Full wwPDB X-ray Structure Validation Report (i)

Mar 16, 2022 – 06:19 PM EDT

PDB ID	:	5ES4
Title	:	RE-REFINEMENT OF INTEGRIN ALPHAXBETA2 ECTODOMAIN IN THE CLOSED/BENT CONFORMATION
Authors	:	Sen, M.; Springer, T.A.
Deposited on	:	2015-11-16
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

The following versions of software and data (see references (i)) were used in the production of this report:

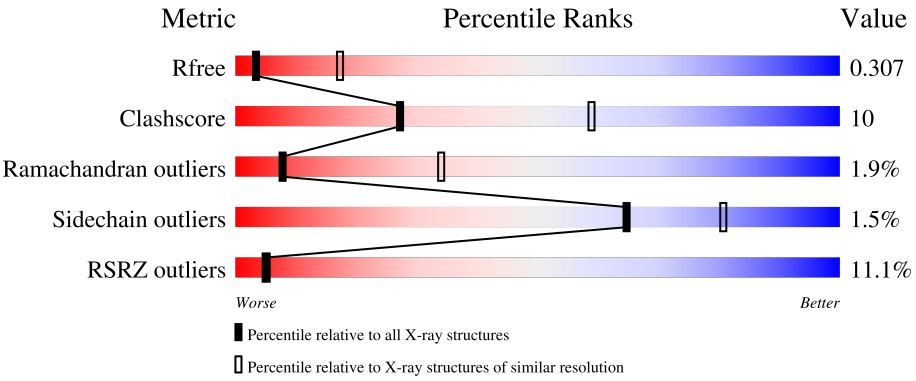
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1137	4% 71% 23% • 5%
1	C	1137	9% 58% 19% • 22%
1	E	1137	5% 55% 21% • 22%
1	G	1137	3% 57% 18% • 22%
2	B	727	11% 74% 18% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	727	27% 71% 20% • 7%
2	F	727	13% 76% 16% • 7%
2	H	727	15% 80% 12% • 7%
3	I	5	80% 20%
4	J	10	10% 70% 20%
5	K	4	100%
5	T	4	25% 75%
5	X	4	25% 75%
6	L	3	33% 33% 33%
7	M	2	50% 50%
8	N	4	50% 50%
8	S	4	25% 50% 25%
9	O	7	43% 57%
10	P	5	60% 40%
11	Q	5	20% 60% 20%
11	U	5	80% 20%
11	V	5	60% 40%
12	R	6	50% 50%
13	W	7	43% 57%
14	Y	5	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MAN	Q	5	-	-	-	X
11	MAN	U	4	-	-	-	X
12	MAN	R	4	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	MAN	W	4	-	-	-	X
13	MAN	W	5	-	-	-	X
14	NAG	Y	2	-	-	-	X
17	NAG	C	3042	-	-	-	X
17	NAG	C	3920	-	-	-	X
17	NAG	D	3232	-	-	-	X
17	NAG	D	3620	-	-	-	X
17	NAG	F	3620	-	-	-	X
17	NAG	H	3620	-	-	-	X
4	MAN	J	9	-	-	-	X
5	BMA	K	3	-	-	-	X
6	BMA	L	3	-	-	-	X
9	MAN	O	5	-	-	-	X
9	MAN	O	6	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 51071 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1080	Total	C	N	O	S	0	0	0
			8371	5289	1451	1593	38			
1	C	884	Total	C	N	O	S	0	3	0
			6834	4314	1188	1298	34			
1	E	884	Total	C	N	O	S	0	3	0
			6838	4317	1187	1300	34			
1	G	883	Total	C	N	O	S	0	1	0
			6787	4287	1170	1296	34			

There are 212 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	expression tag	UNP P20702
A	1086	CYS	-	expression tag	UNP P20702
A	1087	GLY	-	expression tag	UNP P20702
A	1088	GLY	-	expression tag	UNP P20702
A	1089	LEU	-	expression tag	UNP P20702
A	1090	GLU	-	expression tag	UNP P20702
A	1091	ASN	-	expression tag	UNP P20702
A	1092	LEU	-	expression tag	UNP P20702
A	1093	TYR	-	expression tag	UNP P20702
A	1094	PHE	-	expression tag	UNP P20702
A	1095	GLN	-	expression tag	UNP P20702
A	1096	GLY	-	expression tag	UNP P20702
A	1097	GLY	-	expression tag	UNP P20702
A	1098	GLU	-	expression tag	UNP P20702
A	1099	ASN	-	expression tag	UNP P20702
A	1100	ALA	-	expression tag	UNP P20702
A	1101	GLN	-	expression tag	UNP P20702
A	1102	CYS	-	expression tag	UNP P20702
A	1103	GLU	-	expression tag	UNP P20702
A	1104	LYS	-	expression tag	UNP P20702
A	1105	GLU	-	expression tag	UNP P20702

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1106	LEU	-	expression tag	UNP P20702
A	1107	GLN	-	expression tag	UNP P20702
A	1108	ALA	-	expression tag	UNP P20702
A	1109	LEU	-	expression tag	UNP P20702
A	1110	GLU	-	expression tag	UNP P20702
A	1111	LYS	-	expression tag	UNP P20702
A	1112	GLU	-	expression tag	UNP P20702
A	1113	ASN	-	expression tag	UNP P20702
A	1114	ALA	-	expression tag	UNP P20702
A	1115	GLN	-	expression tag	UNP P20702
A	1116	LEU	-	expression tag	UNP P20702
A	1117	GLU	-	expression tag	UNP P20702
A	1118	TRP	-	expression tag	UNP P20702
A	1119	GLU	-	expression tag	UNP P20702
A	1120	LEU	-	expression tag	UNP P20702
A	1121	GLN	-	expression tag	UNP P20702
A	1122	ALA	-	expression tag	UNP P20702
A	1123	LEU	-	expression tag	UNP P20702
A	1124	GLU	-	expression tag	UNP P20702
A	1125	LYS	-	expression tag	UNP P20702
A	1126	GLU	-	expression tag	UNP P20702
A	1127	LEU	-	expression tag	UNP P20702
A	1128	ALA	-	expression tag	UNP P20702
A	1129	GLN	-	expression tag	UNP P20702
A	1130	TRP	-	expression tag	UNP P20702
A	1131	SER	-	expression tag	UNP P20702
A	1132	HIS	-	expression tag	UNP P20702
A	1133	PRO	-	expression tag	UNP P20702
A	1134	GLN	-	expression tag	UNP P20702
A	1135	PHE	-	expression tag	UNP P20702
A	1136	GLU	-	expression tag	UNP P20702
A	1137	LYS	-	expression tag	UNP P20702
C	1085	GLY	-	expression tag	UNP P20702
C	1086	CYS	-	expression tag	UNP P20702
C	1087	GLY	-	expression tag	UNP P20702
C	1088	GLY	-	expression tag	UNP P20702
C	1089	LEU	-	expression tag	UNP P20702
C	1090	GLU	-	expression tag	UNP P20702
C	1091	ASN	-	expression tag	UNP P20702
C	1092	LEU	-	expression tag	UNP P20702
C	1093	TYR	-	expression tag	UNP P20702
C	1094	PHE	-	expression tag	UNP P20702

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	expression tag	UNP P20702
C	1096	GLY	-	expression tag	UNP P20702
C	1097	GLY	-	expression tag	UNP P20702
C	1098	GLU	-	expression tag	UNP P20702
C	1099	ASN	-	expression tag	UNP P20702
C	1100	ALA	-	expression tag	UNP P20702
C	1101	GLN	-	expression tag	UNP P20702
C	1102	CYS	-	expression tag	UNP P20702
C	1103	GLU	-	expression tag	UNP P20702
C	1104	LYS	-	expression tag	UNP P20702
C	1105	GLU	-	expression tag	UNP P20702
C	1106	LEU	-	expression tag	UNP P20702
C	1107	GLN	-	expression tag	UNP P20702
C	1108	ALA	-	expression tag	UNP P20702
C	1109	LEU	-	expression tag	UNP P20702
C	1110	GLU	-	expression tag	UNP P20702
C	1111	LYS	-	expression tag	UNP P20702
C	1112	GLU	-	expression tag	UNP P20702
C	1113	ASN	-	expression tag	UNP P20702
C	1114	ALA	-	expression tag	UNP P20702
C	1115	GLN	-	expression tag	UNP P20702
C	1116	LEU	-	expression tag	UNP P20702
C	1117	GLU	-	expression tag	UNP P20702
C	1118	TRP	-	expression tag	UNP P20702
C	1119	GLU	-	expression tag	UNP P20702
C	1120	LEU	-	expression tag	UNP P20702
C	1121	GLN	-	expression tag	UNP P20702
C	1122	ALA	-	expression tag	UNP P20702
C	1123	LEU	-	expression tag	UNP P20702
C	1124	GLU	-	expression tag	UNP P20702
C	1125	LYS	-	expression tag	UNP P20702
C	1126	GLU	-	expression tag	UNP P20702
C	1127	LEU	-	expression tag	UNP P20702
C	1128	ALA	-	expression tag	UNP P20702
C	1129	GLN	-	expression tag	UNP P20702
C	1130	TRP	-	expression tag	UNP P20702
C	1131	SER	-	expression tag	UNP P20702
C	1132	HIS	-	expression tag	UNP P20702
C	1133	PRO	-	expression tag	UNP P20702
C	1134	GLN	-	expression tag	UNP P20702
C	1135	PHE	-	expression tag	UNP P20702
C	1136	GLU	-	expression tag	UNP P20702

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1137	LYS	-	expression tag	UNP P20702
E	1085	GLY	-	expression tag	UNP P20702
E	1086	CYS	-	expression tag	UNP P20702
E	1087	GLY	-	expression tag	UNP P20702
E	1088	GLY	-	expression tag	UNP P20702
E	1089	LEU	-	expression tag	UNP P20702
E	1090	GLU	-	expression tag	UNP P20702
E	1091	ASN	-	expression tag	UNP P20702
E	1092	LEU	-	expression tag	UNP P20702
E	1093	TYR	-	expression tag	UNP P20702
E	1094	PHE	-	expression tag	UNP P20702
E	1095	GLN	-	expression tag	UNP P20702
E	1096	GLY	-	expression tag	UNP P20702
E	1097	GLY	-	expression tag	UNP P20702
E	1098	GLU	-	expression tag	UNP P20702
E	1099	ASN	-	expression tag	UNP P20702
E	1100	ALA	-	expression tag	UNP P20702
E	1101	GLN	-	expression tag	UNP P20702
E	1102	CYS	-	expression tag	UNP P20702
E	1103	GLU	-	expression tag	UNP P20702
E	1104	LYS	-	expression tag	UNP P20702
E	1105	GLU	-	expression tag	UNP P20702
E	1106	LEU	-	expression tag	UNP P20702
E	1107	GLN	-	expression tag	UNP P20702
E	1108	ALA	-	expression tag	UNP P20702
E	1109	LEU	-	expression tag	UNP P20702
E	1110	GLU	-	expression tag	UNP P20702
E	1111	LYS	-	expression tag	UNP P20702
E	1112	GLU	-	expression tag	UNP P20702
E	1113	ASN	-	expression tag	UNP P20702
E	1114	ALA	-	expression tag	UNP P20702
E	1115	GLN	-	expression tag	UNP P20702
E	1116	LEU	-	expression tag	UNP P20702
E	1117	GLU	-	expression tag	UNP P20702
E	1118	TRP	-	expression tag	UNP P20702
E	1119	GLU	-	expression tag	UNP P20702
E	1120	LEU	-	expression tag	UNP P20702
E	1121	GLN	-	expression tag	UNP P20702
E	1122	ALA	-	expression tag	UNP P20702
E	1123	LEU	-	expression tag	UNP P20702
E	1124	GLU	-	expression tag	UNP P20702
E	1125	LYS	-	expression tag	UNP P20702

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1126	GLU	-	expression tag	UNP P20702
E	1127	LEU	-	expression tag	UNP P20702
E	1128	ALA	-	expression tag	UNP P20702
E	1129	GLN	-	expression tag	UNP P20702
E	1130	TRP	-	expression tag	UNP P20702
E	1131	SER	-	expression tag	UNP P20702
E	1132	HIS	-	expression tag	UNP P20702
E	1133	PRO	-	expression tag	UNP P20702
E	1134	GLN	-	expression tag	UNP P20702
E	1135	PHE	-	expression tag	UNP P20702
E	1136	GLU	-	expression tag	UNP P20702
E	1137	LYS	-	expression tag	UNP P20702
G	1085	GLY	-	expression tag	UNP P20702
G	1086	CYS	-	expression tag	UNP P20702
G	1087	GLY	-	expression tag	UNP P20702
G	1088	GLY	-	expression tag	UNP P20702
G	1089	LEU	-	expression tag	UNP P20702
G	1090	GLU	-	expression tag	UNP P20702
G	1091	ASN	-	expression tag	UNP P20702
G	1092	LEU	-	expression tag	UNP P20702
G	1093	TYR	-	expression tag	UNP P20702
G	1094	PHE	-	expression tag	UNP P20702
G	1095	GLN	-	expression tag	UNP P20702
G	1096	GLY	-	expression tag	UNP P20702
G	1097	GLY	-	expression tag	UNP P20702
G	1098	GLU	-	expression tag	UNP P20702
G	1099	ASN	-	expression tag	UNP P20702
G	1100	ALA	-	expression tag	UNP P20702
G	1101	GLN	-	expression tag	UNP P20702
G	1102	CYS	-	expression tag	UNP P20702
G	1103	GLU	-	expression tag	UNP P20702
G	1104	LYS	-	expression tag	UNP P20702
G	1105	GLU	-	expression tag	UNP P20702
G	1106	LEU	-	expression tag	UNP P20702
G	1107	GLN	-	expression tag	UNP P20702
G	1108	ALA	-	expression tag	UNP P20702
G	1109	LEU	-	expression tag	UNP P20702
G	1110	GLU	-	expression tag	UNP P20702
G	1111	LYS	-	expression tag	UNP P20702
G	1112	GLU	-	expression tag	UNP P20702
G	1113	ASN	-	expression tag	UNP P20702
G	1114	ALA	-	expression tag	UNP P20702

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	1115	GLN	-	expression tag	UNP P20702
G	1116	LEU	-	expression tag	UNP P20702
G	1117	GLU	-	expression tag	UNP P20702
G	1118	TRP	-	expression tag	UNP P20702
G	1119	GLU	-	expression tag	UNP P20702
G	1120	LEU	-	expression tag	UNP P20702
G	1121	GLN	-	expression tag	UNP P20702
G	1122	ALA	-	expression tag	UNP P20702
G	1123	LEU	-	expression tag	UNP P20702
G	1124	GLU	-	expression tag	UNP P20702
G	1125	LYS	-	expression tag	UNP P20702
G	1126	GLU	-	expression tag	UNP P20702
G	1127	LEU	-	expression tag	UNP P20702
G	1128	ALA	-	expression tag	UNP P20702
G	1129	GLN	-	expression tag	UNP P20702
G	1130	TRP	-	expression tag	UNP P20702
G	1131	SER	-	expression tag	UNP P20702
G	1132	HIS	-	expression tag	UNP P20702
G	1133	PRO	-	expression tag	UNP P20702
G	1134	GLN	-	expression tag	UNP P20702
G	1135	PHE	-	expression tag	UNP P20702
G	1136	GLU	-	expression tag	UNP P20702
G	1137	LYS	-	expression tag	UNP P20702

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	S	0	1	0
			5191	3191	932	1004	64			
2	D	674	Total	C	N	O	S	0	0	0
			5178	3183	927	1004	64			
2	F	674	Total	C	N	O	S	0	1	0
			5189	3189	930	1006	64			
2	H	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			

There are 212 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	675	ASP	-	expression tag	UNP P05107
B	676	GLY	-	expression tag	UNP P05107
B	677	CYS	-	expression tag	UNP P05107

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	GLY	-	expression tag	UNP P05107
B	679	LEU	-	expression tag	UNP P05107
B	680	GLU	-	expression tag	UNP P05107
B	681	ASN	-	expression tag	UNP P05107
B	682	LEU	-	expression tag	UNP P05107
B	683	TYR	-	expression tag	UNP P05107
B	684	PHE	-	expression tag	UNP P05107
B	685	GLN	-	expression tag	UNP P05107
B	686	GLY	-	expression tag	UNP P05107
B	687	GLY	-	expression tag	UNP P05107
B	688	LYS	-	expression tag	UNP P05107
B	689	ASN	-	expression tag	UNP P05107
B	690	ALA	-	expression tag	UNP P05107
B	691	GLN	-	expression tag	UNP P05107
B	692	CYS	-	expression tag	UNP P05107
B	693	LYS	-	expression tag	UNP P05107
B	694	LYS	-	expression tag	UNP P05107
B	695	LYS	-	expression tag	UNP P05107
B	696	LEU	-	expression tag	UNP P05107
B	697	GLN	-	expression tag	UNP P05107
B	698	ALA	-	expression tag	UNP P05107
B	699	LEU	-	expression tag	UNP P05107
B	700	LYS	-	expression tag	UNP P05107
B	701	LYS	-	expression tag	UNP P05107
B	702	LYS	-	expression tag	UNP P05107
B	703	ASN	-	expression tag	UNP P05107
B	704	ALA	-	expression tag	UNP P05107
B	705	GLN	-	expression tag	UNP P05107
B	706	LEU	-	expression tag	UNP P05107
B	707	LYS	-	expression tag	UNP P05107
B	708	TRP	-	expression tag	UNP P05107
B	709	LYS	-	expression tag	UNP P05107
B	710	LEU	-	expression tag	UNP P05107
B	711	GLN	-	expression tag	UNP P05107
B	712	ALA	-	expression tag	UNP P05107
B	713	LEU	-	expression tag	UNP P05107
B	714	LYS	-	expression tag	UNP P05107
B	715	LYS	-	expression tag	UNP P05107
B	716	LYS	-	expression tag	UNP P05107
B	717	LEU	-	expression tag	UNP P05107
B	718	ALA	-	expression tag	UNP P05107
B	719	GLN	-	expression tag	UNP P05107

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	720	GLY	-	expression tag	UNP P05107
B	721	GLY	-	expression tag	UNP P05107
B	722	HIS	-	expression tag	UNP P05107
B	723	HIS	-	expression tag	UNP P05107
B	724	HIS	-	expression tag	UNP P05107
B	725	HIS	-	expression tag	UNP P05107
B	726	HIS	-	expression tag	UNP P05107
B	727	HIS	-	expression tag	UNP P05107
D	675	ASP	-	expression tag	UNP P05107
D	676	GLY	-	expression tag	UNP P05107
D	677	CYS	-	expression tag	UNP P05107
D	678	GLY	-	expression tag	UNP P05107
D	679	LEU	-	expression tag	UNP P05107
D	680	GLU	-	expression tag	UNP P05107
D	681	ASN	-	expression tag	UNP P05107
D	682	LEU	-	expression tag	UNP P05107
D	683	TYR	-	expression tag	UNP P05107
D	684	PHE	-	expression tag	UNP P05107
D	685	GLN	-	expression tag	UNP P05107
D	686	GLY	-	expression tag	UNP P05107
D	687	GLY	-	expression tag	UNP P05107
D	688	LYS	-	expression tag	UNP P05107
D	689	ASN	-	expression tag	UNP P05107
D	690	ALA	-	expression tag	UNP P05107
D	691	GLN	-	expression tag	UNP P05107
D	692	CYS	-	expression tag	UNP P05107
D	693	LYS	-	expression tag	UNP P05107
D	694	LYS	-	expression tag	UNP P05107
D	695	LYS	-	expression tag	UNP P05107
D	696	LEU	-	expression tag	UNP P05107
D	697	GLN	-	expression tag	UNP P05107
D	698	ALA	-	expression tag	UNP P05107
D	699	LEU	-	expression tag	UNP P05107
D	700	LYS	-	expression tag	UNP P05107
D	701	LYS	-	expression tag	UNP P05107
D	702	LYS	-	expression tag	UNP P05107
D	703	ASN	-	expression tag	UNP P05107
D	704	ALA	-	expression tag	UNP P05107
D	705	GLN	-	expression tag	UNP P05107
D	706	LEU	-	expression tag	UNP P05107
D	707	LYS	-	expression tag	UNP P05107
D	708	TRP	-	expression tag	UNP P05107

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	709	LYS	-	expression tag	UNP P05107
D	710	LEU	-	expression tag	UNP P05107
D	711	GLN	-	expression tag	UNP P05107
D	712	ALA	-	expression tag	UNP P05107
D	713	LEU	-	expression tag	UNP P05107
D	714	LYS	-	expression tag	UNP P05107
D	715	LYS	-	expression tag	UNP P05107
D	716	LYS	-	expression tag	UNP P05107
D	717	LEU	-	expression tag	UNP P05107
D	718	ALA	-	expression tag	UNP P05107
D	719	GLN	-	expression tag	UNP P05107
D	720	GLY	-	expression tag	UNP P05107
D	721	GLY	-	expression tag	UNP P05107
D	722	HIS	-	expression tag	UNP P05107
D	723	HIS	-	expression tag	UNP P05107
D	724	HIS	-	expression tag	UNP P05107
D	725	HIS	-	expression tag	UNP P05107
D	726	HIS	-	expression tag	UNP P05107
D	727	HIS	-	expression tag	UNP P05107
F	675	ASP	-	expression tag	UNP P05107
F	676	GLY	-	expression tag	UNP P05107
F	677	CYS	-	expression tag	UNP P05107
F	678	GLY	-	expression tag	UNP P05107
F	679	LEU	-	expression tag	UNP P05107
F	680	GLU	-	expression tag	UNP P05107
F	681	ASN	-	expression tag	UNP P05107
F	682	LEU	-	expression tag	UNP P05107
F	683	TYR	-	expression tag	UNP P05107
F	684	PHE	-	expression tag	UNP P05107
F	685	GLN	-	expression tag	UNP P05107
F	686	GLY	-	expression tag	UNP P05107
F	687	GLY	-	expression tag	UNP P05107
F	688	LYS	-	expression tag	UNP P05107
F	689	ASN	-	expression tag	UNP P05107
F	690	ALA	-	expression tag	UNP P05107
F	691	GLN	-	expression tag	UNP P05107
F	692	CYS	-	expression tag	UNP P05107
F	693	LYS	-	expression tag	UNP P05107
F	694	LYS	-	expression tag	UNP P05107
F	695	LYS	-	expression tag	UNP P05107
F	696	LEU	-	expression tag	UNP P05107
F	697	GLN	-	expression tag	UNP P05107

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	698	ALA	-	expression tag	UNP P05107
F	699	LEU	-	expression tag	UNP P05107
F	700	LYS	-	expression tag	UNP P05107
F	701	LYS	-	expression tag	UNP P05107
F	702	LYS	-	expression tag	UNP P05107
F	703	ASN	-	expression tag	UNP P05107
F	704	ALA	-	expression tag	UNP P05107
F	705	GLN	-	expression tag	UNP P05107
F	706	LEU	-	expression tag	UNP P05107
F	707	LYS	-	expression tag	UNP P05107
F	708	TRP	-	expression tag	UNP P05107
F	709	LYS	-	expression tag	UNP P05107
F	710	LEU	-	expression tag	UNP P05107
F	711	GLN	-	expression tag	UNP P05107
F	712	ALA	-	expression tag	UNP P05107
F	713	LEU	-	expression tag	UNP P05107
F	714	LYS	-	expression tag	UNP P05107
F	715	LYS	-	expression tag	UNP P05107
F	716	LYS	-	expression tag	UNP P05107
F	717	LEU	-	expression tag	UNP P05107
F	718	ALA	-	expression tag	UNP P05107
F	719	GLN	-	expression tag	UNP P05107
F	720	GLY	-	expression tag	UNP P05107
F	721	GLY	-	expression tag	UNP P05107
F	722	HIS	-	expression tag	UNP P05107
F	723	HIS	-	expression tag	UNP P05107
F	724	HIS	-	expression tag	UNP P05107
F	725	HIS	-	expression tag	UNP P05107
F	726	HIS	-	expression tag	UNP P05107
F	727	HIS	-	expression tag	UNP P05107
H	675	ASP	-	expression tag	UNP P05107
H	676	GLY	-	expression tag	UNP P05107
H	677	CYS	-	expression tag	UNP P05107
H	678	GLY	-	expression tag	UNP P05107
H	679	LEU	-	expression tag	UNP P05107
H	680	GLU	-	expression tag	UNP P05107
H	681	ASN	-	expression tag	UNP P05107
H	682	LEU	-	expression tag	UNP P05107
H	683	TYR	-	expression tag	UNP P05107
H	684	PHE	-	expression tag	UNP P05107
H	685	GLN	-	expression tag	UNP P05107
H	686	GLY	-	expression tag	UNP P05107

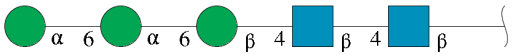
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	687	GLY	-	expression tag	UNP P05107
H	688	LYS	-	expression tag	UNP P05107
H	689	ASN	-	expression tag	UNP P05107
H	690	ALA	-	expression tag	UNP P05107
H	691	GLN	-	expression tag	UNP P05107
H	692	CYS	-	expression tag	UNP P05107
H	693	LYS	-	expression tag	UNP P05107
H	694	LYS	-	expression tag	UNP P05107
H	695	LYS	-	expression tag	UNP P05107
H	696	LEU	-	expression tag	UNP P05107
H	697	GLN	-	expression tag	UNP P05107
H	698	ALA	-	expression tag	UNP P05107
H	699	LEU	-	expression tag	UNP P05107
H	700	LYS	-	expression tag	UNP P05107
H	701	LYS	-	expression tag	UNP P05107
H	702	LYS	-	expression tag	UNP P05107
H	703	ASN	-	expression tag	UNP P05107
H	704	ALA	-	expression tag	UNP P05107
H	705	GLN	-	expression tag	UNP P05107
H	706	LEU	-	expression tag	UNP P05107
H	707	LYS	-	expression tag	UNP P05107
H	708	TRP	-	expression tag	UNP P05107
H	709	LYS	-	expression tag	UNP P05107
H	710	LEU	-	expression tag	UNP P05107
H	711	GLN	-	expression tag	UNP P05107
H	712	ALA	-	expression tag	UNP P05107
H	713	LEU	-	expression tag	UNP P05107
H	714	LYS	-	expression tag	UNP P05107
H	715	LYS	-	expression tag	UNP P05107
H	716	LYS	-	expression tag	UNP P05107
H	717	LEU	-	expression tag	UNP P05107
H	718	ALA	-	expression tag	UNP P05107
H	719	GLN	-	expression tag	UNP P05107
H	720	GLY	-	expression tag	UNP P05107
H	721	GLY	-	expression tag	UNP P05107
H	722	HIS	-	expression tag	UNP P05107
H	723	HIS	-	expression tag	UNP P05107
H	724	HIS	-	expression tag	UNP P05107
H	725	HIS	-	expression tag	UNP P05107
H	726	HIS	-	expression tag	UNP P05107
H	727	HIS	-	expression tag	UNP P05107

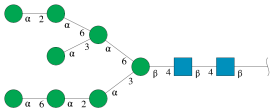
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran

ose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyra nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl ucopyranose.

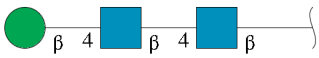


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

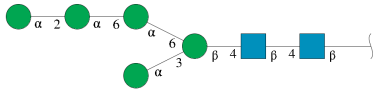
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

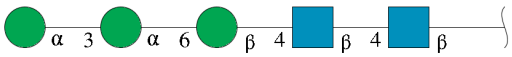
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
8	S	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



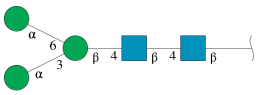
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	O	7	Total C N O 83 46 2 35	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



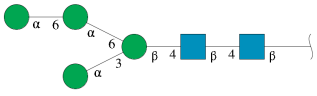
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	P	5	Total C N O 61 34 2 25	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



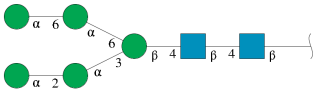
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	Q	5	Total C N O 61 34 2 25	0	0	0
11	U	5	Total C N O 61 34 2 25	0	0	0
11	V	5	Total C N O 61 34 2 25	0	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



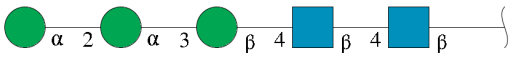
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	R	6	Total C N O 72 40 2 30	0	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	W	7	Total C N O 83 46 2 35	0	0	0

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	Y	5	Total C N O 61 34 2 25	0	0	0

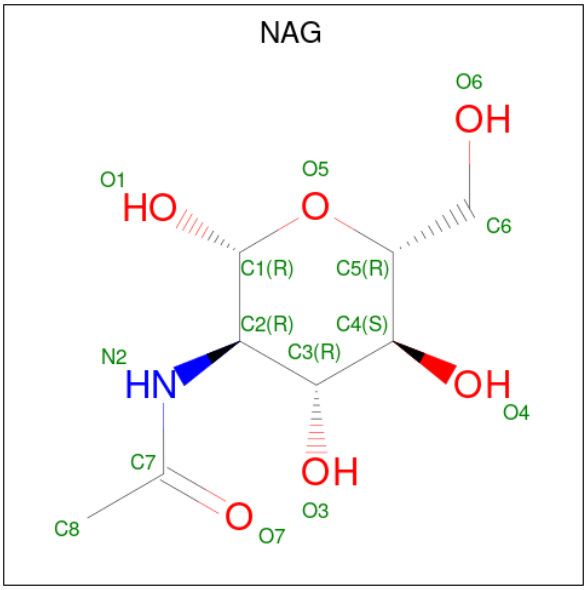
- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	3	Total Ca 3 3	0	0
15	B	1	Total Ca 1 1	0	0
15	C	3	Total Ca 3 3	0	0
15	D	1	Total Ca 1 1	0	0
15	E	3	Total Ca 3 3	0	0
15	F	1	Total Ca 1 1	0	0
15	G	3	Total Ca 3 3	0	0
15	H	1	Total Ca 1 1	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Mg 1 1	0	0

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C N O 14 8 1 5	0	0
17	A	1	Total C N O 14 8 1 5	0	0
17	A	1	Total C N O 14 8 1 5	0	0
17	A	1	Total C N O 14 8 1 5	0	0
17	B	1	Total C N O 14 8 1 5	0	0
17	B	1	Total C N O 14 8 1 5	0	0
17	C	1	Total C N O 14 8 1 5	0	0
17	C	1	Total C N O 14 8 1 5	0	0
17	C	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	C	1	Total	C	N	O	0	0
			14	8	1	5		
17	D	1	Total	C	N	O	0	0
			14	8	1	5		
17	D	1	Total	C	N	O	0	0
			14	8	1	5		
17	E	1	Total	C	N	O	0	0
			14	8	1	5		
17	E	1	Total	C	N	O	0	0
			14	8	1	5		
17	E	1	Total	C	N	O	0	0
			14	8	1	5		
17	E	1	Total	C	N	O	0	0
			14	8	1	5		
17	F	1	Total	C	N	O	0	0
			14	8	1	5		
17	F	1	Total	C	N	O	0	0
			14	8	1	5		
17	F	1	Total	C	N	O	0	0
			14	8	1	5		
17	G	1	Total	C	N	O	0	0
			14	8	1	5		
17	G	1	Total	C	N	O	0	0
			14	8	1	5		
17	G	1	Total	C	N	O	0	0
			14	8	1	5		
17	G	1	Total	C	N	O	0	0
			14	8	1	5		
17	H	1	Total	C	N	O	0	0
			14	8	1	5		
17	H	1	Total	C	N	O	0	0
			14	8	1	5		
17	H	1	Total	C	N	O	0	0
			14	8	1	5		
17	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	29	Total	O	0	0
			29	29		

Continued on next page...

Continued from previous page...

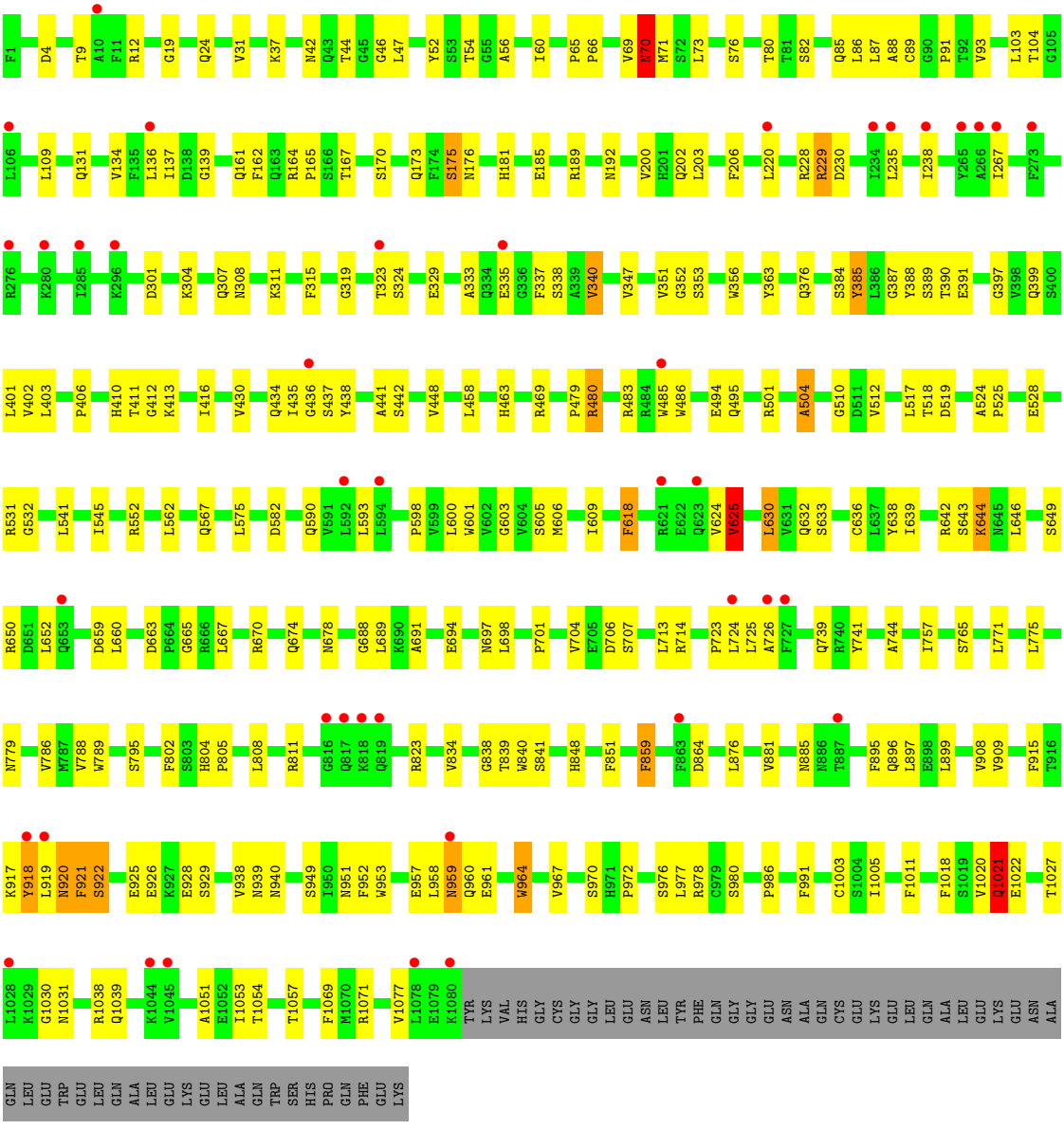
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	B	4	Total O 4 4	0	0
18	C	7	Total O 7 7	0	0
18	D	3	Total O 3 3	0	0
18	E	10	Total O 10 10	0	0
18	F	2	Total O 2 2	0	0
18	G	10	Total O 10 10	0	0
18	H	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

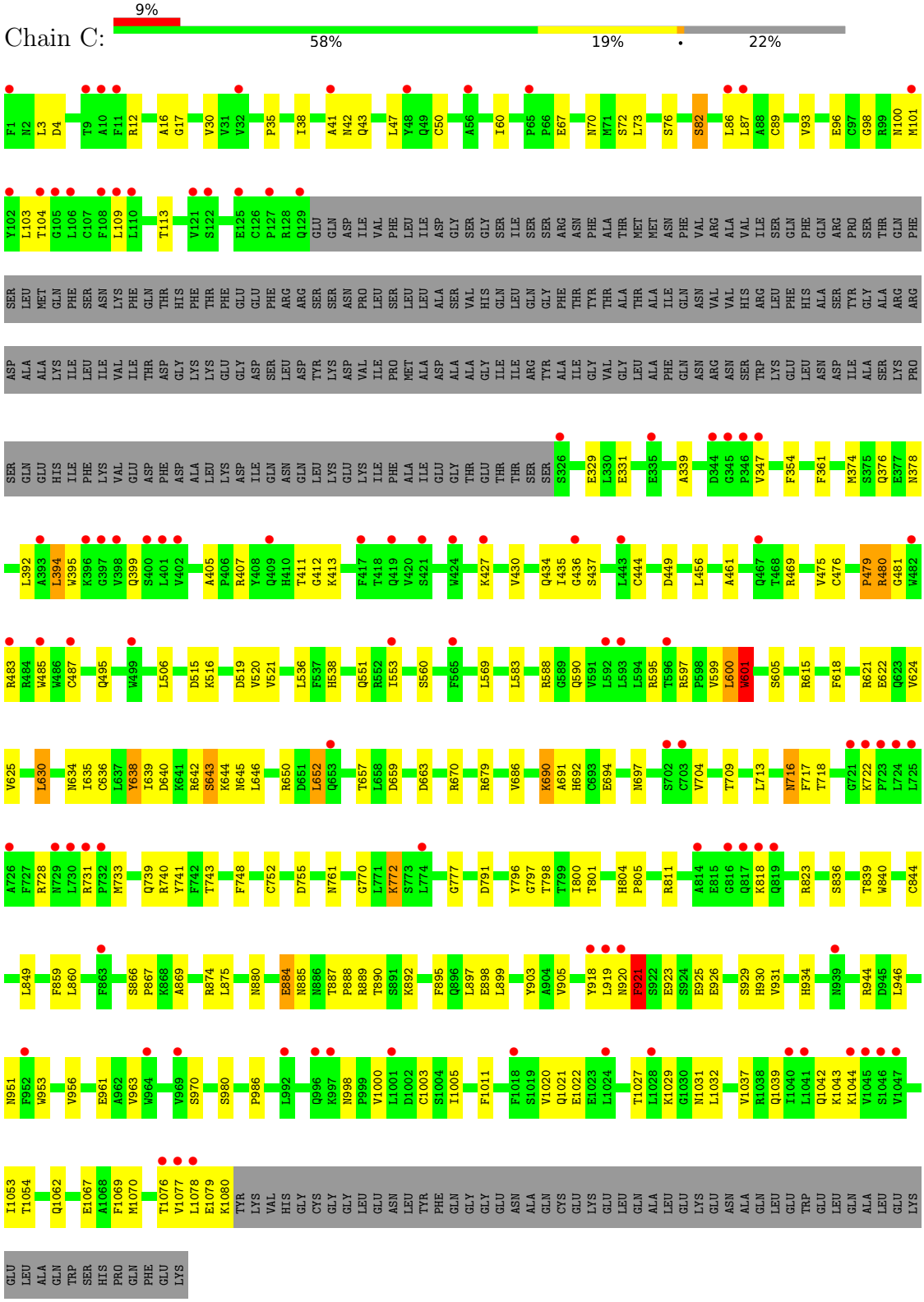
• Molecule 1: Integrin alpha-X

Chain A:



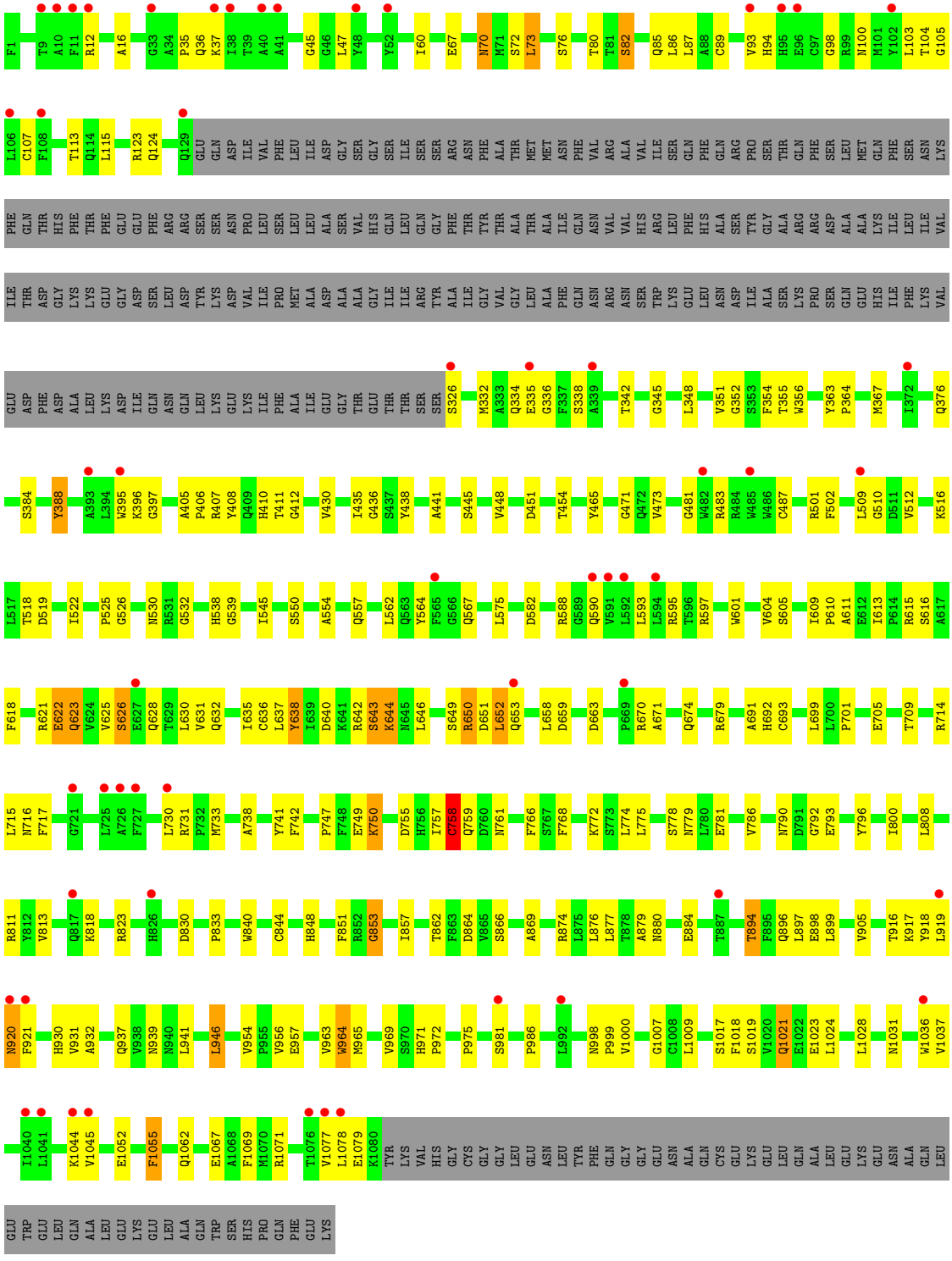
• Molecule 1: Integrin alpha-X

Chain C:



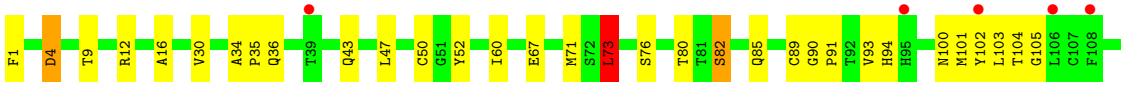
• Molecule 1: Integrin alpha-X

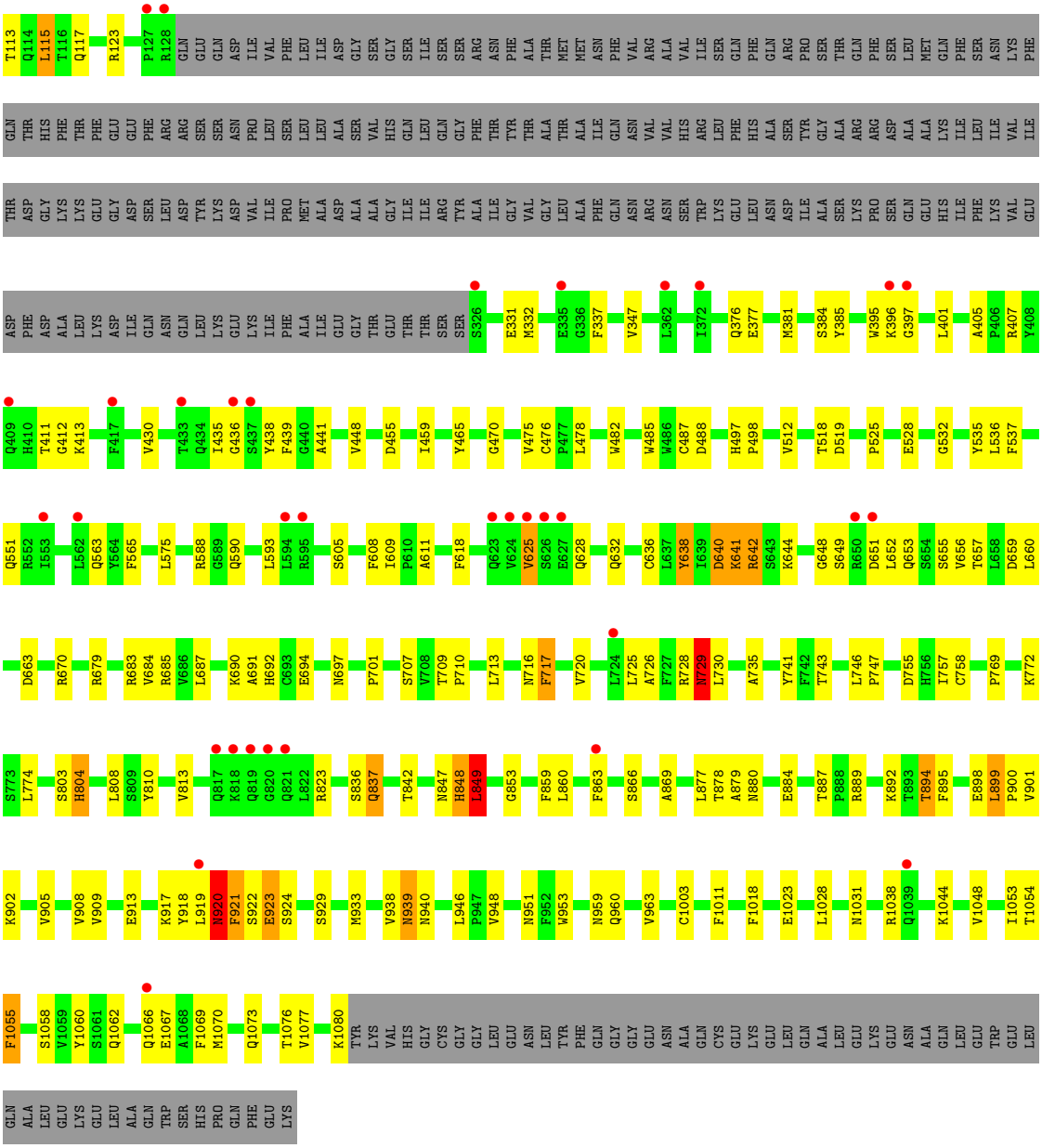
Chain E:



• Molecule 1: Integrin alpha-X

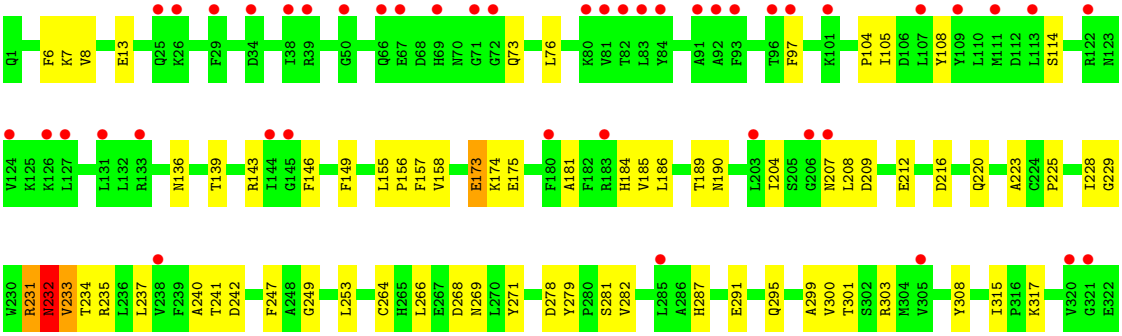
Chain G:

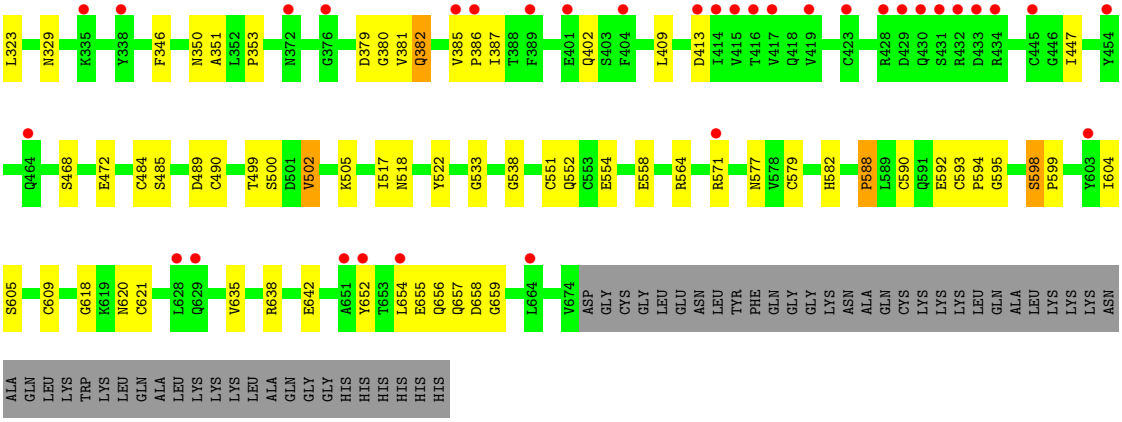




• Molecule 2: Integrin beta-2

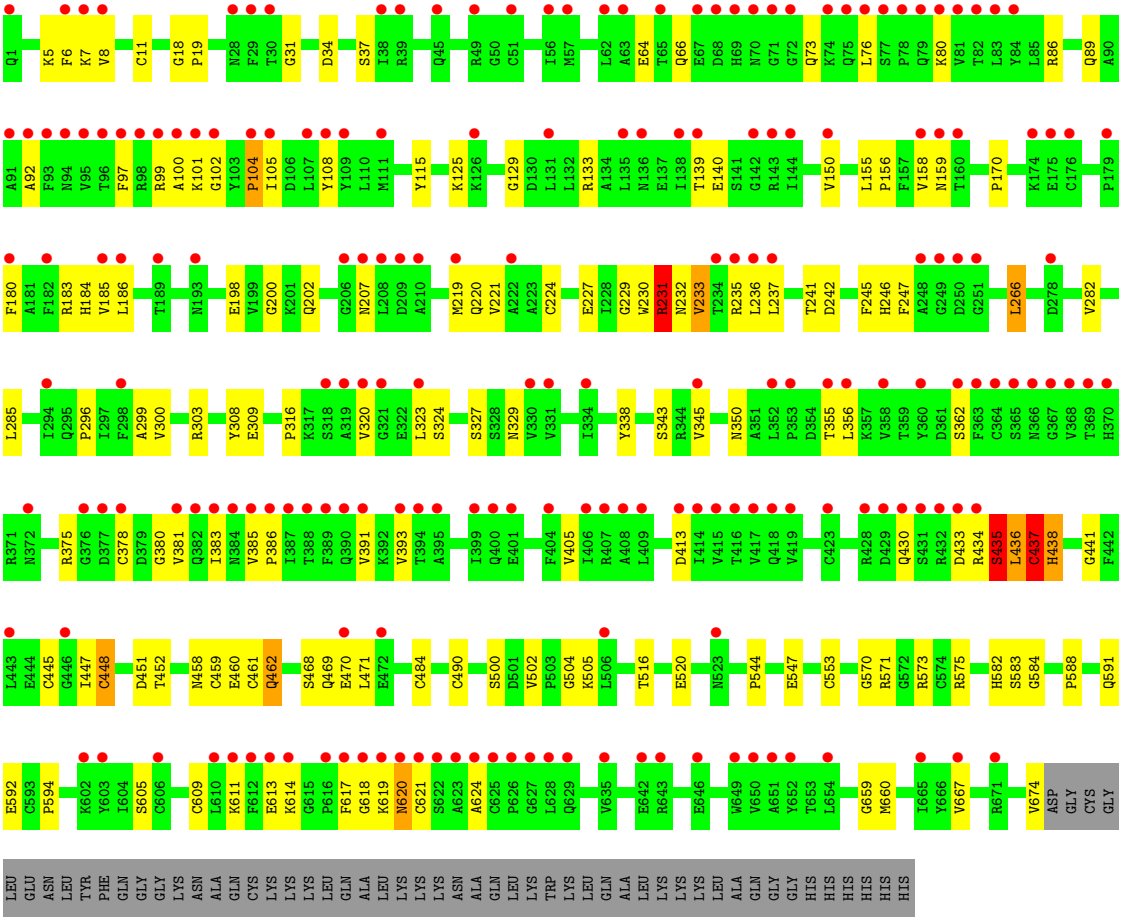
Chain B:





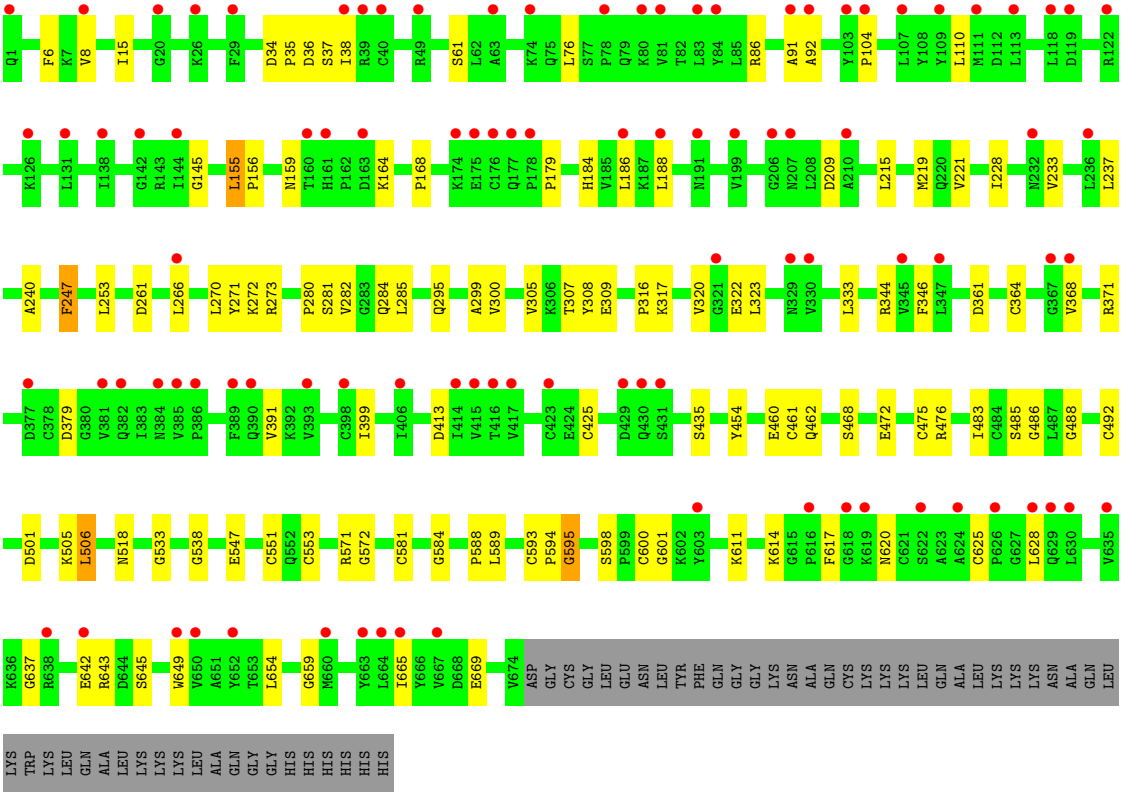
• Molecule 2: Integrin beta-2

Chain D:



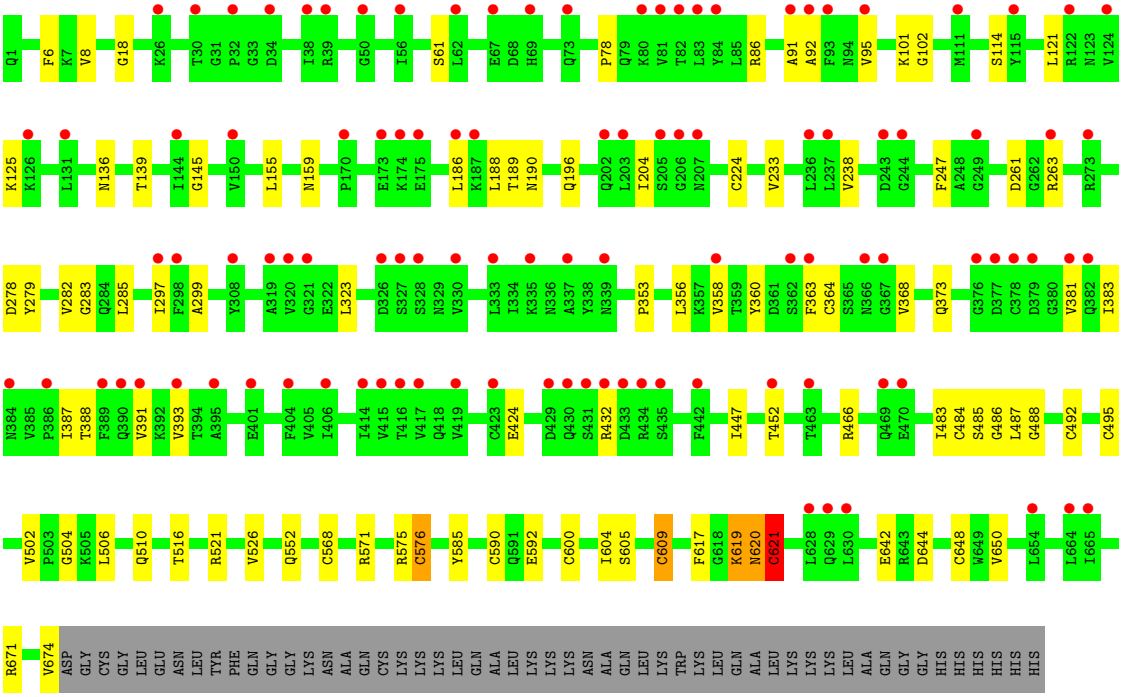
• Molecule 2: Integrin beta-2

Chain F:



• Molecule 2: Integrin beta-2

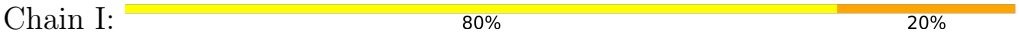
Chain H:



• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra

nose

Chain I:

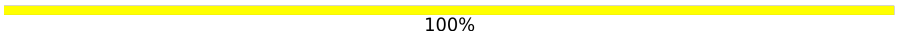


• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

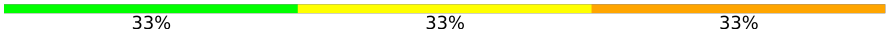
Chain T:

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

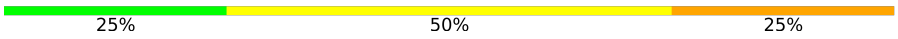
Chain M:

• Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

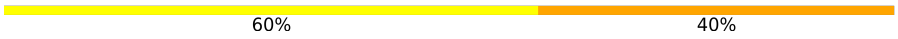


• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

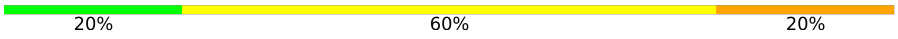
• Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



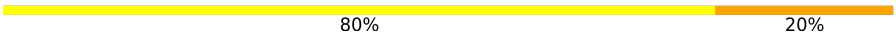
• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 12: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.03Å 163.48Å 536.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 3.30 49.51 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.51-3.30) 97.0 (49.51-3.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.257 , 0.307 0.257 , 0.307	Depositor DCC
R_{free} test set	2041 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	125.2	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 152.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	51071	wwPDB-VP
Average B, all atoms (Å^2)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/8557	0.58	2/11623 (0.0%)
1	C	0.35	1/6997 (0.0%)	0.60	2/9516 (0.0%)
1	E	0.31	0/7004	0.60	3/9526 (0.0%)
1	G	0.32	0/6941	0.60	3/9447 (0.0%)
2	B	0.31	0/5291	0.58	1/7144 (0.0%)
2	D	0.32	0/5274	0.59	2/7122 (0.0%)
2	F	0.29	0/5288	0.55	1/7140 (0.0%)
2	H	0.31	0/5280	0.56	2/7129 (0.0%)
All	All	0.32	1/50632 (0.0%)	0.58	16/68647 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	6
1	E	0	3
1	G	0	3
2	B	0	2
2	D	0	5
All	All	0	23

