



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:38 PM UTC

PDB ID : 5ECU / pdb_00005ecu
Title : The unliganded structure of Caldicellulosiruptor saccharolyticus GH5
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2015-10-20
Resolution : 1.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

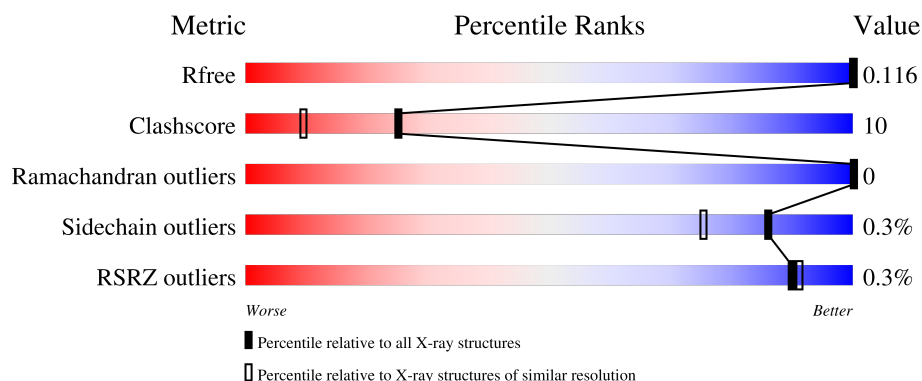
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 ≥ 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	555	

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	607	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	627[B]	-	-	X	-
3	GOL	A	629	-	-	X	-
3	GOL	A	631	-	X	-	-
4	MLI	A	633	-	X	-	-
5	ACT	A	642	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3596 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.

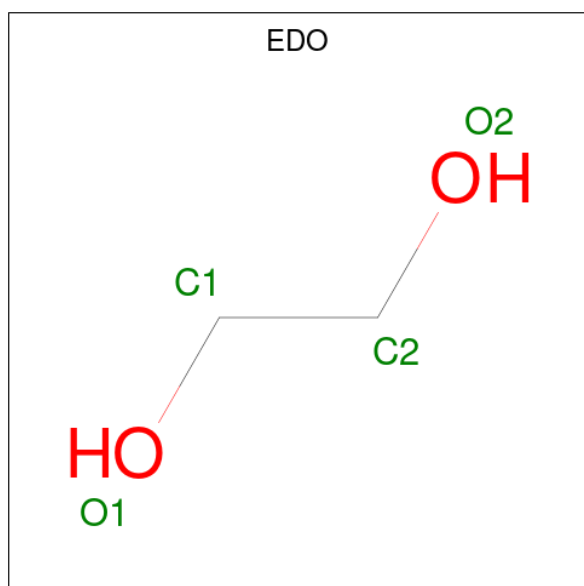
- Molecule 1 is a protein called Cellulase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2950	1878	492	569	11	0	22	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	LEU	PRO	conflict	UNP A4XHB2
A	577	LEU	-	expression tag	UNP A4XHB2
A	578	GLU	-	expression tag	UNP A4XHB2
A	579	HIS	-	expression tag	UNP A4XHB2
A	580	HIS	-	expression tag	UNP A4XHB2
A	581	HIS	-	expression tag	UNP A4XHB2
A	582	HIS	-	expression tag	UNP A4XHB2
A	583	HIS	-	expression tag	UNP A4XHB2
A	584	HIS	-	expression tag	UNP A4XHB2

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



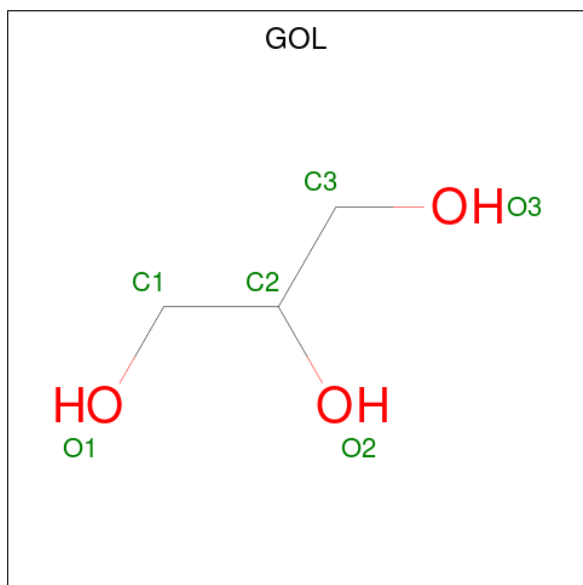
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 8 4 4	0	1
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 8 4 4	0	1
2	A	1	Total C O 8 4 4	0	1
2	A	1	Total C O 8 4 4	0	1
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 8 4 4	0	1

