



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:44 am BST

PDB ID : 1JKV
Title : Crystal Structure of Manganese Catalase from *Lactobacillus plantarum* complexed with azide
Authors : Barynin, V.V.; Whittaker, M.M.; Antonyuk, S.V.; Lamzin, V.S.; Harrison, P.M.; Artymiuk, P.J.; Whittaker, J.W.
Deposited on : 2001-07-13
Resolution : 1.39 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

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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

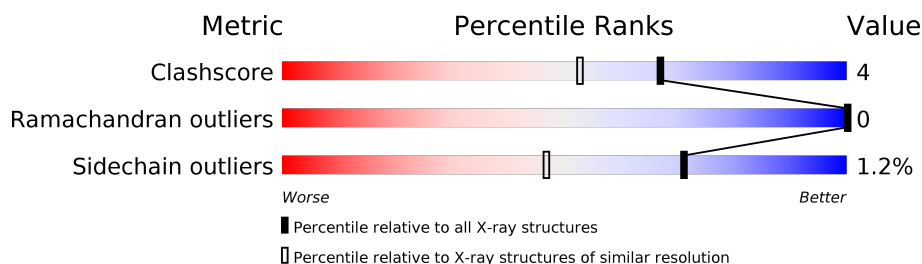
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	266	
1	B	266	
1	C	266	
1	D	266	
1	E	266	
1	F	266	

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
6	EDO	A	4284	-	-	X	-
6	EDO	C	6284	-	-	X	-
6	EDO	E	8284	-	X	-	-
6	EDO	F	9284	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14240 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.

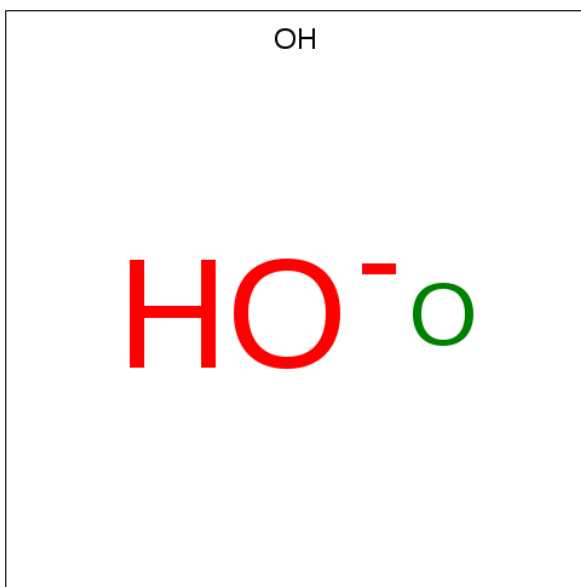
- Molecule 1 is a protein called pseudocatalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	6	0
			2104	1311	362	413	18			
1	B	266	Total	C	N	O	S	0	4	0
			2098	1305	363	412	18			
1	C	266	Total	C	N	O	S	0	5	0
			2100	1307	362	413	18			
1	D	266	Total	C	N	O	S	0	4	0
			2096	1303	362	413	18			
1	E	266	Total	C	N	O	S	0	4	0
			2096	1303	362	413	18			
1	F	266	Total	C	N	O	S	0	4	0
			2098	1306	362	412	18			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



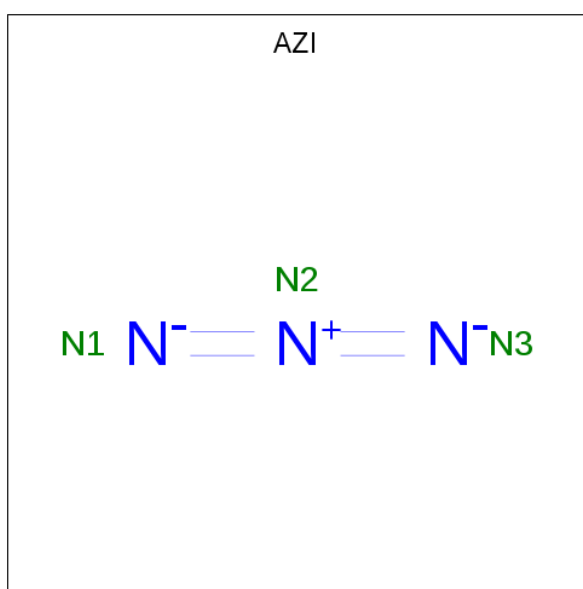
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	A	1	Total O 1 1	0	0
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N₃).

