



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:49 AM BST

PDB ID : 3T5W  
Title : 2ME modified human SOD1  
Authors : Ihara, K.; Yamaguchi, Y.; Torigoe, H.; Wakatsuki, S.; Taniguchi, N.; Suzuki, K.; Fujiwara, N.  
Deposited on : 2011-07-28  
Resolution : 1.80 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

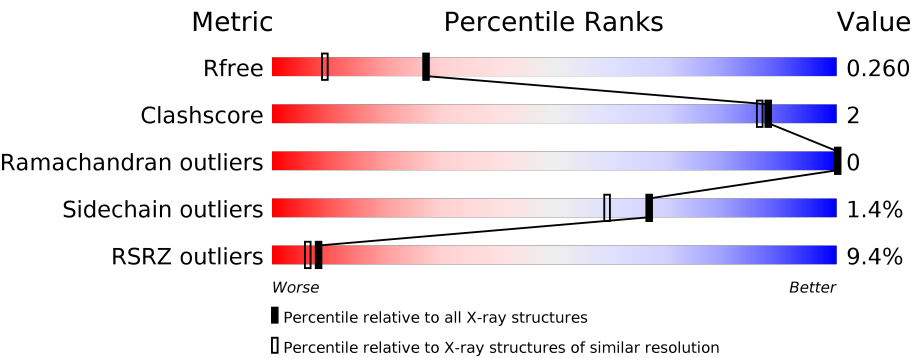
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



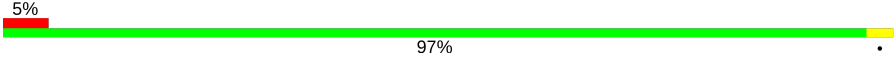
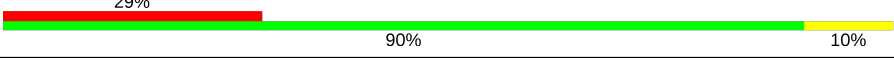
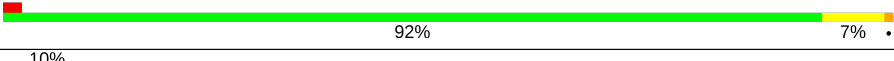
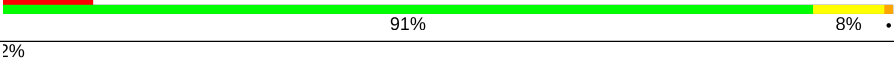
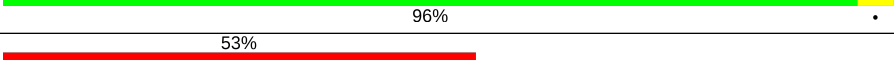
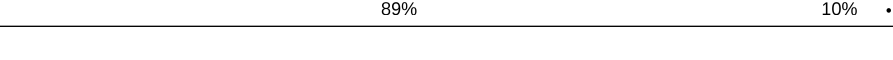
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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><div>%</div><div><div></div><div>98%</div><div>..</div></div></div>
1	B	153	<div><div>%</div><div><div></div><div>96%</div><div>.</div></div></div>
1	D	153	<div><div>3%</div><div><div></div><div>98%</div><div>..</div></div></div>
1	E	153	<div><div>%</div><div><div></div><div>97%</div><div>.</div></div></div>
1	F	153	<div><div>%</div><div><div></div><div>98%</div><div>.</div></div></div>
1	G	153	<div><div>3%</div><div><div></div><div>93%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	H	153	
1	I	153	
1	J	153	
1	K	153	
1	L	153	
1	M	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	L	400	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15198 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
			1114	681	203	225	5			
1	B	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	D	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	E	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	F	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	G	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	H	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	I	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	J	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	K	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	L	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			
1	M	153	Total	C	N	O	S	0	0	0
			1114	681	203	225	5			

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cu	0	0
			1	1		
2	J	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Cu 1	0	0
2	K	1	Total 1	Cu 1	0	0
2	E	1	Total 1	Cu 1	0	0
2	H	1	Total 1	Cu 1	0	0
2	B	1	Total 1	Cu 1	0	0
2	I	1	Total 1	Cu 1	0	0
2	A	1	Total 1	Cu 1	0	0
2	L	1	Total 1	Cu 1	0	0
2	F	1	Total 1	Cu 1	0	0
2	M	1	Total 1	Cu 1	0	0

