



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2017 – 02:36 AM EST

PDB ID : 5K02
Title : Structure of human SOD1 with T2D mutation
Authors : Fay, J.M.; Zhu, C.; Cui, W.; Ke, H.; Dokholyan, N.V.
Deposited on : unknown
Resolution : 1.99 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

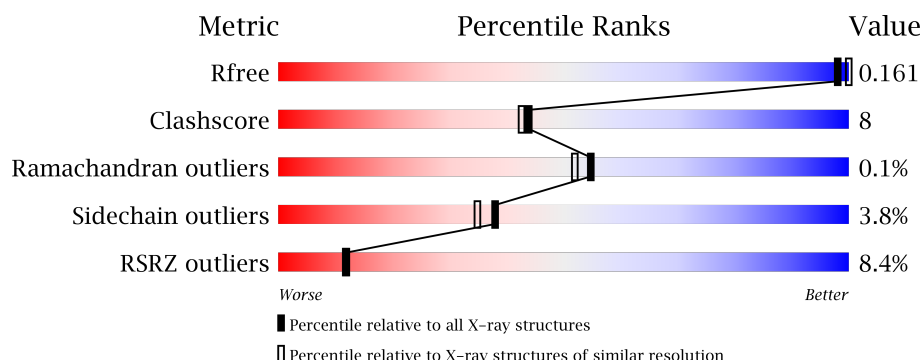
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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.

Mol	Chain	Length	Quality of chain
1	A	153	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>23%</div> <div>.</div> </div> </div>
1	B	153	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
1	C	153	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>
1	D	153	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	E	153	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>21%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	153	
1	G	153	
1	H	153	
1	I	153	
1	J	153	
1	K	153	
1	L	153	
1	M	153	
1	N	153	
1	O	153	
1	P	153	
1	Q	153	
1	R	153	
1	S	153	
1	T	153	
1	U	153	
1	V	153	
1	W	153	
1	X	153	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27396 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	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	B	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	C	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	D	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	E	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	F	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	G	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	H	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	I	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	J	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	K	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	L	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	M	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	N	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	O	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			
1	P	153	Total	C	N	O	S	0	0	0
			1111	679	203	225	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0
1	R	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0
1	S	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0
1	T	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0
1	U	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0
1	V	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0
1	W	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0
1	X	153	Total 1111	C 679	N 203	O 225	S 4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	THR	engineered mutation	UNP P00441
B	2	ASP	THR	engineered mutation	UNP P00441
C	2	ASP	THR	engineered mutation	UNP P00441
D	2	ASP	THR	engineered mutation	UNP P00441
E	2	ASP	THR	engineered mutation	UNP P00441
F	2	ASP	THR	engineered mutation	UNP P00441
G	2	ASP	THR	engineered mutation	UNP P00441
H	2	ASP	THR	engineered mutation	UNP P00441
I	2	ASP	THR	engineered mutation	UNP P00441
J	2	ASP	THR	engineered mutation	UNP P00441
K	2	ASP	THR	engineered mutation	UNP P00441
L	2	ASP	THR	engineered mutation	UNP P00441
M	2	ASP	THR	engineered mutation	UNP P00441
N	2	ASP	THR	engineered mutation	UNP P00441
O	2	ASP	THR	engineered mutation	UNP P00441
P	2	ASP	THR	engineered mutation	UNP P00441
Q	2	ASP	THR	engineered mutation	UNP P00441
R	2	ASP	THR	engineered mutation	UNP P00441
S	2	ASP	THR	engineered mutation	UNP P00441
T	2	ASP	THR	engineered mutation	UNP P00441
U	2	ASP	THR	engineered mutation	UNP P00441
V	2	ASP	THR	engineered mutation	UNP P00441
W	2	ASP	THR	engineered mutation	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
X	2	ASP	THR	engineered mutation	UNP P00441

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	W	1	Total Cu 1 1	0	0
2	N	1	Total Cu 1 1	0	0
2	X	1	Total Cu 1 1	0	0
2	S	1	Total Cu 1 1	0	0
2	J	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	V	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0
2	R	1	Total Cu 1 1	0	0
2	M	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	U	1	Total Cu 1 1	0	0
2	L	1	Total Cu 1 1	0	0
2	G	1	Total Cu 1 1	0	0
2	Q	1	Total Cu 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total 1	Cu 1	0	0
2	C	1	Total 1	Cu 1	0	0
2	T	1	Total 1	Cu 1	0	0
2	O	1	Total 1	Cu 1	0	0
2	F	1	Total 1	Cu 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	W	1	Total 1	Zn 1	0	0
3	N	1	Total 1	Zn 1	0	0
3	X	1	Total 1	Zn 1	0	0
3	S	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	V	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	R	1	Total 1	Zn 1	0	0
3	M	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total 1	Zn 1	0	0
3	U	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	Q	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	T	1	Total 1	Zn 1	0	0
3	O	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	B	26	Total 26	O 26	0	0
4	C	32	Total 32	O 32	0	0
4	D	39	Total 39	O 39	0	0
4	E	25	Total 25	O 25	0	0
4	F	26	Total 26	O 26	0	0
4	G	42	Total 42	O 42	0	0
4	H	20	Total 20	O 20	0	0
4	I	27	Total 27	O 27	0	0

