



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:48 am GMT

PDB ID : 3AK1  
Title : Superoxide dismutase from *Aeropyrum pernix* K1, apo-form  
Authors : Nakamura, T.; Uegaki, K.  
Deposited on : 2010-06-30  
Resolution : 1.57 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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

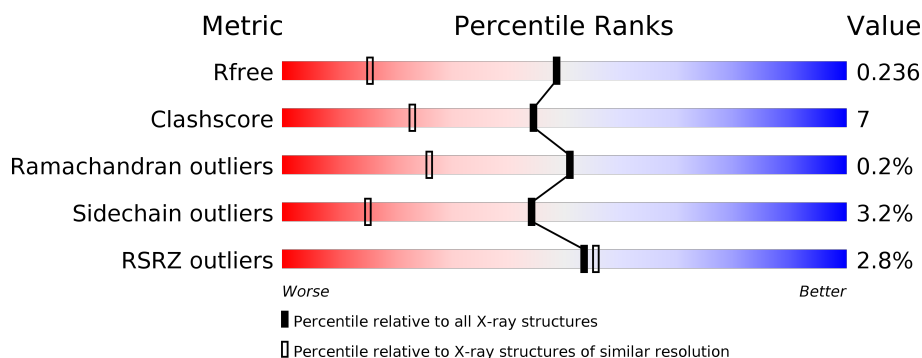
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.57 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	4211 (1.60-1.56)
Clashscore	112137	4539 (1.60-1.56)
Ramachandran outliers	110173	4423 (1.60-1.56)
Sidechain outliers	110143	4420 (1.60-1.56)
RSRZ outliers	101464	4232 (1.60-1.56)

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	214	
1	B	214	
1	C	214	
1	D	214	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	216	-	-	-	X
2	EDO	A	217	-	-	-	X
2	EDO	A	218	-	-	-	X
2	EDO	A	220	-	-	-	X
2	EDO	A	221	-	-	-	X
2	EDO	A	222	-	-	-	X
2	EDO	B	215	-	-	-	X
2	EDO	B	216	-	-	-	X
2	EDO	B	218	-	-	X	X
2	EDO	B	220	-	-	-	X
2	EDO	C	215	-	-	-	X
2	EDO	C	216	-	-	X	X
2	EDO	C	217	-	-	-	X
2	EDO	C	218	-	-	X	X
2	EDO	D	215	-	-	-	X
2	EDO	D	218	-	-	-	X
2	EDO	D	219	-	-	-	X

## 2 Entry composition [i](#)

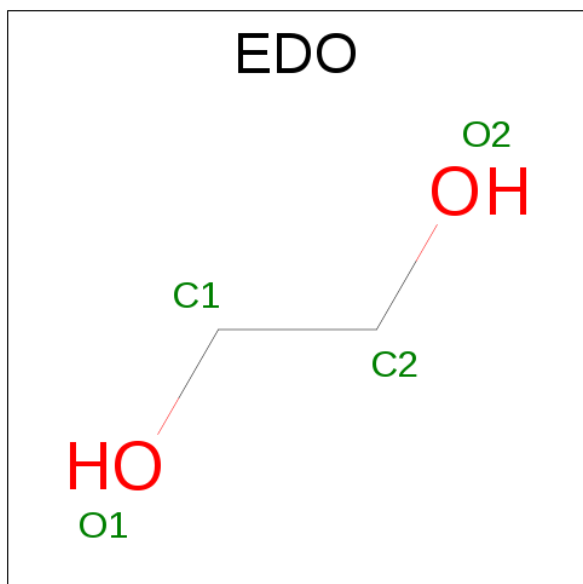
There are 3 unique types of molecules in this entry. The entry contains 7718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 [Mn/Fe].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	3	0
			1740	1136	293	305	6			
1	B	213	Total	C	N	O	S	0	8	0
			1775	1166	296	307	6			
1	C	213	Total	C	N	O	S	0	1	0
			1736	1134	293	303	6			
1	D	212	Total	C	N	O	S	0	2	0
			1733	1130	293	304	6			

- Molecule 2 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
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

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

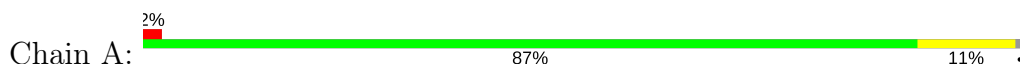
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	161	Total	O	0	0
			161	161		
3	C	156	Total	O	0	0
			156	156		
3	D	149	Total	O	0	0
			149	149		

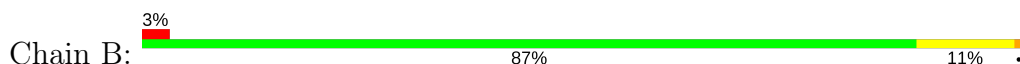
### 3 Residue-property plots [i](#)

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.