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

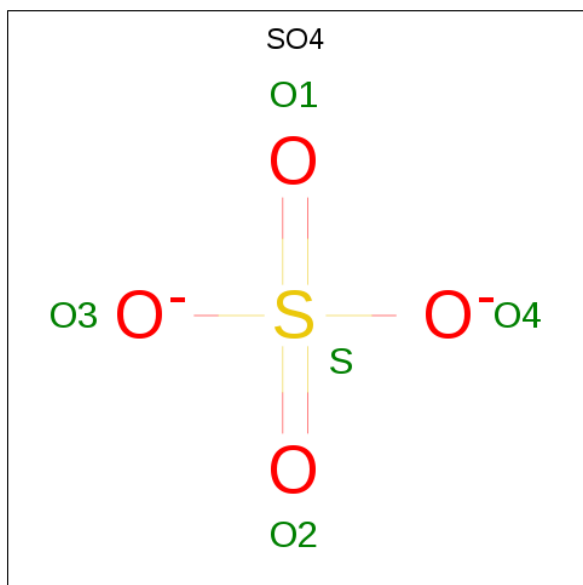
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	M	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	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	G	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		

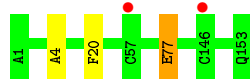
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	209	Total	O	0	0
			209	209		
5	B	226	Total	O	0	0
			226	226		
5	D	204	Total	O	0	0
			204	204		
5	E	228	Total	O	0	0
			228	228		
5	F	165	Total	O	0	0
			165	165		
5	G	123	Total	O	0	0
			123	123		
5	H	128	Total	O	0	0
			128	128		
5	I	52	Total	O	0	0
			52	52		
5	J	152	Total	O	0	0
			152	152		
5	K	65	Total	O	0	0
			65	65		
5	L	166	Total	O	0	0
			166	166		
5	M	28	Total	O	0	0
			28	28		

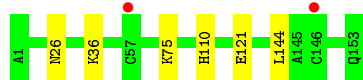
### 3 Residue-property plots [i](#)

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.

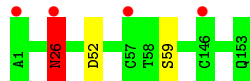
- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



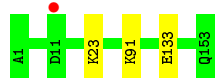
- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]

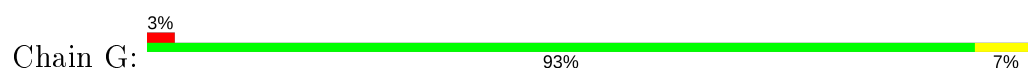


- Molecule 1: Superoxide dismutase [Cu-Zn]

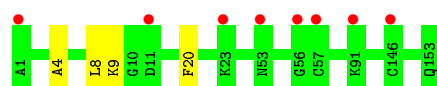


- Molecule 1: Superoxide dismutase [Cu-Zn]

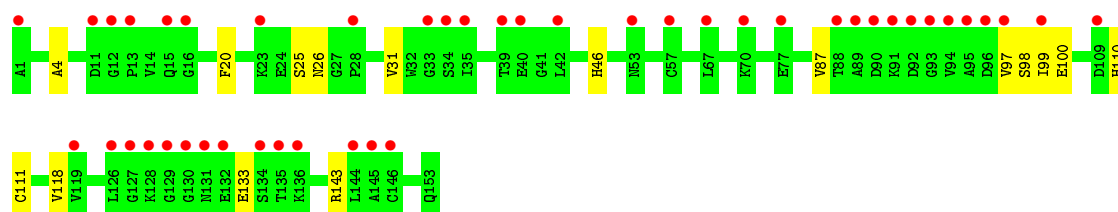
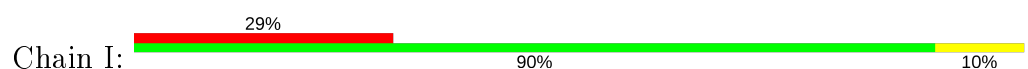




- Molecule 1: Superoxide dismutase [Cu-Zn]