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	722	LYS	C-N	11.19	1.55	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	448	CYS	CA-CB-SG	9.35	130.84	114.00
1	E	115	LEU	CA-CB-CG	8.01	133.71	115.30
2	H	432	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	D	266	LEU	CA-CB-CG	-6.69	99.91	115.30
1	A	663	ASP	CB-CG-OD1	6.29	123.96	118.30
1	G	73	LEU	CA-CB-CG	6.19	129.54	115.30
1	E	73	LEU	CA-CB-CG	6.11	129.35	115.30
2	B	654	LEU	CA-CB-CG	6.08	129.29	115.30
2	H	609	CYS	CA-CB-SG	6.04	124.88	114.00
1	A	663	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	G	899	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	73	LEU	CA-CB-CG	5.39	127.70	115.30
1	G	849	LEU	CA-CB-CG	5.23	127.32	115.30
1	C	752	CYS	CA-CB-SG	-5.13	104.76	114.00
1	E	86	LEU	CA-CB-CG	5.08	126.99	115.30
2	F	492	CYS	CA-CB-SG	-5.02	104.96	114.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	ARG	Peptide
1	A	724	LEU	Peptide
1	A	82	SER	Peptide
1	A	885	ASN	Peptide
2	B	173	GLU	Peptide
2	B	231	ARG	Peptide
1	C	600	LEU	Peptide
1	C	601	TRP	Peptide
1	C	622	GLU	Peptide
1	C	690	LYS	Peptide
1	C	82	SER	Peptide
1	C	884	GLU	Peptide
2	D	102	GLY	Peptide
2	D	433	ASP	Peptide
2	D	436	LEU	Peptide
2	D	437	CYS	Peptide
2	D	620	ASN	Peptide
1	E	465	TYR	Peptide
1	E	640	ASP	Peptide
1	E	82	SER	Peptide
1	G	642	ARG	Peptide
1	G	729	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	G	82	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8371	0	8200	203	1
1	C	6834	0	6700	171	0
1	E	6838	0	6699	194	0
1	G	6787	0	6617	155	0
2	B	5191	0	4979	86	0
2	D	5178	0	4963	118	1
2	F	5189	0	4987	76	0
2	H	5184	0	4971	55	0
3	I	61	0	52	4	0
4	J	116	0	97	2	0
5	K	50	0	43	3	0
5	T	50	0	43	3	1
5	X	50	0	43	4	0
6	L	39	0	34	2	0
7	M	28	0	25	0	0
8	N	50	0	43	5	0
8	S	50	0	43	4	0
9	O	83	0	70	5	0
10	P	61	0	52	4	0
11	Q	61	0	52	1	0
11	U	61	0	52	1	0
11	V	61	0	52	9	0
12	R	72	0	61	2	0
13	W	83	0	69	4	0
14	Y	61	0	52	6	0
15	A	3	0	0	0	0
15	B	1	0	0	0	0
15	C	3	0	0	0	0
15	D	1	0	0	0	0
15	E	3	0	0	0	0
15	F	1	0	0	0	0
15	G	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	1	0	0	0	0
16	A	1	0	0	0	0
17	A	56	0	52	3	0
17	B	28	0	26	0	0
17	C	56	0	52	7	0
17	D	28	0	26	2	0
17	E	56	0	52	1	0
17	F	42	0	39	1	0
17	G	56	0	52	5	0
17	H	56	0	52	2	0
18	A	29	0	0	3	0
18	B	4	0	0	1	0
18	C	7	0	0	4	0
18	D	3	0	0	0	0
18	E	10	0	0	3	0
18	F	2	0	0	2	0
18	G	10	0	0	0	0
18	H	2	0	0	1	0
All	All	51071	0	49350	1016	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1016) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASN:HA	1:A:311:LYS:HD2	1.62	0.80
1:E:481:GLY:HA2	1:E:1021:GLN:HB2	1.66	0.76
1:A:438:TYR:HD1	1:A:441:ALA:HB2	1.54	0.73
1:E:919:LEU:HD21	1:E:930:HIS:HB3	1.70	0.73
2:D:99:ARG:NH2	2:D:338:TYR:OH	2.22	0.73
2:D:185:VAL:HG12	2:D:186:LEU:HG	1.70	0.72
1:A:688:GLY:HA3	1:E:632:GLN:OE1	1.89	0.72
1:E:622:GLU:OE1	1:G:960:GLN:NE2	2.23	0.72
1:G:823:ARG:HG3	1:G:859:PHE:HB2	1.70	0.72
1:G:642:ARG:HA	1:G:644:LYS:HG3	1.71	0.72
2:D:434:ARG:O	2:D:435:SER:HB3	1.91	0.71
1:G:438:TYR:HD1	1:G:441:ALA:HB2	1.56	0.71
1:C:659:ASP:HB2	1:C:716:ASN:HB2	1.71	0.70
1:E:659:ASP:HB2	1:E:716:ASN:OD1	1.91	0.70
1:A:434:GLN:HB3	1:A:437:SER:HB3	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:604:ILE:HD11	2:H:642:GLU:HB2	1.73	0.70
1:E:917:LYS:NZ	2:F:642:GLU:OE1	2.24	0.69
2:B:158:VAL:HG12	2:B:207:ASN:HA	1.72	0.69
1:C:407:ARG:NH2	2:D:245:PHE:O	2.25	0.69
1:E:93:VAL:HB	1:E:104:THR:O	1.93	0.69
1:G:716:ASN:HB3	1:G:741:TYR:CE1	2.28	0.69
11:V:1:NAG:O7	11:V:1:NAG:O3	2.09	0.69
1:A:173:GLN:HE22	1:A:202:GLN:HA	1.58	0.69
1:E:918:TYR:HE1	1:E:1079:GLU:HB3	1.58	0.69
1:E:757:ILE:O	1:E:758:CYS:HB2	1.92	0.68
1:A:161:GLN:HG2	1:A:311:LYS:HD3	1.75	0.68
1:C:739:GLN:HG3	1:C:741:TYR:H	1.58	0.68
1:E:12:ARG:NE	1:E:590:GLN:OE1	2.27	0.68
1:A:307:GLN:HG2	1:A:311:LYS:HE3	1.74	0.68
1:C:741:TYR:OH	10:P:1:NAG:O5	2.11	0.68
1:E:481:GLY:HA2	1:E:1021:GLN:CB	2.23	0.68
1:A:406:PRO:HB3	1:A:438:TYR:CZ	2.30	0.67
11:V:3:BMA:H5	11:V:5:MAN:H3	1.76	0.67
2:B:184:HIS:NE2	2:B:186:LEU:O	2.27	0.67
1:C:748:PHE:O	1:C:885:ASN:ND2	2.24	0.67
2:D:76:LEU:HD21	2:D:97:PHE:HD1	1.60	0.67
1:A:479:PRO:HD3	1:A:485:TRP:CD1	2.29	0.67
2:D:104:PRO:HB3	2:D:139:THR:HB	1.76	0.67
1:C:601:TRP:HZ3	1:C:639:ILE:HG22	1.59	0.67
2:B:379:ASP:OD1	2:B:380:GLY:N	2.28	0.67
1:G:899:LEU:HD12	1:G:900:PRO:HD2	1.77	0.66
1:C:100:ASN:HB2	2:D:159:ASN:ND2	2.11	0.66
1:C:956:VAL:O	1:C:963:VAL:N	2.26	0.66
2:B:232:ASN:O	2:B:233:VAL:HG13	1.95	0.66
2:F:271:TYR:O	2:F:273:ARG:N	2.28	0.66
1:A:311:LYS:HB3	1:A:315:PHE:HE2	1.61	0.66
2:D:343:SER:HA	2:D:381:VAL:O	1.95	0.66
11:V:2:NAG:O7	11:V:2:NAG:O3	2.11	0.65
1:C:638:TYR:HB3	1:C:691:ALA:HB2	1.77	0.65
1:E:410:HIS:CD2	2:F:307:THR:HG21	2.31	0.65
1:A:528:GLU:O	1:A:531:ARG:HG2	1.96	0.65
1:A:71:MET:HB3	1:A:93:VAL:HG22	1.78	0.65
1:C:411:THR:HG22	1:C:435:ILE:HA	1.79	0.65
1:C:521:VAL:HG12	1:C:569:LEU:HD13	1.79	0.65
17:C:3920:NAG:H5	2:D:674:VAL:HG21	1.78	0.64
1:A:517:LEU:HD11	1:A:541:LEU:HD23	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:LYS:NZ	2:B:642:GLU:HB3	2.12	0.64
1:A:329:GLU:OE2	4:J:2:NAG:H5	1.97	0.64
1:G:741:TYR:CD2	2:H:502:VAL:HG12	2.33	0.64
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.33	0.64
2:F:261:ASP:OD1	2:F:261:ASP:N	2.31	0.64
1:G:71:MET:HB3	1:G:93:VAL:HG22	1.80	0.64
1:E:354:PHE:HB3	8:S:1:NAG:H83	1.80	0.64
1:A:929:SER:OG	17:A:3031:NAG:O7	2.15	0.63
2:H:605:SER:O	2:H:609:CYS:HB2	1.98	0.63
13:W:3:BMA:O4	13:W:4:MAN:H3	1.99	0.63
1:E:775:LEU:HB3	1:E:778:SER:HB3	1.79	0.63
1:A:139:GLY:HA3	1:A:173:GLN:HE21	1.62	0.63
1:E:103:LEU:HD21	2:F:155:LEU:HD13	1.81	0.63
1:E:451:ASP:OD2	18:E:4001:HOH:O	2.15	0.63
2:H:619:LYS:O	2:H:621:CYS:N	2.31	0.63
1:E:67:GLU:HG2	1:E:123:ARG:HD3	1.81	0.63
2:F:593:CYS:O	2:F:595:GLY:N	2.32	0.62
1:G:76:SER:HB3	1:G:89:CYS:HB2	1.80	0.62
1:A:436:GLY:HA3	2:B:282:VAL:HG21	1.79	0.62
1:A:1071:ARG:HH21	1:C:755:ASP:HB2	1.64	0.62
1:E:471:GLY:HA3	1:E:502:PHE:HB3	1.81	0.62
1:E:811[B]:ARG:NH1	18:E:4003:HOH:O	2.31	0.62
2:B:225:PRO:HA	2:B:229:GLY:H	1.63	0.62
1:E:407:ARG:O	1:E:410:HIS:N	2.30	0.62
1:A:605:SER:HB3	1:A:636:CYS:HB2	1.82	0.62
1:C:918:TYR:CE1	1:C:1079:GLU:HB3	2.35	0.62
1:C:791:ASP:HB2	18:C:4006:HOH:O	2.00	0.62
1:A:562:LEU:HD21	1:A:590:GLN:HE21	1.65	0.61
1:C:481:GLY:HA3	1:C:1022:GLU:HA	1.83	0.61
1:C:929:SER:OG	17:C:3031:NAG:O7	2.17	0.61
1:A:438:TYR:CD1	1:A:441:ALA:HB2	2.34	0.61
1:A:458:LEU:HD21	1:A:545:ILE:HD12	1.81	0.61
1:C:469:ARG:HH11	1:C:495:GLN:HG2	1.65	0.61
1:C:605:SER:HB3	1:C:636:CYS:HB2	1.83	0.61
1:E:562:LEU:HD21	1:E:590:GLN:NE2	2.16	0.61
2:D:231:ARG:HG2	2:D:231:ARG:HH11	1.65	0.60
1:E:1069:PHE:CE2	2:F:584:GLY:HA3	2.36	0.60
1:G:71:MET:HE2	1:G:73:LEU:HB3	1.83	0.60
1:A:24:GLN:HG2	1:A:575:LEU:HD11	1.84	0.60
1:E:501:ARG:NH1	18:E:4004:HOH:O	2.34	0.60
1:E:750:LYS:HE3	1:E:796:TYR:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:1:NAG:O7	6:L:1:NAG:O3	2.16	0.60
1:C:113:THR:O	1:E:931:VAL:HG21	2.01	0.60
1:G:9:THR:HB	1:G:593:LEU:HB3	1.84	0.60
2:B:323:LEU:HB2	2:B:329:ASN:OD1	2.02	0.60
1:C:601:TRP:HB3	1:C:642:ARG:HH21	1.65	0.60
1:C:925:GLU:OE1	1:C:925:GLU:N	2.35	0.60
1:E:781:GLU:HG2	1:E:811[B]:ARG:HH22	1.67	0.60
1:G:640:ASP:OD1	1:G:641:LYS:N	2.33	0.59
2:H:486:GLY:O	2:H:488:GLY:N	2.34	0.59
1:C:918:TYR:HE2	17:C:3920:NAG:O5	1.84	0.59
2:D:451:ASP:OD1	2:D:452:THR:N	2.33	0.59
2:B:184:HIS:HB3	2:B:269:ASN:HB3	1.84	0.59
2:D:324:SER:H	2:D:329:ASN:HD21	1.50	0.59
1:C:411:THR:O	18:C:4001:HOH:O	2.17	0.59
1:G:659:ASP:OD2	5:X:1:NAG:N2	2.36	0.59
3:I:1:NAG:O7	3:I:1:NAG:O3	2.17	0.59
2:D:502:VAL:O	2:D:505:LYS:HB3	2.03	0.59
1:C:1032:LEU:HD21	1:C:1078:LEU:HD11	1.85	0.59
1:A:54:THR:HG22	1:A:56:ALA:H	1.67	0.58
1:E:354:PHE:CE1	8:S:1:NAG:H4	2.37	0.58
1:C:601:TRP:CH2	1:C:643:SER:HA	2.37	0.58
1:G:880:ASN:ND2	14:Y:1:NAG:O7	2.36	0.58
1:G:909:VAL:HG23	1:G:938:VAL:HB	1.85	0.58
1:A:131:GLN:O	1:A:228:ARG:NH2	2.37	0.58
1:C:1043:LYS:O	1:C:1079:GLU:HA	2.03	0.58
1:E:436:GLY:HA3	2:F:282:VAL:HG21	1.86	0.58
1:E:538:HIS:CD2	1:E:550:SER:HG	2.21	0.58
1:A:575:LEU:N	1:A:582:ASP:OD2	2.37	0.58
2:B:174:LYS:HG3	2:B:175:GLU:H	1.68	0.58
1:C:43:GLN:O	8:N:1:NAG:H82	2.03	0.58
1:E:87:LEU:HD21	1:E:348:LEU:HD21	1.86	0.58
1:A:789:TRP:CE2	1:C:772:LYS:HB3	2.39	0.58
1:C:866:SER:HB3	1:C:869:ALA:HB2	1.85	0.58
2:D:362:SER:OG	2:D:378:CYS:SG	2.61	0.58
2:D:462:GLN:NE2	2:D:462:GLN:H	2.02	0.58
1:E:766:PHE:HB3	1:E:786:VAL:HG22	1.86	0.58
1:E:833:PRO:HA	1:E:840:TRP:CD1	2.38	0.58
1:C:643:SER:O	1:C:645:ASN:N	2.36	0.57
1:A:701:PRO:HG2	1:A:704:VAL:HG22	1.84	0.57
1:C:12:ARG:HB2	1:C:590:GLN:HE21	1.69	0.57
1:G:946:LEU:HD21	1:G:1055:PHE:HD2	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:SER:OG	17:A:3920:NAG:H82	2.04	0.57
1:C:436:GLY:HA3	2:D:282:VAL:HG21	1.85	0.57
1:E:376:GLN:HB2	8:S:1:NAG:H3	1.86	0.57
17:G:3042:NAG:H2	11:V:1:NAG:C8	2.34	0.57
2:B:350:ASN:OD1	2:B:351:ALA:N	2.31	0.57
2:B:579:CYS:HB3	2:B:590:CYS:SG	2.45	0.57
2:D:231:ARG:HG2	2:D:231:ARG:NH1	2.19	0.57
2:F:305:VAL:HG21	2:F:322:GLU:HB2	1.86	0.57
2:F:486:GLY:O	2:F:488:GLY:N	2.37	0.57
1:E:768:PHE:HZ	1:E:877:LEU:HD21	1.70	0.57
2:H:101:LYS:HG3	2:H:383:ILE:HD13	1.86	0.57
1:A:804:HIS:CE1	1:A:840:TRP:HB2	2.40	0.57
1:A:689:LEU:HB2	1:E:609:ILE:HD13	1.86	0.57
1:A:897:LEU:HD13	1:C:897:LEU:HD13	1.85	0.57
1:E:509:LEU:HG	1:E:512:VAL:HG11	1.87	0.57
1:E:516:LYS:HE2	1:E:642:ARG:HH12	1.68	0.57
1:A:670:ARG:HH11	1:A:706:ASP:HB3	1.70	0.56
1:A:964:TRP:CD1	1:A:967:VAL:HG22	2.40	0.56
1:C:113:THR:HA	1:E:1031:ASN:OD1	2.05	0.56
1:C:663:ASP:O	1:C:679:ARG:NH2	2.38	0.56
2:F:61:SER:HB3	2:F:91:ALA:HB2	1.87	0.56
9:O:1:NAG:O4	9:O:2:NAG:O7	2.21	0.56
1:A:925:GLU:O	1:A:925:GLU:HG2	2.05	0.56
1:C:430:VAL:HG11	1:C:487:CYS:SG	2.45	0.56
1:C:630:LEU:HB2	1:G:725:LEU:HD11	1.86	0.56
2:D:224:CYS:SG	2:D:266:LEU:HD11	2.45	0.56
1:E:642:ARG:O	1:E:643:SER:HB2	2.05	0.56
2:B:155:LEU:HD12	2:B:156:PRO:HA	1.86	0.56
1:A:335:GLU:OE2	1:A:363:TYR:OH	2.24	0.56
1:A:486:TRP:HB2	2:B:588:PRO:HD3	1.87	0.56
1:A:659:ASP:CG	5:K:1:NAG:H82	2.26	0.56
1:A:788:VAL:HG21	1:A:881:VAL:HG21	1.88	0.56
1:A:961:GLU:HG3	1:A:1039:GLN:CD	2.25	0.56
1:E:47:LEU:HB3	1:E:60:ILE:HD12	1.88	0.56
1:G:395[B]:TRP:O	1:G:397:GLY:N	2.38	0.56
1:G:455:ASP:HA	1:G:478:LEU:HD23	1.88	0.56
1:G:913:GLU:OE1	1:G:913:GLU:N	2.33	0.56
1:G:115:LEU:HD23	1:G:115:LEU:H	1.70	0.56
2:D:323:LEU:HG	2:D:327:SER:HA	1.85	0.56
1:E:326:SER:O	1:E:355:THR:HB	2.04	0.56
1:E:663:ASP:O	1:E:679:ARG:NH2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLY:O	1:A:567:GLN:NE2	2.38	0.56
1:A:480:ARG:HG3	1:A:1021:GLN:HB2	1.88	0.56
1:E:811[B]:ARG:HH21	1:E:862:THR:HG21	1.71	0.56
1:G:34:ALA:O	1:G:36:GLN:N	2.39	0.56
1:A:411:THR:HG22	1:A:435:ILE:HA	1.88	0.56
5:T:2:NAG:O7	5:T:2:NAG:O3	2.20	0.56
1:E:920:ASN:OD1	17:E:3920:NAG:H82	2.06	0.56
1:C:407:ARG:HD2	2:D:247:PHE:CZ	2.41	0.55
1:G:100:ASN:HB2	2:H:159:ASN:HD21	1.70	0.55
1:G:848:HIS:CG	2:H:485:SER:HB3	2.40	0.55
1:G:939:ASN:HB3	1:G:1023:GLU:HG2	1.87	0.55
2:B:381:VAL:HG21	2:B:387:ILE:HG21	1.88	0.55
1:C:823:ARG:HB3	1:C:859:PHE:HB2	1.87	0.55
1:E:1071[B]:ARG:HH22	1:G:755:ASP:C	2.09	0.55
1:E:716:ASN:HB3	1:E:741:TYR:CE1	2.42	0.55
1:A:600:LEU:HD23	1:A:639:ILE:HD11	1.88	0.55
1:C:329:GLU:HB2	1:C:331:GLU:OE2	2.06	0.55
1:C:718:THR:HB	1:C:740[B]:ARG:HH22	1.72	0.55
2:D:441:GLY:HA3	2:D:459:CYS:SG	2.47	0.55
1:E:76:SER:HB3	1:E:89:CYS:HB2	1.89	0.55
1:E:430:VAL:HG11	1:E:487:CYS:SG	2.46	0.55
2:D:343:SER:HG	2:D:380:GLY:H	1.51	0.55
1:E:921:PHE:CZ	1:E:1037:VAL:HG11	2.42	0.55
2:H:101:LYS:HG2	2:H:102:GLY:H	1.71	0.55
1:A:308:ASN:O	1:A:311:LYS:HB2	2.07	0.55
1:E:781:GLU:CG	1:E:811[B]:ARG:HH22	2.19	0.55
1:A:667:LEU:N	2:B:489:ASP:OD2	2.28	0.55
1:A:674:GLN:HE22	1:E:653:GLN:NE2	2.05	0.55
9:O:3:BMA:O4	9:O:7:MAN:H2	2.07	0.55
1:A:390:THR:HG22	1:A:403:LEU:HG	1.89	0.55
2:B:593:CYS:O	2:B:595:GLY:N	2.39	0.55
2:D:617:PHE:HA	2:D:620:ASN:HB2	1.89	0.55
1:C:811:ARG:HD2	2:D:520:GLU:OE2	2.07	0.55
1:C:923:GLU:O	1:C:926:GLU:HG3	2.07	0.55
1:E:342:THR:HG22	1:E:345:GLY:O	2.07	0.55
2:H:648:CYS:SG	2:H:671:ARG:NH2	2.80	0.55
2:B:346:PHE:HB2	2:B:409:LEU:HB2	1.89	0.54
1:E:406:PRO:HB3	1:E:438:TYR:CE1	2.42	0.54
2:F:295:GLN:HG3	2:F:317:LYS:HB3	1.87	0.54
2:D:324:SER:H	2:D:329:ASN:ND2	2.05	0.54
17:G:3920:NAG:O4	2:H:674:VAL:HG13	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HB	1:A:104:THR:O	2.07	0.54
1:A:897:LEU:HD11	1:C:895:PHE:CZ	2.43	0.54
1:C:413:LYS:HG3	1:C:430:VAL:O	2.07	0.54
1:E:1044:LYS:NZ	1:E:1079:GLU:OE2	2.38	0.54
2:B:571:ARG:NH1	2:B:659:GLY:O	2.39	0.54
1:G:90:GLY:O	1:G:93:VAL:HG23	2.07	0.54
1:A:402:VAL:HG22	1:A:416:ILE:HG12	1.90	0.54
17:G:3042:NAG:H2	11:V:1:NAG:H81	1.89	0.54
12:R:1:NAG:O7	12:R:1:NAG:O3	2.25	0.54
1:C:41:ALA:O	1:C:43:GLN:HG2	2.07	0.54
1:E:866:SER:HB3	1:E:869:ALA:HB2	1.90	0.54
2:D:108:TYR:HB3	2:D:237:LEU:HD23	1.89	0.54
5:K:1:NAG:H4	5:K:2:NAG:HN2	1.73	0.54
1:A:918:TYR:H	1:A:1077:VAL:H	1.56	0.54
2:B:592:GLU:HG2	2:B:594:PRO:HD3	1.90	0.54
1:C:12:ARG:HD2	1:C:590:GLN:HE21	1.72	0.54
17:C:3042:NAG:O7	17:C:3042:NAG:O3	2.23	0.54
2:D:227:GLU:OE1	2:D:227:GLU:N	2.41	0.54
2:D:343:SER:OG	2:D:380:GLY:N	2.33	0.54
1:A:162:PHE:HB3	1:A:167:THR:HG21	1.90	0.53
1:E:916:THR:HG21	1:E:932:ALA:HA	1.90	0.53
1:E:963:VAL:HA	1:E:1036:TRP:CD1	2.42	0.53
1:A:795:SER:HB3	1:A:851:PHE:HB3	1.90	0.53
2:B:287:HIS:HE1	2:B:291:GLU:OE2	1.91	0.53
1:C:354:PHE:CD2	9:O:1:NAG:H2	2.44	0.53
1:C:805:PRO:HA	1:C:839:THR:HA	1.89	0.53
1:C:1029:LYS:HE3	1:E:113:THR:HB	1.89	0.53
17:F:3094:NAG:O7	17:F:3094:NAG:O3	2.23	0.53
1:C:918:TYR:OH	1:C:1079:GLU:HB3	2.09	0.53
1:A:639:ILE:HG22	1:A:688:GLY:O	2.08	0.53
1:A:725:LEU:HD12	1:E:630:LEU:HB2	1.89	0.53
1:C:801:THR:HB	1:C:880:ASN:OD1	2.08	0.53
2:F:168:PRO:HB3	2:F:179:PRO:HG3	1.90	0.53
1:G:642:ARG:HG2	1:G:644:LYS:HE3	1.90	0.53
1:G:1062:GLN:HE21	1:G:1067:GLU:HA	1.73	0.53
1:A:624:VAL:O	1:A:625:VAL:HG12	2.08	0.53
1:C:615:ARG:HA	1:C:618:PHE:CE2	2.43	0.53
1:G:638:TYR:HB3	1:G:691:ALA:HA	1.91	0.53
2:H:585:TYR:HA	2:H:592:GLU:O	2.08	0.53
5:K:2:NAG:O7	5:K:2:NAG:O3	2.25	0.53
1:A:31:VAL:HG11	1:A:86:LEU:HD21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:LEU:O	1:E:332:MET:HA	2.09	0.53
1:E:615:ARG:HA	1:E:618:PHE:CE1	2.44	0.53
1:G:385:TYR:CE2	1:G:407:ARG:HG3	2.44	0.53
17:A:3920:NAG:O7	17:A:3920:NAG:O3	2.21	0.53
1:E:658:LEU:HD23	1:E:715:LEU:HD11	1.90	0.53
1:E:921:PHE:HZ	1:E:1037:VAL:HG11	1.74	0.53
1:G:103:LEU:HD11	2:H:155:LEU:HD13	1.91	0.53
1:A:411:THR:OG1	1:A:412:GLY:N	2.42	0.53
2:D:19:PRO:HB3	2:D:89:GLN:NE2	2.24	0.53
2:H:568:CYS:HB3	2:H:590:CYS:SG	2.49	0.53
2:B:353:PRO:HG2	2:B:402:GLN:NE2	2.23	0.52
2:D:184:HIS:NE2	2:D:266:LEU:HD22	2.24	0.52
2:D:469:GLN:C	2:D:471:LEU:H	2.12	0.52
1:E:714:ARG:NH1	2:F:501:ASP:OD1	2.42	0.52
1:E:759:GLN:O	1:E:793:GLU:N	2.23	0.52
2:F:454:TYR:HA	2:F:462:GLN:HA	1.92	0.52
2:F:460:GLU:HB3	18:F:4002:HOH:O	2.08	0.52
1:A:181:HIS:NE2	1:A:200:VAL:HG13	2.24	0.52
1:C:889:ARG:HH21	1:C:892:LYS:HE2	1.75	0.52
1:C:918:TYR:HE1	1:C:1079:GLU:HB3	1.72	0.52
2:D:383:ILE:O	2:D:385:VAL:HG23	2.09	0.52
1:G:385:TYR:CD2	1:G:407:ARG:HG3	2.45	0.52
1:G:407:ARG:HD2	2:H:247:PHE:CZ	2.45	0.52
1:G:655:SER:OG	1:G:720:VAL:O	2.27	0.52
1:G:716:ASN:ND2	5:X:1:NAG:O7	2.43	0.52
1:A:917:LYS:HZ2	2:B:642:GLU:HB3	1.74	0.52
2:B:564:ARG:NH1	2:B:658:ASP:OD1	2.42	0.52
1:E:605:SER:HB3	1:E:636:CYS:HB2	1.91	0.52
1:G:918:TYR:H	1:G:1077:VAL:H	1.57	0.52
2:H:360:TYR:N	2:H:373:GLN:O	2.42	0.52
1:C:376:GLN:HB3	9:O:1:NAG:H3	1.92	0.52
1:C:716:ASN:ND2	10:P:1:NAG:O7	2.43	0.52
1:E:510:GLY:O	1:E:519:ASP:N	2.43	0.52
1:A:650:ARG:HD3	1:A:726:ALA:HB3	1.92	0.52
2:D:219:MET:HB2	2:D:285:LEU:HD21	1.90	0.52
1:E:388:TYR:CD2	1:E:406:PRO:HG2	2.45	0.52
1:E:800:ILE:O	1:E:844:CYS:N	2.39	0.52
1:G:757:ILE:O	1:G:758:CYS:HB2	2.10	0.52
1:G:929:SER:HB2	1:G:1031:ASN:HB3	1.91	0.52
1:C:444:CYS:HB2	1:C:506:LEU:HB2	1.91	0.52
2:D:350:ASN:HD22	2:D:405:VAL:HG22	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:LEU:HD12	2:F:156:PRO:HB3	1.92	0.52
1:A:137:ILE:HB	1:A:173:GLN:HA	1.91	0.52
1:C:931:VAL:HG22	1:C:1031:ASN:OD1	2.10	0.52
1:E:759:GLN:HG3	1:E:793:GLU:HG2	1.91	0.52
1:E:986:PRO:HD3	1:E:1007:GLY:HA2	1.91	0.52
1:A:47:LEU:HB3	1:A:60:ILE:HD12	1.92	0.52
1:G:9:THR:HG1	1:G:52:TYR:HD1	1.56	0.52
1:G:436:GLY:HA3	2:H:282:VAL:HG21	1.92	0.52
1:G:951:ASN:HA	1:G:1011:PHE:O	2.10	0.52
2:H:299:ALA:HB1	2:H:323:LEU:HD13	1.90	0.52
1:A:229:ARG:NH1	1:A:230:ASP:OD2	2.43	0.52
1:A:632:GLN:HG2	1:A:697:ASN:ND2	2.25	0.52
2:D:92:ALA:HA	2:D:391:VAL:O	2.10	0.52
2:D:104:PRO:HG3	2:D:140:GLU:H	1.75	0.52
1:G:905:VAL:HG11	1:G:946:LEU:HD22	1.91	0.52
2:H:617:PHE:HA	2:H:620:ASN:HB2	1.91	0.52
8:N:2:NAG:O7	8:N:2:NAG:H3	2.09	0.52
1:E:775:LEU:H	1:E:779:ASN:HD22	1.59	0.51
2:F:628:LEU:HD11	2:F:665:ILE:HB	1.91	0.51
1:G:412:GLY:HA3	1:G:439:PHE:HB3	1.92	0.51
1:A:12:ARG:HB3	1:A:590:GLN:OE1	2.10	0.51
1:C:836:SER:HB3	14:Y:5:MAN:O2	2.10	0.51
1:A:479:PRO:HG3	1:A:485:TRP:HB2	1.92	0.51
1:A:823:ARG:HG3	1:A:859:PHE:HB2	1.91	0.51
1:E:1052:GLU:CD	1:E:1071[B]:ARG:NH1	2.64	0.51
1:C:479:PRO:HG3	1:C:485:TRP:HB2	1.91	0.51
2:F:92:ALA:HA	2:F:391:VAL:O	2.11	0.51
1:A:69:VAL:HG12	1:A:70:ASN:OD1	2.11	0.51
2:D:299:ALA:HB1	2:D:323:LEU:HD13	1.92	0.51
2:D:436:LEU:O	2:D:437:CYS:HB2	2.10	0.51
1:E:790:ASN:HB2	1:E:851:PHE:CE2	2.45	0.51
1:E:851:PHE:HE1	1:E:857:ILE:HG12	1.76	0.51
5:T:2:NAG:O3	5:T:3:BMA:O5	2.27	0.51
2:D:617:PHE:HA	2:D:620:ASN:OD1	2.11	0.51
1:E:105:GLY:HA3	1:E:335:GLU:O	2.11	0.51
1:E:628:GLN:HG2	1:E:701:PRO:HA	1.92	0.51
1:A:93:VAL:O	1:A:103:LEU:HA	2.10	0.51
2:B:157:PHE:HA	2:B:209:ASP:HB2	1.92	0.51
1:E:917:LYS:NZ	2:F:642:GLU:HB2	2.26	0.51
1:A:76:SER:HB3	1:A:89:CYS:HB2	1.93	0.51
1:A:480:ARG:HG3	1:A:1021:GLN:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:651:ASP:OD1	1:E:652:LEU:N	2.43	0.51
1:E:705:GLU:N	1:E:705:GLU:OE1	2.44	0.51
1:A:897:LEU:HD11	1:C:895:PHE:CE1	2.46	0.51
1:C:918:TYR:H	1:C:1077:VAL:H	1.58	0.51
2:D:183:ARG:HG2	2:D:202:GLN:HE22	1.76	0.51
1:E:335:GLU:OE2	1:E:363:TYR:OH	2.18	0.51
1:E:649:SER:HA	1:E:652:LEU:HD12	1.92	0.51
2:H:364:CYS:HB3	2:H:368:VAL:HB	1.92	0.51
1:A:665:GLY:HA3	2:B:499:THR:O	2.11	0.50
1:G:923:GLU:OE2	1:G:1038:ARG:NH2	2.35	0.50
1:E:939:ASN:HB3	1:E:1023:GLU:HB2	1.93	0.50
2:H:484:CYS:O	2:H:485:SER:HB2	2.10	0.50
11:Q:1:NAG:H3	11:Q:1:NAG:H83	1.92	0.50
2:D:155:LEU:HD12	2:D:156:PRO:HA	1.93	0.50
1:E:674:GLN:HB2	1:E:699:LEU:HG	1.93	0.50
1:E:880:ASN:HB3	1:E:894:THR:HG22	1.93	0.50
1:E:1069:PHE:HE2	2:F:584:GLY:HA3	1.77	0.50
1:G:866:SER:HB3	1:G:869:ALA:HB2	1.93	0.50
2:D:460:GLU:N	2:D:460:GLU:OE1	2.45	0.50
1:C:601:TRP:HB3	1:C:642:ARG:NH2	2.26	0.50
1:E:897:LEU:HD11	1:G:895:PHE:CZ	2.47	0.50
1:E:918:TYR:CE1	1:E:1079:GLU:HB3	2.43	0.50
2:B:6:PHE:O	2:B:8:VAL:HG23	2.12	0.50
2:B:554:GLU:OE1	2:B:577:ASN:ND2	2.44	0.50
1:C:476:CYS:HA	1:C:487:CYS:HA	1.93	0.50
1:C:692:HIS:CD2	1:G:694:GLU:HA	2.47	0.50
1:G:563:GLN:HG3	1:G:588:ARG:HB3	1.92	0.50
2:F:468:SER:O	2:F:472:GLU:HG3	2.11	0.50
1:G:1:PHE:HA	1:G:551:GLN:HG2	1.93	0.50
2:B:104:PRO:HB2	2:B:233:VAL:HG11	1.94	0.50
2:B:598:SER:OG	2:B:638:ARG:NE	2.45	0.50
1:A:630:LEU:HD22	1:E:653:GLN:HB2	1.93	0.50
1:A:786:VAL:HB	1:A:859:PHE:CE1	2.47	0.50
2:D:356:LEU:HD11	2:D:393:VAL:HG13	1.94	0.50
2:F:309:GLU:HA	2:F:320:VAL:HG11	1.94	0.50
2:B:240:ALA:HA	2:B:299:ALA:O	2.12	0.49
1:C:921:PHE:HE2	1:C:1037:VAL:HG21	1.77	0.49
1:C:970:SER:HB3	1:C:1027:THR:OG1	2.11	0.49
1:C:1062:GLN:HE21	1:C:1067:GLU:HA	1.77	0.49
2:D:183:ARG:HG2	2:D:202:GLN:OE1	2.12	0.49
2:D:469:GLN:O	2:D:471:LEU:N	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:972:PRO:O	1:E:975:PRO:HD3	2.12	0.49
1:G:47:LEU:HB3	1:G:60:ILE:HD12	1.94	0.49
2:B:564:ARG:HH21	2:B:657:GLN:NE2	2.10	0.49
1:C:919:LEU:HB2	1:C:930:HIS:CE1	2.46	0.49
1:E:747:PRO:HB3	1:E:884:GLU:HG2	1.93	0.49
13:W:6:MAN:H62	13:W:7:MAN:H3	1.94	0.49
1:A:340:VAL:HG21	1:A:391:GLU:HA	1.95	0.49
1:A:1020:VAL:O	1:A:1022:GLU:N	2.44	0.49
2:B:174:LYS:CG	2:B:175:GLU:H	2.24	0.49
2:B:618:GLY:C	2:B:620:ASN:H	2.15	0.49
1:C:38:ILE:HG23	8:N:1:NAG:H81	1.95	0.49
1:C:601:TRP:CD2	1:C:601:TRP:N	2.80	0.49
2:D:468:SER:OG	2:D:469:GLN:O	2.23	0.49
2:B:108:TYR:HB3	2:B:237:LEU:HD23	1.94	0.49
1:E:1017:SER:O	1:E:1019:SER:N	2.45	0.49
2:H:278:ASP:OD1	2:H:279:TYR:N	2.45	0.49
13:W:3:BMA:O2	13:W:7:MAN:O6	2.11	0.49
2:D:105:ILE:HD11	2:D:236:LEU:HD12	1.95	0.49
1:E:768:PHE:CZ	1:E:877:LEU:HD21	2.48	0.49
14:Y:2:NAG:H3	14:Y:2:NAG:H83	1.94	0.49
1:A:238:ILE:HG12	1:A:267:ILE:HD12	1.95	0.49
1:A:919:LEU:HD12	1:A:919:LEU:HA	1.62	0.49
2:B:174:LYS:O	2:B:175:GLU:HB2	2.12	0.49
1:E:35:PRO:O	1:E:72:SER:HA	2.12	0.49
1:E:104:THR:HG21	1:E:124:GLN:HB2	1.94	0.49
1:G:609:ILE:HB	1:G:632:GLN:HB2	1.93	0.49
1:G:823:ARG:HB2	1:G:860:LEU:H	1.77	0.49
2:D:104:PRO:CB	2:D:139:THR:HB	2.42	0.49
1:A:47:LEU:HG	1:A:73:LEU:HD13	1.95	0.49
1:C:427:LYS:HE3	1:C:480:ARG:HH21	1.78	0.49
2:D:592:GLU:OE2	2:D:594:PRO:HB3	2.12	0.49
1:E:70:ASN:HB3	1:E:94:HIS:CE1	2.47	0.49
1:G:848:HIS:CD2	2:H:485:SER:HB3	2.48	0.49
1:A:347:VAL:HG21	1:A:401:LEU:HD21	1.95	0.49
1:A:953:TRP:HB3	1:A:1003:CYS:SG	2.53	0.49
1:E:539:GLY:HA2	1:E:545:ILE:HD13	1.93	0.49
2:F:323:LEU:HB3	2:F:333:LEU:HD11	1.95	0.49
1:G:536:LEU:HB3	1:G:551:GLN:HB2	1.95	0.49
1:G:663:ASP:O	1:G:679:ARG:NH2	2.45	0.49
1:G:946:LEU:HD21	1:G:1055:PHE:CD2	2.48	0.49
1:A:351:VAL:HG11	2:B:253:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLU:O	1:A:494:GLU:HG3	2.12	0.48
1:A:601:TRP:CD1	1:A:642:ARG:HB2	2.48	0.48
1:A:644:LYS:HA	1:A:644:LYS:HD3	1.61	0.48
1:A:714:ARG:NH1	1:A:741:TYR:CE1	2.81	0.48
1:C:515:ASP:O	1:C:516:LYS:HG2	2.13	0.48
2:D:18:GLY:O	2:D:86:ARG:NH2	2.46	0.48
1:E:516:LYS:HE2	1:E:642:ARG:NH1	2.28	0.48
1:A:9:THR:OG1	1:A:593:LEU:HB2	2.13	0.48
1:E:67:GLU:HG2	1:E:123:ARG:CD	2.43	0.48
1:E:981:SER:HB3	1:E:1009:LEU:HD11	1.94	0.48
1:E:998:ASN:OD1	1:E:998:ASN:O	2.31	0.48
2:F:364:CYS:HB3	2:F:368:VAL:HB	1.93	0.48
1:G:395[A]:TRP:O	1:G:397:GLY:N	2.46	0.48
2:B:571:ARG:HA	2:B:582[B]:HIS:CE1	2.48	0.48
1:C:87:LEU:HD23	1:C:339:ALA:HB1	1.94	0.48
1:G:920:ASN:C	1:G:920:ASN:OD1	2.51	0.48
1:A:630:LEU:CD2	1:E:653:GLN:HB2	2.44	0.48
2:B:158:VAL:HA	2:B:208:LEU:HB3	1.94	0.48
2:B:484:CYS:SG	18:B:4002:HOH:O	2.61	0.48
2:B:642:GLU:OE2	2:B:652:TYR:OH	2.25	0.48
2:D:97:PHE:O	2:D:386:PRO:HA	2.12	0.48
1:E:67:GLU:OE1	1:E:67:GLU:N	2.37	0.48
2:F:184:HIS:NE2	2:F:186:LEU:O	2.46	0.48
2:F:344:ARG:HD3	2:F:379:ASP:HB3	1.94	0.48
3:I:1:NAG:O3	3:I:2:NAG:O5	2.30	0.48
2:B:220:GLN:OE1	2:B:264:CYS:HA	2.13	0.48
2:D:183:ARG:HG2	2:D:202:GLN:NE2	2.28	0.48
2:F:617:PHE:HA	2:F:620:ASN:HB2	1.94	0.48
2:H:145:GLY:HA3	2:H:188:LEU:HD23	1.94	0.48
2:H:18:GLY:O	2:H:86:ARG:NH2	2.46	0.48
1:A:42:ASN:HA	3:I:1:NAG:C5	2.44	0.48
1:E:438:TYR:HD1	1:E:441:ALA:HB2	1.79	0.48
1:G:953:TRP:HB3	1:G:1003:CYS:SG	2.54	0.48
1:A:618:PHE:CE1	1:A:707:SER:HB3	2.49	0.48
2:D:100:ALA:O	2:D:101:LYS:HB3	2.14	0.48
2:D:620:ASN:HB3	2:D:624:ALA:HB2	1.96	0.48
1:G:656:VAL:HG11	1:G:687:LEU:HG	1.95	0.48
1:A:134:VAL:HG22	1:A:170:SER:HB3	1.95	0.48
1:A:929:SER:HB2	1:A:1031:ASN:HB3	1.95	0.48
1:G:465:TYR:CG	2:H:283:GLY:HA3	2.49	0.48
2:H:388:THR:HG21	17:H:3094:NAG:H61	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:PRO:HB3	1:A:646:LEU:HD11	1.96	0.48
1:A:319:GLY:HA3	4:J:5:MAN:O3	2.14	0.47
1:A:469:ARG:HD3	1:A:495:GLN:HB3	1.96	0.47
1:A:918:TYR:HA	1:A:1077:VAL:O	2.14	0.47
1:A:921:PHE:O	1:A:922:SER:OG	2.26	0.47
1:G:430:VAL:HG11	1:G:487:CYS:SG	2.54	0.47
2:H:114:SER:O	2:H:204:ILE:HD11	2.14	0.47
2:H:261:ASP:OD1	2:H:263:ARG:HB2	2.13	0.47
2:D:158:VAL:HG12	2:D:207:ASN:HA	1.96	0.47
2:F:533:GLY:HA3	2:F:551:CYS:SG	2.54	0.47
2:H:136:ASN:HA	2:H:139:THR:O	2.14	0.47
1:A:352:GLY:HA2	1:A:356:TRP:HA	1.97	0.47
2:D:438:HIS:O	2:D:438:HIS:CD2	2.67	0.47
2:F:571:ARG:NH1	2:F:659:GLY:O	2.47	0.47
2:F:614:LYS:NZ	2:F:645:SER:OG	2.48	0.47
2:B:76:LEU:HD23	2:B:413:ASP:HB3	1.97	0.47
1:C:30:VAL:CG1	1:C:50:CYS:HB2	2.44	0.47
1:C:919:LEU:HD13	1:C:930:HIS:CG	2.49	0.47
2:D:76:LEU:HD21	2:D:97:PHE:CD1	2.45	0.47
2:D:355:THR:HG22	2:D:544:PRO:HG2	1.96	0.47
1:G:103:LEU:H	1:G:332:MET:HG2	1.79	0.47
2:D:447:ILE:HG12	2:D:448:CYS:O	2.14	0.47
1:A:387:GLY:HA2	1:A:403:LEU:HD23	1.95	0.47
1:A:925:GLU:HB2	1:A:928:GLU:HG3	1.97	0.47
2:B:216:ASP:HB3	2:B:271:TYR:CE2	2.49	0.47
2:D:186:LEU:HD21	2:D:198:GLU:HB2	1.97	0.47
2:D:235:ARG:O	2:D:236:LEU:HD23	2.15	0.47
1:E:876:LEU:HD13	1:E:898:GLU:HB2	1.97	0.47
1:E:879:ALA:O	1:E:894:THR:HA	2.15	0.47
1:E:1045:VAL:HG13	1:E:1078:LEU:HB2	1.95	0.47
2:F:461:CYS:SG	18:F:4002:HOH:O	2.61	0.47
1:A:609:ILE:HB	1:A:632:GLN:HB2	1.96	0.47
2:B:149:PHE:HA	2:B:181:ALA:O	2.15	0.47
1:C:1042:GLN:HG3	1:C:1044:LYS:H	1.80	0.47
2:D:232:ASN:HB2	17:D:3232:NAG:H2	1.96	0.47
2:D:500:SER:O	2:D:505:LYS:HB2	2.14	0.47
1:E:757:ILE:HG12	1:G:1054:THR:HG21	1.97	0.47
1:E:917:LYS:HZ3	2:F:642:GLU:HB2	1.80	0.47
1:G:80:THR:HG22	1:G:85:GLN:HB2	1.97	0.47
1:G:100:ASN:HB2	2:H:159:ASN:ND2	2.29	0.47
2:H:424:GLU:H	2:H:424:GLU:CD	2.18	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:HIS:CE1	2:B:291:GLU:OE2	2.67	0.47
1:C:86:LEU:O	1:C:109:LEU:HD12	2.15	0.47
1:C:1069:PHE:CE2	2:D:584:GLY:HA3	2.50	0.47
1:E:998:ASN:O	1:E:1000:VAL:N	2.46	0.47
2:F:215:LEU:HB3	2:F:280:PRO:HG2	1.95	0.47
1:G:438:TYR:CD1	1:G:441:ALA:HB2	2.43	0.47
1:A:660:LEU:HB3	1:A:713:LEU:HD11	1.96	0.47
1:A:757:ILE:HG21	1:C:1054:THR:HG21	1.96	0.47
1:A:958:LEU:HG	1:A:959:ASN:OD1	2.15	0.47
2:B:278:ASP:OD1	2:B:279:TYR:N	2.47	0.47
2:B:295:GLN:HG3	2:B:317:LYS:HB3	1.97	0.47
2:D:220:GLN:O	2:D:224:CYS:SG	2.73	0.47
2:D:350:ASN:ND2	2:D:405:VAL:H	2.13	0.47
2:D:504:GLY:O	2:D:516:THR:OG1	2.32	0.47
2:F:219:MET:HA	2:F:285:LEU:HD21	1.97	0.47
1:G:381:MET:SD	1:G:413:LYS:NZ	2.78	0.47
1:A:385:TYR:HB3	1:A:388:TYR:HB2	1.96	0.47
1:C:887:THR:OG1	18:C:4002:HOH:O	2.20	0.47
2:F:300:VAL:HG11	2:F:308:TYR:CE2	2.50	0.47
1:C:437:SER:O	1:C:461:ALA:HB1	2.14	0.46
1:C:469:ARG:HB3	1:C:495:GLN:HA	1.97	0.46
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.50	0.46
1:E:808:LEU:HA	1:E:864:ASP:O	2.15	0.46
1:G:411:THR:HG22	1:G:435:ILE:HA	1.96	0.46
9:O:2:NAG:O3	9:O:3:BMA:H2	2.15	0.46
11:V:1:NAG:HO3	11:V:1:NAG:C7	2.21	0.46
1:A:961:GLU:HG3	1:A:1039:GLN:NE2	2.30	0.46
1:A:1020:VAL:C	1:A:1022:GLU:H	2.18	0.46
1:C:17:GLY:HA2	1:C:588:ARG:NH1	2.30	0.46
2:F:36[B]:ASP:OD1	2:F:37:SER:N	2.46	0.46
1:G:717:PHE:HA	5:X:1:NAG:H81	1.96	0.46
1:G:892:LYS:NZ	14:Y:1:NAG:H2	2.30	0.46
1:C:951:ASN:HA	1:C:1011:PHE:O	2.15	0.46
2:D:115:TYR:CE1	2:D:170:PRO:HD2	2.51	0.46
2:D:316:PRO:HB3	2:D:375:ARG:NH2	2.30	0.46
1:G:93:VAL:HB	1:G:104:THR:O	2.15	0.46
2:H:552:GLN:O	18:H:4001:HOH:O	2.20	0.46
13:W:3:BMA:O4	13:W:4:MAN:H5	2.15	0.46
1:A:87:LEU:HD12	1:A:109:LEU:HD13	1.97	0.46
1:A:399:GLN:OE1	1:A:399:GLN:N	2.45	0.46
1:C:47:LEU:HB3	1:C:60:ILE:HD12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:THR:O	1:C:717:PHE:HA	2.16	0.46
1:C:659:ASP:OD2	10:P:1:NAG:H82	2.15	0.46
1:G:43:GLN:OE1	1:G:43:GLN:HA	2.15	0.46
1:G:1067:GLU:O	1:G:1070:MET:HG2	2.15	0.46
1:A:185:GLU:OE2	1:A:189:ARG:NH2	2.38	0.46
1:A:1057:THR:HB	1:C:761:ASN:HD22	1.81	0.46
1:E:407:ARG:NH2	2:F:247:PHE:H	2.14	0.46
1:G:12:ARG:HA	1:G:590:GLN:HB3	1.98	0.46
1:G:747:PRO:HB3	1:G:884:GLU:HG2	1.96	0.46
2:H:353:PRO:HD2	2:H:356:LEU:HD21	1.97	0.46
1:A:908:VAL:HG12	1:A:1069:PHE:HB3	1.96	0.46
1:A:980:SER:O	1:A:1011:PHE:HA	2.15	0.46
2:B:212:GLU:OE2	2:B:241:THR:HG21	2.15	0.46
1:C:469:ARG:NH1	1:C:495:GLN:OE1	2.49	0.46
1:C:469:ARG:HD3	1:C:495:GLN:HG2	1.97	0.46
1:C:520:VAL:O	1:C:536:LEU:HD12	2.16	0.46
1:C:1069:PHE:HE2	2:D:584:GLY:HA3	1.78	0.46
1:E:364:PRO:HB2	1:E:367:MET:HG3	1.98	0.46
1:E:613:ILE:O	1:E:749:GLU:HB2	2.16	0.46
1:E:715:LEU:N	1:E:742:PHE:O	2.47	0.46
11:V:2:NAG:HO3	11:V:2:NAG:C7	2.23	0.46
1:A:376:GLN:O	1:A:376:GLN:HG2	2.16	0.46
1:E:874:ARG:HH21	1:E:898:GLU:HG2	1.81	0.46
1:G:683:ARG:CZ	1:G:685:ARG:HH22	2.29	0.46
1:A:789:TRP:CZ2	1:C:772:LYS:HB3	2.51	0.46
1:A:915:PHE:CE2	1:A:917:LYS:HB3	2.51	0.46
2:B:605:SER:O	2:B:609:CYS:HB2	2.16	0.46
1:C:521:VAL:HG11	1:C:583:LEU:HD21	1.98	0.46
2:D:350:ASN:ND2	2:D:405:VAL:HG22	2.31	0.46
2:F:611:LYS:HE2	2:F:669:GLU:HG2	1.96	0.46
2:H:521:ARG:HG2	2:H:526:VAL:HA	1.98	0.46
1:A:91:PRO:HG3	1:A:337:PHE:HA	1.98	0.46
1:A:633:SER:HB2	1:A:698:LEU:HD11	1.98	0.46
2:D:129:GLY:HA3	2:D:133:ARG:HH12	1.80	0.46
2:D:300:VAL:HG11	2:D:308:TYR:CE2	2.51	0.46
1:E:410:HIS:HD2	2:F:307:THR:HG21	1.79	0.46
1:E:716:ASN:HB3	1:E:741:TYR:CD1	2.51	0.46
2:F:240:ALA:HA	2:F:299:ALA:O	2.15	0.46
1:G:608:PHE:CE2	1:G:746:LEU:HB2	2.51	0.46
1:A:510:GLY:O	1:A:519:ASP:N	2.42	0.45
1:A:805:PRO:HA	1:A:839:THR:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:918:TYR:OH	17:C:3920:NAG:H4	2.16	0.45
2:D:6:PHE:CD2	2:D:7:LYS:N	2.83	0.45
2:D:617:PHE:CA	2:D:620:ASN:HB2	2.45	0.45
1:E:790:ASN:HB3	1:E:853:GLY:O	2.16	0.45
1:G:104:THR:HG22	1:G:105:GLY:H	1.81	0.45
1:A:438:TYR:OH	2:B:249:GLY:O	2.34	0.45
1:A:802:PHE:O	1:A:841:SER:HA	2.17	0.45
2:D:227:GLU:HG2	2:D:266:LEU:HD13	1.97	0.45
1:E:642:ARG:HG3	1:E:644:LYS:NZ	2.31	0.45
2:H:121:LEU:HD11	2:H:125:LYS:HE3	1.97	0.45
5:X:3:BMA:O4	5:X:4:MAN:H3	2.16	0.45
1:E:610:PRO:HD2	1:E:631:VAL:HG13	1.98	0.45
1:E:637:LEU:HD11	1:E:658:LEU:HD21	1.99	0.45
1:G:670:ARG:NH2	1:G:710:PRO:O	2.49	0.45
2:B:184:HIS:NE2	2:B:228:ILE:HG12	2.31	0.45
1:C:405:ALA:O	1:C:412:GLY:HA2	2.16	0.45
1:C:521:VAL:HG21	1:C:583:LEU:HD22	1.98	0.45
1:G:475:VAL:O	1:G:488:ASP:N	2.48	0.45
1:A:164:ARG:HB2	1:A:165:PRO:HA	1.98	0.45
1:A:909:VAL:HG23	1:A:938:VAL:HB	1.98	0.45
1:C:434:GLN:O	1:C:437:SER:HB3	2.16	0.45
1:C:480:ARG:HD3	1:C:480:ARG:C	2.36	0.45
1:C:650:ARG:C	1:C:652:LEU:H	2.20	0.45
1:C:934:HIS:HE2	1:C:1076:THR:HB	1.82	0.45
2:D:573:ARG:HD2	2:D:575:ARG:NH2	2.31	0.45
1:E:564:TYR:HB2	1:E:588:ARG:HB2	1.98	0.45
1:E:851:PHE:CE1	1:E:857:ILE:HG12	2.51	0.45
2:F:572:GLY:HA2	2:F:581:CYS:HA	1.99	0.45
1:G:384:SER:HB2	1:G:405:ALA:HB1	1.98	0.45
1:A:389:SER:O	1:A:403:LEU:HA	2.15	0.45
1:E:448:VAL:HA	1:E:518:THR:HB	1.99	0.45
1:G:532:GLY:HA3	1:G:565:PHE:HB3	1.97	0.45
1:A:940:ASN:CG	1:A:1020:VAL:HA	2.37	0.45
2:B:189:THR:OG1	2:B:190:ASN:N	2.50	0.45
2:D:5:LYS:HD2	2:D:37:SER:HB2	1.98	0.45
2:D:309:GLU:HA	2:D:320:VAL:HG21	1.98	0.45
1:G:115:LEU:HG	1:G:117:GLN:NE2	2.31	0.45
1:G:921:PHE:CZ	1:G:1080:LYS:HA	2.52	0.45
1:A:494:GLU:OE2	1:A:552:ARG:CZ	2.65	0.45
1:C:804:HIS:O	1:C:840:TRP:N	2.46	0.45
1:C:919:LEU:HD22	1:C:930:HIS:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1043:LYS:HG2	1:C:1080:LYS:HD3	1.98	0.45
2:D:108:TYR:HB3	2:D:237:LEU:CD2	2.47	0.45
1:E:93:VAL:O	1:E:103:LEU:HA	2.16	0.45
1:E:445:SER:HB2	1:E:454:THR:HG21	1.98	0.45
1:E:638:TYR:HB3	1:E:691:ALA:HB2	1.98	0.45
1:A:638:TYR:HB3	1:A:691:ALA:HB2	1.99	0.45
1:C:918:TYR:CE2	17:C:3920:NAG:O5	2.68	0.45
1:G:67:GLU:HB3	1:G:123:ARG:HD3	1.99	0.45
1:G:729:ASN:N	1:G:729:ASN:HD22	2.15	0.45
1:C:921:PHE:CE2	1:C:1037:VAL:HG21	2.52	0.45
2:D:76:LEU:HD12	2:D:413:ASP:OD2	2.17	0.45
2:D:231:ARG:O	2:D:233:VAL:N	2.48	0.45
1:E:407:ARG:O	1:E:408:TYR:C	2.56	0.45
1:A:80:THR:HG22	1:A:85:GLN:HB2	1.99	0.44
1:A:940:ASN:ND2	1:A:1018:PHE:O	2.43	0.44
1:A:951:ASN:HA	1:A:1011:PHE:O	2.17	0.44
2:B:143:ARG:NH1	2:B:231:ARG:HD3	2.32	0.44
1:C:597:ARG:NH2	1:C:733:MET:SD	2.90	0.44
1:E:411:THR:HG22	1:E:435:ILE:HA	1.99	0.44
1:A:926:GLU:OE2	1:A:1038:ARG:NH2	2.46	0.44
1:A:512:VAL:HB	1:A:519:ASP:OD2	2.16	0.44
1:C:796:TYR:O	1:C:884:GLU:HG3	2.18	0.44
1:E:352:GLY:HA2	1:E:356:TRP:HA	2.00	0.44
1:E:604:VAL:HG21	1:E:742:PHE:CD2	2.52	0.44
1:G:94:HIS:NE2	2:H:155:LEU:HD11	2.32	0.44
2:D:356:LEU:HD11	2:D:393:VAL:CG1	2.47	0.44
2:F:270:LEU:HG	2:F:271:TYR:H	1.82	0.44
1:G:575:LEU:HD12	1:G:593:LEU:HD11	2.00	0.44
1:G:946:LEU:HD13	1:G:1060:TYR:CD2	2.52	0.44
1:A:643:SER:OG	1:A:644:LYS:N	2.50	0.44
1:A:876:LEU:HD11	1:A:896:GLN:HB2	2.00	0.44
1:C:394:LEU:HD22	1:C:395:TRP:H	1.82	0.44
1:C:903:TYR:HD2	1:C:944[B]:ARG:HH12	1.66	0.44
1:C:986:PRO:HG3	1:C:1005:ILE:O	2.18	0.44
1:E:351:VAL:HG11	2:F:253:LEU:HD21	2.00	0.44
1:E:830:ASP:OD1	1:E:830:ASP:N	2.50	0.44
1:E:937:GLN:NE2	1:E:1023:GLU:OE1	2.49	0.44
1:G:618:PHE:CZ	1:G:707:SER:HB3	2.53	0.44
1:C:953:TRP:HB3	1:C:1003:CYS:SG	2.58	0.44
2:D:237:LEU:O	2:D:296:PRO:HA	2.18	0.44
1:G:30:VAL:HB	1:G:50:CYS:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:611:ALA:O	1:G:747:PRO:HD2	2.17	0.44
1:A:12:ARG:HB3	1:A:590:GLN:HB3	1.98	0.44
1:C:1053:ILE:HB	1:C:1070:MET:HB2	2.00	0.44
1:E:80:THR:HG22	1:E:85:GLN:HB2	1.99	0.44
1:E:880:ASN:O	1:E:880:ASN:OD1	2.36	0.44
1:G:459:ILE:HD11	1:G:485:TRP:CZ2	2.53	0.44
1:G:803:SER:HB3	1:G:878:THR:OG1	2.17	0.44
1:A:483:ARG:HH22	1:A:939:ASN:ND2	2.16	0.44
1:C:76:SER:HB3	1:C:89:CYS:HB2	1.99	0.44
2:D:242:ASP:O	2:D:303:ARG:NH2	2.48	0.44
1:E:37:LYS:O	1:E:45:GLY:N	2.46	0.44
1:E:918:TYR:HA	1:E:1077:VAL:O	2.17	0.44
2:F:15:ILE:HG23	2:F:86:ARG:CZ	2.47	0.44
2:F:76:LEU:HD23	2:F:413:ASP:HB3	2.00	0.44
1:C:394:LEU:HD23	1:C:394:LEU:HA	1.59	0.44
2:F:506:LEU:HD23	2:F:506:LEU:HA	1.78	0.44
1:G:920:ASN:HB2	17:G:3920:NAG:O7	2.17	0.44
2:H:504:GLY:O	2:H:516:THR:OG1	2.25	0.44
14:Y:3:BMA:H2	14:Y:4:MAN:H5	2.00	0.44
1:A:181:HIS:CD2	1:A:200:VAL:HG22	2.53	0.43
1:A:632:GLN:HE21	1:A:697:ASN:HD21	1.66	0.43
2:B:301:THR:HG22	2:B:303:ARG:H	1.83	0.43
1:C:905:VAL:HG11	1:C:946:LEU:HD13	2.00	0.43
1:E:761:ASN:H	1:E:792:GLY:HA3	1.83	0.43
1:G:889:ARG:HD2	1:G:889:ARG:HA	1.88	0.43
2:B:447:ILE:HD13	2:B:447:ILE:HA	1.75	0.43
1:C:718:THR:HB	1:C:740[B]:ARG:NH2	2.32	0.43
2:D:436:LEU:HD22	2:D:438:HIS:HB3	2.00	0.43
2:D:484:CYS:SG	2:D:490:CYS:HB2	2.58	0.43
1:E:100:ASN:HB2	2:F:159:ASN:ND2	2.33	0.43
1:E:597:ARG:HD2	1:E:733:MET:SD	2.57	0.43
2:F:34:ASP:HB3	2:F:38:ILE:HG21	2.00	0.43
1:C:519:ASP:OD1	1:C:538:HIS:ND1	2.35	0.43
1:C:692:HIS:HD2	1:G:694:GLU:HA	1.84	0.43
2:F:6:PHE:O	2:F:8:VAL:HG23	2.18	0.43
8:N:2:NAG:O7	8:N:2:NAG:C3	2.67	0.43
1:A:694:GLU:HA	1:E:692:HIS:CD2	2.53	0.43
1:A:949:SER:HB3	1:A:1054:THR:OG1	2.19	0.43
2:D:605:SER:O	2:D:609:CYS:HB2	2.18	0.43
1:E:483:ARG:NH2	1:E:941:LEU:O	2.51	0.43
1:A:562:LEU:HA	1:A:562:LEU:HD23	1.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:VAL:HG11	2:B:308:TYR:CE2	2.54	0.43
2:B:329:ASN:OD1	2:B:329:ASN:N	2.51	0.43
2:B:533:GLY:HA3	2:B:551:CYS:SG	2.59	0.43
1:E:896:GLN:HG2	1:G:898:GLU:HB3	2.01	0.43
1:E:956:VAL:HG12	1:E:957:GLU:HG3	1.99	0.43
1:E:1055:PHE:N	1:E:1055:PHE:CD1	2.87	0.43
2:F:505:LYS:HE3	2:F:505:LYS:HB2	1.85	0.43
1:G:376:GLN:HG3	1:G:377:GLU:N	2.34	0.43
1:G:879:ALA:O	1:G:894:THR:HA	2.18	0.43
1:G:1053:ILE:HB	1:G:1070:MET:HB2	2.01	0.43
2:H:92:ALA:HA	2:H:391:VAL:O	2.19	0.43
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.81	0.43
1:A:991:PHE:HB2	1:A:1005:ILE:HG21	2.00	0.43
1:C:657:THR:HB	1:C:718:THR:HG22	2.01	0.43
1:C:670:ARG:NH1	1:C:709:THR:O	2.48	0.43
1:C:998:ASN:C	1:C:1000:VAL:H	2.22	0.43
2:D:458:ASN:OD1	2:D:460:GLU:HB3	2.19	0.43
2:D:618:GLY:O	2:D:619:LYS:HB2	2.19	0.43
2:F:145:GLY:HA3	2:F:188:LEU:HD23	2.00	0.43
2:F:476:ARG:HB3	2:F:483:ILE:HA	2.00	0.43
1:G:628:GLN:HG2	1:G:701:PRO:HA	2.00	0.43
1:G:659:ASP:HB2	1:G:716:ASN:OD1	2.19	0.43
1:A:775:LEU:H	1:A:779:ASN:HD22	1.67	0.43
1:E:103:LEU:HD13	1:E:334:GLN:HE21	1.84	0.43
2:F:547:GLU:HG3	2:F:553:CYS:HB2	2.01	0.43
2:F:611:LYS:HD2	2:F:611:LYS:HA	1.77	0.43
1:G:813:VAL:O	1:G:823:ARG:NH1	2.51	0.43
1:A:54:THR:HG22	1:A:56:ALA:N	2.34	0.43
1:C:3:LEU:HB3	1:C:553:ILE:HD11	2.01	0.43
1:C:634:ASN:HD22	1:G:690:LYS:HB3	1.83	0.43
1:E:107:CYS:SG	1:E:336:GLY:HA3	2.59	0.43
1:E:406:PRO:HB3	1:E:438:TYR:CZ	2.54	0.43
1:E:670:ARG:NH2	1:E:709:THR:O	2.51	0.43
2:F:221:VAL:HG11	2:F:237:LEU:HD21	2.01	0.43
1:G:497:HIS:CE1	1:G:528:GLU:H	2.37	0.43
1:G:946:LEU:O	1:G:948:VAL:HG13	2.19	0.43
2:H:125:LYS:O	2:H:196:GLN:NE2	2.46	0.43
2:H:381:VAL:HG21	2:H:387:ILE:HD13	2.00	0.43
1:A:175:SER:OG	1:A:176:ASN:N	2.51	0.43
1:A:410:HIS:O	1:A:436:GLY:N	2.45	0.43
1:A:448:VAL:HA	1:A:518:THR:HB	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:SER:HB3	2:B:505:LYS:HG2	2.00	0.43
1:C:103:LEU:HD12	2:D:156:PRO:HB3	1.99	0.43
1:C:551:GLN:HG3	18:C:4005:HOH:O	2.18	0.43
1:C:601:TRP:CZ2	1:C:643:SER:HA	2.53	0.43
2:D:592:GLU:HG2	2:D:594:PRO:HD3	1.99	0.43
1:E:338:SER:HB2	1:E:388:TYR:O	2.19	0.43
1:E:611:ALA:O	1:E:747:PRO:HD2	2.18	0.43
1:E:646:LEU:HD22	1:E:650:ARG:NE	2.33	0.43
1:G:4:ASP:C	1:G:4:ASP:OD1	2.56	0.43
1:G:525:PRO:HA	1:G:532:GLY:HA2	2.01	0.43
1:G:657:THR:HA	1:G:684:VAL:HG22	2.01	0.43
1:G:940:ASN:ND2	1:G:1018:PHE:O	2.44	0.43
1:A:37:LYS:O	1:A:44:THR:HA	2.19	0.43
1:A:739:GLN:HE21	1:A:741:TYR:HB2	1.84	0.43
1:A:976:SER:O	1:A:978:ARG:N	2.52	0.43
1:E:473:VAL:HG21	1:E:522:ILE:HD13	2.01	0.43
1:E:621:ARG:O	1:E:622:GLU:O	2.37	0.43
1:A:4:ASP:HB3	18:A:4001:HOH:O	2.18	0.42
1:A:333:ALA:HB2	1:A:353:SER:HB3	2.01	0.42
2:B:114:SER:O	2:B:204:ILE:HD11	2.19	0.42
1:C:777:GLY:HA2	1:C:867:PRO:HA	2.01	0.42
1:E:601:TRP:CZ3	1:E:738:ALA:HB2	2.54	0.42
1:E:1062:GLN:HE21	1:E:1067:GLU:HA	1.84	0.42
2:F:472:GLU:HA	2:F:475:CYS:HB2	2.01	0.42
1:A:47:LEU:HD11	1:A:88:ALA:CB	2.49	0.42
1:C:411:THR:OG1	1:C:412:GLY:N	2.52	0.42
1:C:920:ASN:HB2	17:C:3920:NAG:H2	1.99	0.42
2:D:125:LYS:HD3	2:D:200:GLY:HA2	2.00	0.42
2:D:241:THR:O	2:D:300:VAL:HA	2.18	0.42
1:E:411:THR:OG1	1:E:412:GLY:N	2.52	0.42
1:E:525:PRO:HA	1:E:532:GLY:HA2	2.01	0.42
1:E:554:ALA:HB3	1:E:557:GLN:HG3	2.01	0.42
2:H:483:ILE:C	2:H:485:SER:H	2.20	0.42
1:A:37:LYS:HD3	1:A:46:GLY:HA3	2.00	0.42
1:A:741:TYR:CD2	2:B:502:VAL:HG12	2.54	0.42
1:A:838:GLY:N	18:A:4005:HOH:O	2.51	0.42
1:A:848:HIS:CD2	2:B:485:SER:HB3	2.55	0.42
1:A:909:VAL:HB	1:A:1053:ILE:HD11	2.00	0.42
2:B:571:ARG:NH1	2:B:656:GLN:NE2	2.68	0.42
1:C:642:ARG:O	1:C:643:SER:HB3	2.20	0.42
1:C:652:LEU:HD23	1:C:652:LEU:HA	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:TRP:CH2	2:F:209:ASP:HA	2.54	0.42
1:E:755:ASP:OD1	1:E:755:ASP:N	2.51	0.42
12:R:3:BMA:H61	12:R:4:MAN:H2	1.57	0.42
1:A:65:PRO:HA	1:A:66:PRO:HD3	1.92	0.42
1:A:1057:THR:HB	1:C:761:ASN:ND2	2.35	0.42
2:D:547:GLU:HG3	2:D:553:CYS:HB2	2.00	0.42
1:E:623:GLN:HB2	1:E:626:SER:HB3	2.01	0.42
1:G:670:ARG:NH1	1:G:709:THR:O	2.48	0.42
3:I:1:NAG:HO3	3:I:1:NAG:C7	2.23	0.42
5:T:2:NAG:H3	5:T:3:BMA:O2	2.19	0.42
1:A:525:PRO:HA	1:A:532:GLY:HA2	2.00	0.42
1:A:1071:ARG:HH21	1:C:755:ASP:CB	2.30	0.42
1:C:980:SER:O	1:C:1011:PHE:HA	2.18	0.42
1:G:847:ASN:O	1:G:849:LEU:N	2.52	0.42
1:G:908:VAL:HG12	1:G:1069:PHE:HB3	2.01	0.42
2:H:61:SER:HB3	2:H:91:ALA:HB2	2.02	0.42
1:C:35:PRO:O	1:C:72:SER:HA	2.20	0.42
1:C:605:SER:O	1:C:635:ILE:HA	2.20	0.42
1:C:918:TYR:CZ	1:C:1079:GLU:HB3	2.54	0.42
1:C:918:TYR:HA	1:C:1077:VAL:O	2.19	0.42
1:E:670:ARG:NH1	1:E:709:THR:O	2.51	0.42
1:G:618:PHE:CE1	1:G:707:SER:HB3	2.55	0.42
1:G:803:SER:O	1:G:877:LEU:HA	2.19	0.42
2:H:575:ARG:O	2:H:576:CYS:HB2	2.19	0.42
1:A:501:ARG:O	1:A:524:ALA:HA	2.20	0.42
1:A:940:ASN:HB2	1:A:1018:PHE:CE2	2.55	0.42
1:A:986:PRO:HG3	18:A:4004:HOH:O	2.19	0.42
1:C:638:TYR:HB3	1:C:691:ALA:CB	2.47	0.42
1:C:697:ASN:HD21	1:G:653:GLN:HG3	1.85	0.42
2:D:430:GLN:H	2:D:430:GLN:CD	2.23	0.42
1:E:593:LEU:HA	1:E:593:LEU:HD23	1.71	0.42
1:E:848:HIS:ND1	2:F:485:SER:HB3	2.34	0.42
2:F:518:ASN:O	2:F:538:GLY:HA2	2.20	0.42
1:G:91:PRO:HG3	1:G:337:PHE:HA	2.02	0.42
1:G:102:TYR:HB2	1:G:331:GLU:O	2.20	0.42
2:H:78:PRO:HD2	2:H:95:VAL:HA	2.00	0.42
1:A:649:SER:O	1:A:650:ARG:HB2	2.19	0.42
2:B:173:GLU:HB3	2:B:174:LYS:O	2.20	0.42
2:B:232:ASN:H	2:B:235:ARG:HH21	1.67	0.42
2:B:468:SER:O	2:B:472:GLU:HG3	2.19	0.42
2:B:518:ASN:O	2:B:538:GLY:HA2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:849:LEU:HD23	1:C:849:LEU:HA	1.77	0.42
2:D:591:GLN:HG3	2:D:592:GLU:N	2.34	0.42
1:E:848:HIS:CG	2:F:485:SER:HB3	2.54	0.42
2:F:281:SER:OG	2:F:284:GLN:HB2	2.19	0.42
2:F:317:LYS:HD2	2:F:317:LYS:HA	1.90	0.42
2:F:643:ARG:HA	2:F:649:TRP:HA	2.02	0.42
1:G:1:PHE:CZ	1:G:735:ALA:HA	2.54	0.42
1:G:717:PHE:N	1:G:717:PHE:CD1	2.88	0.42
1:G:902:LYS:NZ	1:G:1058:SER:HA	2.34	0.42
2:H:495:CYS:HB2	2:H:510:GLN:O	2.20	0.42
1:A:606:MET:HB3	1:A:744:ALA:HB2	2.00	0.42
1:A:811:ARG:HB2	1:A:864:ASP:OD2	2.20	0.42
1:C:12:ARG:HD2	1:C:590:GLN:NE2	2.34	0.42
2:D:183:ARG:HG3	2:D:184:HIS:O	2.20	0.42
1:E:376:GLN:HA	8:S:1:NAG:C7	2.49	0.42
1:A:957:GLU:OE2	1:A:960:GLN:HA	2.20	0.42
2:B:382:GLN:OE1	2:B:385:VAL:HG21	2.20	0.42
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.55	0.42
1:C:392:LEU:HD11	1:C:399:GLN:HB2	2.01	0.42
1:C:600:LEU:HD23	1:C:601:TRP:CH2	2.55	0.42
1:E:625:VAL:HG12	1:E:628:GLN:HG3	2.02	0.42
1:E:965:MET:N	1:E:1031:ASN:O	2.52	0.42
2:F:589:LEU:HD23	2:F:589:LEU:HA	1.85	0.42
2:H:644:ASP:HB3	2:H:650:VAL:HG23	2.00	0.42
10:P:2:NAG:O7	10:P:2:NAG:C3	2.68	0.42
1:A:173:GLN:HB3	1:A:181:HIS:HE1	1.84	0.41
1:A:301:ASP:O	1:A:304:LYS:HG2	2.19	0.41
1:A:1069:PHE:N	1:A:1069:PHE:CD1	2.88	0.41
2:B:105:ILE:HG13	2:B:234:THR:HB	2.02	0.41
2:B:136:ASN:HA	2:B:139:THR:O	2.20	0.41
1:C:407:ARG:NH1	2:D:246:HIS:HA	2.35	0.41
1:C:694:GLU:HA	1:G:692:HIS:CD2	2.55	0.41
2:D:97:PHE:CE2	2:D:345:VAL:HG21	2.54	0.41
2:D:150:VAL:HB	2:D:180:PHE:O	2.20	0.41
2:D:434:ARG:HH11	2:D:434:ARG:HG2	1.84	0.41
2:D:468:SER:HB3	2:D:471:LEU:HD12	2.02	0.41
2:F:316:PRO:HB3	2:F:346:PHE:CE1	2.55	0.41
2:F:399:ILE:H	2:F:399:ILE:HG13	1.69	0.41
1:G:730:LEU:H	1:G:730:LEU:HG	1.59	0.41
1:A:920:ASN:OD1	1:A:920:ASN:C	2.59	0.41
2:B:7:LYS:O	2:B:13:GLU:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:LEU:HD13	1:C:475:VAL:HG13	2.02	0.41
2:D:6:PHE:O	2:D:8:VAL:HG23	2.20	0.41
2:D:230:TRP:CZ3	2:D:235:ARG:HB3	2.55	0.41
1:E:538:HIS:CD2	1:E:550:SER:OG	2.73	0.41
1:E:1052:GLU:CD	1:E:1071[B]:ARG:HH11	2.23	0.41
1:G:347:VAL:HG21	1:G:401:LEU:HD11	2.02	0.41
1:G:713:LEU:O	1:G:743:THR:HA	2.20	0.41
1:G:726:ALA:C	1:G:728:ARG:H	2.23	0.41
1:G:729:ASN:HD22	1:G:729:ASN:H	1.67	0.41
1:G:1066:GLN:CD	1:G:1066:GLN:H	2.23	0.41
2:H:447:ILE:HD13	2:H:447:ILE:HA	1.93	0.41
1:A:442:SER:OG	1:A:504:ALA:O	2.32	0.41
2:B:598:SER:HA	2:B:599:PRO:HD3	1.76	0.41
1:E:16:ALA:HB1	1:E:36:GLN:HB2	2.02	0.41
1:E:564:TYR:CD2	1:E:588:ARG:HD2	2.55	0.41
2:F:361:ASP:HA	2:F:371:ARG:HA	2.02	0.41
11:V:3:BMA:O4	11:V:5:MAN:H2	2.20	0.41
1:A:908:VAL:HA	1:A:1069:PHE:O	2.19	0.41
2:B:484:CYS:SG	2:B:490:CYS:HB2	2.60	0.41
2:B:635:VAL:HB	2:B:655:GLU:OE1	2.20	0.41
1:C:686:VAL:HG11	1:G:697:ASN:HD21	1.86	0.41
2:D:613:GLU:O	2:D:614:LYS:HD2	2.20	0.41
1:E:564:TYR:HB3	1:E:567:GLN:OE1	2.20	0.41
1:E:971:HIS:HE1	1:E:1024:LEU:HB3	1.85	0.41
1:G:660:LEU:HB3	1:G:713:LEU:HD11	2.02	0.41
1:G:836:SER:O	1:G:837:GLN:HB2	2.21	0.41
2:H:363:PHE:HB2	2:H:388:THR:HB	2.02	0.41
1:A:385:TYR:CZ	2:B:253:LEU:HD11	2.56	0.41
1:A:765:SER:HA	1:A:895:PHE:CD2	2.56	0.41
1:C:96:GLU:HG2	1:C:98:GLY:H	1.85	0.41
1:C:897:LEU:HA	1:C:897:LEU:HD12	1.85	0.41
1:E:334:GLN:NE2	2:F:253:LEU:O	2.53	0.41
1:G:115:LEU:H	1:G:115:LEU:CD2	2.34	0.41
2:H:6:PHE:O	2:H:8:VAL:HG23	2.20	0.41
2:H:604:ILE:HD13	2:H:604:ILE:HA	1.82	0.41
14:Y:2:NAG:H83	14:Y:2:NAG:C3	2.50	0.41
1:A:181:HIS:CD2	1:A:200:VAL:HG13	2.56	0.41
1:A:384:SER:O	1:A:385:TYR:HB2	2.20	0.41
1:A:1051:ALA:O	1:A:1071:ARG:HA	2.21	0.41
2:B:146:PHE:HD2	2:B:185:VAL:HG21	1.85	0.41
1:C:887:THR:OG1	1:C:888:PRO:HD2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:611:LYS:HG2	2:D:667:VAL:HB	2.03	0.41
2:F:104:PRO:HB2	2:F:233:VAL:HG11	2.02	0.41
1:G:512:VAL:HG22	1:G:519:ASP:OD2	2.20	0.41
1:C:599:VAL:HG12	1:C:601:TRP:CD1	2.55	0.41
1:C:618:PHE:HB2	1:C:704:VAL:HG22	2.03	0.41
1:C:713:LEU:O	1:C:743:THR:HA	2.20	0.41
1:C:797:GLY:HA3	1:C:884:GLU:HG3	2.03	0.41
2:D:460:GLU:HG2	2:D:461:CYS:N	2.36	0.41
1:E:716:ASN:HB3	1:E:741:TYR:HE1	1.85	0.41
1:E:905:VAL:HG11	1:E:946:LEU:HD22	2.02	0.41
1:G:933:MET:HA	1:G:1028:LEU:O	2.21	0.41
1:A:70:ASN:OD1	1:A:70:ASN:N	2.53	0.41
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	2.03	0.41
2:B:604:ILE:HG12	2:B:642:GLU:HG3	2.03	0.41
1:C:347:VAL:HA	1:C:361:PHE:O	2.21	0.41
1:C:374:MET:HB3	1:C:378:ASN:ND2	2.35	0.41
1:C:875:LEU:O	1:C:898:GLU:HA	2.21	0.41
2:D:469:GLN:C	2:D:471:LEU:N	2.74	0.41
1:E:526:GLY:HA2	1:E:530:ASN:HA	2.03	0.41
1:G:476:CYS:HA	1:G:487:CYS:HA	2.03	0.41
1:G:535:TYR:HB3	1:G:537:PHE:HE1	1.85	0.41
2:H:189:THR:OG1	2:H:190:ASN:N	2.46	0.41
1:A:639:ILE:HG23	1:A:639:ILE:O	2.21	0.41
1:A:970:SER:HB3	1:A:1027:THR:OG1	2.19	0.41
2:B:97:PHE:O	2:B:386:PRO:HA	2.21	0.41
2:B:505:LYS:HD2	2:B:517:ILE:HD12	2.03	0.41
1:C:93:VAL:HB	1:C:104:THR:O	2.21	0.41
1:C:874:ARG:HA	1:C:899:LEU:O	2.21	0.41
2:D:571:ARG:O	2:D:582:HIS:ND1	2.54	0.41
1:E:813:VAL:O	1:E:823:ARG:NH1	2.53	0.41
1:E:954:VAL:HG13	1:E:964:TRP:CE3	2.56	0.41
2:F:184:HIS:CE1	2:F:228:ILE:HG12	2.56	0.41
1:G:47:LEU:HG	1:G:73:LEU:HD13	2.03	0.41
1:G:625:VAL:HG12	1:G:625:VAL:O	2.20	0.41
1:G:649:SER:O	1:G:651:ASP:N	2.50	0.41
1:G:918:TYR:CA	1:G:1077:VAL:HB	2.51	0.41
1:G:1048:VAL:HG11	1:G:1073:GLN:HE21	1.86	0.41
6:L:1:NAG:HO3	6:L:1:NAG:C7	2.26	0.41
1:A:12:ARG:HA	1:A:590:GLN:HB3	2.03	0.41
1:A:307:GLN:O	1:A:311:LYS:HG3	2.21	0.41
1:C:1020:VAL:HG12	1:C:1021:GLN:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:624:ALA:CB	17:D:3620:NAG:H82	2.51	0.41
1:E:969:VAL:HG22	1:E:1028:LEU:HD23	2.03	0.41
2:F:35:PRO:O	2:F:38:ILE:HG12	2.19	0.41
1:G:448:VAL:HA	1:G:518:THR:HB	2.02	0.41
1:G:1044:LYS:HB3	1:G:1044:LYS:HE3	1.90	0.41
17:G:3042:NAG:H2	11:V:1:NAG:H83	2.01	0.41
11:U:1:NAG:H83	11:U:1:NAG:H3	2.01	0.41
1:A:9:THR:HG21	1:A:52:TYR:CE1	2.56	0.40
1:A:413:LYS:HG3	1:A:430:VAL:O	2.22	0.40
1:A:463:HIS:HB3	2:B:281:SER:HB2	2.02	0.40
2:B:242:ASP:HA	2:B:301:THR:OG1	2.21	0.40
1:C:38:ILE:HG12	8:N:1:NAG:H83	2.02	0.40
1:C:67:GLU:OE1	1:C:67:GLU:N	2.45	0.40
1:C:918:TYR:CE2	1:C:920:ASN:HB3	2.56	0.40
1:C:931:VAL:HA	1:C:1031:ASN:HA	2.02	0.40
2:D:430:GLN:OE1	2:D:430:GLN:N	2.49	0.40
1:E:481:GLY:HA2	1:E:1021:GLN:HB3	2.02	0.40
1:E:564:TYR:HD2	1:E:588:ARG:HB2	1.86	0.40
1:E:575:LEU:N	1:E:582:ASP:OD2	2.54	0.40
1:E:963:VAL:HG13	1:E:1036:TRP:NE1	2.35	0.40
1:E:998:ASN:C	1:E:1000:VAL:H	2.24	0.40
1:G:810:TYR:HB2	1:G:842:THR:HG21	2.02	0.40
1:G:917:LYS:HA	1:G:1076:THR:HA	2.03	0.40
2:H:358:VAL:HG22	2:H:393:VAL:HG22	2.03	0.40
17:H:3232:NAG:H83	17:H:3232:NAG:H3	2.02	0.40
1:C:800:ILE:O	1:C:844:CYS:N	2.53	0.40
1:C:961:GLU:OE1	1:C:1039:GLN:HG3	2.21	0.40
2:D:570:GLY:HA3	2:D:659:GLY:CA	2.51	0.40
1:E:635:ILE:O	1:E:693:CYS:HA	2.21	0.40
2:H:238:VAL:HG22	2:H:297:ILE:HB	2.03	0.40
1:A:173:GLN:NE2	1:A:203:LEU:H	2.18	0.40
1:A:739:GLN:NE2	1:A:741:TYR:HB2	2.36	0.40
1:A:1030:GLY:HA2	1:G:113:THR:HG22	2.03	0.40
2:D:571:ARG:HG3	2:D:660:MET:HE3	2.03	0.40
2:F:164:LYS:HD2	2:F:164:LYS:HA	1.88	0.40
2:F:266:LEU:HA	2:F:270:LEU:O	2.21	0.40
2:F:637:GLY:HA3	2:F:654:LEU:O	2.22	0.40
1:G:470:GLY:HA3	1:G:498:PRO:O	2.21	0.40
1:G:774:LEU:HD23	1:G:901:VAL:HG22	2.04	0.40
1:A:917:LYS:HZ1	2:B:642:GLU:HB3	1.83	0.40
2:B:315:ILE:HG23	2:B:315:ILE:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:VAL:HG11	2:D:237:LEU:HD21	2.02	0.40
1:E:582:ASP:OD1	1:E:595:ARG:HG2	2.22	0.40
1:G:959:ASN:O	1:G:960:GLN:HB2	2.22	0.40
1:A:136:LEU:HB2	1:A:235:LEU:HD11	2.02	0.40
1:A:338:SER:HB2	1:A:388:TYR:O	2.21	0.40
1:A:603:GLY:HA3	1:A:638:TYR:CZ	2.56	0.40
2:B:223:ALA:O	2:B:264:CYS:HB2	2.20	0.40
1:C:823:ARG:HD2	1:C:860:LEU:O	2.21	0.40
2:D:31:GLY:H	2:D:34:ASP:HB2	1.86	0.40
2:D:66:GLN:O	2:D:80:LYS:HB3	2.21	0.40
1:E:384:SER:HB2	1:E:405:ALA:HB1	2.03	0.40
1:E:714:ARG:HG2	1:E:715:LEU:N	2.37	0.40
2:F:598:SER:O	2:F:600:CYS:N	2.53	0.40
1:G:605:SER:HB3	1:G:636:CYS:HB2	2.03	0.40
1:G:804:HIS:CD2	1:G:863:PHE:CE2	3.09	0.40
1:G:918:TYR:N	1:G:1077:VAL:HB	2.37	0.40
2:H:285:LEU:HD23	2:H:285:LEU:HA	1.82	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:GLU:OE2	5:T:4:MAN:O4[1_655]	2.02	0.18
1:A:192:ASN:ND2	1:A:986:PRO:O[4_455]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1078/1137 (95%)	958 (89%)	98 (9%)	22 (2%)	7 32
1	C	883/1137 (78%)	792 (90%)	68 (8%)	23 (3%)	5 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	884/1137 (78%)	791 (90%)	73 (8%)	20 (2%)	6 29
1	G	880/1137 (77%)	788 (90%)	71 (8%)	21 (2%)	6 28
2	B	673/727 (93%)	596 (89%)	71 (10%)	6 (1%)	17 48
2	D	672/727 (92%)	616 (92%)	47 (7%)	9 (1%)	12 40
2	F	673/727 (93%)	605 (90%)	60 (9%)	8 (1%)	13 42
2	H	672/727 (92%)	615 (92%)	47 (7%)	10 (2%)	10 38
All	All	6415/7456 (86%)	5761 (90%)	535 (8%)	119 (2%)	8 34

