



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:46 am BST

PDB ID : 2AZU
Title : X-RAY CRYSTAL STRUCTURE OF THE TWO SITE-SPECIFIC MUTANTS HIS35*GLN AND HIS35*LEU OF AZURIN FROM PSEUDOMONAS AERUGINOSA
Authors : Nar, H.; Messerschmidt, A.; Huber, R.
Deposited on : 1991-01-11
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

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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

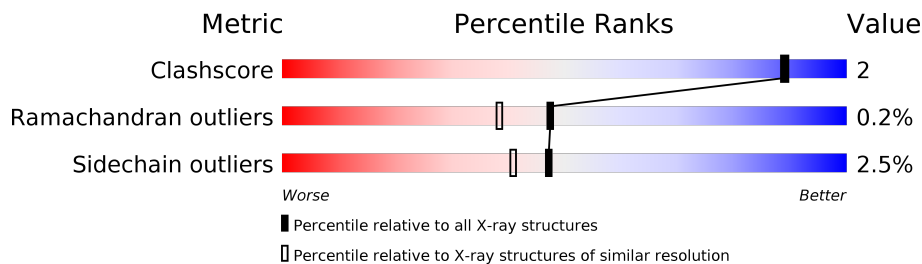
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 ≥ 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	128	
1	B	128	
1	C	128	
1	D	128	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4219 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 AZURIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	128	972	607	163	193	9	0	0	0
1	B	128	972	607	163	193	9	0	0	0
1	C	128	972	607	163	193	9	0	0	0
1	D	128	972	607	163	193	9	0	0	0

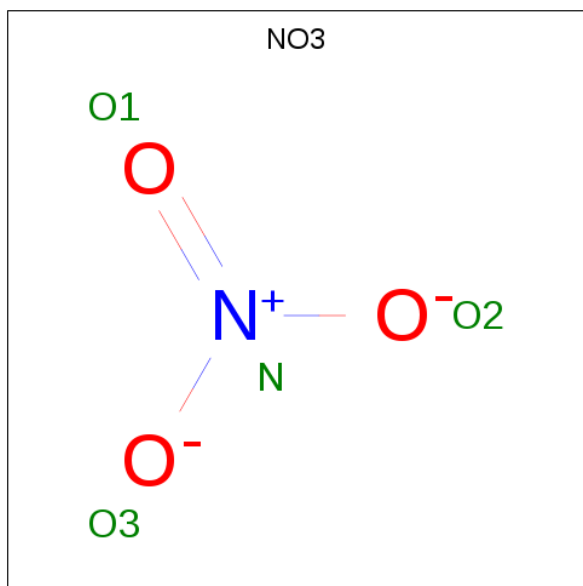
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLN	GLU	CONFLICT	UNP P00282
A	35	LEU	HIS	ENGINEERED MUTATION	UNP P00282
B	2	GLN	GLU	CONFLICT	UNP P00282
B	35	LEU	HIS	ENGINEERED MUTATION	UNP P00282
C	2	GLN	GLU	CONFLICT	UNP P00282
C	35	LEU	HIS	ENGINEERED MUTATION	UNP P00282
D	2	GLN	GLU	CONFLICT	UNP P00282
D	35	LEU	HIS	ENGINEERED MUTATION	UNP P00282

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Cu 1	0	0
2	A	1	Total 1	Cu 1	0	0
2	D	1	Total 1	Cu 1	0	0
2	C	1	Total 1	Cu 1	0	0

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	N O	0	0
			4	1 3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		
4	B	86	Total	O	0	0
			86	86		
4	C	83	Total	O	0	0
			83	83		
4	D	85	Total	O	0	0
			85	85		

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: AZURIN

Chain A:  91% 9%



- Molecule 1: AZURIN

Chain B:  92% 7%




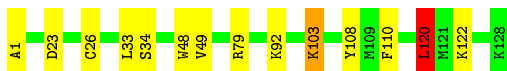
- Molecule 1: AZURIN

Chain C:  91% 8%



- Molecule 1: AZURIN

Chain D:  89% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.82Å 81.06Å 110.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4219	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

