



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:47 AM UTC

PDB ID : 1P7G / pdb_00001p7g
Title : Crystal structure of superoxide dismutase from *Pyrobaculum aerophilum*
Authors : Lee, S.; Sawaya, M.R.; Eisenberg, D.
Deposited on : 2003-05-01
Resolution : 1.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

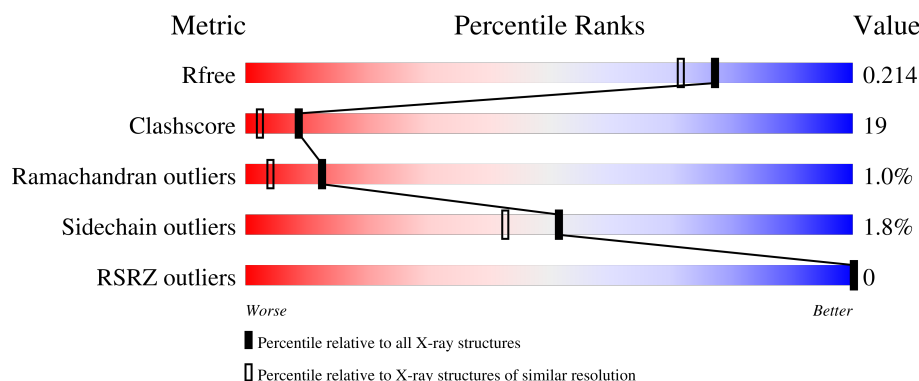
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



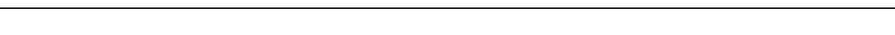
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	222	 64% 27% • 5%
1	B	222	 63% 31% • 5%
1	C	222	 70% 24% • 5%
1	D	222	 64% 28% • 5%
1	E	222	 50% 42% • 5%

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Mol	Chain	Length	Quality of chain
1	F	222	
1	G	222	
1	H	222	
1	I	222	
1	J	222	
1	K	222	
1	L	222	
1	M	222	
1	N	222	
1	O	222	
1	P	222	
1	Q	222	
1	R	222	
1	S	222	
1	T	222	
1	U	222	
1	V	222	
1	W	222	
1	X	222	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	M	313	-	-	X	-
2	ACT	P	316	-	-	X	-
3	BME	B	402	-	X	-	-
3	BME	D	404	-	X	-	-
3	BME	F	406	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BME	H	408	-	X	X	-
3	BME	K	412	-	X	X	-
3	BME	N	414	-	X	-	-
3	BME	P	416	-	X	X	-
3	BME	Q	418	-	X	X	-
3	BME	V	422	-	X	X	-
3	BME	X	424	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43787 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	B	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	C	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	D	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	E	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	F	211	Total	C	N	O	Se	4	0	0
			1714	1109	298	304	3			
1	G	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	H	210	Total	C	N	O	Se	0	0	0
			1705	1103	297	302	3			
1	I	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	J	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	K	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	L	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	M	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	N	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	O	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	P	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	R	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	S	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	T	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	U	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	V	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	W	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			
1	X	211	Total	C	N	O	Se	0	0	0
			1714	1109	298	304	3			