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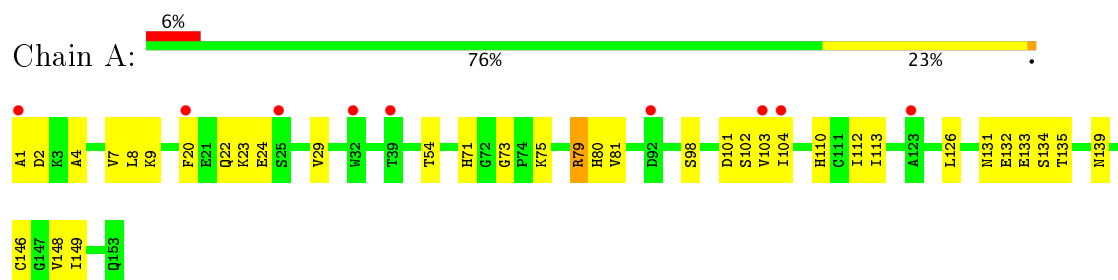
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	26	Total 26	O 26	0	0
4	K	20	Total 20	O 20	0	0
4	L	30	Total 30	O 30	0	0
4	M	34	Total 34	O 34	0	0
4	N	35	Total 35	O 35	0	0
4	O	22	Total 22	O 22	0	0
4	P	31	Total 31	O 31	0	0
4	Q	26	Total 26	O 26	0	0
4	R	20	Total 20	O 20	0	0
4	S	31	Total 31	O 31	0	0
4	T	29	Total 29	O 29	0	0
4	U	29	Total 29	O 29	0	0
4	V	31	Total 31	O 31	0	0
4	W	28	Total 28	O 28	0	0
4	X	19	Total 19	O 19	0	0

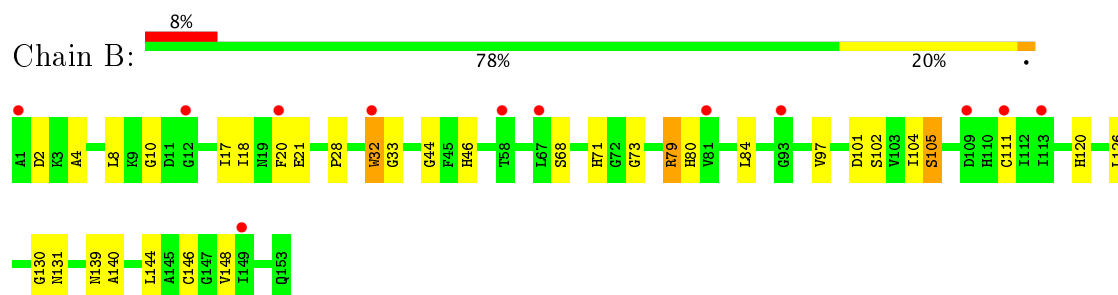
3 Residue-property plots [i](#)

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 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.

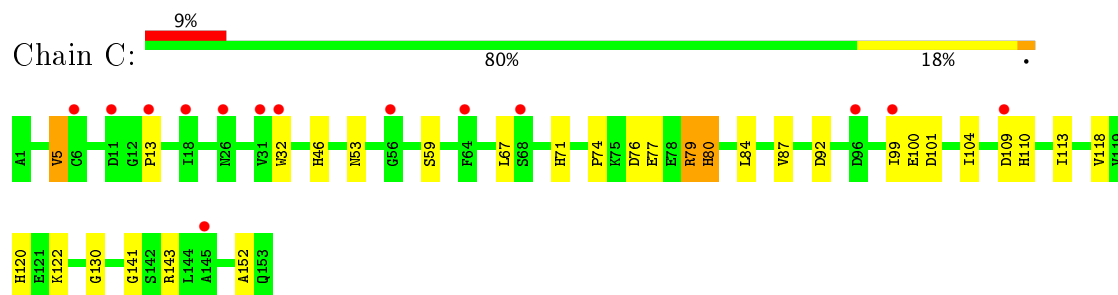
- Molecule 1: Superoxide dismutase [Cu-Zn]



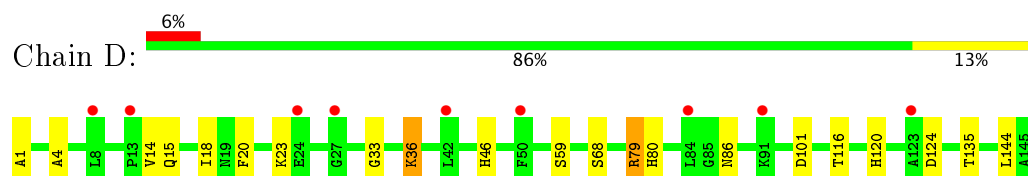
- Molecule 1: Superoxide dismutase [Cu-Zn]



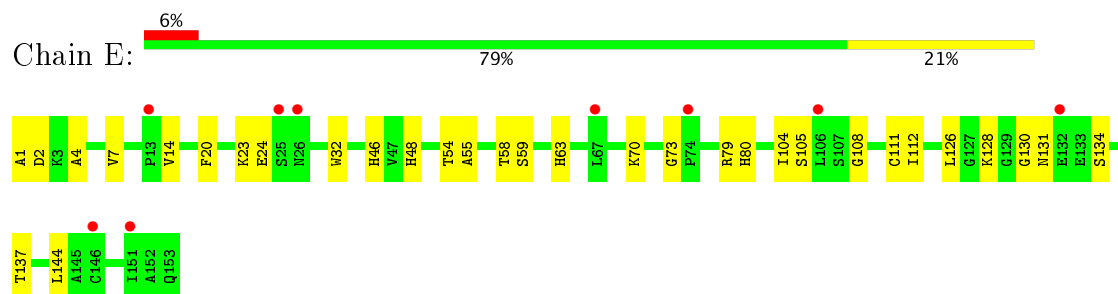
- Molecule 1: Superoxide dismutase [Cu-Zn]



