Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 03:49 PM EDT

PDB ID	:	1MFM
Title	:	MONOMERIC HUMAN SOD MUTANT F50E/G51E/E133Q AT ATOMIC RESOLUTION
Authors	:	Ferraroni, M.; Rypniewski, W.; Wilson, K.S.; Orioli, P.L.; Viezzoli, M.S.; Banci, L.; Bertini, I.; Mangani, S.
Deposited on	:	1999-04-16
Resolution	:	1.02 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

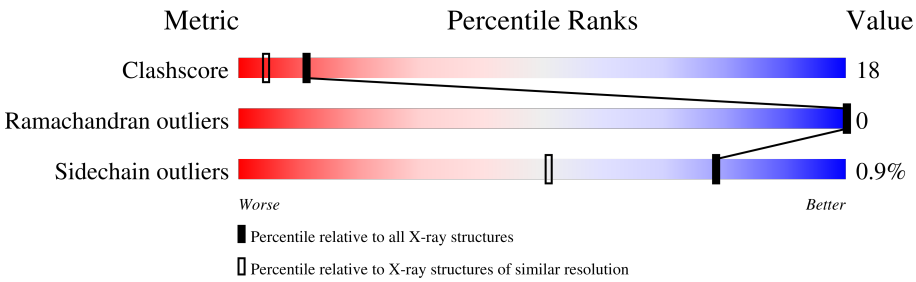
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.02 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	141614	1253 (1.08-0.96)
Ramachandran outliers	138981	1178 (1.08-0.96)
Sidechain outliers	138945	1180 (1.08-0.96)

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 of 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	153	81% 17% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1448 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 PROTEIN (COPPER,ZINC SUPEROXIDE DISMUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1152	707	207	234	4	0	14	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	CYS	engineered mutation	UNP P00441
A	50	GLU	PHE	engineered mutation	UNP P00441
A	51	GLU	GLY	engineered mutation	UNP P00441
A	111	SER	CYS	engineered mutation	UNP P00441
A	133	GLN	GLU	engineered mutation	UNP P00441

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
4	A	9	9	9	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	2	2	2	0	0

- Molecule 6 is water.

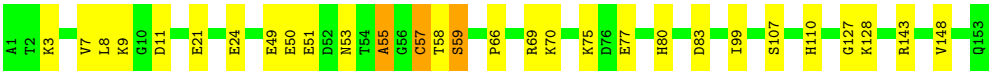
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	283	283	283	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PROTEIN (COPPER,ZINC SUPEROXIDE DISMUTASE)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.99Å 48.11Å 81.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.02 19.82 – 1.02	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-1.02) 95.3 (19.82-1.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.02Å)	Xtriage
Refinement program	SHELXL	Depositor
R, R_{free}	0.118 , (Not available) 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	10.2	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1448	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, ZN, CU, CD

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	0.78	0/1230	1.19	5/1659 (0.3%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	CYS	CA-CB-SG	9.32	130.78	114.00
1	A	55	ALA	C-N-CA	6.46	135.86	122.30
1	A	57	CYS	O-C-N	6.44	133.00	122.70
1	A	21	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	A	11	ASP	CB-CG-OD2	5.90	123.61	118.30

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	1152	0	1101	38	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	9	0	0	0	0
5	A	2	0	0	0	0
6	A	283	0	0	28	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1448	0	1101	39	2

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 18.

All (39) 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:51[A]:GLU:HG2	6:A:333:HOH:O	1.54	1.07
1:A:9:LYS:HG2	6:A:330:HOH:O	1.52	1.06
1:A:9:LYS:HE2	6:A:330:HOH:O	1.64	0.95
1:A:143:ARG:CG	6:A:300:HOH:O	2.25	0.85
1:A:9:LYS:CG	6:A:330:HOH:O	2.16	0.79
1:A:75:LYS:HD3	6:A:332:HOH:O	1.84	0.78
1:A:143:ARG:HD3	6:A:300:HOH:O	1.82	0.78
1:A:49:GLU:OE2	6:A:218:HOH:O	2.03	0.75
1:A:77:GLU:CB	6:A:356:HOH:O	2.36	0.73
1:A:143:ARG:CD	6:A:300:HOH:O	2.37	0.72
1:A:69:ARG:HD2	6:A:322:HOH:O	1.95	0.67
1:A:66:PRO:O	6:A:187:HOH:O	2.12	0.66
1:A:107[A]:SER:OG	6:A:267:HOH:O	2.10	0.65
1:A:75:LYS:CD	6:A:332:HOH:O	2.45	0.64
1:A:128[B]:LYS:HD3	6:A:246:HOH:O	1.98	0.63
1:A:59:SER:O	1:A:59:SER:OG	2.15	0.62
1:A:24[A]:GLU:OE2	6:A:435:HOH:O	2.16	0.61
1:A:80:HIS:HB2	1:A:83:ASP:CG	2.23	0.59
1:A:8:LEU:C	1:A:9:LYS:HG3	2.22	0.58
1:A:148[A]:VAL:HG22	6:A:294:HOH:O	2.04	0.56
1:A:143:ARG:HD3	6:A:169:HOH:O	2.04	0.56
1:A:143:ARG:NH1	6:A:169:HOH:O	2.39	0.56
1:A:8:LEU:O	1:A:9:LYS:HG3	2.04	0.56
1:A:9:LYS:HD2	6:A:402:HOH:O	2.05	0.55
1:A:70:LYS:NZ	6:A:407:HOH:O	2.41	0.54
1:A:57:CYS:O	1:A:143:ARG:NH2	2.42	0.52
1:A:143:ARG:CD	6:A:169:HOH:O	2.57	0.52
1:A:143:ARG:HG2	6:A:300:HOH:O	2.02	0.51
1:A:7:VAL:HG11	1:A:9:LYS:HE3	1.92	0.51
1:A:99:ILE:HD11	6:A:436:HOH:O	2.10	0.51
1:A:69:ARG:CD	6:A:322:HOH:O	2.57	0.47
1:A:143:ARG:CZ	6:A:169:HOH:O	2.63	0.46
1:A:55:ALA:O	1:A:58:THR:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50[B]:GLU:HG2	1:A:59:SER:O	2.18	0.43
1:A:127:GLY:C	1:A:128[B]:LYS:HD2	2.38	0.43
1:A:110[B]:HIS:CD2	6:A:295:HOH:O	2.72	0.43

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	Interatomic distance (Å)	Clash overlap (Å)
6:A:285:HOH:O	6:A:293:HOH:O[4_556]	2.11	0.09
6:A:186:HOH:O	6:A:268:HOH:O[1_455]	2.16	0.04

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	166/153 (108%)	162 (98%)	4 (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	128/118 (108%)	127 (99%)	1 (1%)	81 54

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	153	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 13 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.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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