Integrative Structure Validation Report

July 22, 2024 - 05:36 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	9A47
PDB-Dev ID	PDBDEV_00000228
Structure Title	Man9 fully-glycosylated model of mouse N-cadherin EC4-EC5
Structure Authors	Tsai, Y.-X.; Chang, H.-T.; Wang, Y.-S.; Hsu, M.-F.; Hanus, C.; Sikora, M.; Hsu, S.-T.D.

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

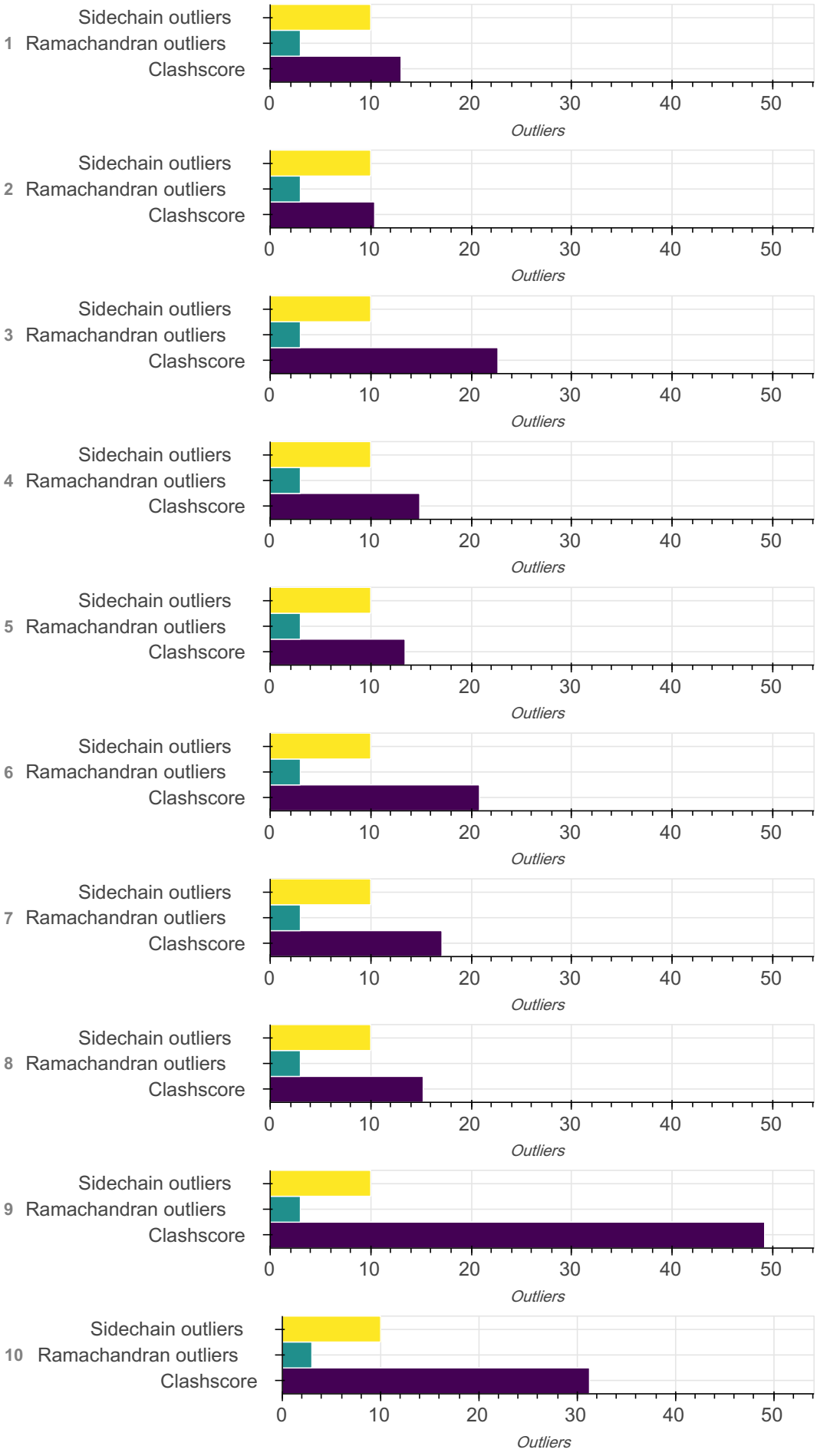
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis


1
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
2
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
3
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
4
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
5
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
6
Sidechain outliers
Ramachandran outliers
Clashscore
0
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20
30
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
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40
50
Outliers
8
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
9
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
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Outliers
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
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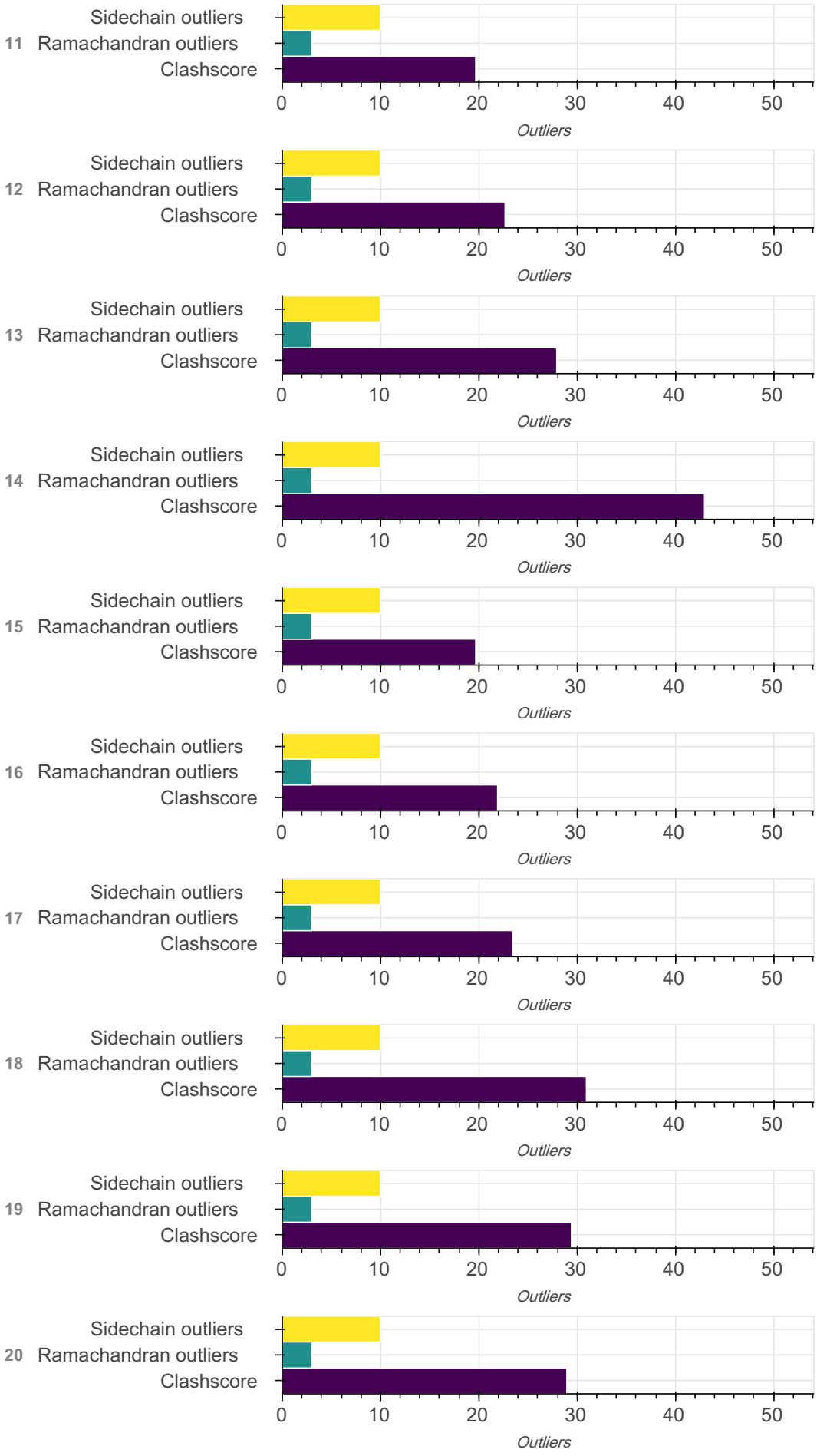
50
Outliers


11
Sidechain outliers
Ramachandran outliers
Clashscore
0
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20
30
40
50
Outliers
12
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
13
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
14
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
15
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
16
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
17
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
18
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
19
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
20
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers

Ensemble information

This entry consists of 1 distinct ensemble(s).

Summary

This entry consists of 20 unique models, with 5 subunits in each model. A total of 2 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 5 flexible or non-rigid units.

Entry composition

There are 20 unique types of models in this entry.These models are titled None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Cadherin-2	A	A	211
1	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
1	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
1	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
2	1	1	Cadherin-2	A	A	211
2	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
2	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
2	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
3	1	1	Cadherin-2	A	A	211

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
3	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
3	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
3	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
3	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
4	1	1	Cadherin-2	A	A	211
4	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
4	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
4	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
5	1	1	Cadherin-2	A	A	211
5	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
5	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
5	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
5	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
6	1	1	Cadherin-2	A	A	211

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
6	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
6	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
7	1	1	Cadherin-2	A	A	211
7	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
7	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
7	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
7	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
8	1	1	Cadherin-2	A	A	211
8	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
8	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
8	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
8	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
9	1	1	Cadherin-2	A	A	211

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
9	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
9	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
9	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
9	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
10	1	1	Cadherin-2	A	A	211
10	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
10	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
10	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
11	1	1	Cadherin-2	A	A	211
11	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
11	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
11	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
11	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
12	1	1	Cadherin-2	A	A	211

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
12	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
12	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
12	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
12	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
13	1	1	Cadherin-2	A	A	211
13	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
13	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
13	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
13	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
14	1	1	Cadherin-2	A	A	211
14	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
14	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
14	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
14	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
15	1	1	Cadherin-2	A	A	211

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
15	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
15	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
15	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
15	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
16	1	1	Cadherin-2	A	A	211
16	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
16	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
16	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
16	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
17	1	1	Cadherin-2	A	A	211
17	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
17	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
17	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
17	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
18	1	1	Cadherin-2	A	A	211

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
18	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
18	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
18	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
18	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
19	1	1	Cadherin-2	A	A	211
19	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11
19	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
19	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
19	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11
20	1	1	Cadherin-2	A	A	211
20	2	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	11

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
20	3	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	11
20	4	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	11
20	5	2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	11

Datasets used for modeling

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code

ID	Dataset type	Database name	Data access code
1	SAS data	SASBDB	SASDT45
2	Other	PDB	3Q2W

Representation

This entry has only one representation and includes 0 rigid bodies and 5 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-211
B	-	1-11
C	-	1-11
D	-	1-11
E	-	1-11

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Use GlycoSHIELD, the tool we have developed, to graft MD-simulated glycan ensemble onto the ectodomains 4 to 5 of x-ray protein structure (PDB ID: 3Q2W).	None	None	20	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	GlycoSHIELD	Not available	model building	https://github.com/GlycoSHIELD-MD/GlycoSHIELD-MD
2	GASBOR	Not available	model building	https://www.embl-hamburg.de/biosaxs/gasbor.html
3	FoXSDock	Not available	data analysis	https://modbase.compbio.ucsf.edu/foxsdock/

Data quality

SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers

There are 87 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	90.63	20
N-CA-C	111.00	133.93	20
C3-C4-O4	107.29	123.59	1
C3-C4-O4	107.29	122.95	1
C3-C4-O4	107.29	122.76	1
C3-C4-O4	107.29	122.63	1
C3-C4-O4	107.29	122.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3-C4-O4	107.29	122.27	1
C3-C4-O4	107.29	122.17	1
C1-O5-C5	118.82	104.20	1
C3-C4-O4	107.29	121.89	1
C1-O5-C5	118.82	104.62	1
C1-C2-O2	106.80	120.59	1
C3-C4-O4	107.29	120.98	1
C3-C4-O4	107.29	120.97	1
C1-C2-O2	106.80	120.45	1
C1-C2-O2	106.80	120.39	1
C3-C4-O4	107.29	120.72	1
C3-C4-O4	107.29	120.69	1
C3-C4-O4	107.29	120.66	1
C3-C4-O4	107.29	120.51	1
C3-C4-O4	107.29	120.44	1
C3-C4-O4	107.29	120.43	1
C3-C4-O4	107.29	120.39	1
C1-C2-O2	106.80	119.75	1
C5-C4-O4	111.70	98.89	1
C3-C4-O4	107.29	119.98	1
C5-C4-O4	111.70	99.05	1
C1-C2-O2	108.40	120.92	1
C3-C4-O4	107.29	119.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-C3-O3	107.58	120.05	1
C3-C4-O4	107.29	119.74	1
C1-C2-O2	108.40	120.85	1
C1-C2-O2	106.80	119.21	1
C4-C5-C6	111.68	124.09	1
C5-C4-O4	111.70	99.32	1
C3-C4-O4	107.29	119.53	1
C3-C4-O4	107.29	119.52	1
C3-C4-O4	107.29	119.47	1
C3-C4-O4	107.29	119.45	1
C1-C2-O2	106.80	118.92	1
C3-C4-O4	107.29	119.38	1
C5-C4-O4	111.70	99.63	1
C1-C2-O2	106.80	118.86	2
C4-C5-O5	109.06	97.01	1
C4-C5-C6	111.68	123.70	1
C5-C4-O4	111.70	99.70	1
C3-C4-O4	107.06	119.06	1

