



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2017 – 01:17 AM EST

PDB ID : 3UBR
Title : Laue structure of Shewanella oneidensis cytochrome-c Nitrite Reductase
Authors : Youngblut, M.; Judd, E.T.; Srajer, V.; Sayed, B.; Goeltzner, T.; Elliott, S.; Schmidt, M.; Pacheco, A.
Deposited on : 2011-10-24
Resolution : 2.59 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

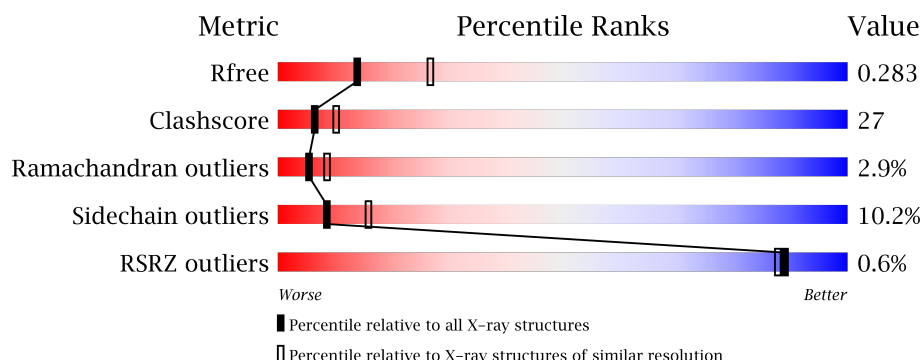
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	439	<div> <div></div> <div> <div></div> <div>63%</div> <div>29%</div> <div>8%</div> </div> </div>
1	B	439	<div> <div></div> <div> <div></div> <div>62%</div> <div>32%</div> <div>7%</div> </div> </div>

2 Entry composition i

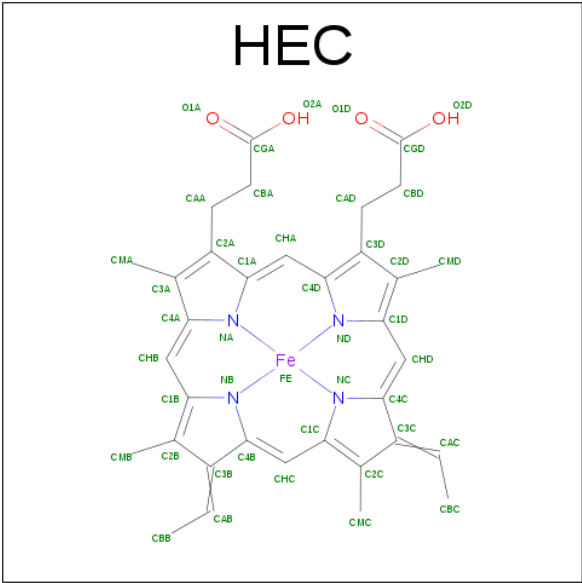
There are 4 unique types of molecules in this entry. The entry contains 7533 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3473	2192	600	656	25			
1	B	439	Total	C	N	O	S	0	0	0
			3473	2192	600	656	25			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total 85	O 85	0	0
4	B	70	Total 70	O 70	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.50 Å 95.90 Å 223.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.56 – 2.59 40.56 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.56-2.59) 73.0 (40.56-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.01 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.285 0.193 , 0.283	Depositor DCC
R_{free} test set	1315 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7533	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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.

5 Model quality

5.1 Standard geometry

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

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	0.63	0/3558	0.72	1/4801 (0.0%)
1	B	0.62	0/3558	0.72	1/4801 (0.0%)
All	All	0.62	0/7116	0.72	2/9602 (0.0%)

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	3
1	B	0	4
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	LYS	N-CA-C	-7.18	91.62	111.00
1	A	228	VAL	N-CA-C	6.08	127.41	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	LYS	Peptide
1	A	228	VAL	Peptide
1	A	468	ALA	Peptide
1	B	209	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	210	LYS	Peptide

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	3473	0	3408	168	0
1	B	3473	0	3409	182	0
2	A	215	0	158	68	0
2	B	215	0	160	66	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	85	0	0	14	0
4	B	70	0	0	15	0
All	All	7533	0	7135	381	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 27.

The worst 5 of 381 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:275:CYS:SG	2:B:474:HEC:HAB	1.48	1.53
1:A:157:CYS:SG	2:A:472:HEC:HAB	1.65	1.34
1:B:119:CYS:SG	2:B:471:HEC:HAB	1.72	1.29
1:A:119:CYS:SG	2:A:471:HEC:CAB	2.23	1.26
1:A:202:CYS:SG	2:A:473:HEC:CAC	2.23	1.26

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	437/439 (100%)	385 (88%)	37 (8%)	15 (3%)	4	6
1	B	437/439 (100%)	385 (88%)	42 (10%)	10 (2%)	7	13
All	All	874/878 (100%)	770 (88%)	79 (9%)	25 (3%)	5	8

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	210	LYS
1	A	211	LYS
1	B	58	LYS
1	B	211	LYS

