



## Full wwPDB EM Validation Report ⓘ

Feb 20, 2025 – 08:00 AM EST

PDB ID : 6QRZ  
Title : Crystal structure of R2-like ligand-binding oxidase from *Sulfolobus acidocaldarius* solved by 3D micro-crystal electron diffraction  
Authors : Xu, H.; Lebrette, H.; Clabbers, M.T.B.; Zhao, J.; Griese, J.J.; Zou, X.; Hogbom, M.  
Deposited on : 2019-02-20  
Resolution : 3.00 Å(reported)  
Based on initial model : 3EE4

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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>.

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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  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

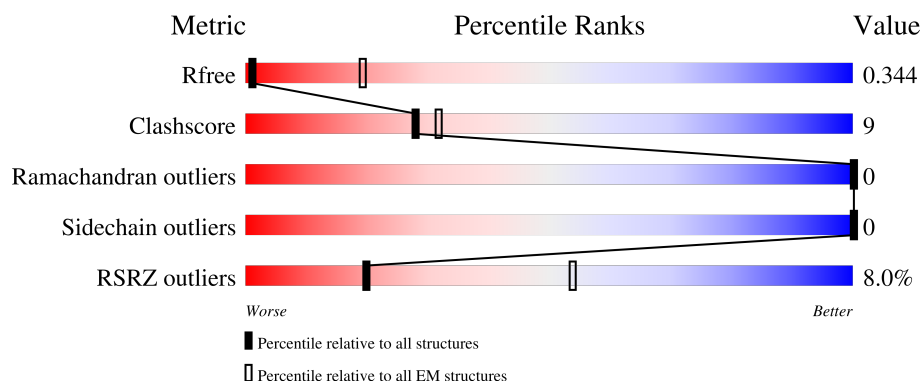
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 3.00 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)	EM structures (#Entries)
$R_{free}$	164678	53
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RSRZ outliers	164674	54

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	328	<div> <div>7%</div> <div>64%</div> <div>20%</div> <div>16%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2243 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ribonucleoside-diphosphate reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	274	Total	C	N	O	S	0	0
			2241	1454	364	416	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q4J6V7
A	-12	ALA	-	expression tag	UNP Q4J6V7
A	-11	HIS	-	expression tag	UNP Q4J6V7
A	-10	HIS	-	expression tag	UNP Q4J6V7
A	-9	HIS	-	expression tag	UNP Q4J6V7
A	-8	HIS	-	expression tag	UNP Q4J6V7
A	-7	HIS	-	expression tag	UNP Q4J6V7
A	-6	HIS	-	expression tag	UNP Q4J6V7
A	-5	VAL	-	expression tag	UNP Q4J6V7
A	-4	ASP	-	expression tag	UNP Q4J6V7
A	-3	ASP	-	expression tag	UNP Q4J6V7
A	-2	ASP	-	expression tag	UNP Q4J6V7
A	-1	ASP	-	expression tag	UNP Q4J6V7
A	0	LYS	-	expression tag	UNP Q4J6V7

- Molecule 2 is MANGANESE (III) ION (three-letter code: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mn	0
			1	1	

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Fe	0
			1	1	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.31Å 108.93Å 48.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 3.00 29.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	62.5 (29.00-3.00) 62.4 (29.00-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.318 , 0.335 0.333 , 0.344	Depositor DCC
$R_{free}$ test set	332 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.3	Xtriage
Anisotropy	1.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	2243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, MN3

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	0.24	0/2293	0.36	0/3104

There are no bond length outliers.

There are no bond angle outliers.

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	2241	0	2240	42	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
All	All	2243	0	2240	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 9.

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:172:THR:HG22	1:A:176:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:HG23	1:A:247:LEU:HD21	1.74	0.69
1:A:146:ILE:HA	1:A:150:GLU:HB2	1.81	0.62
1:A:292:THR:HG22	1:A:294:GLU:H	1.65	0.61
1:A:218:ILE:HD12	1:A:281:ARG:HH22	1.65	0.61
1:A:297:LYS:NZ	1:A:298:SER:OG	2.32	0.60
1:A:226:THR:HG22	1:A:288:ALA:HB2	1.84	0.60
1:A:86:ILE:HD11	1:A:105:LEU:HD22	1.85	0.58
1:A:173:THR:HA	1:A:247:LEU:HD11	1.86	0.57
1:A:176:LEU:HD21	1:A:285:ILE:HD11	1.88	0.56
1:A:74:LEU:HD21	1:A:140:ASN:HD21	1.71	0.54
1:A:92:THR:HG21	1:A:167:LEU:HD21	1.90	0.53
1:A:205:LYS:HE3	1:A:209:LEU:HD11	1.91	0.53
1:A:115:HIS:CD2	1:A:210:ILE:HG12	2.45	0.52
1:A:171:VAL:HG21	1:A:224:LEU:HD22	1.91	0.51
1:A:111:GLU:OE1	1:A:217:HIS:NE2	2.41	0.51
1:A:85:ASP:HB3	1:A:155:MET:HG3	1.92	0.50
1:A:105:LEU:HA	1:A:108:PHE:HB3	1.94	0.50
1:A:75:PHE:O	1:A:79:GLU:HG2	2.12	0.50
1:A:244:PHE:HE2	1:A:278:VAL:HG13	1.79	0.48
1:A:271:ILE:HA	1:A:274:ARG:HG2	1.95	0.48
1:A:86:ILE:HG21	1:A:109:ALA:HB2	1.95	0.47
1:A:225:ILE:O	1:A:229:ILE:HG13	2.14	0.47
1:A:131:ASP:OD1	1:A:132:LEU:N	2.48	0.47
1:A:69:LEU:HD13	1:A:128:ILE:HD13	1.96	0.47
1:A:213:ASP:OD1	1:A:216:ARG:NH2	2.48	0.46
1:A:104:TYR:O	1:A:108:PHE:N	2.31	0.46
1:A:168:ALA:HB2	1:A:236:ILE:HG23	1.98	0.46
1:A:154:VAL:HG21	1:A:173:THR:HB	1.98	0.45
1:A:172:THR:HA	1:A:176:LEU:HD13	1.98	0.45
1:A:244:PHE:CE2	1:A:278:VAL:HG13	2.51	0.45
1:A:15:HIS:ND1	1:A:18:PHE:HE1	2.15	0.44
1:A:74:LEU:O	1:A:143:TYR:OH	2.12	0.44
1:A:144:GLN:O	1:A:148:TYR:HB2	2.17	0.43
1:A:214:GLU:HA	1:A:217:HIS:HB2	2.01	0.42
1:A:98:ARG:HH12	1:A:297:LYS:HE3	1.84	0.42
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.88	0.42
1:A:122:PHE:CZ	1:A:126:LEU:HD11	2.55	0.41
1:A:34:LEU:HD22	1:A:216:ARG:HG2	2.03	0.41
1:A:181:VAL:HG11	1:A:278:VAL:HG23	2.01	0.41
1:A:153:SER:O	1:A:157:LYS:HB2	2.20	0.40
1:A:220:TYR:CE2	1:A:224:LEU:HD12	2.56	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 PDB entries followed by that with respect to all EM entries.

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	270/328 (82%)	261 (97%)	9 (3%)	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 PDB entries followed by that with respect to all EM entries.

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	245/295 (83%)	245 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - 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.

## 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.