



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 27, 2026 – 10:06 AM EDT

PDB ID : 9Z38 / pdb_00009z38
Title : Crystal Structure of CalO4 from Micromonospora echinospora
Authors : Pang, F.; Townsend, C.A.
Deposited on : 2025-11-05
Resolution : 1.64 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

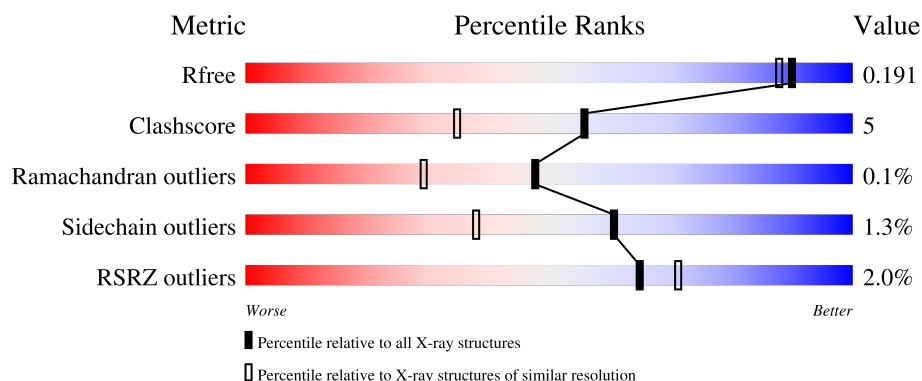
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	358	86% 8% ••
1	C	358	3% 86% 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
3	CL	C	405	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5473 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 3-oxoacyl-[acyl-carrier-protein] synthase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	3	0
			2522	1603	423	478	18			
1	C	342	Total	C	N	O	S	0	4	0
			2524	1604	421	481	18			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLN	ARG	conflict	UNP A0A1C6VYG5
A	49	LEU	MET	conflict	UNP A0A1C6VYG5
A	128	LYS	ARG	conflict	UNP A0A1C6VYG5
A	179	MET	LEU	conflict	UNP A0A1C6VYG5
A	253	GLY	ALA	conflict	UNP A0A1C6VYG5
A	343	GLU	-	expression tag	UNP A0A1C6VYG5
A	344	ARG	-	expression tag	UNP A0A1C6VYG5
A	345	LYS	-	expression tag	UNP A0A1C6VYG5
A	346	LEU	-	expression tag	UNP A0A1C6VYG5
A	347	ALA	-	expression tag	UNP A0A1C6VYG5
A	348	ALA	-	expression tag	UNP A0A1C6VYG5
A	349	ALA	-	expression tag	UNP A0A1C6VYG5
A	350	LEU	-	expression tag	UNP A0A1C6VYG5
A	351	GLU	-	expression tag	UNP A0A1C6VYG5
A	352	HIS	-	expression tag	UNP A0A1C6VYG5
A	353	HIS	-	expression tag	UNP A0A1C6VYG5
A	354	HIS	-	expression tag	UNP A0A1C6VYG5
A	355	HIS	-	expression tag	UNP A0A1C6VYG5
A	356	HIS	-	expression tag	UNP A0A1C6VYG5
A	357	HIS	-	expression tag	UNP A0A1C6VYG5
A	358	VAL	-	expression tag	UNP A0A1C6VYG5
C	27	GLN	ARG	conflict	UNP A0A1C6VYG5
C	49	LEU	MET	conflict	UNP A0A1C6VYG5
C	128	LYS	ARG	conflict	UNP A0A1C6VYG5
C	179	MET	LEU	conflict	UNP A0A1C6VYG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	253	GLY	ALA	conflict	UNP A0A1C6VYG5
C	359	GLU	-	expression tag	UNP A0A1C6VYG5
C	360	ARG	-	expression tag	UNP A0A1C6VYG5
C	361	LYS	-	expression tag	UNP A0A1C6VYG5
C	362	LEU	-	expression tag	UNP A0A1C6VYG5
C	363	ALA	-	expression tag	UNP A0A1C6VYG5
C	364	ALA	-	expression tag	UNP A0A1C6VYG5
C	365	ALA	-	expression tag	UNP A0A1C6VYG5
C	366	LEU	-	expression tag	UNP A0A1C6VYG5
C	367	GLU	-	expression tag	UNP A0A1C6VYG5
C	368	HIS	-	expression tag	UNP A0A1C6VYG5
C	369	HIS	-	expression tag	UNP A0A1C6VYG5
C	370	HIS	-	expression tag	UNP A0A1C6VYG5
C	371	HIS	-	expression tag	UNP A0A1C6VYG5
C	372	HIS	-	expression tag	UNP A0A1C6VYG5
C	373	HIS	-	expression tag	UNP A0A1C6VYG5
C	374	VAL	-	expression tag	UNP A0A1C6VYG5