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	13.02	35

Model ID	Clash score	Number of clashes
2	10.39	28
3	22.66	61
4	14.88	40
5	13.42	36
6	20.82	56
7	17.09	46
8	15.22	41
9	49.20	132
10	31.26	84
11	19.67	53
12	22.66	61
13	27.92	75
14	42.96	115
15	19.67	53
16	21.90	59
17	23.44	63
18	30.94	83
19	29.42	79
20	28.95	78

All 1278 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:187:GLU:CD	B:4:MAN:O6	1.086
1	A:187:GLU:O	B:2:NAG:CT	1.022

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:187:GLU:OE1	B:4:MAN:O6	0.958
1	A:83:ASN:CG	C:1:NAG:C1	0.894
1	A:122:GLU:OE2	E:8:MAN:O4	0.861
1	A:171:ASP:OD2	A:172:PHE:HD2	0.833
1	A:169:ASN:H	A:169:ASN:HD22	0.765
1	A:169:ASN:HD21	A:172:PHE:HB2	0.763
1	A:171:ASP:OD2	A:172:PHE:CD2	0.756
1	A:133:ASN:O	E:1:NAG:O6	0.739
1	A:168:LEU:HB2	A:172:PHE:O	0.691
1	A:83:ASN:CB	C:1:NAG:C1	0.684
1	A:169:ASN:N	A:169:ASN:ND2	0.674
1	A:169:ASN:H	A:169:ASN:ND2	0.671
1	A:11:ASN:HB3	A:12:PRO:HD3	0.610
1	A:79:ASN:HD22	A:80:ASN:H	0.592
1	A:117:LEU:HB3	A:118:PRO:HD3	0.591
1	A:83:ASN:OD1	C:1:NAG:C1	0.584
1	A:187:GLU:OE1	B:4:MAN:C6	0.581
1	A:187:GLU:C	B:2:NAG:CT	0.570
1	A:187:GLU:CD	B:4:MAN:C6	0.564
1	A:61:ASN:HB3	A:63:GLN:HG3	0.560
1	A:158:THR:HG22	A:161:ARG:NH2	0.547
1	A:29:THR:HG22	A:63:GLN:HG2	0.536
1	A:169:ASN:N	A:169:ASN:HD22	0.499

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:93:ILE:HB	A:94:PRO:HD3	0.477
1	A:198:PRO:HA	A:199:PRO:HD3	0.457
1	A:118:PRO:HB3	E:2:NAG:CT	0.451
1	A:11:ASN:CB	A:12:PRO:HD3	0.441
1	A:155:SER:HA	A:156:PRO:C	0.435
1	A:158:THR:OG1	B:1:NAG:H61	0.434
1	A:56:LYS:HD2	A:67:ILE:HD11	0.433
1	A:197:ASN:HA	A:198:PRO:C	0.427
1	A:48:LEU:HD12	A:87:LEU:HG	0.421
1	A:93:ILE:O	A:95:PRO:HD3	0.411
2	A:131:SER:O	E:1:NAG:H61	0.962
2	A:171:ASP:OD2	A:172:PHE:HD2	0.833
2	A:169:ASN:H	A:169:ASN:HD22	0.765
2	A:169:ASN:HD21	A:172:PHE:HB2	0.763
2	A:171:ASP:OD2	A:172:PHE:CD2	0.756
2	A:123:THR:CG2	E:2:NAG:CT	0.699
2	A:168:LEU:HB2	A:172:PHE:O	0.691
2	A:169:ASN:N	A:169:ASN:ND2	0.674
2	A:169:ASN:H	A:169:ASN:ND2	0.671
2	A:11:ASN:HB3	A:12:PRO:HD3	0.610
2	A:79:ASN:HD22	A:80:ASN:H	0.592
2	A:117:LEU:HB3	A:118:PRO:HD3	0.591
2	A:199:PRO:O	D:1:NAG:H61	0.588

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:61:ASN:HB3	A:63:GLN:HG3	0.560
2	A:158:THR:HG22	A:161:ARG:NH2	0.547
2	A:29:THR:HG22	A:63:GLN:HG2	0.536
2	A:169:ASN:N	A:169:ASN:HD22	0.499
2	A:123:THR:HG22	E:2:NAG:CT	0.489
2	A:93:ILE:HB	A:94:PRO:HD3	0.477
2	A:198:PRO:HA	A:199:PRO:HD3	0.457
2	A:123:THR:HG21	E:2:NAG:CT	0.456
2	A:11:ASN:CB	A:12:PRO:HD3	0.441
2	A:155:SER:HA	A:156:PRO:C	0.435
2	A:56:LYS:HD2	A:67:ILE:HD11	0.433
2	A:158:THR:HG21	B:11:MAN:O6	0.427
2	A:197:ASN:HA	A:198:PRO:C	0.427
2	A:48:LEU:HD12	A:87:LEU:HG	0.421
2	A:93:ILE:O	A:95:PRO:HD3	0.411
3	A:154:LEU:HB3	D:5:MAN:O6	1.293
3	A:168:LEU:HD23	E:1:NAG:O	1.243
3	A:182:GLU:OE1	B:8:MAN:O3	1.233
3	A:83:ASN:CG	C:1:NAG:C1	1.078
3	A:182:GLU:HB3	B:8:MAN:O3	1.066
3	A:182:GLU:CB	B:8:MAN:O3	1.026
3	A:168:LEU:CD2	E:1:NAG:O	0.972
3	A:154:LEU:CB	D:5:MAN:O6	0.966

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:154:LEU:HB3	D:5:MAN:HO6	0.953
3	A:183:ALA:N	B:8:MAN:H4	0.944
3	A:182:GLU:OE1	B:8:MAN:C3	0.857
3	A:133:ASN:ND2	E:1:NAG:C1	0.855
3	A:151:ASP:OD2	D:1:NAG:O	0.834
3	A:171:ASP:OD2	A:172:PHE:HD2	0.833
3	A:182:GLU:CD	B:8:MAN:O3	0.805
3	A:133:ASN:CG	E:1:NAG:C1	0.788
3	A:154:LEU:O	D:5:MAN:C6	0.782
3	A:169:ASN:H	A:169:ASN:HD22	0.765
3	A:169:ASN:HD21	A:172:PHE:HB2	0.763
3	A:171:ASP:OD2	A:172:PHE:CD2	0.756
3	A:154:LEU:C	D:5:MAN:O6	0.726
3	A:158:THR:OG1	B:1:NAG:O6	0.700
3	A:133:ASN:CB	E:1:NAG:C1	0.691
3	A:168:LEU:HB2	A:172:PHE:O	0.691
3	A:158:THR:C	B:1:NAG:O6	0.688
3	A:83:ASN:ND2	C:1:NAG:C1	0.684
3	A:169:ASN:N	A:169:ASN:ND2	0.674
3	A:169:ASN:H	A:169:ASN:ND2	0.671
3	A:182:GLU:CG	B:8:MAN:O3	0.659
3	A:158:THR:C	B:1:NAG:HO6	0.646
3	A:182:GLU:CD	B:8:MAN:C3	0.626

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:158:THR:HG1	B:1:NAG:C6	0.623
3	A:154:LEU:O	D:5:MAN:H61	0.617
3	A:83:ASN:OD1	C:1:NAG:C1	0.615
3	A:11:ASN:HB3	A:12:PRO:HD3	0.610
3	A:182:GLU:CD	B:8:MAN:H3	0.600
3	A:79:ASN:HD22	A:80:ASN:H	0.592
3	A:117:LEU:HB3	A:118:PRO:HD3	0.591
3	A:157:VAL:CG2	D:6:MAN:H3	0.589
3	A:158:THR:OG1	B:1:NAG:C6	0.575
3	A:182:GLU:OE1	B:8:MAN:H3	0.573
3	A:168:LEU:CD2	E:1:NAG:C	0.561
3	A:61:ASN:HB3	A:63:GLN:HG3	0.560
3	A:154:LEU:CA	D:5:MAN:O6	0.552
3	A:158:THR:HG22	A:161:ARG:NH2	0.547
3	A:29:THR:HG22	A:63:GLN:HG2	0.536
3	A:157:VAL:HG13	D:5:MAN:O4	0.528
3	A:169:ASN:N	A:169:ASN:HD22	0.499
3	A:93:ILE:HB	A:94:PRO:HD3	0.477
3	A:158:THR:CB	B:1:NAG:O6	0.466
3	A:198:PRO:HA	A:199:PRO:HD3	0.457
3	A:11:ASN:CB	A:12:PRO:HD3	0.441
3	B:2:NAG:H5	B:3:BMA:O5	0.441
3	A:83:ASN:CB	C:1:NAG:C1	0.436

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:155:SER:HA	A:156:PRO:C	0.435
3	A:56:LYS:HD2	A:67:ILE:HD11	0.433
3	A:154:LEU:O	D:5:MAN:O6	0.431
3	A:197:ASN:HA	A:198:PRO:C	0.427
3	A:48:LEU:HD12	A:87:LEU:HG	0.421
3	A:93:ILE:O	A:95:PRO:HD3	0.411
3	A:157:VAL:HG22	D:5:MAN:H4	0.408
4	A:125:GLU:OE2	B:2:NAG:CT	1.348
4	A:78:LYS:N	C:2:NAG:N	1.268
4	A:125:GLU:HG2	B:2:NAG:CT	1.057
4	A:125:GLU:CD	B:2:NAG:CT	1.048
4	A:125:GLU:CG	B:2:NAG:CT	1.014
4	A:125:GLU:OE2	B:2:NAG:C	0.919
4	A:171:ASP:OD2	A:172:PHE:HD2	0.833
4	A:78:LYS:CG	C:3:BMA:C1	0.811
4	A:78:LYS:HG3	C:3:BMA:C1	0.782
4	A:78:LYS:HB3	C:2:NAG:C5	0.768
4	A:169:ASN:H	A:169:ASN:HD22	0.765
4	A:169:ASN:HD21	A:172:PHE:HB2	0.763
4	A:171:ASP:OD2	A:172:PHE:CD2	0.756
4	A:78:LYS:HB3	C:2:NAG:H5	0.754
4	A:168:LEU:HB2	A:172:PHE:O	0.691
4	A:169:ASN:N	A:169:ASN:ND2	0.674

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:169:ASN:H	A:169:ASN:ND2	0.671
4	A:78:LYS:N	C:2:NAG:C	0.639
4	A:11:ASN:HB3	A:12:PRO:HD3	0.610
4	A:79:ASN:HD22	A:80:ASN:H	0.592
4	A:117:LEU:HB3	A:118:PRO:HD3	0.591
4	A:61:ASN:HB3	A:63:GLN:HG3	0.560
4	A:158:THR:HG22	A:161:ARG:NH2	0.547
4	A:161:ARG:HG2	B:1:NAG:C	0.538
4	A:29:THR:HG22	A:63:GLN:HG2	0.536
4	A:78:LYS:N	C:2:NAG:CT	0.527
4	A:133:ASN:ND2	E:1:NAG:C1	0.507
4	A:169:ASN:N	A:169:ASN:HD22	0.499
4	A:161:ARG:NE	B:1:NAG:CT	0.484
4	A:93:ILE:HB	A:94:PRO:HD3	0.477
4	A:198:PRO:HA	A:199:PRO:HD3	0.457
4	A:182:GLU:HG3	B:3:BMA:H5	0.455
4	A:11:ASN:CB	A:12:PRO:HD3	0.441
4	A:155:SER:HA	A:156:PRO:C	0.435
4	A:56:LYS:HD2	A:67:ILE:HD11	0.433
4	A:197:ASN:HA	A:198:PRO:C	0.427
4	A:133:ASN:CB	E:1:NAG:C1	0.426
4	A:161:ARG:HD2	B:1:NAG:CT	0.425
4	A:48:LEU:HD12	A:87:LEU:HG	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:93:ILE:O	A:95:PRO:HD3	0.411
5	A:131:SER:O	E:1:NAG:H61	1.261
5	A:199:PRO:O	D:1:NAG:H61	1.039
5	A:182:GLU:OE1	B:10:MAN:C1	0.906
5	A:131:SER:O	E:1:NAG:C6	0.887
5	A:182:GLU:OE1	B:7:MAN:O6	0.845
5	A:171:ASP:OD2	A:172:PHE:HD2	0.833
5	A:169:ASN:H	A:169:ASN:HD22	0.765
5	A:169:ASN:HD21	A:172:PHE:HB2	0.763
5	A:171:ASP:OD2	A:172:PHE:CD2	0.756
5	A:51:PRO:HB2	C:2:NAG:O	0.736
5	A:199:PRO:O	D:1:NAG:C6	0.727
5	A:83:ASN:HB2	C:1:NAG:C1	0.701
5	A:168:LEU:HB2	A:172:PHE:O	0.691
5	A:83:ASN:ND2	C:1:NAG:C1	0.682
5	A:169:ASN:N	A:169:ASN:ND2	0.674
5	A:169:ASN:H	A:169:ASN:ND2	0.671
5	A:83:ASN:HD22	C:1:NAG:C1	0.617
5	A:11:ASN:HB3	A:12:PRO:HD3	0.610
5	A:79:ASN:HD22	A:80:ASN:H	0.592
5	A:117:LEU:HB3	A:118:PRO:HD3	0.591
5	A:61:ASN:HB3	A:63:GLN:HG3	0.560
5	A:158:THR:HG22	A:161:ARG:NH2	0.547

