



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2025 – 09:06 pm GMT

PDB ID : 9EOB  
Title : Engineered GH181 sialidase from Akkermansia muciniphila  
Authors : Pichler, M.J.; Banerjee, S.; Nielsen, T.S.; Morth, J.P.; Abou Hachem, M.  
Deposited on : 2024-03-14  
Resolution : 1.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

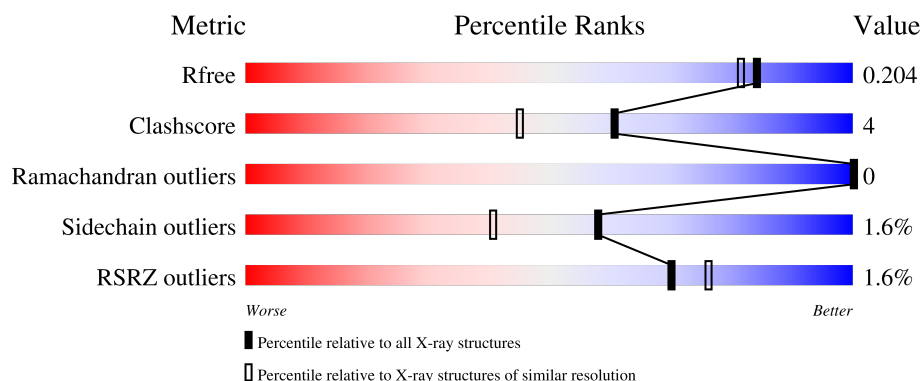
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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))
$R_{free}$	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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  $\geq 3$ , 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	580	

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
5	CL	A	724	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5315 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 exo-alpha-sialidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	11	0
			4659	2927	861	858	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ALA	HIS	conflict	UNP A0A7G6DVF6
A	350	TYR	GLN	conflict	UNP A0A7G6DVF6
A	477	VAL	ALA	conflict	UNP A0A7G6DVF6
A	516	LYS	ARG	conflict	UNP A0A7G6DVF6
A	596	LEU	-	expression tag	UNP A0A7G6DVF6
A	597	GLU	-	expression tag	UNP A0A7G6DVF6
A	598	HIS	-	expression tag	UNP A0A7G6DVF6
A	599	HIS	-	expression tag	UNP A0A7G6DVF6
A	600	HIS	-	expression tag	UNP A0A7G6DVF6
A	601	HIS	-	expression tag	UNP A0A7G6DVF6
A	602	HIS	-	expression tag	UNP A0A7G6DVF6
A	603	HIS	-	expression tag	UNP A0A7G6DVF6

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

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



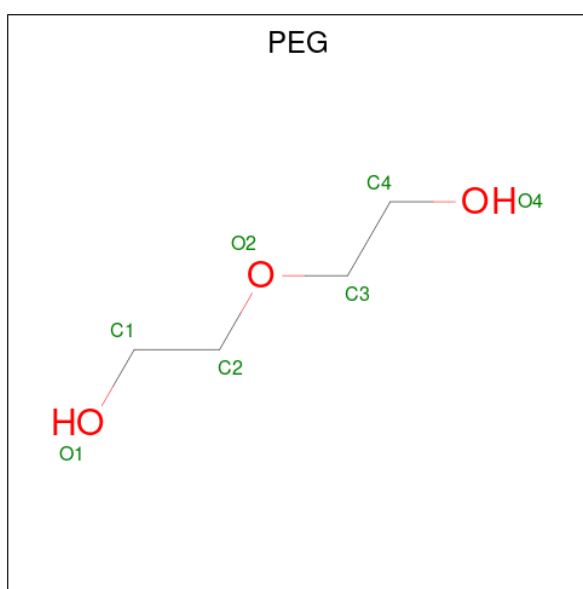
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total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

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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	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	Cl	0	0
			8	8		