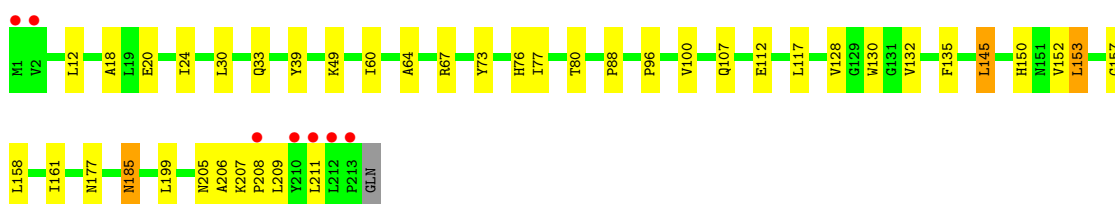
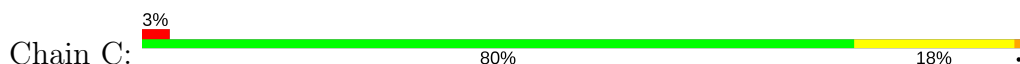
- Molecule 1: Superoxide dismutase [Mn/Fe]



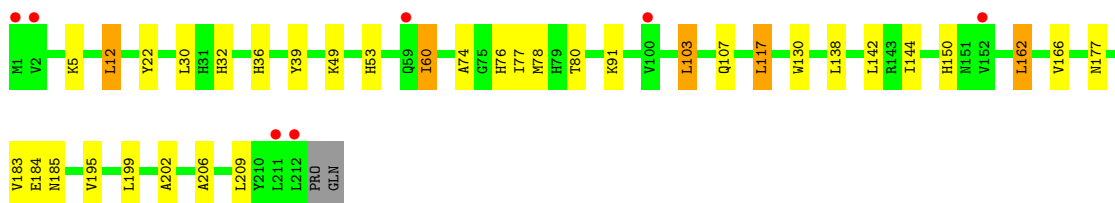
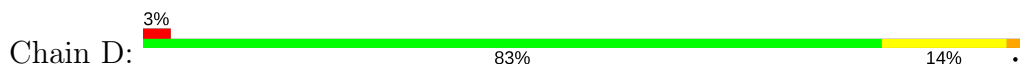
- Molecule 1: Superoxide dismutase [Mn/Fe]



- Molecule 1: Superoxide dismutase [Mn/Fe]