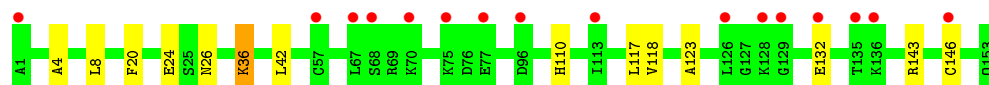
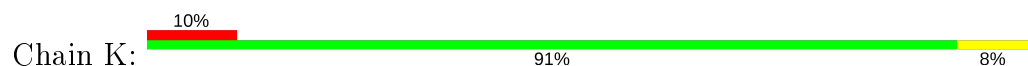
- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



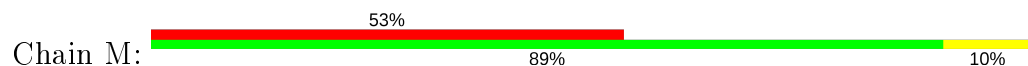
- Molecule 1: Superoxide dismutase [Cu-Zn]

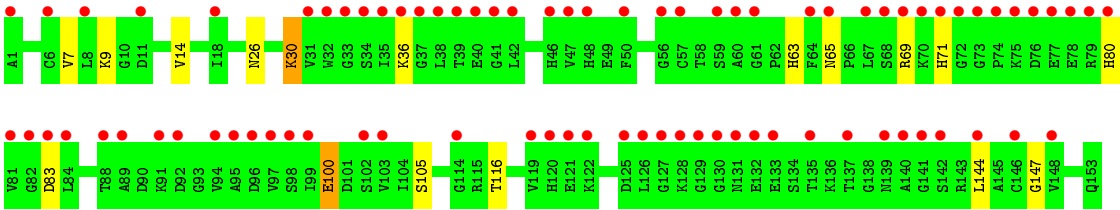


- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.09Å 163.28Å 173.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.04 – 1.80 34.04 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (34.04-1.80) 94.9 (34.04-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.200 , 0.241 0.219 , 0.260	Depositor DCC
$R_{free}$ test set	9252 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, CME, CU1, SO4

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	0.62	0/1121	0.70	0/1509
1	B	0.63	0/1121	0.69	0/1509
1	D	0.67	0/1121	0.70	0/1509
1	E	0.62	0/1121	0.72	1/1509 (0.1%)
1	F	0.59	0/1121	0.63	0/1509
1	G	0.50	0/1121	0.61	0/1509
1	H	0.55	0/1121	0.62	0/1509
1	I	0.44	0/1121	0.56	0/1509
1	J	0.53	0/1121	0.64	0/1509
1	K	0.41	0/1121	0.58	0/1509
1	L	0.52	0/1121	0.65	0/1509
1	M	0.43	0/1121	0.57	0/1509
All	All	0.55	0/13452	0.64	1/18108 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	ASP	CB-CG-OD2	5.29	123.06	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	26	ASN	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	1114	0	1081	2	0
1	B	1114	0	1081	4	0
1	D	1114	0	1081	2	0
1	E	1114	0	1081	3	0
1	F	1114	0	1081	1	0
1	G	1114	0	1081	7	0
1	H	1114	0	1081	1	0
1	I	1114	0	1081	7	0
1	J	1114	0	1081	8	0
1	K	1114	0	1081	8	0
1	L	1114	0	1081	5	0
1	M	1114	0	1081	10	0
2	A	1	0	0	0	0
2	B	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
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
3	A	1	0	0	0	0
3	B	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	1	0
4	K	5	0	0	0	0
4	L	5	0	0	2	0
4	M	5	0	0	0	0
5	A	209	0	0	1	0
5	B	226	0	0	1	0
5	D	204	0	0	0	0
5	E	228	0	0	2	0
5	F	165	0	0	0	0
5	G	123	0	0	2	0
5	H	128	0	0	0	0
5	I	52	0	0	1	0
5	J	152	0	0	2	0
5	K	65	0	0	1	0
5	L	166	0	0	1	0
5	M	28	0	0	1	0
All	All	15198	0	12972	54	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 2.

