



# wwPDB X-ray Structure Validation Summary Report

Dec 7, 2023 – 10:47 pm GMT

PDB ID : 1UXL  
Title : I113T mutant of human SOD1  
Authors : Hough, M.A.; Grossmann, J.G.; Antonyuk, S.V.; Strange, R.W.; Doucette, P.A.; Rodriguez, J.A.; Whitson, L.J.; Hart, P.J.; Hayward, L.J.; Valentine, J.S.; Hasnain, S.S.  
Deposited on : 2004-02-25  
Resolution : 1.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, 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

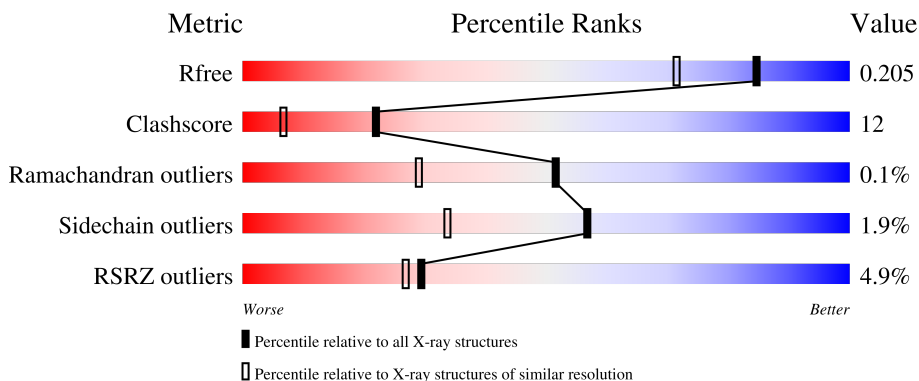
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">87% 10% ..</p>
1	B	153	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">10% 83% 14% ..</p>
1	C	153	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">% 88% 10% .</p>
1	D	153	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">10% 85% 13% .</p>
1	E	153	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">10% 91% 8% .</p>

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Mol	Chain	Length	Quality of chain
1	F	153	
1	G	153	
1	H	153	
1	I	153	
1	J	153	

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	SO4	C	157	-	-	X	-
4	SO4	D	156	-	-	X	-
4	SO4	F	156	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13831 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
			Total	C	N	O	S			
1	A	153	1158	706	210	237	5	22	10	0
1	B	153	1141	694	210	232	5	7	5	0
1	C	153	1113	679	203	226	5	13	2	0
1	D	153	1134	691	205	234	4	23	8	0
1	E	153	1109	677	203	225	4	22	0	0
1	F	153	1129	688	206	231	4	3	6	0
1	G	153	1115	682	203	226	4	12	2	0
1	H	153	1162	705	210	243	4	13	12	0
1	I	153	1146	701	209	231	5	17	5	0
1	J	153	1116	682	203	227	4	25	3	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	THR	ILE	engineered mutation	UNP P00441
B	113	THR	ILE	engineered mutation	UNP P00441
C	113	THR	ILE	engineered mutation	UNP P00441
D	113	THR	ILE	engineered mutation	UNP P00441
E	113	THR	ILE	engineered mutation	UNP P00441
F	113	THR	ILE	engineered mutation	UNP P00441
G	113	THR	ILE	engineered mutation	UNP P00441
H	113	THR	ILE	engineered mutation	UNP P00441
I	113	THR	ILE	engineered mutation	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
J	113	THR	ILE	engineered mutation	UNP P00441

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 2 2	0	1
2	B	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0
2	G	1	Total Cu 1 1	0	0
2	H	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	J	1	Total Cu 1 1	0	0

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

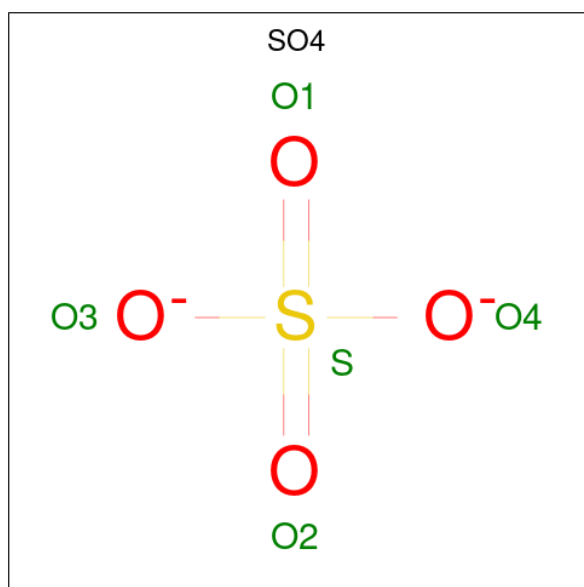
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

