Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 02:21 AM JST

PDB ID	:	5YTU
Title	:	Structure of human SOD1 complexed with isoproteranol in C2221 space group
Authors	:	Manjula, R.; Padmanabhan, B.
Deposited on	:	2017-11-20
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

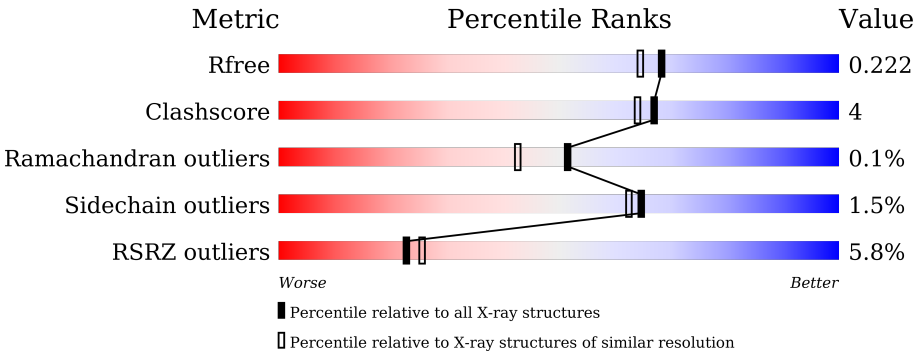
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	180	79% 6% 14%
1	B	180	80% 6% 14%
1	C	180	81% 14%
1	D	180	81% 14%
1	E	180	15% 77% 9% 14%
1	F	180	81% 14%

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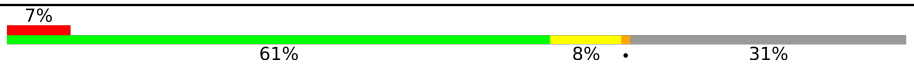
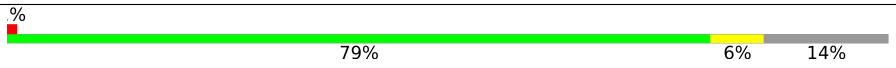
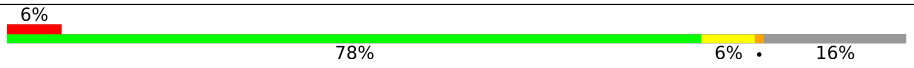
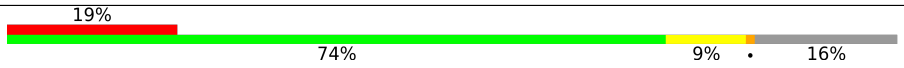
Mol	Chain	Length	Quality of chain
1	G	180	
1	H	180	
1	I	180	
1	J	180	

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
4	TAM	A	203	-	-	X	X
5	S4P	A	204	-	-	X	-
5	S4P	C	202	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12743 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	4	0
			1150	704	209	232	5			
1	H	154	Total	C	N	O	S	0	5	0
			1156	705	210	236	5			
1	B	154	Total	C	N	O	S	0	4	0
			1146	702	208	232	4			
1	C	154	Total	C	N	O	S	0	1	0
			1121	685	205	227	4			
1	D	154	Total	C	N	O	S	0	0	0
			1115	682	204	225	4			
1	E	155	Total	C	N	O	S	0	4	0
			1117	680	204	228	5			
1	F	154	Total	C	N	O	S	0	1	0
			1120	684	204	228	4			
1	G	125	Total	C	N	O	S	0	0	0
			894	554	159	177	4			
1	I	152	Total	C	N	O	S	0	1	0
			1099	671	201	223	4			
1	J	152	Total	C	N	O	S	0	2	0
			1108	678	202	224	4			