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:29:THR:HG22	A:63:GLN:HG2	0.536
5	A:180:LYS:C	B:2:NAG:O3	0.527
5	A:169:ASN:N	A:169:ASN:HD22	0.499
5	A:93:ILE:HB	A:94:PRO:HD3	0.477
5	A:75:PRO:O	C:2:NAG:H3	0.460
5	A:198:PRO:HA	A:199:PRO:HD3	0.457
5	A:78:LYS:HG2	C:3:BMA:H62	0.452
5	A:200:LYS:HA	D:1:NAG:O6	0.443
5	A:11:ASN:CB	A:12:PRO:HD3	0.441
5	A:155:SER:HA	A:156:PRO:C	0.435
5	A:56:LYS:HD2	A:67:ILE:HD11	0.433
5	A:197:ASN:HA	A:198:PRO:C	0.427
5	A:48:LEU:HD12	A:87:LEU:HG	0.421
5	A:93:ILE:O	A:95:PRO:HD3	0.411
6	A:133:ASN:ND2	E:1:NAG:C1	1.504
6	A:158:THR:HG21	B:2:NAG:N	1.386
6	A:158:THR:HG23	B:2:NAG:CT	1.369
6	A:158:THR:CG2	B:2:NAG:N	1.269
6	A:79:ASN:OD1	C:3:BMA:H62	1.076
6	A:79:ASN:HB2	C:2:NAG:C1	1.075
6	A:158:THR:CG2	B:2:NAG:CT	1.006
6	A:158:THR:CG2	B:2:NAG:C	0.982
6	A:133:ASN:CG	E:1:NAG:C1	0.921

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:158:THR:HG23	B:2:NAG:C	0.915
6	A:79:ASN:N	C:2:NAG:N	0.866
6	A:79:ASN:HB3	C:1:NAG:H4	0.837
6	A:171:ASP:OD2	A:172:PHE:HD2	0.833
6	A:158:THR:OG1	B:2:NAG:C	0.785
6	A:133:ASN:ND2	E:1:NAG:O5	0.772
6	A:158:THR:H	B:2:NAG:CT	0.768
6	A:169:ASN:H	A:169:ASN:HD22	0.765
6	A:169:ASN:HD21	A:172:PHE:HB2	0.763
6	A:171:ASP:OD2	A:172:PHE:CD2	0.756
6	A:168:LEU:HB2	A:172:PHE:O	0.691
6	A:79:ASN:HB2	C:2:NAG:N	0.686
6	A:78:LYS:HG2	C:2:NAG:O	0.684
6	A:169:ASN:N	A:169:ASN:ND2	0.674
6	A:169:ASN:H	A:169:ASN:ND2	0.671
6	A:79:ASN:OD1	C:3:BMA:C6	0.643
6	A:79:ASN:HB2	C:1:NAG:O4	0.614
6	A:11:ASN:HB3	A:12:PRO:HD3	0.610
6	A:79:ASN:HD22	A:80:ASN:H	0.592
6	A:117:LEU:HB3	A:118:PRO:HD3	0.591
6	A:61:ASN:HB3	A:63:GLN:HG3	0.560
6	A:158:THR:CB	B:2:NAG:N	0.557
6	A:158:THR:HG22	A:161:ARG:NH2	0.547

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:78:LYS:CG	C:2:NAG:O	0.547
6	A:79:ASN:HB2	C:2:NAG:C2	0.543
6	A:29:THR:HG22	A:63:GLN:HG2	0.536
6	A:158:THR:CB	B:2:NAG:C	0.530
6	A:158:THR:CB	B:1:NAG:O4	0.511
6	A:169:ASN:N	A:169:ASN:HD22	0.499
6	A:79:ASN:HB3	C:1:NAG:C4	0.493
6	A:158:THR:HG21	B:2:NAG:C2	0.493
6	A:79:ASN:CB	C:1:NAG:H4	0.482
6	A:133:ASN:CB	E:1:NAG:C1	0.480
6	A:158:THR:OG1	B:2:NAG:N	0.479
6	A:93:ILE:HB	A:94:PRO:HD3	0.477
6	A:79:ASN:CG	C:3:BMA:H62	0.475
6	A:198:PRO:HA	A:199:PRO:HD3	0.457
6	A:158:THR:HG21	B:2:NAG:C1	0.452
6	A:79:ASN:CB	C:1:NAG:C4	0.449
6	A:79:ASN:CB	C:2:NAG:C1	0.447
6	A:11:ASN:CB	A:12:PRO:HD3	0.441
6	A:155:SER:HA	A:156:PRO:C	0.435
6	A:56:LYS:HD2	A:67:ILE:HD11	0.433
6	A:197:ASN:HA	A:198:PRO:C	0.427
6	A:48:LEU:HD12	A:87:LEU:HG	0.421
6	A:93:ILE:O	A:95:PRO:HD3	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:156:PRO:HB2	B:2:NAG:O	0.411
7	A:130:ASN:OD1	E:1:NAG:CT	1.425
7	A:130:ASN:CG	E:1:NAG:CT	1.226
7	A:78:LYS:HB3	C:11:MAN:C6	1.115
7	A:78:LYS:HB3	C:11:MAN:H61	1.114
7	A:78:LYS:HG3	C:11:MAN:O4	1.107
7	A:130:ASN:OD1	E:1:NAG:C	1.059
7	A:130:ASN:HB3	E:1:NAG:CT	1.055
7	A:130:ASN:CB	E:1:NAG:CT	1.026
7	A:78:LYS:CB	C:11:MAN:H61	1.014
7	A:78:LYS:O	C:11:MAN:H4	0.907
7	A:187:GLU:N	B:2:NAG:CT	0.843
7	A:171:ASP:OD2	A:172:PHE:HD2	0.833
7	A:83:ASN:CG	C:1:NAG:C1	0.830
7	A:78:LYS:C	C:11:MAN:H4	0.782
7	A:169:ASN:H	A:169:ASN:HD22	0.765
7	A:169:ASN:HD21	A:172:PHE:HB2	0.763
7	A:187:GLU:H	B:2:NAG:CT	0.757
7	A:171:ASP:OD2	A:172:PHE:CD2	0.756
7	A:168:LEU:HB2	A:172:PHE:O	0.691
7	A:78:LYS:CG	C:11:MAN:H61	0.690
7	A:169:ASN:N	A:169:ASN:ND2	0.674
7	A:169:ASN:H	A:169:ASN:ND2	0.671

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:78:LYS:CG	C:11:MAN:O4	0.662
7	A:83:ASN:OD1	C:1:NAG:C1	0.650
7	A:78:LYS:HB3	C:11:MAN:O6	0.646
7	A:11:ASN:HB3	A:12:PRO:HD3	0.610
7	A:78:LYS:HG3	C:11:MAN:HO4	0.601
7	A:79:ASN:HD22	A:80:ASN:H	0.592
7	A:117:LEU:HB3	A:118:PRO:HD3	0.591
7	A:61:ASN:HB3	A:63:GLN:HG3	0.560
7	A:158:THR:HG22	A:161:ARG:NH2	0.547
7	A:131:SER:O	E:1:NAG:H61	0.545
7	A:29:THR:HG22	A:63:GLN:HG2	0.536
7	A:187:GLU:O	B:2:NAG:CT	0.504
7	A:169:ASN:N	A:169:ASN:HD22	0.499
7	A:78:LYS:O	C:11:MAN:C4	0.490
7	A:78:LYS:HG2	C:11:MAN:H61	0.489
7	A:93:ILE:HB	A:94:PRO:HD3	0.477
7	A:198:PRO:HA	A:199:PRO:HD3	0.457
7	A:11:ASN:CB	A:12:PRO:HD3	0.441
7	A:79:ASN:N	C:11:MAN:O6	0.436
7	A:155:SER:HA	A:156:PRO:C	0.435
7	A:56:LYS:HD2	A:67:ILE:HD11	0.433
7	A:197:ASN:HA	A:198:PRO:C	0.427
7	A:48:LEU:HD12	A:87:LEU:HG	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:93:ILE:O	A:95:PRO:HD3	0.411
8	A:158:THR:HB	B:1:NAG:C6	1.356
8	A:158:THR:CB	B:1:NAG:H62	1.310
8	A:158:THR:CB	B:1:NAG:C6	1.185
8	A:133:ASN:HD22	E:1:NAG:C1	1.004
8	A:158:THR:HB	B:1:NAG:H62	0.876
8	A:171:ASP:OD2	A:172:PHE:HD2	0.833
8	A:158:THR:HB	B:1:NAG:H61	0.783
8	A:158:THR:HG21	B:2:NAG:N	0.768
8	A:169:ASN:H	A:169:ASN:HD22	0.765
8	A:169:ASN:HD21	A:172:PHE:HB2	0.763
8	A:171:ASP:OD2	A:172:PHE:CD2	0.756
8	A:158:THR:HB	B:1:NAG:C5	0.752
8	A:158:THR:OG1	B:1:NAG:H62	0.740
8	A:133:ASN:HB2	E:1:NAG:C1	0.736
8	A:158:THR:CB	B:1:NAG:H61	0.733
8	A:168:LEU:HB2	A:172:PHE:O	0.691
8	A:133:ASN:ND2	E:1:NAG:C1	0.688
8	A:169:ASN:N	A:169:ASN:ND2	0.674
8	A:169:ASN:H	A:169:ASN:ND2	0.671
8	A:158:THR:HB	B:1:NAG:C4	0.655
8	A:158:THR:HB	B:1:NAG:O4	0.611
8	A:11:ASN:HB3	A:12:PRO:HD3	0.610

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:79:ASN:HD22	A:80:ASN:H	0.592
8	A:117:LEU:HB3	A:118:PRO:HD3	0.591
8	A:61:ASN:HB3	A:63:GLN:HG3	0.560
8	A:158:THR:HG22	A:161:ARG:NH2	0.547
8	A:29:THR:HG22	A:63:GLN:HG2	0.536
8	A:169:ASN:N	A:169:ASN:HD22	0.499
8	A:93:ILE:HB	A:94:PRO:HD3	0.477
8	A:198:PRO:HA	A:199:PRO:HD3	0.457
8	A:11:ASN:CB	A:12:PRO:HD3	0.441
8	C:2:NAG:H5	C:3:BMA:O5	0.439
8	A:155:SER:HA	A:156:PRO:C	0.435
8	A:56:LYS:HD2	A:67:ILE:HD11	0.433
8	A:197:ASN:HA	A:198:PRO:C	0.427
8	A:48:LEU:HD12	A:87:LEU:HG	0.421
8	A:158:THR:OG1	B:2:NAG:CT	0.418
8	A:93:ILE:O	A:95:PRO:HD3	0.411
8	A:158:THR:HA	B:1:NAG:H61	0.411
8	A:158:THR:CG2	B:2:NAG:N	0.409
8	A:161:ARG:HH21	B:1:NAG:C4	0.408
9	A:22:HIS:NE2	D:6:MAN:C2	1.559
9	A:22:HIS:CD2	D:6:MAN:C2	1.546
9	A:83:ASN:ND2	C:1:NAG:C1	1.410
9	A:198:PRO:CD	D:11:MAN:H62	1.370

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:78:LYS:CB	C:2:NAG:N	1.347
9	A:205:ILE:CG2	B:11:MAN:H61	1.323
9	A:141:ILE:HD13	C:10:MAN:C4	1.320
9	A:141:ILE:CD1	C:10:MAN:O4	1.309
9	A:187:GLU:OE2	B:7:MAN:H62	1.294
9	A:126:THR:OG1	E:11:MAN:O6	1.264
9	A:205:ILE:CG2	B:11:MAN:O5	1.263
9	A:141:ILE:HD13	C:10:MAN:O4	1.243
9	A:198:PRO:CG	D:11:MAN:H62	1.235
9	A:205:ILE:CG2	B:11:MAN:C6	1.228
9	A:22:HIS:CG	D:6:MAN:O3	1.205
9	A:141:ILE:HG21	C:10:MAN:O4	1.205
9	A:205:ILE:HG22	B:11:MAN:H61	1.134
9	A:198:PRO:HD3	D:11:MAN:C6	1.122
9	A:78:LYS:HB2	C:2:NAG:N	1.082
9	A:141:ILE:CG2	C:10:MAN:O4	1.067
9	A:141:ILE:CG1	C:10:MAN:O4	1.054
9	A:83:ASN:CG	C:1:NAG:C1	1.048
9	A:198:PRO:HD3	D:11:MAN:H62	1.034
9	A:22:HIS:CD2	D:6:MAN:C3	1.012
9	A:205:ILE:HG21	B:11:MAN:C6	0.991
9	A:80:ASN:OD1	C:11:MAN:H61	0.986
9	A:80:ASN:CG	C:11:MAN:H61	0.975

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:158:THR:C	B:1:NAG:O6	0.940
9	A:205:ILE:HG21	B:11:MAN:O5	0.940
9	A:205:ILE:CD1	B:10:MAN:O2	0.937
9	A:141:ILE:CG2	C:10:MAN:HO4	0.934
9	A:83:ASN:ND2	C:1:NAG:O5	0.923
9	A:187:GLU:N	B:2:NAG:O	0.918
9	A:187:GLU:OE2	B:7:MAN:C6	0.916
9	A:80:ASN:CG	C:11:MAN:C6	0.901
9	A:78:LYS:HD3	C:2:NAG:C	0.893
9	A:22:HIS:CD2	D:6:MAN:O2	0.892
9	A:141:ILE:HG21	C:10:MAN:HO4	0.887
9	A:198:PRO:HG3	D:11:MAN:H62	0.880
9	A:198:PRO:CG	D:11:MAN:C6	0.879
9	A:141:ILE:HD13	C:10:MAN:H4	0.847
9	A:171:ASP:OD2	A:172:PHE:HD2	0.837
9	A:22:HIS:CA	D:6:MAN:O3	0.836
9	A:141:ILE:CB	C:10:MAN:O4	0.836
9	A:22:HIS:CD2	D:6:MAN:O3	0.821
9	A:187:GLU:CD	B:7:MAN:H62	0.817
9	A:22:HIS:HA	D:6:MAN:HO3	0.794
9	A:205:ILE:HD13	B:10:MAN:O2	0.791
9	A:78:LYS:HB2	C:2:NAG:C	0.788
9	A:22:HIS:CE1	D:6:MAN:C2	0.788