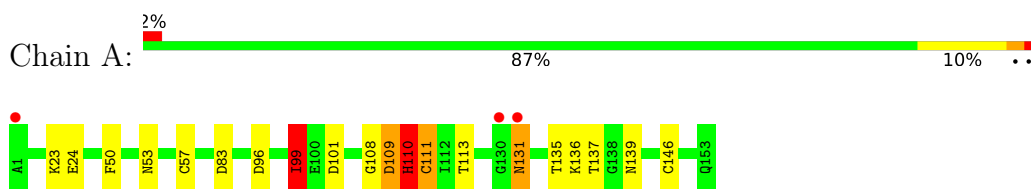
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	248	Total O 248 248	0	0
5	B	197	Total O 197 197	0	0
5	C	263	Total O 263 263	0	0
5	D	178	Total O 178 178	0	0
5	E	179	Total O 179 179	0	0
5	F	304	Total O 304 304	0	0
5	G	270	Total O 270 270	0	0
5	H	316	Total O 316 316	0	0
5	I	246	Total O 246 246	0	0
5	J	246	Total O 246 246	0	0

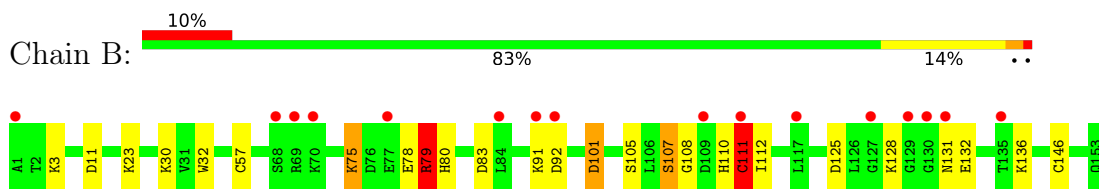
### 3 Residue-property plots [i](#)

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.

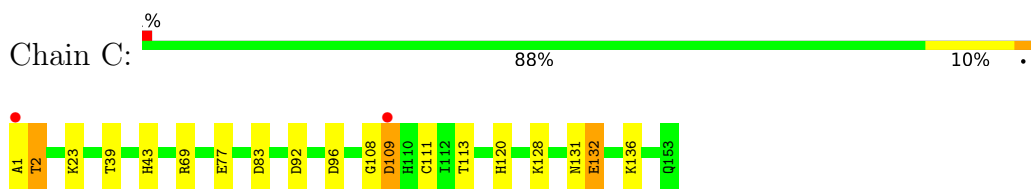
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



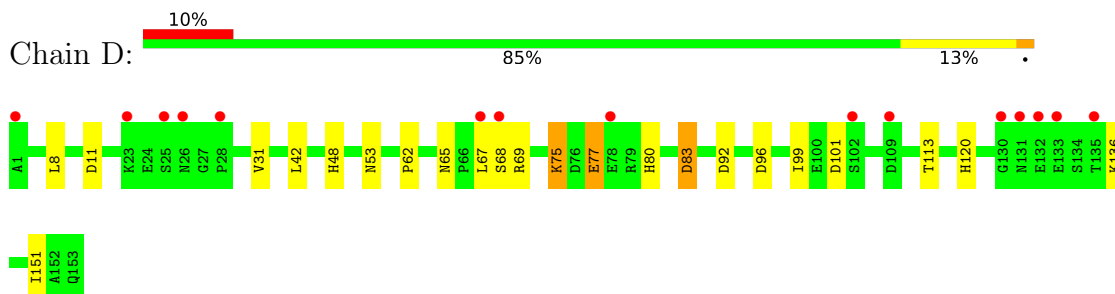
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



