



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 11, 2019 – 03:16 AM EST

PDB ID : 6C13
EMDB ID: : EMD-7327
Title : CryoEM structure of mouse PCDH15-4EC-LHFPL5 complex
Authors : Gouaux, E.; Ge, J.; Elferich, J.
Deposited on : 2018-01-03
Resolution : 11.33 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
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) : 2.4

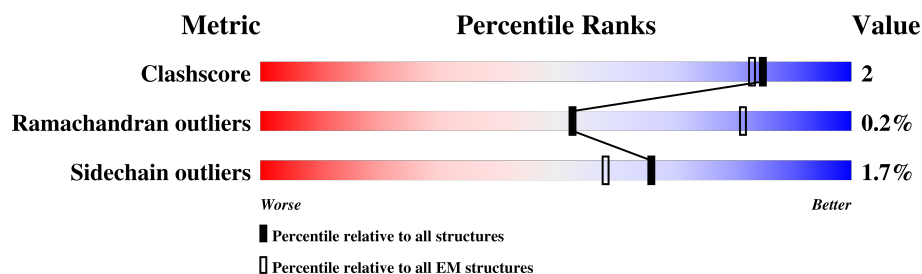
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.33 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)	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	660	 77% 5% 18%
1	B	660	 77% 5% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8862 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 Protocadherin-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	542	Total	C	N	O	S	0	0
			4248	2712	703	822	11		
1	B	542	Total	C	N	O	S	0	0
			4248	2712	703	822	11		

There are 32 discrepancies between the modelled and reference sequences:

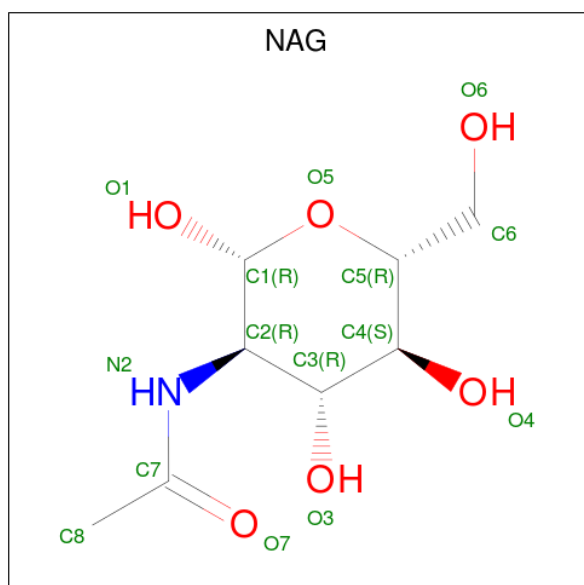
Chain	Residue	Modelled	Actual	Comment	Reference
A	817	GLN	-	expression tag	UNP Q99PJ1
A	818	TYR	-	expression tag	UNP Q99PJ1
A	819	ASP	-	expression tag	UNP Q99PJ1
A	820	ASP	-	expression tag	UNP Q99PJ1
A	901	ALA	VAL	conflict	UNP Q99PJ1
A	1466	THR	-	expression tag	UNP Q99PJ1
A	1467	ALA	-	expression tag	UNP Q99PJ1
A	1468	LEU	-	expression tag	UNP Q99PJ1
A	1469	PHE	-	expression tag	UNP Q99PJ1
A	1470	GLU	-	expression tag	UNP Q99PJ1
A	1471	SER	-	expression tag	UNP Q99PJ1
A	1472	ARG	-	expression tag	UNP Q99PJ1
A	1473	LEU	-	expression tag	UNP Q99PJ1
A	1474	VAL	-	expression tag	UNP Q99PJ1
A	1475	PRO	-	expression tag	UNP Q99PJ1
A	1476	ARG	-	expression tag	UNP Q99PJ1
B	817	GLN	-	expression tag	UNP Q99PJ1
B	818	TYR	-	expression tag	UNP Q99PJ1
B	819	ASP	-	expression tag	UNP Q99PJ1
B	820	ASP	-	expression tag	UNP Q99PJ1
B	901	ALA	VAL	conflict	UNP Q99PJ1
B	1466	THR	-	expression tag	UNP Q99PJ1
B	1467	ALA	-	expression tag	UNP Q99PJ1
B	1468	LEU	-	expression tag	UNP Q99PJ1
B	1469	PHE	-	expression tag	UNP Q99PJ1
B	1470	GLU	-	expression tag	UNP Q99PJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1471	SER	-	expression tag	UNP Q99PJ1
B	1472	ARG	-	expression tag	UNP Q99PJ1
B	1473	LEU	-	expression tag	UNP Q99PJ1
B	1474	VAL	-	expression tag	UNP Q99PJ1
B	1475	PRO	-	expression tag	UNP Q99PJ1
B	1476	ARG	-	expression tag	UNP Q99PJ1

