



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:59 am GMT

PDB ID : 2UXX  
Title : Human LSD1 Histone Demethylase-CoREST in complex with an FAD- tranyl-  
cypromine adduct  
Authors : Yang, M.; Culhane, J.C.; Machius, M.; Cole, P.A.; Yu, H.  
Deposited on : 2007-03-30  
Resolution : 2.74 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

<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

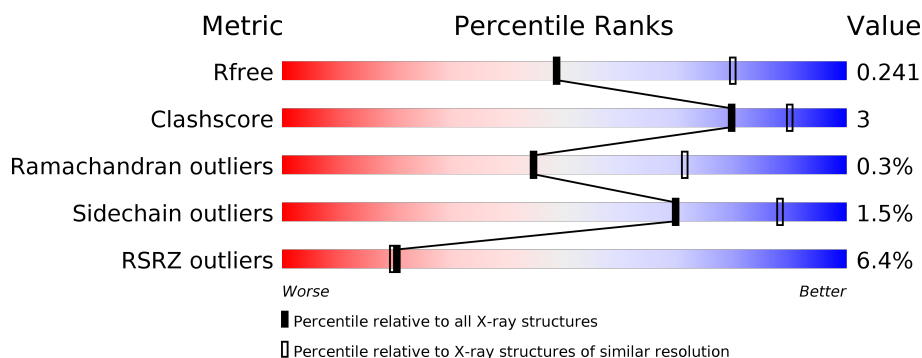
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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	666	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
2	B	235	<div> <div>7%</div> <div> <div></div> <div>55%</div> <div>.</div> <div>43%</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6379 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.

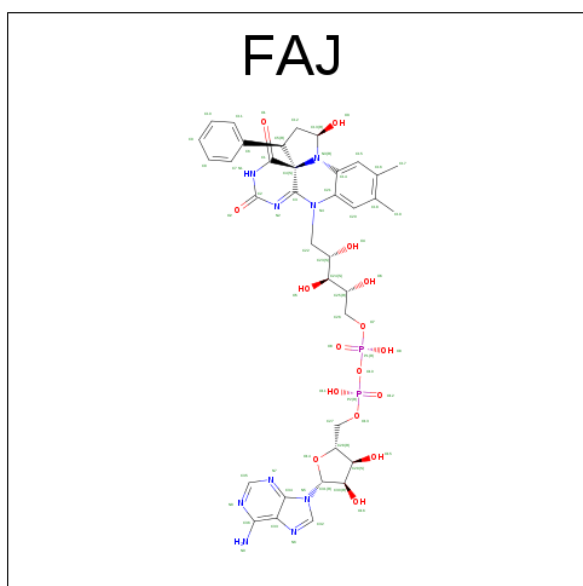
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	665	Total	C	N	O	S	0	0	0
			5209	3318	905	966	20			

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1086	682	197	204	3			

- Molecule 3 is FAD-TRANS-2-PHENYLCYCLOPROPYLAMINE ADDUCT (three-letter code: FAJ) (formula:  $C_{36}H_{43}N_9O_{16}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			63	36	9	16	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	1	Total	O	0	0
			1	1		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.80Å 178.50Å 235.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.74 49.20 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.00-2.74) 97.5 (49.20-2.74)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.235 , 0.260 0.222 , 0.241	Depositor DCC
$R_{free}$ test set	1529 reflections (2.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 81.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: FAJ, GOL, 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	0.56	3/5323 (0.1%)	0.59	4/7221 (0.1%)
2	B	0.32	0/1102	0.46	0/1486
All	All	0.53	3/6425 (0.0%)	0.57	4/8707 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	LYS	C-N	20.70	1.81	1.34
1	A	425	ASP	C-N	19.86	1.79	1.34
1	A	431	TRP	C-N	-16.88	0.95	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	TRP	O-C-N	14.13	145.31	122.70
1	A	431	TRP	CA-C-N	-10.40	94.31	117.20
1	A	431	TRP	C-N-CA	-9.35	98.32	121.70
1	A	424	LYS	O-C-N	-6.32	112.58	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	HIS	Mainchain

## 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	5209	0	5238	40	0
2	B	1086	0	1098	2	0
3	A	63	0	41	2	0
4	A	12	0	16	0	0
5	A	1	0	0	0	0
6	A	7	0	0	0	0
6	B	1	0	0	0	0
All	All	6379	0	6393	41	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 3.

