



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:38 AM BST

PDB ID : 5KC9  
Title : Crystal structure of the amino-terminal domain (ATD) of iGluR Delta-1 (GluD1)  
Authors : Elegheert, J.; Clay, J.E.; Siebold, C.; Aricescu, A.R.  
Deposited on : 2016-06-05  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

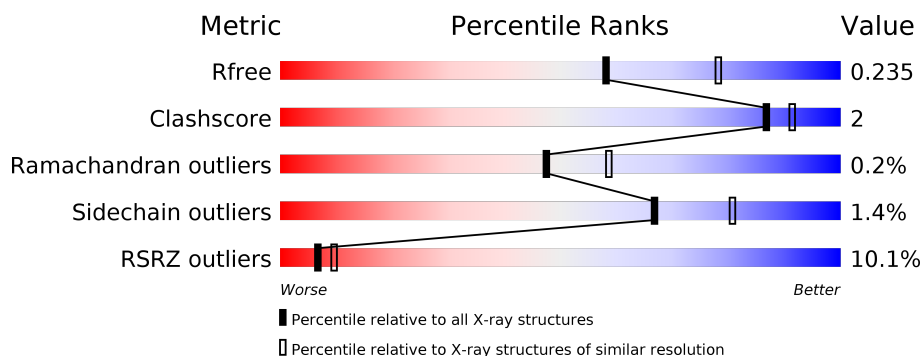
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	428	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	428	<div> <div>16%</div> <div> <div></div> <div>84%</div> <div>•</div> <div>13%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	509	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9483 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 Glutamate receptor ionotropic, delta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3199	2009	561	610	19			
1	B	382	Total	C	N	O	S	0	1	0
			3016	1898	531	570	17			
1	C	372	Total	C	N	O	S	0	0	0
			2892	1817	509	548	18			

There are 36 discrepancies between the modelled and reference sequences:

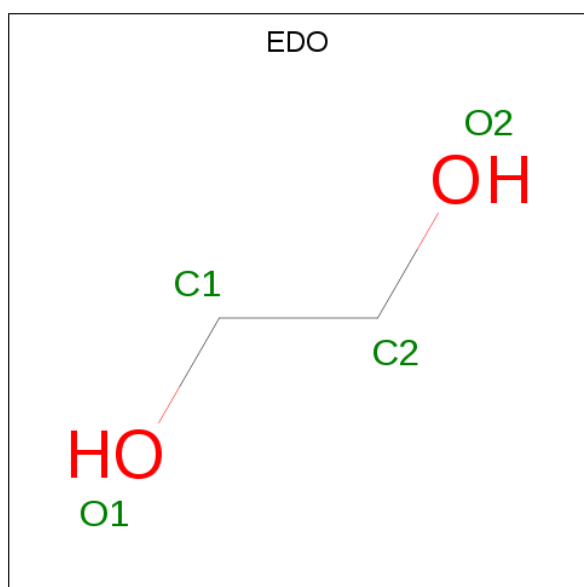
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	expression tag	UNP Q61627
A	19	THR	-	expression tag	UNP Q61627
A	20	GLY	-	expression tag	UNP Q61627
A	437	GLY	-	expression tag	UNP Q61627
A	438	THR	-	expression tag	UNP Q61627
A	439	LYS	-	expression tag	UNP Q61627
A	440	HIS	-	expression tag	UNP Q61627
A	441	HIS	-	expression tag	UNP Q61627
A	442	HIS	-	expression tag	UNP Q61627
A	443	HIS	-	expression tag	UNP Q61627
A	444	HIS	-	expression tag	UNP Q61627
A	445	HIS	-	expression tag	UNP Q61627
B	18	GLU	-	expression tag	UNP Q61627
B	19	THR	-	expression tag	UNP Q61627
B	20	GLY	-	expression tag	UNP Q61627
B	437	GLY	-	expression tag	UNP Q61627
B	438	THR	-	expression tag	UNP Q61627
B	439	LYS	-	expression tag	UNP Q61627
B	440	HIS	-	expression tag	UNP Q61627
B	441	HIS	-	expression tag	UNP Q61627
B	442	HIS	-	expression tag	UNP Q61627
B	443	HIS	-	expression tag	UNP Q61627
B	444	HIS	-	expression tag	UNP Q61627