- Molecule 1: Superoxide dismutase [Mn/Fe]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.26Å 72.25Å 76.65Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	36.13 – 1.57 36.13 – 1.57	Depositor EDS
% Data completeness (in resolution range)	97.8 (36.13-1.57) 97.8 (36.13-1.57)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.236 0.197 , 0.236	Depositor DCC
$R_{free}$ test set	5169 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l 0.012 for k,h,-l 0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0/1800	0.56	1/2442 (0.0%)
1	B	0.40	0/1851	0.54	0/2514
1	C	0.38	0/1791	0.53	0/2432
1	D	0.38	0/1790	0.53	0/2429
All	All	0.40	0/7232	0.54	1/9817 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LEU	CA-CB-CG	5.58	128.14	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1740	0	1732	24	0
1	B	1775	0	1791	24	0
1	C	1736	0	1724	35	0
1	D	1733	0	1719	30	0
2	A	36	0	54	4	0
2	B	24	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	30	14	0
2	D	24	0	36	2	0
3	A	164	0	0	0	0
3	B	161	0	0	1	0
3	C	156	0	0	9	0
3	D	149	0	0	6	0
All	All	7718	0	7122	106	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 7.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:HH11	2:C:216:EDO:H11	1.21	1.05
1:D:103:LEU:HD13	1:D:142:LEU:HD11	1.52	0.91
1:C:77[A]:ILE:HD13	1:D:138:LEU:HD21	1.51	0.91
1:D:130:TRP:HE1	1:D:150:HIS:HD2	1.21	0.89
1:C:67:ARG:HH11	2:C:216:EDO:H22	1.39	0.87
1:C:130:TRP:HE1	1:C:150:HIS:HD2	1.19	0.85
1:C:60:ILE:CG2	3:C:525:HOH:O	2.25	0.83
1:D:49:LYS:HE2	3:D:470:HOH:O	1.78	0.83
1:A:130:TRP:HE1	1:A:150:HIS:HD2	1.27	0.82
1:C:64:ALA:HA	2:C:216:EDO:H21	1.63	0.81
1:D:183:VAL:HG22	3:D:609:HOH:O	1.78	0.81
1:B:130:TRP:HE1	1:B:150:HIS:HD2	1.30	0.78
1:C:128:VAL:H	2:C:218:EDO:H22	1.51	0.76
1:C:49:LYS:HD2	3:C:525:HOH:O	1.86	0.74
1:C:60:ILE:HG22	3:C:525:HOH:O	1.86	0.74
1:B:64:ALA:HA	2:C:216:EDO:H12	1.71	0.73
1:A:149:LYS:HG2	2:C:218:EDO:H21	1.69	0.73
1:A:212:LEU:O	1:B:201:GLN:HG3	1.89	0.71
2:C:215:EDO:H11	2:C:218:EDO:H12	1.71	0.71
1:C:152:VAL:O	1:C:153:LEU:HB2	1.89	0.71
1:D:103:LEU:O	1:D:107[B]:GLN:HG2	1.93	0.69
1:A:124[A]:THR:HG23	1:A:146:GLN:HE22	1.58	0.68
1:A:157:GLY:HA3	1:B:77:ILE:HD13	1.76	0.68
1:D:177:ASN:O	2:D:219:EDO:H22	1.94	0.68
1:B:67:ARG:HH11	2:C:216:EDO:C1	2.03	0.67
1:C:60:ILE:HG21	3:C:525:HOH:O	1.92	0.67
1:A:76:HIS:O	1:A:80:THR:HG23	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:HIS:CG	1:D:60:ILE:HD12	2.31	0.66
1:A:124[A]:THR:HG23	1:A:146:GLN:NE2	2.14	0.63
1:D:103:LEU:HD13	1:D:142:LEU:CD1	2.26	0.63
1:A:208:PRO:HA	1:A:211:LEU:HB2	1.79	0.63
1:D:39:TYR:HD2	3:D:583:HOH:O	1.82	0.63
1:D:22:TYR:HD2	1:D:185:ASN:HD22	1.47	0.63
1:C:130:TRP:HE1	1:C:150:HIS:CD2	2.10	0.62
1:C:67:ARG:HD2	2:C:216:EDO:H22	1.81	0.62
1:C:18:ALA:HB1	1:C:88:PRO:HG3	1.83	0.61
1:D:166:VAL:HG12	3:D:609:HOH:O	2.01	0.61
1:A:211:LEU:O	1:A:212:LEU:HB3	1.99	0.61
1:C:49:LYS:HB3	3:C:525:HOH:O	1.99	0.60
1:B:107:GLN:NE2	1:B:142:LEU:H	2.00	0.60
1:A:212:LEU:HD21	1:B:197:LYS:HD3	1.83	0.58
1:A:120:ALA:O	1:A:124[A]:THR:HG22	2.02	0.58
1:B:107:GLN:HE21	1:B:142:LEU:H	1.54	0.56