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	LEU
1	A	678	ASN
1	A	920	ASN
2	B	233	VAL
2	B	382	GLN
2	B	621	CYS
1	C	624	VAL
1	C	643	SER
1	C	644	LYS
1	C	772	LYS
1	C	921	PHE
2	D	104	PRO
2	D	233	VAL
2	D	588	PRO
1	E	622	GLU
1	E	643	SER
1	E	652	LEU
1	E	920	ASN
2	F	272	LYS
1	G	396	LYS
1	G	482	TRP
1	G	640	ASP
1	G	837	GLN
1	G	848	HIS
1	G	894	THR
1	G	921	PHE
2	H	452	THR
2	H	619	LYS
2	H	620	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	70	ASN
1	A	175	SER
1	A	324	SER
1	A	397	GLY
1	A	921	PHE
1	A	922	SER
1	C	42	ASN
1	C	449	ASP
1	C	621	ARG
1	C	646	LEU
1	C	728	ARG
1	C	818	LYS
2	D	73	GLN
2	D	229	GLY
2	D	231	ARG
2	D	435	SER
1	E	82	SER
1	E	98	GLY
1	E	758	CYS
1	E	818	LYS
1	E	853	GLY
1	E	1018	PHE
2	F	435	SER
2	F	601	GLY
1	G	625	VAL
1	G	648	GLY
1	G	652	LEU
1	G	769	PRO
2	H	487	LEU
1	A	229	ARG
1	A	644	LYS
2	B	558	GLU
1	C	4	ASP
1	C	16	ALA
1	C	82	SER
1	C	560	SER
1	C	640	ASP
1	C	731	ARG
1	C	798	THR
1	C	890	THR
1	E	623	GLN
1	E	772	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	894	THR
1	G	16	ALA
1	G	641	LYS
1	G	772	LYS
1	G	853	GLY
1	G	920	ASN
2	H	466	ARG
2	H	600	CYS
1	A	206	PHE
1	A	323	THR
1	A	385	TYR
1	A	918	TYR
1	A	972	PRO
1	A	1021	GLN
2	B	232	ASN
2	B	588	PRO
2	D	470	GLU
1	E	626	SER
1	E	671	ALA
2	F	506	LEU
2	F	588	PRO
1	G	35	PRO
1	G	887	THR
1	G	922	SER
2	H	576	CYS
1	A	723	PRO
1	A	977	LEU
1	C	483	ARG
1	E	396	LYS
1	E	1021	GLN
1	G	82	SER
2	H	186	LEU
2	H	621	CYS
1	A	504	ALA
1	C	652	LEU
1	C	770	GLY
2	D	583	SER
1	E	731	ARG
1	E	999	PRO
2	H	233	VAL
1	A	625	VAL
1	E	397	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	594	PRO
1	A	340	VAL
1	C	479	PRO
2	F	595	GLY
2	F	625	CYS
1	G	963	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	922/969 (95%)	910 (99%)	12 (1%)	69	82
1	C	756/969 (78%)	744 (98%)	12 (2%)	62	79
1	E	756/969 (78%)	739 (98%)	17 (2%)	52	74
1	G	748/969 (77%)	732 (98%)	16 (2%)	53	75
2	B	584/625 (93%)	577 (99%)	7 (1%)	71	83
2	D	582/625 (93%)	574 (99%)	8 (1%)	67	82
2	F	584/625 (93%)	580 (99%)	4 (1%)	84	90
2	H	583/625 (93%)	578 (99%)	5 (1%)	78	87
All	All	5515/6376 (86%)	5434 (98%)	81 (2%)	65	81

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	618	PHE
1	A	625	VAL
1	A	630	LEU
1	A	771	LEU
1	A	808	LEU
1	A	834	VAL
1	A	859	PHE
1	A	899	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	959	ASN
1	A	964	TRP
1	A	1021	GLN
2	B	73	GLN
2	B	232	ASN
2	B	247	PHE
2	B	266	LEU
2	B	268	ASP
2	B	502	VAL
2	B	598	SER
1	C	70	ASN
1	C	101	MET
1	C	394	LEU
1	C	480	ARG
1	C	595	ARG
1	C	601	TRP
1	C	625	VAL
1	C	630	LEU
1	C	638	TYR
1	C	690	LYS
1	C	716	ASN
1	C	921	PHE
2	D	11	CYS
2	D	231	ARG
2	D	435	SER
2	D	437	CYS
2	D	438	HIS
2	D	445	CYS
2	D	462	GLN
2	D	621	CYS
1	E	70	ASN
1	E	73	LEU
1	E	388	TYR
1	E	395	TRP
1	E	616	SER
1	E	638	TYR
1	E	644	LYS
1	E	650	ARG
1	E	717	PHE
1	E	730	LEU
1	E	750	LYS
1	E	758	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	774	LEU
1	E	899	LEU
1	E	946	LEU
1	E	964	TRP
1	E	1055	PHE
2	F	110	LEU
2	F	155	LEU
2	F	247	PHE
2	F	425	CYS
1	G	4	ASP
1	G	73	LEU
1	G	101	MET
1	G	115	LEU
1	G	638	TYR
1	G	717	PHE
1	G	729	ASN
1	G	804	HIS
1	G	808	LEU
1	G	849	LEU
1	G	919	LEU
1	G	920	ASN
1	G	923	GLU
1	G	924	SER
1	G	939	ASN
1	G	1055	PHE
2	H	224	CYS
2	H	492	CYS
2	H	506	LEU
2	H	571	ARG
2	H	621	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	94	HIS
1	A	114	GLN
1	A	173	GLN
1	A	181	HIS
1	A	697	ASN
1	A	751	ASN
1	A	779	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	848	HIS
1	A	951	ASN
2	B	45	GLN
2	B	167	ASN
2	B	287	HIS
2	B	292	ASN
2	B	400	GLN
2	B	657	GLN
1	C	43	GLN
1	C	590	GLN
1	C	930	HIS
2	D	89	GLN
2	D	438	HIS
1	E	410	HIS
1	E	653	GLN
1	E	697	ASN
1	E	779	ASN
1	E	971	HIS
2	F	45	GLN
1	G	378	ASN
1	G	495	GLN
1	G	692	HIS
1	G	697	ASN
1	G	779	ASN
1	G	848	HIS
1	G	939	ASN
1	G	960	GLN
1	G	994	HIS
1	G	1066	GLN
1	G	1073	GLN
2	H	159	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

85 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	I	1	1,3	14,14,15	0.31	0	17,19,21	0.67	0
3	NAG	I	2	3	14,14,15	0.43	0	17,19,21	1.65	6 (35%)
3	BMA	I	3	3	11,11,12	1.89	3 (27%)	15,15,17	2.99	4 (26%)
3	MAN	I	4	3	11,11,12	0.76	0	15,15,17	1.64	5 (33%)
3	MAN	I	5	3	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.46	0	17,19,21	0.72	0
4	MAN	J	10	4	11,11,12	1.11	1 (9%)	15,15,17	2.03	4 (26%)
4	NAG	J	2	4	14,14,15	1.10	1 (7%)	17,19,21	0.89	0
4	BMA	J	3	4	11,11,12	2.05	2 (18%)	15,15,17	2.38	3 (20%)
4	MAN	J	4	4	11,11,12	1.46	2 (18%)	15,15,17	1.01	2 (13%)
4	MAN	J	5	4	11,11,12	0.75	0	15,15,17	1.27	2 (13%)
4	MAN	J	6	4	11,11,12	0.97	1 (9%)	15,15,17	1.88	4 (26%)
4	MAN	J	7	4	11,11,12	1.84	3 (27%)	15,15,17	1.61	2 (13%)
4	MAN	J	8	4	11,11,12	1.06	1 (9%)	15,15,17	1.05	1 (6%)
4	MAN	J	9	4	11,11,12	0.75	0	15,15,17	0.97	2 (13%)
5	NAG	K	1	5,1	14,14,15	0.51	0	17,19,21	0.82	0
5	NAG	K	2	5	14,14,15	0.42	0	17,19,21	0.70	0
5	BMA	K	3	5	11,11,12	1.56	3 (27%)	15,15,17	2.86	4 (26%)
5	MAN	K	4	5	11,11,12	0.76	0	15,15,17	1.74	3 (20%)
6	NAG	L	1	6,1	14,14,15	0.65	1 (7%)	17,19,21	0.95	1 (5%)
6	NAG	L	2	6	14,14,15	0.43	0	17,19,21	0.49	0
6	BMA	L	3	6	11,11,12	0.74	0	15,15,17	0.97	1 (6%)
7	NAG	M	1	7,2	14,14,15	1.20	1 (7%)	17,19,21	1.74	5 (29%)
7	NAG	M	2	7	14,14,15	0.22	0	17,19,21	0.35	0
8	NAG	N	1	1,8	14,14,15	1.15	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	N	2	8	14,14,15	0.86	1 (7%)	17,19,21	1.49	5 (29%)
8	BMA	N	3	8	11,11,12	2.77	3 (27%)	15,15,17	1.85	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	N	4	8	11,11,12	0.83	0	15,15,17	1.09	2 (13%)
9	NAG	O	1	9,1	14,14,15	0.79	1 (7%)	17,19,21	0.74	0
9	NAG	O	2	9	14,14,15	0.66	0	17,19,21	1.95	6 (35%)
9	BMA	O	3	9	11,11,12	2.29	4 (36%)	15,15,17	1.91	3 (20%)
9	MAN	O	4	9	11,11,12	0.84	1 (9%)	15,15,17	1.02	2 (13%)
9	MAN	O	5	9	11,11,12	1.95	4 (36%)	15,15,17	1.44	2 (13%)
9	MAN	O	6	9	11,11,12	1.10	1 (9%)	15,15,17	1.47	2 (13%)
9	MAN	O	7	9	11,11,12	1.15	2 (18%)	15,15,17	1.38	3 (20%)
10	NAG	P	1	10,1	14,14,15	0.72	1 (7%)	17,19,21	0.87	0
10	NAG	P	2	10	14,14,15	0.45	0	17,19,21	1.34	2 (11%)
10	BMA	P	3	10	11,11,12	0.72	0	15,15,17	1.13	2 (13%)
10	MAN	P	4	10	11,11,12	1.26	1 (9%)	15,15,17	1.61	2 (13%)
10	MAN	P	5	10	11,11,12	1.42	2 (18%)	15,15,17	0.98	1 (6%)
11	NAG	Q	1	11,1	14,14,15	0.50	0	17,19,21	1.16	1 (5%)
11	NAG	Q	2	11	14,14,15	0.55	0	17,19,21	0.53	0
11	BMA	Q	3	11	11,11,12	1.23	1 (9%)	15,15,17	1.06	1 (6%)
11	MAN	Q	4	11	11,11,12	1.79	4 (36%)	15,15,17	2.02	4 (26%)
11	MAN	Q	5	11	11,11,12	0.59	0	15,15,17	2.31	2 (13%)
12	NAG	R	1	12,1	14,14,15	0.80	1 (7%)	17,19,21	0.82	1 (5%)
12	NAG	R	2	12	14,14,15	1.11	2 (14%)	17,19,21	1.03	1 (5%)
12	BMA	R	3	12	11,11,12	2.31	7 (63%)	15,15,17	2.13	6 (40%)
12	MAN	R	4	12	11,11,12	2.79	6 (54%)	15,15,17	1.39	3 (20%)
12	MAN	R	5	12	11,11,12	0.80	0	15,15,17	1.01	1 (6%)
12	MAN	R	6	12	11,11,12	0.74	0	15,15,17	1.05	2 (13%)
8	NAG	S	1	1,8	14,14,15	0.69	0	17,19,21	0.76	1 (5%)
8	NAG	S	2	8	14,14,15	0.31	0	17,19,21	0.44	0
8	BMA	S	3	8	11,11,12	0.99	1 (9%)	15,15,17	1.26	3 (20%)
8	MAN	S	4	8	11,11,12	0.68	0	15,15,17	1.60	4 (26%)
5	NAG	T	1	5,1	14,14,15	0.93	1 (7%)	17,19,21	0.88	0
5	NAG	T	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.74	0
5	BMA	T	3	5	11,11,12	1.01	1 (9%)	15,15,17	1.74	4 (26%)
5	MAN	T	4	5	11,11,12	0.95	1 (9%)	15,15,17	0.92	1 (6%)
11	NAG	U	1	11,1	14,14,15	1.14	1 (7%)	17,19,21	2.09	3 (17%)
11	NAG	U	2	11	14,14,15	0.70	1 (7%)	17,19,21	0.93	1 (5%)
11	BMA	U	3	11	11,11,12	1.81	3 (27%)	15,15,17	2.03	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	U	4	11	11,11,12	0.77	0	15,15,17	1.12	2 (13%)
11	MAN	U	5	11	11,11,12	2.37	2 (18%)	15,15,17	2.03	3 (20%)
11	NAG	V	1	11,1	14,14,15	0.51	0	17,19,21	1.12	0
11	NAG	V	2	11	14,14,15	0.50	0	17,19,21	0.86	0
11	BMA	V	3	11	11,11,12	0.81	0	15,15,17	1.22	1 (6%)
11	MAN	V	4	11	11,11,12	1.00	1 (9%)	15,15,17	2.29	4 (26%)
11	MAN	V	5	11	11,11,12	1.00	0	15,15,17	1.91	2 (13%)
13	NAG	W	1	13,1	14,14,15	1.67	1 (7%)	17,19,21	0.95	1 (5%)
13	NAG	W	2	13	14,14,15	0.64	0	17,19,21	1.29	4 (23%)
13	BMA	W	3	13	11,11,12	1.54	3 (27%)	15,15,17	2.11	7 (46%)
13	MAN	W	4	13	11,11,12	1.70	3 (27%)	15,15,17	1.54	2 (13%)
13	MAN	W	5	13	11,11,12	0.81	0	15,15,17	1.38	2 (13%)
13	MAN	W	6	13	11,11,12	0.98	1 (9%)	15,15,17	1.18	2 (13%)
13	MAN	W	7	13	11,11,12	0.72	0	15,15,17	1.41	3 (20%)
5	NAG	X	1	5,1	14,14,15	0.52	0	17,19,21	1.10	2 (11%)
5	NAG	X	2	5	14,14,15	0.79	1 (7%)	17,19,21	1.15	1 (5%)
5	BMA	X	3	5	11,11,12	1.16	1 (9%)	15,15,17	1.36	1 (6%)
5	MAN	X	4	5	11,11,12	1.05	1 (9%)	15,15,17	0.95	1 (6%)
14	NAG	Y	1	14,1	14,14,15	1.17	1 (7%)	17,19,21	1.15	2 (11%)
14	NAG	Y	2	14	14,14,15	0.74	1 (7%)	17,19,21	2.10	2 (11%)
14	BMA	Y	3	14	11,11,12	1.22	1 (9%)	15,15,17	0.97	1 (6%)
14	MAN	Y	4	14	11,11,12	0.86	1 (9%)	15,15,17	1.84	2 (13%)
14	MAN	Y	5	14	11,11,12	1.37	2 (18%)	15,15,17	1.69	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	MAN	I	4	3	-	1/2/19/22	0/1/1/1
3	MAN	I	5	3	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	MAN	J	10	4	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	MAN	J	6	4	-	0/2/19/22	0/1/1/1
4	MAN	J	7	4	-	2/2/19/22	0/1/1/1
4	MAN	J	8	4	-	0/2/19/22	0/1/1/1
4	MAN	J	9	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	1/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
7	NAG	M	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
8	NAG	N	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	N	2	8	-	1/6/23/26	0/1/1/1
8	BMA	N	3	8	-	2/2/19/22	0/1/1/1
8	MAN	N	4	8	-	1/2/19/22	0/1/1/1
9	NAG	O	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	O	2	9	-	3/6/23/26	0/1/1/1
9	BMA	O	3	9	-	0/2/19/22	0/1/1/1
9	MAN	O	4	9	-	2/2/19/22	0/1/1/1
9	MAN	O	5	9	-	1/2/19/22	0/1/1/1
9	MAN	O	6	9	-	1/2/19/22	0/1/1/1
9	MAN	O	7	9	-	2/2/19/22	0/1/1/1
10	NAG	P	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	P	2	10	-	1/6/23/26	0/1/1/1
10	BMA	P	3	10	-	0/2/19/22	0/1/1/1
10	MAN	P	4	10	-	0/2/19/22	0/1/1/1
10	MAN	P	5	10	-	0/2/19/22	0/1/1/1
11	NAG	Q	1	11,1	-	5/6/23/26	0/1/1/1
11	NAG	Q	2	11	-	0/6/23/26	0/1/1/1
11	BMA	Q	3	11	-	1/2/19/22	0/1/1/1
11	MAN	Q	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	5	11	-	0/2/19/22	0/1/1/1
12	NAG	R	1	12,1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	R	2	12	-	2/6/23/26	0/1/1/1
12	BMA	R	3	12	-	1/2/19/22	0/1/1/1
12	MAN	R	4	12	-	0/2/19/22	0/1/1/1
12	MAN	R	5	12	-	0/2/19/22	0/1/1/1
12	MAN	R	6	12	-	2/2/19/22	0/1/1/1
8	NAG	S	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	T	2	5	-	3/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	MAN	T	4	5	-	0/2/19/22	0/1/1/1
11	NAG	U	1	11,1	-	3/6/23/26	0/1/1/1
11	NAG	U	2	11	-	2/6/23/26	0/1/1/1
11	BMA	U	3	11	-	2/2/19/22	0/1/1/1
11	MAN	U	4	11	-	0/2/19/22	0/1/1/1
11	MAN	U	5	11	-	0/2/19/22	0/1/1/1
11	NAG	V	1	11,1	-	4/6/23/26	0/1/1/1
11	NAG	V	2	11	-	3/6/23/26	0/1/1/1
11	BMA	V	3	11	-	1/2/19/22	0/1/1/1
11	MAN	V	4	11	-	2/2/19/22	0/1/1/1
11	MAN	V	5	11	-	1/2/19/22	0/1/1/1
13	NAG	W	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	W	2	13	-	1/6/23/26	0/1/1/1
13	BMA	W	3	13	-	2/2/19/22	0/1/1/1
13	MAN	W	4	13	-	1/2/19/22	0/1/1/1
13	MAN	W	5	13	-	0/2/19/22	0/1/1/1
13	MAN	W	6	13	-	2/2/19/22	0/1/1/1
13	MAN	W	7	13	-	1/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	X	2	5	-	3/6/23/26	0/1/1/1
5	BMA	X	3	5	-	1/2/19/22	0/1/1/1
5	MAN	X	4	5	-	1/2/19/22	0/1/1/1
14	NAG	Y	1	14,1	-	2/6/23/26	0/1/1/1
14	NAG	Y	2	14	-	4/6/23/26	0/1/1/1
14	BMA	Y	3	14	-	2/2/19/22	0/1/1/1
14	MAN	Y	4	14	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MAN	Y	5	14	-	0/2/19/22	0/1/1/1