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP O93724
A	2	ARG	-	cloning artifact	UNP O93724
A	3	GLY	-	cloning artifact	UNP O93724
A	4	SER	-	cloning artifact	UNP O93724
A	5	HIS	-	cloning artifact	UNP O93724
A	6	HIS	-	cloning artifact	UNP O93724
A	7	HIS	-	cloning artifact	UNP O93724
A	8	HIS	-	cloning artifact	UNP O93724
A	9	HIS	-	cloning artifact	UNP O93724
A	10	HIS	-	cloning artifact	UNP O93724
A	11	GLY	-	cloning artifact	UNP O93724
A	12	SER	-	cloning artifact	UNP O93724
A	39	MSE	MET	modified residue	UNP O93724
A	97	MSE	MET	modified residue	UNP O93724
A	164	MSE	MET	modified residue	UNP O93724
B	1	MET	-	cloning artifact	UNP O93724
B	2	ARG	-	cloning artifact	UNP O93724
B	3	GLY	-	cloning artifact	UNP O93724
B	4	SER	-	cloning artifact	UNP O93724
B	5	HIS	-	cloning artifact	UNP O93724
B	6	HIS	-	cloning artifact	UNP O93724
B	7	HIS	-	cloning artifact	UNP O93724
B	8	HIS	-	cloning artifact	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	cloning artifact	UNP O93724
B	10	HIS	-	cloning artifact	UNP O93724
B	11	GLY	-	cloning artifact	UNP O93724
B	12	SER	-	cloning artifact	UNP O93724
B	39	MSE	MET	modified residue	UNP O93724
B	97	MSE	MET	modified residue	UNP O93724
B	164	MSE	MET	modified residue	UNP O93724
C	1	MET	-	cloning artifact	UNP O93724
C	2	ARG	-	cloning artifact	UNP O93724
C	3	GLY	-	cloning artifact	UNP O93724
C	4	SER	-	cloning artifact	UNP O93724
C	5	HIS	-	cloning artifact	UNP O93724
C	6	HIS	-	cloning artifact	UNP O93724
C	7	HIS	-	cloning artifact	UNP O93724
C	8	HIS	-	cloning artifact	UNP O93724
C	9	HIS	-	cloning artifact	UNP O93724
C	10	HIS	-	cloning artifact	UNP O93724
C	11	GLY	-	cloning artifact	UNP O93724
C	12	SER	-	cloning artifact	UNP O93724
C	39	MSE	MET	modified residue	UNP O93724
C	97	MSE	MET	modified residue	UNP O93724
C	164	MSE	MET	modified residue	UNP O93724
D	1	MET	-	cloning artifact	UNP O93724
D	2	ARG	-	cloning artifact	UNP O93724
D	3	GLY	-	cloning artifact	UNP O93724
D	4	SER	-	cloning artifact	UNP O93724
D	5	HIS	-	cloning artifact	UNP O93724
D	6	HIS	-	cloning artifact	UNP O93724
D	7	HIS	-	cloning artifact	UNP O93724
D	8	HIS	-	cloning artifact	UNP O93724
D	9	HIS	-	cloning artifact	UNP O93724
D	10	HIS	-	cloning artifact	UNP O93724
D	11	GLY	-	cloning artifact	UNP O93724
D	12	SER	-	cloning artifact	UNP O93724
D	39	MSE	MET	modified residue	UNP O93724
D	97	MSE	MET	modified residue	UNP O93724
D	164	MSE	MET	modified residue	UNP O93724
E	1	MET	-	cloning artifact	UNP O93724
E	2	ARG	-	cloning artifact	UNP O93724
E	3	GLY	-	cloning artifact	UNP O93724
E	4	SER	-	cloning artifact	UNP O93724
E	5	HIS	-	cloning artifact	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	HIS	-	cloning artifact	UNP O93724
E	7	HIS	-	cloning artifact	UNP O93724
E	8	HIS	-	cloning artifact	UNP O93724
E	9	HIS	-	cloning artifact	UNP O93724
E	10	HIS	-	cloning artifact	UNP O93724
E	11	GLY	-	cloning artifact	UNP O93724
E	12	SER	-	cloning artifact	UNP O93724
E	39	MSE	MET	modified residue	UNP O93724
E	97	MSE	MET	modified residue	UNP O93724
E	164	MSE	MET	modified residue	UNP O93724
F	1	MET	-	cloning artifact	UNP O93724
F	2	ARG	-	cloning artifact	UNP O93724
F	3	GLY	-	cloning artifact	UNP O93724
F	4	SER	-	cloning artifact	UNP O93724
F	5	HIS	-	cloning artifact	UNP O93724
F	6	HIS	-	cloning artifact	UNP O93724
F	7	HIS	-	cloning artifact	UNP O93724
F	8	HIS	-	cloning artifact	UNP O93724
F	9	HIS	-	cloning artifact	UNP O93724
F	10	HIS	-	cloning artifact	UNP O93724
F	11	GLY	-	cloning artifact	UNP O93724
F	12	SER	-	cloning artifact	UNP O93724
F	39	MSE	MET	modified residue	UNP O93724
F	97	MSE	MET	modified residue	UNP O93724
F	164	MSE	MET	modified residue	UNP O93724
G	1	MET	-	cloning artifact	UNP O93724
G	2	ARG	-	cloning artifact	UNP O93724
G	3	GLY	-	cloning artifact	UNP O93724
G	4	SER	-	cloning artifact	UNP O93724
G	5	HIS	-	cloning artifact	UNP O93724
G	6	HIS	-	cloning artifact	UNP O93724
G	7	HIS	-	cloning artifact	UNP O93724
G	8	HIS	-	cloning artifact	UNP O93724
G	9	HIS	-	cloning artifact	UNP O93724
G	10	HIS	-	cloning artifact	UNP O93724
G	11	GLY	-	cloning artifact	UNP O93724
G	12	SER	-	cloning artifact	UNP O93724
G	39	MSE	MET	modified residue	UNP O93724
G	97	MSE	MET	modified residue	UNP O93724
G	164	MSE	MET	modified residue	UNP O93724
H	1	MET	-	cloning artifact	UNP O93724
H	2	ARG	-	cloning artifact	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLY	-	cloning artifact	UNP O93724
H	4	SER	-	cloning artifact	UNP O93724
H	5	HIS	-	cloning artifact	UNP O93724
H	6	HIS	-	cloning artifact	UNP O93724
H	7	HIS	-	cloning artifact	UNP O93724
H	8	HIS	-	cloning artifact	UNP O93724
H	9	HIS	-	cloning artifact	UNP O93724
H	10	HIS	-	cloning artifact	UNP O93724
H	11	GLY	-	cloning artifact	UNP O93724
H	12	SER	-	cloning artifact	UNP O93724
H	39	MSE	MET	modified residue	UNP O93724
H	97	MSE	MET	modified residue	UNP O93724
H	164	MSE	MET	modified residue	UNP O93724
I	1	MET	-	cloning artifact	UNP O93724
I	2	ARG	-	cloning artifact	UNP O93724
I	3	GLY	-	cloning artifact	UNP O93724
I	4	SER	-	cloning artifact	UNP O93724
I	5	HIS	-	cloning artifact	UNP O93724
I	6	HIS	-	cloning artifact	UNP O93724
I	7	HIS	-	cloning artifact	UNP O93724
I	8	HIS	-	cloning artifact	UNP O93724
I	9	HIS	-	cloning artifact	UNP O93724
I	10	HIS	-	cloning artifact	UNP O93724
I	11	GLY	-	cloning artifact	UNP O93724
I	12	SER	-	cloning artifact	UNP O93724
I	39	MSE	MET	modified residue	UNP O93724
I	97	MSE	MET	modified residue	UNP O93724
I	164	MSE	MET	modified residue	UNP O93724
J	1	MET	-	cloning artifact	UNP O93724
J	2	ARG	-	cloning artifact	UNP O93724
J	3	GLY	-	cloning artifact	UNP O93724
J	4	SER	-	cloning artifact	UNP O93724
J	5	HIS	-	cloning artifact	UNP O93724
J	6	HIS	-	cloning artifact	UNP O93724
J	7	HIS	-	cloning artifact	UNP O93724
J	8	HIS	-	cloning artifact	UNP O93724
J	9	HIS	-	cloning artifact	UNP O93724
J	10	HIS	-	cloning artifact	UNP O93724
J	11	GLY	-	cloning artifact	UNP O93724
J	12	SER	-	cloning artifact	UNP O93724
J	39	MSE	MET	modified residue	UNP O93724
J	97	MSE	MET	modified residue	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
J	164	MSE	MET	modified residue	UNP O93724
K	1	MET	-	cloning artifact	UNP O93724
K	2	ARG	-	cloning artifact	UNP O93724
K	3	GLY	-	cloning artifact	UNP O93724
K	4	SER	-	cloning artifact	UNP O93724
K	5	HIS	-	cloning artifact	UNP O93724
K	6	HIS	-	cloning artifact	UNP O93724
K	7	HIS	-	cloning artifact	UNP O93724
K	8	HIS	-	cloning artifact	UNP O93724
K	9	HIS	-	cloning artifact	UNP O93724
K	10	HIS	-	cloning artifact	UNP O93724
K	11	GLY	-	cloning artifact	UNP O93724
K	12	SER	-	cloning artifact	UNP O93724
K	39	MSE	MET	modified residue	UNP O93724
K	97	MSE	MET	modified residue	UNP O93724
K	164	MSE	MET	modified residue	UNP O93724
L	1	MET	-	cloning artifact	UNP O93724
L	2	ARG	-	cloning artifact	UNP O93724
L	3	GLY	-	cloning artifact	UNP O93724
L	4	SER	-	cloning artifact	UNP O93724
L	5	HIS	-	cloning artifact	UNP O93724
L	6	HIS	-	cloning artifact	UNP O93724
L	7	HIS	-	cloning artifact	UNP O93724
L	8	HIS	-	cloning artifact	UNP O93724
L	9	HIS	-	cloning artifact	UNP O93724
L	10	HIS	-	cloning artifact	UNP O93724
L	11	GLY	-	cloning artifact	UNP O93724
L	12	SER	-	cloning artifact	UNP O93724
L	39	MSE	MET	modified residue	UNP O93724
L	97	MSE	MET	modified residue	UNP O93724
L	164	MSE	MET	modified residue	UNP O93724
M	1	MET	-	cloning artifact	UNP O93724
M	2	ARG	-	cloning artifact	UNP O93724
M	3	GLY	-	cloning artifact	UNP O93724
M	4	SER	-	cloning artifact	UNP O93724
M	5	HIS	-	cloning artifact	UNP O93724
M	6	HIS	-	cloning artifact	UNP O93724
M	7	HIS	-	cloning artifact	UNP O93724
M	8	HIS	-	cloning artifact	UNP O93724
M	9	HIS	-	cloning artifact	UNP O93724
M	10	HIS	-	cloning artifact	UNP O93724
M	11	GLY	-	cloning artifact	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
M	12	SER	-	cloning artifact	UNP O93724
M	39	MSE	MET	modified residue	UNP O93724
M	97	MSE	MET	modified residue	UNP O93724
M	164	MSE	MET	modified residue	UNP O93724
N	1	MET	-	cloning artifact	UNP O93724
N	2	ARG	-	cloning artifact	UNP O93724
N	3	GLY	-	cloning artifact	UNP O93724
N	4	SER	-	cloning artifact	UNP O93724
N	5	HIS	-	cloning artifact	UNP O93724
N	6	HIS	-	cloning artifact	UNP O93724
N	7	HIS	-	cloning artifact	UNP O93724
N	8	HIS	-	cloning artifact	UNP O93724
N	9	HIS	-	cloning artifact	UNP O93724
N	10	HIS	-	cloning artifact	UNP O93724
N	11	GLY	-	cloning artifact	UNP O93724
N	12	SER	-	cloning artifact	UNP O93724
N	39	MSE	MET	modified residue	UNP O93724
N	97	MSE	MET	modified residue	UNP O93724
N	164	MSE	MET	modified residue	UNP O93724
O	1	MET	-	cloning artifact	UNP O93724
O	2	ARG	-	cloning artifact	UNP O93724
O	3	GLY	-	cloning artifact	UNP O93724
O	4	SER	-	cloning artifact	UNP O93724
O	5	HIS	-	cloning artifact	UNP O93724
O	6	HIS	-	cloning artifact	UNP O93724
O	7	HIS	-	cloning artifact	UNP O93724
O	8	HIS	-	cloning artifact	UNP O93724
O	9	HIS	-	cloning artifact	UNP O93724
O	10	HIS	-	cloning artifact	UNP O93724
O	11	GLY	-	cloning artifact	UNP O93724
O	12	SER	-	cloning artifact	UNP O93724
O	39	MSE	MET	modified residue	UNP O93724
O	97	MSE	MET	modified residue	UNP O93724
O	164	MSE	MET	modified residue	UNP O93724
P	1	MET	-	cloning artifact	UNP O93724
P	2	ARG	-	cloning artifact	UNP O93724
P	3	GLY	-	cloning artifact	UNP O93724
P	4	SER	-	cloning artifact	UNP O93724
P	5	HIS	-	cloning artifact	UNP O93724
P	6	HIS	-	cloning artifact	UNP O93724
P	7	HIS	-	cloning artifact	UNP O93724
P	8	HIS	-	cloning artifact	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
P	9	HIS	-	cloning artifact	UNP O93724
P	10	HIS	-	cloning artifact	UNP O93724
P	11	GLY	-	cloning artifact	UNP O93724
P	12	SER	-	cloning artifact	UNP O93724
P	39	MSE	MET	modified residue	UNP O93724
P	97	MSE	MET	modified residue	UNP O93724
P	164	MSE	MET	modified residue	UNP O93724
Q	1	MET	-	cloning artifact	UNP O93724
Q	2	ARG	-	cloning artifact	UNP O93724
Q	3	GLY	-	cloning artifact	UNP O93724
Q	4	SER	-	cloning artifact	UNP O93724
Q	5	HIS	-	cloning artifact	UNP O93724
Q	6	HIS	-	cloning artifact	UNP O93724
Q	7	HIS	-	cloning artifact	UNP O93724
Q	8	HIS	-	cloning artifact	UNP O93724
Q	9	HIS	-	cloning artifact	UNP O93724
Q	10	HIS	-	cloning artifact	UNP O93724
Q	11	GLY	-	cloning artifact	UNP O93724
Q	12	SER	-	cloning artifact	UNP O93724
Q	39	MSE	MET	modified residue	UNP O93724
Q	97	MSE	MET	modified residue	UNP O93724
Q	164	MSE	MET	modified residue	UNP O93724
R	1	MET	-	cloning artifact	UNP O93724
R	2	ARG	-	cloning artifact	UNP O93724
R	3	GLY	-	cloning artifact	UNP O93724
R	4	SER	-	cloning artifact	UNP O93724
R	5	HIS	-	cloning artifact	UNP O93724
R	6	HIS	-	cloning artifact	UNP O93724
R	7	HIS	-	cloning artifact	UNP O93724
R	8	HIS	-	cloning artifact	UNP O93724
R	9	HIS	-	cloning artifact	UNP O93724
R	10	HIS	-	cloning artifact	UNP O93724
R	11	GLY	-	cloning artifact	UNP O93724
R	12	SER	-	cloning artifact	UNP O93724
R	39	MSE	MET	modified residue	UNP O93724
R	97	MSE	MET	modified residue	UNP O93724
R	164	MSE	MET	modified residue	UNP O93724
S	1	MET	-	cloning artifact	UNP O93724
S	2	ARG	-	cloning artifact	UNP O93724
S	3	GLY	-	cloning artifact	UNP O93724
S	4	SER	-	cloning artifact	UNP O93724
S	5	HIS	-	cloning artifact	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
S	6	HIS	-	cloning artifact	UNP O93724
S	7	HIS	-	cloning artifact	UNP O93724
S	8	HIS	-	cloning artifact	UNP O93724
S	9	HIS	-	cloning artifact	UNP O93724
S	10	HIS	-	cloning artifact	UNP O93724
S	11	GLY	-	cloning artifact	UNP O93724
S	12	SER	-	cloning artifact	UNP O93724
S	39	MSE	MET	modified residue	UNP O93724
S	97	MSE	MET	modified residue	UNP O93724
S	164	MSE	MET	modified residue	UNP O93724
T	1	MET	-	cloning artifact	UNP O93724
T	2	ARG	-	cloning artifact	UNP O93724
T	3	GLY	-	cloning artifact	UNP O93724
T	4	SER	-	cloning artifact	UNP O93724
T	5	HIS	-	cloning artifact	UNP O93724
T	6	HIS	-	cloning artifact	UNP O93724
T	7	HIS	-	cloning artifact	UNP O93724
T	8	HIS	-	cloning artifact	UNP O93724
T	9	HIS	-	cloning artifact	UNP O93724
T	10	HIS	-	cloning artifact	UNP O93724
T	11	GLY	-	cloning artifact	UNP O93724
T	12	SER	-	cloning artifact	UNP O93724
T	39	MSE	MET	modified residue	UNP O93724
T	97	MSE	MET	modified residue	UNP O93724
T	164	MSE	MET	modified residue	UNP O93724
U	1	MET	-	cloning artifact	UNP O93724
U	2	ARG	-	cloning artifact	UNP O93724
U	3	GLY	-	cloning artifact	UNP O93724
U	4	SER	-	cloning artifact	UNP O93724
U	5	HIS	-	cloning artifact	UNP O93724
U	6	HIS	-	cloning artifact	UNP O93724
U	7	HIS	-	cloning artifact	UNP O93724
U	8	HIS	-	cloning artifact	UNP O93724
U	9	HIS	-	cloning artifact	UNP O93724
U	10	HIS	-	cloning artifact	UNP O93724
U	11	GLY	-	cloning artifact	UNP O93724
U	12	SER	-	cloning artifact	UNP O93724
U	39	MSE	MET	modified residue	UNP O93724
U	97	MSE	MET	modified residue	UNP O93724
U	164	MSE	MET	modified residue	UNP O93724
V	1	MET	-	cloning artifact	UNP O93724
V	2	ARG	-	cloning artifact	UNP O93724