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



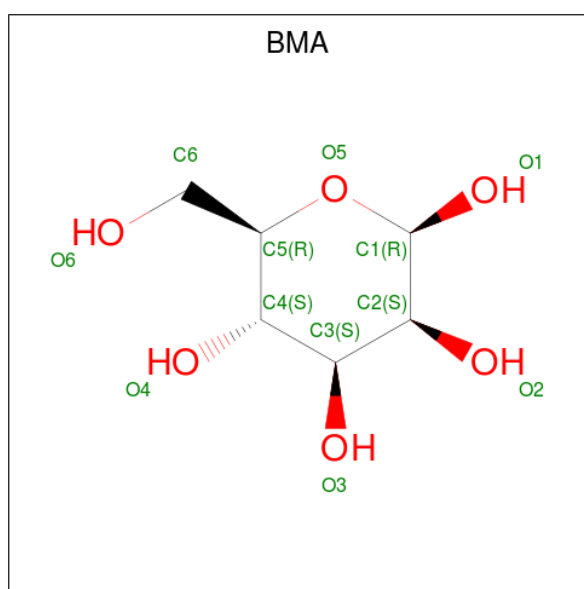
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	

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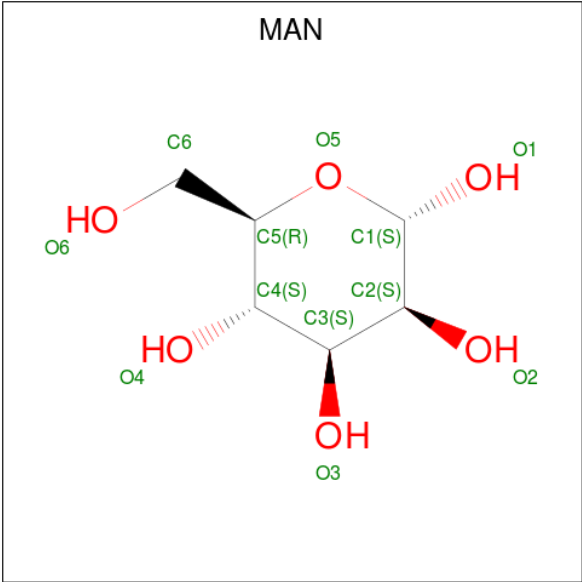
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			84	48	6	30	

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			66	36	30	
4	A	1	Total	C	O	0
			66	36	30	
4	A	1	Total	C	O	0
			66	36	30	
4	A	1	Total	C	O	0
			66	36	30	
4	A	1	Total	C	O	0
			66	36	30	
4	A	1	Total	C	O	0
			66	36	30	
4	B	1	Total	C	O	0
			66	36	30	
4	B	1	Total	C	O	0
			66	36	30	
4	B	1	Total	C	O	0
			66	36	30	
4	B	1	Total	C	O	0
			66	36	30	
4	B	1	Total	C	O	0
			66	36	30	

- Molecule 1: Protocadherin-15



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	16733	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: 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	0.26	0/4339	0.50	0/5908
1	B	0.26	0/4339	0.50	0/5908
All	All	0.26	0/8678	0.50	0/11816

There are no bond length outliers.

There are no bond angle outliers.

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	4248	0	4225	21	0
1	B	4248	0	4225	21	0
2	A	84	0	72	0	0
2	B	84	0	72	0	0
3	A	33	0	24	0	0
3	B	33	0	24	0	0
4	A	66	0	60	0	0
4	B	66	0	60	0	0
All	All	8862	0	8762	42	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 2.

