Integrative Structure Validation Report

July 22, 2024 - 05:30 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	9A41
PDB-Dev ID	PDBDEV_00000222
Structure Title	F1N4 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

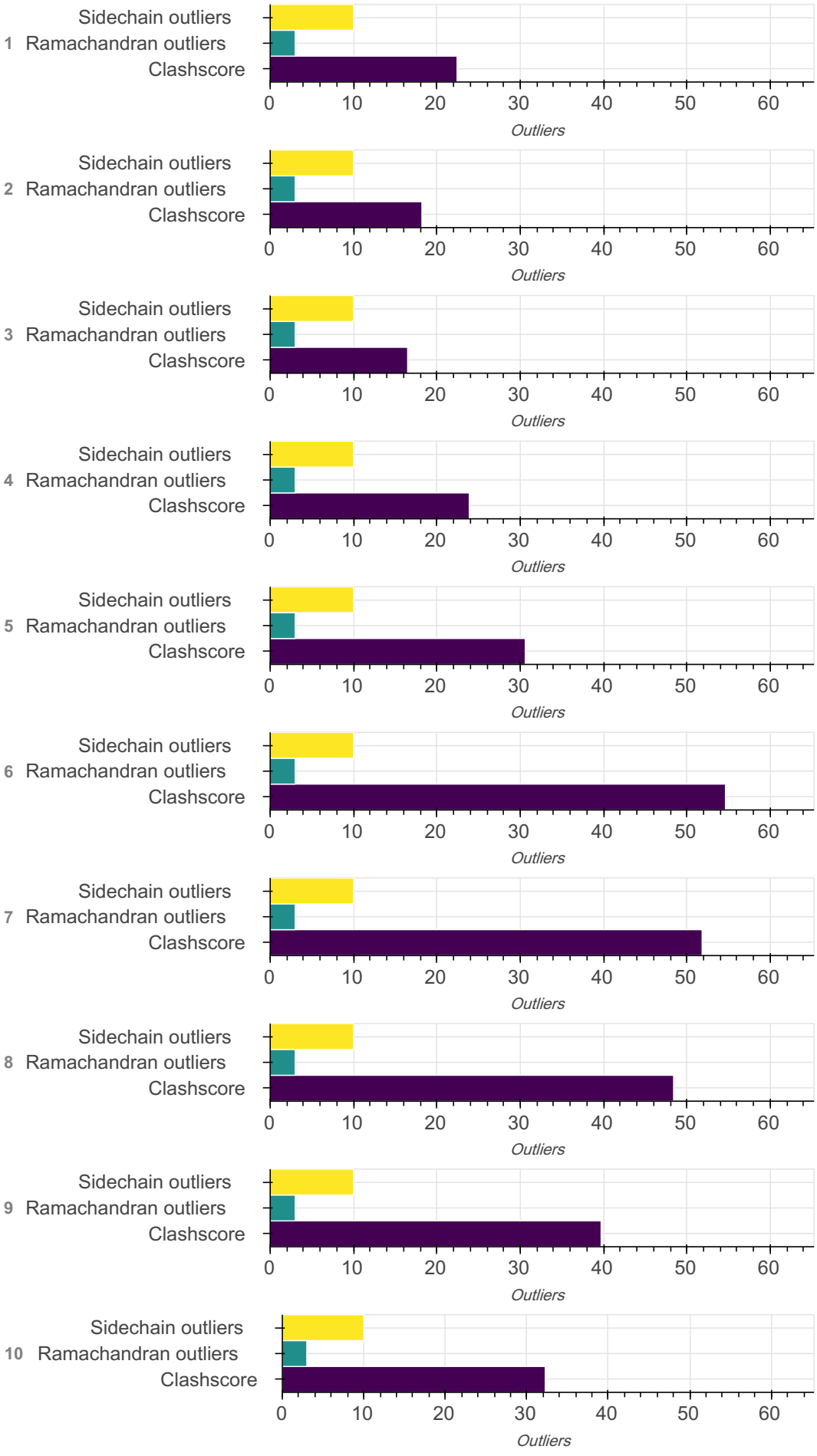
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
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Sidechain outliers
Ramachandran outliers
Clashscore
0
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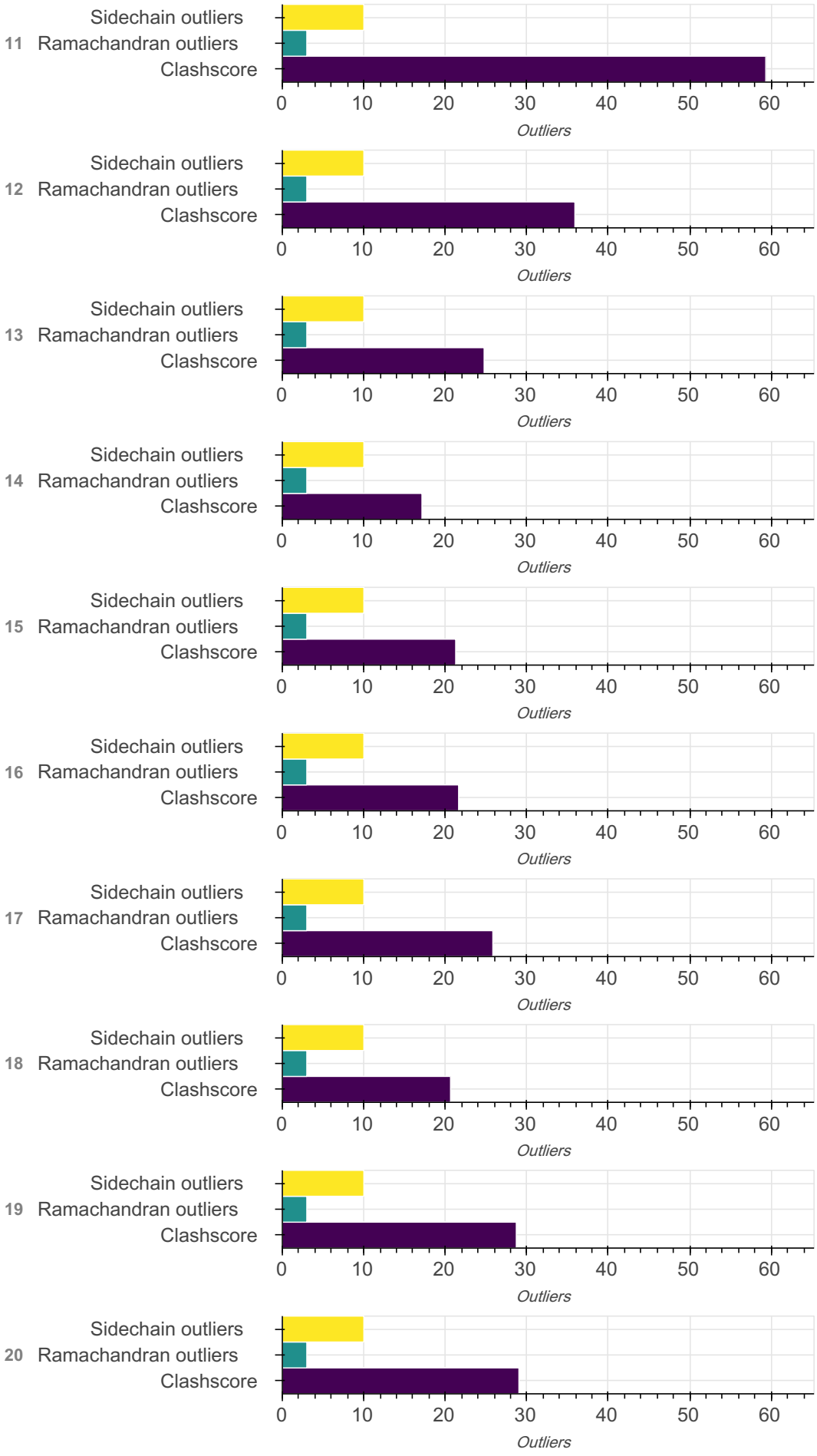
60
Outliers


11
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Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
60
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, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, 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	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
1	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
1	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
2	1	1	Cadherin-2	A	A	211
2	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
2	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
2	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
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	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
3	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
3	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
3	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
4	1	1	Cadherin-2	A	A	211
4	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
4	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
4	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
5	1	1	Cadherin-2	A	A	211
5	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
5	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
5	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
5	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
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	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
6	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
6	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
7	1	1	Cadherin-2	A	A	211
7	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
7	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
7	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
7	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
8	1	1	Cadherin-2	A	A	211
8	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
8	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
8	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
8	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
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	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
9	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
9	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
9	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
10	1	1	Cadherin-2	A	A	211
10	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
10	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
10	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
11	1	1	Cadherin-2	A	A	211
11	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
11	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
11	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
11	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
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	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
12	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
12	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
13	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
13	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
14	1	1	Cadherin-2	A	A	211
14	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
14	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
14	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
14	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
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	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
15	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
15	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
15	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
16	1	1	Cadherin-2	A	A	211
16	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
16	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
16	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
16	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
17	1	1	Cadherin-2	A	A	211
17	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
17	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
17	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
17	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
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	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
18	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
18	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
18	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
19	1	1	Cadherin-2	A	A	211
19	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12
19	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
19	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
19	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12
20	1	1	Cadherin-2	A	A	211
20	2	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	B	B	12

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
20	3	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C	C	12
20	4	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	D	D	12
20	5	2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	E	E	12

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	-	1-12
C	-	1-12
D	-	1-12
E	-	1-12

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 101 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
C2-C3-O3	107.47	125.17	1
C2-C3-O3	107.47	124.90	1
C3-C4-O4	107.29	123.77	1
C3-C4-O4	107.29	123.66	1
C3-C4-O4	107.29	123.29	1
C3-C4-O4	107.29	122.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3-C4-O4	107.29	122.75	1
C3-C4-O4	107.29	122.56	1
C2-C1-O5	110.03	95.24	1
C2-C1-O5	110.03	95.49	1
C1-O5-C5	118.82	104.37	1
C2-C1-O5	110.03	95.60	1
C1-O5-C5	115.81	101.76	1
C1-O5-C5	115.81	101.81	1
C5-C4-O4	106.87	120.86	1
C4-C3-O3	113.26	99.37	1
C4-C3-O3	113.26	99.40	1
C5-C4-O4	106.87	120.72	1
C1-O5-C5	115.81	102.02	1
C1-C2-O6	109.00	122.77	1
C4-C3-O3	113.26	99.56	1
C1-O5-C5	115.81	102.13	1
C1-C2-O6	109.00	122.64	1
C1-C2-O6	109.00	122.58	1
C1-C2-O6	109.00	122.51	1
C1-C2-O2	106.80	120.13	1
C5-C6-O6	109.08	122.26	1
C2-C1-O5	110.03	96.92	1
C1-C2-O2	106.80	119.86	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C2-O2	106.80	119.82	1
C6-C7-C8	111.59	124.59	1
C1-C2-O2	106.80	119.73	1
C3-C4-O4	107.29	120.18	1
C3-C4-O4	107.29	119.94	1
C5-C4-O4	111.70	99.14	1
C5-C4-O4	111.70	99.19	1
C1-C2-O2	106.80	119.30	1
C7-C8-C9	111.05	123.55	1
C7-C8-C9	111.05	123.54	1
C5-C6-C7	110.56	123.05	1
C5-C4-O4	111.70	99.33	1
C5-C6-C7	110.56	122.91	1
C3-C4-O4	107.29	119.58	2
C2-C3-O3	106.67	118.95	1
C2-C1-O5	110.03	97.75	1
C3-C4-O4	107.29	119.57	2
C5-C4-O4	111.70	99.43	1
C7-C6-O6	103.71	115.98	1
C5-C6-O6	109.08	121.34	1
C7-C8-C9	111.05	123.28	1
C5-C4-O4	111.70	99.51	1
C5-C6-C7	110.56	122.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-C3-O3	106.67	118.85	1
C2-C3-O3	106.67	118.79	1
C3-C4-O4	105.79	117.89	1
C3-C4-O4	105.79	117.84	1
C2-C3-O3	106.67	118.70	1
C8-C9-O9	109.54	121.56	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	22.42	64
2	18.20	52
3	16.49	47
4	23.88	68
5	30.60	87
6	54.62	156
7	51.82	148
8	48.40	138
9	39.70	113
10	32.26	92
11	59.32	169
12	35.90	102
13	24.76	71

Model ID	Clash score	Number of clashes
14	17.13	49
15	21.27	61
16	21.63	62
17	25.83	74
18	20.64	59
19	28.71	82
20	29.03	83

All 1777 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:151:ASP:OD2	E:12:FUC:C2	1.413
1	A:158:THR:OG1	D:1:NAG:CT	1.323
1	A:158:THR:CB	D:1:NAG:CT	1.108
1	A:158:THR:HB	D:1:NAG:CT	0.882
1	A:171:ASP:OD2	A:172:PHE:HD2	0.833
1	A:151:ASP:CG	E:12:FUC:C2	0.782
1	A:149:ALA:C	E:12:FUC:O3	0.776
1	A:158:THR:HB	D:1:NAG:C	0.772
1	A:161:ARG:NH1	E:7:SIA:O	0.765
1	A:169:ASN:H	A:169:ASN:HD22	0.765
1	A:169:ASN:HD21	A:172:PHE:HB2	0.763
1	A:151:ASP:HB2	E:12:FUC:O2	0.756
1	A:171:ASP:OD2	A:172:PHE:CD2	0.756
1	A:151:ASP:OD2	E:12:FUC:C3	0.750

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:149:ALA:HB1	E:12:FUC:C4	0.743
1	A:149:ALA:HB1	E:12:FUC:O4	0.717
1	A:181:PHE:CA	D:12:FUC:H2	0.707
1	A:181:PHE:CB	D:12:FUC:H2	0.698
1	A:161:ARG:NH1	E:7:SIA:CT	0.695
1	A:168:LEU:HB2	A:172:PHE:O	0.691
1	A:158:THR:HG1	D:1:NAG:CT	0.681
1	A:181:PHE:N	D:12:FUC:H2	0.681
1	A:169:ASN:N	A:169:ASN:ND2	0.674
1	A:161:ARG:HH11	E:7:SIA:C	0.673
1	A:169:ASN:H	A:169:ASN:ND2	0.671
1	A:149:ALA:CB	E:12:FUC:H4	0.669
1	A:149:ALA:CB	E:12:FUC:C4	0.663
1	A:149:ALA:O	E:12:FUC:O3	0.642
1	A:181:PHE:CB	D:12:FUC:O5	0.637
1	A:133:ASN:ND2	C:1:NAG:C1	0.629
1	A:149:ALA:CB	E:12:FUC:O3	0.627
1	A:161:ARG:NH1	E:7:SIA:C	0.616
1	A:151:ASP:OD2	E:12:FUC:C1	0.615
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:133:ASN:HD22	C:1:NAG:C1	0.579

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:103:GLN:NE2	B:12:FUC:O3	0.569
1	A:151:ASP:HB2	E:12:FUC:C2	0.566
1	A:61:ASN:HB3	A:63:GLN:HG3	0.560
1	A:158:THR:HG22	A:161:ARG:NH2	0.547
1	A:158:THR:HB	D:1:NAG:O	0.544
1	A:29:THR:HG22	A:63:GLN:HG2	0.536
1	A:181:PHE:CB	D:12:FUC:C1	0.533
1	A:157:VAL:HG11	E:7:SIA:C5	0.529
1	A:151:ASP:CB	E:12:FUC:C2	0.512
1	A:169:ASN:N	A:169:ASN:HD22	0.499
1	A:93:ILE:HB	A:94:PRO:HD3	0.477
1	A:198:PRO:HA	A:199:PRO:HD3	0.457
1	A:11:ASN:CB	A:12:PRO:HD3	0.441
1	A:155:SER:HA	A:156:PRO:C	0.435
1	A:56:LYS:HD2	A:67:ILE:HD11	0.433
1	A:79:ASN:OD1	B:11:SIA:CT	0.429
1	A:197:ASN:HA	A:198:PRO:C	0.427
1	D:11:SIA:H91	D:11:SIA:O6	0.423
1	A:151:ASP:OD2	E:12:FUC:O4	0.422
1	A:48:LEU:HD12	A:87:LEU:HG	0.421
1	A:149:ALA:HB3	E:12:FUC:H4	0.417
1	A:149:ALA:HB3	E:12:FUC:O3	0.414
1	C:11:SIA:H91	C:11:SIA:O6	0.413

