



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:14 AM BST

PDB ID : 1H41  
Title : Pseudomonas cellulosa E292A alpha-D-glucuronidase mutant complexed with  
aldotriuronic acid  
Authors : Nurizzo, D.; Nagy, T.; Gilbert, H.J.; Davies, G.J.  
Deposited on : 2002-09-25  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

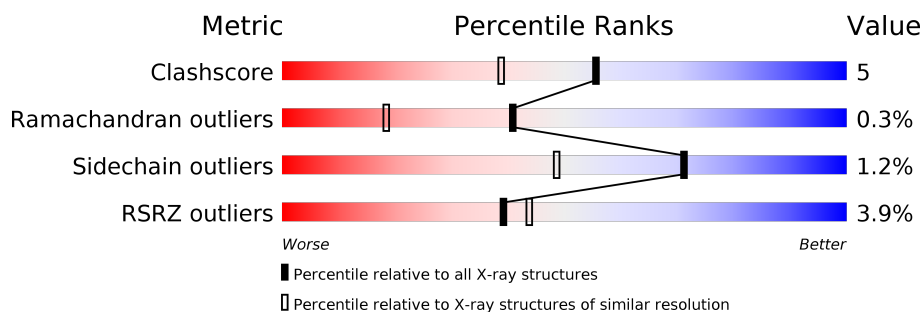
# 1 Overall quality at a glance

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))
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  $\geq 3$ , 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	708	
1	B	708	

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
3	EDO	A	1727	-	X	X	-
3	EDO	B	1722	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13218 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.

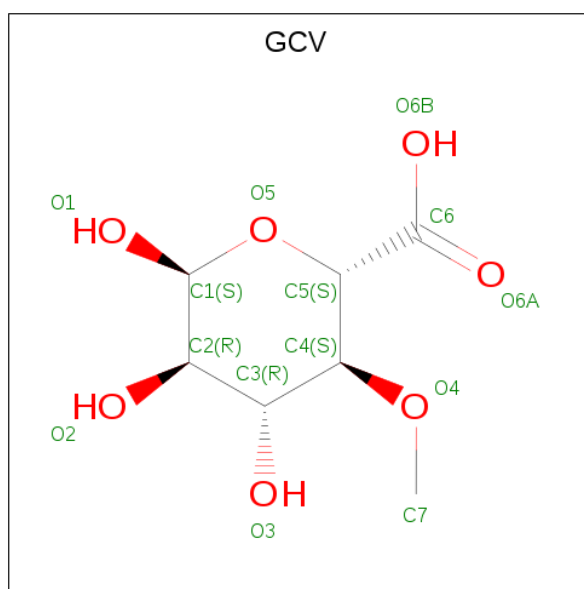
- Molecule 1 is a protein called ALPHA-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	700	Total	C	N	O	S	0	26	0
			5695	3635	1011	1030	19			
1	B	701	Total	C	N	O	S	0	24	0
			5694	3629	1010	1036	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ALA	GLU	engineered mutation	UNP Q8VP74
B	292	ALA	GLU	engineered mutation	UNP Q8VP74

- Molecule 2 is 4-O-methyl-alpha-D-glucopyranuronic acid (three-letter code: GCV) (formula: C<sub>7</sub>H<sub>12</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	7	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			14	7	7		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total Co 5 5	0	0