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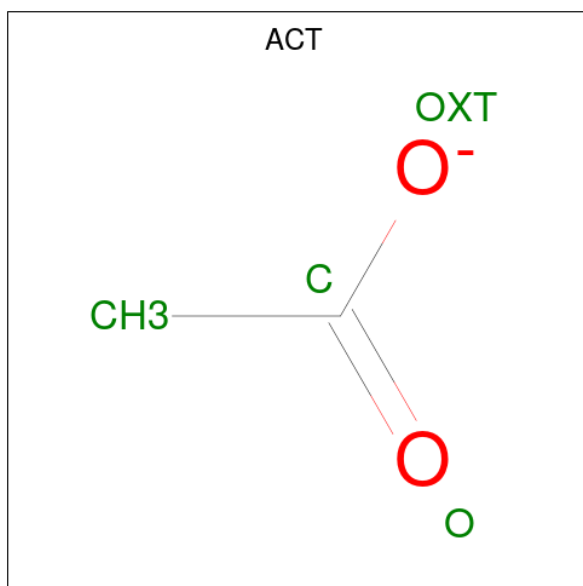
Chain	Residue	Modelled	Actual	Comment	Reference
V	3	GLY	-	cloning artifact	UNP O93724
V	4	SER	-	cloning artifact	UNP O93724
V	5	HIS	-	cloning artifact	UNP O93724
V	6	HIS	-	cloning artifact	UNP O93724
V	7	HIS	-	cloning artifact	UNP O93724
V	8	HIS	-	cloning artifact	UNP O93724
V	9	HIS	-	cloning artifact	UNP O93724
V	10	HIS	-	cloning artifact	UNP O93724
V	11	GLY	-	cloning artifact	UNP O93724
V	12	SER	-	cloning artifact	UNP O93724
V	39	MSE	MET	modified residue	UNP O93724
V	97	MSE	MET	modified residue	UNP O93724
V	164	MSE	MET	modified residue	UNP O93724
W	1	MET	-	cloning artifact	UNP O93724
W	2	ARG	-	cloning artifact	UNP O93724
W	3	GLY	-	cloning artifact	UNP O93724
W	4	SER	-	cloning artifact	UNP O93724
W	5	HIS	-	cloning artifact	UNP O93724
W	6	HIS	-	cloning artifact	UNP O93724
W	7	HIS	-	cloning artifact	UNP O93724
W	8	HIS	-	cloning artifact	UNP O93724
W	9	HIS	-	cloning artifact	UNP O93724
W	10	HIS	-	cloning artifact	UNP O93724
W	11	GLY	-	cloning artifact	UNP O93724
W	12	SER	-	cloning artifact	UNP O93724
W	39	MSE	MET	modified residue	UNP O93724
W	97	MSE	MET	modified residue	UNP O93724
W	164	MSE	MET	modified residue	UNP O93724
X	1	MET	-	cloning artifact	UNP O93724
X	2	ARG	-	cloning artifact	UNP O93724
X	3	GLY	-	cloning artifact	UNP O93724
X	4	SER	-	cloning artifact	UNP O93724
X	5	HIS	-	cloning artifact	UNP O93724
X	6	HIS	-	cloning artifact	UNP O93724
X	7	HIS	-	cloning artifact	UNP O93724
X	8	HIS	-	cloning artifact	UNP O93724
X	9	HIS	-	cloning artifact	UNP O93724
X	10	HIS	-	cloning artifact	UNP O93724
X	11	GLY	-	cloning artifact	UNP O93724
X	12	SER	-	cloning artifact	UNP O93724
X	39	MSE	MET	modified residue	UNP O93724
X	97	MSE	MET	modified residue	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
X	164	MSE	MET	modified residue	UNP O93724