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	445	HIS	-	expression tag	UNP Q61627
C	18	GLU	-	expression tag	UNP Q61627
C	19	THR	-	expression tag	UNP Q61627
C	20	GLY	-	expression tag	UNP Q61627
C	437	GLY	-	expression tag	UNP Q61627
C	438	THR	-	expression tag	UNP Q61627
C	439	LYS	-	expression tag	UNP Q61627
C	440	HIS	-	expression tag	UNP Q61627
C	441	HIS	-	expression tag	UNP Q61627
C	442	HIS	-	expression tag	UNP Q61627
C	443	HIS	-	expression tag	UNP Q61627
C	444	HIS	-	expression tag	UNP Q61627
C	445	HIS	-	expression tag	UNP Q61627

- Molecule 2 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
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

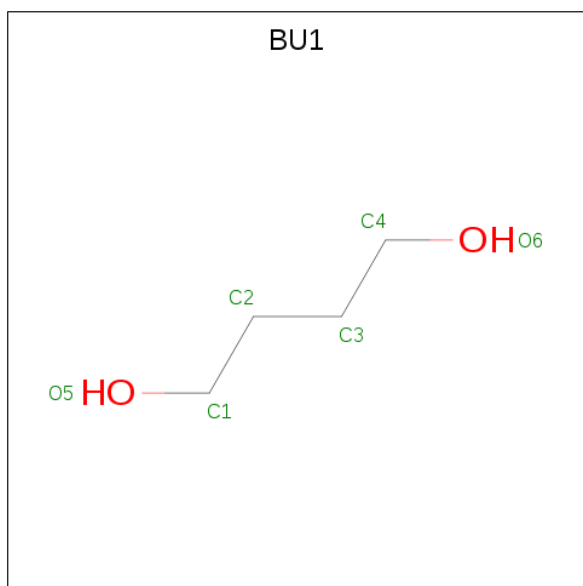
Continued from previous page...

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cl	0	0
			4	4		
3	A	5	Total	Cl	0	0
			5	5		
3	C	5	Total	Cl	0	0
			5	5		

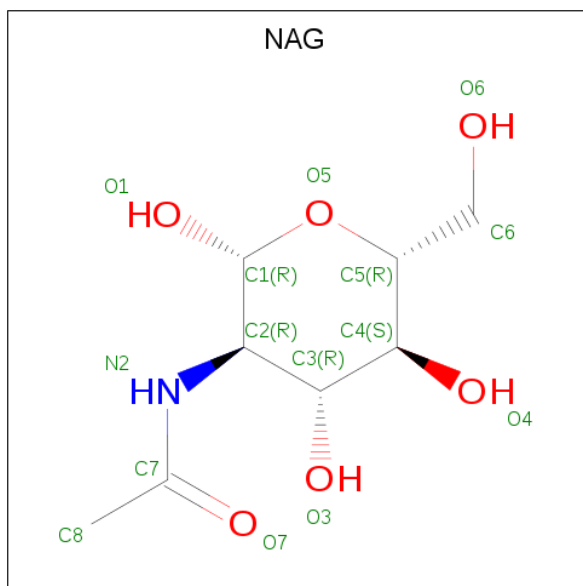
- Molecule 4 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		

