



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 10:36 AM EST

PDB ID : 4OH2  
Title : Crystal Structure of Cu/Zn Superoxide Dismutase I149T  
Authors : Crane, B.R.; Merz, G.E.  
Deposited on : unknown  
Resolution : 2.38 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

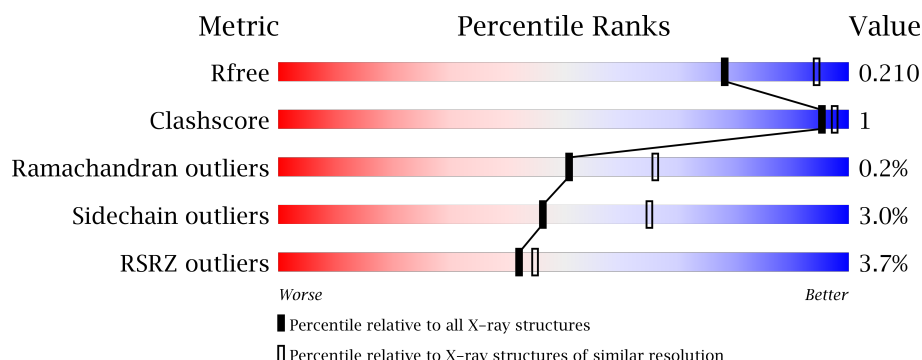
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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))
$R_{free}$	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	153	<div> <div>0.2%</div> <div>93%</div> <div>5%</div> </div>
1	B	153	<div> <div>0.2%</div> <div>97%</div> <div>0.1%</div> </div>
1	C	153	<div> <div>6%</div> <div>93%</div> <div>6%</div> </div>
1	D	153	<div> <div>0.2%</div> <div>99%</div> <div>0.1%</div> </div>
1	E	153	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	153	<div> <div></div> <div>95%</div> <div>..</div> </div>
1	G	153	<div> <div>8%</div> <div>90%</div> <div>9% .</div> </div>
1	H	153	<div> <div></div> <div>99%</div> <div>.</div> </div>
1	I	153	<div> <div>11%</div> <div>90%</div> <div>9% .</div> </div>
1	J	153	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22674 atoms, of which 10860 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	H	N	O	S	7	3	0
			2202	681	1086	204	229	2			
1	B	153	Total	C	H	N	O	S	0	3	0
			2200	680	1085	203	230	2			
1	C	153	Total	C	H	N	O	S	0	3	0
			2202	681	1086	204	229	2			
1	D	153	Total	C	H	N	O	S	10	3	0
			2201	680	1086	203	230	2			
1	E	153	Total	C	H	N	O	S	0	3	0
			2204	681	1088	204	229	2			
1	F	153	Total	C	H	N	O	S	0	3	0
			2200	680	1085	203	230	2			
1	G	153	Total	C	H	N	O	S	0	3	0
			2203	681	1087	204	229	2			
1	H	153	Total	C	H	N	O	S	0	3	0
			2200	680	1085	203	230	2			
1	I	153	Total	C	H	N	O	S	12	3	0
			2203	681	1087	204	229	2			
1	J	153	Total	C	H	N	O	S	0	3	0
			2200	680	1085	203	230	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
A	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
A	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
B	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
B	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
B	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
C	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
C	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
C	149	THR	ILE	ENGINEERED MUTATION	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
D	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
D	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
E	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
E	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
E	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
F	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
F	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
F	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
G	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
G	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
G	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
H	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
H	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
H	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
I	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
I	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
I	149	THR	ILE	ENGINEERED MUTATION	UNP P00441
J	6	ALA	CYS	ENGINEERED MUTATION	UNP P00441
J	111	SER	CYS	ENGINEERED MUTATION	UNP P00441
J	149	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	G	1	Total Cu 1 1	0	0
2	J	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	H	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	Cu	0	0
			1	1		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	95	Total	O	0	0
			95	95		
4	C	57	Total	O	0	0
			57	57		
4	D	90	Total	O	0	0
			90	90		
4	E	48	Total	O	0	0
			48	48		
4	F	89	Total	O	0	0
			89	89		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	33	Total 33	O 33	0	0
4	H	63	Total 63	O 63	0	0
4	I	23	Total 23	O 23	0	0
4	J	47	Total 47	O 47	0	0

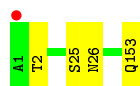
### 3 Residue-property plots [i](#)

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]