All (42) 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:A:1018:GLU:HB3	1:A:1019:PRO:CD	1.33	1.51
1:B:1018:GLU:HB3	1:B:1019:PRO:CD	1.33	1.41
1:A:1018:GLU:CB	1:A:1019:PRO:CD	2.26	1.13
1:B:1018:GLU:HB3	1:B:1019:PRO:HD2	1.15	1.12
1:B:1018:GLU:CB	1:B:1019:PRO:CD	2.26	1.10
1:B:1018:GLU:HB3	1:B:1019:PRO:HD3	1.21	1.08
1:A:1018:GLU:HB3	1:A:1019:PRO:HD3	1.21	1.08
1:A:1018:GLU:HB3	1:A:1019:PRO:HD2	1.15	1.06
1:B:1017:GLY:O	1:B:1018:GLU:O	1.88	0.91
1:A:1017:GLY:O	1:A:1018:GLU:O	1.88	0.90
1:B:1018:GLU:CB	1:B:1019:PRO:HD3	2.01	0.84
1:B:1018:GLU:CB	1:B:1019:PRO:HD2	2.01	0.83
1:A:1018:GLU:CB	1:A:1019:PRO:HD3	2.01	0.82
1:A:1018:GLU:CB	1:A:1019:PRO:HD2	2.01	0.76
1:B:1126:VAL:HG23	1:B:1131:ASN:HD22	1.57	0.69
1:A:1126:VAL:HG23	1:A:1131:ASN:HD22	1.57	0.68
1:B:1110:LEU:HB2	1:B:1135:VAL:HB	1.87	0.56
1:A:1110:LEU:HB2	1:A:1135:VAL:HB	1.88	0.56
1:A:986:VAL:HG22	1:A:993:VAL:HG22	1.90	0.53
1:B:986:VAL:HG22	1:B:993:VAL:HG22	1.90	0.52
1:B:952:THR:OG1	1:B:992:ARG:NH1	2.43	0.52
1:A:952:THR:OG1	1:A:992:ARG:NH1	2.43	0.52
1:B:1283:GLN:HE21	1:B:1338:LYS:HD2	1.75	0.51
1:A:1283:GLN:HE21	1:A:1338:LYS:HD2	1.75	0.50
1:B:1350:TYR:OH	1:B:1355:ARG:NH2	2.44	0.50
1:A:1156:GLY:HA2	1:A:1290:VAL:HG21	1.93	0.50
1:A:1039:ARG:HH22	1:A:1068:ILE:HG12	1.77	0.50
1:B:1156:GLY:HA2	1:B:1290:VAL:HG21	1.93	0.50
1:A:1350:TYR:OH	1:A:1355:ARG:NH2	2.45	0.49
1:B:1039:ARG:HH22	1:B:1068:ILE:HG12	1.77	0.48
1:A:1106:THR:HA	1:A:1139:ILE:HD12	1.96	0.48
1:B:1106:THR:HA	1:B:1139:ILE:HD12	1.96	0.48
1:B:869:LEU:HD22	1:B:885:LEU:HA	1.97	0.47
1:A:869:LEU:HD22	1:A:885:LEU:HA	1.97	0.46
1:A:1298:ARG:HG2	1:A:1305:LEU:HG	1.98	0.46
1:B:1298:ARG:HG2	1:B:1305:LEU:HG	1.98	0.46
1:B:1037:ILE:O	1:B:1039:ARG:NH1	2.48	0.45
1:A:1037:ILE:O	1:A:1039:ARG:NH1	2.49	0.44
1:B:1045:TYR:HB3	1:B:1135:VAL:HG22	2.00	0.44
1:A:1045:TYR:HB3	1:A:1135:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:GLN:HA	1:A:1362:PRO:HD3	2.03	0.41
1:B:1254:GLN:HA	1:B:1362:PRO:HD3	2.03	0.41

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	540/660 (82%)	517 (96%)	22 (4%)	1 (0%)	49	85
1	B	540/660 (82%)	517 (96%)	22 (4%)	1 (0%)	49	85
All	All	1080/1320 (82%)	1034 (96%)	44 (4%)	2 (0%)	53	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	B	1018	GLU