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



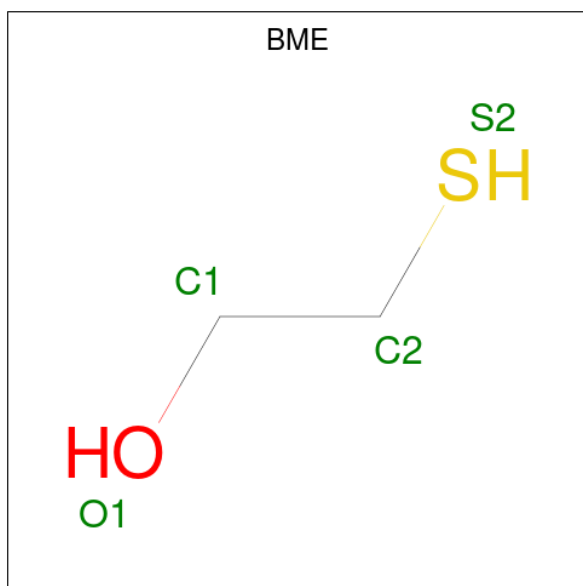
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	M	1	Total	C	O	0	0
			4	2	2		
2	N	1	Total	C	O	0	0
			4	2	2		
2	O	1	Total	C	O	0	0
			4	2	2		
2	P	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	C	O	0	0
			4	2	2		
2	R	1	Total	C	O	0	0
			4	2	2		
2	S	1	Total	C	O	0	0
			4	2	2		
2	T	1	Total	C	O	0	0
			4	2	2		
2	U	1	Total	C	O	0	0
			4	2	2		
2	V	1	Total	C	O	0	0
			4	2	2		
2	W	1	Total	C	O	0	0
			4	2	2		
2	X	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	F	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total 4	C 2	O 1	S 1	0	0
3	I	1	Total 4	C 2	O 1	S 1	0	0
3	K	1	Total 4	C 2	O 1	S 1	0	0
3	N	1	Total 4	C 2	O 1	S 1	0	0
3	P	1	Total 4	C 2	O 1	S 1	0	0
3	Q	1	Total 4	C 2	O 1	S 1	0	0
3	T	1	Total 4	C 2	O 1	S 1	0	0
3	V	1	Total 4	C 2	O 1	S 1	0	0
3	X	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total 118	O 118	0	0
4	B	108	Total 108	O 108	0	0
4	C	110	Total 110	O 110	0	0
4	D	90	Total 90	O 90	0	0
4	E	104	Total 104	O 104	0	0
4	F	69	Total 69	O 69	0	0
4	G	100	Total 100	O 100	0	0
4	H	72	Total 72	O 72	0	0
4	I	113	Total 113	O 113	0	0
4	J	112	Total 112	O 112	0	0

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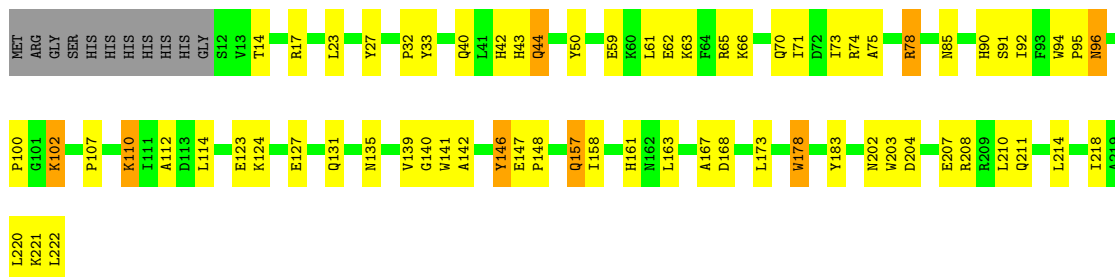
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	119	Total 119	O 119	0	0
4	L	104	Total 104	O 104	0	0
4	M	116	Total 116	O 116	0	0
4	N	117	Total 117	O 117	0	0
4	O	117	Total 117	O 117	0	0
4	P	116	Total 116	O 116	0	0
4	Q	124	Total 124	O 124	0	0
4	R	94	Total 94	O 94	0	0
4	S	109	Total 109	O 109	0	0
4	T	101	Total 101	O 101	0	0
4	U	108	Total 108	O 108	0	0
4	V	104	Total 104	O 104	0	0
4	W	118	Total 118	O 118	0	0
4	X	93	Total 93	O 93	0	0

3 Residue-property plots

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

Chain A: 



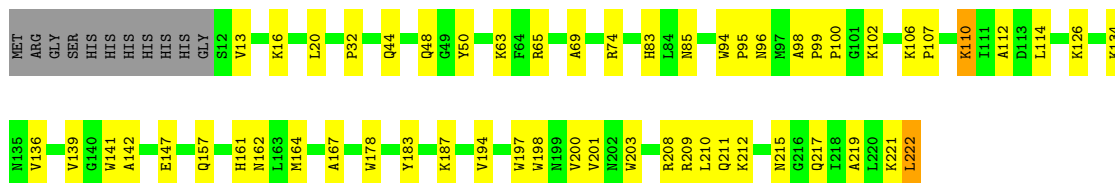
- Molecule 1: Superoxide dismutase

Chain B: 



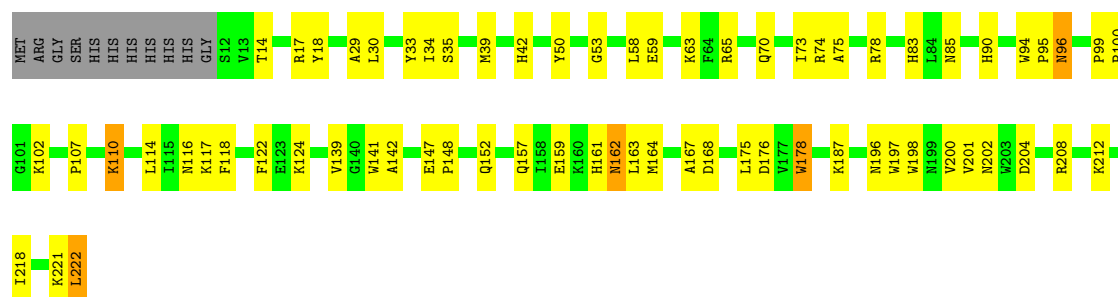
- Molecule 1: Superoxide dismutase

Chain C: 



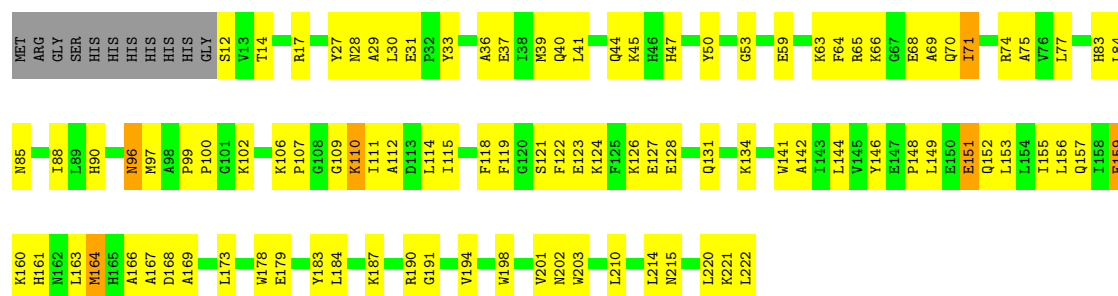
- Molecule 1: Superoxide dismutase

Chain D:  64% 28% • 5%

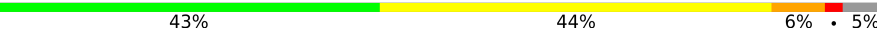


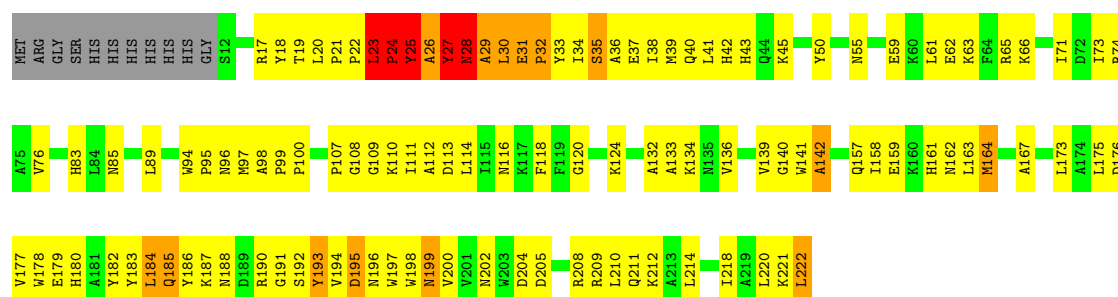
• Molecule 1: Superoxide dismutase

Chain E:  50% 42% • 5%



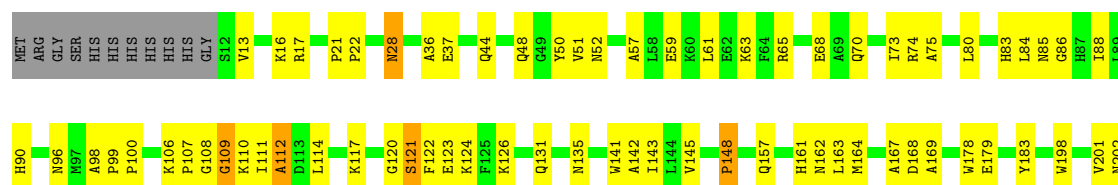
• Molecule 1: Superoxide dismutase

Chain F:  43% 44% 6% • 5%



• Molecule 1: Superoxide dismutase

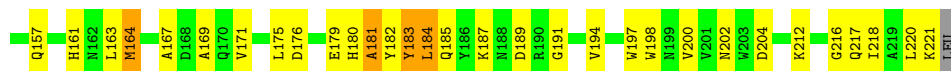
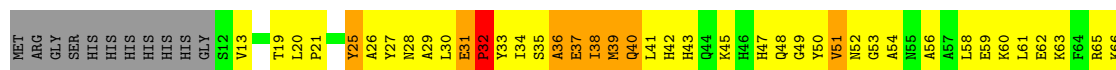
Chain G:  59% 33% • 5%





