



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AOP
Title : SULFITE REDUCTASE HEMOPROTEIN PHOTOREDUCED WITH
PROFLAVINE EDTA, SIROHEME FEII,[4FE-4S] +1, PHOSPHATE
BOUND
Authors : Crane, B.R.; Getzoff, E.D.
Deposited on : 1997-07-09
Resolution : 2.10 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
<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

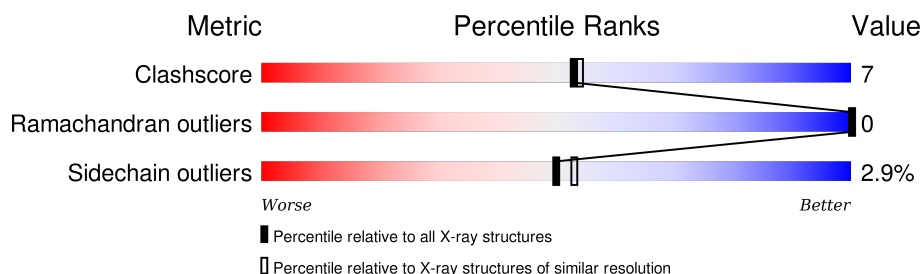
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	497	 77% 13% • 9%

2 Entry composition [i](#)

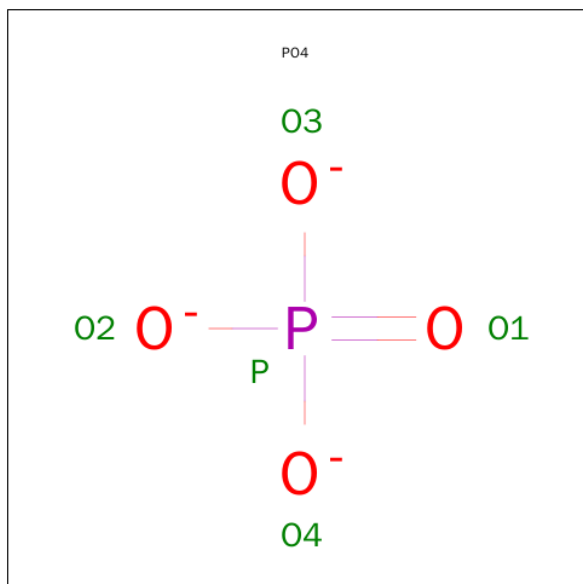
There are 6 unique types of molecules in this entry. The entry contains 4023 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SULFITE REDUCTASE HEMOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3563	2252	644	651	16			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

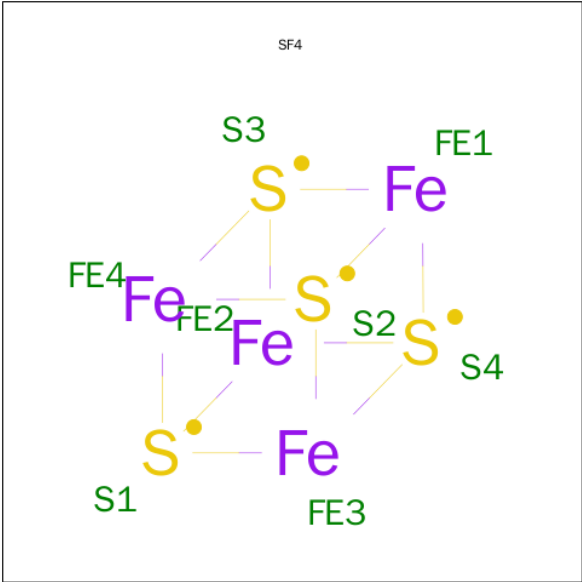


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

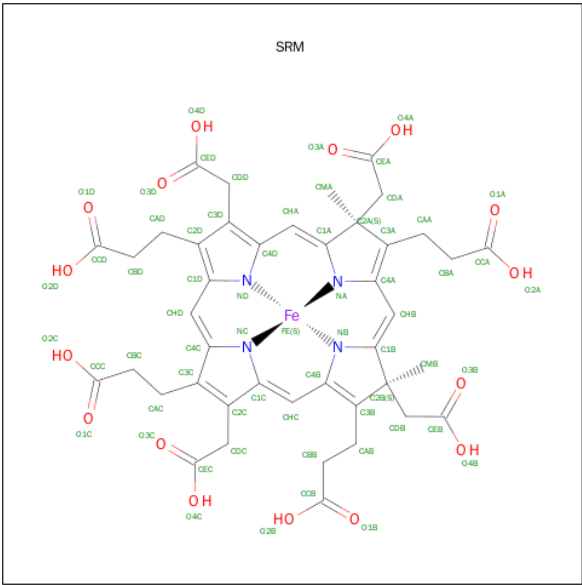
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 5 is SIROHEME (three-letter code: SRM) (formula: C₄₂H₄₂FeN₄O₁₆).