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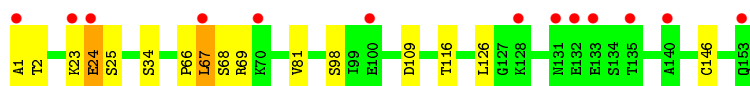
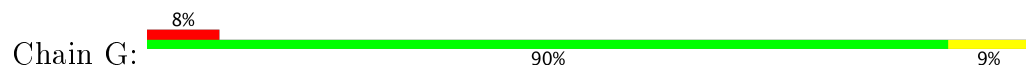
- Molecule 1: Superoxide dismutase [Cu-Zn]



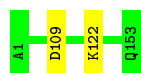
- Molecule 1: Superoxide dismutase [Cu-Zn]



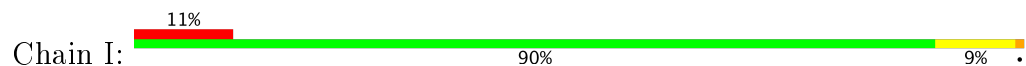
- Molecule 1: Superoxide dismutase [Cu-Zn]



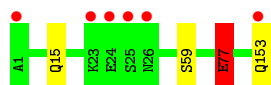
- Molecule 1: Superoxide dismutase [Cu-Zn]



- 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, $\alpha$ , $\beta$ , $\gamma$	165.10Å 203.81Å 144.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.10 – 2.38 48.05 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.3 (36.10-2.38) 93.7 (48.05-2.38)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.163 , 0.216 0.164 , 0.210	Depositor DCC
$R_{free}$ test set	1906 reflections (2.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.75	0/1147	0.73	0/1547
1	B	0.73	0/1147	0.76	0/1546
1	C	0.69	0/1147	0.70	0/1547
1	D	0.78	0/1147	0.75	0/1546
1	E	0.69	0/1147	0.73	0/1547
1	F	0.74	1/1147 (0.1%)	0.74	0/1546
1	G	0.62	0/1147	0.68	0/1547
1	H	0.71	0/1147	0.70	0/1546
1	I	0.59	0/1147	0.69	0/1547
1	J	0.64	1/1147 (0.1%)	0.71	0/1546
All	All	0.70	2/11470 (0.0%)	0.72	0/15465

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	I	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	77	GLU	CG-CD	5.59	1.60	1.51
1	J	77	GLU	CB-CG	5.17	1.61	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	110	HIS	Peptide

## 5.2 Too-close contacts ⓘ

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	1116	1086	1070	6	0
1	B	1115	1085	1077	2	0
1	C	1116	1086	1070	5	0
1	D	1115	1086	1077	1	0
1	E	1116	1088	1070	2	0
1	F	1115	1085	1077	3	0
1	G	1116	1087	1070	5	0
1	H	1115	1085	1077	0	0
1	I	1116	1087	1070	6	0
1	J	1115	1085	1077	3	0
2	A	1	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
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	94	0	0	1	0
4	B	95	0	0	0	0
4	C	57	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	90	0	0	1	0
4	E	48	0	0	1	0
4	F	89	0	0	0	0
4	G	33	0	0	0	0
4	H	63	0	0	0	0
4	I	23	0	0	0	0
4	J	47	0	0	1	0
All	All	11814	10860	10735	30	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 (30) 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:110:HIS:O	1:I:110:HIS:ND1	2.36	0.58
1:A:26:ASN:HA	1:C:26:ASN:HA	1.87	0.56
1:A:136:LYS:NZ	4:A:383:HOH:O	2.40	0.54
1:I:105:SER:O	1:I:111:SER:HA	2.09	0.52
1:F:25:SER:O	1:F:26:ASN:HB3	2.10	0.51
1:I:132:GLU:O	1:I:135:THR:OG1	2.25	0.51
1:G:116:THR:CG2	1:G:146:CYS:HB2	2.41	0.50
1:A:116:THR:CG2	1:A:146:CYS:HB2	2.43	0.49
1:A:132:GLU:H	1:A:132:GLU:CD	2.16	0.49
1:E:129:GLY:N	4:E:348:HOH:O	2.41	0.48
1:C:1:ALA:HB2	1:C:23:LYS:HD3	1.96	0.48
1:J:77:GLU:H	1:J:77:GLU:CD	2.16	0.47
1:G:1:ALA:CB	1:G:23:LYS:HA	2.45	0.47
1:A:2:THR:CG2	1:A:106:LEU:HB2	2.45	0.46
1:B:25:SER:O	1:B:26:ASN:CG	2.55	0.45
1:G:24:GLU:OE2	1:G:25:SER:N	2.51	0.44
1:C:2:THR:HG23	4:C:353:HOH:O	2.16	0.44
1:A:50:PHE:CZ	1:B:153:GLN:HB3	2.53	0.43
1:J:77:GLU:OE1	4:J:335:HOH:O	2.21	0.43
1:C:116:THR:CG2	1:C:146:CYS:HB2	2.49	0.43
1:I:2:THR:HG23	1:I:106:LEU:HD12	2.00	0.43
1:D:132:GLU:HB2	4:D:385:HOH:O	2.18	0.43
1:I:116:THR:CG2	1:I:146:CYS:HB2	2.50	0.42
1:F:121:GLU:HA	1:F:144:LEU:HD11	2.02	0.42
1:G:66:PRO:HD2	1:G:81:VAL:HG23	2.02	0.42
1:I:50:PHE:CZ	1:J:153:GLN:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:SER:O	1:F:111:SER:HA	2.21	0.41
1:G:67:LEU:HB2	1:G:69:ARG:HG2	2.03	0.41
1:E:117:LEU:O	1:E:146:CYS:HA	2.21	0.41