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	367/367 (100%)	332 (90%)	35 (10%)	10	19
1	B	367/367 (100%)	327 (89%)	40 (11%)	7	13
All	All	734/734 (100%)	659 (90%)	75 (10%)	8	16

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	THR
1	B	124	SER
1	B	427	ILE
1	A	470	TYR
1	B	49	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	B	54	HIS
1	B	313	GLN
1	A	339	GLN
1	A	434	GLN

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, 2 are monoatomic - leaving 10 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	$\# Z > 2$
2	HEC	A	471	1,4	28,50,50	2.21	3 (10%)	16,82,82	1.98	4 (25%)
2	HEC	A	472	1	28,50,50	2.34	4 (14%)	16,82,82	1.71	4 (25%)
2	HEC	A	473	1	28,50,50	2.10	4 (14%)	16,82,82	2.18	4 (25%)
2	HEC	A	474	1	28,50,50	2.26	6 (21%)	16,82,82	1.90	6 (37%)
2	HEC	A	475	1	28,50,50	2.16	4 (14%)	16,82,82	2.06	5 (31%)
2	HEC	B	471	1,4	28,50,50	2.34	3 (10%)	16,82,82	1.73	4 (25%)
2	HEC	B	472	1	28,50,50	2.21	3 (10%)	16,82,82	1.77	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	B	473	1	28,50,50	2.39	4 (14%)	16,82,82	1.62	4 (25%)
2	HEC	B	474	1	28,50,50	2.10	3 (10%)	16,82,82	2.00	7 (43%)
2	HEC	B	475	1	28,50,50	2.18	4 (14%)	16,82,82	2.19	8 (50%)

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	HEC	A	471	1,4	-	0/6/54/54	0/0/8/8
2	HEC	A	472	1	-	0/6/54/54	0/0/8/8
2	HEC	A	473	1	-	0/6/54/54	0/0/8/8
2	HEC	A	474	1	-	0/6/54/54	0/0/8/8
2	HEC	A	475	1	-	0/6/54/54	0/0/8/8
2	HEC	B	471	1,4	-	0/6/54/54	0/0/8/8
2	HEC	B	472	1	-	0/6/54/54	0/0/8/8
2	HEC	B	473	1	-	0/6/54/54	0/0/8/8
2	HEC	B	474	1	-	0/6/54/54	0/0/8/8
2	HEC	B	475	1	-	0/6/54/54	0/0/8/8

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	471	HEC	C3B-C2B	-7.48	1.32	1.40
2	B	473	HEC	C3B-C2B	-6.83	1.33	1.40
2	A	471	HEC	C3B-C2B	-6.80	1.33	1.40
2	B	473	HEC	C3C-C2C	-6.76	1.33	1.40
2	A	474	HEC	C3B-C2B	-6.25	1.34	1.40

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	475	HEC	CMC-C2C-C1C	-5.32	120.29	128.46
2	A	471	HEC	CMC-C2C-C1C	-5.20	120.48	128.46
2	A	475	HEC	CMC-C2C-C1C	-5.12	120.59	128.46
2	A	473	HEC	CBD-CAD-C3D	-4.43	104.02	112.48
2	B	471	HEC	CMC-C2C-C1C	-4.25	121.93	128.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	471	HEC	19	0
2	A	472	HEC	13	0
2	A	473	HEC	13	0
2	A	474	HEC	11	0
2	A	475	HEC	12	0
2	B	471	HEC	12	0
2	B	472	HEC	13	0
2	B	473	HEC	17	0
2	B	474	HEC	11	0
2	B	475	HEC	14	0

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 [i](#)

6.1 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	439/439 (100%)	-0.38	3 (0%) 87 85	6, 24, 44, 71	1 (0%)
1	B	439/439 (100%)	-0.37	2 (0%) 90 89	8, 25, 46, 72	1 (0%)
All	All	878/878 (100%)	-0.38	5 (0%) 89 88	6, 24, 44, 72	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	TYR	5.9
1	A	470	TYR	4.9
1	B	468	ALA	2.8
1	A	464	LYS	2.2
1	A	213	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEC	B	474	43/43	0.97	0.14	1.30	16,18,26,31	0
2	HEC	A	474	43/43	0.97	0.14	0.51	14,19,24,26	0
2	HEC	A	472	43/43	0.96	0.14	0.41	27,32,39,43	0
2	HEC	B	473	43/43	0.97	0.13	0.32	17,19,23,25	0
2	HEC	B	471	43/43	0.97	0.14	0.16	15,17,23,25	0
2	HEC	A	473	43/43	0.97	0.12	-0.08	9,13,19,23	0
2	HEC	B	472	43/43	0.97	0.12	-0.32	24,27,30,31	0
2	HEC	B	475	43/43	0.97	0.12	-0.37	5,14,19,21	0
2	HEC	A	471	43/43	0.98	0.12	-0.61	11,14,17,19	0
2	HEC	A	475	43/43	0.97	0.11	-0.62	11,16,24,29	0
3	CA	A	476	1/1	0.97	0.09	-1.86	18,18,18,18	0
3	CA	B	476	1/1	0.99	0.10	-2.76	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.