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

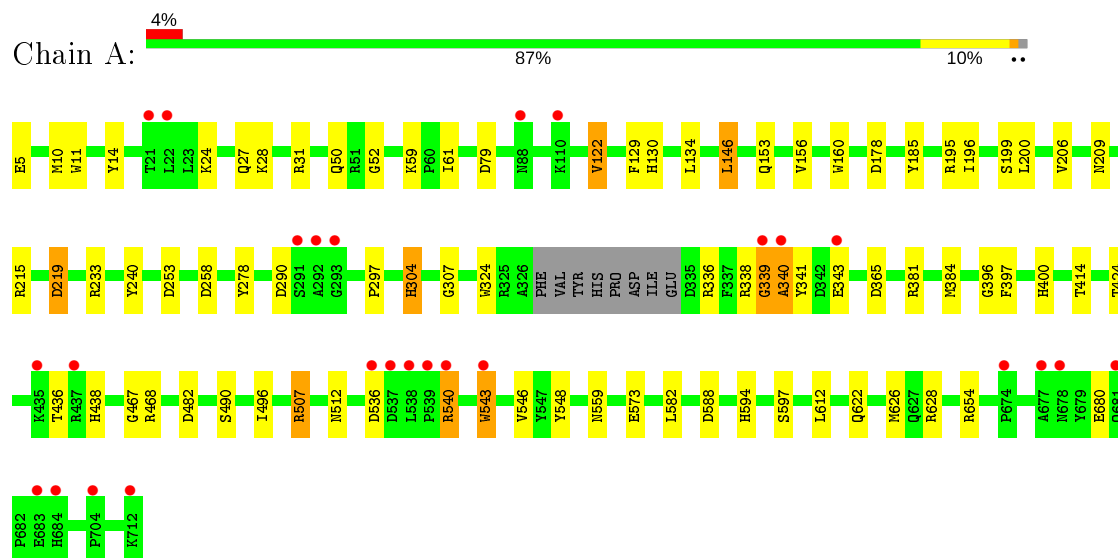
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	824	Total 824	O 824	0	0
5	B	843	Total 843	O 843	0	0

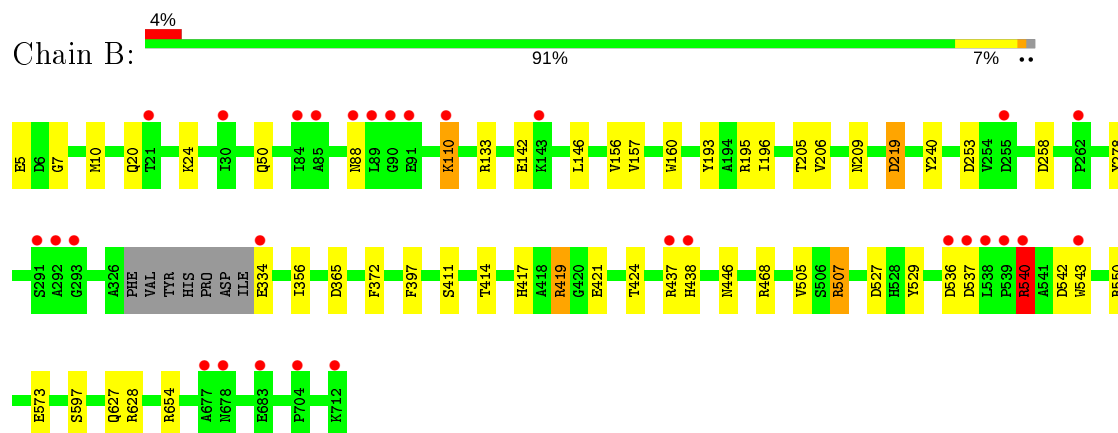
### 3 Residue-property plots [i](#)

