Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 11:22 AM EDT

PDB ID	:	4XXA
Title	:	Crystal structure of a recombinant Vatairea macrocarpa seed lectin
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Deposited on	:	2015-01-30
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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 1.90 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.
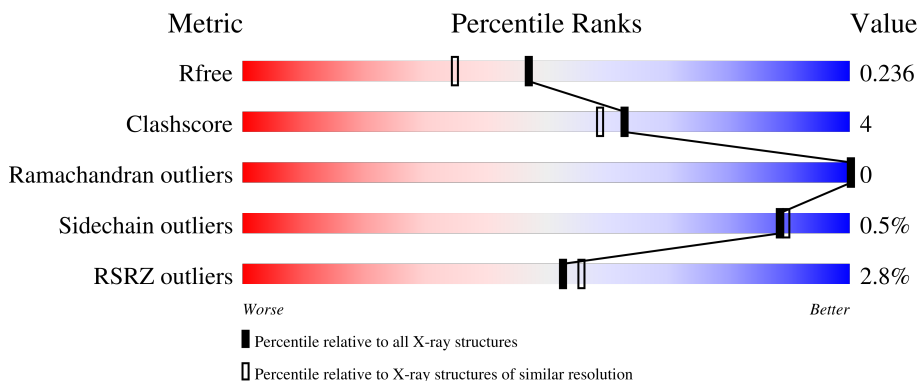
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	250	3% / 86% / 8% / 6%
1	B	250	2% / 84% / 9% / 6%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 3816 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 Seed lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total 1812	C 1157	N 297	O 357	S 1	0	0	0
1	B	234	Total 1814	C 1157	N 297	O 359	S 1	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P81371
A	1	ALA	-	expression tag	UNP P81371
A	242	LEU	-	expression tag	UNP P81371
A	243	GLU	-	expression tag	UNP P81371
A	244	HIS	-	expression tag	UNP P81371
A	245	HIS	-	expression tag	UNP P81371
A	246	HIS	-	expression tag	UNP P81371
A	247	HIS	-	expression tag	UNP P81371
A	248	HIS	-	expression tag	UNP P81371
A	249	HIS	-	expression tag	UNP P81371
B	0	MET	-	initiating methionine	UNP P81371
B	1	ALA	-	expression tag	UNP P81371
B	242	LEU	-	expression tag	UNP P81371
B	243	GLU	-	expression tag	UNP P81371
B	244	HIS	-	expression tag	UNP P81371
B	245	HIS	-	expression tag	UNP P81371
B	246	HIS	-	expression tag	UNP P81371
B	247	HIS	-	expression tag	UNP P81371
B	248	HIS	-	expression tag	UNP P81371
B	249	HIS	-	expression tag	UNP P81371

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0
3	B	1	Total 1	Mn 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
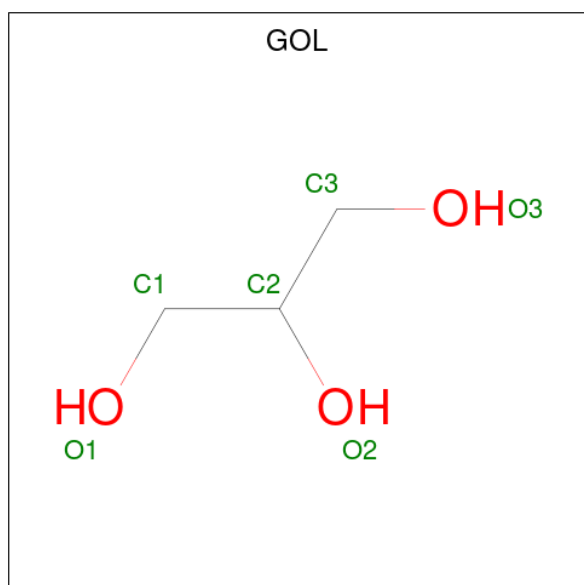
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

1PE

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 11	C 7	O 4	0	0
5	B	1	Total 10	C 6	O 4	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total 67	O 67	0	0
6	B	86	Total 86	O 86	0	0