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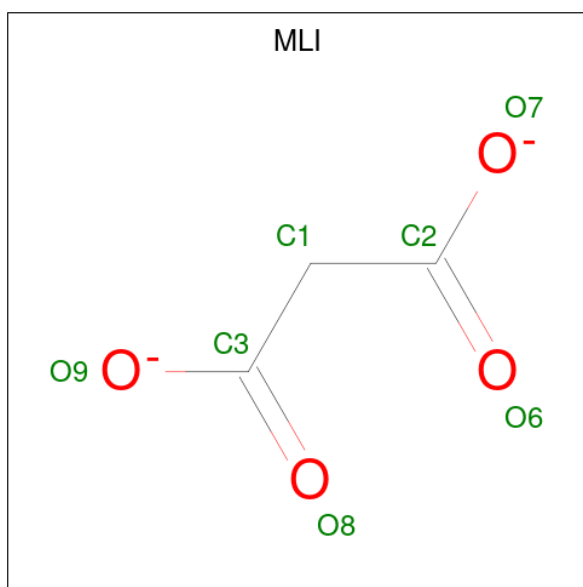
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



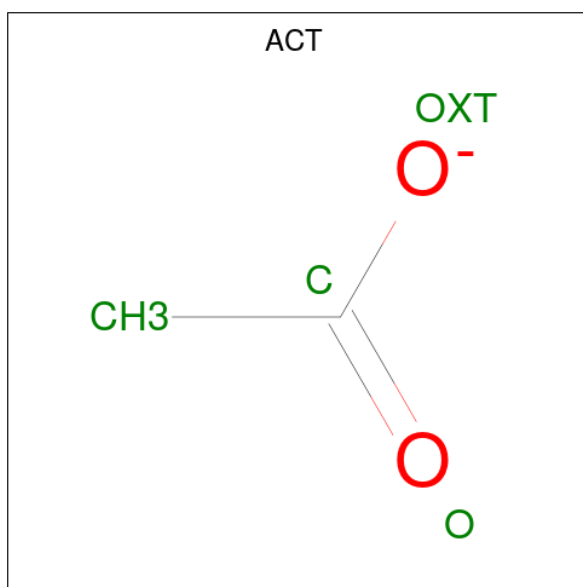
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	A	1	Total	C	O	0	0
			7	3	4		
4	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0

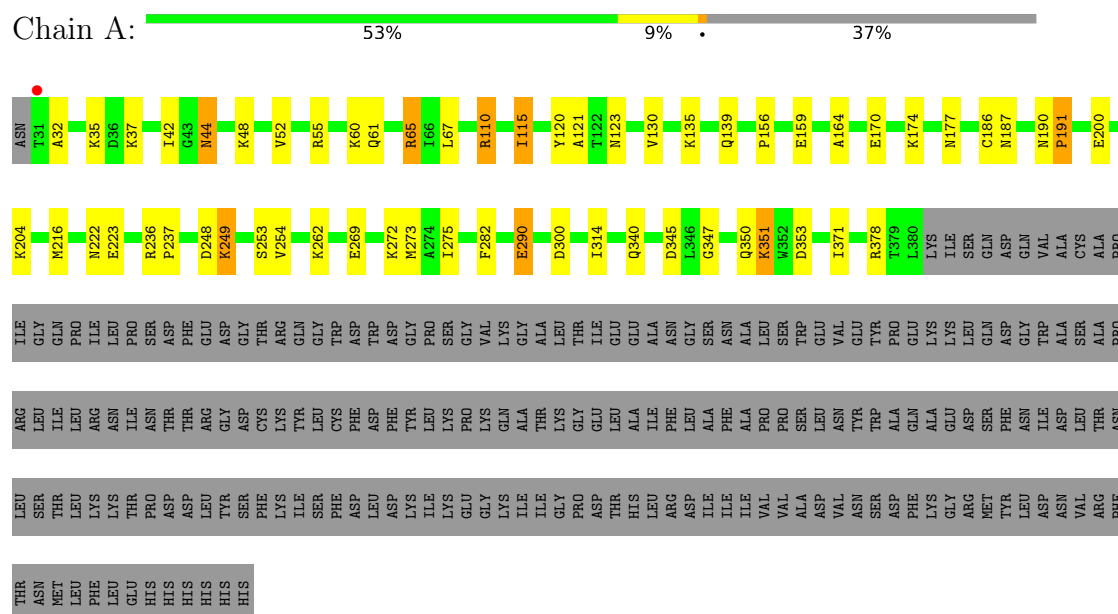
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	392	Total O 427 427	0	35

