wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 01:41 AM UTC

PDB ID	:	8ZD6 / pdb_00008zd6
Title	:	Crystal structure of E40K variant of Cu/Zn-superoxide dismutase from dog (Canis familiaris) in the apo form complexed with 22E1 Fv-clasp
Authors	:	Shino, Y.; Furukawa, Y.; Muraki, N.
Deposited on	:	2024-05-01
Resolution	:	3.29 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

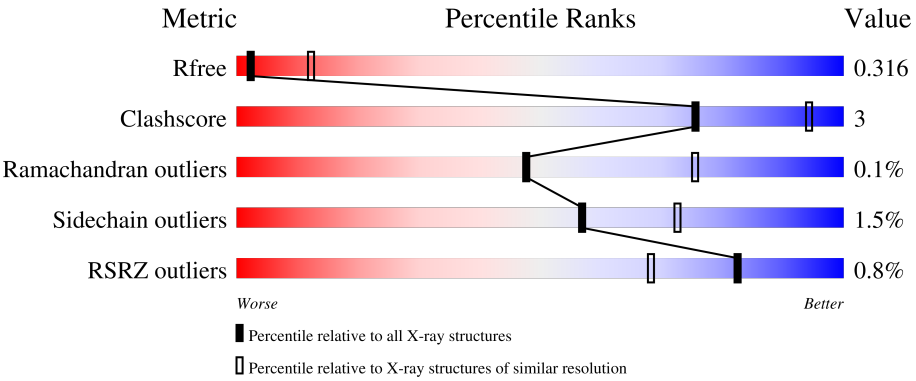
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.29 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	153	80% 5% 15%
1	D	153	90% 9%
1	G	153	77% 18%
1	J	153	90% 9%
2	B	169	5% 91% 5%

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Mol	Chain	Length	Quality of chain
2	E	169	2% 89% 7%
2	H	169	87% 9%
2	K	169	% 83% 5% 12%
3	C	159	% 87% 6% 7%
3	F	159	% 87% 7% 6%
3	I	159	87% 7% 6%
3	L	159	84% 6% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12448 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			946	587	172	181	6			
1	D	153	Total	C	N	O	S	0	0	0
			1105	679	203	217	6			
1	G	125	Total	C	N	O	S	0	0	0
			883	543	162	172	6			
1	J	152	Total	C	N	O	S	0	0	0
			1097	672	201	218	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	LYS	GLU	engineered mutation	UNP Q8WNN6
A	51	GLY	GLU	conflict	UNP Q8WNN6
A	53	ASN	UNK	conflict	UNP Q8WNN6
D	40	LYS	GLU	engineered mutation	UNP Q8WNN6
D	51	GLY	GLU	conflict	UNP Q8WNN6
D	53	ASN	UNK	conflict	UNP Q8WNN6
G	40	LYS	GLU	engineered mutation	UNP Q8WNN6
G	51	GLY	GLU	conflict	UNP Q8WNN6
G	53	ASN	UNK	conflict	UNP Q8WNN6
J	40	LYS	GLU	engineered mutation	UNP Q8WNN6
J	51	GLY	GLU	conflict	UNP Q8WNN6
J	53	ASN	UNK	conflict	UNP Q8WNN6

- Molecule 2 is a protein called 22E1VH-SARAH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	0	0	0
			1113	698	187	224	4			
2	E	162	Total	C	N	O	S	0	0	0
			1094	686	184	220	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	154	Total	C	N	O	S	0	0	0
			1046	653	178	211	4			
2	K	149	Total	C	N	O	S	0	0	0
			1056	663	176	212	5			

- Molecule 3 is a protein called 22E1VL-SARAH.

