



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:07 AM UTC

PDB ID : 4N2O / pdb_00004n2o
Title : Structure of a novel autonomous cohesin protein from *Ruminococcus flavefaciens*
Authors : Frolow, F.; Voronov-Goldman, M.; Levy-Assaraf, M.; Lamed, R.; Bayer, E.; Shimon, L.
Deposited on : 2013-10-05
Resolution : 2.44 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

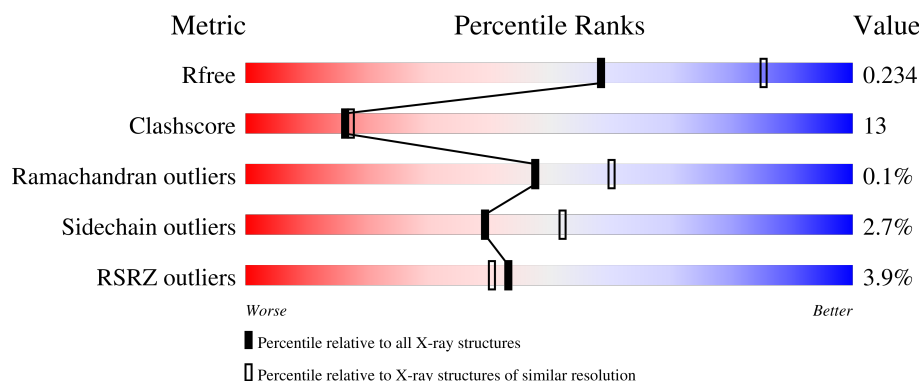
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	201	4% 81% 14% . .
1	B	201	2% 80% 14% . .
1	C	201	4% 79% 13% . 5%
1	D	201	4% 80% 13% . 5%
1	E	201	3% 80% 12% . 5%

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Mol	Chain	Length	Quality of chain
1	F	201	
1	G	201	
1	H	201	

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	H	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12269 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 Autonomous cohesin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	0	0
			1499	941	240	304	3	11			
1	B	193	Total	C	N	O	S	Se	0	0	0
			1489	936	238	301	3	11			
1	C	190	Total	C	N	O	S	Se	0	0	0
			1473	927	237	295	3	11			
1	D	191	Total	C	N	O	S	Se	0	0	0
			1470	925	234	297	3	11			
1	E	190	Total	C	N	O	S	Se	0	0	0
			1467	924	233	296	3	11			
1	F	193	Total	C	N	O	S	Se	0	1	0
			1508	948	245	300	3	12			
1	G	192	Total	C	N	O	S	Se	0	1	0
			1491	938	238	300	3	12			
1	H	191	Total	C	N	O	S	Se	0	1	0
			1485	935	237	298	3	12			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		
2	H	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		

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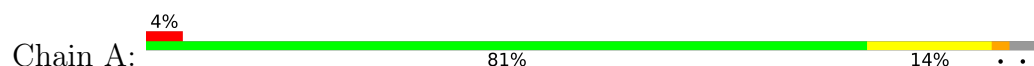
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	58	Total 58	O 58	0	0
3	C	51	Total 51	O 51	0	0
3	D	6	Total 6	O 6	0	0
3	E	8	Total 8	O 8	0	0
3	F	53	Total 53	O 53	0	0
3	G	69	Total 69	O 69	0	0
3	H	64	Total 64	O 64	0	0

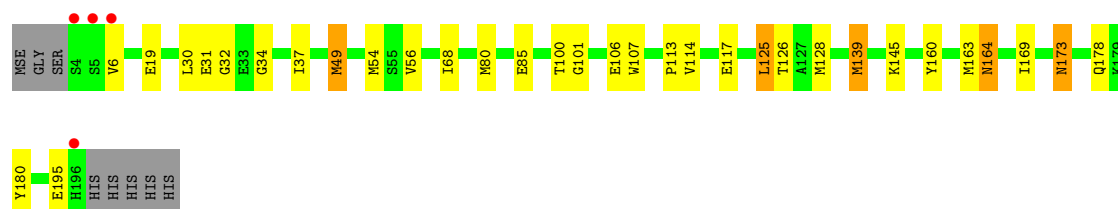
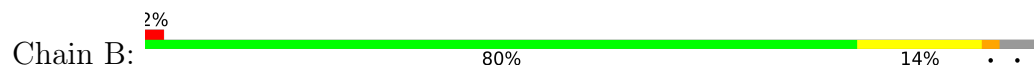
3 Residue-property plots [i](#)

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.