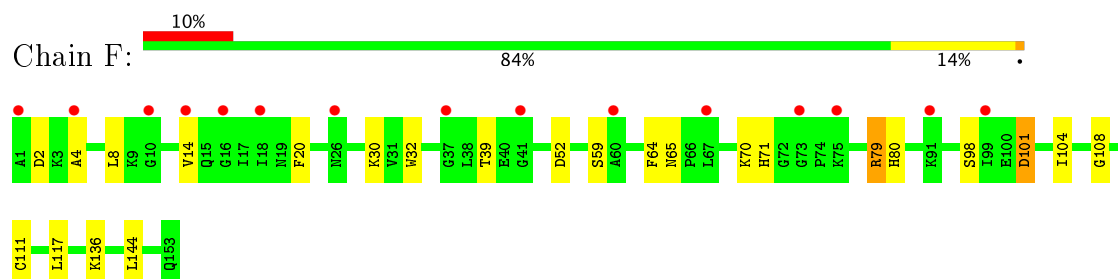
- Molecule 1: Superoxide dismutase [Cu-Zn]



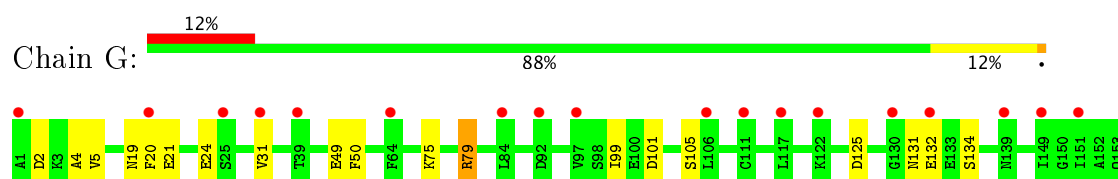
- Molecule 1: Superoxide dismutase [Cu-Zn]



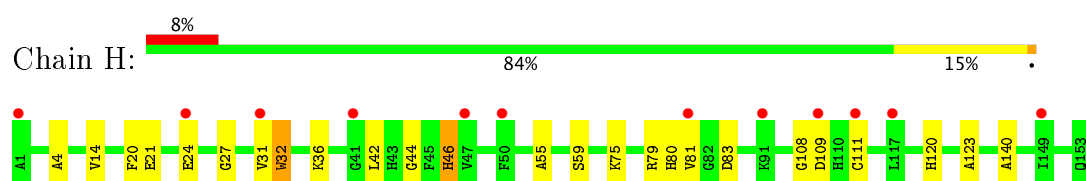
- Molecule 1: Superoxide dismutase [Cu-Zn]



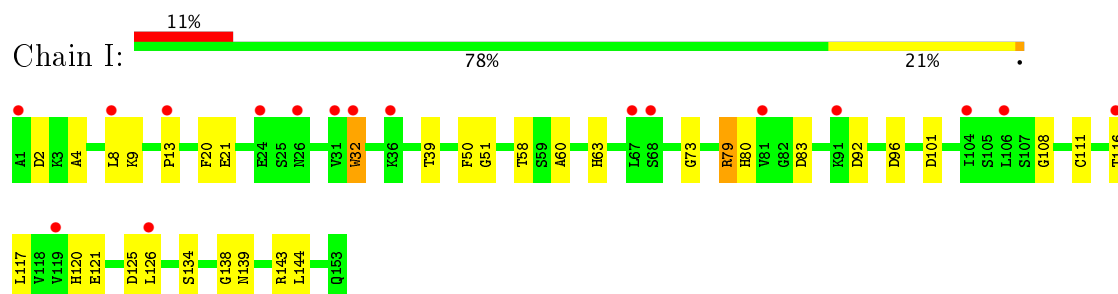
- Molecule 1: Superoxide dismutase [Cu-Zn]



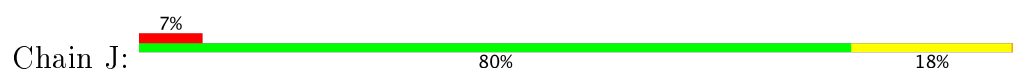
- Molecule 1: Superoxide dismutase [Cu-Zn]

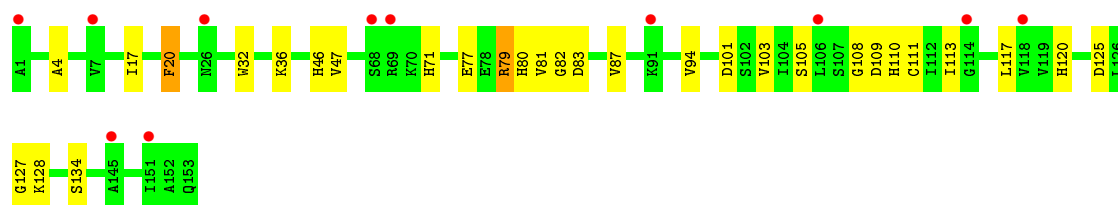


- Molecule 1: Superoxide dismutase [Cu-Zn]

