



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:32 PM GMT

PDB ID : 2V3V
Title : A NEW CATALYTIC MECHANISM OF PERIPLASMIC NITRATE REDUCTASE FROM DESULFOVIBRIO DESULFURICANS ATCC 27774 FROM CRYSTALLOGRAPHIC AND EPR DATA AND BASED ON DETAILED ANALYSIS OF THE SIXTH LIGAND
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Deposited on : 2007-06-22
Resolution : 1.99 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

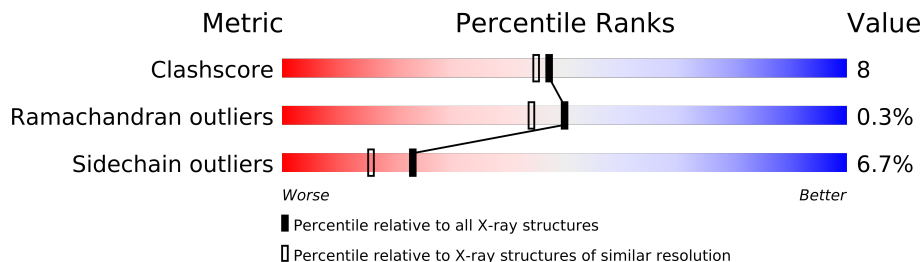
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.99 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	723	

2 Entry composition i

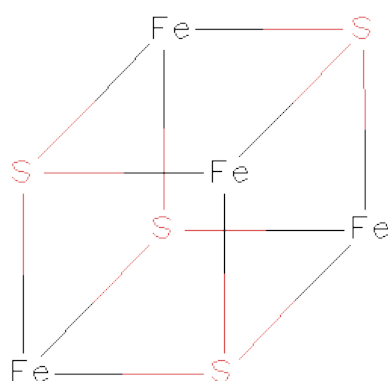
There are 7 unique types of molecules in this entry. The entry contains 6558 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PERIPLASMIC NITRATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	10	0
			5677	3588	1016	1030	43			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



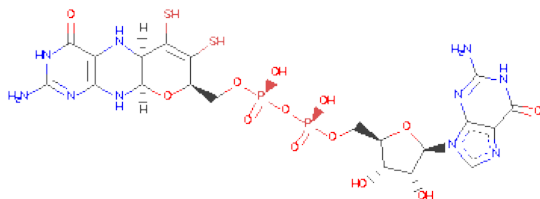
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mo	0	0
			1	1		

- Molecule 4 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA

-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONEGUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).

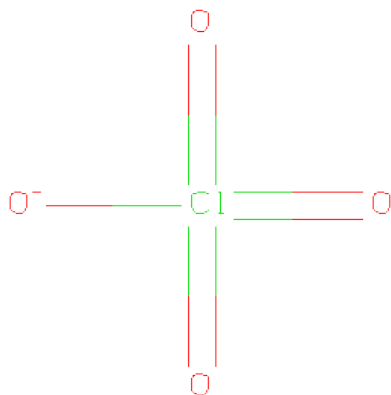


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	X	0	0
			1	1		

- Molecule 6 is PERCHLORATE ION (three-letter code: LCP) (formula: ClO_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Cl	O	0	0
			5	1	4		
6	A	1	Total	Cl	O	0	0
			5	1	4		
6	A	1	Total	Cl	O	0	0
			5	1	4		
6	A	1	Total	Cl	O	0	0
			5	1	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	757	Total	O	0	0
			757	757		

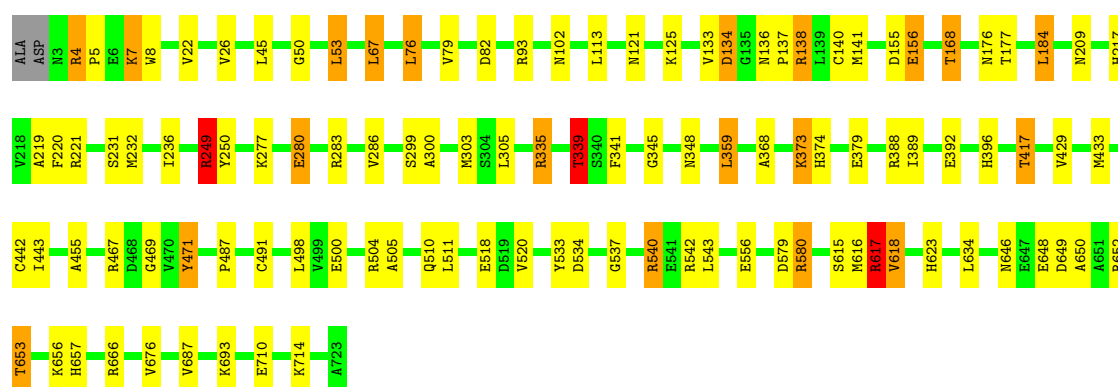
3 Residue-property plots

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 ($RSRZ > 2$). 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 failed to run properly.

• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

Chain A:



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.57Å 106.57Å 135.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.45 – 1.99	Depositor
% Data completeness (in resolution range)	97.1 (92.45-1.99)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.246	Depositor
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.269	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	6 of 63905 reflections (0.009%)	Xtriage
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, MO, SF4, LCP, MGD

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	0.66	2/5853 (0.0%)	0.78	14/7940 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249[A]	ARG	CG-CD	12.52	1.83	1.51
1	A	249[B]	ARG	CG-CD	12.52	1.83	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	617	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	617	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	A	67	LEU	CA-CB-CG	7.17	131.80	115.30
1	A	76	LEU	CA-CB-CG	6.29	129.75	115.30
1	A	249[A]	ARG	CG-CD-NE	6.28	124.98	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5677	0	5597	89	0
2	A	8	0	0	0	0
3	A	1	0	0	0	0
4	A	94	0	44	12	0
5	A	1	0	0	0	0
6	A	20	0	0	6	0
7	A	757	0	0	21	2
All	All	6558	0	5641	91	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 91 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249[A]:ARG:CG	1:A:249[A]:ARG:CD	1.83	1.54
1:A:249[B]:ARG:CG	1:A:249[B]:ARG:CD	1.89	1.49
1:A:249[B]:ARG:CB	1:A:249[B]:ARG:CD	2.37	1.02
1:A:518:GLU:HG3	1:A:540:ARG:HG3	1.50	0.92
1:A:300:ALA:O	1:A:335:ARG:NH2	2.07	0.88

All (2) 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	Distance(Å)	Clash(Å)
7:A:2226:HOH:O	7:A:2227:HOH:O[6_765]	1.98	0.22
7:A:2226:HOH:O	7:A:2239:HOH:O[6_765]	2.06	0.14

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	729/723 (101%)	702 (96%)	25 (3%)	2 (0%)	50 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	156	GLU

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	604/596 (101%)	562 (93%)	42 (7%)	21	14

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	GLU
1	A	417	THR
1	A	648	GLU
1	A	339	THR
1	A	373	LYS

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	A	374	HIS
1	A	657	HIS
1	A	623	HIS
1	A	176	ASN
1	A	490	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 9 ligands modelled in this entry, 1 is unknown and 1 is monoatomic - leaving 7 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	SF4	A	800	1	12,12,12	5.44	9 (75%)	0,24,24	0.00	-
4	MGD	A	811	3	52,52,52	1.63	8 (15%)	72,81,81	3.23	17 (23%)
4	MGD	A	812	3	52,52,52	1.42	8 (15%)	72,81,81	3.44	22 (30%)
6	LCP	A	814	-	4,4,4	7.57	4 (100%)	6,6,6	0.35	0
6	LCP	A	815	-	4,4,4	7.65	4 (100%)	6,6,6	0.29	0
6	LCP	A	816	-	4,4,4	7.58	4 (100%)	6,6,6	0.55	0
6	LCP	A	817	-	4,4,4	7.57	4 (100%)	6,6,6	0.29	0

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	SF4	A	800	1	-	0/0/48/48	0/0/5/5
4	MGD	A	811	3	-	0/22/66/66	0/1/6/6
4	MGD	A	812	3	-	0/22/66/66	0/1/6/6
6	LCP	A	814	-	-	0/0/0/0	0/0/0/0
6	LCP	A	815	-	-	0/0/0/0	0/0/0/0
6	LCP	A	816	-	-	0/0/0/0	0/0/0/0
6	LCP	A	817	-	-	0/0/0/0	0/0/0/0

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	SF4	S2-FE1	-8.99	2.27	2.33
2	A	800	SF4	S1-FE2	-8.59	2.27	2.33
6	A	817	LCP	O4-CL	7.81	1.83	1.40
6	A	815	LCP	O1-CL	7.81	1.85	1.40
2	A	800	SF4	S4-FE3	-7.78	2.28	2.33

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	811	MGD	C6-C5-N7	22.93	137.23	134.14
4	A	812	MGD	C6-C5-N7	21.34	137.01	134.14
4	A	812	MGD	O4'-C1'-N9	11.66	119.29	108.44
4	A	812	MGD	N3-C4-N9	4.77	133.91	126.91
4	A	811	MGD	C14-C23-N22	4.65	116.36	110.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.