



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:28 am BST

PDB ID : 5ECU
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

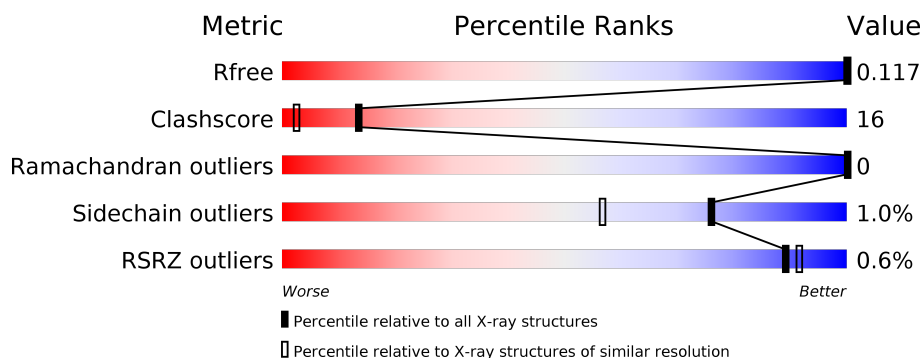
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 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 $\leq 5\%$. 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	<div> <div style="width: 52%; background-color: green;"></div> <div style="width: 9%; background-color: yellow;"></div> <div style="width: 37%; background-color: grey;"></div> </div> <div>52% 9% 37%</div>

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	-
2	EDO	A	609	-	-	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	-	-
5	ACT	A	638	-	-	X	-
5	ACT	A	639	-	-	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 (three-letter code: 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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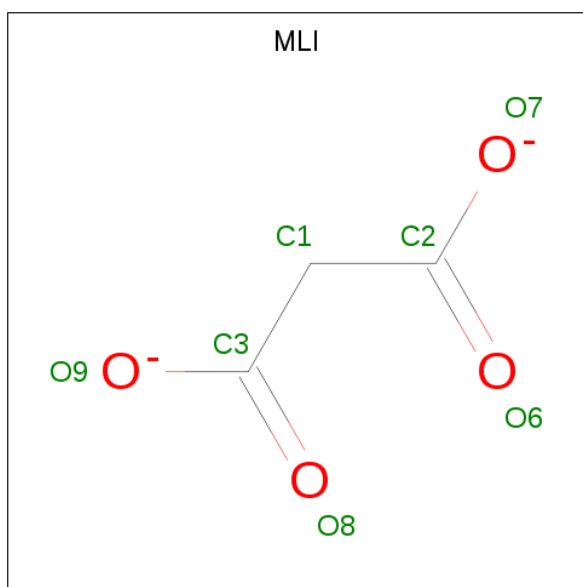
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



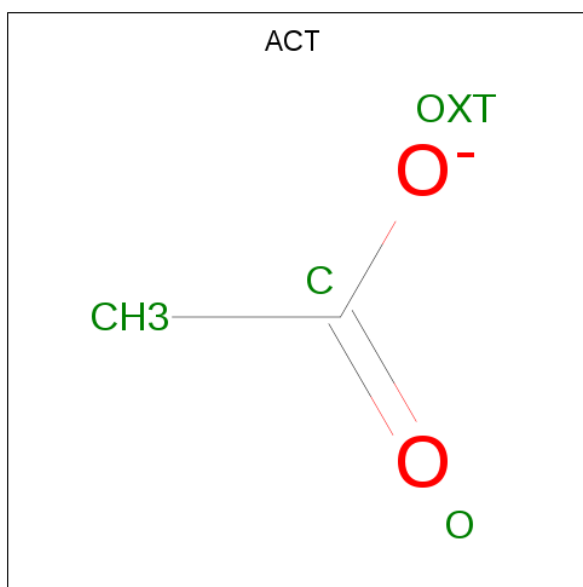
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MALONATE ION (three-letter code: 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 (three-letter code: 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 (three-letter code: CA) (formula: Ca).

