



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2016 – 04:51 PM EDT

PDB ID : 5G0H
Title : Crystal structure of Danio rerio HDAC6 CD2 in complex with (S)- trichostatin A
Authors : Miyake, Y.; Keusch, J.J.; Wang, L.; Saito, M.; Hess, D.; Wang, X.; Melancon, B.J.; Helquist, P.; Gut, H.; Matthias, P.
Deposited on : 2016-03-18
Resolution : 1.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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-20027939

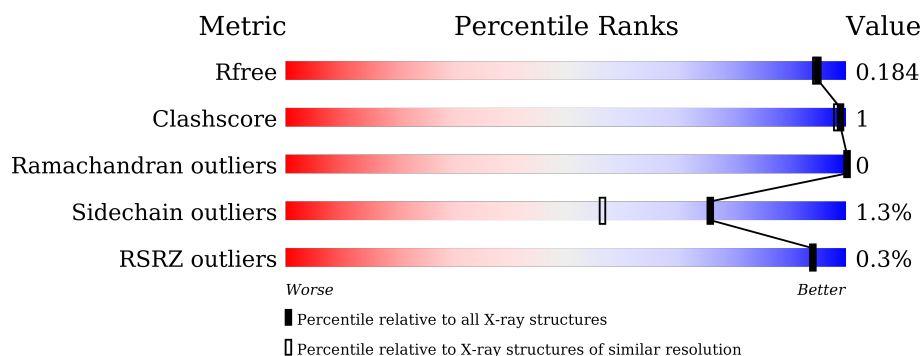
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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 ≥ 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	794	<div> <div style="width: 44%;"></div> <div style="width: 55%;"></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
5	EDO	A	1806	-	-	-	X
5	EDO	A	1808	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1809	-	-	-	X
5	EDO	A	1810	-	-	-	X
5	EDO	A	1811	-	-	-	X
5	EDO	A	1812[A]	-	-	-	X
5	EDO	A	1812[B]	-	-	-	X
5	EDO	A	1814	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3254 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.

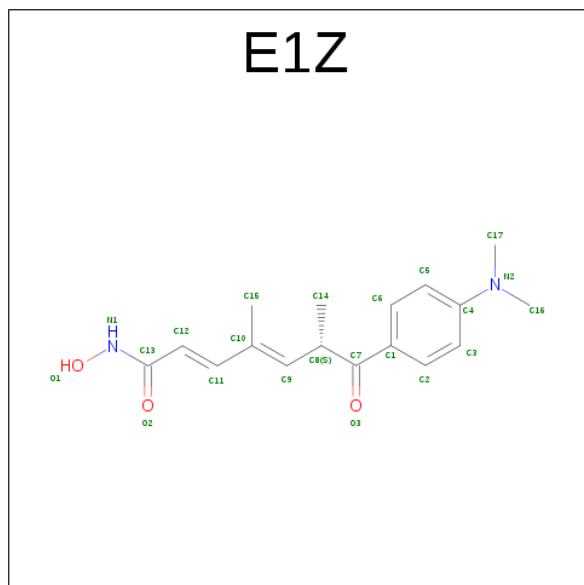
- Molecule 1 is a protein called HDAC6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	3	0
			2832	1779	508	527	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	EXPRESSION TAG	UNP F8W4B7
A	39	PRO	-	EXPRESSION TAG	UNP F8W4B7

- Molecule 2 is S-TRICHOSTATIN A (three-letter code: E1Z) (formula: $C_{17}H_{22}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	17	2	3		

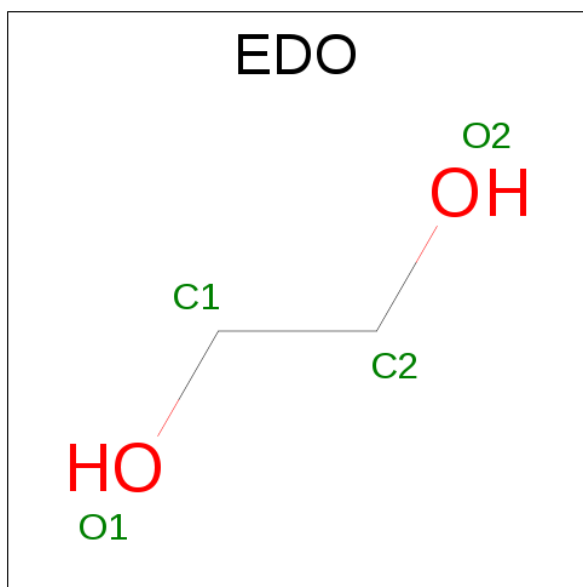
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 8 4 4	0	1

