



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:46 PM GMT

PDB ID : 5AII  
Title : Discovery and characterization of thermophilic limonene-1,2-epoxide hydrolases from hot spring metagenomic libraries. CH55-sample-PEG complex  
Authors : Ferrandi, E.; Sayer, C.; Isupov, M.N.; Annovazzi, C.; Marchesi, C.; Iacobone, G.; Peng, X.; Bonch-Osmolovskaya, E.; Wohlgemuth, R.; Littlechild, J.A.; Montia, D.  
Deposited on : 2015-02-13  
Resolution : 1.47 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20026982

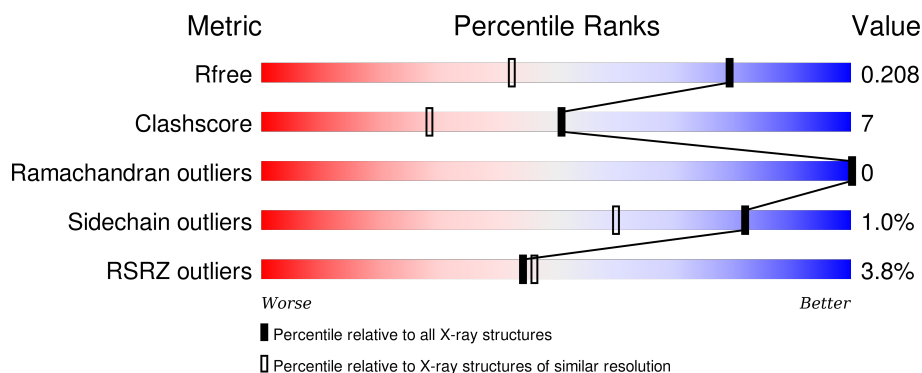
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.47 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))
$R_{free}$	91344	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (1.50-1.46)

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	135	
1	B	135	
1	C	135	
1	D	135	
1	E	135	

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Mol	Chain	Length	Quality of chain
1	F	135	
1	G	135	
1	H	135	
1	I	135	
1	J	135	
1	K	135	
1	L	135	
1	M	135	
1	N	135	
1	O	135	
1	P	135	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	D	1128	-	-	-	X
2	PG4	D	1129	-	-	-	X
2	PG4	F	1128	-	-	-	X
2	PG4	G	1128	-	-	-	X
2	PG4	I	1130	-	-	-	X
2	PG4	O	1129	-	-	-	X
3	PEG	B	1130	-	-	-	X
3	PEG	D	1127	-	-	-	X
3	PEG	F	1126	-	-	-	X
3	PEG	F	1127	-	-	-	X
3	PEG	I	1127	-	-	-	X
3	PEG	I	1128	-	-	-	X
3	PEG	K	1127	-	-	-	X
3	PEG	K	1128	-	-	-	X
3	PEG	O	1128	-	-	-	X
4	ACT	A	1128	-	-	-	X
4	ACT	C	1128	-	-	-	X
4	ACT	G	1127	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	H	1136	-	-	-	X
4	ACT	J	1127	-	-	-	X
4	ACT	K	1129	-	-	-	X
4	ACT	L	1129	-	-	-	X
4	ACT	M	1128	-	-	X	X
4	ACT	P	1128	-	-	X	X
5	EDO	C	1131	-	-	-	X
5	EDO	D	1131	-	-	-	X
5	EDO	M	1130	-	-	-	X
5	EDO	N	1138	-	-	-	X
5	EDO	P	1130	-	-	-	X
5	EDO	P	1131	-	-	-	X
7	PGE	D	1130	-	-	-	X
7	PGE	M	1129	-	-	-	X
7	PGE	N	1137	-	-	-	X
9	PG6	I	1129	-	-	-	X
9	PG6	N	1135	-	-	-	X

## 2 Entry composition

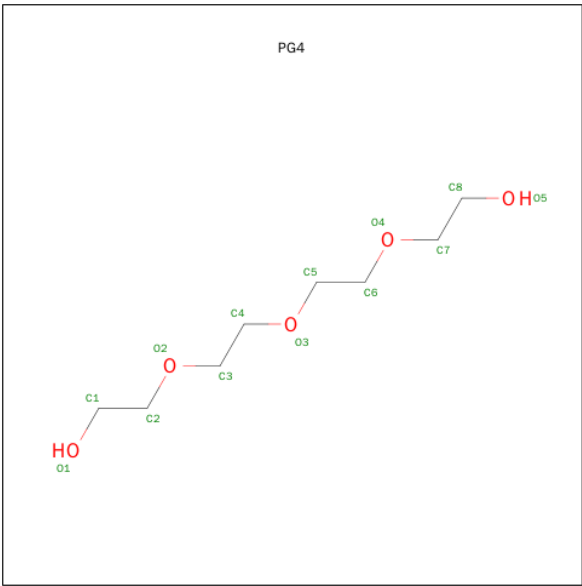
There are 10 unique types of molecules in this entry. The entry contains 18828 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIMONENE-1,2-EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	15	0
			1031	664	177	181	9			
1	B	127	Total	C	N	O	S	0	16	0
			1046	675	176	186	9			
1	C	126	Total	C	N	O	S	0	10	0
			1006	641	172	185	8			
1	D	125	Total	C	N	O	S	0	12	0
			1013	647	175	183	8			
1	E	125	Total	C	N	O	S	0	10	0
			1005	641	174	182	8			
1	F	124	Total	C	N	O	S	0	14	0
			1018	653	176	180	9			
1	G	125	Total	C	N	O	S	0	7	0
			983	623	171	182	7			
1	H	130	Total	C	N	O	S	0	13	1
			1062	679	188	187	8			
1	I	125	Total	C	N	O	S	0	13	0
			1017	651	174	184	8			
1	J	125	Total	C	N	O	S	0	14	0
			1025	654	176	187	8			
1	K	125	Total	C	N	O	S	0	7	0
			980	626	167	180	7			
1	L	125	Total	C	N	O	S	0	12	0
			1015	649	176	182	8			
1	M	125	Total	C	N	O	S	0	11	0
			1009	645	174	182	8			
1	N	130	Total	C	N	O	S	0	17	1
			1078	693	187	190	8			
1	O	125	Total	C	N	O	S	0	12	0
			1018	653	173	183	9			
1	P	126	Total	C	N	O	S	0	14	0
			1029	663	172	185	9			

