE3
B	896	ALA	-	expression tag	UNP Q5ZVE3
B	897	TYR	-	expression tag	UNP Q5ZVE3
B	898	GLN	-	expression tag	UNP Q5ZVE3
B	899	LEU	-	expression tag	UNP Q5ZVE3
B	900	HIS	-	expression tag	UNP Q5ZVE3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

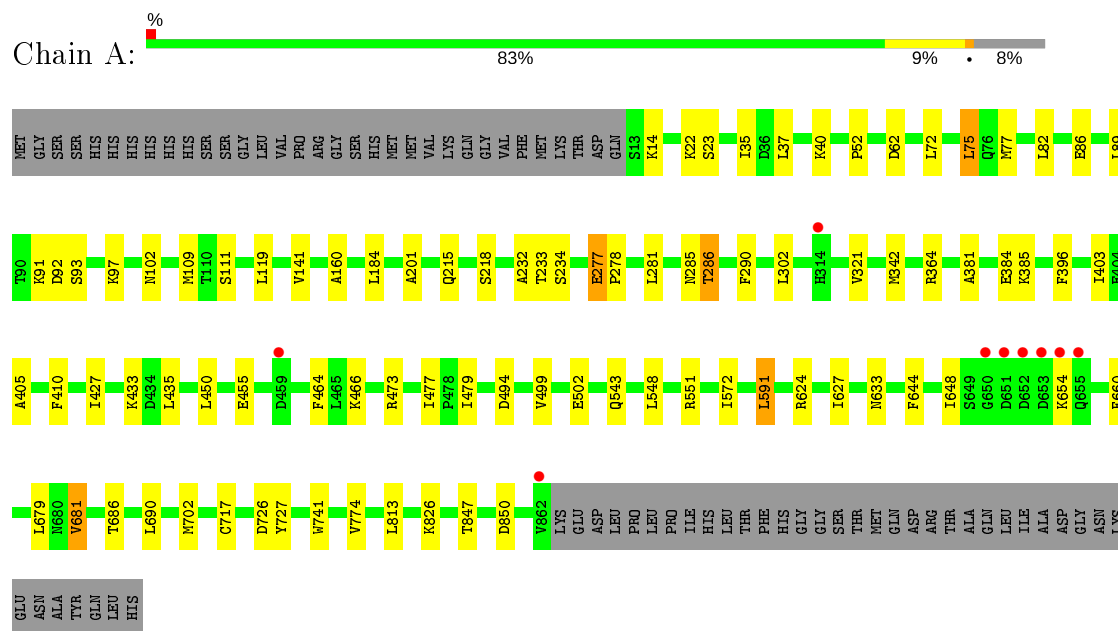
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	12	Total 12	O 12	0	0

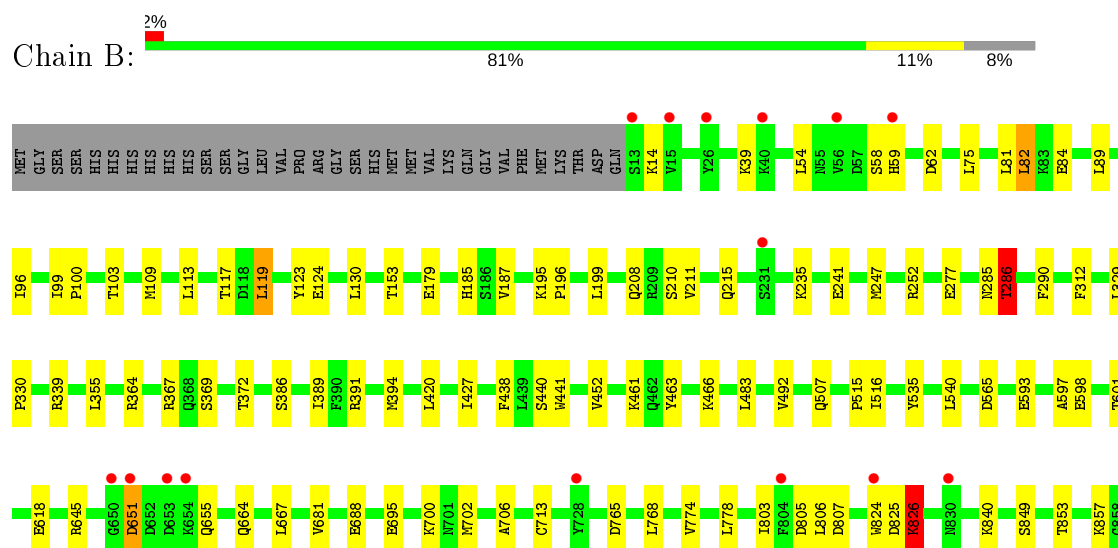
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Aminopeptidase N



