



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 12:16 PM JST

PDB ID : 8IQ0  
Title : Crystal structure of hydrogen sulfide-bound superoxide dismutase in oxidized state  
Authors : Zhou, J.H.; Huang, W.X.; Cheng, R.X.; Zhang, P.J.; Zhu, Y.C.  
Deposited on : 2023-03-15  
Resolution : 1.88 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.

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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
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) : 2.35

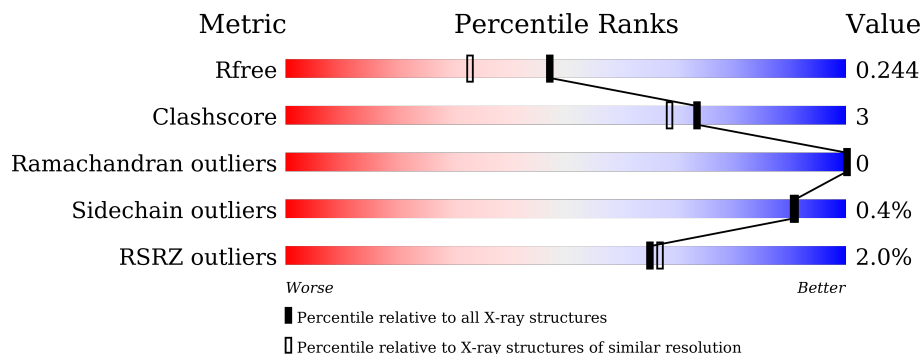
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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.



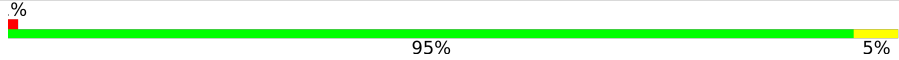
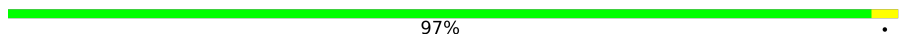
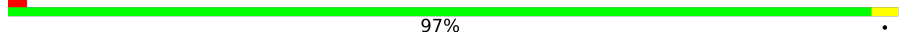
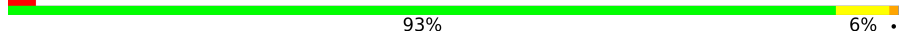
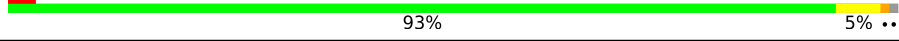
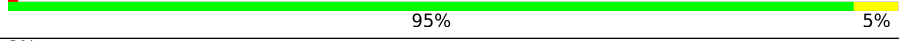

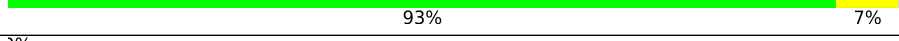
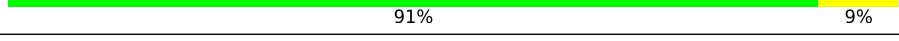
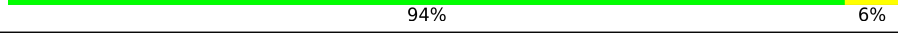
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	151	
1	B	151	
1	C	151	
1	D	151	
1	E	151	
1	F	151	

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Mol	Chain	Length	Quality of chain
1	G	151	 95% 5%
1	H	151	 97% .
1	I	151	 97% .
1	J	151	 93% 6% ..
1	K	151	 93% 5% ..
1	L	151	 95% 5%
1	M	151	 89% 11%
1	N	151	 93% 7%
1	O	151	 91% 9%
1	P	151	 94% 6%

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
5	GOL	F	203	-	-	X	-
8	H2S	M	203	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 18883 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	151	1075	660	196	215	4	0	0	0
1	B	151	1068	659	193	212	4	0	0	0
1	C	151	1084	666	196	218	4	0	0	0
1	D	139	972	602	175	191	4	0	0	0
1	E	151	1089	669	199	216	5	0	1	0
1	F	151	1087	668	198	217	4	0	0	0
1	G	151	1083	666	198	215	4	0	0	0
1	H	151	1083	665	197	217	4	0	0	0
1	I	151	1083	665	197	217	4	0	0	0
1	J	150	1073	661	195	213	4	0	0	0
1	K	149	1072	660	194	214	4	0	0	0
1	L	151	1083	665	197	217	4	0	0	0
1	M	151	1062	654	193	211	4	0	0	0
1	N	151	1093	671	199	218	5	0	1	0
1	O	151	1077	661	193	219	4	0	0	0
1	P	151	1089	670	196	218	5	0	1	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
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 2 2	0	1
2	J	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	L	1	Total Cu 1 1	0	0
2	M	1	Total Cu 2 2	0	1
2	N	1	Total Cu 2 2	0	1
2	O	1	Total Cu 1 1	0	0
2	P	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

