



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:06 PM GMT

PDB ID : 1ILU
Title : X-RAY CRYSTAL STRUCTURE THE TWO SITE-SPECIFIC MUTANTS
ILE7SER AND PHE110SER OF AZURIN FROM PSEUDOMONAS
AERUGINOSA
Authors : Hammann, C.; Nar, H.; Huber, R.; Messerschmidt, A.
Deposited on : 1995-10-12
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

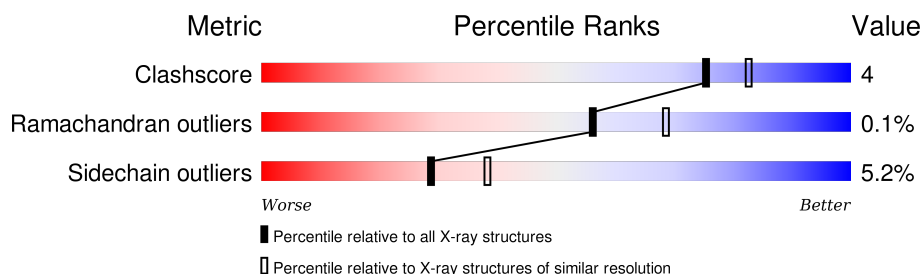
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)






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 $\leq 5\%$. 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.

Note EDS was not executed.

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

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Mol	Chain	Length	Quality of chain
1	H	128	 85% 14% •
1	I	128	 85% 15%
1	K	128	 79% 20% •
1	L	128	 82% 16% •
1	M	128	 89% 10% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16428 atoms, of which 4072 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
1	A	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	B	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	C	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	D	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	E	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	F	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	G	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	H	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	I	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	K	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	L	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	M	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	PHE	ENGINEERED	UNP P00282
B	110	SER	PHE	ENGINEERED	UNP P00282
C	110	SER	PHE	ENGINEERED	UNP P00282
D	110	SER	PHE	ENGINEERED	UNP P00282
E	110	SER	PHE	ENGINEERED	UNP P00282

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Chain	Residue	Modelled	Actual	Comment	Reference
F	110	SER	PHE	ENGINEERED	UNP P00282
G	110	SER	PHE	ENGINEERED	UNP P00282
H	110	SER	PHE	ENGINEERED	UNP P00282
I	110	SER	PHE	ENGINEERED	UNP P00282
K	110	SER	PHE	ENGINEERED	UNP P00282
L	110	SER	PHE	ENGINEERED	UNP P00282
M	110	SER	PHE	ENGINEERED	UNP P00282

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	K	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	H	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	I	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	L	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		
2	M	1	Total	Cu	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	63	Total	H	O	0	0
			189	126	63		
3	B	83	Total	H	O	0	0
			249	166	83		

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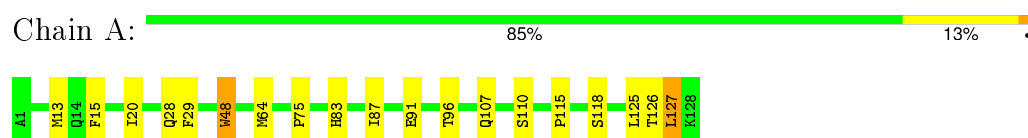
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	63	Total	H	O	0	0
			189	126	63		
3	D	55	Total	H	O	0	0
			165	110	55		
3	E	61	Total	H	O	0	0
			183	122	61		
3	F	47	Total	H	O	0	0
			141	94	47		
3	G	54	Total	H	O	0	0
			162	108	54		
3	H	55	Total	H	O	0	0
			165	110	55		
3	I	52	Total	H	O	0	0
			156	104	52		
3	K	62	Total	H	O	0	0
			186	124	62		
3	L	62	Total	H	O	0	0
			186	124	62		
3	M	59	Total	H	O	0	0
			177	118	59		

3 Residue-property plots

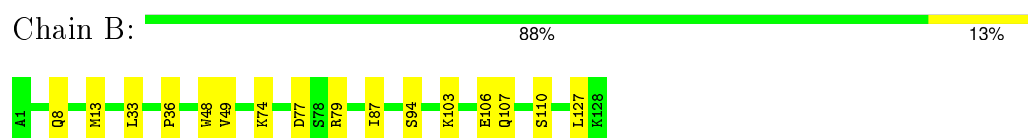
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