1:C:161:ILE:HG21	3:C:575:HOH:O	2.05	0.55
1:C:64:ALA:CA	2:C:216:EDO:H21	2.35	0.55
1:D:76:HIS:O	1:D:80:THR:HG23	2.07	0.55
1:B:67:ARG:NH1	2:C:216:EDO:H11	2.06	0.55
1:B:64:ALA:CB	2:B:218:EDO:H11	2.38	0.54
1:A:157:GLY:HA3	1:B:77:ILE:CD1	2.38	0.54
1:C:96:PRO:HB2	1:C:100:VAL:HG23	1.90	0.53
1:A:130:TRP:HE1	1:A:150:HIS:CD2	2.18	0.52
1:C:76:HIS:O	1:C:80:THR:HG23	2.10	0.52
1:D:130:TRP:HE1	1:D:150:HIS:CD2	2.13	0.52
1:B:39:TYR:CZ	1:B:150:HIS:HE1	2.27	0.52
1:A:77:ILE:HD13	1:B:157:GLY:HA3	1.91	0.51
2:B:218:EDO:H21	3:B:225:HOH:O	2.11	0.51
1:B:64:ALA:HB1	2:B:218:EDO:C1	2.41	0.50
1:D:162:LEU:HG	1:D:195:VAL:HG21	1.93	0.50
1:C:130:TRP:NE1	1:C:150:HIS:HD2	2.00	0.50
1:B:76:HIS:O	1:B:80:THR:HG23	2.11	0.49
1:A:15:ASN:HB2	2:A:217:EDO:H11	1.93	0.49
1:B:64:ALA:HB1	2:B:218:EDO:H11	1.94	0.49
2:A:219:EDO:H12	1:C:177:ASN:HB2	1.93	0.49
1:D:36:HIS:CD2	3:D:583:HOH:O	2.66	0.48
1:A:107:GLN:CD	1:A:141:GLU:HG2	2.33	0.48
1:B:4:PHE:CE1	1:B:6[A]:ARG:HG2	2.47	0.48
1:B:100[B]:VAL:HG23	1:B:196:GLU:OE1	2.14	0.48
1:B:18:ALA:HB1	1:B:88:PRO:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:HD13	1:D:144:ILE:HD12	1.97	0.47
2:A:222:EDO:H22	1:B:47:LEU:CD2	2.45	0.47
3:C:265:HOH:O	1:D:5:LYS:HD2	2.14	0.46
1:C:73:TYR:OH	1:D:138:LEU:HD23	2.15	0.46
1:A:51:GLU:HG2	1:A:55[A]:LYS:HE2	1.97	0.46
1:C:67:ARG:HH11	2:C:216:EDO:C2	2.21	0.46
1:D:107[B]:GLN:HG3	1:D:142:LEU:HB2	1.98	0.45
1:A:135:PHE:CZ	1:A:140:GLU:HA	2.51	0.45
1:A:197:LYS:HA	1:A:200:GLU:HG2	1.97	0.45
1:D:103:LEU:HD11	1:D:199:LEU:CD2	2.47	0.45
1:C:185:ASN:HD22	1:C:185:ASN:HA	1.61	0.45
2:B:220:EDO:H12	3:D:586:HOH:O	2.16	0.45
1:D:206:ALA:O	1:D:209:LEU:HB3	2.16	0.45
1:C:199:LEU:HA	3:C:575:HOH:O	2.17	0.44
1:A:34:LYS:HB3	2:A:219:EDO:H11	2.00	0.44
1:C:132:VAL:HB	1:C:145:LEU:HD12	1.99	0.44
1:C:67:ARG:CD	2:C:216:EDO:H22	2.46	0.44
1:D:12:LEU:HD13	1:D:32:HIS:CD2	2.53	0.43
1:C:205:ASN:HB2	1:D:209:LEU:HD13	1.99	0.43
1:D:39:TYR:CZ	1:D:150:HIS:HE1	2.37	0.42
1:B:2:VAL:O	1:B:3:SER:HB2	2.19	0.42
1:C:209:LEU:CD1	1:D:202:ALA:HA	2.49	0.42
1:A:130:TRP:NE1	1:A:150:HIS:HD2	2.07	0.42
1:D:12:LEU:HB2	2:D:215:EDO:H22	2.02	0.42
1:C:206:ALA:O	1:C:209:LEU:HB3	2.19	0.42
1:C:207:LYS:N	1:C:208:PRO:HD2	2.35	0.42
1:A:207:LYS:HG2	1:A:211:LEU:HG	2.00	0.42
1:B:57[B]:GLU:HG2	1:B:58[B]:ILE:HG13	2.01	0.41
1:B:53:HIS:CG	1:B:60:ILE:HD12	2.55	0.41
1:C:39:TYR:CZ	1:C:150:HIS:HE1	2.38	0.41
1:C:157:GLY:HA3	1:D:77:ILE:HD13	2.02	0.41
1:C:20:GLU:HG2	1:C:24:ILE:HA	2.02	0.41
1:A:149:LYS:CG	2:C:218:EDO:H21	2.45	0.40
1:D:103:LEU:HD11	1:D:199:LEU:HD22	2.03	0.40
1:D:74:ALA:O	1:D:78:MET:HG2	2.21	0.40
1:C:112:GLU:H	1:C:112:GLU:CD	2.24	0.40
1:C:135:PHE:HB2	3:C:575:HOH:O	2.20	0.40
1:A:85:ASN:HA	1:A:85:ASN:HD22	1.71	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	213/214 (100%)	206 (97%)	7 (3%)	0	100	100
1	B	219/214 (102%)	211 (96%)	7 (3%)	1 (0%)	32	11
1	C	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	32	11
1	D	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	856/856 (100%)	824 (96%)	30 (4%)	2 (0%)	51	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	SER
1	C	211	LEU