All (54) 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:J:133:GLU:HG2	4:J:400:SO4:O3	1.81	0.81
1:J:26:ASN:HA	5:J:849:HOH:O	1.91	0.70
1:G:26:ASN:HA	1:I:26:ASN:HA	1.78	0.65
1:B:26:ASN:HA	1:E:26:ASN:HA	1.80	0.62
1:L:133:GLU:HG2	4:L:400:SO4:O3	2.00	0.61
1:J:26:ASN:H	1:J:26:ASN:ND2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:ALA:HB3	1:I:20:PHE:HB2	1.87	0.57
1:H:4:ALA:HB3	1:H:20:PHE:HB2	1.89	0.54
1:L:128:LYS:NZ	5:L:1185:HOH:O	2.40	0.54
1:L:52:ASP:OD2	1:L:54:THR:HG23	2.09	0.52
1:E:3:LYS:HE2	5:E:573:HOH:O	2.10	0.52
1:I:31:VAL:HB	1:I:99:ILE:HB	1.92	0.52
1:L:111:CME:HE3	1:L:113:ILE:HB	1.92	0.51
1:D:52:ASP:O	1:D:59:SER:HB2	2.11	0.51
1:L:133:GLU:CG	4:L:400:SO4:O3	2.59	0.51
1:M:80:HIS:HB2	1:M:83:ASP:OD2	2.11	0.50
1:I:118:VAL:HG11	1:I:143:ARG:HG2	1.94	0.50
1:M:14:VAL:HG21	1:M:144:LEU:HB3	1.94	0.50
1:K:26:ASN:HA	1:M:26:ASN:HA	1.94	0.49
1:J:90:ASP:OD1	5:J:1306:HOH:O	2.20	0.49
1:J:113:ILE:HD13	1:J:151:ILE:HG12	1.95	0.49
1:K:8:LEU:HD11	1:K:117:LEU:HD23	1.93	0.49
1:I:110:HIS:O	5:I:1672:HOH:O	2.19	0.48
1:B:75:LYS:HG2	5:B:896:HOH:O	2.13	0.48
1:D:26:ASN:ND2	1:D:26:ASN:H	2.11	0.48
1:A:4:ALA:HB3	1:A:20:PHE:HB2	1.96	0.48
1:G:30:LYS:HD2	1:G:99:ILE:O	2.14	0.47
1:M:30:LYS:HG3	1:M:100:GLU:OE1	2.14	0.47
1:A:77:GLU:HG3	5:A:1512:HOH:O	2.15	0.47
1:J:121:GLU:HA	1:J:144:LEU:HD11	1.96	0.46
1:B:110:HIS:HE1	5:E:979:HOH:O	1.98	0.46
1:K:36:LYS:HE3	1:K:36:LYS:HB3	1.72	0.46
1:J:4:ALA:HB3	1:J:20:PHE:HB2	1.98	0.45
1:G:22:GLN:HG2	1:G:24:GLU:O	2.16	0.45
1:M:105:SER:N	5:M:1418:HOH:O	2.35	0.45
1:G:101:ASP:HA	5:G:1677:HOH:O	2.16	0.45
1:F:133:GLU:HA	1:F:133:GLU:OE1	2.17	0.45
1:I:87:VAL:HG11	1:I:97:VAL:HG22	1.99	0.44
1:M:65:ASN:HD21	1:M:69:ARG:H	1.65	0.44
1:K:8:LEU:HD23	1:K:146:CYS:HA	1.99	0.43
1:G:100:GLU:HG2	5:G:974:HOH:O	2.20	0.42
1:M:7:VAL:HG12	1:M:9:LYS:HG2	2.01	0.42
1:B:121:GLU:HA	1:B:144:LEU:HD11	2.01	0.42
1:E:121:GLU:HG2	1:E:122:LYS:HG3	2.02	0.41
1:K:118:VAL:HG11	1:K:143:ARG:HG2	2.02	0.41
1:M:63:HIS:CE1	1:M:71:HIS:HE1	2.38	0.41
1:J:133:GLU:HG3	1:J:137:THR:OG1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:GLY:HA3	1:I:25:SER:OG	2.20	0.41
1:M:116:THR:HA	1:M:147:GLY:O	2.20	0.41
1:K:110:HIS:HD2	5:K:1121:HOH:O	2.04	0.41
1:G:4:ALA:HB3	1:G:20:PHE:HB2	2.03	0.41
1:K:4:ALA:HB3	1:K:20:PHE:HB2	2.02	0.41
1:K:42:LEU:HB2	1:K:123:ALA:HB2	2.04	0.40
1:M:14:VAL:HG21	1:M:144:LEU:HD13	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	150/153 (98%)	150 (100%)	0	0	100	100
1	B	150/153 (98%)	150 (100%)	0	0	100	100
1	D	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	E	150/153 (98%)	150 (100%)	0	0	100	100
1	F	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	G	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	H	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	I	150/153 (98%)	146 (97%)	4 (3%)	0	100	100
1	J	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	K	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
1	L	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
1	M	150/153 (98%)	144 (96%)	6 (4%)	0	100	100
All	All	1800/1836 (98%)	1780 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.



