



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 10:00 AM BST

PDB ID : 3VE2
Title : The 2.1 angstrom crystal structure of Transferrin binding protein B (TbpB) from serogroup B M982 *Neisseria meningitidis*
Authors : Calmettes, C.; Moraes, T.F.
Deposited on : 2012-01-06
Resolution : 2.14 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

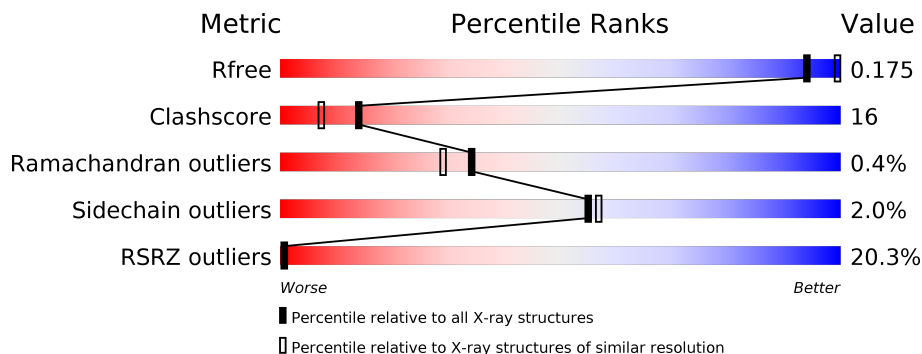
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 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	658	 16% 58% 19% • 22%
1	B	658	 16% 59% 18% • 21%

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
2	GOL	A	704	-	-	X	-
2	GOL	A	705	-	-	X	-
2	GOL	B	701	-	-	X	-
2	GOL	B	702	-	-	X	-
2	GOL	B	703	-	-	X	-
4	ACT	A	708	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8868 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.

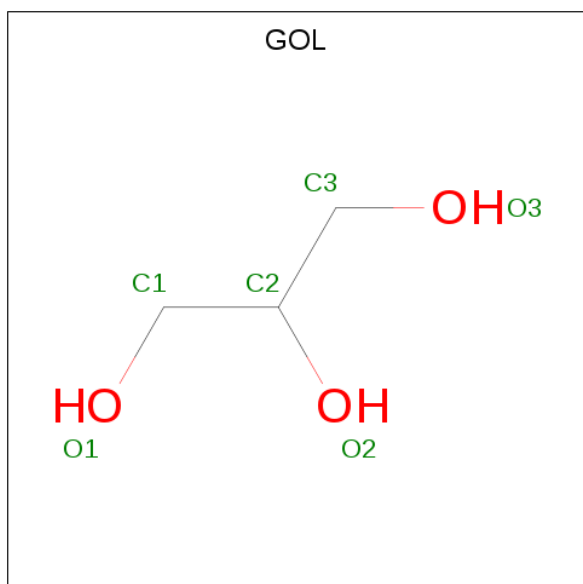
- Molecule 1 is a protein called Transferrin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	Total 4057	C 2557	N 687	O 806	S 7	0	2	0
1	B	519	Total 4087	C 2571	N 695	O 814	S 7	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

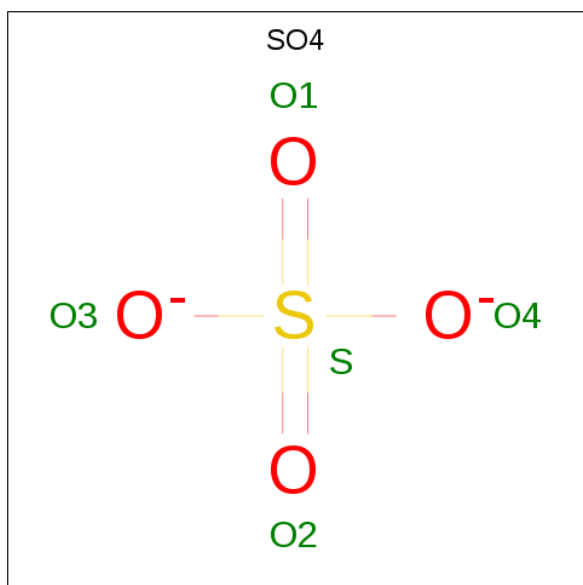
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	EXPRESSION TAG	UNP Q09057
A	35	SER	-	EXPRESSION TAG	UNP Q09057
B	34	GLY	-	EXPRESSION TAG	UNP Q09057
B	35	SER	-	EXPRESSION TAG	UNP Q09057