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



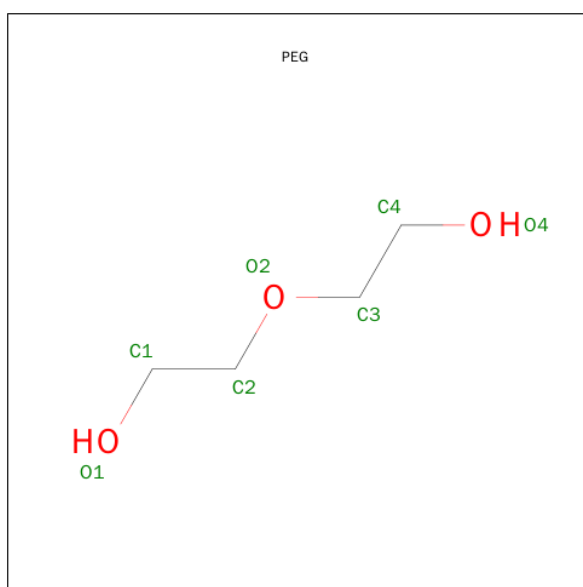
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	E	1	Total	C	O	0	0
			13	8	5		
2	F	1	Total	C	O	0	0
			13	8	5		
2	F	1	Total	C	O	0	0
			13	8	5		
2	G	1	Total	C	O	0	0
			13	8	5		
2	G	1	Total	C	O	0	0
			13	8	5		
2	H	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			13	8	5		
2	I	1	Total	C	O	0	0
			13	8	5		
2	I	1	Total	C	O	0	0
			13	8	5		
2	J	1	Total	C	O	0	0
			13	8	5		
2	K	1	Total	C	O	0	0
			13	8	5		
2	L	1	Total	C	O	0	0
			13	8	5		
2	M	1	Total	C	O	0	0
			13	8	5		
2	N	1	Total	C	O	0	0
			13	8	5		
2	O	1	Total	C	O	0	0
			13	8	5		
2	O	1	Total	C	O	0	0
			13	8	5		
2	P	1	Total	C	O	0	0
			13	8	5		

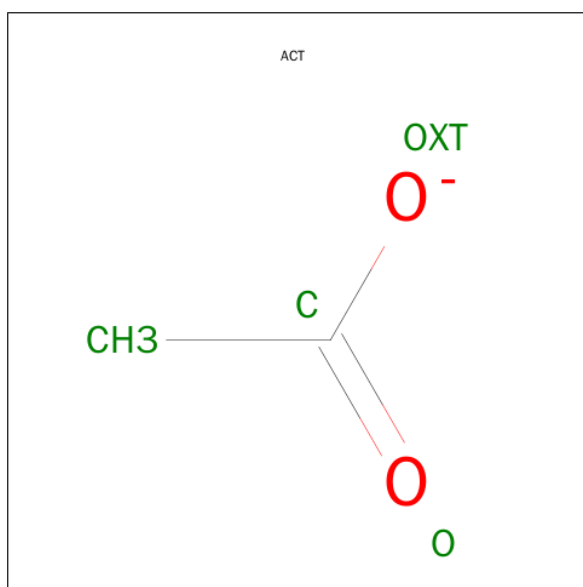
- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0
3	L	1	Total C O 7 4 3	0	0
3	L	1	Total C O 7 4 3	0	0
3	M	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0

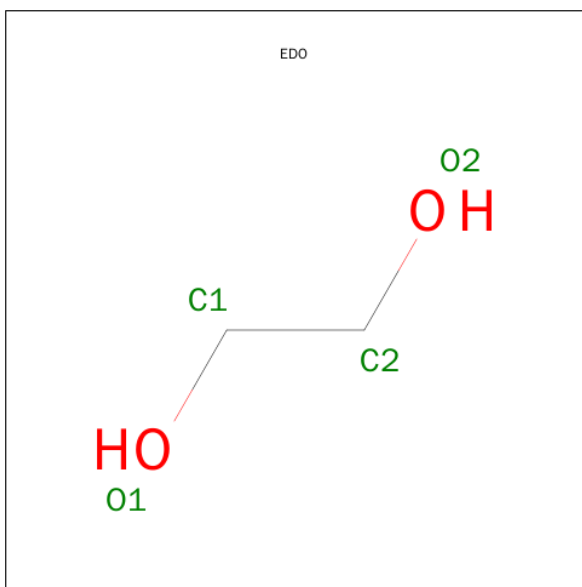
- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



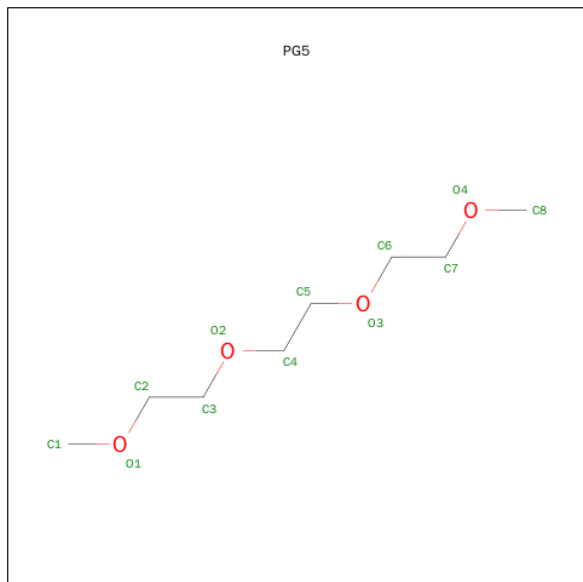
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		

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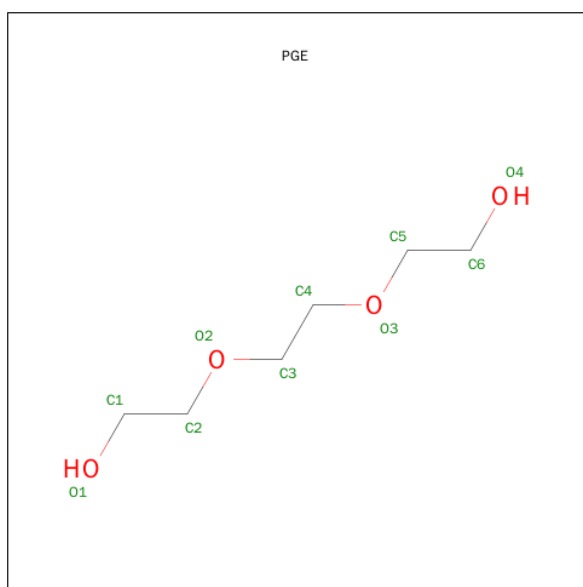
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (three-letter code: PG5) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>4</sub>).