There are 260 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP P00441
A	-25	LYS	-	expression tag	UNP P00441
A	-24	HIS	-	expression tag	UNP P00441
A	-23	HIS	-	expression tag	UNP P00441
A	-22	HIS	-	expression tag	UNP P00441
A	-21	HIS	-	expression tag	UNP P00441
A	-20	HIS	-	expression tag	UNP P00441
A	-19	HIS	-	expression tag	UNP P00441
A	-18	PRO	-	expression tag	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP P00441
A	-16	SER	-	expression tag	UNP P00441
A	-15	ASP	-	expression tag	UNP P00441
A	-14	TYR	-	expression tag	UNP P00441
A	-13	ASP	-	expression tag	UNP P00441
A	-12	ILE	-	expression tag	UNP P00441
A	-11	PRO	-	expression tag	UNP P00441
A	-10	THR	-	expression tag	UNP P00441
A	-9	THR	-	expression tag	UNP P00441
A	-8	GLU	-	expression tag	UNP P00441
A	-7	ASN	-	expression tag	UNP P00441
A	-6	LEU	-	expression tag	UNP P00441
A	-5	TYR	-	expression tag	UNP P00441
A	-4	PHE	-	expression tag	UNP P00441
A	-3	GLN	-	expression tag	UNP P00441
A	-2	GLY	-	expression tag	UNP P00441
A	-1	ALA	-	expression tag	UNP P00441
H	-26	MET	-	initiating methionine	UNP P00441
H	-25	LYS	-	expression tag	UNP P00441
H	-24	HIS	-	expression tag	UNP P00441
H	-23	HIS	-	expression tag	UNP P00441
H	-22	HIS	-	expression tag	UNP P00441
H	-21	HIS	-	expression tag	UNP P00441
H	-20	HIS	-	expression tag	UNP P00441
H	-19	HIS	-	expression tag	UNP P00441
H	-18	PRO	-	expression tag	UNP P00441
H	-17	MET	-	expression tag	UNP P00441
H	-16	SER	-	expression tag	UNP P00441
H	-15	ASP	-	expression tag	UNP P00441
H	-14	TYR	-	expression tag	UNP P00441
H	-13	ASP	-	expression tag	UNP P00441
H	-12	ILE	-	expression tag	UNP P00441
H	-11	PRO	-	expression tag	UNP P00441
H	-10	THR	-	expression tag	UNP P00441
H	-9	THR	-	expression tag	UNP P00441
H	-8	GLU	-	expression tag	UNP P00441
H	-7	ASN	-	expression tag	UNP P00441
H	-6	LEU	-	expression tag	UNP P00441
H	-5	TYR	-	expression tag	UNP P00441
H	-4	PHE	-	expression tag	UNP P00441
H	-3	GLN	-	expression tag	UNP P00441
H	-2	GLY	-	expression tag	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	ALA	-	expression tag	UNP P00441
B	-26	MET	-	initiating methionine	UNP P00441
B	-25	LYS	-	expression tag	UNP P00441
B	-24	HIS	-	expression tag	UNP P00441
B	-23	HIS	-	expression tag	UNP P00441
B	-22	HIS	-	expression tag	UNP P00441
B	-21	HIS	-	expression tag	UNP P00441
B	-20	HIS	-	expression tag	UNP P00441
B	-19	HIS	-	expression tag	UNP P00441
B	-18	PRO	-	expression tag	UNP P00441
B	-17	MET	-	expression tag	UNP P00441
B	-16	SER	-	expression tag	UNP P00441
B	-15	ASP	-	expression tag	UNP P00441
B	-14	TYR	-	expression tag	UNP P00441
B	-13	ASP	-	expression tag	UNP P00441
B	-12	ILE	-	expression tag	UNP P00441
B	-11	PRO	-	expression tag	UNP P00441
B	-10	THR	-	expression tag	UNP P00441
B	-9	THR	-	expression tag	UNP P00441
B	-8	GLU	-	expression tag	UNP P00441
B	-7	ASN	-	expression tag	UNP P00441
B	-6	LEU	-	expression tag	UNP P00441
B	-5	TYR	-	expression tag	UNP P00441
B	-4	PHE	-	expression tag	UNP P00441
B	-3	GLN	-	expression tag	UNP P00441
B	-2	GLY	-	expression tag	UNP P00441
B	-1	ALA	-	expression tag	UNP P00441
C	-26	MET	-	initiating methionine	UNP P00441
C	-25	LYS	-	expression tag	UNP P00441
C	-24	HIS	-	expression tag	UNP P00441
C	-23	HIS	-	expression tag	UNP P00441
C	-22	HIS	-	expression tag	UNP P00441
C	-21	HIS	-	expression tag	UNP P00441
C	-20	HIS	-	expression tag	UNP P00441
C	-19	HIS	-	expression tag	UNP P00441
C	-18	PRO	-	expression tag	UNP P00441
C	-17	MET	-	expression tag	UNP P00441
C	-16	SER	-	expression tag	UNP P00441
C	-15	ASP	-	expression tag	UNP P00441
C	-14	TYR	-	expression tag	UNP P00441
C	-13	ASP	-	expression tag	UNP P00441
C	-12	ILE	-	expression tag	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	PRO	-	expression tag	UNP P00441
C	-10	THR	-	expression tag	UNP P00441
C	-9	THR	-	expression tag	UNP P00441
C	-8	GLU	-	expression tag	UNP P00441
C	-7	ASN	-	expression tag	UNP P00441
C	-6	LEU	-	expression tag	UNP P00441
C	-5	TYR	-	expression tag	UNP P00441
C	-4	PHE	-	expression tag	UNP P00441
C	-3	GLN	-	expression tag	UNP P00441
C	-2	GLY	-	expression tag	UNP P00441
C	-1	ALA	-	expression tag	UNP P00441
D	-26	MET	-	initiating methionine	UNP P00441
D	-25	LYS	-	expression tag	UNP P00441
D	-24	HIS	-	expression tag	UNP P00441
D	-23	HIS	-	expression tag	UNP P00441
D	-22	HIS	-	expression tag	UNP P00441
