



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:33 PM GMT

PDB ID : 1P7G  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

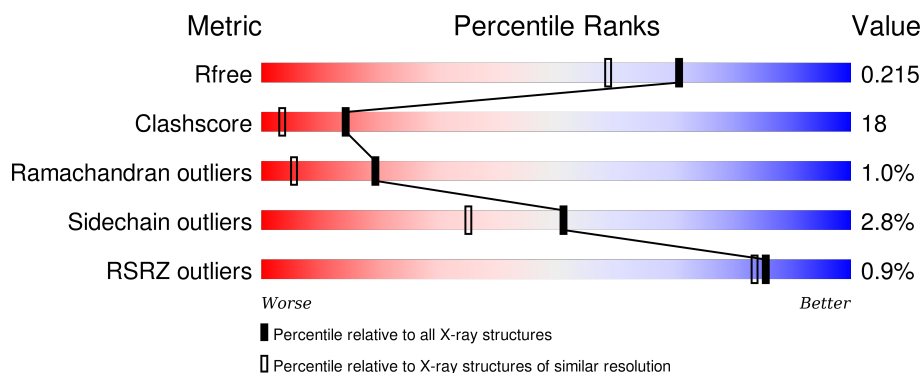
# 1 Overall quality at a glance

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.



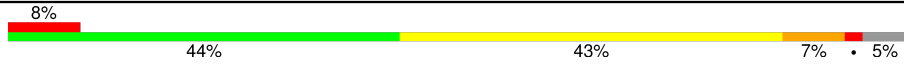




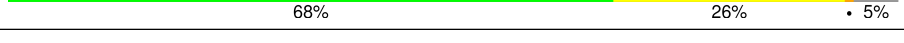
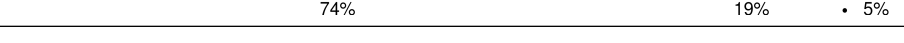
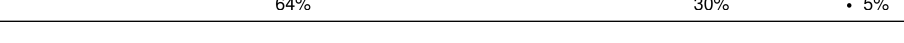
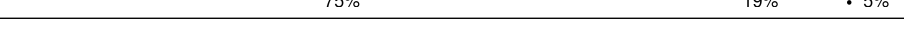
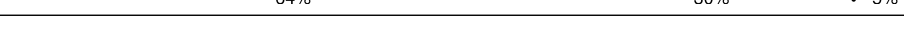


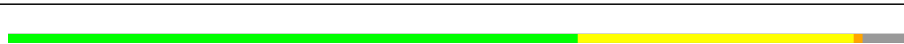






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	222	<div> <div></div> <div>67% 27% • 5%</div> </div>
1	B	222	<div> <div></div> <div>65% 29% 5%</div> </div>
1	C	222	<div> <div></div> <div>73% 21% • 5%</div> </div>
1	D	222	<div> <div></div> <div>68% 26% • 5%</div> </div>
1	E	222	<div> <div></div> <div>51% 41% • 5%</div> </div>

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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	O	315	-	-	-	X
2	ACT	P	316	-	-	X	-
3	BME	B	402	-	-	-	X
3	BME	D	404	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BME	F	406	-	-	-	X
3	BME	H	408	-	-	X	X
3	BME	I	410	-	-	-	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	T	420	-	-	-	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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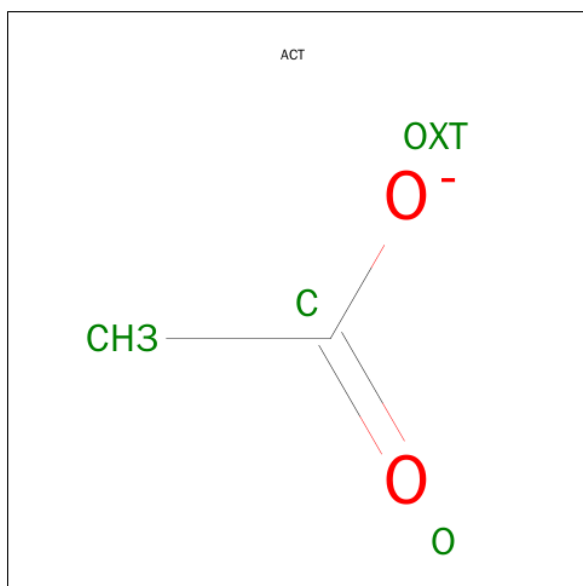
Chain	Residue	Modelled	Actual	Comment	Reference
V	3	GLY	-	CLONING ARTIFACT	UNP O93724
V	4	SER	-	CLONING ARTIFACT	UNP O93724
V	5	HIS	-	CLONING ARTIFACT	UNP O93724
V	6	HIS	-	CLONING ARTIFACT	UNP O93724
V	7	HIS	-	CLONING ARTIFACT	UNP O93724
V	8	HIS	-	CLONING ARTIFACT	UNP O93724
V	9	HIS	-	CLONING ARTIFACT	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 (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



