



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID : 6GEP  
Title : SULFITE REDUCTASE HEMOPROTEIN NITRIC OXIDE COMPLEX REDUCED WITH PROFLAVINE EDTA  
Authors : Crane, B.R.; Getzoff, E.D.  
Deposited on : 1997-07-10  
Resolution : 1.80 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtrriage (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

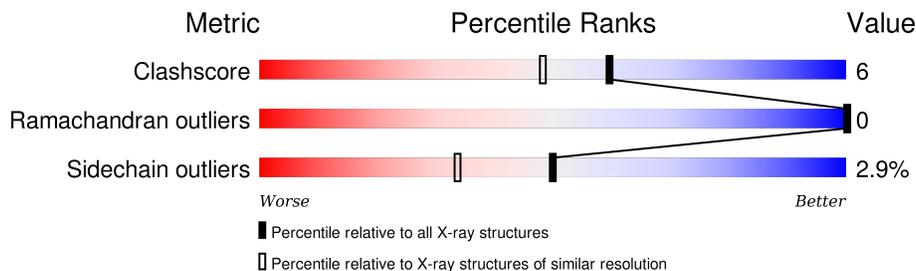
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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  $\geq 3$ , 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	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4015 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.

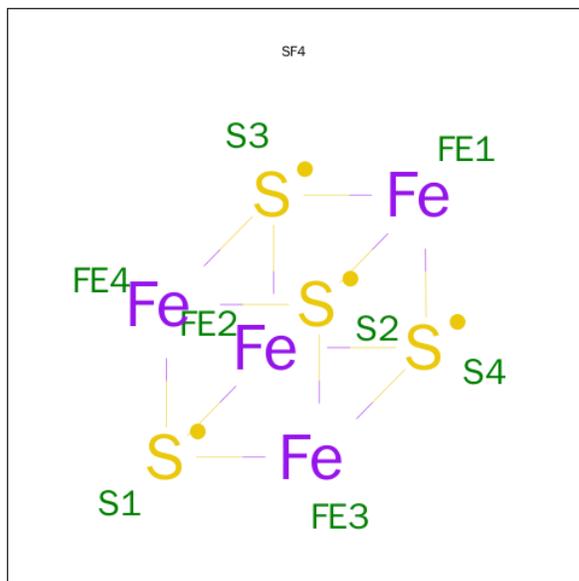
- Molecule 1 is a protein called SULFITE REDUCTASE HEMOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3601	2277	651	657	16	0	1	0

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

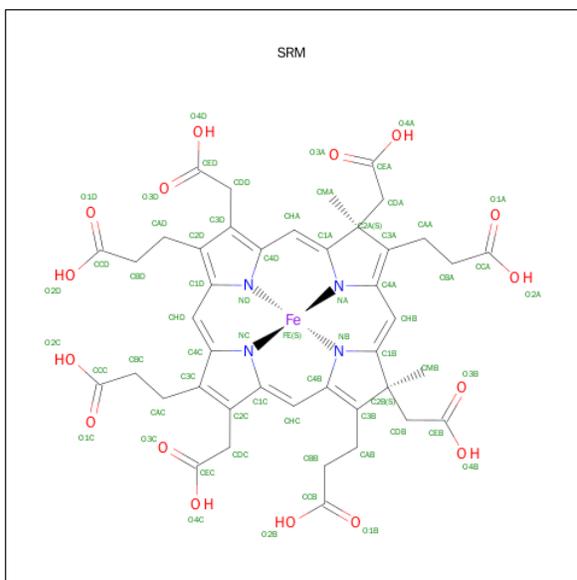
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



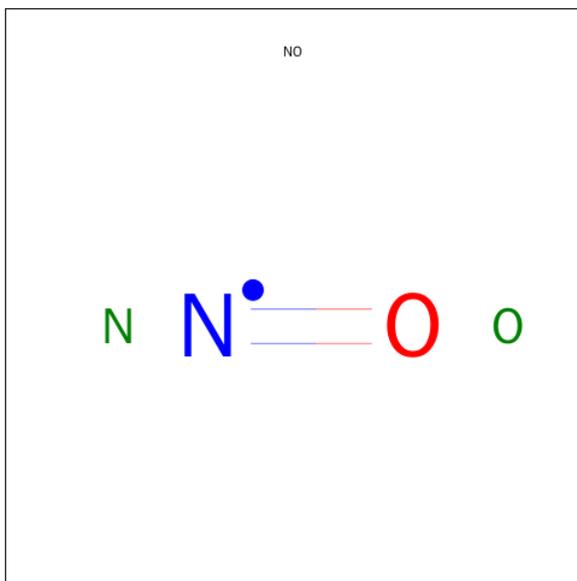
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is SIROHEME (three-letter code: SRM) (formula: C<sub>42</sub>H<sub>42</sub>FeN<sub>4</sub>O<sub>16</sub>).



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

- Molecule 5 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



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

- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	339	Total 340	O 340	0	1



## 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, $\alpha$ , $\beta$ , $\gamma$	69.80Å 77.40Å 87.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.7 (10.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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: SF4, SRM, K, NO

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	0/3675	0.71	1/4966 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LEU	CA-CB-CG	6.58	130.44	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	3601	0	3607	42	0
2	A	1	0	0	0	0
3	A	8	0	0	0	0
4	A	63	0	34	1	0
5	A	2	0	0	0	0
6	A	340	0	0	7	0
All	All	4015	0	3641	42	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 6.