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:198:PRO:CD	D:11:MAN:C6	0.787
9	A:141:ILE:CB	C:10:MAN:HO4	0.783
9	A:22:HIS:NE2	D:6:MAN:C1	0.783
9	A:78:LYS:CD	C:2:NAG:C	0.773
9	A:22:HIS:CG	D:6:MAN:C3	0.767
9	A:169:ASN:H	A:169:ASN:HD22	0.765
9	A:169:ASN:HD21	A:172:PHE:HB2	0.763
9	A:171:ASP:OD2	A:172:PHE:CD2	0.756
9	A:78:LYS:H	C:2:NAG:CT	0.751
9	A:83:ASN:HD21	C:1:NAG:C1	0.739
9	A:22:HIS:NE2	D:6:MAN:C3	0.738
9	A:158:THR:OG1	B:1:NAG:H61	0.728
9	A:78:LYS:HD3	C:2:NAG:O	0.726
9	A:198:PRO:HG3	D:11:MAN:O5	0.724
9	A:141:ILE:HD13	C:10:MAN:HO4	0.718
9	A:141:ILE:CD1	C:10:MAN:HO4	0.715
9	A:22:HIS:CE1	D:6:MAN:H3	0.709
9	A:198:PRO:HG3	D:11:MAN:C6	0.708
9	A:22:HIS:CE1	D:6:MAN:C3	0.704
9	A:22:HIS:CB	D:6:MAN:O3	0.699
9	A:22:HIS:HA	D:6:MAN:O3	0.694
9	A:168:LEU:HB2	A:172:PHE:O	0.691
9	A:158:THR:C	B:1:NAG:HO6	0.687

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:205:ILE:HD11	B:10:MAN:O2	0.687
9	A:169:ASN:N	A:169:ASN:ND2	0.674
9	A:169:ASN:H	A:169:ASN:ND2	0.671
9	A:187:GLU:HG3	B:2:NAG:C	0.657
9	A:78:LYS:HB3	C:2:NAG:C1	0.656
9	A:187:GLU:OE1	B:10:MAN:C1	0.642
9	A:187:GLU:CA	B:2:NAG:O	0.641
9	A:22:HIS:HD2	D:6:MAN:O2	0.639
9	A:205:ILE:HG23	B:11:MAN:O2	0.629
9	A:141:ILE:CD1	C:10:MAN:C4	0.626
9	A:205:ILE:HG23	B:11:MAN:O5	0.624
9	A:78:LYS:N	C:2:NAG:CT	0.613
9	A:11:ASN:HB3	A:12:PRO:HD3	0.610
9	A:141:ILE:HG21	C:10:MAN:C4	0.610
9	A:203:ILE:O	B:11:MAN:O3	0.609
9	A:205:ILE:CG2	B:11:MAN:O2	0.604
9	A:79:ASN:HD22	A:80:ASN:H	0.592
9	A:117:LEU:HB3	A:118:PRO:HD3	0.591
9	A:187:GLU:OE1	B:10:MAN:H2	0.590
9	A:133:ASN:O	E:1:NAG:O6	0.589
9	A:22:HIS:CA	D:6:MAN:HO3	0.579
9	A:205:ILE:HA	B:11:MAN:O2	0.575
9	A:61:ASN:HB3	A:63:GLN:HG3	0.560

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:78:LYS:CA	C:2:NAG:N	0.551
9	A:158:THR:HG22	A:161:ARG:NH2	0.547
9	A:187:GLU:C	B:2:NAG:O	0.546
9	A:205:ILE:CA	B:11:MAN:O2	0.541
9	A:198:PRO:HG3	D:11:MAN:C5	0.540
9	A:198:PRO:HD3	D:11:MAN:O6	0.537
9	A:29:THR:HG22	A:63:GLN:HG2	0.536
9	A:22:HIS:N	D:6:MAN:O3	0.522
9	A:187:GLU:OE1	B:10:MAN:C2	0.512
9	A:187:GLU:CD	B:10:MAN:C1	0.509
9	A:80:ASN:ND2	C:11:MAN:O6	0.502
9	A:169:ASN:N	A:169:ASN:HD22	0.499
9	A:126:THR:HG21	E:11:MAN:O4	0.484
9	A:78:LYS:N	C:2:NAG:N	0.479
9	A:93:ILE:HB	A:94:PRO:HD3	0.477
9	A:80:ASN:HB3	C:11:MAN:H5	0.472
9	D:2:NAG:H5	D:3:BMA:O5	0.461
9	A:120:GLU:O	E:2:NAG:C	0.460
9	A:198:PRO:HA	A:199:PRO:HD3	0.457
9	A:200:LYS:HZ3	D:2:NAG:CT	0.456
9	A:78:LYS:H	C:2:NAG:C	0.455
9	A:187:GLU:OE2	B:10:MAN:C1	0.454
9	A:200:LYS:NZ	D:2:NAG:CT	0.444

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	E:2:NAG:H5	E:3:BMA:O5	0.442
9	A:11:ASN:CB	A:12:PRO:HD3	0.441
9	A:155:SER:HA	A:156:PRO:C	0.435
9	A:56:LYS:HD2	A:67:ILE:HD11	0.433
9	A:197:ASN:HA	A:198:PRO:C	0.427
9	A:78:LYS:CB	C:2:NAG:C	0.422
9	A:48:LEU:HD12	A:87:LEU:HG	0.421
9	A:141:ILE:CD1	C:10:MAN:H4	0.416
9	A:75:PRO:O	C:2:NAG:CT	0.414
9	A:187:GLU:CD	B:7:MAN:C6	0.412
9	A:22:HIS:NE2	D:5:MAN:O2	0.412
9	A:93:ILE:O	A:95:PRO:HD3	0.411
9	A:120:GLU:C	E:2:NAG:O	0.411
10	A:78:LYS:HB2	C:2:NAG:C1	1.408
10	A:79:ASN:OD1	C:11:MAN:C6	1.353
10	A:185:ILE:HD11	B:5:MAN:O6	1.278
10	A:79:ASN:OD1	C:11:MAN:O6	1.268
10	A:83:ASN:ND2	C:1:NAG:C1	1.154
10	A:79:ASN:OD1	C:11:MAN:H62	1.126
10	A:185:ILE:HD11	B:5:MAN:C6	1.120
10	A:185:ILE:CD1	B:5:MAN:H62	1.111
10	A:122:GLU:O	E:2:NAG:O3	1.109
10	A:78:LYS:HE2	C:3:BMA:H2	1.069

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:122:GLU:N	E:2:NAG:C	1.041
10	A:185:ILE:CD1	B:5:MAN:C6	0.996
10	A:78:LYS:CE	C:3:BMA:H2	0.979
10	A:78:LYS:CB	C:2:NAG:C1	0.970
10	A:75:PRO:O	C:2:NAG:O3	0.926
10	A:78:LYS:CE	C:3:BMA:C2	0.915
10	A:78:LYS:N	C:2:NAG:N	0.889
10	A:83:ASN:CG	C:1:NAG:C1	0.851
10	A:78:LYS:NZ	C:3:BMA:C2	0.836
10	A:171:ASP:OD2	A:172:PHE:HD2	0.833
10	A:78:LYS:HE2	C:3:BMA:C2	0.823
10	A:83:ASN:HD22	C:1:NAG:C1	0.812
10	A:75:PRO:O	C:2:NAG:O	0.812
10	A:185:ILE:CG1	B:5:MAN:H62	0.801
10	A:185:ILE:CG1	B:5:MAN:C6	0.774
10	A:169:ASN:H	A:169:ASN:HD22	0.765
10	A:169:ASN:HD21	A:172:PHE:HB2	0.763
10	A:122:GLU:H	E:2:NAG:C	0.763
10	A:187:GLU:O	B:2:NAG:O	0.758
10	A:171:ASP:OD2	A:172:PHE:CD2	0.756
10	A:185:ILE:HG13	B:5:MAN:C6	0.746
10	A:78:LYS:H	C:2:NAG:C2	0.737
10	A:187:GLU:N	B:2:NAG:O	0.730

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:185:ILE:CD1	B:5:MAN:O6	0.728
10	A:130:ASN:CG	E:11:MAN:O3	0.724
10	A:185:ILE:HG13	B:5:MAN:H62	0.709
10	A:185:ILE:HD11	B:5:MAN:HO6	0.709
10	A:168:LEU:HB2	A:172:PHE:O	0.691
10	A:78:LYS:HZ3	C:3:BMA:C2	0.675
10	A:169:ASN:N	A:169:ASN:ND2	0.674
10	A:169:ASN:H	A:169:ASN:ND2	0.671
10	A:75:PRO:C	C:2:NAG:O	0.641
10	A:79:ASN:CG	C:11:MAN:H62	0.640
10	A:83:ASN:HB2	C:1:NAG:C1	0.635
10	A:75:PRO:C	C:2:NAG:C	0.623
10	A:78:LYS:NZ	C:3:BMA:H2	0.612
10	A:11:ASN:HB3	A:12:PRO:HD3	0.610
10	A:185:ILE:HD12	B:5:MAN:H62	0.596
10	A:79:ASN:HD22	A:80:ASN:H	0.592
10	A:117:LEU:HB3	A:118:PRO:HD3	0.591
10	A:129:PRO:HD2	E:10:MAN:O6	0.590
10	A:130:ASN:ND2	E:11:MAN:O3	0.586
10	A:83:ASN:CB	C:1:NAG:C1	0.582
10	A:78:LYS:HB2	C:2:NAG:C2	0.573
10	A:61:ASN:HB3	A:63:GLN:HG3	0.560
10	A:131:SER:O	E:11:MAN:C6	0.560

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:124:CYS:SG	E:5:MAN:H61	0.554
10	A:158:THR:HG22	A:161:ARG:NH2	0.547
10	A:78:LYS:HZ3	C:3:BMA:H2	0.539
10	A:29:THR:HG22	A:63:GLN:HG2	0.536
10	A:122:GLU:N	E:2:NAG:CT	0.536
10	A:78:LYS:H	C:2:NAG:C1	0.504
10	A:169:ASN:N	A:169:ASN:HD22	0.499
10	A:131:SER:O	E:11:MAN:H61	0.498
10	A:75:PRO:C	C:2:NAG:O3	0.489
10	A:93:ILE:HB	A:94:PRO:HD3	0.477
10	A:187:GLU:O	B:2:NAG:CT	0.463
10	A:187:GLU:C	B:2:NAG:O	0.457
10	A:198:PRO:HA	A:199:PRO:HD3	0.457
10	A:185:ILE:HG13	B:5:MAN:H61	0.447
10	A:187:GLU:O	B:2:NAG:C	0.446
10	A:78:LYS:NZ	C:3:BMA:O2	0.444
10	A:11:ASN:CB	A:12:PRO:HD3	0.441
10	A:185:ILE:O	B:2:NAG:H4	0.438
10	A:155:SER:HA	A:156:PRO:C	0.435
10	A:56:LYS:HD2	A:67:ILE:HD11	0.433
10	A:75:PRO:O	C:2:NAG:C	0.432
10	A:197:ASN:HA	A:198:PRO:C	0.427
10	A:129:PRO:CD	E:10:MAN:O6	0.423

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:48:LEU:HD12	A:87:LEU:HG	0.421
10	A:78:LYS:N	C:2:NAG:C2	0.417
10	A:78:LYS:CA	C:2:NAG:C3	0.411
10	A:93:ILE:O	A:95:PRO:HD3	0.411
10	A:123:THR:CG2	E:2:NAG:H3	0.410
11	A:185:ILE:CD1	B:11:MAN:H62	1.136
11	A:185:ILE:HD12	B:11:MAN:H62	1.133
11	A:185:ILE:CD1	B:11:MAN:O4	1.084
11	A:126:THR:HG21	E:11:MAN:H4	1.060
11	A:103:GLN:CD	C:1:NAG:H3	1.049
11	A:185:ILE:HD11	B:11:MAN:O4	1.047
11	A:133:ASN:O	E:1:NAG:O6	1.034
11	A:126:THR:HG21	E:11:MAN:C4	1.023
11	A:126:THR:CG2	E:11:MAN:H4	1.023
11	A:185:ILE:HD12	B:11:MAN:C6	0.897
11	A:185:ILE:HD13	B:11:MAN:O4	0.879
11	A:171:ASP:OD2	A:172:PHE:HD2	0.833
11	A:103:GLN:NE2	C:1:NAG:H3	0.817
11	A:128:GLU:CD	E:11:MAN:O2	0.812
11	A:169:ASN:H	A:169:ASN:HD22	0.765
11	A:169:ASN:HD21	A:172:PHE:HB2	0.763
11	A:171:ASP:OD2	A:172:PHE:CD2	0.756
11	A:185:ILE:CD1	B:11:MAN:C6	0.734

