



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2018 – 01:38 am GMT

PDB ID : 1X0R
Title : Thioredoxin Peroxidase from *Aeropyrum pernix* K1
Authors : Nakamura, T.; Yamamoto, T.; Inoue, T.; Matsumura, H.; Kobayashi, A.;
Hagihara, Y.; Uegaki, K.; Ataka, M.; Kai, Y.; Ishikawa, K.
Deposited on : 2005-03-28
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

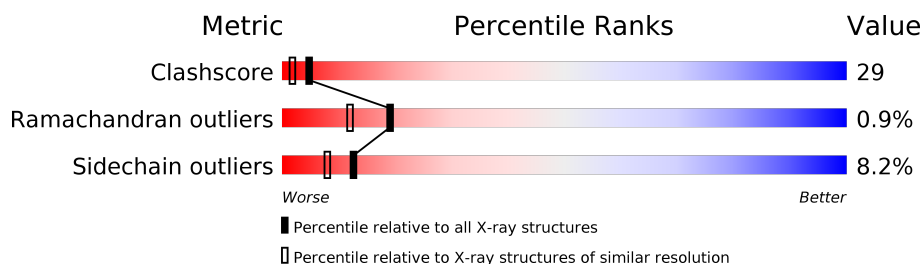
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	122078	8264 (2.00-2.00)
Ramachandran outliers	120005	8163 (2.00-2.00)
Sidechain outliers	119972	8162 (2.00-2.00)


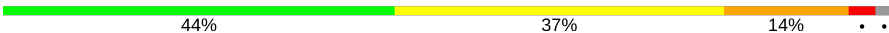
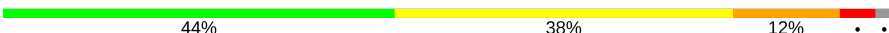
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	249	
1	B	249	
1	C	249	
1	D	249	
1	E	249	
1	F	249	
1	G	249	

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Mol	Chain	Length	Quality of chain
1	H	249	
1	I	249	
1	J	249	

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
2	EDO	A	2001	-	-	X	-
2	EDO	A	2012	-	-	X	-
2	EDO	A	2029	-	-	X	-
2	EDO	A	2063	-	-	X	-
2	EDO	A	2065	-	-	X	-
2	EDO	A	2122	-	-	X	-
2	EDO	A	2124	-	-	X	-
2	EDO	B	2002	-	-	X	-
2	EDO	B	2021	-	-	X	-
2	EDO	B	2028	-	-	X	-
2	EDO	B	2030	-	-	X	-
2	EDO	B	2125	-	X	X	-
2	EDO	C	2004	-	-	X	-
2	EDO	C	2024	-	-	X	-
2	EDO	C	2067	-	-	X	-
2	EDO	C	2075	-	-	X	-
2	EDO	C	2081	-	X	-	-
2	EDO	C	2085	-	X	X	-
2	EDO	C	2126	-	X	X	-
2	EDO	C	2128	-	-	X	-
2	EDO	D	2003	-	-	X	-
2	EDO	D	2031	-	-	X	-
2	EDO	D	2035	-	-	X	-
2	EDO	D	2118	-	-	X	-
2	EDO	E	2005	-	-	X	-
2	EDO	E	2076	-	-	X	-
2	EDO	E	2089	-	-	X	-
2	EDO	E	2090	-	-	X	-
2	EDO	E	2091	-	-	X	-
2	EDO	E	2120	-	-	X	-
2	EDO	E	2127	-	X	X	-
2	EDO	F	2006	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	F	2034	-	-	X	-
2	EDO	F	2038	-	-	X	-
2	EDO	F	2043	-	-	X	-
2	EDO	F	2086	-	X	X	-
2	EDO	F	2094	-	X	-	-
2	EDO	F	2097	-	-	X	-
2	EDO	G	2009	-	-	X	-
2	EDO	G	2050	-	-	X	-
2	EDO	G	2056	-	-	X	-
2	EDO	G	2057	-	-	X	-
2	EDO	G	2093	-	-	X	-
2	EDO	G	2101	-	X	-	-
2	EDO	H	2010	-	-	X	-
2	EDO	H	2044	-	-	X	-
2	EDO	H	2058	-	X	X	-
2	EDO	H	2059	-	X	-	-
2	EDO	H	2060	-	-	X	-
2	EDO	H	2111	-	X	-	-
2	EDO	H	2113	-	-	X	-
2	EDO	I	2007	-	X	X	-
2	EDO	I	2046	-	-	X	-
2	EDO	I	2051	-	-	X	-
2	EDO	I	2099	-	X	-	-
2	EDO	I	2103	-	X	X	-
2	EDO	I	2107	-	-	X	-
2	EDO	I	2115	-	-	X	-
2	EDO	I	2121	-	-	X	-
2	EDO	J	2008	-	-	X	-
2	EDO	J	2049	-	-	X	-
2	EDO	J	2068	-	-	X	-
2	EDO	J	2104	-	X	X	-
2	EDO	J	2105	-	-	X	-
2	EDO	J	2109	-	-	X	-
2	EDO	J	2123	-	X	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21431 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	B	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	C	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	D	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	E	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	F	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	G	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	H	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	I	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0
1	J	244	Total 1973	C 1268	N 347	O 352	S 2	Se 4	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

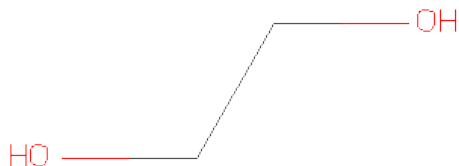
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
B	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
C	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
D	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
E	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
F	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
G	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
H	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
I	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
J	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	207	SER	CYS	ENGINEERED	UNP Q9Y9L0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
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	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is water.