D	-21	HIS	-	expression tag	UNP P00441
D	-20	HIS	-	expression tag	UNP P00441
D	-19	HIS	-	expression tag	UNP P00441
D	-18	PRO	-	expression tag	UNP P00441
D	-17	MET	-	expression tag	UNP P00441
D	-16	SER	-	expression tag	UNP P00441
D	-15	ASP	-	expression tag	UNP P00441
D	-14	TYR	-	expression tag	UNP P00441
D	-13	ASP	-	expression tag	UNP P00441
D	-12	ILE	-	expression tag	UNP P00441
D	-11	PRO	-	expression tag	UNP P00441
D	-10	THR	-	expression tag	UNP P00441
D	-9	THR	-	expression tag	UNP P00441
D	-8	GLU	-	expression tag	UNP P00441
D	-7	ASN	-	expression tag	UNP P00441
D	-6	LEU	-	expression tag	UNP P00441
D	-5	TYR	-	expression tag	UNP P00441
D	-4	PHE	-	expression tag	UNP P00441
D	-3	GLN	-	expression tag	UNP P00441
D	-2	GLY	-	expression tag	UNP P00441
D	-1	ALA	-	expression tag	UNP P00441
E	-26	MET	-	initiating methionine	UNP P00441
E	-25	LYS	-	expression tag	UNP P00441
E	-24	HIS	-	expression tag	UNP P00441
E	-23	HIS	-	expression tag	UNP P00441
E	-22	HIS	-	expression tag	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	HIS	-	expression tag	UNP P00441
E	-20	HIS	-	expression tag	UNP P00441
E	-19	HIS	-	expression tag	UNP P00441
E	-18	PRO	-	expression tag	UNP P00441
E	-17	MET	-	expression tag	UNP P00441
E	-16	SER	-	expression tag	UNP P00441
E	-15	ASP	-	expression tag	UNP P00441
E	-14	TYR	-	expression tag	UNP P00441
E	-13	ASP	-	expression tag	UNP P00441
E	-12	ILE	-	expression tag	UNP P00441
E	-11	PRO	-	expression tag	UNP P00441
E	-10	THR	-	expression tag	UNP P00441
E	-9	THR	-	expression tag	UNP P00441
E	-8	GLU	-	expression tag	UNP P00441
E	-7	ASN	-	expression tag	UNP P00441
E	-6	LEU	-	expression tag	UNP P00441
E	-5	TYR	-	expression tag	UNP P00441
E	-4	PHE	-	expression tag	UNP P00441
E	-3	GLN	-	expression tag	UNP P00441
E	-2	GLY	-	expression tag	UNP P00441
E	-1	ALA	-	expression tag	UNP P00441
F	-26	MET	-	initiating methionine	UNP P00441
F	-25	LYS	-	expression tag	UNP P00441
F	-24	HIS	-	expression tag	UNP P00441
F	-23	HIS	-	expression tag	UNP P00441
F	-22	HIS	-	expression tag	UNP P00441
F	-21	HIS	-	expression tag	UNP P00441
F	-20	HIS	-	expression tag	UNP P00441
F	-19	HIS	-	expression tag	UNP P00441
F	-18	PRO	-	expression tag	UNP P00441
F	-17	MET	-	expression tag	UNP P00441
F	-16	SER	-	expression tag	UNP P00441
F	-15	ASP	-	expression tag	UNP P00441
F	-14	TYR	-	expression tag	UNP P00441
F	-13	ASP	-	expression tag	UNP P00441
F	-12	ILE	-	expression tag	UNP P00441
F	-11	PRO	-	expression tag	UNP P00441
F	-10	THR	-	expression tag	UNP P00441
F	-9	THR	-	expression tag	UNP P00441
F	-8	GLU	-	expression tag	UNP P00441
F	-7	ASN	-	expression tag	UNP P00441
F	-6	LEU	-	expression tag	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	TYR	-	expression tag	UNP P00441
F	-4	PHE	-	expression tag	UNP P00441
F	-3	GLN	-	expression tag	UNP P00441
F	-2	GLY	-	expression tag	UNP P00441
F	-1	ALA	-	expression tag	UNP P00441
G	-26	MET	-	initiating methionine	UNP P00441
G	-25	LYS	-	expression tag	UNP P00441
G	-24	HIS	-	expression tag	UNP P00441
G	-23	HIS	-	expression tag	UNP P00441
G	-22	HIS	-	expression tag	UNP P00441
G	-21	HIS	-	expression tag	UNP P00441
G	-20	HIS	-	expression tag	UNP P00441
G	-19	HIS	-	expression tag	UNP P00441
G	-18	PRO	-	expression tag	UNP P00441
G	-17	MET	-	expression tag	UNP P00441
G	-16	SER	-	expression tag	UNP P00441
G	-15	ASP	-	expression tag	UNP P00441
G	-14	TYR	-	expression tag	UNP P00441
G	-13	ASP	-	expression tag	UNP P00441
G	-12	ILE	-	expression tag	UNP P00441
G	-11	PRO	-	expression tag	UNP P00441
G	-10	THR	-	expression tag	UNP P00441
G	-9	THR	-	expression tag	UNP P00441
G	-8	GLU	-	expression tag	UNP P00441
G	-7	ASN	-	expression tag	UNP P00441
G	-6	LEU	-	expression tag	UNP P00441
G	-5	TYR	-	expression tag	UNP P00441
G	-4	PHE	-	expression tag	UNP P00441
G	-3	GLN	-	expression tag	UNP P00441
G	-2	GLY	-	expression tag	UNP P00441
G	-1	ALA	-	expression tag	UNP P00441
I	-26	MET	-	initiating methionine	UNP P00441
I	-25	LYS	-	expression tag	UNP P00441
I	-24	HIS	-	expression tag	UNP P00441
I	-23	HIS	-	expression tag	UNP P00441
I	-22	HIS	-	expression tag	UNP P00441
I	-21	HIS	-	expression tag	UNP P00441
I	-20	HIS	-	expression tag	UNP P00441
I	-19	HIS	-	expression tag	UNP P00441
I	-18	PRO	-	expression tag	UNP P00441
I	-17	MET	-	expression tag	UNP P00441
I	-16	SER	-	expression tag	UNP P00441

