Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:33 pm BST

PDB ID	:	6FP6
Title	:	Complex of human Cu,Zn SOD1 with the human copper chaperone for SOD1 in a compact conformation
Authors	:	Sala, F.A.; Wright, G.S.A.; Antonyuk, S.V.; Garratt, R.C.; Hasnain, S.S.
Deposited on	:	2018-02-09
Resolution	:	3.00 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 ⓘ symbol.

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

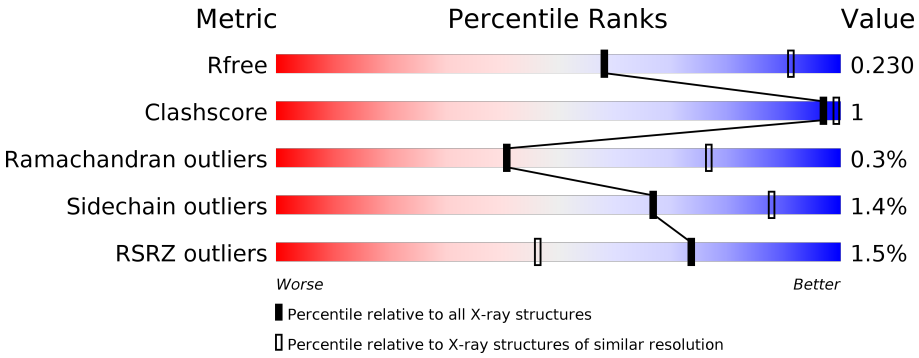
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	153	99%
1	C	153	98%
1	E	153	99%
1	G	153	99%
1	I	153	% 97%
1	K	153	% 98%

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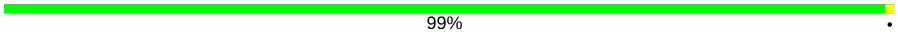
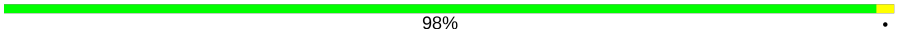
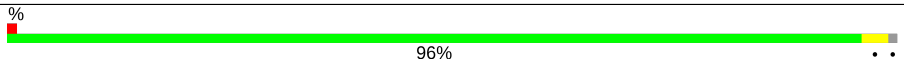
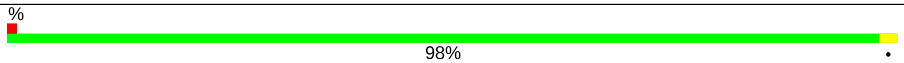
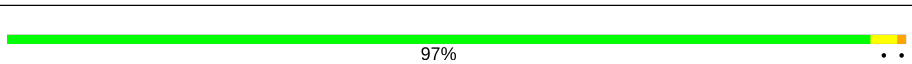
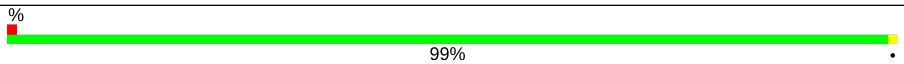
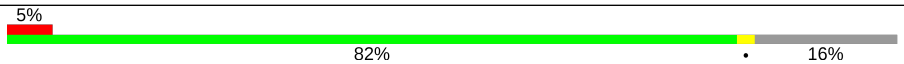
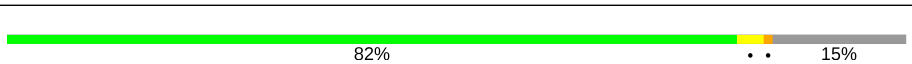
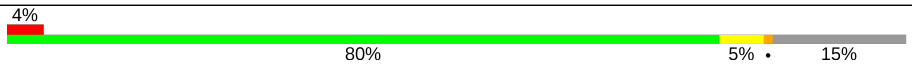
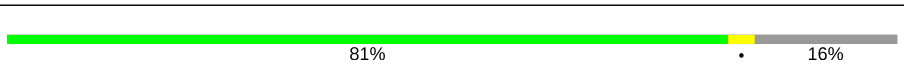
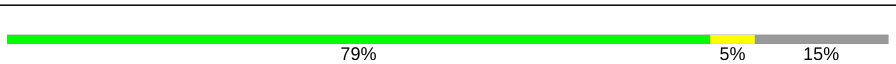
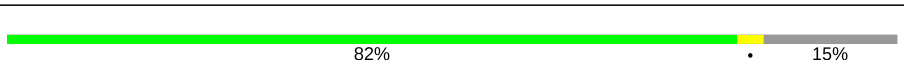
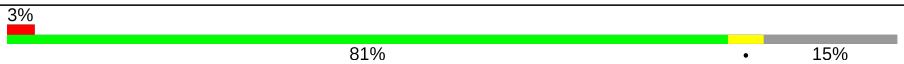
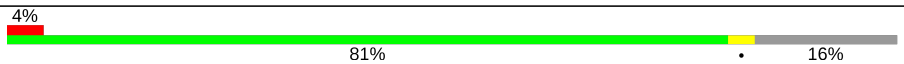
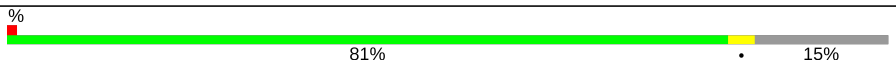
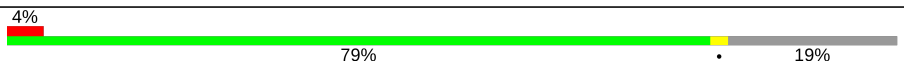
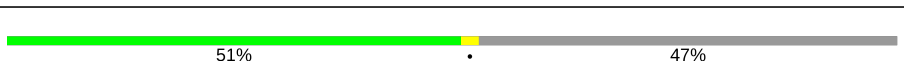
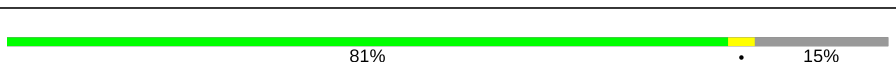
Mol	Chain	Length	Quality of chain
1	M	153	
1	O	153	
1	Q	153	
1	S	153	
1	U	153	
1	W	153	
2	B	274	
2	D	274	
2	F	274	
2	H	274	
2	J	274	
2	L	274	
2	N	274	
2	P	274	
2	R	274	
2	T	274	
2	V	274	
2	X	274	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 33247 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1104	676	202	224	2			
1	C	153	Total	C	N	O	S	0	0	0
			1108	679	203	224	2			
1	E	153	Total	C	N	O	S	0	0	0
			1108	679	203	224	2			
1	G	153	Total	C	N	O	S	0	0	0
			1108	679	203	224	2			
1	I	153	Total	C	N	O	S	0	1	0
			1119	689	204	224	2			
1	K	153	Total	C	N	O	S	0	0	0
			1108	679	203	224	2			
1	M	153	Total	C	N	O	S	0	0	0
			1108	679	203	224	2			
1	O	153	Total	C	N	O	S	0	0	0
			1104	677	203	222	2			
1	Q	151	Total	C	N	O	S	0	0	0
			1085	666	197	220	2			
1	S	153	Total	C	N	O	S	0	0	0
			1108	679	203	224	2			
1	U	153	Total	C	N	O	S	0	0	0
			1108	679	203	224	2			
1	W	153	Total	C	N	O	S	0	0	0
			1104	676	202	224	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	CYS	engineered mutation	UNP P00441
A	146	ALA	CYS	engineered mutation	UNP P00441
C	57	ALA	CYS	engineered mutation	UNP P00441
C	146	ALA	CYS	engineered mutation	UNP P00441
E	57	ALA	CYS	engineered mutation	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
E	146	ALA	CYS	engineered mutation	UNP P00441
G	57	ALA	CYS	engineered mutation	UNP P00441
G	146	ALA	CYS	engineered mutation	UNP P00441
I	57	ALA	CYS	engineered mutation	UNP P00441
I	146	ALA	CYS	engineered mutation	UNP P00441
K	57	ALA	CYS	engineered mutation	UNP P00441
K	146	ALA	CYS	engineered mutation	UNP P00441
M	57	ALA	CYS	engineered mutation	UNP P00441
M	146	ALA	CYS	engineered mutation	UNP P00441
O	57	ALA	CYS	engineered mutation	UNP P00441
O	146	ALA	CYS	engineered mutation	UNP P00441
Q	57	ALA	CYS	engineered mutation	UNP P00441
Q	146	ALA	CYS	engineered mutation	UNP P00441
S	57	ALA	CYS	engineered mutation	UNP P00441
S	146	ALA	CYS	engineered mutation	UNP P00441
U	57	ALA	CYS	engineered mutation	UNP P00441
U	146	ALA	CYS	engineered mutation	UNP P00441
W	57	ALA	CYS	engineered mutation	UNP P00441
W	146	ALA	CYS	engineered mutation	UNP P00441