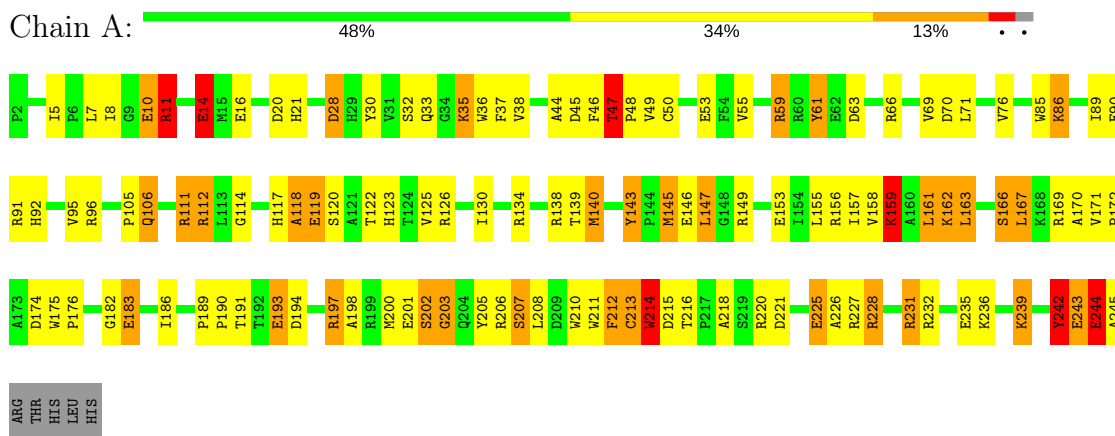
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	140	Total O 140 140	0	0
3	B	120	Total O 120 120	0	0
3	C	136	Total O 136 136	0	0
3	D	132	Total O 132 132	0	0
3	E	133	Total O 133 133	0	0
3	F	115	Total O 115 115	0	0
3	G	98	Total O 98 98	0	0
3	H	94	Total O 94 94	0	0
3	I	106	Total O 106 106	0	0
3	J	115	Total O 115 115	0	0

3 Residue-property plots

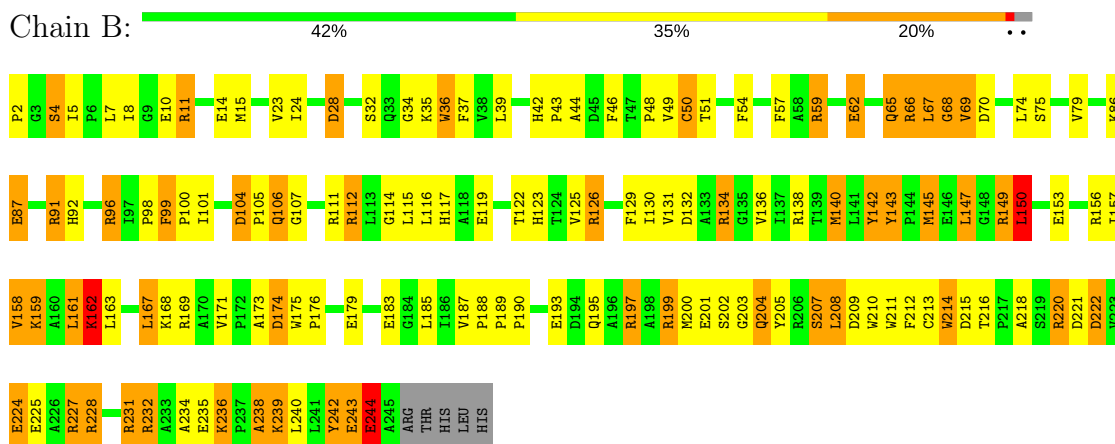
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

