Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jun 13, 2018 – 12:53 AM EDT

Deposition ID : D_1000231110
PDB ID : *(not yet assigned)*

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

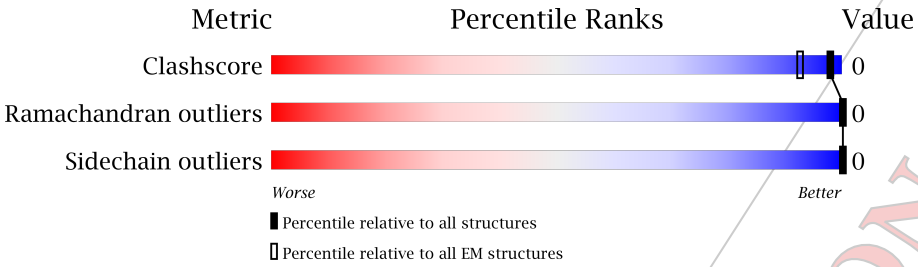
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031172

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	965	61% 39%
2	B	639	55% 45%
3	C	213	55% 45%
4	D	213	49% . 50%
5	E	212	54% 46%
6	F	214	50% . 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7338 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	593	2982	1784	599	599	0	0

- Molecule 2 is a protein called Integrin beta-8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	353	1791	1075	358	358	0	0

- Molecule 3 is a protein called 8B8 heavy chain Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	117	585	351	117	117	0	0

- Molecule 4 is a protein called 8B8 light chain Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	107	536	322	107	107	0	0

- Molecule 5 is a protein called 68 heavy chain Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	115	569	339	115	115	0	0

- Molecule 6 is a protein called 68 light chain Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	108	540	324	108	108	0	0

- Molecule 7 is a ligand with the chemical component id NAG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for NAG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	A	1	Total C N O 154 88 11 55	0
7	B	1	Total C N O 126 72 9 45	0
7	B	1	Total C N O 126 72 9 45	0
7	B	1	Total C N O 126 72 9 45	0
7	B	1	Total C N O 126 72 9 45	0
7	B	1	Total C N O 126 72 9 45	0
7	B	1	Total C N O 126 72 9 45	0
7	B	1	Total C N O 126 72 9 45	0
7	B	1	Total C N O 126 72 9 45	0

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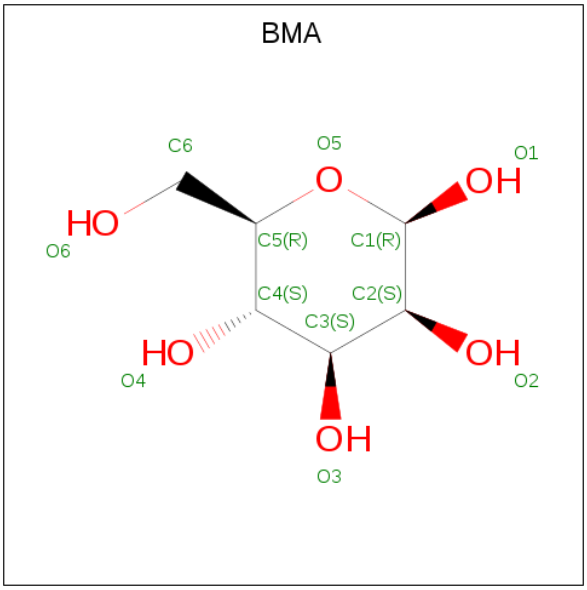
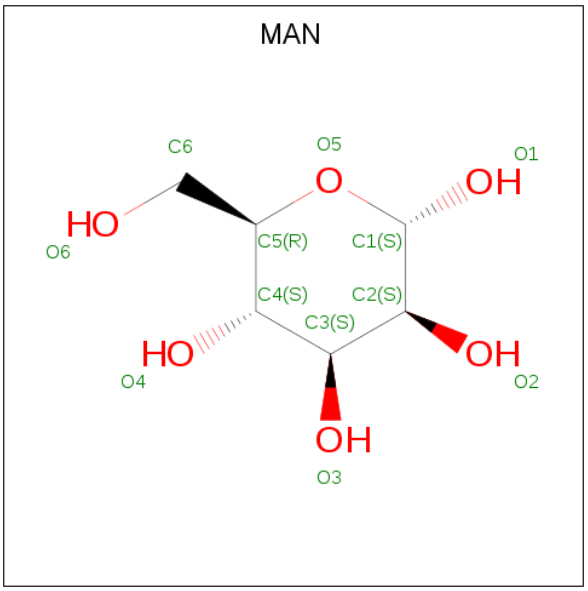
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			126	72	9	45	