3 Residue-property plots

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: Cellulase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	146.66Å 146.66Å 146.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 1.50 19.96 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-1.50) 99.8 (19.96-1.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.15 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.085 , 0.115 0.086 , 0.116	Depositor DCC
R_{free} test set	4156 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3596	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, EDO, MLI, ACT, GOL

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	1.46	22/3022 (0.7%)	1.34	14/4105 (0.3%)

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	GLY	C-O	9.58	1.34	1.23
1	A	350	GLN	CA-C	-7.90	1.43	1.53
1	A	345	ASP	C-O	-7.14	1.15	1.24
1	A	61	GLN	N-CA	7.13	1.55	1.46
1	A	351	LYS	CA-C	6.67	1.61	1.52
1	A	44	ASN	CG-OD1	6.66	1.36	1.23
1	A	37	LYS	CA-C	6.51	1.61	1.52
1	A	67	LEU	CB-CG	-6.26	1.41	1.53
1	A	65	ARG	CZ-NH2	6.24	1.41	1.33
1	A	32	ALA	C-O	6.11	1.31	1.23
1	A	290	GLU	CD-OE2	-6.08	1.13	1.25
1	A	351	LYS	C-O	-6.07	1.16	1.23
1	A	191	PRO	CA-C	6.03	1.59	1.52
1	A	353	ASP	CG-OD1	-5.92	1.14	1.25
1	A	223	GLU	CD-OE1	5.74	1.36	1.25
1	A	42	ILE	CA-CB	-5.72	1.47	1.54
1	A	159	GLU	CD-OE2	5.67	1.36	1.25
1	A	139	GLN	CA-CB	5.31	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	ASP	CG-OD2	5.21	1.35	1.25
1	A	115	ILE	CB-CG1	5.06	1.63	1.53
1	A	378	ARG	CG-CD	-5.05	1.37	1.52
1	A	353	ASP	CA-CB	-5.05	1.44	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ARG	NE-CZ-NH1	-6.26	115.23	121.50
1	A	110	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	A	236	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	A	353	ASP	CB-CG-OD1	5.86	131.89	118.40
1	A	35	LYS	CB-CG-CD	5.82	124.69	111.30
1	A	65	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	130	VAL	N-CA-C	-5.34	105.50	110.53
1	A	55	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	115	ILE	CB-CA-C	5.10	116.05	111.71
1	A	60	LYS	CB-CG-CD	5.09	123.00	111.30
1	A	204	LYS	CB-CG-CD	5.05	122.91	111.30
1	A	37	LYS	N-CA-CB	-5.02	102.74	110.42
1	A	249[A]	LYS	CD-CE-NZ	5.00	127.92	111.90
1	A	249[B]	LYS	CD-CE-NZ	5.00	127.92	111.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	290	GLU	Sidechain

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	2950	0	2842	56	1
2	A	120	0	166	20	0
3	A	48	0	56	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	21	0	4	2	0
5	A	28	0	19	5	0
6	A	2	0	0	0	0
7	A	427	0	0	15	0
All	All	3596	0	3087	61	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 10.