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:93:ILE:O	A:95:PRO:HD3	0.411
1	E:11:SIA:H91	E:11:SIA:O6	0.407
1	A:181:PHE:CB	D:12:FUC:C2	0.405
1	B:11:SIA:H91	B:11:SIA:O6	0.401
2	A:85:THR:CG2	B:1:NAG:H3	1.419
2	A:101:THR:HA	B:1:NAG:CT	1.226
2	A:154:LEU:HD11	E:11:SIA:O4	1.218
2	A:85:THR:HG22	B:1:NAG:C3	1.182
2	A:101:THR:OG1	B:1:NAG:O3	1.164
2	A:154:LEU:CD1	E:11:SIA:O4	1.119
2	A:101:THR:CA	B:1:NAG:CT	1.101
2	A:101:THR:HA	B:1:NAG:C	1.101
2	A:130:ASN:OD1	C:1:NAG:H3	1.042
2	A:101:THR:C	B:1:NAG:CT	1.031
2	A:130:ASN:OD1	C:1:NAG:C3	0.961
2	A:85:THR:HG22	B:1:NAG:H3	0.884
2	A:154:LEU:HD11	E:11:SIA:HO4	0.869
2	A:130:ASN:HB3	C:1:NAG:O3	0.843
2	A:101:THR:CA	B:1:NAG:C	0.833
2	A:171:ASP:OD2	A:172:PHE:HD2	0.833
2	A:85:THR:CG2	B:1:NAG:C3	0.777
2	A:169:ASN:H	A:169:ASN:HD22	0.765
2	A:169:ASN:HD21	A:172:PHE:HB2	0.763

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:171:ASP:OD2	A:172:PHE:CD2	0.756
2	A:168:LEU:HB2	A:172:PHE:O	0.691
2	A:161:ARG:HE	D:1:NAG:C2	0.681
2	A:169:ASN:N	A:169:ASN:ND2	0.674
2	A:169:ASN:H	A:169:ASN:ND2	0.671
2	A:85:THR:HG21	B:1:NAG:H3	0.643
2	A:154:LEU:HD12	E:11:SIA:C	0.640
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:161:ARG:NE	D:1:NAG:C2	0.571
2	A:61:ASN:HB3	A:63:GLN:HG3	0.560
2	A:182:GLU:OE2	D:10:GAL:O3	0.556
2	A:158:THR:HG22	A:161:ARG:NH2	0.547
2	A:183:ALA:O	D:11:SIA:N	0.546
2	A:130:ASN:CB	C:1:NAG:O3	0.545
2	A:101:THR:OG1	B:1:NAG:C	0.541
2	A:29:THR:HG22	A:63:GLN:HG2	0.536
2	A:182:GLU:HB3	D:11:SIA:N	0.509
2	A:169:ASN:N	A:169:ASN:HD22	0.499
2	A:85:THR:CG2	B:1:NAG:C2	0.483
2	A:93:ILE:HB	A:94:PRO:HD3	0.477
2	A:85:THR:HG22	B:1:NAG:C2	0.461

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:198:PRO:HA	A:199:PRO:HD3	0.457
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:197:ASN:HA	A:198:PRO:C	0.427
2	A:199:PRO:C	E:1:NAG:C	0.423
2	A:48:LEU:HD12	A:87:LEU:HG	0.421
2	A:93:ILE:O	A:95:PRO:HD3	0.411
2	A:85:THR:HG22	B:1:NAG:N	0.406
2	A:101:THR:OG1	B:1:NAG:C3	0.405
3	A:79:ASN:OD1	B:2:NAG:C5	1.329
3	A:79:ASN:OD1	B:2:NAG:H5	1.070
3	A:199:PRO:HD2	E:12:FUC:H63	1.061
3	A:83:ASN:ND2	B:1:NAG:N	0.987
3	A:83:ASN:ND2	B:1:NAG:C1	0.942
3	A:79:ASN:OD1	B:2:NAG:C6	0.932
3	A:131:SER:C	C:12:FUC:H4	0.911
3	A:171:ASP:OD2	A:172:PHE:HD2	0.833
3	A:199:PRO:HD2	E:12:FUC:C6	0.790
3	A:199:PRO:O	E:12:FUC:C4	0.783
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

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:78:LYS:HG3	B:8:MAN:H62	0.752
3	A:133:ASN:HD22	C:1:NAG:C1	0.752
3	A:168:LEU:HB2	A:172:PHE:O	0.691
3	A:199:PRO:O	E:12:FUC:H62	0.683
3	A:169:ASN:N	A:169:ASN:ND2	0.674
3	A:161:ARG:NH1	D:12:FUC:O4	0.673
3	A:169:ASN:H	A:169:ASN:ND2	0.671
3	A:133:ASN:ND2	C:1:NAG:C1	0.662
3	A:79:ASN:CB	B:1:NAG:O3	0.641
3	A:11:ASN:HB3	A:12:PRO:HD3	0.610
3	A:79:ASN:HD22	A:80:ASN:H	0.592
3	A:133:ASN:ND2	C:1:NAG:O5	0.592
3	A:117:LEU:HB3	A:118:PRO:HD3	0.591
3	A:61:ASN:HB3	A:63:GLN:HG3	0.560
3	A:83:ASN:ND2	B:1:NAG:C2	0.555
3	A:78:LYS:CG	B:8:MAN:H62	0.554
3	A:158:THR:HG22	A:161:ARG:NH2	0.547
3	A:29:THR:HG22	A:63:GLN:HG2	0.536
3	A:79:ASN:HB2	B:1:NAG:O3	0.524
3	A:199:PRO:HG2	E:12:FUC:O5	0.512
3	A:169:ASN:N	A:169:ASN:HD22	0.499
3	A:199:PRO:HG2	E:12:FUC:C1	0.483
3	A:199:PRO:O	E:12:FUC:C6	0.479

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:93:ILE:HB	A:94:PRO:HD3	0.477
3	A:79:ASN:HB3	B:1:NAG:O3	0.462
3	A:198:PRO:HA	A:199:PRO:HD3	0.457
3	A:11:ASN:CB	A:12:PRO:HD3	0.441
3	A:155:SER:HA	A:156:PRO:C	0.435
3	A:56:LYS:HD2	A:67:ILE:HD11	0.433
3	A:197:ASN:HA	A:198:PRO:C	0.427
3	A:48:LEU:HD12	A:87:LEU:HG	0.421
3	A:83:ASN:CG	B:1:NAG:C1	0.415
3	A:93:ILE:O	A:95:PRO:HD3	0.411
3	A:161:ARG:HD2	D:12:FUC:C2	0.411
4	A:85:THR:OG1	B:12:FUC:H4	1.370
4	A:187:GLU:OE2	E:11:SIA:CT	1.233
4	A:48:LEU:HD22	B:12:FUC:O4	1.143
4	A:154:LEU:HD12	E:2:NAG:H4	1.112
4	A:85:THR:HG21	B:12:FUC:H5	1.076
4	A:85:THR:OG1	B:12:FUC:C4	1.035
4	A:169:ASN:O	C:10:GAL:H61	1.021
4	A:154:LEU:HD12	E:2:NAG:C4	1.010
4	A:161:ARG:HB3	D:12:FUC:O2	0.980
4	A:85:THR:CB	B:12:FUC:H4	0.978
4	A:85:THR:HG21	B:12:FUC:C5	0.950
4	A:172:PHE:HE2	C:2:NAG:CT	0.906

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:161:ARG:CB	D:12:FUC:O2	0.903
4	A:172:PHE:CE2	C:2:NAG:CT	0.879
4	A:187:GLU:CD	E:11:SIA:CT	0.869
4	A:48:LEU:CD2	B:12:FUC:O4	0.861
4	A:171:ASP:OD2	A:172:PHE:HD2	0.837
4	A:172:PHE:CD1	C:1:NAG:H5	0.821
4	A:169:ASN:O	C:10:GAL:C6	0.806
4	A:154:LEU:CD1	E:2:NAG:H4	0.805
4	A:154:LEU:HD12	E:3:BMA:C1	0.795
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:172:PHE:CD1	C:1:NAG:C5	0.749
4	A:49:SER:O	B:12:FUC:O3	0.727
4	A:168:LEU:HB2	A:172:PHE:O	0.691
4	A:130:ASN:OD1	C:1:NAG:CT	0.691
4	A:169:ASN:N	A:169:ASN:ND2	0.674
4	A:169:ASN:H	A:169:ASN:ND2	0.671
4	A:154:LEU:CD1	E:3:BMA:C1	0.666
4	A:85:THR:CG2	B:12:FUC:H4	0.664
4	A:85:THR:HG21	B:12:FUC:C4	0.611
4	A:172:PHE:CE1	C:12:FUC:C3	0.611
4	A:11:ASN:HB3	A:12:PRO:HD3	0.610

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:49:SER:OG	B:12:FUC:C2	0.593
4	A:79:ASN:HD22	A:80:ASN:H	0.592
4	A:117:LEU:HB3	A:118:PRO:HD3	0.591
4	A:85:THR:CG2	B:12:FUC:C4	0.579
4	A:172:PHE:CG	C:1:NAG:H5	0.567
4	A:61:ASN:HB3	A:63:GLN:HG3	0.560
4	A:168:LEU:HD21	C:1:NAG:N	0.550
4	A:172:PHE:CE2	C:2:NAG:C	0.550
4	A:85:THR:CG2	B:12:FUC:H5	0.543
4	A:29:THR:HG22	A:63:GLN:HG2	0.536
4	A:48:LEU:HD22	B:12:FUC:C4	0.521
4	A:187:GLU:OE1	E:11:SIA:CT	0.519
4	A:85:THR:OG1	B:12:FUC:C3	0.519
4	A:49:SER:OG	B:12:FUC:O2	0.503
4	A:169:ASN:N	A:169:ASN:HD22	0.499
4	A:154:LEU:HB2	E:2:NAG:O3	0.497
4	A:154:LEU:HB2	E:2:NAG:H4	0.492
4	A:168:LEU:CD2	C:1:NAG:N	0.485
4	A:93:ILE:HB	A:94:PRO:HD3	0.477
4	A:49:SER:CB	B:12:FUC:O4	0.474
4	A:198:PRO:HA	A:199:PRO:HD3	0.457
4	A:158:THR:HB	D:12:FUC:H3	0.454
4	A:207:ARG:HH12	E:11:SIA:CT	0.447

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:49:SER:HB3	B:12:FUC:O4	0.447
4	A:11:ASN:CB	A:12:PRO:HD3	0.441
4	A:154:LEU:HD12	E:2:NAG:O4	0.440
4	A:155:SER:C	E:8:MAN:O3	0.440
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:154:LEU:CG	E:2:NAG:H4	0.426
4	A:48:LEU:HD12	A:87:LEU:HG	0.421
4	A:93:ILE:O	A:95:PRO:HD3	0.411
5	C:10:GAL:C4	E:6:GAL:H61	1.507
5	A:199:PRO:HD2	E:12:FUC:C2	1.506
5	A:199:PRO:CD	E:12:FUC:H2	1.505
5	C:10:GAL:C5	E:6:GAL:H61	1.430
5	A:168:LEU:CB	C:12:FUC:O4	1.330
5	A:199:PRO:CD	E:12:FUC:C2	1.329
5	A:168:LEU:HB2	C:12:FUC:O4	1.265
5	A:83:ASN:CG	B:1:NAG:C1	1.239
5	A:83:ASN:ND2	B:1:NAG:C1	1.211
5	A:199:PRO:HG2	E:12:FUC:C1	1.203
5	C:10:GAL:H62	E:6:GAL:C5	1.154
5	A:83:ASN:OD1	B:1:NAG:C1	1.145
5	A:199:PRO:CG	E:12:FUC:C1	1.113

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:168:LEU:CB	C:12:FUC:HO4	1.113
5	A:199:PRO:CG	E:12:FUC:C2	1.052
5	A:199:PRO:CG	E:12:FUC:H2	1.016
5	A:158:THR:HG22	D:12:FUC:H4	1.005
5	C:10:GAL:H62	E:6:GAL:O5	0.996
5	A:168:LEU:HB3	C:12:FUC:O4	0.995
5	A:161:ARG:CB	D:12:FUC:O3	0.993
5	A:199:PRO:N	E:12:FUC:H2	0.990
5	A:167:ARG:CD	E:4:MAN:H61	0.983
5	A:167:ARG:HD2	E:4:MAN:H61	0.944
5	C:10:GAL:H4	E:6:GAL:H61	0.932
5	A:83:ASN:HD21	B:1:NAG:C1	0.929
5	A:167:ARG:NH1	E:4:MAN:O4	0.925
5	A:161:ARG:HB3	D:12:FUC:O3	0.896
5	A:83:ASN:HD21	B:1:NAG:C2	0.874
5	A:199:PRO:CB	E:12:FUC:C2	0.866
5	A:79:ASN:HB3	B:1:NAG:O	0.834
5	A:171:ASP:OD2	A:172:PHE:HD2	0.833
5	A:199:PRO:HD2	E:12:FUC:C3	0.827
5	C:10:GAL:O4	E:6:GAL:C6	0.823
5	A:168:LEU:HB2	C:12:FUC:HO4	0.815
5	A:199:PRO:HD2	E:12:FUC:C1	0.806
5	C:10:GAL:O4	E:6:GAL:H62	0.795

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:161:ARG:HB2	D:12:FUC:O3	0.791
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	C:10:GAL:C4	E:6:GAL:C6	0.753
5	A:158:THR:HA	D:12:FUC:C3	0.745
5	A:199:PRO:CD	E:12:FUC:C1	0.727
5	A:172:PHE:O	C:12:FUC:O4	0.705
5	A:199:PRO:CB	E:12:FUC:C1	0.696
5	A:161:ARG:HB3	D:12:FUC:C3	0.694
5	A:168:LEU:HB2	A:172:PHE:O	0.691
5	A:158:THR:HA	D:12:FUC:O3	0.679
5	A:161:ARG:CB	D:12:FUC:C3	0.675
5	A:169:ASN:N	A:169:ASN:ND2	0.674
5	A:169:ASN:H	A:169:ASN:ND2	0.671
5	A:158:THR:CG2	D:12:FUC:H4	0.649
5	A:83:ASN:ND2	B:1:NAG:C2	0.639
5	A:168:LEU:HD21	C:1:NAG:H5	0.637
5	A:199:PRO:HB2	E:12:FUC:C1	0.625
5	A:199:PRO:HD2	E:12:FUC:C4	0.620
5	A:83:ASN:ND2	B:1:NAG:N	0.617
5	A:11:ASN:HB3	A:12:PRO:HD3	0.610
5	A:199:PRO:HD2	E:12:FUC:H2	0.604

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:168:LEU:CB	C:12:FUC:C4	0.597
5	C:10:GAL:C5	E:6:GAL:C6	0.594
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:151:ASP:HB2	E:1:NAG:CT	0.560
5	A:158:THR:HG22	A:161:ARG:NH2	0.541
5	A:29:THR:HG22	A:63:GLN:HG2	0.536
5	A:172:PHE:C	C:12:FUC:O4	0.504
5	A:149:ALA:HB2	E:2:NAG:H62	0.503
5	A:169:ASN:N	A:169:ASN:HD22	0.499
5	A:199:PRO:N	E:12:FUC:C2	0.482
5	A:93:ILE:HB	A:94:PRO:HD3	0.477
5	A:172:PHE:C	C:12:FUC:HO4	0.475
5	A:79:ASN:CB	B:1:NAG:O	0.466
5	A:198:PRO:HA	A:199:PRO:HD3	0.457
5	A:172:PHE:CB	C:12:FUC:O4	0.450
5	A:151:ASP:OD2	E:1:NAG:O	0.442
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:169:ASN:OD1	C:12:FUC:H2	0.428
5	A:197:ASN:HA	A:198:PRO:C	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:48:LEU:HD12	A:87:LEU:HG	0.421
5	A:93:ILE:O	A:95:PRO:HD3	0.411
5	A:172:PHE:HB2	C:12:FUC:O4	0.411
5	A:167:ARG:HD3	E:4:MAN:H4	0.404
5	A:157:VAL:O	D:12:FUC:O3	0.404
6	A:49:SER:HB3	B:12:FUC:C2	1.588
6	A:199:PRO:HB2	E:1:NAG:C6	1.586
6	A:161:ARG:CD	D:10:GAL:H2	1.574
6	A:161:ARG:HD2	D:10:GAL:C2	1.567
6	A:161:ARG:HD2	D:10:GAL:C3	1.521
6	A:49:SER:HB3	B:12:FUC:C1	1.513
6	A:199:PRO:CB	E:1:NAG:H61	1.507
6	A:199:PRO:HD2	E:12:FUC:C1	1.415
6	A:161:ARG:NE	D:10:GAL:H2	1.415
6	A:161:ARG:CG	D:10:GAL:O3	1.406
6	A:161:ARG:NH2	D:1:NAG:C	1.361
6	A:158:THR:HA	D:1:NAG:CT	1.345
6	A:161:ARG:HD3	D:10:GAL:O4	1.299
6	A:49:SER:CB	B:12:FUC:C1	1.285
6	A:161:ARG:CZ	D:1:NAG:CT	1.265
6	A:161:ARG:O	D:11:SIA:H31	1.256
6	A:161:ARG:CD	D:10:GAL:C3	1.244
6	A:49:SER:CB	B:12:FUC:C2	1.241