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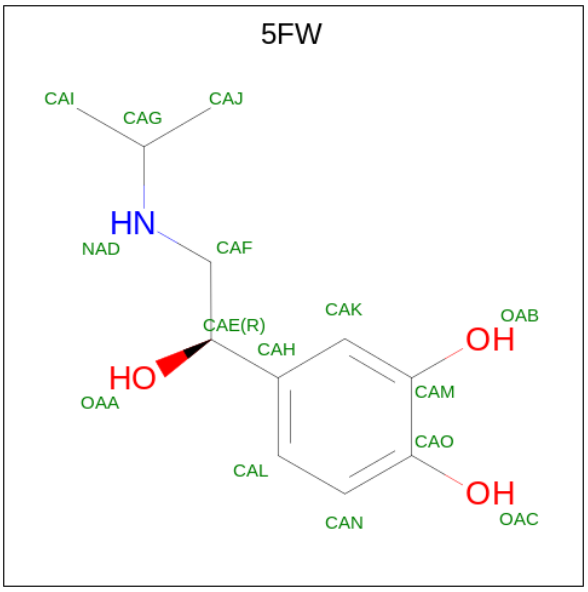
Chain	Residue	Modelled	Actual	Comment	Reference
I	-15	ASP	-	expression tag	UNP P00441
I	-14	TYR	-	expression tag	UNP P00441
I	-13	ASP	-	expression tag	UNP P00441
I	-12	ILE	-	expression tag	UNP P00441
I	-11	PRO	-	expression tag	UNP P00441
I	-10	THR	-	expression tag	UNP P00441
I	-9	THR	-	expression tag	UNP P00441
I	-8	GLU	-	expression tag	UNP P00441
I	-7	ASN	-	expression tag	UNP P00441
I	-6	LEU	-	expression tag	UNP P00441
I	-5	TYR	-	expression tag	UNP P00441
I	-4	PHE	-	expression tag	UNP P00441
I	-3	GLN	-	expression tag	UNP P00441
I	-2	GLY	-	expression tag	UNP P00441
I	-1	ALA	-	expression tag	UNP P00441
J	-26	MET	-	initiating methionine	UNP P00441
J	-25	LYS	-	expression tag	UNP P00441
J	-24	HIS	-	expression tag	UNP P00441
J	-23	HIS	-	expression tag	UNP P00441
J	-22	HIS	-	expression tag	UNP P00441
J	-21	HIS	-	expression tag	UNP P00441
J	-20	HIS	-	expression tag	UNP P00441
J	-19	HIS	-	expression tag	UNP P00441
J	-18	PRO	-	expression tag	UNP P00441
J	-17	MET	-	expression tag	UNP P00441
J	-16	SER	-	expression tag	UNP P00441
J	-15	ASP	-	expression tag	UNP P00441
J	-14	TYR	-	expression tag	UNP P00441
J	-13	ASP	-	expression tag	UNP P00441
J	-12	ILE	-	expression tag	UNP P00441
J	-11	PRO	-	expression tag	UNP P00441
J	-10	THR	-	expression tag	UNP P00441
J	-9	THR	-	expression tag	UNP P00441
J	-8	GLU	-	expression tag	UNP P00441
J	-7	ASN	-	expression tag	UNP P00441
J	-6	LEU	-	expression tag	UNP P00441
J	-5	TYR	-	expression tag	UNP P00441
J	-4	PHE	-	expression tag	UNP P00441
J	-3	GLN	-	expression tag	UNP P00441
J	-2	GLY	-	expression tag	UNP P00441
J	-1	ALA	-	expression tag	UNP P00441