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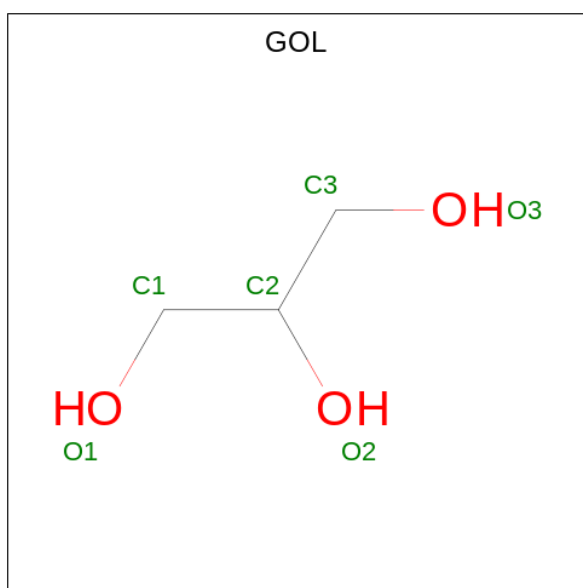
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	K	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0
3	M	1	Total Zn 1 1	0	0
3	N	1	Total Zn 1 1	0	0
3	O	1	Total Zn 1 1	0	0
3	P	1	Total Zn 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	N	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



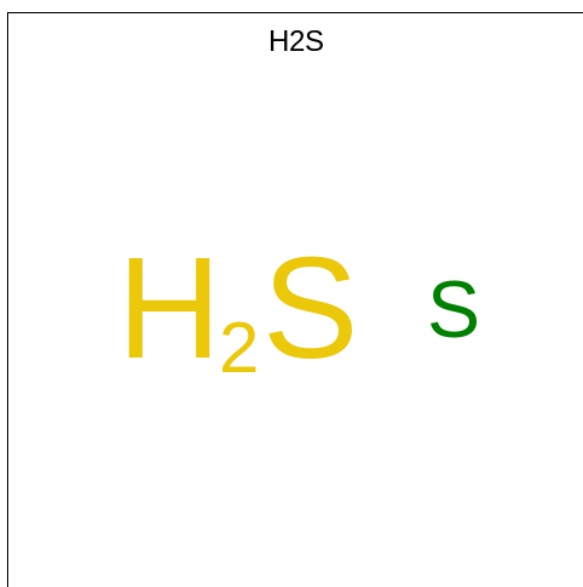
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total O S 5 4 1	0	0
6	I	1	Total O S 5 4 1	0	0
6	K	1	Total O S 5 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total Cl 1 1	0	0
7	P	1	Total Cl 1 1	0	0

- Molecule 8 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total S 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	128	Total O 128 128	0	0
9	B	88	Total O 88 88	0	0
9	C	100	Total O 100 100	0	0
9	D	66	Total O 66 66	0	0
9	E	111	Total O 111 111	0	0
9	F	123	Total O 123 123	0	0
9	G	92	Total O 92 92	0	0
9	H	152	Total O 152 152	0	0
9	I	89	Total O 89 89	0	0
9	J	75	Total O 75 75	0	0
9	K	92	Total O 92 92	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	102	Total 102	O 102	0	0
9	M	86	Total 86	O 86	0	0
9	N	88	Total 88	O 88	0	0
9	O	102	Total 102	O 102	0	0
9	P	149	Total 149	O 149	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]

Chain A:  92% 8%




- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  95% 5% 2%




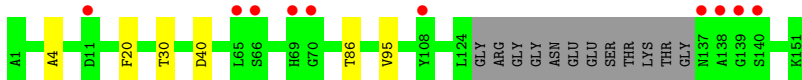
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain C:  91% 9% 5%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain D:  88% 8% 7%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain E:  93% 7%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain F:  92% 8%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain G:  95% 5%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain H:  97% .

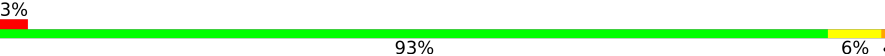


- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain I:  97% .



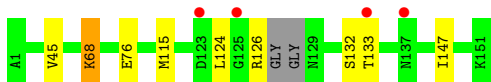
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain J:  93% 6% ..



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain K:  93% 5% ..