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:161:ARG:CD	D:10:GAL:O4	1.233
6	A:180:LYS:N	D:12:FUC:O3	1.228
6	A:199:PRO:O	E:12:FUC:C1	1.227
6	A:158:THR:CA	D:1:NAG:CT	1.214
6	A:199:PRO:CG	E:1:NAG:H61	1.213
6	A:161:ARG:HG3	D:10:GAL:O3	1.199
6	A:149:ALA:O	E:1:NAG:CT	1.199
6	A:199:PRO:CD	E:12:FUC:C1	1.196
6	A:199:PRO:HD2	E:12:FUC:O5	1.188
6	A:161:ARG:CD	D:10:GAL:C2	1.179
6	A:161:ARG:HD2	D:10:GAL:C4	1.169
6	A:199:PRO:CB	E:1:NAG:C6	1.147
6	A:172:PHE:CZ	C:12:FUC:H5	1.146
6	A:181:PHE:CB	D:12:FUC:H2	1.134
6	A:199:PRO:CD	E:12:FUC:O5	1.126
6	A:161:ARG:CZ	D:1:NAG:C	1.124
6	A:161:ARG:NE	D:1:NAG:N	1.106
6	A:199:PRO:CG	E:1:NAG:C6	1.102
6	A:147:PRO:HG2	E:4:MAN:O6	1.090
6	A:161:ARG:NE	D:1:NAG:CT	1.066
6	A:49:SER:O	B:12:FUC:O2	1.045
6	A:49:SER:HB3	B:12:FUC:H2	1.043
6	A:172:PHE:CE2	C:12:FUC:H5	1.043

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:161:ARG:O	D:11:SIA:C3	1.003
6	A:161:ARG:HH21	D:1:NAG:C	0.996
6	A:199:PRO:HG2	E:1:NAG:H62	0.983
6	A:161:ARG:CD	D:10:GAL:C4	0.982
6	A:199:PRO:O	E:1:NAG:O6	0.965
6	A:199:PRO:HB2	E:1:NAG:C5	0.964
6	A:172:PHE:CZ	C:12:FUC:C5	0.942
6	A:49:SER:CB	B:12:FUC:H2	0.941
6	A:161:ARG:NH2	D:1:NAG:N	0.940
6	A:49:SER:HB3	B:12:FUC:O2	0.935
6	A:161:ARG:NH2	D:1:NAG:O3	0.920
6	A:199:PRO:O	E:12:FUC:O2	0.887
6	A:199:PRO:O	E:12:FUC:C2	0.884
6	A:199:PRO:HG2	E:1:NAG:C6	0.883
6	A:161:ARG:HG2	D:10:GAL:O3	0.875
6	A:161:ARG:CZ	D:1:NAG:N	0.866
6	A:161:ARG:CG	D:10:GAL:C3	0.852
6	A:180:LYS:N	D:12:FUC:HO3	0.850
6	A:48:LEU:HD13	B:12:FUC:C4	0.848
6	A:161:ARG:NE	D:1:NAG:C	0.846
6	A:149:ALA:HB3	E:1:NAG:CT	0.845
6	A:149:ALA:HB3	E:1:NAG:C	0.837
6	A:171:ASP:OD2	A:172:PHE:HD2	0.837

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:149:ALA:C	E:1:NAG:CT	0.831
6	A:139:TYR:HA	C:11:SIA:H4	0.830
6	A:199:PRO:N	E:12:FUC:C1	0.807
6	A:171:ASP:O	C:12:FUC:H4	0.798
6	A:139:TYR:CA	C:11:SIA:H4	0.788
6	A:172:PHE:CE2	C:12:FUC:C5	0.778
6	A:161:ARG:HD3	D:10:GAL:HO4	0.777
6	A:49:SER:N	B:12:FUC:H2	0.777
6	A:199:PRO:CA	E:1:NAG:H61	0.770
6	A:169:ASN:H	A:169:ASN:HD22	0.765
6	A:169:ASN:HD21	A:172:PHE:HB2	0.763
6	A:137:LEU:HD23	C:11:SIA:O8	0.761
6	A:171:ASP:OD2	A:172:PHE:CD2	0.756
6	A:161:ARG:HH21	D:1:NAG:C2	0.743
6	A:49:SER:CB	B:12:FUC:O2	0.735
6	A:139:TYR:HA	C:11:SIA:C4	0.734
6	A:161:ARG:HG3	D:11:SIA:C2	0.722
6	A:199:PRO:CG	E:1:NAG:H62	0.715
6	A:161:ARG:CZ	D:10:GAL:H2	0.709
6	A:168:LEU:HB2	A:172:PHE:O	0.691
6	A:199:PRO:C	E:12:FUC:C1	0.690
6	A:161:ARG:NE	D:10:GAL:C2	0.685
6	A:169:ASN:N	A:169:ASN:ND2	0.674

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:49:SER:C	B:12:FUC:O2	0.674
6	A:149:ALA:CB	E:1:NAG:CT	0.672
6	A:169:ASN:H	A:169:ASN:ND2	0.671
6	A:172:PHE:CE1	C:12:FUC:H5	0.669
6	A:161:ARG:HH21	D:1:NAG:C3	0.667
6	A:199:PRO:HB2	E:1:NAG:C4	0.664
6	A:161:ARG:CG	D:10:GAL:C2	0.658
6	A:172:PHE:CE2	C:12:FUC:C6	0.653
6	A:49:SER:HB2	B:12:FUC:C1	0.639
6	A:199:PRO:CG	E:2:NAG:N	0.629
6	A:49:SER:CA	B:12:FUC:O2	0.628
6	A:48:LEU:HD22	B:12:FUC:C2	0.627
6	A:172:PHE:CD1	C:1:NAG:C1	0.618
6	A:48:LEU:HD22	B:12:FUC:H2	0.617
6	A:161:ARG:NH2	D:1:NAG:O	0.616
6	A:161:ARG:NH2	D:1:NAG:C3	0.613
6	A:49:SER:CA	B:12:FUC:H2	0.611
6	A:11:ASN:HB3	A:12:PRO:HD3	0.610
6	A:199:PRO:CD	E:1:NAG:C6	0.605
6	A:48:LEU:HB3	B:12:FUC:O3	0.599
6	A:199:PRO:HG3	E:2:NAG:N	0.597
6	A:49:SER:CA	B:12:FUC:C2	0.594
6	A:85:THR:HG21	B:12:FUC:H5	0.592

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:79:ASN:HD22	A:80:ASN:H	0.592
6	A:117:LEU:HB3	A:118:PRO:HD3	0.591
6	A:199:PRO:HB2	E:1:NAG:H61	0.568
6	A:199:PRO:CA	E:12:FUC:C1	0.564
6	A:147:PRO:CG	E:4:MAN:O6	0.562
6	A:61:ASN:HB3	A:63:GLN:HG3	0.560
6	A:199:PRO:HG2	E:2:NAG:N	0.552
6	A:158:THR:HG22	A:161:ARG:NH2	0.547
6	A:172:PHE:CE2	C:12:FUC:H61	0.543
6	A:29:THR:HG22	A:63:GLN:HG2	0.536
6	A:161:ARG:CG	D:11:SIA:C2	0.523
6	A:171:ASP:O	C:12:FUC:C4	0.513
6	A:181:PHE:CB	D:12:FUC:C2	0.508
6	A:169:ASN:N	A:169:ASN:HD22	0.499
6	A:151:ASP:CB	E:11:SIA:O4	0.493
6	A:161:ARG:HG3	D:10:GAL:C3	0.492
6	A:199:PRO:CB	E:1:NAG:C4	0.482
6	A:172:PHE:CZ	C:12:FUC:O5	0.480
6	A:48:LEU:HD13	B:12:FUC:H4	0.477
6	A:93:ILE:HB	A:94:PRO:HD3	0.477
6	A:199:PRO:CB	E:1:NAG:H4	0.468
6	A:161:ARG:HB3	D:1:NAG:CT	0.459
6	A:199:PRO:HG2	E:2:NAG:C	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:198:PRO:HA	A:199:PRO:HD3	0.457
6	A:49:SER:N	B:12:FUC:C2	0.450
6	A:178:LYS:HG2	D:11:SIA:O	0.444
6	A:11:ASN:CB	A:12:PRO:HD3	0.441
6	A:151:ASP:HB3	E:11:SIA:O4	0.440
6	A:171:ASP:HB2	C:12:FUC:H62	0.439
6	A:155:SER:HA	A:156:PRO:C	0.435
6	A:56:LYS:HD2	A:67:ILE:HD11	0.433
6	A:151:ASP:HB2	E:11:SIA:O4	0.432
6	A:171:ASP:CG	C:12:FUC:H62	0.427
6	A:197:ASN:HA	A:198:PRO:C	0.427
6	A:48:LEU:HD22	B:12:FUC:O5	0.423
6	A:161:ARG:CG	D:11:SIA:C3	0.422
6	A:48:LEU:HD12	A:87:LEU:HG	0.421
6	A:172:PHE:CD2	C:12:FUC:H5	0.416
6	A:161:ARG:HG3	D:11:SIA:C3	0.415
6	A:151:ASP:OD2	E:11:SIA:H31	0.415
6	A:199:PRO:HB2	E:1:NAG:H4	0.412
6	A:49:SER:HB3	B:12:FUC:HO2	0.411
6	A:93:ILE:O	A:95:PRO:HD3	0.411
6	A:161:ARG:CD	D:1:NAG:CT	0.407
6	A:181:PHE:CA	D:12:FUC:H2	0.407
6	A:161:ARG:HH21	D:1:NAG:N	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:168:LEU:CD2	C:1:NAG:C	1.621
7	A:103:GLN:CD	B:12:FUC:C5	1.575
7	A:103:GLN:CG	B:12:FUC:C3	1.532
7	A:103:GLN:CG	B:12:FUC:H3	1.505
7	A:103:GLN:HG3	B:12:FUC:C3	1.480
7	A:130:ASN:OD1	C:1:NAG:C5	1.435
7	A:158:THR:HA	D:1:NAG:CT	1.405
7	A:103:GLN:OE1	B:12:FUC:C5	1.387
7	A:161:ARG:CZ	D:10:GAL:H2	1.386
7	A:79:ASN:HD21	B:11:SIA:C6	1.377
7	A:79:ASN:ND2	B:11:SIA:H6	1.362
7	A:79:ASN:OD1	B:11:SIA:H7	1.322
7	A:12:PRO:CB	B:12:FUC:H2	1.253
7	A:168:LEU:HD23	C:1:NAG:C	1.250
7	A:79:ASN:OD1	B:11:SIA:C7	1.239
7	A:161:ARG:CZ	D:1:NAG:CT	1.229
7	A:130:ASN:OD1	C:1:NAG:C4	1.224
7	A:103:GLN:CD	B:12:FUC:H3	1.222
7	A:158:THR:CA	D:1:NAG:CT	1.192
7	A:161:ARG:NH1	D:10:GAL:H2	1.183
7	A:130:ASN:OD1	C:1:NAG:C6	1.182
7	A:83:ASN:OD1	B:1:NAG:C1	1.179
7	A:12:PRO:HB2	B:12:FUC:O4	1.160

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:161:ARG:NH1	D:10:GAL:O4	1.154
7	A:12:PRO:HB3	B:12:FUC:H2	1.148
7	A:199:PRO:HG3	E:11:SIA:CT	1.145
7	A:130:ASN:OD1	C:1:NAG:H4	1.116
7	A:103:GLN:HB2	B:12:FUC:C4	1.109
7	A:130:ASN:OD1	C:1:NAG:O5	1.100
7	A:103:GLN:CD	B:12:FUC:C4	1.097
7	A:131:SER:CA	C:12:FUC:O2	1.071
7	A:168:LEU:CG	C:1:NAG:O	1.062
7	A:131:SER:C	C:12:FUC:O2	1.061
7	A:130:ASN:CG	C:1:NAG:H61	1.035
7	A:198:PRO:HA	E:11:SIA:N	1.034
7	A:103:GLN:CD	B:12:FUC:C3	1.027
7	A:103:GLN:CB	B:12:FUC:H4	1.027
7	A:130:ASN:CB	C:1:NAG:H61	1.023
7	A:80:ASN:ND2	B:11:SIA:O11	1.022
7	A:161:ARG:CZ	D:10:GAL:C2	1.020
7	A:103:GLN:HB2	B:12:FUC:H4	1.016
7	A:199:PRO:O	E:11:SIA:H32	0.999
7	A:198:PRO:HA	E:11:SIA:C	0.990
7	A:168:LEU:HD21	C:1:NAG:O	0.990
7	A:130:ASN:HB3	C:1:NAG:H61	0.989
7	A:168:LEU:HD22	C:1:NAG:O	0.983

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:12:PRO:HB3	B:12:FUC:C2	0.962
7	A:130:ASN:CG	C:1:NAG:C6	0.957
7	A:83:ASN:OD1	B:1:NAG:O5	0.952
7	A:83:ASN:CG	B:1:NAG:C1	0.951
7	A:79:ASN:OD1	B:11:SIA:C8	0.945
7	A:130:ASN:OD1	C:1:NAG:H61	0.933
7	A:168:LEU:CD2	C:1:NAG:O	0.933
7	A:178:LYS:C	D:11:SIA:CT	0.927
7	A:199:PRO:CG	E:11:SIA:CT	0.927
7	A:198:PRO:HA	E:11:SIA:O	0.919
7	A:168:LEU:HD22	C:1:NAG:C	0.916
7	A:79:ASN:CG	B:11:SIA:C8	0.910
7	A:103:GLN:CG	B:12:FUC:C4	0.904
7	A:103:GLN:N	B:12:FUC:O3	0.892
7	A:103:GLN:CB	B:12:FUC:C3	0.891
7	A:103:GLN:OE1	B:12:FUC:C6	0.891
7	A:103:GLN:CB	B:12:FUC:C4	0.868
7	A:198:PRO:CA	E:11:SIA:O	0.866
7	A:79:ASN:CG	B:11:SIA:C7	0.861
7	A:103:GLN:HG3	B:12:FUC:O3	0.861
7	A:12:PRO:CB	B:12:FUC:C2	0.852
7	A:198:PRO:CA	E:11:SIA:C	0.839
7	A:131:SER:HA	C:12:FUC:C2	0.835

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:171:ASP:OD2	A:172:PHE:HD2	0.833
7	A:79:ASN:ND2	B:11:SIA:H8	0.821
7	A:199:PRO:O	E:11:SIA:C3	0.814
7	A:161:ARG:NE	D:1:NAG:CT	0.811
7	A:161:ARG:NE	D:10:GAL:C2	0.803
7	A:161:ARG:NE	D:10:GAL:H2	0.792
7	A:131:SER:O	C:12:FUC:O3	0.780
7	A:101:THR:HG22	B:12:FUC:O3	0.772
7	A:83:ASN:ND2	B:1:NAG:C1	0.767
7	A:169:ASN:H	A:169:ASN:HD22	0.765
7	A:169:ASN:HD21	A:172:PHE:HB2	0.763
7	A:158:THR:HG22	D:1:NAG:CT	0.759
7	A:171:ASP:OD2	A:172:PHE:CD2	0.756
7	A:79:ASN:OD1	B:11:SIA:O8	0.752
7	A:79:ASN:ND2	B:11:SIA:C6	0.743
7	A:79:ASN:CG	B:11:SIA:H8	0.739
7	A:12:PRO:CB	B:12:FUC:O4	0.723
7	A:197:ASN:N	E:11:SIA:CT	0.716
7	A:103:GLN:HG3	B:12:FUC:H3	0.710
7	A:161:ARG:HH11	D:10:GAL:C4	0.710
7	A:79:ASN:CG	B:11:SIA:H7	0.707
7	A:80:ASN:CG	B:11:SIA:O11	0.699
7	A:131:SER:CA	C:12:FUC:C2	0.698