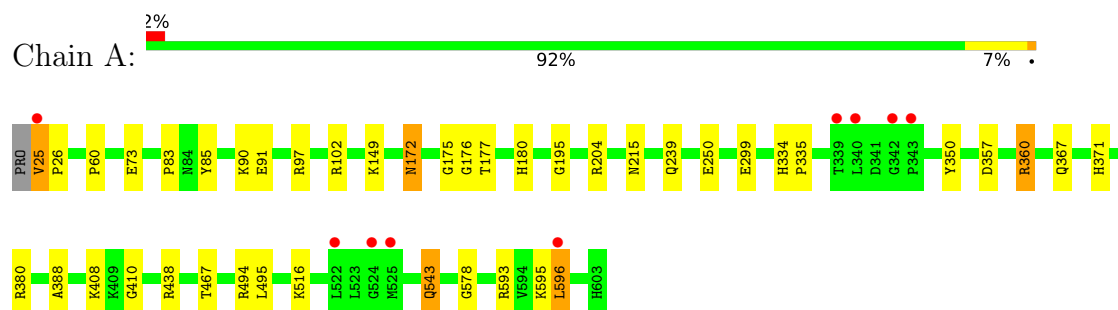
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	566	Total	O	0	2
			568	568		

### 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: exo-alpha-sialidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.67Å 88.19Å 99.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.02 – 1.77 66.02 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.5 (66.02-1.77) 99.5 (66.02-1.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.155 , 0.195 0.166 , 0.204	Depositor DCC
$R_{free}$ test set	3285 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PEG, NI, 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	0.49	1/4781 (0.0%)	0.80	1/6482 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	GLU	CD-OE1	-6.38	1.18	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	ARG	NE-CZ-NH2	-5.88	117.36	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ARG	Sidechain
1	A	97	ARG	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	4659	0	4565	35	0
2	A	1	0	0	0	0
3	A	72	0	108	9	0
4	A	7	0	10	0	0
5	A	8	0	0	3	0
6	A	568	0	0	12	0
All	All	5315	0	4683	39	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 4.

The worst 5 of 39 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:438[B]:ARG:NH2	6:A:801:HOH:O	1.59	1.28
1:A:467[A]:THR:CG2	1:A:543[A]:GLN:HG2	1.94	0.98
1:A:467[A]:THR:HG22	1:A:543[A]:GLN:HG2	1.58	0.86
1:A:25:VAL:HG13	1:A:26:PRO:HD2	1.61	0.83
1:A:467[A]:THR:HG21	1:A:543[A]:GLN:HG2	1.61	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	588/580 (101%)	564 (96%)	24 (4%)	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	497/487 (102%)	488 (98%)	9 (2%)	54 36

