



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:48 AM UTC

PDB ID : 3H3Z / pdb_00003h3z
Title : Crystal structure of a putative cyclic nucleotide binding protein (spoa0323) from ruegeria pomeroyi dss-3 at 2.35 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2009-04-17
Resolution : 2.35 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 ⓘ 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

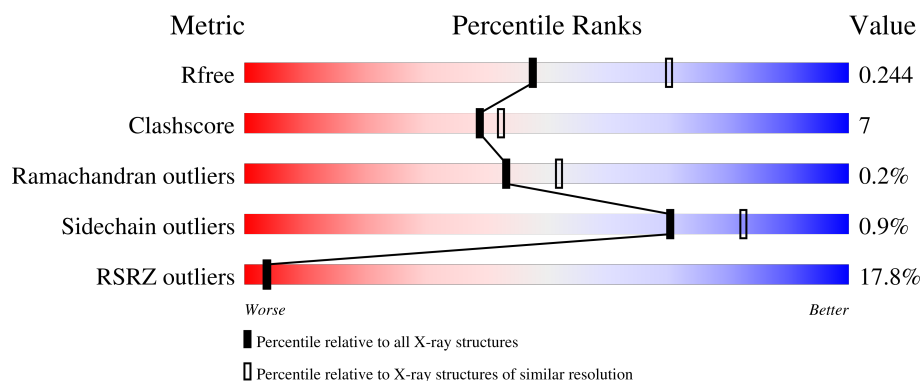
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 ≥ 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	235	18% 81% 14% .
1	B	235	16% 80% 16% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3588 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 Cyclic nucleotide-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	Se	0	7	0
			1744	1107	304	321	5	7			
1	B	228	Total	C	N	O	S	Se	0	4	0
			1744	1111	296	326	6	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q5LKQ8
B	0	GLY	-	expression tag	UNP Q5LKQ8

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

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

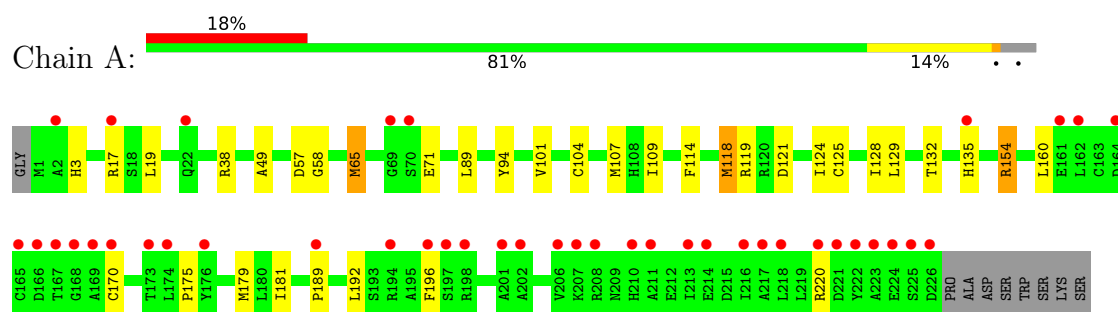
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	35	Total	O	0	0
			35	35		

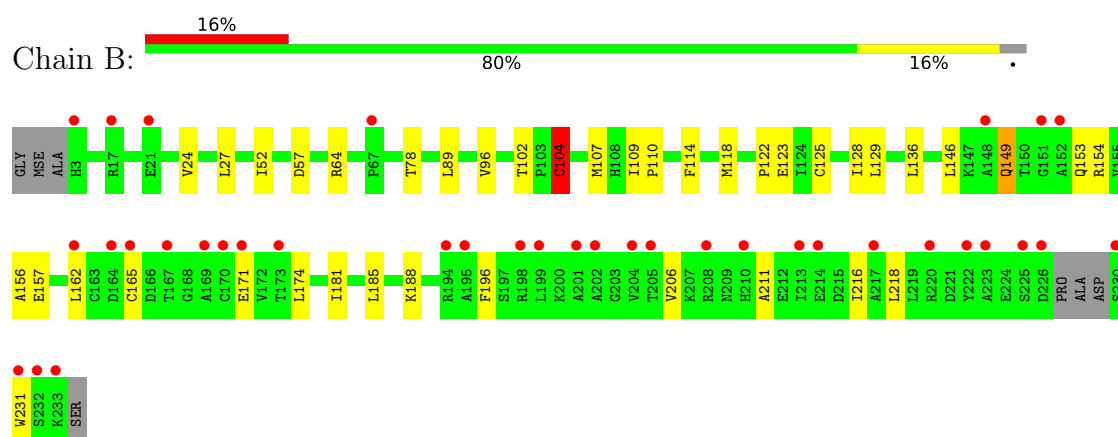
3 Residue-property plots [i](#)