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	471/566 (83%)	463 (98%)	8 (2%)	63	83
1	B	471/566 (83%)	463 (98%)	8 (2%)	63	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	942/1132 (83%)	926 (98%)	16 (2%)	66	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	910	MET
1	A	924	MET
1	A	939	MET
1	A	963	MET
1	A	1018	GLU
1	A	1097	ASN
1	A	1219	ARG
1	A	1249	ASN
1	B	910	MET
1	B	924	MET
1	B	939	MET
1	B	963	MET
1	B	1018	GLU
1	B	1097	ASN
1	B	1219	ARG
1	B	1249	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	873	HIS
1	A	1097	ASN
1	A	1131	ASN
1	A	1249	ASN
1	A	1283	GLN
1	A	1343	ASN
1	B	873	HIS
1	B	1097	ASN
1	B	1131	ASN
1	B	1249	ASN
1	B	1283	GLN
1	B	1343	ASN

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 ⓘ

30 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
2	NAG	A	1501	1,2	14,14,15	0.47	0	17,19,21	0.57	0
2	NAG	A	1502	3,2	14,14,15	0.30	0	17,19,21	0.48	0
3	BMA	A	1503	2,4	11,11,12	0.73	0	15,15,17	0.91	0
4	MAN	A	1504	3	11,11,12	0.88	1 (9%)	15,15,17	1.26	2 (13%)
4	MAN	A	1505	3	11,11,12	0.82	0	15,15,17	1.04	2 (13%)
2	NAG	A	1506	1,2	14,14,15	0.54	0	17,19,21	0.76	1 (5%)
2	NAG	A	1507	3,2	14,14,15	0.35	0	17,19,21	0.42	0
3	BMA	A	1508	2,4	11,11,12	0.78	0	15,15,17	0.87	0
4	MAN	A	1509	3	11,11,12	0.85	1 (9%)	15,15,17	1.21	2 (13%)
4	MAN	A	1510	3	11,11,12	0.83	0	15,15,17	1.10	2 (13%)
2	NAG	A	1511	1,2	14,14,15	0.78	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	A	1512	3,2	14,14,15	0.45	0	17,19,21	0.39	0
3	BMA	A	1513	2,4	11,11,12	0.80	0	15,15,17	0.84	0
4	MAN	A	1514	3	11,11,12	0.85	1 (9%)	15,15,17	1.18	2 (13%)
4	MAN	A	1515	3	11,11,12	0.81	0	15,15,17	1.06	2 (13%)
2	NAG	B	1501	1,2	14,14,15	0.47	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1502	3,2	14,14,15	0.29	0	17,19,21	0.47	0
3	BMA	B	1503	2,4	11,11,12	0.73	0	15,15,17	0.91	0
4	MAN	B	1504	3	11,11,12	0.87	1 (9%)	15,15,17	1.25	2 (13%)
4	MAN	B	1505	3	11,11,12	0.82	0	15,15,17	1.04	2 (13%)
2	NAG	B	1506	1,2	14,14,15	0.54	0	17,19,21	0.77	1 (5%)
2	NAG	B	1507	3,2	14,14,15	0.34	0	17,19,21	0.42	0
3	BMA	B	1508	2,4	11,11,12	0.77	0	15,15,17	0.87	0
4	MAN	B	1509	3	11,11,12	0.86	1 (9%)	15,15,17	1.22	2 (13%)
4	MAN	B	1510	3	11,11,12	0.82	0	15,15,17	1.10	2 (13%)
2	NAG	B	1511	1,2	14,14,15	0.78	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	B	1512	3,2	14,14,15	0.43	0	17,19,21	0.40	0
3	BMA	B	1513	2,4	11,11,12	0.80	0	15,15,17	0.84	0
4	MAN	B	1514	3	11,11,12	0.84	0	15,15,17	1.19	2 (13%)
4	MAN	B	1515	3	11,11,12	0.81	0	15,15,17	1.07	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
2	NAG	A	1501	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	1502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1503	2,4	-	2/2/19/22	0/1/1/1
4	MAN	A	1504	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1505	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1507	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1508	2,4	-	2/2/19/22	0/1/1/1
4	MAN	A	1509	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1510	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1511	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	1512	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1513	2,4	-	2/2/19/22	0/1/1/1
