



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:19 am GMT

PDB ID : 5FIP  
Title : Discovery and characterization of a novel thermostable and highly halotolerant GH5 cellulase from an Icelandic hot spring isolate  
Authors : Zarafeta, D.; Kissas, D.; Sayer, C.; Gudbergisdottir, S.R.; Ladoukakis, E.; Isupov, M.N.; Chatziioannou, A.; Peng, X.; Littlechild, J.A.; Skretas, G.; Kolisis, F.N.  
Deposited on : 2015-10-01  
Resolution : 1.88 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

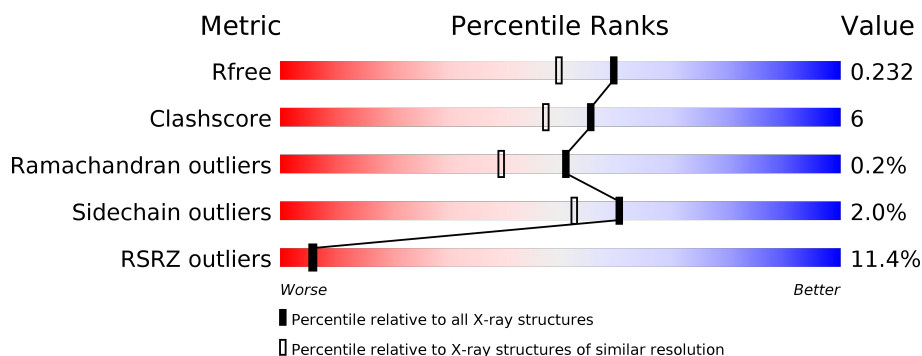
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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))
$R_{free}$	100719	7505 (1.90-1.86)
Clashscore	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)
RSRZ outliers	101464	7571 (1.90-1.86)

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. 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	334	<div> <div>5%</div> <div>86%</div> <div>13%</div> <div>..</div> </div>
1	B	334	<div> <div>6%</div> <div>93%</div> <div>6%</div> <div>..</div> </div>
1	C	334	<div> <div>15%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	D	334	<div> <div>19%</div> <div>86%</div> <div>12%</div> <div>..</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	A	1386	-	-	X	X
2	PEG	B	1382	-	-	-	X
3	PGE	B	1384	-	-	-	X
4	EDO	A	1393	-	-	-	X
4	EDO	B	1385	-	-	-	X
4	EDO	B	1386	-	-	-	X
4	EDO	B	1389	-	-	-	X
4	EDO	B	1390	-	-	-	X
4	EDO	B	1392	-	-	-	X
4	EDO	D	1385	-	-	-	X
5	IPA	A	1394	-	-	-	X
5	IPA	A	1395	-	-	X	X
5	IPA	B	1394	-	-	X	-
5	IPA	B	1395	-	-	X	-
5	IPA	B	1399	-	-	-	X
5	IPA	C	1384	-	-	X	-
5	IPA	D	1391	-	-	X	-
5	IPA	D	1393	-	-	-	X
6	CL	B	1401	-	-	-	X

## 2 Entry composition [i](#)

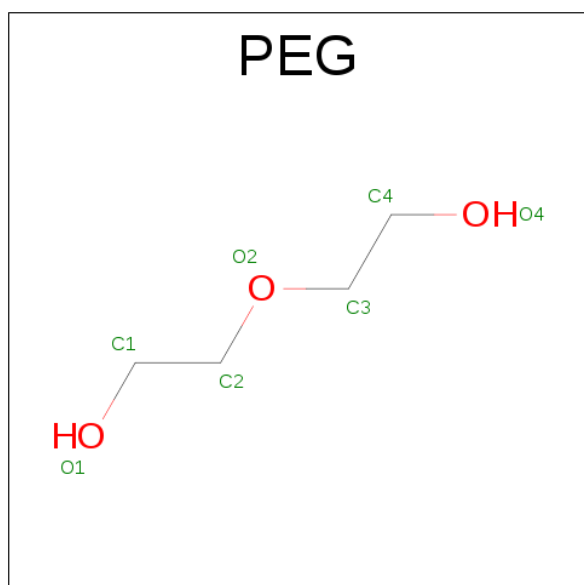
There are 9 unique types of molecules in this entry. The entry contains 11615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GH5 CELLULASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	20	0
			2715	1736	454	516	9			
1	B	332	Total	C	N	O	S	0	19	0
			2711	1737	454	511	9			
1	C	331	Total	C	N	O	S	0	14	0
			2677	1710	449	510	8			
1	D	328	Total	C	N	O	S	0	10	0
			2648	1690	450	499	9			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