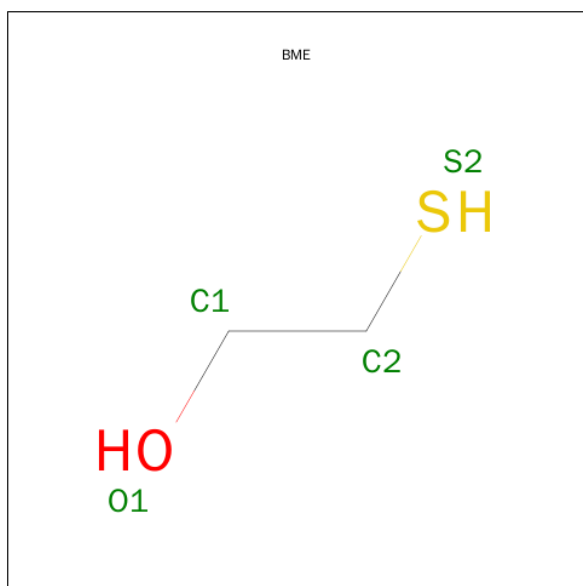
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	M	1	Total	C	O	0	0
			4	2	2		
2	N	1	Total	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 (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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.

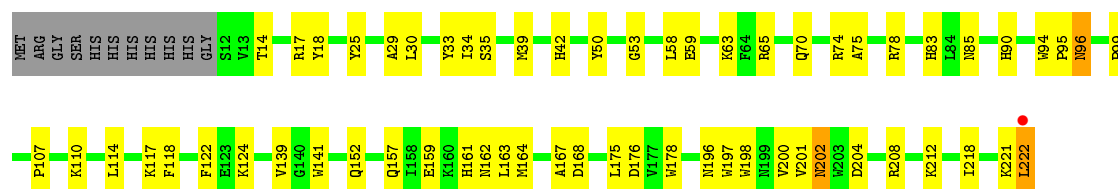
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total 118	O 118	0	0
4	B	108	Total 108	O 108	0	0
4	C	110	Total 110	O 110	0	0
4	D	90	Total 90	O 90	0	0
4	E	104	Total 104	O 104	0	0
4	F	69	Total 69	O 69	0	0
4	G	100	Total 100	O 100	0	0
4	H	72	Total 72	O 72	0	0
4	I	113	Total 113	O 113	0	0
4	J	112	Total 112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

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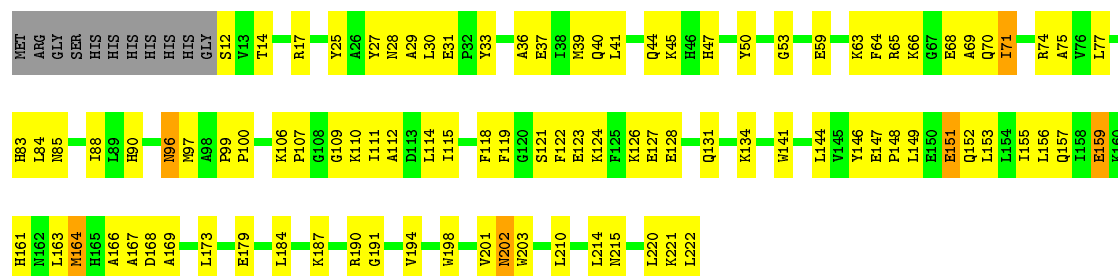
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	119	Total 119	O 119	0	0
4	L	104	Total 104	O 104	0	0
4	M	116	Total 116	O 116	0	0
4	N	117	Total 117	O 117	0	0
4	O	117	Total 117	O 117	0	0
4	P	116	Total 116	O 116	0	0
4	Q	124	Total 124	O 124	0	0
4	R	94	Total 94	O 94	0	0
4	S	109	Total 109	O 109	0	0
4	T	101	Total 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





