



Full wwPDB X-ray Structure Validation Report ⓘ

PDB ID : 3NP4 / pdb_00003np4
Title : C112D/M121E Pseudomonas aeruginosa Azurin
Authors : Lancaster, K.M.; Gray, H.B.
Deposited on : 2010-06-27
Resolution : 2.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

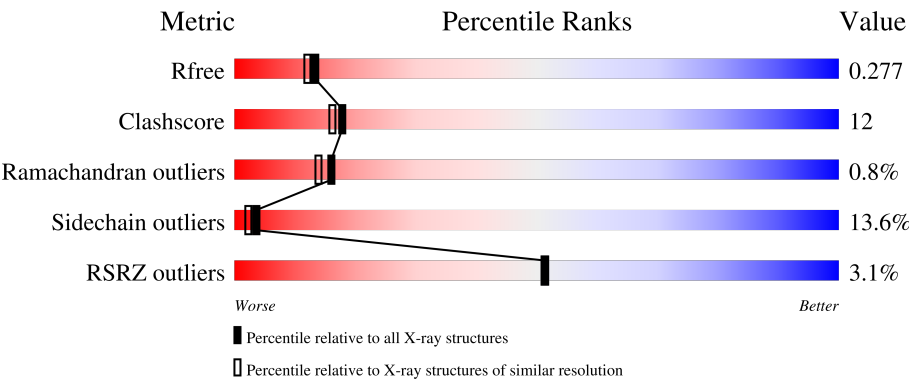
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	48.41Å 55.03Å 94.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.92 – 2.25 33.92 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.1 (33.92-2.25) 94.0 (33.92-2.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.42 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.276 0.213 , 0.277	Depositor DCC
R_{free} test set	289 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1046	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% 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.

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, 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	1.04	0/993	1.26	9/1340 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	SER	CA-C-N	-8.35	112.73	122.83
1	A	66	SER	C-N-CA	-8.35	112.73	122.83
1	A	8	GLN	N-CA-C	6.66	120.36	109.24
1	A	35	HIS	CA-C-N	5.93	125.69	119.76
1	A	35	HIS	C-N-CA	5.93	125.69	119.76
1	A	66	SER	N-CA-C	-5.84	102.27	110.50
1	A	39	LEU	CA-C-N	5.73	125.64	119.85
1	A	39	LEU	C-N-CA	5.73	125.64	119.85
1	A	19	ALA	N-CA-C	5.39	118.17	108.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ASN	Peptide

3.2 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	976	0	949	24	1
2	A	2	0	0	0	0
3	A	8	0	11	0	0
4	A	60	0	0	5	1
All	All	1046	0	960	24	1

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.

All (24) 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:A:11:ASP:O	1:A:12:GLN:HB3	1.88	0.71
1:A:13:MET:O	1:A:120:LEU:HD23	1.91	0.70
1:A:11:ASP:O	4:A:176:HOH:O	2.10	0.68
1:A:37:GLY:O	1:A:89:SER:HB2	1.95	0.66
1:A:35:HIS:CD2	1:A:46:HIS:HD2	2.14	0.65
1:A:52:THR:HG22	1:A:55:ASP:H	1.62	0.65
1:A:119:ALA:O	1:A:122:LYS:HE3	2.00	0.61
1:A:88:GLY:O	1:A:91:GLU:HB2	2.06	0.55
1:A:124:THR:HG23	4:A:160:HOH:O	2.07	0.53
1:A:11:ASP:OD1	1:A:44:MET:HG2	2.10	0.52
1:A:53:ALA:HB2	1:A:107:GLN:HG3	1.92	0.50
1:A:107:GLN:NE2	1:A:108:TYR:O	2.44	0.50
1:A:35:HIS:CD2	1:A:46:HIS:CD2	2.99	0.48
1:A:117:HIS:HB3	1:A:121:GLU:OE1	2.15	0.46
1:A:25:SER:HB3	4:A:191:HOH:O	2.17	0.45
1:A:49:VAL:O	1:A:110:PHE:HA	2.17	0.44
1:A:9:GLY:O	1:A:36:PRO:HD2	2.18	0.42
1:A:56:MET:HG3	1:A:111:PHE:CE2	2.54	0.42
1:A:23:ASP:OD2	1:A:25:SER:HB2	2.18	0.42
1:A:24:LYS:HA	1:A:127:LEU:HD11	2.01	0.42
1:A:31:VAL:O	1:A:94:SER:HA	2.20	0.42
1:A:13:MET:C	1:A:120:LEU:HD23	2.44	0.41
1:A:12:GLN:NE2	4:A:185:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:ND2	4:A:186:HOH:O	2.54	0.40

All (1) 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:A:83:HIS:NE2	4:A:180:HOH:O[8_555]	2.07	0.13

3.3 Torsion angles [i](#)

3.3.1 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%)	122 (97%)	3 (2%)	1 (1%)	16 14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLN

3.3.2 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%)	95 (86%)	15 (14%)	3 2

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	8	GLN
1	A	12	GLN
1	A	17	THR
1	A	21	THR
1	A	25	SER
1	A	30	THR
1	A	43	VAL
1	A	52	THR
1	A	92	LYS
1	A	103	LYS
1	A	115	PRO
1	A	124	THR
1	A	126	THR
1	A	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

3.7 Other polymers

There are no such residues in this entry.

3.8 Polymer linkage issues

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 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	128/128 (100%)	0.09	4 (3%) 51 51	27, 41, 69, 86	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	GLY	3.0
1	A	13	MET	2.9
1	A	10	ASN	2.9
1	A	15	PHE	2.7

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

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

4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

4.4 Other polymers [i](#)

There are no such residues in this entry.