All (61) 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:A:275:ILE:HD13	1:A:314[B]:ILE:HD11	1.39	1.05
1:A:249[B]:LYS:HE3	7:A:1029[B]:HOH:O	1.53	1.04
1:A:275:ILE:CD1	1:A:314[B]:ILE:HD11	1.92	0.98
1:A:249[B]:LYS:CE	7:A:1029[B]:HOH:O	2.07	0.95
1:A:249[B]:LYS:HD2	7:A:1029[B]:HOH:O	1.70	0.92
1:A:314[A]:ILE:CD1	2:A:607:EDO:C2	2.54	0.85
1:A:164:ALA:HB3	3:A:631:GOL:H11	1.60	0.83
1:A:314[A]:ILE:CD1	2:A:607:EDO:H22	2.11	0.80
1:A:314[A]:ILE:HD11	2:A:607:EDO:H11	1.64	0.77
1:A:314[A]:ILE:HD13	2:A:607:EDO:C2	2.18	0.74
1:A:314[A]:ILE:HD13	2:A:607:EDO:H21	1.71	0.73
1:A:249[B]:LYS:CD	7:A:1029[B]:HOH:O	2.19	0.73
1:A:314[A]:ILE:HD12	2:A:607:EDO:H22	1.71	0.70
1:A:120:TYR:HD2	5:A:642:ACT:H2	1.60	0.65
1:A:273[B]:MET:HE2	3:A:627[B]:GOL:H31	1.78	0.65
1:A:275:ILE:HD11	1:A:314[B]:ILE:HD11	1.79	0.64
1:A:275:ILE:HD11	1:A:314[B]:ILE:CD1	2.29	0.62
1:A:314[A]:ILE:CD1	2:A:607:EDO:H11	2.30	0.62
1:A:273[B]:MET:CE	3:A:627[B]:GOL:O1	2.48	0.62
2:A:609:EDO:H12	7:A:1031:HOH:O	2.01	0.61
1:A:340[A]:GLN:HE21	3:A:629:GOL:H2	1.65	0.60
4:A:634:MLI:O7	4:A:634:MLI:O9	2.09	0.59
1:A:340[A]:GLN:HE21	3:A:629:GOL:C3	2.15	0.59
1:A:300:ASP:OD1	4:A:635:MLI:O9	2.21	0.58
1:A:275:ILE:CD1	1:A:314[B]:ILE:CD1	2.72	0.58
1:A:314[A]:ILE:CD1	2:A:607:EDO:C1	2.84	0.56
1:A:314[A]:ILE:HD11	2:A:607:EDO:C1	2.36	0.55
1:A:121:ALA:HB2	5:A:642:ACT:H3	1.88	0.55
2:A:615[A]:EDO:C2	7:A:793[A]:HOH:O	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:615[A]:EDO:H21	7:A:793[A]:HOH:O	2.07	0.54
1:A:170[B]:GLU:OE2	1:A:174:LYS:HE3	2.09	0.52
1:A:48:LYS:HA	2:A:621:EDO:H12	1.91	0.52
1:A:174:LYS:HE2	7:A:948:HOH:O	2.10	0.51
1:A:340[A]:GLN:HE21	3:A:629:GOL:H31	1.76	0.51
1:A:177:ASN:H	1:A:222:ASN:ND2	2.07	0.51
1:A:273[B]:MET:CE	3:A:627[B]:GOL:H31	2.40	0.50
1:A:121:ALA:HA	5:A:642:ACT:H1	1.93	0.49
1:A:123:ASN:HB2	7:A:944:HOH:O	2.11	0.49
1:A:200[A]:GLU:H	1:A:200[A]:GLU:CD	2.21	0.49
1:A:65:ARG:HD3	2:A:622[B]:EDO:O2	2.13	0.48
1:A:371:ILE:HD11	2:A:623:EDO:H21	1.95	0.48
1:A:170[B]:GLU:HG3	7:A:948:HOH:O	2.13	0.47
1:A:340[A]:GLN:HE21	3:A:629:GOL:C2	2.28	0.46
1:A:115:ILE:HG23	5:A:642:ACT:CH3	2.46	0.45
1:A:52:VAL:HG21	2:A:621:EDO:H22	1.99	0.45
1:A:174:LYS:HG3	7:A:948:HOH:O	2.16	0.44
1:A:351:LYS:HE2	7:A:747[B]:HOH:O	2.17	0.44
1:A:190:ASN:HB2	1:A:191:PRO:HD2	1.99	0.43
1:A:275:ILE:HG12	2:A:607:EDO:H11	2.00	0.43
1:A:272:LYS:CE	7:A:893[A]:HOH:O	2.66	0.43
1:A:156:PRO:O	3:A:631:GOL:H32	2.18	0.43
1:A:120:TYR:CD2	5:A:642:ACT:H2	2.47	0.43
1:A:262:LYS:HG2	7:A:832[B]:HOH:O	2.18	0.42
1:A:237:PRO:HG3	1:A:254[A]:VAL:CG2	2.50	0.42
1:A:52:VAL:HG21	2:A:621:EDO:H11	2.01	0.42
2:A:616[B]:EDO:H11	7:A:1027:HOH:O	2.20	0.41
1:A:170[B]:GLU:CG	1:A:174:LYS:HE2	2.49	0.41
1:A:216:MET:HG3	2:A:616[A]:EDO:H12	2.02	0.41
1:A:186:CYS:O	1:A:187:ASN:C	2.64	0.41
1:A:253:SER:HA	1:A:282:PHE:O	2.20	0.41
1:A:273[B]:MET:HE3	3:A:627[B]:GOL:O1	2.20	0.40