- Molecule 2 is a protein called Copper chaperone for superoxide dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	231	Total	C	N	O	S	0	0	0
			1699	1039	315	337	8			
2	D	234	Total	C	N	O	S	0	0	0
			1724	1056	322	338	8			
2	F	234	Total	C	N	O	S	0	0	0
			1724	1056	319	341	8			
2	H	230	Total	C	N	O	S	0	0	0
			1692	1037	313	334	8			
2	J	232	Total	C	N	O	S	0	0	0
			1709	1046	318	337	8			
2	L	234	Total	C	N	O	S	0	0	0
			1731	1059	323	341	8			
2	N	234	Total	C	N	O	S	0	0	0
			1723	1055	322	338	8			
2	P	231	Total	C	N	O	S	0	0	0
			1702	1043	315	336	8			
2	R	232	Total	C	N	O	S	0	0	0
			1700	1040	315	337	8			
2	T	223	Total	C	N	O	S	0	0	0
			1638	1002	308	321	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	146	Total	C	N	O	S	0	0	0
			1091	663	209	214	5			
2	X	232	Total	C	N	O	S	0	0	0
			1707	1046	316	337	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	CYS	engineered mutation	UNP O14618
B	22	ALA	CYS	engineered mutation	UNP O14618
B	25	ALA	CYS	engineered mutation	UNP O14618
D	12	ALA	CYS	engineered mutation	UNP O14618
D	22	ALA	CYS	engineered mutation	UNP O14618
D	25	ALA	CYS	engineered mutation	UNP O14618
F	12	ALA	CYS	engineered mutation	UNP O14618
F	22	ALA	CYS	engineered mutation	UNP O14618
F	25	ALA	CYS	engineered mutation	UNP O14618
H	12	ALA	CYS	engineered mutation	UNP O14618
H	22	ALA	CYS	engineered mutation	UNP O14618
H	25	ALA	CYS	engineered mutation	UNP O14618
J	12	ALA	CYS	engineered mutation	UNP O14618
J	22	ALA	CYS	engineered mutation	UNP O14618
J	25	ALA	CYS	engineered mutation	UNP O14618
L	12	ALA	CYS	engineered mutation	UNP O14618
L	22	ALA	CYS	engineered mutation	UNP O14618
L	25	ALA	CYS	engineered mutation	UNP O14618
N	12	ALA	CYS	engineered mutation	UNP O14618
N	22	ALA	CYS	engineered mutation	UNP O14618
N	25	ALA	CYS	engineered mutation	UNP O14618
P	12	ALA	CYS	engineered mutation	UNP O14618
P	22	ALA	CYS	engineered mutation	UNP O14618
P	25	ALA	CYS	engineered mutation	UNP O14618
R	12	ALA	CYS	engineered mutation	UNP O14618
R	22	ALA	CYS	engineered mutation	UNP O14618
R	25	ALA	CYS	engineered mutation	UNP O14618
T	12	ALA	CYS	engineered mutation	UNP O14618
T	22	ALA	CYS	engineered mutation	UNP O14618
T	25	ALA	CYS	engineered mutation	UNP O14618
V	12	ALA	CYS	engineered mutation	UNP O14618
V	22	ALA	CYS	engineered mutation	UNP O14618
V	25	ALA	CYS	engineered mutation	UNP O14618
X	12	ALA	CYS	engineered mutation	UNP O14618

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Chain	Residue	Modelled	Actual	Comment	Reference
X	22	ALA	CYS	engineered mutation	UNP O14618
X	25	ALA	CYS	engineered mutation	UNP O14618

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

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

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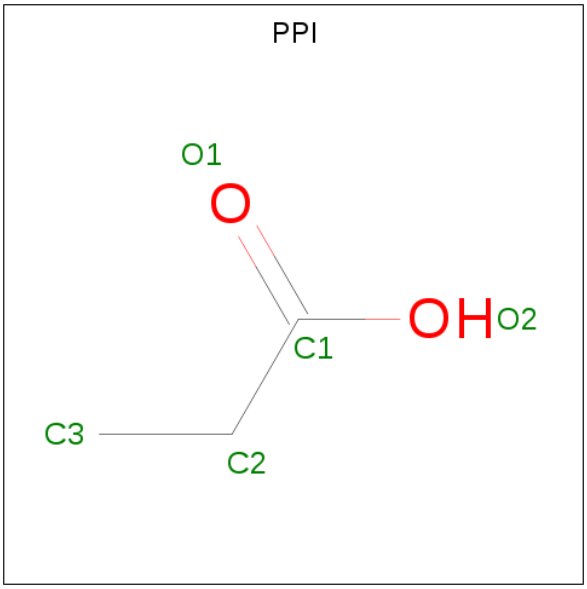
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Q	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	T	1	Total Zn 1 1	0	0
3	O	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is PROPANOIC ACID (three-letter code: PPI) (formula: $C_3H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	I	1	Total C O 5 3 2	0	0
4	K	1	Total C O 5 3 2	0	0
4	K	1	Total C O 5 3 2	0	0