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: Cyclic nucleotide-binding protein



• Molecule 1: Cyclic nucleotide-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	137.05Å 137.05Å 94.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.72 – 2.35 28.72 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.72-2.35) 99.7 (28.72-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.202 , 0.236 0.211 , 0.244	Depositor DCC
R_{free} test set	1409 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3588	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.01	1/1771 (0.1%)	1.06	2/2397 (0.1%)
1	B	0.96	0/1772	1.12	7/2401 (0.3%)
All	All	0.99	1/3543 (0.0%)	1.09	9/4798 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	MSE	SE-CE	5.77	2.12	1.95

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	THR	CA-C-N	-7.70	111.85	119.78
1	B	102	THR	C-N-CA	-7.70	111.85	119.78
1	B	149	GLN	N-CA-C	6.34	118.48	110.24
1	B	104	CYS	N-CA-C	6.24	118.26	108.96
1	A	170	CYS	N-CA-C	5.88	117.46	108.52
1	B	52	ILE	N-CA-C	-5.88	100.01	108.53
1	B	188	LYS	N-CA-C	-5.44	102.92	109.83
1	B	27	LEU	N-CA-C	-5.30	104.93	111.40
1	A	118	MSE	CA-CB-CG	-5.12	103.87	114.10

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	1744	0	1689	25	0
1	B	1744	0	1684	28	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
3	A	63	0	0	1	0
3	B	35	0	0	0	0
All	All	3588	0	3373	46	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 7.

All (46) 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:57:ASP:O	1:A:104:CYS:HB2	1.95	0.66
1:A:179[A]:MSE:SE	1:A:189:PRO:HB3	2.48	0.64
1:A:125[A]:CYS:CB	1:B:125[A]:CYS:HG	2.11	0.63
1:A:107:MSE:HE3	1:A:109:ILE:HD11	1.80	0.63
1:B:196:PHE:CD1	1:B:206:VAL:HG21	2.35	0.61
1:B:118:MSE:SE	1:B:125[B]:CYS:HB3	2.50	0.60
1:B:57:ASP:O	1:B:104:CYS:HB3	2.03	0.59
1:A:3:HIS:HD2	3:A:264:HOH:O	1.85	0.58
1:B:165:CYS:O	1:B:216:ILE:HD13	2.03	0.58
1:B:174:LEU:HD22	1:B:181:ILE:HD11	1.86	0.58
1:B:89:LEU:HD21	1:B:114:PHE:CD2	2.39	0.57
1:B:107:MSE:HE3	1:B:109:ILE:HD11	1.86	0.57
1:A:128:ILE:O	1:A:132:THR:HG23	2.05	0.56
1:B:165:CYS:SG	1:B:216:ILE:HD11	2.47	0.55
1:A:154:ARG:HG3	1:B:146:LEU:HD13	1.90	0.54
1:A:38[A]:ARG:NE	2:A:235:CL:CL	2.78	0.53
1:B:89:LEU:HD21	1:B:114:PHE:CE2	2.44	0.52
1:A:192:LEU:HG	1:A:196:PHE:CE2	2.45	0.51
1:A:65:MSE:SE	1:A:71:GLU:HG2	2.61	0.51
1:B:64:ARG:HG3	1:B:96:VAL:HG12	1.94	0.48
1:A:179[A]:MSE:SE	1:A:189:PRO:HG3	2.64	0.48
1:A:154:ARG:CG	1:B:146:LEU:HD13	2.44	0.47
1:A:49:ALA:HA	1:A:94:TYR:CZ	2.50	0.47
1:A:58:GLY:HA3	1:A:104:CYS:HB3	1.97	0.47
1:B:153:GLN:O	1:B:156:ALA:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLN:NE2	1:B:157:GLU:OE2	2.39	0.45
1:B:154:ARG:NH1	1:B:185:LEU:O	2.50	0.45
1:A:89:LEU:HD21	1:A:118:MSE:HE1	1.98	0.45
1:A:129:LEU:HD11	1:B:128:ILE:HG22	2.00	0.44
1:A:128:ILE:HG22	1:B:129:LEU:HD11	2.00	0.44
1:B:174:LEU:HD22	1:B:181:ILE:CD1	2.49	0.43
1:A:121:ASP:HB3	1:A:124:ILE:HD12	1.99	0.43
1:B:171:GLU:HA	1:B:211:ALA:O	2.18	0.43
1:A:175:PRO:HD2	1:A:181:ILE:HD11	2.01	0.42
1:B:109:ILE:O	1:B:110:PRO:C	2.61	0.42
1:B:218:LEU:HD11	1:B:231:TRP:CH2	2.55	0.42
1:B:122:PRO:HA	1:B:125[B]:CYS:SG	2.59	0.42
1:B:57:ASP:O	1:B:104:CYS:CB	2.67	0.42
1:A:19:LEU:HD21	1:A:114:PHE:HE1	1.85	0.42
1:A:160:LEU:HD11	1:A:220:ARG:HA	2.02	0.41
1:A:118:MSE:HB3	1:A:125[B]:CYS:SG	2.61	0.41
1:B:78:THR:HG21	1:B:162:LEU:HD21	2.02	0.41
1:A:38[A]:ARG:HG3	1:A:101:VAL:O	2.19	0.41
1:A:135[B]:HIS:HB3	1:B:136:LEU:HD21	2.03	0.41
1:B:218:LEU:HD11	1:B:231:TRP:HH2	1.85	0.41
1:A:119:ARG:NE	1:B:123:GLU:OE2	2.50	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	231/235 (98%)	223 (96%)	8 (4%)	0	100	100
1	B	228/235 (97%)	222 (97%)	5 (2%)	1 (0%)	30	34
All	All	459/470 (98%)	445 (97%)	13 (3%)	1 (0%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	VAL

