



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 12:30 PM JST

PDB ID : 7WOI
Title : Structure of the shaft pilin Spa2 from *Corynebacterium glutamicum*
Authors : Wu, Y.F.; Wang, L.T.; Huang, Y.Y.; Zhong, C.; Zhou, J.
Deposited on : 2022-01-21
Resolution : 2.73 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

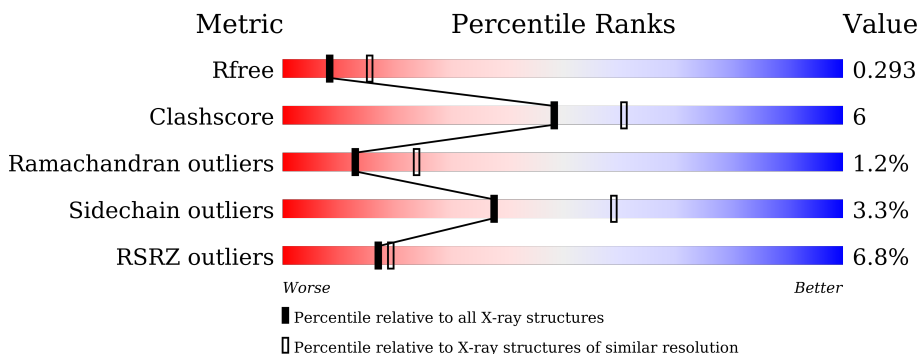
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	509	 3% 69% 14% • 16%
1	B	509	 8% 72% 11% • 16%

2 Entry composition [i](#)

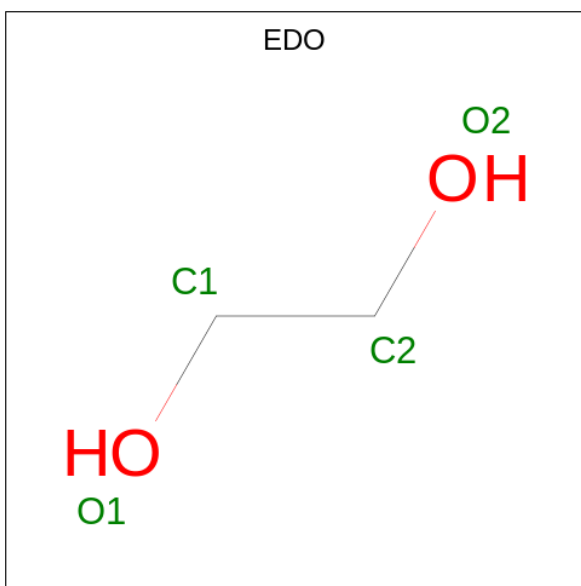
There are 4 unique types of molecules in this entry. The entry contains 6454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Spa2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	Total 3176	C 1987	N 518	O 666	S 5	0	0	0
1	B	429	Total 3179	C 1987	N 520	O 667	S 5	0	1	0

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



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	46	Total O 46 46	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.65Å 64.09Å 441.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.43 – 2.73 63.43 – 2.73	Depositor EDS
% Data completeness (in resolution range)	73.7 (63.43-2.73) 73.7 (63.43-2.73)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.266 , 0.293 0.266 , 0.293	Depositor DCC
R_{free} test set	1320 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtrriage
Anisotropy	0.448	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6454	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/3250	0.53	0/4465
1	B	0.28	0/3253	0.50	0/4469
All	All	0.30	0/6503	0.52	0/8934

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3176	0	2981	39	0
1	B	3179	0	2972	35	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0
3	B	6	0	8	0	0
4	A	35	0	0	0	0
4	B	46	0	0	0	0
All	All	6454	0	5979	74	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 6.