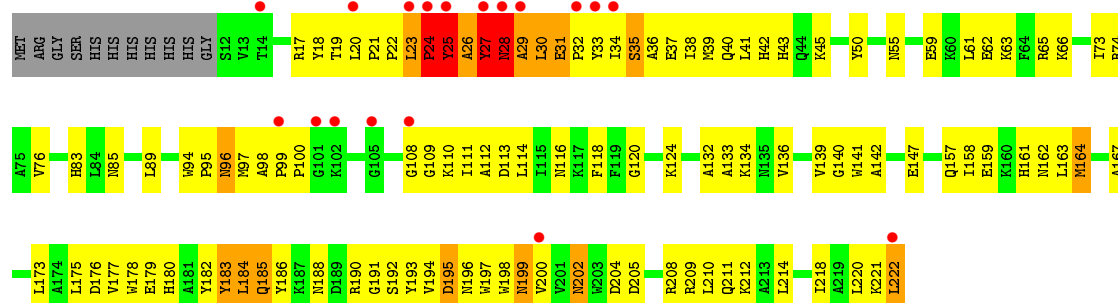
• Molecule 1: Superoxide dismutase

Chain E: 51% 41% 5%



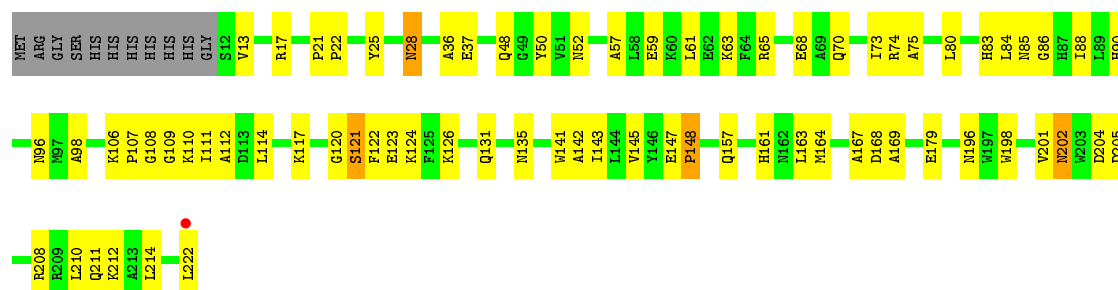
• Molecule 1: Superoxide dismutase

Chain F: 8% 44% 43% 7% 5%



• Molecule 1: Superoxide dismutase

Chain G: 62% 31% 5%



• Molecule 1: Superoxide dismutase

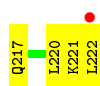
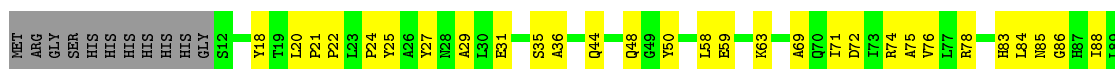
Chain H: 4% 48% 41% 5% 5%





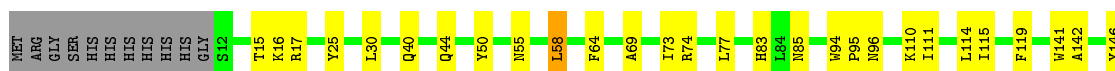
- Molecule 1: Superoxide dismutase

Chain M: 64% 30% 5%



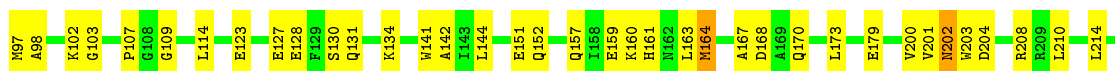
- Molecule 1: Superoxide dismutase

Chain N: 75% 19% 5%



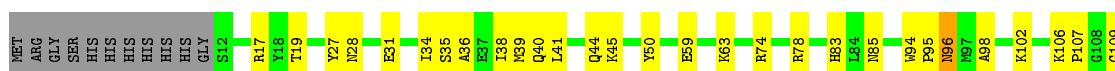
- Molecule 1: Superoxide dismutase

Chain O: 64% 30% 5%

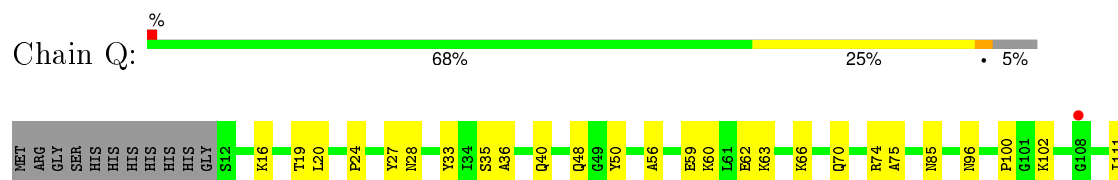


- Molecule 1: Superoxide dismutase

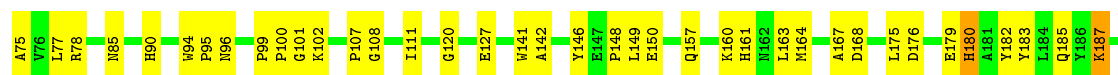
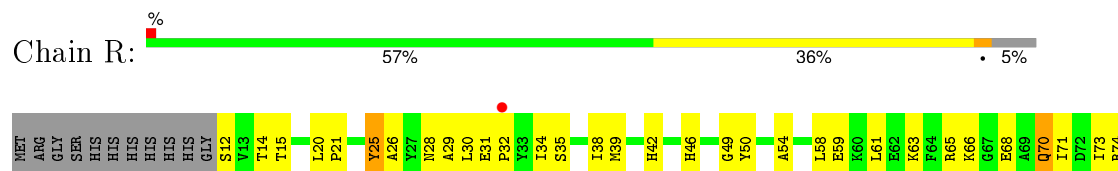
Chain P: 68% 26% 5%