### 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	117/117 (100%)	116 (99%)	1 (1%)	78	75
1	B	117/117 (100%)	116 (99%)	1 (1%)	78	75
1	D	117/117 (100%)	116 (99%)	1 (1%)	78	75
1	E	117/117 (100%)	117 (100%)	0	100	100
1	F	117/117 (100%)	115 (98%)	2 (2%)	60	51
1	G	117/117 (100%)	117 (100%)	0	100	100
1	H	117/117 (100%)	115 (98%)	2 (2%)	60	51
1	I	117/117 (100%)	113 (97%)	4 (3%)	37	22
1	J	117/117 (100%)	114 (97%)	3 (3%)	46	32
1	K	117/117 (100%)	114 (97%)	3 (3%)	46	32
1	L	117/117 (100%)	117 (100%)	0	100	100
1	M	117/117 (100%)	114 (97%)	3 (3%)	46	32
All	All	1404/1404 (100%)	1384 (99%)	20 (1%)	67	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	B	36	LYS
1	D	26	ASN
1	F	23	LYS
1	F	91	LYS
1	H	8	LEU
1	H	9	LYS
1	I	46	HIS
1	I	98	SER
1	I	100	GLU
1	I	133	GLU
1	J	3	LYS
1	J	25	SER
1	J	26	ASN

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Mol	Chain	Res	Type
1	K	24	GLU
1	K	36	LYS
1	K	132	GLU
1	M	30	LYS
1	M	36	LYS
1	M	100	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	B	110	HIS
1	D	15	GLN
1	D	26	ASN
1	D	53	ASN
1	E	53	ASN
1	F	53	ASN
1	H	53	ASN
1	H	153	GLN
1	I	15	GLN
1	J	26	ASN
1	J	53	ASN
1	K	53	ASN
1	L	15	GLN
1	L	53	ASN
1	M	63	HIS
1	M	65	ASN
1	M	110	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CME	B	111	1	8,9,10	0.79	0	5,9,11	0.33	0
1	CME	M	111	1	8,9,10	0.76	0	5,9,11	0.66	0
1	CME	H	111	1	8,9,10	0.82	0	5,9,11	0.63	0
1	CME	K	111	1	8,9,10	0.79	0	5,9,11	0.39	0
1	CME	I	111	1	8,9,10	0.85	0	5,9,11	0.98	1 (20%)
1	CME	D	111	1	8,9,10	0.73	0	5,9,11	0.97	0
1	CME	G	111	1	8,9,10	0.79	0	5,9,11	0.36	0
1	CME	E	111	1	8,9,10	0.75	0	5,9,11	0.56	0
1	CME	F	111	1	8,9,10	0.66	0	5,9,11	0.88	0
1	CME	A	111	1	8,9,10	0.75	0	5,9,11	0.79	0
1	CME	J	111	1	8,9,10	0.71	0	5,9,11	0.86	0
1	CME	L	111	1	8,9,10	0.87	0	5,9,11	1.11	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
1	CME	B	111	1	-	0/5/8/10	-
1	CME	M	111	1	-	0/5/8/10	-
1	CME	H	111	1	-	1/5/8/10	-
1	CME	K	111	1	-	0/5/8/10	-
1	CME	I	111	1	-	1/5/8/10	-
1	CME	D	111	1	-	2/5/8/10	-
1	CME	G	111	1	-	0/5/8/10	-
1	CME	E	111	1	-	2/5/8/10	-
1	CME	F	111	1	-	1/5/8/10	-
1	CME	A	111	1	-	1/5/8/10	-
1	CME	J	111	1	-	2/5/8/10	-
1	CME	L	111	1	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	I	111	CME	CB-SG-SD	2.02	109.05	103.82