- Molecule 2 is ISOPRENALINE (three-letter code: 5FW) (formula: $C_{11}H_{17}NO_3$).

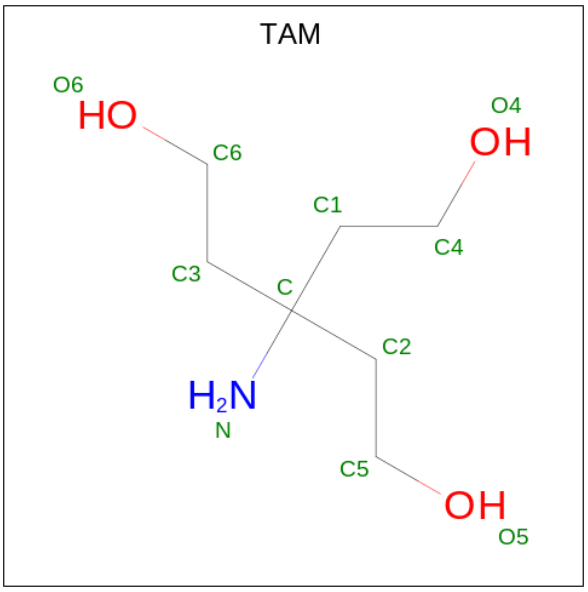


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 7 3	0	0

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

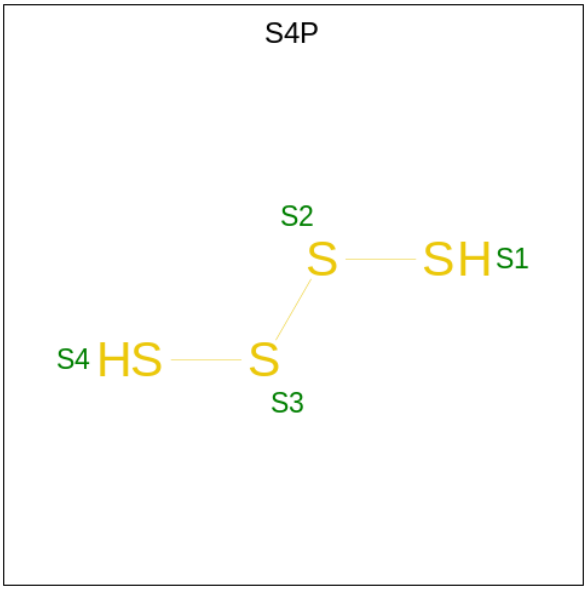
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



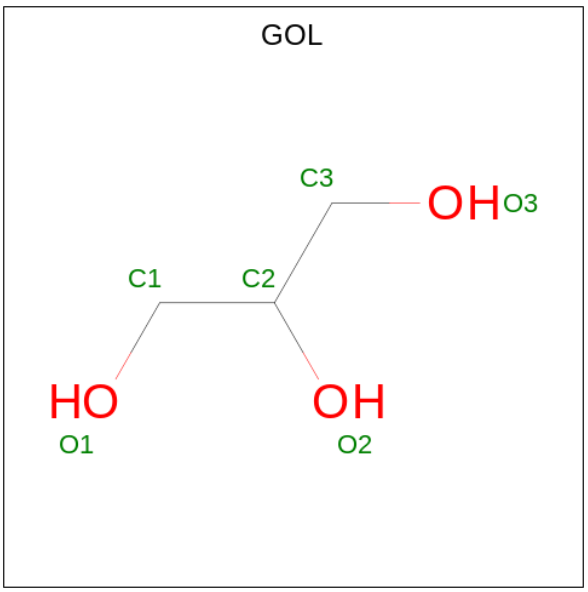
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 11 7 1 3	0	0

- Molecule 5 is Dihydrogen tetrasulfide (three-letter code: S4P) (formula: H_2S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 4 4	0	0
5	C	1	Total S 4 4	0	0
5	E	1	Total S 4 4	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	244	Total O 248 248	0	4
7	H	170	Total O 173 173	0	3
7	B	228	Total O 236 236	0	8
7	C	165	Total O 171 171	0	6
7	D	241	Total O 246 246	0	5
7	E	127	Total O 128 128	0	1
7	F	178	Total O 180 180	0	2
7	G	77	Total O 78 78	0	1
7	I	101	Total O 102 102	0	1

