wwPDB EM Validation Summary Report

May 21, 2024 – 10:09 AM JST

PDB ID	:	8HFS
EMDB ID	:	EMD-34726
Title	:	The structure of LcnA, LciA, and the man-PTS of Lactococcus lactis
Authors	:	Wang, J.W.
Deposited on	:	2022-11-12
Resolution	:	2.98 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

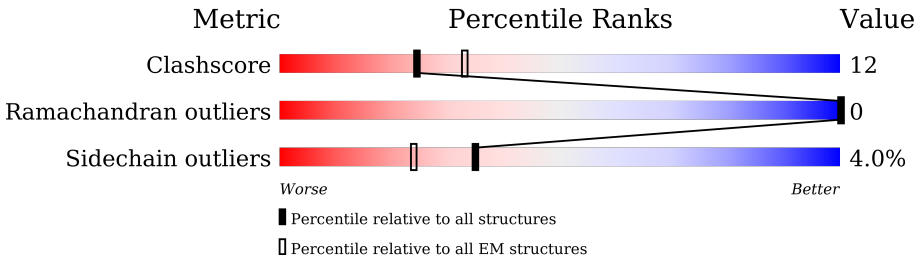
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.98 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	C	270	60% 31% • 8%
1	E	270	65% 26% • 8%
1	Y	270	69% 23% 8%
2	D	307	64% 34% • •
2	F	307	69% 28% • •
2	Z	307	66% 33% •
3	B	98	68% 23% • 6%
4	A	54	70% 24% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16216 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 Mannose-specific PTS system, IIC component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	249	Total	C	N	O	S	0	0
			1799	1184	291	314	10		
1	E	248	Total	C	N	O	S	0	0
			1795	1182	290	313	10		
1	C	248	Total	C	N	O	S	179	0
			3092	2029	504	542	17		

- Molecule 2 is a protein called Mannose-specific PTS system, IID component.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	303	Total	C	N	O	S	0	0
			2341	1541	390	401	9		
2	F	302	Total	C	N	O	S	0	0
			2332	1535	388	400	9		
2	D	302	Total	C	N	O	S	172	0
			3669	2410	612	633	14		

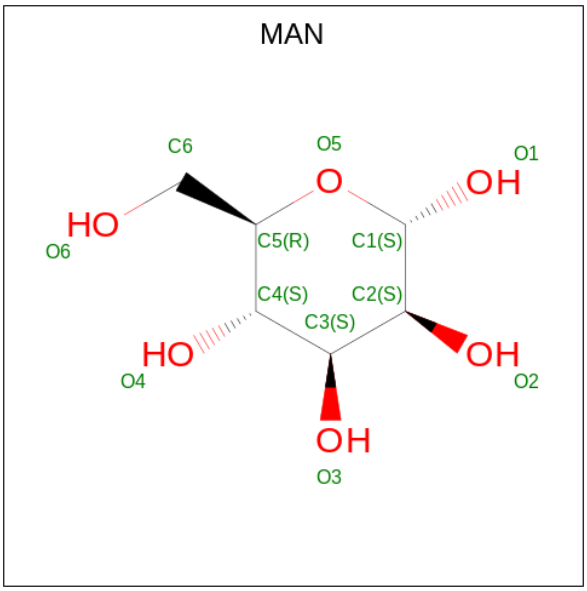
- Molecule 3 is a protein called Lactococcin-A immunity protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	92	Total	C	N	O	S	0	0
			731	462	127	140	2		

- Molecule 4 is a protein called Bacteriocin lactococcin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	54	Total	C	N	O	S	0	0
			409	260	72	76	1		

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



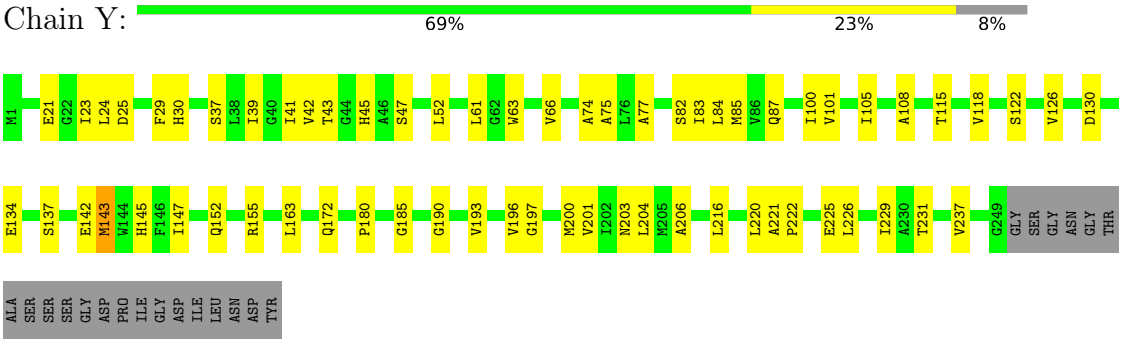
Mol	Chain	Residues	Atoms	AltConf
5	Z	1	Total C O 12 6 6	0
5	F	1	Total C O 12 6 6	0
5	D	1	Total C O 24 12 12	1

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. 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.