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

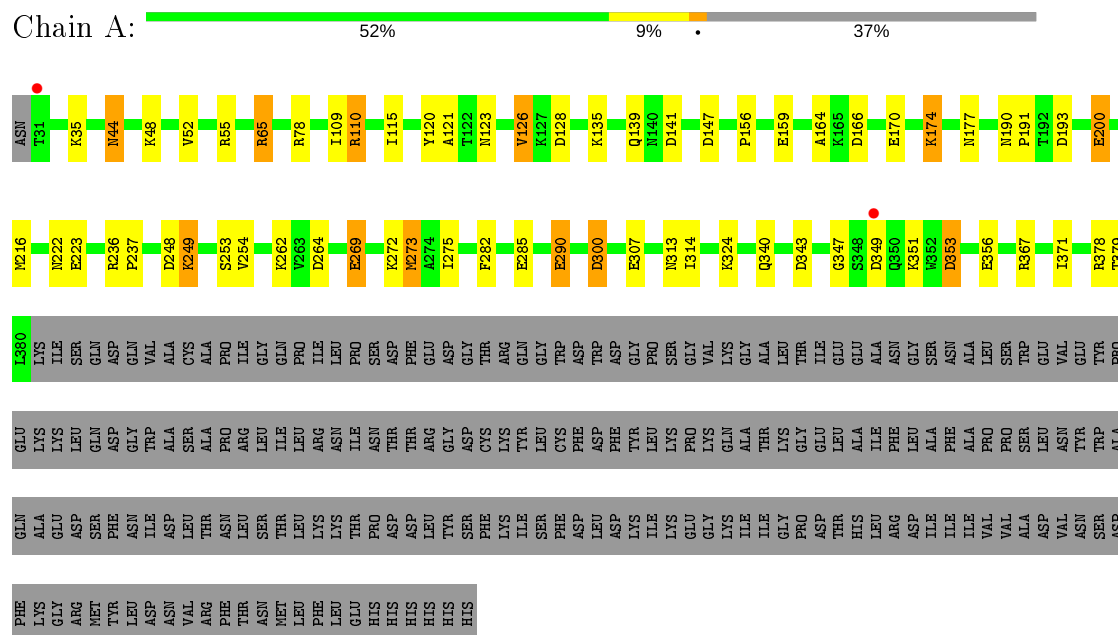
- Molecule 7 is water.

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

3 Residue-property plots [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: 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) 99.9 (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 0.087 , 0.117	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)	0.39 , 57.1	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, MLI, EDO, ACT

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	1.33	18/3022 (0.6%)	1.39	33/4105 (0.8%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	GLU	CD-OE2	-10.78	1.13	1.25
1	A	223	GLU	CD-OE1	9.64	1.36	1.25
1	A	159	GLU	CD-OE2	9.52	1.36	1.25
1	A	200[A]	GLU	CB-CG	8.28	1.67	1.52
1	A	200[B]	GLU	CB-CG	8.28	1.67	1.52
1	A	159	GLU	CD-OE1	8.15	1.34	1.25
1	A	223	GLU	CG-CD	7.03	1.62	1.51
1	A	347	GLY	C-O	6.94	1.34	1.23
1	A	285	GLU	CD-OE2	6.67	1.32	1.25
1	A	200[A]	GLU	CG-CD	6.64	1.61	1.51
1	A	200[B]	GLU	CG-CD	6.64	1.61	1.51
1	A	65	ARG	CZ-NH2	6.54	1.41	1.33
1	A	307	GLU	CD-OE1	6.22	1.32	1.25
1	A	378	ARG	CG-CD	-5.86	1.37	1.51
1	A	44	ASN	CG-OD1	5.57	1.36	1.24
1	A	269[A]	GLU	CD-OE1	5.49	1.31	1.25
1	A	269[B]	GLU	CD-OE1	5.49	1.31	1.25
1	A	139	GLN	CB-CG	-5.39	1.38	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ASP	CB-CG-OD1	15.10	131.89	118.30
1	A	349[A]	ASP	CB-CG-OD2	-12.12	107.39	118.30
1	A	349[B]	ASP	CB-CG-OD2	-12.12	107.39	118.30
1	A	367	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	A	110	ARG	NE-CZ-NH1	-10.13	115.23	120.30
1	A	166[A]	ASP	CB-CG-OD2	-10.12	109.19	118.30
1	A	166[B]	ASP	CB-CG-OD2	-10.12	109.19	118.30
1	A	378	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	A	110	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	A	236	ARG	NE-CZ-NH2	8.68	124.64	120.30
1	A	264	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	55	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	65	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	A	249[A]	LYS	CD-CE-NZ	7.05	127.92	111.70
1	A	249[B]	LYS	CD-CE-NZ	7.05	127.92	111.70
1	A	193[A]	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	193[B]	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	378	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	141	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	248	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	126[A]	VAL	CG1-CB-CG2	6.13	120.71	110.90
1	A	126[B]	VAL	CG1-CB-CG2	6.13	120.71	110.90
1	A	353	ASP	OD1-CG-OD2	-5.99	111.91	123.30
1	A	174	LYS	CD-CE-NZ	-5.67	98.67	111.70
1	A	166[A]	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	166[B]	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	300	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	65	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
1	A	78	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	343	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	128	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	147	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	35	LYS	CB-CG-CD	5.03	124.69	111.60