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	154/153 (101%)	152 (99%)	2 (1%)	0	100	100
1	B	154/153 (101%)	151 (98%)	3 (2%)	0	100	100
1	C	154/153 (101%)	153 (99%)	1 (1%)	0	100	100
1	D	154/153 (101%)	153 (99%)	1 (1%)	0	100	100
1	E	154/153 (101%)	145 (94%)	8 (5%)	1 (1%)	28	39
1	F	154/153 (101%)	151 (98%)	3 (2%)	0	100	100
1	G	154/153 (101%)	145 (94%)	9 (6%)	0	100	100
1	H	154/153 (101%)	153 (99%)	1 (1%)	0	100	100
1	I	154/153 (101%)	146 (95%)	6 (4%)	2 (1%)	14	18
1	J	154/153 (101%)	153 (99%)	1 (1%)	0	100	100
All	All	1540/1530 (101%)	1502 (98%)	35 (2%)	3 (0%)	51	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	123	ALA
1	I	111	SER
1	I	68	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/117 (103%)	116 (97%)	4 (3%)	43	61
1	B	120/117 (103%)	119 (99%)	1 (1%)	85	93
1	C	120/117 (103%)	115 (96%)	5 (4%)	34	51
1	D	120/117 (103%)	119 (99%)	1 (1%)	85	93
1	E	120/117 (103%)	113 (94%)	7 (6%)	23	34
1	F	120/117 (103%)	119 (99%)	1 (1%)	85	93
1	G	120/117 (103%)	111 (92%)	9 (8%)	16	22
1	H	120/117 (103%)	118 (98%)	2 (2%)	66	81
1	I	120/117 (103%)	115 (96%)	5 (4%)	34	51
1	J	120/117 (103%)	117 (98%)	3 (2%)	53	71
All	All	1200/1170 (103%)	1162 (97%)	38 (3%)	46	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	132	GLU
1	A	135	THR
1	A	136	LYS
1	B	2	THR
1	C	2	THR
1	C	68	SER
1	C	99[A]	ILE
1	C	99[B]	ILE
1	C	132	GLU
1	D	68	SER
1	E	2	THR
1	E	21	GLU
1	E	68	SER
1	E	99[A]	ILE
1	E	99[B]	ILE

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Mol	Chain	Res	Type
1	E	122	LYS
1	E	128	LYS
1	F	26	ASN
1	G	2	THR
1	G	24	GLU
1	G	34	SER
1	G	67	LEU
1	G	68	SER
1	G	98[A]	SER
1	G	98[B]	SER
1	G	109	ASP
1	G	126	LEU
1	H	109	ASP
1	H	122	LYS
1	I	25	SER
1	I	59	SER
1	I	70	LYS
1	I	77	GLU
1	I	142	SER
1	J	15	GLN
1	J	59	SER
1	J	77	GLU

