



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 02:32 AM EDT

PDB ID : 4QQ1
Title : Crystal structure of the isotype 1 Transferrin binding protein B (TbpB) from serogroup B *Neisseria meningitidis*
Authors : Calmettes, C.; Moraes, T.F.
Deposited on : 2014-06-26
Resolution : 3.33 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

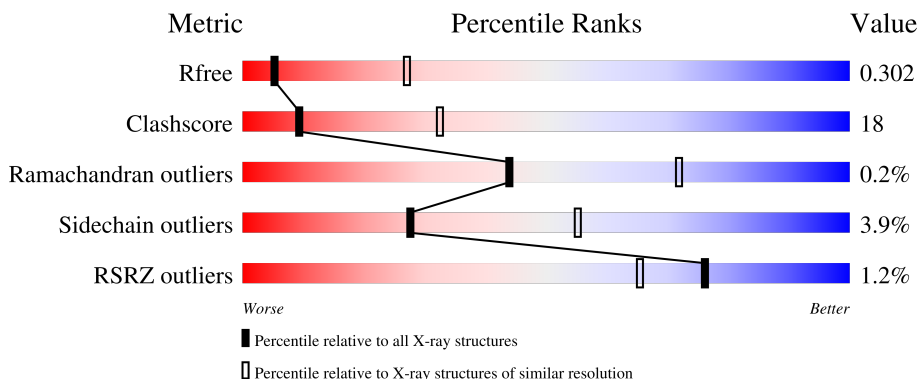
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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	1325 (3.38-3.30)
Clashscore	180529	1376 (3.38-3.30)
Ramachandran outliers	177936	1376 (3.38-3.30)
Sidechain outliers	177891	1375 (3.38-3.30)
RSRZ outliers	164620	1325 (3.38-3.30)

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	543	
1	B	543	
1	C	543	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11828 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
1	A	521	Total	C	N	O	S	129	0	0
			4023	2514	700	800	9			
1	B	485	Total	C	N	O	S	145	0	0
			3768	2368	651	740	9			
1	C	515	Total	C	N	O	S	109	0	0
			3982	2494	689	790	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	-	expression tag	UNP Q06988
B	37	SER	-	expression tag	UNP Q06988
C	37	SER	-	expression tag	UNP Q06988

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cs	0	0
			4	4		
2	B	2	Total	Cs	0	0
			2	2		
2	C	2	Total	Cs	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

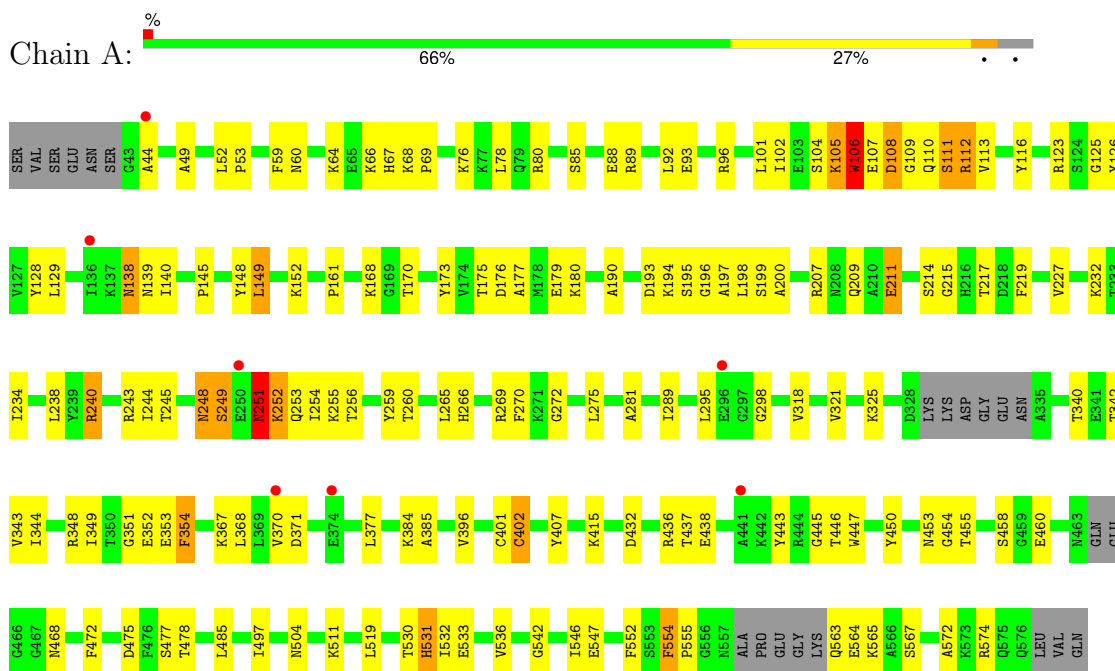
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0
5	B	5	Total 5	O 5	0	0
5	C	10	Total 10	O 10	0	0