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	75	1
2	A	120	0	166	29	0
3	A	48	0	56	21	0
4	A	21	0	4	3	0
5	A	28	0	19	12	0
6	A	2	0	0	0	0
7	A	427	0	0	47	0
All	All	3596	0	3087	101	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 16.

All (101) 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)
5:A:638:ACT:H1	5:A:639:ACT:O	1.28	1.33
1:A:109[B]:ILE:HD13	7:A:840:HOH:O	1.32	1.28
1:A:351:LYS:NZ	7:A:722[A]:HOH:O	1.67	1.23
3:A:632:GOL:O1	7:A:721[A]:HOH:O	1.57	1.23
1:A:351:LYS:CE	7:A:722[A]:HOH:O	1.78	1.22
1:A:356[B]:GLU:HG2	3:A:629:GOL:H12	1.27	1.12
3:A:631:GOL:O3	7:A:724:HOH:O	1.70	1.07
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
2:A:609:EDO:C2	7:A:729:HOH:O	2.08	1.00
1:A:351:LYS:HE2	7:A:722[A]:HOH:O	1.47	1.00
1:A:275:ILE:CD1	1:A:314[B]:ILE:HD11	1.92	0.98
5:A:639:ACT:H1	7:A:932:HOH:O	1.63	0.96
1:A:249[B]:LYS:CE	7:A:1029[B]:HOH:O	2.07	0.95
1:A:356[B]:GLU:HG2	3:A:629:GOL:C1	1.97	0.93
1:A:249[B]:LYS:HD2	7:A:1029[B]:HOH:O	1.70	0.92
2:A:609:EDO:H21	7:A:729:HOH:O	1.68	0.89
2:A:609:EDO:O2	7:A:729:HOH:O	1.89	0.89
3:A:632:GOL:O2	7:A:731:HOH:O	1.93	0.86
5:A:639:ACT:CH3	7:A:932:HOH:O	2.18	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356[A]:GLU:HG2	3:A:629:GOL:H12	1.58	0.86
3:A:630:GOL:O3	7:A:732:HOH:O	1.94	0.86
1:A:314[A]:ILE:CD1	2:A:607:EDO:C2	2.54	0.85
1:A:379[B]:THR:OG1	7:A:734:HOH:O	1.95	0.85
1:A:269[A]:GLU:OE1	7:A:733:HOH:O	1.94	0.83
1:A:164:ALA:HB3	3:A:631:GOL:H11	1.60	0.83
1:A:126[B]:VAL:HG23	7:A:944:HOH:O	1.77	0.82
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
2:A:611:EDO:H11	7:A:1077[B]:HOH:O	1.86	0.76
1:A:314[A]:ILE:HD13	2:A:607:EDO:C2	2.18	0.74
1:A:126[B]:VAL:CG2	7:A:944:HOH:O	2.32	0.73
1:A:314[A]:ILE:HD13	2:A:607:EDO:H21	1.71	0.73
5:A:638:ACT:CH3	5:A:639:ACT:O	2.22	0.73
2:A:625:EDO:C1	7:A:809:HOH:O	2.37	0.73