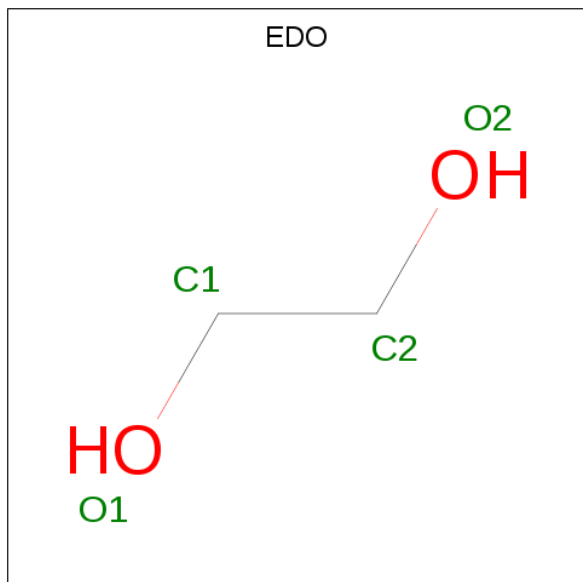


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 3 3	0	0
4	B	1	Total N 3 3	0	0
4	C	1	Total N 3 3	0	0
4	D	1	Total N 3 3	0	0
4	E	1	Total N 3 3	0	0
4	F	1	Total N 3 3	0	0

- Molecule 5 is MANGANESE (III) ION (three-letter code: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total Mn 2 2	0	0
5	E	2	Total Mn 2 2	0	0
5	B	2	Total Mn 2 2	0	0
5	C	2	Total Mn 2 2	0	0
5	A	2	Total Mn 2 2	0	0
5	F	2	Total Mn 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	258	Total 258	O 258	0	0
7	B	267	Total 267	O 267	0	0
7	C	259	Total 259	O 259	0	0
7	D	245	Total 245	O 245	0	0
7	E	244	Total 244	O 244	0	0
7	F	261	Total 261	O 261	0	0

3 Residue-property plots [i](#)

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

Chain A: 



- Molecule 1: pseudocatalase

Chain B: 



- Molecule 1: pseudocatalase

Chain C: 



- Molecule 1: pseudocatalase

Chain D: 

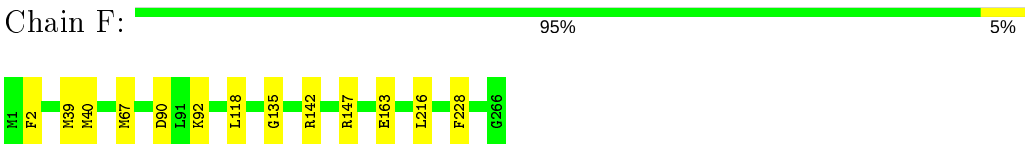


- Molecule 1: pseudocatalase

Chain E: 



- Molecule 1: pseudocatalase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.21Å 95.55Å 106.11Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	17.00 – 1.39	Depositor
% Data completeness (in resolution range)	97.2 (17.00-1.39)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	5.00	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.104 , 0.130	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14240	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: AZI, CA, MN3, EDO, OH

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	0.66	0/2172	0.80	2/2923 (0.1%)
1	B	0.64	0/2159	0.80	2/2904 (0.1%)
1	C	0.69	0/2164	0.81	3/2912 (0.1%)
1	D	0.67	0/2156	0.82	3/2901 (0.1%)
1	E	0.68	0/2156	0.87	6/2901 (0.2%)
1	F	0.67	0/2158	0.80	2/2904 (0.1%)
All	All	0.67	0/12965	0.82	18/17445 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	D	93	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	E	93	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	C	93	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	F	90	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	94	ASP	CB-CG-OD2	6.37	124.03	118.30
1	D	260	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	E	57	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	260	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	169	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	142	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	E	223	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	90	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	249	GLY	N-CA-C	5.08	125.81	113.10
1	B	24	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	E	260	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	E	147	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	93	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	2104	0	2025	16	1
1	B	2098	0	2019	25	0
1	C	2100	0	2018	29	0
1	D	2096	0	2011	16	0
1	E	2096	0	2011	8	0
1	F	2098	0	2017	16	1
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
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
6	A	12	0	18	7	0
6	B	4	0	6	0	0
6	C	12	0	18	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	8	0	12	0	0
6	E	12	0	13	0	0
6	F	12	0	18	6	0
7	A	258	0	0	3	0
7	B	267	0	0	15	0
7	C	259	0	0	8	0
7	D	245	0	0	9	1
7	E	244	0	0	2	0
7	F	261	0	0	3	0
All	All	14240	0	12186	96	2

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 4.