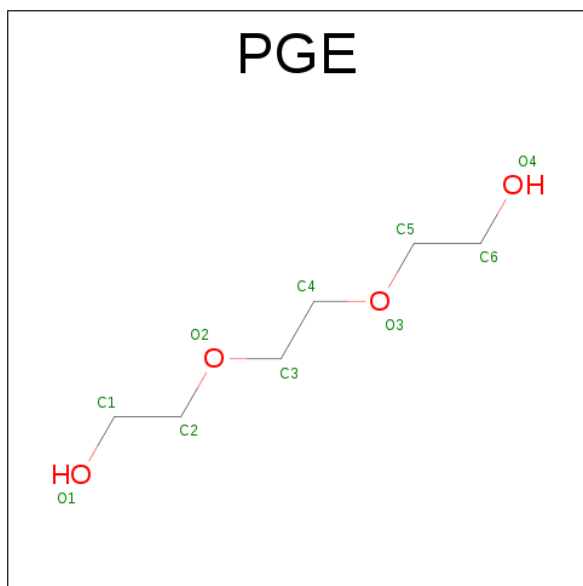
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



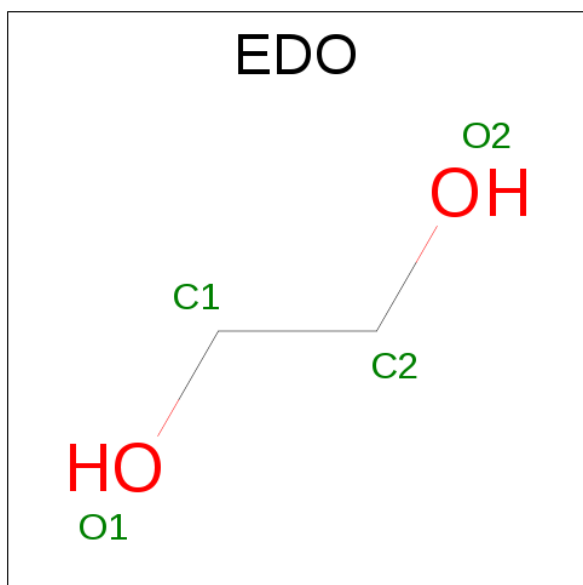
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



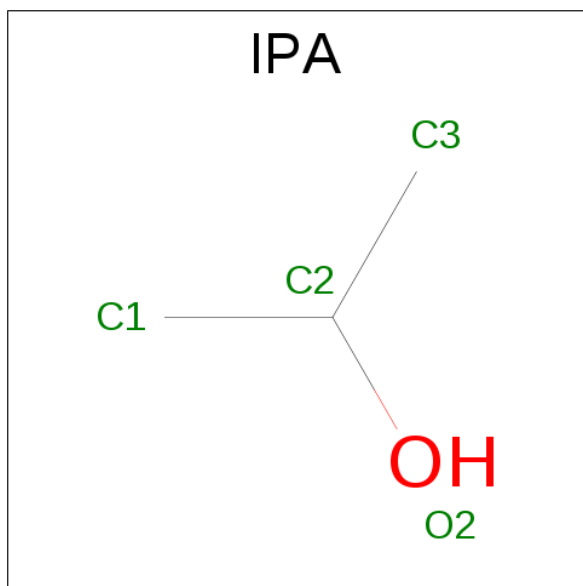
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