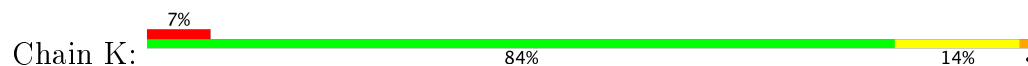


- Molecule 1: Superoxide dismutase [Cu-Zn]

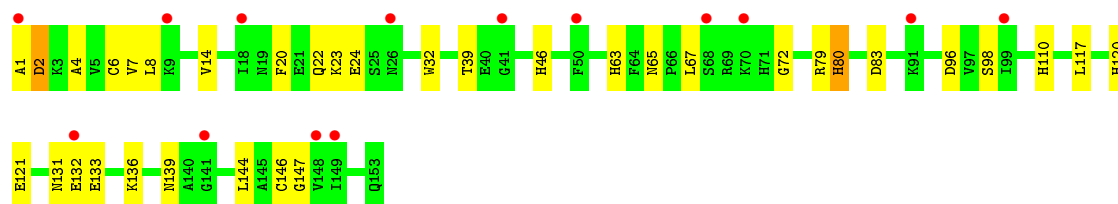
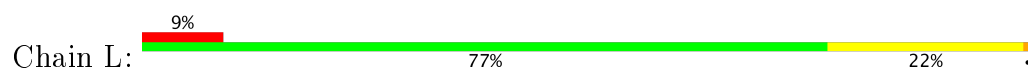




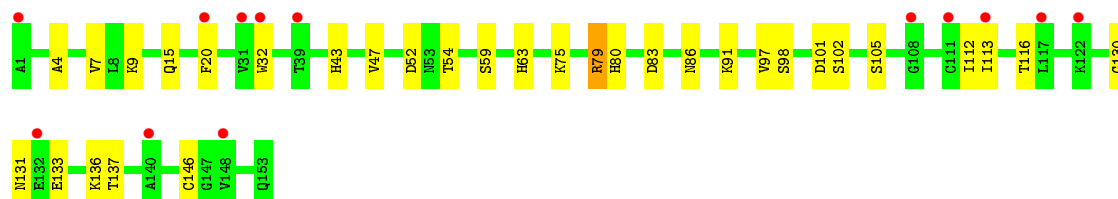
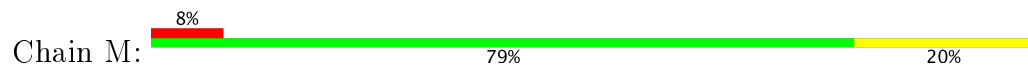
- Molecule 1: Superoxide dismutase [Cu-Zn]



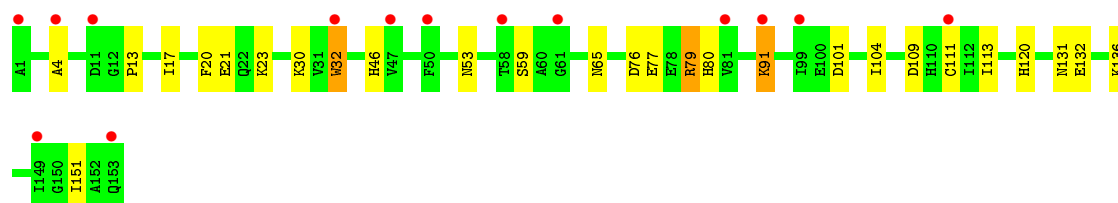
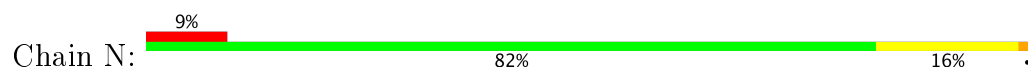
- Molecule 1: Superoxide dismutase [Cu-Zn]



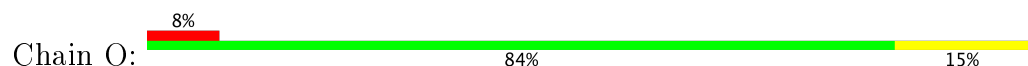
- Molecule 1: Superoxide dismutase [Cu-Zn]

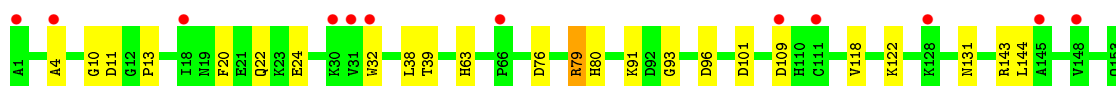


- Molecule 1: Superoxide dismutase [Cu-Zn]

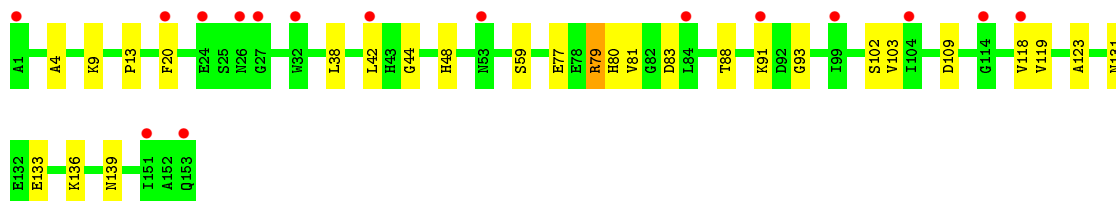
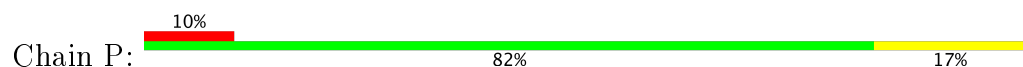