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, 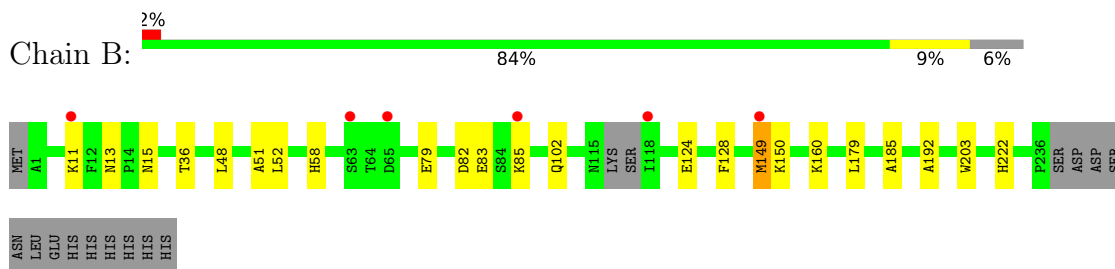yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Seed lectin

Chain A:

- Molecule 1: Seed lectin

Chain B:
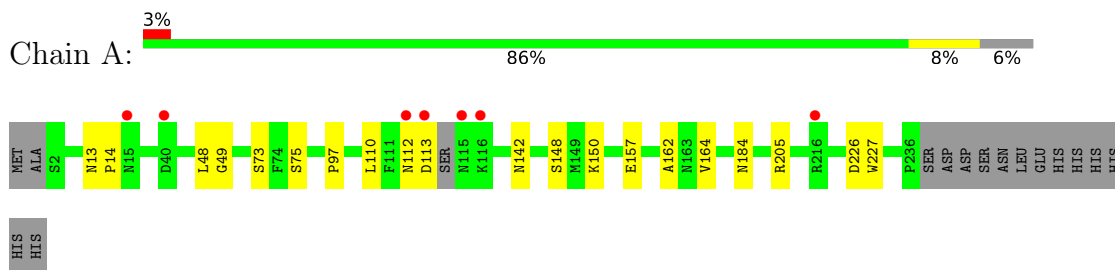
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.08Å 96.08Å 85.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.21 – 1.90 48.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.21-1.90) 99.9 (48.04-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.94 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.192 , 0.235 0.199 , 0.236	Depositor DCC
R_{free} test set	1764 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3816	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 1PE, CA, MN, GOL

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	0.88	0/1859	0.91	0/2535
1	B	0.95	2/1861 (0.1%)	0.94	0/2539
All	All	0.92	2/3720 (0.1%)	0.93	0/5074

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	GLU	CD-OE2	-5.27	1.19	1.25
1	B	83	GLU	CD-OE1	5.22	1.31	1.25

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	1812	0	1750	12	0
1	B	1814	0	1749	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	2	0
5	A	11	0	13	0	0
5	B	10	0	13	3	0
6	A	67	0	0	1	0
6	B	86	0	0	2	0
All	All	3816	0	3541	31	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.

All (31) 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:B:149:MET:SD	1:B:192:ALA:HB1	2.05	0.96
1:B:52:LEU:HD12	1:B:52:LEU:N	1.99	0.76
1:B:128:PHE:CE2	4:B:303:GOL:H31	2.27	0.69
1:B:149:MET:SD	1:B:192:ALA:CB	2.84	0.66
1:A:157:GLU:HG2	6:A:420:HOH:O	1.99	0.62
1:B:51:ALA:C	1:B:52:LEU:HD12	2.20	0.62
1:A:48:LEU:C	1:A:48:LEU:HD23	2.25	0.56
1:B:82:ASP:OD2	1:B:85:LYS:HE3	2.07	0.54
1:B:128:PHE:CD2	4:B:303:GOL:H31	2.45	0.52
1:B:79:GLU:OE2	5:B:304:1PE:H231	2.09	0.51
1:A:112:ASN:OD1	1:A:113:ASP:N	2.44	0.51
5:B:304:1PE:C24	5:B:304:1PE:OH3	2.59	0.51
1:A:157:GLU:CD	1:A:184:ASN:HD22	2.15	0.49
1:B:13:ASN:ND2	1:B:15:ASN:H	2.11	0.48
1:B:36:THR:OG1	1:B:222:HIS:HD2	1.99	0.45
1:A:97:PRO:HA	1:A:205:ARG:HG3	2.00	0.44
1:A:48:LEU:HD23	1:A:49:GLY:N	2.33	0.43
1:A:150:LYS:NZ	1:B:185:ALA:O	2.51	0.43
1:A:226:ASP:O	1:A:227:TRP:HB2	2.18	0.42
5:B:304:1PE:OH3	5:B:304:1PE:H241	2.19	0.42
1:B:149:MET:HG3	1:B:150:LYS:N	2.33	0.42
1:A:75:SER:HA	1:A:162:ALA:O	2.20	0.42
1:B:11:LYS:HG2	6:B:436:HOH:O	2.19	0.42
1:B:52:LEU:N	1:B:52:LEU:CD1	2.70	0.42
1:B:179:LEU:C	1:B:179:LEU:HD23	2.40	0.42
1:B:48:LEU:HD11	1:B:102:GLN:O	2.20	0.41
1:B:160:LYS:HE3	6:B:425:HOH:O	2.20	0.41
1:B:58:HIS:HB2	1:B:203:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ASN:OD1	1:A:14:PRO:O	2.39	0.41
1:A:142:ASN:ND2	1:A:148:SER:OG	2.52	0.41
1:A:73:SER:HA	1:A:164:VAL:O	2.21	0.40