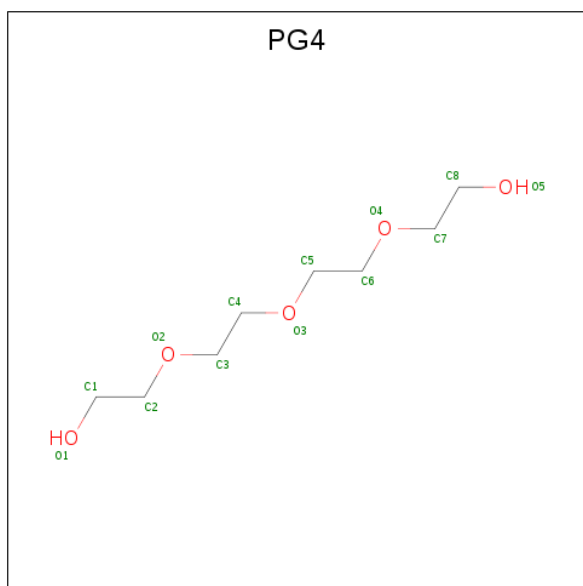
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 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
6	A	1	Total	C	O	0	0
			13	8	5		

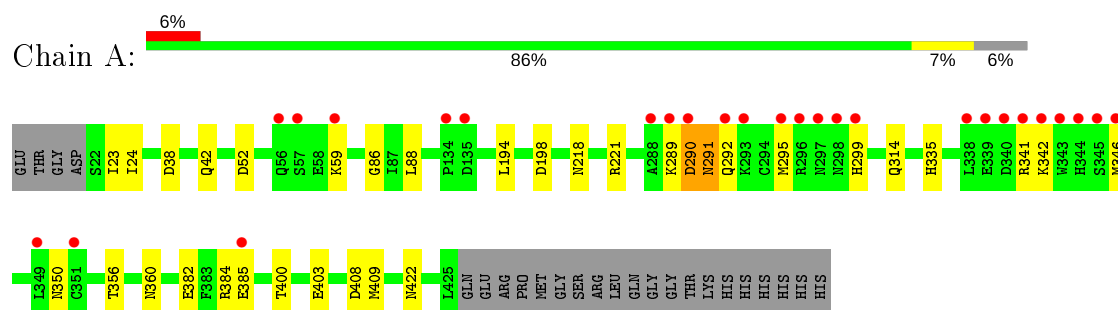
- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	89	Total	O		0	0
			89	89			
7	B	58	Total	O		0	0
			58	58			
7	C	32	Total	O		0	0
			32	32			

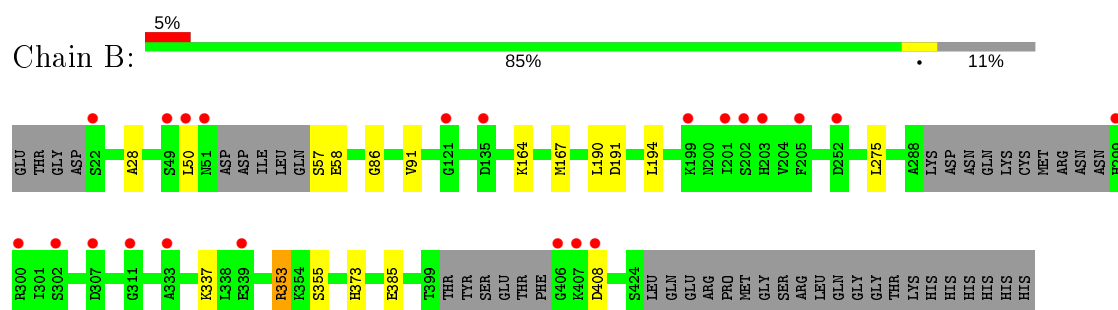
### 3 Residue-property plots [i](#)

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.