- Molecule 1: Superoxide dismutase [Cu-Zn]

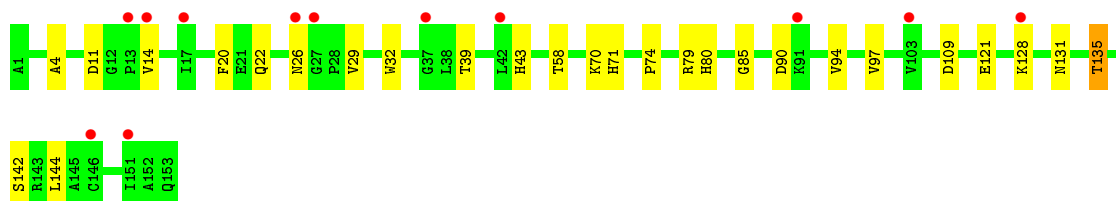
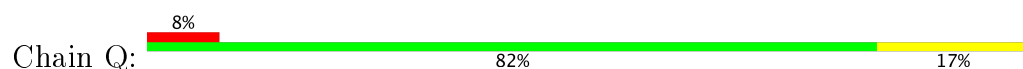




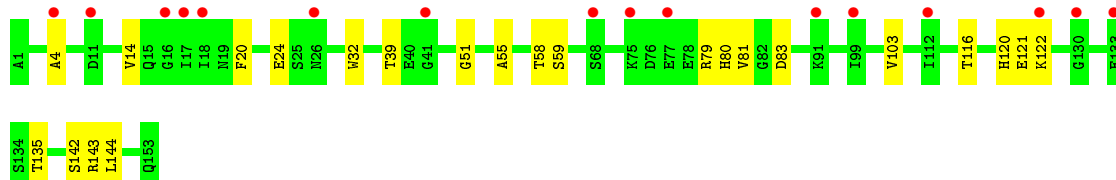
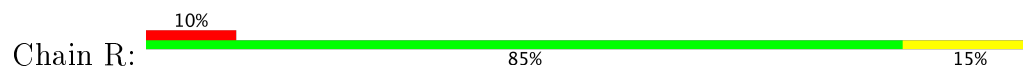
- Molecule 1: Superoxide dismutase [Cu-Zn]



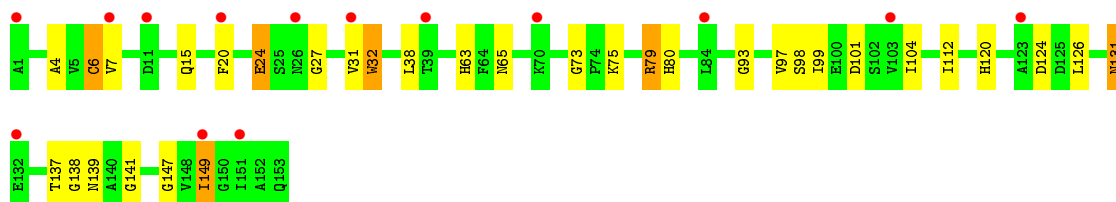
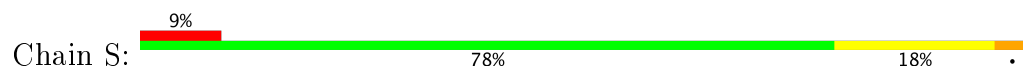
- Molecule 1: Superoxide dismutase [Cu-Zn]



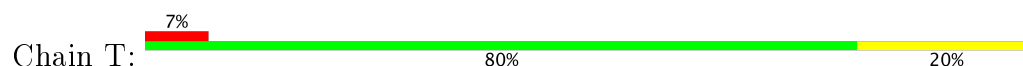
- Molecule 1: Superoxide dismutase [Cu-Zn]

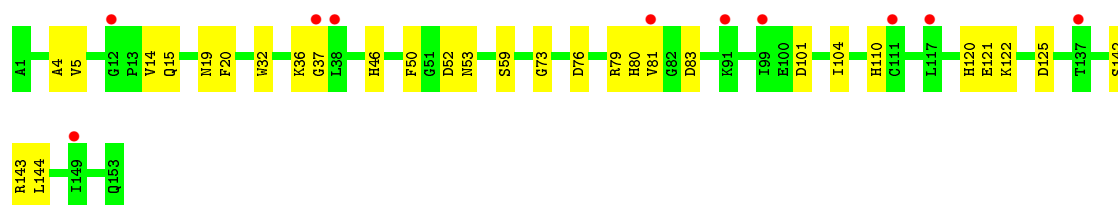


- Molecule 1: Superoxide dismutase [Cu-Zn]

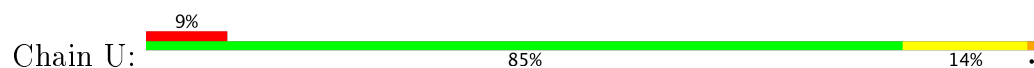


- Molecule 1: Superoxide dismutase [Cu-Zn]