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: ALPHA-GLUCURONIDASE



#### • Molecule 1: ALPHA-GLUCURONIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.41Å 74.39Å 87.46Å 115.09° 93.04° 109.44°	Depositor
Resolution (Å)	20.00 – 1.50 19.74 – 1.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (20.00-1.50) 91.2 (19.74-1.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, $R_{free}$	0.118 , 0.153 0.152 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.5	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.78	6/5987 (0.1%)	0.90	17/8133 (0.2%)
1	B	0.78	5/5977 (0.1%)	0.91	23/8120 (0.3%)
All	All	0.78	11/11964 (0.1%)	0.90	40/16253 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	TRP	NE1-CE2	8.76	1.49	1.37
1	B	156[A]	VAL	CB-CG2	-6.19	1.39	1.52
1	B	156[B]	VAL	CB-CG2	-6.19	1.39	1.52
1	B	142	GLU	CD-OE1	5.94	1.32	1.25
1	A	597[A]	SER	CB-OG	-5.93	1.34	1.42
1	A	597[B]	SER	CB-OG	-5.93	1.34	1.42
1	B	505	VAL	CB-CG1	-5.62	1.41	1.52
1	A	156[A]	VAL	CB-CG2	-5.39	1.41	1.52
1	A	156[B]	VAL	CB-CG2	-5.39	1.41	1.52
1	A	626	MET	SD-CE	-5.26	1.48	1.77
1	B	529	TYR	CD2-CE2	-5.17	1.31	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419[A]	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	B	419[B]	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	B	628	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	626	MET	CG-SD-CE	-7.50	88.21	100.20
1	A	628	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	628	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	381	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	628	ARG	NE-CZ-NH2	-6.76	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536[A]	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	536[B]	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	468	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	233	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	253	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	540	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	537	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	79	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	527	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	258	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	215	ARG	O-C-N	-5.68	113.61	122.70
1	B	542	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	178	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	482	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	219[A]	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	219[B]	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	397	PHE	CB-CG-CD1	5.41	124.59	120.80
1	B	133	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	195	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	397	PHE	CB-CG-CD1	5.33	124.53	120.80
1	B	654	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	253	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	258	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	219[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	219[B]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	654	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	7	GLY	O-C-N	-5.08	114.57	122.70
1	A	588	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	654	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	419[A]	ARG	CD-NE-CZ	5.04	130.66	123.60
1	B	419[B]	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	397	PHE	CB-CG-CD2	-5.03	117.28	120.80