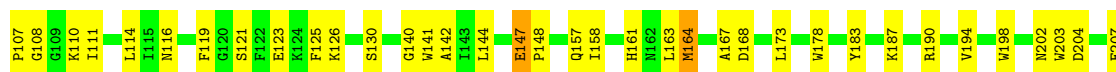
- Molecule 1: Superoxide dismutase

Chain H: 45% 40% 9% 5%



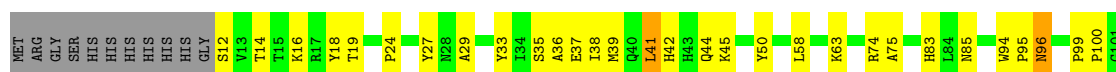
- Molecule 1: Superoxide dismutase

Chain I: 61% 32% 5%



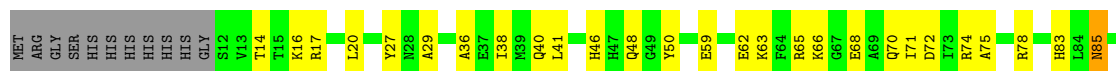
- Molecule 1: Superoxide dismutase

Chain J: 65% 27% 5%



- Molecule 1: Superoxide dismutase

Chain K: 64% 29% 5%



L222

- Molecule 1: Superoxide dismutase

Chain L:  71% 23% 5%

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	S12	V13	T14	T15	Y18	L23	A29	P32	K39	H46	Y50	L58	E62	R65	K66	G67	E68	I71	D72	R73	R74	A75	V76	R78	N85	N96	P99	K102	G108	G109	K110	I111
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A112	F118	G140	W141	A142	E147	E150	Q157	I158	K160	H161	N162	L163	M164	A167	D168	D176	V177	W178	Y183	W198	V201	N202	N203	D204	R208	Q211	K221	L222
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- Molecule 1: Superoxide dismutase

Chain M:  63% 32% 5%

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	S12	Y18	T19	L20	P21	P22	L23	P24	Y27	N28	A29	L30	E31	S35	A36	Q44	Q48	G49	Y50	L58	E59	K63	A69	Q70	I71	D72	I73	R74	A75	V76	L77	R78	H83	L84	N85	G86	H87	L89	H90
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W94	P95	P99	P100	G101	K102	P107	K110	I111	A112	D113	K126	K134	H135	V136	W141	A142	I143	L144	V145	E147	P148	E151	Q157	H161	N162	L163	M164	A167	D168	L173	W178	E179	H180	Y183	K187	G191	D195	N202	R208
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R209	L210	Q211	K212	Q217	L220	K221	L222
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- Molecule 1: Superoxide dismutase

Chain N:  72% 22% 5%

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	S12	T15	K16	R17	A29	L30	Q40	Q44	Y50	N55	L58	F64	A69	I73	R74	L77	R78	H83	L84	N85	W94	P95	N96	P99	P100	G101	K102	K110	I111	L114	I115	F119
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V136	W141	A142	Y146	E150	E151	Q157	H161	N162	L163	M164	A167	D168	D176	V177	W178	E179	H180	Y183	K187	W197	V200	L210	K221	L222
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- Molecule 1: Superoxide dismutase

Chain O:  62% 31% 5%

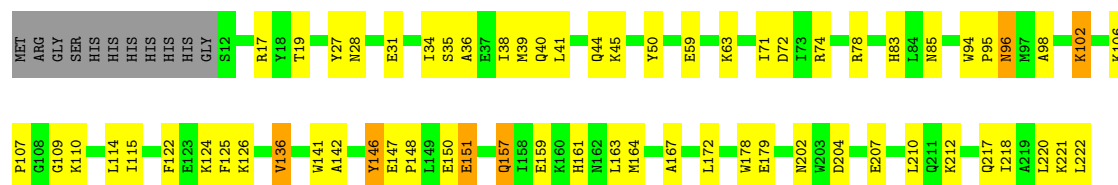
MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	GLY	S12	V13	K16	R17	Y18	Y27	N28	A29	L30	E31	I34	E37	I38	K39	Q40	L41	H42	H43	Q44	X45	H46	Y50	E59	F64	R65	K66	A69	Q70	I71	R74	A75	V76	L77	R78	A79	Y183	V200	V201	N202	N203	D204	R208
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H90	N97	A98	K102	G103	P107	G108	G109	L114	E127	E128	F129	S130	Q131	K134	W141	A142	I143	L144	E147	E151	Q152	Q157	I158	E159	K160	H161	N162	L163	M164	A167	D168	A169	Q170	L173	W178	E179	Y183	V200	V201	N202	N203	D204	R208
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R209	L210	L214	L220	K221	L222
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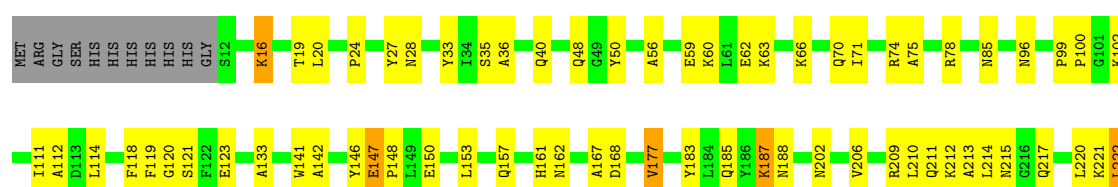
- Molecule 1: Superoxide dismutase