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	173/190 (91%)	170 (98%)	3 (2%)	53	68
1	B	176/190 (93%)	175 (99%)	1 (1%)	78	87
All	All	349/380 (92%)	345 (99%)	4 (1%)	70	79

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17[A]	ARG
1	A	17[B]	ARG
1	A	154	ARG
1	B	104	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	B	12	ASN
1	B	142	GLN

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 2 ligands modelled in this entry, 2 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

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	220/235 (93%)	0.90	42 (19%)	3 3	28, 64, 108, 118	6 (2%)
1	B	223/235 (94%)	0.98	37 (16%)	4 5	27, 69, 104, 118	4 (1%)
All	All	443/470 (94%)	0.94	79 (17%)	4 4	27, 67, 107, 118	10 (2%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	7.7
1	B	226	ASP	6.3
1	B	230	SER	5.8
1	B	167	THR	4.3
1	A	211	ALA	4.2
1	A	135[A]	HIS	4.1
1	B	233	LYS	4.0
1	B	164	ASP	4.0
1	A	170	CYS	3.9
1	A	167	THR	3.7
1	A	164	ASP	3.7
1	A	166	ASP	3.7
1	A	225	SER	3.7
1	B	204	VAL	3.6
1	B	223	ALA	3.6
1	A	224	GLU	3.6
1	A	220	ARG	3.6
1	A	176	TYR	3.5
1	B	231	TRP	3.5
1	A	207	LYS	3.4
1	A	22[A]	GLN	3.4
1	A	208	ARG	3.2
1	A	213	ILE	3.2
1	A	2	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	225	SER	3.2
1	B	208	ARG	3.2
1	A	217	ALA	3.2
1	A	218	LEU	3.2
1	A	196	PHE	3.2
1	A	201	ALA	3.1
1	B	17[A]	ARG	3.1
1	A	210	HIS	3.0
1	B	165	CYS	3.0
1	A	169	ALA	2.9
1	A	214	GLU	2.9
1	B	152	ALA	2.9
1	A	206	VAL	2.9
1	A	223	ALA	2.8
1	B	3	HIS	2.8
1	A	17[A]	ARG	2.8
1	B	195	ALA	2.8
1	B	194	ARG	2.7
1	B	170	CYS	2.7
1	A	222	TYR	2.7
1	B	169	ALA	2.6
1	B	148	ALA	2.6
1	B	199	LEU	2.5
1	B	202	ALA	2.5
1	B	21	GLU	2.5
1	B	162	LEU	2.5
1	A	198	ARG	2.4
1	A	165	CYS	2.4
1	B	171	GLU	2.4
1	B	232	SER	2.4
1	A	189	PRO	2.3
1	B	222	TYR	2.3
1	A	69	GLY	2.3
1	B	201	ALA	2.3
1	A	194	ARG	2.3
1	B	198	ARG	2.3
1	A	168	GLY	2.3
1	A	161	GLU	2.3
1	B	213	ILE	2.3
1	B	220	ARG	2.2
1	A	202	ALA	2.2
1	B	210	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	173	THR	2.2
1	B	217	ALA	2.2
1	A	197	SER	2.2
1	B	214	GLU	2.2
1	B	151	GLY	2.2
1	A	221	ASP	2.1
1	A	173	THR	2.1
1	A	174	LEU	2.1
1	A	216	ILE	2.1
1	A	70	SER	2.0
1	B	205	THR	2.0
1	B	67	PRO	2.0
1	A	162	LEU	2.0

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	235	1/1	0.83	0.24	107,107,107,107	0
2	CL	B	235	1/1	0.96	0.19	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.