• Molecule 1: Aminopeptidase N



I859	LYS
D860	GLU
F861	ASP
V862	LEU
	PRO
	LEU
	PRO
	ILE
	HIS
	LEU
	THR
	PHE
	HIS
	GLY
	GLY
	SER
	THR
	MET
	GLN
	ASP
	ARG
	THR
	ALA
	GLN
	LEU
	ILE
	ALA
	ASP
	GLY
	ASN
	LYS
	GLU
	ASN
	ALA
	TYR
	GLN
	LEU
	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.54Å 101.45Å 129.59Å 90.00° 99.29° 90.00°	Depositor
Resolution (Å)	33.05 – 2.60 33.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (33.05-2.60) 97.7 (33.05-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.216 , 0.308 0.217 , 0.306	Depositor DCC
R_{free} test set	2534 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13662	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	0/6954	0.75	1/9416 (0.0%)
1	B	0.54	0/6954	0.73	2/9416 (0.0%)
All	All	0.55	0/13908	0.74	3/18832 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	624	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	252	ARG	NE-CZ-NH2	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6815	0	6793	35	0
1	B	6815	0	6793	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	0	0	0
3	B	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13662	0	13586	63	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 2.

The worst 5 of 63 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:372:THR:HG21	1:B:853:THR:HG21	1.60	0.84
1:B:651:ASP:OD1	1:B:664:GLN:NE2	2.22	0.72
1:A:82:LEU:HD22	1:A:86:GLU:HG2	1.74	0.68
1:B:355:LEU:HD13	1:B:598:GLU:HG2	1.78	0.64
1:A:75:LEU:HD13	1:A:82:LEU:HD12	1.84	0.59

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	848/921 (92%)	784 (92%)	58 (7%)	6 (1%)	22	43
1	B	848/921 (92%)	776 (92%)	63 (7%)	9 (1%)	14	30
All	All	1696/1842 (92%)	1560 (92%)	121 (7%)	15 (1%)	17	35

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	THR
1	A	286	THR
1	B	286	THR
1	A	679	LEU

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Mol	Chain	Res	Type
1	B	285	ASN

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	755/816 (92%)	721 (96%)	34 (4%)	27	52
1	B	755/816 (92%)	707 (94%)	48 (6%)	17	35
All	All	1510/1632 (92%)	1428 (95%)	82 (5%)	22	44

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	HIS
1	B	109	MET
1	B	700	LYS
1	B	62	ASP
1	B	82	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	501	GLN
1	A	512	GLN
1	A	655	GLN
1	B	740	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	850/921 (92%)	-0.34	9 (1%) 80 78	34, 54, 88, 151	0
1	B	850/921 (92%)	-0.16	17 (2%) 65 60	37, 63, 108, 143	0
All	All	1700/1842 (92%)	-0.25	26 (1%) 73 70	34, 58, 101, 151	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	650	GLY	7.5
1	A	651	ASP	7.4
1	B	13	SER	5.1
1	B	650	GLY	4.5
1	B	26	TYR	3.2