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

Mol	Chain	Res	Type
1	G	63	HIS

### 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 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

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

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<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%)	-0.06	2 (1%) 77 78	16, 25, 47, 61	1 (0%)
1	B	153/153 (100%)	-0.03	1 (0%) 87 88	14, 21, 46, 60	1 (0%)
1	C	153/153 (100%)	0.27	9 (5%) 23 25	19, 30, 69, 90	0
1	D	153/153 (100%)	-0.10	1 (0%) 87 88	14, 21, 51, 60	1 (0%)
1	E	153/153 (100%)	0.25	6 (3%) 40 43	20, 37, 66, 85	1 (0%)
1	F	153/153 (100%)	-0.07	2 (1%) 77 78	15, 22, 45, 62	0
1	G	153/153 (100%)	0.54	13 (8%) 11 12	24, 41, 82, 103	1 (0%)
1	H	153/153 (100%)	-0.03	0 100 100	18, 29, 51, 68	1 (0%)
1	I	153/153 (100%)	0.65	17 (11%) 6 6	28, 47, 76, 95	3 (1%)
1	J	153/153 (100%)	0.27	6 (3%) 40 43	25, 35, 65, 79	0
All	All	1530/1530 (100%)	0.17	57 (3%) 42 45	14, 31, 67, 103	9 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1	ALA	9.7
1	E	1	ALA	7.4
1	J	1	ALA	7.3
1	I	130	GLY	6.1
1	C	1	ALA	5.6
1	I	70	LYS	5.1
1	A	1	ALA	5.0
1	D	1	ALA	5.0
1	I	1	ALA	4.5
1	J	153	GLN	4.5
1	I	133	GLU	4.3
1	G	23	LYS	4.2
1	C	131	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	4.0
1	I	132	GLU	3.9
1	G	153	GLN	3.9
1	C	132	GLU	3.8
1	I	135	THR	3.6
1	G	131	ASN	3.4
1	C	133	GLU	3.3
1	J	26	ASN	3.3
1	I	57	CYS	3.3
1	I	136	LYS	3.2
1	E	132	GLU	3.2
1	I	153	GLN	3.1
1	G	133	GLU	3.0
1	I	129	GLY	3.0
1	G	67	LEU	2.9
1	G	24	GLU	2.9
1	I	68	SER	2.9
1	C	128	LYS	2.9
1	A	153	GLN	2.8
1	E	131	ASN	2.8
1	C	135	THR	2.8
1	F	1	ALA	2.8
1	G	70	LYS	2.7
1	I	26	ASN	2.7
1	C	127	GLY	2.6
1	G	140	ALA	2.6
1	E	70	LYS	2.5
1	I	110	HIS	2.5
1	I	131	ASN	2.4
1	E	129	GLY	2.4
1	G	132	GLU	2.4
1	G	135	THR	2.2
1	J	24	GLU	2.2
1	F	153	GLN	2.2
1	J	23	LYS	2.2
1	C	77	GLU	2.1
1	I	67	LEU	2.1
1	I	66	PRO	2.1
1	E	133	GLU	2.1
1	C	68	SER	2.1
1	G	100	GLU	2.1
1	J	25	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	23	LYS	2.0
1	G	128	LYS	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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	D	202	1/1	1.00	0.14	0.08	21,21,21,21	0
3	ZN	B	202	1/1	1.00	0.14	0.03	21,21,21,21	0
3	ZN	A	202	1/1	1.00	0.11	-0.52	28,28,28,28	0
3	ZN	H	202	1/1	1.00	0.12	-0.74	27,27,27,27	0
3	ZN	J	202	1/1	1.00	0.10	-0.81	31,31,31,31	0
3	ZN	F	202	1/1	1.00	0.11	-1.01	22,22,22,22	0
3	ZN	E	202	1/1	0.98	0.09	-1.29	42,42,42,42	0
3	ZN	I	202	1/1	0.95	0.07	-1.55	53,53,53,53	0
3	ZN	G	202	1/1	0.96	0.09	-2.42	66,66,66,66	0
3	ZN	C	202	1/1	1.00	0.07	-2.48	42,42,42,42	0
2	CU	C	201	1/1	0.99	0.10	-2.56	39,39,39,39	0
2	CU	I	201	1/1	0.98	0.05	-3.27	62,62,62,62	0
2	CU	G	201	1/1	0.99	0.10	-3.32	59,59,59,59	0
2	CU	H	201	1/1	0.99	0.08	-3.87	39,39,39,39	0
2	CU	B	201	1/1	1.00	0.09	-4.22	34,34,34,34	0
2	CU	A	201	1/1	1.00	0.09	-5.08	36,36,36,36	0
2	CU	J	201	1/1	1.00	0.06	-	42,42,42,42	0
2	CU	E	201	1/1	0.99	0.09	-	50,50,50,50	0
2	CU	D	201	1/1	1.00	0.10	-	32,32,32,32	0
2	CU	F	201	1/1	0.99	0.08	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.