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	351	Total	O	0	4
			353	353		

- Molecule 1: HDAC6

L761	LEV	GLU	GLN	ARG	PHE	THR	GLY	PRO	GLY
F793	LEV	PHE	TYR	ARG	SER	GLY	GLY	GLY	THR
M800	ILE	ILE	ASN	GLN	CYS	LEU	LEU	GLU	GLY
	THR	THR	THR	VAL	SER	ARG	ARG	GLU	GLY
	PRO	ILE	PRO	LEU	VAL	VAL	CYS	GLU	GLY
	GLU	SER	MET	TRP	ILE	GLY	VAL	VAL	VAL
	SER	ASP	ASN	VAL	SER	GLN	GLN	ASN	ASN
	LEU	LYS	LYS	ASP	VAL	VAL	VAL	GLU	GLU
ARG	TRP	GLY	VAL	TRP	ASP	GLU	GLU	LEU	LEU
	PRO	VAL	GLY	VAL	GLN	ALA	ALA	ASN	GLN
	THR	PHE	MET	VAL	LEU	ARG	ARG	ASN	THR
	TRP	GLN	GLU	HIS	VAL	VAL	VAL	ALA	THR
	LYS	GLY	SER	HIS	GLY	LYS	LYS	ASP	VAL
	PRO	ARG	LEU	GLN	GLY	VAL	THR	VAL	VAL
	SER	LEU	ASP	PHE	ILE	LEU	LEU	ALA	SER
	PRO	LEU	VAL	ILE	ASN	ARG	ASN	GLN	THR
	GLN	VAL	GLN	PHE	ILE	LEU	LEU	VAL	THR
CYS	GLY	GLY	GLN	PHE	ILE	LEU	LEU	VAL	THR
THR	PRO	PRO	GLN	GLU	GLU	GLU	GLU	VAL	GLY
PRO	PRO	LEU	TYR	GLU	ASP	GLY	LYS	ASP	GLY
LYS	GLY	GLU	LEU	TYR	SER	SER	TYR	GLU	GLY
LYS	VAL	GLN	PRO	SER	ILE	TYR	TYR	VAL	TYR
GLY	SER	SER	VAL	VAL	ASN	ASN	ARG	GLU	VAL
LYS	VAL	THR	ALA	ALA	PRO	PRO	GLU	LEU	VAL
LYS	LEU	ALA	TYR	TYR	TYR	PRO	PHE	LEU	VAL
SER	PRO	GLU	GLU	PHE	SER	GLY	GLY	MET	ALA
PRO	ALA	VAL	PHE	VAL	HIS	HIS	LYS	SER	THR
ARG	VAL	CYS	PRO	HIS	HIS	ARG	THR	THR	ARG
GLN	VAL	VAL	VAL	ASP	ASP	ASP	THR	LEU	GLY
SER	VAL	SER	LEU	GLY	LYS	GLU	GLU	ASP	ASP
	VAL	LEU	ALA	SER	MET	GLU	GLU	ALA	ALA
	SER	LEU	ALA	PHE	ASN	GLY	LEU	LEU	SER
	S441	ASP	GLY	TRP	PRO	PHE	LYS	LYS	SER
	E465	PRO	CYS	LEU	MET	MET	CYS	LEU	GLY
	I489	PRO	PRO	ALA	ASP	ASP	GLY	ALA	CYS
	S852	PRO	HIS	LEU	GLY	ILE	LYS	PHE	GLY
	V565	PRO	SER	ASP	PRO	SER	ASP	ASN	LYS
	H573	GLY	SER	SER	LYS	SER	ILE	VAL	THR
	M611	ALA	ALA	VAL	GLY	GLY	VAL	ARG	VAL
	S701	CYS	GLN	SER	TYR	ARG	TYR	HIS	GLY
	TH60	GLU	VAL	GLY	ALA	ALA	ALA	PRO	GLY
		SER	SER	ALA	GLN	GLY	GLY	GLY	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.98Å 48.23Å 73.78Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	23.43 – 1.60 48.66 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (23.43-1.60) 96.8 (48.66-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.60Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.150 , 0.174 0.156 , 0.184	Depositor DCC
R_{free} test set	2204 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3254	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, E1Z, K, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/2903	0.60	0/3940