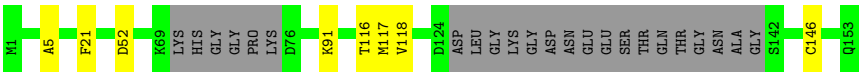
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	148	Total	C	N	O	S	0	0	0
			1034	642	179	209	4			
3	F	150	Total	C	N	O	S	0	0	0
			1034	642	177	211	4			
3	I	149	Total	C	N	O	S	0	0	0
			1026	633	179	210	4			
3	L	142	Total	C	N	O	S	0	0	0
			1014	634	175	201	4			

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

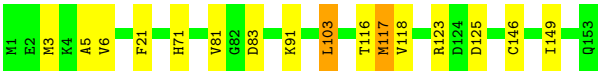
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



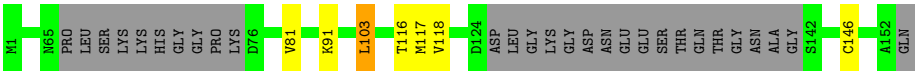
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain D:



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain G:

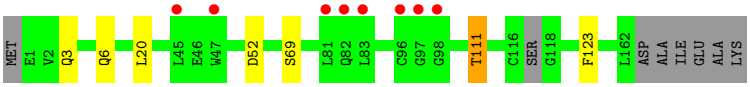


• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain J:

• Molecule 2: 22E1VH-SARAH

Chain B:

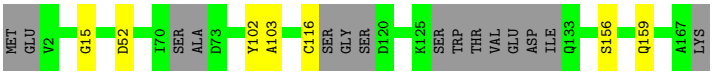


• Molecule 2: 22E1VH-SARAH

Chain E:

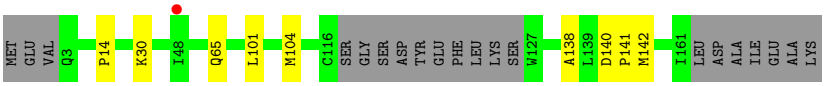
• Molecule 2: 22E1VH-SARAH

Chain H:



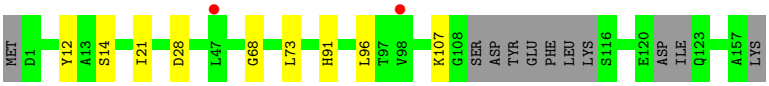
• Molecule 2: 22E1VH-SARAH

Chain K:



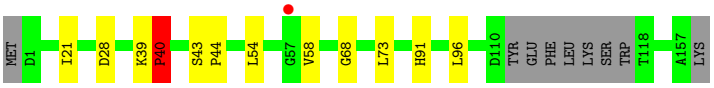
• Molecule 3: 22E1VL-SARAH

Chain C:



• Molecule 3: 22E1VL-SARAH

Chain F:

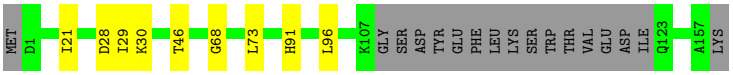


• Molecule 3: 22E1VL-SARAH

Chain I:

• Molecule 3: 22E1VL-SARAH

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.62Å 83.60Å 185.75Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	43.94 – 3.29 43.94 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.94-3.29) 99.2 (43.94-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.277 , 0.326 0.272 , 0.316	Depositor DCC
R_{free} test set	1918 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	120.0	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 198.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12448	wwPDB-VP
Average B, all atoms (Å^2)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

5.1 Standard geometry

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	0.51	0/959	0.78	0/1290
1	D	0.52	0/1122	0.81	0/1511
1	G	0.48	0/894	0.76	0/1204
1	J	0.49	0/1114	0.81	0/1500
2	B	0.50	0/1137	0.86	0/1559
2	E	0.52	0/1115	0.88	0/1530
2	H	0.46	0/1066	0.81	0/1460
2	K	0.48	0/1078	0.82	0/1473
3	C	0.50	0/1052	0.86	0/1434
3	F	0.51	0/1053	0.90	1/1440 (0.1%)
3	I	0.47	0/1044	0.84	0/1427
3	L	0.47	0/1033	0.82	0/1407
All	All	0.49	0/12667	0.83	1/17235 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	40	PRO	N-CA-CB	-5.09	97.90	103.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	53	ARG	Sidechain

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	946	0	940	5	0
1	D	1105	0	1085	10	0
1	G	883	0	849	4	0
1	J	1097	0	1073	7	0
2	B	1113	0	916	7	0
2	E	1094	0	896	9	0
2	H	1046	0	837	9	0
2	K	1056	0	903	11	0
3	C	1034	0	896	5	0
3	F	1034	0	873	10	0
3	I	1026	0	872	8	0
3	L	1014	0	909	6	0
All	All	12448	0	11049	70	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 3.

