



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 06:08 PM EDT

PDB ID : 2OJ1  
Title : Disulfide-linked dimer of azurin N42C/M64E double mutant  
Authors : de Jongh, T.E.; Hoffmann, M.; Einsle, O.; Cavazzini, D.; Rossi, G.L.; Ubbink, M.; Canters, G.W.  
Deposited on : 2007-01-12  
Resolution : 2.30 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  
Xtrriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

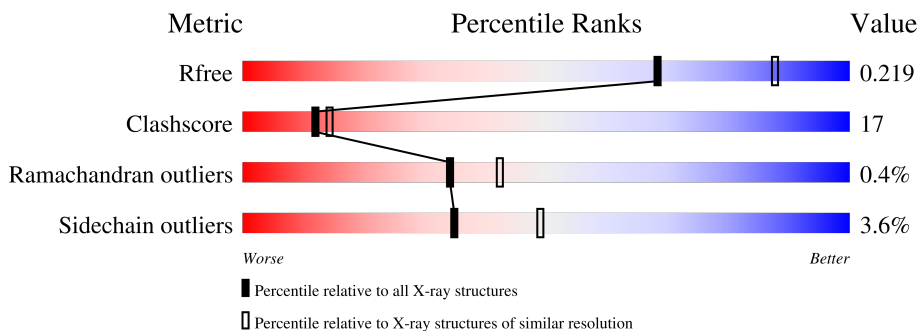
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 of 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	128	62% 34% 5%
1	B	128	59% 35% 5%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2100 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	973	606	163	195	9	0	0	0
1	B	128	973	606	163	195	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	CYS	ASN	engineered mutation	UNP P00282
A	64	GLU	MET	engineered mutation	UNP P00282
B	42	CYS	ASN	engineered mutation	UNP P00282
B	64	GLU	MET	engineered mutation	UNP P00282

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

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

- Molecule 3 is water.

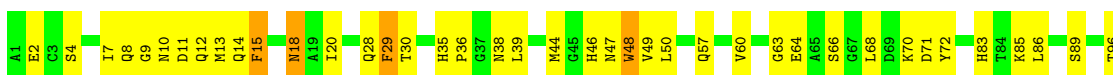
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	61	Total	O	0	0
			61	61		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

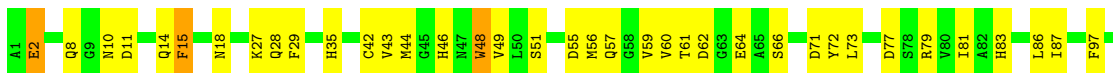
- Molecule 1: Azurin

Chain A: 



- Molecule 1: Azurin

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.57Å 116.98Å 30.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.30 – 2.30 34.28 – 2.21	Depositor EDS
% Data completeness (in resolution range)	95.1 (34.30-2.30) 88.9 (34.28-2.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1, REFMAC 5.0	Depositor
R, $R_{free}$	0.208 , 0.281 0.238 , 0.219	Depositor DCC
$R_{free}$ test set	551 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtrriage
Anisotropy	0.616	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 66.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5160e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	1.10	27/990 (2.7%)	0.75	0/1334
1	B	1.08	24/990 (2.4%)	0.74	0/1334
All	All	1.09	51/1980 (2.6%)	0.75	0/2668