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	111	CME	SD-CE-CZ-OH
1	D	111	CME	SD-CE-CZ-OH
1	F	111	CME	SD-CE-CZ-OH
1	A	111	CME	SD-CE-CZ-OH
1	J	111	CME	SD-CE-CZ-OH
1	L	111	CME	SD-CE-CZ-OH
1	I	111	CME	CE-SD-SG-CB
1	E	111	CME	CZ-CE-SD-SG
1	D	111	CME	CA-CB-SG-SD
1	E	111	CME	CA-CB-SG-SD
1	J	111	CME	CA-CB-SG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	111	CME	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	G	400	-	4,4,4	0.16	0	6,6,6	0.32	0
4	SO4	M	400	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	K	400	-	4,4,4	0.14	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	400	-	4,4,4	0.18	0	6,6,6	0.37	0
4	SO4	B	400	-	4,4,4	0.15	0	6,6,6	0.32	0
4	SO4	F	400	-	4,4,4	0.21	0	6,6,6	0.19	0
4	SO4	I	400	-	4,4,4	0.16	0	6,6,6	0.13	0
4	SO4	D	400	-	4,4,4	0.15	0	6,6,6	0.29	0
4	SO4	J	400	-	4,4,4	0.17	0	6,6,6	0.33	0
4	SO4	H	400	-	4,4,4	0.17	0	6,6,6	0.32	0
4	SO4	L	400	-	4,4,4	0.21	0	6,6,6	0.44	0
4	SO4	E	400	-	4,4,4	0.11	0	6,6,6	0.33	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	400	SO4	1	0
4	L	400	SO4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	152/153 (99%)	0.02	2 (1%) 77 74	2, 6, 15, 19	2 (1%)
1	B	152/153 (99%)	-0.23	2 (1%) 77 74	2, 6, 15, 19	2 (1%)
1	D	152/153 (99%)	-0.13	4 (2%) 56 51	2, 6, 15, 25	2 (1%)
1	E	152/153 (99%)	-0.09	2 (1%) 77 74	2, 7, 16, 20	2 (1%)
1	F	152/153 (99%)	0.14	1 (0%) 87 86	7, 12, 22, 28	2 (1%)
1	G	152/153 (99%)	0.49	5 (3%) 46 40	15, 20, 31, 33	2 (1%)
1	H	152/153 (99%)	0.24	8 (5%) 26 21	7, 17, 26, 31	2 (1%)
1	I	152/153 (99%)	1.56	45 (29%) 0 0	20, 33, 45, 49	2 (1%)
1	J	152/153 (99%)	0.05	3 (1%) 65 61	7, 14, 24, 29	2 (1%)
1	K	152/153 (99%)	0.83	16 (10%) 6 4	16, 29, 40, 46	2 (1%)
1	L	152/153 (99%)	0.15	3 (1%) 65 61	5, 15, 27, 33	2 (1%)
1	M	152/153 (99%)	2.40	81 (53%) 0 0	23, 40, 51, 56	2 (1%)
All	All	1824/1836 (99%)	0.45	172 (9%) 8 6	2, 15, 41, 56	24 (1%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	144	LEU	9.2
1	M	1	ALA	7.6
1	M	57	CYS	6.0
1	M	129	GLY	5.9
1	I	11	ASP	5.5
1	M	142	SER	5.4
1	I	95	ALA	5.4
1	M	70	LYS	5.2
1	M	77	GLU	5.2
1	I	39	THR	5.1
1	I	94	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	M	146	CYS	5.1
1	M	135	THR	4.9
1	I	34	SER	4.9
1	M	76	ASP	4.8
1	I	88	THR	4.8
1	M	131	ASN	4.7
1	M	42	LEU	4.6
1	M	141	GLY	4.6
1	I	13	PRO	4.6
1	M	39	THR	4.6
1	M	84	LEU	4.6
1	M	91	LYS	4.5
1	I	33	GLY	4.5
1	B	146	CYS	4.4
1	I	128	LYS	4.4
1	I	67	LEU	4.3
1	M	130	GLY	4.3
1	M	95	ALA	4.2
1	M	128	LYS	4.2
1	M	140	ALA	4.1
1	K	129	GLY	4.1
1	H	57	CYS	4.0
1	E	146	CYS	4.0
1	M	67	LEU	4.0
1	I	35	ILE	3.9
1	M	121	GLU	3.9
1	D	146	CYS	3.9
1	M	126	LEU	3.9
1	I	91	LYS	3.9
1	M	40	GLU	3.9
1	I	132	GLU	3.9
1	M	82	GLY	3.8
1	E	57	CYS	3.7
1	M	127	GLY	3.6