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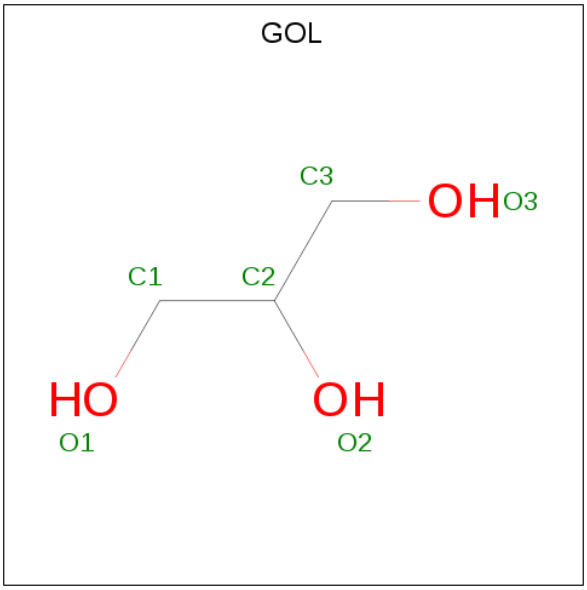
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	1	Total C O 5 3 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	4	Total O 4 4	0	0
6	C	2	Total O 2 2	0	0
6	D	5	Total O 5 5	0	0
6	E	2	Total O 2 2	0	0
6	F	5	Total O 5 5	0	0
6	G	8	Total O 8 8	0	0

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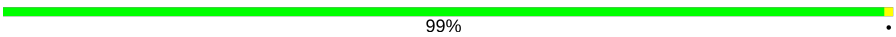
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	8	Total O 8 8	0	0
6	J	6	Total O 6 6	0	0
6	K	3	Total O 3 3	0	0
6	L	3	Total O 3 3	0	0
6	N	2	Total O 2 2	0	0
6	O	4	Total O 4 4	0	0
6	P	3	Total O 3 3	0	0
6	R	2	Total O 2 2	0	0
6	V	3	Total O 3 3	0	0
6	X	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

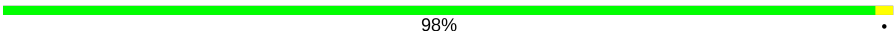
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



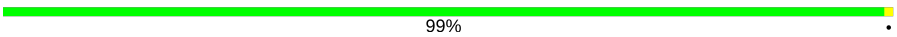
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain C:



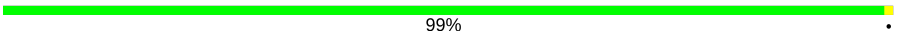
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain E:



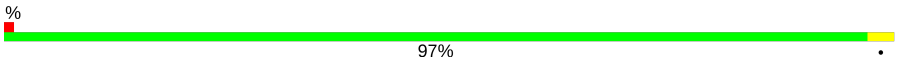
- Molecule 1: Superoxide dismutase [Cu-Zn]

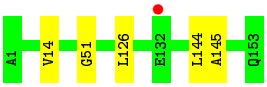
Chain G:



- Molecule 1: Superoxide dismutase [Cu-Zn]

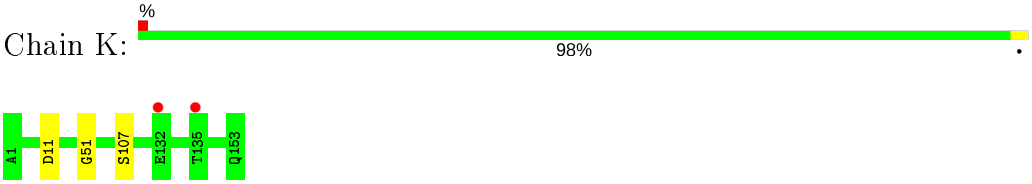
Chain I:





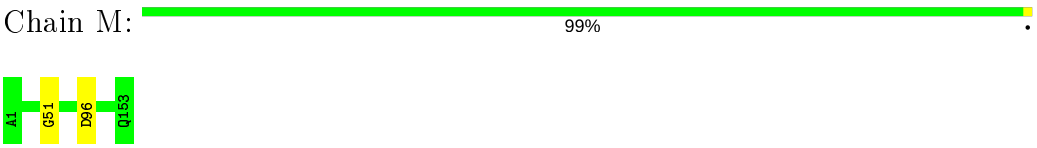
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain K:



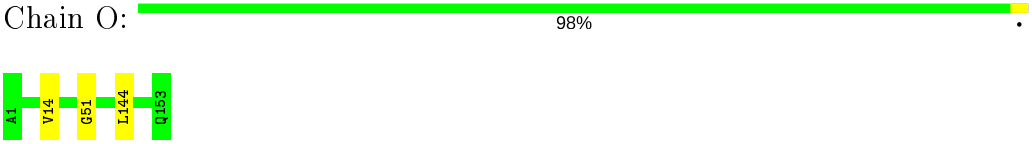
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain M:



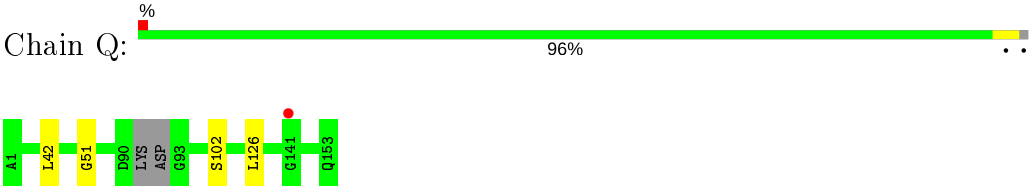
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain O:



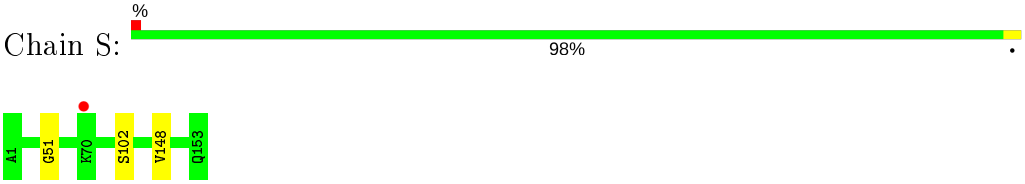
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain Q:



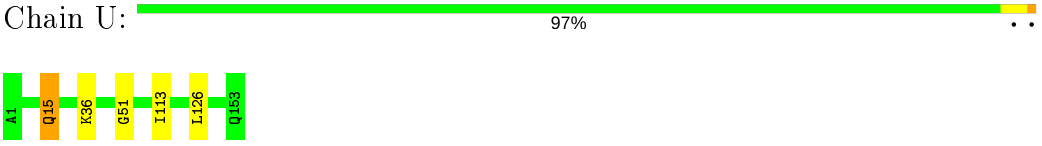
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain S:



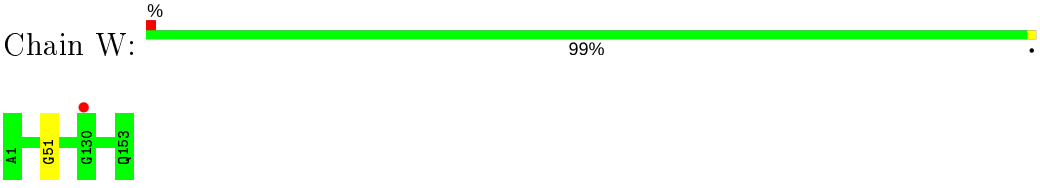
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain U:



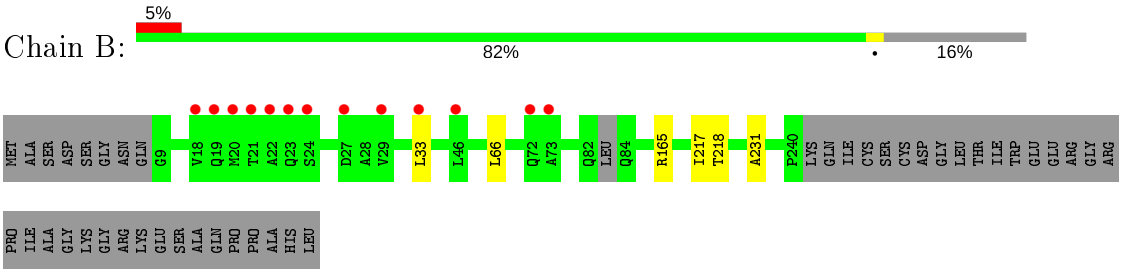
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain W:



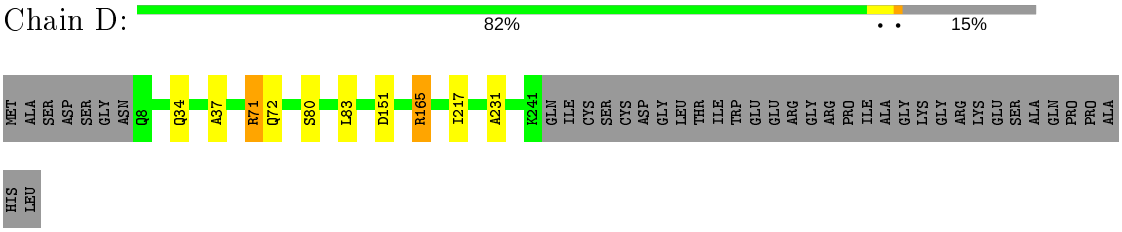
• Molecule 2: Copper chaperone for superoxide dismutase

Chain B:



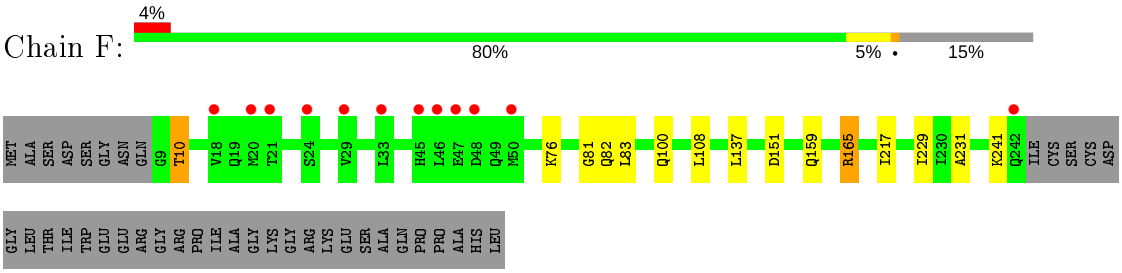
- Molecule 2: Copper chaperone for superoxide dismutase

Chain D:



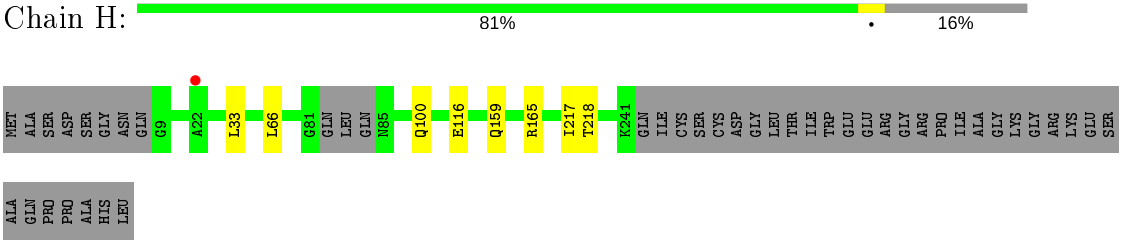
- Molecule 2: Copper chaperone for superoxide dismutase

Chain F:



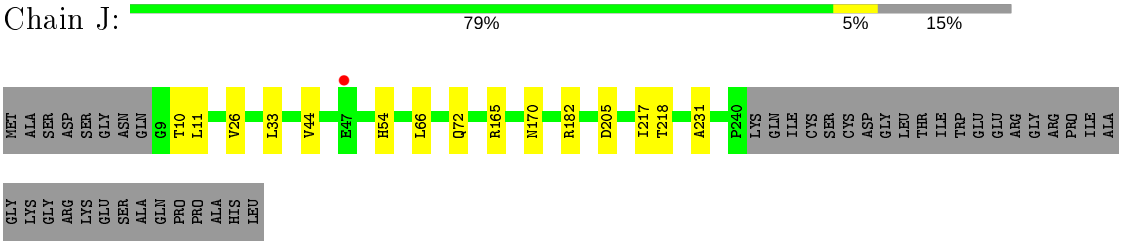
- Molecule 2: Copper chaperone for superoxide dismutase

Chain H:



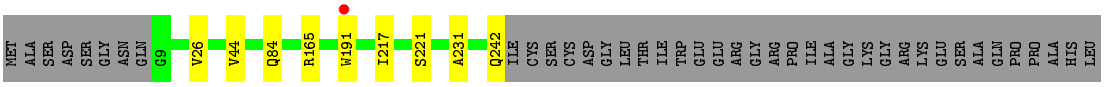
- Molecule 2: Copper chaperone for superoxide dismutase

Chain J:

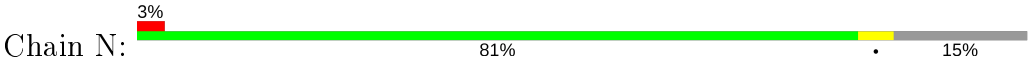


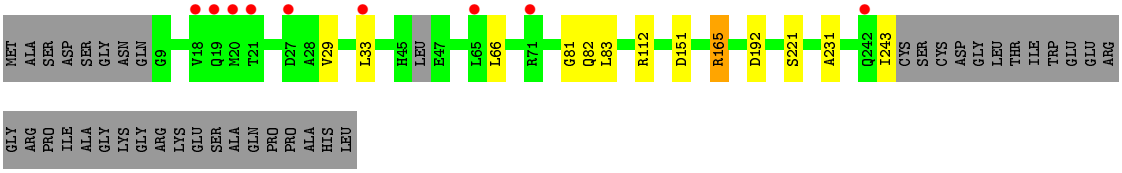
- Molecule 2: Copper chaperone for superoxide dismutase