All (41) 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:425:ASP:C	1:A:426:GLU:N	1.79	1.35
1:A:424:LYS:C	1:A:425:ASP:N	1.81	1.33
1:A:427:GLN:O	1:A:431:TRP:CD1	2.18	0.97
1:A:427:GLN:O	1:A:431:TRP:HD1	1.64	0.78
1:A:695:TRP:HE1	1:A:706:LEU:HD11	1.54	0.71
1:A:801:GLU:HG2	1:A:809:ALA:H	1.54	0.70
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.74	0.68
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.78	0.64
1:A:801:GLU:CG	1:A:809:ALA:H	2.16	0.59
1:A:479:LEU:O	1:A:480:VAL:HB	2.05	0.57
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.38	0.54
1:A:360:CYS:SG	1:A:677:LEU:HD22	2.48	0.54
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.45	0.51
1:A:415:VAL:O	1:A:419:GLN:HG2	2.12	0.50
1:A:677:LEU:HD23	1:A:693:LEU:HD11	1.94	0.49
1:A:801:GLU:CG	1:A:809:ALA:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PRO:HB2	1:A:176:GLY:HA2	1.97	0.47
1:A:431:TRP:CE3	1:A:434:ILE:HD12	2.50	0.47
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.96	0.47
1:A:624:THR:HG22	1:A:799:ALA:HB3	1.96	0.47
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.49	0.46
1:A:458:LEU:HD12	1:A:490:LEU:HD12	1.98	0.46
1:A:425:ASP:C	1:A:426:GLU:CA	2.79	0.46
1:A:425:ASP:CA	1:A:426:GLU:N	2.74	0.46
1:A:463:LYS:O	1:A:467:GLU:HG3	2.16	0.45
1:A:665:CYS:HB2	1:A:745:GLU:HB2	1.99	0.45
1:A:541:ALA:O	1:A:657:GLY:HA3	2.17	0.45
1:A:174:VAL:HB	1:A:215:ASN:HB3	1.99	0.44
1:A:793:ILE:H	1:A:793:ILE:HD12	1.83	0.44
1:A:662:VAL:HB	1:A:705:ALA:HB3	2.00	0.43
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.92	0.43
1:A:335:THR:HG21	3:A:900:FAJ:H7	2.00	0.43
1:A:707:VAL:HG11	1:A:715:MET:HG3	2.01	0.43
1:A:388:ALA:HB1	2:B:316:LEU:HD11	1.99	0.43
1:A:820:ARG:NE	1:A:821:GLU:OE2	2.47	0.42
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.00	0.42
1:A:632:GLN:CD	1:A:758:ARG:HE	2.23	0.42
1:A:432:LYS:HA	1:A:435:VAL:HG22	2.02	0.42
1:A:801:GLU:HG2	1:A:809:ALA:N	2.27	0.41
3:A:900:FAJ:H5	3:A:900:FAJ:H10	1.87	0.41
1:A:501:GLN:O	1:A:505:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	663/666 (100%)	644 (97%)	17 (3%)	2 (0%)	44 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	132/235 (56%)	128 (97%)	4 (3%)	0	100	100
All	All	795/901 (88%)	772 (97%)	21 (3%)	2 (0%)	44	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLY
1	A	701	PRO

