



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 7N6H / pdb_00007n6h
Title : The crystal structure of the GH30 subfamily 10 enzyme, AcXbh30A from *Acetivibrio clariflavus*
Authors : Tan, K.; St John, F.J.
Deposited on : 2021-06-08
Resolution : 1.28 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

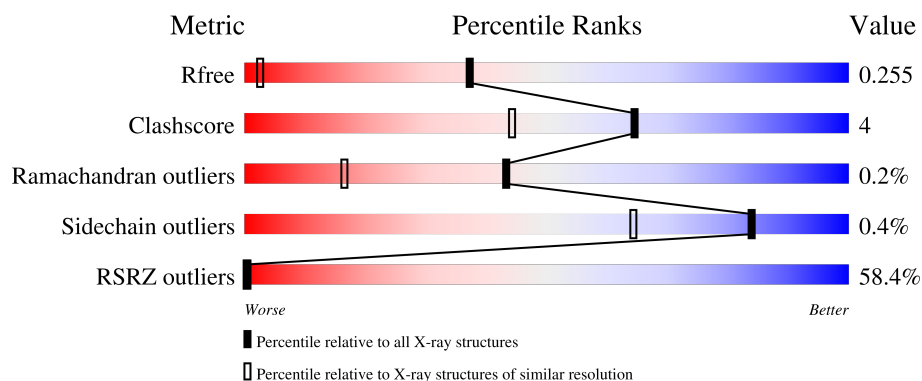
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.28 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}	180053	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	444	61% 89% 8%
1	B	444	53% 88% 9%

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	CL	A	508	-	-	X	-
2	CL	A	515	-	-	X	-
2	CL	B	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7649 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 AcXbh30A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	3	0
			3454	2194	570	679	11			
1	B	433	Total	C	N	O	S	0	1	0
			3443	2187	569	676	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP G8LU16
A	464	LEU	-	expression tag	UNP G8LU16
A	465	GLU	-	expression tag	UNP G8LU16
A	466	HIS	-	expression tag	UNP G8LU16
A	467	HIS	-	expression tag	UNP G8LU16
A	468	HIS	-	expression tag	UNP G8LU16
A	469	HIS	-	expression tag	UNP G8LU16
A	470	HIS	-	expression tag	UNP G8LU16
A	471	HIS	-	expression tag	UNP G8LU16
B	28	MET	-	initiating methionine	UNP G8LU16
B	464	LEU	-	expression tag	UNP G8LU16
B	465	GLU	-	expression tag	UNP G8LU16
B	466	HIS	-	expression tag	UNP G8LU16
B	467	HIS	-	expression tag	UNP G8LU16
B	468	HIS	-	expression tag	UNP G8LU16
B	469	HIS	-	expression tag	UNP G8LU16
B	470	HIS	-	expression tag	UNP G8LU16
B	471	HIS	-	expression tag	UNP G8LU16

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	Cl	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total	Cl	0	0
			8	8		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

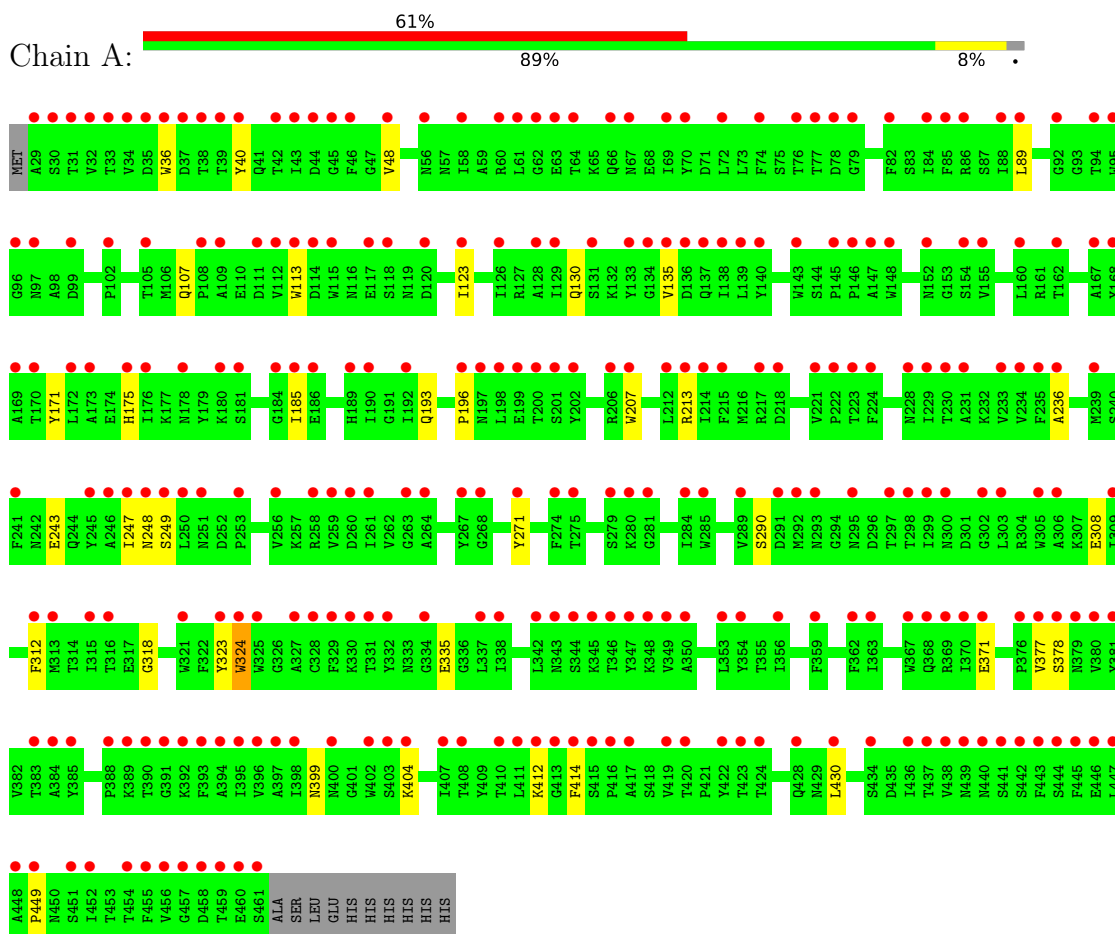
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	388	Total	O	0	0
			388	388		
4	B	329	Total	O	0	0
			329	329		