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			11	6	5	
8	B	1	Total	C	O	0
			11	6	5	

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



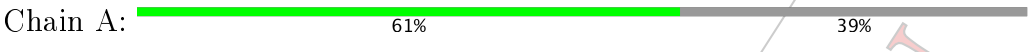
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	A	1	33	18	15	0
			Total	C	O	
9	A	1	33	18	15	0
			Total	C	O	
9	A	1	33	18	15	0

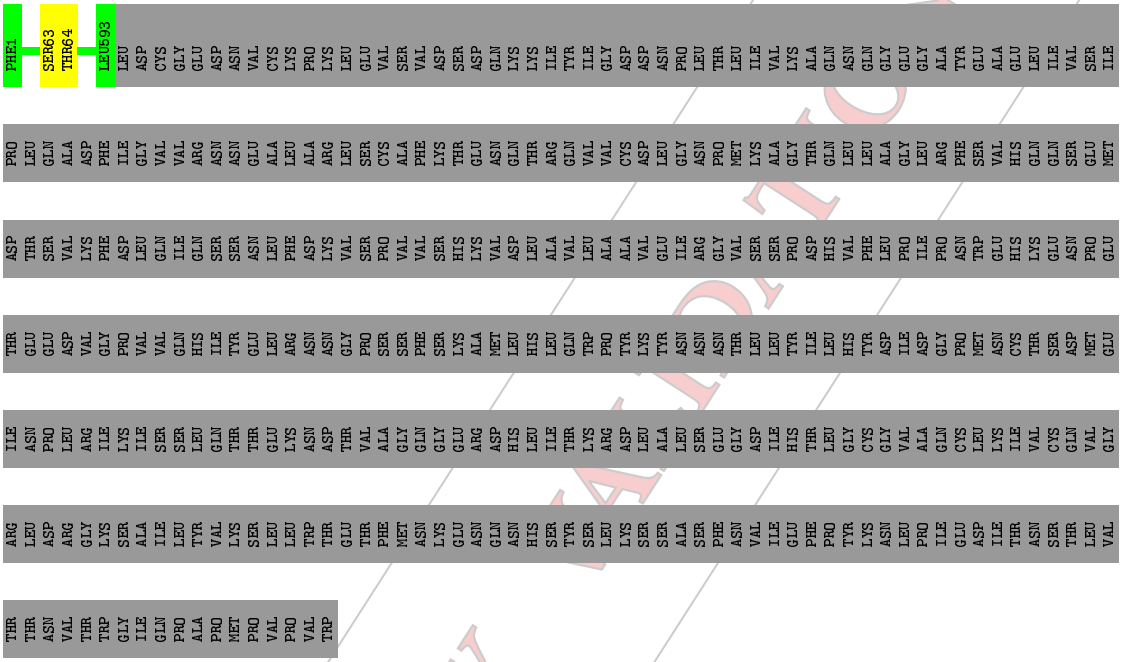
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Integrin alpha-V