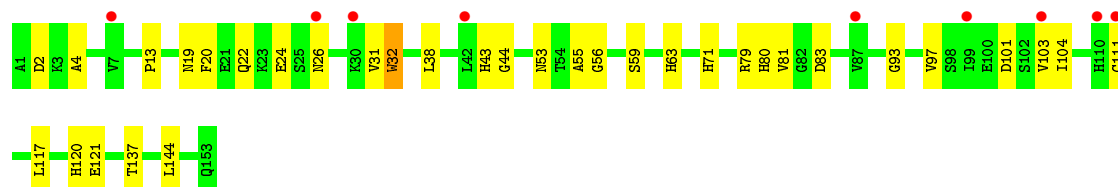
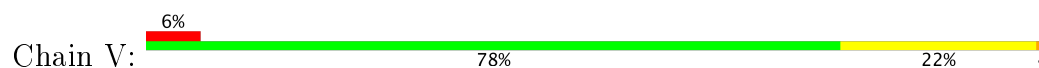




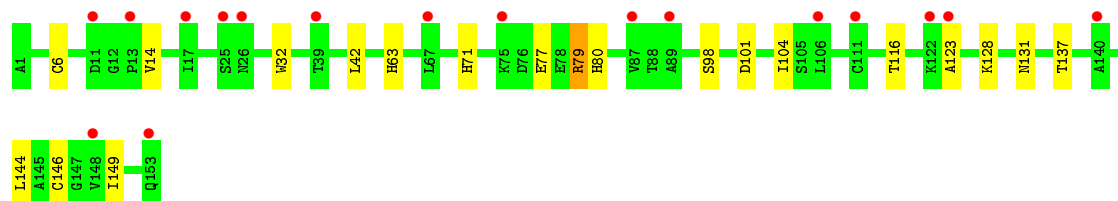
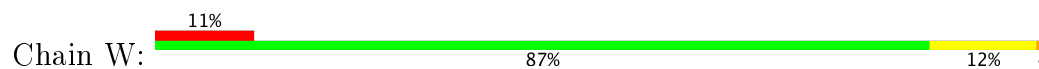
- Molecule 1: Superoxide dismutase [Cu-Zn]



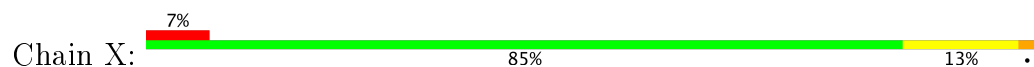
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	111.98Å 111.96Å 149.88Å 89.86° 89.85° 60.13°	Depositor
Resolution (Å)	149.92 – 1.99 37.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	80.4 (149.92-1.99) 81.0 (37.33-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.146 , 0.162 0.145 , 0.161	Depositor DCC
R_{free} test set	17442 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.427 for h-k,h,l 0.427 for k,-h+k,l 0.426 for -k,h-k,l 0.426 for -h+k,-h,l 0.427 for -h+k,k,-l 0.467 for h,h-k,-l 0.469 for -h,-k,l 0.428 for k,h,-l 0.430 for -k,-h,-l 0.427 for h-k,-k,-l 0.459 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	27396	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0.46	0/1129	0.60	0/1521
1	B	0.46	1/1129 (0.1%)	0.61	0/1521
1	C	0.48	1/1129 (0.1%)	0.59	0/1521
1	D	0.46	0/1129	0.59	0/1521
1	E	0.46	1/1129 (0.1%)	0.54	0/1521
1	F	0.45	1/1129 (0.1%)	0.55	0/1521
1	G	0.44	0/1129	0.53	0/1521
1	H	0.46	1/1129 (0.1%)	0.54	0/1521
1	I	0.46	1/1129 (0.1%)	0.56	0/1521
1	J	0.46	1/1129 (0.1%)	0.57	0/1521
1	K	0.46	0/1129	0.56	0/1521
1	L	0.47	1/1129 (0.1%)	0.60	0/1521
1	M	0.48	0/1129	0.59	0/1521
1	N	0.46	1/1129 (0.1%)	0.57	0/1521
1	O	0.47	1/1129 (0.1%)	0.56	0/1521
1	P	0.46	0/1129	0.54	0/1521
1	Q	0.46	0/1129	0.57	0/1521
1	R	0.46	1/1129 (0.1%)	0.57	0/1521
1	S	0.47	1/1129 (0.1%)	0.56	0/1521
1	T	0.46	1/1129 (0.1%)	0.56	0/1521
1	U	0.47	0/1129	0.59	0/1521
1	V	0.48	1/1129 (0.1%)	0.59	0/1521
1	W	0.46	1/1129 (0.1%)	0.57	0/1521
1	X	0.46	0/1129	0.56	0/1521
All	All	0.46	15/27096 (0.1%)	0.57	0/36504

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	32	TRP	CD2-CE2	5.41	1.47	1.41
1	B	32	TRP	CD2-CE2	5.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	32	TRP	CD2-CE2	5.14	1.47	1.41
1	I	32	TRP	CD2-CE2	5.13	1.47	1.41
1	R	32	TRP	CD2-CE2	5.12	1.47	1.41