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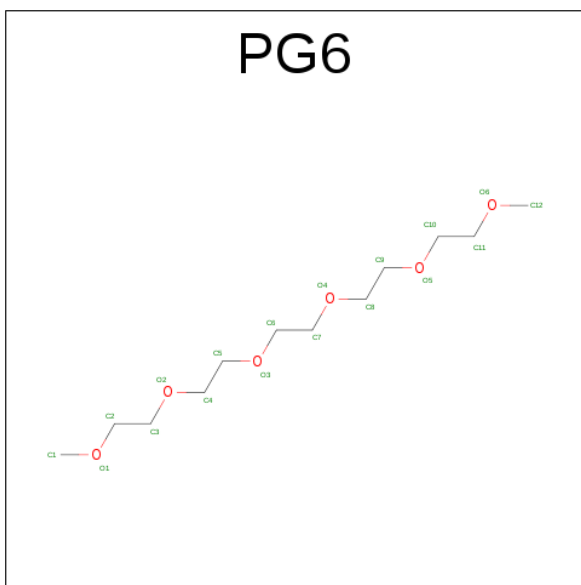
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	C	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Cl 2 2	0	0
6	A	3	Total Cl 3 3	0	0
6	D	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0

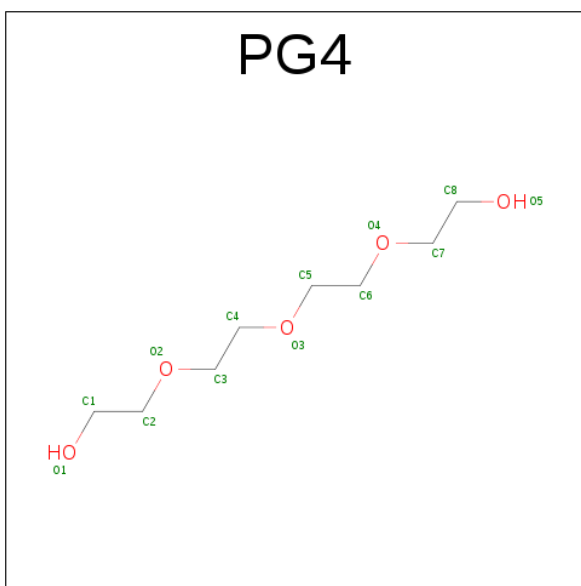
- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			18	12	6		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			13	8	5		

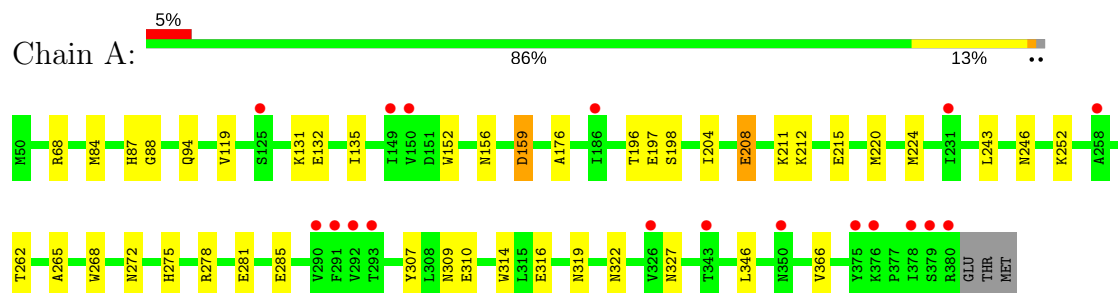
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	206	Total 206	O 206	0	0
9	B	196	Total 196	O 196	0	0
9	C	94	Total 94	O 94	0	0
9	D	89	Total 89	O 89	0	0

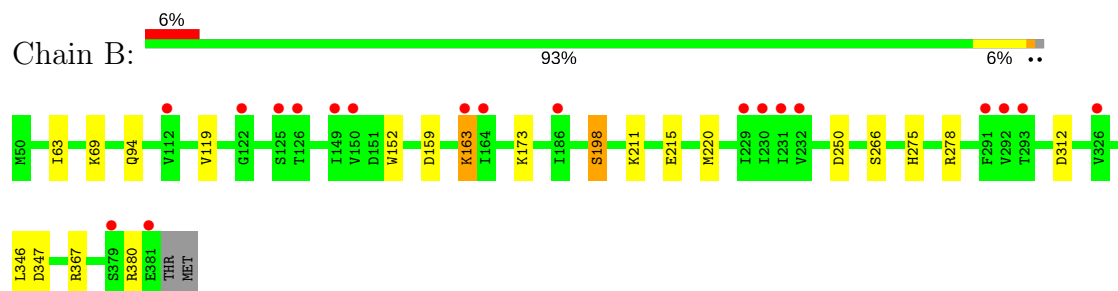
### 3 Residue-property plots

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.