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:126:THR:HG1	E:11:MAN:C4	0.733
11	A:168:LEU:HB2	A:172:PHE:O	0.691
11	A:103:GLN:OE1	C:1:NAG:H3	0.690
11	A:169:ASN:N	A:169:ASN:ND2	0.674
11	A:169:ASN:H	A:169:ASN:ND2	0.671
11	A:128:GLU:CD	E:11:MAN:HO2	0.649
11	A:126:THR:CB	E:11:MAN:H4	0.640
11	A:11:ASN:HB3	A:12:PRO:HD3	0.610
11	A:79:ASN:HD22	A:80:ASN:H	0.592
11	A:117:LEU:HB3	A:118:PRO:HD3	0.591
11	A:128:GLU:CG	E:11:MAN:O2	0.586
11	A:61:ASN:HB3	A:63:GLN:HG3	0.560
11	A:158:THR:HG22	A:161:ARG:NH2	0.547
11	A:185:ILE:HD13	B:11:MAN:H62	0.539
11	A:29:THR:HG22	A:63:GLN:HG2	0.536
11	A:169:ASN:N	A:169:ASN:HD22	0.499
11	A:126:THR:CG2	E:11:MAN:C4	0.491
11	A:126:THR:OG1	E:11:MAN:O4	0.488
11	A:103:GLN:OE1	C:1:NAG:C3	0.480
11	A:93:ILE:HB	A:94:PRO:HD3	0.477
11	A:128:GLU:HB2	E:11:MAN:HO2	0.469
11	A:198:PRO:HA	A:199:PRO:HD3	0.457
11	A:128:GLU:HB2	E:11:MAN:O2	0.455

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:128:GLU:OE1	E:11:MAN:O5	0.444
11	A:11:ASN:CB	A:12:PRO:HD3	0.441
11	A:155:SER:HA	A:156:PRO:C	0.435
11	A:128:GLU:OE1	E:11:MAN:C1	0.434
11	A:56:LYS:HD2	A:67:ILE:HD11	0.433
11	A:185:ILE:CD1	B:11:MAN:C5	0.431
11	A:197:ASN:HA	A:198:PRO:C	0.427
11	A:126:THR:CB	E:11:MAN:C4	0.422
11	A:48:LEU:HD12	A:87:LEU:HG	0.421
11	A:93:ILE:O	A:95:PRO:HD3	0.411
11	A:128:GLU:CD	E:11:MAN:C1	0.406
11	A:126:THR:HG21	E:11:MAN:C3	0.401
12	A:211:CYS:SG	E:11:MAN:H4	1.424
12	A:211:CYS:SG	E:11:MAN:C4	1.364
12	A:118:PRO:HB3	E:2:NAG:C	1.195
12	A:211:CYS:HG	E:11:MAN:C4	1.139
12	A:211:CYS:SG	E:11:MAN:C6	0.985
12	A:118:PRO:CB	E:2:NAG:C	0.979
12	A:118:PRO:CB	E:2:NAG:CT	0.957
12	A:118:PRO:HB3	E:2:NAG:O	0.947
12	A:118:PRO:HB2	E:2:NAG:CT	0.920
12	A:198:PRO:HD3	D:11:MAN:H61	0.916
12	A:83:ASN:ND2	C:1:NAG:N	0.915

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:211:CYS:SG	E:11:MAN:H61	0.905
12	A:158:THR:HB	B:1:NAG:O6	0.877
12	A:197:ASN:OD1	D:11:MAN:O2	0.866
12	A:118:PRO:HA	E:2:NAG:O	0.860
12	A:171:ASP:OD2	A:172:PHE:HD2	0.833
12	A:118:PRO:CA	E:2:NAG:O	0.808
12	A:118:PRO:CB	E:2:NAG:O	0.771
12	A:169:ASN:H	A:169:ASN:HD22	0.765
12	A:169:ASN:HD21	A:172:PHE:HB2	0.763
12	A:171:ASP:OD2	A:172:PHE:CD2	0.756
12	A:83:ASN:OD1	C:1:NAG:H3	0.739
12	A:211:CYS:CB	E:11:MAN:H4	0.723
12	A:211:CYS:SG	E:11:MAN:H62	0.693
12	A:168:LEU:HB2	A:172:PHE:O	0.691
12	A:169:ASN:N	A:169:ASN:ND2	0.674
12	A:169:ASN:H	A:169:ASN:ND2	0.671
12	A:211:CYS:SG	E:11:MAN:O4	0.670
12	A:211:CYS:SG	E:11:MAN:C5	0.662
12	A:197:ASN:O	D:11:MAN:H61	0.649
12	A:11:ASN:HB3	A:12:PRO:HD3	0.610
12	A:211:CYS:HG	E:11:MAN:HO4	0.601
12	A:79:ASN:HD22	A:80:ASN:H	0.592
12	A:117:LEU:HB3	A:118:PRO:HD3	0.591

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:83:ASN:OD1	C:1:NAG:C3	0.580
12	A:61:ASN:HB3	A:63:GLN:HG3	0.560
12	A:158:THR:HG22	A:161:ARG:NH2	0.547
12	A:118:PRO:C	E:2:NAG:CT	0.545
12	A:29:THR:HG22	A:63:GLN:HG2	0.536
12	A:198:PRO:CD	D:11:MAN:H61	0.519
12	A:197:ASN:O	D:11:MAN:C6	0.514
12	A:198:PRO:HD3	D:11:MAN:C6	0.501
12	A:169:ASN:N	A:169:ASN:HD22	0.499
12	A:133:ASN:O	E:1:NAG:O6	0.495
12	A:211:CYS:CB	E:11:MAN:HO4	0.481
12	A:93:ILE:HB	A:94:PRO:HD3	0.477
12	A:118:PRO:CA	E:2:NAG:C	0.466
12	A:198:PRO:HA	A:199:PRO:HD3	0.457
12	A:83:ASN:OD1	C:1:NAG:N	0.449
12	A:118:PRO:O	E:2:NAG:CT	0.448
12	A:11:ASN:CB	A:12:PRO:HD3	0.441
12	A:103:GLN:NE2	C:1:NAG:H3	0.441
12	A:211:CYS:HB2	E:11:MAN:H4	0.440
12	A:155:SER:HA	A:156:PRO:C	0.435
12	A:118:PRO:CA	E:2:NAG:CT	0.435
12	A:56:LYS:HD2	A:67:ILE:HD11	0.433
12	A:200:LYS:HZ1	D:2:NAG:CT	0.432

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:197:ASN:HA	A:198:PRO:C	0.427
12	A:200:LYS:NZ	D:2:NAG:CT	0.427
12	A:48:LEU:HD12	A:87:LEU:HG	0.421
12	A:93:ILE:O	A:95:PRO:HD3	0.411
13	A:78:LYS:HZ1	C:7:MAN:C1	1.486
13	A:78:LYS:NZ	C:7:MAN:C1	1.431
13	A:51:PRO:HG2	C:1:NAG:C6	1.386
13	A:158:THR:OG1	B:1:NAG:O6	1.243
13	A:207:ARG:NH2	B:10:MAN:O6	1.163
13	A:187:GLU:OE2	B:3:BMA:H62	1.162
13	A:51:PRO:HG2	C:1:NAG:O6	1.144
13	A:51:PRO:CG	C:1:NAG:C6	1.117
13	A:78:LYS:NZ	C:7:MAN:C2	1.110
13	A:126:THR:HG23	E:11:MAN:H4	1.092
13	A:51:PRO:CG	C:1:NAG:H61	1.084
13	A:126:THR:CG2	E:11:MAN:O5	1.079
13	A:126:THR:HG21	E:11:MAN:O5	1.051
13	A:78:LYS:NZ	C:7:MAN:O2	1.047
13	A:51:PRO:HG2	C:1:NAG:H61	1.037
13	A:126:THR:CG2	E:11:MAN:H4	1.028
13	A:200:LYS:HZ3	D:2:NAG:CT	1.002
13	A:78:LYS:HZ2	C:7:MAN:C1	0.924
13	A:207:ARG:NH2	B:10:MAN:C6	0.909

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	A:126:THR:HG23	E:11:MAN:C4	0.896
13	A:75:PRO:HG3	C:11:MAN:C1	0.894
13	A:78:LYS:NZ	C:7:MAN:O5	0.891
13	A:200:LYS:NZ	D:2:NAG:CT	0.889
13	A:126:THR:HG21	E:11:MAN:C1	0.880
13	A:207:ARG:CZ	B:10:MAN:H62	0.862
13	A:171:ASP:OD2	A:172:PHE:HD2	0.833
13	A:120:GLU:O	E:2:NAG:CT	0.821
13	A:78:LYS:HZ1	C:7:MAN:C2	0.813
13	A:158:THR:OG1	B:1:NAG:C6	0.787
13	A:207:ARG:CZ	B:10:MAN:C6	0.782
13	A:169:ASN:H	A:169:ASN:HD22	0.765
13	A:169:ASN:HD21	A:172:PHE:HB2	0.763
13	A:51:PRO:HG3	C:1:NAG:H61	0.756
13	A:171:ASP:OD2	A:172:PHE:CD2	0.756
13	A:207:ARG:CZ	B:10:MAN:O6	0.724
13	A:126:THR:CG2	E:11:MAN:C4	0.717
13	A:187:GLU:HG3	B:2:NAG:O	0.696
13	A:187:GLU:OE2	B:3:BMA:C6	0.696
13	A:168:LEU:HB2	A:172:PHE:O	0.691
13	A:169:ASN:N	A:169:ASN:ND2	0.674
13	A:169:ASN:H	A:169:ASN:ND2	0.671
13	A:75:PRO:HG3	C:11:MAN:O5	0.657

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	A:187:GLU:CG	B:2:NAG:O3	0.633
13	A:11:ASN:HB3	A:12:PRO:HD3	0.610
13	A:79:ASN:HD22	A:80:ASN:H	0.592
13	A:117:LEU:HB3	A:118:PRO:HD3	0.591
13	A:187:GLU:CD	B:3:BMA:H62	0.582
13	A:78:LYS:CE	C:7:MAN:O5	0.572
13	A:61:ASN:HB3	A:63:GLN:HG3	0.560
13	A:158:THR:HG22	A:161:ARG:NH2	0.547
13	A:126:THR:HG21	E:11:MAN:C2	0.546
13	A:75:PRO:CG	C:11:MAN:O5	0.545
13	A:29:THR:HG22	A:63:GLN:HG2	0.536
13	A:51:PRO:CD	C:1:NAG:H62	0.535
13	A:207:ARG:NE	B:10:MAN:O6	0.524
13	A:51:PRO:CD	C:1:NAG:C6	0.519
13	A:207:ARG:NE	B:10:MAN:C6	0.518
13	A:187:GLU:OE1	B:2:NAG:O3	0.514
13	A:158:THR:CB	B:1:NAG:O6	0.506
13	A:169:ASN:N	A:169:ASN:HD22	0.499
13	A:207:ARG:NE	B:10:MAN:H62	0.498
13	A:187:GLU:CD	B:2:NAG:O3	0.485
13	A:93:ILE:HB	A:94:PRO:HD3	0.477
13	A:126:THR:CG2	E:11:MAN:O2	0.470
13	A:187:GLU:HG3	B:2:NAG:O3	0.466

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	A:78:LYS:HZ2	C:7:MAN:C2	0.463
13	A:198:PRO:HA	A:199:PRO:HD3	0.457
13	A:51:PRO:CG	C:1:NAG:H62	0.445
13	A:11:ASN:CB	A:12:PRO:HD3	0.441
13	A:158:THR:OG1	B:1:NAG:H62	0.437
13	A:155:SER:HA	A:156:PRO:C	0.435
13	A:56:LYS:HD2	A:67:ILE:HD11	0.433
13	A:197:ASN:HA	A:198:PRO:C	0.427
13	A:48:LEU:HD12	A:87:LEU:HG	0.421
13	A:93:ILE:O	A:95:PRO:HD3	0.411
14	A:185:ILE:CG2	B:3:BMA:H61	1.568
14	A:207:ARG:CG	B:11:MAN:H5	1.561
14	A:207:ARG:HG2	B:11:MAN:C5	1.437
14	A:185:ILE:CG2	B:3:BMA:C6	1.346
14	A:207:ARG:HG3	B:10:MAN:C1	1.323
14	A:185:ILE:HG22	B:3:BMA:C6	1.321
14	A:207:ARG:HG3	B:10:MAN:C2	1.272
14	A:205:ILE:O	B:11:MAN:C6	1.247
14	A:207:ARG:CG	B:10:MAN:C1	1.183
14	A:187:GLU:CB	B:7:MAN:H2	1.177
14	A:187:GLU:HB3	B:7:MAN:H2	1.129
14	A:120:GLU:HA	B:11:MAN:C3	1.116
14	A:185:ILE:HB	B:3:BMA:C5	1.104

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:185:ILE:HG22	B:3:BMA:H62	1.084
14	A:120:GLU:CG	B:11:MAN:H2	1.075
14	A:120:GLU:HA	B:11:MAN:O3	1.058
14	A:205:ILE:O	B:11:MAN:H62	1.055
14	A:185:ILE:HB	B:3:BMA:H5	1.035
14	A:78:LYS:N	C:2:NAG:CT	1.023
14	A:185:ILE:HG21	B:3:BMA:H61	1.005
14	A:207:ARG:CD	B:7:MAN:O5	0.999
14	A:120:GLU:CA	B:11:MAN:O3	0.990
14	A:207:ARG:CB	B:11:MAN:H5	0.989
14	A:187:GLU:OE2	B:8:MAN:O5	0.987
14	A:187:GLU:N	B:2:NAG:O3	0.987
14	A:130:ASN:HB3	E:1:NAG:CT	0.984
14	A:187:GLU:HB3	B:7:MAN:C2	0.966
14	A:187:GLU:HB2	B:8:MAN:H5	0.928
14	A:207:ARG:HB2	B:11:MAN:H3	0.926
14	A:207:ARG:CG	B:11:MAN:C5	0.917
14	A:205:ILE:O	B:11:MAN:H61	0.902
14	A:187:GLU:HB2	B:8:MAN:C5	0.876
14	A:74:SER:O	C:2:NAG:CT	0.871
14	A:120:GLU:HG2	B:11:MAN:H2	0.864
14	A:207:ARG:HG3	B:10:MAN:H2	0.862
14	A:78:LYS:HB2	C:2:NAG:C1	0.860