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)
1:A:135:LYS:NZ	1:A:269[B]:GLU:OE2[23_455]	2.15	0.05

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	370/555 (67%)	359 (97%)	11 (3%)	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	317/474 (67%)	316 (100%)	1 (0%)	86	75

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	61	GLN
1	A	123	ASN
1	A	139	GLN
1	A	140	ASN
1	A	222	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 2 are monoatomic - leaving 48 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
2	EDO	A	601	-	3,3,3	0.75	0	2,2,2	0.48	0
2	EDO	A	617	-	3,3,3	0.57	0	2,2,2	0.78	0
3	GOL	A	629	-	5,5,5	1.20	1 (20%)	5,5,5	2.11	2 (40%)
2	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.11	0
2	EDO	A	608	-	3,3,3	0.88	0	2,2,2	0.80	0
2	EDO	A	619	-	3,3,3	0.47	0	2,2,2	0.63	0
4	MLI	A	633	-	6,6,6	3.01	5 (83%)	7,7,7	2.94	4 (57%)
5	ACT	A	637	-	3,3,3	1.08	0	3,3,3	1.14	0
2	EDO	A	612[B]	-	3,3,3	0.61	0	2,2,2	0.46	0
3	GOL	A	627[B]	-	5,5,5	0.89	0	5,5,5	1.36	1 (20%)
2	EDO	A	625	-	3,3,3	0.78	0	2,2,2	1.24	0
2	EDO	A	605	-	3,3,3	0.77	0	2,2,2	2.11	1 (50%)
2	EDO	A	622[B]	-	3,3,3	0.59	0	2,2,2	0.26	0
2	EDO	A	610	-	3,3,3	0.52	0	2,2,2	0.75	0
2	EDO	A	614[A]	6	3,3,3	0.89	0	2,2,2	0.84	0
3	GOL	A	632	-	5,5,5	0.62	0	5,5,5	1.38	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	615[B]	-	3,3,3	0.41	0	2,2,2	0.36	0
3	GOL	A	628	-	5,5,5	1.15	0	5,5,5	1.72	2 (40%)
5	ACT	A	640	-	3,3,3	0.89	0	3,3,3	2.40	2 (66%)
4	MLI	A	635	-	6,6,6	1.56	2 (33%)	7,7,7	0.74	0
2	EDO	A	616[B]	-	3,3,3	0.51	0	2,2,2	0.23	0
5	ACT	A	641	-	3,3,3	0.70	0	3,3,3	0.68	0
2	EDO	A	613	-	3,3,3	0.44	0	2,2,2	0.28	0
2	EDO	A	620	-	3,3,3	0.51	0	2,2,2	1.50	0
2	EDO	A	602	-	3,3,3	0.41	0	2,2,2	0.51	0
2	EDO	A	621	-	3,3,3	1.76	1 (33%)	2,2,2	0.78	0
2	EDO	A	609	-	3,3,3	1.19	0	2,2,2	0.38	0
3	GOL	A	626	-	5,5,5	0.74	0	5,5,5	1.81	2 (40%)
4	MLI	A	634	-	6,6,6	2.39	3 (50%)	7,7,7	1.67	1 (14%)
2	EDO	A	623	-	3,3,3	1.16	0	2,2,2	0.48	0
5	ACT	A	639	-	3,3,3	1.39	0	3,3,3	0.44	0
2	EDO	A	612[A]	-	3,3,3	0.20	0	2,2,2	0.22	0
3	GOL	A	627[A]	-	5,5,5	0.81	0	5,5,5	2.10	2 (40%)
2	EDO	A	607	-	3,3,3	0.34	0	2,2,2	0.80	0
2	EDO	A	618	-	3,3,3	0.82	0	2,2,2	0.60	0
2	EDO	A	624	-	3,3,3	0.78	0	2,2,2	0.49	0
5	ACT	A	638	-	3,3,3	0.91	0	3,3,3	1.86	2 (66%)
5	ACT	A	636	-	3,3,3	0.51	0	3,3,3	0.47	0
2	EDO	A	614[B]	6	3,3,3	1.11	0	2,2,2	0.18	0
2	EDO	A	622[A]	-	3,3,3	0.29	0	2,2,2	1.36	0
2	EDO	A	611	-	3,3,3	0.74	0	2,2,2	0.75	0
2	EDO	A	606	-	3,3,3	0.57	0	2,2,2	0.81	0
2	EDO	A	603	-	3,3,3	1.17	0	2,2,2	0.58	0
3	GOL	A	630	-	5,5,5	0.25	0	5,5,5	0.89	0
2	EDO	A	615[A]	-	3,3,3	0.58	0	2,2,2	0.86	0
3	GOL	A	631	-	5,5,5	1.93	1 (20%)	5,5,5	2.92	2 (40%)
5	ACT	A	642	-	3,3,3	1.13	0	3,3,3	2.89	2 (66%)
2	EDO	A	616[A]	-	3,3,3	0.92	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