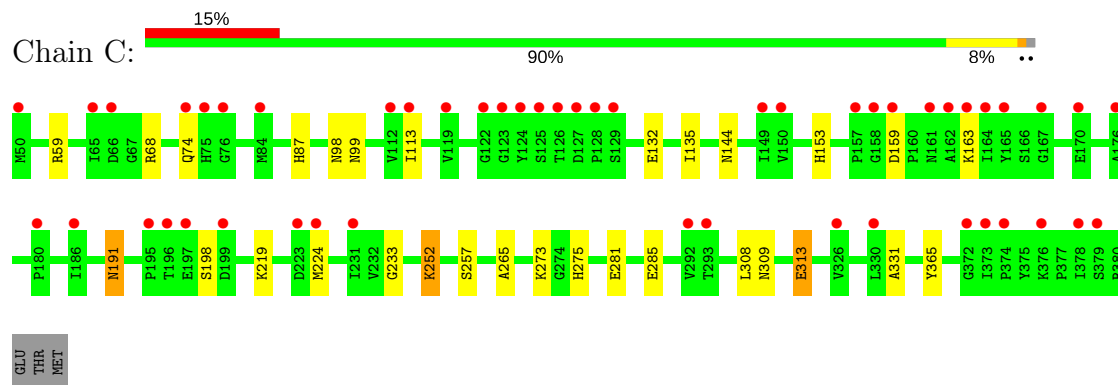
#### • Molecule 1: GH5 CELLULASE



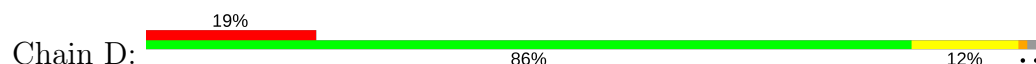
#### • Molecule 1: GH5 CELLULASE

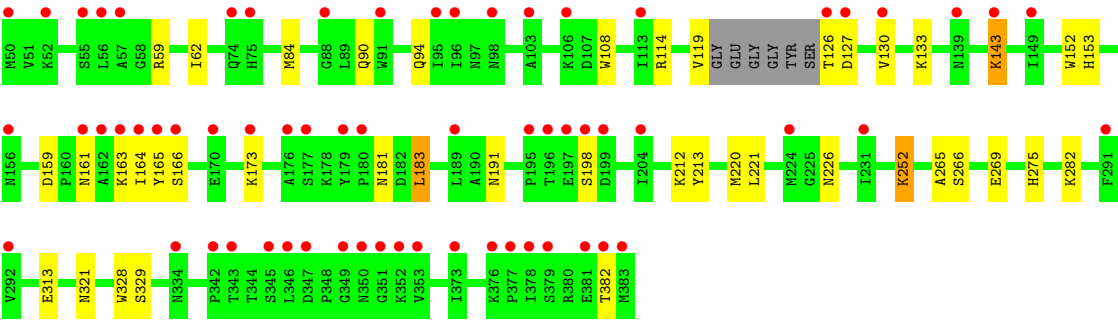


#### • Molecule 1: GH5 CELLULASE



#### • Molecule 1: GH5 CELLULASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.34Å 137.45Å 121.34Å 90.00° 114.44° 90.00°	Depositor
Resolution (Å)	36.38 – 1.88 36.38 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.4 (36.38-1.88) 97.4 (36.38-1.88)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.193 , 0.234 0.192 , 0.232	Depositor DCC
$R_{free}$ test set	6406 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: PGE, CL, EDO, PG6, PG4, IPA, PEG