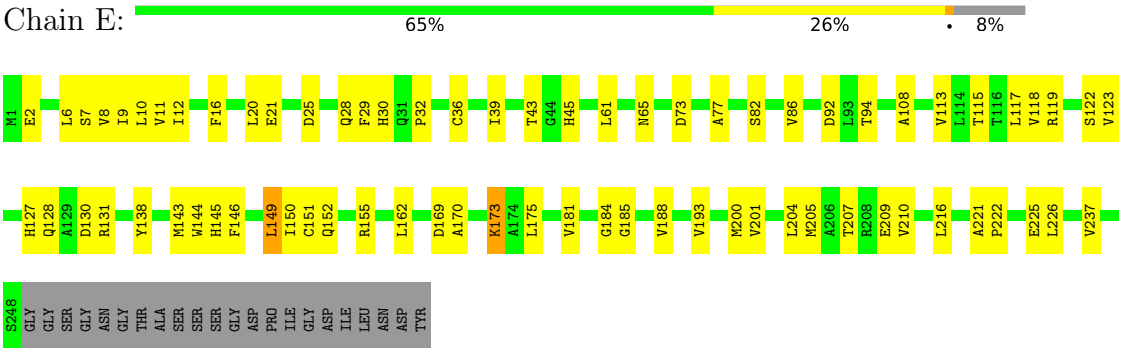
• Molecule 1: Mannose-specific PTS system, IIC component

Chain Y:



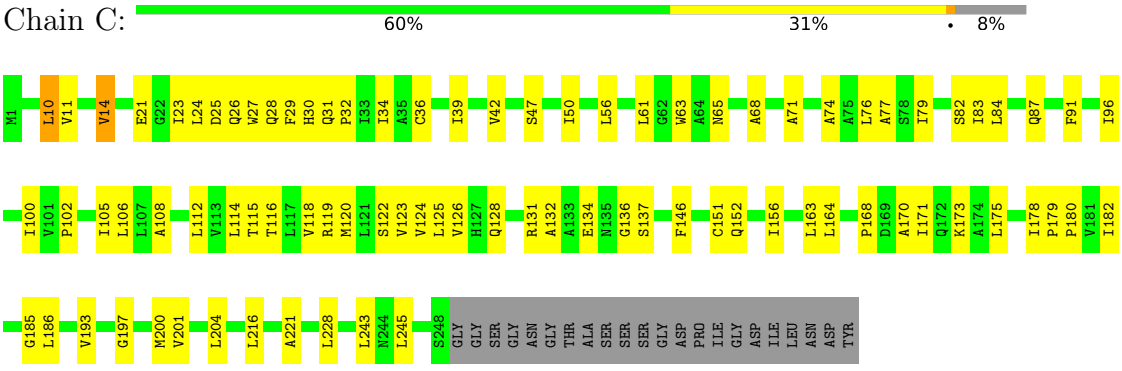
• Molecule 1: Mannose-specific PTS system, IIC component

Chain E:



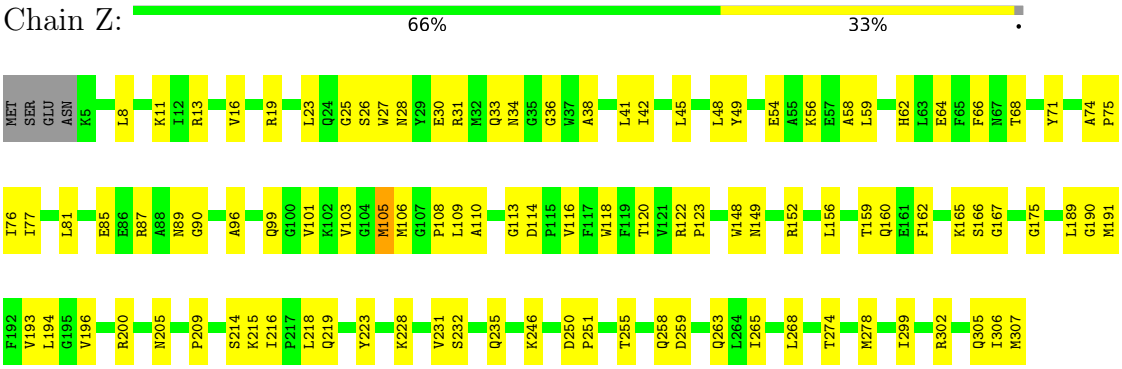
• Molecule 1: Mannose-specific PTS system, IIC component