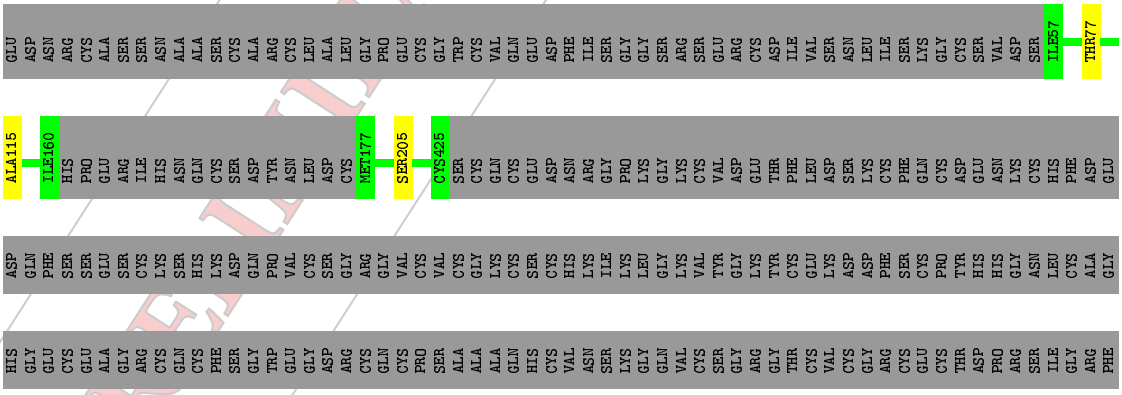
Chain A:





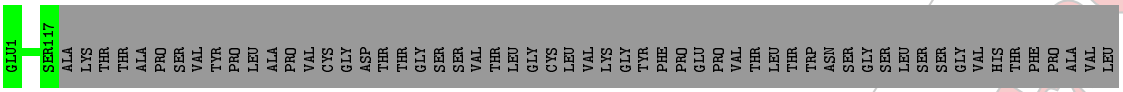
- Molecule 2: Integrin beta-8

Chain B:



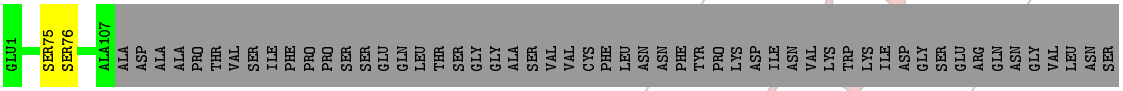
- Molecule 3: 8B8 heavy chain Fab

Chain C:



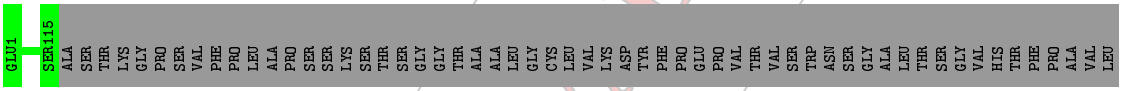
- Molecule 4: 8B8 light chain Fab

Chain D:



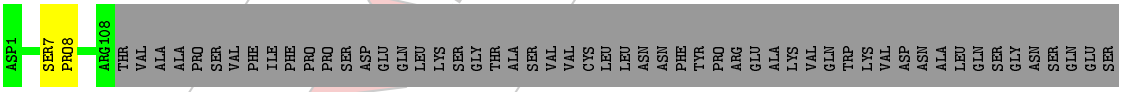
- Molecule 5: 68 heavy chain Fab

Chain E:



- Molecule 6: 68 light chain Fab

Chain F:



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.55	0/3009	0.85	0/4198
2	B	0.54	0/1806	0.88	1/2524 (0.0%)
3	C	0.56	0/588	0.92	0/820
4	D	0.58	0/540	0.90	0/753
5	E	0.59	0/571	0.86	0/793
6	F	0.54	0/544	0.92	0/758
All	All	0.55	0/7058	0.88	1/9846 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	77	THR	N-CA-C	5.95	127.05	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2982	0	1553	1	0
2	B	1791	0	884	1	0
3	C	585	0	267	0	0
4	D	536	0	280	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	569	0	283	0	0
6	F	540	0	262	1	0
7	A	154	0	93	0	0
7	B	126	0	76	0	0
8	A	11	0	7	0	0
8	B	11	0	9	0	0
9	A	33	0	26	0	0
All	All	7338	0	3740	4	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 0.