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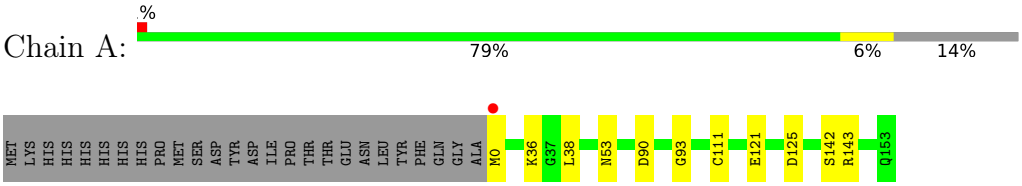
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	100	Total O 101 101	0	1

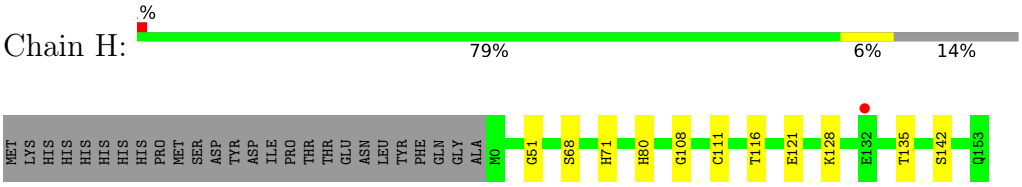
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

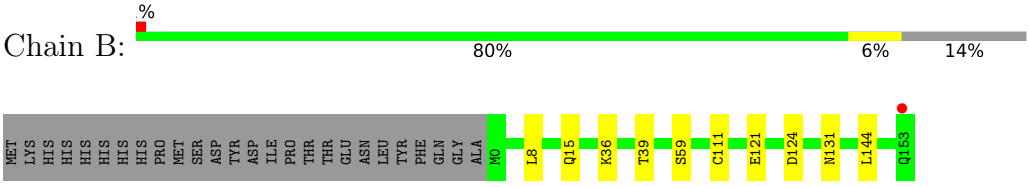
• Molecule 1: Superoxide dismutase [Cu-Zn]



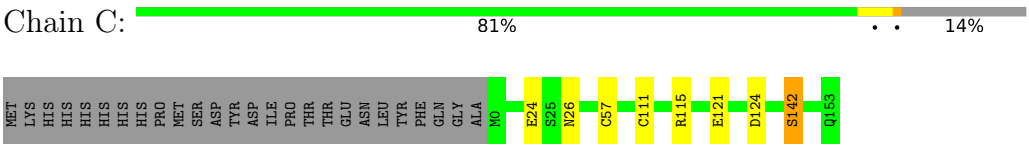
• Molecule 1: Superoxide dismutase [Cu-Zn]



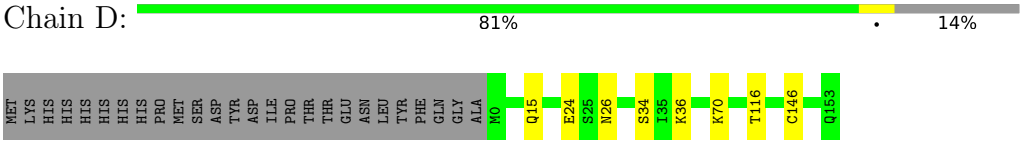
• Molecule 1: Superoxide dismutase [Cu-Zn]



• Molecule 1: Superoxide dismutase [Cu-Zn]

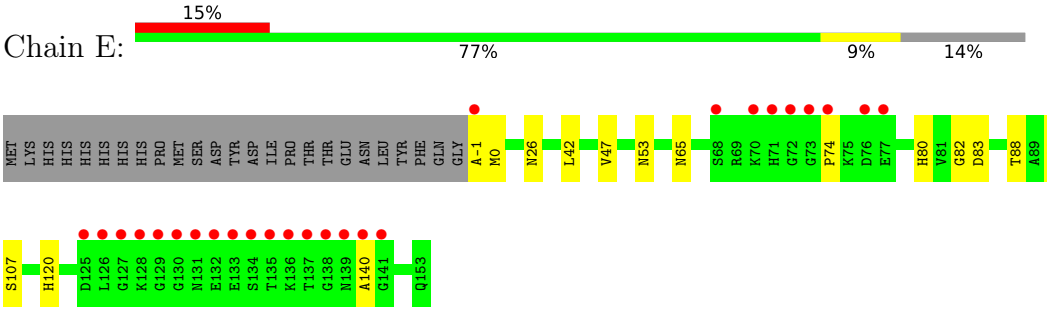


• Molecule 1: Superoxide dismutase [Cu-Zn]



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain E:



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain F:

• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain G:

• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain I:

• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain J:

• Molecule 1: Superoxide dismutase [Cu-Zn]

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	164.52Å 203.79Å 144.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 47.95 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-1.90) 95.8 (47.95-1.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.221 0.179 , 0.222	Depositor DCC
R_{free} test set	9225 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12743	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5FW, TAM, S4P, GOL