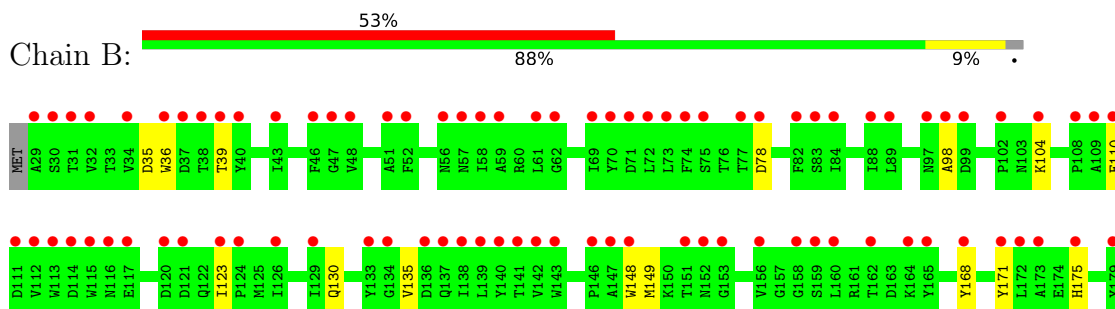
3 Residue-property plots

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: AcXbh30A



• Molecule 1: AcXbh30A



HIS	K404	A327	N251	K180
	Q405	C328	D252	S181
HIS	S406	F329	P253	K182
	I407		I254	F183
	T408	Y332	A255	G184
	Y409		V256	I185
	T410	E335	K257	E186
	L411		N258	I187
	K412	D341		T188
	G413	L342	I261	H189
	F414	N343		I190
	S415	S344	A264	G191
	P416	K345	H265	I192
	A417	T346	N266	Q193
		Y347	Y267	
	T420		G268	P196
	P421	A350	S269	N197
	Y422		S270	L198
	T423	L353	Y271	
	T424	Y354	I272	V202
	S425		P273	
	S426	Q358	F274	R206
	T427		T275	W207
		F362	T276	S208
	L430	I363	T277	P209
		R364	K278	
	G433	P365	S279	L212
	S434	G366		R213
	D435	W367	I284	I214
	I436	Q368	W285	F215
	T437	R369		M216
	V438	I370	V288	R217
	N439	E371	S290	D218
	N440			Y219
	S441	K374	N293	L220
	S442	N375		
	F443	P376	T297	T223
	S444	V377	T298	F224
	F445	S378	I299	D225
	E446	N379		K226
	L447	V380	L303	E227
		Y381	R304	N228
	I452	T383	W305	I229
	T453	A384	A306	T230
	T454	T385		
	F455		I309	V233
	V456			V234
	D458	P388	F312	F235
	T459	K389		A236
	E460	T390	T316	
	S461	G391	F317	F241
		K392	G318	E242
ALA		F393	N319	E243
SER			A320	Q244
LEU		I398	W321	Y245
GLU		N399	F322	A246
HIS		N400	Y323	I247
HIS		G401	W324	N248
		W402	W325	S249
HIS		S403	G326	L250