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:205:ILE:C	B:11:MAN:H62	0.847
14	A:187:GLU:CD	B:8:MAN:O5	0.845
14	A:130:ASN:OD1	E:1:NAG:C	0.843
14	A:185:ILE:CB	B:3:BMA:C6	0.838
14	A:171:ASP:OD2	A:172:PHE:HD2	0.833
14	A:185:ILE:CB	B:3:BMA:H5	0.822
14	A:120:GLU:CD	B:10:MAN:H4	0.813
14	A:119:GLN:HG2	B:11:MAN:C1	0.798
14	A:187:GLU:HB2	B:7:MAN:H2	0.789
14	A:187:GLU:O	B:2:NAG:CT	0.786
14	A:131:SER:O	E:1:NAG:H61	0.783
14	A:119:GLN:HG2	B:11:MAN:O5	0.782
14	A:207:ARG:HD2	B:7:MAN:O5	0.779
14	A:169:ASN:H	A:169:ASN:HD22	0.765
14	A:169:ASN:HD21	A:172:PHE:HB2	0.763
14	A:207:ARG:CD	B:10:MAN:C1	0.762
14	A:171:ASP:OD2	A:172:PHE:CD2	0.756
14	A:78:LYS:N	C:2:NAG:N	0.743
14	A:185:ILE:HB	B:3:BMA:C6	0.735
14	A:120:GLU:CG	B:11:MAN:C2	0.707
14	A:120:GLU:HG2	B:11:MAN:C2	0.706
14	A:187:GLU:HB3	B:7:MAN:C1	0.704
14	A:168:LEU:HB2	A:172:PHE:O	0.691

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:207:ARG:CB	B:10:MAN:C1	0.682
14	A:207:ARG:HG2	B:11:MAN:C6	0.682
14	A:169:ASN:N	A:169:ASN:ND2	0.674
14	A:185:ILE:CB	B:3:BMA:H61	0.672
14	A:169:ASN:H	A:169:ASN:ND2	0.671
14	A:78:LYS:HB2	C:2:NAG:N	0.670
14	A:75:PRO:O	C:2:NAG:O3	0.670
14	A:78:LYS:CB	C:2:NAG:N	0.666
14	A:187:GLU:C	B:2:NAG:CT	0.666
14	A:207:ARG:HG2	B:11:MAN:H5	0.662
14	A:130:ASN:CB	E:1:NAG:CT	0.651
14	A:78:LYS:N	C:2:NAG:C	0.646
14	A:11:ASN:HB3	A:12:PRO:HD3	0.610
14	A:120:GLU:CD	B:10:MAN:C4	0.609
14	A:185:ILE:CB	B:3:BMA:C5	0.592
14	A:79:ASN:HD22	A:80:ASN:H	0.592
14	A:117:LEU:HB3	A:118:PRO:HD3	0.591
14	A:78:LYS:HG3	C:3:BMA:H62	0.588
14	A:207:ARG:CG	B:10:MAN:C2	0.588
14	A:78:LYS:HD2	C:2:NAG:C	0.573
14	A:61:ASN:HB3	A:63:GLN:HG3	0.560
14	A:158:THR:HG22	A:161:ARG:NH2	0.547
14	A:29:THR:HG22	A:63:GLN:HG2	0.536

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:207:ARG:CB	B:11:MAN:C5	0.534
14	A:187:GLU:HB3	B:3:BMA:O6	0.513
14	A:185:ILE:CG2	B:3:BMA:H62	0.512
14	A:199:PRO:O	D:1:NAG:H61	0.510
14	A:169:ASN:N	A:169:ASN:HD22	0.499
14	A:207:ARG:HD2	B:10:MAN:C1	0.492
14	A:78:LYS:HB2	C:2:NAG:C2	0.481
14	A:120:GLU:C	B:11:MAN:O3	0.481
14	A:187:GLU:N	B:2:NAG:C	0.479
14	A:93:ILE:HB	A:94:PRO:HD3	0.477
14	A:207:ARG:NH2	B:8:MAN:H2	0.476
14	A:78:LYS:HE2	C:3:BMA:H5	0.473
14	A:207:ARG:HG3	B:10:MAN:O2	0.472
14	A:187:GLU:OE2	B:8:MAN:C1	0.471
14	A:198:PRO:HA	A:199:PRO:HD3	0.457
14	A:130:ASN:OD1	E:1:NAG:CT	0.453
14	A:78:LYS:CA	C:2:NAG:N	0.449
14	A:11:ASN:CB	A:12:PRO:HD3	0.441
14	A:155:SER:HA	A:156:PRO:C	0.435
14	A:187:GLU:HG2	B:2:NAG:O3	0.434
14	A:56:LYS:HD2	A:67:ILE:HD11	0.433
14	A:78:LYS:CG	C:3:BMA:H62	0.430
14	A:197:ASN:HA	A:198:PRO:C	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:207:ARG:CA	B:7:MAN:O2	0.424
14	A:120:GLU:N	B:11:MAN:O3	0.424
14	A:48:LEU:HD12	A:87:LEU:HG	0.421
14	A:120:GLU:HA	B:11:MAN:H3	0.417
14	A:207:ARG:HB2	B:11:MAN:C3	0.416
14	A:78:LYS:N	C:1:NAG:O6	0.416
14	A:130:ASN:CG	E:1:NAG:CT	0.413
14	A:93:ILE:O	A:95:PRO:HD3	0.411
14	A:78:LYS:H	C:2:NAG:C	0.410
14	A:207:ARG:CB	B:11:MAN:H3	0.405
15	A:187:GLU:OE2	B:7:MAN:H2	1.266
15	A:187:GLU:OE1	B:8:MAN:C6	1.195
15	A:207:ARG:NH1	B:7:MAN:O2	1.193
15	A:187:GLU:OE1	B:8:MAN:O6	1.127
15	A:187:GLU:OE2	B:7:MAN:C2	1.075
15	A:83:ASN:CG	C:1:NAG:C1	1.031
15	A:187:GLU:HG2	B:2:NAG:O3	1.007
15	A:199:PRO:O	D:1:NAG:C6	0.993
15	A:199:PRO:O	D:1:NAG:H61	0.935
15	A:130:ASN:ND2	E:1:NAG:C1	0.918
15	A:187:GLU:OE1	B:8:MAN:H62	0.891
15	A:187:GLU:HG2	B:2:NAG:HO3	0.887
15	A:187:GLU:CG	B:2:NAG:O3	0.838

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	A:171:ASP:OD2	A:172:PHE:HD2	0.833
15	A:169:ASN:H	A:169:ASN:HD22	0.765
15	A:169:ASN:HD21	A:172:PHE:HB2	0.763
15	A:187:GLU:N	B:2:NAG:O3	0.762
15	A:171:ASP:OD2	A:172:PHE:CD2	0.756
15	A:131:SER:O	E:1:NAG:C6	0.756
15	A:131:SER:O	E:1:NAG:O6	0.727
15	A:83:ASN:OD1	C:1:NAG:C1	0.712
15	A:131:SER:O	E:1:NAG:H61	0.711
15	A:130:ASN:HD21	E:1:NAG:C1	0.708
15	A:130:ASN:O	E:1:NAG:H4	0.702
15	A:168:LEU:HB2	A:172:PHE:O	0.691
15	A:169:ASN:N	A:169:ASN:ND2	0.674
15	A:169:ASN:H	A:169:ASN:ND2	0.671
15	A:205:ILE:HD11	B:8:MAN:O4	0.625
15	A:11:ASN:HB3	A:12:PRO:HD3	0.610
15	A:199:PRO:O	D:1:NAG:O6	0.610
15	A:79:ASN:HD22	A:80:ASN:H	0.592
15	A:117:LEU:HB3	A:118:PRO:HD3	0.591
15	A:205:ILE:CD1	B:8:MAN:O4	0.572
15	A:61:ASN:HB3	A:63:GLN:HG3	0.560
15	A:187:GLU:OE1	B:8:MAN:C5	0.559
15	A:158:THR:HG22	A:161:ARG:NH2	0.547

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	A:29:THR:HG22	A:63:GLN:HG2	0.536
15	A:207:ARG:CZ	B:7:MAN:O2	0.517
15	A:83:ASN:ND2	C:1:NAG:C1	0.515
15	A:169:ASN:N	A:169:ASN:HD22	0.499
15	A:200:LYS:HA	D:1:NAG:HO6	0.481
15	A:93:ILE:HB	A:94:PRO:HD3	0.477
15	A:187:GLU:CD	B:7:MAN:H2	0.467
15	A:198:PRO:HA	A:199:PRO:HD3	0.457
15	A:207:ARG:HH12	B:7:MAN:HO2	0.453
15	A:11:ASN:CB	A:12:PRO:HD3	0.441
15	A:155:SER:HA	A:156:PRO:C	0.435
15	A:56:LYS:HD2	A:67:ILE:HD11	0.433
15	A:199:PRO:O	D:1:NAG:C5	0.431
15	A:197:ASN:HA	A:198:PRO:C	0.427
15	A:48:LEU:HD12	A:87:LEU:HG	0.421
15	A:187:GLU:OE2	B:7:MAN:O2	0.412
15	A:93:ILE:O	A:95:PRO:HD3	0.411
16	A:78:LYS:HB2	C:2:NAG:C2	1.275
16	A:78:LYS:HZ3	C:3:BMA:H2	1.094
16	A:78:LYS:HB2	C:2:NAG:N	1.044
16	A:83:ASN:ND2	C:1:NAG:C1	1.042
16	A:133:ASN:ND2	E:1:NAG:C1	1.021
16	A:78:LYS:HB2	C:2:NAG:C3	1.016

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	A:78:LYS:HG2	C:3:BMA:C1	1.004
16	A:78:LYS:N	C:2:NAG:N	0.995
16	A:78:LYS:NZ	C:3:BMA:H2	0.985
16	A:78:LYS:CB	C:2:NAG:C3	0.953
16	A:78:LYS:CB	C:2:NAG:H3	0.950
16	A:83:ASN:CG	C:1:NAG:C1	0.918
16	A:75:PRO:C	C:2:NAG:CT	0.870
16	A:78:LYS:HB2	C:2:NAG:C1	0.864
16	A:171:ASP:OD2	A:172:PHE:HD2	0.833
16	A:78:LYS:CB	C:2:NAG:N	0.817
16	A:78:LYS:N	C:2:NAG:CT	0.816
16	A:181:PHE:N	B:1:NAG:O	0.805
16	A:78:LYS:HZ3	C:3:BMA:C2	0.800
16	A:169:ASN:H	A:169:ASN:HD22	0.765
16	A:169:ASN:HD21	A:172:PHE:HB2	0.763
16	A:182:GLU:N	B:2:NAG:HO6	0.763
16	A:78:LYS:H	C:2:NAG:C	0.758
16	A:171:ASP:OD2	A:172:PHE:CD2	0.756
16	A:133:ASN:CG	E:1:NAG:C1	0.739
16	A:83:ASN:HB2	C:1:NAG:C1	0.700
16	A:168:LEU:HB2	A:172:PHE:O	0.691
16	A:182:GLU:N	B:2:NAG:O6	0.679
16	A:169:ASN:N	A:169:ASN:ND2	0.674

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	A:169:ASN:H	A:169:ASN:ND2	0.671
16	A:83:ASN:CB	C:1:NAG:C1	0.661
16	A:78:LYS:NZ	C:3:BMA:C2	0.659
16	A:181:PHE:CB	B:1:NAG:O	0.640
16	A:11:ASN:HB3	A:12:PRO:HD3	0.610
16	A:78:LYS:N	C:2:NAG:C	0.608
16	A:83:ASN:HD22	C:1:NAG:C1	0.601
16	A:79:ASN:HD22	A:80:ASN:H	0.592
16	A:117:LEU:HB3	A:118:PRO:HD3	0.591
16	A:61:ASN:HB3	A:63:GLN:HG3	0.560
16	A:78:LYS:CA	C:2:NAG:N	0.556
16	A:158:THR:HG22	A:161:ARG:NH2	0.547
16	A:29:THR:HG22	A:63:GLN:HG2	0.536
16	A:83:ASN:ND2	C:1:NAG:O5	0.534
16	A:181:PHE:CB	B:1:NAG:C	0.529
16	A:78:LYS:HE2	C:5:MAN:O6	0.501
16	A:181:PHE:CA	B:1:NAG:O	0.499
16	A:169:ASN:N	A:169:ASN:HD22	0.499
16	A:133:ASN:ND2	E:1:NAG:O5	0.490
16	A:93:ILE:HB	A:94:PRO:HD3	0.477
16	A:198:PRO:HA	A:199:PRO:HD3	0.457
16	A:11:ASN:CB	A:12:PRO:HD3	0.441
16	A:155:SER:HA	A:156:PRO:C	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	A:56:LYS:HD2	A:67:ILE:HD11	0.433
16	A:78:LYS:HZ2	C:3:BMA:C1	0.431
16	A:197:ASN:HA	A:198:PRO:C	0.427
16	A:78:LYS:HG2	C:2:NAG:C4	0.424
16	A:48:LEU:HD12	A:87:LEU:HG	0.421
16	A:93:ILE:O	A:95:PRO:HD3	0.411
16	A:78:LYS:NZ	C:3:BMA:C1	0.402
17	A:78:LYS:NZ	C:3:BMA:C1	1.417
17	A:78:LYS:HZ2	C:3:BMA:C1	1.412
17	A:78:LYS:HD3	C:2:NAG:C3	1.406
17	A:78:LYS:CD	C:2:NAG:H3	1.285
17	A:154:LEU:HD11	D:8:MAN:C4	1.138
17	A:78:LYS:NZ	C:3:BMA:H5	1.134
17	A:154:LEU:CD1	D:8:MAN:H4	1.124
17	A:78:LYS:CG	C:3:BMA:H62	1.113
17	A:78:LYS:HG2	C:3:BMA:H62	1.078
17	A:78:LYS:NZ	C:3:BMA:C5	1.056
17	A:78:LYS:HZ2	C:3:BMA:C5	0.977
17	A:78:LYS:HG2	C:3:BMA:C6	0.946
17	A:154:LEU:HD11	D:8:MAN:H4	0.944
17	A:78:LYS:HD3	C:2:NAG:C2	0.908
17	A:78:LYS:HD3	C:2:NAG:H3	0.905
17	A:78:LYS:HZ3	C:3:BMA:H5	0.888