2	EDO	A	601	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	617	-	-	1/1/1/1	-
3	GOL	A	629	-	-	2/4/4/4	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	A	608	-	-	0/1/1/1	-
2	EDO	A	619	-	-	1/1/1/1	-
4	MLI	A	633	-	-	2/4/4/4	-
2	EDO	A	612[B]	-	-	1/1/1/1	-
3	GOL	A	627[B]	-	-	1/4/4/4	-
2	EDO	A	625	-	-	1/1/1/1	-
2	EDO	A	605	-	-	0/1/1/1	-
2	EDO	A	622[B]	-	-	0/1/1/1	-
2	EDO	A	610	-	-	0/1/1/1	-
2	EDO	A	614[A]	6	-	0/1/1/1	-
3	GOL	A	632	-	-	3/4/4/4	-
2	EDO	A	615[B]	-	-	0/1/1/1	-
3	GOL	A	628	-	-	2/4/4/4	-
4	MLI	A	635	-	-	4/4/4/4	-
2	EDO	A	616[B]	-	-	1/1/1/1	-
2	EDO	A	613	-	-	1/1/1/1	-
2	EDO	A	620	-	-	1/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	A	621	-	-	1/1/1/1	-
2	EDO	A	609	-	-	0/1/1/1	-
3	GOL	A	626	-	-	0/4/4/4	-
4	MLI	A	634	-	-	2/4/4/4	-
2	EDO	A	623	-	-	1/1/1/1	-
2	EDO	A	612[A]	-	-	0/1/1/1	-
3	GOL	A	627[A]	-	-	2/4/4/4	-
2	EDO	A	607	-	-	0/1/1/1	-
2	EDO	A	618	-	-	0/1/1/1	-
2	EDO	A	624	-	-	1/1/1/1	-
2	EDO	A	614[B]	6	-	1/1/1/1	-
2	EDO	A	622[A]	-	-	1/1/1/1	-
2	EDO	A	611	-	-	1/1/1/1	-
2	EDO	A	606	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
3	GOL	A	630	-	-	2/4/4/4	-
2	EDO	A	615[A]	-	-	1/1/1/1	-
3	GOL	A	631	-	-	4/4/4/4	-
2	EDO	A	616[A]	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	633	MLI	O9-C3	4.18	1.44	1.30
4	A	634	MLI	C1-C3	-3.82	1.45	1.51
4	A	633	MLI	O6-C2	3.54	1.33	1.22
4	A	633	MLI	O8-C3	3.28	1.32	1.22
4	A	634	MLI	O9-C3	-3.08	1.20	1.30
3	A	631	GOL	O2-C2	-3.06	1.34	1.43
2	A	621	EDO	O1-C1	2.90	1.56	1.42
4	A	634	MLI	O8-C3	-2.82	1.12	1.22
4	A	633	MLI	C1-C2	-2.69	1.46	1.51
3	A	629	GOL	C3-C2	2.53	1.61	1.51
4	A	635	MLI	O9-C3	-2.33	1.23	1.30
4	A	635	MLI	O7-C2	-2.32	1.23	1.30
4	A	633	MLI	C1-C3	-2.28	1.47	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	631	GOL	O2-C2-C1	-5.52	86.33	109.18
4	A	633	MLI	O9-C3-O8	4.46	134.80	123.33
5	A	642	ACT	OXT-C-O	4.10	137.25	122.03
4	A	633	MLI	O7-C2-O6	4.04	133.71	123.33
3	A	629	GOL	C3-C2-C1	3.92	126.18	111.80
4	A	633	MLI	O9-C3-C1	-3.67	103.14	114.51
3	A	627[A]	GOL	O2-C2-C1	-3.46	94.85	109.18
3	A	626	GOL	O1-C1-C2	-3.09	96.47	110.38
2	A	605	EDO	O1-C1-C2	-2.95	89.92	112.39
5	A	640	ACT	OXT-C-CH3	2.93	127.35	115.05
5	A	640	ACT	OXT-C-O	-2.93	111.16	122.03
3	A	631	GOL	C3-C2-C1	2.79	122.04	111.80
3	A	627[A]	GOL	O2-C2-C3	2.73	120.47	109.18
5	A	642	ACT	O-C-CH3	-2.67	111.57	122.53
4	A	634	MLI	C3-C1-C2	-2.54	103.99	112.95
3	A	626	GOL	C3-C2-C1	-2.47	102.75	111.80
3	A	629	GOL	O2-C2-C1	-2.46	98.98	109.18
5	A	638	ACT	OXT-C-CH3	2.36	124.96	115.05
3	A	627[B]	GOL	C3-C2-C1	2.34	120.37	111.80
3	A	628	GOL	C3-C2-C1	-2.28	103.43	111.80
3	A	628	GOL	O2-C2-C3	2.20	118.30	109.18
5	A	638	ACT	O-C-CH3	-2.19	113.53	122.53
4	A	633	MLI	O7-C2-C1	-2.17	107.77	114.51
3	A	632	GOL	C3-C2-C1	-2.15	103.92	111.80