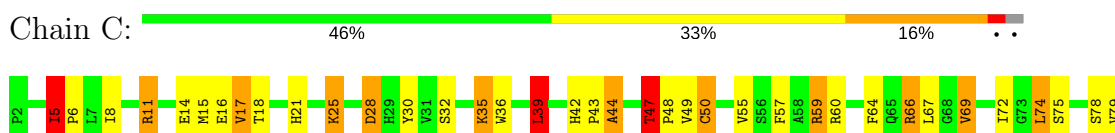
- Molecule 1: Probable peroxiredoxin

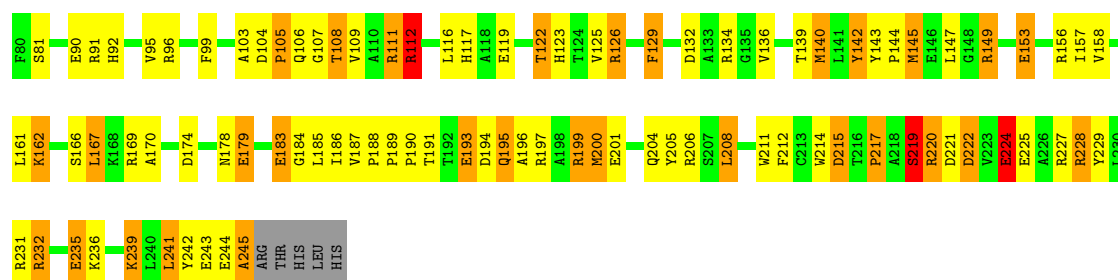


- Molecule 1: Probable peroxiredoxin



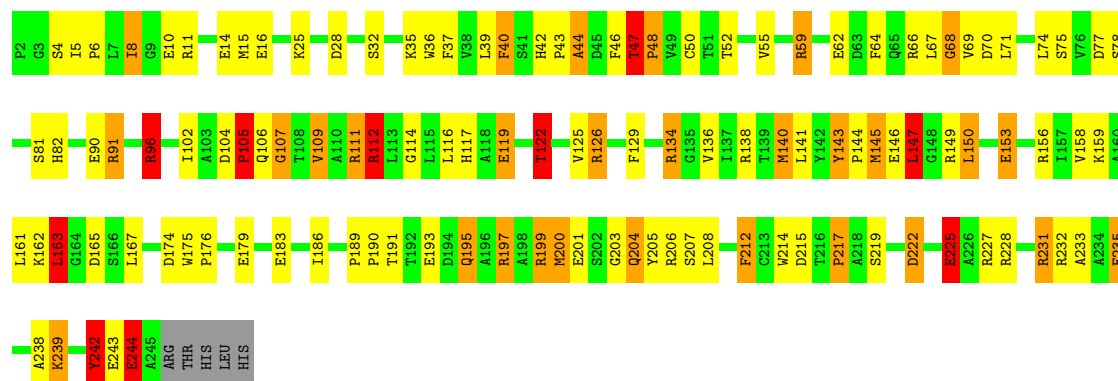
- Molecule 1: Probable peroxiredoxin





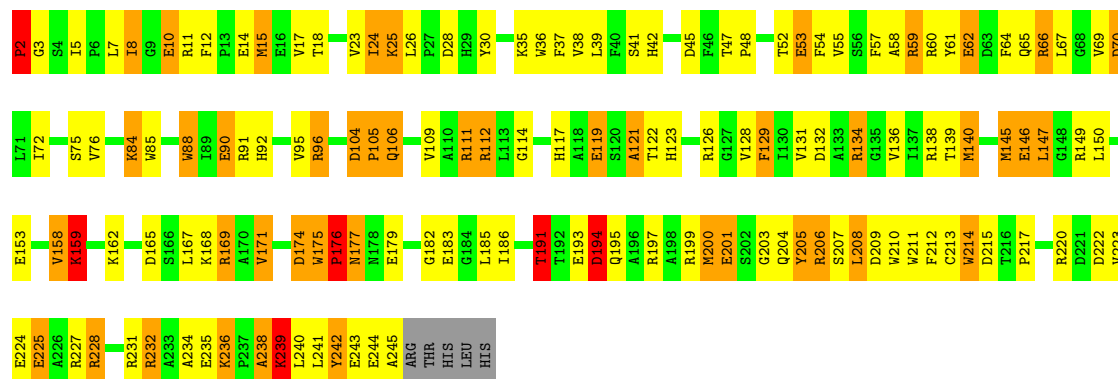
- Molecule 1: Probable peroxiredoxin

Chain D: 50% 33% 12% . .



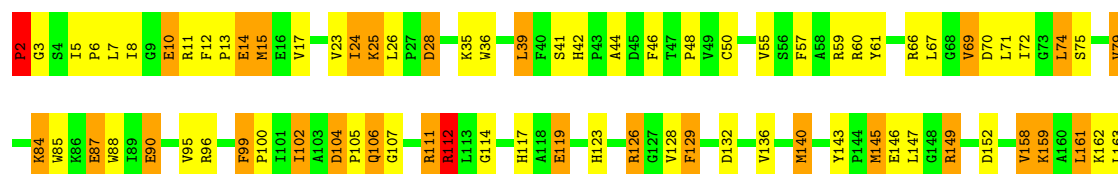
- Molecule 1: Probable peroxiredoxin

Chain E: 41% 37% 18% . .



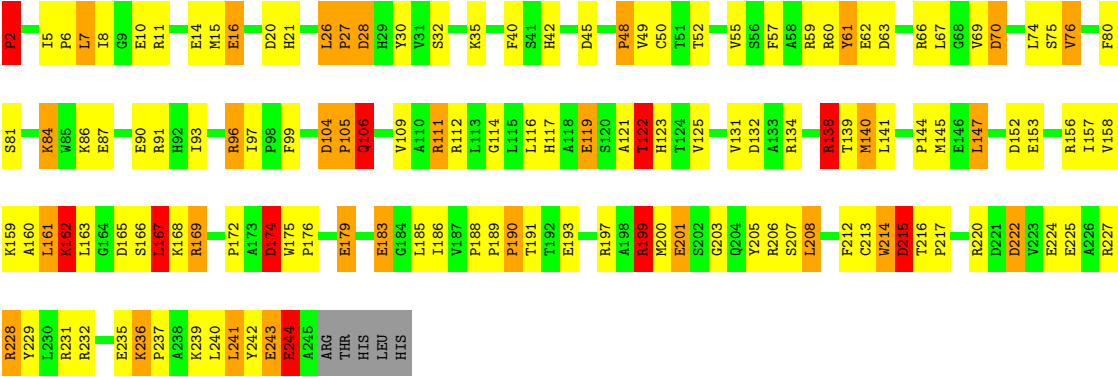
- Molecule 1: Probable peroxiredoxin

Chain F: 44% 35% 17% . .