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	LYS
1	A	596	LEU
1	A	350	TYR
1	A	494	ARG
1	A	543[A]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	239	GLN
1	A	331	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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	706	-	3,3,3	0.18	0	2,2,2	0.33	0
3	EDO	A	714	-	3,3,3	0.23	0	2,2,2	0.15	0
3	EDO	A	716	-	3,3,3	0.12	0	2,2,2	0.19	0
3	EDO	A	713	-	3,3,3	0.38	0	2,2,2	0.62	0
3	EDO	A	703	-	3,3,3	0.15	0	2,2,2	0.44	0
3	EDO	A	707	-	3,3,3	0.14	0	2,2,2	0.13	0
3	EDO	A	708	-	3,3,3	0.26	0	2,2,2	0.34	0
3	EDO	A	702	-	3,3,3	0.33	0	2,2,2	0.16	0
3	EDO	A	710	-	3,3,3	0.20	0	2,2,2	0.25	0
3	EDO	A	712	-	3,3,3	0.23	0	2,2,2	0.41	0
3	EDO	A	717	-	3,3,3	0.14	0	2,2,2	0.32	0
3	EDO	A	705	-	3,3,3	0.53	0	2,2,2	0.33	0
4	PEG	A	711	-	6,6,6	0.16	0	5,5,5	0.13	0
3	EDO	A	709	-	3,3,3	0.13	0	2,2,2	0.29	0
3	EDO	A	720	-	3,3,3	0.21	0	2,2,2	0.40	0
3	EDO	A	704	-	3,3,3	0.60	0	2,2,2	0.51	0
3	EDO	A	719	-	3,3,3	0.15	0	2,2,2	0.20	0
3	EDO	A	715	-	3,3,3	0.14	0	2,2,2	0.13	0
3	EDO	A	718	-	3,3,3	0.37	0	2,2,2	0.61	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	706	-	-	0/1/1/1	-
3	EDO	A	714	-	-	0/1/1/1	-
3	EDO	A	716	-	-	1/1/1/1	-
3	EDO	A	713	-	-	1/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	A	707	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	708	-	-	1/1/1/1	-
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	A	710	-	-	1/1/1/1	-
3	EDO	A	712	-	-	1/1/1/1	-
3	EDO	A	717	-	-	0/1/1/1	-
3	EDO	A	705	-	-	1/1/1/1	-
4	PEG	A	711	-	-	1/4/4/4	-
3	EDO	A	709	-	-	1/1/1/1	-
3	EDO	A	720	-	-	1/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	A	719	-	-	0/1/1/1	-
3	EDO	A	715	-	-	1/1/1/1	-
3	EDO	A	718	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	708	EDO	O1-C1-C2-O2
3	A	720	EDO	O1-C1-C2-O2
3	A	712	EDO	O1-C1-C2-O2
3	A	705	EDO	O1-C1-C2-O2
3	A	718	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	706	EDO	2	0
3	A	712	EDO	1	0
3	A	717	EDO	1	0
3	A	705	EDO	2	0
3	A	718	EDO	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	579/580 (99%)	-0.22	9 (1%) 70 76	11, 23, 41, 82	11 (1%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	PRO	4.5
1	A	340	LEU	4.2
1	A	596	LEU	3.6
1	A	25	VAL	3.5
1	A	342	GLY	3.0

### 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, 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	A	720	4/4	0.73	0.17	59,60,61,63	0
3	EDO	A	710	4/4	0.75	0.20	52,52,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	714	4/4	0.76	0.22	54,55,56,64	0
5	CL	A	725	1/1	0.77	0.19	70,70,70,70	0
3	EDO	A	718	4/4	0.78	0.17	51,57,57,60	0
5	CL	A	728	1/1	0.79	0.16	70,70,70,70	0
3	EDO	A	706	4/4	0.80	0.14	41,42,46,49	0
4	PEG	A	711	7/7	0.81	0.17	54,57,63,63	0
3	EDO	A	708	4/4	0.84	0.16	51,53,53,60	0
3	EDO	A	705	4/4	0.84	0.14	42,47,48,49	0
3	EDO	A	713	4/4	0.84	0.18	42,48,51,51	0
3	EDO	A	709	4/4	0.85	0.16	37,40,43,51	0
5	CL	A	726	1/1	0.88	0.20	63,63,63,63	0
3	EDO	A	712	4/4	0.88	0.12	47,53,56,57	0
3	EDO	A	707	4/4	0.89	0.13	42,46,50,54	0
3	EDO	A	716	4/4	0.89	0.11	47,49,51,51	0
5	CL	A	727	1/1	0.90	0.13	50,50,50,50	0
3	EDO	A	719	4/4	0.90	0.14	48,49,52,55	0
3	EDO	A	717	4/4	0.91	0.12	39,43,50,53	0
3	EDO	A	704	4/4	0.93	0.09	28,30,32,33	0
3	EDO	A	702	4/4	0.93	0.11	25,37,43,46	0
3	EDO	A	715	4/4	0.93	0.12	44,45,48,52	0
5	CL	A	724	1/1	0.93	0.28	56,56,56,56	0
5	CL	A	723	1/1	0.95	0.08	50,50,50,50	0
3	EDO	A	703	4/4	0.97	0.05	21,23,23,26	0
5	CL	A	722	1/1	0.97	0.27	50,50,50,50	0
5	CL	A	721	1/1	0.99	0.04	21,21,21,21	0
2	NI	A	701	1/1	1.00	0.03	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.