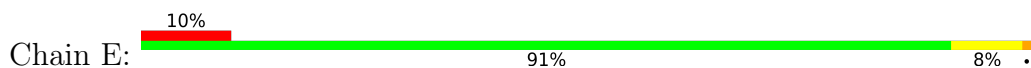
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



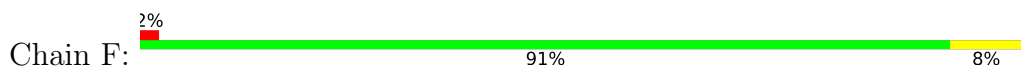
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]







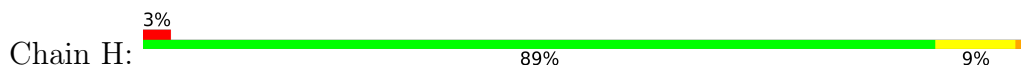
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



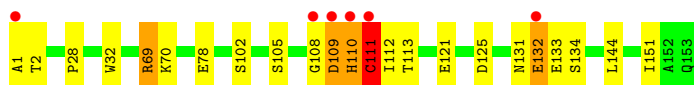
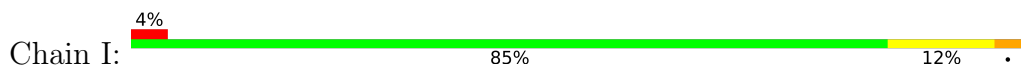
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



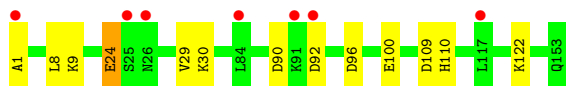
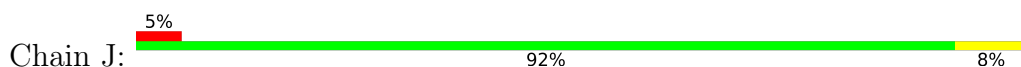
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.04Å 203.55Å 144.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 23.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.60) 99.6 (23.99-1.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.170 , 0.196 0.181 , 0.205	Depositor DCC
$R_{free}$ test set	15965 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	2/1200 (0.2%)	1.29	14/1619 (0.9%)
1	B	0.86	1/1162 (0.1%)	0.98	10/1563 (0.6%)
1	C	0.58	1/1140 (0.1%)	0.90	4/1537 (0.3%)
1	D	0.47	0/1188	0.90	7/1602 (0.4%)
1	E	0.46	1/1127 (0.1%)	0.79	3/1519 (0.2%)
1	F	0.56	0/1173	0.86	1/1581 (0.1%)
1	G	0.61	1/1142 (0.1%)	0.83	1/1540 (0.1%)
1	H	1.10	2/1221 (0.2%)	1.02	3/1647 (0.2%)
1	I	0.77	3/1175 (0.3%)	1.09	9/1586 (0.6%)
1	J	0.56	1/1148 (0.1%)	0.88	4/1548 (0.3%)
All	All	0.69	12/11676 (0.1%)	0.97	56/15742 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	H	0	1
1	I	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	133[A]	GLU	C-N	23.15	1.87	1.34
1	H	133[B]	GLU	C-N	23.15	1.87	1.34
1	B	107	SER	C-N	22.68	1.73	1.33
1	I	111[A]	CYS	C-N	13.17	1.64	1.34
1	I	111[B]	CYS	C-N	13.17	1.64	1.34

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110[A]	HIS	O-C-N	-17.30	95.02	122.70
1	A	110[B]	HIS	O-C-N	-17.30	95.02	122.70
1	I	111[A]	CYS	O-C-N	-16.54	96.23	122.70
1	I	111[B]	CYS	O-C-N	-16.54	96.23	122.70
1	H	133[A]	GLU	O-C-N	-13.81	100.60	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109[A]	ASP	Sidechain
1	A	110[A]	HIS	Mainchain
1	A	99[A]	ILE	Mainchain
1	H	130	GLY	Mainchain
1	I	111[A]	CYS	Mainchain

## 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	1158	0	1118	26	0
1	B	1141	0	1093	33	0
1	C	1113	0	1077	30	0
1	D	1134	0	1093	24	0
1	E	1109	0	1073	9	0
1	F	1129	0	1092	22	0
1	G	1115	0	1083	16	0
1	H	1162	0	1107	25	0
1	I	1146	0	1099	52	1
1	J	1116	0	1084	12	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
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
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	2	0
4	D	5	0	0	7	0
4	E	5	0	0	1	0
4	F	5	0	0	2	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
5	A	248	0	0	21	1
5	B	197	0	0	17	0
5	C	263	0	0	22	2
5	D	178	0	0	15	2
5	E	179	0	0	7	0
5	F	304	0	0	20	0
5	G	270	0	0	16	0
5	H	316	0	0	16	0
5	I	246	0	0	30	0
5	J	246	0	0	10	2
All	All	13831	0	10919	254	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 12.