All (4) 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)
4:D:75:SER:O	4:D:76:SER:C	2.51	0.48
1:A:63:SER:O	1:A:64:THR:C	2.56	0.44
6:F:7:SER:N	6:F:8:PRO:CD	2.80	0.44
2:B:115:ALA:N	2:B:205:SER:O	2.54	0.40

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 PDB entries followed by that with respect to all EM entries.

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	591/965 (61%)	570 (96%)	21 (4%)	0	100	100
2	B	349/639 (55%)	334 (96%)	15 (4%)	0	100	100
3	C	115/213 (54%)	104 (90%)	11 (10%)	0	100	100
4	D	105/213 (49%)	98 (93%)	7 (7%)	0	100	100
5	E	113/212 (53%)	110 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	106/214 (50%)	99 (93%)	7 (7%)	0	100	100
All	All	1379/2456 (56%)	1315 (95%)	64 (5%)	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 PDB entries followed by that with respect to all EM entries.

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	34/819 (4%)	34 (100%)	0	100	100
2	B	22/561 (4%)	22 (100%)	0	100	100
3	C	4/192 (2%)	4 (100%)	0	100	100
4	D	5/185 (3%)	5 (100%)	0	100	100
5	E	3/178 (2%)	3 (100%)	0	100	100
6	F	5/190 (3%)	5 (100%)	0	100	100
All	All	73/2125 (3%)	73 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 20 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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	$\#\|Z\| > 2$
8	BMA	A	2268	9,7	11,11,12	1.80	2 (18%)	15,15,17	0.99	1 (6%)
9	MAN	A	2269	8	11,11,12	1.77	2 (18%)	15,15,17	1.16	2 (13%)
9	MAN	A	2270	9,8	11,11,12	1.81	3 (27%)	15,15,17	1.19	1 (6%)
9	MAN	A	2271	9	11,11,12	1.77	2 (18%)	15,15,17	1.23	3 (20%)
8	BMA	B	2416	7	11,11,12	1.78	2 (18%)	15,15,17	1.10	2 (13%)

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
8	BMA	A	2268	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	2269	8	-	0/2/19/22	0/1/1/1
9	MAN	A	2270	9,8	-	0/2/19/22	0/1/1/1
9	MAN	A	2271	9	-	0/2/19/22	0/1/1/1
8	BMA	B	2416	7	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2271	MAN	O2-C2	-4.06	1.34	1.43
9	A	2269	MAN	O2-C2	-4.03	1.34	1.43
9	A	2270	MAN	O2-C2	-3.99	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	2416	BMA	O2-C2	-3.98	1.34	1.43
8	A	2268	BMA	O2-C2	-3.94	1.34	1.43
8	B	2416	BMA	C2-C3	-2.32	1.49	1.52
9	A	2270	MAN	C2-C3	-2.28	1.49	1.52
9	A	2269	MAN	C2-C3	-2.28	1.49	1.52
9	A	2271	MAN	C2-C3	-2.27	1.49	1.52
8	A	2268	BMA	C2-C3	-2.25	1.49	1.52
9	A	2270	MAN	C4-C5	2.32	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2271	MAN	C2-C3-C4	-2.41	106.69	110.87
8	A	2268	BMA	C2-C3-C4	-2.32	106.83	110.87
9	A	2269	MAN	C2-C3-C4	-2.27	106.92	110.87
8	B	2416	BMA	O5-C1-C2	-2.23	107.30	110.78
9	A	2271	MAN	O5-C1-C2	-2.23	107.30	110.78
8	B	2416	BMA	C2-C3-C4	-2.17	107.10	110.87
9	A	2270	MAN	C3-C4-C5	-2.15	106.40	110.24
9	A	2269	MAN	C1-C2-C3	2.40	112.69	109.66
9	A	2271	MAN	C1-C2-C3	2.47	112.78	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.