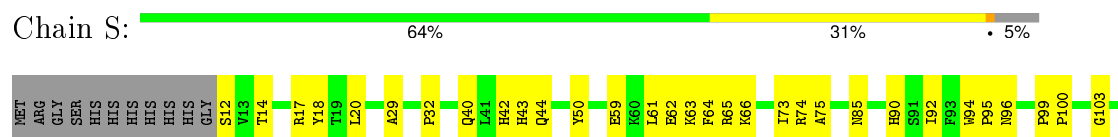
- Molecule 1: Superoxide dismutase



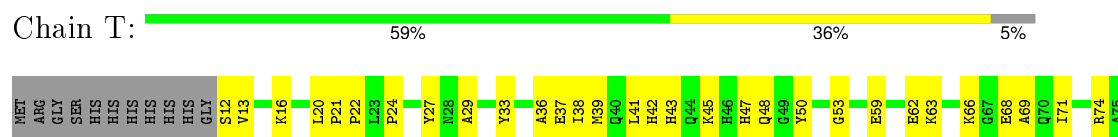
- Molecule 1: Superoxide dismutase



- Molecule 1: Superoxide dismutase

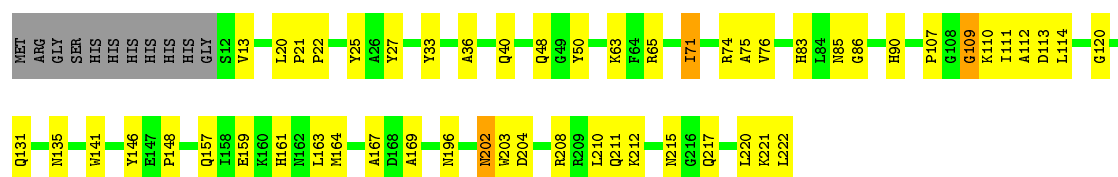


- Molecule 1: Superoxide dismutase



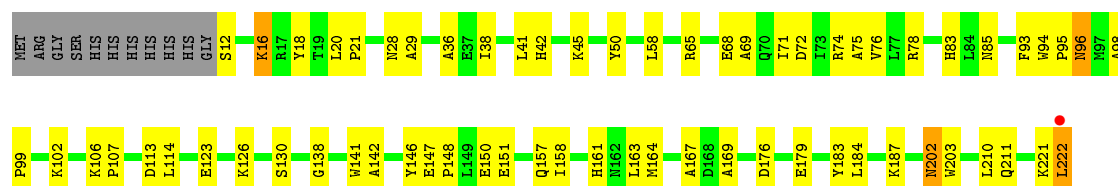
- Molecule 1: Superoxide dismutase





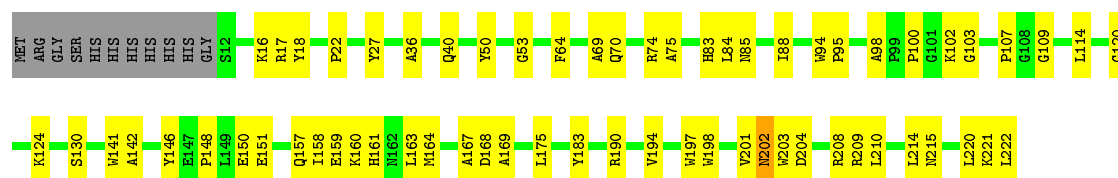
- Molecule 1: Superoxide dismutase

Chain V: 66% 27% 5%



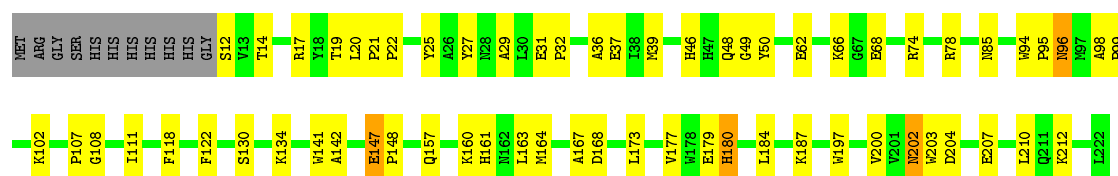
- Molecule 1: Superoxide dismutase

Chain W: 66% 28% 5%



- Molecule 1: Superoxide dismutase

Chain X: 67% 27% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.43Å 163.43Å 172.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.45 – 1.80 36.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (36.45-1.80) 97.6 (36.44-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.05 (at 1.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.162 , 0.217 0.161 , 0.215	Depositor DCC
$R_{free}$ test set	37229 reflections (8.70%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 35.9	EDS
Estimated twinning fraction	0.028 for -h,-k,l 0.029 for h,-h-k,-l 0.449 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 465035 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	43787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ACT, BME