All (96) 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:190:GLU:OE2	7:B:9448:HOH:O	1.61	1.15
1:F:118[B]:LEU:CD2	6:F:9284:EDO:H12	1.77	1.12
1:C:118[A]:LEU:CD2	6:C:6284:EDO:H21	1.78	1.12
1:A:118[A]:LEU:CD2	6:A:4284:EDO:H12	1.82	1.10
1:D:165:GLU:OE2	7:D:7478:HOH:O	1.69	1.10
1:C:93:ARG:NH2	7:C:6377:HOH:O	1.61	1.09
1:C:93:ARG:C	7:C:6444:HOH:O	1.96	1.03
1:C:118[A]:LEU:HD21	6:C:6284:EDO:H21	1.43	0.99
1:F:118[B]:LEU:HD21	6:F:9284:EDO:H12	1.52	0.89
1:A:118[A]:LEU:HD21	6:A:4284:EDO:H12	1.54	0.87
1:B:190:GLU:CD	7:B:9448:HOH:O	2.07	0.82
1:F:118[B]:LEU:HD23	6:F:9284:EDO:H12	1.60	0.81
1:B:187:LYS:HE2	7:B:9482:HOH:O	1.84	0.78
1:B:187:LYS:HE2	7:B:9535:HOH:O	1.83	0.77
1:B:253:HIS:CD2	7:B:9459:HOH:O	2.39	0.76
1:C:94:ASP:N	7:C:6444:HOH:O	2.16	0.75
1:A:118[A]:LEU:HD23	6:A:4284:EDO:H12	1.69	0.73
1:C:93:ARG:HD2	7:C:6431:HOH:O	1.93	0.69
1:C:95:PRO:HD3	7:C:6444:HOH:O	1.93	0.69
1:C:118[A]:LEU:CG	6:C:6284:EDO:H21	2.22	0.68
1:B:253:HIS:HD2	7:B:9459:HOH:O	1.73	0.68
1:A:7:LYS:HD3	7:A:5510:HOH:O	1.93	0.68
1:B:187:LYS:NZ	1:B:191:GLU:OE2	2.32	0.63
1:B:187:LYS:NZ	1:C:231:GLN:NE2	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67[A]:MET:SD	7:D:7518:HOH:O	1.03	0.60
1:C:118[A]:LEU:HD23	6:C:6284:EDO:H21	1.79	0.60
1:C:93:ARG:HH11	1:C:94:ASP:HB2	1.67	0.60
1:A:7:LYS:HE3	7:F:9452:HOH:O	2.01	0.60
1:A:118[A]:LEU:CG	6:A:4284:EDO:H12	2.31	0.58
1:C:93:ARG:HH11	1:C:94:ASP:CB	2.15	0.58
1:F:118[B]:LEU:HG	6:F:9284:EDO:O1	2.04	0.58
1:F:118[B]:LEU:CG	6:F:9284:EDO:H12	2.35	0.56
1:B:187:LYS:HD3	7:B:9482:HOH:O	2.06	0.55
1:B:187:LYS:NZ	7:B:9444:HOH:O	2.39	0.55
1:B:187:LYS:CE	7:B:9482:HOH:O	2.51	0.54
1:A:92:LYS:NZ	1:C:163:GLU:OE2	2.37	0.54
1:C:118[A]:LEU:HG	6:C:6284:EDO:H21	1.90	0.53
1:D:190:GLU:HB2	7:D:7520:HOH:O	2.09	0.53
1:B:206:GLU:HG3	7:B:9547:HOH:O	2.08	0.53
1:C:93:ARG:CD	1:C:93:ARG:C	2.76	0.53
1:B:187:LYS:HZ2	1:C:231:GLN:NE2	2.07	0.52
1:C:67[A]:MET:HG3	1:E:2:PHE:CE1	2.44	0.52
1:E:135:GLY:HA2	7:E:8457:HOH:O	2.08	0.52
1:D:190:GLU:CG	7:D:7520:HOH:O	2.57	0.52
1:F:39[B]:MET:SD	1:F:40:MET:SD	3.07	0.52
1:B:187:LYS:CD	7:B:9482:HOH:O	2.57	0.51
1:D:67[A]:MET:HG3	1:F:2:PHE:CE1	2.45	0.51
