



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:43 AM GMT

PDB ID : 3BX1  
Title : Complex between the Barley alpha-Amylase/Subtilisin Inhibitor and the subtilisin Savinase  
Authors : Micheelsen, P.O.; Vevodova, J.; Wilson, K.; Skjot, M.  
Deposited on : 2008-01-11  
Resolution : 1.85 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

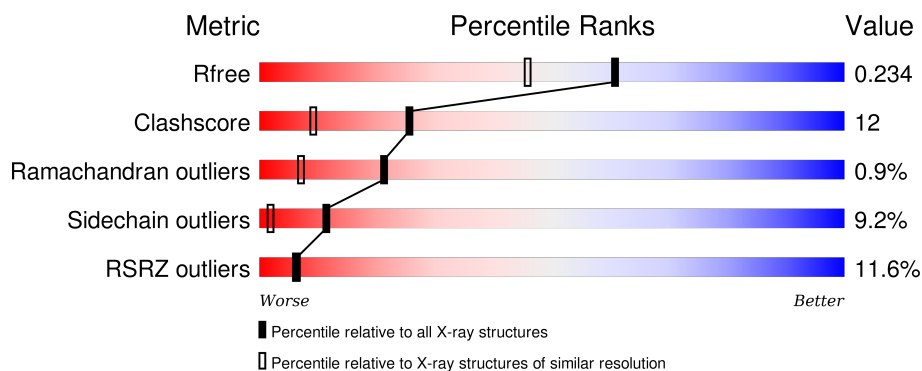
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	269	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
1	B	269	<div> <div>11%</div> <div>87%</div> <div>11%</div> </div>
2	C	181	<div> <div>14%</div> <div>67%</div> <div>21%</div> <div>8%</div> </div>
2	D	181	<div> <div>19%</div> <div>69%</div> <div>18%</div> <div>10%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	B	282	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7228 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 Subtilisin Savinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	1	6	0
			1903	1165	349	386	3			
1	B	269	Total	C	N	O	S	1	3	0
			1889	1156	347	383	3			

- Molecule 2 is a protein called Alpha-amylase/subtilisin inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	181	Total	C	N	O	S	0	1	0
			1407	887	255	259	6			
2	C	181	Total	C	N	O	S	0	3	0
			1421	897	259	259	6			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	Cl	0	0
			6	6		
4	A	11	Total	Cl	0	0
			11	11		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Cl 3	0	0
4	C	4	Total 4	Cl 4	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Na 2	0	0
5	A	3	Total 3	Na 3	0	0
5	C	1	Total 1	Na 1	0	0

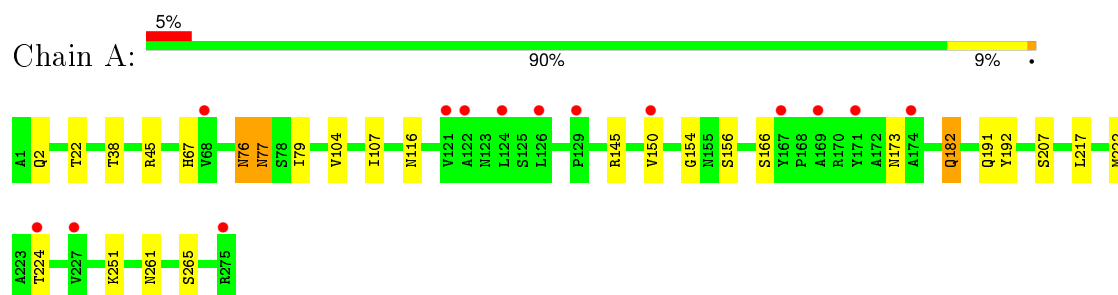
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	211	Total 211	O 211	0	0
6	B	127	Total 127	O 127	0	0
6	C	140	Total 140	O 140	0	0
6	D	96	Total 96	O 96	0	0

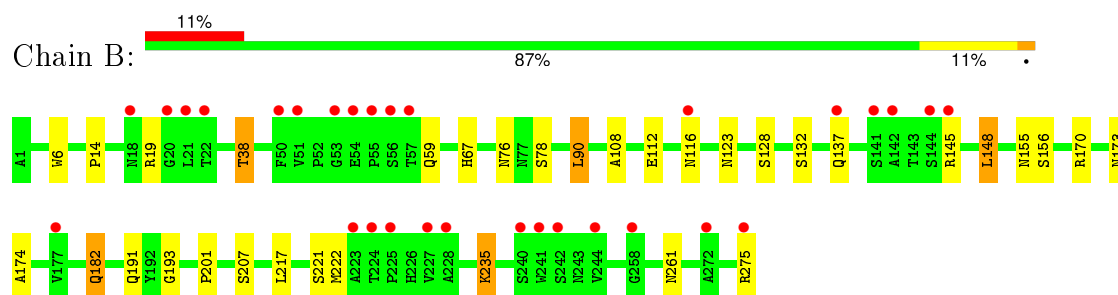
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