Chain C:



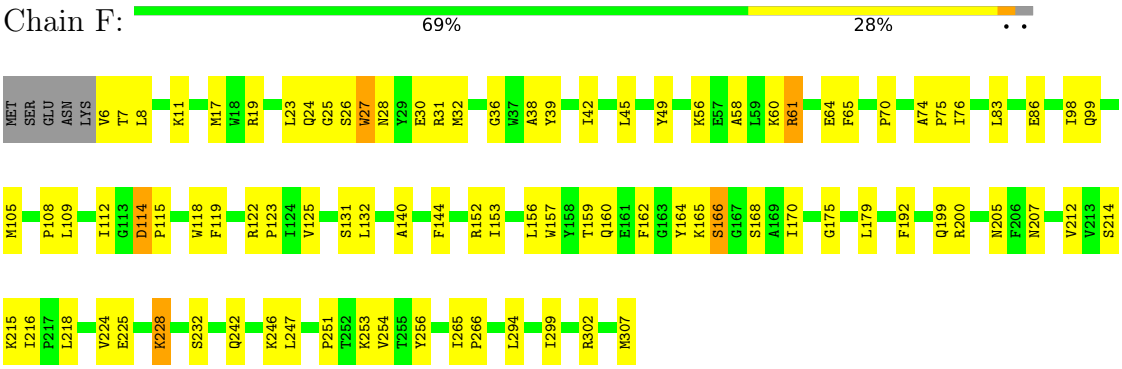
• Molecule 2: Mannose-specific PTS system, IID component

Chain Z:



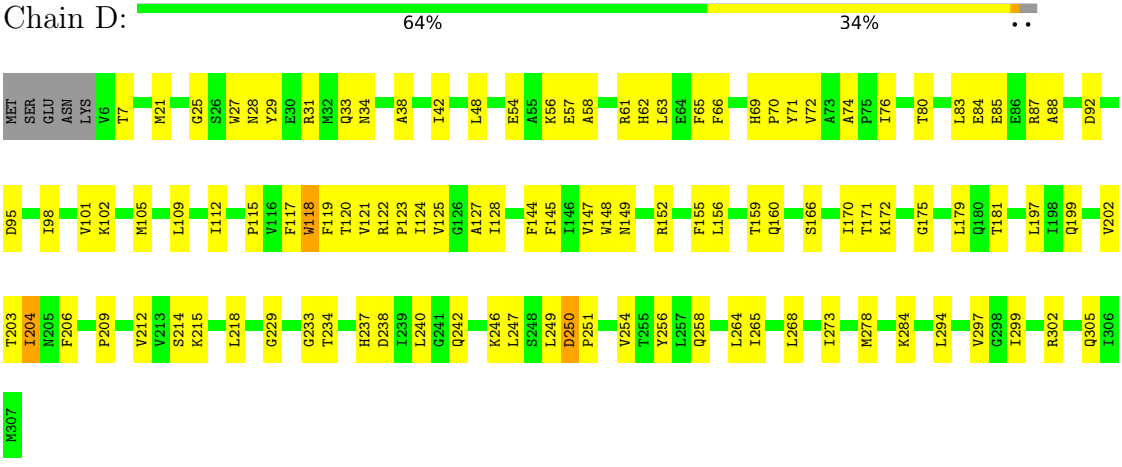
• Molecule 2: Mannose-specific PTS system, IID component

Chain F:



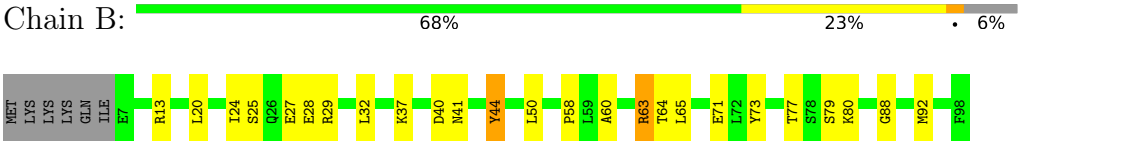
• Molecule 2: Mannose-specific PTS system, IID component

Chain D:



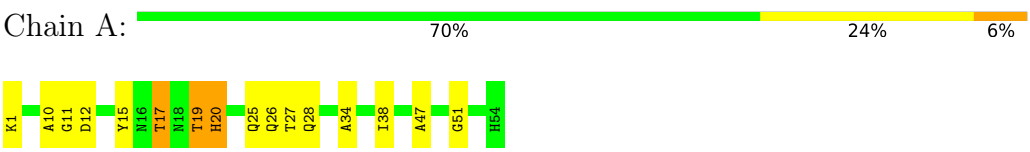
• Molecule 3: Lactococcin-A immunity protein

Chain B:



• Molecule 4: Bacteriocin lactococcin-A

Chain A:


70%
24%
6%
K1
A10
G11
D12
Y15
N16
T17
N18
T19
H20
Q25
Q26
T27
Q28
A34
I38
A47
G51
HE4

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1529899	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.24	0/3148	0.43	0/4312
1	E	0.26	0/1828	0.49	1/2503 (0.0%)
1	Y	0.27	0/1832	0.48	0/2508
2	D	0.25	0/3764	0.47	1/5110 (0.0%)
2	F	0.26	0/2389	0.48	0/3244
2	Z	0.27	0/2398	0.47	0/3255
3	B	0.29	0/740	0.55	0/995
4	A	0.26	0/420	0.44	0/570
All	All	0.26	0/16519	0.47	2/22497 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	204	ILE	CG1-CB-CG2	-6.86	96.32	111.40
1	E	25	ASP	CB-CG-OD2	5.23	123.01	118.30

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	C	3092	0	3244	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1795	0	1902	54	0
1	Y	1799	0	1905	46	0
2	D	3669	0	3720	103	0
2	F	2332	0	2420	71	0
2	Z	2341	0	2433	71	0
3	B	731	0	750	20	0
4	A	409	0	381	11	0
5	D	24	0	20	4	0
5	F	12	0	12	4	0
5	Z	12	0	12	3	0
All	All	16216	0	16799	388	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 12.

The worst 5 of 388 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:F:58:ALA:HA	2:F:61:ARG:HE	1.35	0.92
1:Y:23:ILE:HD12	2:Z:25:GLY:HA2	1.60	0.81
2:Z:190:GLY:O	2:Z:194:LEU:HB2	1.83	0.78
1:Y:21:GLU:HG2	1:Y:29:PHE:H	1.49	0.76
1:C:26[A]:GLN:O	2:D:152[A]:ARG:NH2	2.20	0.75

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	C	424/270 (157%)	402 (95%)	22 (5%)	0	100	100
1	E	246/270 (91%)	231 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	247/270 (92%)	237 (96%)	10 (4%)	0	100	100
2	D	471/307 (153%)	432 (92%)	39 (8%)	0	100	100
2	F	300/307 (98%)	274 (91%)	26 (9%)	0	100	100
2	Z	301/307 (98%)	268 (89%)	33 (11%)	0	100	100
3	B	90/98 (92%)	80 (89%)	10 (11%)	0	100	100
4	A	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
All	All	2131/1883 (113%)	1974 (93%)	157 (7%)	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	C	321/201 (160%)	312 (97%)	9 (3%)	43	75
1	E	186/201 (92%)	177 (95%)	9 (5%)	25	60
1	Y	186/201 (92%)	180 (97%)	6 (3%)	39	72
2	D	377/249 (151%)	365 (97%)	12 (3%)	39	72
2	F	244/249 (98%)	230 (94%)	14 (6%)	20	54
2	Z	245/249 (98%)	237 (97%)	8 (3%)	38	71
3	B	80/86 (93%)	77 (96%)	3 (4%)	33	67
4	A	38/38 (100%)	34 (90%)	4 (10%)	7	25
All	All	1677/1474 (114%)	1612 (96%)	65 (4%)	35	66

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	63[A]	LEU
2	D	118[A]	TRP
1	E	143	MET
1	E	65	ASN

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Mol	Chain	Res	Type
2	D	118[B]	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	28	ASN
2	F	67	ASN
2	F	99	GLN
2	F	205	ASN
2	F	207	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	MAN	D	401[B]	-	12,12,12	0.49	0	17,17,17	0.88	0
5	MAN	Z	401	-	12,12,12	0.55	0	17,17,17	1.31	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	F	401	-	12,12,12	0.44	0	17,17,17	0.90	1 (5%)
5	MAN	D	401[A]	-	12,12,12	0.44	0	17,17,17	0.86	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
5	MAN	D	401[B]	-	-	1/2/22/22	0/1/1/1
5	MAN	Z	401	-	-	2/2/22/22	0/1/1/1
5	MAN	F	401	-	-	1/2/22/22	0/1/1/1
5	MAN	D	401[A]	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Z	401	MAN	O5-C1-C2	3.22	116.03	110.28
5	Z	401	MAN	C1-O5-C5	2.61	118.58	113.66
5	Z	401	MAN	O2-C2-C3	-2.14	105.40	110.35
5	F	401	MAN	O2-C2-C3	-2.13	105.42	110.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	401	MAN	O5-C5-C6-O6
5	Z	401	MAN	C4-C5-C6-O6
5	D	401[B]	MAN	O5-C5-C6-O6
5	F	401	MAN	O5-C5-C6-O6
5	D	401[A]	MAN	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401[B]	MAN	2	0
5	Z	401	MAN	3	0
5	F	401	MAN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401[A]	MAN	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.