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	3	BMA	O5-C1	-6.94	1.32	1.43
11	U	5	MAN	O5-C5	6.28	1.56	1.43
13	W	1	NAG	O5-C1	-6.03	1.34	1.43
4	J	3	BMA	O5-C1	-5.51	1.34	1.43
3	I	3	BMA	O5-C1	-4.85	1.36	1.43
12	R	4	MAN	C1-C2	4.74	1.63	1.52
4	J	7	MAN	O5-C1	-4.61	1.36	1.43
12	R	4	MAN	C2-C3	4.57	1.59	1.52
9	O	3	BMA	C1-C2	4.41	1.62	1.52
8	N	3	BMA	C1-C2	4.28	1.62	1.52
12	R	3	BMA	O5-C1	-4.24	1.36	1.43
9	O	5	MAN	O2-C2	4.13	1.52	1.43
14	Y	1	NAG	O5-C1	-4.07	1.37	1.43
4	J	2	NAG	O5-C1	-3.98	1.37	1.43
5	K	3	BMA	O5-C1	-3.88	1.37	1.43
12	R	4	MAN	O5-C1	-3.84	1.37	1.43
11	U	1	NAG	O5-C1	-3.83	1.37	1.43
11	U	5	MAN	O5-C1	3.76	1.49	1.43
12	R	4	MAN	O2-C2	3.74	1.51	1.43
4	J	4	MAN	C2-C3	3.72	1.58	1.52
8	N	1	NAG	O5-C1	-3.65	1.37	1.43
9	O	5	MAN	C2-C3	3.53	1.57	1.52
5	T	1	NAG	O5-C1	-3.43	1.38	1.43
7	M	1	NAG	C1-C2	3.40	1.57	1.52
13	W	4	MAN	C1-C2	3.38	1.59	1.52
9	O	3	BMA	O3-C3	3.37	1.50	1.43
9	O	3	BMA	O5-C1	-3.33	1.38	1.43
11	Q	4	MAN	O5-C5	3.25	1.50	1.43
4	J	10	MAN	C1-C2	3.09	1.59	1.52
13	W	4	MAN	C2-C3	3.07	1.57	1.52
8	N	2	NAG	O5-C1	-3.05	1.38	1.43
14	Y	5	MAN	C1-C2	3.04	1.59	1.52
11	U	3	BMA	C6-C5	3.01	1.61	1.51
14	Y	3	BMA	O5-C1	-3.00	1.38	1.43
12	R	3	BMA	O5-C5	-2.96	1.37	1.43
11	Q	4	MAN	C1-C2	2.92	1.58	1.52
11	Q	3	BMA	C4-C3	2.86	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	3	BMA	C6-C5	-2.86	1.42	1.51
9	O	3	BMA	C2-C3	2.85	1.56	1.52
9	O	6	MAN	O5-C5	2.84	1.49	1.43
5	X	4	MAN	O5-C1	-2.84	1.39	1.43
11	Q	4	MAN	O5-C1	2.82	1.48	1.43
8	N	3	BMA	C4-C3	2.80	1.59	1.52
9	O	1	NAG	O5-C1	-2.76	1.39	1.43
3	I	3	BMA	C4-C5	2.74	1.58	1.53
11	U	3	BMA	C1-C2	2.73	1.58	1.52
10	P	4	MAN	O3-C3	2.73	1.49	1.43
13	W	3	BMA	O4-C4	-2.67	1.36	1.43
12	R	4	MAN	O5-C5	2.66	1.48	1.43
4	J	6	MAN	C1-C2	2.66	1.58	1.52
13	W	3	BMA	C4-C3	2.65	1.59	1.52
3	I	3	BMA	C4-C3	2.63	1.59	1.52
5	T	2	NAG	O5-C1	-2.63	1.39	1.43
12	R	2	NAG	C1-C2	-2.62	1.48	1.52
13	W	6	MAN	O5-C1	-2.59	1.39	1.43
9	O	7	MAN	C1-C2	2.58	1.58	1.52
5	T	4	MAN	O5-C1	-2.55	1.39	1.43
4	J	8	MAN	O5-C1	-2.55	1.39	1.43
4	J	3	BMA	C2-C3	2.54	1.56	1.52
11	U	3	BMA	O6-C6	2.53	1.53	1.42
10	P	1	NAG	C1-C2	2.53	1.56	1.52
11	U	2	NAG	O5-C1	-2.51	1.39	1.43
4	J	7	MAN	C4-C3	2.50	1.58	1.52
5	T	3	BMA	C1-C2	2.49	1.57	1.52
5	K	3	BMA	C4-C3	2.48	1.58	1.52
5	X	2	NAG	O5-C1	-2.46	1.39	1.43
10	P	5	MAN	C1-C2	2.46	1.57	1.52
12	R	3	BMA	C4-C5	2.45	1.58	1.53
13	W	3	BMA	C1-C2	2.45	1.57	1.52
14	Y	4	MAN	O5-C5	2.44	1.48	1.43
12	R	3	BMA	C2-C3	2.42	1.56	1.52
12	R	2	NAG	O5-C1	-2.41	1.39	1.43
11	V	4	MAN	C1-C2	2.40	1.57	1.52
9	O	4	MAN	O5-C1	-2.38	1.39	1.43
9	O	7	MAN	O5-C5	2.37	1.48	1.43
9	O	5	MAN	C4-C3	2.30	1.58	1.52
6	L	1	NAG	O5-C1	-2.25	1.40	1.43
9	O	5	MAN	C1-C2	2.22	1.57	1.52
14	Y	2	NAG	O5-C1	-2.22	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	4	MAN	C1-C2	2.19	1.57	1.52
11	Q	4	MAN	C2-C3	2.19	1.55	1.52
8	S	3	BMA	O5-C1	-2.16	1.40	1.43
12	R	3	BMA	O3-C3	2.16	1.48	1.43
13	W	4	MAN	O2-C2	2.14	1.47	1.43
10	P	5	MAN	O5-C5	2.13	1.47	1.43
4	J	7	MAN	C1-C2	2.11	1.57	1.52
12	R	1	NAG	O5-C1	-2.10	1.40	1.43
12	R	4	MAN	C4-C3	2.05	1.57	1.52
5	X	3	BMA	C2-C3	-2.05	1.49	1.52
12	R	3	BMA	C1-C2	2.04	1.56	1.52
14	Y	5	MAN	C2-C3	2.03	1.55	1.52
5	K	3	BMA	C4-C5	2.02	1.57	1.53

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3	BMA	C1-C2-C3	-8.96	98.66	109.67
5	K	3	BMA	C1-C2-C3	-7.53	100.41	109.67
11	Q	5	MAN	C1-O5-C5	6.94	121.59	112.19
11	V	4	MAN	C1-O5-C5	6.75	121.34	112.19
14	Y	2	NAG	C2-N2-C7	6.74	132.50	122.90
11	U	1	NAG	C2-N2-C7	6.69	132.42	122.90
5	K	3	BMA	C1-O5-C5	-6.62	103.22	112.19
11	U	5	MAN	C1-O5-C5	6.35	120.80	112.19
11	Q	4	MAN	C1-O5-C5	6.02	120.34	112.19
4	J	3	BMA	C1-O5-C5	6.00	120.32	112.19
14	Y	4	MAN	C1-O5-C5	5.95	120.25	112.19
11	V	5	MAN	C1-O5-C5	5.87	120.15	112.19
3	I	3	BMA	C1-O5-C5	-5.71	104.46	112.19
11	U	3	BMA	O5-C5-C6	5.57	115.93	107.20
4	J	3	BMA	O5-C5-C6	-5.43	98.70	107.20
4	J	10	MAN	C1-O5-C5	5.39	119.50	112.19
5	K	4	MAN	C1-O5-C5	5.01	118.98	112.19
12	R	3	BMA	O3-C3-C2	4.97	119.52	109.99
9	O	3	BMA	O3-C3-C2	4.89	119.36	109.99
4	J	6	MAN	C1-O5-C5	4.81	118.71	112.19
11	Q	5	MAN	O5-C1-C2	4.72	118.06	110.77
10	P	2	NAG	C2-N2-C7	4.41	129.18	122.90
13	W	4	MAN	O3-C3-C2	4.40	118.42	109.99
9	O	6	MAN	C1-O5-C5	4.27	117.98	112.19
14	Y	5	MAN	C1-O5-C5	4.20	117.89	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	4	MAN	C1-O5-C5	4.19	117.87	112.19
11	Q	1	NAG	C2-N2-C7	4.18	128.85	122.90
9	O	2	NAG	C2-N2-C7	4.15	128.81	122.90
10	P	4	MAN	C1-O5-C5	4.02	117.63	112.19
14	Y	2	NAG	C1-C2-N2	3.88	117.11	110.49
5	T	3	BMA	C1-O5-C5	3.85	117.41	112.19
3	I	4	MAN	C1-O5-C5	3.82	117.37	112.19
5	X	3	BMA	O2-C2-C3	-3.78	102.57	110.14
7	M	1	NAG	C2-N2-C7	-3.77	117.53	122.90
9	O	2	NAG	C1-C2-N2	3.73	116.86	110.49
13	W	3	BMA	O5-C5-C6	3.72	113.04	107.20
11	V	4	MAN	O5-C1-C2	3.67	116.43	110.77
8	N	3	BMA	O2-C2-C3	-3.59	102.95	110.14
13	W	5	MAN	C1-O5-C5	3.58	117.05	112.19
9	O	3	BMA	C2-C3-C4	-3.56	104.74	110.89
9	O	7	MAN	C1-O5-C5	3.52	116.96	112.19
5	X	2	NAG	C2-N2-C7	3.50	127.88	122.90
13	W	6	MAN	C1-O5-C5	3.48	116.90	112.19
10	P	4	MAN	O3-C3-C2	3.47	116.65	109.99
4	J	6	MAN	O5-C1-C2	3.45	116.10	110.77
12	R	4	MAN	O2-C2-C3	-3.45	103.23	110.14
4	J	7	MAN	O2-C2-C3	-3.44	103.24	110.14
4	J	10	MAN	C1-C2-C3	3.42	113.87	109.67
8	N	2	NAG	C2-N2-C7	3.35	127.68	122.90
13	W	7	MAN	C1-O5-C5	3.27	116.62	112.19
5	X	1	NAG	C1-O5-C5	3.26	116.61	112.19
11	V	5	MAN	O5-C1-C2	3.23	115.76	110.77
4	J	7	MAN	C1-C2-C3	3.20	113.60	109.67
4	J	5	MAN	C1-O5-C5	3.16	116.48	112.19
13	W	3	BMA	O4-C4-C5	-3.15	101.47	109.30
8	N	3	BMA	O5-C5-C6	3.14	112.12	107.20
12	R	3	BMA	O5-C5-C6	-3.07	102.40	107.20
9	O	5	MAN	O2-C2-C1	3.03	115.36	109.15
12	R	3	BMA	C3-C4-C5	3.02	115.62	110.24
11	U	4	MAN	C1-O5-C5	3.02	116.28	112.19
11	U	3	BMA	O2-C2-C3	-3.01	104.11	110.14
5	T	3	BMA	O2-C2-C3	-2.99	104.15	110.14
9	O	2	NAG	O3-C3-C4	2.98	117.23	110.35
14	Y	5	MAN	O2-C2-C3	-2.96	104.21	110.14
4	J	6	MAN	C1-C2-C3	2.94	113.28	109.67
4	J	10	MAN	O5-C1-C2	2.93	115.30	110.77
9	O	5	MAN	C1-O5-C5	2.90	116.13	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	U	1	NAG	C1-C2-N2	2.90	115.45	110.49
13	W	7	MAN	O2-C2-C3	-2.90	104.33	110.14
13	W	3	BMA	C2-C3-C4	-2.90	105.88	110.89
8	S	3	BMA	C1-O5-C5	2.89	116.11	112.19
3	I	4	MAN	O2-C2-C3	-2.89	104.34	110.14
11	Q	4	MAN	C1-C2-C3	2.88	113.20	109.67
9	O	6	MAN	O2-C2-C3	-2.87	104.39	110.14
10	P	3	BMA	C1-O5-C5	2.84	116.04	112.19
6	L	1	NAG	C1-O5-C5	-2.83	108.36	112.19
13	W	2	NAG	O3-C3-C4	2.82	116.87	110.35
5	K	4	MAN	O5-C1-C2	2.80	115.09	110.77
5	T	3	BMA	O5-C1-C2	2.79	115.08	110.77
9	O	3	BMA	C1-C2-C3	-2.77	106.26	109.67
12	R	6	MAN	C1-O5-C5	2.77	115.95	112.19
8	N	4	MAN	O2-C2-C3	-2.77	104.59	110.14
3	I	2	NAG	C1-O5-C5	2.75	115.92	112.19
3	I	2	NAG	O4-C4-C3	2.74	116.68	110.35
7	M	1	NAG	O4-C4-C3	-2.74	104.02	110.35
14	Y	1	NAG	C2-N2-C7	2.72	126.77	122.90
13	W	3	BMA	C1-C2-C3	-2.72	106.33	109.67
12	R	3	BMA	C1-O5-C5	-2.71	108.53	112.19
11	V	4	MAN	C1-C2-C3	2.71	112.99	109.67
3	I	2	NAG	C1-C2-N2	2.69	115.08	110.49
3	I	2	NAG	C4-C3-C2	-2.68	107.09	111.02
13	W	3	BMA	C1-O5-C5	-2.66	108.59	112.19
11	Q	4	MAN	O5-C1-C2	2.64	114.84	110.77
7	M	1	NAG	C1-O5-C5	-2.62	108.64	112.19
4	J	8	MAN	O2-C2-C3	-2.62	104.90	110.14
8	N	3	BMA	C1-O5-C5	-2.61	108.65	112.19
4	J	10	MAN	O2-C2-C3	-2.61	104.90	110.14
11	U	3	BMA	O5-C1-C2	2.61	114.80	110.77
9	O	2	NAG	C4-C3-C2	-2.60	107.21	111.02
7	M	1	NAG	C4-C3-C2	2.58	114.80	111.02
8	N	2	NAG	O3-C3-C2	-2.57	104.15	109.47
8	S	4	MAN	O2-C2-C3	-2.55	105.03	110.14
3	I	3	BMA	O2-C2-C1	2.55	114.37	109.15
11	V	4	MAN	O2-C2-C3	-2.55	105.03	110.14
11	U	2	NAG	C2-N2-C7	2.53	126.50	122.90
13	W	4	MAN	O5-C5-C6	2.51	111.13	107.20
11	U	1	NAG	O4-C4-C3	-2.50	104.57	110.35
7	M	1	NAG	C1-C2-N2	2.50	114.76	110.49
14	Y	5	MAN	O5-C1-C2	2.49	114.61	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	3	BMA	O5-C1-C2	-2.48	106.94	110.77
9	O	7	MAN	C1-C2-C3	2.47	112.70	109.67
12	R	1	NAG	O4-C4-C3	2.47	116.06	110.35
3	I	5	MAN	C1-O5-C5	2.43	115.49	112.19
8	N	3	BMA	O6-C6-C5	-2.43	102.94	111.29
11	U	4	MAN	O2-C2-C3	-2.43	105.27	110.14
12	R	2	NAG	O3-C3-C2	-2.42	104.45	109.47
12	R	5	MAN	O2-C2-C3	-2.42	105.29	110.14
3	I	4	MAN	O5-C1-C2	2.42	114.50	110.77
4	J	6	MAN	O2-C2-C3	-2.41	105.31	110.14
11	Q	3	BMA	O2-C2-C3	-2.39	105.36	110.14
3	I	2	NAG	O3-C3-C4	2.37	115.83	110.35
4	J	9	MAN	O2-C2-C3	-2.36	105.40	110.14
11	V	3	BMA	O2-C2-C3	-2.36	105.41	110.14
10	P	3	BMA	O2-C2-C3	-2.36	105.42	110.14
3	I	4	MAN	C1-C2-C3	2.34	112.54	109.67
12	R	4	MAN	C1-C2-C3	2.33	112.54	109.67
4	J	3	BMA	O6-C6-C5	-2.32	103.33	111.29
3	I	3	BMA	O3-C3-C2	2.32	114.43	109.99
11	U	5	MAN	O2-C2-C3	-2.30	105.54	110.14
5	K	4	MAN	O2-C2-C3	-2.29	105.54	110.14
13	W	2	NAG	C4-C3-C2	-2.29	107.66	111.02
12	R	6	MAN	O2-C2-C3	-2.29	105.55	110.14
11	Q	4	MAN	O2-C2-C3	-2.29	105.56	110.14
14	Y	4	MAN	O5-C1-C2	2.28	114.29	110.77
8	S	4	MAN	C1-C2-C3	2.28	112.47	109.67
5	X	1	NAG	C1-C2-N2	2.28	114.38	110.49
14	Y	5	MAN	C1-C2-C3	2.26	112.45	109.67
9	O	4	MAN	O2-C2-C3	-2.25	105.62	110.14
10	P	5	MAN	O2-C2-C3	-2.25	105.62	110.14
9	O	4	MAN	C1-O5-C5	2.24	115.23	112.19
8	S	3	BMA	O2-C2-C3	-2.24	105.66	110.14
5	X	4	MAN	O2-C2-C3	-2.23	105.66	110.14
5	K	3	BMA	O2-C2-C3	-2.23	105.68	110.14
5	T	4	MAN	O2-C2-C3	-2.22	105.68	110.14
9	O	2	NAG	C3-C4-C5	-2.21	106.29	110.24
13	W	5	MAN	O5-C1-C2	2.20	114.17	110.77
13	W	3	BMA	O2-C2-C3	-2.20	105.73	110.14
5	T	3	BMA	O2-C2-C1	2.20	113.65	109.15
8	N	4	MAN	C1-O5-C5	2.19	115.16	112.19
13	W	6	MAN	O2-C2-C3	-2.17	105.80	110.14
3	I	2	NAG	C3-C4-C5	-2.16	106.38	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	U	5	MAN	O5-C5-C6	2.16	110.59	107.20
8	S	4	MAN	O5-C1-C2	2.15	114.10	110.77
4	J	4	MAN	O3-C3-C2	2.15	114.11	109.99
13	W	1	NAG	O3-C3-C2	-2.14	105.04	109.47
8	S	3	BMA	C1-C2-C3	2.14	112.29	109.67
8	S	1	NAG	C2-N2-C7	2.14	125.95	122.90
4	J	5	MAN	C1-C2-C3	-2.13	107.04	109.67
4	J	9	MAN	C1-O5-C5	2.13	115.08	112.19
9	O	2	NAG	C1-O5-C5	2.13	115.07	112.19
5	K	3	BMA	O5-C5-C6	2.12	110.52	107.20
13	W	3	BMA	O2-C2-C1	2.11	113.47	109.15
14	Y	3	BMA	O2-C2-C3	-2.11	105.92	110.14
12	R	3	BMA	O3-C3-C4	-2.08	105.54	110.35
13	W	2	NAG	O3-C3-C2	-2.08	105.16	109.47
8	N	2	NAG	O4-C4-C3	-2.08	105.54	110.35
6	L	3	BMA	O2-C2-C3	-2.07	105.99	110.14
11	U	3	BMA	O2-C2-C1	2.07	113.38	109.15
10	P	2	NAG	C1-O5-C5	2.05	114.96	112.19
8	N	2	NAG	C4-C3-C2	2.04	114.01	111.02
13	W	7	MAN	O6-C6-C5	-2.04	104.30	111.29
4	J	4	MAN	O5-C5-C4	-2.04	105.87	110.83
8	N	2	NAG	C1-C2-N2	2.03	113.96	110.49
3	I	4	MAN	O5-C5-C6	-2.03	104.02	107.20
13	W	2	NAG	C1-C2-N2	2.02	113.94	110.49
8	N	1	NAG	C1-O5-C5	-2.02	109.46	112.19
12	R	4	MAN	O3-C3-C2	2.01	113.85	109.99
9	O	7	MAN	O2-C2-C1	2.01	113.27	109.15
14	Y	1	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	2	NAG	C1-C2-N2-C7
5	X	1	NAG	C3-C2-N2-C7
8	N	2	NAG	C3-C2-N2-C7
10	P	2	NAG	C3-C2-N2-C7
12	R	1	NAG	C1-C2-N2-C7
14	Y	1	NAG	C3-C2-N2-C7
14	Y	2	NAG	C3-C2-N2-C7
5	T	2	NAG	C1-C2-N2-C7
11	V	2	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	V	1	NAG	O5-C5-C6-O6
12	R	1	NAG	O5-C5-C6-O6
4	J	7	MAN	O5-C5-C6-O6
4	J	9	MAN	O5-C5-C6-O6
9	O	4	MAN	O5-C5-C6-O6
13	W	3	BMA	O5-C5-C6-O6
12	R	6	MAN	O5-C5-C6-O6
11	V	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
12	R	1	NAG	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
11	U	3	BMA	O5-C5-C6-O6
12	R	2	NAG	O5-C5-C6-O6
14	Y	3	BMA	O5-C5-C6-O6
4	J	7	MAN	C4-C5-C6-O6
13	W	3	BMA	C4-C5-C6-O6
8	N	3	BMA	O5-C5-C6-O6
3	I	1	NAG	C1-C2-N2-C7
9	O	1	NAG	C1-C2-N2-C7
4	J	3	BMA	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
4	J	9	MAN	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
5	X	2	NAG	C8-C7-N2-C2
5	X	2	NAG	O7-C7-N2-C2
8	S	1	NAG	C8-C7-N2-C2
8	S	1	NAG	O7-C7-N2-C2
11	Q	1	NAG	C8-C7-N2-C2
11	Q	1	NAG	O7-C7-N2-C2
11	U	1	NAG	C8-C7-N2-C2
11	U	1	NAG	O7-C7-N2-C2
11	U	2	NAG	C8-C7-N2-C2
11	U	2	NAG	O7-C7-N2-C2
14	Y	2	NAG	C8-C7-N2-C2
14	Y	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C4-C5-C6-O6
14	Y	3	BMA	C4-C5-C6-O6
8	N	3	BMA	C4-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
11	V	4	MAN	O5-C5-C6-O6
12	R	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	V	1	NAG	C1-C2-N2-C7
11	U	3	BMA	C4-C5-C6-O6
12	R	6	MAN	C4-C5-C6-O6
8	N	1	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
9	O	2	NAG	C1-C2-N2-C7
9	O	4	MAN	C4-C5-C6-O6
11	Q	3	BMA	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
6	L	1	NAG	C1-C2-N2-C7
3	I	4	MAN	O5-C5-C6-O6
14	Y	2	NAG	O5-C5-C6-O6
13	W	7	MAN	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	I	5	MAN	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
13	W	6	MAN	O5-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
9	O	5	MAN	O5-C5-C6-O6
11	V	5	MAN	O5-C5-C6-O6
13	W	2	NAG	O5-C5-C6-O6
13	W	4	MAN	O5-C5-C6-O6
5	X	4	MAN	O5-C5-C6-O6
13	W	6	MAN	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
4	J	10	MAN	O5-C5-C6-O6
8	N	4	MAN	O5-C5-C6-O6
9	O	6	MAN	O5-C5-C6-O6
11	V	3	BMA	O5-C5-C6-O6
11	Q	1	NAG	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	L	1	NAG	C3-C2-N2-C7
11	U	1	NAG	C3-C2-N2-C7
11	V	1	NAG	C3-C2-N2-C7
9	O	7	MAN	C4-C5-C6-O6
8	N	1	NAG	C1-C2-N2-C7
10	P	1	NAG	C4-C5-C6-O6
8	N	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	P	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
9	O	1	NAG	C3-C2-N2-C7
10	P	1	NAG	C3-C2-N2-C7
11	V	2	NAG	C3-C2-N2-C7
12	R	1	NAG	C3-C2-N2-C7
4	J	2	NAG	C4-C5-C6-O6
12	R	3	BMA	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
8	S	3	BMA	C4-C5-C6-O6
11	V	2	NAG	C4-C5-C6-O6
9	O	7	MAN	O5-C5-C6-O6
5	X	1	NAG	C1-C2-N2-C7
8	S	3	BMA	O5-C5-C6-O6
9	O	2	NAG	C3-C2-N2-C7
11	Q	1	NAG	C3-C2-N2-C7
11	V	4	MAN	C4-C5-C6-O6
14	Y	1	NAG	C1-C2-N2-C7
11	Q	1	NAG	C1-C2-N2-C7

There are no ring outliers.

40 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	2	0
14	Y	2	NAG	2	0
4	J	2	NAG	1	0
14	Y	3	BMA	1	0
12	R	3	BMA	1	0
5	X	4	MAN	1	0
10	P	1	NAG	3	0
12	R	4	MAN	1	0
14	Y	4	MAN	1	0
4	J	5	MAN	1	0
6	L	1	NAG	2	0
3	I	1	NAG	4	0
3	I	2	NAG	1	0
5	K	2	NAG	2	0
8	N	1	NAG	3	0
14	Y	5	MAN	1	0

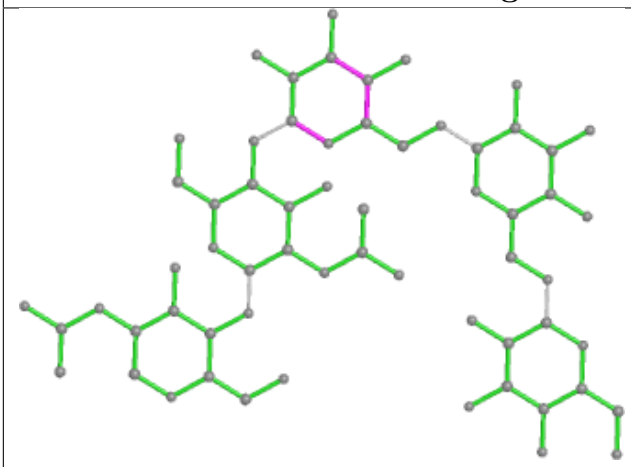
Continued on next page...

Continued from previous page...

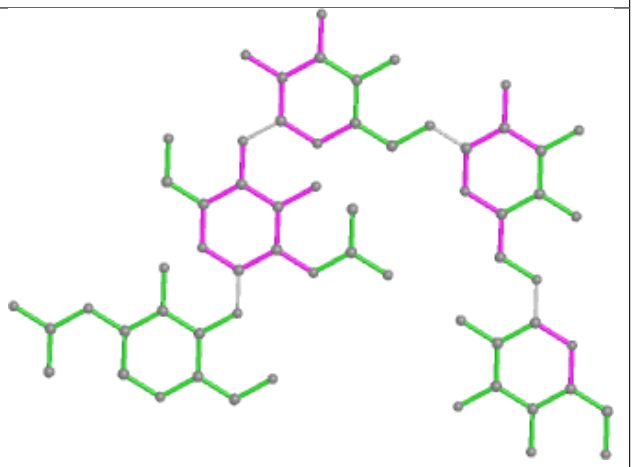
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	2	NAG	2	0
11	U	1	NAG	1	0
13	W	7	MAN	2	0
11	V	3	BMA	2	0
11	V	5	MAN	2	0
8	S	1	NAG	4	0
13	W	4	MAN	2	0
5	T	4	MAN	0	1
14	Y	1	NAG	2	0
11	V	1	NAG	5	0
9	O	1	NAG	3	0
9	O	2	NAG	2	0
13	W	6	MAN	1	0
11	V	2	NAG	2	0
9	O	7	MAN	1	0
10	P	2	NAG	1	0
13	W	3	BMA	3	0
5	X	1	NAG	3	0
12	R	1	NAG	1	0
9	O	3	BMA	2	0
5	X	3	BMA	1	0
5	T	2	NAG	3	0
11	Q	1	NAG	1	0
5	T	3	BMA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