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



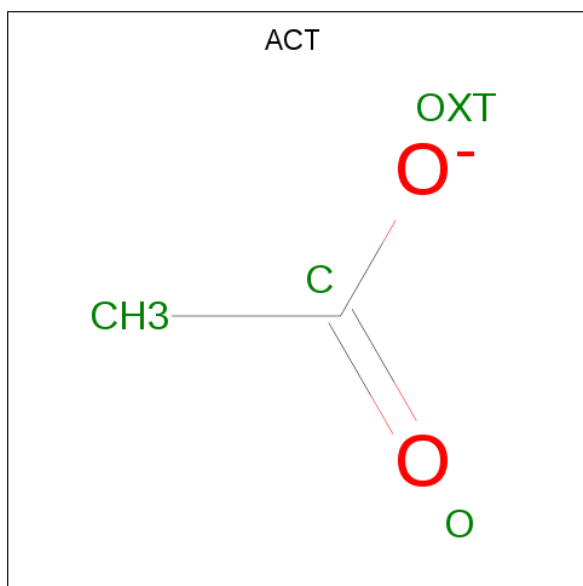
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	299	Total 299	O 299	0	0
6	B	319	Total 319	O 319	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	46.60Å 149.34Å 199.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.38 – 2.14 46.60 – 2.14	Depositor EDS
% Data completeness (in resolution range)	93.4 (45.38-2.14) 93.4 (46.60-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.14Å)	Xtrriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.171 , 0.209 0.170 , 0.175	Depositor DCC
R_{free} test set	3667 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8868	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: GOL, ACT, SO4, NA

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	0.44	0/4147	0.63	3/5573 (0.1%)
1	B	0.45	0/4176	0.63	4/5611 (0.1%)
All	All	0.44	0/8323	0.63	7/11184 (0.1%)

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
1	B	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	A	330	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	B	330	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	A	330	ARG	NE-CZ-NH2	10.03	125.31	120.30
1	B	330	ARG	CD-NE-CZ	5.61	131.45	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ASN	Peptide

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	4057	0	3902	126	0
1	B	4087	0	3927	127	0
2	A	36	0	48	17	0
2	B	30	0	40	19	0
3	A	5	0	0	0	0
3	B	30	0	0	1	0
4	A	4	0	3	5	0
5	B	1	0	0	0	0
6	A	299	0	0	14	0
6	B	319	0	0	15	0
All	All	8868	0	7920	254	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 16.

The worst 5 of 254 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:46:ARG:HH22	2:B:702:GOL:H32	1.14	1.09
1:B:302:GLU:HB3	1:B:303:THR:CA	1.82	1.07
1:A:46:ARG:HH22	2:A:704:GOL:H32	1.19	1.05
1:B:302:GLU:CB	1:B:303:THR:HA	1.87	1.04
1:B:615:GLU:O	1:B:615:GLU:HG2	1.57	1.02

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	496/658 (75%)	465 (94%)	29 (6%)	2 (0%)	34	29
1	B	501/658 (76%)	467 (93%)	32 (6%)	2 (0%)	34	29
All	All	997/1316 (76%)	932 (94%)	61 (6%)	4 (0%)	34	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	LYS
1	B	476	LYS
1	B	615	GLU
1	A	678	ALA

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	434/533 (81%)	424 (98%)	10 (2%)	50	51
1	B	437/533 (82%)	429 (98%)	8 (2%)	59	60
All	All	871/1066 (82%)	853 (98%)	18 (2%)	55	54

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	582	ILE
1	A	635	ASP
1	B	288	ARG
1	A	301	ASN
1	A	394	ILE