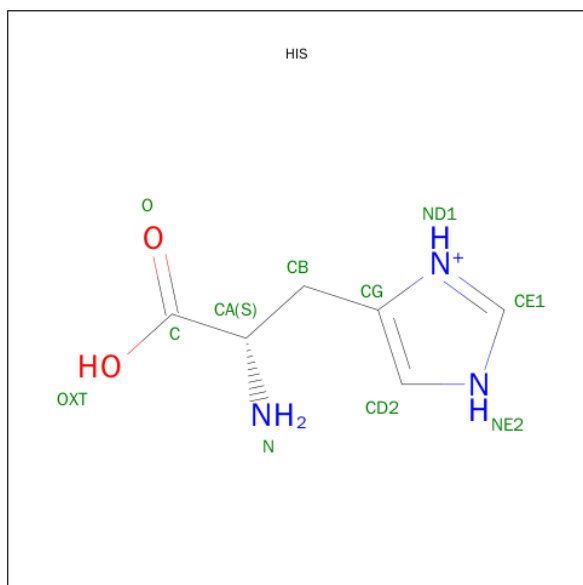
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



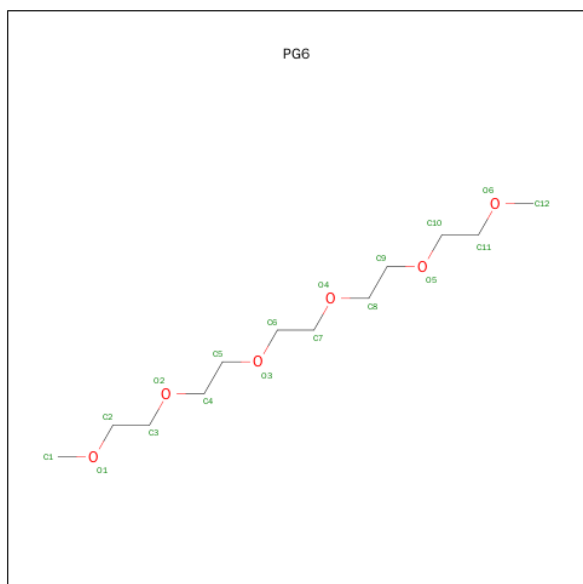
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		
7	K	1	Total	C	O	0	0
			10	6	4		
7	M	1	Total	C	O	0	0
			10	6	4		
7	N	1	Total	C	O	0	0
			10	6	4		
7	N	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is HISTIDINE (three-letter code: HIS) (formula:  $C_6H_{10}N_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 9 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
9	I	1	Total	C	O	0	0
			18	12	6		
9	N	1	Total	C	O	0	0
			18	12	6		

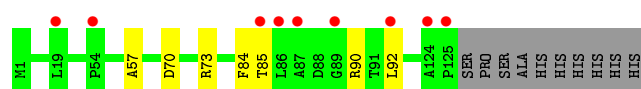
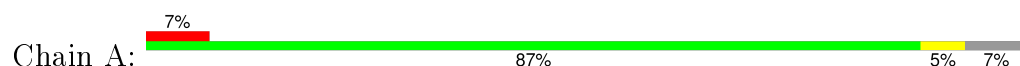
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	124	Total 124	O 124	0	0
10	B	114	Total 114	O 114	0	0
10	C	146	Total 146	O 146	0	0
10	D	140	Total 140	O 140	0	0
10	E	84	Total 84	O 84	0	0
10	F	94	Total 94	O 94	0	0
10	G	126	Total 126	O 126	0	0
10	H	97	Total 97	O 97	0	0
10	I	137	Total 137	O 137	0	0
10	J	95	Total 95	O 95	0	0
10	K	109	Total 109	O 109	0	0
10	L	80	Total 80	O 80	0	0
10	M	126	Total 126	O 126	0	0
10	N	137	Total 137	O 137	0	0
10	O	114	Total 114	O 114	0	0
10	P	107	Total 107	O 107	0	0

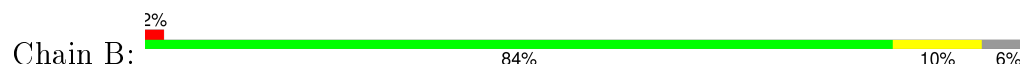
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

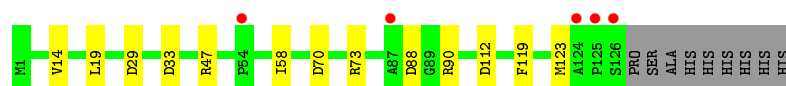
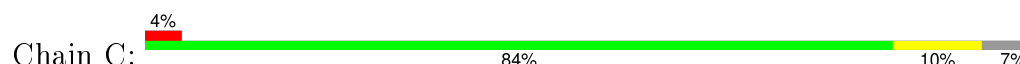
#### • Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



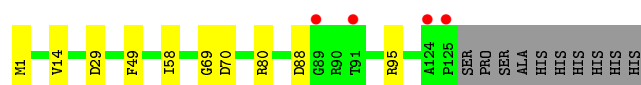
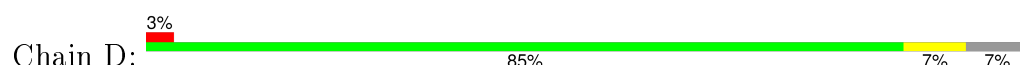
#### • Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



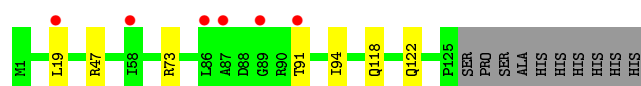
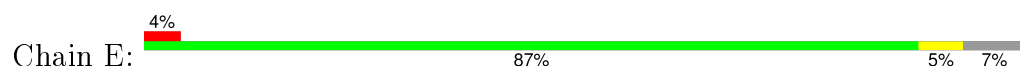
#### • Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



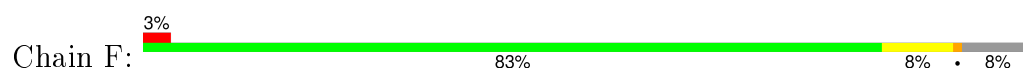
#### • Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



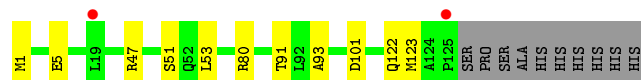
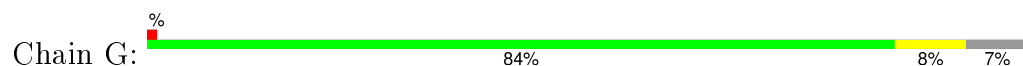
#### • Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



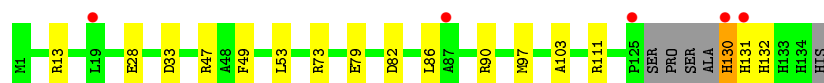
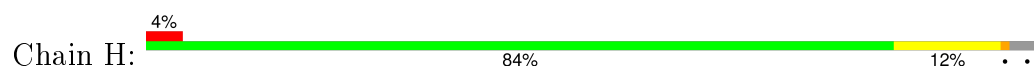
#### • Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



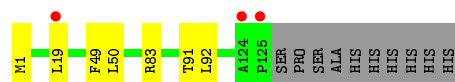
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