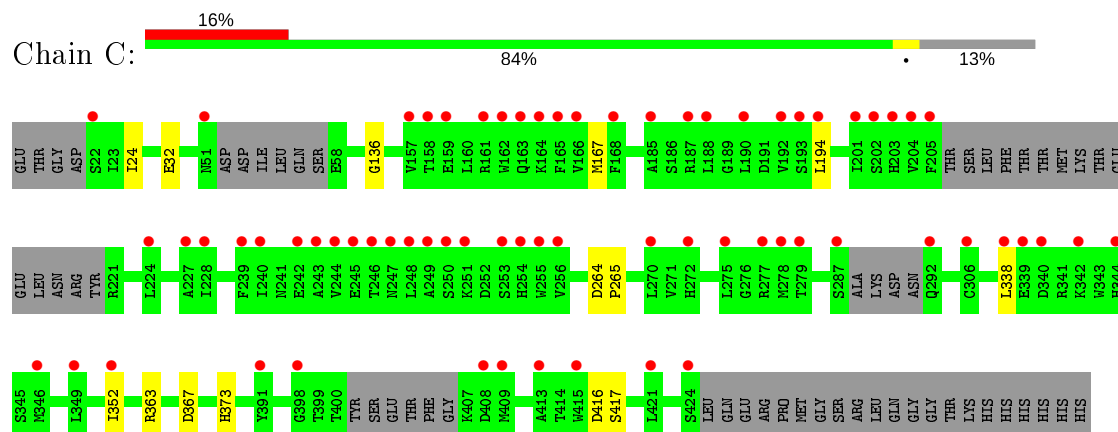
- Molecule 1: Glutamate receptor ionotropic, delta-1



- Molecule 1: Glutamate receptor ionotropic, delta-1



- Molecule 1: Glutamate receptor ionotropic, delta-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.42Å 128.42Å 153.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.22 – 2.30 59.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.22-2.30) 99.7 (59.22-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_1772	Depositor
R, $R_{free}$	0.199 , 0.227 0.206 , 0.235	Depositor DCC
$R_{free}$ test set	3276 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: PG4, BU1, EDO, NAG, CL

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	0.27	0/3260	0.47	0/4411
1	B	0.25	0/3071	0.44	0/4152
1	C	0.24	0/2943	0.43	0/3980
All	All	0.26	0/9274	0.45	0/12543

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	3199	0	3166	21	0
1	B	3016	0	2994	8	0
1	C	2892	0	2833	8	1
2	A	56	0	84	0	0
2	B	36	0	54	0	0
2	C	24	0	36	0	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	5	0	0	0	0
4	A	6	0	10	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	0	10	2	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
6	A	13	0	18	5	0
7	A	89	0	0	0	0
7	B	58	0	0	0	0
7	C	32	0	0	0	0
All	All	9483	0	9244	39	1

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 2.

All (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:382:GLU:OE2	1:A:384:ARG:NH2	2.29	0.66
1:A:422:ASN:ND2	5:A:522:NAG:O7	2.30	0.64
1:C:416:ASP:OD1	1:C:417:SER:N	2.36	0.59
1:A:23:ILE:HD12	1:A:24:ILE:H	1.74	0.52
1:A:218:ASN:OD1	1:A:221:ARG:NH2	2.43	0.52
1:C:24:ILE:HD11	1:C:338:LEU:HD13	1.91	0.52
1:B:57:SER:OG	1:B:58:GLU:N	2.39	0.51
1:A:194:LEU:H	6:A:523:PG4:H31	1.74	0.51
1:A:38:ASP:OD1	1:A:42:GLN:NE2	2.43	0.51
1:A:23:ILE:HD13	1:A:59:LYS:HB3	1.92	0.51
1:A:360:ASN:N	1:A:360:ASN:OD1	2.43	0.51
1:C:32:GLU:HG3	4:C:512:BU1:C4	2.42	0.50
1:A:52:ASP:CG	1:A:335:HIS:HE2	2.14	0.50
1:A:350:ASN:O	1:A:356:THR:OG1	2.25	0.50
1:A:24:ILE:HG23	1:A:88:LEU:HD12	1.95	0.49
1:C:167:MET:HB2	1:C:194:LEU:HD23	1.95	0.48
1:C:136:GLY:O	1:C:363:ARG:NH1	2.47	0.48
1:A:314:GLN:N	1:A:314:GLN:OE1	2.45	0.47
1:A:23:ILE:HD13	1:A:59:LYS:HG2	1.96	0.47
1:A:385:GLU:N	1:A:385:GLU:OE1	2.46	0.46
6:A:523:PG4:H11	1:B:190:LEU:O	2.15	0.46
6:A:523:PG4:H72	1:B:194:LEU:H	1.81	0.46
1:B:353:ARG:C	1:B:355:SER:H	2.19	0.46
1:B:164:LYS:HG2	1:B:191:ASP:HB2	1.98	0.45
1:B:385:GLU:OE1	1:B:385:GLU:N	2.46	0.45
1:C:363:ARG:NH2	1:C:367:ASP:OD1	2.50	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LYS:O	1:A:291:ASN:N	2.47	0.44
1:A:23:ILE:HD12	1:A:24:ILE:N	2.33	0.44
6:A:523:PG4:H42	6:A:523:PG4:H12	2.00	0.44
1:A:23:ILE:HD13	1:A:59:LYS:CB	2.49	0.43
1:A:86:GLY:HA2	1:A:346:MET:HG3	2.00	0.43
1:C:264:ASP:HB2	1:C:265:PRO:HD3	2.01	0.43
1:C:32:GLU:HG3	4:C:512:BU1:H42	2.00	0.43
1:A:403:GLU:OE1	1:A:403:GLU:N	2.50	0.42
1:A:400:THR:N	1:A:408:ASP:O	2.50	0.42
1:A:292:GLN:HA	1:A:295:MET:HB2	2.03	0.41
1:B:167:MET:HB2	1:B:194:LEU:HD23	2.03	0.41
6:A:523:PG4:C1	6:A:523:PG4:H42	2.51	0.40
1:B:28:ALA:HA	1:B:91:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ILE:CG2	1:C:352:ILE:CG2[6_555]	1.97	0.23