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: CU, NO3

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	0.67	0/988	1.26	6/1331 (0.5%)
1	B	0.68	0/988	1.25	6/1331 (0.5%)
1	C	0.67	0/988	1.27	5/1331 (0.4%)
1	D	0.69	0/988	1.27	10/1331 (0.8%)
All	All	0.68	0/3952	1.26	27/5324 (0.5%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	D	48	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	C	79	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	48	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	D	103	LYS	CA-CB-CG	7.33	129.53	113.40
1	C	48	TRP	CD1-CG-CD2	7.18	112.04	106.30
1	B	48	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	C	48	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	D	48	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	B	79	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	79	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	79	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	48	TRP	CE2-CD2-CG	-6.09	102.42	107.30
1	B	48	TRP	CG-CD1-NE1	-6.00	104.10	110.10
1	C	79	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	79	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	127	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	79	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	121	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	2	GLN	N-CA-C	-5.46	96.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	A	59	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	D	120	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	72	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	D	108	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	D	103	LYS	CB-CA-C	-5.13	100.14	110.40
1	D	48	TRP	CG-CD1-NE1	-5.07	105.03	110.10

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	972	0	958	4	0
1	B	972	0	958	2	0
1	C	972	0	958	4	0
1	D	972	0	958	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	0	0	0
4	A	69	0	0	0	0
4	B	86	0	0	0	0
4	C	83	0	0	1	0
4	D	85	0	0	1	0
All	All	4219	0	3832	15	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.

All (15) 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:47:ASN:HD21	1:C:113:THR:H	1.45	0.64
1:D:23:ASP:HB3	1:D:26:CYS:SG	2.43	0.58
1:C:54:ALA:HB1	4:C:839:HOH:O	2.05	0.56
1:D:34:SER:HB3	1:D:92:LYS:HD3	1.87	0.55
1:A:43:VAL:HG23	1:C:114:PHE:CZ	2.46	0.51
1:A:53:ALA:HA	1:A:109:MET:HG2	1.94	0.49
1:D:1:ALA:N	4:D:822:HOH:O	2.46	0.48
1:B:23:ASP:HA	1:B:128:LYS:O	2.17	0.45
1:B:49:VAL:O	1:B:110:PHE:HA	2.17	0.45
1:A:34:SER:HB3	1:A:92:LYS:HD2	2.00	0.44
1:D:49:VAL:O	1:D:110:PHE:HA	2.19	0.42
1:D:33:LEU:O	1:D:92:LYS:HD2	2.21	0.41
1:A:120:LEU:HD22	1:D:120:LEU:HD22	2.03	0.41
1:C:49:VAL:O	1:C:110:PHE:HA	2.21	0.41
1:D:103:LYS:HB3	1:D:103:LYS:HE2	1.66	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	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
1	B	126/128 (98%)	124 (98%)	1 (1%)	1 (1%)	19	9
1	C	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
1	D	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
All	All	504/512 (98%)	493 (98%)	10 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	GLN

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	110/110 (100%)	107 (97%)	3 (3%)	44	38
1	B	110/110 (100%)	107 (97%)	3 (3%)	44	38
1	C	110/110 (100%)	107 (97%)	3 (3%)	44	38
1	D	110/110 (100%)	108 (98%)	2 (2%)	59	55
All	All	440/440 (100%)	429 (98%)	11 (2%)	47	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	GLU
1	A	122	LYS
1	A	127	LEU
1	B	2	GLN
1	B	78	SER
1	B	127	LEU
1	C	4	SER
1	C	21	THR
1	C	47	ASN
1	D	120	LEU
1	D	122	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	47	ASN
1	C	107	GLN
1	D	8	GLN
1	D	57	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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	NO3	A	130	-	1,3,3	0.25	0	0,3,3	0.00	-

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

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.