All (74) 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:262:SER:HA	1:A:267:PRO:HA	1.62	0.80
1:A:261:VAL:HG13	1:A:268:LEU:HB3	1.65	0.79
1:B:294:LYS:HD3	1:B:295:ALA:H	1.49	0.78
1:B:283:TRP:CZ3	1:B:301:VAL:HB	2.23	0.74
1:B:82:ALA:H	1:B:138:THR:HG22	1.53	0.73
1:A:247:VAL:HB	1:A:327:PRO:HA	1.70	0.71
1:B:261:VAL:HG12	1:B:301:VAL:HG12	1.71	0.71
1:A:312:GLU:HA	1:A:456:THR:HG22	1.74	0.70
1:B:247:VAL:HB	1:B:327:PRO:HA	1.77	0.66
1:B:312:GLU:HA	1:B:456:THR:HG22	1.76	0.66
1:A:261:VAL:HG13	1:A:268:LEU:CB	2.29	0.62
1:A:83:GLU:HB3	1:A:160:ASP:HB3	1.82	0.61
1:A:261:VAL:CG1	1:A:268:LEU:HD13	2.31	0.60
1:B:166:VAL:HG12	1:B:336:GLY:HA3	1.83	0.60
1:B:83:GLU:HB2	1:B:137:THR:HG22	1.84	0.58
1:B:247:VAL:HG22	1:B:280:VAL:HG13	1.88	0.56
1:A:368:GLU:HG2	1:A:394:VAL:HG12	1.88	0.55
1:B:283:TRP:CD1	1:B:283:TRP:N	2.74	0.55
1:B:280:VAL:HG12	1:B:280:VAL:O	2.05	0.55
1:B:269:VAL:HG12	1:B:270:GLU:H	1.73	0.53
1:B:67:THR:HB	1:B:69:GLU:OE1	2.08	0.53
1:B:228:GLN:HE21	1:B:229:THR:N	2.08	0.52
1:A:263:LEU:N	1:A:266:THR:O	2.33	0.51
1:A:247:VAL:HG22	1:A:280:VAL:HG13	1.92	0.50
1:B:283:TRP:CH2	1:B:301:VAL:HB	2.45	0.50
1:A:56:HIS:HB2	1:A:192:TYR:CD1	2.47	0.50
1:B:87:TRP:HZ3	1:B:157:GLN:HG2	1.77	0.49
1:B:368:GLU:HG2	1:B:394:VAL:HG12	1.93	0.49
1:B:54:THR:HG22	1:B:145:THR:HG23	1.93	0.49
1:B:321:SER:HB2	1:B:328:GLY:HA3	1.93	0.49
1:A:228:GLN:HE21	1:A:229:THR:N	2.11	0.49
1:B:56:HIS:HB2	1:B:192:TYR:CD1	2.47	0.48
1:A:275:THR:HA	1:A:283:TRP:HD1	1.78	0.48
1:A:419:SER:HB2	1:A:424:ILE:HD11	1.96	0.48
1:B:287:GLU:HA	1:B:290:LEU:HD12	1.96	0.47
1:A:59:VAL:HB	1:A:77:GLN:HG2	1.95	0.47
1:B:83:GLU:HA	1:B:137:THR:HA	1.95	0.47
1:A:166:VAL:HG12	1:A:336:GLY:HA3	1.97	0.47
1:A:56:HIS:HB2	1:A:192:TYR:HD1	1.79	0.47
1:B:151:LEU:HD22	1:B:177:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:HB	1:A:346:THR:HG23	1.97	0.46
1:A:55:VAL:O	1:A:143:GLU:HA	2.16	0.46
1:B:364:LEU:HD23	1:B:439:PRO:HG2	1.96	0.46
1:A:167:SER:HB3	1:A:196:GLN:HB2	1.98	0.46
1:A:198:VAL:HA	1:A:231:PRO:HB3	1.98	0.46
1:A:221:VAL:HG12	1:A:306:THR:HA	1.98	0.45
1:A:225:THR:HG22	1:A:302:VAL:HG22	1.98	0.45
1:B:351:LEU:HD12	1:B:460:LEU:HD23	1.98	0.45
1:A:272:THR:HG21	1:A:288:LYS:HD2	1.97	0.45
1:B:262:SER:HA	1:B:267:PRO:HA	1.99	0.45
1:A:268:LEU:H	1:A:268:LEU:HD23	1.82	0.44
1:A:70:GLU:HB2	1:A:190:HIS:CG	2.52	0.44
1:B:198:VAL:HA	1:B:231:PRO:HB3	1.99	0.44
1:A:245:TRP:HA	1:A:282:SER:HA	1.99	0.44
1:A:87:TRP:HZ3	1:A:157:GLN:HG2	1.82	0.44
1:A:321:SER:HB2	1:A:328:GLY:HA3	2.00	0.44
1:A:51:GLY:HA3	1:A:176:ILE:HG21	2.00	0.43
1:B:71:ILE:HG13	1:B:73:VAL:H	1.83	0.43
1:B:211:GLN:HG2	1:B:415:TRP:CE2	2.54	0.42
1:B:282:SER:C	1:B:283:TRP:CD1	2.93	0.42
1:B:102:LEU:HG	1:B:152:GLY:HA2	2.00	0.42
1:B:468:LYS:HE2	1:B:468:LYS:HB3	1.84	0.42
1:B:201:PRO:HB3	1:B:228:GLN:HB2	2.01	0.42
1:A:203:LYS:HG2	1:A:344:PRO:HG3	2.01	0.42
1:A:258:THR:HA	1:A:303:PHE:HA	2.01	0.42
1:A:272:THR:HG22	1:A:289:LYS:HG2	2.01	0.42
1:A:438:ALA:HB2	1:A:444:ALA:HB2	2.02	0.42
1:A:66:GLY:O	1:A:67:THR:HB	2.20	0.41
1:A:287:GLU:HA	1:A:290:LEU:HD12	2.01	0.41
1:A:233:LEU:HD21	1:A:334:ASN:HD21	1.86	0.41
1:B:83:GLU:HB3	1:B:160:ASP:HB3	2.02	0.41
1:A:268:LEU:HB2	1:A:273:ASP:OD2	2.20	0.40
1:B:69:GLU:H	1:B:69:GLU:HG3	1.61	0.40
1:A:287:GLU:HA	1:A:290:LEU:HB2	2.03	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	423/509 (83%)	391 (92%)	27 (6%)	5 (1%)	13	24
1	B	424/509 (83%)	397 (94%)	22 (5%)	5 (1%)	13	24
All	All	847/1018 (83%)	788 (93%)	49 (6%)	10 (1%)	13	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	184	ASN
1	A	74	PRO
1	B	267	PRO
1	A	267	PRO
1	A	276	ILE
1	B	277	ASP
1	B	74	PRO
1	B	276	ILE
1	B	280	VAL