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](#)

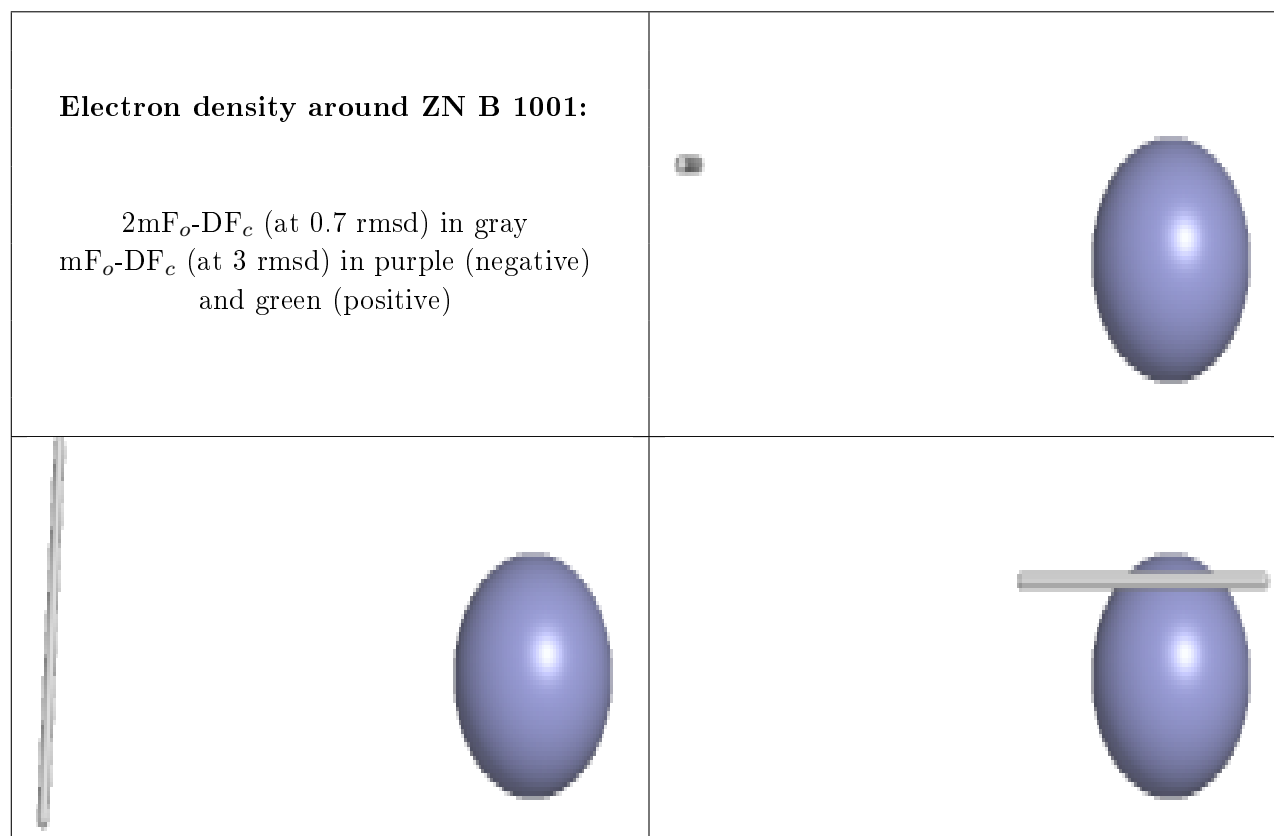
There are no carbohydrates in this entry.

