



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:18 pm BST

PDB ID : 2CAK
Title : 1.27Angstrom Structure of Rusticyanin from Thiobacillus ferrooxidans
Authors : Barrett, M.L.; Harvey, I.; Sundararajan, M.; Surendran, R.; Hall, J.F.; Ellis, M.J.; Hough, M.A.; Strange, R.W.; Hillier, I.H.; Hasnain, S.S.
Deposited on : 2005-12-21
Resolution : 1.27 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

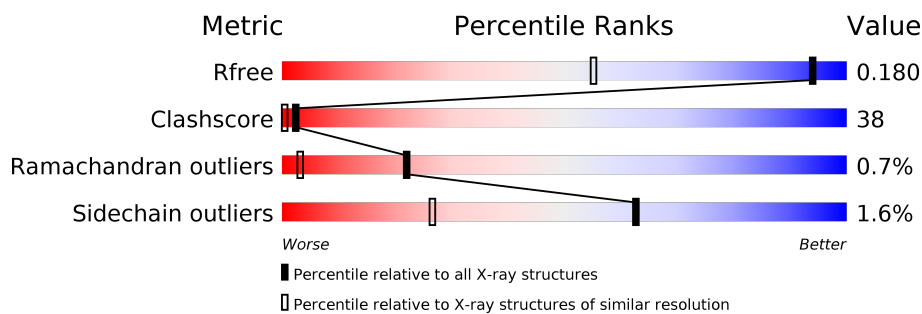
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.27 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}	130704	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)

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 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	154	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1279 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 RUSTICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	8	0
			1192	782	194	212	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P24930
A	58	GLY	ASP	conflict	UNP P24930
A	65	ASP	GLU	conflict	UNP P24930
A	68	GLY	ALA	conflict	UNP P24930
A	91	GLN	LYS	conflict	UNP P24930
A	93	VAL	GLY	conflict	UNP P24930
A	124	ASN	ASP	conflict	UNP P24930
A	153	ILE	VAL	conflict	UNP P24930

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

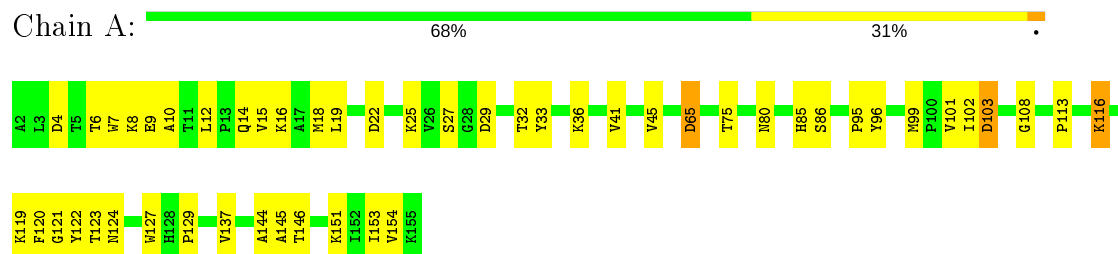
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	4
			86	86		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

• Molecule 1: RUSTICYANIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	32.47Å 60.82Å 38.12Å 90.00° 108.01° 90.00°	Depositor
Resolution (Å)	12.00 – 1.27 12.85 – 1.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-1.27) 98.1 (12.85-1.27)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.120 , 0.138 0.189 , 0.180	Depositor DCC
R_{free} test set	1834 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 54.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1279	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

¹Theoretical 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: CU1

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	0.70	0/1268	1.11	6/1723 (0.3%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	29	ASP	CB-CG-OD1	8.68	126.11	118.30
1	A	65	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	103	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	99	MET	CG-SD-CE	6.65	110.85	100.20
1	A	4	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	4	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1192	0	1192	90	0
2	A	1	0	0	0	0
3	A	86	0	0	85	1
All	All	1279	0	1192	91	1

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 38.