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	0.39	0/1759	0.62	0/2378
1	B	0.39	0/1759	0.61	0/2378
1	C	0.39	0/1759	0.62	1/2378 (0.0%)
1	D	0.37	0/1759	0.61	0/2378
1	E	0.36	0/1759	0.60	0/2378
1	F	0.36	0/1759	0.70	3/2378 (0.1%)
1	G	0.38	0/1759	0.59	1/2378 (0.0%)
1	H	0.35	0/1750	0.79	3/2367 (0.1%)
1	I	0.39	0/1759	0.62	1/2378 (0.0%)
1	J	0.39	0/1759	0.61	0/2378
1	K	0.40	0/1759	0.63	0/2378
1	L	0.40	0/1759	0.62	0/2378
1	M	0.39	0/1759	0.61	1/2378 (0.0%)
1	N	0.40	0/1759	0.62	1/2378 (0.0%)
1	O	0.39	0/1759	0.63	1/2378 (0.0%)
1	P	0.40	0/1759	0.62	0/2378
1	Q	0.37	0/1759	0.61	0/2378
1	R	0.37	0/1759	0.62	1/2378 (0.0%)
1	S	0.38	0/1759	0.62	0/2378
1	T	0.37	0/1759	0.59	0/2378
1	U	0.38	0/1759	0.61	0/2378
1	V	0.39	0/1759	0.63	1/2378 (0.0%)
1	W	0.37	0/1759	0.62	1/2378 (0.0%)
1	X	0.38	0/1759	0.59	1/2378 (0.0%)
All	All	0.38	0/42207	0.62	16/57061 (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
1	B	0	1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	31	GLU	C-N-CD	-21.47	73.37	120.60
1	H	31	GLU	C-N-CA	10.42	165.77	122.00
1	F	29	ALA	N-CA-C	-9.90	84.26	111.00
1	H	32	PRO	CA-N-CD	-7.14	101.50	111.50
1	F	25	TYR	N-CA-C	-6.34	93.88	111.00

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	64	0
1	B	1714	0	1688	58	0
1	C	1714	0	1688	49	0
1	D	1714	0	1688	63	0
1	E	1714	0	1688	92	0
1	F	1714	0	1688	161	0
1	G	1714	0	1688	71	0
1	H	1705	0	1677	130	0
1	I	1714	0	1688	62	0
1	J	1714	0	1688	60	0
1	K	1714	0	1688	59	0
1	L	1714	0	1688	50	0
1	M	1714	0	1688	64	0
1	N	1714	0	1688	48	0
1	O	1714	0	1688	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1714	0	1688	77	0
1	Q	1714	0	1688	65	0
1	R	1714	0	1688	77	0
1	S	1714	0	1688	59	0
1	T	1714	0	1688	76	0
1	U	1714	0	1688	53	0
1	V	1714	0	1688	63	0
1	W	1714	0	1688	55	0
1	X	1714	0	1688	52	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	4	0
4	W	118	0	0	8	0
4	X	93	0	0	2	0
All	All	43787	0	40618	1480	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 18.

The worst 5 of 1480 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%)	34	17
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%)	10	2
1	F	209/222 (94%)	168 (80%)	27 (13%)	14 (7%)	1	0
1	G	209/222 (94%)	191 (91%)	13 (6%)	5 (2%)	7	1
1	H	208/222 (94%)	171 (82%)	27 (13%)	10 (5%)	3	0
1	I	209/222 (94%)	194 (93%)	15 (7%)	0	100	100
1	J	209/222 (94%)	195 (93%)	13 (6%)	1 (0%)	34	17
1	K	209/222 (94%)	196 (94%)	13 (6%)	0	100	100
1	L	209/222 (94%)	196 (94%)	12 (6%)	1 (0%)	34	17
1	M	209/222 (94%)	193 (92%)	16 (8%)	0	100	100
1	N	209/222 (94%)	195 (93%)	13 (6%)	1 (0%)	34	17
1	O	209/222 (94%)	196 (94%)	8 (4%)	5 (2%)	7	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%)	19	5
1	S	209/222 (94%)	198 (95%)	10 (5%)	1 (0%)	34	17
1	T	209/222 (94%)	191 (91%)	17 (8%)	1 (0%)	34	17
1	U	209/222 (94%)	194 (93%)	13 (6%)	2 (1%)	19	5
1	V	209/222 (94%)	197 (94%)	12 (6%)	0	100	100
1	W	209/222 (94%)	197 (94%)	10 (5%)	2 (1%)	19	5
1	X	209/222 (94%)	193 (92%)	16 (8%)	0	100	100
All	All	5015/5328 (94%)	4635 (92%)	330 (7%)	50 (1%)	19	5