### 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	182/181 (101%)	179 (98%)	3 (2%)	68	43
1	B	188/181 (104%)	184 (98%)	4 (2%)	59	30
1	C	181/181 (100%)	172 (95%)	9 (5%)	28	6
1	D	181/181 (100%)	173 (96%)	8 (4%)	33	8
All	All	732/724 (101%)	708 (97%)	24 (3%)	44	15

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	158	LEU
1	A	212	LEU
1	B	30[A]	LEU
1	B	30[B]	LEU
1	B	60	ILE
1	B	107	GLN
1	C	12	LEU
1	C	30	LEU
1	C	33	GLN
1	C	107	GLN
1	C	117	LEU
1	C	145	LEU
1	C	153	LEU
1	C	158	LEU
1	C	185	ASN
1	D	12	LEU
1	D	30	LEU
1	D	60	ILE
1	D	91	LYS
1	D	103	LEU
1	D	117	LEU
1	D	162	LEU
1	D	184	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	150	HIS
1	A	204	ASN
1	B	33	GLN
1	B	107	GLN
1	B	150	HIS
1	B	201	GLN
1	C	150	HIS
1	C	185	ASN
1	D	15	ASN
1	D	150	HIS
1	D	185	ASN
1	D	201	GLN

### 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 ⓘ

26 ligands 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	$\# Z  > 2$
2	EDO	A	215	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	A	216	-	3,3,3	0.47	0	2,2,2	0.42	0
2	EDO	A	217	-	3,3,3	0.47	0	2,2,2	0.11	0
2	EDO	A	218	-	3,3,3	0.29	0	2,2,2	0.74	0
2	EDO	A	219	-	3,3,3	0.42	0	2,2,2	0.28	0
2	EDO	A	220	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	A	221	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	A	222	-	3,3,3	0.36	0	2,2,2	0.45	0
2	EDO	A	223	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	215	-	3,3,3	0.43	0	2,2,2	0.45	0
2	EDO	B	216	-	3,3,3	0.42	0	2,2,2	0.42	0
2	EDO	B	217	-	3,3,3	0.49	0	2,2,2	0.36	0
2	EDO	B	218	-	3,3,3	0.45	0	2,2,2	0.21	0
2	EDO	B	219	-	3,3,3	0.48	0	2,2,2	0.13	0
2	EDO	B	220	-	3,3,3	0.44	0	2,2,2	0.42	0
2	EDO	C	215	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	C	216	-	3,3,3	0.36	0	2,2,2	0.14	0
2	EDO	C	217	-	3,3,3	0.40	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	C	218	-	3,3,3	0.40	0	2,2,2	0.36	0
2	EDO	C	219	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	D	215	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	D	216	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	D	217	-	3,3,3	0.44	0	2,2,2	0.26	0
2	EDO	D	218	-	3,3,3	0.44	0	2,2,2	0.42	0
2	EDO	D	219	-	3,3,3	0.40	0	2,2,2	0.32	0
2	EDO	D	220	-	3,3,3	0.47	0	2,2,2	0.29	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
2	EDO	A	215	-	-	0/1/1/1	0/0/0/0
2	EDO	A	216	-	-	0/1/1/1	0/0/0/0
2	EDO	A	217	-	-	0/1/1/1	0/0/0/0
2	EDO	A	218	-	-	0/1/1/1	0/0/0/0
2	EDO	A	219	-	-	0/1/1/1	0/0/0/0
2	EDO	A	220	-	-	0/1/1/1	0/0/0/0
2	EDO	A	221	-	-	0/1/1/1	0/0/0/0
2	EDO	A	222	-	-	0/1/1/1	0/0/0/0
2	EDO	A	223	-	-	0/1/1/1	0/0/0/0
2	EDO	B	215	-	-	0/1/1/1	0/0/0/0
2	EDO	B	216	-	-	0/1/1/1	0/0/0/0
2	EDO	B	217	-	-	0/1/1/1	0/0/0/0
2	EDO	B	218	-	-	0/1/1/1	0/0/0/0
2	EDO	B	219	-	-	0/1/1/1	0/0/0/0
2	EDO	B	220	-	-	0/1/1/1	0/0/0/0
2	EDO	C	215	-	-	0/1/1/1	0/0/0/0
2	EDO	C	216	-	-	0/1/1/1	0/0/0/0
2	EDO	C	217	-	-	0/1/1/1	0/0/0/0
2	EDO	C	218	-	-	0/1/1/1	0/0/0/0
2	EDO	C	219	-	-	0/1/1/1	0/0/0/0
2	EDO	D	215	-	-	0/1/1/1	0/0/0/0
2	EDO	D	216	-	-	0/1/1/1	0/0/0/0
2	EDO	D	217	-	-	0/1/1/1	0/0/0/0
2	EDO	D	218	-	-	0/1/1/1	0/0/0/0
2	EDO	D	219	-	-	0/1/1/1	0/0/0/0
2	EDO	D	220	-	-	0/1/1/1	0/0/0/0