All (91) 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:145:ALA:CA	3:A:2078:HOH:O	1.66	1.28
1:A:145:ALA:CB	3:A:2078:HOH:O	1.68	1.27
1:A:22:ASP:HA	3:A:2025:HOH:O	1.18	1.27
1:A:102:ILE:HG12	3:A:2047:HOH:O	1.31	1.26
1:A:32:THR:CG2	3:A:2022:HOH:O	1.72	1.25
1:A:7:TRP:HA	3:A:2003:HOH:O	1.40	1.20
1:A:145:ALA:HB3	3:A:2078:HOH:O	1.28	1.19
1:A:122:TYR:CE2	3:A:2065:HOH:O	1.97	1.17
1:A:154:VAL:N	3:A:2086:HOH:O	1.76	1.17
1:A:121:GLY:N	3:A:2061:HOH:O	1.77	1.13
1:A:120:PHE:HE1	3:A:2007:HOH:O	1.31	1.10
1:A:32:THR:HG23	3:A:2022:HOH:O	1.28	1.10
1:A:86:SER:HB3	3:A:2036:HOH:O	1.52	1.09
1:A:41:VAL:HG23	3:A:2027:HOH:O	1.47	1.08
1:A:15:VAL:CA	3:A:2009:HOH:O	1.94	1.08
1:A:96:TYR:HA	3:A:2040:HOH:O	1.55	1.07
1:A:120:PHE:O	3:A:2060:HOH:O	1.73	1.04
1:A:145:ALA:O	3:A:2080:HOH:O	1.74	1.03
1:A:19:LEU:N	3:A:2011:HOH:O	1.91	1.02
1:A:145:ALA:N	3:A:2078:HOH:O	1.66	1.01
1:A:120:PHE:CE1	3:A:2007:HOH:O	2.06	1.01
1:A:122:TYR:HE2	3:A:2065:HOH:O	1.33	1.00
1:A:95:PRO:O	3:A:2041:HOH:O	1.79	0.99
1:A:86:SER:CB	3:A:2036:HOH:O	2.07	0.98
1:A:14:GLN:OE1	3:A:2008:HOH:O	1.81	0.96
1:A:80:ASN:HD22	1:A:85:HIS:HE2	1.01	0.94
1:A:9:GLU:OE1	3:A:2004:HOH:O	1.86	0.93
1:A:41:VAL:CG2	3:A:2027:HOH:O	1.88	0.92
1:A:6:THR:O	3:A:2003:HOH:O	1.89	0.90
1:A:15:VAL:HA	3:A:2009:HOH:O	1.60	0.90
1:A:108:GLY:O	3:A:2053[B]:HOH:O	1.90	0.88
1:A:153:ILE:CG2	3:A:2086:HOH:O	2.20	0.88
1:A:116:LYS:HA	3:A:2057:HOH:O	1.73	0.87
1:A:123:THR:HB	3:A:2003:HOH:O	1.75	0.86
1:A:153:ILE:C	3:A:2086:HOH:O	2.11	0.80
1:A:27:SER:HA	3:A:2019:HOH:O	1.83	0.78
1:A:8:LYS:O	3:A:2064:HOH:O	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:CA	3:A:2086:HOH:O	2.34	0.74
1:A:120:PHE:HB2	3:A:2060:HOH:O	1.89	0.72
1:A:32:THR:HG22	3:A:2022:HOH:O	1.56	0.72
1:A:103:ASP:OD1	3:A:2049:HOH:O	2.08	0.71
1:A:123:THR:CB	3:A:2003:HOH:O	2.37	0.70
1:A:151:LYS:HB3	3:A:2033:HOH:O	1.92	0.69
1:A:102:ILE:HG23	3:A:2046:HOH:O	1.93	0.69
1:A:153:ILE:HG23	3:A:2086:HOH:O	1.87	0.68
1:A:95:PRO:HG2	3:A:2041:HOH:O	1.94	0.68
1:A:102:ILE:N	3:A:2047:HOH:O	2.27	0.66
1:A:14:GLN:CD	3:A:2008:HOH:O	2.24	0.66
1:A:96:TYR:C	3:A:2043:HOH:O	2.34	0.65
1:A:14:GLN:NE2	3:A:2008:HOH:O	2.31	0.63
1:A:120:PHE:CA	3:A:2060:HOH:O	2.47	0.62
1:A:19:LEU:CA	3:A:2011:HOH:O	2.37	0.62
1:A:146:THR:N	3:A:2078:HOH:O	2.27	0.61