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	627[A]	GOL	C1-C2-C3-O3
3	A	628	GOL	C1-C2-C3-O3
3	A	630	GOL	C1-C2-C3-O3
3	A	631	GOL	O1-C1-C2-C3
3	A	631	GOL	C1-C2-C3-O3
3	A	632	GOL	C1-C2-C3-O3
3	A	627[A]	GOL	O2-C2-C3-O3
3	A	629	GOL	O1-C1-C2-O2
3	A	631	GOL	O1-C1-C2-O2
3	A	631	GOL	O2-C2-C3-O3
3	A	629	GOL	O1-C1-C2-C3
3	A	628	GOL	O2-C2-C3-O3
3	A	630	GOL	O2-C2-C3-O3
3	A	632	GOL	O2-C2-C3-O3
2	A	617	EDO	O1-C1-C2-O2
2	A	622[A]	EDO	O1-C1-C2-O2
4	A	635	MLI	C2-C1-C3-O9
2	A	615[A]	EDO	O1-C1-C2-O2
2	A	616[B]	EDO	O1-C1-C2-O2
2	A	621	EDO	O1-C1-C2-O2
2	A	625	EDO	O1-C1-C2-O2
4	A	633	MLI	C2-C1-C3-O9
4	A	635	MLI	C3-C1-C2-O7
4	A	635	MLI	C2-C1-C3-O8
4	A	634	MLI	C3-C1-C2-O6
2	A	616[A]	EDO	O1-C1-C2-O2
2	A	619	EDO	O1-C1-C2-O2
2	A	620	EDO	O1-C1-C2-O2
2	A	624	EDO	O1-C1-C2-O2
4	A	633	MLI	C2-C1-C3-O8
2	A	623	EDO	O1-C1-C2-O2
3	A	627[B]	GOL	O2-C2-C3-O3
2	A	611	EDO	O1-C1-C2-O2
2	A	613	EDO	O1-C1-C2-O2
2	A	614[B]	EDO	O1-C1-C2-O2
3	A	632	GOL	O1-C1-C2-C3
4	A	634	MLI	C3-C1-C2-O7
2	A	601	EDO	O1-C1-C2-O2
2	A	612[B]	EDO	O1-C1-C2-O2
4	A	635	MLI	C3-C1-C2-O6

There are no ring outliers.