Chain L:

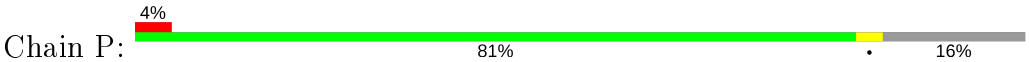


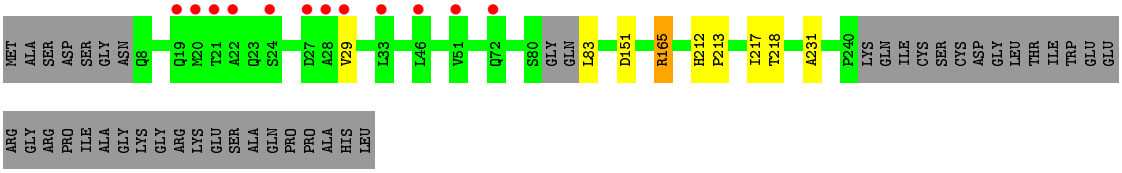
• Molecule 2: Copper chaperone for superoxide dismutase



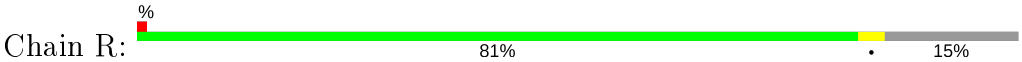


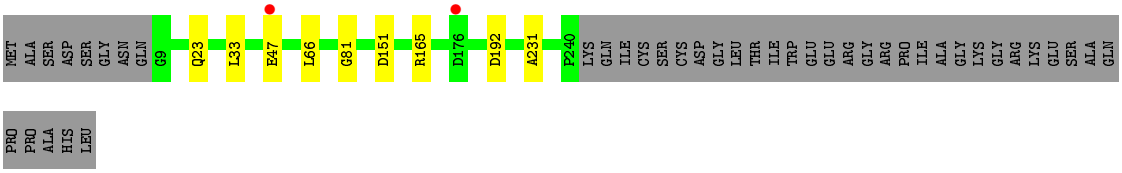
• Molecule 2: Copper chaperone for superoxide dismutase



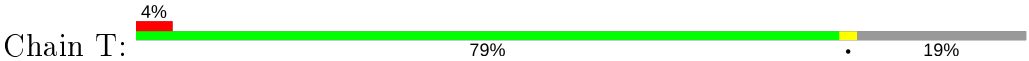


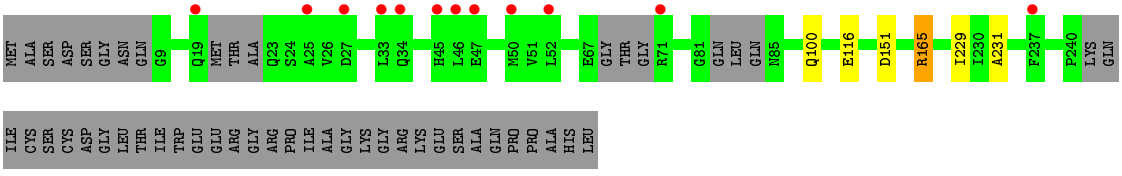
• Molecule 2: Copper chaperone for superoxide dismutase



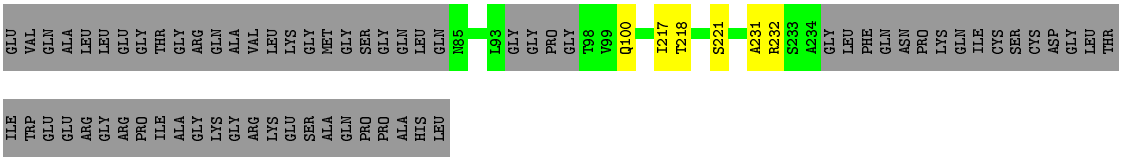


• Molecule 2: Copper chaperone for superoxide dismutase



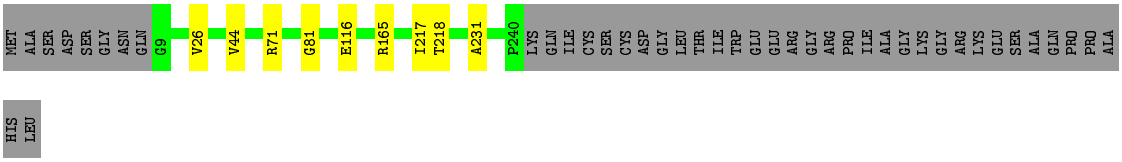


• Molecule 2: Copper chaperone for superoxide dismutase



• Molecule 2: Copper chaperone for superoxide dismutase

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	181.05Å 181.05Å 141.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 3.00 49.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.01-3.00) 100.0 (49.01-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.189 , 0.230 0.194 , 0.230	Depositor DCC
R_{free} test set	5115 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.023 for h,-h-k,-l 0.020 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33247	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: GOL, ZN, PPI

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	0.35	0/1122	0.57	0/1514
1	C	0.34	0/1126	0.55	0/1518
1	E	0.34	0/1126	0.56	0/1518
1	G	0.35	0/1126	0.59	0/1518
1	I	0.34	0/1142	0.54	0/1541
1	K	0.34	0/1126	0.57	0/1518
1	M	0.35	0/1126	0.56	0/1518
1	O	0.36	0/1122	0.57	0/1513
1	Q	0.36	0/1102	0.52	0/1486
1	S	0.36	0/1126	0.56	0/1518
1	U	0.36	0/1126	0.57	0/1518
1	W	0.34	0/1122	0.55	0/1514
2	B	0.37	0/1722	0.62	0/2329
2	D	0.36	0/1748	0.64	0/2364
2	F	0.37	0/1748	0.63	0/2365
2	H	0.37	0/1715	0.62	0/2318
2	J	0.36	0/1733	0.64	0/2345
2	L	0.36	0/1755	0.63	0/2373
2	N	0.37	0/1746	0.62	0/2360
2	P	0.37	0/1725	0.60	0/2334
2	R	0.37	0/1724	0.61	0/2334
2	T	0.37	0/1659	0.61	0/2241
2	V	0.37	0/1107	0.67	0/1494
2	X	0.38	0/1731	0.63	0/2342
All	All	0.36	0/33605	0.60	0/45393