The worst 5 of 254 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:B:107:SER:C	1:B:108[A]:GLY:N	1.73	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133[A]:GLU:C	1:H:134:SER:N	1.87	1.28
4:F:156:SO4:O4	5:F:2301:HOH:O	1.52	1.25
4:C:157:SO4:O2	5:C:2263:HOH:O	1.55	1.24
1:A:53:ASN:ND2	5:A:2119:HOH:O	1.68	1.24

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)
1:I:110[B]:HIS:CB	5:D:2090:HOH:O[3_755]	2.03	0.17
5:C:2229:HOH:O	5:J:2141:HOH:O[5_545]	2.15	0.05
5:A:2075:HOH:O	5:D:2152:HOH:O[5_445]	2.18	0.02
5:C:2231:HOH:O	5:J:2215:HOH:O[5_545]	2.19	0.01

## 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	161/153 (105%)	159 (99%)	2 (1%)	0	100	100
1	B	156/153 (102%)	156 (100%)	0	0	100	100
1	C	153/153 (100%)	153 (100%)	0	0	100	100
1	D	159/153 (104%)	156 (98%)	3 (2%)	0	100	100
1	E	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	F	157/153 (103%)	156 (99%)	1 (1%)	0	100	100
1	G	153/153 (100%)	151 (99%)	2 (1%)	0	100	100
1	H	163/153 (106%)	163 (100%)	0	0	100	100
1	I	156/153 (102%)	154 (99%)	0	2 (1%)	12	2
1	J	154/153 (101%)	154 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1563/1530 (102%)	1552 (99%)	9 (1%)	2 (0%)	51	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	110[A]	HIS
1	I	110[B]	HIS

### 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	127/118 (108%)	123 (97%)	4 (3%)	40	15
1	B	122/118 (103%)	117 (96%)	5 (4%)	30	9
1	C	120/118 (102%)	118 (98%)	2 (2%)	60	38
1	D	126/118 (107%)	124 (98%)	2 (2%)	62	41
1	E	118/118 (100%)	114 (97%)	4 (3%)	37	13
1	F	124/118 (105%)	123 (99%)	1 (1%)	81	70
1	G	120/118 (102%)	120 (100%)	0	100	100
1	H	130/118 (110%)	127 (98%)	3 (2%)	50	25
1	I	123/118 (104%)	119 (97%)	4 (3%)	38	14
1	J	121/118 (102%)	119 (98%)	2 (2%)	60	38
All	All	1231/1180 (104%)	1204 (98%)	27 (2%)	57	27

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	77	GLU
1	F	26	ASN
1	I	132	GLU
1	E	135	THR
1	H	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	131	ASN
1	F	153	GLN
1	E	53	ASN
1	C	43	HIS
1	F	110	HIS

### 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 29 ligands modelled in this entry, 21 are monoatomic - leaving 8 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	SO4	F	156	-	4,4,4	0.56	0	6,6,6	0.37	0
4	SO4	H	156	-	4,4,4	0.60	0	6,6,6	0.52	0
4	SO4	D	156	2	4,4,4	0.35	0	6,6,6	0.70	0
4	SO4	A	156	-	4,4,4	0.18	0	6,6,6	0.46	0
4	SO4	E	156	-	4,4,4	0.11	0	6,6,6	0.33	0
4	SO4	I	156	-	4,4,4	0.22	0	6,6,6	0.30	0
4	SO4	B	156	2	4,4,4	0.18	0	6,6,6	0.32	0
4	SO4	C	157	-	4,4,4	0.33	0	6,6,6	0.30	0