1:A:39[B]:MET:SD	1:A:40:MET:SD	3.08	0.51
1:D:39[A]:MET:SD	1:D:40:MET:SD	3.08	0.51
1:F:135:GLY:HA2	7:F:9471:HOH:O	2.10	0.51
1:D:16:ARG:CZ	7:D:7487:HOH:O	2.60	0.50
1:F:118[B]:LEU:HG	6:F:9284:EDO:C1	2.42	0.49
1:B:187:LYS:CE	7:B:9535:HOH:O	2.51	0.49
1:C:135:GLY:HA2	7:C:6424:HOH:O	2.10	0.49
1:A:67[B]:MET:CE	1:B:43:LEU:CD1	2.91	0.49
1:D:190:GLU:CD	7:D:7520:HOH:O	2.51	0.48
1:F:216:LEU:CD1	1:F:228:PHE:HB2	2.42	0.48
1:D:16:ARG:NH1	7:D:7487:HOH:O	2.47	0.48
1:F:216:LEU:HD12	1:F:228:PHE:HB2	1.96	0.48
1:C:2:PHE:CE1	1:E:67[B]:MET:HG3	2.49	0.47
1:D:2:PHE:CE1	1:F:67[B]:MET:HG3	2.48	0.47
1:F:163:GLU:HG2	7:F:9477:HOH:O	2.14	0.47
1:D:135:GLY:HA2	7:D:7431:HOH:O	2.14	0.47
1:A:67[B]:MET:CE	1:B:43:LEU:HD13	2.44	0.47
1:C:93:ARG:O	1:C:93:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASN:CG	7:B:9431:HOH:O	2.51	0.47
1:B:39[A]:MET:SD	1:B:40:MET:SD	3.13	0.46
1:B:187:LYS:HZ1	1:C:231:GLN:NE2	2.12	0.46
1:E:39[B]:MET:SD	1:E:40:MET:SD	3.14	0.46
1:A:135:GLY:HA2	7:A:5395:HOH:O	2.15	0.46
1:C:118[A]:LEU:HG	6:C:6284:EDO:C2	2.46	0.46
1:E:93:ARG:NH2	7:E:8438:HOH:O	2.07	0.46
1:E:191:GLU:HA	1:E:194:GLU:HG2	1.98	0.46
1:A:118[A]:LEU:HG	6:A:4284:EDO:O1	2.16	0.45
1:C:39[A]:MET:SD	1:C:40:MET:SD	3.14	0.45
1:D:198:ILE:O	1:E:186:MET:HE1	2.17	0.45
1:C:39[B]:MET:SD	1:C:67[B]:MET:HG2	2.57	0.45
1:A:118[A]:LEU:HG	6:A:4284:EDO:C1	2.46	0.45
1:C:93:ARG:CD	7:C:6431:HOH:O	2.61	0.43
1:D:39[B]:MET:SD	1:D:67[B]:MET:HG2	2.58	0.43
1:F:39[A]:MET:SD	1:F:67[A]:MET:HG2	2.58	0.43
1:A:39[A]:MET:SD	1:A:67[A]:MET:HG2	2.59	0.43
1:B:11:ASN:ND2	7:B:9431:HOH:O	2.52	0.43
1:B:39[B]:MET:SD	1:B:67[B]:MET:HG2	2.59	0.42
1:E:190:GLU:O	1:E:194:GLU:HG2	2.20	0.42
1:D:165:GLU:CD	7:D:7478:HOH:O	2.39	0.42
1:B:187:LYS:NZ	1:C:231:GLN:HE22	2.17	0.42
1:A:118[A]:LEU:HG	6:A:4284:EDO:H12	2.00	0.42
1:D:138:VAL:HG22	1:D:192:LEU:HB3	2.01	0.42
1:A:180:GLN:NE2	1:F:216:LEU:HG	2.35	0.41
1:B:89:GLU:HG2	7:B:9521:HOH:O	2.21	0.40
1:B:187:LYS:HZ2	1:C:231:GLN:CD	2.24	0.40
1:C:118[A]:LEU:CD2	6:C:6284:EDO:C2	2.71	0.40
7:A:5320:HOH:O	1:F:216:LEU:HD23	2.20	0.40
1:C:89:GLU:HG3	7:C:6495:HOH:O	2.21	0.40
1:D:120:ASN:HB2	1:D:121:PRO:CD	2.52	0.40