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	0.68	1/2841 (0.0%)	0.73	1/3855 (0.0%)
1	B	0.69	0/2833	0.74	5/3843 (0.1%)
1	C	0.55	0/2784	0.71	0/3781
1	D	0.57	0/2742	0.69	1/3720 (0.0%)
All	All	0.62	1/11200 (0.0%)	0.72	7/15199 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLU	CD-OE2	-5.18	1.20	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	278	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	278	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	347	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	159	ASP	CB-CG-OD1	5.70	123.43	118.30

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	2715	0	2706	50	0
1	B	2711	0	2722	16	0
1	C	2677	0	2656	22	0
1	D	2648	0	2630	33	0
2	A	49	0	70	14	0
2	B	14	0	20	1	0
2	C	7	0	10	0	0
2	D	7	0	10	0	0
3	A	20	0	28	4	0
3	B	10	0	14	0	0
3	C	10	0	14	1	0
4	A	16	0	24	0	0
4	B	32	0	48	0	0
4	C	4	0	6	0	0
4	D	20	0	30	0	0
5	A	8	0	16	6	0
5	B	24	0	48	10	0
5	C	4	0	8	5	0
5	D	16	0	32	13	0
6	A	3	0	0	1	0
6	B	2	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	18	0	26	3	0
8	D	13	0	18	0	0
9	A	206	0	0	14	0
9	B	196	0	0	4	0
9	C	94	0	0	2	0
9	D	89	0	0	3	0
All	All	11615	0	11136	130	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.

The worst 5 of 130 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:132[A]:GLU:OE1	9:A:2075:HOH:O	1.59	1.18
9:A:2023:HOH:O	1:C:313[B]:GLU:OE1	1.62	1.17
1:C:309[B]:ASN:OD1	9:C:2074:HOH:O	1.62	1.16
1:A:132[A]:GLU:CD	9:A:2075:HOH:O	1.80	1.15
1:A:197[B]:GLU:OE2	6:A:1397:CL:CL	2.13	1.04

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	349/334 (104%)	340 (97%)	9 (3%)	0	100	100
1	B	349/334 (104%)	336 (96%)	13 (4%)	0	100	100
1	C	343/334 (103%)	331 (96%)	11 (3%)	1 (0%)	44	32
1	D	334/334 (100%)	321 (96%)	11 (3%)	2 (1%)	28	15
All	All	1375/1336 (103%)	1328 (97%)	44 (3%)	3 (0%)	51	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS
1	C	191	ASN
1	D	152	TRP

### 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	299/282 (106%)	299 (100%)	0	100	100
1	B	299/282 (106%)	294 (98%)	5 (2%)	66	59
1	C	293/282 (104%)	284 (97%)	9 (3%)	45	33
1	D	289/282 (102%)	275 (95%)	14 (5%)	30	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1180/1128 (105%)	1152 (98%)	28 (2%)	60 44

