



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:47 pm GMT

PDB ID : 2QTW
Title : The Crystal Structure of PCSK9 at 1.9 Angstroms Resolution Reveals structural homology to Resistin within the C-terminal domain
Authors : Hampton, E.N.; Knuth, M.W.; Li, J.; Harris, J.L.; Lesley, S.A.; Spraggon, G.
Deposited on : 2007-08-02
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

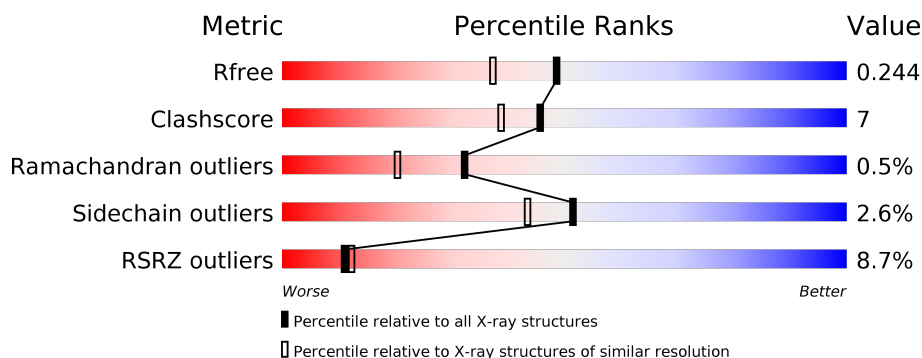
1 Overall quality at a glance

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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	124	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>6%</div> <div>26%</div> </div> </div>
2	B	546	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>• 11%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4697 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 Proprotein convertase subtilisin/kexin type 9 Propeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	1	0
			748	479	136	131	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	486	Total	C	N	O	S	0	1	0
			3614	2229	668	685	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	693	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	694	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	695	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	696	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	697	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	698	HIS	-	EXPRESSION TAG	UNP Q8NBP7

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	B	254	Total	O	0	0
			254	254		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.43Å 70.15Å 148.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 47.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.90) 99.8 (47.79-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.239 0.197 , 0.244	Depositor DCC
R_{free} test set	2654 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4697	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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: CA, NAG

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	0.80	0/768	0.77	0/1037
2	B	0.73	3/3682 (0.1%)	0.75	1/4996 (0.0%)
All	All	0.74	3/4450 (0.1%)	0.75	1/6033 (0.0%)

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
2	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	654	CYS	CB-SG	-6.35	1.71	1.82
2	B	255	CYS	C-N	-5.62	1.21	1.34
2	B	256	GLN	C-N	-5.29	1.23	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	LEU	CA-CB-CG	6.44	130.11	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	494	LYS	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	748	0	763	4	1
2	B	3614	0	3522	60	1
3	B	14	0	13	1	0
4	B	1	0	0	0	0
5	A	66	0	0	1	0
5	B	254	0	0	7	0
All	All	4697	0	4298	63	1