All (42) 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:288:ALA:O	1:A:292:THR:HG23	1.90	0.71
1:A:151:MET:HB2	1:A:212:LEU:HB2	1.74	0.70
1:A:213:PRO:HG3	1:A:299:ARG:NH2	2.10	0.67
1:A:161:PRO:HA	1:A:225:GLN:HE22	1.60	0.65
1:A:151:MET:HG3	1:A:212:LEU:O	1.99	0.62
1:A:350:LYS:HG3	6:A:711:HOH:O	2.00	0.61
1:A:352:ILE:HG12	6:A:670:HOH:O	2.00	0.60
1:A:299:ARG:HA	1:A:299:ARG:HE	1.65	0.60
1:A:161:PRO:HA	1:A:225:GLN:NE2	2.18	0.58
1:A:83:ARG:HD3	4:A:580:SRM:O1B	2.03	0.58
1:A:524:GLU:HB3	1:A:525:PRO:HD3	1.85	0.58
1:A:475:ARG:HD2	1:A:489:ALA:HB2	1.85	0.57
1:A:212:LEU:HD21	1:A:290:VAL:HG13	1.86	0.56
1:A:92:THR:HA	1:A:389:ASP:HB3	1.89	0.54
1:A:102:PHE:CZ	1:A:133:VAL:HG22	2.44	0.53
1:A:278:PRO:HD2	1:A:281:HIS:HD2	1.74	0.52
1:A:151:MET:CB	1:A:212:LEU:HB2	2.39	0.52
1:A:137:LEU:CD1	1:A:144:ALA:HB2	2.39	0.52
1:A:182:LEU:HD12	1:A:183:PRO:HD2	1.91	0.51
1:A:91:ILE:O	1:A:389:ASP:HB2	2.12	0.49
1:A:85:ARG:HB2	1:A:145:LEU:HG	1.93	0.49
1:A:213:PRO:HG3	1:A:299:ARG:HH22	1.76	0.48
1:A:221:VAL:HG22	1:A:228:ILE:HD11	1.95	0.48
1:A:177:ILE:O	1:A:181:LEU:HG	2.14	0.47
1:A:479:CYS:HB2	1:A:480:PRO:HD2	1.96	0.47
1:A:150:ASP:OD1	1:A:152:ASN:HB2	2.15	0.46
1:A:524:GLU:HG2	1:A:528:LEU:HD22	1.97	0.46
1:A:103:ALA:O	1:A:110:GLY:HA2	2.16	0.45
1:A:210:THR:HB	1:A:294:ARG:HD3	1.98	0.45
1:A:360:LEU:HD11	1:A:400:ILE:HD11	1.98	0.45
1:A:313:ARG:HD3	6:A:871:HOH:O	2.14	0.45
1:A:469:ASP:HB2	6:A:797:HOH:O	2.17	0.44
1:A:212:LEU:HD13	1:A:216:PHE:HB2	2.00	0.44
1:A:182:LEU:CD1	1:A:183:PRO:HD2	2.49	0.43
1:A:95:GLN:NE2	1:A:142:LEU:HD13	2.34	0.42
1:A:507:GLY:O	1:A:549:GLY:HA3	2.20	0.42
1:A:278:PRO:HD2	1:A:281:HIS:CD2	2.53	0.42
1:A:345:ARG:NH2	6:A:892:HOH:O	2.50	0.42
1:A:498:PRO:HD2	6:A:720:HOH:O	2.19	0.42
1:A:292:THR:HG22	1:A:326:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD12	6:A:798:HOH:O	2.21	0.41
1:A:293:GLN:NE2	1:A:305:ALA:O	2.54	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	449/497 (90%)	439 (98%)	10 (2%)	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	380/413 (92%)	369 (97%)	11 (3%)	50 34

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

Mol	Chain	Res	Type
1	A	126	LEU
1	A	142	LEU
1	A	214	ARG
1	A	229	ASP

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Mol	Chain	Res	Type
1	A	230	LEU
1	A	246	LEU
1	A	277	LEU
1	A	292	THR
1	A	338	GLU
1	A	389	ASP
1	A	528	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	149	ASN
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
3	SF4	A	575	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SRM	A	580	5	29,70,70	1.24	2 (6%)	29,112,112	4.36	12 (41%)
5	NO	A	585	4	0,1,1	0.00	-	0,0,0	0.00	-

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
3	SF4	A	575	1	-	0/0/48/48	0/6/5/5
4	SRM	A	580	5	-	0/22/126/126	0/0/8/8
5	NO	A	585	4	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	580	SRM	FE-NA	2.95	2.07	1.95
4	A	580	SRM	FE-NB	3.08	2.08	1.95

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	580	SRM	CAB-C3B-C2B	-16.19	105.23	123.46
4	A	580	SRM	CAA-C3A-C2A	-9.74	112.49	123.46
4	A	580	SRM	CED-CDD-C3D	-4.05	108.57	116.31
4	A	580	SRM	C3B-C4B-NB	-2.96	106.79	110.09
4	A	580	SRM	CDD-C3D-C4D	-2.88	122.66	127.34
4	A	580	SRM	CBD-CAD-C2D	-2.64	107.80	112.53
4	A	580	SRM	CDC-C2C-C1C	-2.42	123.47	127.38
4	A	580	SRM	C3A-C4A-NA	-2.04	107.82	110.09
4	A	580	SRM	C4B-NB-C1B	5.01	109.62	106.90
4	A	580	SRM	CMB-C2B-CDB	5.35	116.13	109.76
4	A	580	SRM	C4A-NA-C1A	5.86	110.08	106.90
4	A	580	SRM	CMA-C2A-CDA	5.91	116.79	109.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	580	SRM	1	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

### 6.1 Protein, DNA and RNA chains

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

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

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

### 6.3 Carbohydrates

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

### 6.4 Ligands

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

### 6.5 Other polymers

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