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:168:LEU:HB2	A:172:PHE:O	0.691
7	A:12:PRO:O	B:12:FUC:O4	0.686
7	A:169:ASN:N	A:169:ASN:ND2	0.674
7	A:169:ASN:H	A:169:ASN:ND2	0.671
7	A:12:PRO:HB3	B:12:FUC:C1	0.665
7	A:130:ASN:CG	C:1:NAG:O5	0.655
7	A:168:LEU:HD21	C:1:NAG:C2	0.652
7	A:161:ARG:NH1	D:10:GAL:C2	0.636
7	A:149:ALA:H	E:12:FUC:C2	0.635
7	A:79:ASN:ND2	B:11:SIA:C7	0.626
7	A:161:ARG:HD3	D:10:GAL:O4	0.617
7	A:158:THR:CG2	D:1:NAG:CT	0.616
7	A:149:ALA:N	E:12:FUC:H2	0.614
7	A:11:ASN:HB3	A:12:PRO:HD3	0.610
7	A:130:ASN:HB3	C:1:NAG:C6	0.606
7	A:12:PRO:CA	B:12:FUC:H2	0.603
7	A:131:SER:N	C:12:FUC:O2	0.600
7	A:83:ASN:HD21	B:1:NAG:C1	0.597
7	A:130:ASN:CB	C:1:NAG:C6	0.596
7	A:79:ASN:HD22	A:80:ASN:H	0.592
7	A:117:LEU:HB3	A:118:PRO:HD3	0.591
7	A:79:ASN:HD21	B:11:SIA:H6	0.591
7	A:161:ARG:NH1	D:1:NAG:CT	0.573

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:149:ALA:N	E:12:FUC:C2	0.573
7	A:12:PRO:HB2	B:12:FUC:H2	0.566
7	A:61:ASN:HB3	A:63:GLN:HG3	0.560
7	A:103:GLN:HB2	B:12:FUC:C3	0.557
7	A:79:ASN:ND2	B:11:SIA:C8	0.549
7	A:12:PRO:HB2	B:12:FUC:C4	0.544
7	A:29:THR:HG22	A:63:GLN:HG2	0.536
7	A:198:PRO:C	E:11:SIA:C	0.531
7	A:79:ASN:CG	B:11:SIA:O8	0.519
7	A:80:ASN:ND2	B:11:SIA:C1	0.518
7	A:169:ASN:N	A:169:ASN:HD22	0.499
7	A:161:ARG:CD	D:10:GAL:O4	0.496
7	A:161:ARG:NE	D:10:GAL:O2	0.495
7	A:93:ILE:HB	A:94:PRO:HD3	0.477
7	A:149:ALA:N	E:12:FUC:O2	0.473
7	A:172:PHE:HB3	C:1:NAG:CT	0.467
7	A:158:THR:HG22	A:161:ARG:NH2	0.459
7	A:158:THR:N	D:1:NAG:CT	0.456
7	A:161:ARG:HG3	D:11:SIA:O11	0.452
7	A:181:PHE:CB	D:12:FUC:O2	0.450
7	A:103:GLN:CB	B:12:FUC:O3	0.448
7	A:79:ASN:CG	B:11:SIA:C6	0.442
7	A:131:SER:O	C:12:FUC:O2	0.442

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:11:ASN:CB	A:12:PRO:HD3	0.441
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:12:PRO:CB	B:12:FUC:C1	0.427
7	A:12:PRO:HB2	B:12:FUC:C2	0.427
7	A:48:LEU:HD12	A:87:LEU:HG	0.421
7	A:93:ILE:O	A:95:PRO:HD3	0.411
7	A:149:ALA:H	E:12:FUC:H2	0.411
7	A:130:ASN:HB3	C:12:FUC:C1	0.407
8	A:101:THR:HG23	B:11:SIA:C4	1.618
8	A:168:LEU:HD21	C:1:NAG:C6	1.616
8	A:101:THR:CG2	B:11:SIA:H4	1.589
8	A:168:LEU:CD2	C:1:NAG:H61	1.579
8	A:101:THR:CG2	B:11:SIA:C4	1.399
8	A:161:ARG:CG	D:11:SIA:H32	1.363
8	A:174:GLN:CG	C:12:FUC:O2	1.332
8	A:161:ARG:HG2	D:11:SIA:C3	1.331
8	A:128:GLU:C	C:11:SIA:CT	1.329
8	A:197:ASN:CB	E:10:GAL:H62	1.266
8	A:161:ARG:HD2	D:10:GAL:O3	1.261
8	A:85:THR:HG22	B:11:SIA:O	1.234
8	A:101:THR:HG23	B:11:SIA:C5	1.222

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:161:ARG:CG	D:11:SIA:C3	1.144
8	A:161:ARG:CD	D:10:GAL:O3	1.143
8	A:161:ARG:HG3	D:11:SIA:H32	1.133
8	A:161:ARG:HD2	D:10:GAL:C3	1.120
8	A:168:LEU:CG	C:1:NAG:H61	1.117
8	A:101:THR:CG2	B:11:SIA:C5	1.116
8	A:161:ARG:HH21	D:1:NAG:C2	1.094
8	A:85:THR:CG2	B:11:SIA:O	1.092
8	A:161:ARG:NH2	D:1:NAG:N	1.072
8	A:174:GLN:HG2	C:12:FUC:O2	1.068
8	A:161:ARG:HH21	D:1:NAG:C3	1.063
8	A:101:THR:HG22	B:11:SIA:H4	1.049
8	A:161:ARG:HG2	D:11:SIA:H31	1.047
8	A:168:LEU:CD2	C:1:NAG:C6	1.046
8	A:168:LEU:HD21	C:1:NAG:C5	1.039
8	A:161:ARG:NH2	D:1:NAG:C3	1.023
8	A:161:ARG:NH2	D:1:NAG:H3	1.022
8	A:101:THR:HG23	B:11:SIA:N	1.012
8	A:101:THR:CG2	B:11:SIA:N	1.010
8	A:174:GLN:HG2	C:12:FUC:HO2	1.004
8	A:197:ASN:HB3	E:10:GAL:H62	0.997
8	A:168:LEU:HD23	C:1:NAG:H61	0.969
8	A:197:ASN:CB	E:10:GAL:C6	0.968

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:101:THR:HG21	B:11:SIA:H6	0.960
8	A:128:GLU:OE2	C:11:SIA:H7	0.958
8	A:161:ARG:CD	D:10:GAL:O4	0.954
8	A:161:ARG:HD2	D:10:GAL:O4	0.942
8	A:101:THR:OG1	B:11:SIA:N	0.938
8	A:85:THR:HG23	B:11:SIA:CT	0.924
8	A:85:THR:HG22	B:11:SIA:C	0.909
8	A:199:PRO:C	E:11:SIA:H32	0.894
8	A:161:ARG:HD2	D:10:GAL:C4	0.893
8	A:198:PRO:HA	E:10:GAL:O4	0.880
8	A:161:ARG:CG	D:10:GAL:O3	0.871
8	A:174:GLN:CG	C:12:FUC:HO2	0.859
8	A:174:GLN:CD	C:12:FUC:O2	0.857
8	A:197:ASN:HB2	E:10:GAL:C6	0.854
8	A:161:ARG:CZ	D:10:GAL:H2	0.851
8	A:101:THR:HG21	B:11:SIA:C5	0.848
8	A:174:GLN:CB	C:12:FUC:O2	0.844
8	A:83:ASN:ND2	B:1:NAG:N	0.838
8	A:171:ASP:OD2	A:172:PHE:HD2	0.833
8	A:101:THR:HG21	B:11:SIA:C4	0.826
8	A:197:ASN:HB3	E:10:GAL:C6	0.825
8	A:200:LYS:O	E:11:SIA:O4	0.824
8	A:101:THR:HG21	B:11:SIA:C6	0.815

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:101:THR:HG21	B:11:SIA:H4	0.798
8	A:133:ASN:ND2	C:1:NAG:C1	0.797
8	A:83:ASN:ND2	B:1:NAG:C1	0.795
8	A:85:THR:CG2	B:11:SIA:CT	0.788
8	A:168:LEU:HD11	C:12:FUC:O2	0.781
8	A:130:ASN:CG	C:12:FUC:H3	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:168:LEU:CD2	C:1:NAG:C5	0.754
8	A:168:LEU:HD21	C:1:NAG:O5	0.750
8	A:85:THR:CG2	B:11:SIA:C	0.738
8	A:128:GLU:O	C:11:SIA:CT	0.737
8	A:198:PRO:CA	E:10:GAL:O4	0.736
8	A:161:ARG:HG3	D:11:SIA:C3	0.735
8	A:161:ARG:NE	D:10:GAL:H2	0.735
8	A:79:ASN:CB	B:1:NAG:O3	0.729
8	A:200:LYS:N	E:11:SIA:H32	0.726
8	A:168:LEU:HD21	C:1:NAG:O6	0.719
8	A:161:ARG:HD3	D:10:GAL:O4	0.708
8	A:12:PRO:HB2	B:11:SIA:O12	0.706
8	A:197:ASN:HB2	E:10:GAL:H61	0.697
8	A:174:GLN:HB3	C:12:FUC:O2	0.692

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:168:LEU:HB2	A:172:PHE:O	0.691
8	A:168:LEU:HD11	C:12:FUC:C1	0.691
8	A:199:PRO:C	E:11:SIA:C3	0.691
8	A:101:THR:CB	B:11:SIA:N	0.684
8	A:101:THR:HG23	B:11:SIA:O4	0.676
8	A:169:ASN:N	A:169:ASN:ND2	0.674
8	A:169:ASN:H	A:169:ASN:ND2	0.671
8	A:199:PRO:O	E:1:NAG:CT	0.657
8	A:130:ASN:H	C:11:SIA:CT	0.655
8	A:168:LEU:CD2	C:1:NAG:O5	0.647
8	A:168:LEU:HG	C:1:NAG:H61	0.620
8	A:149:ALA:O	E:11:SIA:O	0.611
8	A:11:ASN:HB3	A:12:PRO:HD3	0.610
8	A:79:ASN:HD22	A:80:ASN:H	0.592
8	A:117:LEU:HB3	A:118:PRO:HD3	0.591
8	A:129:PRO:N	C:11:SIA:CT	0.590
8	A:79:ASN:HB2	B:1:NAG:O3	0.589
8	A:168:LEU:HD23	C:1:NAG:H4	0.585
8	A:161:ARG:CG	D:11:SIA:C2	0.583
8	A:12:PRO:HB3	B:11:SIA:O11	0.579
8	A:133:ASN:CG	C:1:NAG:C1	0.578
8	A:12:PRO:CB	B:11:SIA:O12	0.574
8	A:101:THR:OG1	B:11:SIA:C	0.565

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:61:ASN:HB3	A:63:GLN:HG3	0.560
8	A:161:ARG:CD	D:10:GAL:C3	0.557
8	A:158:THR:HG22	A:161:ARG:NH2	0.547
8	A:12:PRO:HB2	B:11:SIA:C1	0.540
8	A:168:LEU:CG	C:1:NAG:C6	0.539
8	A:161:ARG:HH21	D:1:NAG:H3	0.539
8	A:12:PRO:CB	B:11:SIA:O11	0.538
8	A:29:THR:HG22	A:63:GLN:HG2	0.536
8	A:12:PRO:CB	B:11:SIA:C1	0.516
8	A:181:PHE:CB	D:12:FUC:H2	0.506
8	A:169:ASN:N	A:169:ASN:HD22	0.499
8	A:168:LEU:HD23	C:1:NAG:C6	0.489
8	A:168:LEU:HD11	C:12:FUC:C2	0.478
8	A:93:ILE:HB	A:94:PRO:HD3	0.477
8	A:131:SER:HA	C:11:SIA:N	0.470
8	A:161:ARG:NH1	D:10:GAL:O4	0.469
8	A:161:ARG:NH2	D:1:NAG:O3	0.468
8	A:79:ASN:HB3	B:1:NAG:O3	0.466
8	A:130:ASN:N	C:11:SIA:CT	0.446
8	A:168:LEU:CD1	C:12:FUC:C1	0.446
8	A:11:ASN:CB	A:12:PRO:HD3	0.441
8	A:149:ALA:HB3	E:11:SIA:O	0.441
8	A:83:ASN:ND2	B:1:NAG:C2	0.437

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:155:SER:HA	A:156:PRO:C	0.435
8	A:56:LYS:HD2	A:67:ILE:HD11	0.433
8	A:161:ARG:CZ	D:1:NAG:N	0.428
8	A:197:ASN:HA	A:198:PRO:C	0.427
8	A:101:THR:HG1	B:11:SIA:C	0.425
8	A:12:PRO:HB3	B:11:SIA:C1	0.422
8	A:48:LEU:HD12	A:87:LEU:HG	0.421
8	A:93:ILE:O	A:95:PRO:HD3	0.411
8	A:161:ARG:HD2	D:10:GAL:C2	0.409
8	A:83:ASN:OD1	B:11:SIA:O6	0.402
9	A:101:THR:HG23	B:11:SIA:C4	1.564
9	A:101:THR:CG2	B:11:SIA:H4	1.536
9	A:130:ASN:HD22	C:1:NAG:CT	1.292
9	A:172:PHE:HD1	C:11:SIA:CT	1.264
9	A:101:THR:CG2	B:11:SIA:C4	1.227
9	A:172:PHE:CD1	C:11:SIA:CT	1.202
9	A:199:PRO:CB	E:10:GAL:O3	1.198
9	A:149:ALA:O	E:11:SIA:O	1.164
9	A:180:LYS:N	D:11:SIA:H6	1.157
9	A:180:LYS:H	D:11:SIA:H6	1.152
9	A:79:ASN:HB3	B:1:NAG:O3	1.123
9	A:101:THR:HG21	B:11:SIA:H4	1.091
9	A:180:LYS:H	D:11:SIA:C6	1.061

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:161:ARG:NH1	D:2:NAG:H62	1.055
9	A:130:ASN:ND2	C:1:NAG:CT	1.053
9	A:180:LYS:HG3	D:11:SIA:O11	1.029
9	A:79:ASN:CB	B:1:NAG:O3	1.019
9	A:181:PHE:H	D:11:SIA:H7	1.006
9	A:130:ASN:OD1	C:1:NAG:H3	0.998
9	A:168:LEU:HB2	C:11:SIA:H6	0.992
9	A:174:GLN:HG2	C:11:SIA:C1	0.979
9	A:199:PRO:HB2	E:10:GAL:O3	0.969
9	A:199:PRO:HB2	E:11:SIA:C2	0.964
9	A:83:ASN:ND2	B:1:NAG:N	0.933
9	A:130:ASN:CG	C:10:GAL:H2	0.912
9	A:130:ASN:OD1	C:1:NAG:C3	0.901
9	A:83:ASN:ND2	B:1:NAG:C1	0.898
9	A:181:PHE:H	D:11:SIA:C7	0.886
9	A:180:LYS:N	D:11:SIA:C6	0.860
9	A:161:ARG:HH12	D:2:NAG:H62	0.857
9	A:199:PRO:CB	E:11:SIA:C2	0.849
9	A:199:PRO:HB3	E:11:SIA:O11	0.840
9	A:171:ASP:OD2	A:172:PHE:HD2	0.837
9	A:180:LYS:CA	D:11:SIA:H6	0.828
9	A:161:ARG:NE	D:1:NAG:C2	0.828
9	A:174:GLN:N	C:11:SIA:O12	0.828

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:130:ASN:ND2	C:10:GAL:H2	0.824
9	A:181:PHE:N	D:11:SIA:H7	0.821
9	A:181:PHE:CB	D:11:SIA:H7	0.816
9	A:180:LYS:N	D:11:SIA:N	0.804
9	A:161:ARG:HE	D:1:NAG:C2	0.795
9	A:130:ASN:OD1	C:10:GAL:O2	0.794
9	A:199:PRO:HB2	E:11:SIA:C3	0.793
9	A:101:THR:HG23	B:11:SIA:O4	0.790
9	A:12:PRO:HB2	B:11:SIA:O12	0.783
9	A:181:PHE:N	D:11:SIA:N	0.781
9	A:149:ALA:C	E:11:SIA:O	0.768
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:199:PRO:HB3	E:11:SIA:C1	0.750
9	A:130:ASN:CG	C:10:GAL:C2	0.749
9	A:168:LEU:HB2	A:172:PHE:O	0.691
9	A:133:ASN:OD1	C:11:SIA:H31	0.685
9	A:180:LYS:HB2	D:11:SIA:H6	0.682
9	A:149:ALA:HB3	E:11:SIA:N	0.680
9	A:169:ASN:N	A:169:ASN:ND2	0.674
9	A:169:ASN:H	A:169:ASN:ND2	0.671
9	A:180:LYS:CB	D:11:SIA:H6	0.658