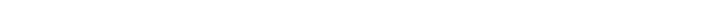


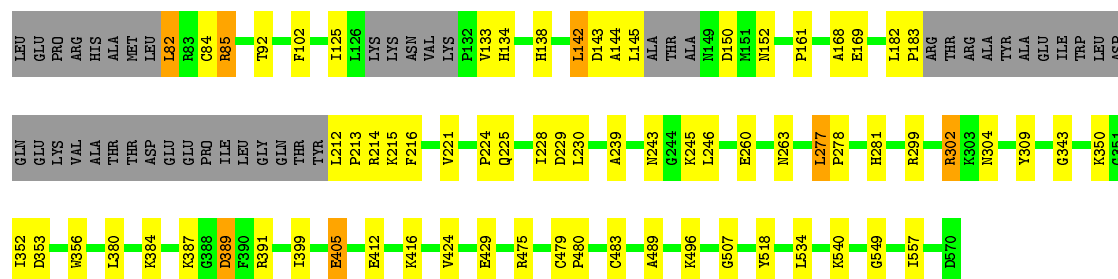
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	383	Total 383	O 383	0	0

Note EDS was not executed.

- Chain A:  77% 13% • 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.80 Å 77.40 Å 87.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.2 (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4023	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: PO4, K, SF4, SRM

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	0.43	0/3636	0.70	1/4913 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	277	LEU	CA-CB-CG	7.46	132.47	115.30

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	3563	0	3568	46	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
5	A	63	0	34	4	0
6	A	383	0	0	14	0
All	All	4023	0	3602	48	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 7.

All (48) 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:299:ARG:NE	1:A:299:ARG:HA	2.03	0.73
1:A:356:TRP:HE1	1:A:405:GLU:HG3	1.56	0.69
1:A:239:ALA:HB1	1:A:246:LEU:HD11	1.75	0.67
1:A:138:HIS:HB2	6:A:946:HOH:O	1.97	0.63
1:A:152:ASN:HB2	6:A:844:HOH:O	2.00	0.61
1:A:102:PHE:CZ	1:A:133:VAL:HG22	2.35	0.61
1:A:182:LEU:HD12	1:A:183:PRO:HD2	1.85	0.58
1:A:496:LYS:HE2	6:A:635:HOH:O	2.04	0.58
1:A:479:CYS:HB2	1:A:480:PRO:HD2	1.87	0.56
1:A:213:PRO:HG3	6:A:964:HOH:O	2.05	0.55
1:A:243:ASN:HB3	6:A:742:HOH:O	2.07	0.53
1:A:169:GLU:HG3	6:A:891:HOH:O	2.09	0.52
1:A:352:ILE:HG12	6:A:880:HOH:O	2.10	0.51
1:A:412:GLU:O	1:A:416:LYS:HB2	2.12	0.50
1:A:125:ILE:HD13	1:A:133:VAL:HG21	1.93	0.50
1:A:221:VAL:HG22	1:A:228:ILE:HD11	1.94	0.50
1:A:82:LEU:HB2	1:A:125:ILE:CD1	2.42	0.49
1:A:84:CYS:SG	1:A:142:LEU:HG	2.52	0.49
1:A:92:THR:HA	1:A:389:ASP:HB3	1.95	0.49
1:A:380:LEU:O	1:A:384:LYS:HG3	2.14	0.48
1:A:278:PRO:HD2	1:A:281:HIS:HD2	1.79	0.47
1:A:224:PRO:HB3	6:A:897:HOH:O	2.14	0.47
1:A:540:LYS:HE2	6:A:896:HOH:O	2.15	0.47
1:A:356:TRP:NE1	1:A:405:GLU:HG3	2.28	0.45
1:A:353:ASP:HA	6:A:971:HOH:O	2.15	0.45
5:A:580:SRM:HAB1	5:A:580:SRM:HMB3	1.69	0.45
1:A:343:GLY:HA2	6:A:958:HOH:O	2.15	0.45
1:A:299:ARG:NE	1:A:299:ARG:CA	2.78	0.45
1:A:260:GLU:HB3	1:A:263:ASN:HB3	1.98	0.45
1:A:85:ARG:HD3	1:A:143:ASP:OD1	2.17	0.45
1:A:475:ARG:HD2	1:A:489:ALA:HB2	1.98	0.45
1:A:215:LYS:HE2	5:A:580:SRM:HBD2	2.00	0.43
5:A:580:SRM:HDD1	5:A:580:SRM:HHA	1.89	0.43
1:A:507:GLY:O	1:A:549:GLY:HA3	2.19	0.43
1:A:391:ARG:HB2	1:A:399:ILE:HB	2.01	0.42
1:A:214:ARG:HD2	1:A:302:ARG:HH21	1.85	0.42
1:A:212:LEU:HD13	1:A:216:PHE:HB2	2.02	0.42
1:A:161:PRO:HA	1:A:225:GLN:NE2	2.34	0.41
1:A:483:CYS:HA	5:A:580:SRM:C2C	2.51	0.41
1:A:85:ARG:HB2	1:A:145:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:TYR:HA	6:A:970:HOH:O	2.21	0.41
1:A:534:LEU:HD22	1:A:557:ILE:HD13	2.01	0.41
1:A:304:ASN:HA	1:A:309:TYR:CD2	2.56	0.41
1:A:134:HIS:NE2	1:A:144:ALA:HB3	2.35	0.41
1:A:424:VAL:HG23	1:A:429:GLU:HG3	2.03	0.40
1:A:350:LYS:HG3	6:A:744:HOH:O	2.19	0.40
1:A:168:ALA:HB3	6:A:891:HOH:O	2.21	0.40
1:A:145:LEU:HD22	1:A:150:ASP:OD2	2.21	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	445/497 (90%)	427 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	376/413 (91%)	365 (97%)	11 (3%)	50	53