Chain P:  66% 27% 5%



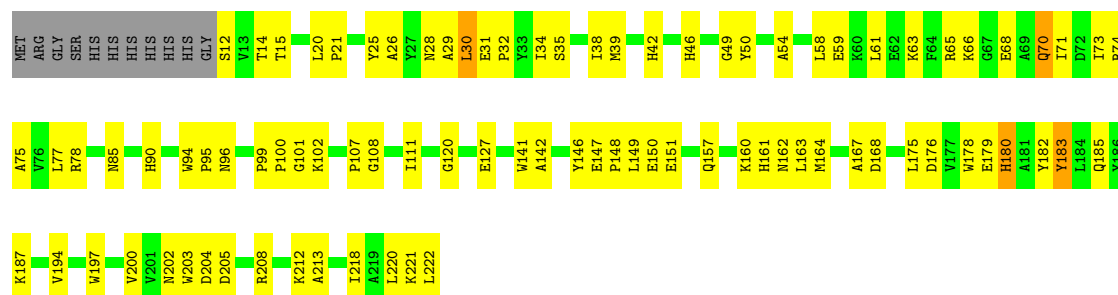
- Molecule 1: Superoxide dismutase

Chain Q:  65% 28% 5%



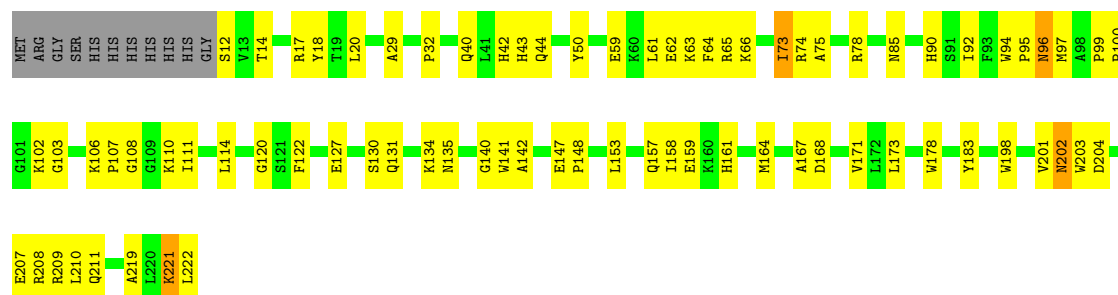
- Molecule 1: Superoxide dismutase

Chain R:  55% 38% 5%



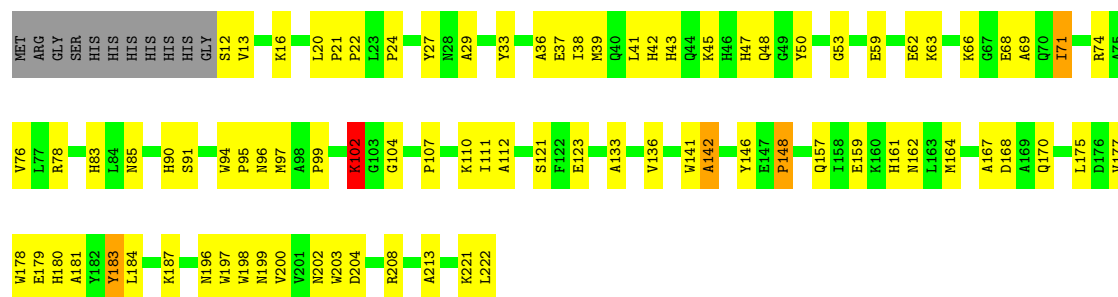
- Molecule 1: Superoxide dismutase

Chain S:  60% 33% 5%



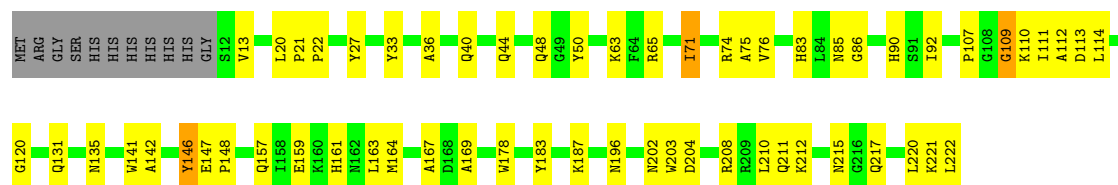
- Molecule 1: Superoxide dismutase

Chain T:  57% 36% 5%



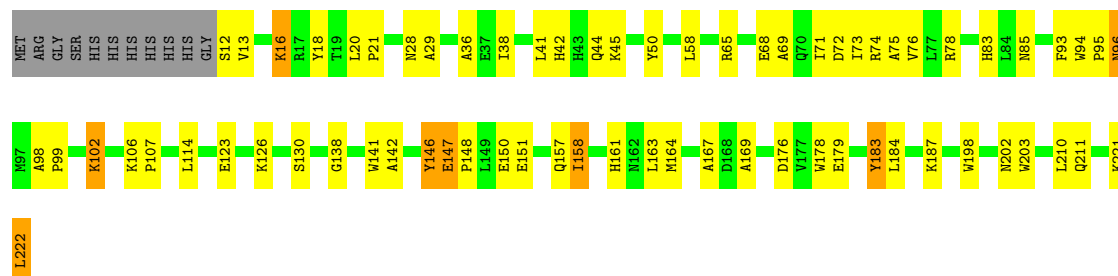
• Molecule 1: Superoxide dismutase

Chain U: 68% 26% 5%



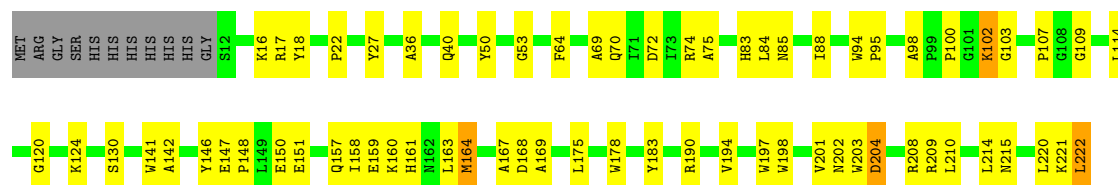
• Molecule 1: Superoxide dismutase

Chain V: 64% 27% 5%



• Molecule 1: Superoxide dismutase

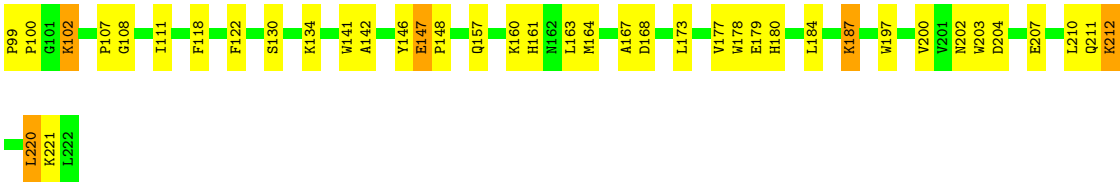
Chain W: 65% 28% 5%



• Molecule 1: Superoxide dismutase

Chain X: 64% 29% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	163.43Å 163.43Å 172.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.45 – 1.80 36.45 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (36.45-1.80) 97.6 (36.45-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 1.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.162 , 0.217 0.161 , 0.214	Depositor DCC
R_{free} test set	37229 reflections (8.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.029 for h,-h-k,-l 0.449 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	43787	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0145e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BME, ACT

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	0.45	0/1759	0.97	13/2378 (0.5%)
1	B	0.44	0/1759	0.94	6/2378 (0.3%)
1	C	0.43	0/1759	0.95	9/2378 (0.4%)
1	D	0.44	0/1759	0.94	9/2378 (0.4%)
1	E	0.41	0/1759	0.91	5/2378 (0.2%)
1	F	0.43	0/1759	1.09	11/2378 (0.5%)
1	G	0.42	0/1759	0.92	8/2378 (0.3%)
1	H	0.40	0/1750	1.48	20/2367 (0.8%)
1	I	0.44	0/1759	0.96	8/2378 (0.3%)
1	J	0.45	0/1759	0.96	7/2378 (0.3%)
1	K	0.44	0/1759	0.94	8/2378 (0.3%)
1	L	0.44	0/1759	0.96	9/2378 (0.4%)
1	M	0.44	0/1759	0.94	6/2378 (0.3%)
1	N	0.45	0/1759	0.94	7/2378 (0.3%)
1	O	0.45	0/1759	0.93	7/2378 (0.3%)
1	P	0.44	0/1759	0.95	10/2378 (0.4%)
1	Q	0.41	0/1759	0.96	7/2378 (0.3%)
1	R	0.43	0/1759	0.97	8/2378 (0.3%)
1	S	0.44	0/1759	0.95	9/2378 (0.4%)
1	T	0.41	0/1759	0.92	7/2378 (0.3%)
1	U	0.45	0/1759	0.95	9/2378 (0.4%)
1	V	0.45	0/1759	0.97	10/2378 (0.4%)
1	W	0.43	0/1759	0.95	9/2378 (0.4%)
1	X	0.45	0/1759	0.91	7/2378 (0.3%)
All	All	0.44	0/42207	0.98	209/57061 (0.4%)

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
1	B	0	1

There are no bond length outliers.