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:174:GLN:CG	C:11:SIA:C1	0.654
9	A:130:ASN:CG	C:10:GAL:HO2	0.645
9	A:101:THR:HG23	B:11:SIA:H4	0.642
9	A:130:ASN:CG	C:10:GAL:O2	0.634
9	A:12:PRO:CB	B:11:SIA:O12	0.630
9	A:181:PHE:H	D:11:SIA:C6	0.629
9	A:149:ALA:HB3	E:11:SIA:C	0.619
9	A:199:PRO:CB	E:11:SIA:C1	0.619
9	A:11:ASN:HB3	A:12:PRO:HD3	0.610
9	A:101:THR:HG21	B:11:SIA:C1	0.610
9	A:161:ARG:HH12	D:2:NAG:C6	0.601
9	A:79:ASN:HD22	A:80:ASN:H	0.592
9	A:117:LEU:HB3	A:118:PRO:HD3	0.591
9	A:172:PHE:HB3	C:11:SIA:H7	0.591
9	A:197:ASN:CB	E:10:GAL:O6	0.574
9	A:181:PHE:N	D:11:SIA:H91	0.569
9	A:168:LEU:CB	C:11:SIA:H6	0.565
9	A:197:ASN:HB3	E:10:GAL:O6	0.563
9	A:61:ASN:HB3	A:63:GLN:HG3	0.560
9	A:158:THR:HG22	A:161:ARG:NH2	0.547
9	A:130:ASN:ND2	C:10:GAL:C2	0.545
9	A:101:THR:CG2	B:11:SIA:C3	0.541
9	A:172:PHE:CB	C:11:SIA:H7	0.539

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:101:THR:HG21	B:11:SIA:C4	0.538
9	A:29:THR:HG22	A:63:GLN:HG2	0.536
9	A:83:ASN:ND2	B:1:NAG:C2	0.525
9	A:172:PHE:HB3	C:11:SIA:C7	0.507
9	A:149:ALA:HB2	E:11:SIA:H91	0.499
9	A:169:ASN:N	A:169:ASN:HD22	0.499
9	A:149:ALA:HB3	E:11:SIA:O	0.498
9	A:180:LYS:C	D:11:SIA:N	0.495
9	A:83:ASN:OD1	B:11:SIA:O6	0.481
9	A:93:ILE:HB	A:94:PRO:HD3	0.477
9	A:79:ASN:CG	B:1:NAG:O3	0.471
9	A:180:LYS:CB	D:11:SIA:H91	0.469
9	A:199:PRO:CB	E:11:SIA:C3	0.464
9	A:161:ARG:NH1	D:2:NAG:C6	0.464
9	A:83:ASN:HD21	B:1:NAG:C1	0.463
9	A:181:PHE:CA	D:11:SIA:H7	0.461
9	A:197:ASN:HB2	E:10:GAL:O6	0.457
9	A:198:PRO:HA	A:199:PRO:HD3	0.457
9	A:174:GLN:HG2	C:11:SIA:O12	0.454
9	A:11:ASN:CB	A:12:PRO:HD3	0.441
9	A:199:PRO:HD3	E:10:GAL:O6	0.441
9	A:83:ASN:OD1	B:11:SIA:C3	0.438
9	A:155:SER:HA	A:156:PRO:C	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:56:LYS:HD2	A:67:ILE:HD11	0.433
9	A:168:LEU:HB2	C:11:SIA:C6	0.431
9	A:197:ASN:HA	A:198:PRO:C	0.427
9	A:180:LYS:CG	D:11:SIA:O11	0.427
9	A:79:ASN:HA	B:2:NAG:H62	0.423
9	A:48:LEU:HD12	A:87:LEU:HG	0.421
9	A:93:ILE:O	A:95:PRO:HD3	0.411
9	A:180:LYS:HB2	D:11:SIA:H91	0.408
10	A:85:THR:HG22	B:11:SIA:O	1.297
10	A:130:ASN:HD22	C:1:NAG:CT	1.264
10	A:130:ASN:CG	C:1:NAG:N	1.226
10	A:79:ASN:OD1	B:2:NAG:H62	1.198
10	A:79:ASN:OD1	B:2:NAG:C6	1.155
10	A:12:PRO:HB2	B:11:SIA:O12	1.117
10	A:85:THR:CG2	B:11:SIA:O	1.117
10	A:128:GLU:OE2	C:2:NAG:C6	1.090
10	A:130:ASN:ND2	C:1:NAG:N	1.068
10	A:130:ASN:ND2	C:1:NAG:CT	1.031
10	A:12:PRO:HB2	B:11:SIA:C1	1.025
10	A:79:ASN:HB2	B:1:NAG:O3	1.015
10	A:128:GLU:OE2	C:2:NAG:O6	0.983
10	A:161:ARG:HD2	D:10:GAL:O4	0.970
10	A:158:THR:HG21	D:1:NAG:O3	0.964

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:199:PRO:O	E:1:NAG:O	0.944
10	A:12:PRO:CB	B:11:SIA:C1	0.901
10	A:12:PRO:CB	B:11:SIA:O11	0.866
10	A:79:ASN:O	B:1:NAG:CT	0.866
10	A:130:ASN:ND2	C:1:NAG:C	0.863
10	A:12:PRO:HB3	B:11:SIA:O11	0.858
10	A:171:ASP:OD2	A:172:PHE:HD2	0.833
10	A:158:THR:CG2	D:1:NAG:O3	0.825
10	A:83:ASN:ND2	B:1:NAG:C1	0.794
10	A:128:GLU:OE2	C:2:NAG:H62	0.784
10	A:79:ASN:CB	B:1:NAG:O3	0.775
10	A:169:ASN:H	A:169:ASN:HD22	0.765
10	A:79:ASN:OD1	B:2:NAG:O6	0.764
10	A:169:ASN:HD21	A:172:PHE:HB2	0.763
10	A:178:LYS:N	D:11:SIA:CT	0.758
10	A:171:ASP:OD2	A:172:PHE:CD2	0.756
10	A:12:PRO:CB	B:11:SIA:O12	0.731
10	A:101:THR:OG1	B:11:SIA:N	0.730
10	A:130:ASN:CG	C:1:NAG:C	0.724
10	A:157:VAL:C	D:1:NAG:CT	0.709
10	A:168:LEU:HB2	A:172:PHE:O	0.691
10	A:79:ASN:N	B:1:NAG:O	0.684
10	A:169:ASN:N	A:169:ASN:ND2	0.674

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:169:ASN:H	A:169:ASN:ND2	0.671
10	A:161:ARG:CZ	D:10:GAL:H2	0.667
10	A:12:PRO:HB3	B:11:SIA:C1	0.640
10	A:161:ARG:HG2	D:11:SIA:H31	0.640
10	A:151:ASP:OD2	E:11:SIA:H6	0.632
10	A:131:SER:C	C:1:NAG:O	0.631
10	A:151:ASP:OD2	E:11:SIA:H4	0.623
10	A:161:ARG:HH21	D:1:NAG:H3	0.618
10	A:11:ASN:HB3	A:12:PRO:HD3	0.610
10	A:161:ARG:CD	D:10:GAL:O4	0.608
10	A:199:PRO:O	E:1:NAG:C	0.598
10	A:161:ARG:HH21	D:1:NAG:C3	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:157:VAL:O	D:1:NAG:CT	0.578
10	A:130:ASN:OD1	C:10:GAL:H2	0.564
10	A:61:ASN:HB3	A:63:GLN:HG3	0.560
10	A:168:LEU:HD11	C:11:SIA:H32	0.560
10	A:161:ARG:NH2	D:1:NAG:H3	0.549
10	A:158:THR:HG22	A:161:ARG:NH2	0.547
10	A:161:ARG:HG2	D:11:SIA:C3	0.540
10	A:29:THR:HG22	A:63:GLN:HG2	0.536
10	A:79:ASN:CG	B:2:NAG:H62	0.534

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:85:THR:CG2	B:11:SIA:C	0.532
10	A:79:ASN:C	B:1:NAG:CT	0.519
10	A:101:THR:HG1	B:11:SIA:C	0.514
10	A:169:ASN:N	A:169:ASN:HD22	0.499
10	A:130:ASN:CB	C:1:NAG:N	0.498
10	A:178:LYS:H	D:11:SIA:CT	0.491
10	A:130:ASN:OD1	C:10:GAL:C2	0.478
10	A:93:ILE:HB	A:94:PRO:HD3	0.477
10	A:161:ARG:NH2	D:1:NAG:C3	0.475
10	A:130:ASN:CB	C:10:GAL:H2	0.469
10	A:149:ALA:HB3	E:11:SIA:H32	0.467
10	A:161:ARG:HH21	D:1:NAG:C2	0.463
10	A:79:ASN:HB3	B:1:NAG:C	0.461
10	A:161:ARG:NE	D:10:GAL:H2	0.460
10	A:198:PRO:HA	A:199:PRO:HD3	0.457
10	A:130:ASN:OD1	C:1:NAG:N	0.452
10	A:85:THR:HG23	B:11:SIA:O	0.446
10	A:85:THR:HG23	B:11:SIA:CT	0.445
10	A:11:ASN:CB	A:12:PRO:HD3	0.441
10	A:101:THR:CB	B:11:SIA:N	0.438
10	A:79:ASN:CB	B:1:NAG:C	0.437
10	A:131:SER:C	C:1:NAG:C	0.437
10	A:155:SER:HA	A:156:PRO:C	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:161:ARG:NH2	D:1:NAG:N	0.434
10	A:128:GLU:OE2	C:2:NAG:H61	0.434
10	A:56:LYS:HD2	A:67:ILE:HD11	0.433
10	A:197:ASN:HA	A:198:PRO:C	0.427
10	A:48:LEU:HD12	A:87:LEU:HG	0.421
10	A:101:THR:HG21	B:11:SIA:H6	0.413
10	A:93:ILE:O	A:95:PRO:HD3	0.411
10	A:168:LEU:HG	C:11:SIA:C1	0.402
11	A:129:PRO:CG	C:9:NAG:CT	1.483
11	A:129:PRO:HG2	C:9:NAG:CT	1.446
11	A:130:ASN:HD22	C:1:NAG:CT	1.430
11	A:174:GLN:CB	C:10:GAL:O3	1.408
11	A:130:ASN:ND2	C:1:NAG:N	1.407
11	A:130:ASN:CG	C:1:NAG:N	1.404
11	A:172:PHE:HD1	C:11:SIA:CT	1.366
11	A:172:PHE:CA	C:11:SIA:O	1.359
11	A:172:PHE:CB	C:11:SIA:C	1.308
11	A:172:PHE:HB3	C:11:SIA:N	1.305
11	A:168:LEU:CB	C:11:SIA:O9	1.301
11	A:172:PHE:C	C:11:SIA:N	1.289
11	A:172:PHE:CA	C:11:SIA:C	1.288
11	A:172:PHE:HA	C:11:SIA:C	1.262
11	A:129:PRO:CB	C:9:NAG:CT	1.255

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:172:PHE:CA	C:11:SIA:N	1.246
11	A:172:PHE:CB	C:11:SIA:N	1.231
11	A:168:LEU:HB3	C:11:SIA:O9	1.221
11	A:130:ASN:OD1	C:1:NAG:H3	1.208
11	A:172:PHE:CD1	C:11:SIA:CT	1.179
11	A:130:ASN:ND2	C:1:NAG:CT	1.175
11	A:172:PHE:CD1	C:11:SIA:C	1.167
11	A:172:PHE:HA	C:11:SIA:O	1.154
11	A:130:ASN:HB3	C:1:NAG:O3	1.121
11	A:151:ASP:CG	E:11:SIA:H6	1.113
11	A:174:GLN:NE2	C:10:GAL:C2	1.097
11	A:174:GLN:HB3	C:10:GAL:O3	1.094
11	A:174:GLN:HE21	C:10:GAL:H2	1.086
11	A:166:ASN:O	C:11:SIA:O12	1.081
11	A:149:ALA:CB	E:10:GAL:H4	1.076
11	A:130:ASN:ND2	C:1:NAG:C	1.076
11	A:199:PRO:O	E:1:NAG:C	1.070
11	A:79:ASN:ND2	B:9:NAG:O3	1.066
11	A:174:GLN:HE21	C:10:GAL:C2	1.054
11	A:174:GLN:NE2	C:10:GAL:H2	1.040
11	A:149:ALA:HB1	E:11:SIA:O12	1.024
11	A:151:ASP:CG	E:11:SIA:C6	1.018
11	A:78:LYS:HB2	B:1:NAG:O	1.008

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:172:PHE:CG	C:11:SIA:C	1.008
11	A:172:PHE:CG	C:11:SIA:O	0.992
11	A:149:ALA:HB3	E:10:GAL:H4	0.986
11	A:174:GLN:CG	C:10:GAL:O3	0.985
11	A:168:LEU:CB	C:11:SIA:HO9	0.985
11	A:83:ASN:OD1	B:11:SIA:O7	0.979
11	A:151:ASP:OD1	E:11:SIA:H6	0.978
11	A:130:ASN:OD1	C:1:NAG:C3	0.974
11	A:172:PHE:HB3	C:11:SIA:C	0.964
11	A:78:LYS:CB	B:1:NAG:O	0.963
11	A:161:ARG:NH2	D:1:NAG:N	0.962
11	A:78:LYS:N	B:1:NAG:CT	0.956
11	A:80:ASN:ND2	B:10:GAL:H62	0.947
11	A:158:THR:OG1	D:1:NAG:H4	0.947
11	A:182:GLU:N	D:11:SIA:H7	0.943
11	A:130:ASN:CG	C:10:GAL:H2	0.938
11	A:174:GLN:HB3	C:11:SIA:C2	0.927
11	A:80:ASN:HD21	B:10:GAL:C6	0.914
11	A:80:ASN:CG	B:10:GAL:H62	0.899
11	A:172:PHE:CD1	C:11:SIA:O	0.898
11	A:172:PHE:HD1	C:11:SIA:C	0.895
11	A:80:ASN:OD1	B:10:GAL:H62	0.888
11	A:130:ASN:CG	C:1:NAG:C2	0.887

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:79:ASN:H	B:1:NAG:C	0.883
11	A:129:PRO:HB3	C:9:NAG:CT	0.881
11	A:149:ALA:CB	E:11:SIA:O12	0.876
11	A:129:PRO:CB	C:9:NAG:C	0.875
11	A:125:GLU:OE2	D:11:SIA:H4	0.871
11	A:199:PRO:O	E:1:NAG:O	0.838
11	A:171:ASP:OD2	A:172:PHE:HD2	0.837
11	A:172:PHE:CB	C:11:SIA:O	0.828
11	A:130:ASN:CG	C:1:NAG:C3	0.817
11	A:130:ASN:OD1	C:1:NAG:C2	0.809
11	A:130:ASN:ND2	C:10:GAL:H2	0.806
11	A:199:PRO:HD2	E:1:NAG:O	0.803
11	A:130:ASN:CG	C:1:NAG:H3	0.798
11	A:168:LEU:CG	C:11:SIA:O9	0.793
11	A:168:LEU:HB3	C:11:SIA:C9	0.791
11	A:130:ASN:CG	C:10:GAL:C2	0.790
11	A:174:GLN:HG2	C:11:SIA:O12	0.788
11	A:129:PRO:HB3	C:9:NAG:C	0.785
11	A:130:ASN:CG	C:1:NAG:C	0.783
11	A:169:ASN:H	A:169:ASN:HD22	0.765
11	A:130:ASN:OD1	C:10:GAL:O2	0.765
11	A:169:ASN:HD21	A:172:PHE:HB2	0.763
11	A:182:GLU:N	D:11:SIA:C7	0.757

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:149:ALA:HB1	E:11:SIA:C1	0.756
11	A:171:ASP:OD2	A:172:PHE:CD2	0.756
11	A:133:ASN:OD1	C:11:SIA:H31	0.751
11	A:103:GLN:OE1	B:11:SIA:C2	0.750
11	A:80:ASN:HD21	B:10:GAL:H62	0.749
11	A:80:ASN:OD1	B:10:GAL:O4	0.748
11	A:168:LEU:CA	C:11:SIA:O11	0.735
11	A:174:GLN:HG2	C:10:GAL:O3	0.723
11	A:172:PHE:HB3	C:11:SIA:H7	0.722
11	A:182:GLU:HB2	D:11:SIA:H7	0.699
11	A:174:GLN:NE2	C:10:GAL:O5	0.698
11	A:158:THR:HG22	D:1:NAG:C	0.692
11	A:168:LEU:HB2	A:172:PHE:O	0.691
11	A:130:ASN:CB	C:1:NAG:O3	0.690
11	A:129:PRO:HG3	C:9:NAG:CT	0.685
11	A:168:LEU:HB3	C:11:SIA:HO9	0.680
11	A:79:ASN:HB2	B:1:NAG:O3	0.679
11	A:169:ASN:N	A:169:ASN:ND2	0.674
11	A:169:ASN:H	A:169:ASN:ND2	0.671
11	A:129:PRO:HB2	C:9:NAG:C	0.641
11	A:78:LYS:CA	B:1:NAG:O	0.637
11	A:130:ASN:HB3	C:1:NAG:C3	0.624
11	A:78:LYS:N	B:1:NAG:O	0.618