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 (63) 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)
2:B:201:MET:HE1	2:B:203:THR:HG22	1.44	0.98
2:B:615:ILE:HD12	2:B:619:GLN:HE21	1.34	0.91
2:B:615:ILE:HD12	2:B:619:GLN:NE2	1.95	0.81
2:B:446:PRO:HB2	2:B:448:THR:HG22	1.63	0.78
2:B:185:LEU:HD11	2:B:271:ILE:HD11	1.65	0.77
2:B:186:ASP:OD2	2:B:230:LEU:HD12	1.85	0.76
2:B:302:GLN:HE21	2:B:306:ARG:HH21	1.34	0.76
2:B:529:LEU:HG	2:B:532:ALA:HB2	1.75	0.68
2:B:201:MET:HE1	2:B:203:THR:CG2	2.23	0.68
2:B:435:VAL:HG23	5:B:1061:HOH:O	1.94	0.68
2:B:343:ASP:HB3	2:B:423:VAL:HG12	1.76	0.66
2:B:437:THR:O	5:B:1167:HOH:O	2.15	0.64
2:B:612:GLU:HG2	2:B:675:VAL:HG22	1.81	0.62
2:B:176:GLY:O	2:B:244:GLY:HA3	2.00	0.61
2:B:343:ASP:OD2	2:B:423:VAL:HG11	2.00	0.61
2:B:343:ASP:CB	2:B:423:VAL:HG12	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:CYS:HB3	2:B:557[B]:HIS:CE1	2.39	0.58
2:B:615:ILE:CD1	2:B:619:GLN:HE21	2.13	0.58
2:B:638:LEU:HD13	2:B:675:VAL:HG21	1.86	0.56
2:B:189:ILE:CD1	2:B:200:VAL:HG11	2.37	0.55
2:B:638:LEU:HD22	2:B:673:THR:HG21	1.90	0.54
2:B:469:ARG:HD2	2:B:515:PHE:CD1	2.44	0.53
2:B:549:ARG:HG2	2:B:589:VAL:HG22	1.91	0.53
1:A:97:ARG:CZ	5:A:202:HOH:O	2.57	0.53
2:B:201:MET:CE	2:B:203:THR:HG22	2.29	0.52
2:B:345:PRO:HD3	2:B:424:ILE:HG23	1.91	0.52
1:A:67:CYS:SG	5:B:1256:HOH:O	2.04	0.52
2:B:343:ASP:CB	2:B:423:VAL:CG1	2.88	0.51
2:B:179:LEU:HD22	2:B:401:SER:HA	1.93	0.51
2:B:468:THR:OG1	2:B:471:ALA:HB2	2.11	0.50
2:B:177:GLY:HA2	2:B:401:SER:OG	2.12	0.50
2:B:632:LEU:HD13	2:B:676:ALA:HB1	1.95	0.49
2:B:193:HIS:HD2	2:B:195:GLU:H	1.61	0.49
2:B:531:GLN:O	3:B:1001:NAG:H82	2.13	0.49
2:B:632:LEU:CD1	2:B:676:ALA:HB1	2.43	0.48
2:B:455:LEU:HD22	2:B:606:LEU:HD11	1.96	0.47
2:B:186:ASP:OD1	2:B:226:HIS:ND1	2.36	0.47
2:B:201:MET:CE	2:B:203:THR:CG2	2.91	0.46
2:B:554:GLN:HB2	2:B:557[B]:HIS:CE1	2.51	0.46
2:B:435:VAL:HG12	2:B:461:TRP:CZ2	2.51	0.46
1:A:152:GLN:C	2:B:386:SER:OG	2.54	0.46
2:B:557[A]:HIS:CE1	2:B:602:HIS:HB2	2.52	0.45
2:B:410:GLU:HA	2:B:528:LEU:HD11	1.99	0.44
2:B:493:GLY:CA	2:B:645:LEU:HD12	2.48	0.44
2:B:200:VAL:HG22	2:B:247:MET:HB2	2.00	0.44
2:B:493:GLY:HA3	2:B:645:LEU:HD12	1.99	0.43
2:B:417:HIS:ND1	5:B:1181:HOH:O	2.36	0.42
2:B:495:ARG:CG	5:B:1133:HOH:O	2.66	0.42
2:B:194:ARG:HG3	2:B:377:THR:HG22	2.02	0.42
2:B:557[B]:HIS:HB2	2:B:601:CYS:O	2.20	0.42
2:B:201:MET:HE2	2:B:201:MET:HB3	1.95	0.42
2:B:289:LEU:HD12	2:B:289:LEU:C	2.41	0.42
2:B:302:GLN:O	2:B:306:ARG:HG3	2.19	0.41
2:B:166:TYR:HA	2:B:447:SER:OG	2.20	0.41
2:B:359:VAL:O	2:B:438:PRO:HG2	2.20	0.41
2:B:495:ARG:HG2	5:B:1133:HOH:O	2.19	0.41
1:A:70:ASP:N	1:A:71:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:CYS:HB2	2:B:586:ASN:HB3	2.02	0.41
2:B:490:SER:OG	2:B:493:GLY:N	2.51	0.41
2:B:554:GLN:H	2:B:557[B]:HIS:CE1	2.39	0.41
2:B:243:LYS:O	2:B:244:GLY:C	2.58	0.41
2:B:680:ARG:NE	5:B:1185:HOH:O	2.52	0.40
2:B:499:ARG:HD3	2:B:512:HIS:NE2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:OH	2:B:405:GLU:OE2[3_655]	2.17	0.03