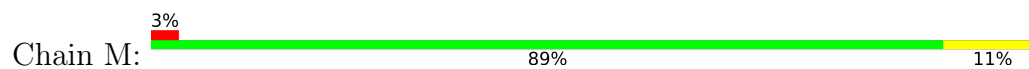


- Molecule 1: Superoxide dismutase [Cu-Zn]

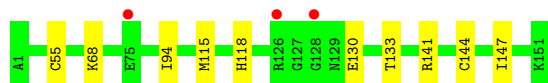
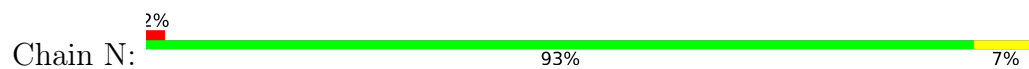
Chain L:  95% 5%



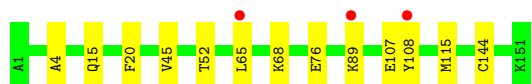
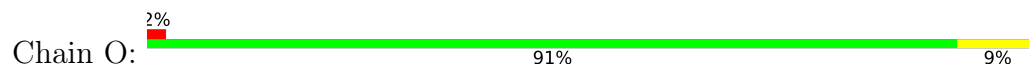
- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.35Å 91.47Å 91.16Å 85.00° 78.06° 66.76°	Depositor
Resolution (Å)	30.68 – 1.88 30.68 – 1.88	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.68-1.88) 88.4 (30.68-1.88)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 1.88Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.201 , 0.244 0.201 , 0.244	Depositor DCC
$R_{free}$ test set	7837 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtrriage
Anisotropy	0.095	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for -h,-h+k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 84.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8274e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, H2S, GOL, SO4, CL, EDO, 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	0.41	0/1093	0.60	0/1481
1	B	0.38	0/1086	0.62	0/1471
1	C	0.41	0/1102	0.61	0/1491
1	D	0.39	0/989	0.62	0/1345
1	E	0.39	0/1107	0.62	0/1497
1	F	0.40	0/1105	0.61	0/1494
1	G	0.39	0/1101	0.62	0/1489
1	H	0.39	0/1101	0.64	0/1490
1	I	0.35	0/1101	0.59	0/1490
1	J	0.33	0/1090	0.58	0/1474
1	K	0.38	0/1089	0.58	0/1473
1	L	0.38	0/1101	0.60	0/1490
1	M	0.39	0/1080	0.59	0/1465
1	N	0.40	0/1111	0.58	0/1502
1	O	0.40	0/1095	0.61	0/1484
1	P	0.43	0/1107	0.60	0/1497
All	All	0.39	0/17458	0.60	0/23633

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

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	1075	0	1037	8	0
1	B	1068	0	1033	4	0
1	C	1084	0	1052	12	0
1	D	972	0	918	3	0
1	E	1089	0	1063	7	0
1	F	1087	0	1063	11	0
1	G	1083	0	1059	5	0
1	H	1083	0	1052	2	0
1	I	1083	0	1052	2	0
1	J	1073	0	1042	8	0
1	K	1072	0	1041	7	0
1	L	1083	0	1052	4	0
1	M	1062	0	1020	12	0
1	N	1093	0	1067	8	0
1	O	1077	0	1034	11	0
1	P	1089	0	1060	9	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	2	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	2	0	0	0	0
2	N	2	0	0	0	0
2	O	1	0	0	0	0
2	P	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
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	C	4	0	6	0	0
4	N	4	0	6	2	0
5	F	6	0	8	4	0
6	F	5	0	0	0	0
6	I	5	0	0	0	0
6	K	5	0	0	0	0
7	L	1	0	0	0	0
7	P	1	0	0	0	0
8	M	1	0	0	2	0
9	A	128	0	0	0	0
9	B	88	0	0	1	0
9	C	100	0	0	2	0
9	D	66	0	0	0	0
9	E	111	0	0	0	0
9	F	123	0	0	1	0
9	G	92	0	0	1	0
9	H	152	0	0	0	0
9	I	89	0	0	0	0
9	J	75	0	0	1	0
9	K	92	0	0	0	0
9	L	102	0	0	0	0
9	M	86	0	0	1	0
9	N	88	0	0	1	0
9	O	102	0	0	1	0
9	P	149	0	0	2	0
All	All	18883	0	16665	108	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 3.