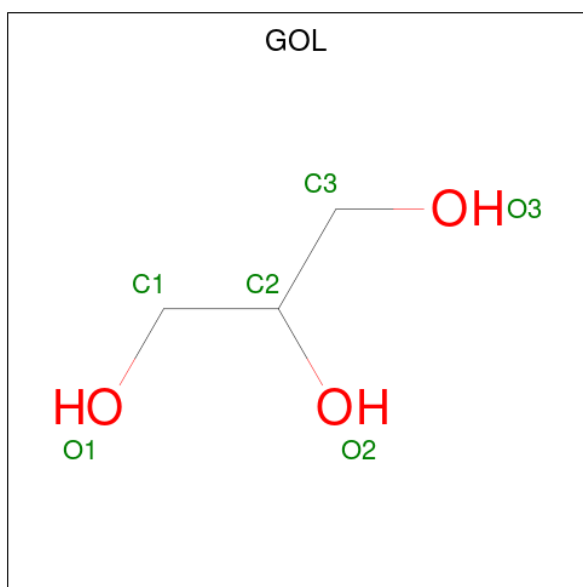
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	C	3	Total Mg 3 3	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	C	3	Total Cl 3 3	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		

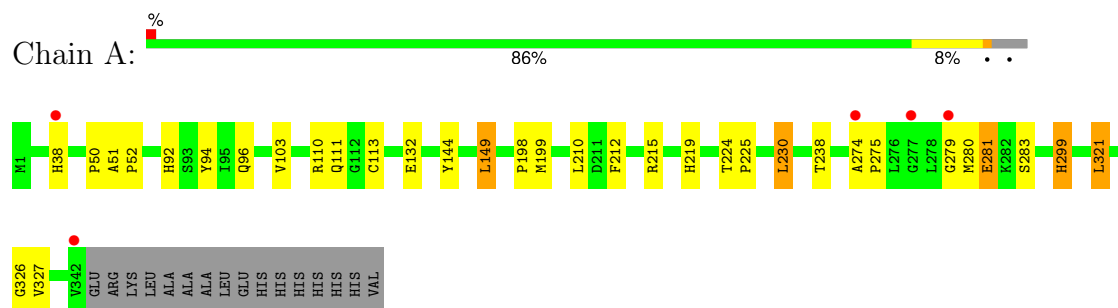
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	204	Total	O	0	0
			204	204		
6	C	203	Total	O	0	0
			203	203		

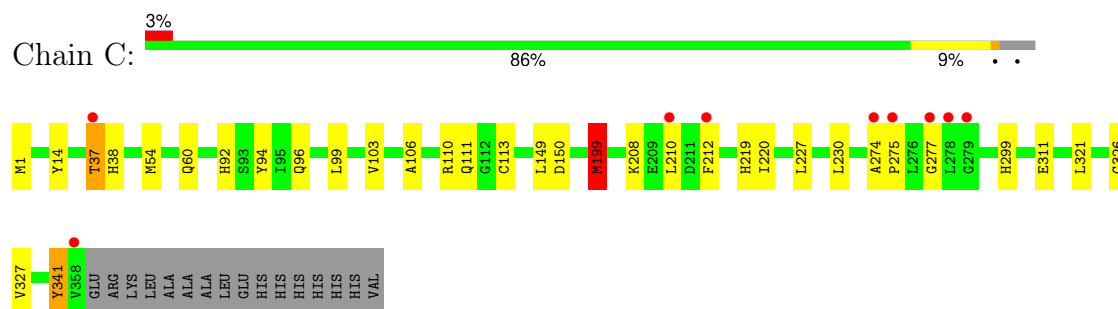
3 Residue-property plots

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: 3-oxoacyl-[acyl-carrier-protein] synthase-3