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:103:GLN:OE1	B:11:SIA:C1	0.617
11	A:78:LYS:N	B:1:NAG:C	0.613
11	A:149:ALA:C	E:11:SIA:O12	0.612
11	A:11:ASN:HB3	A:12:PRO:HD3	0.610
11	A:130:ASN:HB2	C:9:NAG:C3	0.609
11	A:103:GLN:HE21	B:11:SIA:CT	0.606
11	A:129:PRO:HB2	C:9:NAG:CT	0.604
11	A:130:ASN:HB2	C:9:NAG:O4	0.598
11	A:79:ASN:HD22	A:80:ASN:H	0.592
11	A:117:LEU:HB3	A:118:PRO:HD3	0.591
11	A:174:GLN:HB3	C:10:GAL:C3	0.591
11	A:130:ASN:OD1	C:10:GAL:C2	0.591
11	A:182:GLU:CB	D:11:SIA:H7	0.588
11	A:130:ASN:CB	C:9:NAG:O4	0.574
11	A:130:ASN:CG	C:9:NAG:O4	0.571
11	A:168:LEU:N	C:11:SIA:O11	0.569
11	A:158:THR:OG1	D:1:NAG:C4	0.566
11	A:130:ASN:OD1	C:9:NAG:O4	0.561
11	A:61:ASN:HB3	A:63:GLN:HG3	0.560
11	A:12:PRO:CB	B:11:SIA:O	0.558
11	A:130:ASN:HB2	C:9:NAG:H3	0.549
11	A:174:GLN:HG2	C:11:SIA:C1	0.549
11	A:79:ASN:N	B:1:NAG:C	0.548

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:130:ASN:CB	C:1:NAG:C3	0.547
11	A:131:SER:C	C:1:NAG:O	0.547
11	A:158:THR:HG22	A:161:ARG:NH2	0.547
11	A:174:GLN:NE2	C:10:GAL:C1	0.545
11	A:174:GLN:CB	C:10:GAL:C3	0.543
11	A:29:THR:HG22	A:63:GLN:HG2	0.536
11	A:130:ASN:CB	C:1:NAG:N	0.534
11	A:130:ASN:OD1	C:1:NAG:C1	0.518
11	A:158:THR:O	D:1:NAG:C1	0.512
11	A:83:ASN:ND2	B:1:NAG:C1	0.510
11	A:12:PRO:CA	B:11:SIA:O	0.504
11	A:182:GLU:CA	D:11:SIA:H7	0.502
11	A:151:ASP:OD1	E:11:SIA:C6	0.500
11	A:199:PRO:CD	E:1:NAG:O	0.500
11	A:169:ASN:N	A:169:ASN:HD22	0.499
11	A:131:SER:C	C:1:NAG:C	0.494
11	A:151:ASP:OD1	E:11:SIA:N	0.494
11	A:149:ALA:HB3	E:10:GAL:C4	0.485
11	A:130:ASN:CG	C:10:GAL:HO2	0.485
11	A:130:ASN:ND2	C:10:GAL:C2	0.480
11	A:93:ILE:HB	A:94:PRO:HD3	0.477
11	A:79:ASN:HB2	B:1:NAG:C3	0.473
11	A:198:PRO:HA	A:199:PRO:HD3	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	A:12:PRO:HA	B:11:SIA:O	0.449
11	A:174:GLN:CB	C:11:SIA:C2	0.448
11	A:78:LYS:H	B:1:NAG:CT	0.443
11	A:11:ASN:CB	A:12:PRO:HD3	0.441
11	A:172:PHE:CB	C:11:SIA:H7	0.441
11	A:172:PHE:C	C:11:SIA:C5	0.436
11	A:155:SER:HA	A:156:PRO:C	0.435
11	A:56:LYS:HD2	A:67:ILE:HD11	0.433
11	A:158:THR:O	D:1:NAG:C2	0.433
11	A:105:TYR:CE2	B:11:SIA:O12	0.430
11	A:197:ASN:HA	A:198:PRO:C	0.427
11	A:48:LEU:HD12	A:87:LEU:HG	0.421
11	A:149:ALA:HB1	E:10:GAL:H4	0.420
11	A:93:ILE:O	A:95:PRO:HD3	0.411
11	A:129:PRO:HB2	C:9:NAG:N	0.410
11	A:181:PHE:CB	D:11:SIA:O12	0.403
12	A:199:PRO:HB2	E:1:NAG:C	1.610
12	A:131:SER:CA	C:1:NAG:CT	1.516
12	A:199:PRO:HB2	E:1:NAG:CT	1.402
12	A:79:ASN:OD1	B:9:NAG:C	1.400
12	A:199:PRO:CB	E:1:NAG:O	1.386
12	A:149:ALA:O	E:11:SIA:N	1.347
12	A:199:PRO:CB	E:1:NAG:CT	1.314

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:131:SER:HA	C:1:NAG:CT	1.302
12	A:131:SER:C	C:1:NAG:CT	1.289
12	A:199:PRO:HB2	E:1:NAG:O	1.210
12	A:169:ASN:ND2	C:11:SIA:H92	1.127
12	A:79:ASN:OD1	B:9:NAG:O3	1.083
12	A:199:PRO:CB	E:1:NAG:C	1.082
12	A:169:ASN:N	C:11:SIA:C9	1.077
12	A:199:PRO:HB3	E:1:NAG:CT	1.007
12	A:172:PHE:HD1	C:11:SIA:CT	0.968
12	A:79:ASN:OD1	B:9:NAG:N	0.959
12	A:149:ALA:C	E:11:SIA:N	0.896
12	A:78:LYS:HG2	B:2:NAG:H5	0.885
12	A:131:SER:O	C:1:NAG:CT	0.882
12	A:169:ASN:ND2	C:11:SIA:C9	0.869
12	A:79:ASN:OD1	B:9:NAG:O	0.868
12	A:130:ASN:OD1	C:1:NAG:H3	0.858
12	A:172:PHE:CD1	C:11:SIA:CT	0.847
12	A:171:ASP:OD2	A:172:PHE:HD2	0.837
12	A:78:LYS:CG	B:2:NAG:H5	0.829
12	A:199:PRO:CG	E:1:NAG:O	0.820
12	A:169:ASN:CG	C:11:SIA:H92	0.807
12	A:79:ASN:O	B:1:NAG:O	0.795
12	A:79:ASN:CG	B:9:NAG:C	0.789

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:149:ALA:O	E:11:SIA:C	0.786
12	A:79:ASN:CG	B:9:NAG:HO3	0.780
12	A:166:ASN:HB2	C:11:SIA:O12	0.773
12	A:169:ASN:H	A:169:ASN:HD22	0.765
12	A:79:ASN:CG	B:9:NAG:O3	0.763
12	A:169:ASN:HD21	A:172:PHE:HB2	0.763
12	A:171:ASP:OD2	A:172:PHE:CD2	0.756
12	A:130:ASN:OD1	C:10:GAL:O2	0.738
12	A:130:ASN:CG	C:10:GAL:O2	0.730
12	A:199:PRO:CA	E:1:NAG:O	0.718
12	A:166:ASN:CB	C:11:SIA:O12	0.702
12	A:79:ASN:C	B:1:NAG:CT	0.701
12	A:79:ASN:OD1	B:9:NAG:C3	0.696
12	A:168:LEU:HB2	A:172:PHE:O	0.691
12	A:151:ASP:OD2	E:11:SIA:O11	0.680
12	A:169:ASN:N	A:169:ASN:ND2	0.674
12	A:169:ASN:H	A:169:ASN:ND2	0.671
12	A:169:ASN:N	C:11:SIA:H91	0.661
12	A:199:PRO:C	E:1:NAG:O	0.657
12	A:79:ASN:OD1	B:9:NAG:C2	0.655
12	A:167:ARG:C	C:11:SIA:O11	0.652
12	A:172:PHE:HB3	C:11:SIA:CT	0.634
12	A:78:LYS:HB3	B:2:NAG:H5	0.616

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:11:ASN:HB3	A:12:PRO:HD3	0.610
12	A:172:PHE:O	C:11:SIA:O9	0.602
12	A:199:PRO:O	E:1:NAG:O	0.602
12	A:78:LYS:CB	B:2:NAG:H5	0.592
12	A:79:ASN:HD22	A:80:ASN:H	0.592
12	A:117:LEU:HB3	A:118:PRO:HD3	0.591
12	A:79:ASN:O	B:1:NAG:CT	0.591
12	A:151:ASP:OD2	E:11:SIA:C6	0.589
12	A:79:ASN:O	B:1:NAG:C	0.583
12	A:79:ASN:HB3	B:1:NAG:CT	0.572
12	A:172:PHE:HB3	C:11:SIA:H7	0.564
12	A:151:ASP:OD2	E:11:SIA:H6	0.561
12	A:61:ASN:HB3	A:63:GLN:HG3	0.560
12	A:199:PRO:CG	E:1:NAG:C	0.558
12	A:169:ASN:CG	C:11:SIA:C9	0.547
12	A:79:ASN:N	B:1:NAG:O3	0.539
12	A:78:LYS:HB3	B:2:NAG:C5	0.537
12	A:29:THR:HG22	A:63:GLN:HG2	0.536
12	A:79:ASN:HB2	B:1:NAG:O3	0.532
12	A:130:ASN:OD1	C:1:NAG:C3	0.522
12	A:79:ASN:CG	B:9:NAG:CT	0.514
12	A:79:ASN:HB3	B:1:NAG:C	0.514
12	A:130:ASN:CG	C:10:GAL:HO2	0.500

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:169:ASN:H	C:11:SIA:C9	0.499
12	A:169:ASN:N	A:169:ASN:HD22	0.499
12	A:79:ASN:C	B:1:NAG:C	0.493
12	A:169:ASN:HD21	C:11:SIA:H92	0.487
12	A:172:PHE:CB	C:11:SIA:H7	0.486
12	A:93:ILE:HB	A:94:PRO:HD3	0.477
12	A:199:PRO:CD	E:1:NAG:O	0.463
12	A:161:ARG:HB2	D:12:FUC:O4	0.462
12	A:79:ASN:N	B:1:NAG:O	0.462
12	A:83:ASN:ND2	B:1:NAG:C1	0.459
12	A:198:PRO:HA	A:199:PRO:HD3	0.457
12	A:130:ASN:CG	C:1:NAG:N	0.449
12	A:158:THR:HG22	A:161:ARG:NH2	0.442
12	A:11:ASN:CB	A:12:PRO:HD3	0.441
12	A:172:PHE:C	C:11:SIA:H7	0.439
12	A:172:PHE:CB	C:11:SIA:CT	0.438
12	A:155:SER:HA	A:156:PRO:C	0.435
12	A:56:LYS:HD2	A:67:ILE:HD11	0.433
12	A:130:ASN:OD1	C:1:NAG:C1	0.433
12	A:174:GLN:CG	C:11:SIA:O12	0.431
12	A:197:ASN:HA	A:198:PRO:C	0.427
12	A:151:ASP:CG	E:11:SIA:O11	0.427
12	A:79:ASN:CB	B:1:NAG:C	0.423

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:48:LEU:HD12	A:87:LEU:HG	0.421
12	A:130:ASN:ND2	C:10:GAL:O2	0.414
12	A:93:ILE:O	A:95:PRO:HD3	0.411
13	A:133:ASN:HD22	C:1:NAG:C1	1.447
13	A:168:LEU:HD23	C:11:SIA:C3	1.311
13	A:133:ASN:ND2	C:1:NAG:C1	1.303
13	A:79:ASN:HB2	B:1:NAG:O3	1.265
13	A:168:LEU:CD2	C:11:SIA:H32	1.253
13	A:103:GLN:HE22	B:11:SIA:C5	1.094
13	A:168:LEU:HD23	C:11:SIA:C2	1.083
13	A:168:LEU:HD23	C:11:SIA:H32	1.079
13	A:161:ARG:CZ	D:1:NAG:O3	1.058
13	A:101:THR:CG2	B:11:SIA:O	1.057
13	A:79:ASN:HB2	B:1:NAG:HO3	1.006
13	A:79:ASN:CB	B:1:NAG:O3	0.927
13	A:168:LEU:CD2	C:11:SIA:C3	0.905
13	A:101:THR:HG21	B:11:SIA:O	0.896
13	A:161:ARG:HE	D:1:NAG:C2	0.885
13	A:160:LYS:NZ	E:4:MAN:O6	0.880
13	A:168:LEU:CD2	C:11:SIA:C2	0.873
13	A:160:LYS:NZ	E:4:MAN:C6	0.860
13	A:168:LEU:HD22	C:11:SIA:H32	0.853
13	A:130:ASN:OD1	C:10:GAL:O4	0.848

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	A:160:LYS:HZ1	E:4:MAN:H62	0.833
13	A:171:ASP:OD2	A:172:PHE:HD2	0.833
13	A:160:LYS:NZ	E:4:MAN:H62	0.831
13	A:103:GLN:OE1	B:11:SIA:O4	0.796
13	A:161:ARG:NE	D:1:NAG:C2	0.794
13	A:79:ASN:OD1	B:2:NAG:H62	0.770
13	A:169:ASN:H	A:169:ASN:HD22	0.765
13	A:169:ASN:HD21	A:172:PHE:HB2	0.763
13	A:160:LYS:HZ1	E:4:MAN:C6	0.758
13	A:171:ASP:OD2	A:172:PHE:CD2	0.756
13	A:161:ARG:HH12	D:2:NAG:H62	0.732
13	A:161:ARG:NE	D:1:NAG:O3	0.699
13	A:168:LEU:HB2	A:172:PHE:O	0.691
13	A:103:GLN:HE22	B:11:SIA:C4	0.687
13	A:160:LYS:HZ3	E:4:MAN:C6	0.686
13	A:103:GLN:NE2	B:11:SIA:C5	0.684
13	A:169:ASN:N	A:169:ASN:ND2	0.674
13	A:169:ASN:H	A:169:ASN:ND2	0.671
13	A:83:ASN:ND2	B:1:NAG:C1	0.662
13	A:133:ASN:HD21	C:1:NAG:C1	0.654
13	A:168:LEU:CD2	C:10:GAL:O3	0.641
13	A:168:LEU:HD21	C:10:GAL:O3	0.633
13	A:101:THR:HG23	B:11:SIA:O	0.616

Model ID	Atom-1	Atom-2	Clash overlap (Å)
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:130:ASN:HB2	C:10:GAL:H61	0.590
13	A:161:ARG:NH1	D:2:NAG:H62	0.564
13	A:61:ASN:HB3	A:63:GLN:HG3	0.560
13	A:83:ASN:OD1	B:11:SIA:CT	0.558
13	A:83:ASN:ND2	B:1:NAG:N	0.548
13	A:158:THR:HG22	A:161:ARG:NH2	0.547
13	A:29:THR:HG22	A:63:GLN:HG2	0.536
13	A:161:ARG:NH2	D:1:NAG:H4	0.535
13	A:169:ASN:N	A:169:ASN:HD22	0.499
13	A:93:ILE:HB	A:94:PRO:HD3	0.477
13	A:203:ILE:HG12	E:1:NAG:CT	0.461
13	A:198:PRO:HA	A:199:PRO:HD3	0.457
13	A:11:ASN:CB	A:12:PRO:HD3	0.441
13	A:79:ASN:OD1	B:2:NAG:C6	0.437
13	A:131:SER:C	C:1:NAG:C	0.435
13	A:155:SER:HA	A:156:PRO:C	0.435
13	A:56:LYS:HD2	A:67:ILE:HD11	0.433
13	A:130:ASN:CG	C:10:GAL:H61	0.433
13	A:130:ASN:CB	C:10:GAL:H61	0.431
13	A:131:SER:O	C:1:NAG:O	0.431