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1104	0	1068	1	0
1	C	1108	0	1079	2	0
1	E	1108	0	1079	1	0
1	G	1108	0	1079	1	0
1	I	1119	0	1089	3	0
1	K	1108	0	1079	1	0
1	M	1108	0	1079	1	0
1	O	1104	0	1075	2	0
1	Q	1085	0	1050	1	0
1	S	1108	0	1079	2	0
1	U	1108	0	1079	4	0
1	W	1104	0	1068	1	0
2	B	1699	0	1649	4	0
2	D	1724	0	1685	4	0
2	F	1724	0	1680	6	0
2	H	1692	0	1650	3	0
2	J	1709	0	1666	8	0
2	L	1731	0	1693	3	0
2	N	1723	0	1682	4	0
2	P	1702	0	1654	5	0
2	R	1700	0	1646	3	0
2	T	1638	0	1582	3	0
2	V	1091	0	1045	3	0
2	X	1707	0	1663	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	10	0	10	0	0
4	I	5	0	5	0	0
4	K	10	0	10	0	0
4	R	5	0	5	0	0
5	A	6	0	8	0	0
6	A	7	0	0	0	0
6	B	4	0	0	0	0
6	C	2	0	0	0	0
6	D	5	0	0	0	0
6	E	2	0	0	0	0
6	F	5	0	0	0	0
6	G	8	0	0	0	0
6	H	8	0	0	0	0
6	J	6	0	0	0	0
6	K	3	0	0	0	0
6	L	3	0	0	0	0
6	N	2	0	0	0	0
6	O	4	0	0	0	0
6	P	3	0	0	0	0
6	R	2	0	0	0	0
6	V	3	0	0	0	0
6	X	8	0	0	0	0
All	All	33247	0	32236	56	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 1.

All (56) 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:I:14:VAL:HG13	1:I:145:ALA:HB2	1.84	0.60
1:S:51:GLY:HA3	2:T:231:ALA:HB1	1.84	0.59
1:I:14:VAL:HG11	1:I:144:LEU:HB3	1.83	0.59
2:F:10:THR:HG21	2:F:108:LEU:HD13	1.86	0.56
1:U:113:ILE:O	2:V:232:ARG:NH1	2.38	0.55
2:N:151:ASP:OD2	2:N:165:ARG:NH1	2.40	0.55
2:J:217:ILE:HG22	2:J:218:THR:HG23	1.89	0.52
2:X:26:VAL:HG13	2:X:44:VAL:HG11	1.92	0.52
2:L:26:VAL:HG13	2:L:44:VAL:HG11	1.92	0.51
2:P:217:ILE:HG22	2:P:218:THR:HG23	1.93	0.51
1:M:51:GLY:HA3	2:N:231:ALA:HB1	1.93	0.50
1:Q:51:GLY:HA3	2:R:231:ALA:HB1	1.94	0.48
1:W:51:GLY:HA3	2:X:231:ALA:HB1	1.95	0.48
1:O:51:GLY:HA3	2:P:231:ALA:HB1	1.95	0.48
2:V:217:ILE:HG22	2:V:218:THR:HG23	1.96	0.48
2:B:217:ILE:HG22	2:B:218:THR:HG23	1.96	0.48
1:U:51:GLY:HA3	2:V:231:ALA:HB1	1.95	0.48
2:X:217:ILE:HD12	2:X:217:ILE:N	2.28	0.47
1:U:15:GLN:HE22	1:U:36:LYS:CE	2.28	0.47
2:H:217:ILE:HG22	2:H:218:THR:HG23	1.97	0.47
2:F:137:LEU:HD11	2:F:229:ILE:HG13	1.97	0.46
2:D:151:ASP:OD2	2:D:165:ARG:NH1	2.48	0.46
2:N:33:LEU:HD11	2:N:66:LEU:HD21	1.97	0.45
2:J:26:VAL:HG13	2:J:44:VAL:HG11	1.97	0.45
2:R:151:ASP:OD1	2:R:165:ARG:NH1	2.49	0.45
1:U:15:GLN:HE22	1:U:36:LYS:HE3	1.82	0.45
2:X:217:ILE:HG22	2:X:218:THR:HG23	1.99	0.45
1:C:51:GLY:HA3	2:D:231:ALA:HB1	1.98	0.45
1:C:5:VAL:HG12	1:C:152:ALA:HB2	1.98	0.44
2:F:151:ASP:OD2	2:F:165:ARG:NH1	2.51	0.44
2:D:217:ILE:N	2:D:217:ILE:HD12	2.33	0.44
1:I:51:GLY:HA3	2:J:231:ALA:HB1	2.00	0.43
2:J:217:ILE:N	2:J:217:ILE:HD12	2.33	0.43
2:F:217:ILE:N	2:F:217:ILE:HD12	2.33	0.43
1:A:51:GLY:HA3	2:B:231:ALA:HB1	2.01	0.42
2:H:217:ILE:HD12	2:H:217:ILE:N	2.34	0.42
1:K:51:GLY:HA3	2:L:231:ALA:HB1	2.01	0.42
1:G:109:ASP:OD2	2:N:112:ARG:NH1	2.53	0.42
2:F:76:LYS:NZ	2:F:241:LYS:O	2.51	0.42
2:P:217:ILE:N	2:P:217:ILE:HD12	2.35	0.42
1:S:148:VAL:HB	2:T:229:ILE:HD12	2.01	0.42
2:B:217:ILE:N	2:B:217:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:GLY:HA3	2:F:231:ALA:HB1	2.01	0.41
2:J:10:THR:O	2:J:182:ARG:NH2	2.52	0.41
2:H:33:LEU:HD11	2:H:66:LEU:HD21	2.02	0.41
2:L:217:ILE:N	2:L:217:ILE:HD12	2.35	0.41
2:P:212:HIS:CD2	2:P:213:PRO:HD2	2.56	0.41
2:B:33:LEU:HD11	2:B:66:LEU:HD21	2.03	0.41
1:O:14:VAL:HG21	1:O:144:LEU:HB3	2.03	0.41
2:R:33:LEU:HD11	2:R:66:LEU:HD21	2.03	0.40
2:J:33:LEU:HD11	2:J:66:LEU:HD21	2.04	0.40
2:P:151:ASP:OD2	2:P:165:ARG:NH1	2.55	0.40
2:J:170:ASN:HD21	2:J:205:ASP:H	1.68	0.40
2:T:151:ASP:OD2	2:T:165:ARG:NH1	2.54	0.40
2:D:80:SER:HB3	2:D:83:LEU:CD2	2.52	0.40
2:J:11:LEU:HD12	2:J:54:HIS:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	C	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	E	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	G	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	I	152/153 (99%)	150 (99%)	2 (1%)	0	100	100
1	K	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	M	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	O	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	Q	147/153 (96%)	141 (96%)	5 (3%)	1 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	U	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	W	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
2	B	227/274 (83%)	217 (96%)	10 (4%)	0	100	100
2	D	232/274 (85%)	215 (93%)	15 (6%)	2 (1%)	17	55
2	F	232/274 (85%)	219 (94%)	9 (4%)	4 (2%)	9	39
2	H	226/274 (82%)	218 (96%)	8 (4%)	0	100	100
2	J	230/274 (84%)	220 (96%)	10 (4%)	0	100	100
2	L	232/274 (85%)	217 (94%)	15 (6%)	0	100	100
2	N	230/274 (84%)	217 (94%)	10 (4%)	3 (1%)	12	45
2	P	227/274 (83%)	216 (95%)	11 (5%)	0	100	100
2	R	230/274 (84%)	215 (94%)	14 (6%)	1 (0%)	34	72
2	T	215/274 (78%)	208 (97%)	7 (3%)	0	100	100
2	V	142/274 (52%)	137 (96%)	5 (4%)	0	100	100
2	X	230/274 (84%)	219 (95%)	9 (4%)	2 (1%)	17	55
All	All	4462/5124 (87%)	4286 (96%)	163 (4%)	13 (0%)	41	76