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	5695	0	5567	72	0
1	B	5694	0	5548	38	0
2	A	14	0	11	0	0
2	B	14	0	11	0	0
3	A	64	0	95	14	0
3	B	60	0	90	13	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	824	0	0	6	0
5	B	843	0	0	14	0
All	All	13218	0	11322	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (117) 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:573[B]:GLU:OE1	5:B:2639:HOH:O	1.64	1.14
1:B:372:PHE:HB3	3:B:1722:EDO:H11	1.41	1.02
1:B:411[B]:SER:OG	3:B:1722:EDO:H21	1.61	1.01
1:A:573:GLU:OE1	5:A:2633:HOH:O	1.79	1.00
1:A:11:TRP:HZ2	1:A:200[B]:LEU:HD21	1.43	0.84
1:A:11:TRP:CZ2	1:A:200[B]:LEU:HD21	2.12	0.84
1:A:304[B]:HIS:HE1	1:A:343[B]:GLU:HG3	1.44	0.82
1:A:384:MET:H	3:A:1727:EDO:H21	1.43	0.81
1:A:304[A]:HIS:CD2	1:A:324:TRP:HE1	2.01	0.79
3:B:1722:EDO:H22	5:B:2469:HOH:O	1.82	0.78
1:A:10[A]:MET:SD	1:A:196:ILE:HD13	2.24	0.77
1:A:512:ASN:HD22	1:A:622:GLN:HE22	1.33	0.76
1:B:219[B]:ASP:OD1	1:B:278:TYR:OH	2.04	0.74
1:B:540:ARG:HD3	1:B:543:TRP:CE2	2.23	0.74
1:A:540:ARG:HG3	1:A:543:TRP:CD2	2.24	0.72
1:A:304[B]:HIS:HE1	1:A:343[B]:GLU:CG	2.04	0.70
3:B:1727:EDO:H21	5:B:2839:HOH:O	1.92	0.70
1:A:436:THR:OG1	3:A:1727:EDO:H22	1.94	0.68
1:B:372:PHE:CB	3:B:1722:EDO:H11	2.22	0.68
1:A:5:GLU:HA	5:A:2008:HOH:O	1.95	0.67
3:B:1722:EDO:O1	5:B:2829:HOH:O	2.13	0.66
3:B:1727:EDO:H12	5:B:2232:HOH:O	1.95	0.66
1:B:157:VAL:CG2	1:B:205[B]:THR:HG22	2.26	0.66
1:A:28[A]:LYS:HG2	1:A:31:ARG:HH21	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1714:EDO:H22	5:B:2819:HOH:O	1.96	0.65
1:B:334:GLU:HG2	5:B:2435:HOH:O	1.97	0.63
1:B:10[A]:MET:SD	1:B:196:ILE:HD13	2.39	0.63
1:A:536[B]:ASP:OD2	1:A:546[B]:VAL:HG21	2.00	0.62
1:A:384:MET:H	3:A:1727:EDO:C2	2.12	0.61
1:A:540:ARG:HD3	1:A:543:TRP:CZ2	2.35	0.61
1:B:411[B]:SER:OG	3:B:1722:EDO:C2	2.45	0.61
1:A:304[B]:HIS:CE1	1:A:343[B]:GLU:HG3	2.32	0.61
1:A:384:MET:N	3:A:1727:EDO:H21	2.15	0.61
1:A:290:ASP:OD2	1:A:304[A]:HIS:HE1	1.83	0.59
1:A:185:TYR:CD2	3:A:1717[B]:EDO:H22	2.38	0.59
1:A:24[A]:LYS:HD3	1:A:27:GLN:OE1	2.03	0.59
1:B:356:ILE:CD1	1:B:438:HIS:HB3	2.34	0.58
1:A:594:HIS:HA	3:A:1724:EDO:H22	1.86	0.58
1:A:540:ARG:HG3	1:A:543:TRP:CE2	2.39	0.57
1:A:340:ALA:O	1:A:341:TYR:C	2.42	0.57
1:A:28[A]:LYS:HG2	1:A:31:ARG:NH2	2.20	0.56
1:A:546[A]:VAL:HG13	5:A:2605:HOH:O	2.04	0.56
1:A:304[A]:HIS:HD2	1:A:324:TRP:HE1	1.51	0.56
1:B:110[A]:LYS:HD3	5:B:2192:HOH:O	2.06	0.55
1:B:356:ILE:HD11	1:B:438:HIS:HB3	1.87	0.55
1:A:339:GLY:O	1:A:340:ALA:C	2.44	0.55
1:A:340:ALA:HB3	5:A:2439:HOH:O	2.06	0.55
1:B:193:TYR:OH	1:B:205[B]:THR:HG21	2.07	0.55
1:A:146:LEU:C	1:A:146:LEU:HD12	2.28	0.54
1:A:219[B]:ASP:CG	1:A:278:TYR:HH	2.10	0.54
1:B:193:TYR:OH	1:B:205[B]:THR:CG2	2.55	0.54
1:B:540:ARG:HG3	1:B:543:TRP:CG	2.44	0.53
1:A:10[A]:MET:SD	1:A:196:ILE:CD1	2.97	0.52
1:A:219[B]:ASP:CG	1:A:278:TYR:OH	2.48	0.52
1:A:134:LEU:HD23	3:A:1726:EDO:H11	1.91	0.51