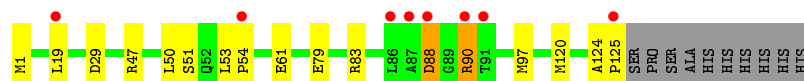
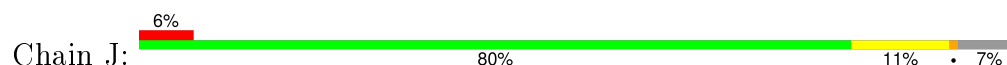
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



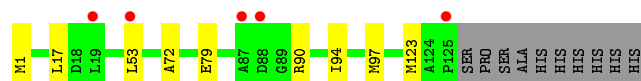
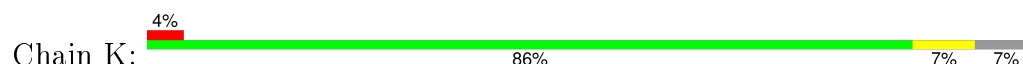
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



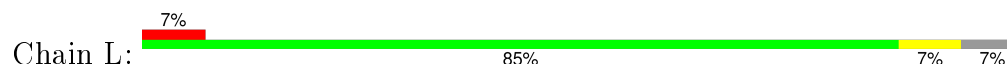
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE

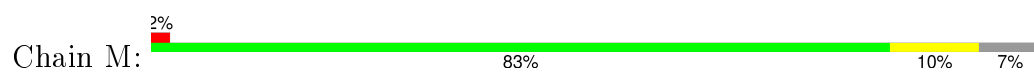


- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE

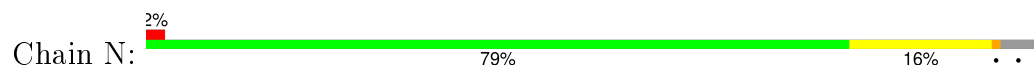


- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE

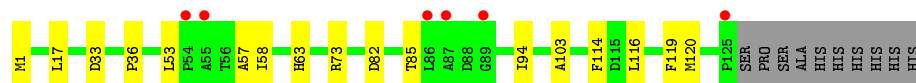
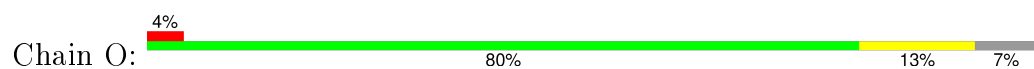




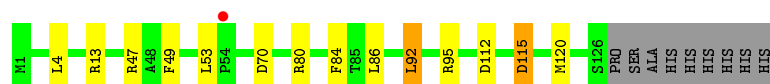
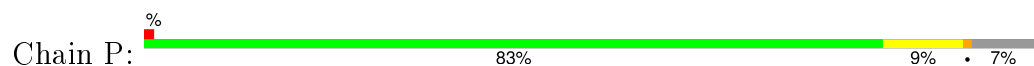
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.97Å 104.23Å 148.00Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	104.23 – 1.47 84.54 – 1.47	Depositor EDS
% Data completeness (in resolution range)	97.4 (104.23-1.47) 97.4 (84.54-1.47)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.175 , 0.208 0.175 , 0.208	Depositor DCC
$R_{free}$ test set	16691 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.8	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 336937 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.72 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.0485e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: PGE, EDO, PG6, PG4, PG5, ACT, 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	0.64	0/1094	0.86	1/1489 (0.1%)
1	B	0.63	0/1113	0.82	0/1517
1	C	0.73	0/1054	0.94	3/1435 (0.2%)
1	D	0.73	0/1068	0.92	4/1453 (0.3%)
1	E	0.64	0/1053	0.82	0/1433
1	F	0.65	0/1077	0.80	0/1464
1	G	0.71	0/1022	0.87	2/1392 (0.1%)
1	H	0.68	0/1124	0.88	3/1529 (0.2%)
1	I	0.63	0/1074	0.78	0/1463
1	J	0.63	0/1085	0.84	1/1475 (0.1%)
1	K	0.66	0/1019	0.84	0/1390
1	L	0.60	0/1069	0.81	2/1453 (0.1%)
1	M	0.68	0/1060	0.82	1/1442 (0.1%)
1	N	0.72	0/1152	0.96	4/1568 (0.3%)
1	O	0.75	0/1067	0.90	2/1452 (0.1%)
1	P	0.73	0/1090	0.99	8/1484 (0.5%)
All	All	0.68	0/17221	0.87	31/23439 (0.1%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	80	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	C	33	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	G	80	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	P	70	ASP	CB-CG-OD1	7.37	124.93	118.30
1	P	95	ARG	NE-CZ-NH1	7.04	123.82	120.30

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	1031	0	1087	6	0
1	B	1046	0	1103	13	0
1	C	1006	0	1028	17	0
1	D	1013	0	1044	10	0
1	E	1005	0	1031	13	0
1	F	1018	0	1069	12	0
1	G	983	0	995	8	0
1	H	1062	0	1080	15	0
1	I	1017	0	1056	8	0
1	J	1025	0	1060	20	0
1	K	980	0	998	14	0
1	L	1015	0	1052	9	0
1	M	1009	0	1038	11	0
1	N	1078	0	1105	37	0
1	O	1018	0	1046	21	0
1	P	1029	0	1068	21	0
2	A	13	0	18	0	0
2	B	26	0	36	3	0
2	C	13	0	18	0	0
2	D	39	0	54	7	0
2	E	13	0	18	0	0
2	F	26	0	36	1	0
2	G	26	0	36	0	0
2	H	26	0	36	3	0
2	I	26	0	36	5	0
2	J	13	0	18	0	0
2	K	13	0	18	3	0
2	L	13	0	18	0	0
2	M	13	0	18	1	0
2	N	13	0	18	2	0
2	O	26	0	36	2	0
2	P	13	0	18	5	0
3	A	7	0	10	0	0
3	B	14	0	20	0	0
3	D	7	0	10	1	0
3	F	14	0	20	1	0
3	H	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	14	0	20	0	0
3	K	14	0	20	3	0
3	L	14	0	20	1	0
3	M	7	0	10	2	0
3	O	14	0	20	1	0
4	A	4	0	3	0	0
4	C	8	0	6	1	0
4	G	4	0	3	0	0
4	H	8	0	6	0	0
4	J	4	0	3	0	0
4	K	4	0	3	0	0
4	L	4	0	3	0	0
4	M	4	0	3	2	0
4	P	4	0	3	10	0
5	A	4	0	6	0	0
5	C	4	0	6	3	0
5	D	16	0	24	0	0
5	F	4	0	6	0	0
5	G	8	0	12	0	0
5	H	4	0	6	1	0
5	L	4	0	6	0	0
5	M	8	0	12	0	0
5	N	4	0	6	0	0
5	P	20	0	30	5	0
6	A	12	0	18	0	0
7	C	10	0	14	0	0
7	D	10	0	14	1	0
7	K	10	0	14	0	0
7	M	10	0	14	0	0
7	N	20	0	28	3	0
8	F	11	0	6	0	0
9	I	18	0	26	2	0
9	N	18	0	26	3	0
10	A	124	0	0	1	0
10	B	114	0	0	4	0
10	C	146	0	0	5	0
10	D	140	0	0	6	0
10	E	84	0	0	1	0
10	F	94	0	0	3	0
10	G	126	0	0	2	0
10	H	97	0	0	3	0
10	I	137	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	95	0	0	3	0
10	K	109	0	0	5	0
10	L	80	0	0	1	0
10	M	126	0	0	3	0
10	N	137	0	0	6	0
10	O	114	0	0	4	0
10	P	107	0	0	3	0
All	All	18828	0	17759	239	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 7.