All (108) 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:M:118:HIS:CE1	8:M:203:H2S:S	2.63	0.90
1:N:141:ARG:HH21	4:N:203:EDO:H21	1.48	0.78
1:F:141:ARG:HH21	5:F:203:GOL:H2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:HIS:NE2	8:M:203:H2S:S	2.56	0.77
1:F:65:LEU:HD21	1:F:108:TYR:HE1	1.55	0.71
1:A:130:GLU:O	1:A:133:THR:HG22	1.92	0.70
1:F:141:ARG:NH2	5:F:203:GOL:H2	2.10	0.66
1:P:119:GLU:HG3	1:P:120:LYS:HG3	1.79	0.64
1:O:107:GLU:HG3	1:O:108:TYR:CD1	2.34	0.63
1:N:130:GLU:O	1:N:133:THR:HG22	1.98	0.62
1:A:133:THR:HG23	1:A:134:LYS:HD3	1.82	0.61
1:D:40:ASP:OD1	1:D:86:THR:HG22	2.01	0.60
1:F:141:ARG:HH21	5:F:203:GOL:C2	2.12	0.60
1:E:8:LEU:O	1:E:9:LYS:HD3	2.02	0.59
1:M:119:GLU:HA	1:M:142:LEU:HD11	1.84	0.58
1:K:126:ARG:N	1:K:132:SER:OG	2.37	0.58
1:L:34:THR:HG22	1:L:92:VAL:HG22	1.86	0.58
1:B:119:GLU:HA	1:B:142:LEU:HD11	1.86	0.57
1:K:68:LYS:HE2	1:K:133:THR:HB	1.86	0.57
1:O:107:GLU:HG3	1:O:108:TYR:HD1	1.69	0.57
1:G:73:LYS:NZ	9:G:303:HOH:O	2.37	0.57
1:N:115:MET:HG2	1:N:147:ILE:HD11	1.87	0.56
1:A:3:LYS:HE2	1:A:151:LYS:O	2.06	0.55
1:O:65:LEU:HD21	1:O:108:TYR:OH	2.07	0.55
1:K:115:MET:HE1	1:K:147:ILE:HD11	1.90	0.54
1:G:45:VAL:HG22	1:G:115:MET:SD	2.48	0.54
1:O:65:LEU:HD21	1:O:108:TYR:CZ	2.43	0.54
1:C:45:VAL:HG22	1:C:115:MET:CE	2.38	0.54
1:O:89:LYS:HE2	9:O:384:HOH:O	2.09	0.53
1:O:45:VAL:HG22	1:O:115:MET:SD	2.49	0.53
1:M:4:ALA:HB3	1:M:20:PHE:HB2	1.91	0.52
1:C:119:GLU:HA	1:C:142:LEU:HD11	1.91	0.52
1:F:119:GLU:HG2	1:F:120:LYS:HG3	1.92	0.52
1:H:94:ILE:HD12	1:N:94:ILE:HG23	1.92	0.51
1:C:3:LYS:NZ	9:C:309:HOH:O	2.43	0.51
1:P:119:GLU:HA	1:P:142:LEU:HD11	1.93	0.51
1:C:67:LYS:HG3	1:C:76:GLU:OE2	2.12	0.50
1:N:68:LYS:HA	9:N:332:HOH:O	2.12	0.50
1:F:135:THR:HG22	5:F:203:GOL:H11	1.94	0.49
1:D:4:ALA:HB3	1:D:20:PHE:HB2	1.94	0.49
1:E:119:GLU:HA	1:E:142:LEU:HD11	1.94	0.49
1:O:68:LYS:HG2	1:O:76:GLU:OE2	2.12	0.49
1:F:69:HIS:HB2	1:F:78:HIS:CE1	2.47	0.48
1:I:8:LEU:C	1:I:9:LYS:HG3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:LEU:HD21	1:F:108:TYR:CE1	2.44	0.47
1:G:7:VAL:HG11	1:G:9:LYS:NZ	2.29	0.47
1:M:56:THR:OG1	1:P:130:GLU:OE2	2.20	0.47
1:E:7:VAL:HG12	1:E:9:LYS:HE3	1.96	0.47
1:F:64:PRO:HG2	1:F:65:LEU:HD22	1.96	0.47
1:D:30:THR:HA	1:D:95:VAL:O	2.14	0.47
1:M:8:LEU:O	1:M:15:GLN:HG3	2.15	0.47
1:E:7:VAL:CG1	1:E:9:LYS:HE3	2.45	0.47
1:J:45:VAL:HG22	1:J:115:MET:CE	2.44	0.46
1:A:119:GLU:HA	1:A:142:LEU:HD11	1.97	0.46
1:M:45:VAL:HG22	1:M:115:MET:SD	2.55	0.46
1:C:68:LYS:N	1:C:68:LYS:HD3	2.30	0.46
1:J:119:GLU:HA	1:J:142:LEU:HD11	1.97	0.46
1:K:45:VAL:HG22	1:K:115:MET:CE	2.46	0.46
1:A:130:GLU:O	1:A:134:LYS:HG2	2.16	0.46
1:P:134:LYS:HE2	9:P:416:HOH:O	2.16	0.45
1:B:127:GLY:HA3	1:E:37:THR:HB	1.98	0.45
1:N:118:HIS:HE1	4:N:203:EDO:H12	1.81	0.45
1:C:45:VAL:HG22	1:C:115:MET:HE1	1.98	0.45
1:K:124:LEU:HD23	1:K:124:LEU:N	2.31	0.45
1:L:4:ALA:HB3	1:L:20:PHE:HB2	1.99	0.45
1:A:4:ALA:HB3	1:A:20:PHE:HB2	1.99	0.45
1:P:89:LYS:HG3	9:P:400:HOH:O	2.17	0.45
1:C:134:LYS:NZ	9:C:311:HOH:O	2.47	0.45
1:B:61:HIS:NE2	9:B:302:HOH:O	2.34	0.44
1:C:67:LYS:HE3	1:C:67:LYS:HB2	1.67	0.44
1:L:43:PHE:CE2	1:L:115:MET:HE2	2.53	0.44
1:M:35:GLY:O	9:M:301:HOH:O	2.21	0.44
1:C:67:LYS:HD3	1:C:76:GLU:HA	1.99	0.43
1:J:119:GLU:HB2	1:J:142:LEU:HD21	2.00	0.43
1:O:4:ALA:HB3	1:O:20:PHE:HB2	2.00	0.43
