



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2024 – 09:42 PM EST

PDB ID : 1SDD
Title : Crystal Structure of Bovine Factor Vai
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Deposited on : 2004-02-13
Resolution : 2.80 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

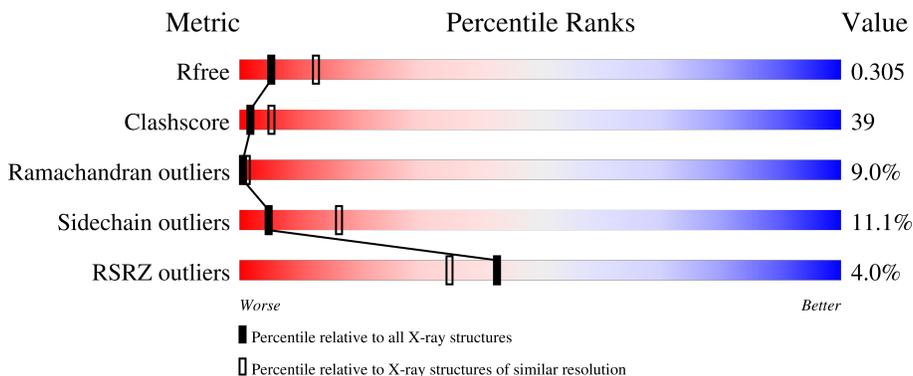
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	306	
2	B	647	

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	NAG	B	2187	X	-	-	-
3	NAG	B	2189	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7271 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.

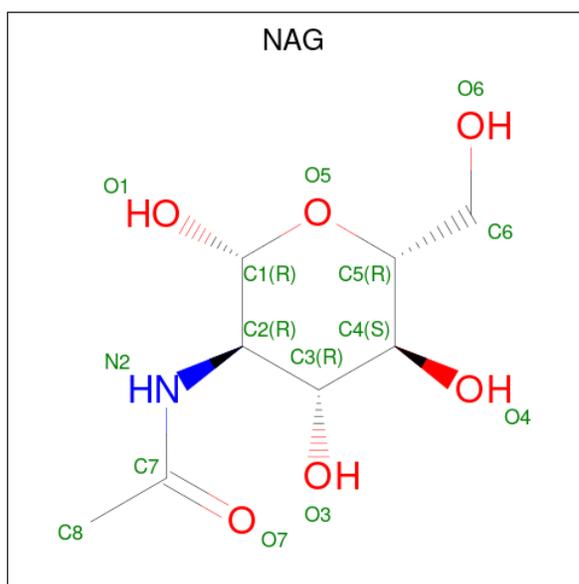
- Molecule 1 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2132	1366	356	398	12	0	0	0

- Molecule 2 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	601	4878	3127	840	888	23	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cu	0	0
			1	1		

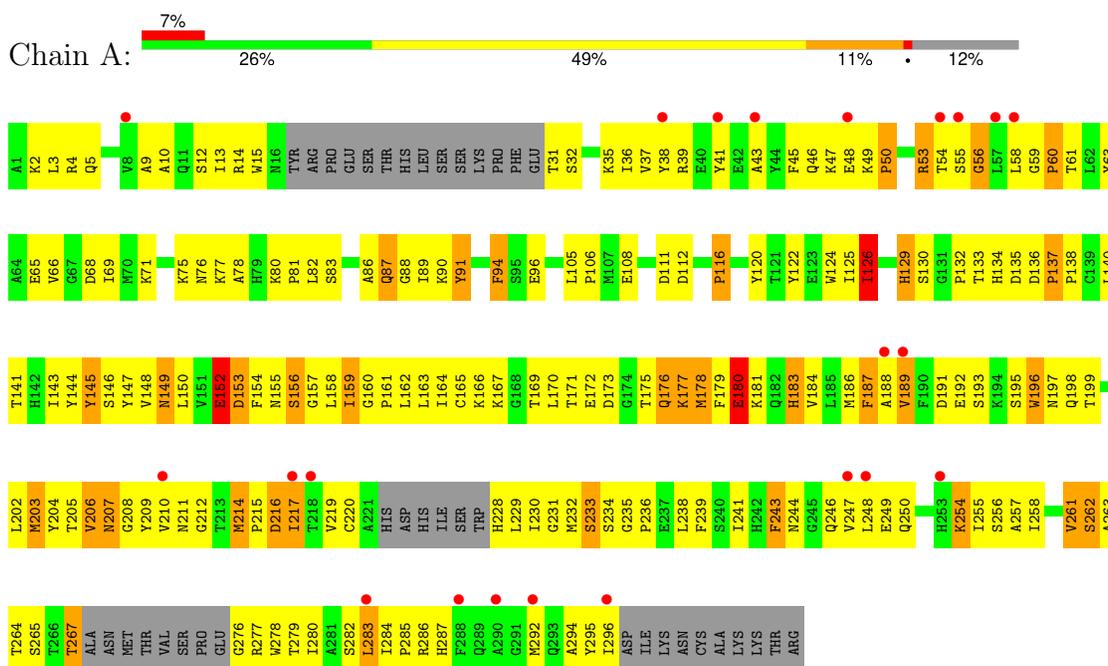
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	142	Total	O	0	0
			142	142		