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.87Å 108.02Å 66.84Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	41.18 – 1.28 41.18 – 1.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (41.18-1.28) 96.3 (41.18-1.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.51 (at 1.28Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.202 , 0.254 0.202 , 0.255	Depositor DCC
R_{free} test set	10529 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.387 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: ACT, 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	0.07	0/3544	0.22	0/4821
1	B	0.07	0/3533	0.21	0/4806
All	All	0.07	0/7077	0.22	0/9627

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	3454	0	3292	24	0
1	B	3443	0	3281	24	0
2	A	15	0	0	8	0
2	B	8	0	0	5	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	388	0	0	4	0
4	B	329	0	0	3	0
All	All	7649	0	6582	53	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 4.

The worst 5 of 53 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:A:510:CL:CL	4:A:896:HOH:O	2.38	0.78
1:A:213:ARG:NE	2:A:503:CL:CL	2.50	0.73
2:A:515:CL:CL	4:A:860:HOH:O	2.43	0.73
2:A:514:CL:CL	4:A:952:HOH:O	2.53	0.61
1:A:404:LYS:HG3	1:A:449:PRO:HD3	1.85	0.59

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	433/444 (98%)	418 (96%)	14 (3%)	1 (0%)	43	16
1	B	432/444 (97%)	418 (97%)	13 (3%)	1 (0%)	43	16
All	All	865/888 (97%)	836 (97%)	27 (3%)	2 (0%)	43	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	TRP
1	B	324	TRP

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	376/384 (98%)	374 (100%)	2 (0%)	81	59
1	B	374/384 (97%)	373 (100%)	1 (0%)	86	66
All	All	750/768 (98%)	747 (100%)	3 (0%)	84	64

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	TRP
1	A	430	LEU
1	B	378	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	ASN
1	B	166	GLN
1	B	358	GLN
1	B	339	GLN
1	A	375	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 23 are 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	$\# Z > 2$
3	ACT	A	517	-	3,3,3	1.33	0	3,3,3	1.30	0
3	ACT	A	516	-	3,3,3	1.35	0	3,3,3	1.39	0
3	ACT	B	509	-	3,3,3	1.36	0	3,3,3	1.26	0

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, 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	433/444 (97%)	2.56	270 (62%) 0 0	7, 15, 21, 38	2 (0%)
1	B	433/444 (97%)	2.41	236 (54%) 0 0	8, 14, 21, 34	1 (0%)
All	All	866/888 (97%)	2.49	506 (58%) 0 0	7, 14, 21, 38	3 (0%)

The worst 5 of 506 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	ALA	8.1
1	B	123	ILE	8.0
1	A	456[A]	VAL	7.6
1	B	108	PRO	7.4
1	A	329	PHE	7.3

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	509	1/1	0.88	0.26	68,68,68,68	0
2	CL	A	503	1/1	0.90	0.18	52,52,52,52	0
2	CL	A	514	1/1	0.91	0.21	45,45,45,45	0
2	CL	B	501	1/1	0.91	0.26	33,33,33,33	0
3	ACT	B	509	4/4	0.91	0.24	24,24,26,27	0
3	ACT	A	516	4/4	0.92	0.18	17,18,20,21	0
2	CL	A	510	1/1	0.93	0.17	50,50,50,50	0
2	CL	B	505	1/1	0.94	0.11	38,38,38,38	0
2	CL	A	515	1/1	0.95	0.15	26,26,26,26	0
2	CL	A	507	1/1	0.95	0.10	23,23,23,23	0
2	CL	A	511	1/1	0.95	0.17	33,33,33,33	0
2	CL	A	513	1/1	0.95	0.17	49,49,49,49	0
2	CL	A	501	1/1	0.95	0.12	39,39,39,39	0
2	CL	A	505	1/1	0.96	0.20	29,29,29,29	0
2	CL	B	506	1/1	0.96	0.08	27,27,27,27	0
2	CL	A	512	1/1	0.96	0.12	40,40,40,40	0
3	ACT	A	517	4/4	0.96	0.15	21,21,22,22	0
2	CL	A	502	1/1	0.96	0.12	31,31,31,31	0
2	CL	B	504	1/1	0.97	0.23	39,39,39,39	0
2	CL	A	508	1/1	0.97	0.12	22,22,22,22	0
2	CL	A	506	1/1	0.97	0.21	45,45,45,45	0
2	CL	A	504	1/1	0.97	0.20	48,48,48,48	0
2	CL	B	502	1/1	0.97	0.17	23,23,23,23	0
2	CL	B	503	1/1	0.97	0.09	24,24,24,24	0
2	CL	B	508	1/1	0.98	0.24	45,45,45,45	0
2	CL	B	507	1/1	0.98	0.28	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.