● Molecule 1: Probable peroxiredoxin



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.63Å 101.79Å 102.89Å 105.37° 105.28° 93.32°	Depositor
Resolution (Å)	29.89 – 2.00	Depositor
% Data completeness (in resolution range)	89.9 (29.89-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.164 , 0.171	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21431	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	2.20	78/2024 (3.9%)	1.70	37/2745 (1.3%)
1	B	2.16	79/2024 (3.9%)	1.91	55/2745 (2.0%)
1	C	2.16	79/2024 (3.9%)	1.76	55/2745 (2.0%)
1	D	2.17	68/2024 (3.4%)	1.68	39/2745 (1.4%)
1	E	2.25	96/2024 (4.7%)	1.91	51/2745 (1.9%)
1	F	2.14	74/2024 (3.7%)	1.78	50/2745 (1.8%)
1	G	2.12	65/2024 (3.2%)	1.74	36/2745 (1.3%)
1	H	2.15	74/2024 (3.7%)	1.62	28/2745 (1.0%)
1	I	2.12	74/2024 (3.7%)	1.75	43/2745 (1.6%)
1	J	2.21	63/2024 (3.1%)	2.32	78/2745 (2.8%)
All	All	2.17	750/20240 (3.7%)	1.83	472/27450 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	D	0	2
1	E	0	1
1	G	0	3
1	H	0	1
1	I	0	2
1	J	0	4
All	All	0	16

The worst 5 of 750 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	GLU	CG-CD	15.52	1.75	1.51
1	H	62	GLU	CD-OE2	15.03	1.42	1.25
1	B	162	LYS	CE-NZ	14.24	1.84	1.49
1	J	214	TRP	CG-CD1	14.23	1.56	1.36
1	D	68	GLY	N-CA	13.91	1.67	1.46

The worst 5 of 472 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	138	ARG	NE-CZ-NH2	-36.48	102.06	120.30
1	J	138	ARG	NE-CZ-NH1	34.23	137.42	120.30
1	B	104	ASP	CB-CG-OD2	-32.90	88.69	118.30
1	G	26	LEU	C-N-CD	-31.81	50.61	120.60
1	J	26	LEU	C-N-CD	-28.89	57.03	120.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Sidechain
1	A	242	TYR	Sidechain
1	B	143	TYR	Sidechain
1	D	242	TYR	Sidechain
1	D	82	HIS	Sidechain

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	1973	0	1959	108	0
1	B	1973	0	1959	123	0
1	C	1973	0	1959	113	0
1	D	1973	0	1959	104	0
1	E	1973	0	1959	138	0
1	F	1973	0	1959	128	0
1	G	1973	0	1959	98	0
1	H	1973	0	1959	99	0
1	I	1973	0	1959	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1973	0	1959	119	0
2	A	56	0	84	55	0
2	B	56	0	84	46	0
2	C	64	0	96	68	0
2	D	40	0	60	33	0
2	E	68	0	101	57	0
2	F	48	0	72	43	0
2	G	36	0	54	36	0
2	H	36	0	54	37	1
2	I	44	0	66	56	0
2	J	64	0	96	79	0
3	A	140	0	0	9	0
3	B	120	0	0	9	0
3	C	136	0	0	3	1
3	D	132	0	0	9	0
3	E	133	0	0	7	0
3	F	115	0	0	9	0
3	G	98	0	0	4	0
3	H	94	0	0	3	0
3	I	106	0	0	9	0
3	J	115	0	0	6	0
All	All	21431	0	20357	1196	1

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 29.

The worst 5 of 1196 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:ILE:CG1	1:I:102:ILE:CD1	1.76	1.60
1:E:145:MSE:CB	1:E:145:MSE:CG	1.81	1.58
1:D:145:MSE:CG	1:D:145:MSE:CB	1.77	1.56
1:H:145:MSE:CG	1:H:145:MSE:CB	1.82	1.56
1:E:25:LYS:NZ	1:E:25:LYS:CE	1.67	1.56

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2114:EDO:O1	3:C:2190:HOH:O[1_556]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	242/249 (97%)	229 (95%)	10 (4%)	3 (1%)	14	7
1	B	242/249 (97%)	234 (97%)	6 (2%)	2 (1%)	21	14
1	C	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	36	31
1	D	242/249 (97%)	231 (96%)	9 (4%)	2 (1%)	21	14
1	E	242/249 (97%)	233 (96%)	6 (2%)	3 (1%)	14	7
1	F	242/249 (97%)	235 (97%)	6 (2%)	1 (0%)	36	31
1	G	242/249 (97%)	232 (96%)	7 (3%)	3 (1%)	14	7
1	H	242/249 (97%)	233 (96%)	7 (3%)	2 (1%)	21	14
1	I	242/249 (97%)	234 (97%)	7 (3%)	1 (0%)	36	31
1	J	242/249 (97%)	236 (98%)	3 (1%)	3 (1%)	14	7
All	All	2420/2490 (97%)	2332 (96%)	67 (3%)	21 (1%)	19	12