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%)	58	42
1	B	176/182 (97%)	172 (98%)	4 (2%)	58	42
1	C	176/182 (97%)	169 (96%)	7 (4%)	38	20
1	D	176/182 (97%)	172 (98%)	4 (2%)	58	42
1	E	176/182 (97%)	171 (97%)	5 (3%)	51	35
1	F	176/182 (97%)	164 (93%)	12 (7%)	20	6
1	G	176/182 (97%)	170 (97%)	6 (3%)	44	26
1	H	175/182 (96%)	168 (96%)	7 (4%)	38	20
1	I	176/182 (97%)	172 (98%)	4 (2%)	58	42
1	J	176/182 (97%)	170 (97%)	6 (3%)	44	26
1	K	176/182 (97%)	171 (97%)	5 (3%)	51	35
1	L	176/182 (97%)	172 (98%)	4 (2%)	58	42
1	M	176/182 (97%)	172 (98%)	4 (2%)	58	42
1	N	176/182 (97%)	170 (97%)	6 (3%)	44	26
1	O	176/182 (97%)	174 (99%)	2 (1%)	80	74
1	P	176/182 (97%)	173 (98%)	3 (2%)	68	57
1	Q	176/182 (97%)	169 (96%)	7 (4%)	38	20
1	R	176/182 (97%)	170 (97%)	6 (3%)	44	26
1	S	176/182 (97%)	173 (98%)	3 (2%)	68	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	176/182 (97%)	173 (98%)	3 (2%)	68	57
1	U	176/182 (97%)	174 (99%)	2 (1%)	80	74
1	V	176/182 (97%)	171 (97%)	5 (3%)	51	35
1	W	176/182 (97%)	173 (98%)	3 (2%)	68	57
1	X	176/182 (97%)	171 (97%)	5 (3%)	51	35
All	All	4223/4368 (97%)	4106 (97%)	117 (3%)	51	35

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	215	ASN
1	L	202	ASN
1	V	222	LEU
1	J	147	GLU
1	K	85	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 206 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	211	GLN
1	N	85	ASN
1	W	44	GLN
1	L	44	GLN
1	M	85	ASN