1:M:68:LYS:CE	1:M:133:THR:HB	2.48	0.43
1:M:68:LYS:HB3	1:M:68:LYS:HE3	1.86	0.43
1:A:45:VAL:HG22	1:A:115:MET:CE	2.48	0.43
1:G:4:ALA:HB3	1:G:20:PHE:HB2	2.01	0.43
1:J:56:THR:HG21	1:K:76:GLU:OE1	2.18	0.43
1:F:3:LYS:HE3	9:F:383:HOH:O	2.18	0.42
1:I:45:VAL:HG22	1:I:115:MET:SD	2.59	0.42
1:K:45:VAL:HG22	1:K:115:MET:HE1	2.00	0.42
1:P:119:GLU:CG	1:P:120:LYS:HG3	2.46	0.42
1:F:115:MET:O	1:F:144:CYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:MET:HG2	1:M:147:ILE:HD11	2.02	0.42
1:C:132:SER:HB2	1:C:137:ASN:ND2	2.35	0.42
1:C:55:CYS:SG	1:C:144:CYS:CB	3.08	0.42
1:P:55:CYS:SG	1:P:144[B]:CYS:HB3	2.60	0.42
1:L:101:LEU:HD23	1:L:101:LEU:HA	1.95	0.41
1:E:55:CYS:SG	1:E:144[B]:CYS:HB3	2.60	0.41
1:H:69:HIS:HB2	1:H:78:HIS:CE1	2.55	0.41
1:J:79:VAL:HA	1:J:101:LEU:HD13	2.03	0.41
1:J:1:ALA:HB1	9:J:318:HOH:O	2.20	0.41
1:M:30:THR:HA	1:M:95:VAL:O	2.21	0.41
1:O:52:THR:HG22	1:P:17:THR:HG21	2.03	0.41
1:A:115:MET:HE2	1:A:147:ILE:HD11	2.02	0.41
1:C:45:VAL:HG22	1:C:115:MET:HE2	2.03	0.41
1:J:4:ALA:HB3	1:J:20:PHE:HB2	2.01	0.41
1:B:32:SER:HB3	1:B:94:ILE:HD13	2.02	0.41
1:N:55:CYS:SG	1:N:144[B]:CYS:HB3	2.60	0.40
1:G:115:MET:HG2	1:G:147:ILE:HD11	2.03	0.40
1:O:115:MET:O	1:O:144:CYS:HA	2.21	0.40
1:J:101:LEU:HD23	1:J:101:LEU:HA	1.92	0.40
1:E:4:ALA:HB3	1:E:20:PHE:HB2	2.03	0.40
1:N:115:MET:O	1:N:144[A]:CYS:HA	2.22	0.40
1:O:65:LEU:HD22	1:O:65:LEU:N	2.36	0.40
1:P:89:LYS:HE2	1:P:89:LYS:HB2	1.73	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	149/151 (99%)	147 (99%)	2 (1%)	0	100 100
1	B	149/151 (99%)	147 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
1	D	135/151 (89%)	133 (98%)	2 (2%)	0	100	100
1	E	150/151 (99%)	149 (99%)	1 (1%)	0	100	100
1	F	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
1	G	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
1	H	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
1	I	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
1	J	146/151 (97%)	143 (98%)	3 (2%)	0	100	100
1	K	145/151 (96%)	142 (98%)	3 (2%)	0	100	100
1	L	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
1	M	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
1	N	150/151 (99%)	148 (99%)	2 (1%)	0	100	100
1	O	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
1	P	150/151 (99%)	148 (99%)	2 (1%)	0	100	100
All	All	2366/2416 (98%)	2327 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	113/117 (97%)	113 (100%)	0	100	100
1	B	111/117 (95%)	110 (99%)	1 (1%)	78	76
1	C	115/117 (98%)	113 (98%)	2 (2%)	60	54
1	D	99/117 (85%)	99 (100%)	0	100	100
1	E	116/117 (99%)	116 (100%)	0	100	100
1	F	116/117 (99%)	116 (100%)	0	100	100
1	G	115/117 (98%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	115/117 (98%)	114 (99%)	1 (1%)	78	76
1	I	115/117 (98%)	115 (100%)	0	100	100
1	J	113/117 (97%)	112 (99%)	1 (1%)	78	76
1	K	114/117 (97%)	113 (99%)	1 (1%)	78	76
1	L	115/117 (98%)	115 (100%)	0	100	100
1	M	110/117 (94%)	110 (100%)	0	100	100
1	N	117/117 (100%)	117 (100%)	0	100	100
1	O	114/117 (97%)	113 (99%)	1 (1%)	78	76
1	P	116/117 (99%)	116 (100%)	0	100	100
All	All	1814/1872 (97%)	1807 (100%)	7 (0%)	91	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	89	LYS
1	C	68	LYS
1	C	129	ASN
1	H	68	LYS
1	J	101	LEU
1	K	68	LYS
1	O	15	GLN