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	31	GLU	CA-C-N	36.74	165.77	119.84
1	H	31	GLU	C-N-CA	36.74	165.77	119.84
1	F	29	ALA	N-CA-C	-17.06	84.26	110.70
1	H	31	GLU	C-N-CD	-12.59	73.37	125.00
1	F	32	PRO	N-CA-C	-9.64	102.63	114.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	18	TYR	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	1714	0	1688	65	0
1	B	1714	0	1688	62	0
1	C	1714	0	1688	49	0
1	D	1714	0	1688	66	0
1	E	1714	0	1688	94	0
1	F	1714	0	1688	167	0
1	G	1714	0	1688	75	0
1	H	1705	0	1677	134	0
1	I	1714	0	1688	65	0
1	J	1714	0	1688	61	0
1	K	1714	0	1688	62	0
1	L	1714	0	1688	51	0
1	M	1714	0	1688	65	0
1	N	1714	0	1688	50	0
1	O	1714	0	1688	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1714	0	1688	78	0
1	Q	1714	0	1688	66	0
1	R	1714	0	1688	78	0
1	S	1714	0	1688	60	0
1	T	1714	0	1688	82	0
1	U	1714	0	1688	53	0
1	V	1714	0	1688	64	0
1	W	1714	0	1688	55	0
1	X	1714	0	1688	54	0
2	B	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	1	0
2	H	4	0	3	0	0
2	J	4	0	3	1	0
2	L	4	0	3	0	0
2	M	4	0	3	2	0
2	N	4	0	3	0	0
2	O	4	0	3	0	0
2	P	4	0	3	2	0
2	Q	4	0	3	1	0
2	R	4	0	3	0	0
2	S	4	0	3	0	0
2	T	4	0	3	0	0
2	U	4	0	3	1	0
2	V	4	0	3	0	0
2	W	4	0	3	1	0
2	X	4	0	3	0	0
3	B	4	0	5	3	0
3	D	4	0	5	3	0
3	F	4	0	5	3	0
3	H	4	0	5	6	0
3	I	4	0	5	3	0
3	K	4	0	5	8	0
3	N	4	0	5	3	0
3	P	4	0	5	4	0
3	Q	4	0	5	5	0
3	T	4	0	5	2	0
3	V	4	0	5	6	0
3	X	4	0	5	3	0
4	A	118	0	0	3	0
4	B	108	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	110	0	0	1	0
4	D	90	0	0	2	0
4	E	104	0	0	1	0
4	F	69	0	0	10	0
4	G	100	0	0	5	0
4	H	72	0	0	8	0
4	I	113	0	0	5	0
4	J	112	0	0	3	0
4	K	119	0	0	5	0
4	L	104	0	0	2	0
4	M	116	0	0	8	0
4	N	117	0	0	2	0
4	O	117	0	0	6	0
4	P	116	0	0	8	0
4	Q	124	0	0	5	0
4	R	94	0	0	7	0
4	S	109	0	0	3	0
4	T	101	0	0	10	0
4	U	108	0	0	3	0
4	V	104	0	0	5	0
4	W	118	0	0	8	0
4	X	93	0	0	2	0
All	All	43787	0	40618	1529	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 19.

The worst 5 of 1529 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:F:30:LEU:HD12	1:F:200:VAL:HG11	1.37	1.04
1:F:157:GLN:HE22	1:G:74:ARG:HG3	1.24	0.98
1:E:141:TRP:HE1	1:E:161:HIS:HD2	1.12	0.98
1:F:30:LEU:CD1	1:F:200:VAL:HG11	1.94	0.97
1:A:141:TRP:HE1	1:A:161:HIS:HD2	0.99	0.96

There are no symmetry-related clashes.

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	209/222 (94%)	201 (96%)	8 (4%)	0	100	100
1	B	209/222 (94%)	197 (94%)	11 (5%)	1 (0%)	24	14
1	C	209/222 (94%)	201 (96%)	8 (4%)	0	100	100
1	D	209/222 (94%)	195 (93%)	14 (7%)	0	100	100
1	E	209/222 (94%)	191 (91%)	14 (7%)	4 (2%)	6	1
1	F	209/222 (94%)	168 (80%)	27 (13%)	14 (7%)	1	0
1	G	209/222 (94%)	191 (91%)	13 (6%)	5 (2%)	4	1
1	H	208/222 (94%)	171 (82%)	27 (13%)	10 (5%)	2	0
1	I	209/222 (94%)	194 (93%)	15 (7%)	0	100	100
1	J	209/222 (94%)	195 (93%)	13 (6%)	1 (0%)	24	14
1	K	209/222 (94%)	196 (94%)	13 (6%)	0	100	100
1	L	209/222 (94%)	196 (94%)	12 (6%)	1 (0%)	24	14
1	M	209/222 (94%)	193 (92%)	16 (8%)	0	100	100
1	N	209/222 (94%)	195 (93%)	13 (6%)	1 (0%)	24	14
1	O	209/222 (94%)	196 (94%)	8 (4%)	5 (2%)	4	1
1	P	209/222 (94%)	198 (95%)	11 (5%)	0	100	100
1	Q	209/222 (94%)	196 (94%)	13 (6%)	0	100	100
1	R	209/222 (94%)	191 (91%)	16 (8%)	2 (1%)	12	4
1	S	209/222 (94%)	198 (95%)	10 (5%)	1 (0%)	24	14
1	T	209/222 (94%)	191 (91%)	17 (8%)	1 (0%)	24	14
1	U	209/222 (94%)	194 (93%)	13 (6%)	2 (1%)	12	4
1	V	209/222 (94%)	197 (94%)	12 (6%)	0	100	100
1	W	209/222 (94%)	197 (94%)	10 (5%)	2 (1%)	12	4
1	X	209/222 (94%)	193 (92%)	16 (8%)	0	100	100
All	All	5015/5328 (94%)	4635 (92%)	330 (7%)	50 (1%)	12	4

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	109	GLY
1	F	23	LEU
1	F	25	TYR
1	F	26	ALA
1	F	27	TYR

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	176/182 (97%)	172 (98%)	4 (2%)	44	33
1	B	176/182 (97%)	174 (99%)	2 (1%)	65	60
1	C	176/182 (97%)	171 (97%)	5 (3%)	38	26
1	D	176/182 (97%)	172 (98%)	4 (2%)	44	33
1	E	176/182 (97%)	173 (98%)	3 (2%)	53	45
1	F	176/182 (97%)	169 (96%)	7 (4%)	28	15
1	G	176/182 (97%)	173 (98%)	3 (2%)	53	45
1	H	175/182 (96%)	170 (97%)	5 (3%)	37	25
1	I	176/182 (97%)	175 (99%)	1 (1%)	78	77
1	J	176/182 (97%)	172 (98%)	4 (2%)	44	33
1	K	176/182 (97%)	172 (98%)	4 (2%)	44	33
1	L	176/182 (97%)	172 (98%)	4 (2%)	44	33
1	M	176/182 (97%)	175 (99%)	1 (1%)	78	77
1	N	176/182 (97%)	173 (98%)	3 (2%)	53	45
1	O	176/182 (97%)	175 (99%)	1 (1%)	78	77
1	P	176/182 (97%)	174 (99%)	2 (1%)	65	60
1	Q	176/182 (97%)	171 (97%)	5 (3%)	38	26
1	R	176/182 (97%)	173 (98%)	3 (2%)	53	45
1	S	176/182 (97%)	173 (98%)	3 (2%)	53	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	176/182 (97%)	174 (99%)	2 (1%)	65	60
1	U	176/182 (97%)	176 (100%)	0	100	100
1	V	176/182 (97%)	172 (98%)	4 (2%)	44	33
1	W	176/182 (97%)	174 (99%)	2 (1%)	65	60
1	X	176/182 (97%)	170 (97%)	6 (3%)	32	20
All	All	4223/4368 (97%)	4145 (98%)	78 (2%)	51	43