### 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 carbohydrates 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$
2	ACT	B	302	-	1,3,3	1.28	0	0,3,3	0.00	-
3	BME	B	402	-	3,3,3	1.95	1 (33%)	2,2,2	1.70	1 (50%)
2	ACT	D	304	-	1,3,3	0.92	0	0,3,3	0.00	-
3	BME	D	404	-	3,3,3	1.95	1 (33%)	2,2,2	1.79	1 (50%)
2	ACT	E	305	-	1,3,3	0.83	0	0,3,3	0.00	-
2	ACT	F	306	-	1,3,3	0.90	0	0,3,3	0.00	-
3	BME	F	406	-	3,3,3	1.98	1 (33%)	2,2,2	1.77	1 (50%)
2	ACT	H	308	-	1,3,3	1.22	0	0,3,3	0.00	-
3	BME	H	408	-	3,3,3	1.94	1 (33%)	2,2,2	1.81	1 (50%)
3	BME	I	410	-	3,3,3	2.00	1 (33%)	2,2,2	1.74	1 (50%)
2	ACT	J	310	-	1,3,3	0.94	0	0,3,3	0.00	-
3	BME	K	412	-	3,3,3	1.94	1 (33%)	2,2,2	1.79	1 (50%)
2	ACT	L	312	-	1,3,3	1.32	0	0,3,3	0.00	-
2	ACT	M	313	-	1,3,3	0.55	0	0,3,3	0.00	-
2	ACT	N	314	-	1,3,3	1.00	0	0,3,3	0.00	-
3	BME	N	414	-	3,3,3	1.99	1 (33%)	2,2,2	1.67	1 (50%)
2	ACT	O	315	-	1,3,3	1.00	0	0,3,3	0.00	-
2	ACT	P	316	-	1,3,3	0.46	0	0,3,3	0.00	-
3	BME	P	416	-	3,3,3	2.03	1 (33%)	2,2,2	1.75	1 (50%)
2	ACT	Q	317	-	1,3,3	1.18	0	0,3,3	0.00	-
3	BME	Q	418	-	3,3,3	1.98	1 (33%)	2,2,2	1.78	1 (50%)
2	ACT	R	318	-	1,3,3	0.98	0	0,3,3	0.00	-
2	ACT	S	319	-	1,3,3	0.42	0	0,3,3	0.00	-
2	ACT	T	320	-	1,3,3	0.95	0	0,3,3	0.00	-
3	BME	T	420	-	3,3,3	1.96	1 (33%)	2,2,2	1.78	1 (50%)
2	ACT	U	321	-	1,3,3	0.94	0	0,3,3	0.00	-
2	ACT	V	322	-	1,3,3	0.91	0	0,3,3	0.00	-
3	BME	V	422	-	3,3,3	1.93	1 (33%)	2,2,2	1.80	1 (50%)
2	ACT	W	323	-	1,3,3	1.54	0	0,3,3	0.00	-
2	ACT	X	324	-	1,3,3	1.34	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BME	X	424	-	3,3,3	2.01	1 (33%)	2,2,2	1.79	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
2	ACT	B	302	-	-	0/0/0/0	0/0/0/0
3	BME	B	402	-	-	0/1/1/1	0/0/0/0
2	ACT	D	304	-	-	0/0/0/0	0/0/0/0
3	BME	D	404	-	-	0/1/1/1	0/0/0/0
2	ACT	E	305	-	-	0/0/0/0	0/0/0/0
2	ACT	F	306	-	-	0/0/0/0	0/0/0/0
3	BME	F	406	-	-	0/1/1/1	0/0/0/0
2	ACT	H	308	-	-	0/0/0/0	0/0/0/0
3	BME	H	408	-	-	0/1/1/1	0/0/0/0
3	BME	I	410	-	-	0/1/1/1	0/0/0/0
2	ACT	J	310	-	-	0/0/0/0	0/0/0/0
3	BME	K	412	-	-	0/1/1/1	0/0/0/0
2	ACT	L	312	-	-	0/0/0/0	0/0/0/0
2	ACT	M	313	-	-	0/0/0/0	0/0/0/0
2	ACT	N	314	-	-	0/0/0/0	0/0/0/0
3	BME	N	414	-	-	0/1/1/1	0/0/0/0
2	ACT	O	315	-	-	0/0/0/0	0/0/0/0
2	ACT	P	316	-	-	0/0/0/0	0/0/0/0
3	BME	P	416	-	-	0/1/1/1	0/0/0/0
2	ACT	Q	317	-	-	0/0/0/0	0/0/0/0
3	BME	Q	418	-	-	0/1/1/1	0/0/0/0
2	ACT	R	318	-	-	0/0/0/0	0/0/0/0
2	ACT	S	319	-	-	0/0/0/0	0/0/0/0
2	ACT	T	320	-	-	0/0/0/0	0/0/0/0
3	BME	T	420	-	-	0/1/1/1	0/0/0/0
2	ACT	U	321	-	-	0/0/0/0	0/0/0/0
2	ACT	V	322	-	-	0/0/0/0	0/0/0/0
3	BME	V	422	-	-	0/1/1/1	0/0/0/0
2	ACT	W	323	-	-	0/0/0/0	0/0/0/0
2	ACT	X	324	-	-	0/0/0/0	0/0/0/0
3	BME	X	424	-	-	0/1/1/1	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	416	BME	O1-C1	-3.49	1.23	1.42
3	X	424	BME	O1-C1	-3.45	1.23	1.42
3	I	410	BME	O1-C1	-3.44	1.23	1.42
3	N	414	BME	O1-C1	-3.42	1.23	1.42
3	F	406	BME	O1-C1	-3.39	1.23	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	414	BME	O1-C1-C2	2.31	120.93	110.83
3	B	402	BME	O1-C1-C2	2.34	121.08	110.83
3	I	410	BME	O1-C1-C2	2.39	121.32	110.83
3	V	422	BME	O1-C1-C2	2.41	121.40	110.83
3	P	416	BME	O1-C1-C2	2.42	121.42	110.83

There are no chirality outliers.

There are no torsion outliers.