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.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	217	EDO	1	0
2	A	219	EDO	2	0
2	A	222	EDO	1	0
2	B	218	EDO	4	0
2	B	220	EDO	1	0
2	C	215	EDO	1	0
2	C	216	EDO	10	0
2	C	218	EDO	4	0
2	D	215	EDO	1	0
2	D	219	EDO	1	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	212/214 (99%)	-0.15	4 (1%) 67 69	14, 22, 30, 41	0
1	B	213/214 (99%)	-0.02	6 (2%) 53 55	14, 22, 34, 47	0
1	C	213/214 (99%)	0.19	7 (3%) 47 48	16, 25, 38, 49	0
1	D	212/214 (99%)	0.27	7 (3%) 47 48	16, 26, 39, 53	0
All	All	850/856 (99%)	0.07	24 (2%) 53 55	14, 23, 37, 53	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	LEU	9.3
1	C	212	LEU	6.4
1	D	212	LEU	6.0
1	B	2	VAL	5.8
1	B	3	SER	5.5
1	C	211	LEU	4.9
1	C	213	PRO	4.0
1	C	1	MET	3.8
1	C	2	VAL	3.8
1	A	211	LEU	3.7
1	A	1	MET	3.2
1	B	58[A]	ILE	3.2
1	B	1	MET	3.0
1	D	211	LEU	2.8
1	C	208	PRO	2.8
1	D	59	GLN	2.6
1	D	2	VAL	2.5
1	B	4	PHE	2.4
1	D	1	MET	2.4
1	C	210	TYR	2.4
1	B	213	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	100	VAL	2.3
1	D	152	VAL	2.1
1	A	2	VAL	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
2	EDO	A	217	4/4	0.66	0.45	38.34	68,68,68,68	0
2	EDO	A	218	4/4	0.90	0.16	12.66	18,22,24,27	0
2	EDO	B	218	4/4	0.80	0.18	9.78	44,44,45,45	0
2	EDO	D	219	4/4	0.73	0.22	9.62	32,34,35,36	0
2	EDO	C	216	4/4	0.93	0.16	8.62	28,29,29,30	0
2	EDO	A	216	4/4	0.71	0.22	6.47	44,45,45,45	0
2	EDO	D	215	4/4	0.94	0.19	5.08	42,43,43,43	0
2	EDO	B	215	4/4	0.83	0.20	4.74	35,37,38,39	0
2	EDO	A	220	4/4	0.81	0.17	4.31	43,43,44,44	0
2	EDO	B	216	4/4	0.91	0.12	4.09	27,28,28,30	0
2	EDO	C	217	4/4	0.91	0.14	3.97	32,33,33,35	0
2	EDO	A	221	4/4	0.72	0.15	3.48	48,49,49,51	0
2	EDO	A	222	4/4	0.86	0.14	3.06	28,30,30,31	0
2	EDO	C	215	4/4	0.92	0.14	2.95	24,25,25,26	0
2	EDO	B	220	4/4	0.84	0.15	2.76	40,40,40,41	0
2	EDO	C	218	4/4	0.88	0.15	2.53	28,29,29,32	0
2	EDO	D	218	4/4	0.92	0.15	2.37	35,37,37,38	0
2	EDO	B	219	4/4	0.93	0.17	1.71	29,29,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	215	4/4	0.87	0.08	1.38	33,34,34,36	0
2	EDO	A	223	4/4	0.88	0.10	1.31	32,33,33,33	0
2	EDO	C	219	4/4	0.87	0.16	1.11	39,40,42,42	0
2	EDO	D	217	4/4	0.93	0.10	0.68	33,34,34,34	0
2	EDO	D	220	4/4	0.88	0.11	0.33	46,47,47,47	0
2	EDO	A	219	4/4	0.92	0.12	-	43,43,43,43	0
2	EDO	D	216	4/4	0.90	0.08	-	43,43,44,44	0
2	EDO	B	217	4/4	0.48	0.20	-	51,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.