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:78:LYS:HZ1	C:3:BMA:C1	0.868
17	A:78:LYS:CG	C:3:BMA:C6	0.851
17	A:171:ASP:OD2	A:172:PHE:HD2	0.833
17	A:78:LYS:CE	C:3:BMA:H5	0.797
17	A:78:LYS:CD	C:2:NAG:C3	0.793
17	A:169:ASN:H	A:169:ASN:HD22	0.765
17	A:169:ASN:HD21	A:172:PHE:HB2	0.763
17	A:171:ASP:OD2	A:172:PHE:CD2	0.756
17	A:78:LYS:HG2	C:3:BMA:C5	0.729
17	A:156:PRO:HG3	B:2:NAG:CT	0.718
17	A:78:LYS:HG3	C:3:BMA:H62	0.715
17	A:168:LEU:HB2	A:172:PHE:O	0.691
17	A:169:ASN:N	A:169:ASN:ND2	0.674
17	A:169:ASN:H	A:169:ASN:ND2	0.671
17	A:78:LYS:HB2	C:2:NAG:C1	0.658
17	A:78:LYS:CE	C:2:NAG:H3	0.638
17	A:78:LYS:HG3	C:3:BMA:C6	0.626
17	A:11:ASN:HB3	A:12:PRO:HD3	0.610
17	A:78:LYS:HZ3	C:3:BMA:C5	0.599
17	A:79:ASN:HD22	A:80:ASN:H	0.592
17	A:117:LEU:HB3	A:118:PRO:HD3	0.591
17	A:78:LYS:HZ3	C:3:BMA:C1	0.589
17	A:78:LYS:CG	C:3:BMA:C5	0.583

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:78:LYS:CG	C:2:NAG:H3	0.575
17	A:61:ASN:HB3	A:63:GLN:HG3	0.560
17	A:78:LYS:HG2	C:3:BMA:O5	0.559
17	A:158:THR:HG22	A:161:ARG:NH2	0.547
17	A:154:LEU:HD11	D:8:MAN:O4	0.546
17	A:29:THR:HG22	A:63:GLN:HG2	0.536
17	A:169:ASN:N	A:169:ASN:HD22	0.499
17	A:156:PRO:CG	B:2:NAG:CT	0.490
17	A:93:ILE:HB	A:94:PRO:HD3	0.477
17	A:78:LYS:HD3	C:2:NAG:N	0.473
17	A:198:PRO:HA	A:199:PRO:HD3	0.457
17	A:78:LYS:NZ	C:2:NAG:H3	0.454
17	D:2:NAG:H5	D:3:BMA:O5	0.448
17	A:11:ASN:CB	A:12:PRO:HD3	0.441
17	E:2:NAG:H5	E:3:BMA:O5	0.438
17	A:155:SER:HA	A:156:PRO:C	0.435
17	A:56:LYS:HD2	A:67:ILE:HD11	0.433
17	A:78:LYS:HZ3	C:3:BMA:C3	0.431
17	A:197:ASN:HA	A:198:PRO:C	0.427
17	A:78:LYS:CE	C:2:NAG:C3	0.427
17	A:48:LEU:HD12	A:87:LEU:HG	0.421
17	A:93:ILE:O	A:95:PRO:HD3	0.411
17	A:78:LYS:HE2	C:3:BMA:H5	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:78:LYS:NZ	C:2:NAG:C3	0.400
18	A:129:PRO:CG	E:11:MAN:O6	1.334
18	A:126:THR:CG2	E:10:MAN:O6	1.258
18	A:182:GLU:N	B:2:NAG:O6	1.224
18	A:78:LYS:HD3	C:2:NAG:H3	1.175
18	A:126:THR:HG21	E:10:MAN:O6	1.167
18	A:128:GLU:HG3	E:11:MAN:C5	1.153
18	A:129:PRO:HG2	E:11:MAN:O6	1.153
18	A:129:PRO:CD	E:11:MAN:O6	1.126
18	A:197:ASN:HB3	D:11:MAN:H5	1.113
18	A:128:GLU:CG	E:11:MAN:H5	1.113
18	A:126:THR:HG21	E:10:MAN:C6	1.100
18	A:197:ASN:OD1	D:10:MAN:H4	0.985
18	A:197:ASN:CB	D:11:MAN:H5	0.949
18	A:126:THR:HG21	E:10:MAN:HO6	0.940
18	A:197:ASN:N	D:11:MAN:O4	0.933
18	A:129:PRO:CB	E:11:MAN:O6	0.860
18	A:128:GLU:N	E:11:MAN:O3	0.855
18	A:197:ASN:CG	D:10:MAN:O2	0.840
18	A:128:GLU:CA	E:11:MAN:O3	0.837
18	A:197:ASN:ND2	D:11:MAN:C5	0.835
18	A:171:ASP:OD2	A:172:PHE:HD2	0.833
18	A:197:ASN:HB3	D:11:MAN:C5	0.832

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	A:78:LYS:CD	C:2:NAG:H3	0.816
18	A:128:GLU:HG3	E:11:MAN:H5	0.786
18	A:169:ASN:H	A:169:ASN:HD22	0.765
18	A:169:ASN:HD21	A:172:PHE:HB2	0.763
18	A:171:ASP:OD2	A:172:PHE:CD2	0.756
18	A:182:GLU:HB3	B:4:MAN:O6	0.755
18	A:128:GLU:CG	E:11:MAN:C5	0.753
18	A:129:PRO:HG2	E:11:MAN:HO6	0.745
18	A:197:ASN:ND2	D:11:MAN:H5	0.718
18	A:182:GLU:N	B:2:NAG:C6	0.708
18	A:197:ASN:OD1	D:10:MAN:O6	0.700
18	A:168:LEU:HB2	A:172:PHE:O	0.691
18	A:181:PHE:CB	B:1:NAG:O	0.674
18	A:169:ASN:N	A:169:ASN:ND2	0.674
18	A:169:ASN:H	A:169:ASN:ND2	0.671
18	A:126:THR:CB	E:10:MAN:O6	0.659
18	A:197:ASN:CG	D:11:MAN:H5	0.655
18	A:78:LYS:HG2	C:3:BMA:C6	0.653
18	A:129:PRO:HB2	E:11:MAN:O6	0.652
18	A:183:ALA:O	B:3:BMA:H2	0.645
18	A:182:GLU:CA	B:2:NAG:O6	0.644
18	A:197:ASN:CB	D:11:MAN:C4	0.634
18	A:197:ASN:HB3	D:11:MAN:C4	0.630

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	A:78:LYS:HD2	C:2:NAG:O	0.624
18	A:11:ASN:HB3	A:12:PRO:HD3	0.610
18	A:79:ASN:HD22	A:80:ASN:H	0.592
18	A:117:LEU:HB3	A:118:PRO:HD3	0.591
18	A:78:LYS:CD	C:2:NAG:O	0.588
18	A:78:LYS:HD3	C:2:NAG:C3	0.587
18	A:126:THR:CG2	E:10:MAN:C6	0.580
18	A:197:ASN:HB3	D:11:MAN:O4	0.575
18	A:197:ASN:CB	D:11:MAN:O4	0.571
18	A:182:GLU:CB	B:4:MAN:O6	0.563
18	A:61:ASN:HB3	A:63:GLN:HG3	0.560
18	A:182:GLU:C	B:2:NAG:O6	0.557
18	A:128:GLU:HG3	E:11:MAN:C4	0.556
18	A:158:THR:HG22	A:161:ARG:NH2	0.547
18	A:182:GLU:O	B:2:NAG:O6	0.543
18	A:29:THR:HG22	A:63:GLN:HG2	0.536
18	A:78:LYS:HG2	C:3:BMA:H62	0.536
18	A:128:GLU:CB	E:11:MAN:H3	0.522
18	A:126:THR:CG2	E:10:MAN:H4	0.513
18	A:197:ASN:CA	D:11:MAN:O4	0.511
18	A:197:ASN:OD1	D:10:MAN:C4	0.503
18	A:182:GLU:HB3	B:4:MAN:HO6	0.499
18	A:169:ASN:N	A:169:ASN:HD22	0.499

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	A:197:ASN:H	D:11:MAN:C3	0.485
18	A:93:ILE:HB	A:94:PRO:HD3	0.477
18	A:198:PRO:HA	A:199:PRO:HD3	0.457
18	A:182:GLU:OE1	B:4:MAN:O6	0.457
18	A:11:ASN:CB	A:12:PRO:HD3	0.441
18	A:78:LYS:CE	C:2:NAG:H3	0.436
18	A:126:THR:CG2	E:10:MAN:HO6	0.436
18	A:128:GLU:CG	E:11:MAN:C4	0.435
18	A:155:SER:HA	A:156:PRO:C	0.435
18	A:56:LYS:HD2	A:67:ILE:HD11	0.433
18	A:182:GLU:CB	B:4:MAN:HO6	0.432
18	A:197:ASN:HA	A:198:PRO:C	0.427
18	A:48:LEU:HD12	A:87:LEU:HG	0.421
18	A:197:ASN:H	D:11:MAN:C4	0.419
18	A:93:ILE:O	A:95:PRO:HD3	0.411
19	A:158:THR:CG2	B:2:NAG:C1	1.637
19	A:158:THR:HG21	B:2:NAG:C1	1.633
19	A:158:THR:HB	B:1:NAG:C4	1.531
19	A:156:PRO:HG2	B:2:NAG:CT	1.467
19	A:158:THR:CB	B:2:NAG:C1	1.422
19	A:78:LYS:HB2	C:2:NAG:C1	1.410
19	A:78:LYS:HG2	C:3:BMA:O5	1.271
19	A:78:LYS:CG	C:3:BMA:O5	1.226

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:78:LYS:HG3	C:3:BMA:C5	1.218
19	A:156:PRO:CG	B:2:NAG:CT	1.217
19	A:158:THR:HB	B:1:NAG:H4	1.187
19	A:78:LYS:HB2	C:2:NAG:C2	1.153
19	A:155:SER:HB2	B:8:MAN:H61	1.137
19	A:78:LYS:CG	C:3:BMA:C1	1.120
19	A:158:THR:CB	B:1:NAG:C4	1.109
19	A:78:LYS:HG2	C:3:BMA:C1	1.100
19	A:78:LYS:N	C:2:NAG:N	1.099
19	A:158:THR:HB	B:1:NAG:O4	1.050
19	A:158:THR:CB	B:1:NAG:O4	0.980
19	A:78:LYS:CB	C:2:NAG:C1	0.954
19	A:158:THR:HG21	B:2:NAG:O5	0.950
19	A:158:THR:HB	B:1:NAG:C5	0.947
19	A:78:LYS:HG3	C:3:BMA:H5	0.931
19	A:78:LYS:CG	C:3:BMA:C5	0.924
19	A:158:THR:HG21	B:2:NAG:C5	0.919
19	A:78:LYS:HG2	C:2:NAG:H5	0.846
19	A:78:LYS:CB	C:2:NAG:C2	0.839
19	A:171:ASP:OD2	A:172:PHE:HD2	0.833
19	A:155:SER:HB2	B:8:MAN:C6	0.816
19	A:158:THR:CB	B:1:NAG:H4	0.803
19	A:169:ASN:H	A:169:ASN:HD22	0.765

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:169:ASN:HD21	A:172:PHE:HB2	0.763
19	A:158:THR:CG2	B:2:NAG:C2	0.759
19	A:171:ASP:OD2	A:172:PHE:CD2	0.756
19	A:158:THR:HG21	B:2:NAG:H5	0.755
19	A:158:THR:HG21	B:2:NAG:C2	0.706
19	A:168:LEU:HB2	A:172:PHE:O	0.691
19	A:169:ASN:N	A:169:ASN:ND2	0.674
19	A:169:ASN:H	A:169:ASN:ND2	0.671
19	A:75:PRO:O	C:2:NAG:O3	0.650
19	A:78:LYS:HG3	C:3:BMA:C6	0.639
19	A:78:LYS:HB2	C:2:NAG:N	0.626
19	A:75:PRO:O	C:2:NAG:O	0.624
19	A:156:PRO:HG3	B:2:NAG:CT	0.615
19	A:75:PRO:C	C:2:NAG:C	0.613
19	A:161:ARG:HH21	B:1:NAG:H4	0.612
19	A:11:ASN:HB3	A:12:PRO:HD3	0.610
19	A:158:THR:OG1	B:1:NAG:O4	0.605
19	A:130:ASN:OD1	E:1:NAG:CT	0.599
19	A:78:LYS:CG	C:2:NAG:H5	0.595
19	A:79:ASN:HD22	A:80:ASN:H	0.592
19	A:117:LEU:HB3	A:118:PRO:HD3	0.591
19	A:156:PRO:CB	B:2:NAG:CT	0.574
19	A:158:THR:HB	B:2:NAG:C1	0.567