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313[A]	GLU
1	D	94	GLN
1	D	252[A]	LYS
1	C	313[B]	GLU
1	D	90	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	275	HIS
1	C	275	HIS
1	C	98	ASN
1	A	139	ASN
1	C	99	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 55 ligands modelled in this entry, 7 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PEG	A	1381	-	6,6,6	0.47	0	5,5,5	0.31	0
2	PEG	A	1382	-	6,6,6	0.44	0	5,5,5	0.45	0
2	PEG	A	1383	-	6,6,6	0.36	0	5,5,5	0.57	0
2	PEG	A	1384	-	6,6,6	0.40	0	5,5,5	0.41	0
2	PEG	A	1385	-	6,6,6	0.40	0	5,5,5	0.39	0
2	PEG	A	1386	-	6,6,6	0.29	0	5,5,5	0.82	0
2	PEG	A	1387	-	6,6,6	0.78	0	5,5,5	0.69	0
3	PGE	A	1388	-	9,9,9	0.62	0	8,8,8	0.55	0
3	PGE	A	1389	-	9,9,9	0.58	0	8,8,8	0.87	0
4	EDO	A	1390	-	3,3,3	0.47	0	2,2,2	0.40	0
4	EDO	A	1391	-	3,3,3	0.47	0	2,2,2	0.15	0
4	EDO	A	1392	-	3,3,3	0.42	0	2,2,2	0.44	0
4	EDO	A	1393	-	3,3,3	0.56	0	2,2,2	0.39	0
5	IPA	A	1394	-	3,3,3	0.55	0	3,3,3	0.52	0
5	IPA	A	1395	-	3,3,3	0.29	0	3,3,3	0.63	0
2	PEG	B	1382	-	6,6,6	0.49	0	5,5,5	0.25	0
2	PEG	B	1383	-	6,6,6	0.48	0	5,5,5	0.33	0
3	PGE	B	1384	-	9,9,9	0.53	0	8,8,8	0.35	0
4	EDO	B	1385	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	B	1386	-	3,3,3	0.51	0	2,2,2	0.36	0
4	EDO	B	1387	-	3,3,3	0.39	0	2,2,2	0.53	0
4	EDO	B	1388	-	3,3,3	0.37	0	2,2,2	0.61	0
4	EDO	B	1389	-	3,3,3	0.52	0	2,2,2	0.35	0
4	EDO	B	1390	-	3,3,3	0.55	0	2,2,2	0.16	0
4	EDO	B	1391	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	B	1392	-	3,3,3	0.41	0	2,2,2	0.59	0
7	PG6	B	1393	-	17,17,17	0.57	0	16,16,16	0.39	0
5	IPA	B	1394	-	3,3,3	0.45	0	3,3,3	0.63	0
5	IPA	B	1395	-	3,3,3	0.47	0	3,3,3	0.77	0
5	IPA	B	1396	-	3,3,3	0.50	0	3,3,3	0.46	0
5	IPA	B	1397	-	3,3,3	0.48	0	3,3,3	0.20	0
5	IPA	B	1398	-	3,3,3	0.55	0	3,3,3	0.17	0
5	IPA	B	1399	-	3,3,3	0.38	0	3,3,3	0.71	0
2	PEG	C	1381	-	6,6,6	0.44	0	5,5,5	0.28	0
3	PGE	C	1382	-	9,9,9	0.57	0	8,8,8	0.50	0
4	EDO	C	1383	-	3,3,3	0.44	0	2,2,2	0.54	0
5	IPA	C	1384	-	3,3,3	0.43	0	3,3,3	0.84	0
2	PEG	D	1384	-	6,6,6	0.49	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	D	1385	-	3,3,3	0.44	0	2,2,2	0.28	0
4	EDO	D	1386	-	3,3,3	0.41	0	2,2,2	0.47	0
4	EDO	D	1387	-	3,3,3	0.46	0	2,2,2	0.53	0
4	EDO	D	1388	-	3,3,3	0.48	0	2,2,2	0.42	0
4	EDO	D	1389	-	3,3,3	0.39	0	2,2,2	0.50	0
8	PG4	D	1390	-	12,12,12	0.46	0	11,11,11	0.26	0
5	IPA	D	1391	-	3,3,3	0.87	0	3,3,3	0.64	0
5	IPA	D	1392	-	3,3,3	0.54	0	3,3,3	0.20	0
5	IPA	D	1393	-	3,3,3	0.48	0	3,3,3	0.36	0
5	IPA	D	1394	-	3,3,3	0.41	0	3,3,3	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	1381	-	-	0/4/4/4	0/0/0/0
2	PEG	A	1382	-	-	0/4/4/4	0/0/0/0
2	PEG	A	1383	-	-	0/4/4/4	0/0/0/0
2	PEG	A	1384	-	-	0/4/4/4	0/0/0/0
2	PEG	A	1385	-	-	0/4/4/4	0/0/0/0
2	PEG	A	1386	-	-	0/4/4/4	0/0/0/0
2	PEG	A	1387	-	-	0/4/4/4	0/0/0/0