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	1111	0	1074	26	0
1	B	1111	0	1074	24	0
1	C	1111	0	1073	19	0
1	D	1111	0	1074	13	0
1	E	1111	0	1074	18	0
1	F	1111	0	1074	16	0
1	G	1111	0	1074	14	0
1	H	1111	0	1074	18	0
1	I	1111	0	1074	21	0
1	J	1111	0	1074	19	0
1	K	1111	0	1074	17	0
1	L	1111	0	1074	20	0
1	M	1111	0	1074	22	0
1	N	1111	0	1074	21	0
1	O	1111	0	1074	12	0
1	P	1111	0	1074	17	0
1	Q	1111	0	1074	18	0
1	R	1111	0	1074	13	0
1	S	1111	0	1074	21	0
1	T	1111	0	1074	21	0
1	U	1111	0	1074	13	0
1	V	1111	0	1074	20	0
1	W	1111	0	1074	13	0
1	X	1111	0	1073	18	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	36	0	0	3	0
4	B	26	0	0	3	0
4	C	32	0	0	0	0
4	D	39	0	0	0	0
4	E	25	0	0	1	0
4	F	26	0	0	1	0
4	G	42	0	0	1	0
4	H	20	0	0	1	0
4	I	27	0	0	0	0
4	J	26	0	0	1	0
4	K	20	0	0	0	0
4	L	30	0	0	3	0
4	M	34	0	0	1	0
4	N	35	0	0	4	0
4	O	22	0	0	0	0
4	P	31	0	0	2	0
4	Q	26	0	0	1	0
4	R	20	0	0	0	0
4	S	31	0	0	0	0
4	T	29	0	0	1	0
4	U	29	0	0	0	0
4	V	31	0	0	0	0
4	W	28	0	0	0	0
4	X	19	0	0	1	0
All	All	27396	0	25774	401	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 8.

The worst 5 of 401 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:X:8:LEU:HD21	1:X:117:LEU:HD23	1.37	1.07
1:A:29:VAL:HG13	4:A:303:HOH:O	1.53	1.07
1:X:131:ASN:HD21	1:X:139:ASN:HD21	1.09	0.98
1:A:75:LYS:HG3	1:K:128:LYS:HA	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:CYS:HA	4:B:301:HOH:O	1.75	0.86

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	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	B	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	C	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	D	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	E	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
1	F	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	G	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	H	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
1	I	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
1	J	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	K	151/153 (99%)	146 (97%)	4 (3%)	1 (1%)	25	18
1	L	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	M	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	N	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
1	O	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	P	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	Q	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
1	R	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
1	S	151/153 (99%)	146 (97%)	4 (3%)	1 (1%)	25	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
1	U	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
1	V	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	W	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	X	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
All	All	3624/3672 (99%)	3479 (96%)	143 (4%)	2 (0%)	55	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	140	ALA
1	S	149	ILE

5.3.2 Protein sidechains ⓘ

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	118/118 (100%)	111 (94%)	7 (6%)	23	17
1	B	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	C	118/118 (100%)	109 (92%)	9 (8%)	15	10
1	D	118/118 (100%)	113 (96%)	5 (4%)	34	30
1	E	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	F	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	G	118/118 (100%)	115 (98%)	3 (2%)	53	54
1	H	118/118 (100%)	117 (99%)	1 (1%)	85	88
1	I	118/118 (100%)	113 (96%)	5 (4%)	34	30
1	J	118/118 (100%)	111 (94%)	7 (6%)	23	17
1	K	118/118 (100%)	113 (96%)	5 (4%)	34	30
1	L	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	M	118/118 (100%)	113 (96%)	5 (4%)	34	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	O	118/118 (100%)	112 (95%)	6 (5%)	28	22
1	P	118/118 (100%)	111 (94%)	7 (6%)	23	17
1	Q	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	R	118/118 (100%)	115 (98%)	3 (2%)	53	54
1	S	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	T	118/118 (100%)	117 (99%)	1 (1%)	85	88
1	U	118/118 (100%)	114 (97%)	4 (3%)	42	40
1	V	118/118 (100%)	115 (98%)	3 (2%)	53	54
1	W	118/118 (100%)	116 (98%)	2 (2%)	66	70
1	X	118/118 (100%)	112 (95%)	6 (5%)	28	22
All	All	2832/2832 (100%)	2725 (96%)	107 (4%)	38	35

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	113	ILE
1	M	79	ARG
1	V	111	CYS
1	K	15	GLN
1	L	2	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	110	HIS
1	Q	19	ASN
1	V	53	ASN
1	O	19	ASN
1	Q	53	ASN

5.3.3 RNA ⓘ

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 48 ligands modelled in this entry, 48 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 ⓘ

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, 95th 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	153/153 (100%)	0.76	9 (5%)	23 23	23, 32, 43, 46	0
1	B	153/153 (100%)	0.91	12 (7%)	14 14	24, 36, 47, 52	0
1	C	153/153 (100%)	0.97	14 (9%)	10 10	24, 36, 48, 58	0
1	D	153/153 (100%)	0.87	9 (5%)	23 23	24, 33, 44, 49	0
1	E	153/153 (100%)	0.96	9 (5%)	23 23	28, 37, 46, 55	0
1	F	153/153 (100%)	1.00	15 (9%)	8 8	27, 37, 47, 56	0
1	G	153/153 (100%)	1.00	18 (11%)	5 5	26, 36, 45, 52	0
1	H	153/153 (100%)	0.96	12 (7%)	14 14	25, 36, 47, 54	0
1	I	153/153 (100%)	1.11	17 (11%)	6 6	25, 37, 49, 54	0
1	J	153/153 (100%)	0.86	11 (7%)	16 16	25, 34, 44, 58	0
1	K	153/153 (100%)	0.88	10 (6%)	20 20	25, 36, 47, 53	0
1	L	153/153 (100%)	0.92	14 (9%)	10 10	27, 36, 44, 48	0
1	M	153/153 (100%)	0.90	13 (8%)	11 11	22, 32, 43, 49	0
1	N	153/153 (100%)	0.99	14 (9%)	10 10	24, 35, 49, 58	0
1	O	153/153 (100%)	0.95	12 (7%)	14 14	27, 36, 46, 54	0
1	P	153/153 (100%)	0.99	16 (10%)	7 7	26, 35, 46, 53	0
1	Q	153/153 (100%)	1.02	12 (7%)	14 14	26, 36, 43, 47	0
1	R	153/153 (100%)	1.01	16 (10%)	7 7	25, 37, 46, 53	0
1	S	153/153 (100%)	0.88	14 (9%)	10 10	24, 34, 43, 49	0
1	T	153/153 (100%)	0.89	10 (6%)	20 20	26, 36, 50, 55	0
1	U	153/153 (100%)	1.00	14 (9%)	10 10	25, 35, 47, 51	0
1	V	153/153 (100%)	0.81	9 (5%)	23 23	24, 32, 42, 46	0
1	W	153/153 (100%)	1.03	17 (11%)	6 6	28, 37, 49, 57	0
1	X	153/153 (100%)	1.04	11 (7%)	16 16	26, 37, 47, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3672/3672 (100%)	0.95	308 (8%) 12 12	22, 35, 46, 58	0