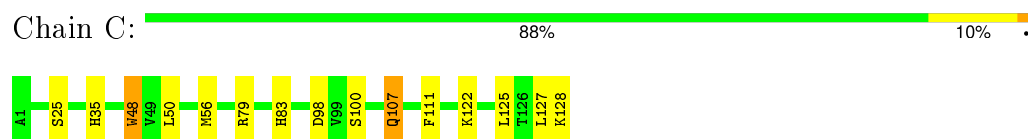
- Molecule 1: AZURIN



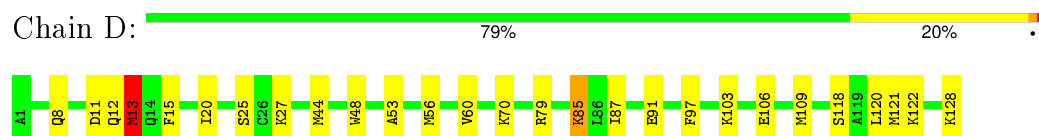
- Molecule 1: AZURIN



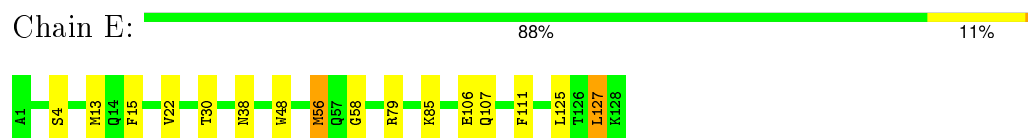
- Molecule 1: AZURIN



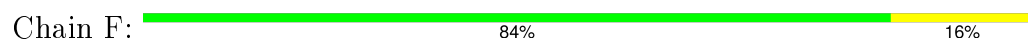
- Molecule 1: AZURIN

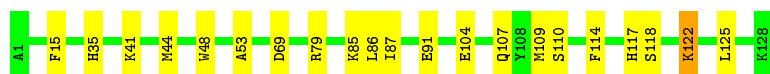


- Molecule 1: AZURIN

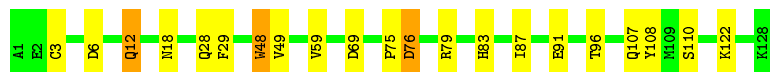
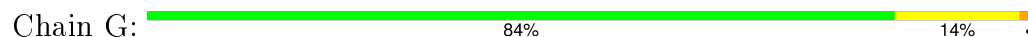


- Molecule 1: AZURIN

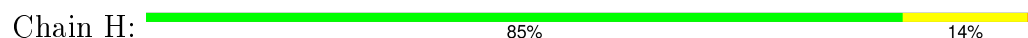




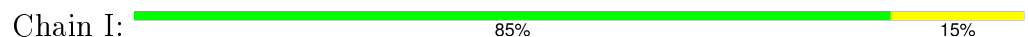
- Molecule 1: AZURIN



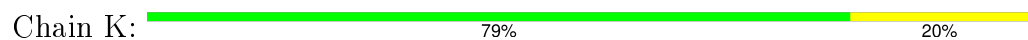
- Molecule 1: AZURIN



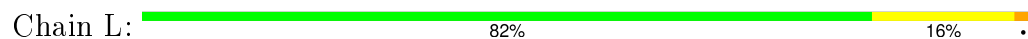
- Molecule 1: AZURIN



- Molecule 1: AZURIN



- Molecule 1: AZURIN



- Molecule 1: AZURIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.40 Å 170.10 Å 99.70 Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16428	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: CU