1:B:540:ARG:HG3	1:B:543:TRP:CD1	2.46	0.51
1:B:540:ARG:HD3	1:B:543:TRP:CZ2	2.46	0.51
1:A:304[B]:HIS:CE1	1:A:343[B]:GLU:CG	2.92	0.51
1:B:417:HIS:CE1	1:B:421[A]:GLU:OE1	2.65	0.50
1:A:206:VAL:HG22	1:A:240:TYR:HB2	1.94	0.49
1:A:336:ARG:HD3	1:A:548:TYR:OH	2.11	0.49
1:A:438:HIS:O	3:A:1727:EDO:O2	2.31	0.49
1:A:199:SER:OG	1:A:200[B]:LEU:HD22	2.12	0.49
1:A:153[B]:GLN:NE2	1:A:438:HIS:HA	2.28	0.49
1:A:196:ILE:O	1:A:200[B]:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TRP:HA	1:A:209:ASN:HA	1.95	0.48
1:A:297:PRO:HG3	1:A:307:GLY:HA3	1.96	0.47
1:A:219[B]:ASP:OD1	1:A:278:TYR:OH	2.31	0.47
3:B:1714:EDO:C2	5:B:2819:HOH:O	2.60	0.46
1:B:157:VAL:HG23	1:B:205[B]:THR:HG22	1.96	0.46
1:A:559:ASN:CG	3:A:1724:EDO:H21	2.37	0.45
1:B:146:LEU:C	1:B:146:LEU:HD12	2.36	0.45
1:A:185:TYR:CD2	3:A:1717[A]:EDO:H22	2.52	0.45
1:A:507:ARG:C	1:A:507:ARG:HD3	2.37	0.45
1:B:411[B]:SER:HG	3:B:1722:EDO:H21	1.77	0.45
1:A:396:GLY:HA3	1:A:400:HIS:CG	2.52	0.45
1:A:219[B]:ASP:OD2	1:A:278:TYR:OH	2.35	0.45
1:A:195:ARG:HH11	1:A:195:ARG:HD3	1.56	0.44
1:A:130:HIS:CE1	3:A:1715:EDO:H12	2.53	0.44
1:A:490:SER:O	1:A:496[B]:ILE:HD11	2.18	0.44
1:A:129:PHE:CG	1:A:199:SER:HA	2.53	0.43
1:B:507:ARG:HD3	1:B:507:ARG:C	2.38	0.43
1:A:196:ILE:O	1:A:200[B]:LEU:CD2	2.67	0.43
1:A:200[A]:LEU:HD13	1:A:467:GLY:HA3	2.01	0.43
1:A:536[B]:ASP:CG	1:A:546[B]:VAL:HG21	2.38	0.43
1:A:50:GLN:HG3	1:A:61:ILE:O	2.19	0.43
1:A:540:ARG:HG3	1:A:543:TRP:CG	2.54	0.42
1:B:550:ARG:HG2	1:B:550:ARG:NH1	2.33	0.42
1:B:160:TRP:HA	1:B:209:ASN:HA	2.02	0.42
1:A:436:THR:CB	3:A:1727:EDO:H22	2.49	0.42
1:A:196:ILE:HD11	3:A:1716:EDO:H22	2.02	0.42
1:B:196:ILE:HD11	3:B:1718:EDO:C2	2.49	0.42
1:A:338:ARG:HH11	1:A:338:ARG:HD2	1.60	0.42
1:B:20:GLN:O	1:B:24:LYS:HG2	2.19	0.42
1:B:206:VAL:HG22	1:B:240:TYR:HB2	2.02	0.42
1:A:559:ASN:OD1	3:A:1724:EDO:H21	2.20	0.41
1:B:627:GLN:NE2	5:B:2703:HOH:O	2.53	0.41
1:A:612:LEU:HD23	1:A:612:LEU:C	2.41	0.41
1:A:304[A]:HIS:CD2	1:A:324:TRP:NE1	2.81	0.41
1:B:110[A]:LYS:CE	5:B:2192:HOH:O	2.68	0.41
1:B:446:ASN:HA	5:B:2244:HOH:O	2.21	0.41
1:B:110[A]:LYS:CD	5:B:2192:HOH:O	2.68	0.41
1:B:414:THR:O	1:B:424:THR:HA	2.21	0.41
1:B:540:ARG:HD3	1:B:543:TRP:NE1	2.34	0.41
1:B:219[B]:ASP:CG	1:B:278:TYR:OH	2.59	0.41
1:A:14:TYR:CG	1:A:52:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LEU:HA	1:A:582:LEU:HD23	1.93	0.41
1:A:122[B]:VAL:HG11	5:A:2065:HOH:O	2.21	0.40
1:A:468:ARG:HD2	5:A:2296:HOH:O	2.21	0.40
1:A:414:THR:O	1:A:424:THR:HA	2.22	0.40
1:B:24:LYS:HA	1:B:24:LYS:HD3	1.95	0.40
1:B:597[A]:SER:HB2	5:B:2617:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/708 (102%)	703 (97%)	16 (2%)	3 (0%)	34	13
1	B	721/708 (102%)	700 (97%)	20 (3%)	1 (0%)	51	25
All	All	1443/1416 (102%)	1403 (97%)	36 (2%)	4 (0%)	41	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	GLY
1	A	340	ALA
1	B	365	ASP
1	A	365	ASP