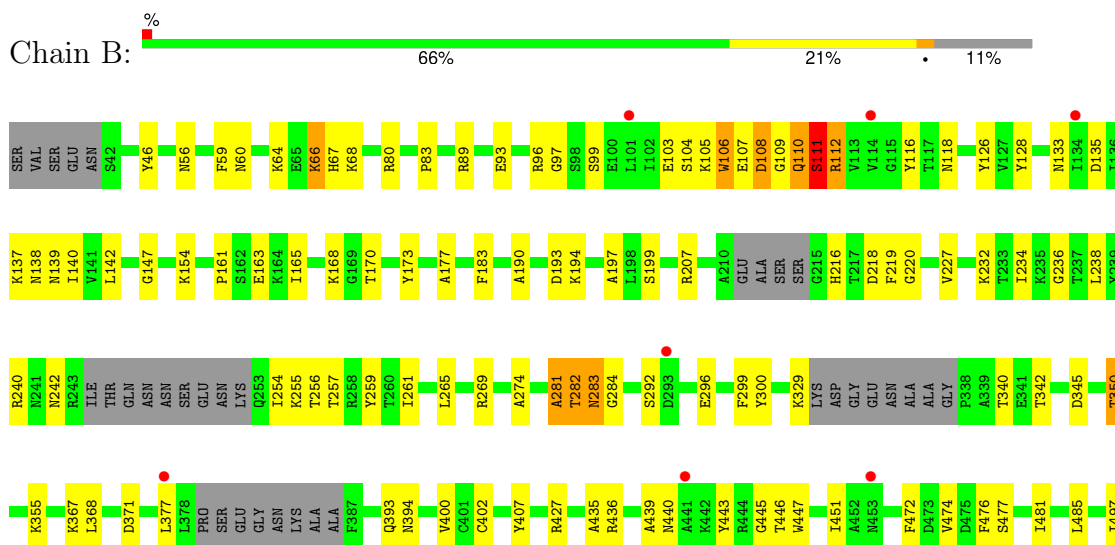
3 Residue-property plots

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: Transferrin-binding protein 2

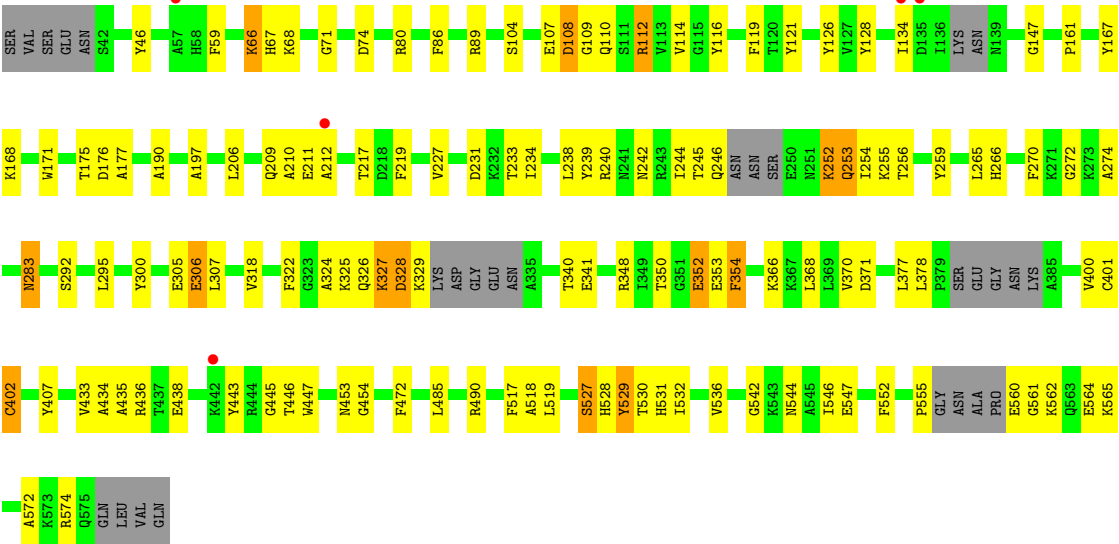


• Molecule 1: Transferrin-binding protein 2





● Molecule 1: Transferrin-binding protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.33Å 99.97Å 160.16Å 90.00° 93.47° 90.00°	Depositor
Resolution (Å)	45.17 – 3.33 45.17 – 3.33	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.17-3.33) 91.0 (45.17-3.33)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.249 , 0.301 0.252 , 0.302	Depositor DCC
R_{free} test set	1527 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 149.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11828	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, SO4, CS