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

Mol	Chain	Res	Type
1	A	15	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 37 are monoatomic and 1 is modelled with single atom - leaving 6 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	EDO	N	203	-	3,3,3	0.53	0	2,2,2	0.17	0
6	SO4	K	203	-	4,4,4	0.16	0	6,6,6	0.23	0
6	SO4	I	203	-	4,4,4	0.17	0	6,6,6	0.20	0
4	EDO	C	203	-	3,3,3	0.53	0	2,2,2	0.16	0
5	GOL	F	203	-	5,5,5	0.11	0	5,5,5	0.44	0
6	SO4	F	204	-	4,4,4	0.12	0	6,6,6	0.19	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	EDO	C	203	-	-	0/1/1/1	-
4	EDO	N	203	-	-	1/1/1/1	-
5	GOL	F	203	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	203	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	203	EDO	2	0
5	F	203	GOL	4	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 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	151/151 (100%)	-0.09	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	13, 21, 36, 44	0
1	B	151/151 (100%)	-0.02	3 (1%) <span style="border: 1px solid blue; padding: 0 2px;">65</span> <span style="border: 1px solid blue; padding: 0 2px;">67</span>	14, 25, 36, 42	0
1	C	151/151 (100%)	0.35	8 (5%) <span style="border: 1px solid red; padding: 0 2px;">26</span> <span style="border: 1px solid red; padding: 0 2px;">28</span>	12, 26, 46, 62	0
1	D	139/151 (92%)	0.28	10 (7%) <span style="border: 1px solid red; padding: 0 2px;">15</span> <span style="border: 1px solid red; padding: 0 2px;">16</span>	13, 30, 49, 57	0
1	E	151/151 (100%)	-0.34	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	12, 20, 33, 42	0
1	F	151/151 (100%)	-0.10	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	14, 23, 34, 44	0
1	G	151/151 (100%)	-0.04	1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">87</span> <span style="border: 1px solid blue; padding: 0 2px;">88</span>	12, 26, 41, 49	0
1	H	151/151 (100%)	-0.22	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	11, 18, 32, 38	0
1	I	151/151 (100%)	-0.03	3 (1%) <span style="border: 1px solid blue; padding: 0 2px;">65</span> <span style="border: 1px solid blue; padding: 0 2px;">67</span>	16, 29, 43, 49	0
1	J	150/151 (99%)	0.26	5 (3%) <span style="border: 1px solid blue; padding: 0 2px;">46</span> <span style="border: 1px solid blue; padding: 0 2px;">47</span>	20, 31, 48, 58	0
1	K	149/151 (98%)	-0.04	4 (2%) <span style="border: 1px solid blue; padding: 0 2px;">54</span> <span style="border: 1px solid blue; padding: 0 2px;">56</span>	13, 26, 47, 57	0
1	L	151/151 (100%)	0.09	2 (1%) <span style="border: 1px solid blue; padding: 0 2px;">77</span> <span style="border: 1px solid blue; padding: 0 2px;">79</span>	12, 24, 41, 49	0
1	M	151/151 (100%)	0.41	5 (3%) <span style="border: 1px solid blue; padding: 0 2px;">46</span> <span style="border: 1px solid blue; padding: 0 2px;">47</span>	18, 33, 52, 64	0
1	N	151/151 (100%)	0.12	3 (1%) <span style="border: 1px solid blue; padding: 0 2px;">65</span> <span style="border: 1px solid blue; padding: 0 2px;">67</span>	16, 28, 46, 54	0
1	O	151/151 (100%)	-0.07	3 (1%) <span style="border: 1px solid blue; padding: 0 2px;">65</span> <span style="border: 1px solid blue; padding: 0 2px;">67</span>	11, 24, 40, 53	0
1	P	151/151 (100%)	-0.35	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	10, 16, 28, 40	0
All	All	2401/2416 (99%)	0.01	47 (1%) <span style="border: 1px solid blue; padding: 0 2px;">65</span> <span style="border: 1px solid blue; padding: 0 2px;">67</span>	10, 25, 44, 64	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	127	GLY	5.1
1	B	128	GLY	4.5
1	B	127	GLY	3.7
1	L	128	GLY	3.4
1	C	130	GLU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	O	108	TYR	3.3
1	D	108	TYR	2.9
1	C	128	GLY	2.9
1	M	108	TYR	2.9
1	D	140	SER	2.9
1	J	129	ASN	2.9
1	N	75	GLU	2.8
1	J	126	ARG	2.8
1	M	127	GLY	2.8
1	I	127	GLY	2.8
1	D	66	SER	2.7
1	D	137	ASN	2.7
1	D	11	ASP	2.7
1	B	108	TYR	2.7
1	D	69	HIS	2.6
1	C	13	PRO	2.6
1	M	91	GLY	2.6
1	J	147	ILE	2.6
1	N	128	GLY	2.5
1	C	127	GLY	2.5
1	M	37	THR	2.5
1	I	129	ASN	2.4
1	K	125	GLY	2.4
1	D	138	ALA	2.3
1	C	11	ASP	2.3
1	J	124	LEU	2.3
1	K	123	ASP	2.2
1	D	65	LEU	2.2
1	C	37	THR	2.2
1	D	70	GLY	2.2
1	D	139	GLY	2.2
1	C	129	ASN	2.2
1	O	65	LEU	2.2
1	K	133	THR	2.2
1	N	126	ARG	2.2
1	K	137	ASN	2.1
1	M	65	LEU	2.1
1	G	11	ASP	2.1
1	C	65	LEU	2.1
1	I	37	THR	2.0
1	J	146	VAL	2.0
1	O	89	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 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.