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	0.73	1/985 (0.1%)	1.38	7/1327 (0.5%)
1	B	0.69	0/985	1.35	9/1327 (0.7%)
1	C	0.71	0/985	1.28	5/1327 (0.4%)
1	D	0.68	0/985	1.31	6/1327 (0.5%)
1	E	0.70	0/985	1.34	7/1327 (0.5%)
1	F	0.68	0/985	1.33	9/1327 (0.7%)
1	G	0.71	0/985	1.38	8/1327 (0.6%)
1	H	0.71	0/985	1.29	6/1327 (0.5%)
1	I	0.70	0/985	1.34	8/1327 (0.6%)
1	K	0.68	0/985	1.30	5/1327 (0.4%)
1	L	0.70	0/985	1.34	10/1327 (0.8%)
1	M	0.70	0/985	1.32	6/1327 (0.5%)
All	All	0.70	1/11820 (0.0%)	1.33	86/15924 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLN	CB-CG	-5.78	1.36	1.52

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	48	TRP	CD1-CG-CD2	9.40	113.82	106.30
1	E	56	MET	CG-SD-CE	-9.31	85.30	100.20
1	A	48	TRP	CD1-CG-CD2	8.96	113.46	106.30
1	I	79	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	H	48	TRP	CD1-CG-CD2	8.72	113.28	106.30

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	969	220	949	7	0
1	B	969	220	948	7	0
1	C	969	220	948	4	1
1	D	969	220	948	12	1
1	E	969	220	948	5	0
1	F	969	220	948	5	0
1	G	969	220	948	7	1
1	H	969	220	948	8	0
1	I	969	220	948	5	1
1	K	969	220	948	14	0
1	L	969	220	948	9	0
1	M	969	220	948	6	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
3	A	63	126	0	1	0
3	B	83	166	0	2	0
3	C	63	126	0	1	0
3	D	55	110	0	4	1
3	E	61	122	0	2	0
3	F	47	94	0	1	0
3	G	54	108	0	3	0
3	H	55	110	0	2	0
3	I	52	104	0	0	0
3	K	62	124	0	2	1
3	L	62	124	0	2	0
3	M	59	118	0	1	0
All	All	12356	4072	11377	89	3

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 4.

The worst 5 of 89 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:I:32:ASN:HB3	1:I:92:LYS:HZ2	1.58	0.67
1:G:87:ILE:HB	1:G:91:GLU:HB2	1.81	0.63
1:M:34:SER:HB3	1:M:92:LYS:HD2	1.79	0.63
1:I:32:ASN:HB3	1:I:92:LYS:NZ	2.14	0.62
1:L:13:MET:HE3	1:L:117:HIS:HA	1.82	0.62

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LYS:HZ2	3:D:1944:HOH:H2[1_455]	1.32	0.28
1:C:79:ARG:HH12	3:K:2351:HOH:H1[2_646]	1.34	0.26
1:G:12:GLN:HE21	1:I:85:LYS:HZ3[1_554]	1.34	0.26

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	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
1	B	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
1	C	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
1	D	126/128 (98%)	122 (97%)	3 (2%)	1 (1%)	24	27
1	E	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
1	F	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
1	G	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	24	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
1	I	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
1	K	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
1	L	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
1	M	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
All	All	1512/1536 (98%)	1450 (96%)	60 (4%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	3	CYS
1	D	13	MET

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	110/110 (100%)	104 (94%)	6 (6%)	27	36
1	B	110/110 (100%)	109 (99%)	1 (1%)	84	93
1	C	110/110 (100%)	102 (93%)	8 (7%)	17	22
1	D	110/110 (100%)	102 (93%)	8 (7%)	17	22
1	E	110/110 (100%)	104 (94%)	6 (6%)	27	36
1	F	110/110 (100%)	102 (93%)	8 (7%)	17	22
1	G	110/110 (100%)	104 (94%)	6 (6%)	27	36
1	H	110/110 (100%)	103 (94%)	7 (6%)	22	28
1	I	110/110 (100%)	103 (94%)	7 (6%)	22	28
1	K	110/110 (100%)	108 (98%)	2 (2%)	66	82
1	L	110/110 (100%)	103 (94%)	7 (6%)	22	28
1	M	110/110 (100%)	108 (98%)	2 (2%)	66	82
All	All	1320/1320 (100%)	1252 (95%)	68 (5%)	29	38

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	35	HIS
1	G	28	GLN
1	L	38	ASN
1	F	69	ASP
1	F	118	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	28	GLN
1	L	8	GLN
1	G	107	GLN
1	C	107	GLN
1	F	32	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.