## 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	402/428 (94%)	391 (97%)	10 (2%)	1 (0%)	47	58
1	B	375/428 (88%)	364 (97%)	10 (3%)	1 (0%)	41	50
1	C	362/428 (85%)	351 (97%)	11 (3%)	0	100	100
All	All	1139/1284 (89%)	1106 (97%)	31 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	ASP
1	B	86	GLY

### 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	358/378 (95%)	351 (98%)	7 (2%)	55	72
1	B	335/378 (89%)	329 (98%)	6 (2%)	59	75
1	C	316/378 (84%)	315 (100%)	1 (0%)	92	97
All	All	1009/1134 (89%)	995 (99%)	14 (1%)	67	81

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	290	ASP
1	A	291	ASN
1	A	299	HIS
1	A	341	ARG
1	A	342	LYS
1	A	409	MET
1	B	50	LEU
1	B	275	LEU
1	B	337	LYS
1	B	353	ARG
1	B	373	HIS
1	B	408	ASP
1	C	373	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	241	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	283	GLN
1	A	373	HIS
1	B	195	GLN
1	C	241	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 14 are monoatomic - leaving 35 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	$\# Z  > 2$
5	NAG	A	522	1	14,14,15	0.55	0	17,19,21	0.53	0
2	EDO	A	514	-	3,3,3	0.47	0	2,2,2	0.31	0
4	BU1	C	512	-	5,5,5	0.37	0	4,4,4	0.40	0
2	EDO	A	507	-	3,3,3	0.46	0	2,2,2	0.36	0
5	NAG	B	514	1	14,14,15	0.28	0	17,19,21	0.58	0
2	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	B	507	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	A	505	-	3,3,3	0.50	0	2,2,2	0.43	0
2	EDO	A	513	-	3,3,3	0.48	0	2,2,2	0.28	0
6	PG4	A	523	-	12,12,12	0.50	0	11,11,11	0.52	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	521	1	14,14,15	0.20	0	17,19,21	0.39	0
2	EDO	B	501	-	3,3,3	0.50	0	2,2,2	0.33	0
2	EDO	A	509	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.16	0
2	EDO	A	511	-	3,3,3	0.48	0	2,2,2	0.27	0
4	BU1	A	520	-	5,5,5	0.28	0	4,4,4	0.49	0
2	EDO	C	504	-	3,3,3	0.50	0	2,2,2	0.19	0
2	EDO	A	503	-	3,3,3	0.45	0	2,2,2	0.33	0
2	EDO	A	510	-	3,3,3	0.48	0	2,2,2	0.25	0
2	EDO	B	502	-	3,3,3	0.52	0	2,2,2	0.24	0
2	EDO	A	502	-	3,3,3	0.43	0	2,2,2	0.22	0
2	EDO	B	506	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	C	501	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	A	501	-	3,3,3	0.52	0	2,2,2	0.26	0
2	EDO	C	505	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	A	512	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	B	508	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	C	503	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.20	0