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	176	PRO
1	G	27	PRO
1	J	27	PRO
1	A	106	GLN
1	A	244	GLU

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	210/211 (100%)	190 (90%)	20 (10%)	9	5
1	B	210/211 (100%)	193 (92%)	17 (8%)	13	8
1	C	210/211 (100%)	189 (90%)	21 (10%)	8	4
1	D	210/211 (100%)	193 (92%)	17 (8%)	13	8
1	E	210/211 (100%)	197 (94%)	13 (6%)	20	15
1	F	210/211 (100%)	193 (92%)	17 (8%)	13	8
1	G	210/211 (100%)	195 (93%)	15 (7%)	16	11
1	H	210/211 (100%)	197 (94%)	13 (6%)	20	15
1	I	210/211 (100%)	190 (90%)	20 (10%)	9	5
1	J	210/211 (100%)	190 (90%)	20 (10%)	9	5
All	All	2100/2110 (100%)	1927 (92%)	173 (8%)	12	8

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	70	ASP
1	F	161	LEU
1	J	122	THR
1	E	147	LEU
1	E	212	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	106	GLN
1	F	117	HIS
1	J	92	HIS
1	E	123	HIS
1	B	117	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

128 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	2001	-	3,3,3	2.51	2 (66%)	2,2,2	0.26	0
2	EDO	A	2011	-	3,3,3	2.67	2 (66%)	2,2,2	1.35	0
2	EDO	A	2012	-	3,3,3	3.98	2 (66%)	2,2,2	0.33	0
2	EDO	A	2016	-	3,3,3	2.15	2 (66%)	2,2,2	0.58	0
2	EDO	A	2017	-	3,3,3	2.03	2 (66%)	2,2,2	0.99	0
2	EDO	A	2019	-	3,3,3	2.68	2 (66%)	2,2,2	0.78	0
2	EDO	A	2022	-	3,3,3	2.03	1 (33%)	2,2,2	1.08	0
2	EDO	A	2029	-	3,3,3	3.21	2 (66%)	2,2,2	0.77	0
2	EDO	A	2063	-	3,3,3	3.35	2 (66%)	2,2,2	1.09	0
2	EDO	A	2065	-	3,3,3	2.58	2 (66%)	2,2,2	0.74	0
2	EDO	A	2066	-	3,3,3	2.96	2 (66%)	2,2,2	0.48	0
2	EDO	A	2116	-	3,3,3	3.03	2 (66%)	2,2,2	0.53	0
2	EDO	A	2122	-	3,3,3	3.10	1 (33%)	2,2,2	1.32	0
2	EDO	A	2124	-	3,3,3	4.36	2 (66%)	2,2,2	0.82	0
2	EDO	B	2002	-	3,3,3	4.57	2 (66%)	2,2,2	1.25	0
2	EDO	B	2013	-	3,3,3	2.42	2 (66%)	2,2,2	0.75	0
2	EDO	B	2015	-	3,3,3	2.35	2 (66%)	2,2,2	0.72	0
2	EDO	B	2018	-	3,3,3	2.12	2 (66%)	2,2,2	0.89	0
2	EDO	B	2020	-	3,3,3	2.94	2 (66%)	2,2,2	0.79	0
2	EDO	B	2021	-	3,3,3	3.99	2 (66%)	2,2,2	0.17	0
2	EDO	B	2023	-	3,3,3	3.20	2 (66%)	2,2,2	1.01	0
2	EDO	B	2025	-	3,3,3	2.90	2 (66%)	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	2027	-	3,3,3	1.70	1 (33%)	2,2,2	1.16	0
2	EDO	B	2028	-	3,3,3	2.29	2 (66%)	2,2,2	1.27	0
2	EDO	B	2030	-	3,3,3	1.03	0	2,2,2	0.36	0
2	EDO	B	2062	-	3,3,3	1.85	1 (33%)	2,2,2	1.10	0
2	EDO	B	2070	-	3,3,3	2.80	2 (66%)	2,2,2	0.94	0
2	EDO	B	2125	-	3,3,3	2.78	3 (100%)	2,2,2	1.05	0
2	EDO	C	2004	-	3,3,3	4.42	2 (66%)	2,2,2	0.49	0
2	EDO	C	2024	-	3,3,3	3.39	2 (66%)	2,2,2	0.87	0
2	EDO	C	2026	-	3,3,3	1.06	0	2,2,2	0.79	0
2	EDO	C	2036	-	3,3,3	2.67	2 (66%)	2,2,2	1.14	0
2	EDO	C	2064	-	3,3,3	2.68	2 (66%)	2,2,2	0.59	0
2	EDO	C	2067	-	3,3,3	2.81	1 (33%)	2,2,2	0.43	0
2	EDO	C	2075	-	3,3,3	2.16	2 (66%)	2,2,2	1.30	0
2	EDO	C	2080	-	3,3,3	2.72	2 (66%)	2,2,2	0.52	0
2	EDO	C	2081	-	3,3,3	2.84	3 (100%)	2,2,2	0.92	0
2	EDO	C	2082	-	3,3,3	3.25	1 (33%)	2,2,2	0.62	0
2	EDO	C	2083	-	3,3,3	2.75	2 (66%)	2,2,2	1.28	0
2	EDO	C	2084	-	3,3,3	3.12	2 (66%)	2,2,2	1.29	0
2	EDO	C	2085	-	3,3,3	3.98	2 (66%)	2,2,2	1.44	1 (50%)
2	EDO	C	2117	-	3,3,3	2.38	2 (66%)	2,2,2	0.49	0
2	EDO	C	2126	-	3,3,3	3.27	3 (100%)	2,2,2	0.66	0
2	EDO	C	2128	-	3,3,3	3.37	2 (66%)	2,2,2	1.01	0
2	EDO	D	2003	-	3,3,3	2.76	2 (66%)	2,2,2	0.96	0
2	EDO	D	2031	-	3,3,3	2.96	2 (66%)	2,2,2	0.60	0
2	EDO	D	2033	-	3,3,3	2.29	2 (66%)	2,2,2	1.03	0
2	EDO	D	2035	-	3,3,3	1.27	0	2,2,2	0.29	0
2	EDO	D	2071	-	3,3,3	2.90	2 (66%)	2,2,2	0.54	0
2	EDO	D	2072	-	3,3,3	2.63	2 (66%)	2,2,2	0.61	0
2	EDO	D	2073	-	3,3,3	2.07	2 (66%)	2,2,2	0.66	0
2	EDO	D	2074	-	3,3,3	3.72	2 (66%)	2,2,2	1.49	0
2	EDO	D	2118	-	3,3,3	3.15	2 (66%)	2,2,2	0.25	0
2	EDO	D	2119	-	3,3,3	2.56	2 (66%)	2,2,2	1.04	0
2	EDO	E	2005	-	3,3,3	4.43	2 (66%)	2,2,2	0.49	0