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	222	LEU
1	W	222	LEU
1	R	96	ASN
1	T	102	LYS
1	X	211	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 217 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	215	ASN
1	P	199	ASN
1	V	161	HIS
1	N	83	HIS
1	O	157	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	BME	B	402	-	3,3,3	2.07	1 (33%)	2,2,2	1.90	1 (50%)
2	ACT	F	306	-	3,3,3	1.37	1 (33%)	3,3,3	0.78	0
2	ACT	T	320	-	3,3,3	1.29	1 (33%)	3,3,3	0.75	0
3	BME	D	404	-	3,3,3	2.07	1 (33%)	2,2,2	2.01	1 (50%)
2	ACT	E	305	-	3,3,3	1.32	1 (33%)	3,3,3	0.74	0
2	ACT	M	313	-	3,3,3	1.23	1 (33%)	3,3,3	0.79	0
2	ACT	S	319	-	3,3,3	1.33	1 (33%)	3,3,3	0.81	0
3	BME	N	414	-	3,3,3	2.11	1 (33%)	2,2,2	1.87	1 (50%)
3	BME	X	424	-	3,3,3	2.14	1 (33%)	2,2,2	2.01	1 (50%)
2	ACT	X	324	-	3,3,3	1.36	1 (33%)	3,3,3	0.74	0
2	ACT	R	318	-	3,3,3	1.29	1 (33%)	3,3,3	0.76	0
2	ACT	L	312	-	3,3,3	1.25	1 (33%)	3,3,3	0.73	0
2	ACT	Q	317	-	3,3,3	1.41	1 (33%)	3,3,3	0.78	0
2	ACT	V	322	-	3,3,3	1.31	1 (33%)	3,3,3	0.77	0
2	ACT	B	302	-	3,3,3	1.25	1 (33%)	3,3,3	0.68	0
3	BME	Q	418	-	3,3,3	2.10	1 (33%)	2,2,2	1.98	1 (50%)
2	ACT	U	321	-	3,3,3	1.32	1 (33%)	3,3,3	0.76	0
2	ACT	N	314	-	3,3,3	1.29	1 (33%)	3,3,3	0.78	0
2	ACT	P	316	-	3,3,3	1.23	1 (33%)	3,3,3	0.73	0
2	ACT	O	315	-	3,3,3	1.42	1 (33%)	3,3,3	0.79	0
3	BME	F	406	-	3,3,3	2.10	1 (33%)	2,2,2	1.99	1 (50%)
3	BME	P	416	-	3,3,3	2.15	1 (33%)	2,2,2	1.96	1 (50%)
3	BME	I	410	-	3,3,3	2.13	1 (33%)	2,2,2	1.94	1 (50%)
2	ACT	W	323	-	3,3,3	1.41	1 (33%)	3,3,3	0.73	0
2	ACT	J	310	-	3,3,3	1.26	1 (33%)	3,3,3	0.75	0
3	BME	K	412	-	3,3,3	2.06	1 (33%)	2,2,2	1.99	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	H	308	-	3,3,3	1.33	1 (33%)	3,3,3	0.70	0
3	BME	V	422	-	3,3,3	2.05	1 (33%)	2,2,2	1.99	1 (50%)
3	BME	H	408	-	3,3,3	2.06	1 (33%)	2,2,2	2.02	1 (50%)
2	ACT	D	304	-	3,3,3	1.38	1 (33%)	3,3,3	0.79	0
3	BME	T	420	-	3,3,3	2.08	1 (33%)	2,2,2	1.99	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	V	422	-	-	1/1/1/1	-
3	BME	B	402	-	-	1/1/1/1	-
3	BME	H	408	-	-	1/1/1/1	-
3	BME	D	404	-	-	1/1/1/1	-
3	BME	N	414	-	-	1/1/1/1	-
3	BME	X	424	-	-	1/1/1/1	-
3	BME	F	406	-	-	1/1/1/1	-
3	BME	P	416	-	-	1/1/1/1	-
3	BME	I	410	-	-	0/1/1/1	-
3	BME	Q	418	-	-	1/1/1/1	-
3	BME	T	420	-	-	0/1/1/1	-
3	BME	K	412	-	-	1/1/1/1	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	416	BME	O1-C1	-3.71	1.23	1.42
3	X	424	BME	O1-C1	-3.67	1.23	1.42
3	I	410	BME	O1-C1	-3.66	1.23	1.42
3	N	414	BME	O1-C1	-3.64	1.23	1.42
3	F	406	BME	O1-C1	-3.61	1.23	1.42

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	424	BME	O1-C1-C2	2.80	121.74	110.82
3	D	404	BME	O1-C1-C2	2.78	121.67	110.82
3	H	408	BME	O1-C1-C2	2.77	121.63	110.82
3	F	406	BME	O1-C1-C2	2.76	121.60	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	420	BME	O1-C1-C2	2.75	121.55	110.82

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	BME	O1-C1-C2-S2
3	D	404	BME	O1-C1-C2-S2
3	H	408	BME	O1-C1-C2-S2
3	K	412	BME	O1-C1-C2-S2
3	N	414	BME	O1-C1-C2-S2

There are no ring outliers.

19 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	BME	3	0
2	F	306	ACT	1	0
3	D	404	BME	3	0
2	M	313	ACT	2	0
3	N	414	BME	3	0
3	X	424	BME	3	0
2	Q	317	ACT	1	0
3	Q	418	BME	5	0
2	U	321	ACT	1	0
2	P	316	ACT	2	0
3	F	406	BME	3	0
3	P	416	BME	4	0
3	I	410	BME	3	0
2	W	323	ACT	1	0
2	J	310	ACT	1	0
3	K	412	BME	8	0
3	V	422	BME	6	0
3	H	408	BME	6	0
3	T	420	BME	2	0

5.7 Other polymers [i](#)

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 ⓘ

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	208/222 (93%)	-1.33	0 100 100	7, 18, 33, 44	0
1	B	208/222 (93%)	-1.25	0 100 100	11, 19, 33, 45	0
1	C	208/222 (93%)	-1.34	0 100 100	8, 19, 30, 39	0
1	D	208/222 (93%)	-1.17	0 100 100	10, 22, 38, 42	0
1	E	208/222 (93%)	-1.23	0 100 100	9, 22, 40, 52	0
1	F	208/222 (93%)	-0.76	0 100 100	15, 37, 57, 66	1 (0%)
1	G	208/222 (93%)	-1.25	0 100 100	10, 21, 41, 49	0
1	H	207/222 (93%)	-0.90	0 100 100	14, 32, 51, 56	0
1	I	208/222 (93%)	-1.38	0 100 100	8, 17, 32, 44	0
1	J	208/222 (93%)	-1.35	0 100 100	10, 17, 33, 42	0
1	K	208/222 (93%)	-1.40	0 100 100	7, 17, 31, 40	0
1	L	208/222 (93%)	-1.38	0 100 100	9, 17, 31, 39	0
1	M	208/222 (93%)	-1.37	0 100 100	8, 17, 31, 42	0
1	N	208/222 (93%)	-1.37	0 100 100	9, 16, 28, 40	0
1	O	208/222 (93%)	-1.37	0 100 100	8, 17, 31, 41	0
1	P	208/222 (93%)	-1.35	0 100 100	9, 18, 30, 43	0
1	Q	208/222 (93%)	-1.34	0 100 100	8, 18, 35, 45	0
1	R	208/222 (93%)	-1.28	0 100 100	11, 22, 38, 46	0
1	S	208/222 (93%)	-1.39	0 100 100	8, 18, 33, 41	0
1	T	208/222 (93%)	-1.29	0 100 100	14, 22, 37, 50	0
1	U	208/222 (93%)	-1.37	0 100 100	7, 18, 32, 40	0
1	V	208/222 (93%)	-1.39	0 100 100	9, 17, 30, 43	0
1	W	208/222 (93%)	-1.40	0 100 100	8, 17, 31, 40	0
1	X	208/222 (93%)	-1.24	0 100 100	10, 21, 36, 42	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4991/5328 (93%)	-1.29	0 100 100	7, 19, 39, 66	1 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	ACT	F	306	4/4	0.96	0.05	37,37,37,37	0
2	ACT	Q	317	4/4	0.97	0.10	49,49,49,50	0
2	ACT	W	323	4/4	0.97	0.06	27,28,29,29	0
2	ACT	B	302	4/4	0.98	0.04	27,28,29,30	0
2	ACT	S	319	4/4	0.98	0.04	28,29,30,30	0
2	ACT	U	321	4/4	0.98	0.07	42,42,42,43	0
2	ACT	H	308	4/4	0.98	0.06	38,39,39,41	0
2	ACT	X	324	4/4	0.98	0.04	21,22,22,23	0
3	BME	D	404	4/4	0.98	0.09	32,37,37,41	0
3	BME	H	408	4/4	0.98	0.07	36,37,38,39	0
3	BME	I	410	4/4	0.98	0.07	21,27,28,35	0
3	BME	N	414	4/4	0.98	0.07	49,50,51,56	0
3	BME	T	420	4/4	0.98	0.06	32,33,33,39	0
2	ACT	E	305	4/4	0.99	0.03	19,20,21,21	0
2	ACT	T	320	4/4	0.99	0.03	25,27,27,27	0
2	ACT	J	310	4/4	0.99	0.04	29,30,30,30	0
2	ACT	V	322	4/4	0.99	0.03	20,21,21,22	0
2	ACT	L	312	4/4	0.99	0.02	20,20,21,22	0
2	ACT	M	313	4/4	0.99	0.04	23,23,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BME	B	402	4/4	0.99	0.07	26,30,30,34	0
2	ACT	N	314	4/4	0.99	0.04	20,21,22,22	0
3	BME	F	406	4/4	0.99	0.06	24,24,25,32	0
2	ACT	O	315	4/4	0.99	0.06	43,43,44,45	0
2	ACT	P	316	4/4	0.99	0.04	24,25,26,28	0
3	BME	K	412	4/4	0.99	0.06	32,33,33,33	0
2	ACT	D	304	4/4	0.99	0.04	26,27,28,29	0
3	BME	P	416	4/4	0.99	0.06	20,22,23,29	0
3	BME	Q	418	4/4	0.99	0.06	29,34,35,38	0
2	ACT	R	318	4/4	0.99	0.04	28,28,28,29	0
3	BME	V	422	4/4	0.99	0.08	41,43,43,43	0
3	BME	X	424	4/4	0.99	0.07	30,32,34,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.