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

Mol	Chain	Res	Type
1	A	125	GLN
1	A	590	ASN
1	B	594	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	GOL	A	701	-	5,5,5	0.44	0	5,5,5	0.57	0
2	GOL	B	701	-	5,5,5	0.46	0	5,5,5	0.45	0
3	SO4	B	708	-	4,4,4	0.12	0	6,6,6	0.15	0
2	GOL	A	705	-	5,5,5	0.33	0	5,5,5	0.32	0
2	GOL	B	705	-	5,5,5	0.33	0	5,5,5	0.40	0
2	GOL	B	702	-	5,5,5	0.34	0	5,5,5	0.26	0
3	SO4	B	707	-	4,4,4	0.18	0	6,6,6	0.18	0
3	SO4	B	709	-	4,4,4	0.11	0	6,6,6	0.11	0
2	GOL	A	703	-	5,5,5	0.35	0	5,5,5	0.34	0
2	GOL	A	704	-	5,5,5	0.32	0	5,5,5	0.41	0
4	ACT	A	708	-	1,3,3	1.23	0	0,3,3	0.00	-
2	GOL	B	703	-	5,5,5	0.35	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	706	-	4,4,4	0.18	0	6,6,6	0.12	0
2	GOL	A	702	-	5,5,5	0.44	0	5,5,5	0.17	0
2	GOL	B	704	-	5,5,5	0.32	0	5,5,5	0.24	0
3	SO4	B	711	-	4,4,4	0.18	0	6,6,6	0.08	0
2	GOL	A	706	-	5,5,5	0.37	0	5,5,5	0.25	0
3	SO4	A	707	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	710	-	4,4,4	0.15	0	6,6,6	0.15	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	GOL	A	701	-	-	2/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-
2	GOL	A	705	-	-	2/4/4/4	-
2	GOL	B	705	-	-	2/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	A	703	-	-	2/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-
2	GOL	B	703	-	-	2/4/4/4	-
2	GOL	A	702	-	-	2/4/4/4	-
2	GOL	B	704	-	-	2/4/4/4	-
2	GOL	A	706	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-C3
2	B	701	GOL	O1-C1-C2-C3
2	A	705	GOL	O1-C1-C2-O2
2	A	705	GOL	O1-C1-C2-C3
2	B	702	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GOL	1	0
2	B	701	GOL	6	0
2	A	705	GOL	4	0
2	B	702	GOL	7	0
2	A	703	GOL	2	0
2	A	704	GOL	6	0
4	A	708	ACT	5	0
2	B	703	GOL	4	0
3	B	706	SO4	1	0
2	A	702	GOL	2	0
2	B	704	GOL	2	0
2	A	706	GOL	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	514/658 (78%)	1.00	108 (21%) 1 1	16, 51, 132, 194	0
1	B	519/658 (78%)	0.90	102 (19%) 1 1	15, 47, 129, 179	0
All	All	1033/1316 (78%)	0.95	210 (20%) 1 1	15, 49, 131, 194	0

The worst 5 of 210 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	PRO	20.1
1	B	614	ALA	12.0
1	A	618	PHE	9.3
1	A	264	LEU	9.1
1	B	615	GLU	9.0

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 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
2	GOL	A	702	6/6	0.61	0.21	40,62,65,74	0
2	GOL	A	706	6/6	0.67	0.25	68,82,91,92	0
2	GOL	A	705	6/6	0.75	0.30	56,69,75,88	0
2	GOL	B	705	6/6	0.76	0.20	63,76,81,84	0
2	GOL	B	703	6/6	0.82	0.25	64,81,87,87	0
2	GOL	B	701	6/6	0.84	0.20	44,67,72,82	0
2	GOL	B	704	6/6	0.85	0.39	58,78,96,105	0
3	SO4	B	709	5/5	0.85	0.12	91,113,118,124	0
2	GOL	A	703	6/6	0.88	0.18	47,76,85,87	0
2	GOL	B	702	6/6	0.91	0.17	31,46,72,80	0
3	SO4	B	711	5/5	0.92	0.17	59,122,134,139	0
4	ACT	A	708	4/4	0.94	0.21	36,37,50,82	0
3	SO4	B	708	5/5	0.94	0.15	52,85,109,122	0
2	GOL	A	704	6/6	0.94	0.16	35,52,59,68	0
3	SO4	A	707	5/5	0.96	0.17	56,96,119,121	0
3	SO4	B	706	5/5	0.97	0.15	47,59,90,125	0
3	SO4	B	707	5/5	0.98	0.16	47,49,79,91	0
2	GOL	A	701	6/6	0.98	0.25	22,64,76,77	0
3	SO4	B	710	5/5	0.98	0.17	51,65,98,98	0
5	NA	B	712	1/1	0.99	0.19	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.