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

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/222 (93%)	-0.53	2 (0%) 84 82	7, 18, 33, 44	0
1	B	208/222 (93%)	-0.51	1 (0%) 91 90	11, 19, 33, 45	0
1	C	208/222 (93%)	-0.52	0 100 100	8, 19, 30, 39	0
1	D	208/222 (93%)	-0.28	1 (0%) 91 90	10, 22, 38, 42	0
1	E	208/222 (93%)	-0.36	0 100 100	9, 22, 40, 52	0
1	F	208/222 (93%)	0.60	18 (8%) 13 10	15, 37, 57, 66	1 (0%)
1	G	208/222 (93%)	-0.35	1 (0%) 91 90	10, 21, 41, 49	0
1	H	207/222 (93%)	0.24	8 (3%) 43 37	14, 32, 51, 56	0
1	I	208/222 (93%)	-0.58	0 100 100	8, 17, 32, 44	0
1	J	208/222 (93%)	-0.55	1 (0%) 91 90	10, 17, 33, 42	0
1	K	208/222 (93%)	-0.59	1 (0%) 91 90	7, 17, 31, 40	0
1	L	208/222 (93%)	-0.58	1 (0%) 91 90	9, 17, 31, 39	0
1	M	208/222 (93%)	-0.59	1 (0%) 91 90	8, 17, 31, 42	0
1	N	208/222 (93%)	-0.60	1 (0%) 91 90	9, 16, 28, 40	0
1	O	208/222 (93%)	-0.59	0 100 100	8, 17, 31, 41	0
1	P	208/222 (93%)	-0.55	1 (0%) 91 90	9, 18, 30, 43	0
1	Q	208/222 (93%)	-0.43	2 (0%) 84 82	8, 18, 35, 45	0
1	R	208/222 (93%)	-0.36	2 (0%) 84 82	11, 22, 38, 46	0
1	S	208/222 (93%)	-0.55	1 (0%) 91 90	8, 18, 33, 41	0
1	T	208/222 (93%)	-0.36	1 (0%) 91 90	14, 22, 37, 50	0
1	U	208/222 (93%)	-0.56	0 100 100	7, 18, 32, 40	0
1	V	208/222 (93%)	-0.60	1 (0%) 91 90	9, 17, 30, 43	0
1	W	208/222 (93%)	-0.58	0 100 100	8, 17, 31, 40	0
1	X	208/222 (93%)	-0.37	0 100 100	10, 21, 36, 42	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4991/5328 (93%)	-0.42	44 (0%) 85 83	7, 19, 40, 66	1 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	29	ALA	12.8
1	F	23	LEU	4.8
1	N	222	LEU	4.7
1	T	222	LEU	4.7
1	F	33	TYR	4.6

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	BME	N	414	4/4	0.74	0.18	13.28	49,50,51,56	0
3	BME	D	404	4/4	0.88	0.22	10.82	32,37,37,41	0
3	BME	Q	418	4/4	0.91	0.15	10.11	29,34,35,38	0
3	BME	X	424	4/4	0.90	0.16	10.05	30,32,34,40	0
3	BME	K	412	4/4	0.94	0.12	8.84	32,33,33,33	0
3	BME	T	420	4/4	0.85	0.14	7.71	32,33,33,39	0
3	BME	I	410	4/4	0.91	0.12	6.67	21,27,28,35	0
3	BME	B	402	4/4	0.94	0.12	6.64	26,30,30,34	0
3	BME	P	416	4/4	0.97	0.10	5.09	20,22,23,29	0
3	BME	H	408	4/4	0.88	0.17	4.99	36,37,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BME	V	422	4/4	0.88	0.17	4.83	41,43,43,43	0
3	BME	F	406	4/4	0.93	0.12	2.39	24,24,25,32	0
2	ACT	O	315	4/4	0.85	0.19	2.04	43,43,44,45	0
2	ACT	Q	317	4/4	0.80	0.26	1.61	49,49,49,50	0
2	ACT	H	308	4/4	0.82	0.16	1.49	38,39,39,41	0
2	ACT	U	321	4/4	0.82	0.17	1.24	42,42,42,43	0
2	ACT	J	310	4/4	0.95	0.13	0.31	29,30,30,30	0
2	ACT	P	316	4/4	0.94	0.13	0.08	24,25,26,28	0
2	ACT	E	305	4/4	0.98	0.10	0.03	19,20,21,21	0
2	ACT	W	323	4/4	0.87	0.11	0.03	27,28,29,29	0
2	ACT	D	304	4/4	0.88	0.11	-0.05	26,27,28,29	0
2	ACT	B	302	4/4	0.92	0.10	-0.16	27,28,29,30	0
2	ACT	T	320	4/4	0.91	0.09	-0.35	25,27,27,27	0
2	ACT	R	318	4/4	0.95	0.09	-0.36	28,28,28,29	0
2	ACT	V	322	4/4	0.97	0.09	-0.38	20,21,21,22	0
2	ACT	S	319	4/4	0.95	0.07	-0.44	28,29,30,30	0
2	ACT	M	313	4/4	0.97	0.08	-0.50	23,23,24,24	0
2	ACT	N	314	4/4	0.96	0.07	-0.56	20,21,22,22	0
2	ACT	F	306	4/4	0.91	0.11	-0.64	37,37,37,37	0
2	ACT	L	312	4/4	0.97	0.06	-0.77	20,20,21,22	0
2	ACT	X	324	4/4	0.98	0.07	-0.85	21,22,22,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.