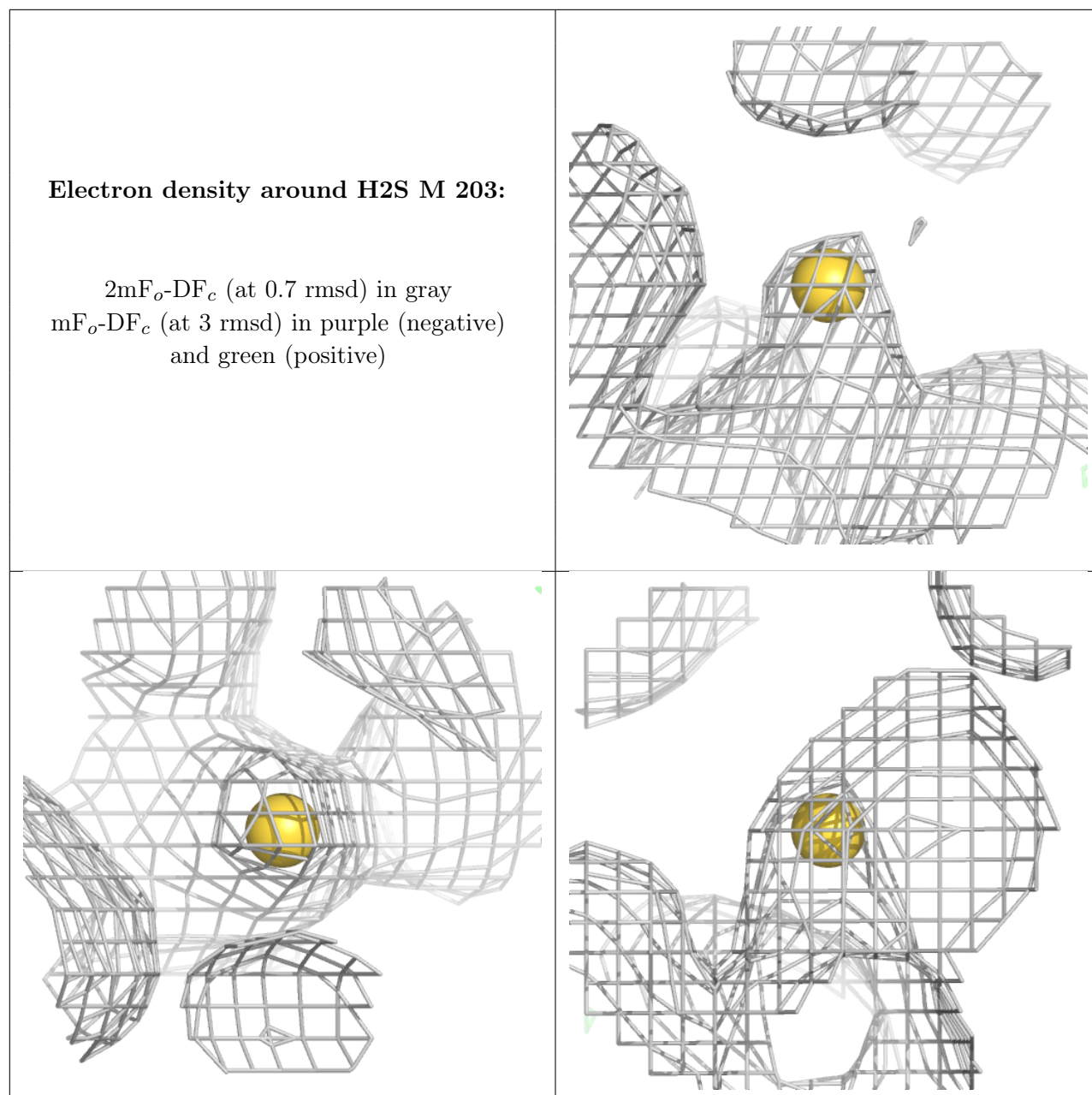
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	H2S	M	203	1/1	0.75	0.29	32,32,32,32	1
4	EDO	C	203	4/4	0.81	0.17	29,31,31,32	0
4	EDO	N	203	4/4	0.84	0.20	34,35,36,36	0
5	GOL	F	203	6/6	0.91	0.17	27,28,30,30	0
7	CL	L	203	1/1	0.93	0.06	47,47,47,47	0
6	SO4	I	203	5/5	0.96	0.12	33,37,38,40	0
6	SO4	F	204	5/5	0.97	0.23	29,32,34,38	0
3	ZN	G	202	1/1	0.97	0.06	22,22,22,22	0
6	SO4	K	203	5/5	0.98	0.13	31,35,36,38	0
2	CU	C	201	1/1	0.98	0.04	28,28,28,28	0
2	CU	D	201	1/1	0.98	0.04	39,39,39,39	0
3	ZN	D	202	1/1	0.99	0.04	35,35,35,35	0
3	ZN	E	202	1/1	0.99	0.06	18,18,18,18	0
2	CU	A	201	1/1	0.99	0.06	22,22,22,22	0
3	ZN	I	202	1/1	0.99	0.07	27,27,27,27	0
3	ZN	J	202	1/1	0.99	0.04	33,33,33,33	0
3	ZN	N	202	1/1	0.99	0.06	27,27,27,27	0
3	ZN	O	202	1/1	0.99	0.04	24,24,24,24	0
2	CU	G	201	1/1	0.99	0.07	24,24,24,24	0
2	CU	J	201	1/1	0.99	0.06	34,34,34,34	0
2	CU	K	201	1/1	0.99	0.04	30,30,30,30	0
2	CU	L	201	1/1	0.99	0.06	23,23,23,23	0