2	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.28	0
2	EDO	C	506	-	3,3,3	0.34	0	2,2,2	0.45	0
2	EDO	B	509	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	A	506	-	3,3,3	0.49	0	2,2,2	0.36	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
5	NAG	A	522	1	-	2/6/23/26	0/1/1/1
2	EDO	A	514	-	-	1/1/1/1	-
4	BU1	C	512	-	-	2/3/3/3	-
2	EDO	A	507	-	-	0/1/1/1	-
5	NAG	B	514	1	-	2/6/23/26	0/1/1/1
2	EDO	A	508	-	-	1/1/1/1	-
2	EDO	B	507	-	-	1/1/1/1	-
2	EDO	A	505	-	-	0/1/1/1	-
2	EDO	A	513	-	-	1/1/1/1	-
6	PG4	A	523	-	-	3/10/10/10	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	521	1	-	4/6/23/26	0/1/1/1
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	A	509	-	-	1/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	A	511	-	-	1/1/1/1	-
4	BU1	A	520	-	-	2/3/3/3	-
2	EDO	C	504	-	-	0/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	A	510	-	-	1/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	B	506	-	-	0/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	C	505	-	-	1/1/1/1	-
2	EDO	A	512	-	-	1/1/1/1	-
2	EDO	A	504	-	-	1/1/1/1	-
2	EDO	B	504	-	-	1/1/1/1	-
2	EDO	B	508	-	-	0/1/1/1	-
2	EDO	C	503	-	-	1/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	B	505	-	-	1/1/1/1	-
2	EDO	C	506	-	-	0/1/1/1	-
2	EDO	B	509	-	-	1/1/1/1	-
2	EDO	A	506	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	522	NAG	C3-C2-N2-C7
5	B	514	NAG	O5-C5-C6-O6
5	B	514	NAG	C4-C5-C6-O6
6	A	523	PG4	O1-C1-C2-O2
6	A	523	PG4	O3-C5-C6-O4
2	B	507	EDO	O1-C1-C2-O2
2	A	511	EDO	O1-C1-C2-O2
2	A	510	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	504	EDO	O1-C1-C2-O2
2	B	505	EDO	O1-C1-C2-O2
2	B	509	EDO	O1-C1-C2-O2
4	A	520	BU1	O5-C1-C2-C3
2	A	513	EDO	O1-C1-C2-O2
2	C	503	EDO	O1-C1-C2-O2
2	A	509	EDO	O1-C1-C2-O2
4	C	512	BU1	C1-C2-C3-C4
4	A	520	BU1	C1-C2-C3-C4
2	A	514	EDO	O1-C1-C2-O2
2	A	508	EDO	O1-C1-C2-O2
2	A	504	EDO	O1-C1-C2-O2
5	A	521	NAG	C4-C5-C6-O6
4	C	512	BU1	O5-C1-C2-C3
2	C	505	EDO	O1-C1-C2-O2
5	A	521	NAG	C1-C2-N2-C7
6	A	523	PG4	O2-C3-C4-O3
5	A	521	NAG	O5-C5-C6-O6
5	A	522	NAG	C1-C2-N2-C7
5	A	521	NAG	C3-C2-N2-C7
2	A	512	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	522	NAG	1	0
4	C	512	BU1	2	0