### 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	605/587 (103%)	595 (98%)	10 (2%)	60	33
1	B	604/587 (103%)	594 (98%)	10 (2%)	60	33
All	All	1209/1174 (103%)	1189 (98%)	20 (2%)	71	33

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	122[A]	VAL
1	A	122[B]	VAL
1	A	146	LEU
1	A	304[A]	HIS
1	A	304[B]	HIS
1	A	507	ARG
1	A	540	ARG
1	A	680[A]	GLU
1	A	680[B]	GLU
1	B	5	GLU
1	B	88[A]	ASN
1	B	88[B]	ASN
1	B	110[A]	LYS
1	B	110[B]	LYS
1	B	419[A]	ARG
1	B	419[B]	ARG
1	B	437	ARG
1	B	507	ARG
1	B	540	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	294	GLN
1	A	618	GLN
1	A	622	GLN
1	A	627	GLN
1	B	525	GLN
1	B	618	GLN
1	B	627	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 10 are monoatomic - leaving 33 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	EDO	A	1716	-	3,3,3	0.34	0	2,2,2	0.19	0
3	EDO	B	1724	-	3,3,3	0.40	0	2,2,2	0.41	0
3	EDO	A	1724	-	3,3,3	0.29	0	2,2,2	0.86	0
3	EDO	B	1725	-	3,3,3	0.38	0	2,2,2	0.92	0
2	GCV	B	1713	-	11,14,14	0.57	0	14,20,20	0.88	0
3	EDO	A	1721	-	3,3,3	0.29	0	2,2,2	0.73	0
3	EDO	B	1723	-	3,3,3	0.55	0	2,2,2	0.43	0
3	EDO	A	1725	-	3,3,3	0.34	0	2,2,2	0.27	0
3	EDO	B	1727	-	3,3,3	0.35	0	2,2,2	0.16	0
3	EDO	A	1723[A]	-	3,3,3	0.29	0	2,2,2	0.65	0
3	EDO	B	1721	-	3,3,3	0.70	0	2,2,2	0.51	0
3	EDO	A	1723[B]	-	3,3,3	0.29	0	2,2,2	0.72	0
3	EDO	A	1722	-	3,3,3	0.35	0	2,2,2	0.51	0
3	EDO	A	1727	-	3,3,3	1.78	1 (33%)	2,2,2	2.01	1 (50%)
3	EDO	B	1722	-	3,3,3	0.72	0	2,2,2	1.11	0
3	EDO	A	1726	-	3,3,3	0.64	0	2,2,2	0.89	0
3	EDO	B	1720	-	3,3,3	0.24	0	2,2,2	0.82	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	B	1719	-	3,3,3	0.35	0	2,2,2	0.33	0
3	EDO	A	1719	-	3,3,3	0.27	0	2,2,2	0.46	0
3	EDO	A	1717[A]	-	3,3,3	0.40	0	2,2,2	0.15	0
3	EDO	B	1718	-	3,3,3	0.43	0	2,2,2	0.14	0
3	EDO	B	1726[B]	-	3,3,3	0.29	0	2,2,2	0.13	0
3	EDO	A	1717[B]	-	3,3,3	0.41	0	2,2,2	0.18	0
2	GCV	A	1713	-	11,14,14	0.82	0	14,20,20	0.99	1 (7%)
3	EDO	B	1717	-	3,3,3	0.19	0	2,2,2	0.53	0
3	EDO	B	1726[A]	-	3,3,3	0.37	0	2,2,2	0.54	0
3	EDO	A	1715	-	3,3,3	0.38	0	2,2,2	0.78	0
3	EDO	A	1718	-	3,3,3	0.49	0	2,2,2	0.70	0
3	EDO	A	1720	-	3,3,3	0.32	0	2,2,2	0.61	0
3	EDO	B	1715	-	3,3,3	0.49	0	2,2,2	0.35	0
3	EDO	B	1714	-	3,3,3	0.28	0	2,2,2	0.56	0
3	EDO	A	1714	-	3,3,3	0.36	0	2,2,2	0.84	0
3	EDO	B	1716	-	3,3,3	0.37	0	2,2,2	0.44	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
3	EDO	A	1716	-	-	0/1/1/1	-
3	EDO	B	1724	-	-	0/1/1/1	-