1:A:249[B]:LYS:CD	7:A:1029[B]:HOH:O	2.19	0.73
2:A:625:EDO:O2	7:A:702:HOH:O	0.72	0.71
1:A:314[A]:ILE:HD12	2:A:607:EDO:H22	1.71	0.70
1:A:313[A]:ASN:HD21	5:A:638:ACT:C	2.08	0.67
1:A:120:TYR:HD2	5:A:642:ACT:H2	1.60	0.65
2:A:618:EDO:O2	7:A:734:HOH:O	2.15	0.65
3:A:627[B]:GOL:O2	7:A:735:HOH:O	2.13	0.65
1:A:275:ILE:HD11	1:A:314[B]:ILE:HD11	1.79	0.64
1:A:273[B]:MET:HE2	3:A:627[B]:GOL:H31	1.79	0.64
2:A:625:EDO:C2	7:A:809:HOH:O	2.44	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
2:A:614[B]:EDO:C2	7:A:738:HOH:O	2.48	0.60
1:A:109[B]:ILE:CD1	7:A:840:HOH:O	2.12	0.60
4:A:634:MLI:O9	4:A:634:MLI:O7	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:249[B]:LYS:HD2	7:A:1008:HOH:O	2.05	0.56
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
2:A:615[A]:EDO:C2	7:A:793[A]:HOH:O	2.53	0.55
1:A:121:ALA:HB2	5:A:642:ACT:H3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356[B]:GLU:CG	3:A:629:GOL:H12	2.18	0.55
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:324[B]:LYS:HE2	3:A:626:GOL:O2	2.09	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
5:A:638:ACT:CH3	7:A:763:HOH:O	0.79	0.48
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:126[B]:VAL:HG21	7:A:944:HOH:O	2.09	0.44
1:A:200[A]:GLU:CD	1:A:200[A]:GLU:H	2.21	0.44
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
5:A:638:ACT:H3	7:A:763:HOH:O	0.77	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
1:A:126[B]:VAL:HG23	7:A:1061:HOH:O	2.20	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:313[B]:ASN:CG	7:A:822:HOH:O	2.59	0.41
1:A:253:SER:HA	1:A:282:PHE:O	2.20	0.41
1:A:356[B]:GLU:HG2	3:A:629:GOL:H11	1.97	0.41
4:A:633:MLI:O8	7:A:782:HOH:O	0.41	0.41
1:A:273[B]:MET:HE3	3:A:627[B]:GOL:O1	2.20	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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%)	313 (99%)	4 (1%)	69	44