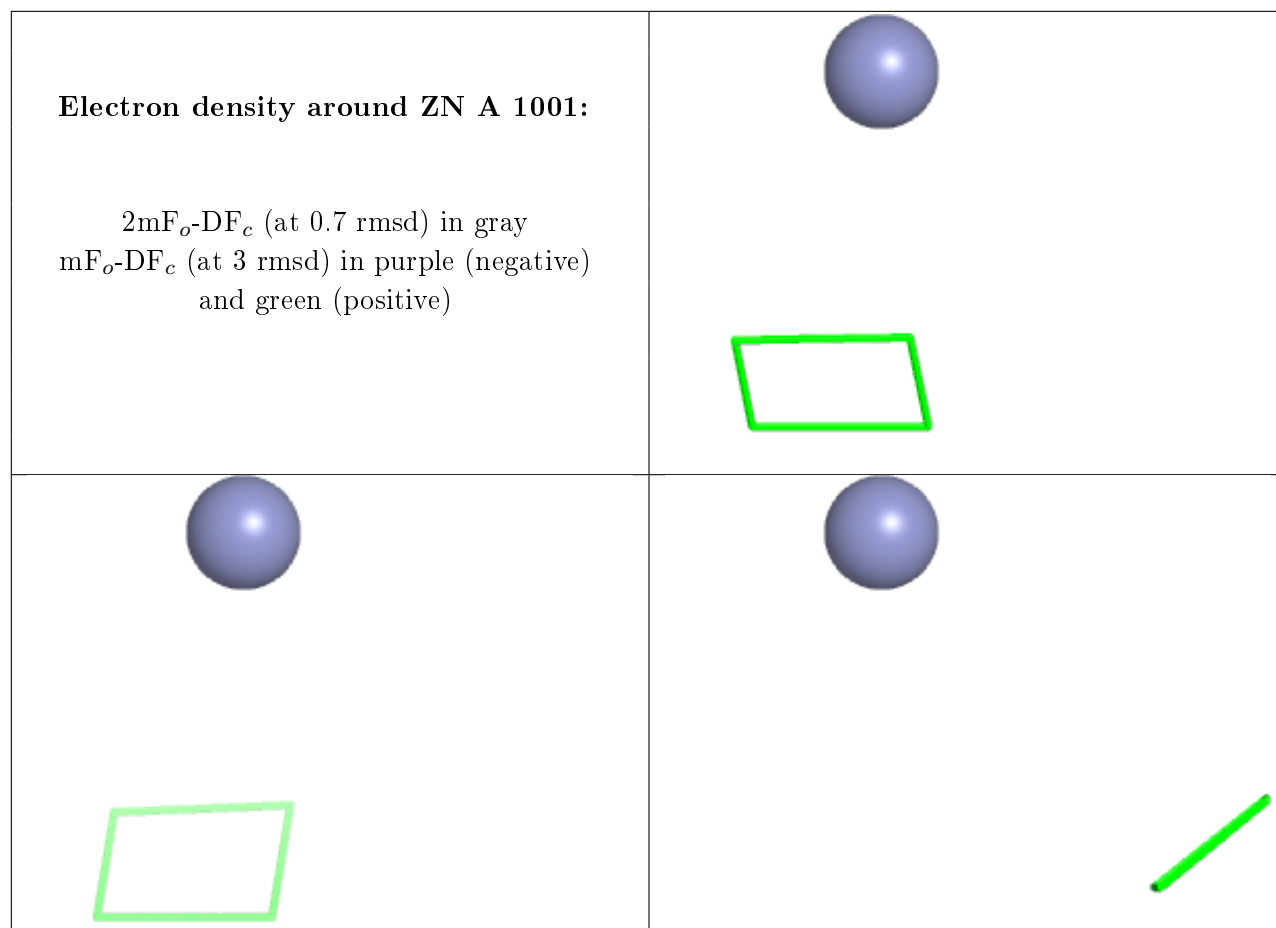
6.4 Ligands [i](#)

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, 95th 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(\AA^2)	Q<0.9
2	ZN	B	1001	1/1	0.99	0.13	46,46,46,46	0
2	ZN	A	1001	1/1	1.00	0.15	43,43,43,43	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.