



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 27, 2016 – 11:10 AM EDT

PDB ID : 5F4Q
Title : Crystal structure of the human egg surface protein Juno
Authors : Aydin, H.; Sultana, A.; Lee, J.E.
Deposited on : 2015-12-03
Resolution : 1.80 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
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027790

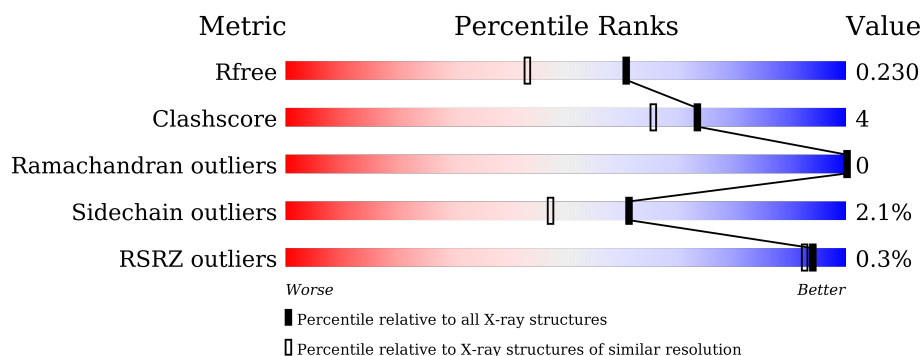
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 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	215	 85% 7% 8%
1	B	215	 83% 9% 7%
1	C	215	 82% 8% 9%
1	D	215	 84% 7% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	301	-	-	-	X
2	NAG	B	301	-	-	-	X
2	NAG	D	301	-	-	-	X
4	GOL	D	303	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13337 atoms, of which 5743 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 Sperm-egg fusion protein Juno.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	1	0
			2997	999	1420	276	283	19			
1	B	201	Total	C	H	N	O	S	0	2	0
			3059	1021	1449	283	287	19			
1	C	195	Total	C	H	N	O	S	0	1	0
			2974	997	1407	275	276	19			
1	D	197	Total	C	H	N	O	S	0	0	0
			2956	997	1390	272	278	19			

There are 24 discrepancies between the modelled and reference sequences:

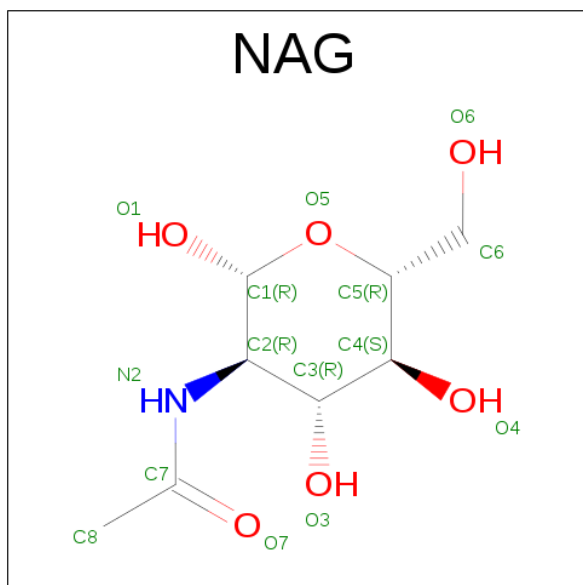
Chain	Residue	Modelled	Actual	Comment	Reference
A	229	GLY	-	expression tag	UNP A6ND01
A	230	ARG	-	expression tag	UNP A6ND01
A	231	LEU	-	expression tag	UNP A6ND01
A	232	VAL	-	expression tag	UNP A6ND01
A	233	PRO	-	expression tag	UNP A6ND01
A	234	ARG	-	expression tag	UNP A6ND01
B	229	GLY	-	expression tag	UNP A6ND01
B	230	ARG	-	expression tag	UNP A6ND01
B	231	LEU	-	expression tag	UNP A6ND01
B	232	VAL	-	expression tag	UNP A6ND01
B	233	PRO	-	expression tag	UNP A6ND01
B	234	ARG	-	expression tag	UNP A6ND01
C	229	GLY	-	expression tag	UNP A6ND01
C	230	ARG	-	expression tag	UNP A6ND01
C	231	LEU	-	expression tag	UNP A6ND01
C	232	VAL	-	expression tag	UNP A6ND01
C	233	PRO	-	expression tag	UNP A6ND01
C	234	ARG	-	expression tag	UNP A6ND01
D	229	GLY	-	expression tag	UNP A6ND01
D	230	ARG	-	expression tag	UNP A6ND01
D	231	LEU	-	expression tag	UNP A6ND01