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	273[A]	MET
1	A	273[B]	MET
1	A	353	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) 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	222	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
3	GOL	A	626	-	5,5,5	0.73	0	5,5,5	1.68	2 (40%)
2	EDO	A	618	-	3,3,3	0.84	0	2,2,2	0.70	0
3	GOL	A	631	-	5,5,5	1.88	1 (20%)	5,5,5	2.75	2 (40%)
5	ACT	A	641	-	1,3,3	1.18	0	0,3,3	0.00	-
5	ACT	A	639	-	1,3,3	2.29	1 (100%)	0,3,3	0.00	-
2	EDO	A	607	-	3,3,3	0.37	0	2,2,2	0.90	0
2	EDO	A	604	-	3,3,3	0.47	0	2,2,2	0.06	0
4	MLI	A	633	-	0,6,6	0.00	-	0,7,7	0.00	-
2	EDO	A	605	-	3,3,3	0.79	0	2,2,2	2.19	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	640	-	1,3,3	3.20	1 (100%)	0,3,3	0.00	-
2	EDO	A	601	-	3,3,3	0.77	0	2,2,2	0.58	0
2	EDO	A	624	-	3,3,3	0.82	0	2,2,2	0.58	0
3	GOL	A	632	-	5,5,5	0.61	0	5,5,5	1.31	1 (20%)
3	GOL	A	629	-	5,5,5	1.13	1 (20%)	5,5,5	2.00	2 (40%)
5	ACT	A	642	-	1,3,3	4.67	1 (100%)	0,3,3	0.00	-
2	EDO	A	616[A]	-	3,3,3	0.99	0	2,2,2	0.65	0
2	EDO	A	617	-	3,3,3	0.59	0	2,2,2	0.81	0
2	EDO	A	620	-	3,3,3	0.54	0	2,2,2	1.57	0
2	EDO	A	616[B]	-	3,3,3	0.57	0	2,2,2	0.24	0
2	EDO	A	615[B]	-	3,3,3	0.43	0	2,2,2	0.33	0
3	GOL	A	630	-	5,5,5	0.25	0	5,5,5	0.85	0
2	EDO	A	619	-	3,3,3	0.49	0	2,2,2	0.60	0
2	EDO	A	615[A]	-	3,3,3	0.60	0	2,2,2	0.85	0
2	EDO	A	610	-	3,3,3	0.52	0	2,2,2	0.73	0
5	ACT	A	638	-	1,3,3	1.84	0	0,3,3	0.00	-
2	EDO	A	622[A]	-	3,3,3	0.29	0	2,2,2	1.41	0
2	EDO	A	623	-	3,3,3	1.22	0	2,2,2	0.57	0
2	EDO	A	622[B]	-	3,3,3	0.66	0	2,2,2	0.34	0
4	MLI	A	634	-	0,6,6	0.00	-	0,7,7	0.00	-
2	EDO	A	611	-	3,3,3	0.78	0	2,2,2	0.80	0
4	MLI	A	635	-	0,6,6	0.00	-	0,7,7	0.00	-
3	GOL	A	628	-	5,5,5	1.11	0	5,5,5	1.62	2 (40%)
2	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.47	0
3	GOL	A	627[A]	-	5,5,5	0.77	0	5,5,5	1.97	2 (40%)
2	EDO	A	625	-	3,3,3	0.80	0	2,2,2	1.25	0
2	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.23	0
2	EDO	A	608	-	3,3,3	0.94	0	2,2,2	0.79	0
2	EDO	A	603	-	3,3,3	1.16	0	2,2,2	0.67	0
2	EDO	A	612[A]	-	3,3,3	0.20	0	2,2,2	0.17	0
2	EDO	A	609	-	3,3,3	1.23	0	2,2,2	0.45	0
2	EDO	A	614[B]	6	3,3,3	1.16	0	2,2,2	0.23	0
3	GOL	A	627[B]	-	5,5,5	0.86	0	5,5,5	1.29	1 (20%)
2	EDO	A	614[A]	6	3,3,3	0.97	0	2,2,2	0.83	0
2	EDO	A	612[B]	-	3,3,3	0.63	0	2,2,2	0.43	0
5	ACT	A	637	-	1,3,3	1.64	0	0,3,3	0.00	-
2	EDO	A	606	-	3,3,3	0.56	0	2,2,2	0.80	0
2	EDO	A	621	-	3,3,3	1.77	1 (33%)	2,2,2	0.78	0
5	ACT	A	636	-	1,3,3	0.45	0	0,3,3	0.00	-