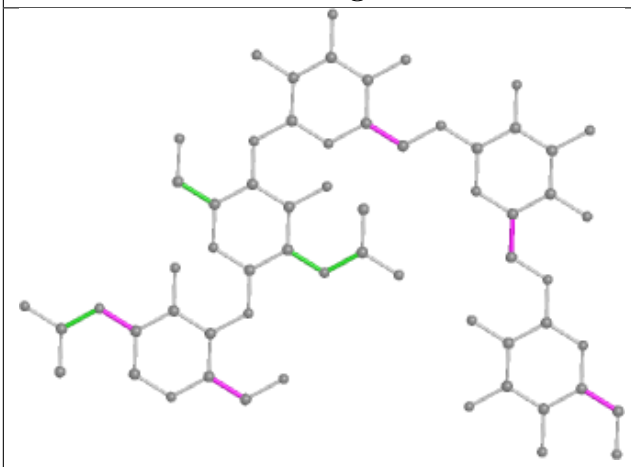
Oligosaccharide Chain I



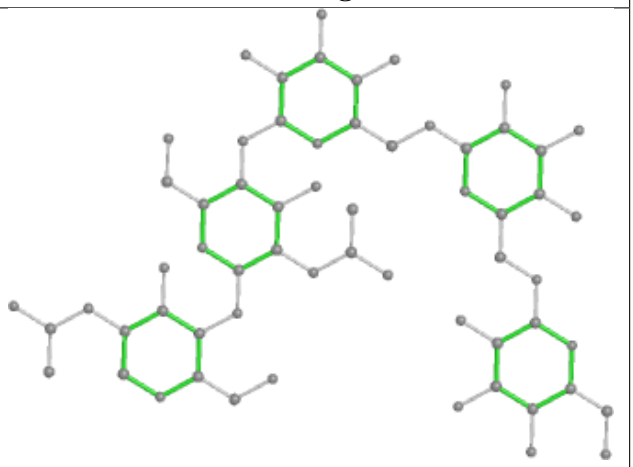
Bond lengths



Bond angles

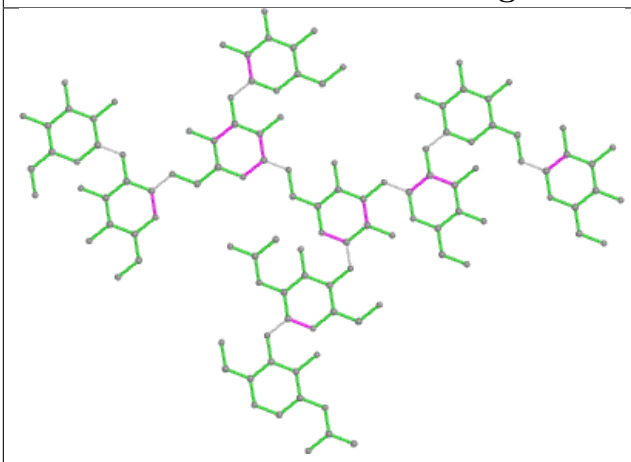


Torsions

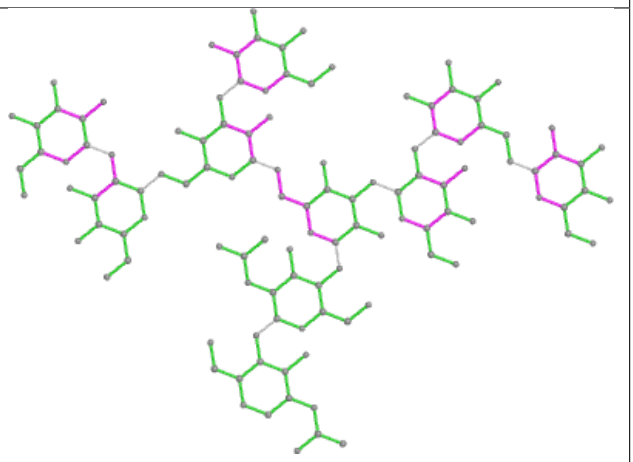


Rings

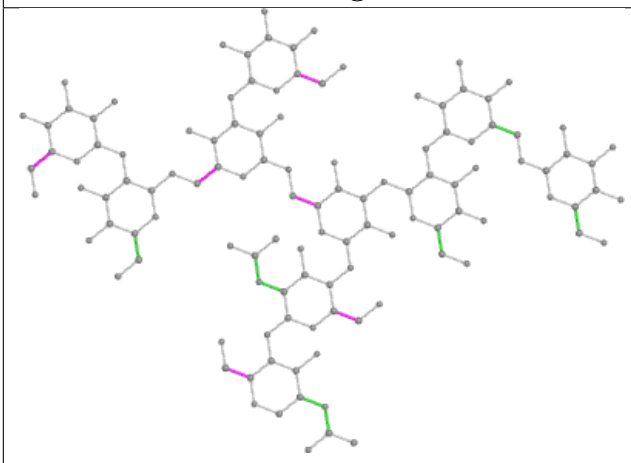
Oligosaccharide Chain J



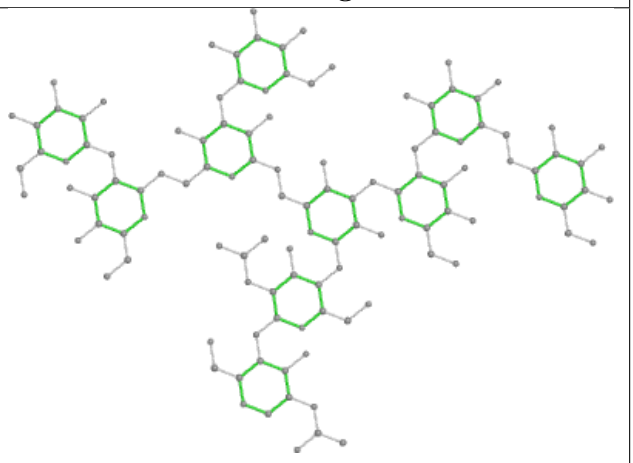
Bond lengths



Bond angles

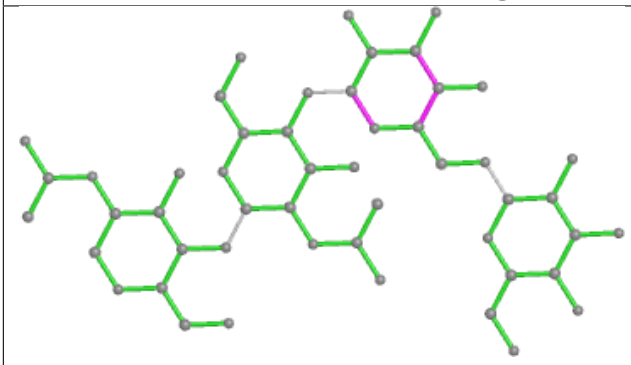


Torsions

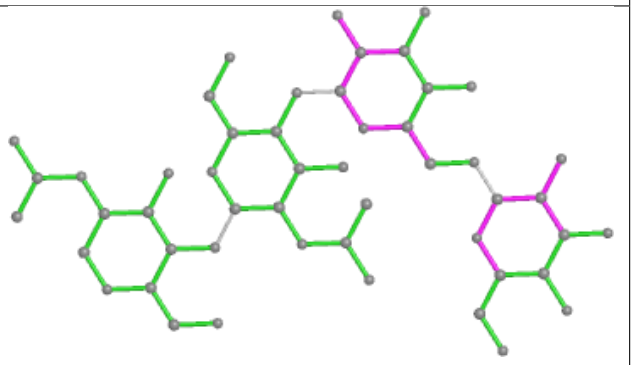


Rings

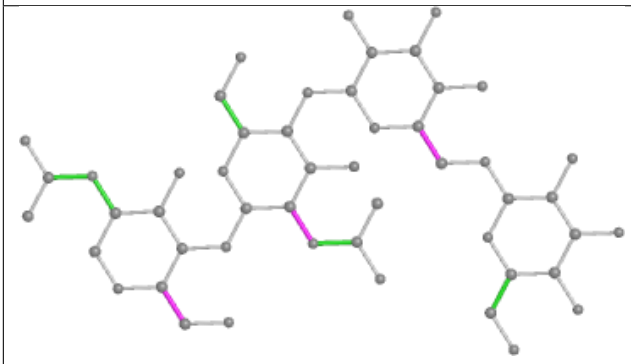
Oligosaccharide Chain K



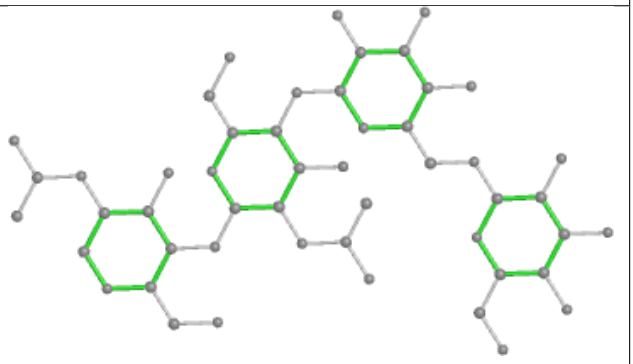
Bond lengths



Bond angles

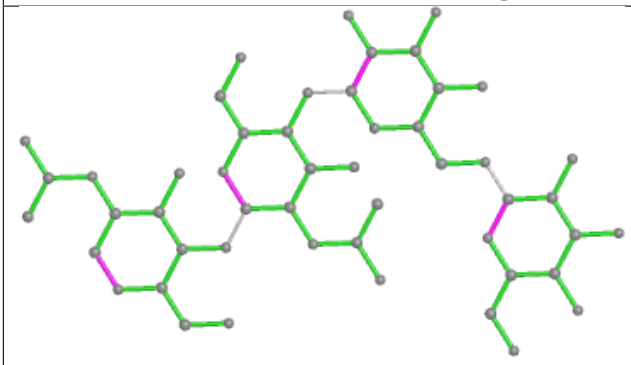


Torsions

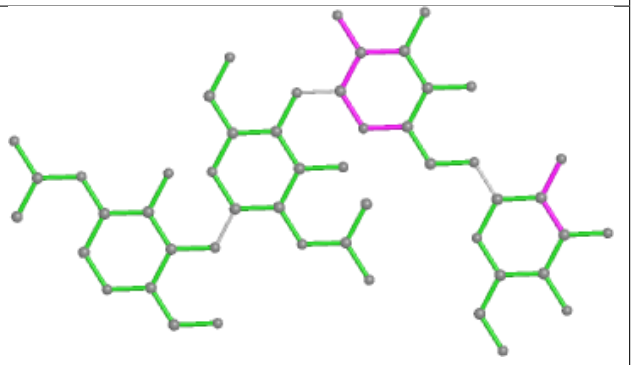


Rings

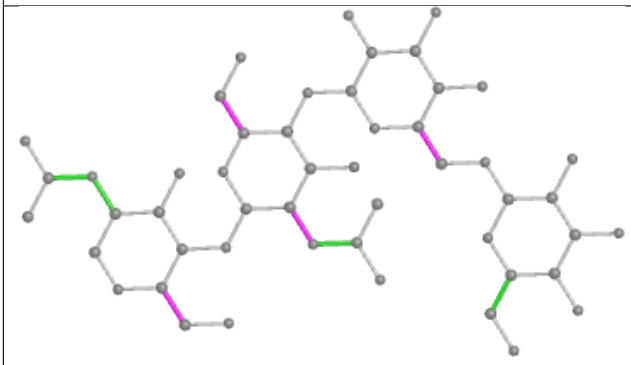
Oligosaccharide Chain T



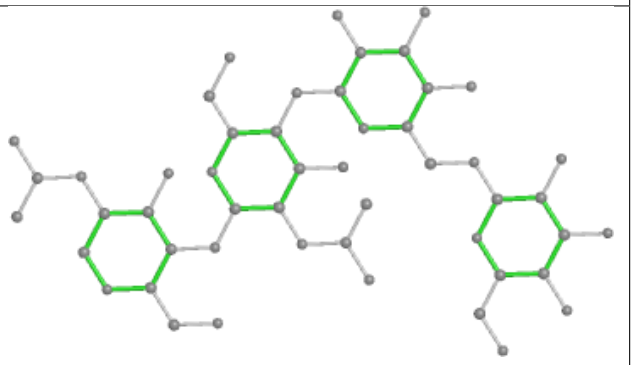
Bond lengths



Bond angles

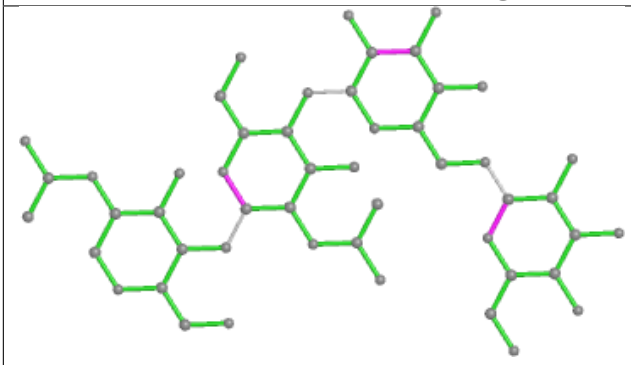


Torsions

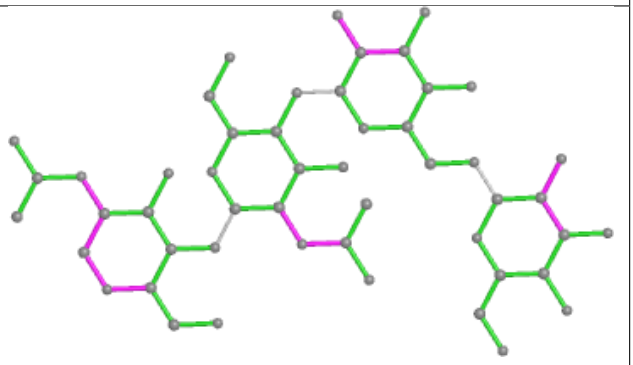


Rings

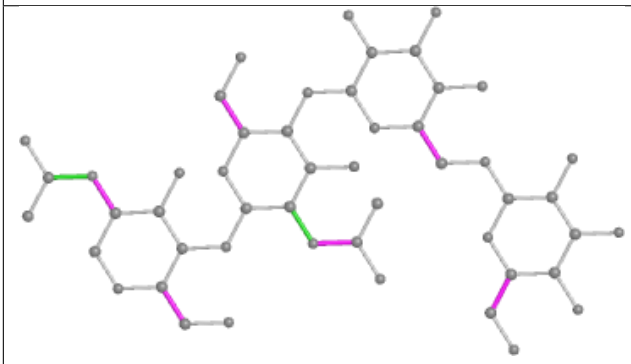
Oligosaccharide Chain X



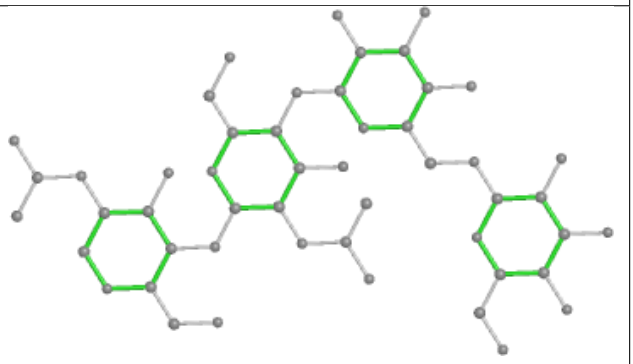
Bond lengths



Bond angles

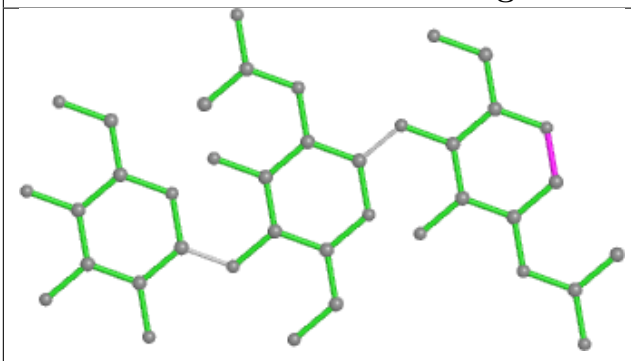


Torsions

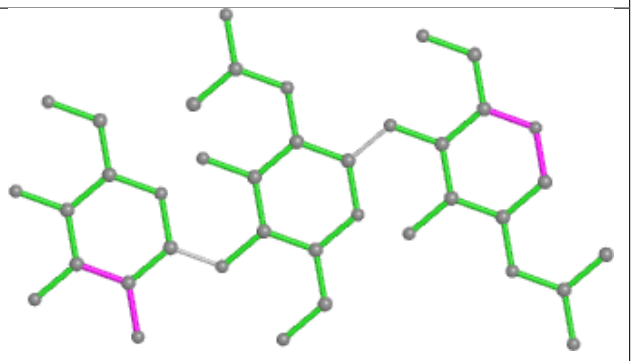


Rings

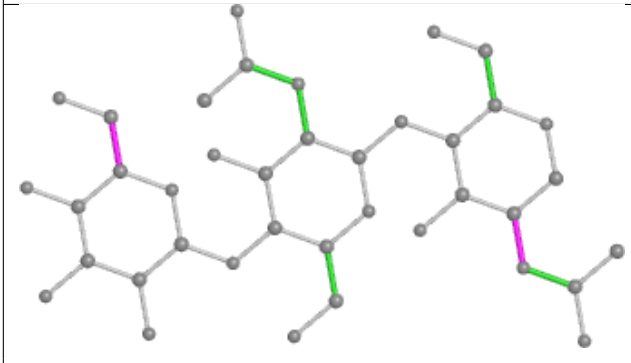
Oligosaccharide Chain L



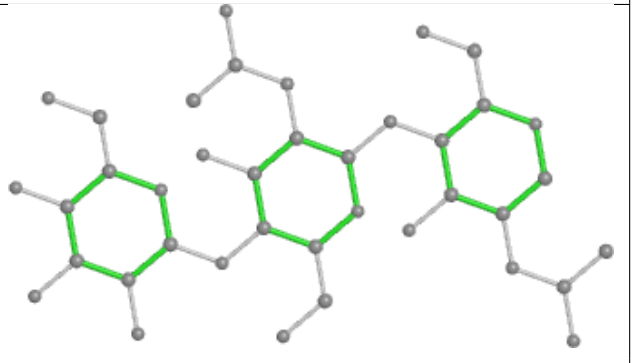
Bond lengths



Bond angles

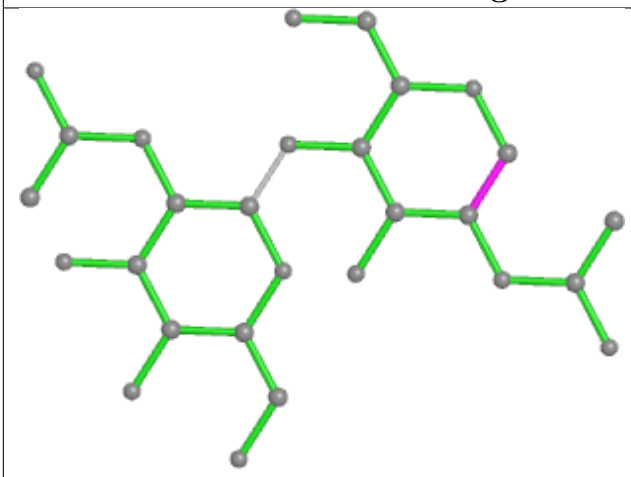


Torsions

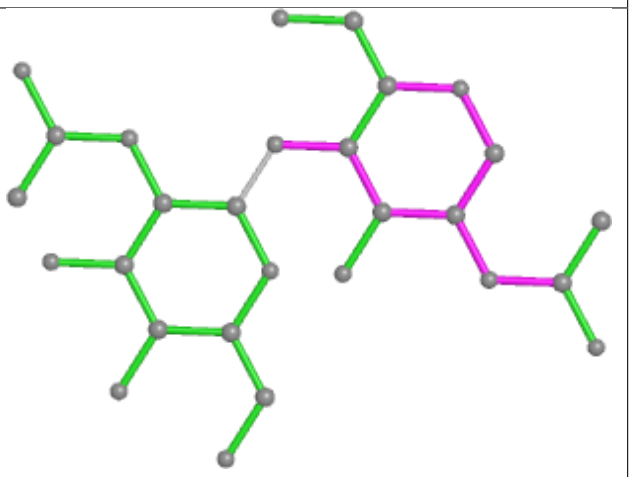


Rings

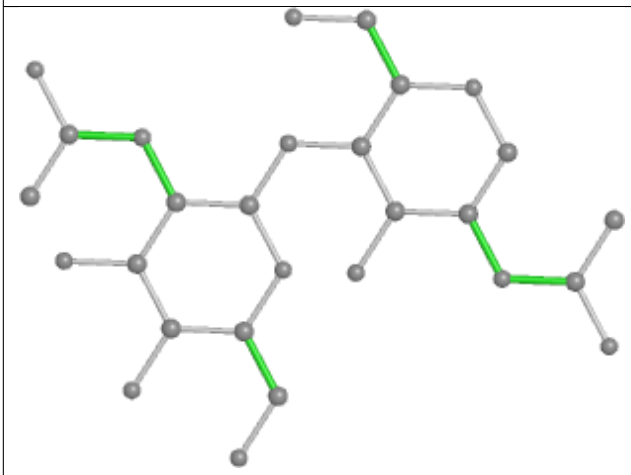
Oligosaccharide Chain M



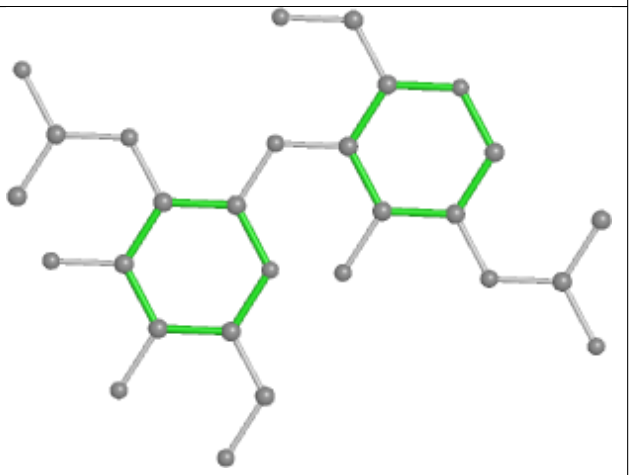
Bond lengths



Bond angles

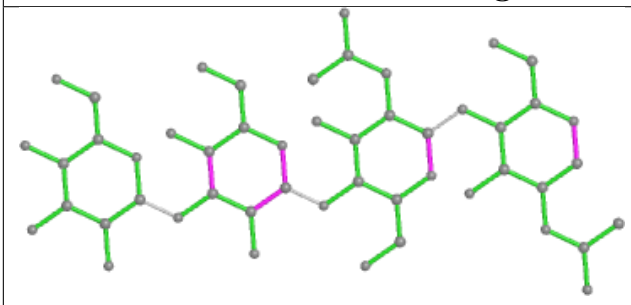


Torsions

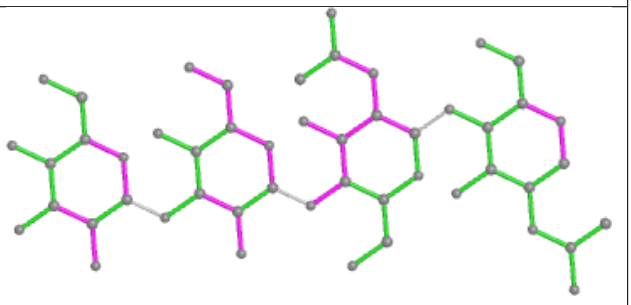


Rings

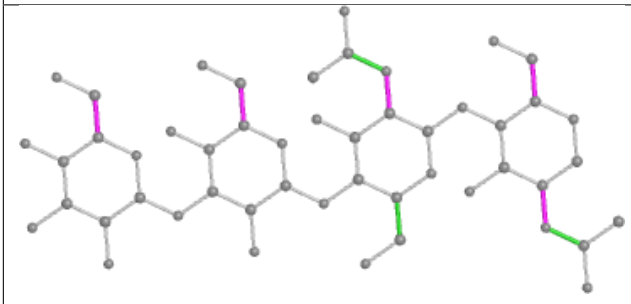
Oligosaccharide Chain N



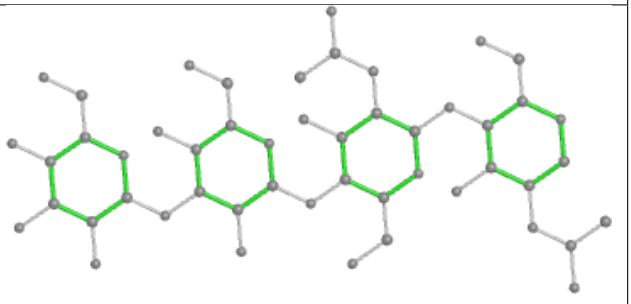
Bond lengths



Bond angles

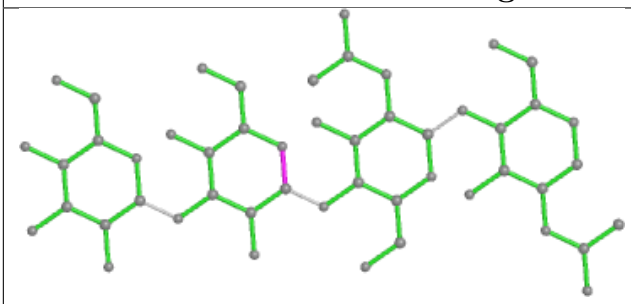


Torsions

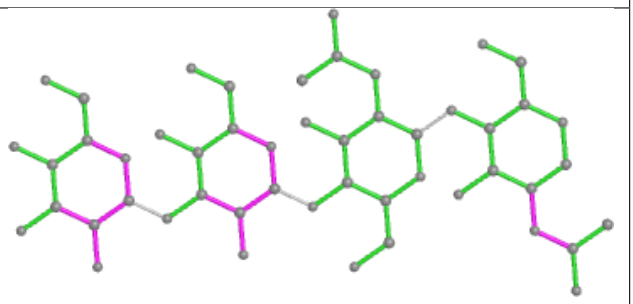


Rings

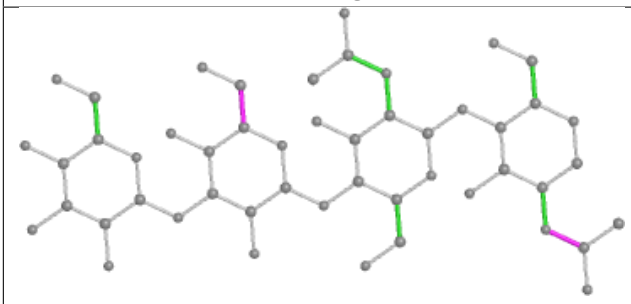
Oligosaccharide Chain S



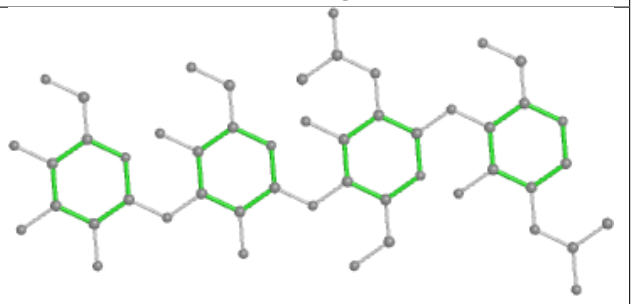
Bond lengths



Bond angles

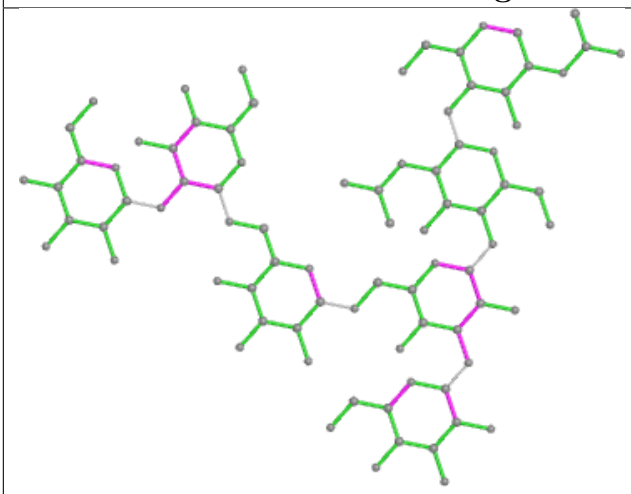


Torsions

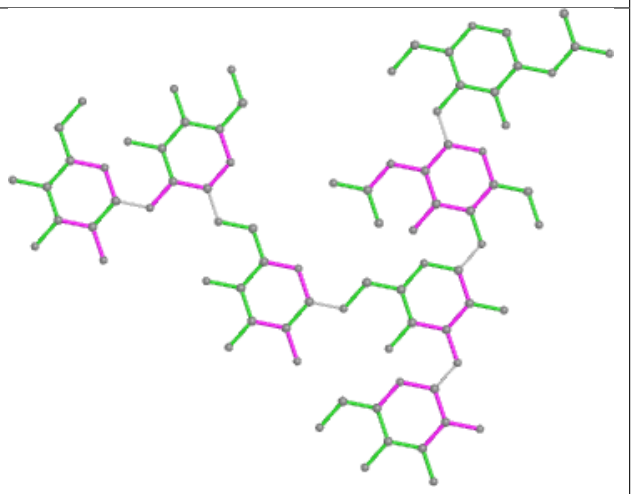


Rings

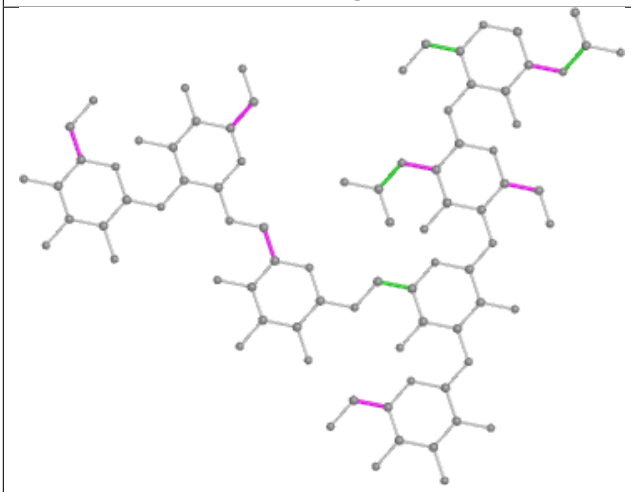
Oligosaccharide Chain O



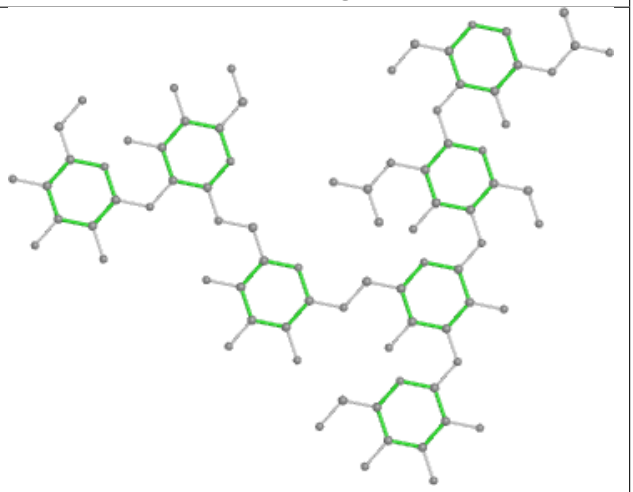
Bond lengths



Bond angles

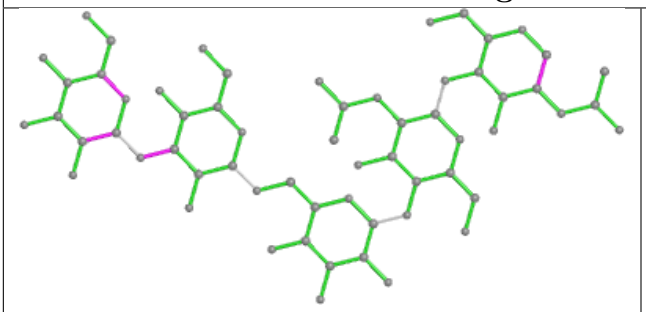


Torsions

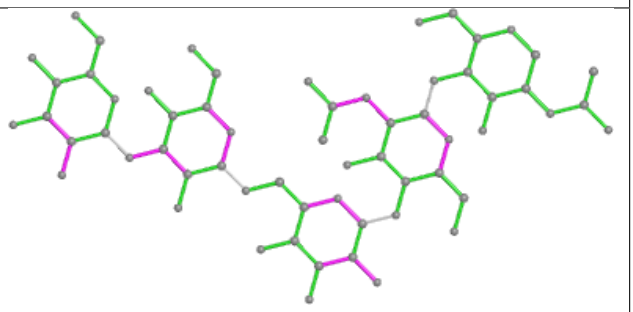


Rings

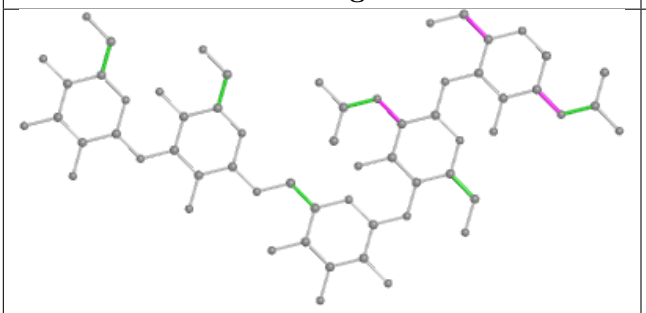
Oligosaccharide Chain P



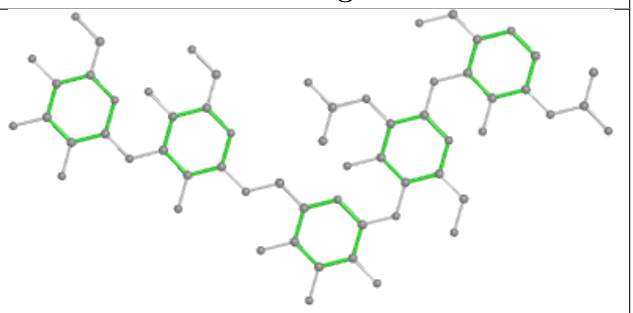
Bond lengths



Bond angles

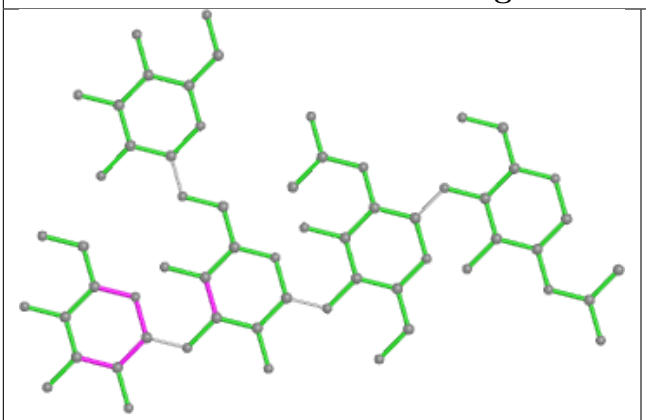


Torsions

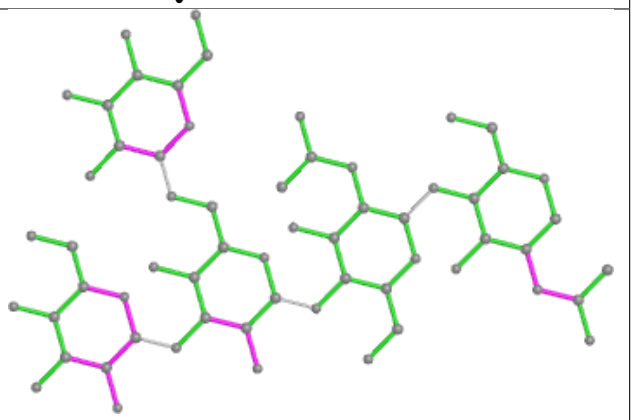


Rings

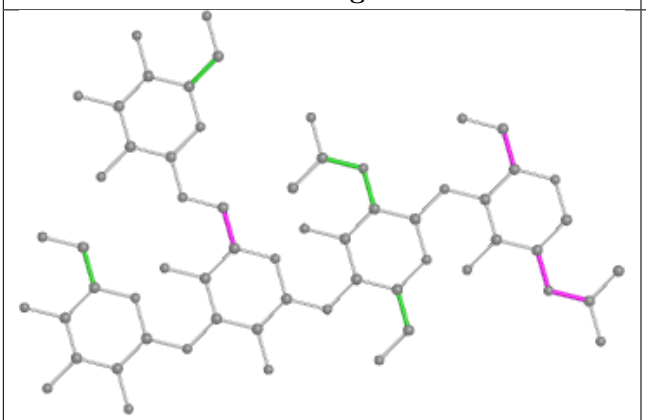
Oligosaccharide Chain Q



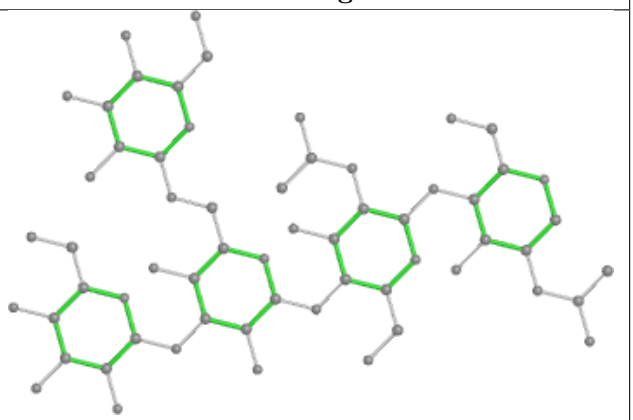
Bond lengths



Bond angles

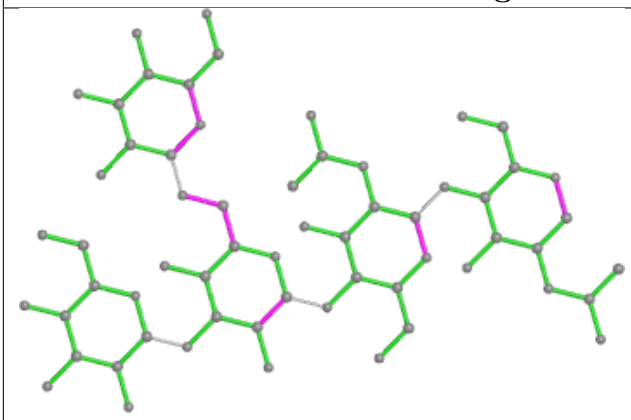


Torsions

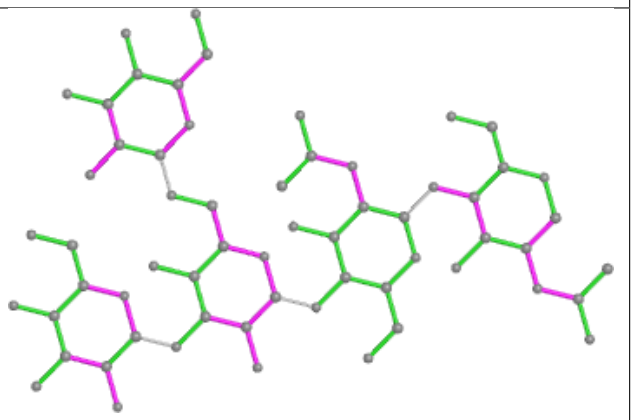


Rings

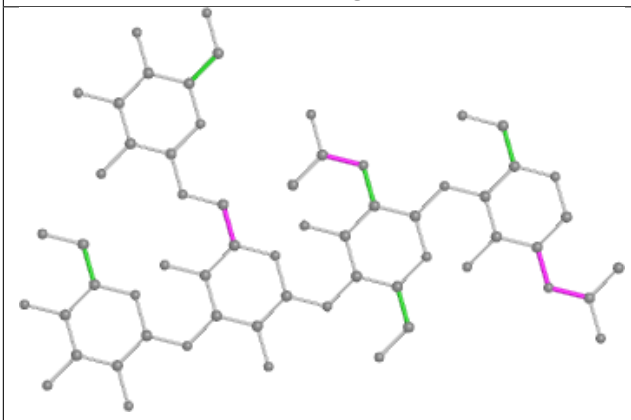
Oligosaccharide Chain U



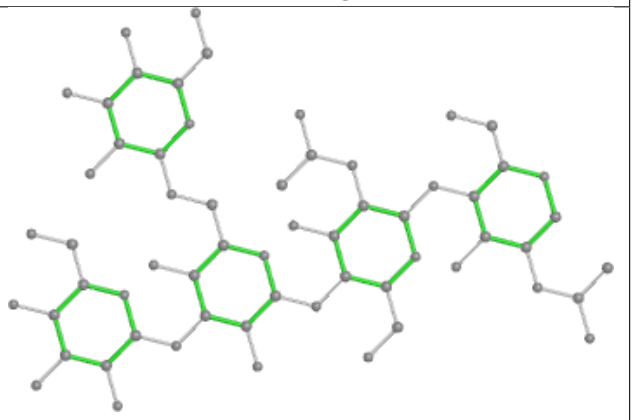
Bond lengths



Bond angles

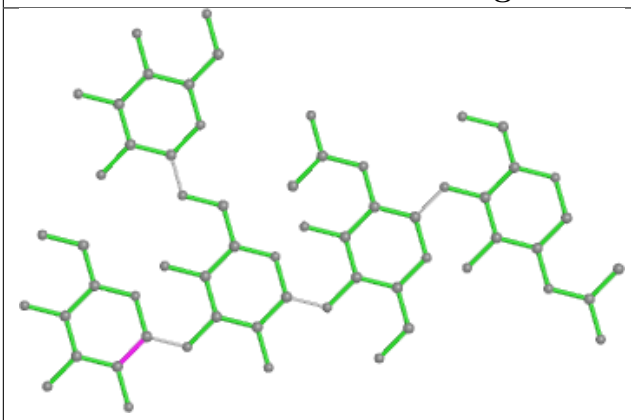


Torsions

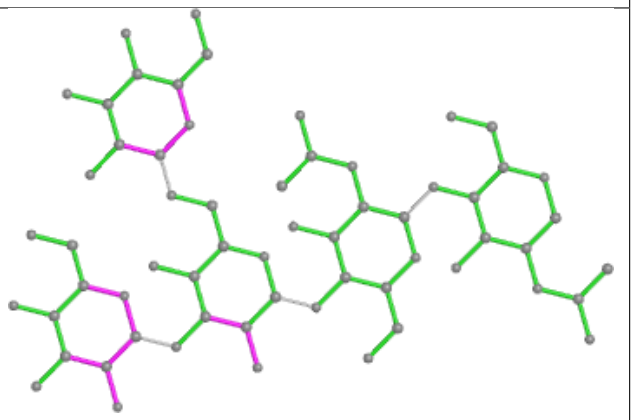


Rings

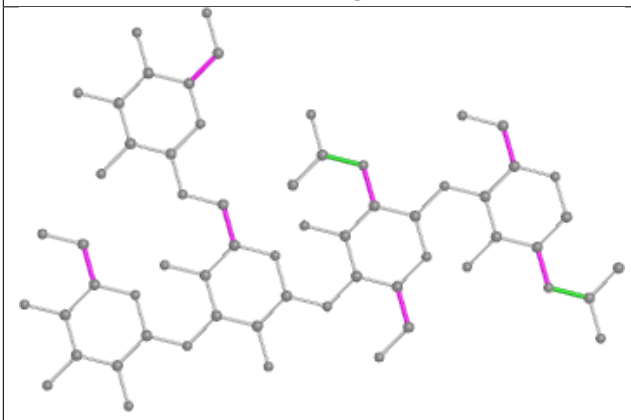
Oligosaccharide Chain V



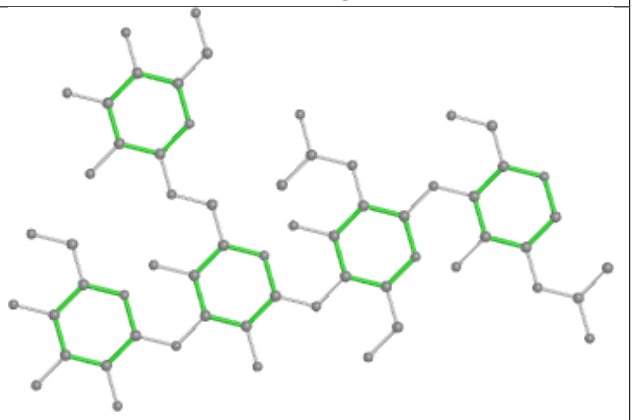
Bond lengths



Bond angles

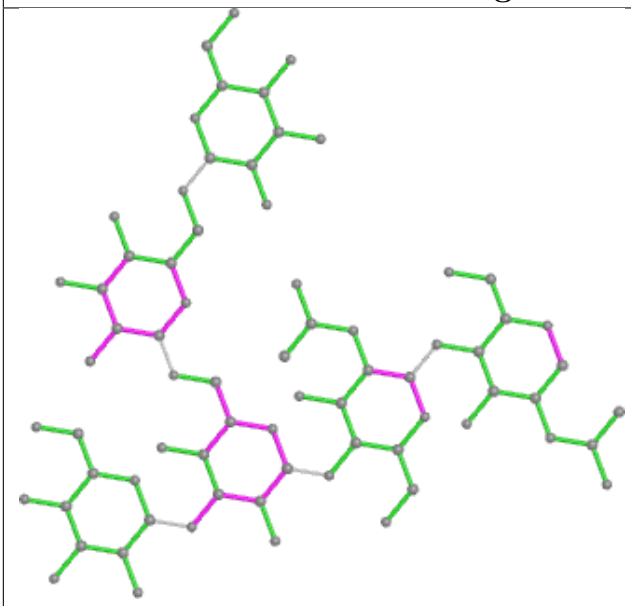


Torsions

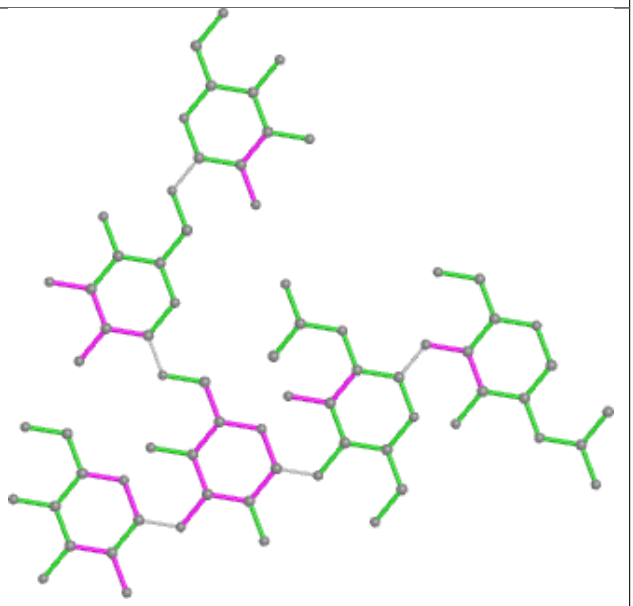


Rings

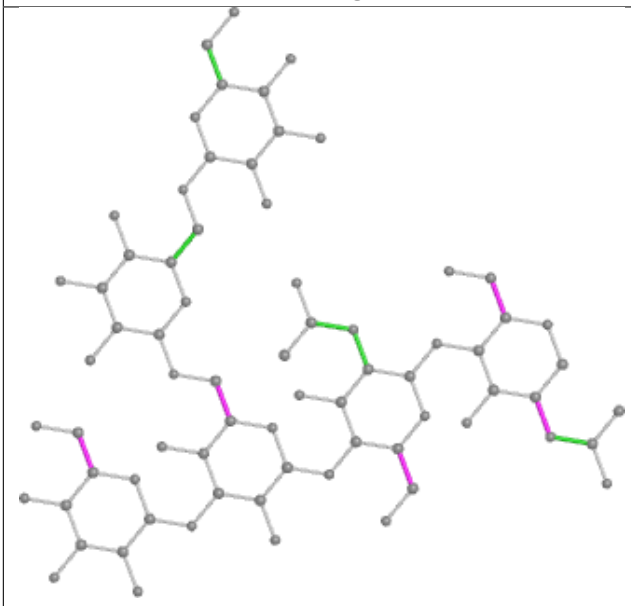
Oligosaccharide Chain R



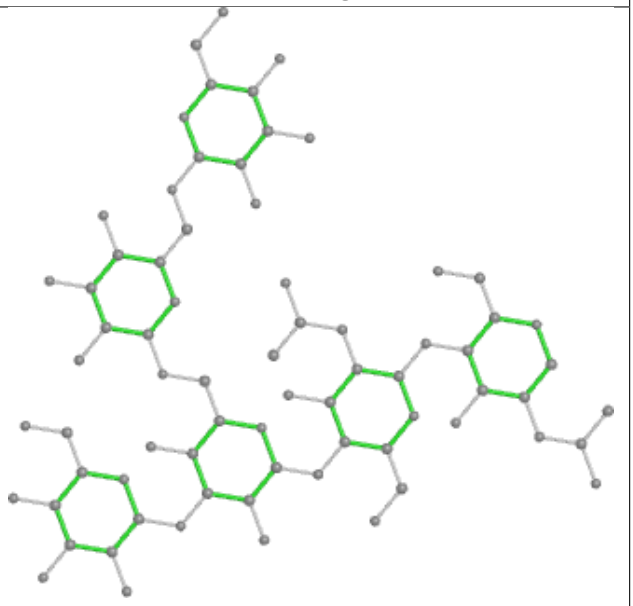
Bond lengths



Bond angles

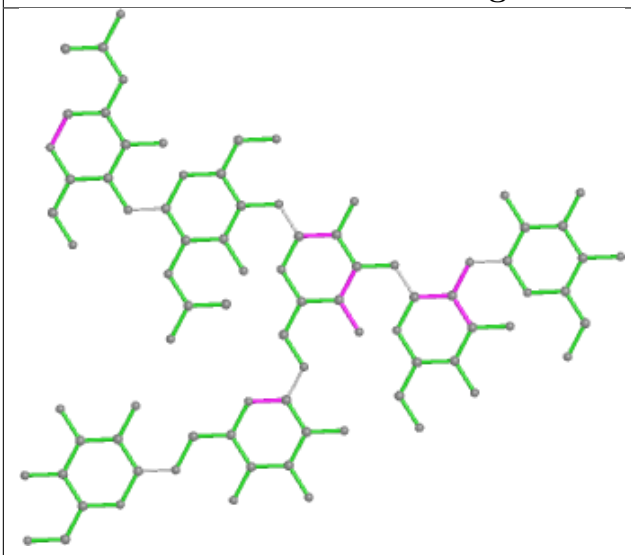


Torsions

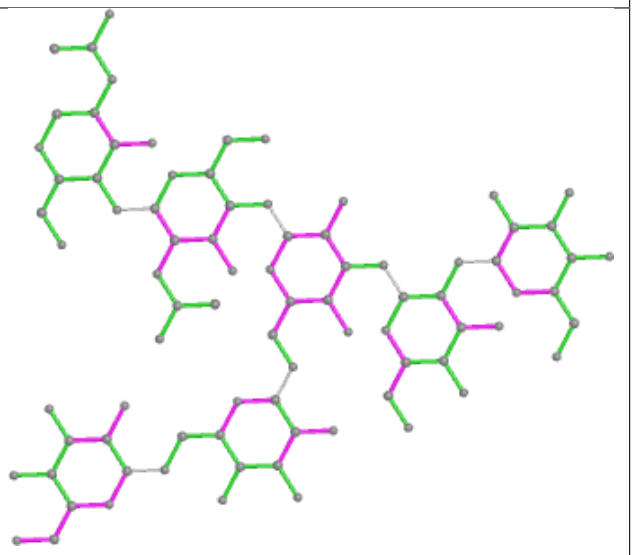


Rings

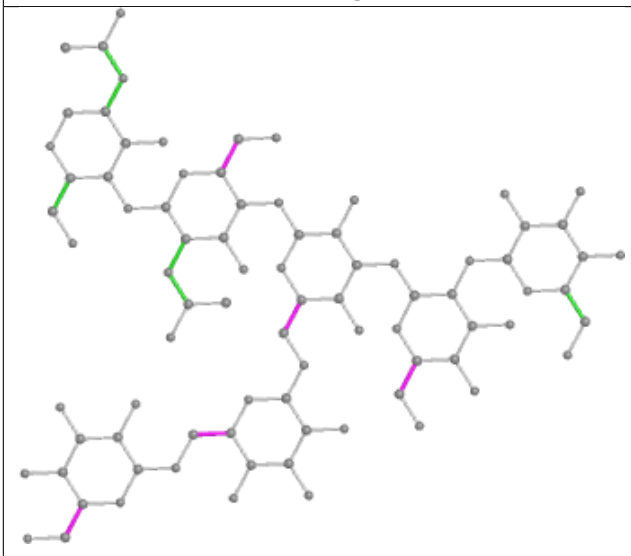
Oligosaccharide Chain W



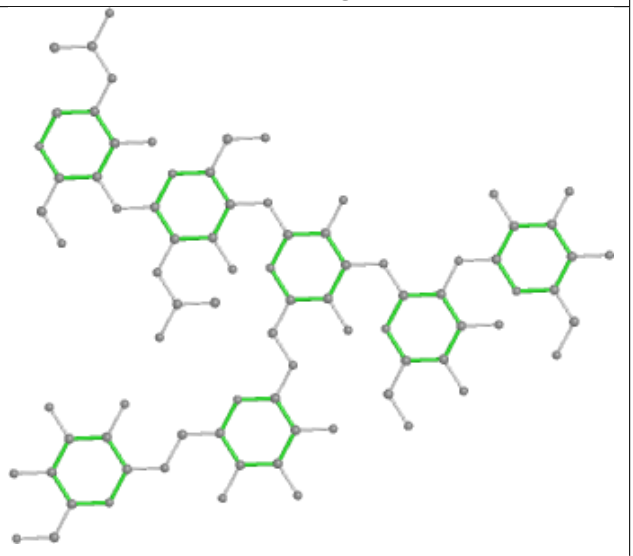
Bond lengths



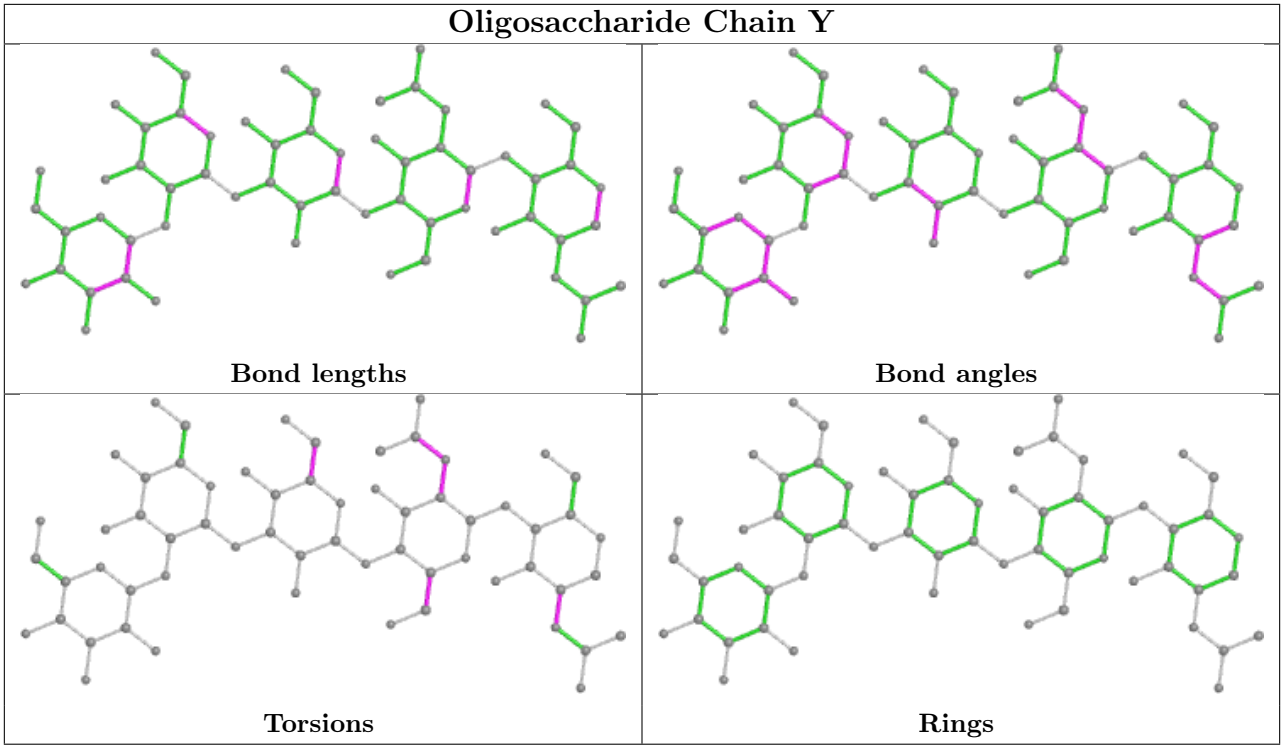
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 17 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	NAG	C	3678	1	14,14,15	0.82	1 (7%)	17,19,21	1.36	2 (11%)
17	NAG	G	3042	1	14,14,15	0.79	1 (7%)	17,19,21	0.55	0
17	NAG	F	3190	2	14,14,15	0.35	0	17,19,21	0.95	1 (5%)
17	NAG	E	3920	1	14,14,15	0.75	1 (7%)	17,19,21	3.90	3 (17%)
17	NAG	G	3031	1	14,14,15	0.35	0	17,19,21	0.55	0
17	NAG	H	3190	2	14,14,15	1.17	1 (7%)	17,19,21	0.93	1 (5%)
17	NAG	G	3678	1	14,14,15	0.74	1 (7%)	17,19,21	0.64	0
17	NAG	E	3042	1	14,14,15	0.43	0	17,19,21	0.66	1 (5%)
17	NAG	E	3031	1	14,14,15	0.33	0	17,19,21	0.43	0
17	NAG	H	3620	2	14,14,15	0.39	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	NAG	D	3620	2	14,14,15	0.40	0	17,19,21	0.41	0
17	NAG	H	3232	2	14,14,15	0.88	1 (7%)	17,19,21	2.47	3 (17%)
17	NAG	G	3920	1	14,14,15	0.91	1 (7%)	17,19,21	0.60	0
17	NAG	C	3031	1	14,14,15	0.27	0	17,19,21	0.54	0
17	NAG	A	3920	1	14,14,15	0.75	1 (7%)	17,19,21	0.52	0
17	NAG	F	3620	2	14,14,15	0.55	0	17,19,21	0.55	0
17	NAG	A	3042	1	14,14,15	0.74	1 (7%)	17,19,21	1.38	1 (5%)
17	NAG	B	3620	2	14,14,15	0.42	0	17,19,21	0.49	0
17	NAG	B	3232	2	14,14,15	1.03	1 (7%)	17,19,21	1.74	2 (11%)
17	NAG	E	3678	1	14,14,15	0.36	0	17,19,21	1.13	1 (5%)
17	NAG	C	3920	1	14,14,15	0.76	1 (7%)	17,19,21	0.82	0
17	NAG	A	3678	1	14,14,15	0.71	1 (7%)	17,19,21	0.64	0
17	NAG	H	3094	2	14,14,15	0.57	1 (7%)	17,19,21	0.41	0
17	NAG	A	3031	1	14,14,15	0.27	0	17,19,21	0.52	0
17	NAG	D	3232	2	14,14,15	0.84	1 (7%)	17,19,21	0.85	1 (5%)
17	NAG	C	3042	1	14,14,15	1.07	2 (14%)	17,19,21	0.47	0
17	NAG	F	3094	2	14,14,15	0.44	0	17,19,21	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	C	3678	1	-	2/6/23/26	0/1/1/1
17	NAG	G	3042	1	-	0/6/23/26	0/1/1/1
17	NAG	F	3190	2	-	2/6/23/26	0/1/1/1
17	NAG	E	3920	1	-	3/6/23/26	0/1/1/1
17	NAG	G	3031	1	-	2/6/23/26	0/1/1/1
17	NAG	H	3190	2	-	2/6/23/26	0/1/1/1
17	NAG	G	3678	1	-	0/6/23/26	0/1/1/1
17	NAG	E	3042	1	-	3/6/23/26	0/1/1/1
17	NAG	E	3031	1	-	2/6/23/26	0/1/1/1
17	NAG	H	3620	2	-	2/6/23/26	0/1/1/1
17	NAG	D	3620	2	-	1/6/23/26	0/1/1/1
17	NAG	H	3232	2	-	3/6/23/26	0/1/1/1
17	NAG	G	3920	1	-	2/6/23/26	0/1/1/1
17	NAG	C	3031	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	A	3920	1	-	2/6/23/26	0/1/1/1
17	NAG	F	3620	2	-	2/6/23/26	0/1/1/1
17	NAG	A	3042	1	-	1/6/23/26	0/1/1/1
17	NAG	B	3620	2	-	2/6/23/26	0/1/1/1
17	NAG	B	3232	2	-	3/6/23/26	0/1/1/1
17	NAG	E	3678	1	-	4/6/23/26	0/1/1/1
17	NAG	C	3920	1	-	2/6/23/26	0/1/1/1
17	NAG	A	3678	1	-	2/6/23/26	0/1/1/1
17	NAG	H	3094	2	-	1/6/23/26	0/1/1/1
17	NAG	A	3031	1	-	2/6/23/26	0/1/1/1
17	NAG	D	3232	2	-	2/6/23/26	0/1/1/1
17	NAG	C	3042	1	-	4/6/23/26	0/1/1/1
17	NAG	F	3094	2	-	4/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	3190	NAG	O5-C1	-4.22	1.37	1.43
17	B	3232	NAG	O5-C1	-3.42	1.38	1.43
17	G	3920	NAG	O5-C1	-3.19	1.38	1.43
17	C	3042	NAG	C1-C2	3.06	1.56	1.52
17	G	3042	NAG	C1-C2	2.82	1.56	1.52
17	D	3232	NAG	C1-C2	2.81	1.56	1.52
17	H	3232	NAG	O5-C1	2.70	1.48	1.43
17	G	3678	NAG	O5-C1	-2.69	1.39	1.43
17	A	3678	NAG	O5-C1	-2.58	1.39	1.43
17	A	3042	NAG	O5-C1	2.40	1.47	1.43
17	A	3920	NAG	C1-C2	2.40	1.55	1.52
17	C	3042	NAG	O5-C1	2.31	1.47	1.43
17	E	3920	NAG	O5-C1	2.30	1.47	1.43
17	C	3920	NAG	C1-C2	2.15	1.55	1.52
17	C	3678	NAG	C1-C2	2.13	1.55	1.52
17	H	3094	NAG	O5-C1	-2.06	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	E	3920	NAG	C1-O5-C5	11.00	127.09	112.19
17	E	3920	NAG	C2-N2-C7	9.81	136.87	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	3232	NAG	C2-N2-C7	7.38	133.41	122.90
17	B	3232	NAG	C1-O5-C5	-5.42	104.85	112.19
17	E	3920	NAG	C1-C2-N2	5.21	119.39	110.49
17	A	3042	NAG	C2-N2-C7	4.88	129.84	122.90
17	H	3232	NAG	C1-O5-C5	4.44	118.21	112.19
17	E	3678	NAG	C1-O5-C5	4.23	117.92	112.19
17	H	3232	NAG	C1-C2-N2	4.07	117.44	110.49
17	C	3678	NAG	C1-O5-C5	3.91	117.49	112.19
17	F	3190	NAG	C1-O5-C5	3.59	117.06	112.19
17	B	3232	NAG	C2-N2-C7	3.03	127.22	122.90
17	C	3678	NAG	C2-N2-C7	2.55	126.54	122.90
17	H	3620	NAG	C1-O5-C5	2.54	115.63	112.19
17	H	3190	NAG	C1-O5-C5	2.34	115.36	112.19
17	D	3232	NAG	C1-O5-C5	-2.18	109.24	112.19
17	E	3042	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	3042	NAG	C3-C2-N2-C7
17	E	3920	NAG	C1-C2-N2-C7
17	H	3232	NAG	C3-C2-N2-C7
17	F	3620	NAG	O5-C5-C6-O6
17	G	3031	NAG	O5-C5-C6-O6
17	A	3920	NAG	C1-C2-N2-C7
17	B	3232	NAG	C1-C2-N2-C7
17	F	3094	NAG	C1-C2-N2-C7
17	A	3031	NAG	O5-C5-C6-O6
17	C	3031	NAG	O5-C5-C6-O6
17	E	3678	NAG	O5-C5-C6-O6
17	H	3190	NAG	O5-C5-C6-O6
17	F	3620	NAG	C4-C5-C6-O6
17	G	3031	NAG	C4-C5-C6-O6
17	C	3042	NAG	C1-C2-N2-C7
17	E	3678	NAG	C4-C5-C6-O6
17	A	3031	NAG	C4-C5-C6-O6
17	H	3190	NAG	C4-C5-C6-O6
17	C	3031	NAG	C4-C5-C6-O6
17	C	3678	NAG	C8-C7-N2-C2
17	C	3678	NAG	O7-C7-N2-C2
17	D	3232	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	D	3232	NAG	O7-C7-N2-C2
17	E	3042	NAG	C8-C7-N2-C2
17	E	3042	NAG	O7-C7-N2-C2
17	E	3678	NAG	C8-C7-N2-C2
17	E	3678	NAG	O7-C7-N2-C2
17	E	3920	NAG	C8-C7-N2-C2
17	E	3920	NAG	O7-C7-N2-C2
17	H	3232	NAG	C8-C7-N2-C2
17	H	3232	NAG	O7-C7-N2-C2
17	A	3678	NAG	O5-C5-C6-O6
17	F	3190	NAG	O5-C5-C6-O6
17	H	3620	NAG	O5-C5-C6-O6
17	F	3094	NAG	C4-C5-C6-O6
17	H	3094	NAG	O5-C5-C6-O6
17	B	3620	NAG	O5-C5-C6-O6
17	A	3678	NAG	C4-C5-C6-O6
17	G	3920	NAG	O5-C5-C6-O6
17	F	3190	NAG	C4-C5-C6-O6
17	F	3094	NAG	O5-C5-C6-O6
17	H	3620	NAG	C4-C5-C6-O6
17	E	3042	NAG	O5-C5-C6-O6
17	C	3042	NAG	O5-C5-C6-O6
17	D	3620	NAG	O5-C5-C6-O6
17	E	3031	NAG	C4-C5-C6-O6
17	B	3232	NAG	C4-C5-C6-O6
17	E	3031	NAG	O5-C5-C6-O6
17	B	3620	NAG	C4-C5-C6-O6
17	C	3920	NAG	C1-C2-N2-C7
17	A	3920	NAG	C3-C2-N2-C7
17	B	3232	NAG	C3-C2-N2-C7
17	C	3042	NAG	C3-C2-N2-C7
17	F	3094	NAG	C3-C2-N2-C7
17	C	3920	NAG	O5-C5-C6-O6
17	C	3042	NAG	C4-C5-C6-O6
17	G	3920	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	3042	NAG	3	0
17	E	3920	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	3620	NAG	1	0
17	H	3232	NAG	1	0
17	G	3920	NAG	2	0
17	C	3031	NAG	1	0
17	A	3920	NAG	2	0
17	C	3920	NAG	5	0
17	H	3094	NAG	1	0
17	A	3031	NAG	1	0
17	D	3232	NAG	1	0
17	C	3042	NAG	1	0
17	F	3094	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1080/1137 (94%)	0.20	41 (3%) 40 37	86, 154, 246, 360	0
1	C	884/1137 (77%)	0.62	99 (11%) 5 5	90, 184, 288, 417	0
1	E	884/1137 (77%)	0.32	56 (6%) 20 20	84, 163, 267, 405	0
1	G	883/1137 (77%)	0.27	39 (4%) 34 33	86, 148, 255, 387	0
2	B	674/727 (92%)	0.58	79 (11%) 4 4	120, 217, 318, 438	0
2	D	674/727 (92%)	1.41	198 (29%) 0 0	136, 266, 376, 453	0
2	F	674/727 (92%)	0.68	97 (14%) 2 2	105, 213, 308, 375	0
2	H	674/727 (92%)	0.78	106 (15%) 2 2	101, 222, 327, 434	0
All	All	6427/7456 (86%)	0.56	715 (11%) 5 5	84, 188, 313, 453	0

All (715) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	433	ASP	20.6
2	D	92	ALA	19.9
2	B	92	ALA	16.7
2	D	91	ALA	15.7
2	D	82	THR	14.9
2	D	416	THR	12.7
2	H	432	ARG	11.5
1	C	817	GLN	10.6
2	H	92	ALA	10.5
2	F	91	ALA	10.2
2	D	189	THR	10.2
2	D	83	LEU	10.1
1	C	818	LYS	10.0
2	B	433	ASP	10.0
2	D	393	VAL	9.8
2	F	92	ALA	9.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	430	GLN	9.6
2	B	430	GLN	9.3
2	D	433	ASP	9.1
2	H	91	ALA	8.9
2	D	610	LEU	8.9
2	D	97	PHE	8.5
2	H	417	VAL	8.5
2	D	650	VAL	8.3
2	B	432	ARG	8.1
2	D	144	ILE	7.8
2	B	431	SER	7.8
1	A	727	PHE	7.8
2	B	72	GLY	7.7
2	D	207	ASN	7.5
2	D	443	LEU	7.4
2	D	143	ARG	7.3
1	E	727	PHE	7.1
2	H	80	LYS	7.1
2	H	416	THR	7.1
1	C	335	GLU	7.0
2	F	206	GLY	7.0
2	D	78	PRO	6.9
2	F	163	ASP	6.9
2	D	105	ILE	6.8
2	D	345	VAL	6.8
2	D	109	TYR	6.7
1	G	817	GLN	6.6
1	C	397	GLY	6.6
2	F	176	CYS	6.6
2	D	135	LEU	6.6
2	D	654	LEU	6.6
2	H	321	GLY	6.5
1	C	816	GLY	6.5
2	D	415	VAL	6.4
2	H	175	GLU	6.4
1	E	102	TYR	6.3
2	D	432	ARG	6.3
2	D	206	GLY	6.3
2	H	434	ARG	6.3
1	C	106	LEU	6.2
1	C	398	VAL	6.1
1	G	626	SER	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	321	GLY	6.0
2	D	107	LEU	6.0
2	D	63	ALA	6.0
1	G	624	VAL	5.9
2	D	62	LEU	5.9
2	D	29	PHE	5.8
1	A	1044	LYS	5.8
1	C	819	GLN	5.8
1	C	653	GLN	5.8
2	H	469	GLN	5.8
2	D	68	ASP	5.7
1	A	10	ALA	5.7
2	B	91	ALA	5.7
2	D	401	GLU	5.7
2	H	470	GLU	5.7
1	C	393	ALA	5.7
2	H	431	SER	5.6
1	C	723	PRO	5.6
2	B	144	ILE	5.6
2	H	393	VAL	5.5
2	F	160	THR	5.5
2	H	207	ASN	5.5
2	F	81	VAL	5.5
2	F	207	ASN	5.5
2	D	417	VAL	5.5
1	G	818	LYS	5.4
2	D	603	TYR	5.4
2	F	629	GLN	5.4
1	A	817	GLN	5.4
1	C	326	SER	5.4
2	F	1	GLN	5.4
2	D	384	ASN	5.4
2	D	160	THR	5.4
2	D	628	LEU	5.3
2	D	430	GLN	5.3
2	H	389	PHE	5.3
2	D	101	LYS	5.3
1	C	102	TYR	5.3
2	D	131	LEU	5.2
2	B	417	VAL	5.2
2	D	67	GLU	5.2
1	G	326	SER	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	452	THR	5.2
2	D	399	ILE	5.1
2	F	26	LYS	5.1
2	D	1	GLN	5.1
1	C	485	TRP	5.0
2	D	606	CYS	5.0
2	D	175	GLU	5.0
2	H	328	SER	5.0
1	C	919	LEU	5.0
2	B	131	LEU	4.9
2	D	391	VAL	4.9
1	C	1078	LEU	4.9