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

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	2832	0	2744	4	0
2	A	22	0	0	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	44	0	66	1	0
6	A	353	0	0	1	0
All	All	3254	0	2810	4	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 1.

All (4) 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:793:PHE:HB3	5:A:1810:EDO:H22	1.81	0.63
1:A:752[B]:GLU:HG2	6:A:2316:HOH:O	2.03	0.58
1:A:565[B]:VAL:HG23	1:A:761:LEU:HD12	1.86	0.56
1:A:489:ILE:HD13	1:A:552:SER:HA	2.03	0.41

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	361/794 (46%)	355 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/672 (46%)	303 (99%)	4 (1%)	76	56

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	GLU
1	A	573	HIS
1	A	611	TRP

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Mol	Chain	Res	Type
1	A	701	SER

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

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 ⓘ

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	E1Z	A	1801	4	22,22,22	0.92	0	24,29,29	0.97	1 (4%)
5	EDO	A	1805	-	3,3,3	0.52	0	2,2,2	0.42	0
5	EDO	A	1806	-	3,3,3	0.35	0	2,2,2	0.38	0
5	EDO	A	1807	-	3,3,3	0.50	0	2,2,2	0.46	0
5	EDO	A	1808	-	3,3,3	0.56	0	2,2,2	0.48	0
5	EDO	A	1809	-	3,3,3	0.40	0	2,2,2	0.69	0
5	EDO	A	1810	-	3,3,3	0.52	0	2,2,2	0.13	0
5	EDO	A	1811	-	3,3,3	0.57	0	2,2,2	0.39	0
5	EDO	A	1812[A]	-	3,3,3	0.52	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1812[B]	-	3,3,3	0.54	0	2,2,2	0.33	0
5	EDO	A	1813	-	3,3,3	0.48	0	2,2,2	0.77	0
5	EDO	A	1814	-	3,3,3	0.25	0	2,2,2	0.65	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	E1Z	A	1801	4	-	0/23/23/23	0/1/1/1
5	EDO	A	1805	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1806	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1807	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1808	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1809	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1810	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1811	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1812[A]	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1812[B]	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1813	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1814	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1801	E1Z	C12-C11-C10	-2.96	121.74	126.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1810	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	360/794 (45%)	-0.60	1 (0%) 94 94	12, 16, 31, 57	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	SER	3.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	A	1811	4/4	0.72	0.16	13.69	50,51,51,51	0
5	EDO	A	1814	4/4	0.91	0.16	12.81	24,24,24,25	4
5	EDO	A	1809	4/4	0.92	0.16	7.87	21,31,37,42	0
5	EDO	A	1810	4/4	0.91	0.14	7.72	28,28,29,31	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	1808	4/4	0.92	0.12	5.44	20,25,29,34	0
5	EDO	A	1806	4/4	0.87	0.11	3.35	34,34,36,37	0
5	EDO	A	1812[B]	4/4	0.82	0.18	3.28	33,35,37,39	4
5	EDO	A	1812[A]	4/4	0.82	0.18	3.08	68,68,68,68	4
5	EDO	A	1805	4/4	0.95	0.08	1.16	24,27,28,28	4
2	E1Z	A	1801	22/22	0.93	0.11	0.92	15,20,25,27	0
3	K	A	1803	1/1	1.00	0.06	-0.13	14,14,14,14	0
3	K	A	1802	1/1	1.00	0.04	-2.98	14,14,14,14	0
4	ZN	A	1804	1/1	1.00	0.04	-5.39	16,16,16,16	0
5	EDO	A	1813	4/4	0.82	0.26	-	25,32,36,40	4
5	EDO	A	1807	4/4	0.92	0.14	-	25,31,37,42	4

6.5 Other polymers ⓘ

There are no such residues in this entry.