3	EDO	A	1724	-	-	0/1/1/1	-
3	EDO	B	1725	-	-	0/1/1/1	-
2	GCV	B	1713	-	-	0/2/26/26	0/1/1/1
3	EDO	A	1721	-	-	0/1/1/1	-
3	EDO	B	1723	-	-	0/1/1/1	-
3	EDO	A	1725	-	-	0/1/1/1	-
3	EDO	B	1727	-	-	1/1/1/1	-
3	EDO	A	1723[A]	-	-	1/1/1/1	-
3	EDO	B	1721	-	-	0/1/1/1	-
3	EDO	A	1723[B]	-	-	0/1/1/1	-
3	EDO	A	1722	-	-	0/1/1/1	-
3	EDO	A	1727	-	-	1/1/1/1	-
3	EDO	B	1722	-	-	0/1/1/1	-
3	EDO	A	1726	-	-	1/1/1/1	-
3	EDO	B	1720	-	-	0/1/1/1	-
3	EDO	B	1719	-	-	0/1/1/1	-
3	EDO	A	1719	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1717[A]	-	-	0/1/1/1	-
3	EDO	B	1718	-	-	0/1/1/1	-
3	EDO	B	1726[B]	-	-	0/1/1/1	-
3	EDO	A	1717[B]	-	-	0/1/1/1	-
2	GCV	A	1713	-	-	0/2/26/26	0/1/1/1
3	EDO	B	1717	-	-	1/1/1/1	-
3	EDO	B	1726[A]	-	-	1/1/1/1	-
3	EDO	A	1715	-	-	0/1/1/1	-
3	EDO	A	1718	-	-	0/1/1/1	-
3	EDO	A	1720	-	-	0/1/1/1	-
3	EDO	B	1715	-	-	0/1/1/1	-
3	EDO	B	1714	-	-	0/1/1/1	-
3	EDO	A	1714	-	-	1/1/1/1	-
3	EDO	B	1716	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1727	EDO	O2-C2	-2.24	1.30	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1727	EDO	O1-C1-C2	-2.32	95.20	111.91
2	A	1713	GCV	C2-C3-C4	2.10	114.47	109.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1727	EDO	O1-C1-C2-O2
3	A	1726	EDO	O1-C1-C2-O2
3	B	1717	EDO	O1-C1-C2-O2
3	B	1726[A]	EDO	O1-C1-C2-O2
3	B	1727	EDO	O1-C1-C2-O2
3	A	1723[A]	EDO	O1-C1-C2-O2
3	A	1714	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1716	EDO	1	0
3	A	1724	EDO	3	0
3	B	1727	EDO	2	0
3	A	1727	EDO	6	0
3	B	1722	EDO	8	0
3	A	1726	EDO	1	0
3	A	1717[A]	EDO	1	0
3	B	1718	EDO	1	0
3	A	1717[B]	EDO	1	0
3	A	1715	EDO	1	0
3	B	1714	EDO	2	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	700/708 (98%)	0.20	26 (3%)	41 46	8, 13, 25, 42	1 (0%)
1	B	701/708 (99%)	0.19	29 (4%)	37 41	7, 12, 25, 39	0
All	All	1401/1416 (98%)	0.20	55 (3%)	39 44	7, 12, 25, 42	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	ALA	6.5
1	B	537	ASP	6.3
1	A	543	TRP	6.2
1	A	537	ASP	6.1
1	B	437	ARG	6.0
1	B	292	ALA	5.6
1	B	543	TRP	5.6
1	A	293	GLY	5.4
1	B	88[A]	ASN	5.0
1	B	539	PRO	4.2
1	A	340	ALA	4.2
1	A	437	ARG	4.1
1	B	540	ARG	4.0
1	A	539	PRO	4.0
1	B	334	GLU	4.0
1	B	538	LEU	3.9
1	A	540	ARG	3.8
1	A	291	SER	3.8
1	B	677	ALA	3.7
1	A	435[A]	LYS	3.7
1	B	291	SER	3.7
1	B	293	GLY	3.6
1	B	89	LEU	3.6
1	B	712	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	538	LEU	3.6
1	B	438	HIS	3.4
1	A	684	HIS	3.3
1	B	683	GLU	3.3
1	A	683	GLU	3.1
1	A	339	GLY	2.9