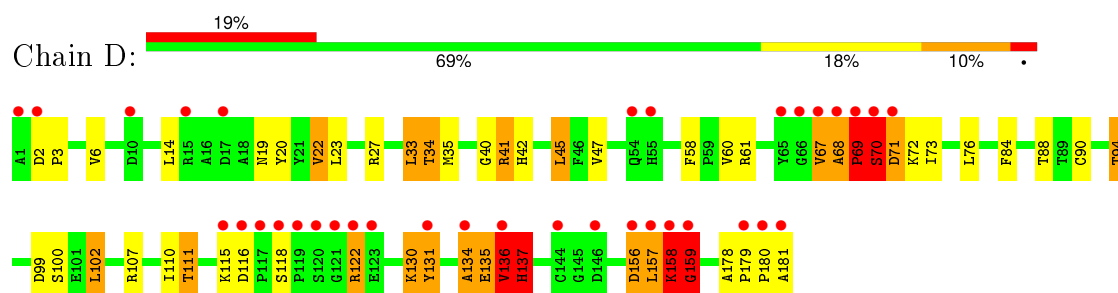
#### • Molecule 1: Subtilisin Savinase



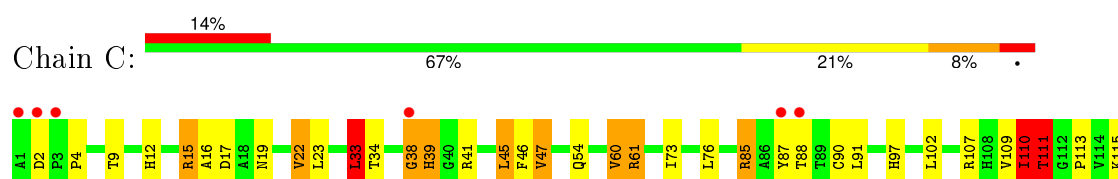
#### • Molecule 1: Subtilisin Savinase

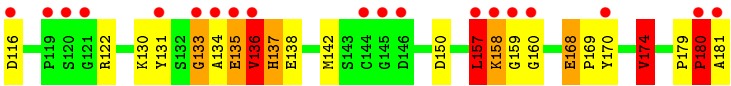


#### • Molecule 2: Alpha-amylase/subtilisin inhibitor



#### • Molecule 2: Alpha-amylase/subtilisin inhibitor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.64Å 100.64Å 216.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.11 – 1.85 35.11 – 1.85	Depositor EDS
% Data completeness (in resolution range)	87.3 (35.11-1.85) 87.3 (35.11-1.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.239 0.200 , 0.234	Depositor DCC
$R_{free}$ test set	4203 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 83612 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, CA, 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	0.82	0/1955	0.78	1/2669 (0.0%)
1	B	0.70	0/1932	0.79	4/2638 (0.2%)
2	C	0.88	0/1474	1.24	18/2005 (0.9%)
2	D	0.84	1/1454 (0.1%)	0.96	2/1980 (0.1%)
All	All	0.81	1/6815 (0.0%)	0.94	25/9292 (0.3%)

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
1	B	0	1
2	C	0	6
2	D	0	9
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	69	PRO	N-CA	6.65	1.58	1.47

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	107	ARG	NE-CZ-NH1	13.40	127.00	120.30
2	C	85	ARG	NE-CZ-NH1	10.84	125.72	120.30
2	C	107	ARG	NE-CZ-NH2	-10.66	114.97	120.30
2	C	85	ARG	NE-CZ-NH2	-9.92	115.34	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	61	ARG	NE-CZ-NH1	9.70	125.15	120.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ASN	Peptide
1	B	173	ASN	Peptide
2	D	67	VAL	Peptide
2	D	68	ALA	Peptide
2	D	69	PRO	Peptide

## 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	1903	0	1870	25	0
1	B	1889	0	1851	19	0
2	C	1421	0	1369	54	1
2	D	1407	0	1344	69	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	0	0	0
4	B	6	0	0	4	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
6	A	211	0	0	4	0
6	B	127	0	0	0	0
6	C	140	0	0	10	0
6	D	96	0	0	3	0
All	All	7228	0	6434	163	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 12.