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	339/397 (85%)	328 (97%)	11 (3%)	39	59
1	B	338/397 (85%)	326 (96%)	12 (4%)	35	55
All	All	677/794 (85%)	654 (97%)	23 (3%)	38	58

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	95	ASP
1	A	123	VAL
1	A	186	LEU
1	A	204	THR
1	A	224	TRP
1	A	261	VAL
1	A	262	SER
1	A	299	ILE
1	A	303	PHE
1	A	388	ASP
1	B	54	THR
1	B	69	GLU
1	B	120	LEU
1	B	186	LEU
1	B	224	TRP
1	B	276	ILE
1	B	283	TRP
1	B	303	PHE
1	B	351	LEU
1	B	362[A]	ASN
1	B	362[B]	ASN
1	B	388	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	602	-	5,5,5	0.91	0	5,5,5	0.99	0
2	EDO	A	601	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	A	602	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	B	601	-	3,3,3	0.46	0	2,2,2	0.34	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	GOL	B	602	-	-	2/4/4/4	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	429/509 (84%)	0.42	17 (3%) 38 42	16, 49, 96, 130	0
1	B	429/509 (84%)	0.75	41 (9%) 8 8	19, 62, 121, 165	0
All	All	858/1018 (84%)	0.59	58 (6%) 17 19	16, 54, 110, 165	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	ALA	4.5
1	B	273	ASP	4.5
1	B	65	ALA	4.4
1	B	274	TYR	4.1
1	A	283	TRP	3.9
1	B	275	THR	3.7
1	B	242	ALA	3.7
1	A	268	LEU	3.6
1	B	66	GLY	3.6
1	B	75	GLY	3.6
1	B	293	ILE	3.5
1	B	241	SER	3.2
1	B	72	SER	3.2
1	B	46	GLY	3.1
1	A	292	GLU	3.1
1	B	70	GLU	3.0
1	A	397	ALA	3.0
1	A	269	VAL	3.0
1	A	379	VAL	2.9
1	B	73	VAL	2.9
1	B	269	VAL	2.9
1	B	299	ILE	2.9
1	B	110	GLN	2.8
1	B	77	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLY	2.8
1	A	281	VAL	2.7
1	A	372	PHE	2.7
1	A	273	ASP	2.7
1	A	275	THR	2.7
1	A	242	ALA	2.5
1	B	47	ALA	2.5
1	B	283	TRP	2.5
1	B	58	TYR	2.5
1	B	187	TYR	2.5
1	B	102	LEU	2.5
1	B	124	GLN	2.4
1	B	74	PRO	2.4
1	B	40	VAL	2.4
1	B	114	GLY	2.3
1	B	280	VAL	2.3
1	B	121	SER	2.3
1	B	155	TYR	2.3
1	A	72	SER	2.3
1	B	292	GLU	2.3
1	B	84	PHE	2.2
1	B	147	GLY	2.2
1	B	174	VAL	2.2
1	B	308	LEU	2.1
1	A	265	GLY	2.1
1	B	276	ILE	2.1
1	B	301	VAL	2.1
1	B	125	ASN	2.1
1	B	270	GLU	2.1
1	B	71	ILE	2.1
1	A	257	GLY	2.1
1	B	86	ILE	2.1
1	B	281	VAL	2.0
1	A	222	VAL	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 monosaccharides 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	B	601	4/4	0.83	0.33	50,52,53,54	0
2	EDO	A	602	4/4	0.86	0.25	36,40,41,44	0
3	GOL	B	602	6/6	0.86	0.14	21,39,41,42	0
2	EDO	A	601	4/4	0.93	0.19	27,29,35,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.