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	83	LEU
1	Q	42	LEU
2	D	37	ALA
2	D	71	ARG
2	F	10	THR
2	F	81	GLY
2	F	82	GLN
2	F	83	LEU
2	N	82	GLN
2	X	81	GLY
2	X	71	ARG
2	R	81	GLY
2	N	81	GLY

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	115/116 (99%)	115 (100%)	0	100	100
1	C	116/116 (100%)	116 (100%)	0	100	100
1	E	116/116 (100%)	115 (99%)	1 (1%)	78	92
1	G	116/116 (100%)	116 (100%)	0	100	100
1	I	117/116 (101%)	116 (99%)	1 (1%)	78	92
1	K	116/116 (100%)	114 (98%)	2 (2%)	60	85
1	M	116/116 (100%)	115 (99%)	1 (1%)	78	92
1	O	115/116 (99%)	115 (100%)	0	100	100
1	Q	113/116 (97%)	111 (98%)	2 (2%)	59	85
1	S	116/116 (100%)	115 (99%)	1 (1%)	78	92
1	U	116/116 (100%)	114 (98%)	2 (2%)	60	85
1	W	115/116 (99%)	115 (100%)	0	100	100
2	B	178/213 (84%)	177 (99%)	1 (1%)	86	95
2	D	180/213 (84%)	176 (98%)	4 (2%)	52	81
2	F	181/213 (85%)	178 (98%)	3 (2%)	60	85
2	H	177/213 (83%)	173 (98%)	4 (2%)	50	80
2	J	179/213 (84%)	177 (99%)	2 (1%)	73	90
2	L	182/213 (85%)	177 (97%)	5 (3%)	44	77
2	N	180/213 (84%)	175 (97%)	5 (3%)	43	77
2	P	178/213 (84%)	175 (98%)	3 (2%)	60	85
2	R	177/213 (83%)	174 (98%)	3 (2%)	60	85
2	T	170/213 (80%)	167 (98%)	3 (2%)	59	85
2	V	114/213 (54%)	112 (98%)	2 (2%)	59	85
2	X	178/213 (84%)	176 (99%)	2 (1%)	73	90
All	All	3461/3948 (88%)	3414 (99%)	47 (1%)	67	88

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	165	ARG
2	D	34	GLN
2	D	71	ARG
2	D	72	GLN
2	D	165	ARG
1	E	32	TRP
2	F	100	GLN
2	F	159	GLN
2	F	165	ARG
2	H	100	GLN
2	H	116	GLU
2	H	159	GLN
2	H	165	ARG
1	I	126	LEU
2	J	72	GLN
2	J	165	ARG
1	K	11	ASP
1	K	107	SER
2	L	84	GLN
2	L	165	ARG
2	L	191	TRP
2	L	221	SER
2	L	242	GLN
1	M	96	ASP
2	N	29	VAL
2	N	165	ARG
2	N	192	ASP
2	N	221	SER
2	N	243	ILE
2	P	29	VAL
2	P	83	LEU
2	P	165	ARG
1	Q	102	SER
1	Q	126	LEU
2	R	23	GLN
2	R	47	GLU
2	R	192	ASP
1	S	102	SER
2	T	100	GLN
2	T	116	GLU
2	T	165	ARG
1	U	15	GLN
1	U	126	LEU

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Mol	Chain	Res	Type
2	V	100	GLN
2	V	221	SER
2	X	116	GLU
2	X	165	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	212	HIS
1	C	15	GLN
2	D	127	HIS
2	D	170	ASN
2	D	212	HIS
1	E	53	ASN
1	E	86	ASN
2	F	82	GLN
2	F	85	ASN
2	F	127	HIS
2	F	170	ASN
2	F	242	GLN
1	G	15	GLN
1	G	43	HIS
1	G	53	ASN
2	H	132	HIS
2	H	170	ASN
2	H	212	HIS
1	I	15	GLN
1	I	86	ASN
2	J	127	HIS
2	J	170	ASN
2	J	212	HIS
1	K	15	GLN
1	K	86	ASN
2	L	84	GLN
2	L	127	HIS
2	L	170	ASN
2	L	212	HIS
1	M	46	HIS
1	M	63	HIS
2	N	100	GLN
2	N	127	HIS
2	N	170	ASN

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Mol	Chain	Res	Type
2	N	212	HIS
1	O	15	GLN
1	O	43	HIS
1	O	53	ASN
1	O	86	ASN
1	O	139	ASN
2	P	170	ASN
2	R	170	ASN
2	R	212	HIS
1	S	15	GLN
1	S	43	HIS
1	S	86	ASN
2	T	107	GLN
1	U	15	GLN
2	V	170	ASN
2	V	212	HIS
1	W	15	GLN
1	W	86	ASN
1	W	139	ASN
2	X	170	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