All (2) 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)
7:D:7468:HOH:O	7:D:7488:HOH:O[1_655]	2.07	0.13
1:A:194:GLU:CD	1:F:92:LYS:NZ[2_545]	2.12	0.08

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	270/266 (102%)	264 (98%)	6 (2%)	0	100	100
1	B	268/266 (101%)	263 (98%)	5 (2%)	0	100	100
1	C	269/266 (101%)	264 (98%)	5 (2%)	0	100	100
1	D	268/266 (101%)	262 (98%)	6 (2%)	0	100	100
1	E	268/266 (101%)	264 (98%)	4 (2%)	0	100	100
1	F	268/266 (101%)	261 (97%)	7 (3%)	0	100	100
All	All	1611/1596 (101%)	1578 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	228/222 (103%)	223 (98%)	5 (2%)	52	19
1	B	226/222 (102%)	223 (99%)	3 (1%)	69	42
1	C	227/222 (102%)	225 (99%)	2 (1%)	78	58
1	D	226/222 (102%)	224 (99%)	2 (1%)	78	58
1	E	226/222 (102%)	222 (98%)	4 (2%)	59	28
1	F	226/222 (102%)	225 (100%)	1 (0%)	91	78
All	All	1359/1332 (102%)	1342 (99%)	17 (1%)	71	42

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	A	205	LYS
1	A	206	GLU
1	A	216[A]	LEU
1	A	216[B]	LEU
1	B	147	ARG
1	B	201	PRO
1	B	216	LEU
1	C	93	ARG
1	C	147	ARG
1	D	147	ARG
1	D	216	LEU
1	E	16	ARG
1	E	147	ARG
1	E	216	LEU
1	E	246	GLU
1	F	147	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	HIS
1	B	11	ASN
1	B	253	HIS
1	C	231	GLN
1	D	11	ASN
1	E	253	HIS
1	F	253	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 57 ligands modelled in this entry, 18 are modelled with single atom and 18 are monoatomic - leaving 21 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	$\# Z > 2$
6	EDO	C	6283	-	3,3,3	0.50	0	2,2,2	0.49	0
6	EDO	F	9284	-	3,3,3	0.41	0	2,2,2	0.40	0
6	EDO	F	4285	-	3,3,3	0.49	0	2,2,2	0.86	0
6	EDO	B	5283	-	3,3,3	0.41	0	2,2,2	0.24	0
4	AZI	D	7281	5	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	E	8283	-	3,3,3	0.49	0	2,2,2	0.26	0
6	EDO	D	7284	-	3,3,3	0.34	0	2,2,2	0.09	0
4	AZI	B	5281	5	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	C	6284	-	3,3,3	0.50	0	2,2,2	0.09	0
6	EDO	D	7283	-	3,3,3	0.58	0	2,2,2	0.29	0
6	EDO	A	4284	-	3,3,3	0.52	0	2,2,2	0.13	0
6	EDO	C	6285	-	3,3,3	0.82	0	2,2,2	0.88	0
4	AZI	E	8281	5	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	4283	-	3,3,3	0.38	0	2,2,2	0.14	0
6	EDO	F	9283	-	3,3,3	0.60	0	2,2,2	0.35	0
4	AZI	C	6281	5	0,2,2	0.00	-	0,1,1	0.00	-
4	AZI	F	9281	5	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	5284	-	3,3,3	0.43	0	2,2,2	0.12	0
6	EDO	E	8284	-	3,3,3	12.70	2 (66%)	2,2,2	10.11	2 (100%)
4	AZI	A	4281	5	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	E	7285	-	3,3,3	0.33	0	2,2,2	0.55	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
6	EDO	C	6283	-	-	0/1/1/1	-
6	EDO	F	9284	-	-	0/1/1/1	-
6	EDO	F	4285	-	-	0/1/1/1	-
6	EDO	E	8283	-	-	0/1/1/1	-
6	EDO	B	5283	-	-	0/1/1/1	-
6	EDO	D	7284	-	-	0/1/1/1	-
6	EDO	A	4283	-	-	0/1/1/1	-
6	EDO	C	6284	-	-	0/1/1/1	-
6	EDO	D	7283	-	-	0/1/1/1	-
6	EDO	A	4284	-	-	0/1/1/1	-
6	EDO	C	6285	-	-	1/1/1/1	-
6	EDO	E	7285	-	-	0/1/1/1	-
6	EDO	F	9283	-	-	0/1/1/1	-
6	EDO	A	5284	-	-	0/1/1/1	-
6	EDO	E	8284	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	8284	EDO	O2-C2	20.93	2.50	1.42
6	E	8284	EDO	C2-C1	-6.75	1.01	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	8284	EDO	O2-C2-C1	-12.91	19.05	111.91
6	E	8284	EDO	O1-C1-C2	-6.15	67.64	111.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	8284	EDO	O1-C1-C2-O2
6	C	6285	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	9284	EDO	6	0
6	C	6284	EDO	7	0
6	A	4284	EDO	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.