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Chain	Residue	Modelled	Actual	Comment	Reference
D	232	VAL	-	expression tag	UNP A6ND01
D	233	PRO	-	expression tag	UNP A6ND01
D	234	ARG	-	expression tag	UNP A6ND01

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		


- Molecule 5 is water.

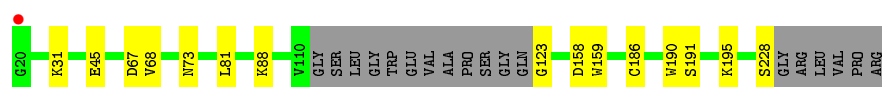
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	308	Total	O	0	0
			308	308		
5	B	293	Total	O	0	0
			293	293		
5	C	302	Total	O	0	0
			302	302		
5	D	293	Total	O	0	0
			293	293		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

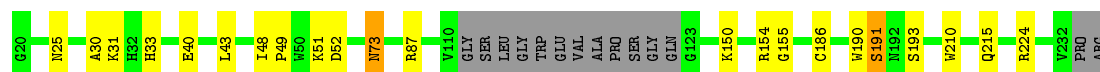
- Molecule 1: Sperm-egg fusion protein Juno

Chain A: 




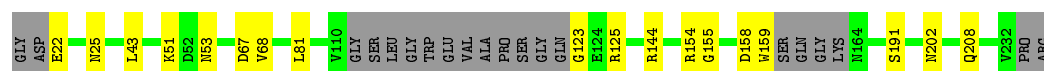
- Molecule 1: Sperm-egg fusion protein Juno

Chain B: 




- Molecule 1: Sperm-egg fusion protein Juno

Chain C: 



- Molecule 1: Sperm-egg fusion protein Juno

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	73.15Å 73.15Å 163.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 1.80 43.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.68-1.80) 88.9 (43.68-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.196 , 0.227 0.198 , 0.230	Depositor DCC
R_{free} test set	1816 reflections (2.65%)	DCC
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.489 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for k,h,-l	Depositor
Outliers	1 of 78747 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13337	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.49 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3112e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, NAG, 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	0.50	0/1634	0.59	1/2226 (0.0%)
1	B	0.54	0/1670	0.66	2/2273 (0.1%)
1	C	0.51	0/1623	0.62	1/2210 (0.0%)
1	D	0.50	0/1619	0.58	0/2205
All	All	0.51	0/6546	0.61	4/8914 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASP	C-N-CA	7.50	140.44	121.70
1	B	87[A]	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	87[B]	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	67	ASP	CB-CG-OD1	5.03	122.82	118.30

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	1577	1420	1444	9	0
1	B	1610	1449	1490	14	0
1	C	1567	1407	1448	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1566	1390	1440	13	0
2	A	14	13	13	1	0
2	B	14	13	13	2	0
2	C	14	14	13	0	0
2	D	14	13	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	8	8	0	0
4	C	6	8	8	0	0
4	D	6	8	8	0	0
5	A	308	0	0	7	0
5	B	293	0	0	5	1
5	C	302	0	0	9	0
5	D	293	0	0	4	1
All	All	7594	5743	5898	50	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 4.