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.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	156	SO4	2	0
4	H	156	SO4	1	0
4	D	156	SO4	7	0
4	A	156	SO4	1	0
4	E	156	SO4	1	0
4	B	156	SO4	1	0
4	C	157	SO4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	3
1	B	3
1	A	2
1	H	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	111[B]:CYS	C	112:ILE	N	2.30
1	B	107:SER	C	108[B]:GLY	N	2.13
1	B	111[A]:CYS	C	112:ILE	N	2.07
1	H	133[A]:GLU	C	134:SER	N	1.87
1	B	107:SER	C	108[A]:GLY	N	1.73

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	153/153 (100%)	-0.16	3 (1%) 65 64	10, 14, 22, 30	9 (5%)
1	B	153/153 (100%)	0.55	16 (10%) 6 5	13, 19, 30, 37	4 (2%)
1	C	153/153 (100%)	-0.15	2 (1%) 77 77	9, 13, 20, 26	7 (4%)
1	D	153/153 (100%)	0.55	15 (9%) 7 6	13, 19, 31, 36	7 (4%)
1	E	153/153 (100%)	0.41	15 (9%) 7 6	11, 19, 29, 34	6 (3%)
1	F	153/153 (100%)	-0.16	3 (1%) 65 64	9, 12, 21, 28	4 (2%)
1	G	153/153 (100%)	-0.11	4 (2%) 56 53	7, 13, 22, 26	7 (4%)
1	H	153/153 (100%)	-0.11	4 (2%) 56 53	8, 12, 21, 25	6 (3%)
1	I	153/153 (100%)	-0.00	6 (3%) 39 36	9, 15, 26, 30	9 (5%)
1	J	153/153 (100%)	0.10	7 (4%) 32 29	9, 16, 24, 29	12 (7%)
All	All	1530/1530 (100%)	0.09	75 (4%) 29 27	7, 15, 26, 37	71 (4%)

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	ALA	6.4
1	D	1	ALA	5.7
1	J	25	SER	5.2
1	E	132	GLU	4.8
1	E	130	GLY	4.8

### 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	D	155	1/1	0.82	0.16	21,21,21,21	0
4	SO4	H	156	5/5	0.82	0.25	15,21,25,26	5
2	CU	F	154	1/1	0.90	0.06	23,23,23,23	0
4	SO4	I	156	5/5	0.90	0.33	38,41,43,44	0
4	SO4	D	156	5/5	0.91	0.21	15,26,30,31	5
4	SO4	E	156	5/5	0.91	0.17	32,33,34,34	5
4	SO4	C	157	5/5	0.92	0.22	24,27,30,31	5
4	SO4	F	156	5/5	0.93	0.16	14,19,21,22	5
2	CU	B	154	1/1	0.94	0.15	24,24,24,24	0
2	CU	D	154	1/1	0.94	0.18	21,21,21,21	0
2	CU	I	154	1/1	0.95	0.09	24,24,24,24	0
3	ZN	B	155	1/1	0.95	0.16	18,18,18,18	0
2	CU	E	154	1/1	0.95	0.14	30,30,30,30	0
4	SO4	B	156	5/5	0.95	0.17	26,26,28,28	5
2	CU	C	154	1/1	0.95	0.08	25,25,25,25	0
2	CU	H	154	1/1	0.96	0.06	22,22,22,22	0
3	ZN	E	155	1/1	0.97	0.15	17,17,17,17	0
2	CU	G	154	1/1	0.97	0.16	14,14,14,14	1
4	SO4	A	156	5/5	0.98	0.07	21,23,29,30	5
3	ZN	A	155	1/1	0.99	0.04	14,14,14,14	0
3	ZN	H	155	1/1	0.99	0.02	12,12,12,12	0
2	CU	A	154[A]	1/1	0.99	0.04	17,17,17,17	1
3	ZN	C	155	1/1	0.99	0.03	12,12,12,12	0
2	CU	A	154[B]	1/1	0.99	0.04	11,11,11,11	1
3	ZN	I	155	1/1	1.00	0.06	13,13,13,13	0
3	ZN	J	155	1/1	1.00	0.04	13,13,13,13	0
3	ZN	F	155	1/1	1.00	0.02	12,12,12,12	0
3	ZN	G	155	1/1	1.00	0.02	12,12,12,12	0
2	CU	J	154	1/1	1.00	0.09	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.