2	H	69	HIS	4.9
2	H	186	LEU	4.9
1	C	108	PHE	4.9
1	C	725	LEU	4.9
2	D	378	CYS	4.9
2	D	49	ARG	4.9
2	D	331	VAL	4.8
2	F	83	LEU	4.8
2	B	386	PRO	4.8
2	D	126	LYS	4.8
1	C	122	SER	4.8
2	F	628	LEU	4.7
2	H	335	LYS	4.7
1	C	419	GLN	4.7
2	D	159	ASN	4.7
1	C	10	ALA	4.7
1	C	1045	VAL	4.7
2	F	385	VAL	4.7
2	D	102	GLY	4.7
2	B	127	LEU	4.6
2	B	429	ASP	4.6
2	D	77	SER	4.6
2	D	75	GLN	4.6
2	D	236	LEU	4.6
2	D	104	PRO	4.6
2	D	208	LEU	4.6
2	F	78	PRO	4.6
2	H	244	GLY	4.5
2	D	408	ALA	4.5
2	D	431	SER	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	623	ALA	4.5
2	H	206	GLY	4.5
2	D	626	PRO	4.5
2	H	126	LYS	4.5
1	G	335	GLU	4.5
2	B	81	VAL	4.5
2	D	404	PHE	4.5
2	D	72	GLY	4.4
2	D	625	CYS	4.4
2	F	650	VAL	4.4
1	E	40	ALA	4.4
1	E	129	GLN	4.4
2	H	67	GLU	4.4
1	A	726	ALA	4.4
2	D	651	ALA	4.4
1	A	819	GLN	4.3
2	D	470	GLU	4.3
1	C	87	LEU	4.3
2	D	406	ILE	4.3
2	D	390	GLN	4.3
2	D	363	PHE	4.3
2	D	94	ASN	4.3
2	D	81	VAL	4.3
1	E	591	VAL	4.2
1	E	1077	VAL	4.2
1	C	424	TRP	4.2
2	D	318	SER	4.2
2	F	393	VAL	4.2
2	H	73	GLN	4.2
2	D	622	SER	4.2
2	D	365	SER	4.1
2	D	176	CYS	4.1
1	G	108	PHE	4.1
2	H	423	CYS	4.1
1	C	724	LEU	4.1
2	F	39	ARG	4.1
1	E	95	HIS	4.1
2	H	377	ASP	4.1
2	F	603	TYR	4.1
2	F	423	CYS	4.1
2	B	71	GLY	4.1
1	C	726	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	726	ALA	4.0
1	E	1044	LYS	4.0
2	B	415	VAL	4.0
1	C	996	GLN	4.0
1	G	625	VAL	4.0
2	B	145	GLY	4.0
2	B	389	PHE	4.0
2	B	80	LYS	4.0
2	D	369	THR	4.0
2	D	667	VAL	4.0
1	G	128	ARG	4.0
2	F	415	VAL	4.0
2	B	203	LEU	4.0
2	B	206	GLY	4.0
2	B	414	ILE	4.0
2	H	115	TYR	3.9
1	E	721	GLY	3.9
1	G	127	PRO	3.9
2	B	97	PHE	3.9
1	E	921	PHE	3.9
1	E	10	ALA	3.9
1	E	41	ALA	3.9
1	C	1044	LYS	3.9
2	D	65	THR	3.9
2	D	100	ALA	3.9
2	B	434	ARG	3.9
2	B	445	CYS	3.9
2	B	651	ALA	3.9
2	D	237	LEU	3.9
2	D	366	ASN	3.9
1	C	48	TYR	3.8
2	D	38	ILE	3.8
1	C	593	LEU	3.8
2	B	416	THR	3.8
2	B	26	LYS	3.8
2	D	74	LYS	3.8
2	D	70	ASN	3.8
2	H	379	ASP	3.8
1	E	817	GLN	3.8
2	F	175	GLU	3.8
1	C	1	PHE	3.8
2	D	142	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	724	LEU	3.8
2	D	382	GLN	3.8
2	F	329	ASN	3.8
2	D	627	GLY	3.8
1	E	9	THR	3.8
2	H	378	CYS	3.8
2	H	32	PRO	3.8
2	B	628	LEU	3.8
2	H	415	VAL	3.7
2	B	69	HIS	3.7
2	D	56	ILE	3.7
2	D	620	ASN	3.7
2	B	83	LEU	3.7
1	E	11	PHE	3.7
2	B	335	LYS	3.7
2	B	111	MET	3.7
2	B	25	GLN	3.7
1	A	621	ARG	3.7
1	E	108	PHE	3.7
2	H	327	SER	3.7
2	H	243	ASP	3.7
2	D	381	VAL	3.7
2	F	186	LEU	3.7
1	C	920	ASN	3.7
2	B	124	VAL	3.6
2	B	385	VAL	3.6
2	D	621	CYS	3.6
2	D	652	TYR	3.6
2	F	74	LYS	3.6
2	D	602	LYS	3.6
2	D	358	VAL	3.6
2	H	391	VAL	3.6
1	C	483	ARG	3.6
2	F	118	LEU	3.6
2	H	26	LYS	3.6
2	D	352	LEU	3.6
2	H	366	ASN	3.6
1	C	9	THR	3.6
2	D	386	PRO	3.6
2	F	236	LEU	3.6
2	D	370	HIS	3.5
2	F	142	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	649	TRP	3.5
2	F	429	ASP	3.5
1	E	395	TRP	3.5
2	D	611	LYS	3.5
1	C	721	GLY	3.5
1	G	651	ASP	3.5
2	H	81	VAL	3.5
2	H	333	LEU	3.5
2	H	93	PHE	3.5
2	H	376	GLY	3.5
2	D	320	VAL	3.5
2	B	305	VAL	3.5
2	F	107	LEU	3.5
1	E	482	TRP	3.4
2	D	84	TYR	3.4
2	D	388	THR	3.4
2	D	419	VAL	3.4
2	D	98	ARG	3.4
1	C	41	ALA	3.4
1	C	105	GLY	3.4
2	B	126	LYS	3.4
2	D	138	ILE	3.4
2	D	394	THR	3.4
2	F	49	ARG	3.4
2	H	320	VAL	3.4
2	H	174	LYS	3.4
2	H	382	GLN	3.4
1	G	409	GLN	3.3
2	H	84	TYR	3.3
2	F	345	VAL	3.3
1	G	1039	GLN	3.3
2	B	413	ASP	3.3
2	H	442	PHE	3.3
2	D	99	ARG	3.3
1	C	104	THR	3.3
2	F	188	LEU	3.3
2	F	619	LYS	3.3
2	B	93	PHE	3.3
1	C	1040	ILE	3.3
2	B	67	GLU	3.3
2	F	80	LYS	3.3
2	B	133	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	663	TYR	3.3
2	H	298	PHE	3.3
2	D	613	GLU	3.3
1	E	1078	LEU	3.3
2	D	294	ILE	3.3
1	C	345	GLY	3.3
2	F	406	ILE	3.3
1	E	48	TYR	3.3
2	D	180	PHE	3.3
2	D	71	GLY	3.2
2	B	238	VAL	3.2
2	D	665	ILE	3.2
1	C	731	ARG	3.2
2	B	571	ARG	3.2
2	D	30	THR	3.2
1	C	997	LYS	3.2
1	E	592	LEU	3.2
1	C	482	TRP	3.2
2	H	82	THR	3.2
2	D	377	ASP	3.2
2	D	330	VAL	3.2
2	D	193	ASN	3.2
2	B	404	PHE	3.2
1	C	109	LEU	3.2
1	E	730	LEU	3.2
2	D	446	GLY	3.2
1	G	820	GLY	3.1
2	F	177	GLN	3.1
2	D	616	PRO	3.1
2	F	330	VAL	3.1
2	B	50	GLY	3.1
1	A	623	GLN	3.1
2	D	79	GLN	3.1
2	D	210	ALA	3.1
2	H	83	LEU	3.1
2	H	56	ILE	3.1
2	D	7	LYS	3.1
2	B	419	VAL	3.1
2	D	95	VAL	3.1
1	G	819	GLN	3.1
2	H	654	LEU	3.1
1	C	400	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	34	ASP	3.1
2	F	664	LEU	3.1
2	B	423	CYS	3.1
1	A	265	TYR	3.1
2	F	622	SER	3.1
2	D	387	ILE	3.1
2	H	50	GLY	3.0
2	B	664	LEU	3.0
2	D	235	ARG	3.0
1	A	266	ALA	3.0
2	H	404	PHE	3.0
1	G	623	GLN	3.0
2	D	372	ASN	3.0
2	H	429	ASP	3.0
2	H	664	LEU	3.0
1	E	326	SER	3.0
1	E	920	ASN	3.0
2	D	414	ILE	3.0
1	G	95	HIS	3.0
1	E	594	LEU	3.0
2	H	30	THR	3.0
2	H	629	GLN	3.0
2	B	180	PHE	3.0
2	H	39	ARG	3.0
2	D	179	PRO	3.0
1	C	1001	LEU	3.0
1	G	919	LEU	3.0
1	G	102	TYR	3.0
2	D	635	VAL	3.0
2	D	472	GLU	3.0
1	C	722	LYS	3.0
2	F	103	TYR	2.9
2	H	628	LEU	2.9
2	H	363	PHE	2.9
1	G	433	THR	2.9
1	E	106	LEU	2.9
2	F	178	PRO	2.9
2	D	182	PHE	2.9
2	D	39	ARG	2.9
1	A	816	GLY	2.9
2	H	122	ARG	2.9
2	B	338	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	436	GLY	2.9
1	C	436	GLY	2.9
2	B	376	GLY	2.9
1	E	1040	ILE	2.9
2	H	173	GLU	2.9
1	C	730	LEU	2.9
2	B	107	LEU	2.9
2	D	395	ALA	2.8
2	D	506	LEU	2.8
1	C	65	PRO	2.8
2	F	122	ARG	2.8
1	C	1046	SER	2.8
2	D	418	GLN	2.8
2	H	381	VAL	2.8
2	D	249	GLY	2.8
2	D	353	PRO	2.8
1	G	372	ILE	2.8
2	D	624	ALA	2.8
1	A	592	LEU	2.8
1	E	393	ALA	2.8
2	F	113	LEU	2.8
1	C	129	GLN	2.8
1	E	335	GLU	2.8
2	D	51	CYS	2.8
2	B	84	TYR	2.8
2	B	39	ARG	2.8
2	D	93	PHE	2.8
2	F	199	VAL	2.8
1	C	1028	LEU	2.8
1	C	121	VAL	2.8
2	D	643	ARG	2.8
2	D	646	GLU	2.7
2	F	386	PRO	2.7
2	D	80	LYS	2.7
2	D	617	PHE	2.7
2	D	523	ASN	2.7
1	C	487	CYS	2.7
1	A	594	LEU	2.7
1	C	11	PHE	2.7
2	D	383	ILE	2.7
1	C	344	ASP	2.7
2	H	395	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	38	ILE	2.7
2	D	355	THR	2.7
2	H	367	GLY	2.7
1	C	814	ALA	2.7
2	F	624	ALA	2.7
2	H	297	ILE	2.7
2	H	111	MET	2.7
2	D	618	GLY	2.7
2	D	321	GLY	2.7
2	H	319	ALA	2.7
2	H	358	VAL	2.7
2	B	96	THR	2.7
2	D	186	LEU	2.7
1	C	467	GLN	2.7
1	C	347	VAL	2.7
1	A	918	TYR	2.6
2	F	161	HIS	2.7
1	A	724	LEU	2.6
1	C	443	LEU	2.6
1	G	594	LEU	2.6
2	F	119	ASP	2.6
1	E	826	HIS	2.6
2	F	660	MET	2.6
1	G	553	ILE	2.6
2	F	377	ASP	2.6
2	D	96	THR	2.6
2	F	430	GLN	2.6
2	D	319	ALA	2.6
2	D	356	LEU	2.6
1	C	702	SER	2.6
2	D	139	THR	2.6
2	F	384	ASN	2.6
1	C	596	THR	2.6
1	E	339	ALA	2.6
1	A	220	LEU	2.6
1	C	553	ILE	2.6
2	F	626	PRO	2.6
2	H	463	THR	2.6
2	F	8	VAL	2.6
2	D	57	MET	2.6
2	F	266	LEU	2.6
2	F	347	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	665	ILE	2.6
1	C	56	ALA	2.6
2	D	248	ALA	2.6
1	C	101	MET	2.6
2	F	144	ILE	2.6
2	D	389	PHE	2.6
1	A	818	LYS	2.6
2	H	435	SER	2.6
2	F	616	PRO	2.6
2	D	367	GLY	2.5
1	C	863	PHE	2.5
2	D	434	ARG	2.5
1	G	595	ARG	2.5
2	D	69	HIS	2.5
2	H	339	ASN	2.5
1	E	590	GLN	2.5
2	H	150	VAL	2.5
2	F	29	PHE	2.5
1	A	276	ARG	2.5
2	F	652	TYR	2.5
2	D	8	VAL	2.5
2	D	219	MET	2.5
2	D	334	ILE	2.5
2	F	111	MET	2.5
1	E	96	GLU	2.5
1	C	964	TRP	2.5
1	E	1076	THR	2.5
2	B	113	LEU	2.5
2	H	38	ILE	2.5
1	C	409	GLN	2.5
2	D	376	GLY	2.5
2	B	372	ASN	2.5
1	E	52	TYR	2.5
2	H	330	VAL	2.5
2	B	464	GLN	2.5
2	D	45	GLN	2.5
2	H	630	LEU	2.5
1	C	565	PHE	2.5
1	A	296	LYS	2.5
2	B	101	LYS	2.5
2	H	124	VAL	2.5
2	H	236	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	406	ILE	2.5
2	F	232	ASN	2.5
1	E	38	ILE	2.5
2	H	263	ARG	2.5
2	D	250	ASP	2.4
2	F	642	GLU	2.4
2	H	203	LEU	2.4
1	C	918	TYR	2.4
2	F	20	GLY	2.4
1	A	887	THR	2.4
2	D	174	LYS	2.4
2	D	108	TYR	2.4
1	C	1076	THR	2.4
1	A	1078	LEU	2.4
1	C	992	LEU	2.4
2	D	423	CYS	2.4
1	A	1080	LYS	2.4
2	D	362	SER	2.4
1	A	267	ILE	2.4
2	D	642	GLU	2.4
1	C	401	LEU	2.4
2	H	386	PRO	2.4
1	A	273	PHE	2.4
1	E	653	GLN	2.4
2	D	150	VAL	2.4
2	F	321	GLY	2.4
2	F	618	GLY	2.4
2	B	454	TYR	2.4
2	F	638	ARG	2.4
1	E	37	LYS	2.4
1	C	1077	VAL	2.4
2	D	6	PHE	2.4
1	A	1028	LEU	2.4
1	A	959	ASN	2.4
1	C	729	ASN	2.4
2	H	414	ILE	2.4
2	D	76	LEU	2.4
1	G	821	GLN	2.3
1	G	437	SER	2.3
1	C	110	LEU	2.3
2	F	635	VAL	2.3
2	H	273	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	485	TRP	2.3
2	H	401	GLU	2.3
1	C	592	LEU	2.3
1	E	372	ILE	2.3
1	C	1047	VAL	2.3
1	A	335	GLU	2.3
2	F	398	CYS	2.3
2	B	109	TYR	2.3
1	E	93	VAL	2.3
2	F	414	ILE	2.3
1	C	346	PRO	2.3
1	E	1045	VAL	2.3
2	H	249	GLY	2.3
1	A	323	THR	2.3
1	E	887	THR	2.3
2	B	603	TYR	2.3
2	D	360	TYR	2.3
2	F	368	VAL	2.3
1	A	436	GLY	2.3
2	D	364	CYS	2.3
2	F	40	CYS	2.3
2	H	187	LYS	2.3
1	C	1041	LEU	2.3
2	F	131	LEU	2.3
1	A	280	LYS	2.3
1	G	106	LEU	2.3
2	D	671	ARG	2.3
2	F	665	ILE	2.3
2	B	652	TYR	2.3
2	F	210	ALA	2.3
2	D	619	LYS	2.3
2	H	170	PRO	2.3
1	E	981	SER	2.3
1	E	485	TRP	2.3
2	B	29	PHE	2.3
2	D	368	VAL	2.3
2	F	417	VAL	2.3
2	F	649	TRP	2.3
2	H	95	VAL	2.3
2	D	28	ASN	2.3
2	F	191	ASN	2.3
2	D	409	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	38	ILE	2.3
1	A	1045	VAL	2.3
2	F	381	VAL	2.3
1	C	703	CYS	2.2
2	B	207	ASN	2.2
2	D	209	ASP	2.2
1	C	1018	PHE	2.2
2	B	66	GLN	2.2
1	E	919	LEU	2.2
2	D	428	ARG	2.2
2	F	630	LEU	2.2
1	E	33	GLY	2.2
2	D	614	LYS	2.2
1	A	234	ILE	2.2
1	C	939	ASN	2.2
2	F	84	TYR	2.2
2	H	237	LEU	2.2
1	E	1036	TRP	2.2
1	G	417	PHE	2.2
2	D	429	ASP	2.2
2	B	285	LEU	2.2
2	D	629	GLN	2.2
2	F	416	THR	2.2
2	F	431	SER	2.2
1	C	127	PRO	2.2
2	D	111	MET	2.2
2	D	385	VAL	2.2
2	B	34	ASP	2.2
2	F	174	LYS	2.2
1	C	417	PHE	2.2
2	H	384	ASN	2.2
1	C	125	GLU	2.2
1	C	969	VAL	2.2
2	B	320	VAL	2.2
1	G	562	LEU	2.2
1	C	732	PRO	2.2
1	A	136	LEU	2.2
1	E	992	LEU	2.2
1	G	362	LEU	2.2
2	H	131	LEU	2.2
2	B	629	GLN	2.2
1	G	627	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	413	ASP	2.2
1	C	774	LEU	2.1
2	D	407	ARG	2.1
2	H	419	VAL	2.1
1	A	863	PHE	2.1
1	C	421	SER	2.1
2	F	390	GLN	2.1
1	A	919	LEU	2.1
2	D	612	PHE	2.1
2	F	382	GLN	2.1
1	E	725	LEU	2.1
1	C	952	PHE	2.1
1	G	650	ARG	2.1
2	D	222	ALA	2.1
1	G	396	LYS	2.1
2	H	390	GLN	2.1
1	G	397	GLY	2.1
2	D	251	GLY	2.1
1	C	396	LYS	2.1
2	F	109	TYR	2.1
1	C	499	TRP	2.1
2	D	185	VAL	2.1
2	B	401	GLU	2.1
2	H	202	GLN	2.1
1	C	32	VAL	2.1
2	H	144	ILE	2.1
2	D	323	LEU	2.1
2	H	62	LEU	2.1
1	E	627	GLU	2.1
2	H	308	TYR	2.1
2	H	205	SER	2.1
1	C	86	LEU	2.1
1	E	509	LEU	2.1
2	F	367	GLY	2.1
2	H	326	ASP	2.1
1	E	565	PHE	2.1
2	D	298	PHE	2.1
2	F	63	ALA	2.1
2	F	667	VAL	2.1
2	F	138	ILE	2.1
1	G	863	PHE	2.1
2	D	400	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	389	PHE	2.1
1	A	238	ILE	2.1
2	B	654	LEU	2.1
2	B	428	ARG	2.0
2	F	104	PRO	2.0
2	H	337	ALA	2.0
1	A	285	ILE	2.0
1	C	427	LYS	2.0
2	D	278	ASP	2.0
2	H	362	SER	2.0
1	C	1024	LEU	2.0
1	E	669	PRO	2.0
2	D	136	ASN	2.0
2	D	234	THR	2.0
1	A	653	GLN	2.0
1	C	402	VAL	2.0
1	A	235	LEU	2.0
2	B	122	ARG	2.0
1	A	106	LEU	2.0
1	E	1041	LEU	2.0
1	G	39	THR	2.0
2	B	82	THR	2.0
1	G	1066	GLN	2.0
2	D	158	VAL	2.0
1	E	12	ARG	2.0
2	F	126	LYS	2.0
2	B	183	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MAN	O	4	11/12	0.02	0.26	288,304,311,317	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BMA	N	3	11/12	0.27	0.39	297,334,341,350	0
9	NAG	O	1	14/15	0.39	0.35	257,282,326,328	0
9	NAG	O	2	14/15	0.41	0.34	229,298,329,346	0
14	NAG	Y	2	14/15	0.43	0.41	239,315,332,345	0
14	BMA	Y	3	11/12	0.44	0.33	261,315,353,371	0
6	BMA	L	3	11/12	0.47	0.47	252,306,330,335	0
5	BMA	X	3	11/12	0.49	0.26	337,345,352,353	0
9	MAN	O	6	11/12	0.49	0.51	274,292,298,299	0
8	NAG	N	1	14/15	0.55	0.25	220,240,264,265	0
13	MAN	W	4	11/12	0.61	0.49	346,370,378,391	0
6	NAG	L	2	14/15	0.63	0.29	225,301,319,329	0
5	BMA	K	3	11/12	0.63	0.43	313,322,328,341	0
11	MAN	U	4	11/12	0.63	0.44	246,284,314,321	0
13	MAN	W	7	11/12	0.64	0.19	230,289,305,305	0
5	BMA	T	3	11/12	0.64	0.14	329,335,342,344	0
4	MAN	J	9	11/12	0.64	0.43	263,300,333,333	0
9	BMA	O	3	11/12	0.66	0.31	336,352,372,394	0
3	MAN	I	5	11/12	0.66	0.26	261,289,311,344	0
8	BMA	S	3	11/12	0.69	0.29	320,330,340,343	0
13	BMA	W	3	11/12	0.70	0.29	328,334,347,350	0
5	MAN	T	4	11/12	0.70	0.17	268,299,311,315	0
9	MAN	O	5	11/12	0.70	0.46	273,287,297,298	0
8	MAN	N	4	11/12	0.70	0.35	251,320,334,336	0
8	NAG	N	2	14/15	0.70	0.31	219,269,303,323	0
5	MAN	X	4	11/12	0.71	0.34	270,309,322,327	0
10	BMA	P	3	11/12	0.72	0.29	305,318,338,338	0
11	BMA	Q	3	11/12	0.72	0.31	287,305,328,361	0
12	NAG	R	1	14/15	0.73	0.32	212,243,256,277	0
11	BMA	U	3	11/12	0.73	0.27	260,320,325,331	0
11	NAG	Q	2	14/15	0.73	0.23	261,295,308,310	0
11	NAG	U	2	14/15	0.74	0.39	285,304,339,371	0
4	MAN	J	7	11/12	0.74	0.23	309,311,326,327	0
13	MAN	W	5	11/12	0.74	0.59	307,322,345,358	0
7	NAG	M	1	14/15	0.75	0.30	252,275,300,325	0
13	MAN	W	6	11/12	0.75	0.37	309,319,344,347	0
12	MAN	R	6	11/12	0.75	0.33	230,277,297,301	0
4	MAN	J	8	11/12	0.75	0.37	308,325,333,336	0
11	MAN	V	5	11/12	0.75	0.20	237,293,323,332	0
4	BMA	J	3	11/12	0.76	0.15	260,272,289,292	0
11	MAN	V	4	11/12	0.76	0.25	263,276,302,308	0
3	BMA	I	3	11/12	0.76	0.22	291,299,315,325	0
12	MAN	R	4	11/12	0.77	0.69	243,252,266,272	0

Continued on next page...