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:61:ASN:HB3	A:63:GLN:HG3	0.560
19	A:158:THR:HG22	A:161:ARG:NH2	0.547
19	A:83:ASN:HB2	C:1:NAG:C1	0.546
19	A:29:THR:HG22	A:63:GLN:HG2	0.536
19	A:158:THR:CG2	B:2:NAG:H5	0.517
19	A:75:PRO:O	C:2:NAG:C	0.516
19	A:169:ASN:N	A:169:ASN:HD22	0.499
19	A:93:ILE:HB	A:94:PRO:HD3	0.477
19	A:78:LYS:CB	C:2:NAG:N	0.469
19	A:198:PRO:HA	A:199:PRO:HD3	0.457
19	A:158:THR:HG21	B:2:NAG:C3	0.443
19	A:78:LYS:CA	C:2:NAG:N	0.443
19	A:11:ASN:CB	A:12:PRO:HD3	0.441
19	A:155:SER:HA	A:156:PRO:C	0.435
19	A:78:LYS:CB	C:2:NAG:H5	0.434
19	A:56:LYS:HD2	A:67:ILE:HD11	0.433
19	A:78:LYS:CG	C:3:BMA:H62	0.428
19	A:197:ASN:HA	A:198:PRO:C	0.427
19	A:83:ASN:ND2	C:1:NAG:C1	0.425
19	A:48:LEU:HD12	A:87:LEU:HG	0.421
19	A:131:SER:O	E:1:NAG:H61	0.418
19	A:93:ILE:O	A:95:PRO:HD3	0.411
19	A:156:PRO:HB2	B:2:NAG:CT	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:78:LYS:N	C:2:NAG:CT	0.408
19	A:83:ASN:CG	C:1:NAG:C1	0.403
20	A:78:LYS:HZ3	C:3:BMA:C1	1.303
20	A:124:CYS:SG	E:11:MAN:H62	1.253
20	A:124:CYS:HB2	E:11:MAN:C6	1.241
20	A:78:LYS:HB2	C:2:NAG:C1	1.235
20	A:78:LYS:HG3	C:3:BMA:C6	1.204
20	A:22:HIS:NE2	D:6:MAN:H2	1.204
20	A:83:ASN:ND2	C:1:NAG:C1	1.197
20	A:78:LYS:CG	C:3:BMA:H62	1.186
20	A:78:LYS:CD	C:2:NAG:H3	1.168
20	A:78:LYS:HD3	C:2:NAG:C3	1.136
20	A:124:CYS:HB2	E:11:MAN:H61	1.128
20	A:78:LYS:HD3	C:2:NAG:H3	1.099
20	A:78:LYS:HG2	C:3:BMA:O5	1.078
20	A:78:LYS:NZ	C:3:BMA:C1	1.050
20	A:22:HIS:NE2	D:6:MAN:C2	1.003
20	A:124:CYS:CB	E:11:MAN:C6	0.969
20	A:124:CYS:CB	E:11:MAN:H62	0.963
20	A:78:LYS:HG3	C:3:BMA:H62	0.960
20	A:78:LYS:CG	C:2:NAG:H3	0.907
20	A:78:LYS:NZ	C:3:BMA:H5	0.896
20	A:83:ASN:HD22	C:1:NAG:C1	0.889

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	A:79:ASN:CB	C:1:NAG:CT	0.874
20	A:78:LYS:CE	C:3:BMA:H5	0.848
20	A:124:CYS:HB2	E:11:MAN:H62	0.845
20	A:171:ASP:OD2	A:172:PHE:HD2	0.833
20	A:78:LYS:HZ3	C:3:BMA:C5	0.808
20	A:78:LYS:CG	C:3:BMA:C5	0.805
20	A:78:LYS:CG	C:3:BMA:C6	0.785
20	A:124:CYS:SG	E:11:MAN:C6	0.774
20	A:169:ASN:H	A:169:ASN:HD22	0.765
20	A:169:ASN:HD21	A:172:PHE:HB2	0.763
20	A:158:THR:C	B:1:NAG:C6	0.762
20	A:79:ASN:HB2	C:1:NAG:CT	0.760
20	A:118:PRO:HB3	E:2:NAG:O	0.760
20	A:171:ASP:OD2	A:172:PHE:CD2	0.756
20	A:124:CYS:CB	E:11:MAN:H61	0.734
20	A:78:LYS:HG2	C:3:BMA:C5	0.724
20	A:78:LYS:HZ3	C:3:BMA:H5	0.710
20	A:78:LYS:HG3	C:3:BMA:C5	0.707
20	A:78:LYS:CB	C:2:NAG:C1	0.699
20	A:124:CYS:HG	E:11:MAN:H62	0.697
20	A:168:LEU:HB2	A:172:PHE:O	0.691
20	A:78:LYS:HE2	C:3:BMA:H5	0.689
20	A:169:ASN:N	A:169:ASN:ND2	0.674

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	A:169:ASN:H	A:169:ASN:ND2	0.671
20	A:22:HIS:CE1	D:6:MAN:H2	0.664
20	A:78:LYS:CG	C:3:BMA:O5	0.635
20	A:78:LYS:HD3	C:2:NAG:C2	0.623
20	A:78:LYS:HD3	C:2:NAG:N	0.621
20	A:79:ASN:HB3	C:1:NAG:CT	0.620
20	A:11:ASN:HB3	A:12:PRO:HD3	0.610
20	A:78:LYS:HG2	C:2:NAG:H3	0.592
20	A:79:ASN:HD22	A:80:ASN:H	0.592
20	A:117:LEU:HB3	A:118:PRO:HD3	0.591
20	A:83:ASN:CG	C:1:NAG:C1	0.588
20	A:141:ILE:HG23	C:11:MAN:H61	0.579
20	A:187:GLU:O	B:2:NAG:O	0.575
20	A:61:ASN:HB3	A:63:GLN:HG3	0.560
20	A:158:THR:HG22	A:161:ARG:NH2	0.547
20	A:29:THR:HG22	A:63:GLN:HG2	0.536
20	A:158:THR:C	B:1:NAG:H62	0.505
20	A:169:ASN:N	A:169:ASN:HD22	0.499
20	A:133:ASN:O	E:1:NAG:O6	0.494
20	A:118:PRO:CB	E:2:NAG:O	0.489
20	A:78:LYS:HG2	C:3:BMA:C1	0.488
20	A:22:HIS:NE2	D:6:MAN:O2	0.487
20	A:93:ILE:HB	A:94:PRO:HD3	0.477

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	A:78:LYS:HD3	C:2:NAG:O3	0.472
20	A:198:PRO:HA	A:199:PRO:HD3	0.457
20	A:79:ASN:CG	C:1:NAG:CT	0.449
20	A:78:LYS:NZ	C:3:BMA:C5	0.444
20	A:11:ASN:CB	A:12:PRO:HD3	0.441
20	A:155:SER:HA	A:156:PRO:C	0.435
20	A:78:LYS:HB2	C:2:NAG:C2	0.434
20	A:56:LYS:HD2	A:67:ILE:HD11	0.433
20	A:197:ASN:HA	A:198:PRO:C	0.427
20	A:48:LEU:HD12	A:87:LEU:HG	0.421
20	A:93:ILE:O	A:95:PRO:HD3	0.411

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	207	178	26	3
2	207	178	26	3
3	207	178	26	3
4	207	178	26	3
5	207	178	26	3
6	207	178	26	3
7	207	178	26	3
8	207	178	26	3
9	207	178	26	3

Model ID	Analyzed	Favored	Allowed	Outliers
10	207	178	26	3
11	207	178	26	3
12	207	178	26	3
13	207	178	26	3
14	207	178	26	3
15	207	178	26	3
16	207	178	26	3
17	207	178	26	3
18	207	178	26	3
19	207	178	26	3
20	207	178	26	3

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	185	144	31	10
2	185	144	31	10
3	185	144	31	10
4	185	144	31	10
5	185	144	31	10
6	185	144	31	10
7	185	144	31	10
8	185	144	31	10
9	185	144	31	10

Model ID	Analyzed	Favored	Allowed	Outliers
10	185	144	31	10
11	185	144	31	10
12	185	144	31	10
13	185	144	31	10
14	185	144	31	10
15	185	144	31	10
16	185	144	31	10
17	185	144	31	10
18	185	144	31	10
19	185	144	31	10
20	185	144	31	10

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	8	PHE
1	A	18	GLU
1	A	43	ILE
1	A	73	GLU
1	A	79	ASN
1	A	135	THR
1	A	152	LEU
1	A	169	ASN
1	A	177	LEU
1	A	185	ILE

Model ID	Chain	Residue ID	Residue type
2	A	8	PHE
2	A	18	GLU
2	A	43	ILE
2	A	73	GLU
2	A	79	ASN
2	A	135	THR
2	A	152	LEU
2	A	169	ASN
2	A	177	LEU
2	A	185	ILE
3	A	8	PHE
3	A	18	GLU
3	A	43	ILE
3	A	73	GLU
3	A	79	ASN
3	A	135	THR
3	A	152	LEU
3	A	169	ASN
3	A	177	LEU
3	A	185	ILE
4	A	8	PHE
4	A	18	GLU
4	A	43	ILE

Model ID	Chain	Residue ID	Residue type
4	A	73	GLU
4	A	79	ASN
4	A	135	THR
4	A	152	LEU
4	A	169	ASN
4	A	177	LEU
4	A	185	ILE
5	A	8	PHE
5	A	18	GLU
5	A	43	ILE
5	A	73	GLU
5	A	79	ASN
5	A	135	THR
5	A	152	LEU
5	A	169	ASN
5	A	177	LEU
5	A	185	ILE
6	A	8	PHE
6	A	18	GLU
6	A	43	ILE
6	A	73	GLU
6	A	79	ASN
6	A	135	THR

Model ID	Chain	Residue ID	Residue type
6	A	152	LEU
6	A	169	ASN
6	A	177	LEU
6	A	185	ILE
7	A	8	PHE
7	A	18	GLU
7	A	43	ILE
7	A	73	GLU
7	A	79	ASN
7	A	135	THR
7	A	152	LEU
7	A	169	ASN
7	A	177	LEU
7	A	185	ILE
8	A	8	PHE
8	A	18	GLU
8	A	43	ILE
8	A	73	GLU
8	A	79	ASN
8	A	135	THR
8	A	152	LEU
8	A	169	ASN
8	A	177	LEU

Model ID	Chain	Residue ID	Residue type
8	A	185	ILE
9	A	8	PHE
9	A	18	GLU
9	A	43	ILE
9	A	73	GLU
9	A	79	ASN
9	A	135	THR
9	A	152	LEU
9	A	169	ASN
9	A	177	LEU
9	A	185	ILE
10	A	8	PHE
10	A	18	GLU
10	A	43	ILE
10	A	73	GLU
10	A	79	ASN
10	A	135	THR
10	A	152	LEU
10	A	169	ASN
10	A	177	LEU
10	A	185	ILE
11	A	8	PHE
11	A	18	GLU

Model ID	Chain	Residue ID	Residue type
11	A	43	ILE
11	A	73	GLU
11	A	79	ASN
11	A	135	THR
11	A	152	LEU
11	A	169	ASN
11	A	177	LEU
11	A	185	ILE
12	A	8	PHE
12	A	18	GLU
12	A	43	ILE
12	A	73	GLU
12	A	79	ASN
12	A	135	THR
12	A	152	LEU
12	A	169	ASN
12	A	177	LEU
12	A	185	ILE
13	A	8	PHE
13	A	18	GLU
13	A	43	ILE
13	A	73	GLU
13	A	79	ASN

Model ID	Chain	Residue ID	Residue type
13	A	135	THR
13	A	152	LEU
13	A	169	ASN
13	A	177	LEU
13	A	185	ILE
14	A	8	PHE
14	A	18	GLU
14	A	43	ILE
14	A	73	GLU
14	A	79	ASN
14	A	135	THR
14	A	152	LEU
14	A	169	ASN
14	A	177	LEU
14	A	185	ILE
15	A	8	PHE
15	A	18	GLU
15	A	43	ILE
15	A	73	GLU
15	A	79	ASN
15	A	135	THR
15	A	152	LEU
15	A	169	ASN

Model ID	Chain	Residue ID	Residue type
15	A	177	LEU
15	A	185	ILE
16	A	8	PHE
16	A	18	GLU
16	A	43	ILE
16	A	73	GLU
16	A	79	ASN
16	A	135	THR
16	A	152	LEU
16	A	169	ASN
16	A	177	LEU
16	A	185	ILE
17	A	8	PHE
17	A	18	GLU
17	A	43	ILE
17	A	73	GLU
17	A	79	ASN
17	A	135	THR
17	A	152	LEU
17	A	169	ASN
17	A	177	LEU
17	A	185	ILE
18	A	8	PHE

Model ID	Chain	Residue ID	Residue type
18	A	18	GLU
18	A	43	ILE
18	A	73	GLU
18	A	79	ASN
18	A	135	THR
18	A	152	LEU
18	A	169	ASN
18	A	177	LEU
18	A	185	ILE
19	A	8	PHE
19	A	18	GLU
19	A	43	ILE
19	A	73	GLU
19	A	79	ASN
19	A	135	THR
19	A	152	LEU
19	A	169	ASN
19	A	177	LEU
19	A	185	ILE
20	A	8	PHE
20	A	18	GLU
20	A	43	ILE
20	A	73	GLU

Model ID	Chain	Residue ID	Residue type
20	A	79	ASN
20	A	135	THR
20	A	152	LEU
20	A	169	ASN
20	A	177	LEU
20	A	185	ILE

Fit of model to data used for modeling

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

Fit of model to data used for validation

Validation for this section is under development.

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