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	85	ARG
1	A	142	LEU
1	A	229	ASP
1	A	230	LEU
1	A	245	LYS
1	A	277	LEU
1	A	302	ARG
1	A	387	LYS
1	A	389	ASP
1	A	405	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	281	HIS
1	A	355	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	SF4	A	575	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SRM	A	580	2	29,70,70	1.59	7 (24%)	29,112,112	3.95	13 (44%)
2	PO4	A	585	5	4,4,4	2.89	1 (25%)	6,6,6	0.34	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
4	SF4	A	575	1	-	0/0/48/48	0/6/5/5
5	SRM	A	580	2	-	0/22/126/126	0/0/8/8
2	PO4	A	585	5	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	580	SRM	C1C-NC	-3.48	1.32	1.36
5	A	580	SRM	CDC-C2C	-2.43	1.49	1.52
5	A	580	SRM	CMA-C2A	2.42	1.59	1.54
5	A	580	SRM	C4C-NC	2.49	1.40	1.36
5	A	580	SRM	FE-NA	2.55	2.05	1.95
5	A	580	SRM	C1A-NA	2.60	1.42	1.38
5	A	580	SRM	CDB-C2B	3.53	1.62	1.56
2	A	585	PO4	P-O2	5.45	1.73	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	580	SRM	CAB-C3B-C2B	-12.83	109.01	123.46
5	A	580	SRM	CAA-C3A-C2A	-12.31	109.60	123.46
5	A	580	SRM	CDD-C3D-C4D	-4.91	119.36	127.34
5	A	580	SRM	C3B-C4B-NB	-3.91	105.74	110.09
5	A	580	SRM	CBD-CAD-C2D	-2.58	107.90	112.53
5	A	580	SRM	CAC-C3C-C2C	-2.44	123.32	129.38
5	A	580	SRM	CMA-C2A-CDA	2.30	112.50	109.76
5	A	580	SRM	CHC-C4B-NB	2.34	128.27	123.70
5	A	580	SRM	CAC-C3C-C4C	2.42	129.63	127.01
5	A	580	SRM	C2A-CDA-CEA	2.52	119.36	115.45

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	580	SRM	C4B-NB-C1B	3.55	108.83	106.90
5	A	580	SRM	C4A-NA-C1A	3.80	108.97	106.90
5	A	580	SRM	CBC-CAC-C3C	4.54	120.67	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	580	SRM	4	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](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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