The worst 5 of 239 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:N:92[B]:LEU:HD11	1:N:123[B]:MET:CE	1.36	1.53
1:J:120[B]:MET:HE3	10:J:2094:HOH:O	1.20	1.33
1:N:91[A]:THR:HG22	10:N:2097:HOH:O	1.23	1.28
1:B:1[A]:MET:HE2	10:B:2003:HOH:O	1.13	1.26
1:F:1[A]:MET:HE2	10:F:2002:HOH:O	1.17	1.25

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	138/135 (102%)	135 (98%)	3 (2%)	0	100	100
1	B	140/135 (104%)	138 (99%)	2 (1%)	0	100	100
1	C	134/135 (99%)	133 (99%)	1 (1%)	0	100	100
1	D	134/135 (99%)	133 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
1	F	135/135 (100%)	134 (99%)	1 (1%)	0	100	100
1	G	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
1	H	138/135 (102%)	133 (96%)	5 (4%)	0	100	100
1	I	135/135 (100%)	133 (98%)	2 (2%)	0	100	100
1	J	136/135 (101%)	132 (97%)	4 (3%)	0	100	100
1	K	130/135 (96%)	129 (99%)	1 (1%)	0	100	100
1	L	135/135 (100%)	132 (98%)	3 (2%)	0	100	100
1	M	134/135 (99%)	131 (98%)	3 (2%)	0	100	100
1	N	142/135 (105%)	141 (99%)	1 (1%)	0	100	100
1	O	134/135 (99%)	133 (99%)	1 (1%)	0	100	100
1	P	138/135 (102%)	136 (99%)	2 (1%)	0	100	100
All	All	2165/2160 (100%)	2129 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	109/103 (106%)	109 (100%)	0	100	100
1	B	112/103 (109%)	112 (100%)	0	100	100
1	C	105/103 (102%)	105 (100%)	0	100	100
1	D	106/103 (103%)	105 (99%)	1 (1%)	84	64
1	E	104/103 (101%)	103 (99%)	1 (1%)	82	60
1	F	107/103 (104%)	105 (98%)	2 (2%)	65	30
1	G	101/103 (98%)	101 (100%)	0	100	100
1	H	111/103 (108%)	109 (98%)	2 (2%)	66	33
1	I	107/103 (104%)	105 (98%)	2 (2%)	65	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	108/103 (105%)	100 (93%)	8 (7%)	17	1
1	K	101/103 (98%)	100 (99%)	1 (1%)	82	60
1	L	106/103 (103%)	104 (98%)	2 (2%)	65	30
1	M	105/103 (102%)	105 (100%)	0	100	100
1	N	115/103 (112%)	110 (96%)	5 (4%)	35	6
1	O	106/103 (103%)	106 (100%)	0	100	100
1	P	109/103 (106%)	109 (100%)	0	100	100
All	All	1712/1648 (104%)	1688 (99%)	24 (1%)	82	46

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	51[A]	SER
1	J	88[B]	ASP
1	N	119[B]	PHE
1	J	51[B]	SER
1	J	88[A]	ASP

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

Mol	Chain	Res	Type
1	G	122	GLN
1	H	52	GLN
1	N	118	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 carbohydrates in this entry.