4	MAN	A	1514	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1515	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1501	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	1502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1503	2,4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	1504	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1505	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1507	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1508	2,4	-	2/2/19/22	0/1/1/1
4	MAN	B	1509	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1510	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1511	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	1512	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1513	2,4	-	2/2/19/22	0/1/1/1
4	MAN	B	1514	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1515	3	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1511	NAG	C1-C2	2.43	1.56	1.52
2	B	1511	NAG	C1-C2	2.43	1.56	1.52
4	B	1509	MAN	C1-C2	2.04	1.56	1.52
4	A	1504	MAN	C1-C2	2.03	1.56	1.52
4	B	1504	MAN	C1-C2	2.02	1.56	1.52
4	A	1509	MAN	C1-C2	2.01	1.56	1.52
4	A	1514	MAN	C1-C2	2.00	1.56	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1504	MAN	C1-O5-C5	3.60	117.10	112.20
4	B	1504	MAN	C1-O5-C5	3.57	117.06	112.20
4	B	1509	MAN	C1-O5-C5	3.43	116.87	112.20
4	A	1509	MAN	C1-O5-C5	3.38	116.80	112.20
4	B	1514	MAN	C1-O5-C5	3.30	116.69	112.20
4	A	1514	MAN	C1-O5-C5	3.25	116.62	112.20
2	A	1511	NAG	C1-O5-C5	2.88	116.12	112.20
4	B	1510	MAN	C1-O5-C5	2.85	116.08	112.20
2	B	1511	NAG	C1-O5-C5	2.84	116.06	112.20
4	A	1510	MAN	C1-O5-C5	2.83	116.05	112.20
4	B	1515	MAN	C1-O5-C5	2.69	115.86	112.20
4	A	1515	MAN	C1-O5-C5	2.68	115.84	112.20
4	A	1505	MAN	C1-O5-C5	2.58	115.70	112.20
4	B	1505	MAN	C1-O5-C5	2.56	115.69	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1506	NAG	C1-O5-C5	2.43	115.51	112.20
2	A	1506	NAG	C1-O5-C5	2.41	115.47	112.20
4	B	1504	MAN	O2-C2-C3	-2.29	105.69	110.16
4	A	1514	MAN	O2-C2-C3	-2.28	105.72	110.16
4	A	1504	MAN	O2-C2-C3	-2.27	105.73	110.16
4	B	1514	MAN	O2-C2-C3	-2.27	105.73	110.16
4	B	1505	MAN	O2-C2-C3	-2.26	105.74	110.16
4	A	1505	MAN	O2-C2-C3	-2.25	105.76	110.16
4	A	1510	MAN	O2-C2-C3	-2.25	105.76	110.16
4	B	1509	MAN	O2-C2-C3	-2.25	105.77	110.16
4	B	1515	MAN	O2-C2-C3	-2.24	105.78	110.16
4	A	1509	MAN	O2-C2-C3	-2.24	105.79	110.16
4	A	1515	MAN	O2-C2-C3	-2.24	105.79	110.16
4	B	1510	MAN	O2-C2-C3	-2.23	105.80	110.16

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1503	BMA	O5-C5-C6-O6
3	A	1503	BMA	O5-C5-C6-O6
3	A	1513	BMA	O5-C5-C6-O6
3	B	1513	BMA	O5-C5-C6-O6
3	B	1503	BMA	C4-C5-C6-O6
3	A	1503	BMA	C4-C5-C6-O6
3	B	1508	BMA	O5-C5-C6-O6
3	A	1508	BMA	O5-C5-C6-O6
3	A	1513	BMA	C4-C5-C6-O6
3	B	1513	BMA	C4-C5-C6-O6
3	B	1508	BMA	C4-C5-C6-O6
3	A	1508	BMA	C4-C5-C6-O6
2	B	1501	NAG	O5-C5-C6-O6
2	A	1501	NAG	O5-C5-C6-O6
2	B	1501	NAG	C4-C5-C6-O6
2	A	1501	NAG	C4-C5-C6-O6
2	A	1511	NAG	O5-C5-C6-O6
2	B	1511	NAG	O5-C5-C6-O6
2	A	1511	NAG	C4-C5-C6-O6
2	B	1511	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.