Of 31 ligands modelled in this entry, 24 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	$\#\|Z\| > 2$
4	PPI	A	202	-	1,4,4	0.24	0	1,4,4	1.95	0
4	PPI	K	203	-	1,4,4	0.32	0	1,4,4	1.53	0
5	GOL	A	204	-	5,5,5	0.35	0	5,5,5	0.29	0
4	PPI	R	302	-	1,4,4	0.34	0	1,4,4	0.70	0
4	PPI	A	203	-	1,4,4	0.29	0	1,4,4	1.14	0
4	PPI	K	202	-	1,4,4	0.26	0	1,4,4	0.21	0
4	PPI	I	202	-	1,4,4	0.31	0	1,4,4	0.89	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
4	PPI	A	202	-	-	0/0/2/2	-
4	PPI	K	203	-	-	0/0/2/2	-
5	GOL	A	204	-	-	0/4/4/4	-
4	PPI	R	302	-	-	0/0/2/2	-
4	PPI	A	203	-	-	0/0/2/2	-
4	PPI	K	202	-	-	0/0/2/2	-
4	PPI	I	202	-	-	0/0/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	153/153 (100%)	-0.31	0 100 100	48, 55, 73, 84	0
1	C	153/153 (100%)	-0.17	0 100 100	59, 73, 90, 100	0
1	E	153/153 (100%)	-0.27	0 100 100	51, 57, 70, 79	0
1	G	153/153 (100%)	-0.26	0 100 100	50, 56, 62, 68	0
1	I	153/153 (100%)	-0.04	1 (0%) 87 69	58, 72, 97, 112	0
1	K	153/153 (100%)	-0.13	2 (1%) 77 51	52, 60, 79, 92	0
1	M	153/153 (100%)	-0.15	0 100 100	55, 71, 91, 99	0
1	O	153/153 (100%)	-0.37	0 100 100	53, 58, 70, 77	0
1	Q	151/153 (98%)	0.17	1 (0%) 87 69	82, 104, 122, 128	0
1	S	153/153 (100%)	-0.13	1 (0%) 87 69	61, 71, 95, 104	0
1	U	153/153 (100%)	0.04	0 100 100	63, 81, 104, 114	0
1	W	153/153 (100%)	-0.10	1 (0%) 87 69	57, 70, 89, 99	0
2	B	231/274 (84%)	0.11	13 (5%) 24 8	50, 67, 132, 142	0
2	D	234/274 (85%)	-0.07	0 100 100	51, 65, 105, 118	0
2	F	234/274 (85%)	0.13	12 (5%) 28 10	51, 69, 142, 152	0
2	H	230/274 (83%)	-0.08	1 (0%) 92 79	50, 64, 114, 127	0
2	J	232/274 (84%)	-0.08	1 (0%) 92 79	50, 61, 93, 106	0
2	L	234/274 (85%)	-0.14	1 (0%) 92 79	53, 68, 91, 115	0
2	N	234/274 (85%)	0.11	9 (3%) 40 16	51, 67, 129, 136	0
2	P	231/274 (84%)	0.15	12 (5%) 27 10	58, 75, 141, 153	0
2	R	232/274 (84%)	-0.01	2 (0%) 84 63	63, 87, 117, 124	0
2	T	223/274 (81%)	0.12	12 (5%) 25 9	63, 90, 147, 159	0
2	V	146/274 (53%)	-0.17	0 100 100	53, 63, 74, 87	0
2	X	232/274 (84%)	-0.19	0 100 100	55, 67, 93, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	4527/5124 (88%)	-0.06	69 (1%) 73 46	48, 68, 117, 159	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	33	LEU	4.9
2	B	21	THR	4.2
2	T	46	LEU	4.2
2	B	19	GLN	3.7
2	P	21	THR	3.7
2	P	22	ALA	3.5
2	N	33	LEU	3.4
2	T	25	ALA	3.4
2	T	45	HIS	3.4
2	T	34	GLN	3.3
2	F	33	LEU	3.2
2	B	72	GLN	3.2
2	B	33	LEU	3.1
2	P	33	LEU	3.0
2	F	45	HIS	3.0
2	N	71	ARG	3.0
2	N	242	GLN	3.0
2	P	46	LEU	3.0
2	T	19	GLN	3.0
2	P	72	GLN	3.0
2	H	22	ALA	2.9
2	F	20	MET	2.8
2	B	46	LEU	2.8
2	B	27	ASP	2.8
2	T	47	GLU	2.8
2	B	24	SER	2.8
1	K	132	GLU	2.7
2	N	21	THR	2.7
2	F	47	GLU	2.7
2	T	50	MET	2.6
2	F	242	GLN	2.6
2	B	18	VAL	2.6
2	B	20	MET	2.6
2	F	50	MET	2.6
2	R	47	GLU	2.6
2	N	19	GLN	2.5
2	R	176	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	27	ASP	2.5
2	B	23	GLN	2.5
1	Q	141	GLY	2.5
1	W	130	GLY	2.5
2	P	51	VAL	2.5
2	N	18	VAL	2.4
2	F	18	VAL	2.4
2	F	46	LEU	2.4
2	P	19	GLN	2.4
1	K	135	THR	2.4
2	P	28	ALA	2.4
1	I	132	GLU	2.3
2	F	24	SER	2.3
2	P	29	VAL	2.3
2	B	29	VAL	2.3
2	F	29	VAL	2.3
2	T	71	ARG	2.2
1	S	70	LYS	2.2
2	P	20	MET	2.2
2	N	65	LEU	2.2
2	T	52	LEU	2.2
2	F	48	ASP	2.2
2	N	20	MET	2.2
2	T	27	ASP	2.1
2	F	21	THR	2.1
2	P	24	SER	2.1
2	B	22	ALA	2.1
2	L	191	TRP	2.1
2	P	27	ASP	2.1
2	T	237	PHE	2.0
2	B	73	ALA	2.0
2	J	47	GLU	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 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. 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
4	PPI	I	202	5/5	0.76	0.28	93,93,94,95	0
4	PPI	A	202	5/5	0.79	0.33	74,77,78,80	0
4	PPI	A	203	5/5	0.79	0.28	75,78,78,79	0
4	PPI	K	203	5/5	0.80	0.32	76,79,80,80	0
4	PPI	K	202	5/5	0.80	0.32	56,56,58,60	0
4	PPI	R	302	5/5	0.86	0.24	67,68,70,72	0
5	GOL	A	204	6/6	0.89	0.24	63,64,65,67	0
3	ZN	E	201	1/1	0.98	0.17	56,56,56,56	0
3	ZN	A	201	1/1	0.98	0.18	55,55,55,55	0
3	ZN	U	201	1/1	0.98	0.13	78,78,78,78	0
3	ZN	W	201	1/1	0.98	0.13	67,67,67,67	0
3	ZN	K	201	1/1	0.98	0.13	56,56,56,56	0
3	ZN	T	400	1/1	0.99	0.17	68,68,68,68	0
3	ZN	L	400	1/1	0.99	0.17	49,49,49,49	0
3	ZN	C	201	1/1	0.99	0.15	67,67,67,67	0
3	ZN	B	400	1/1	0.99	0.20	49,49,49,49	0
3	ZN	D	400	1/1	0.99	0.16	48,48,48,48	0
3	ZN	H	400	1/1	0.99	0.18	48,48,48,48	0
3	ZN	N	400	1/1	0.99	0.17	49,49,49,49	0
3	ZN	M	201	1/1	0.99	0.15	67,67,67,67	0
3	ZN	X	400	1/1	0.99	0.19	53,53,53,53	0
3	ZN	V	400	1/1	0.99	0.17	50,50,50,50	0
3	ZN	F	400	1/1	0.99	0.17	53,53,53,53	0
3	ZN	S	201	1/1	0.99	0.16	72,72,72,72	0
3	ZN	J	400	1/1	0.99	0.18	47,47,47,47	0
3	ZN	R	301	1/1	0.99	0.18	61,61,61,61	0
3	ZN	G	201	1/1	0.99	0.17	48,48,48,48	0
3	ZN	P	400	1/1	1.00	0.17	55,55,55,55	0
3	ZN	Q	201	1/1	1.00	0.13	96,96,96,96	0
3	ZN	I	201	1/1	1.00	0.16	66,66,66,66	0
3	ZN	O	201	1/1	1.00	0.19	52,52,52,52	0

6.5 Other polymers

There are no such residues in this entry.