## 5.6 Ligand geometry

80 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	$\# Z  > 2$
2	PG4	A	1126	-	12,12,12	0.50	0	11,11,11	0.44	0
3	PEG	A	1127	-	6,6,6	0.33	0	5,5,5	0.82	0
4	ACT	A	1128	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	A	1129	-	3,3,3	0.44	0	2,2,2	0.45	0
6	PG5	A	1130	-	11,11,11	0.59	0	10,10,10	0.39	0
2	PG4	B	1128	-	12,12,12	0.55	0	11,11,11	0.35	0
2	PG4	B	1129	-	12,12,12	0.56	0	11,11,11	0.33	0
3	PEG	B	1130	-	6,6,6	0.48	0	5,5,5	0.28	0
3	PEG	B	1131	-	6,6,6	0.53	0	5,5,5	0.48	0
2	PG4	C	1127	-	12,12,12	0.59	0	11,11,11	0.53	0
4	ACT	C	1128	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	C	1129	-	0,3,3	0.00	-	0,3,3	0.00	-
7	PGE	C	1130	-	9,9,9	0.57	0	8,8,8	0.45	0
5	EDO	C	1131	-	3,3,3	0.31	0	2,2,2	0.97	0
2	PG4	D	1126	-	12,12,12	0.60	0	11,11,11	0.54	0
3	PEG	D	1127	-	6,6,6	0.48	0	5,5,5	0.59	0
2	PG4	D	1128	-	12,12,12	0.55	0	11,11,11	0.37	0
2	PG4	D	1129	-	12,12,12	0.52	0	11,11,11	0.51	0
7	PGE	D	1130	-	9,9,9	0.75	0	8,8,8	1.14	1 (12%)
5	EDO	D	1131	-	3,3,3	0.40	0	2,2,2	0.35	0
5	EDO	D	1132	-	3,3,3	0.42	0	2,2,2	0.51	0
5	EDO	D	1133	-	3,3,3	0.46	0	2,2,2	0.41	0
5	EDO	D	1134	-	3,3,3	0.47	0	2,2,2	0.34	0
2	PG4	E	1126	-	12,12,12	0.57	0	11,11,11	0.47	0
2	PG4	F	1125	-	12,12,12	0.56	0	11,11,11	0.40	0
3	PEG	F	1126	-	6,6,6	0.38	0	5,5,5	0.55	0
3	PEG	F	1127	-	6,6,6	0.54	0	5,5,5	0.34	0
2	PG4	F	1128	-	12,12,12	0.57	0	11,11,11	0.40	0
5	EDO	F	1129	-	3,3,3	0.46	0	2,2,2	0.39	0
8	HIS	F	1130	-	4,11,11	0.46	0	3,14,14	1.27	1 (33%)
2	PG4	G	1126	-	12,12,12	0.63	0	11,11,11	0.51	0
4	ACT	G	1127	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PG4	G	1128	-	12,12,12	0.50	0	11,11,11	0.68	0
5	EDO	G	1129	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	G	1130	-	3,3,3	0.44	0	2,2,2	0.18	0
2	PG4	H	1134	-	12,12,12	0.50	0	11,11,11	0.46	0
3	PEG	H	1135	-	6,6,6	0.46	0	5,5,5	0.34	0
4	ACT	H	1136	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	H	1137	-	0,3,3	0.00	-	0,3,3	0.00	-
2	PG4	H	1138	-	12,12,12	0.53	0	11,11,11	0.27	0
5	EDO	H	1139	-	3,3,3	0.29	0	2,2,2	0.84	0
2	PG4	I	1126	-	12,12,12	0.50	0	11,11,11	0.45	0
3	PEG	I	1127	-	6,6,6	0.54	0	5,5,5	0.29	0
3	PEG	I	1128	-	6,6,6	0.51	0	5,5,5	0.24	0
9	PG6	I	1129	-	17,17,17	0.67	0	16,16,16	0.51	0
2	PG4	I	1130	-	12,12,12	0.55	0	11,11,11	0.20	0
2	PG4	J	1126	-	12,12,12	0.51	0	11,11,11	0.56	0
4	ACT	J	1127	-	0,3,3	0.00	-	0,3,3	0.00	-
2	PG4	K	1126	-	12,12,12	0.51	0	11,11,11	0.49	0
3	PEG	K	1127	-	6,6,6	0.46	0	5,5,5	0.55	0
3	PEG	K	1128	-	6,6,6	0.48	0	5,5,5	0.25	0
4	ACT	K	1129	-	0,3,3	0.00	-	0,3,3	0.00	-
7	PGE	K	1130	-	9,9,9	0.44	0	8,8,8	0.50	0
2	PG4	L	1126	-	12,12,12	0.45	0	11,11,11	0.52	0
3	PEG	L	1127	-	6,6,6	0.47	0	5,5,5	0.39	0
3	PEG	L	1128	-	6,6,6	0.49	0	5,5,5	0.41	0
4	ACT	L	1129	-	0,3,3	0.00	-	0,3,3	0.00	-
5	EDO	L	1130	-	3,3,3	0.44	0	2,2,2	0.40	0
2	PG4	M	1126	-	12,12,12	0.58	0	11,11,11	0.65	0
3	PEG	M	1127	-	6,6,6	0.44	0	5,5,5	0.74	0
4	ACT	M	1128	-	0,3,3	0.00	-	0,3,3	0.00	-
7	PGE	M	1129	-	9,9,9	0.42	0	8,8,8	0.74	0
5	EDO	M	1130	-	3,3,3	0.46	0	2,2,2	0.39	0
5	EDO	M	1131	-	3,3,3	0.39	0	2,2,2	0.49	0
2	PG4	N	1134	-	12,12,12	0.50	0	11,11,11	0.40	0
9	PG6	N	1135	-	17,17,17	0.56	0	16,16,16	0.51	0
7	PGE	N	1136	-	9,9,9	0.50	0	8,8,8	0.56	0
7	PGE	N	1137	-	9,9,9	0.46	0	8,8,8	0.37	0
5	EDO	N	1138	-	3,3,3	0.49	0	2,2,2	0.40	0
2	PG4	O	1126	-	12,12,12	0.59	0	11,11,11	0.41	0
3	PEG	O	1127	-	6,6,6	0.42	0	5,5,5	0.38	0
3	PEG	O	1128	-	6,6,6	0.50	0	5,5,5	0.35	0
2	PG4	O	1129	-	12,12,12	0.68	0	11,11,11	0.73	0
2	PG4	P	1127	-	12,12,12	0.47	0	11,11,11	0.79	0
4	ACT	P	1128	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	P	1129	-	3,3,3	0.35	0	2,2,2	0.44	0
5	EDO	P	1130	-	3,3,3	0.51	0	2,2,2	0.13	0
5	EDO	P	1131	-	3,3,3	0.66	0	2,2,2	0.41	0
5	EDO	P	1132	-	3,3,3	0.47	0	2,2,2	0.16	0
5	EDO	P	1133	-	3,3,3	0.46	0	2,2,2	0.38	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	PG4	A	1126	-	-	0/10/10/10	0/0/0/0
3	PEG	A	1127	-	-	0/4/4/4	0/0/0/0
4	ACT	A	1128	-	-	0/0/0/0	0/0/0/0
5	EDO	A	1129	-	-	0/1/1/1	0/0/0/0
6	PG5	A	1130	-	-	0/9/9/9	0/0/0/0
2	PG4	B	1128	-	-	0/10/10/10	0/0/0/0
2	PG4	B	1129	-	-	0/10/10/10	0/0/0/0
3	PEG	B	1130	-	-	0/4/4/4	0/0/0/0
3	PEG	B	1131	-	-	0/4/4/4	0/0/0/0
2	PG4	C	1127	-	-	0/10/10/10	0/0/0/0
4	ACT	C	1128	-	-	0/0/0/0	0/0/0/0
4	ACT	C	1129	-	-	0/0/0/0	0/0/0/0
7	PGE	C	1130	-	-	0/7/7/7	0/0/0/0
5	EDO	C	1131	-	-	0/1/1/1	0/0/0/0