3	PGE	A	1388	-	-	0/7/7/7	0/0/0/0
3	PGE	A	1389	-	-	0/7/7/7	0/0/0/0
4	EDO	A	1390	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1391	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1392	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1393	-	-	0/1/1/1	0/0/0/0
5	IPA	A	1394	-	-	0/0/0/0	0/0/0/0
5	IPA	A	1395	-	-	0/0/0/0	0/0/0/0
2	PEG	B	1382	-	-	0/4/4/4	0/0/0/0
2	PEG	B	1383	-	-	0/4/4/4	0/0/0/0
3	PGE	B	1384	-	-	0/7/7/7	0/0/0/0
4	EDO	B	1385	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1386	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1387	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1388	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1389	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1390	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1391	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1392	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG6	B	1393	-	-	0/15/15/15	0/0/0/0
5	IPA	B	1394	-	-	0/0/0/0	0/0/0/0
5	IPA	B	1395	-	-	0/0/0/0	0/0/0/0
5	IPA	B	1396	-	-	0/0/0/0	0/0/0/0
5	IPA	B	1397	-	-	0/0/0/0	0/0/0/0
5	IPA	B	1398	-	-	0/0/0/0	0/0/0/0
5	IPA	B	1399	-	-	0/0/0/0	0/0/0/0
2	PEG	C	1381	-	-	0/4/4/4	0/0/0/0
3	PGE	C	1382	-	-	0/7/7/7	0/0/0/0
4	EDO	C	1383	-	-	0/1/1/1	0/0/0/0
5	IPA	C	1384	-	-	0/0/0/0	0/0/0/0
2	PEG	D	1384	-	-	0/4/4/4	0/0/0/0
4	EDO	D	1385	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1386	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1387	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1388	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1389	-	-	0/1/1/1	0/0/0/0
8	PG4	D	1390	-	-	0/10/10/10	0/0/0/0
5	IPA	D	1391	-	-	0/0/0/0	0/0/0/0
5	IPA	D	1392	-	-	0/0/0/0	0/0/0/0
5	IPA	D	1393	-	-	0/0/0/0	0/0/0/0
5	IPA	D	1394	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1381	PEG	2	0
2	A	1382	PEG	3	0
2	A	1384	PEG	2	0
2	A	1386	PEG	5	0
2	A	1387	PEG	2	0
3	A	1388	PGE	1	0
3	A	1389	PGE	3	0
5	A	1395	IPA	6	0
2	B	1382	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1383	PEG	1	0
7	B	1393	PG6	3	0
5	B	1394	IPA	4	0
5	B	1395	IPA	5	0
5	B	1397	IPA	1	0
3	C	1382	PGE	1	0
5	C	1384	IPA	5	0
5	D	1391	IPA	8	0
5	D	1392	IPA	1	0
5	D	1393	IPA	2	0
5	D	1394	IPA	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 [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	331/334 (99%)	0.10	18 (5%) 26 29	19, 33, 53, 72	0
1	B	332/334 (99%)	0.04	19 (5%) 24 26	20, 30, 53, 93	0
1	C	331/334 (99%)	0.56	50 (15%) 3 3	29, 45, 80, 110	0
1	D	328/334 (98%)	0.84	64 (19%) 1 1	23, 51, 93, 132	0
All	All	1322/1336 (98%)	0.38	151 (11%) 6 6	19, 39, 74, 132	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	THR	6.5
1	D	383	MET	6.1
1	C	50	MET	5.7
1	D	349	GLY	5.7
1	D	197	GLU	5.3

