



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2018 – 09:45 AM EDT

PDB ID : 1B0V
Title : I40N MUTANT OF AZOTOBACTER VINELANDII FDI
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Deposited on : 1998-11-12
Resolution : 2.80 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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031021

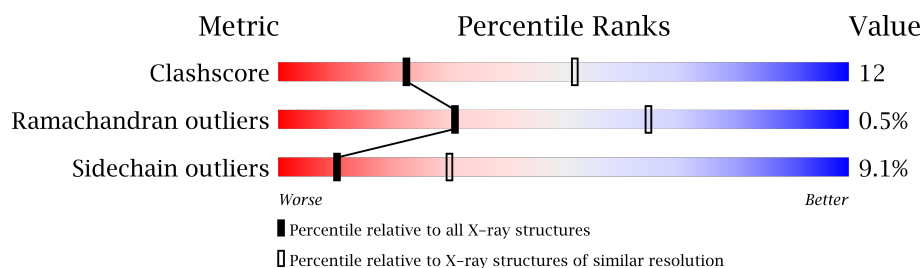
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)

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. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	106	
1	B	106	
1	C	106	
1	D	106	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	107	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	B	307	-	-	X	-
3	F3S	B	308	-	-	X	-
3	F3S	C	508	-	-	X	-
3	F3S	D	708	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3424 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 PROTEIN (FERREDOXIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			
1	B	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			
1	C	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			
1	D	106	Total	C	N	O	S	0	0	0
			841	529	130	172	10			

There are 4 discrepancies between the modelled and reference sequences:

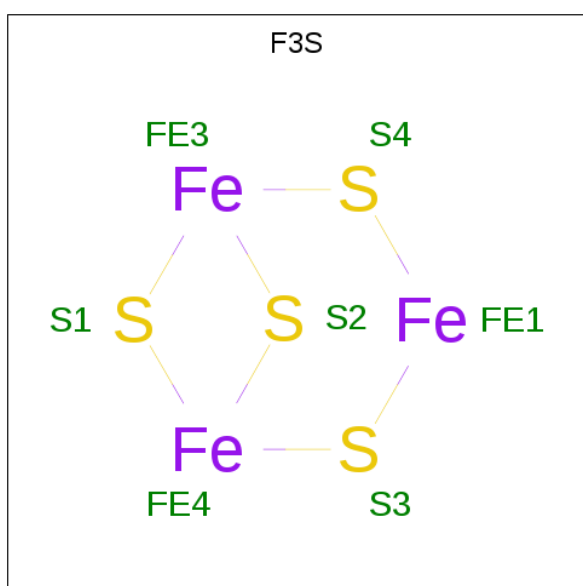
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ILE	ENGINEERED	UNP P00214
B	240	ASN	ILE	ENGINEERED	UNP P00214
C	440	ASN	ILE	ENGINEERED	UNP P00214
D	640	ASN	ILE	ENGINEERED	UNP P00214

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is 2,4,6,7-tetrathia-1 λ^3 ,3 λ^2 ,5 λ^3 -triferrabicyclo[3.1.1]heptane (three-letter code: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	Fe 3	S 4	0	0
3	B	1	Total 7	Fe 3	S 4	0	0
3	C	1	Total 7	Fe 3	S 4	0	0
3	D	1	Total 7	Fe 3	S 4	0	0

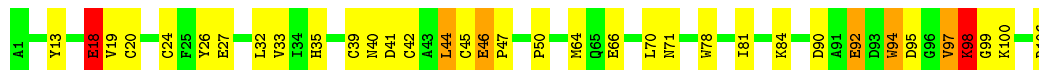
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (FERREDOXIN)

Chain A: 



• Molecule 1: PROTEIN (FERREDOXIN)

Chain B: 



• Molecule 1: PROTEIN (FERREDOXIN)

Chain C: 



• Molecule 1: PROTEIN (FERREDOXIN)

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.00 Å 55.30 Å 62.30 Å 78.10° 85.20° 71.90°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	87.3 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3424	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S