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	A:197:ASN:HA	A:198:PRO:C	0.427
13	A:48:LEU:HD12	A:87:LEU:HG	0.421
13	A:161:ARG:NE	D:1:NAG:C3	0.421
13	A:93:ILE:O	A:95:PRO:HD3	0.411
13	A:161:ARG:NH2	D:1:NAG:O3	0.410
14	A:161:ARG:HG2	D:1:NAG:O	1.277
14	A:125:GLU:OE2	D:12:FUC:O3	1.199
14	A:161:ARG:CG	D:1:NAG:O	1.088
14	A:181:PHE:CB	D:12:FUC:H3	0.988
14	A:181:PHE:CB	D:12:FUC:H5	0.975
14	A:161:ARG:O	D:1:NAG:C	0.948
14	A:125:GLU:CD	D:12:FUC:O3	0.911
14	A:171:ASP:OD2	A:172:PHE:HD2	0.833
14	A:78:LYS:HG2	B:12:FUC:O3	0.794
14	A:169:ASN:H	A:169:ASN:HD22	0.765
14	A:169:ASN:HD21	A:172:PHE:HB2	0.763
14	A:171:ASP:OD2	A:172:PHE:CD2	0.756
14	A:181:PHE:CB	D:12:FUC:C3	0.742
14	A:181:PHE:CB	D:12:FUC:C5	0.707
14	A:78:LYS:CG	B:12:FUC:O3	0.698
14	A:182:GLU:HG3	D:12:FUC:O4	0.693
14	A:168:LEU:HB2	A:172:PHE:O	0.691
14	A:174:GLN:HG2	C:11:SIA:O4	0.685

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:169:ASN:N	A:169:ASN:ND2	0.674
14	A:169:ASN:H	A:169:ASN:ND2	0.671
14	A:181:PHE:CB	D:12:FUC:C4	0.662
14	A:161:ARG:O	D:1:NAG:O	0.662
14	A:161:ARG:O	D:1:NAG:CT	0.658
14	A:125:GLU:OE2	D:12:FUC:C3	0.655
14	A:11:ASN:HB3	A:12:PRO:HD3	0.610
14	A:79:ASN:HD22	A:80:ASN:H	0.592
14	A:117:LEU:HB3	A:118:PRO:HD3	0.591
14	A:125:GLU:OE1	D:12:FUC:O3	0.571
14	A:78:LYS:CB	B:12:FUC:O3	0.567
14	A:133:ASN:OD1	C:11:SIA:CT	0.562
14	A:61:ASN:HB3	A:63:GLN:HG3	0.560
14	A:158:THR:HG22	A:161:ARG:NH2	0.547
14	A:78:LYS:HB2	B:12:FUC:O2	0.542
14	A:29:THR:HG22	A:63:GLN:HG2	0.536
14	A:78:LYS:CB	B:12:FUC:O2	0.528
14	A:174:GLN:CD	C:11:SIA:O4	0.527
14	A:174:GLN:CG	C:11:SIA:O4	0.507
14	A:169:ASN:N	A:169:ASN:HD22	0.499
14	A:93:ILE:HB	A:94:PRO:HD3	0.477
14	A:78:LYS:HB3	B:12:FUC:C2	0.467
14	A:198:PRO:HA	A:199:PRO:HD3	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:11:ASN:CB	A:12:PRO:HD3	0.441
14	A:155:SER:HA	A:156:PRO:C	0.435
14	A:56:LYS:HD2	A:67:ILE:HD11	0.433
14	A:197:ASN:HA	A:198:PRO:C	0.427
14	A:48:LEU:HD12	A:87:LEU:HG	0.421
14	A:78:LYS:HB2	B:12:FUC:O3	0.411
14	A:93:ILE:O	A:95:PRO:HD3	0.411
14	A:78:LYS:HB3	B:12:FUC:O2	0.405
15	A:130:ASN:O	C:1:NAG:H61	1.198
15	A:130:ASN:O	C:1:NAG:H4	1.181
15	A:83:ASN:HD21	B:1:NAG:C2	1.161
15	A:130:ASN:O	C:1:NAG:C6	1.116
15	A:123:THR:HG21	C:12:FUC:H2	1.091
15	A:130:ASN:O	C:1:NAG:C4	1.084
15	A:131:SER:O	C:12:FUC:O2	1.081
15	A:133:ASN:ND2	C:1:NAG:C1	1.011
15	A:161:ARG:O	D:1:NAG:O	0.982
15	A:130:ASN:OD1	C:1:NAG:O	0.971
15	A:83:ASN:ND2	B:1:NAG:C2	0.970
15	A:133:ASN:HD22	C:1:NAG:C1	0.960
15	A:83:ASN:ND2	B:1:NAG:C	0.952
15	A:131:SER:HA	C:1:NAG:H61	0.946
15	A:131:SER:O	C:12:FUC:C1	0.936

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	A:83:ASN:HD21	B:1:NAG:C	0.912
15	A:130:ASN:OD1	C:1:NAG:C2	0.884
15	A:130:ASN:O	C:1:NAG:C5	0.879
15	A:131:SER:HA	C:12:FUC:C1	0.872
15	A:171:ASP:OD2	A:172:PHE:HD2	0.833
15	A:83:ASN:ND2	B:1:NAG:N	0.813
15	A:133:ASN:HD21	C:1:NAG:C2	0.812
15	A:131:SER:CA	C:1:NAG:H61	0.809
15	A:130:ASN:C	C:1:NAG:H61	0.785
15	A:169:ASN:H	A:169:ASN:HD22	0.765
15	A:169:ASN:HD21	A:172:PHE:HB2	0.763
15	A:131:SER:HA	C:1:NAG:C6	0.758
15	A:171:ASP:OD2	A:172:PHE:CD2	0.756
15	A:83:ASN:ND2	B:1:NAG:O	0.745
15	A:131:SER:O	C:12:FUC:C2	0.742
15	A:131:SER:CA	C:12:FUC:C1	0.708
15	A:130:ASN:HB3	C:1:NAG:H4	0.704
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:83:ASN:CG	B:1:NAG:N	0.665
15	A:131:SER:C	C:12:FUC:C1	0.613
15	A:11:ASN:HB3	A:12:PRO:HD3	0.610

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	A:131:SER:O	C:1:NAG:O6	0.604
15	A:133:ASN:ND2	C:1:NAG:C2	0.602
15	A:130:ASN:CB	C:1:NAG:H4	0.599
15	A:79:ASN:HD22	A:80:ASN:H	0.592
15	A:117:LEU:HB3	A:118:PRO:HD3	0.591
15	A:123:THR:HG21	C:12:FUC:C2	0.590
15	A:83:ASN:CG	B:1:NAG:C	0.572
15	A:61:ASN:HB3	A:63:GLN:HG3	0.560
15	A:158:THR:HG22	A:161:ARG:NH2	0.547
15	A:29:THR:HG22	A:63:GLN:HG2	0.536
15	A:103:GLN:CD	B:1:NAG:N	0.524
15	A:169:ASN:N	A:169:ASN:HD22	0.499
15	A:130:ASN:C	C:1:NAG:H4	0.497
15	A:93:ILE:HB	A:94:PRO:HD3	0.477
15	A:130:ASN:OD1	C:1:NAG:C	0.470
15	A:198:PRO:HA	A:199:PRO:HD3	0.457
15	A:123:THR:CG2	C:12:FUC:H2	0.443
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:197:ASN:HA	A:198:PRO:C	0.427
15	A:48:LEU:HD12	A:87:LEU:HG	0.421
15	A:93:ILE:O	A:95:PRO:HD3	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	A:105:TYR:CZ	B:2:NAG:H61	1.452
16	A:83:ASN:OD1	B:1:NAG:C1	1.344
16	A:147:PRO:HD2	E:4:MAN:O6	1.218
16	A:105:TYR:OH	B:2:NAG:C5	1.209
16	A:181:PHE:CB	D:12:FUC:O4	1.207
16	A:105:TYR:OH	B:2:NAG:O6	1.132
16	A:83:ASN:CG	B:1:NAG:C1	1.117
16	A:105:TYR:OH	B:2:NAG:C6	1.102
16	A:147:PRO:CD	E:4:MAN:O6	1.086
16	A:105:TYR:CE2	B:2:NAG:H61	0.996
16	A:83:ASN:ND2	B:1:NAG:C1	0.995
16	A:105:TYR:OH	B:2:NAG:H62	0.980
16	A:103:GLN:OE1	B:1:NAG:C3	0.953
16	A:103:GLN:OE1	B:1:NAG:O3	0.936
16	A:83:ASN:HD21	B:1:NAG:C1	0.919
16	A:105:TYR:HH	B:2:NAG:C6	0.895
16	A:147:PRO:HD3	E:4:MAN:C6	0.853
16	A:105:TYR:CE2	B:2:NAG:C6	0.844
16	A:105:TYR:CZ	B:2:NAG:C6	0.839
16	A:171:ASP:OD2	A:172:PHE:HD2	0.833
16	A:105:TYR:CZ	B:2:NAG:H62	0.803
16	A:147:PRO:CD	E:4:MAN:C6	0.770
16	A:169:ASN:H	A:169:ASN:HD22	0.765

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	A:169:ASN:HD21	A:172:PHE:HB2	0.763
16	A:181:PHE:CB	D:12:FUC:HO4	0.760
16	A:171:ASP:OD2	A:172:PHE:CD2	0.756
16	A:83:ASN:OD1	B:1:NAG:C2	0.756
16	A:147:PRO:HD3	E:4:MAN:H61	0.727
16	A:105:TYR:CZ	B:2:NAG:C5	0.724
16	A:103:GLN:OE1	B:1:NAG:H3	0.694
16	A:168:LEU:HB2	A:172:PHE:O	0.691
16	A:83:ASN:HD21	B:1:NAG:C2	0.687
16	A:125:GLU:OE2	D:12:FUC:O3	0.676
16	A:169:ASN:N	A:169:ASN:ND2	0.674
16	A:169:ASN:H	A:169:ASN:ND2	0.671
16	A:105:TYR:HH	B:2:NAG:H62	0.665
16	A:83:ASN:ND2	B:1:NAG:C2	0.650
16	A:182:GLU:N	D:12:FUC:O3	0.647
16	A:105:TYR:CE2	B:2:NAG:H62	0.641
16	A:11:ASN:HB3	A:12:PRO:HD3	0.610
16	A:83:ASN:CG	B:1:NAG:C2	0.598
16	A:79:ASN:HD22	A:80:ASN:H	0.592
16	A:117:LEU:HB3	A:118:PRO:HD3	0.591
16	A:105:TYR:CZ	B:2:NAG:H5	0.590
16	A:79:ASN:OD1	B:2:NAG:CT	0.582
16	A:172:PHE:HB3	C:1:NAG:O	0.571

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	A:61:ASN:HB3	A:63:GLN:HG3	0.560
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:OD1	B:1:NAG:N	0.526
16	A:169:ASN:N	A:169:ASN:HD22	0.499
16	A:93:ILE:HB	A:94:PRO:HD3	0.477
16	A:198:PRO:HA	A:199:PRO:HD3	0.457
16	A:181:PHE:C	D:12:FUC:O4	0.446
16	A:11:ASN:CB	A:12:PRO:HD3	0.441
16	A:149:ALA:O	E:1:NAG:CT	0.440
16	A:155:SER:HA	A:156:PRO:C	0.435
16	A:105:TYR:OH	B:2:NAG:H61	0.434
16	A:56:LYS:HD2	A:67:ILE:HD11	0.433
16	A:197:ASN:HA	A:198:PRO:C	0.427
16	A:48:LEU:HD12	A:87:LEU:HG	0.421
16	A:93:ILE:O	A:95:PRO:HD3	0.411
17	A:199:PRO:HB2	E:1:NAG:CT	1.555
17	A:130:ASN:ND2	C:1:NAG:CT	1.549
17	A:79:ASN:CG	B:2:NAG:H62	1.344
17	A:199:PRO:CB	E:1:NAG:CT	1.329
17	A:79:ASN:OD1	B:2:NAG:C6	1.281
17	A:79:ASN:OD1	B:2:NAG:H62	1.252
17	A:199:PRO:HB2	E:1:NAG:C	1.251

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:133:ASN:ND2	C:1:NAG:C1	1.244
17	A:161:ARG:NH1	D:2:NAG:H62	1.145
17	A:133:ASN:HD22	C:1:NAG:C1	1.132
17	A:83:ASN:ND2	B:1:NAG:N	1.111
17	A:131:SER:C	C:1:NAG:O	1.095
17	A:79:ASN:HB2	B:1:NAG:O3	1.028
17	A:161:ARG:CZ	D:2:NAG:H62	0.998
17	A:161:ARG:HH12	D:2:NAG:H62	0.993
17	A:130:ASN:CG	C:1:NAG:N	0.976
17	A:161:ARG:HH12	D:2:NAG:C6	0.921
17	A:161:ARG:NH2	D:2:NAG:H62	0.896
17	A:131:SER:CA	C:1:NAG:O	0.867
17	A:83:ASN:ND2	B:1:NAG:C	0.865
17	A:130:ASN:ND2	C:1:NAG:C	0.850
17	A:171:ASP:OD2	A:172:PHE:HD2	0.833
17	A:133:ASN:HD21	C:1:NAG:C1	0.792
17	A:79:ASN:OD1	B:2:NAG:O6	0.786
17	A:161:ARG:HH22	D:2:NAG:C5	0.783
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:79:ASN:CB	B:2:NAG:H62	0.755
17	A:79:ASN:CB	B:1:NAG:O3	0.748

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:161:ARG:HH22	D:2:NAG:C6	0.734
17	A:161:ARG:HH22	D:2:NAG:H62	0.732
17	A:199:PRO:HB3	E:1:NAG:CT	0.717
17	A:79:ASN:CG	B:2:NAG:C6	0.700
17	A:168:LEU:HB2	A:172:PHE:O	0.691
17	A:199:PRO:HB2	E:1:NAG:O	0.675
17	A:169:ASN:N	A:169:ASN:ND2	0.674
17	A:128:GLU:OE2	C:2:NAG:O6	0.674
17	A:169:ASN:H	A:169:ASN:ND2	0.671
17	A:131:SER:O	C:1:NAG:O	0.646
17	A:161:ARG:NH1	D:2:NAG:C6	0.633
17	A:83:ASN:HD21	B:1:NAG:C	0.624
17	A:83:ASN:HD22	B:1:NAG:C	0.611
17	A:11:ASN:HB3	A:12:PRO:HD3	0.610
17	A:161:ARG:NH2	D:2:NAG:O5	0.606
17	A:199:PRO:CB	E:1:NAG:C	0.596
17	A:79:ASN:HD22	A:80:ASN:H	0.592
17	A:117:LEU:HB3	A:118:PRO:HD3	0.591
17	A:133:ASN:ND2	C:1:NAG:C2	0.578
17	A:130:ASN:OD1	C:1:NAG:N	0.573
17	A:161:ARG:NH2	D:2:NAG:C6	0.561
17	A:130:ASN:ND2	C:1:NAG:N	0.561
17	A:61:ASN:HB3	A:63:GLN:HG3	0.560

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:158:THR:HG22	A:161:ARG:NH2	0.547
17	A:83:ASN:ND2	B:1:NAG:C1	0.547
17	A:29:THR:HG22	A:63:GLN:HG2	0.536
17	A:133:ASN:ND2	C:1:NAG:N	0.533
17	A:161:ARG:NH2	D:2:NAG:C5	0.520
17	A:199:PRO:CB	E:1:NAG:O	0.516
17	A:130:ASN:O	C:1:NAG:O	0.501
17	A:169:ASN:N	A:169:ASN:HD22	0.499
17	A:128:GLU:OE2	C:2:NAG:C6	0.493
17	A:83:ASN:ND2	B:1:NAG:C2	0.490
17	A:93:ILE:HB	A:94:PRO:HD3	0.477
17	A:198:PRO:HA	A:199:PRO:HD3	0.457
17	A:11:ASN:CB	A:12:PRO:HD3	0.441
17	A:155:SER:HA	A:156:PRO:C	0.435
17	A:56:LYS:HD2	A:67:ILE:HD11	0.433
17	A:197:ASN:HA	A:198:PRO:C	0.427
17	A:199:PRO:C	E:1:NAG:CT	0.425
17	A:83:ASN:ND2	B:1:NAG:CT	0.425
17	A:48:LEU:HD12	A:87:LEU:HG	0.421
17	A:83:ASN:HD21	B:1:NAG:CT	0.415
17	A:93:ILE:O	A:95:PRO:HD3	0.411
18	A:83:ASN:HD21	B:1:NAG:C	1.611
18	A:174:GLN:CA	C:1:NAG:CT	1.448