2	EDO	E	2032	-	3,3,3	3.03	1 (33%)	2,2,2	0.86	0
2	EDO	E	2039	-	3,3,3	2.10	2 (66%)	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	E	2040	-	3,3,3	2.62	2 (66%)	2,2,2	0.87	0
2	EDO	E	2041	-	3,3,3	1.69	1 (33%)	2,2,2	1.10	0
2	EDO	E	2042	-	3,3,3	2.16	2 (66%)	2,2,2	0.88	0
2	EDO	E	2076	-	3,3,3	2.56	2 (66%)	2,2,2	0.99	0
2	EDO	E	2077	-	3,3,3	2.69	2 (66%)	2,2,2	0.95	0
2	EDO	E	2078	-	3,3,3	2.40	1 (33%)	2,2,2	1.38	0
2	EDO	E	2079	-	3,3,3	2.68	2 (66%)	2,2,2	1.19	0
2	EDO	E	2088	-	3,3,3	2.81	2 (66%)	2,2,2	1.24	0
2	EDO	E	2089	-	3,3,3	3.45	2 (66%)	2,2,2	0.28	0
2	EDO	E	2090	-	3,3,3	2.66	2 (66%)	2,2,2	0.62	0
2	EDO	E	2091	-	3,3,3	3.25	2 (66%)	2,2,2	1.30	0
2	EDO	E	2092	-	3,3,3	1.81	2 (66%)	2,2,2	1.28	0
2	EDO	E	2120	-	3,3,3	2.95	2 (66%)	2,2,2	0.76	0
2	EDO	E	2127	-	3,3,3	2.60	2 (66%)	2,2,2	1.53	1 (50%)
2	EDO	F	2006	-	3,3,3	3.53	3 (100%)	2,2,2	0.94	0
2	EDO	F	2034	-	3,3,3	2.17	1 (33%)	2,2,2	0.26	0
2	EDO	F	2037	-	3,3,3	2.47	2 (66%)	2,2,2	1.08	0
2	EDO	F	2038	-	3,3,3	2.46	2 (66%)	2,2,2	0.75	0
2	EDO	F	2043	-	3,3,3	3.02	2 (66%)	2,2,2	1.41	0
2	EDO	F	2086	-	3,3,3	2.46	2 (66%)	2,2,2	1.50	1 (50%)
2	EDO	F	2087	-	3,3,3	1.64	1 (33%)	2,2,2	0.83	0
2	EDO	F	2094	-	3,3,3	2.97	2 (66%)	2,2,2	1.46	1 (50%)
2	EDO	F	2095	-	3,3,3	3.04	2 (66%)	2,2,2	1.01	0
2	EDO	F	2096	-	3,3,3	2.38	2 (66%)	2,2,2	0.99	0
2	EDO	F	2097	-	3,3,3	2.94	2 (66%)	2,2,2	0.13	0
2	EDO	F	2098	-	3,3,3	4.13	2 (66%)	2,2,2	0.80	0
2	EDO	G	2009	-	3,3,3	3.70	2 (66%)	2,2,2	1.29	0
2	EDO	G	2047	-	3,3,3	2.79	2 (66%)	2,2,2	0.80	0
2	EDO	G	2050	-	3,3,3	2.95	1 (33%)	2,2,2	0.36	0
2	EDO	G	2056	-	3,3,3	3.14	2 (66%)	2,2,2	0.98	0
2	EDO	G	2057	-	3,3,3	1.44	1 (33%)	2,2,2	0.92	0
2	EDO	G	2093	-	3,3,3	3.00	2 (66%)	2,2,2	1.19	0
2	EDO	G	2101	-	3,3,3	2.25	2 (66%)	2,2,2	1.94	1 (50%)
2	EDO	G	2102	-	3,3,3	3.04	2 (66%)	2,2,2	0.78	0
2	EDO	G	2112	-	3,3,3	2.64	2 (66%)	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	H	2010	-	3,3,3	3.92	2 (66%)	2,2,2	0.45	0
2	EDO	H	2044	-	3,3,3	2.18	1 (33%)	2,2,2	0.29	0
2	EDO	H	2054	-	3,3,3	2.23	2 (66%)	2,2,2	0.96	0
2	EDO	H	2058	-	3,3,3	3.29	2 (66%)	2,2,2	1.56	1 (50%)
2	EDO	H	2059	-	3,3,3	4.02	3 (100%)	2,2,2	0.60	0
2	EDO	H	2060	-	3,3,3	1.00	0	2,2,2	0.22	0
2	EDO	H	2111	-	3,3,3	2.54	3 (100%)	2,2,2	1.11	0
2	EDO	H	2113	-	3,3,3	2.49	1 (33%)	2,2,2	0.89	0
2	EDO	H	2114	-	3,3,3	3.15	2 (66%)	2,2,2	0.96	0
2	EDO	I	2007	-	3,3,3	3.76	2 (66%)	2,2,2	1.49	1 (50%)
2	EDO	I	2045	-	3,3,3	2.95	2 (66%)	2,2,2	0.50	0
2	EDO	I	2046	-	3,3,3	2.21	1 (33%)	2,2,2	1.06	0
2	EDO	I	2051	-	3,3,3	1.99	1 (33%)	2,2,2	1.13	0
2	EDO	I	2052	-	3,3,3	2.57	2 (66%)	2,2,2	1.05	0
2	EDO	I	2099	-	3,3,3	2.48	2 (66%)	2,2,2	1.90	1 (50%)
2	EDO	I	2100	-	3,3,3	1.80	1 (33%)	2,2,2	0.81	0
2	EDO	I	2103	-	3,3,3	2.81	2 (66%)	2,2,2	1.93	1 (50%)
2	EDO	I	2107	-	3,3,3	1.52	1 (33%)	2,2,2	0.67	0
2	EDO	I	2115	-	3,3,3	3.65	2 (66%)	2,2,2	0.97	0
2	EDO	I	2121	-	3,3,3	1.24	0	2,2,2	0.80	0
2	EDO	J	2008	-	3,3,3	4.91	2 (66%)	2,2,2	1.25	0
2	EDO	J	2014	-	3,3,3	3.39	2 (66%)	2,2,2	0.75	0
2	EDO	J	2048	-	3,3,3	3.04	2 (66%)	2,2,2	0.94	0
2	EDO	J	2049	-	3,3,3	2.92	2 (66%)	2,2,2	0.90	0
2	EDO	J	2053	-	3,3,3	3.34	2 (66%)	2,2,2	0.37	0
2	EDO	J	2055	-	3,3,3	2.09	1 (33%)	2,2,2	0.87	0
2	EDO	J	2061	-	3,3,3	2.21	1 (33%)	2,2,2	1.01	0
2	EDO	J	2068	-	3,3,3	2.85	2 (66%)	2,2,2	0.03	0
2	EDO	J	2069	-	3,3,3	2.83	2 (66%)	2,2,2	0.50	0
2	EDO	J	2104	-	3,3,3	3.76	2 (66%)	2,2,2	2.11	1 (50%)
2	EDO	J	2105	-	3,3,3	2.99	2 (66%)	2,2,2	0.54	0
2	EDO	J	2106	-	3,3,3	2.36	1 (33%)	2,2,2	1.00	0
2	EDO	J	2108	-	3,3,3	1.61	1 (33%)	2,2,2	0.83	0
2	EDO	J	2109	-	3,3,3	1.28	1 (33%)	2,2,2	1.20	0
2	EDO	J	2110	-	3,3,3	2.46	2 (66%)	2,2,2	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	J	2123	-	3,3,3	3.41	2 (66%)	2,2,2	2.01	1 (50%)