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	1.00	1/862 (0.1%)	1.67	17/1175 (1.4%)
1	B	0.96	1/862 (0.1%)	1.71	22/1175 (1.9%)
1	C	1.03	2/862 (0.2%)	1.74	23/1175 (2.0%)
1	D	1.02	1/862 (0.1%)	1.73	19/1175 (1.6%)
All	All	1.00	5/3448 (0.1%)	1.71	81/4700 (1.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	698	LYS	CB-CG	6.17	1.69	1.52
1	B	298	LYS	CB-CG	5.47	1.67	1.52
1	A	98	LYS	CB-CG	5.47	1.67	1.52
1	C	498	LYS	CD-CE	5.30	1.64	1.51
1	C	498	LYS	CB-CG	5.11	1.66	1.52

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	706	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	D	698	LYS	CA-CB-CG	12.87	141.71	113.40
1	C	498	LYS	CA-CB-CG	10.98	137.56	113.40
1	B	298	LYS	CA-CB-CG	10.31	136.08	113.40
1	A	98	LYS	CB-CG-CD	10.20	138.11	111.60

There are no chirality outliers.

There are no planarity outliers.

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	841	0	773	29	0
1	B	841	0	770	27	0
1	C	841	0	770	29	0
1	D	841	0	770	25	0
2	A	8	0	0	2	0
2	B	8	0	0	3	0
2	C	8	0	0	1	0
2	D	8	0	0	0	0
3	A	7	0	0	1	0
3	B	7	0	0	2	0
3	C	7	0	0	4	0
3	D	7	0	0	2	0
All	All	3424	0	3083	81	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 12.

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LYS:HB2	1:D:698:LYS:HZ3	1.36	0.90
1:C:498:LYS:HB3	1:D:698:LYS:HB3	1.54	0.89
1:C:498:LYS:NZ	1:D:698:LYS:HB2	1.90	0.85
1:A:98:LYS:HB2	1:B:298:LYS:NZ	1.92	0.84
1:B:240:ASN:HB2	2:B:307:SF4:S3	2.17	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	104/106 (98%)	96 (92%)	8 (8%)	0	100	100
1	B	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	17	48
1	C	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	17	48
1	D	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
All	All	416/424 (98%)	390 (94%)	24 (6%)	2 (0%)	31	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	441	ASP
1	B	241	ASP

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	96/96 (100%)	86 (90%)	10 (10%)	8	23
1	B	96/96 (100%)	86 (90%)	10 (10%)	8	23
1	C	96/96 (100%)	88 (92%)	8 (8%)	12	34
1	D	96/96 (100%)	89 (93%)	7 (7%)	15	41
All	All	384/384 (100%)	349 (91%)	35 (9%)	10	30

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	270	LEU
1	B	298	LYS
1	D	670	LEU
1	B	280	ASN
1	B	292	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	502	GLN
1	D	669	GLN

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](#)

8 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	SF4	A	107	1	0,12,12	0.00	-	0,24,24	0.00	-
3	F3S	A	108	1	0,8,8	0.00	-	0,11,11	0.00	-
2	SF4	B	307	1	0,12,12	0.00	-	0,24,24	0.00	-
3	F3S	B	308	1	0,8,8	0.00	-	0,11,11	0.00	-
2	SF4	C	507	1	0,12,12	0.00	-	0,24,24	0.00	-
3	F3S	C	508	1	0,8,8	0.00	-	0,11,11	0.00	-
2	SF4	D	707	1	0,12,12	0.00	-	0,24,24	0.00	-
3	F3S	D	708	1	0,8,8	0.00	-	0,11,11	0.00	-

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	SF4	A	107	1	-	0/0/48/48	0/6/5/5
3	F3S	A	108	1	-	0/0/14/14	1/1/2/2
2	SF4	B	307	1	-	0/0/48/48	0/6/5/5
3	F3S	B	308	1	-	0/0/14/14	1/1/2/2
2	SF4	C	507	1	-	0/0/48/48	0/6/5/5
3	F3S	C	508	1	-	0/0/14/14	1/1/2/2
2	SF4	D	707	1	-	0/0/48/48	0/6/5/5
3	F3S	D	708	1	-	0/0/14/14	1/1/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	508	F3S	FE3-FE4-S1-S2
3	A	108	F3S	FE3-FE4-S1-S2
3	B	308	F3S	FE3-FE4-S1-S2
3	D	708	F3S	FE3-FE4-S1-S2

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	107	SF4	2	0
3	A	108	F3S	1	0
2	B	307	SF4	3	0
3	B	308	F3S	2	0
2	C	507	SF4	1	0
3	C	508	F3S	4	0
3	D	708	F3S	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.