1	A	712	LYS	2.8
1	B	704	PRO	2.7
1	A	536[A]	ASP	2.7
1	B	91	GLU	2.6
1	A	22[A]	LEU	2.6
1	B	678	ASN	2.6
1	A	704	PRO	2.5
1	B	143	LYS	2.5
1	A	681	GLN	2.4
1	B	536[A]	ASP	2.4
1	B	110[A]	LYS	2.4
1	A	110	LYS	2.4
1	A	674	PRO	2.3
1	B	30[A]	ILE	2.3
1	B	255	ASP	2.3
1	B	21	THR	2.2
1	A	21	THR	2.2
1	B	262	PRO	2.2
1	B	84	ILE	2.2
1	A	343[A]	GLU	2.1
1	A	678	ASN	2.1
1	B	90	GLY	2.0
1	A	88	ASN	2.0
1	A	677	ALA	2.0
1	B	85	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	B	1723	4/4	0.74	0.19	35,37,37,43	0
3	EDO	B	1724	4/4	0.77	0.16	39,41,42,42	0
3	EDO	A	1727	4/4	0.77	0.25	19,20,22,24	0
3	EDO	B	1727	4/4	0.83	0.31	20,20,20,20	0
3	EDO	B	1719	4/4	0.84	0.15	35,36,37,39	0
3	EDO	A	1720	4/4	0.86	0.21	29,31,32,33	0
3	EDO	A	1721	4/4	0.88	0.17	33,34,34,36	0
3	EDO	B	1722	4/4	0.88	0.18	18,20,21,22	0
3	EDO	B	1714	4/4	0.88	0.16	32,34,35,37	0
3	EDO	A	1723[B]	4/4	0.89	0.16	16,19,19,20	4
3	EDO	A	1723[A]	4/4	0.89	0.16	13,15,17,20	4
3	EDO	B	1725	4/4	0.90	0.18	21,25,27,31	0
3	EDO	A	1714	4/4	0.91	0.17	17,25,27,28	0
3	EDO	A	1722	4/4	0.92	0.18	23,24,26,27	0
3	EDO	A	1726	4/4	0.92	0.15	15,20,23,23	0
4	CO	B	1732	1/1	0.92	0.27	32,32,32,32	1
3	EDO	B	1726[A]	4/4	0.93	0.13	11,14,15,18	4
3	EDO	A	1717[A]	4/4	0.93	0.13	23,24,24,24	4
3	EDO	B	1726[B]	4/4	0.93	0.13	16,16,17,19	4
3	EDO	A	1717[B]	4/4	0.93	0.13	19,21,23,23	4
3	EDO	A	1718	4/4	0.94	0.18	12,20,22,25	0
3	EDO	B	1715	4/4	0.94	0.12	12,20,22,24	0
3	EDO	A	1715	4/4	0.95	0.10	17,17,18,18	0
3	EDO	B	1717	4/4	0.95	0.11	17,23,23,24	0
3	EDO	A	1724	4/4	0.95	0.13	22,25,28,29	0
2	GCV	A	1713	14/14	0.96	0.09	10,12,20,20	0
2	GCV	B	1713	14/14	0.97	0.08	8,10,18,18	0
3	EDO	A	1719	4/4	0.97	0.10	13,16,18,20	0
4	CO	A	1732	1/1	0.97	0.24	25,25,25,25	1
3	EDO	B	1716	4/4	0.97	0.11	14,15,17,19	0
3	EDO	B	1720	4/4	0.97	0.08	16,17,18,19	0
4	CO	A	1730	1/1	0.98	0.09	18,18,18,18	1
3	EDO	B	1718	4/4	0.98	0.07	10,13,13,13	0
4	CO	B	1731	1/1	0.99	0.09	19,19,19,19	1
3	EDO	B	1721	4/4	0.99	0.07	9,10,11,11	0
3	EDO	A	1725	4/4	0.99	0.07	11,11,12,14	0
3	EDO	A	1716	4/4	0.99	0.06	12,12,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CO	A	1731	1/1	0.99	0.05	16,16,16,16	1
4	CO	B	1728	1/1	1.00	0.05	14,14,14,14	1
4	CO	B	1729	1/1	1.00	0.06	11,11,11,11	1
4	CO	A	1728	1/1	1.00	0.06	15,15,15,15	1
4	CO	B	1730	1/1	1.00	0.05	16,16,16,16	1
4	CO	A	1729	1/1	1.00	0.05	12,12,12,12	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.