2	CU	M	201[A]	1/1	0.99	0.06	20,20,20,20	1
2	CU	M	201[B]	1/1	0.99	0.06	23,23,23,23	1
3	ZN	B	202	1/1	0.99	0.04	25,25,25,25	0
7	CL	P	203	1/1	0.99	0.06	41,41,41,41	0
3	ZN	C	202	1/1	0.99	0.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	I	201[A]	1/1	1.00	0.05	23,23,23,23	1
2	CU	N	201[A]	1/1	1.00	0.06	30,30,30,30	1
3	ZN	K	202	1/1	1.00	0.05	29,29,29,29	0
3	ZN	L	202	1/1	1.00	0.04	18,18,18,18	0
3	ZN	M	202	1/1	1.00	0.04	23,23,23,23	0
2	CU	N	201[B]	1/1	1.00	0.06	29,29,29,29	1
2	CU	O	201	1/1	1.00	0.04	26,26,26,26	0
3	ZN	P	202	1/1	1.00	0.06	12,12,12,12	0
2	CU	P	201	1/1	1.00	0.04	17,17,17,17	0
3	ZN	A	202	1/1	1.00	0.04	19,19,19,19	0
2	CU	I	201[B]	1/1	1.00	0.05	24,24,24,24	1
2	CU	E	201	1/1	1.00	0.05	21,21,21,21	0
2	CU	F	201	1/1	1.00	0.06	22,22,22,22	0
2	CU	B	201	1/1	1.00	0.06	26,26,26,26	0
3	ZN	F	202	1/1	1.00	0.04	21,21,21,21	0
2	CU	H	201	1/1	1.00	0.06	19,19,19,19	0
3	ZN	H	202	1/1	1.00	0.05	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.