1	H	11	ASP	3.5
1	M	68	SER	3.5
1	M	94	VAL	3.5
1	I	131	ASN	3.4
1	J	26	ASN	3.4
1	I	57	CYS	3.4
1	I	12	GLY	3.3
1	A	146	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	74	PRO	3.3
1	K	135	THR	3.3
1	J	146	CYS	3.3
1	M	69	ARG	3.3
1	M	132	GLU	3.3
1	M	133	GLU	3.3
1	M	36	LYS	3.2
1	M	96	ASP	3.2
1	M	137	THR	3.2
1	I	89	ALA	3.2
1	G	11	ASP	3.2
1	I	93	GLY	3.2
1	M	119	VAL	3.1
1	M	81	VAL	3.1
1	H	146	CYS	3.0
1	K	68	SER	3.0
1	M	99	ILE	3.0
1	M	92	ASP	3.0
1	H	56	GLY	3.0
1	A	57	CYS	3.0
1	M	32	TRP	2.9
1	L	1	ALA	2.9
1	M	38	LEU	2.9
1	I	136	LYS	2.9
1	M	125	ASP	2.9
1	I	129	GLY	2.9
1	F	11	ASP	2.9
1	M	33	GLY	2.8
1	M	75	LYS	2.8
1	M	122	LYS	2.8
1	K	1	ALA	2.8
1	M	46	HIS	2.8
1	I	145	ALA	2.8
1	M	35	ILE	2.8
1	K	146	CYS	2.8
1	G	12	GLY	2.7
1	I	42	LEU	2.7
1	I	92	ASP	2.7
1	I	40	GLU	2.7
1	I	96	ASP	2.7
1	M	11	ASP	2.7
1	M	97	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	103	VAL	2.6
1	M	71	HIS	2.6
1	I	90	ASP	2.6
1	I	146	CYS	2.6
1	J	57	CYS	2.6
1	M	31	VAL	2.6
1	G	1	ALA	2.6
1	B	57	CYS	2.6
1	I	16	GLY	2.6
1	M	73	GLY	2.6
1	M	102	SER	2.6
1	G	91	LYS	2.5
1	M	47	VAL	2.5
1	D	26	ASN	2.5
1	I	77	GLU	2.5
1	L	146	CYS	2.5
1	I	15	GLN	2.5
1	M	18	ILE	2.5
1	I	127	GLY	2.5
1	M	61	GLY	2.5
1	M	139	ASN	2.4
1	K	128	LYS	2.4
1	H	1	ALA	2.4
1	I	70	LYS	2.4
1	M	78	GLU	2.4
1	I	130	GLY	2.4
1	D	1	ALA	2.4
1	M	60	ALA	2.4
1	K	75	LYS	2.4
1	M	88	THR	2.4
1	I	109	ASP	2.4
1	M	8	LEU	2.4
1	M	48	HIS	2.4
1	K	132	GLU	2.4
1	H	23	LYS	2.4
1	I	23	LYS	2.4
1	M	59	SER	2.3
1	M	98	SER	2.3
1	I	53	ASN	2.3
1	M	79	ARG	2.3
1	I	135	THR	2.3
1	K	70	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	113	ILE	2.3
1	M	65	ASN	2.3
1	M	64	PHE	2.3
1	I	28	PRO	2.2
1	K	126	LEU	2.2
1	M	41	GLY	2.2
1	D	57	CYS	2.2
1	L	57	CYS	2.2
1	M	6	CYS	2.2
1	M	34	SER	2.2
1	I	97	VAL	2.2
1	M	83	ASP	2.2
1	M	37	GLY	2.2
1	M	80	HIS	2.2
1	H	91	LYS	2.2
1	M	120	HIS	2.1
1	K	77	GLU	2.1
1	M	148	VAL	2.1
1	K	57	CYS	2.1
1	K	136	LYS	2.1
1	I	119	VAL	2.1
1	M	72	GLY	2.1
1	I	144	LEU	2.1
1	M	56	GLY	2.1
1	M	50	PHE	2.0
1	I	1	ALA	2.0
1	M	89	ALA	2.0
1	K	96	ASP	2.0
1	M	114	GLY	2.0
1	G	8	LEU	2.0
1	H	53	ASN	2.0
1	I	99	ILE	2.0
1	I	126	LEU	2.0
1	K	67	LEU	2.0
1	I	134	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	CME	M	111	10/11	0.85	0.13	29,31,34,37	0
1	CME	G	111	10/11	0.85	0.15	20,22,32,33	0
1	CME	I	111	10/11	0.88	0.16	25,27,36,39	0
1	CME	H	111	10/11	0.92	0.12	15,17,32,35	0
1	CME	K	111	10/11	0.93	0.12	25,28,33,36	0
1	CME	L	111	10/11	0.93	0.10	12,15,29,30	0
1	CME	F	111	10/11	0.95	0.10	11,14,31,35	0
1	CME	J	111	10/11	0.95	0.12	11,13,25,29	0
1	CME	B	111	10/11	0.95	0.09	6,10,20,21	0
1	CME	E	111	10/11	0.96	0.09	5,7,18,22	0
1	CME	D	111	10/11	0.98	0.07	5,7,18,20	0
1	CME	A	111	10/11	0.98	0.09	3,5,18,20	0