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	0.28	0/4101	0.50	1/5510 (0.0%)
1	B	0.28	0/3840	0.48	2/5149 (0.0%)
1	C	0.27	0/4058	0.56	4/5448 (0.1%)
All	All	0.28	0/11999	0.52	7/16107 (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
1	A	0	3
1	B	0	3
All	All	0	6

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	C	352	GLU	CB-CA-C	-12.73	84.94	110.40
1	C	353	GLU	N-CA-C	-8.78	87.31	111.00
1	C	352	GLU	N-CA-C	-7.54	90.63	111.00
1	A	249	SER	N-CA-C	5.91	126.96	111.00
1	C	327	LYS	N-CA-CB	-5.33	101.01	110.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LYS	Peptide
1	A	106	TRP	Peptide
1	A	251	ASN	Peptide
1	B	106	TRP	Peptide
1	B	281	ALA	Mainchain

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	4023	0	3879	156	0
1	B	3768	0	3647	114	0
1	C	3982	0	3846	126	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
4	C	5	0	0	0	0
5	A	15	0	0	5	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
All	All	11828	0	11388	394	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 18.

The worst 5 of 394 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:C:325:LYS:CE	1:C:328:ASP:HB2	1.77	1.13
1:B:281:ALA:CB	1:B:282:THR:HA	1.79	1.12
1:A:107:GLU:HG2	1:A:110:GLN:H	1.11	1.10
1:B:135:ASP:CB	1:B:140:ILE:HG22	1.81	1.09
1:B:107:GLU:HG2	1:B:110:GLN:H	1.14	1.08

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	513/543 (94%)	432 (84%)	80 (16%)	1 (0%)	44	72
1	B	471/543 (87%)	414 (88%)	57 (12%)	0	100	100
1	C	503/543 (93%)	435 (86%)	66 (13%)	2 (0%)	30	61
All	All	1487/1629 (91%)	1281 (86%)	203 (14%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	GLN
1	C	527	SER
1	A	138	ASN

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	420/439 (96%)	397 (94%)	23 (6%)	18	46
1	B	393/439 (90%)	382 (97%)	11 (3%)	38	64
1	C	415/439 (94%)	401 (97%)	14 (3%)	32	59
All	All	1228/1317 (93%)	1180 (96%)	48 (4%)	27	55

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	111	SER
1	C	66	LYS
1	B	112	ARG
1	B	402	CYS
1	C	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	531	HIS
1	B	424	GLN
1	C	424	GLN
1	A	181	GLN
1	A	118	ASN

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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
4	SO4	C	603	-	4,4,4	0.23	0	6,6,6	0.07	0
3	GOL	A	605	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	B	603	-	5,5,5	0.37	0	5,5,5	0.30	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	GOL	A	605	-	-	2/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	GOL	O1-C1-C2-C3
3	B	603	GOL	O1-C1-C2-C3
3	B	603	GOL	O1-C1-C2-O2
3	A	605	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	GOL	1	0
3	B	603	GOL	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 [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	521/543 (95%)	-0.09	7 (1%) 74 63	46, 95, 178, 280	35 (6%)
1	B	485/543 (89%)	0.05	7 (1%) 73 61	50, 118, 243, 487	39 (8%)
1	C	515/543 (94%)	-0.06	5 (0%) 79 69	42, 120, 218, 312	29 (5%)
All	All	1521/1629 (93%)	-0.03	19 (1%) 76 65	42, 112, 214, 487	103 (6%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	441	ALA	3.9
1	A	250	GLU	3.0
1	B	101	LEU	2.8
1	A	296	GLU	2.7
1	B	114	VAL	2.6

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	GOL	A	605	6/6	0.64	0.16	81,85,103,119	0
4	SO4	C	603	5/5	0.70	0.11	226,227,227,227	5
2	CS	A	604	1/1	0.82	0.15	231,231,231,231	0
2	CS	C	602	1/1	0.84	0.17	262,262,262,262	0
2	CS	A	603	1/1	0.89	0.11	200,200,200,200	0
3	GOL	B	603	6/6	0.90	0.18	62,94,110,122	0
2	CS	B	602	1/1	0.90	0.14	192,192,192,192	0
2	CS	B	601	1/1	0.91	0.18	177,177,177,177	0
2	CS	C	601	1/1	0.91	0.12	196,196,196,196	0
2	CS	A	602	1/1	0.92	0.07	190,190,190,190	0
2	CS	A	601	1/1	0.92	0.10	179,179,179,179	0

6.5 Other polymers [i](#)

There are no such residues in this entry.