The worst 5 of 70 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)
2:B:123:PHE:HA	2:H:15:GLY:HA3	1.09	1.08
2:B:123:PHE:HA	2:H:15:GLY:CA	1.92	0.99
2:B:123:PHE:CA	2:H:15:GLY:HA3	2.03	0.80
2:B:6:GLN:HE21	2:B:111:THR:HG22	1.57	0.69
2:B:6:GLN:NE2	2:B:111:THR:HG22	2.07	0.69

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	124/153 (81%)	122 (98%)	2 (2%)	0	100	100
1	D	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	G	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
1	J	150/153 (98%)	145 (97%)	5 (3%)	0	100	100
2	B	157/169 (93%)	151 (96%)	6 (4%)	0	100	100
2	E	158/169 (94%)	153 (97%)	5 (3%)	0	100	100
2	H	146/169 (86%)	141 (97%)	5 (3%)	0	100	100
2	K	145/169 (86%)	142 (98%)	3 (2%)	0	100	100
3	C	142/159 (89%)	139 (98%)	3 (2%)	0	100	100
3	F	146/159 (92%)	141 (97%)	4 (3%)	1 (1%)	18	49
3	I	145/159 (91%)	142 (98%)	3 (2%)	0	100	100
3	L	138/159 (87%)	135 (98%)	3 (2%)	0	100	100
All	All	1721/1924 (89%)	1674 (97%)	46 (3%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	40	PRO

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	102/119 (86%)	101 (99%)	1 (1%)	68	76
1	D	117/119 (98%)	115 (98%)	2 (2%)	53	71
1	G	91/119 (76%)	89 (98%)	2 (2%)	45	66
1	J	117/119 (98%)	114 (97%)	3 (3%)	40	64
2	B	94/146 (64%)	91 (97%)	3 (3%)	34	60
2	E	90/146 (62%)	87 (97%)	3 (3%)	33	59
2	H	84/146 (58%)	83 (99%)	1 (1%)	63	75
2	K	95/146 (65%)	95 (100%)	0	100	100
3	C	94/142 (66%)	93 (99%)	1 (1%)	65	76
3	F	91/142 (64%)	90 (99%)	1 (1%)	65	76
3	I	91/142 (64%)	91 (100%)	0	100	100
3	L	95/142 (67%)	95 (100%)	0	100	100
All	All	1161/1628 (71%)	1144 (98%)	17 (2%)	57	72

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	1	MET
1	J	134	SER
2	E	63	LYS
2	E	96	CYS
2	E	117	SER

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

Mol	Chain	Res	Type
1	A	53	ASN
3	C	37	GLN
3	L	37	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	130/153 (84%)	-0.35	0 100 100	105, 148, 212, 273	0
1	D	153/153 (100%)	-0.36	0 100 100	100, 142, 189, 224	0
1	G	125/153 (81%)	-0.51	0 100 100	144, 201, 240, 286	0
1	J	152/153 (99%)	-0.47	0 100 100	141, 179, 230, 264	0
2	B	161/169 (95%)	0.00	8 (4%) 34 23	44, 155, 241, 272	0
2	E	162/169 (95%)	-0.30	3 (1%) 66 48	108, 161, 212, 257	0
2	H	154/169 (91%)	-0.24	0 100 100	151, 223, 272, 320	0
2	K	149/169 (88%)	-0.48	1 (0%) 84 70	117, 163, 229, 254	0
3	C	148/159 (93%)	-0.29	2 (1%) 73 55	103, 160, 239, 280	0
3	F	150/159 (94%)	-0.40	1 (0%) 84 70	107, 162, 231, 278	0
3	I	149/159 (93%)	-0.38	0 100 100	140, 198, 261, 296	0
3	L	142/159 (89%)	-0.46	0 100 100	98, 168, 212, 232	0
All	All	1775/1924 (92%)	-0.35	15 (0%) 82 68	44, 171, 246, 320	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	104	MET	4.9
2	B	97	GLY	4.8
2	B	96	CYS	4.0
2	E	107	TRP	3.1
2	B	81	LEU	2.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.