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	91/124 (73%)	90 (99%)	1 (1%)	0	100	100
2	B	471/546 (86%)	459 (98%)	9 (2%)	3 (1%)	28	16
All	All	562/670 (84%)	549 (98%)	10 (2%)	3 (0%)	32	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	GLY
2	B	545	SER
2	B	280	VAL

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	80/104 (77%)	79 (99%)	1 (1%)	73	72
2	B	389/437 (89%)	378 (97%)	11 (3%)	49	40
All	All	469/541 (87%)	457 (97%)	12 (3%)	51	43

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
2	B	201	MET
2	B	278	GLN
2	B	375	CYS
2	B	490	SER
2	B	571	LEU
2	B	615	ILE
2	B	623	THR
2	B	638	LEU
2	B	644	VAL
2	B	645	LEU
2	B	659	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	116	HIS
2	B	193	HIS
2	B	302	GLN
2	B	449	HIS
2	B	537	HIS
2	B	554	GLN
2	B	602	HIS
2	B	619	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
3	NAG	B	1001	2	14,14,15	0.52	0	15,19,21	1.08	1 (6%)

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
3	NAG	B	1001	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	NAG	C3-C4-C5	2.20	114.10	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	NAG	1	0

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	92/124 (74%)	0.07	5 (5%)	26 30	17, 23, 37, 44	0
2	B	486/546 (89%)	0.62	45 (9%)	9 10	13, 26, 53, 74	0
All	All	578/670 (86%)	0.54	50 (8%)	11 12	13, 25, 52, 74	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	515	PHE	10.4
2	B	546	MET	7.2
2	B	642	SER	6.1
2	B	449	HIS	5.3
2	B	568	VAL	5.2
2	B	659	ARG	5.1
2	B	616	PRO	5.1
2	B	671	ALA	5.0
2	B	212	ASP	5.0
2	B	220	ALA	5.0
2	B	470	MET	4.8
2	B	448	THR	4.7
2	B	469	ARG	4.7
2	B	447	SER	4.7
2	B	570	ASP	4.7
2	B	571	LEU	4.2
2	B	167	ARG	4.1
2	B	620	GLU	4.1
2	B	221	SER	4.1
2	B	584	GLN	4.0
2	B	505	GLY	3.9
2	B	453	TRP	3.9
2	B	530	PRO	3.8
2	B	569	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	643	HIS	3.7
1	A	61	THR	3.6
2	B	555	GLN	3.5
2	B	503	GLN	3.5
2	B	615	ILE	3.4
1	A	103	ALA	3.2
2	B	531	GLN	3.2
2	B	604	PRO	3.1
1	A	104	ARG	3.1
2	B	543	GLU	3.1
2	B	672	VAL	3.0
2	B	194	ARG	3.0
2	B	658	SER	3.0
2	B	516	GLY	2.9
2	B	452	GLY	2.9
2	B	237	ARG	2.5
1	A	85	GLU	2.4
1	A	108	LEU	2.4
2	B	557[A]	HIS	2.3
2	B	545	SER	2.2
2	B	471	ALA	2.2
2	B	192	ASP	2.1
2	B	619	GLN	2.1
2	B	153	SER	2.1
2	B	644	VAL	2.0
2	B	494	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	B	1	1/1	0.91	0.17	0.62	61,61,61,61	0
3	NAG	B	1001	14/15	0.71	0.30	-	57,62,65,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.