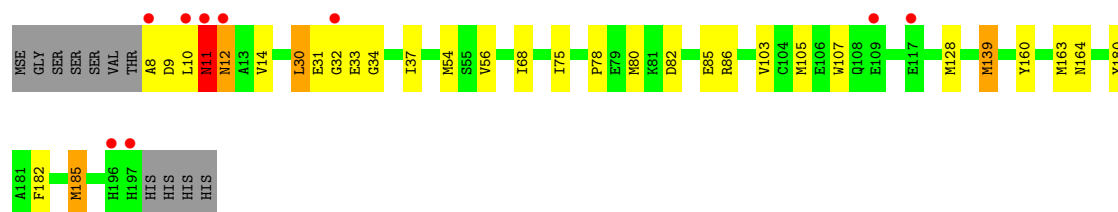
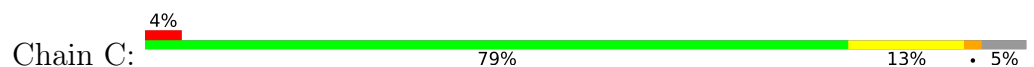
• Molecule 1: Autonomous cohesin



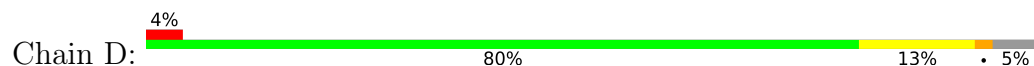
• Molecule 1: Autonomous cohesin



• Molecule 1: Autonomous cohesin



• Molecule 1: Autonomous cohesin



GLU
HIS
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HIS

• Molecule 1: Autonomous cohesin

Chain E: 3% 80% 12% 5%

RSE GLY SER SER V6 E19 L30 E31 G32 E33 G34 I37 K45 M54 S55 V56 Q62 I68 P78 E79 M80 K81 D82 P83 E84 E85 R86 E87 W107 L125 T126 A127 M128 E136 M139 R143 P152 Y160 M163 M164 P175

Y180 E193 E194 E195 HIS HIS HIS HIS HIS

• Molecule 1: Autonomous cohesin

Chain F: 5% 77% 16% 2%

RSE GLY SER SER VAL T7 A8 D9 L10 N11 N12 N21 P28 D29 L30 E31 G32 E33 G34 M49 M54 A59 D60 M61 Q62 M65 I68 P78 E79 M80 K81 D82 P83 E84 E85 W107 Q108 E109 M128 K145 D148 Y160 M163 M164

I169 Q172 M173 M174 P175 T176 Y177 K178 Y179 Y180 A181 F182 M185 H197 H198 H199 HIS HIS

• Molecule 1: Autonomous cohesin

Chain G: 3% 77% 15% 5%

RSE GLY SER SER S5 V6 T7 A8 D9 L10 N11 N12 E19 D29 L30 E31 G32 E33 G34 I37 K45 M49 M54 S55 V56 S57 M58 M61 M65 E85 R86 G101 M107 Q108 E109 T126 A127 M128 M139 K145 M163 M164 I169

M173 I174 P175 Q178 K179 Y180 A181 F182 M185 H196 HIS HIS HIS HIS

• Molecule 1: Autonomous cohesin

Chain H: 2% 82% 12% 5%

RSE GLY SER SER V6 T7 E19 E31 G32 E33 G34 M49 M54 M58 D82 P83 E84 E85 R86 G101 M107 Q108 E109 V114 L125 M128 K145 M163 M164 I169 M173 Q178 K179 Y180 H196 HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.24Å 67.73Å 258.91Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	22.77 – 2.44 22.77 – 2.44	Depositor EDS
% Data completeness (in resolution range)	96.8 (22.77-2.44) 90.9 (22.77-2.44)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.8.0049, PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.229 0.213 , 0.234	Depositor DCC
R_{free} test set	3683 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.025 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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:
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	0.85	0/1520	0.90	2/2045 (0.1%)
1	B	0.79	0/1510	0.88	2/2032 (0.1%)
1	C	0.78	0/1495	0.92	4/2011 (0.2%)
1	D	0.71	0/1490	0.90	3/2005 (0.1%)
1	E	0.78	0/1487	0.95	4/2001 (0.2%)
1	F	0.80	0/1532	0.97	4/2061 (0.2%)
1	G	0.87	0/1512	0.95	4/2034 (0.2%)
1	H	0.75	0/1506	0.85	1/2026 (0.0%)
All	All	0.79	0/12052	0.92	24/16215 (0.1%)