The worst 5 of 308 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	13	PRO	5.6
1	N	1	ALA	5.1
1	I	1	ALA	5.1
1	N	81	VAL	4.6
1	J	26	ASN	4.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	V	202	1/1	0.99	0.12	-0.56	37,37,37,37	0
3	ZN	P	202	1/1	0.95	0.11	-0.97	31,31,31,31	0
3	ZN	K	202	1/1	0.98	0.11	-1.04	37,37,37,37	0
3	ZN	Q	202	1/1	0.99	0.10	-1.07	33,33,33,33	0
3	ZN	J	202	1/1	0.95	0.11	-1.24	32,32,32,32	0
3	ZN	M	202	1/1	0.94	0.09	-1.52	33,33,33,33	0
3	ZN	R	202	1/1	0.98	0.07	-1.54	32,32,32,32	0
3	ZN	O	202	1/1	0.97	0.11	-1.60	38,38,38,38	0
3	ZN	H	202	1/1	0.98	0.09	-1.78	36,36,36,36	0
3	ZN	E	202	1/1	0.94	0.06	-1.85	33,33,33,33	0
3	ZN	B	202	1/1	0.99	0.08	-1.86	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	W	202	1/1	0.96	0.09	-1.96	37,37,37,37	0
3	ZN	F	202	1/1	0.99	0.07	-2.02	31,31,31,31	0
3	ZN	N	202	1/1	0.96	0.08	-2.19	31,31,31,31	0
3	ZN	I	202	1/1	0.93	0.09	-2.44	32,32,32,32	0
3	ZN	D	202	1/1	0.98	0.07	-2.46	28,28,28,28	0
3	ZN	L	202	1/1	0.94	0.05	-2.53	32,32,32,32	0
2	CU	B	201	1/1	0.95	0.08	-3.00	38,38,38,38	0
3	ZN	U	202	1/1	0.99	0.10	-3.05	31,31,31,31	0
3	ZN	G	202	1/1	0.99	0.07	-3.13	32,32,32,32	0
2	CU	J	201	1/1	0.94	0.10	-3.18	36,36,36,36	0
3	ZN	S	202	1/1	0.98	0.08	-3.21	31,31,31,31	0
2	CU	A	201	1/1	0.98	0.10	-3.34	38,38,38,38	0
3	ZN	A	202	1/1	0.95	0.08	-3.37	30,30,30,30	0
3	ZN	T	202	1/1	0.99	0.07	-3.59	36,36,36,36	0
2	CU	F	201	1/1	0.99	0.06	-3.69	35,35,35,35	0
3	ZN	X	202	1/1	0.97	0.05	-3.80	36,36,36,36	0
2	CU	K	201	1/1	0.97	0.05	-3.92	34,34,34,34	0
3	ZN	C	202	1/1	0.97	0.11	-3.95	26,26,26,26	0
2	CU	E	201	1/1	0.94	0.07	-6.40	33,33,33,33	0
2	CU	C	201	1/1	0.98	0.03	-6.50	35,35,35,35	0
2	CU	X	201	1/1	0.98	0.04	-8.09	35,35,35,35	0
2	CU	P	201	1/1	0.96	0.07	-	33,33,33,33	0
2	CU	U	201	1/1	0.99	0.04	-	32,32,32,32	0
2	CU	V	201	1/1	0.99	0.13	-	31,31,31,31	0
2	CU	I	201	1/1	0.98	0.12	-	44,44,44,44	0
2	CU	O	201	1/1	0.97	0.07	-	35,35,35,35	0
2	CU	M	201	1/1	0.98	0.09	-	34,34,34,34	0
2	CU	R	201	1/1	0.99	0.10	-	37,37,37,37	0
2	CU	N	201	1/1	0.93	0.11	-	40,40,40,40	0
2	CU	L	201	1/1	0.98	0.05	-	31,31,31,31	0
2	CU	S	201	1/1	0.99	0.10	-	30,30,30,30	0
2	CU	H	201	1/1	0.94	0.08	-	33,33,33,33	0
2	CU	G	201	1/1	0.98	0.10	-	37,37,37,37	0
2	CU	D	201	1/1	0.96	0.11	-	36,36,36,36	0
2	CU	W	201	1/1	0.96	0.10	-	39,39,39,39	0
2	CU	T	201	1/1	0.97	0.10	-	35,35,35,35	0
2	CU	Q	201	1/1	0.97	0.06	-	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.