



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2025 – 01:10 PM EST

PDB ID : 9YHC / pdb\_00009yhc  
Title : Crystal structure of Chikungunya virus nsP3 macrodomain D31H mutant (P31 crystal form)  
Authors : Correy, G.J.; Fraser, J.S.  
Deposited on : 2025-09-30  
Resolution : 1.35 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

<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>.

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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

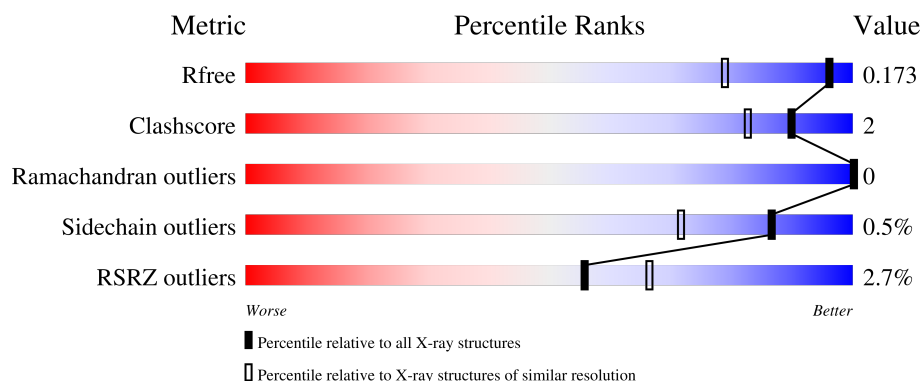
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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))
$R_{free}$	164625	1089 (1.36-1.36)
Clashscore	180529	1157 (1.36-1.36)
Ramachandran outliers	177936	1146 (1.36-1.36)
Sidechain outliers	177891	1146 (1.36-1.36)
RSRZ outliers	164620	1088 (1.36-1.36)

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  $\geq 3$ , 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	168	<div> <div>2%</div> <div>92%</div> <div>• •</div> </div>
1	B	168	<div> <div>3%</div> <div>93%</div> <div>• 5%</div> </div>
1	C	168	<div> <div>%</div> <div>95%</div> <div>5%</div> </div>
1	D	168	<div> <div>5%</div> <div>99%</div> <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
4	CL	A	205	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11174 atoms, of which 5253 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	H	N	O	S	0	9	0
			2575	802	1287	232	246	8			
1	B	160	Total	C	H	N	O	S	0	5	0
			2510	784	1254	223	240	9			
1	C	168	Total	C	H	N	O	S	0	12	0
			2719	850	1355	248	256	10			
1	D	168	Total	C	H	N	O	S	0	7	0
			2668	835	1327	246	250	10			

There are 36 discrepancies between the modelled and reference sequences:

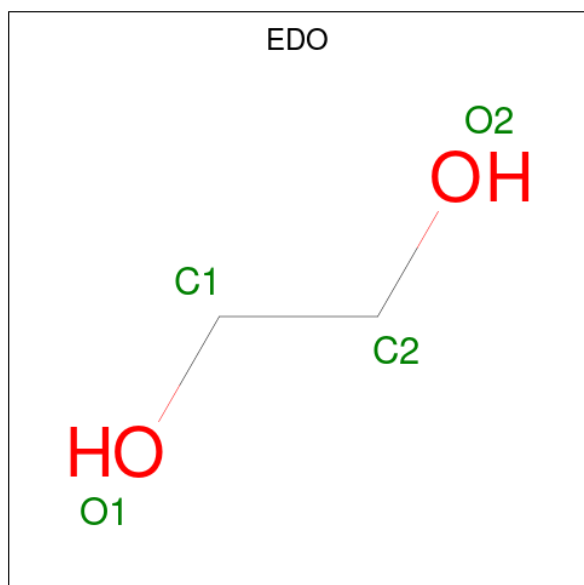
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q8JUX6
A	-6	LYS	-	expression tag	UNP Q8JUX6
A	-5	HIS	-	expression tag	UNP Q8JUX6
A	-4	HIS	-	expression tag	UNP Q8JUX6
A	-3	HIS	-	expression tag	UNP Q8JUX6
A	-2	HIS	-	expression tag	UNP Q8JUX6
A	-1	HIS	-	expression tag	UNP Q8JUX6
A	0	HIS	-	expression tag	UNP Q8JUX6
A	31	HIS	ASP	engineered mutation	UNP Q8JUX6
B	-7	MET	-	initiating methionine	UNP Q8JUX6
B	-6	LYS	-	expression tag	UNP Q8JUX6
B	-5	HIS	-	expression tag	UNP Q8JUX6
B	-4	HIS	-	expression tag	UNP Q8JUX6
B	-3	HIS	-	expression tag	UNP Q8JUX6
B	-2	HIS	-	expression tag	UNP Q8JUX6
B	-1	HIS	-	expression tag	UNP Q8JUX6
B	0	HIS	-	expression tag	UNP Q8JUX6
B	31	HIS	ASP	engineered mutation	UNP Q8JUX6
C	-7	MET	-	initiating methionine	UNP Q8JUX6
C	-6	LYS	-	expression tag	UNP Q8JUX6
C	-5	HIS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q8JUX6
C	-3	HIS	-	expression tag	UNP Q8JUX6
C	-2	HIS	-	expression tag	UNP Q8JUX6
C	-1	HIS	-	expression tag	UNP Q8JUX6
C	0	HIS	-	expression tag	UNP Q8JUX6
C	31	HIS	ASP	engineered mutation	UNP Q8JUX6
D	-7	MET	-	initiating methionine	UNP Q8JUX6
D	-6	LYS	-	expression tag	UNP Q8JUX6
D	-5	HIS	-	expression tag	UNP Q8JUX6
D	-4	HIS	-	expression tag	UNP Q8JUX6
D	-3	HIS	-	expression tag	UNP Q8JUX6
D	-2	HIS	-	expression tag	UNP Q8JUX6
D	-1	HIS	-	expression tag	UNP Q8JUX6
D	0	HIS	-	expression tag	UNP Q8JUX6
D	31	HIS	ASP	engineered mutation	UNP Q8JUX6

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: 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	H	O	0	1
			10	2	6	2		
2	B	1	Total	C	H	O	0	1
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cl	0	0
			5	5		
4	B	3	Total	Cl	0	0
			3	3		
4	C	3	Total	Cl	0	0
			3	3		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O	0	2
			179	179		
5	B	126	Total	O	0	2
			127	127		
5	C	187	Total	O	0	2
			187	187		
5	D	141	Total	O	0	3
			142	142		

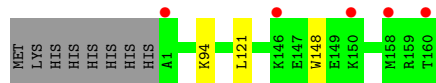
### 3 Residue-property plots [i](#)

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.

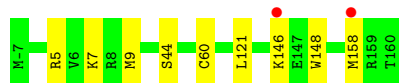
- Molecule 1: Non-structural protein 3



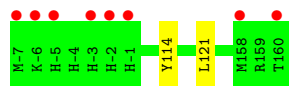
- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.44Å 87.44Å 85.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.91 – 1.35 38.91 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.91-1.35) 99.6 (38.91-1.35)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 1.35Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.136 , 0.172 0.139 , 0.173	Depositor DCC
$R_{free}$ test set	8267 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.027 for h,-h-k,-l 0.002 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	11174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8110e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: EDO, 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	0.32	0/1346	0.50	0/1819
1	B	0.27	0/1292	0.45	0/1749
1	C	0.33	0/1432	0.51	0/1936
1	D	0.28	0/1399	0.47	0/1893
All	All	0.30	0/5469	0.48	0/7397

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	1288	1287	1254	6	0
1	B	1256	1254	1247	2	0
1	C	1364	1355	1317	7	0
1	D	1341	1327	1307	2	0
2	A	4	6	6	0	0
2	B	4	6	6	0	0
2	C	4	6	6	0	0
2	D	8	12	10	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	3	0
4	B	3	0	0	1	0
4	C	3	0	0	0	0
4	D	2	0	0	1	0
5	A	179	0	0	1	0
5	B	127	0	0	1	0
5	C	187	0	0	2	0
5	D	142	0	0	0	0
All	All	5921	5253	5153	18	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 2.