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	2001	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2011	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2012	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2016	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2017	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2019	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2022	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2029	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2063	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2065	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2066	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2116	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2122	-	-	0/1/1/1	0/0/0/0
2	EDO	A	2124	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2002	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2013	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2015	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2018	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2020	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2021	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2023	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2025	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2027	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2028	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2030	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2062	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2070	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2125	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2004	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2024	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2026	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2036	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2064	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2067	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	2075	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2080	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2081	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2082	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2083	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2084	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2085	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2117	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2126	-	-	0/1/1/1	0/0/0/0
2	EDO	C	2128	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2003	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2031	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2033	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2035	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2071	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2072	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2073	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2074	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2118	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2119	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2005	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2032	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2039	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2040	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2041	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2042	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2076	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2077	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2078	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2079	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2088	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2089	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2090	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2091	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2092	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2120	-	-	0/1/1/1	0/0/0/0
2	EDO	E	2127	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2006	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2034	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2037	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2038	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2043	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	F	2086	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2087	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2094	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2095	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2096	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2097	-	-	0/1/1/1	0/0/0/0
2	EDO	F	2098	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2009	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2047	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2050	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2056	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2057	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2093	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2101	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2102	-	-	0/1/1/1	0/0/0/0
2	EDO	G	2112	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2010	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2044	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2054	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2058	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2059	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2060	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2111	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2113	-	-	0/1/1/1	0/0/0/0
2	EDO	H	2114	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2007	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2045	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2046	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2051	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2052	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2099	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2100	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2103	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2107	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2115	-	-	0/1/1/1	0/0/0/0
2	EDO	I	2121	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2008	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2014	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2048	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2049	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2053	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2055	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	J	2061	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2068	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2069	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2104	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2105	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2106	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2108	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2109	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2110	-	-	0/1/1/1	0/0/0/0
2	EDO	J	2123	-	-	0/1/1/1	0/0/0/0