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	TYR	CD2-CE2	8.44	1.52	1.39
1	B	108	TYR	CD1-CE1	7.63	1.50	1.39
1	B	72	TYR	CD1-CE1	7.62	1.50	1.39
1	A	72	TYR	CD1-CE1	6.97	1.49	1.39
1	B	108	TYR	CD2-CE2	6.83	1.49	1.39
1	A	29	PHE	CD2-CE2	6.82	1.52	1.39
1	A	108	TYR	CD2-CE2	6.79	1.49	1.39
1	B	72	TYR	CD2-CE2	6.74	1.49	1.39
1	A	110	PHE	CE2-CZ	6.70	1.50	1.37
1	B	110	PHE	CE1-CZ	6.67	1.50	1.37
1	A	108	TYR	CD1-CE1	6.62	1.49	1.39
1	B	111	PHE	CD2-CE2	6.38	1.52	1.39
1	B	15	PHE	CD2-CE2	6.37	1.51	1.39
1	A	29	PHE	CE1-CZ	6.29	1.49	1.37
1	A	97	PHE	CE1-CZ	6.29	1.49	1.37
1	B	48	TRP	CE3-CZ3	6.28	1.49	1.38
1	B	97	PHE	CE1-CZ	6.18	1.49	1.37
1	A	110	PHE	CD1-CE1	6.12	1.51	1.39
1	B	111	PHE	CD1-CE1	6.05	1.51	1.39
1	A	48	TRP	CE3-CZ3	6.04	1.48	1.38
1	B	97	PHE	CE2-CZ	6.03	1.48	1.37
1	A	111	PHE	CD2-CE2	5.98	1.51	1.39
1	A	29	PHE	CD1-CE1	5.94	1.51	1.39
1	A	110	PHE	CE1-CZ	5.93	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	PHE	CE1-CZ	5.93	1.48	1.37
1	A	97	PHE	CD1-CE1	5.92	1.51	1.39
1	B	111	PHE	CE1-CZ	5.92	1.48	1.37
1	B	15	PHE	CE1-CZ	5.92	1.48	1.37
1	B	97	PHE	CD2-CE2	5.92	1.51	1.39
1	A	29	PHE	CE2-CZ	5.91	1.48	1.37
1	A	110	PHE	CD2-CE2	5.88	1.51	1.39
1	A	111	PHE	CD1-CE1	5.81	1.50	1.39
1	A	97	PHE	CE2-CZ	5.78	1.48	1.37
1	A	114	PHE	CD2-CE2	5.62	1.50	1.39
1	A	114	PHE	CE1-CZ	5.61	1.48	1.37
1	B	110	PHE	CD1-CE1	5.56	1.50	1.39
1	A	97	PHE	CD2-CE2	5.53	1.50	1.39
1	B	15	PHE	CD1-CE1	5.51	1.50	1.39
1	A	15	PHE	CD2-CE2	5.49	1.50	1.39
1	B	114	PHE	CE1-CZ	5.43	1.47	1.37
1	B	110	PHE	CE2-CZ	5.43	1.47	1.37
1	A	114	PHE	CD1-CE1	5.39	1.50	1.39
1	B	29	PHE	CD2-CE2	5.35	1.50	1.39
1	A	111	PHE	CE1-CZ	5.31	1.47	1.37
1	B	29	PHE	CD1-CE1	5.27	1.49	1.39
1	B	110	PHE	CD2-CE2	5.24	1.49	1.39
1	A	15	PHE	CD1-CE1	5.21	1.49	1.39
1	B	114	PHE	CD2-CE2	5.10	1.49	1.39
1	B	97	PHE	CD1-CE1	5.08	1.49	1.39
1	A	111	PHE	CE2-CZ	5.06	1.47	1.37
1	B	29	PHE	CE2-CZ	5.00	1.46	1.37

There are no bond angle outliers.

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	973	0	947	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	973	0	947	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	91	0	0	3	0
3	B	61	0	0	1	0
All	All	2100	0	1894	66	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 17.