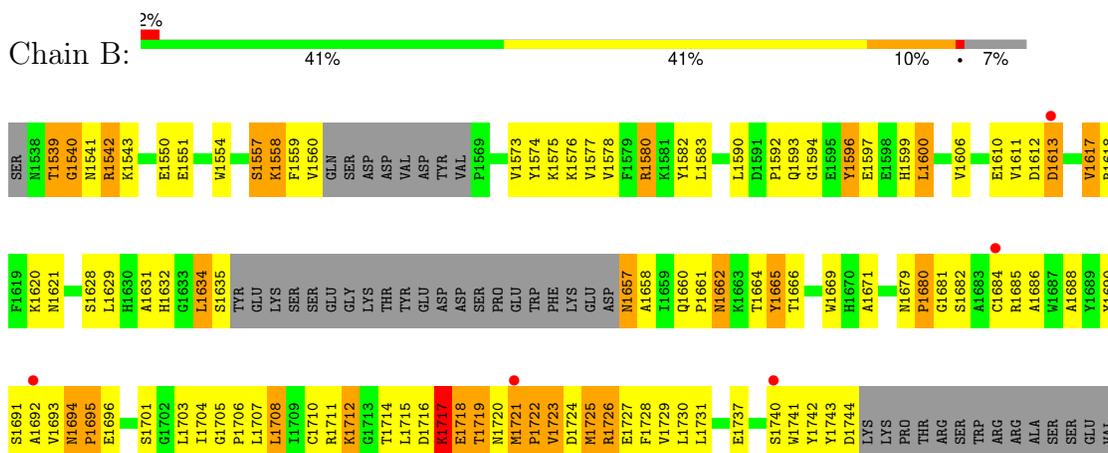
3 Residue-property plots [i](#)

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: Coagulation factor V



• Molecule 2: Coagulation factor V



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.37Å 86.56Å 229.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.80) 90.5 (30.00-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.296 0.248 , 0.305	Depositor DCC
R_{free} test set	918 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: CA, NAG, CU

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	0.35	0/2188	0.60	0/2960
2	B	0.46	0/5012	0.70	2/6792 (0.0%)
All	All	0.43	0/7200	0.67	2/9752 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1847	VAL	N-CA-C	-6.63	93.11	111.00
2	B	2014	ARG	N-CA-C	-6.47	93.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1890	TYR	Sidechain

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	2132	0	2074	198	0
2	B	4878	0	4767	357	0
3	A	28	0	26	3	0
3	B	42	0	39	11	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	47	0	0	1	0
6	B	142	0	0	3	0
All	All	7271	0	6906	549	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 39.

The worst 5 of 549 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:1992:ASP:HB3	2:B:1993:PRO:HD3	1.13	1.13
2:B:2152:ASN:HB2	2:B:2153:PRO:HD3	1.22	1.10
2:B:1721:MET:HG3	2:B:1786:ARG:HH22	1.01	1.08
2:B:1914:THR:HB	2:B:1920:PRO:HD2	1.38	1.05
1:A:264:THR:HG21	2:B:1822:PRO:HG3	1.44	0.98

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	260/306 (85%)	178 (68%)	46 (18%)	36 (14%)	0 0
2	B	593/647 (92%)	479 (81%)	73 (12%)	41 (7%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	853/953 (90%)	657 (77%)	119 (14%)	77 (9%)	0 1

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	A	60	PRO
1	A	180	GLU
1	A	187	PHE
1	A	206	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	233/269 (87%)	208 (89%)	25 (11%)	5 17
2	B	526/570 (92%)	467 (89%)	59 (11%)	5 16
All	All	759/839 (90%)	675 (89%)	84 (11%)	5 16

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1895	LEU
2	B	2079	ASN
2	B	1900	ASN
2	B	1921	TRP
2	B	2113	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1804	HIS
2	B	2083	GLN
2	B	1817	GLN

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Mol	Chain	Res	Type
2	B	2168	ASN
2	B	2065	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	A	2186	1	14,14,15	0.53	0	17,19,21	0.70	0
3	NAG	A	2185	1	14,14,15	0.67	0	17,19,21	0.70	0
3	NAG	B	2187	2	14,14,15	0.61	0	17,19,21	0.79	0
3	NAG	B	2188	2	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
3	NAG	B	2189	2	14,14,15	0.66	0	17,19,21	0.68	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
3	NAG	A	2186	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2185	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2187	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	2188	2	-	2/6/23/26	0/1/1/1
3	NAG	B	2189	2	1/1/5/7	2/6/23/26	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	2188	NAG	C2-N2-C7	-2.21	119.94	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	2187	NAG	C1
3	B	2189	NAG	C1

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2185	NAG	C8-C7-N2-C2
3	A	2185	NAG	O7-C7-N2-C2
3	A	2186	NAG	C8-C7-N2-C2
3	A	2186	NAG	O7-C7-N2-C2
3	B	2187	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2185	NAG	3	0
3	B	2187	NAG	4	0
3	B	2188	NAG	4	0
3	B	2189	NAG	3	0

5.7 Other polymers [i](#)

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 [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	268/306 (87%)	0.81	22 (8%) 19 14	48, 89, 127, 136	0
2	B	601/647 (92%)	-0.05	13 (2%) 62 53	26, 54, 91, 112	0
All	All	869/953 (91%)	0.22	35 (4%) 43 35	26, 64, 116, 136	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	5.6
2	B	1721	MET	4.3
1	A	217	ILE	3.7
1	A	188	ALA	3.4
1	A	54	THR	3.3

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 monosaccharides 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(\AA^2)	Q<0.9
3	NAG	A	2185	14/15	0.28	0.14	127,128,129,130	0
3	NAG	B	2187	14/15	0.66	0.12	94,98,101,101	0
3	NAG	A	2186	14/15	0.80	0.12	86,88,90,91	0
3	NAG	B	2189	14/15	0.82	0.12	70,72,74,76	0
3	NAG	B	2188	14/15	0.88	0.10	73,74,76,78	0
4	CA	A	2184	1/1	0.93	0.07	68,68,68,68	0
5	CU	B	2190	1/1	0.96	0.09	65,65,65,65	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.