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	A:83:ASN:ND2	B:1:NAG:C	1.425
18	A:174:GLN:CG	C:1:NAG:CT	1.422
18	A:174:GLN:HB2	C:1:NAG:C	1.371
18	A:174:GLN:CB	C:1:NAG:C	1.336
18	A:83:ASN:ND2	B:1:NAG:N	1.254
18	A:133:ASN:CG	C:1:NAG:C1	1.251
18	A:133:ASN:OD1	C:1:NAG:C1	1.207
18	A:133:ASN:OD1	C:1:NAG:N	1.086
18	A:133:ASN:ND2	C:1:NAG:C1	1.063
18	A:133:ASN:OD1	C:1:NAG:C2	1.040
18	A:133:ASN:HD21	C:1:NAG:C2	1.040
18	A:182:GLU:N	D:12:FUC:HO3	1.017
18	A:133:ASN:ND2	C:1:NAG:C2	0.971
18	A:83:ASN:CG	B:1:NAG:N	0.945
18	A:174:GLN:HB3	C:1:NAG:N	0.933
18	A:174:GLN:HB3	C:1:NAG:CT	0.903
18	A:133:ASN:CG	C:1:NAG:C2	0.885
18	A:174:GLN:HB3	C:1:NAG:C	0.876
18	A:171:ASP:OD2	A:172:PHE:HD2	0.833
18	A:199:PRO:HB2	E:1:NAG:CT	0.798
18	A:174:GLN:CB	C:1:NAG:CT	0.795
18	A:174:GLN:CD	C:1:NAG:CT	0.790
18	A:169:ASN:H	A:169:ASN:HD22	0.765

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	A:169:ASN:HD21	A:172:PHE:HB2	0.763
18	A:171:ASP:OD2	A:172:PHE:CD2	0.756
18	A:83:ASN:ND2	B:1:NAG:C2	0.729
18	A:83:ASN:ND2	B:1:NAG:O	0.715
18	A:182:GLU:N	D:12:FUC:O3	0.706
18	A:133:ASN:OD1	C:1:NAG:C	0.698
18	A:168:LEU:HB2	A:172:PHE:O	0.691
18	A:83:ASN:HD21	B:1:NAG:CT	0.689
18	A:169:ASN:N	A:169:ASN:ND2	0.674
18	A:169:ASN:H	A:169:ASN:ND2	0.671
18	A:174:GLN:C	C:1:NAG:CT	0.647
18	A:174:GLN:HA	C:1:NAG:CT	0.613
18	A:11:ASN:HB3	A:12:PRO:HD3	0.610
18	A:199:PRO:CB	E:1:NAG:CT	0.594
18	A:79:ASN:HD22	A:80:ASN:H	0.592
18	A:117:LEU:HB3	A:118:PRO:HD3	0.591
18	A:61:ASN:HB3	A:63:GLN:HG3	0.560
18	A:168:LEU:HD21	C:1:NAG:C1	0.559
18	A:158:THR:HG22	A:161:ARG:NH2	0.547
18	A:29:THR:HG22	A:63:GLN:HG2	0.536
18	A:83:ASN:ND2	B:1:NAG:CT	0.510
18	A:169:ASN:N	A:169:ASN:HD22	0.499
18	A:174:GLN:NE2	C:1:NAG:CT	0.492

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	A:174:GLN:HE21	C:1:NAG:C	0.485
18	A:93:ILE:HB	A:94:PRO:HD3	0.477
18	A:174:GLN:HB2	C:1:NAG:CT	0.457
18	A:198:PRO:HA	A:199:PRO:HD3	0.457
18	A:11:ASN:CB	A:12:PRO:HD3	0.441
18	A:155:SER:HA	A:156:PRO:C	0.435
18	A:56:LYS:HD2	A:67:ILE:HD11	0.433
18	A:174:GLN:NE2	C:1:NAG:C	0.433
18	A:197:ASN:HA	A:198:PRO:C	0.427
18	A:48:LEU:HD12	A:87:LEU:HG	0.421
18	A:93:ILE:O	A:95:PRO:HD3	0.411
19	A:83:ASN:HD21	B:1:NAG:C	1.399
19	A:130:ASN:C	C:1:NAG:CT	1.260
19	A:11:ASN:OD1	B:11:SIA:H4	1.232
19	A:11:ASN:CG	B:11:SIA:H4	1.225
19	A:11:ASN:OD1	B:11:SIA:C1	1.160
19	A:130:ASN:CA	C:1:NAG:CT	1.115
19	A:12:PRO:HA	B:11:SIA:C	1.106
19	A:197:ASN:OD1	E:5:NAG:CT	1.094
19	A:83:ASN:ND2	B:1:NAG:C	1.089
19	A:11:ASN:OD1	B:11:SIA:C4	1.088
19	A:83:ASN:ND2	B:1:NAG:N	1.057
19	A:130:ASN:O	C:1:NAG:C	0.920

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:130:ASN:CG	C:1:NAG:N	0.913
19	A:11:ASN:OD1	B:11:SIA:C3	0.900
19	A:130:ASN:C	C:1:NAG:C	0.863
19	A:130:ASN:HA	C:1:NAG:CT	0.855
19	A:130:ASN:OD1	C:1:NAG:N	0.850
19	A:11:ASN:OD1	B:11:SIA:C2	0.847
19	A:178:LYS:C	D:1:NAG:CT	0.839
19	A:171:ASP:OD2	A:172:PHE:HD2	0.833
19	A:130:ASN:O	C:1:NAG:O	0.827
19	A:11:ASN:OD1	B:11:SIA:O12	0.820
19	A:83:ASN:ND2	B:1:NAG:C2	0.801
19	A:182:GLU:N	D:12:FUC:O5	0.799
19	A:199:PRO:HB2	E:1:NAG:O	0.790
19	A:83:ASN:CG	B:1:NAG:C1	0.787
19	A:11:ASN:ND2	B:11:SIA:H6	0.777
19	A:169:ASN:H	A:169:ASN:HD22	0.765
19	A:169:ASN:HD21	A:172:PHE:HB2	0.763
19	A:83:ASN:CG	B:1:NAG:N	0.757
19	A:171:ASP:OD2	A:172:PHE:CD2	0.756
19	A:11:ASN:OD1	B:11:SIA:H6	0.754
19	A:83:ASN:OD1	B:1:NAG:C1	0.752
19	A:12:PRO:HA	B:11:SIA:CT	0.748
19	A:11:ASN:HD21	B:11:SIA:H6	0.731

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:199:PRO:HG2	E:2:NAG:H62	0.716
19	A:11:ASN:CG	B:11:SIA:H6	0.715
19	A:168:LEU:HB2	A:172:PHE:O	0.691
19	A:83:ASN:OD1	B:1:NAG:N	0.681
19	A:169:ASN:N	A:169:ASN:ND2	0.674
19	A:169:ASN:H	A:169:ASN:ND2	0.671
19	A:131:SER:N	C:1:NAG:CT	0.658
19	A:199:PRO:CG	E:2:NAG:H62	0.647
19	A:12:PRO:CB	B:11:SIA:CT	0.630
19	A:12:PRO:HB3	B:11:SIA:CT	0.628
19	A:11:ASN:OD1	B:11:SIA:C6	0.613
19	A:11:ASN:HB3	A:12:PRO:HD3	0.610
19	A:199:PRO:CD	E:2:NAG:H62	0.608
19	A:12:PRO:CA	B:11:SIA:CT	0.602
19	A:11:ASN:CG	B:11:SIA:C4	0.600
19	A:83:ASN:CG	B:1:NAG:C2	0.599
19	A:79:ASN:HD22	A:80:ASN:H	0.592
19	A:117:LEU:HB3	A:118:PRO:HD3	0.591
19	A:83:ASN:HD21	B:1:NAG:C2	0.570
19	A:181:PHE:CB	D:2:NAG:O	0.567
19	A:199:PRO:CB	E:1:NAG:O	0.566
19	A:61:ASN:HB3	A:63:GLN:HG3	0.560
19	A:12:PRO:CA	B:11:SIA:C	0.554

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:131:SER:C	C:1:NAG:O	0.551
19	A:158:THR:HG22	A:161:ARG:NH2	0.547
19	A:12:PRO:HA	B:11:SIA:N	0.539
19	A:103:GLN:OE1	B:1:NAG:CT	0.538
19	A:29:THR:HG22	A:63:GLN:HG2	0.536
19	A:130:ASN:C	C:1:NAG:O	0.534
19	A:181:PHE:CB	D:2:NAG:C	0.507
19	A:181:PHE:CB	D:2:NAG:C2	0.504
19	A:169:ASN:N	A:169:ASN:HD22	0.499
19	A:93:ILE:HB	A:94:PRO:HD3	0.477
19	A:161:ARG:O	D:1:NAG:O	0.471
19	A:181:PHE:C	D:12:FUC:C6	0.468
19	A:198:PRO:HA	A:199:PRO:HD3	0.457
19	A:11:ASN:CB	B:11:SIA:H4	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:56:LYS:HD2	A:67:ILE:HD11	0.433
19	A:197:ASN:HA	A:198:PRO:C	0.427
19	A:125:GLU:HG3	D:12:FUC:H4	0.423
19	A:48:LEU:HD12	A:87:LEU:HG	0.421
19	A:181:PHE:CB	D:1:NAG:O4	0.416
19	A:12:PRO:CA	B:11:SIA:N	0.416
19	A:11:ASN:O	B:11:SIA:N	0.414

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:93:ILE:O	A:95:PRO:HD3	0.411
20	A:199:PRO:HB2	E:1:NAG:C	1.453
20	A:168:LEU:CD2	C:1:NAG:H5	1.342
20	A:168:LEU:HD23	C:1:NAG:H5	1.206
20	A:133:ASN:CG	C:1:NAG:C1	1.201
20	A:199:PRO:HB2	E:1:NAG:CT	1.186
20	A:199:PRO:CB	E:1:NAG:CT	1.182
20	A:133:ASN:OD1	C:1:NAG:C1	1.171
20	A:83:ASN:ND2	B:1:NAG:N	1.126
20	A:133:ASN:HD21	C:1:NAG:C2	1.070
20	A:133:ASN:ND2	C:1:NAG:C2	1.046
20	A:133:ASN:OD1	C:1:NAG:N	1.004
20	A:199:PRO:CB	E:1:NAG:C	0.971
20	A:199:PRO:O	E:1:NAG:O	0.968
20	A:199:PRO:C	E:1:NAG:O	0.962
20	A:168:LEU:HD21	C:1:NAG:H5	0.959
20	A:168:LEU:CD2	C:1:NAG:C5	0.941
20	A:199:PRO:HB2	E:1:NAG:O	0.927
20	A:199:PRO:HB3	E:1:NAG:CT	0.924
20	A:83:ASN:ND2	B:1:NAG:C	0.905
20	A:83:ASN:ND2	B:1:NAG:C1	0.893
20	A:83:ASN:ND2	B:1:NAG:C2	0.882
20	A:130:ASN:OD1	C:1:NAG:O3	0.875

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	A:83:ASN:HD21	B:1:NAG:C2	0.874
20	A:83:ASN:HD21	B:1:NAG:C	0.861
20	A:79:ASN:ND2	B:2:NAG:O6	0.854
20	A:171:ASP:OD2	A:172:PHE:HD2	0.837
20	A:79:ASN:ND2	B:2:NAG:C6	0.815
20	A:133:ASN:CG	C:1:NAG:N	0.811
20	A:181:PHE:CB	D:12:FUC:O4	0.803
20	A:133:ASN:ND2	C:1:NAG:N	0.798
20	A:133:ASN:CG	C:1:NAG:C2	0.797
20	A:79:ASN:HB3	B:1:NAG:O3	0.795
20	A:133:ASN:HD21	C:1:NAG:C	0.783
20	A:169:ASN:H	A:169:ASN:HD22	0.765
20	A:169:ASN:HD21	A:172:PHE:HB2	0.763
20	A:171:ASP:OD2	A:172:PHE:CD2	0.756
20	A:79:ASN:CB	B:1:NAG:O3	0.752
20	A:168:LEU:HD21	C:1:NAG:H3	0.732
20	A:133:ASN:OD1	C:1:NAG:C2	0.732
20	A:133:ASN:ND2	C:1:NAG:C	0.718
20	A:79:ASN:CG	B:2:NAG:O6	0.705
20	A:133:ASN:ND2	C:1:NAG:C1	0.698
20	A:168:LEU:HB2	A:172:PHE:O	0.691
20	A:168:LEU:HD21	C:1:NAG:C1	0.688
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:181:PHE:CA	D:12:FUC:O4	0.666
20	A:83:ASN:CG	B:1:NAG:C1	0.665
20	A:168:LEU:HD21	C:1:NAG:C5	0.647
20	A:79:ASN:HD21	B:2:NAG:H62	0.621
20	A:133:ASN:ND2	C:1:NAG:O	0.617
20	A:168:LEU:CD2	C:1:NAG:C1	0.615
20	A:11:ASN:HB3	A:12:PRO:HD3	0.610
20	A:79:ASN:HD21	B:2:NAG:C6	0.605
20	A:168:LEU:HD21	C:1:NAG:C3	0.596
20	A:79:ASN:HD22	A:80:ASN:H	0.592
20	A:117:LEU:HB3	A:118:PRO:HD3	0.591
20	A:199:PRO:CB	E:1:NAG:O	0.583
20	A:172:PHE:CB	C:12:FUC:H3	0.574
20	A:61:ASN:HB3	A:63:GLN:HG3	0.560
20	A:158:THR:HG22	A:161:ARG:NH2	0.547
20	A:168:LEU:HD23	C:1:NAG:C5	0.541
20	A:180:LYS:N	D:12:FUC:H3	0.540
20	A:29:THR:HG22	A:63:GLN:HG2	0.536
20	A:161:ARG:O	D:1:NAG:C	0.533
20	A:169:ASN:N	A:169:ASN:HD22	0.499
20	A:130:ASN:OD1	C:1:NAG:C3	0.494
20	A:181:PHE:HA	D:12:FUC:O4	0.482

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	A:93:ILE:HB	A:94:PRO:HD3	0.477
20	A:181:PHE:O	D:12:FUC:O2	0.460
20	A:198:PRO:HA	A:199:PRO:HD3	0.457
20	A:83:ASN:HD21	B:1:NAG:C1	0.443
20	A:180:LYS:H	D:12:FUC:H3	0.442
20	A:11:ASN:CB	A:12:PRO:HD3	0.441
20	A:130:ASN:C	C:1:NAG:CT	0.436
20	A:155:SER:HA	A:156:PRO:C	0.435
20	A:172:PHE:HB2	C:12:FUC:H3	0.435
20	A:56:LYS:HD2	A:67:ILE:HD11	0.433
20	A:180:LYS:N	D:12:FUC:C3	0.430
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
20	A:79:ASN:HB2	B:1:NAG:O3	0.404

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

Model ID	Analyzed	Favored	Allowed	Outliers
6	207	178	26	3
7	207	178	26	3
8	207	178	26	3
9	207	178	26	3
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

Model ID	Analyzed	Favored	Allowed	Outliers
6	185	144	31	10
7	185	144	31	10
8	185	144	31	10
9	185	144	31	10
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

Model ID	Chain	Residue ID	Residue type
1	A	152	LEU
1	A	169	ASN
1	A	177	LEU
1	A	185	ILE
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

Model ID	Chain	Residue ID	Residue type
3	A	185	ILE
4	A	8	PHE
4	A	18	GLU
4	A	43	ILE
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

Model ID	Chain	Residue ID	Residue type
6	A	43	ILE
6	A	73	GLU
6	A	79	ASN
6	A	135	THR
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

Model ID	Chain	Residue ID	Residue type
8	A	135	THR
8	A	152	LEU
8	A	169	ASN
8	A	177	LEU
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

Model ID	Chain	Residue ID	Residue type
10	A	177	LEU
10	A	185	ILE
11	A	8	PHE
11	A	18	GLU
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

Model ID	Chain	Residue ID	Residue type
13	A	18	GLU
13	A	43	ILE
13	A	73	GLU
13	A	79	ASN
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

Model ID	Chain	Residue ID	Residue type
15	A	79	ASN
15	A	135	THR
15	A	152	LEU
15	A	169	ASN
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

Model ID	Chain	Residue ID	Residue type
17	A	169	ASN
17	A	177	LEU
17	A	185	ILE
18	A	8	PHE
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

Model ID	Chain	Residue ID	Residue type
20	A	8	PHE
20	A	18	GLU
20	A	43	ILE
20	A	73	GLU
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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