The worst 5 of 163 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)
2:D:135:GLU:HB3	2:D:136:VAL:CG1	1.58	1.32
1:A:116:ASN:ND2	1:A:145:ARG:HH22	1.32	1.26
2:D:136:VAL:CG2	2:D:137:HIS:N	1.96	1.24
1:B:116:ASN:ND2	1:B:145:ARG:HH12	1.39	1.21
2:D:136:VAL:HG22	2:D:137:HIS:N	1.40	1.16

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)
2:D:131:TYR:OH	2:C:131:TYR:OH[3_545]	1.78	0.42

## 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	273/269 (102%)	266 (97%)	7 (3%)	0	100	100
1	B	270/269 (100%)	263 (97%)	7 (3%)	0	100	100
2	C	182/181 (101%)	169 (93%)	10 (6%)	3 (2%)	12	3
2	D	180/181 (99%)	166 (92%)	9 (5%)	5 (3%)	6	0
All	All	905/900 (101%)	864 (96%)	33 (4%)	8 (1%)	21	7

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	159	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	136	VAL
2	C	158	LYS
2	D	69	PRO
2	D	136	VAL

### 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	200/194 (103%)	195 (98%)	5 (2%)	55	37
1	B	197/194 (102%)	182 (92%)	15 (8%)	16	3
2	C	150/147 (102%)	130 (87%)	20 (13%)	5	0
2	D	148/147 (101%)	124 (84%)	24 (16%)	3	0
All	All	695/682 (102%)	631 (91%)	64 (9%)	11	2

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	60	VAL
2	D	116	ASP
2	C	135	GLU
2	D	70	SER
2	D	102	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	ASN
1	B	191	GLN
2	C	29	HIS
1	B	173	ASN
1	B	182	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 34 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	269/269 (100%)	0.34	14 (5%) 31 29	20, 28, 38, 49	1 (0%)
1	B	269/269 (100%)	0.61	30 (11%) 7 6	23, 34, 45, 54	2 (0%)
2	C	181/181 (100%)	0.70	25 (13%) 4 4	21, 32, 52, 58	7 (3%)
2	D	181/181 (100%)	1.18	35 (19%) 2 1	24, 35, 58, 65	4 (2%)
All	All	900/900 (100%)	0.66	104 (11%) 6 6	20, 32, 49, 65	14 (1%)

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	70	SER	12.0
2	C	181	ALA	11.9
2	D	1	ALA	10.9
2	D	157	LEU	10.7
2	C	1	ALA	10.5

### 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
3	CA	A	276	1/1	0.99	0.10	0.64	25,25,25,25	0
3	CA	D	182	1/1	0.96	0.12	-0.25	59,59,59,59	0
4	CL	A	281	1/1	0.92	0.11	-0.50	56,56,56,56	0
5	NA	C	187	1/1	0.85	0.17	-0.51	58,58,58,58	0
4	CL	A	283	1/1	0.99	0.09	-0.86	27,27,27,27	0
4	CL	C	186	1/1	0.99	0.06	-0.86	38,38,38,38	0
4	CL	C	183	1/1	0.90	0.08	-0.98	69,69,69,69	0
4	CL	D	185	1/1	0.84	0.10	-1.46	78,78,78,78	0
5	NA	A	290	1/1	0.98	0.10	-1.47	27,27,27,27	0
5	NA	B	284	1/1	0.97	0.07	-1.52	36,36,36,36	0
3	CA	C	182	1/1	0.94	0.08	-1.57	70,70,70,70	0
4	CL	B	281	1/1	0.99	0.08	-1.61	31,31,31,31	0
4	CL	A	284	1/1	1.00	0.06	-1.63	29,29,29,29	0
3	CA	B	276	1/1	0.97	0.07	-1.91	36,36,36,36	0
4	CL	C	184	1/1	0.99	0.06	-2.28	35,35,35,35	0
5	NA	A	288	1/1	0.98	0.07	-2.36	32,32,32,32	0
4	CL	D	183	1/1	0.99	0.04	-2.54	34,34,34,34	0
4	CL	C	185	1/1	0.98	0.05	-2.97	41,41,41,41	0
4	CL	B	282	1/1	0.98	0.04	-3.02	45,45,45,45	0
4	CL	A	278	1/1	0.99	0.12	-	38,38,38,38	0
4	CL	A	282	1/1	0.86	0.14	-	71,71,71,71	0
4	CL	A	280	1/1	0.99	0.04	-	30,30,30,30	0
4	CL	A	287	1/1	0.89	0.09	-	75,75,75,75	0
4	CL	A	286	1/1	0.99	0.05	-	36,36,36,36	0
4	CL	B	280	1/1	0.95	0.13	-	58,58,58,58	0
4	CL	D	184	1/1	0.92	0.10	-	74,74,74,74	0
5	NA	A	289	1/1	0.99	0.08	-	23,23,23,23	0
4	CL	B	278	1/1	0.94	0.27	-	67,67,67,67	0
5	NA	B	283	1/1	0.99	0.04	-	31,31,31,31	0
4	CL	B	277	1/1	0.99	0.06	-	37,37,37,37	0
4	CL	A	277	1/1	0.99	0.07	-	40,40,40,40	0
4	CL	A	285	1/1	0.96	0.16	-	54,54,54,54	0
4	CL	A	279	1/1	0.95	0.22	-	53,53,53,53	0
4	CL	B	279	1/1	0.98	0.14	-	40,40,40,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.