### 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	565/566 (100%)	558 (99%)	7 (1%)	75	90
2	B	118/203 (58%)	115 (98%)	3 (2%)	53	80
All	All	683/769 (89%)	673 (98%)	10 (2%)	70	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	MET
1	A	475	THR
1	A	538	PHE
1	A	571	TYR
1	A	677	LEU
1	A	721	ASP
1	A	801	GLU
2	B	314	MET
2	B	368	GLU
2	B	371	ARG

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
4	GOL	A	1837	-	5,5,5	0.35	0	5,5,5	0.26	0
4	GOL	A	1838	-	5,5,5	0.33	0	5,5,5	0.26	0
3	FAJ	A	900	-	62,70,70	0.97	4 (6%)	64,109,109	1.57	5 (7%)

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
4	GOL	A	1837	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1838	-	-	0/4/4/4	0/0/0/0
3	FAJ	A	900	-	-	0/34/106/106	0/8/8/8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAJ	C1-N1	2.09	1.40	1.37
3	A	900	FAJ	O14-C31	2.12	1.44	1.41
3	A	900	FAJ	C3-N4	2.16	1.40	1.36
3	A	900	FAJ	C3-N2	3.51	1.41	1.31

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAJ	N7-C35-N8	-8.76	121.23	128.86
3	A	900	FAJ	C12-C5-C6	-4.24	107.80	115.66
3	A	900	FAJ	C28-O14-C31	-3.74	105.79	109.77
3	A	900	FAJ	C15-C14-N3	-2.17	117.20	121.59
3	A	900	FAJ	C4-C1-N1	2.46	120.24	116.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAJ	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

### 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	665/666 (99%)	0.65	35 (5%) 27 27	70, 100, 117, 125	0
2	B	134/235 (57%)	0.76	16 (11%) 5 4	77, 98, 117, 126	0
All	All	799/901 (88%)	0.67	51 (6%) 20 19	70, 99, 118, 126	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	378	LYS	5.4
1	A	171	PRO	4.4
2	B	375	VAL	4.3
1	A	172	SER	4.0
2	B	422	VAL	3.9
2	B	312	LYS	3.9
2	B	376	ILE	3.4
1	A	504	LEU	3.3
1	A	480	VAL	3.2
2	B	395	ILE	3.0
1	A	834	TYR	2.8
2	B	402	PHE	2.8
1	A	242	TYR	2.8
1	A	238	LEU	2.8
1	A	467	GLU	2.8
2	B	399	GLY	2.7
2	B	414	VAL	2.7
2	B	308	ARG	2.6
1	A	271	LYS	2.6
1	A	398	PHE	2.6
1	A	274	PRO	2.5
1	A	174	VAL	2.5
1	A	698	TYR	2.4
1	A	273	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	372	LEU	2.3
2	B	342	LEU	2.3
1	A	431	TRP	2.3
1	A	506	GLU	2.3
1	A	476	ALA	2.3
1	A	239	GLU	2.3
1	A	455	ILE	2.3
1	A	528	ILE	2.3
1	A	739	ALA	2.3
1	A	474	ILE	2.3
1	A	539	ALA	2.2
2	B	316	LEU	2.2
1	A	762	SER	2.2
1	A	275	THR	2.2
1	A	392	LEU	2.1
2	B	421	PHE	2.1
1	A	809	ALA	2.1
1	A	508	LEU	2.1
1	A	268	LYS	2.1
1	A	740	VAL	2.1
1	A	808	PRO	2.1
1	A	656	PHE	2.1
1	A	655	GLY	2.1
2	B	408	VAL	2.0
2	B	367	ILE	2.0
1	A	175	GLU	2.0
1	A	377	MET	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 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
4	GOL	A	1838	6/6	0.85	0.26	0.76	133,134,134,134	0
4	GOL	A	1837	6/6	0.94	0.18	-1.49	83,84,85,85	0
3	FAJ	A	900	63/63	0.96	0.13	-3.03	58,67,74,74	0
5	CL	A	1840	1/1	0.67	0.16	-	109,109,109,109	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.