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase-3



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	47.70Å 95.64Å 172.58Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	29.24 – 1.64 29.24 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.24-1.64) 98.7 (29.24-1.64)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.163 , 0.193 0.162 , 0.191	Depositor DCC
R_{free} test set	4745 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5473	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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: MG, GOL, CL, CA

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	0.81	0/2581	1.29	11/3519 (0.3%)
1	C	0.86	1/2582 (0.0%)	1.32	11/3521 (0.3%)
All	All	0.84	1/5163 (0.0%)	1.31	22/7040 (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	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	341	TYR	C-N	15.73	1.55	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	TYR	O-C-N	-9.53	109.56	122.33
1	C	37	THR	CA-CB-OG1	-9.33	95.61	109.60
1	C	208	LYS	N-CA-CB	-8.08	97.81	109.85
1	A	149	LEU	N-CA-CB	-7.23	97.92	111.00
1	C	212	PHE	N-CA-CB	-7.01	99.90	110.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	C	110	ARG	Sidechain
1	C	341	TYR	Mainchain

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	2522	0	2420	25	0
1	C	2524	0	2423	26	0
2	A	4	0	0	0	0
2	C	3	0	0	0	0
3	A	3	0	0	1	0
3	C	3	0	0	3	0
4	C	6	0	8	0	0
5	C	1	0	0	0	0
6	A	204	0	0	6	0
6	C	203	0	0	4	0
All	All	5473	0	4851	47	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 5.

The worst 5 of 47 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:198:PRO:HG2	6:A:526:HOH:O	1.61	1.01
1:A:92:HIS:HE1	1:C:111:GLN:HE22	1.20	0.90
1:C:275:PRO:C	1:C:277:GLY:H	1.88	0.81
1:C:299:HIS:HD2	6:C:664:HOH:O	1.67	0.78
1:A:299:HIS:HD2	6:A:675:HOH:O	1.68	0.74

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	343/358 (96%)	332 (97%)	10 (3%)	1 (0%)	36	20
1	C	344/358 (96%)	332 (96%)	12 (4%)	0	100	100
All	All	687/716 (96%)	664 (97%)	22 (3%)	1 (0%)	48	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	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	241/270 (89%)	238 (99%)	3 (1%)	63	41
1	C	243/270 (90%)	240 (99%)	3 (1%)	63	41
All	All	484/540 (90%)	478 (99%)	6 (1%)	61	41

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	37	THR
1	C	199	MET
1	C	230	LEU
1	A	230	LEU
1	A	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	111	GLN
1	C	243	GLN
1	C	299	HIS
1	A	223	GLN
1	A	299	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 14 are monoatomic - leaving 1 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	C	401	-	5,5,5	0.25	0	5,5,5	0.76	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
4	GOL	C	401	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	GOL	O1-C1-C2-C3

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	342/358 (95%)	-0.46	5 (1%) 72 77	6, 14, 28, 49	3 (0%)
1	C	342/358 (95%)	-0.42	9 (2%) 57 62	5, 14, 27, 48	4 (1%)
All	All	684/716 (95%)	-0.44	14 (2%) 65 71	5, 14, 28, 49	7 (1%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	279	GLY	3.9
1	C	274	ALA	3.3
1	A	342	VAL	3.2
1	A	279	GLY	3.2
1	C	212	PHE	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, 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
3	CL	C	407	1/1	0.80	0.18	69,69,69,69	0
3	CL	C	405	1/1	0.83	0.21	66,66,66,66	0
3	CL	A	407	1/1	0.86	0.15	52,52,52,52	0
5	CA	C	408	1/1	0.87	0.13	74,74,74,74	0
2	MG	A	403	1/1	0.88	0.11	43,43,43,43	0
4	GOL	C	401	6/6	0.88	0.12	25,31,35,36	0
3	CL	C	406	1/1	0.88	0.12	50,50,50,50	0
2	MG	A	402	1/1	0.90	0.11	43,43,43,43	0
2	MG	C	403	1/1	0.91	0.18	36,36,36,36	0
2	MG	A	404	1/1	0.92	0.10	36,36,36,36	0
3	CL	A	405	1/1	0.92	0.11	51,51,51,51	0
3	CL	A	406	1/1	0.93	0.21	51,51,51,51	1
2	MG	A	401	1/1	0.96	0.16	37,37,37,37	0
2	MG	C	402	1/1	0.98	0.05	26,26,26,26	0
2	MG	C	404	1/1	0.99	0.06	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.