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	0.82	0/1168	0.80	2/1572 (0.1%)
1	B	0.76	0/1164	0.83	1/1569 (0.1%)
1	C	0.69	0/1139	0.81	3/1535 (0.2%)
1	D	0.73	0/1133	0.77	0/1527
1	E	0.62	0/1135	0.75	1/1536 (0.1%)
1	F	0.63	0/1138	0.74	0/1535
1	G	0.51	0/908	0.68	0/1228
1	H	0.71	0/1174	0.84	0/1581
1	I	0.54	0/1117	0.68	0/1508
1	J	0.52	0/1126	0.66	0/1521
All	All	0.66	0/11202	0.76	7/15112 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	115	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	115	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	124	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	125	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	124	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	90	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	90	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1150	0	1117	10	0
1	B	1146	0	1108	7	0
1	C	1121	0	1083	8	0
1	D	1115	0	1079	4	0
1	E	1117	0	1038	14	0
1	F	1120	0	1073	5	0
1	G	894	0	854	8	0
1	H	1156	0	1114	9	0
1	I	1099	0	1047	9	0
1	J	1108	0	1053	10	0
2	A	10	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	11	0	17	8	0
5	A	4	0	0	4	0
5	C	4	0	0	6	0
5	E	4	0	0	0	0
6	B	6	0	8	2	0
6	H	6	0	8	0	0
7	A	248	0	0	4	2
7	B	236	0	0	1	0
7	C	171	0	0	2	2
7	D	246	0	0	1	1
7	E	128	0	0	6	0
7	F	180	0	0	2	1
7	G	78	0	0	0	0
7	H	173	0	0	3	1
7	I	102	0	0	6	1
7	J	101	0	0	1	0
All	All	12743	0	10603	85	4

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 4.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HE	4:A:203:TAM:H12	1.02	1.15
1:I:6:CYS:SG	7:I:317:HOH:O	2.12	1.06
1:B:39:THR:HA	6:B:202:GOL:H32	1.41	1.01
1:A:143:ARG:NE	4:A:203:TAM:H12	1.87	0.89
1:A:111:CYS:SG	5:A:204:S4P:S1	2.75	0.85
5:A:204:S4P:S4	1:H:111:CYS:SG	2.74	0.84
1:E:42:LEU:HD23	1:E:88[A]:THR:HG22	1.57	0.84
1:C:111:CYS:SG	5:C:202:S4P:S4	2.75	0.84
1:J:2:THR:HG22	1:J:22:GLN:O	1.81	0.79
1:E:88[A]:THR:HG23	7:E:353:HOH:O	1.83	0.78
1:F:2:THR:CG2	7:F:444:HOH:O	2.32	0.78
1:A:111:CYS:SG	5:A:204:S4P:S2	2.83	0.76
1:E:83:ASP:HB3	7:E:329:HOH:O	1.87	0.75
1:E:42:LEU:CD2	1:E:88[A]:THR:HG22	2.21	0.70
1:J:2:THR:HG23	1:J:106:LEU:HD12	1.74	0.70
7:A:463:HOH:O	1:B:131:ASN:HB3	1.93	0.67
1:A:142:SER:HA	4:A:203:TAM:H22	1.77	0.67
1:H:121:GLU:HB2	1:H:142:SER:HB3	1.76	0.66
1:I:153:GLN:HB3	1:J:50:PHE:CZ	2.31	0.66
1:C:111:CYS:SG	5:C:202:S4P:S3	2.87	0.66
1:D:15:GLN:OE1	1:D:36:LYS:HE2	2.00	0.62
1:A:143:ARG:HE	4:A:203:TAM:C1	1.96	0.61
4:A:203:TAM:H41	4:A:203:TAM:O6	2.02	0.60
1:H:68[B]:SER:O	1:H:68[B]:SER:OG	2.18	0.59
1:E:53[A]:ASN:ND2	7:E:301:HOH:O	2.29	0.59
1:C:26:ASN:HA	1:E:26:ASN:HA	1.86	0.58
1:G:121:GLU:HG2	1:G:122:LYS:HE3	1.88	0.55
1:A:143:ARG:HH21	4:A:203:TAM:H41	1.72	0.55
1:C:121:GLU:HB2	1:C:142:SER:HB2	1.88	0.55
5:A:204:S4P:S3	1:H:111:CYS:SG	3.05	0.54
1:G:1:ALA:O	1:G:2:THR:HB	2.08	0.53
1:C:24:GLU:HG3	7:C:453:HOH:O	2.08	0.53
1:E:42:LEU:HD23	1:E:88[B]:THR:HB	1.90	0.52
1:G:105:SER:O	1:G:111:CYS:HA	2.10	0.51
6:B:202:GOL:H31	1:G:13:PRO:HA	1.93	0.50
1:F:75:LYS:NZ	7:F:303:HOH:O	2.44	0.50
1:A:121:GLU:HG3	7:A:480:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:CYS:SG	5:C:202:S4P:S1	3.10	0.49
1:A:38:LEU:O	1:A:93:GLY:HA2	2.12	0.49
1:A:53:ASN:ND2	7:A:308:HOH:O	2.46	0.49
1:J:136:LYS:HA	7:J:368:HOH:O	2.12	0.48
1:J:80:HIS:HB2	1:J:83:ASP:OD1	2.14	0.47
1:I:91:LYS:HD2	7:I:382:HOH:O	2.15	0.46
1:C:57:CYS:HB2	7:C:429:HOH:O	2.15	0.46
1:I:8:LEU:HD23	7:I:317:HOH:O	2.16	0.46
1:I:121:GLU:HA	1:I:144:LEU:HD11	1.97	0.46
1:E:47:VAL:HB	1:E:82:GLY:HA2	1.97	0.46
4:A:203:TAM:O6	4:A:203:TAM:C4	2.64	0.45
1:J:117:LEU:O	1:J:146:CYS:HA	2.17	0.45
1:E:120:HIS:HB3	1:E:140:ALA:O	2.16	0.45
1:B:8[B]:LEU:HD12	1:B:8[B]:LEU:N	2.32	0.45
1:B:111:CYS:SG	5:C:202:S4P:S2	3.06	0.44
1:F:121:GLU:HA	1:F:144:LEU:HD11	1.99	0.44
4:A:203:TAM:H32	7:A:485:HOH:O	2.17	0.44
1:D:24:GLU:HB3	1:D:26:ASN:OD1	2.18	0.44
1:B:15:GLN:HG2	7:B:346[B]:HOH:O	2.17	0.43
1:E:65:ASN:HA	7:E:305:HOH:O	2.16	0.43
1:G:80:HIS:ND1	1:G:81:VAL:O	2.49	0.43
1:D:116:THR:CG2	1:D:146:CYS:HB2	2.49	0.43
1:E:-1:ALA:HA	1:E:107:SER:CB	2.48	0.43
1:G:122:LYS:HA	1:G:122:LYS:HD3	1.82	0.43
1:J:127:GLY:HA2	1:J:134:SER:O	2.18	0.43
1:G:80:HIS:CD2	1:G:83:ASP:HB2	2.53	0.43
1:B:121:GLU:HA	1:B:144:LEU:HD11	1.99	0.43
1:I:7:VAL:C	7:I:317:HOH:O	2.57	0.43
1:J:121:GLU:HB2	1:J:144:LEU:HD21	2.00	0.43
1:H:135:THR:HA	7:H:350:HOH:O	2.18	0.42
1:C:111:CYS:HB3	5:C:202:S4P:S4	2.59	0.42
1:F:118:VAL:HG22	1:F:146:CYS:HB3	2.01	0.42
1:H:108:GLY:C	7:H:315:HOH:O	2.58	0.41
1:H:128:LYS:HD2	7:H:421:HOH:O	2.20	0.41
1:E:88[B]:THR:HG22	7:E:353:HOH:O	2.18	0.41
1:G:49:GLU:O	1:G:115:ARG:HD3	2.19	0.41
1:J:25:SER:C	1:J:27:GLY:H	2.23	0.41
1:I:92:ASP:HB2	7:I:367:HOH:O	2.20	0.41
1:J:15:GLN:HG3	1:J:36:LYS:HZ3	1.86	0.41
1:H:71:HIS:HB2	1:H:80:HIS:CE1	2.56	0.41
1:D:70:LYS:HE3	7:D:501:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:GLY:O	1:F:139:ASN:HB2	2.20	0.41
1:I:5:VAL:HG22	1:I:6:CYS:N	2.35	0.41
1:C:111:CYS:CB	5:C:202:S4P:S4	3.09	0.40
1:H:51:GLY:HA2	1:H:116:THR:OG1	2.22	0.40
1:E:80:HIS:HB2	1:E:83:ASP:OD1	2.22	0.40
1:I:9:LYS:HD2	7:I:306:HOH:O	2.21	0.40
1:E:74:PRO:HD2	7:E:377:HOH:O	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:380:HOH:O	7:D:414:HOH:O[3_455]	2.09	0.11
7:A:498:HOH:O	7:H:431:HOH:O[4_555]	2.14	0.06
7:C:431:HOH:O	7:F:457:HOH:O[8_555]	2.14	0.06
7:C:351:HOH:O	7:I:370:HOH:O[7_455]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/180 (87%)	155 (99%)	1 (1%)	0	100	100
1	B	156/180 (87%)	156 (100%)	0	0	100	100
1	C	153/180 (85%)	150 (98%)	3 (2%)	0	100	100
1	D	152/180 (84%)	151 (99%)	1 (1%)	0	100	100
1	E	157/180 (87%)	150 (96%)	7 (4%)	0	100	100
1	F	153/180 (85%)	152 (99%)	1 (1%)	0	100	100
1	G	119/180 (66%)	115 (97%)	3 (2%)	1 (1%)	19	9
1	H	157/180 (87%)	157 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	151/180 (84%)	148 (98%)	3 (2%)	0	100 100
1	J	152/180 (84%)	149 (98%)	3 (2%)	0	100 100
All	All	1506/1800 (84%)	1483 (98%)	22 (2%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	2	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	123/143 (86%)	120 (98%)	3 (2%)	49 43
1	B	122/143 (85%)	120 (98%)	2 (2%)	62 60
1	C	119/143 (83%)	118 (99%)	1 (1%)	81 82
1	D	118/143 (82%)	117 (99%)	1 (1%)	81 82
1	E	114/143 (80%)	113 (99%)	1 (1%)	78 79
1	F	118/143 (82%)	118 (100%)	0	100 100
1	G	94/143 (66%)	91 (97%)	3 (3%)	39 30
1	H	124/143 (87%)	124 (100%)	0	100 100
1	I	116/143 (81%)	113 (97%)	3 (3%)	46 39
1	J	116/143 (81%)	112 (97%)	4 (3%)	37 28
All	All	1164/1430 (81%)	1146 (98%)	18 (2%)	65 62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	36[A]	LYS
1	A	36[B]	LYS