The worst 5 of 18 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:C:158:MET:SD	5:C:480:HOH:O	2.55	0.64
1:D:121:LEU:HD23	1:D:121:LEU:C	2.30	0.56
1:A:138:ASP:OD2	4:A:205:CL:CL	2.63	0.53
1:A:83[B]:ARG:NH2	5:A:301:HOH:O	2.43	0.50
1:C:7:LYS:HE2	1:C:9:MET:SD	2.55	0.47

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	168/168 (100%)	168 (100%)	0	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/168 (97%)	161 (99%)	2 (1%)	0	100	100
1	C	178/168 (106%)	178 (100%)	0	0	100	100
1	D	173/168 (103%)	172 (99%)	1 (1%)	0	100	100
All	All	682/672 (102%)	679 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	143/141 (101%)	142 (99%)	1 (1%)	81	62
1	B	137/141 (97%)	136 (99%)	1 (1%)	81	62
1	C	152/141 (108%)	151 (99%)	1 (1%)	81	62
1	D	148/141 (105%)	148 (100%)	0	100	100
All	All	580/564 (103%)	577 (100%)	3 (0%)	86	72

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

Mol	Chain	Res	Type
1	A	159	ARG
1	B	94	LYS
1	C	146	LYS

Sometimes 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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 17 are monoatomic - leaving 5 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	EDO	D	201	3	3,3,3	0.34	0	2,2,2	0.31	0
2	EDO	A	201[A]	-	3,3,3	0.35	0	2,2,2	0.26	0
2	EDO	D	202	-	3,3,3	0.28	0	2,2,2	0.29	0
2	EDO	B	201[A]	-	3,3,3	0.26	0	2,2,2	0.10	0
2	EDO	C	201	-	3,3,3	0.31	0	2,2,2	0.28	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	EDO	D	201	3	-	1/1/1/1	-
2	EDO	A	201[A]	-	-	1/1/1/1	-
2	EDO	D	202	-	-	0/1/1/1	-
2	EDO	B	201[A]	-	-	1/1/1/1	-
2	EDO	C	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201[A]	EDO	O1-C1-C2-O2
2	A	201[A]	EDO	O1-C1-C2-O2
2	D	201	EDO	O1-C1-C2-O2

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	161/168 (95%)	-0.43	3 (1%) 66 76	8, 20, 37, 64	5 (3%)
1	B	160/168 (95%)	-0.13	5 (3%) 51 61	11, 25, 59, 82	3 (1%)
1	C	168/168 (100%)	-0.30	2 (1%) 76 86	9, 20, 40, 60	7 (4%)
1	D	168/168 (100%)	-0.02	8 (4%) 36 46	10, 24, 57, 80	4 (2%)
All	All	657/672 (97%)	-0.22	18 (2%) 56 66	8, 22, 52, 82	19 (2%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	THR	5.2
1	D	160	THR	3.4
1	D	-1	HIS	3.2
1	B	1	ALA	3.2
1	D	-3	HIS	3.1

### 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, 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( $\text{\AA}^2$ )	Q<0.9
3	CA	A	202	1/1	0.90	0.18	64,64,64,64	0
2	EDO	D	202	4/4	0.93	0.10	45,54,55,55	0
4	CL	B	205	1/1	0.93	0.11	64,64,64,64	0
2	EDO	A	201[A]	4/4	0.94	0.10	25,33,34,39	10
2	EDO	B	201[A]	4/4	0.94	0.13	31,38,38,39	10
2	EDO	C	201	4/4	0.94	0.08	22,27,28,28	0
4	CL	C	205	1/1	0.94	0.10	50,50,50,50	0
4	CL	A	205	1/1	0.96	0.10	57,57,57,57	0
2	EDO	D	201	4/4	0.97	0.07	23,29,33,34	0
4	CL	A	207	1/1	0.97	0.10	44,44,44,44	0
4	CL	D	205	1/1	0.97	0.08	48,48,48,48	0
4	CL	B	204	1/1	0.99	0.08	29,29,29,29	0
4	CL	A	204	1/1	0.99	0.05	27,27,27,27	0
3	CA	D	203	1/1	1.00	0.04	19,19,19,19	1
4	CL	B	203	1/1	1.00	0.05	22,22,22,22	0
4	CL	A	203	1/1	1.00	0.01	19,19,19,19	0
3	CA	B	202	1/1	1.00	0.12	22,22,22,22	1
4	CL	C	203	1/1	1.00	0.02	17,17,17,17	0
4	CL	C	204	1/1	1.00	0.05	24,24,24,24	0
3	CA	C	202	1/1	1.00	0.04	17,17,17,17	0
4	CL	D	204	1/1	1.00	0.04	25,25,25,25	0
4	CL	A	206	1/1	1.00	0.06	25,25,25,25	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.