14 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	629	GOL	4	0
3	A	627[B]	GOL	4	0
2	A	622[B]	EDO	1	0
4	A	635	MLI	1	0
2	A	616[B]	EDO	1	0
2	A	621	EDO	3	0
2	A	609	EDO	1	0
4	A	634	MLI	1	0
2	A	623	EDO	1	0
2	A	607	EDO	10	0
2	A	615[A]	EDO	2	0
3	A	631	GOL	2	0
5	A	642	ACT	5	0
2	A	616[A]	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, 95th 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 ²)	Q<0.9
1	A	350/555 (63%)	-0.85	1 (0%) 90 91	5, 14, 29, 68	22 (6%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	THR	3.8

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	EDO	A	625	4/4	0.58	0.26	22,26,29,37	4
5	ACT	A	640	4/4	0.69	0.22	30,34,38,42	4
5	ACT	A	639	4/4	0.70	0.25	35,47,47,51	4
2	EDO	A	624	4/4	0.71	0.27	26,26,29,30	4
5	ACT	A	638	4/4	0.71	0.26	27,29,34,34	4
5	ACT	A	637	4/4	0.73	0.23	45,46,47,49	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	629	6/6	0.75	0.23	23,28,31,34	6
2	EDO	A	615[B]	4/4	0.76	0.17	27,28,29,31	4
2	EDO	A	615[A]	4/4	0.76	0.17	36,37,41,54	4
4	MLI	A	635	7/7	0.78	0.21	30,35,41,54	7
2	EDO	A	618	4/4	0.80	0.17	39,46,47,48	4
3	GOL	A	630	6/6	0.82	0.19	41,44,46,50	6
2	EDO	A	622[B]	4/4	0.84	0.16	19,23,26,34	4
2	EDO	A	622[A]	4/4	0.84	0.16	35,36,36,37	4
5	ACT	A	641	4/4	0.84	0.20	40,41,42,44	4
3	GOL	A	632	6/6	0.86	0.16	23,34,35,43	6
2	EDO	A	620	4/4	0.87	0.17	40,54,58,59	0
2	EDO	A	617	4/4	0.87	0.16	19,21,23,24	4
2	EDO	A	613	4/4	0.88	0.13	45,45,46,54	0
2	EDO	A	619	4/4	0.88	0.17	24,39,41,41	4
3	GOL	A	631	6/6	0.89	0.17	17,27,29,31	6
2	EDO	A	606	4/4	0.90	0.12	36,38,45,54	0
3	GOL	A	628	6/6	0.90	0.14	15,24,25,27	6
3	GOL	A	626	6/6	0.91	0.14	19,22,22,23	6
2	EDO	A	605	4/4	0.91	0.12	21,30,37,70	0
4	MLI	A	634	7/7	0.91	0.13	23,35,49,52	7
2	EDO	A	623	4/4	0.92	0.11	18,18,19,20	4
2	EDO	A	621	4/4	0.92	0.16	22,23,26,29	4
2	EDO	A	616[A]	4/4	0.92	0.08	22,24,25,27	4
2	EDO	A	616[B]	4/4	0.92	0.08	22,22,22,26	4
3	GOL	A	627[A]	6/6	0.92	0.11	24,34,38,40	6
3	GOL	A	627[B]	6/6	0.92	0.11	35,45,53,53	6
2	EDO	A	609	4/4	0.93	0.12	24,27,27,33	4
5	ACT	A	636	4/4	0.94	0.12	22,25,25,37	4
2	EDO	A	614[B]	4/4	0.94	0.10	29,34,37,37	4
2	EDO	A	612[A]	4/4	0.94	0.11	26,38,41,54	4
2	EDO	A	612[B]	4/4	0.94	0.11	26,34,38,39	4
2	EDO	A	611	4/4	0.94	0.09	24,27,27,28	4
2	EDO	A	614[A]	4/4	0.94	0.10	20,21,24,27	4
5	ACT	A	642	4/4	0.94	0.21	19,20,25,31	4
2	EDO	A	610	4/4	0.95	0.10	23,24,27,31	4
2	EDO	A	608	4/4	0.95	0.09	30,35,38,48	4
4	MLI	A	633	7/7	0.96	0.08	11,20,31,38	7
2	EDO	A	604	4/4	0.96	0.07	17,20,22,24	4
2	EDO	A	607	4/4	0.97	0.06	17,18,19,20	4
2	EDO	A	601	4/4	0.98	0.04	13,14,15,19	4
6	CA	A	644	1/1	0.98	0.09	24,24,24,24	1
2	EDO	A	602	4/4	0.99	0.03	12,13,13,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	603	4/4	0.99	0.04	17,19,27,30	0
6	CA	A	643	1/1	1.00	0.10	17,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.