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	230/250 (92%)	223 (97%)	7 (3%)	0	100	100
1	B	231/250 (92%)	225 (97%)	6 (3%)	0	100	100
All	All	461/500 (92%)	448 (97%)	13 (3%)	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	201/216 (93%)	200 (100%)	1 (0%)	88	89
1	B	201/216 (93%)	200 (100%)	1 (0%)	88	89
All	All	402/432 (93%)	400 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	B	149	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	142	ASN
1	B	13	ASN
1	B	130	ASN
1	B	142	ASN
1	B	222	HIS

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	B	303	-	5,5,5	0.83	0	5,5,5	1.40	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	303	-	5,5,5	0.18	0	5,5,5	1.32	1 (20%)
5	1PE	A	304	-	10,10,15	1.13	0	9,9,14	0.92	0
5	1PE	B	304	-	9,9,15	0.97	0	8,8,14	1.41	1 (12%)

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	B	303	-	-	0/4/4/4	-
4	GOL	A	303	-	-	0/4/4/4	-
5	1PE	A	304	-	-	5/8/8/13	-
5	1PE	B	304	-	-	2/7/7/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	304	1PE	OH3-C23-C13	3.38	125.65	110.39
4	B	303	GOL	C3-C2-C1	-2.58	101.69	111.70
4	A	303	GOL	O2-C2-C3	2.01	117.98	109.12

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	304	1PE	C23-C13-OH4-C24
5	B	304	1PE	C12-C22-OH3-C23
5	A	304	1PE	OH2-C12-C22-OH3
5	A	304	1PE	C13-C23-OH3-C22
5	A	304	1PE	C23-C13-OH4-C24
5	A	304	1PE	OH4-C13-C23-OH3
5	A	304	1PE	OH5-C14-C24-OH4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	1PE	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	234/250 (93%)	0.04	7 (2%)	50	53	24, 35, 48, 54	0
1	B	234/250 (93%)	-0.08	6 (2%)	56	58	25, 33, 45, 51	0
All	All	468/500 (93%)	-0.02	13 (2%)	53	56	24, 34, 46, 54	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	ASN	3.6
1	B	118	ILE	3.6
1	A	216	ARG	3.6
1	B	65	ASP	3.3
1	A	116	LYS	3.3
1	A	40	ASP	2.8
1	B	149	MET	2.8
1	B	63	SER	2.7
1	A	113	ASP	2.6
1	A	112	ASN	2.2
1	B	85	LYS	2.2
1	A	15	ASN	2.1
1	B	11	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($\mathring{A}^2$)	Q<0.9
5	1PE	A	304	11/16	0.79	0.23	35,35,35,35	0
5	1PE	B	304	10/16	0.80	0.22	35,35,35,35	0
4	GOL	B	303	6/6	0.84	0.24	35,35,35,35	0
4	GOL	A	303	6/6	0.86	0.21	35,35,35,35	0
3	MN	B	302	1/1	0.90	0.24	35,35,35,35	0
3	MN	A	302	1/1	0.91	0.22	35,35,35,35	0
2	CA	B	301	1/1	0.94	0.07	35,35,35,35	0
2	CA	A	301	1/1	0.97	0.04	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.