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
3	GOL	A	626	-	-	0/4/4/4	-
2	EDO	A	618	-	-	0/1/1/1	-
3	GOL	A	631	-	-	4/4/4/4	-
2	EDO	A	621	-	-	1/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-
4	MLI	A	633	-	-	0/0/4/4	-
2	EDO	A	605	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
3	GOL	A	632	-	-	3/4/4/4	-
3	GOL	A	629	-	-	2/4/4/4	-
2	EDO	A	616[A]	-	-	1/1/1/1	-
2	EDO	A	617	-	-	1/1/1/1	-
2	EDO	A	620	-	-	1/1/1/1	-
2	EDO	A	616[B]	-	-	1/1/1/1	-
2	EDO	A	615[B]	-	-	0/1/1/1	-
3	GOL	A	630	-	-	2/4/4/4	-
2	EDO	A	619	-	-	1/1/1/1	-
2	EDO	A	615[A]	-	-	1/1/1/1	-
2	EDO	A	610	-	-	0/1/1/1	-
2	EDO	A	622[A]	-	-	1/1/1/1	-
2	EDO	A	607	-	-	0/1/1/1	-
2	EDO	A	623	-	-	1/1/1/1	-
2	EDO	A	622[B]	-	-	0/1/1/1	-
4	MLI	A	634	-	-	0/0/4/4	-
2	EDO	A	611	-	-	1/1/1/1	-
4	MLI	A	635	-	-	0/0/4/4	-
3	GOL	A	628	-	-	2/4/4/4	-
2	EDO	A	624	-	-	1/1/1/1	-
3	GOL	A	627[A]	-	-	2/4/4/4	-
2	EDO	A	625	-	-	1/1/1/1	-
2	EDO	A	613	-	-	1/1/1/1	-
2	EDO	A	608	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	A	612[A]	-	-	0/1/1/1	-
2	EDO	A	609	-	-	0/1/1/1	-
2	EDO	A	614[B]	6	-	1/1/1/1	-
3	GOL	A	627[B]	-	-	1/4/4/4	-
2	EDO	A	614[A]	6	-	0/1/1/1	-
2	EDO	A	612[B]	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	606	-	-	0/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	642	ACT	CH3-C	-4.67	1.42	1.48
5	A	640	ACT	CH3-C	3.20	1.52	1.48
3	A	631	GOL	O2-C2	-2.99	1.34	1.43
2	A	621	EDO	O1-C1	2.87	1.56	1.42
3	A	629	GOL	C3-C2	2.36	1.61	1.51
5	A	639	ACT	CH3-C	2.29	1.51	1.48

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	631	GOL	O2-C2-C1	-5.17	86.33	109.12
3	A	629	GOL	C3-C2-C1	3.72	126.18	111.70
3	A	627[A]	GOL	O2-C2-C1	-3.24	94.85	109.12
2	A	605	EDO	O1-C1-C2	-3.06	89.92	111.91
3	A	626	GOL	O1-C1-C2	-2.86	96.47	110.20
3	A	631	GOL	C3-C2-C1	2.66	122.04	111.70
3	A	627[A]	GOL	O2-C2-C3	2.58	120.47	109.12
3	A	626	GOL	C3-C2-C1	-2.30	102.75	111.70
3	A	629	GOL	O2-C2-C1	-2.30	98.98	109.12
3	A	627[B]	GOL	C3-C2-C1	2.23	120.37	111.70
3	A	628	GOL	C3-C2-C1	-2.13	103.43	111.70
3	A	628	GOL	O2-C2-C3	2.08	118.30	109.12
3	A	632	GOL	C3-C2-C1	-2.00	103.92	111.70

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	630	GOL	C1-C2-C3-O3
3	A	628	GOL	C1-C2-C3-O3
3	A	627[A]	GOL	C1-C2-C3-O3
3	A	631	GOL	O1-C1-C2-O2

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

There are no ring outliers.