6	A	523	PG4	5	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	404/428 (94%)	0.39	27 (6%)	17 23	39, 58, 130, 177	0
1	B	382/428 (89%)	0.50	22 (5%)	23 29	45, 70, 115, 164	0
1	C	372/428 (86%)	0.88	68 (18%)	1 1	42, 88, 144, 165	0
All	All	1158/1284 (90%)	0.58	117 (10%)	7 9	39, 68, 135, 177	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ALA	7.1
1	A	346	MET	6.2
1	C	244	VAL	6.2
1	B	406	GLY	5.9
1	C	161	ARG	5.8
1	C	278	MET	5.7
1	C	248	LEU	5.7
1	C	409	MET	5.5
1	A	344	HIS	5.4
1	C	275	LEU	5.4
1	C	168	PHE	5.3
1	C	255	TRP	5.3
1	C	340	ASP	5.2
1	A	339	GLU	5.1
1	A	343	TRP	5.1
1	C	166	VAL	4.8
1	C	227	ALA	4.7
1	C	190	LEU	4.5
1	C	247	ASN	4.5
1	C	243	ALA	4.5
1	A	296	ARG	4.3
1	C	249	ALA	4.3
1	C	415	TRP	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	165	PHE	4.1
1	C	277	ARG	4.1
1	C	240	ILE	4.1
1	C	162	TRP	3.9
1	B	50	LEU	3.9
1	C	188	LEU	3.9
1	A	298	ASN	3.8
1	A	340	ASP	3.8
1	C	239	PHE	3.8
1	C	201	ILE	3.8
1	B	299	HIS	3.8
1	A	290	ASP	3.7
1	C	192	VAL	3.7
1	C	202	SER	3.6
1	C	157	VAL	3.6
1	A	341	ARG	3.5
1	A	289	LYS	3.5
1	A	349	LEU	3.5
1	C	413	ALA	3.5
1	A	338	LEU	3.4
1	B	49	SER	3.4
1	A	345	SER	3.4
1	C	22	SER	3.3
1	C	270	LEU	3.3
1	C	342	LYS	3.2
1	A	351	CYS	3.1
1	C	253	SER	3.1
1	C	256	VAL	3.1
1	C	272	HIS	3.1
1	C	246	THR	3.0
1	C	187	ARG	3.0
1	C	306	CYS	3.0
1	A	342	LYS	3.0
1	C	279	THR	3.0
1	C	398	GLY	2.9
1	C	424	SER	2.9
1	B	121	GLY	2.9
1	C	346	MET	2.8
1	C	349	LEU	2.8
1	B	135	ASP	2.8
1	A	385	GLU	2.8
1	B	201	ILE	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	224	LEU	2.8
1	C	159	GLU	2.7
1	B	199	LYS	2.7
1	A	292	GLN	2.6
1	C	163	GLN	2.6
1	B	51	ASN	2.6
1	B	205	PHE	2.6
1	B	307	ASP	2.6
1	C	338	LEU	2.6
1	C	352	ILE	2.5
1	B	407	LYS	2.5
1	A	299	HIS	2.5
1	C	164	LYS	2.5
1	A	295	MET	2.5
1	C	203	HIS	2.4
1	A	293	LYS	2.4
1	A	135	ASP	2.4
1	B	203	HIS	2.4
1	C	194	LEU	2.4
1	A	297	ASN	2.4
1	C	205	PHE	2.3
1	A	57	SER	2.3
1	C	251	LYS	2.3
1	B	311	GLY	2.3
1	C	158	THR	2.3
1	C	51	ASN	2.3
1	B	22	SER	2.3
1	A	134	PRO	2.2
1	B	302	SER	2.2
1	C	408	ASP	2.2
1	C	245	GLU	2.2
1	C	185	ALA	2.2
1	B	202	SER	2.2
1	C	287	SER	2.2
1	B	252	ASP	2.2
1	C	344	HIS	2.2
1	C	339	GLU	2.2
1	C	228	ILE	2.1
1	B	300	ARG	2.1
1	C	204	VAL	2.1
1	A	56	GLN	2.1
1	C	421	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	193	SER	2.1
1	C	250	SER	2.1
1	A	59	LYS	2.1
1	C	254	HIS	2.1
1	C	242	GLU	2.1
1	C	391	TYR	2.1
1	B	408	ASP	2.0
1	B	339	GLU	2.0