2	PG4	D	1126	-	-	0/10/10/10	0/0/0/0
3	PEG	D	1127	-	-	0/4/4/4	0/0/0/0
2	PG4	D	1128	-	-	0/10/10/10	0/0/0/0
2	PG4	D	1129	-	-	0/10/10/10	0/0/0/0
7	PGE	D	1130	-	-	0/7/7/7	0/0/0/0
5	EDO	D	1131	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1132	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1133	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1134	-	-	0/1/1/1	0/0/0/0
2	PG4	E	1126	-	-	0/10/10/10	0/0/0/0
2	PG4	F	1125	-	-	0/10/10/10	0/0/0/0
3	PEG	F	1126	-	-	0/4/4/4	0/0/0/0
3	PEG	F	1127	-	-	0/4/4/4	0/0/0/0
2	PG4	F	1128	-	-	0/10/10/10	0/0/0/0
5	EDO	F	1129	-	-	0/1/1/1	0/0/0/0
8	HIS	F	1130	-	-	0/4/8/8	0/1/1/1
2	PG4	G	1126	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACT	G	1127	-	-	0/0/0/0	0/0/0/0
2	PG4	G	1128	-	-	0/10/10/10	0/0/0/0
5	EDO	G	1129	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1130	-	-	0/1/1/1	0/0/0/0
2	PG4	H	1134	-	-	0/10/10/10	0/0/0/0
3	PEG	H	1135	-	-	0/4/4/4	0/0/0/0
4	ACT	H	1136	-	-	0/0/0/0	0/0/0/0
4	ACT	H	1137	-	-	0/0/0/0	0/0/0/0
2	PG4	H	1138	-	-	0/10/10/10	0/0/0/0
5	EDO	H	1139	-	-	0/1/1/1	0/0/0/0
2	PG4	I	1126	-	-	0/10/10/10	0/0/0/0
3	PEG	I	1127	-	-	0/4/4/4	0/0/0/0
3	PEG	I	1128	-	-	0/4/4/4	0/0/0/0
9	PG6	I	1129	-	-	0/15/15/15	0/0/0/0
2	PG4	I	1130	-	-	0/10/10/10	0/0/0/0
2	PG4	J	1126	-	-	0/10/10/10	0/0/0/0
4	ACT	J	1127	-	-	0/0/0/0	0/0/0/0
2	PG4	K	1126	-	-	0/10/10/10	0/0/0/0
3	PEG	K	1127	-	-	0/4/4/4	0/0/0/0
3	PEG	K	1128	-	-	0/4/4/4	0/0/0/0
4	ACT	K	1129	-	-	0/0/0/0	0/0/0/0
7	PGE	K	1130	-	-	0/7/7/7	0/0/0/0
2	PG4	L	1126	-	-	0/10/10/10	0/0/0/0
3	PEG	L	1127	-	-	0/4/4/4	0/0/0/0
3	PEG	L	1128	-	-	0/4/4/4	0/0/0/0
4	ACT	L	1129	-	-	0/0/0/0	0/0/0/0
5	EDO	L	1130	-	-	0/1/1/1	0/0/0/0
2	PG4	M	1126	-	-	0/10/10/10	0/0/0/0
3	PEG	M	1127	-	-	0/4/4/4	0/0/0/0
4	ACT	M	1128	-	-	0/0/0/0	0/0/0/0
7	PGE	M	1129	-	-	0/7/7/7	0/0/0/0
5	EDO	M	1130	-	-	0/1/1/1	0/0/0/0
5	EDO	M	1131	-	-	0/1/1/1	0/0/0/0
2	PG4	N	1134	-	-	0/10/10/10	0/0/0/0
9	PG6	N	1135	-	-	0/15/15/15	0/0/0/0
7	PGE	N	1136	-	-	0/7/7/7	0/0/0/0
7	PGE	N	1137	-	-	0/7/7/7	0/0/0/0
5	EDO	N	1138	-	-	0/1/1/1	0/0/0/0
2	PG4	O	1126	-	-	0/10/10/10	0/0/0/0
3	PEG	O	1127	-	-	0/4/4/4	0/0/0/0
3	PEG	O	1128	-	-	0/4/4/4	0/0/0/0
2	PG4	O	1129	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	P	1127	-	-	0/10/10/10	0/0/0/0
4	ACT	P	1128	-	-	0/0/0/0	0/0/0/0
5	EDO	P	1129	-	-	0/1/1/1	0/0/0/0
5	EDO	P	1130	-	-	0/1/1/1	0/0/0/0
5	EDO	P	1131	-	-	0/1/1/1	0/0/0/0
5	EDO	P	1132	-	-	0/1/1/1	0/0/0/0
5	EDO	P	1133	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1130	PGE	O2-C3-C4	2.00	119.28	110.40
8	F	1130	HIS	CD2-NE2-CE1	2.03	109.14	105.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1128	PG4	3	0
4	C	1129	ACT	1	0
5	C	1131	EDO	3	0
2	D	1126	PG4	2	0
3	D	1127	PEG	1	0
2	D	1129	PG4	5	0
7	D	1130	PGE	1	0
3	F	1126	PEG	1	0
2	F	1128	PG4	1	0
2	H	1134	PG4	3	0
5	H	1139	EDO	1	0
2	I	1126	PG4	2	0
9	I	1129	PG6	2	0
2	I	1130	PG4	3	0
2	K	1126	PG4	3	0
3	K	1128	PEG	3	0
3	L	1127	PEG	1	0
2	M	1126	PG4	1	0
3	M	1127	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1128	ACT	2	0
2	N	1134	PG4	2	0
9	N	1135	PG6	3	0
7	N	1137	PGE	3	0
2	O	1126	PG4	2	0
3	O	1128	PEG	1	0
2	P	1127	PG4	5	0
4	P	1128	ACT	10	0
5	P	1130	EDO	2	0
5	P	1131	EDO	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	125/135 (92%)	0.08	9 (7%) 18 19	16, 25, 51, 94	0
1	B	127/135 (94%)	-0.07	3 (2%) 62 65	16, 26, 46, 71	0
1	C	126/135 (93%)	-0.18	5 (3%) 42 44	10, 17, 45, 86	0
1	D	125/135 (92%)	-0.25	4 (3%) 51 53	11, 17, 44, 85	0
1	E	125/135 (92%)	0.32	6 (4%) 34 35	17, 31, 56, 76	0
1	F	124/135 (91%)	-0.09	4 (3%) 51 53	16, 25, 54, 72	0
1	G	125/135 (92%)	-0.26	2 (1%) 74 78	13, 19, 41, 82	0
1	H	130/135 (96%)	-0.10	5 (3%) 44 46	13, 25, 45, 67	0
1	I	125/135 (92%)	-0.26	3 (2%) 62 65	14, 21, 44, 96	0
1	J	125/135 (92%)	-0.16	8 (6%) 23 23	14, 23, 59, 76	0
1	K	125/135 (92%)	-0.14	5 (4%) 42 44	14, 23, 49, 79	0
1	L	125/135 (92%)	0.14	10 (8%) 15 15	15, 26, 62, 90	0
1	M	125/135 (92%)	-0.23	3 (2%) 62 65	12, 21, 38, 55	0
1	N	130/135 (96%)	-0.18	3 (2%) 64 67	12, 19, 37, 81	0
1	O	125/135 (92%)	-0.17	6 (4%) 34 35	10, 17, 46, 70	0
1	P	126/135 (93%)	-0.37	1 (0%) 87 89	10, 16, 32, 61	0
All	All	2013/2160 (93%)	-0.12	77 (3%) 44 46	10, 22, 49, 96	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	87	ALA	7.5
1	N	125	PRO	5.9
1	I	125	PRO	5.4
1	A	87	ALA	5.3
1	K	125	PRO	4.7