24 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	626	GOL	1	0
2	A	618	EDO	1	0
3	A	631	GOL	3	0
5	A	639	ACT	4	0
2	A	607	EDO	10	0
4	A	633	MLI	1	0
3	A	632	GOL	2	0
3	A	629	GOL	9	0
5	A	642	ACT	5	0
2	A	616[A]	EDO	1	0
2	A	616[B]	EDO	1	0
3	A	630	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	615[A]	EDO	2	0
5	A	638	ACT	5	0
2	A	623	EDO	1	0
2	A	622[B]	EDO	1	0
4	A	634	MLI	1	0
2	A	611	EDO	1	0
4	A	635	MLI	1	0
2	A	625	EDO	3	0
2	A	609	EDO	4	0
2	A	614[B]	EDO	1	0
3	A	627[B]	GOL	5	0
2	A	621	EDO	3	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%)	-0.65	2 (0%) 89 91	9, 14, 30, 68	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	THR	6.5
1	A	349[A]	ASP	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. 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	0.66	0.21	22,26,29,37	4
5	ACT	A	640	4/4	0.72	0.17	30,34,38,42	4
3	GOL	A	630	6/6	0.77	0.19	41,44,46,50	6
4	MLI	A	635	7/7	0.80	0.33	30,35,41,54	7
2	EDO	A	622[B]	4/4	0.81	0.20	19,23,26,34	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	639	4/4	0.81	0.14	35,47,47,51	4
2	EDO	A	622[A]	4/4	0.81	0.20	35,36,36,37	4
2	EDO	A	618	4/4	0.82	0.12	39,46,47,48	4
3	GOL	A	627[A]	6/6	0.84	0.22	24,34,38,40	6
3	GOL	A	627[B]	6/6	0.84	0.22	35,45,53,53	6
5	ACT	A	637	4/4	0.84	0.22	45,46,47,49	4
5	ACT	A	641	4/4	0.85	0.14	40,41,42,44	4
3	GOL	A	629	6/6	0.86	0.27	23,28,31,34	6
4	MLI	A	634	7/7	0.89	0.19	23,35,49,52	7
2	EDO	A	613	4/4	0.91	0.11	45,45,46,54	0
2	EDO	A	606	4/4	0.91	0.11	36,38,45,54	0
2	EDO	A	620	4/4	0.92	0.12	40,54,58,59	0
2	EDO	A	619	4/4	0.92	0.15	24,39,41,41	4
2	EDO	A	624	4/4	0.93	0.15	26,26,29,30	4
2	EDO	A	614[A]	4/4	0.93	0.15	20,21,24,27	4
5	ACT	A	638	4/4	0.93	0.11	27,29,34,34	4
2	EDO	A	614[B]	4/4	0.93	0.15	29,34,37,37	4
2	EDO	A	612[A]	4/4	0.94	0.19	26,38,41,54	4
2	EDO	A	605	4/4	0.94	0.08	21,30,37,70	0
2	EDO	A	615[B]	4/4	0.94	0.22	27,28,29,31	4
3	GOL	A	631	6/6	0.94	0.16	17,27,29,31	6
2	EDO	A	612[B]	4/4	0.94	0.19	26,34,38,39	4
3	GOL	A	632	6/6	0.94	0.17	23,34,35,43	6
2	EDO	A	615[A]	4/4	0.94	0.22	36,37,41,54	4
2	EDO	A	617	4/4	0.95	0.14	19,21,23,24	4
2	EDO	A	608	4/4	0.95	0.07	30,35,38,48	4
2	EDO	A	611	4/4	0.95	0.18	24,27,27,28	4
3	GOL	A	628	6/6	0.96	0.14	15,24,25,27	6
2	EDO	A	609	4/4	0.96	0.10	24,27,27,33	4
2	EDO	A	610	4/4	0.96	0.11	23,24,27,31	4
2	EDO	A	604	4/4	0.96	0.14	17,20,22,24	4
5	ACT	A	636	4/4	0.96	0.10	22,25,25,37	4
2	EDO	A	616[A]	4/4	0.97	0.13	22,24,25,27	4
2	EDO	A	621	4/4	0.97	0.26	22,23,26,29	4
2	EDO	A	616[B]	4/4	0.97	0.13	22,22,22,26	4
2	EDO	A	603	4/4	0.98	0.06	17,19,27,30	0
2	EDO	A	601	4/4	0.98	0.05	13,14,15,19	4
2	EDO	A	623	4/4	0.98	0.13	18,18,19,20	4
5	ACT	A	642	4/4	0.98	0.12	19,20,25,31	4
3	GOL	A	626	6/6	0.98	0.07	19,22,22,23	6
6	CA	A	644	1/1	0.99	0.14	24,24,24,24	1
4	MLI	A	633	7/7	0.99	0.07	11,20,31,38	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	A	643	1/1	0.99	0.09	17,17,17,17	1
2	EDO	A	602	4/4	0.99	0.07	12,13,13,14	0
2	EDO	A	607	4/4	0.99	0.11	17,18,19,20	4

6.5 Other polymers [i](#)

There are no such residues in this entry.