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	IPA	D	1393	4/4	0.86	0.18	13.77	37,45,53,62	0
4	EDO	D	1385	4/4	0.85	0.20	6.34	49,56,62,63	0
5	IPA	A	1394	4/4	0.82	0.30	5.56	37,47,51,53	4
5	IPA	B	1399	4/4	0.97	0.26	5.41	33,36,40,45	0
4	EDO	B	1390	4/4	0.88	0.17	5.28	42,62,62,74	0
4	EDO	B	1392	4/4	0.87	0.12	4.90	55,61,62,75	0
4	EDO	B	1385	4/4	0.88	0.19	4.42	43,60,64,73	0
2	PEG	B	1382	7/7	0.73	0.18	3.63	63,66,77,78	0
2	PEG	A	1386	7/7	0.79	0.23	3.25	40,49,72,80	0
4	EDO	B	1386	4/4	0.75	0.14	3.07	60,67,69,70	0
5	IPA	A	1395	4/4	0.94	0.16	2.69	22,23,27,42	0
4	EDO	A	1393	4/4	0.83	0.15	2.28	49,51,68,74	0
4	EDO	B	1389	4/4	0.68	0.23	2.28	63,72,72,78	0
6	CL	B	1401	1/1	0.98	0.13	2.23	39,39,39,39	1
3	PGE	B	1384	10/10	0.70	0.21	2.18	68,77,85,85	0
8	PG4	D	1390	13/13	0.94	0.14	1.73	43,51,61,63	0
2	PEG	A	1381	7/7	0.90	0.15	1.67	31,49,53,57	0
2	PEG	A	1387	7/7	0.71	0.17	1.62	36,47,57,61	0
2	PEG	B	1383	7/7	0.86	0.26	1.33	58,62,69,83	0
5	IPA	B	1395	4/4	0.94	0.11	1.31	26,35,41,41	0
4	EDO	D	1386	4/4	0.89	0.11	1.26	53,59,64,64	0
3	PGE	A	1389	10/10	0.88	0.14	1.08	34,50,59,62	0
5	IPA	C	1384	4/4	0.95	0.13	0.96	31,33,36,37	0
2	PEG	D	1384	7/7	0.85	0.17	0.60	52,70,76,79	0
7	PG6	B	1393	18/18	0.91	0.09	0.53	44,52,78,78	0
5	IPA	B	1394	4/4	0.93	0.10	0.50	19,29,29,42	0
2	PEG	A	1384	7/7	0.90	0.14	0.46	49,59,67,78	0
3	PGE	A	1388	10/10	0.87	0.10	0.46	50,60,69,70	0
5	IPA	D	1391	4/4	0.81	0.15	0.43	29,29,37,51	0
3	PGE	C	1382	10/10	0.84	0.16	0.41	43,51,64,71	0
4	EDO	C	1383	4/4	0.84	0.13	0.29	50,53,59,63	0
4	EDO	D	1389	4/4	0.93	0.12	-0.99	58,62,64,75	0
2	PEG	A	1382	7/7	0.98	0.08	-1.41	26,31,45,48	7
6	CL	A	1397	1/1	0.93	0.07	-	30,30,30,30	1
4	EDO	B	1387	4/4	0.92	0.08	-	46,52,57,65	0
4	EDO	D	1387	4/4	0.74	0.17	-	45,58,65,72	0
6	CL	D	1395	1/1	0.96	0.09	-	52,52,52,52	1
5	IPA	B	1398	4/4	0.92	0.14	-	50,57,74,78	0
4	EDO	B	1391	4/4	0.87	0.38	-	70,71,73,78	0
5	IPA	B	1396	4/4	0.91	0.14	-	48,49,50,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	A	1383	7/7	0.92	0.17	-	45,49,58,72	0
6	CL	A	1396	1/1	0.93	0.06	-	53,53,53,53	0
4	EDO	B	1388	4/4	0.92	0.13	-	37,47,50,61	0
6	CL	C	1385	1/1	0.92	0.06	-	56,56,56,56	1
5	IPA	B	1397	4/4	0.95	0.09	-	42,46,54,61	0
2	PEG	C	1381	7/7	0.81	0.12	-	59,61,64,68	0
5	IPA	D	1394	4/4	0.94	0.11	-	38,41,44,46	0
5	IPA	D	1392	4/4	0.90	0.11	-	49,55,57,59	0
4	EDO	A	1390	4/4	0.66	0.19	-	75,77,80,82	0
4	EDO	D	1388	4/4	0.66	0.23	-	71,79,79,81	0
4	EDO	A	1392	4/4	0.76	0.17	-	72,80,82,91	0
4	EDO	A	1391	4/4	0.72	0.25	-	59,59,66,81	0
6	CL	B	1400	1/1	0.98	0.03	-	47,47,47,47	0
6	CL	A	1400	1/1	0.91	0.13	-	59,59,59,59	1
2	PEG	A	1385	7/7	0.89	0.12	-	57,72,77,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.