### 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	M	300	1/1	0.65	0.10	38,38,38,38	0
4	SO4	M	400	5/5	0.67	0.24	83,83,84,84	0
2	CU1	M	200	1/1	0.78	0.09	48,48,48,48	0
4	SO4	I	400	5/5	0.81	0.27	63,63,63,64	0
4	SO4	K	400	5/5	0.89	0.17	69,69,70,70	0
3	ZN	K	300	1/1	0.94	0.05	31,31,31,31	0
2	CU1	I	200	1/1	0.95	0.06	34,34,34,34	0
4	SO4	L	400	5/5	0.95	0.11	33,34,35,36	0
4	SO4	F	400	5/5	0.96	0.18	30,32,32,33	0
2	CU1	K	200	1/1	0.96	0.07	33,33,33,33	0
4	SO4	G	400	5/5	0.97	0.09	26,27,28,28	0
4	SO4	D	400	5/5	0.97	0.12	22,22,23,23	0
3	ZN	I	300	1/1	0.97	0.04	27,27,27,27	0
4	SO4	J	400	5/5	0.97	0.10	33,33,34,35	0
4	SO4	A	400	5/5	0.98	0.08	17,17,20,20	0
2	CU1	G	200	1/1	0.98	0.05	23,23,23,23	0
2	CU1	F	200	1/1	0.98	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	H	400	5/5	0.98	0.13	25,25,26,27	0
3	ZN	F	300	1/1	0.98	0.04	11,11,11,11	0
2	CU1	J	200	1/1	0.99	0.07	13,13,13,13	0
2	CU1	L	200	1/1	0.99	0.07	11,11,11,11	0
3	ZN	G	300	1/1	0.99	0.06	16,16,16,16	0
2	CU1	H	200	1/1	0.99	0.04	18,18,18,18	0
3	ZN	H	300	1/1	0.99	0.09	11,11,11,11	0
4	SO4	B	400	5/5	0.99	0.05	13,14,15,16	0
3	ZN	J	300	1/1	0.99	0.09	9,9,9,9	0
2	CU1	E	200	1/1	0.99	0.08	7,7,7,7	0
3	ZN	L	300	1/1	0.99	0.08	7,7,7,7	0
4	SO4	E	400	5/5	0.99	0.05	18,19,20,21	0
3	ZN	B	300	1/1	1.00	0.09	4,4,4,4	0
3	ZN	D	300	1/1	1.00	0.09	5,5,5,5	0
2	CU1	D	200	1/1	1.00	0.07	6,6,6,6	0
2	CU1	B	200	1/1	1.00	0.07	6,6,6,6	0
3	ZN	E	300	1/1	1.00	0.07	5,5,5,5	0
2	CU1	A	200	1/1	1.00	0.09	6,6,6,6	0
3	ZN	A	300	1/1	1.00	0.09	5,5,5,5	0

## 6.5 Other polymers

There are no such residues in this entry.