1:A:121:GLY:CA	3:A:2061:HOH:O	2.31	0.61
1:A:27:SER:CA	3:A:2019:HOH:O	2.47	0.61
1:A:27:SER:CB	3:A:2019:HOH:O	2.41	0.60
1:A:145:ALA:N	3:A:2081:HOH:O	2.34	0.60
1:A:16[B]:LYS:HE2	1:A:19:LEU:HD12	1.84	0.59
1:A:95:PRO:CG	3:A:2041:HOH:O	2.49	0.59
1:A:80:ASN:ND2	1:A:85:HIS:HE2	1.85	0.58
1:A:15:VAL:C	3:A:2009:HOH:O	2.28	0.58
1:A:102:ILE:CG2	3:A:2046:HOH:O	2.51	0.58
1:A:33:TYR:N	3:A:2022:HOH:O	2.37	0.57
1:A:12:LEU:N	3:A:2007:HOH:O	2.37	0.57
1:A:153:ILE:CB	3:A:2085:HOH:O	2.54	0.56
1:A:116:LYS:CA	3:A:2057:HOH:O	2.45	0.56
1:A:96:TYR:HB2	3:A:2081:HOH:O	2.06	0.56
1:A:116:LYS:HB2	3:A:2057:HOH:O	2.06	0.55
1:A:153:ILE:HB	3:A:2085:HOH:O	2.04	0.55
1:A:102:ILE:CG1	3:A:2047:HOH:O	2.13	0.55
1:A:10:ALA:O	3:A:2060:HOH:O	2.19	0.52
1:A:96:TYR:CB	3:A:2081:HOH:O	2.58	0.51
1:A:153:ILE:HG22	3:A:2086:HOH:O	1.97	0.50
1:A:120:PHE:N	3:A:2060:HOH:O	2.43	0.49
1:A:145:ALA:C	3:A:2078:HOH:O	2.23	0.49
1:A:95:PRO:CD	3:A:2041:HOH:O	2.60	0.49
1:A:120:PHE:CD1	3:A:2007:HOH:O	2.50	0.49
1:A:153:ILE:HA	3:A:2086:HOH:O	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:OH	3:A:2062:HOH:O	0.47	0.46
1:A:65:ASP:HA	3:A:2085:HOH:O	2.15	0.46
1:A:18:MET:C	3:A:2011:HOH:O	2.44	0.45
1:A:25[A]:LYS:HE2	3:A:2018:HOH:O	2.16	0.45
1:A:127:TRP:CZ2	1:A:129:PRO:HB3	2.51	0.44
1:A:101:VAL:C	3:A:2046:HOH:O	2.56	0.44
1:A:75:THR:OG1	1:A:124:ASN:ND2	2.50	0.44
1:A:113:PRO:HD2	3:A:2055:HOH:O	2.17	0.43
1:A:119:LYS:HB2	3:A:2004:HOH:O	2.20	0.42
1:A:19:LEU:HA	3:A:2011:HOH:O	2.13	0.42
1:A:137[B]:VAL:HG12	1:A:144:ALA:HB2	2.03	0.41
1:A:151:LYS:CE	3:A:2033:HOH:O	2.69	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:2002:HOH:O	3:A:2018:HOH:O[2_556]	1.26	0.94

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	159/154 (103%)	157 (99%)	1 (1%)	1 (1%)	25 5

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	VAL

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	131/125 (105%)	128 (98%)	3 (2%)	50 12

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36[A]	LYS
1	A	36[B]	LYS
1	A	116	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	80	ASN
1	A	124	ASN
1	A	128	HIS

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

Of 1 ligands modelled in this entry, 1 is 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

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.