## 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( $\text{\AA}^2$ )	Q<0.9
5	EDO	D	1131	4/4	0.91	0.12	20.12	39,43,49,54	0
3	PEG	F	1126	7/7	0.89	0.14	13.83	38,50,56,65	0
3	PEG	I	1127	7/7	0.89	0.10	10.68	31,43,50,50	0
7	PGE	D	1130	10/10	0.83	0.14	9.85	22,34,45,47	0
4	ACT	K	1129	4/4	0.84	0.15	9.34	47,50,50,56	0
3	PEG	D	1127	7/7	0.91	0.10	8.14	35,48,54,60	0
5	EDO	P	1131	4/4	0.94	0.16	8.03	18,32,33,37	0
4	ACT	P	1128	4/4	0.95	0.18	7.36	24,28,36,42	0
5	EDO	P	1130	4/4	0.97	0.17	6.97	21,21,22,60	0
4	ACT	L	1129	4/4	0.92	0.11	6.80	30,30,32,34	0
4	ACT	M	1128	4/4	0.94	0.10	6.31	18,20,22,25	0
5	EDO	C	1131	4/4	0.95	0.26	5.92	21,22,33,35	0
9	PG6	N	1135	18/18	0.86	0.13	5.90	28,46,60,64	0
2	PG4	F	1128	13/13	0.83	0.13	5.65	31,42,51,57	13
2	PG4	G	1128	13/13	0.82	0.17	5.63	27,31,43,45	13
3	PEG	I	1128	7/7	0.87	0.10	5.28	43,54,58,64	0
4	ACT	J	1127	4/4	0.94	0.09	5.04	30,32,33,33	0
3	PEG	O	1128	7/7	0.90	0.10	5.02	44,47,55,58	0
2	PG4	D	1128	13/13	0.83	0.14	4.20	33,41,53,55	0
5	EDO	M	1130	4/4	0.73	0.12	4.10	52,58,62,67	0
3	PEG	K	1128	7/7	0.79	0.16	4.04	44,52,56,58	0
4	ACT	A	1128	4/4	0.93	0.12	3.63	37,37,41,42	0
4	ACT	C	1128	4/4	0.93	0.09	3.28	26,27,28,29	0
3	PEG	F	1127	7/7	0.87	0.12	3.24	39,46,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	N	1138	4/4	0.81	0.10	3.18	42,45,46,51	0
4	ACT	G	1127	4/4	0.82	0.16	3.06	48,53,55,61	0
7	PGE	M	1129	10/10	0.95	0.09	2.98	27,30,49,50	0
2	PG4	D	1129	13/13	0.89	0.12	2.88	27,42,54,56	0
3	PEG	B	1130	7/7	0.91	0.08	2.88	41,48,56,59	0
2	PG4	I	1130	13/13	0.81	0.13	2.85	43,51,57,60	0
4	ACT	H	1136	4/4	0.97	0.08	2.37	20,25,25,25	0
2	PG4	O	1129	13/13	0.87	0.10	2.32	30,37,42,45	0
9	PG6	I	1129	18/18	0.88	0.11	2.30	26,35,45,62	0
7	PGE	N	1137	10/10	0.90	0.15	2.22	28,35,42,52	10
3	PEG	K	1127	7/7	0.87	0.09	2.04	45,54,59,61	0
2	PG4	H	1138	13/13	0.91	0.10	1.60	30,41,57,66	0
7	PGE	K	1130	10/10	0.93	0.10	1.37	32,42,44,57	0
3	PEG	A	1127	7/7	0.90	0.14	1.20	33,51,65,70	0
5	EDO	G	1130	4/4	0.86	0.12	1.14	38,39,45,46	0
2	PG4	B	1129	13/13	0.85	0.12	1.10	32,45,53,57	0
7	PGE	N	1136	10/10	0.92	0.11	1.06	29,37,50,51	0
3	PEG	M	1127	7/7	0.88	0.10	1.00	34,40,52,53	0
2	PG4	D	1126	13/13	0.94	0.10	0.96	18,34,52,53	0
3	PEG	L	1128	7/7	0.85	0.12	0.86	31,37,40,49	7
2	PG4	K	1126	13/13	0.95	0.14	0.78	22,41,72,76	0
3	PEG	L	1127	7/7	0.92	0.10	0.77	36,40,49,56	0
4	ACT	C	1129	4/4	0.96	0.11	0.67	23,34,38,56	0
2	PG4	L	1126	13/13	0.93	0.09	0.64	27,37,61,64	0
3	PEG	O	1127	7/7	0.92	0.10	0.63	32,47,55,59	0
5	EDO	H	1139	4/4	0.86	0.13	0.63	39,43,49,50	0
2	PG4	A	1126	13/13	0.94	0.12	0.62	26,48,81,81	0
2	PG4	M	1126	13/13	0.94	0.09	0.57	18,26,39,44	0
2	PG4	F	1125	13/13	0.92	0.12	0.57	29,44,99,106	0
3	PEG	B	1131	7/7	0.81	0.16	0.54	41,54,63,72	0
2	PG4	C	1127	13/13	0.93	0.09	0.48	19,29,48,49	0
7	PGE	C	1130	10/10	0.90	0.10	0.47	25,35,49,54	0
2	PG4	E	1126	13/13	0.91	0.12	0.44	27,51,68,72	0
2	PG4	B	1128	13/13	0.91	0.14	0.43	26,38,76,79	0
6	PG5	A	1130	12/12	0.88	0.09	0.33	33,40,49,55	0
2	PG4	P	1127	13/13	0.96	0.10	0.29	17,29,53,55	0
2	PG4	G	1126	13/13	0.94	0.11	0.25	18,31,57,63	0
5	EDO	D	1133	4/4	0.89	0.10	0.19	35,46,53,57	0
4	ACT	H	1137	4/4	0.85	0.09	0.18	43,46,54,62	0
5	EDO	P	1133	4/4	0.88	0.11	0.12	44,48,56,62	0
2	PG4	I	1126	13/13	0.95	0.10	0.09	22,41,62,70	0
2	PG4	O	1126	13/13	0.94	0.10	0.07	21,36,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PG4	N	1134	13/13	0.95	0.09	0.04	18,34,46,61	0
2	PG4	J	1126	13/13	0.95	0.07	0.01	22,32,56,61	0
5	EDO	A	1129	4/4	0.73	0.14	-0.40	57,60,64,67	0
5	EDO	D	1134	4/4	0.78	0.11	-0.41	48,51,57,59	0
5	EDO	P	1132	4/4	0.90	0.08	-0.60	35,42,43,46	0
5	EDO	F	1129	4/4	0.83	0.10	-0.65	46,50,52,59	0
2	PG4	H	1134	13/13	0.95	0.07	-0.90	21,28,48,57	0
5	EDO	D	1132	4/4	0.87	0.07	-1.42	45,48,50,54	0
8	HIS	F	1130	11/11	0.84	0.12	-	36,42,64,70	0
3	PEG	H	1135	7/7	0.92	0.14	-	49,54,62,67	0
5	EDO	L	1130	4/4	0.87	0.11	-	37,52,55,62	0
5	EDO	M	1131	4/4	0.88	0.08	-	49,50,54,62	0
5	EDO	G	1129	4/4	0.91	0.08	-	44,44,47,54	0
5	EDO	P	1129	4/4	0.95	0.09	-	28,29,37,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.