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Mol	Chain	Res	Type
1	B	36	LYS
1	B	59	SER
1	C	142	SER
1	D	34	SER
1	E	0	MET
1	G	34	SER
1	G	99	ILE
1	G	124	ASP
1	I	9	LYS
1	I	59	SER
1	I	68	SER
1	J	2	THR
1	J	25	SER
1	J	59	SER
1	J	100	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	15	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
5	S4P	C	202	-	1,3,3	1.50	0	0,2,2	-	-
5	S4P	A	204	-	1,3,3	1.48	0	0,2,2	-	-
2	5FW	A	201	-	10,10,15	0.76	0	13,13,20	0.65	0
6	GOL	B	202	-	5,5,5	0.34	0	5,5,5	1.05	0
4	TAM	A	203	-	7,10,10	1.02	1 (14%)	9,12,12	1.78	3 (33%)
5	S4P	E	202	-	1,3,3	0.55	0	0,2,2	-	-
6	GOL	H	202	-	5,5,5	0.33	0	5,5,5	0.28	0

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
5	S4P	C	202	-	-	0/0/1/1	-
5	S4P	A	204	-	-	0/0/1/1	-
2	5FW	A	201	-	-	0/2/2/9	0/1/1/1
6	GOL	B	202	-	-	2/4/4/4	-
4	TAM	A	203	-	-	3/12/12/12	-
5	S4P	E	202	-	-	0/0/1/1	-
6	GOL	H	202	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	TAM	C1-C4	2.04	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	203	TAM	O4-C4-C1	3.65	121.14	111.39
4	A	203	TAM	C2-C-C1	2.50	114.91	110.50
4	A	203	TAM	C3-C-C2	-2.04	106.91	110.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	TAM	C1-C-C3-C6
4	A	203	TAM	C2-C-C3-C6
4	A	203	TAM	N-C-C3-C6
6	B	202	GOL	O1-C1-C2-C3
6	B	202	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	202	S4P	6	0
5	A	204	S4P	4	0
6	B	202	GOL	2	0
4	A	203	TAM	8	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	154/180 (85%)	-0.17	1 (0%) 89 90	16, 21, 36, 60	0
1	B	154/180 (85%)	-0.00	1 (0%) 89 90	16, 23, 42, 56	0
1	C	154/180 (85%)	-0.07	0 100 100	19, 32, 48, 60	0
1	D	154/180 (85%)	-0.04	0 100 100	18, 24, 43, 55	0
1	E	155/180 (86%)	0.58	27 (17%) 1 1	22, 36, 75, 88	0
1	F	154/180 (85%)	-0.23	0 100 100	23, 33, 52, 66	0
1	G	125/180 (69%)	0.24	12 (9%) 8 9	29, 40, 65, 77	0
1	H	154/180 (85%)	0.09	1 (0%) 89 90	17, 30, 51, 69	0
1	I	152/180 (84%)	0.33	11 (7%) 15 17	29, 43, 65, 80	0
1	J	152/180 (84%)	0.95	34 (22%) 0 0	33, 48, 69, 78	0
All	All	1508/1800 (83%)	0.17	87 (5%) 23 25	16, 33, 61, 88	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	130	GLY	6.8
1	E	135	THR	5.9
1	G	1	ALA	5.8
1	I	25	SER	5.0
1	J	129	GLY	4.8
1	E	131	ASN	4.7
1	J	131	ASN	4.6
1	E	68	SER	4.6
1	E	137	THR	4.5
1	J	135	THR	4.5
1	J	130	GLY	4.4
1	E	129	GLY	4.2
1	E	132	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	132	GLU	4.1
1	J	67	LEU	4.0
1	J	68	SER	4.0
1	E	138	GLY	4.0
1	E	76	ASP	4.0
1	I	153	GLN	3.9
1	J	110	HIS	3.9
1	I	26	ASN	3.9
1	E	126	LEU	3.8
1	G	28	PRO	3.7
1	G	25	SER	3.7
1	J	77	GLU	3.7
1	J	26	ASN	3.7
1	J	69	ARG	3.7
1	E	136	LYS	3.6
1	E	133	GLU	3.6
1	E	71	HIS	3.5
1	J	109	ASP	3.5
1	G	27	GLY	3.3
1	J	55	ALA	3.2
1	E	139	ASN	3.2
1	H	132	GLU	3.2
1	J	128	LYS	3.2
1	G	23	LYS	3.1
1	J	133	GLU	3.1
1	G	153	GLN	3.0
1	E	140	ALA	3.0
1	A	0	MET	3.0
1	J	137	THR	2.9
1	E	128	LYS	2.9
1	E	127	GLY	2.9
1	J	134	SER	2.9
1	I	28	PRO	2.9
1	J	136	LYS	2.9
1	J	127	GLY	2.9
1	J	140	ALA	2.9
1	I	23	LYS	2.8
1	I	109	ASP	2.8
1	J	27	GLY	2.8
1	I	102	SER	2.8
1	E	74	PRO	2.8
1	E	125	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	134	SER	2.8
1	J	70	LYS	2.7
1	G	109	ASP	2.7
1	E	70	LYS	2.7
1	I	110	HIS	2.6
1	J	57	CYS	2.6
1	J	138	GLY	2.6
1	I	27	GLY	2.6
1	G	125	ASP	2.5
1	E	77	GLU	2.5
1	J	80	HIS	2.5
1	E	96	ASP	2.4
1	E	-1	ALA	2.4
1	J	58	THR	2.4
1	E	72	GLY	2.4
1	J	62	PRO	2.4
1	J	71	HIS	2.3
1	J	72	GLY	2.3
1	E	141	GLY	2.3
1	G	30	LYS	2.3
1	B	153	GLN	2.3
1	J	108	GLY	2.2
1	J	11	ASP	2.2
1	E	73	GLY	2.2
1	G	82	GLY	2.2
1	J	106	LEU	2.1
1	J	78	GLU	2.1
1	G	102	SER	2.1
1	J	139	ASN	2.0
1	G	24	GLU	2.0
1	I	11	ASP	2.0
1	I	67	LEU	2.0

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 monosaccharides 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, 95^{th} 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
6	GOL	H	202	6/6	0.75	0.26	63,66,68,71	0
4	TAM	A	203	11/11	0.78	0.42	39,56,61,66	0
6	GOL	B	202	6/6	0.85	0.32	39,43,50,57	0
5	S4P	C	202	4/4	0.90	0.16	69,69,70,85	0
5	S4P	E	202	4/4	0.90	0.17	55,59,63,72	0
5	S4P	A	204	4/4	0.91	0.23	70,75,79,89	0
2	5FW	A	201	10/15	0.92	0.15	32,45,60,67	0
3	ZN	E	201	1/1	0.96	0.15	61,61,61,61	0
3	ZN	F	201	1/1	0.97	0.06	35,35,35,35	0
3	ZN	H	201	1/1	0.98	0.04	37,37,37,37	0
3	ZN	J	201	1/1	0.98	0.09	60,60,60,60	0
3	ZN	I	201	1/1	0.99	0.03	39,39,39,39	0
3	ZN	C	201	1/1	0.99	0.04	41,41,41,41	0
3	ZN	A	202	1/1	1.00	0.06	24,24,24,24	0
3	ZN	D	201	1/1	1.00	0.08	25,25,25,25	0
3	ZN	B	201	1/1	1.00	0.07	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.