The worst 5 of 50 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:150:LYS:NZ	1:B:155:GLY:O	2.17	0.76
1:C:154:ARG:HD2	1:C:191:SER:HB3	1.67	0.75
1:A:123:GLY:N	5:A:403:HOH:O	2.20	0.73
1:D:154:ARG:HD2	1:D:191:SER:HB2	1.72	0.70
1:B:52:ASP:OD1	5:B:401:HOH:O	2.09	0.69

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)
5:B:547:HOH:O	5:D:539:HOH:O[1_565]	2.11	0.09

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	194/215 (90%)	188 (97%)	6 (3%)	0	100	100
1	B	199/215 (93%)	195 (98%)	4 (2%)	0	100	100
1	C	190/215 (88%)	186 (98%)	4 (2%)	0	100	100
1	D	191/215 (89%)	188 (98%)	3 (2%)	0	100	100
All	All	774/860 (90%)	757 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	171/188 (91%)	166 (97%)	5 (3%)	50	34
1	B	175/188 (93%)	171 (98%)	4 (2%)	58	42
1	C	170/188 (90%)	168 (99%)	2 (1%)	78	71
1	D	169/188 (90%)	166 (98%)	3 (2%)	66	54
All	All	685/752 (91%)	671 (98%)	14 (2%)	61	49

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	ASN
1	B	186	CYS
1	D	43	LEU

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Mol	Chain	Res	Type
1	B	43	LEU
1	C	81	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
2	NAG	A	301	1	14,14,15	1.41	1 (7%)	15,19,21	1.03	1 (6%)
4	GOL	A	303	-	5,5,5	0.29	0	5,5,5	0.36	0
2	NAG	B	301	1	14,14,15	1.18	1 (7%)	15,19,21	0.78	1 (6%)
2	NAG	C	301	1	14,14,15	0.29	0	15,19,21	0.38	0
4	GOL	C	303	-	5,5,5	0.53	0	5,5,5	0.54	0
2	NAG	D	301	1	14,14,15	0.32	0	15,19,21	0.28	0
4	GOL	D	303	-	5,5,5	0.48	0	5,5,5	0.60	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
2	NAG	A	301	1	-	0/6/23/26	0/1/1/1
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	NAG	B	301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	301	1	-	0/6/23/26	0/1/1/1
4	GOL	C	303	-	-	0/4/4/4	0/0/0/0
2	NAG	D	301	1	-	0/6/23/26	0/1/1/1
4	GOL	D	303	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAG	O5-C1	-5.17	1.35	1.43
2	B	301	NAG	O5-C1	-4.25	1.36	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAG	C1-O5-C5	-2.37	108.65	112.14
2	A	301	NAG	C2-N2-C7	2.58	126.46	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAG	1	0
2	B	301	NAG	2	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 [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	197/215 (91%)	-0.39	1 (0%) 91 90	7, 14, 31, 47	0
1	B	201/215 (93%)	-0.38	0 100 100	8, 14, 30, 42	0
1	C	195/215 (90%)	-0.41	0 100 100	8, 13, 24, 31	0
1	D	197/215 (91%)	-0.38	1 (0%) 91 90	7, 14, 27, 33	0
All	All	790/860 (91%)	-0.39	2 (0%) 94 92	7, 14, 28, 47	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	GLY	2.8
1	D	214	ALA	2.1

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 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
2	NAG	A	301	14/15	0.62	0.23	5.74	40,41,49,50	0
2	NAG	B	301	14/15	0.74	0.19	4.03	38,43,52,52	0
2	NAG	D	301	14/15	0.70	0.18	3.76	51,52,63,63	0
4	GOL	D	303	6/6	0.91	0.12	2.09	17,21,21,21	0
2	NAG	C	301	14/15	0.78	0.16	1.69	42,45,53,54	0
4	GOL	A	303	6/6	0.96	0.10	0.67	17,21,21,21	0
4	GOL	C	303	6/6	0.92	0.09	-0.27	17,21,21,21	0
3	CL	C	302	1/1	0.99	0.07	-1.16	10,10,10,10	0
3	CL	B	302	1/1	1.00	0.06	-1.57	7,7,7,7	0
3	CL	A	302	1/1	0.99	0.04	-5.56	10,10,10,10	0
3	CL	D	302	1/1	0.99	0.03	-5.76	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.