All (66) 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:10:ASN:HD21	1:B:14:GLN:HE21	1.11	0.94
1:A:10:ASN:HD21	1:A:14:GLN:HE21	1.17	0.86
1:A:18:ASN:H	1:A:18:ASN:HD22	1.29	0.81
1:A:35:HIS:HE1	1:A:44:MET:O	1.64	0.80
1:A:39:LEU:O	1:A:89:SER:HB2	1.83	0.78
1:A:18:ASN:H	1:A:18:ASN:ND2	1.91	0.69
1:B:10:ASN:HD21	1:B:14:GLN:NE2	1.90	0.66
1:A:57:GLN:HG3	3:A:201:HOH:O	1.96	0.65
1:A:2:GLU:HA	1:A:2:GLU:OE1	1.98	0.64
1:A:49:VAL:O	1:A:110:PHE:HA	1.99	0.62
1:A:8:GLN:O	1:A:15:PHE:HA	2.01	0.60
1:B:10:ASN:ND2	1:B:14:GLN:HE21	1.91	0.59
1:A:7:ILE:HD11	1:A:20:ILE:HD11	1.83	0.58
1:A:18:ASN:ND2	1:A:18:ASN:N	2.50	0.58
1:B:11:ASP:HA	1:B:44:MET:HG2	1.88	0.55
1:A:28:GLN:HA	1:A:99:VAL:HG23	1.89	0.54
1:B:60:VAL:O	1:B:64:GLU:HG3	2.08	0.53
1:B:46:HIS:C	1:B:86:LEU:HD12	2.29	0.53
1:B:48:TRP:O	1:B:83:HIS:HA	2.08	0.53
1:B:35:HIS:HB2	1:B:87:ILE:HD12	1.91	0.52
1:A:63:GLY:O	1:A:66:SER:HB2	2.10	0.52
1:B:49:VAL:O	1:B:110:PHE:HA	2.10	0.52
1:B:8:GLN:O	1:B:15:PHE:HA	2.09	0.52
1:B:55:ASP:O	1:B:59:VAL:HG23	2.11	0.51
1:B:125:LEU:C	1:B:125:LEU:HD23	2.31	0.50
1:B:56:MET:HG3	1:B:111:PHE:CE1	2.46	0.50
1:A:15:PHE:CE2	1:A:121:MET:HB3	2.46	0.49
1:A:9:GLY:HA2	1:A:14:GLN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TRP:O	1:A:83:HIS:HA	2.12	0.49
1:A:18:ASN:HD22	1:A:18:ASN:N	1.94	0.49
1:A:14:GLN:HB3	3:A:213:HOH:O	2.13	0.48
1:A:11:ASP:HA	1:A:44:MET:HG2	1.95	0.47
1:A:47:ASN:HB3	1:A:86:LEU:HA	1.95	0.47
1:A:7:ILE:HG22	1:A:8:GLN:N	2.29	0.47
1:B:103:LYS:HG2	1:B:108:TYR:OH	2.14	0.47
1:B:42:CYS:SG	1:B:43:VAL:HG23	2.55	0.47
1:A:4:SER:HA	1:A:30:THR:O	2.15	0.47
1:A:12:GLN:O	1:A:13:MET:HB3	2.15	0.47
1:A:60:VAL:O	1:A:64:GLU:HG3	2.15	0.47
1:B:71:ASP:OD1	1:B:86:LEU:HB3	2.14	0.47
1:A:10:ASN:HD21	1:A:14:GLN:NE2	1.99	0.46
1:A:29:PHE:O	1:A:96:THR:HA	2.16	0.46
1:B:125:LEU:HD23	1:B:125:LEU:O	2.15	0.46
1:B:46:HIS:HA	1:B:112:CYS:SG	2.55	0.46
1:B:71:ASP:O	1:B:73:LEU:HG	2.16	0.46
1:B:118:SER:O	1:B:119:ALA:C	2.54	0.46
1:A:106:GLU:HG2	1:A:108:TYR:CE2	2.51	0.45
1:B:51:SER:HA	1:B:81:ILE:HG13	1.98	0.45
1:A:11:ASP:OD2	1:A:38:ASN:N	2.41	0.43
1:B:106:GLU:OE1	1:B:108:TYR:CZ	2.71	0.43
1:A:35:HIS:CE1	1:A:44:MET:O	2.56	0.43
1:A:46:HIS:HA	1:A:112:CYS:SG	2.58	0.43
1:A:68:LEU:C	1:A:70:LYS:N	2.72	0.43
1:A:68:LEU:C	1:A:70:LYS:H	2.22	0.43
1:B:18:ASN:ND2	3:B:143:HOH:O	2.52	0.43
1:B:77:ASP:OD1	1:B:79:ARG:HB2	2.19	0.42
1:B:102:LEU:HD22	1:B:108:TYR:CZ	2.53	0.42
1:A:35:HIS:CD2	1:A:35:HIS:C	2.93	0.42
1:A:85:LYS:HG3	3:A:169:HOH:O	2.20	0.41
1:B:27:LYS:HA	1:B:27:LYS:HD3	1.87	0.41
1:B:57:GLN:NE2	1:B:61:THR:OG1	2.54	0.41
1:B:114:PHE:CD1	1:B:114:PHE:C	2.94	0.41
1:B:62:ASP:O	1:B:66:SER:OG	2.33	0.40
1:A:35:HIS:HD2	1:A:36:PRO:O	2.04	0.40
1:A:71:ASP:CG	1:A:86:LEU:H	2.24	0.40
1:B:103:LYS:HG2	1:B:103:LYS:H	1.76	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%)	114 (90%)	12 (10%)	0	100	100
1	B	126/128 (98%)	117 (93%)	8 (6%)	1 (1%)	19	23
All	All	252/256 (98%)	231 (92%)	20 (8%)	1 (0%)	34	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	GLU

### 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%)	108 (98%)	2 (2%)	59	75
1	B	110/110 (100%)	104 (94%)	6 (6%)	21	30
All	All	220/220 (100%)	212 (96%)	8 (4%)	35	49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	50	LEU
1	B	2	GLU
1	B	28	GLN
1	B	100	SER

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Mol	Chain	Res	Type
1	B	104	GLU
1	B	107	GLN
1	B	120	LEU

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

Mol	Chain	Res	Type
1	A	8	GLN
1	A	14	GLN
1	A	18	ASN
1	A	28	GLN
1	A	35	HIS
1	B	8	GLN
1	B	14	GLN
1	B	18	ASN
1	B	28	GLN
1	B	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 monosaccharides 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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.