1	B	333	ALA	2.0
1	C	292	GLN	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, 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
2	EDO	B	507	4/4	0.43	0.34	109,110,112,113	0
2	EDO	B	508	4/4	0.59	0.28	93,94,94,94	0
2	EDO	B	506	4/4	0.60	0.35	82,83,85,87	0
3	CL	B	511	1/1	0.63	0.13	86,86,86,86	0
2	EDO	C	504	4/4	0.63	0.37	89,90,92,92	0
2	EDO	C	505	4/4	0.64	0.30	72,74,76,77	0
3	CL	C	507	1/1	0.70	0.12	90,90,90,90	0
2	EDO	A	509	4/4	0.71	0.28	95,98,101,103	0
3	CL	C	510	1/1	0.73	0.25	100,100,100,100	0
6	PG4	A	523	13/13	0.73	0.24	56,64,73,75	0
2	EDO	B	509	4/4	0.73	0.51	103,104,105,105	0
3	CL	B	513	1/1	0.73	0.19	101,101,101,101	0
4	BU1	C	512	6/6	0.74	0.20	53,56,60,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	C	503	4/4	0.74	0.25	71,74,76,78	0
2	EDO	B	503	4/4	0.78	0.37	75,76,76,77	0
2	EDO	B	505	4/4	0.78	0.28	70,76,84,88	0
2	EDO	A	506	4/4	0.78	0.24	68,72,77,80	0
2	EDO	A	511	4/4	0.79	0.14	95,96,98,100	0
2	EDO	A	507	4/4	0.81	0.19	87,88,91,94	0
4	BU1	A	520	6/6	0.81	0.43	63,71,78,79	0
3	CL	C	509	1/1	0.81	0.21	100,100,100,100	0
2	EDO	A	514	4/4	0.82	0.15	95,97,100,101	0
2	EDO	A	508	4/4	0.83	0.19	102,103,107,109	0
2	EDO	B	504	4/4	0.83	0.28	81,84,88,90	0
3	CL	B	510	1/1	0.84	0.34	87,87,87,87	0
2	EDO	C	502	4/4	0.85	0.42	85,87,89,91	0
5	NAG	A	521	14/15	0.86	0.15	86,100,106,111	0
2	EDO	A	513	4/4	0.87	0.18	82,84,87,89	0
5	NAG	A	522	14/15	0.87	0.23	107,117,131,140	0
3	CL	B	512	1/1	0.89	0.64	101,101,101,101	0
3	CL	A	518	1/1	0.89	0.16	108,108,108,108	0
2	EDO	A	512	4/4	0.89	0.23	75,77,80,82	0
3	CL	C	511	1/1	0.89	0.30	109,109,109,109	0
2	EDO	A	510	4/4	0.90	0.25	94,97,102,103	0
3	CL	A	516	1/1	0.90	0.24	96,96,96,96	0
3	CL	A	519	1/1	0.90	0.14	100,100,100,100	0
5	NAG	B	514	14/15	0.91	0.19	79,94,101,103	0
3	CL	C	508	1/1	0.91	0.07	97,97,97,97	0
3	CL	A	517	1/1	0.91	0.17	90,90,90,90	0
2	EDO	A	503	4/4	0.93	0.12	84,85,88,90	0
2	EDO	C	501	4/4	0.93	0.15	69,69,69,69	0
2	EDO	A	502	4/4	0.94	0.23	67,67,69,70	0
3	CL	A	515	1/1	0.94	0.22	93,93,93,93	0
2	EDO	A	504	4/4	0.94	0.34	71,73,77,80	0
2	EDO	C	506	4/4	0.94	0.32	59,61,63,64	0
2	EDO	B	501	4/4	0.95	0.17	48,48,48,51	0
2	EDO	B	502	4/4	0.96	0.15	46,47,47,49	0
2	EDO	A	501	4/4	0.96	0.19	43,45,46,46	0
2	EDO	A	505	4/4	0.98	0.10	44,45,46,46	0

## 6.5 Other polymers

There are no such residues in this entry.