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	C	0	2
1	G	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	49	MSE	CG-SE-CE	9.32	119.42	98.92
1	G	49	MSE	CG-SE-CE	8.53	117.70	98.92
1	E	30	LEU	N-CA-CB	7.58	121.81	110.29
1	B	49	MSE	CG-SE-CE	7.50	115.43	98.92
1	D	185	MSE	CG-SE-CE	-7.44	82.56	98.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11	ASN	Peptide
1	C	12	ASN	Peptide
1	G	10	LEU	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	1499	0	1420	43	0
1	B	1489	0	1412	51	0
1	C	1473	0	1393	40	0
1	D	1470	0	1399	40	0
1	E	1467	0	1395	34	0
1	F	1508	0	1422	57	0
1	G	1491	0	1415	48	0
1	H	1485	0	1410	36	0
2	A	2	0	0	1	0
2	B	1	0	0	0	0
2	H	1	0	0	2	0
3	A	74	0	0	3	0
3	B	58	0	0	3	0
3	C	51	0	0	1	0
3	D	6	0	0	1	0
3	E	8	0	0	0	0
3	F	53	0	0	0	0
3	G	69	0	0	5	0
3	H	64	0	0	2	0
All	All	12269	0	11266	301	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 13.

The worst 5 of 301 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:G:128[B]:MSE:HG3	1:H:128[B]:MSE:CE	1.55	1.36
1:A:128:MSE:HE3	1:A:129:PHE:O	1.23	1.29
1:G:128[B]:MSE:CG	1:H:128[B]:MSE:HE3	1.71	1.18
1:F:49:MSE:HE2	1:F:145:LYS:HD3	1.33	1.10
1:B:49:MSE:HE2	1:B:145:LYS:HD3	1.13	1.08

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	193/201 (96%)	186 (96%)	7 (4%)	0	100	100
1	B	191/201 (95%)	185 (97%)	6 (3%)	0	100	100
1	C	188/201 (94%)	180 (96%)	8 (4%)	0	100	100
1	D	189/201 (94%)	183 (97%)	6 (3%)	0	100	100
1	E	188/201 (94%)	183 (97%)	5 (3%)	0	100	100
1	F	192/201 (96%)	183 (95%)	8 (4%)	1 (0%)	24	29
1	G	191/201 (95%)	185 (97%)	6 (3%)	0	100	100
1	H	190/201 (94%)	185 (97%)	5 (3%)	0	100	100
All	All	1522/1608 (95%)	1470 (97%)	51 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	197	HIS

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	162/156 (104%)	158 (98%)	4 (2%)	42	54
1	B	161/156 (103%)	158 (98%)	3 (2%)	50	63
1	C	158/156 (101%)	154 (98%)	4 (2%)	42	54
1	D	159/156 (102%)	155 (98%)	4 (2%)	42	54
1	E	158/156 (101%)	153 (97%)	5 (3%)	34	46
1	F	162/156 (104%)	156 (96%)	6 (4%)	30	41
1	G	161/156 (103%)	156 (97%)	5 (3%)	35	47
1	H	160/156 (103%)	157 (98%)	3 (2%)	50	63
All	All	1281/1248 (103%)	1247 (97%)	34 (3%)	39	52

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	12	ASN
1	G	164	ASN
1	H	173	ASN
1	D	164	ASN
1	D	125	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	157	ASN
1	G	173	ASN
1	H	173	ASN
1	H	41	ASN
1	G	41	ASN

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 4 ligands modelled in this entry, 4 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, 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	184/201 (91%)	-0.10	8 (4%) 40 37	22, 30, 63, 95	0
1	B	182/201 (90%)	-0.02	4 (2%) 62 63	24, 37, 64, 125	0
1	C	179/201 (89%)	0.29	9 (5%) 34 31	27, 44, 92, 108	0
1	D	180/201 (89%)	0.67	9 (5%) 34 31	38, 57, 100, 126	0
1	E	179/201 (89%)	0.62	7 (3%) 43 40	40, 59, 86, 110	0
1	F	182/201 (90%)	0.37	10 (5%) 30 28	24, 45, 91, 132	0
1	G	181/201 (90%)	-0.10	6 (3%) 49 48	21, 30, 61, 90	0
1	H	180/201 (89%)	-0.02	4 (2%) 62 63	25, 37, 63, 114	0
All	All	1447/1608 (89%)	0.21	57 (3%) 43 40	21, 42, 84, 132	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	LEU	6.2
1	F	7	THR	5.3
1	E	6	VAL	5.3
1	F	8	ALA	4.8
1	D	6	VAL	4.6

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(Å ²)	Q<0.9
2	CL	A	302	1/1	0.85	0.12	56,56,56,56	0
2	CL	A	301	1/1	0.91	0.16	53,53,53,53	0
2	CL	B	301	1/1	0.93	0.16	71,71,71,71	0
2	CL	H	301	1/1	0.94	0.10	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.