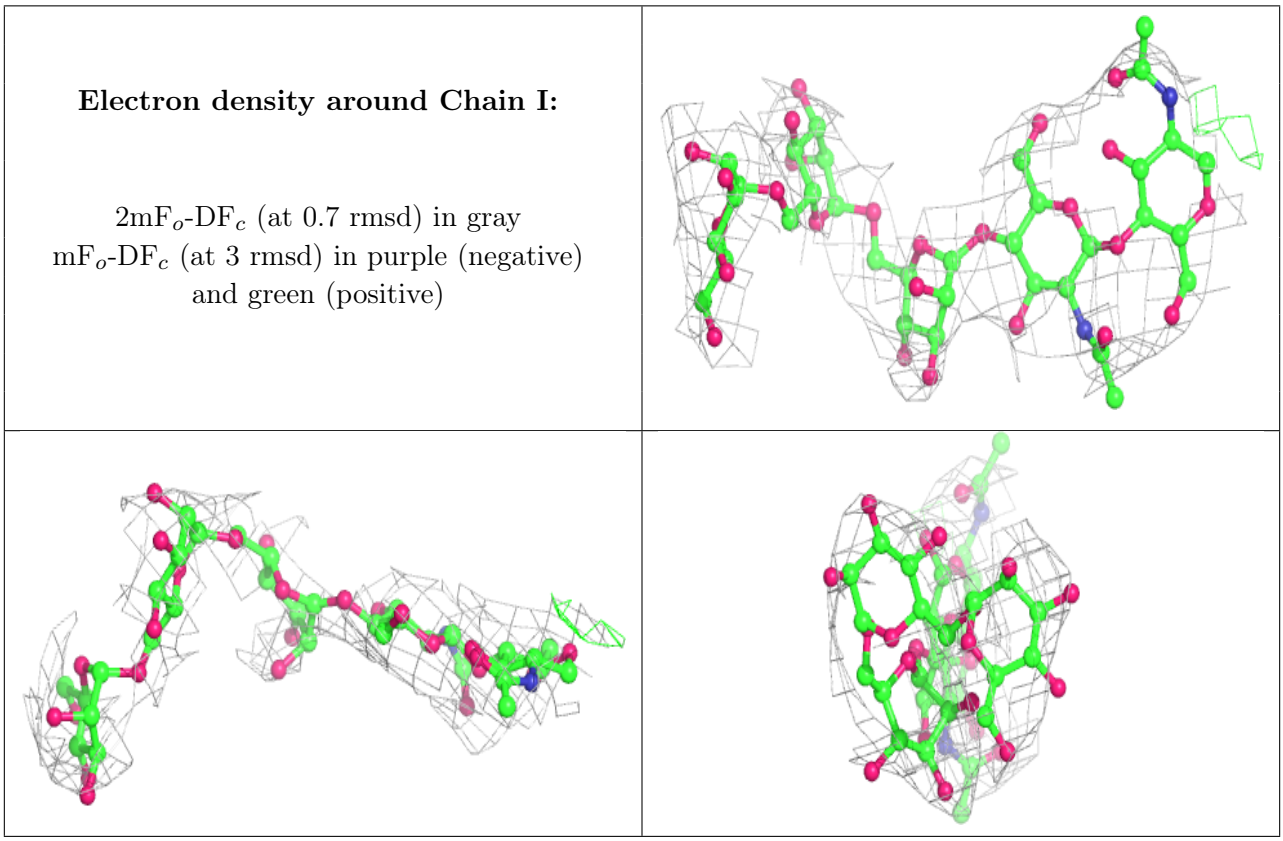
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	MAN	Q	5	11/12	0.78	0.78	249,281,295,299	0
8	MAN	S	4	11/12	0.78	0.24	269,325,347,348	0
4	MAN	J	6	11/12	0.80	0.18	219,247,260,292	0
11	NAG	Q	1	14/15	0.80	0.20	167,216,284,298	0
11	BMA	V	3	11/12	0.80	0.18	310,323,330,334	0
9	MAN	O	7	11/12	0.81	0.37	317,336,352,359	0
8	NAG	S	2	14/15	0.81	0.33	233,292,313,337	0
10	MAN	P	5	11/12	0.81	0.32	186,218,245,252	0
12	MAN	R	5	11/12	0.81	0.86	214,236,249,250	0
5	MAN	K	4	11/12	0.82	0.48	265,290,297,302	0
10	MAN	P	4	11/12	0.82	0.25	287,306,320,322	0
4	MAN	J	10	11/12	0.82	0.39	280,311,318,330	0
14	MAN	Y	5	11/12	0.82	0.13	178,213,255,260	0
12	BMA	R	3	11/12	0.83	0.46	274,304,315,326	0
14	MAN	Y	4	11/12	0.83	0.21	217,278,294,299	0
13	NAG	W	2	14/15	0.83	0.30	242,271,298,315	0
5	NAG	X	2	14/15	0.84	0.20	260,287,322,339	0
8	NAG	S	1	14/15	0.84	0.26	222,248,291,302	0
11	MAN	Q	4	11/12	0.85	0.30	205,224,243,264	0
14	NAG	Y	1	14/15	0.85	0.27	162,214,255,297	0
3	MAN	I	4	11/12	0.85	0.22	282,287,289,290	0
3	NAG	I	2	14/15	0.86	0.15	201,244,258,278	0
7	NAG	M	2	14/15	0.86	0.64	273,334,340,343	0
11	NAG	V	2	14/15	0.86	0.19	225,265,287,289	0
10	NAG	P	2	14/15	0.86	0.23	276,297,343,352	0
13	NAG	W	1	14/15	0.86	0.29	253,265,294,302	0
6	NAG	L	1	14/15	0.86	0.24	213,237,268,301	0
4	NAG	J	1	14/15	0.86	0.38	214,248,299,302	0
4	NAG	J	2	14/15	0.86	0.29	230,288,304,324	0
4	MAN	J	5	11/12	0.87	0.28	269,291,305,306	0
5	NAG	K	2	14/15	0.87	0.29	271,296,314,323	0
11	MAN	U	5	11/12	0.88	0.27	200,226,241,242	0
5	NAG	X	1	14/15	0.88	0.17	130,217,244,263	0
4	MAN	J	4	11/12	0.90	0.19	253,283,295,302	0
5	NAG	T	2	14/15	0.91	0.17	233,281,330,342	0
12	NAG	R	2	14/15	0.91	0.24	219,262,289,297	0
3	NAG	I	1	14/15	0.91	0.18	182,238,254,256	0
11	NAG	V	1	14/15	0.92	0.28	208,268,306,312	0
11	NAG	U	1	14/15	0.93	0.22	194,219,246,273	0
5	NAG	K	1	14/15	0.94	0.10	105,177,205,238	0
10	NAG	P	1	14/15	0.95	0.16	116,173,218,249	0
5	NAG	T	1	14/15	0.96	0.21	92,173,221,231	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

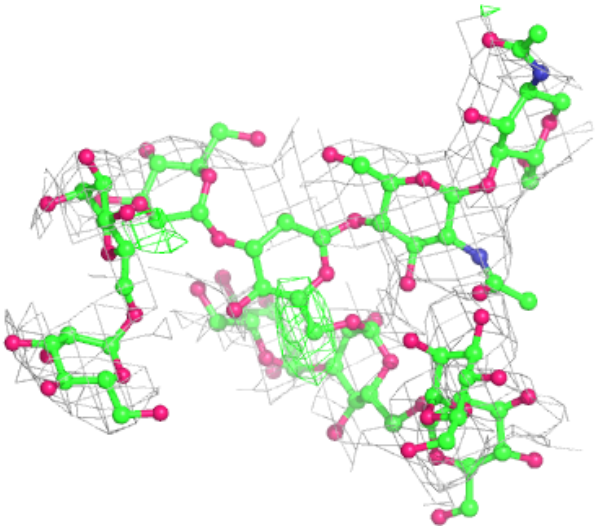
Electron density around Chain I:

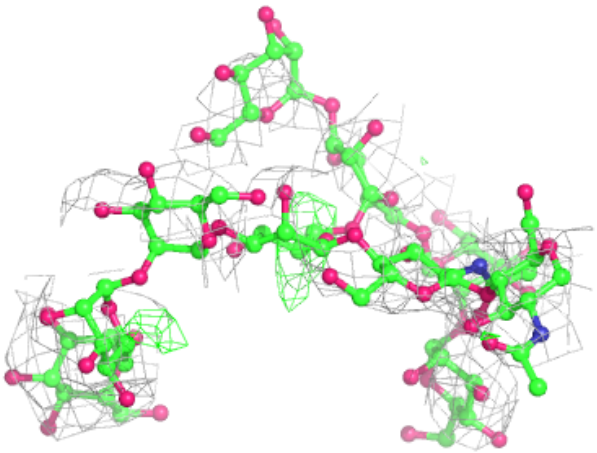
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

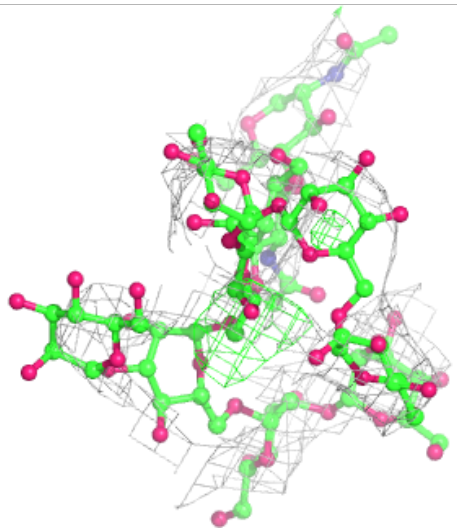


Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

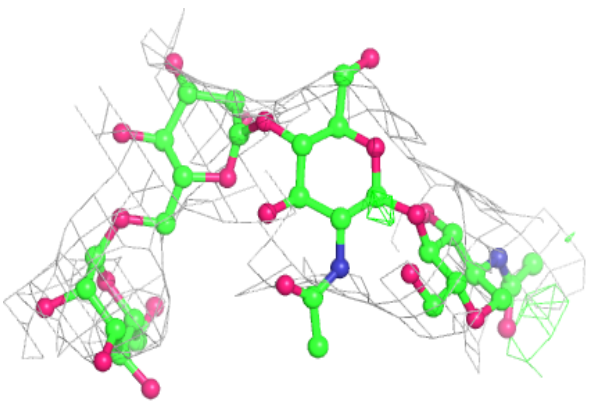


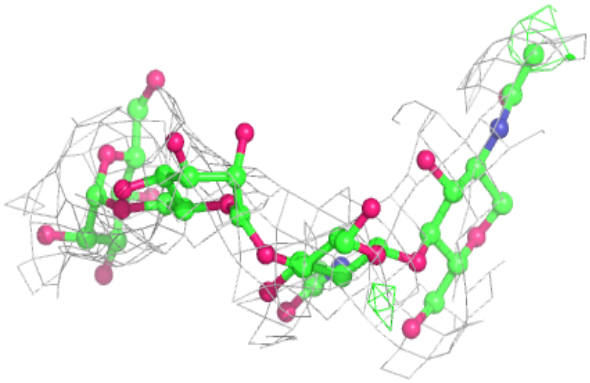


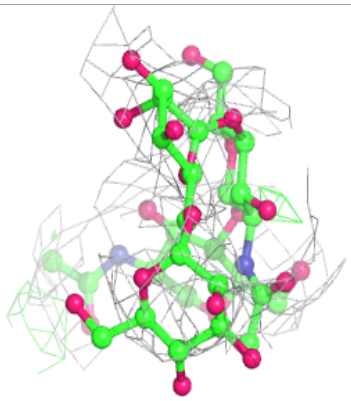


Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

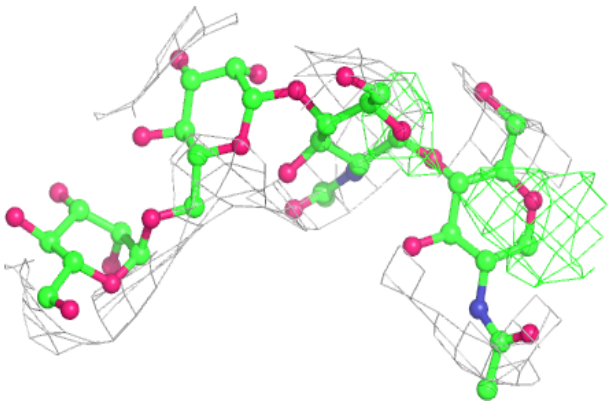


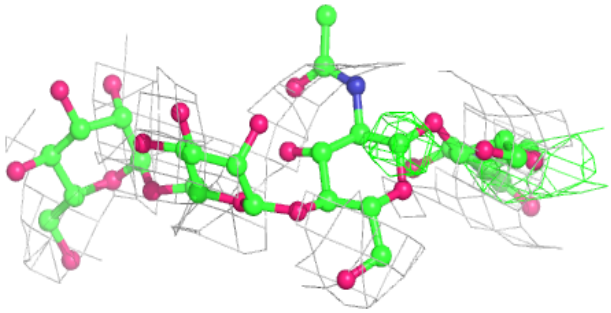


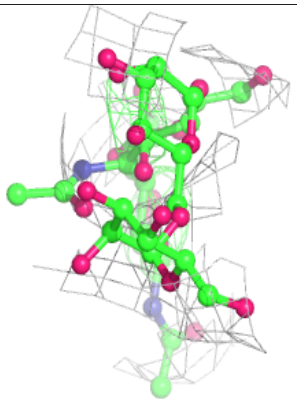


Electron density around Chain T:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

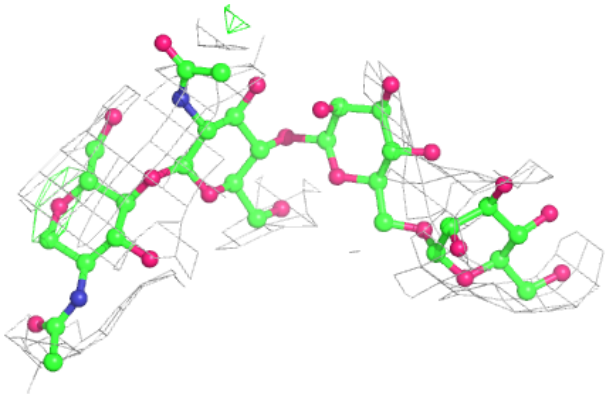


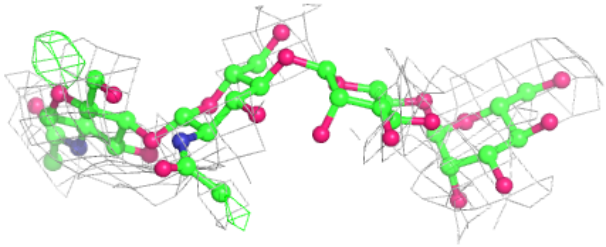


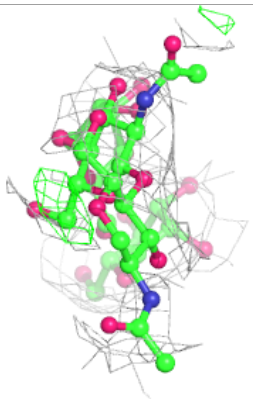


Electron density around Chain X:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

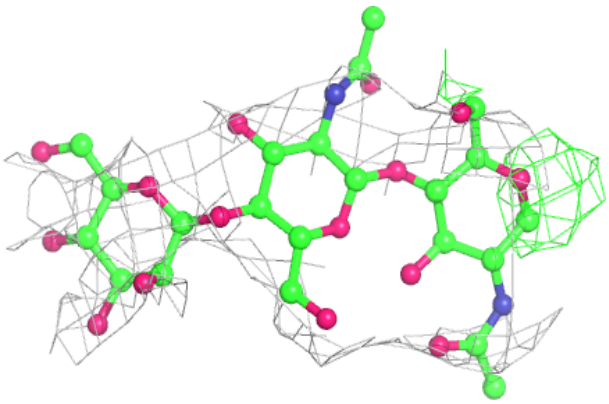


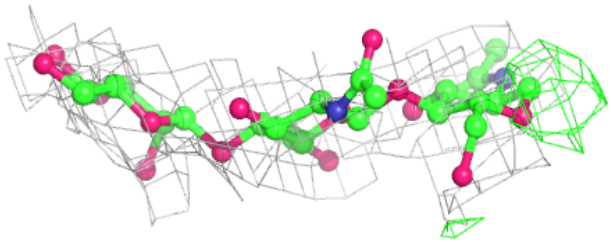


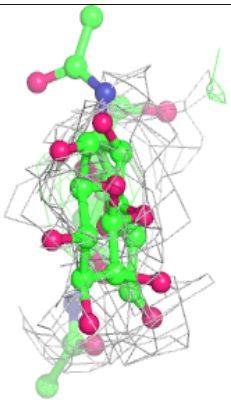


Electron density around Chain L:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

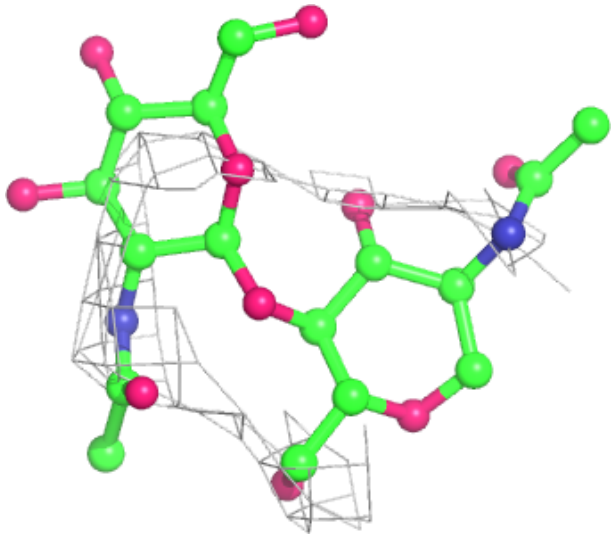


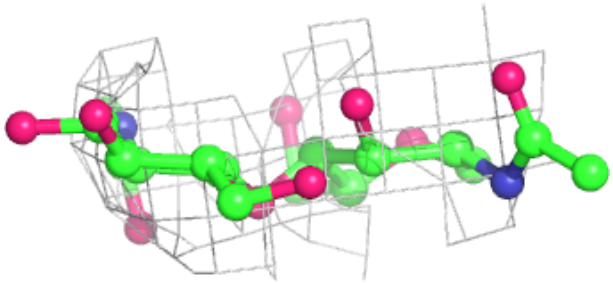


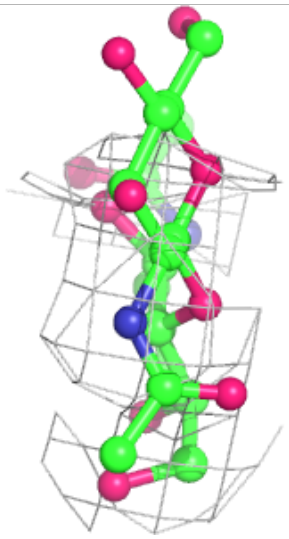


Electron density around Chain M:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

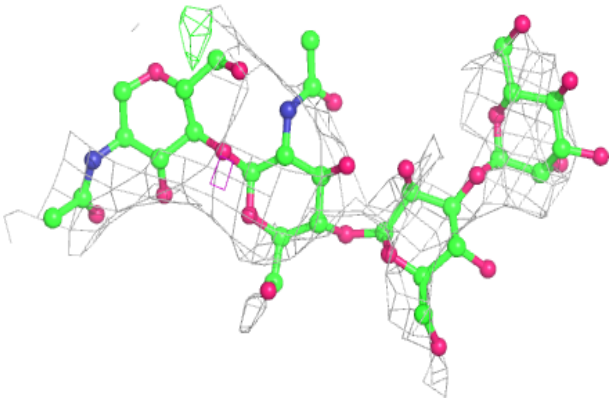


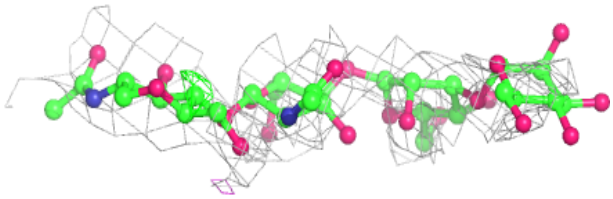


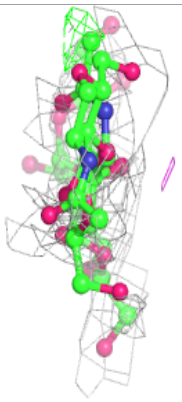


Electron density around Chain N:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

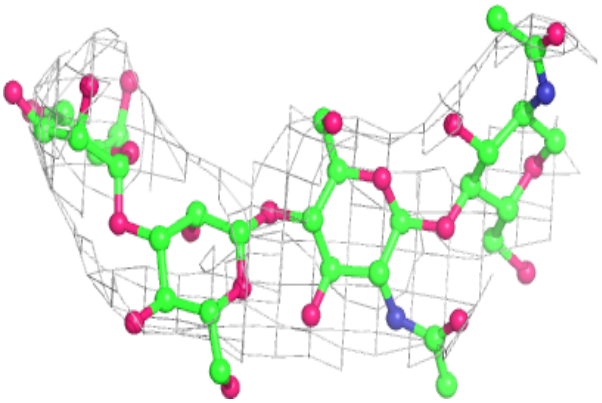


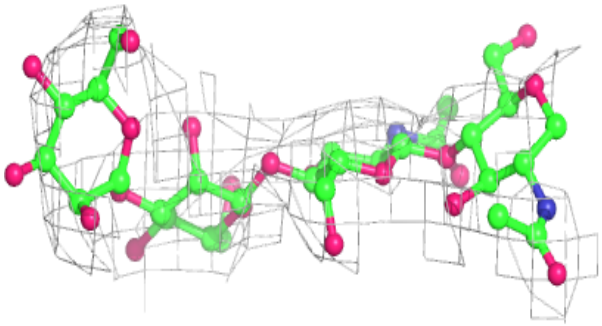


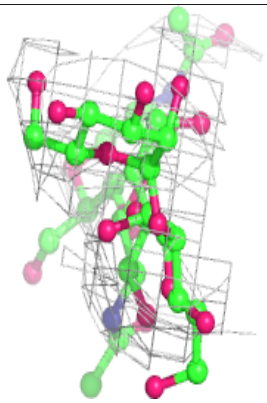


Electron density around Chain S:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

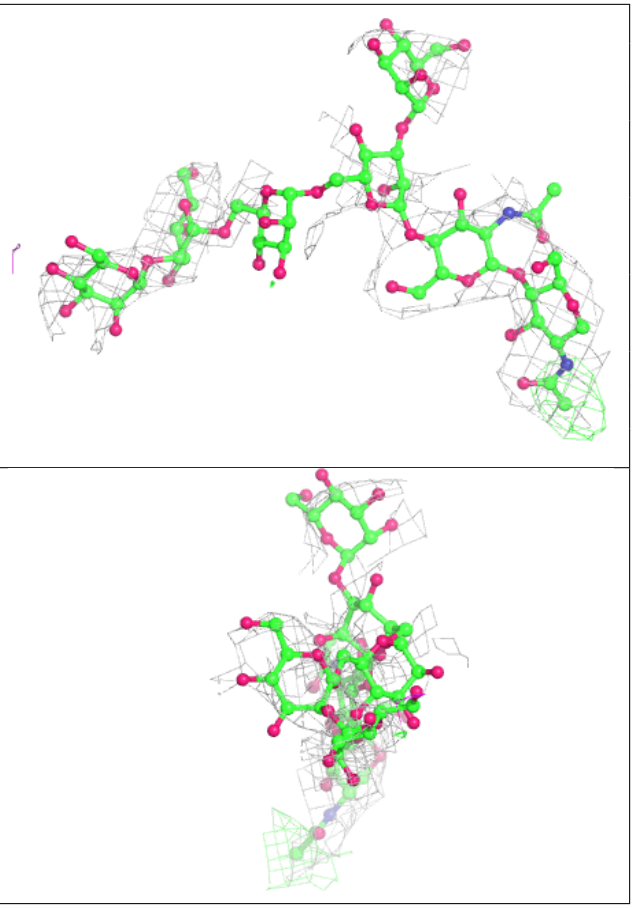


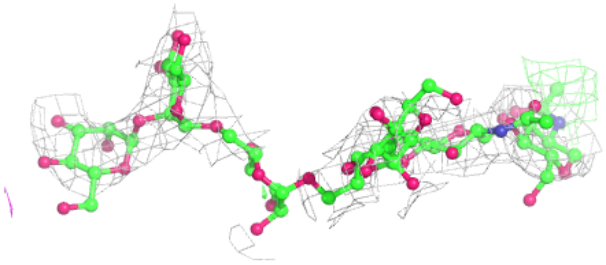




Electron density around Chain O:

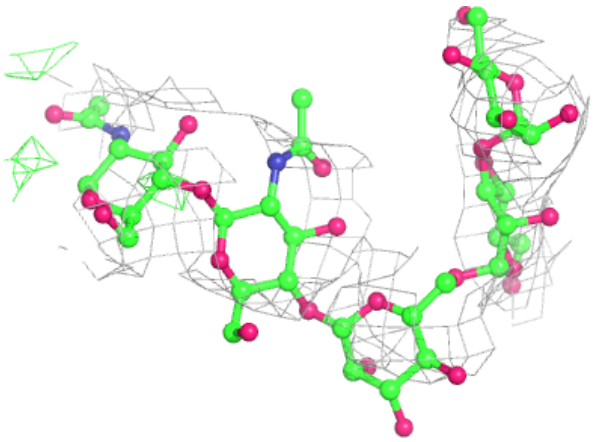
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

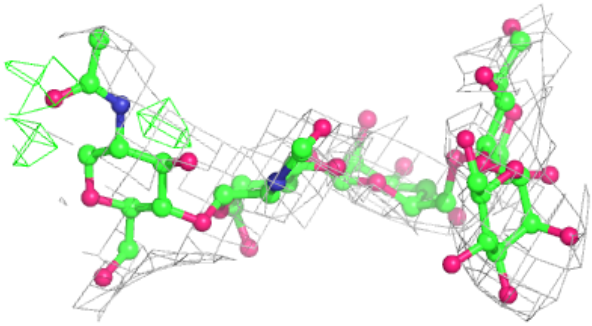


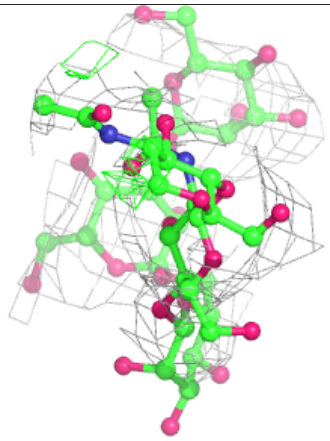


Electron density around Chain P:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

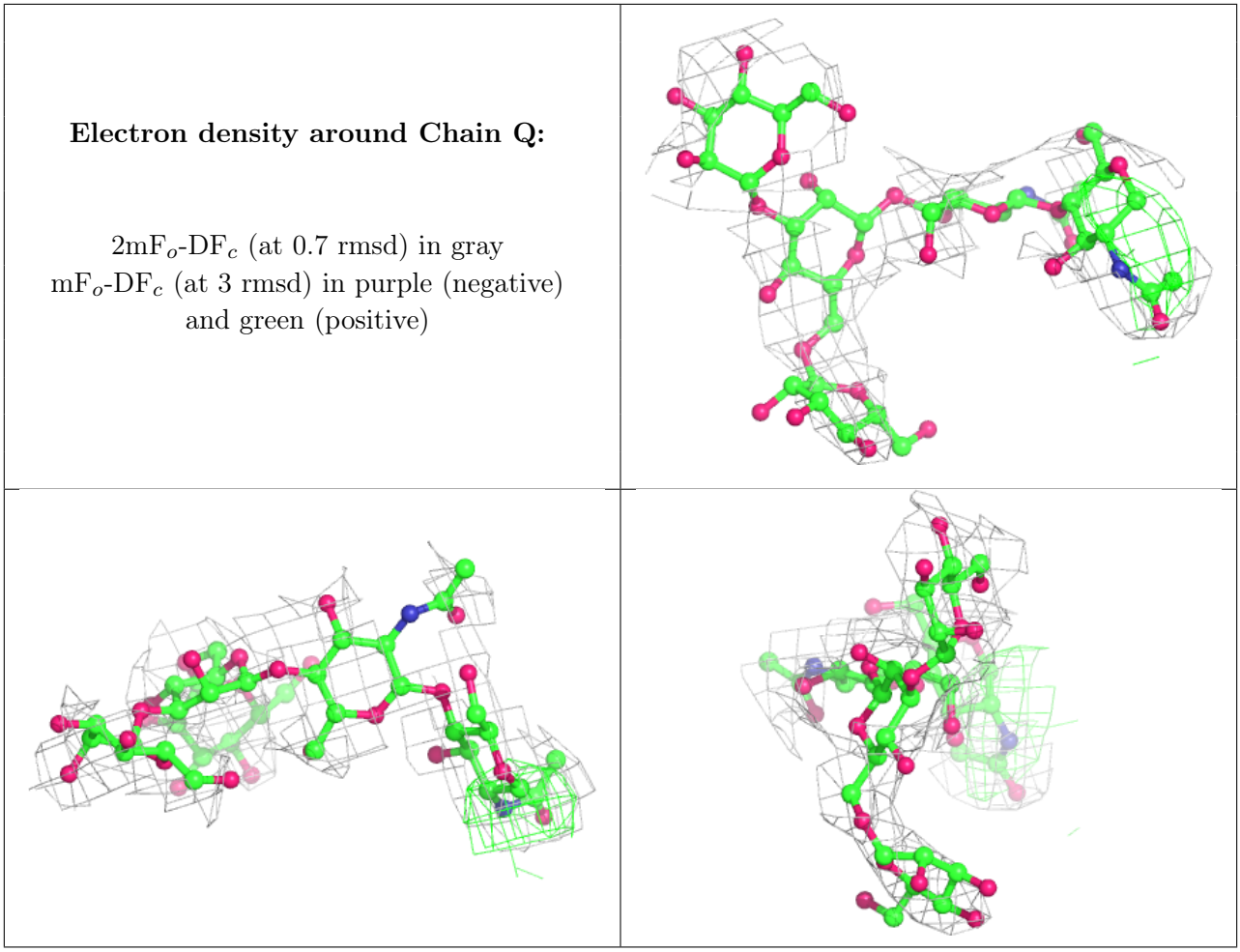






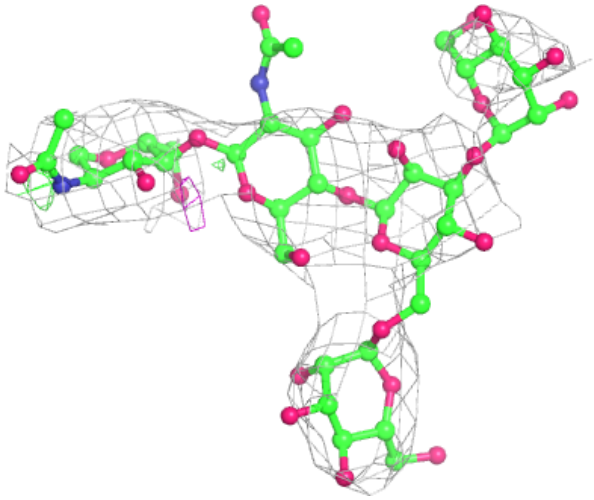
Electron density around Chain Q:

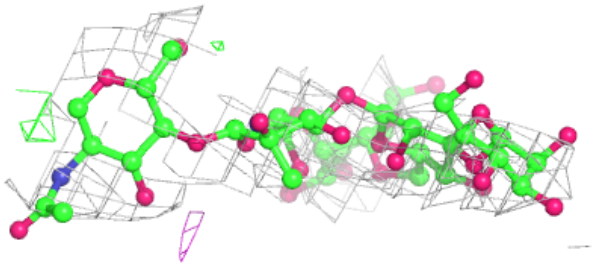
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

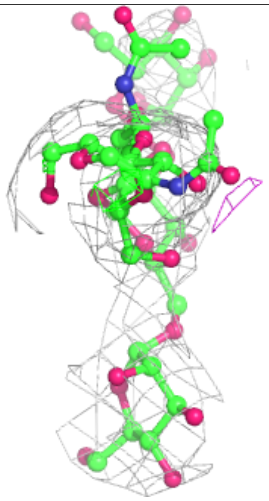


Electron density around Chain U:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

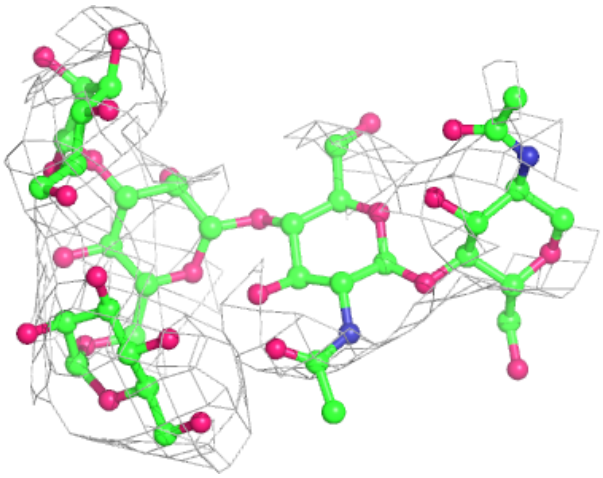


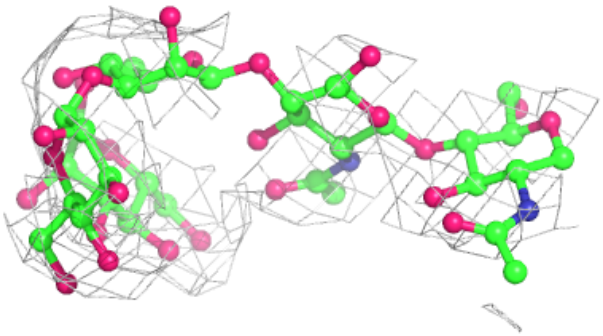


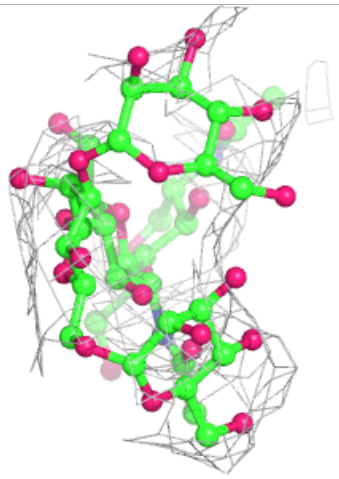


Electron density around Chain V:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

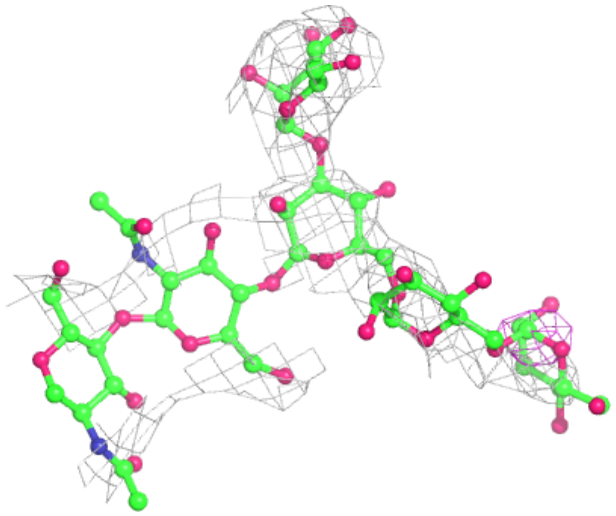


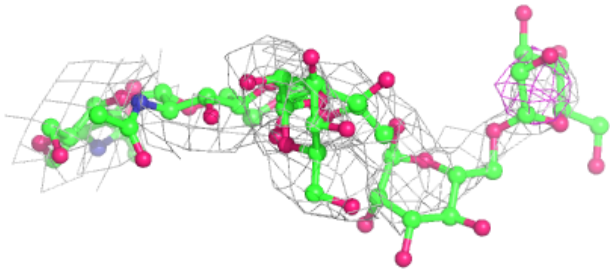




Electron density around Chain R:

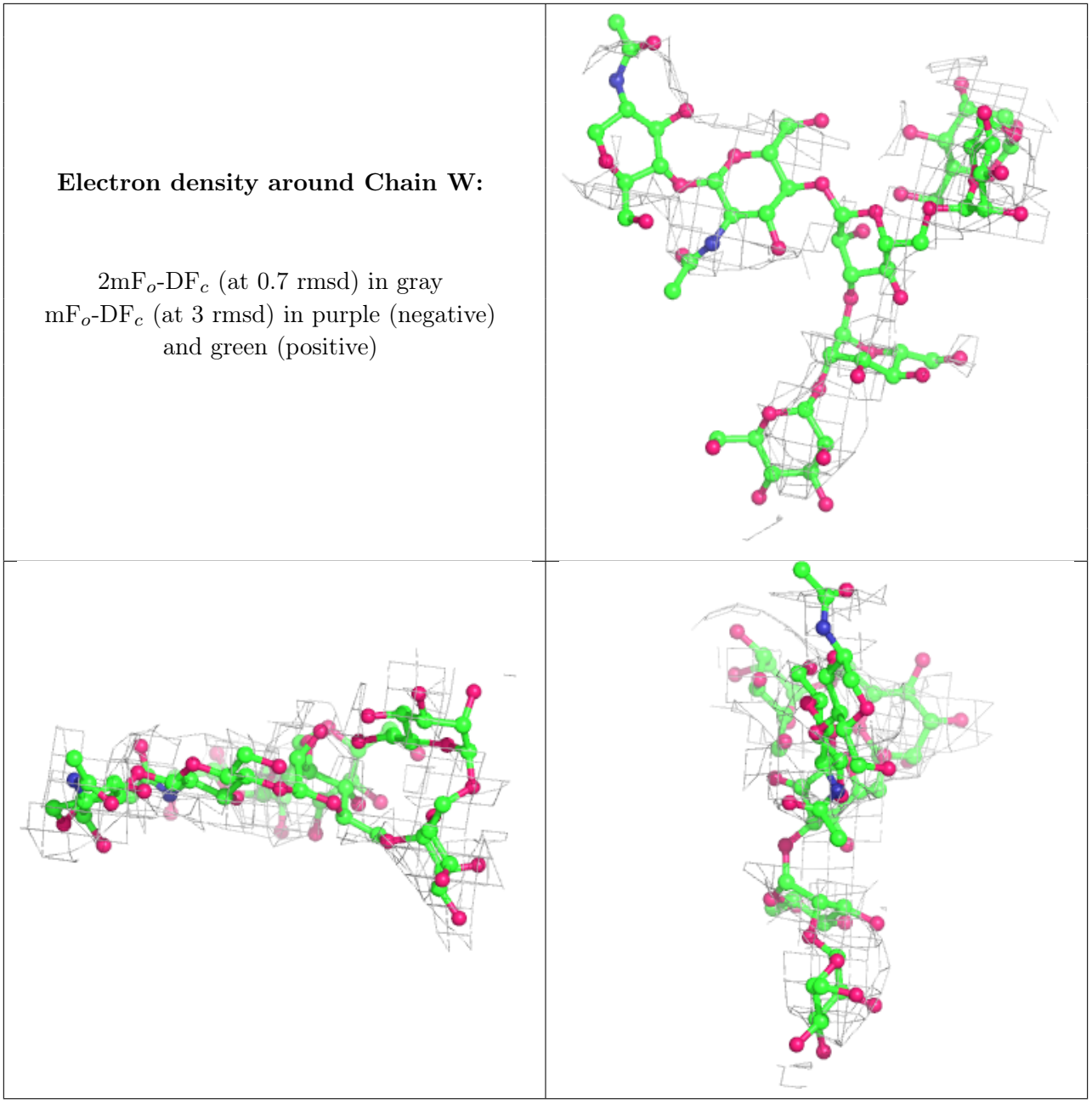
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





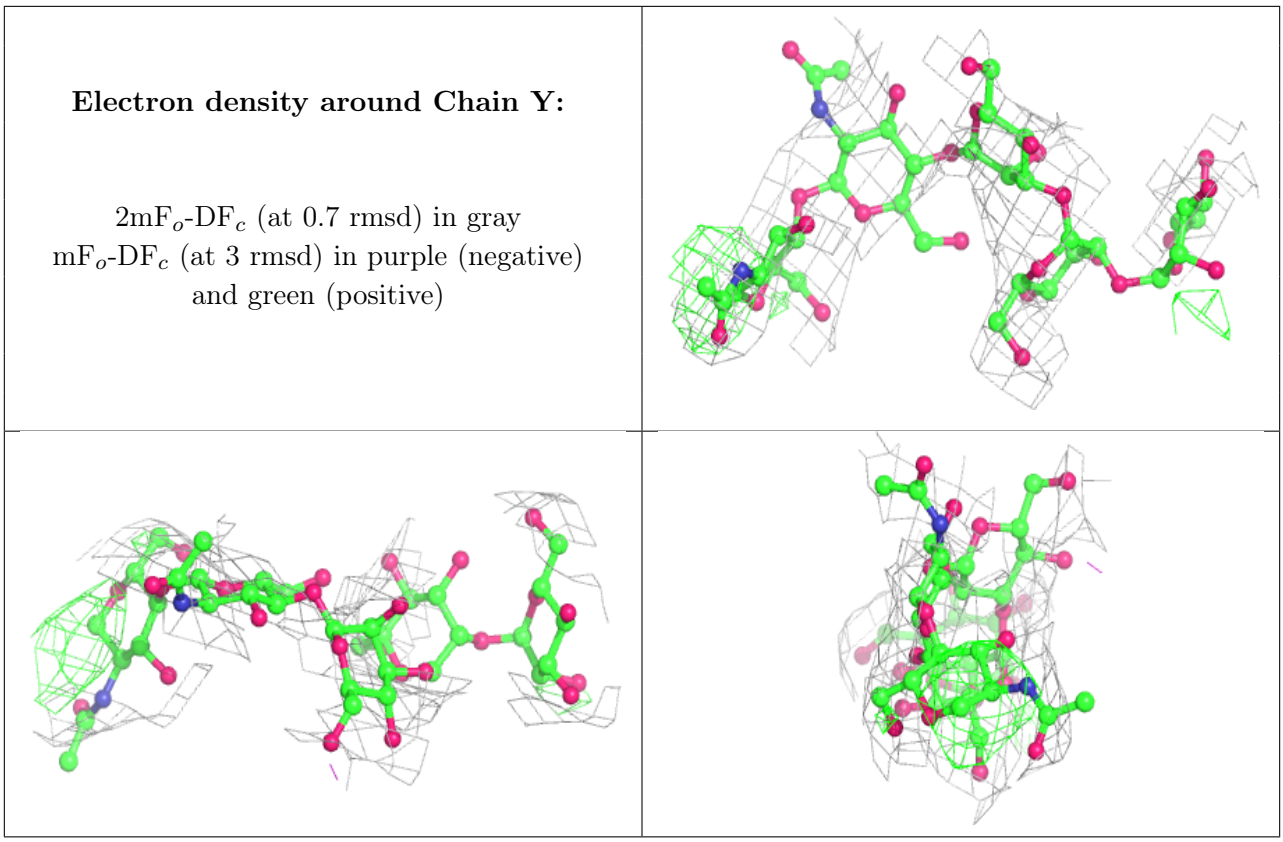
Electron density around Chain W:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain Y:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	NAG	D	3620	14/15	0.51	0.84	259,279,292,296	0
17	NAG	D	3232	14/15	0.54	0.40	220,239,242,244	0
17	NAG	C	3920	14/15	0.60	0.47	261,304,317,320	0
17	NAG	F	3190	14/15	0.62	0.36	235,263,275,278	0
15	CA	A	2005	1/1	0.66	0.14	282,282,282,282	0
17	NAG	F	3620	14/15	0.68	0.57	281,300,312,313	0
17	NAG	B	3232	14/15	0.69	0.31	192,229,251,259	0
15	CA	C	2007	1/1	0.69	0.06	311,311,311,311	0
17	NAG	E	3042	14/15	0.70	0.35	205,258,290,292	0
17	NAG	H	3232	14/15	0.70	0.34	189,210,226,226	0
15	CA	G	2006	1/1	0.73	0.17	214,214,214,214	0
15	CA	D	2002	1/1	0.75	0.15	715,715,715,715	0
17	NAG	G	3678	14/15	0.75	0.34	196,238,257,263	0
17	NAG	A	3920	14/15	0.75	0.23	165,310,345,346	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	NAG	C	3042	14/15	0.76	0.62	195,241,267,281	0
17	NAG	E	3920	14/15	0.76	0.23	230,286,310,319	0
17	NAG	H	3094	14/15	0.78	0.22	239,260,312,313	0
17	NAG	A	3042	14/15	0.78	0.30	237,241,277,278	0
17	NAG	H	3620	14/15	0.78	0.59	203,255,288,311	0
17	NAG	E	3678	14/15	0.79	0.28	188,244,283,300	0
17	NAG	G	3920	14/15	0.80	0.29	152,193,229,237	0
15	CA	A	2007	1/1	0.80	0.04	238,238,238,238	0
15	CA	E	2006	1/1	0.81	0.13	242,242,242,242	0
17	NAG	H	3190	14/15	0.81	0.17	215,264,276,276	0
17	NAG	C	3678	14/15	0.82	0.35	225,273,310,321	0
17	NAG	G	3042	14/15	0.82	0.29	206,259,269,270	0
17	NAG	G	3031	14/15	0.84	0.23	139,227,255,259	0
17	NAG	B	3620	14/15	0.85	0.47	221,253,270,280	0
17	NAG	F	3094	14/15	0.85	0.34	221,279,292,292	0
17	NAG	E	3031	14/15	0.86	0.16	172,223,244,254	0
15	CA	H	2002	1/1	0.87	0.09	448,448,448,448	0
15	CA	E	2007	1/1	0.88	0.17	246,246,246,246	0
17	NAG	A	3031	14/15	0.88	0.14	126,244,266,274	0
15	CA	E	2005	1/1	0.88	0.07	276,276,276,276	0
17	NAG	C	3031	14/15	0.88	0.21	200,248,281,285	0
15	CA	A	2006	1/1	0.89	0.07	234,234,234,234	0
17	NAG	A	3678	14/15	0.89	0.16	162,236,250,253	0
15	CA	C	2006	1/1	0.92	0.15	232,232,232,232	0
15	CA	B	2002	1/1	0.93	0.14	457,457,457,457	0
15	CA	F	2002	1/1	0.94	0.14	505,505,505,505	0
15	CA	G	2007	1/1	0.96	0.11	189,189,189,189	0
15	CA	G	2005	1/1	0.97	0.10	240,240,240,240	0
15	CA	C	2005	1/1	0.97	0.04	236,236,236,236	0
16	MG	A	2009	1/1	0.97	0.07	370,370,370,370	0

6.5 Other polymers (i)

There are no such residues in this entry.