The worst 5 of 228 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2092	EDO	O2-C2	2.00	1.52	1.42
2	F	2006	EDO	C2-C1	2.05	1.62	1.48
2	A	2065	EDO	O2-C2	2.07	1.52	1.42
2	B	2023	EDO	O1-C1	2.09	1.53	1.42
2	I	2107	EDO	O1-C1	2.10	1.53	1.42

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2101	EDO	O2-C2-C1	-2.72	92.91	112.09
2	J	2123	EDO	O2-C2-C1	-2.67	93.21	112.09
2	I	2099	EDO	O2-C2-C1	-2.63	93.54	112.09
2	J	2104	EDO	O2-C2-C1	-2.27	96.06	112.09
2	H	2058	EDO	O2-C2-C1	-2.20	96.52	112.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

107 monomers are involved in 502 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	EDO	6	0
2	A	2011	EDO	1	0
2	A	2012	EDO	11	0
2	A	2017	EDO	2	0
2	A	2022	EDO	3	0
2	A	2029	EDO	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2063	EDO	7	0
2	A	2065	EDO	5	0
2	A	2066	EDO	1	0
2	A	2116	EDO	1	0
2	A	2122	EDO	4	0
2	A	2124	EDO	7	0
2	B	2002	EDO	5	0
2	B	2018	EDO	1	0
2	B	2020	EDO	2	0
2	B	2021	EDO	4	0
2	B	2023	EDO	3	0
2	B	2025	EDO	2	0
2	B	2028	EDO	11	0
2	B	2030	EDO	10	0
2	B	2125	EDO	8	0
2	C	2004	EDO	11	0
2	C	2024	EDO	12	0
2	C	2036	EDO	1	0
2	C	2064	EDO	2	0
2	C	2067	EDO	4	0
2	C	2075	EDO	7	0
2	C	2080	EDO	2	0
2	C	2082	EDO	2	0
2	C	2084	EDO	1	0
2	C	2085	EDO	10	0
2	C	2117	EDO	3	0
2	C	2126	EDO	6	0
2	C	2128	EDO	8	0
2	D	2003	EDO	4	0
2	D	2031	EDO	4	0
2	D	2035	EDO	11	0
2	D	2072	EDO	3	0
2	D	2074	EDO	2	0
2	D	2118	EDO	7	0
2	D	2119	EDO	2	0
2	E	2005	EDO	5	0
2	E	2032	EDO	3	0
2	E	2039	EDO	2	0
2	E	2040	EDO	1	0
2	E	2042	EDO	2	0
2	E	2076	EDO	7	0
2	E	2077	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2078	EDO	1	0
2	E	2079	EDO	2	0
2	E	2088	EDO	3	0
2	E	2089	EDO	4	0
2	E	2090	EDO	5	0
2	E	2091	EDO	5	0
2	E	2092	EDO	1	0
2	E	2120	EDO	6	0
2	E	2127	EDO	9	0
2	F	2006	EDO	2	0
2	F	2034	EDO	5	0
2	F	2038	EDO	4	0
2	F	2043	EDO	13	0
2	F	2086	EDO	7	0
2	F	2087	EDO	2	0
2	F	2095	EDO	2	0
2	F	2097	EDO	5	0
2	F	2098	EDO	3	0
2	G	2009	EDO	4	0
2	G	2047	EDO	2	0
2	G	2050	EDO	5	0
2	G	2056	EDO	7	0
2	G	2057	EDO	7	0
2	G	2093	EDO	6	0
2	G	2102	EDO	3	0
2	G	2112	EDO	2	0
2	H	2010	EDO	8	0
2	H	2044	EDO	4	0
2	H	2054	EDO	1	0
2	H	2058	EDO	11	0
2	H	2059	EDO	2	0
2	H	2060	EDO	4	0
2	H	2111	EDO	3	0
2	H	2113	EDO	4	0
2	H	2114	EDO	0	1
2	I	2007	EDO	5	0
2	I	2045	EDO	2	0
2	I	2046	EDO	4	0
2	I	2051	EDO	6	0
2	I	2099	EDO	3	0
2	I	2100	EDO	2	0
2	I	2103	EDO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2107	EDO	11	0
2	I	2115	EDO	7	0
2	I	2121	EDO	12	0
2	J	2008	EDO	7	0
2	J	2014	EDO	3	0
2	J	2049	EDO	10	0
2	J	2053	EDO	3	0
2	J	2055	EDO	2	0
2	J	2061	EDO	2	0
2	J	2068	EDO	6	0
2	J	2104	EDO	14	0
2	J	2105	EDO	4	0
2	J	2106	EDO	2	0
2	J	2108	EDO	3	0
2	J	2109	EDO	14	0
2	J	2110	EDO	3	0
2	J	2123	EDO	6	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.