



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 04:34 PM UTC

PDB ID : 5ES4 / pdb_00005es4
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

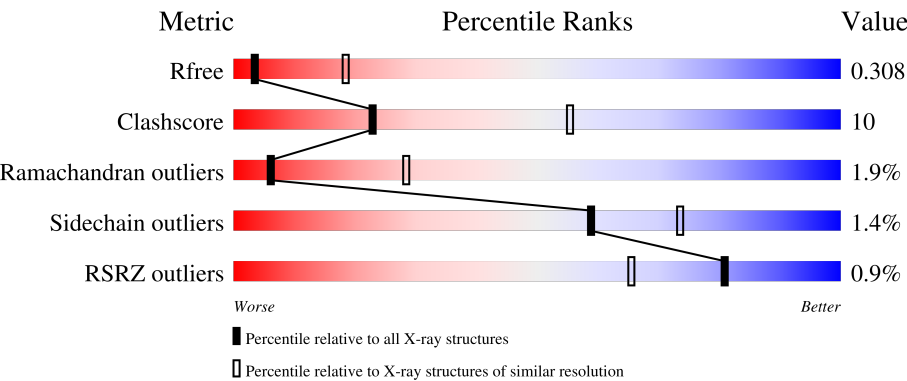
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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.



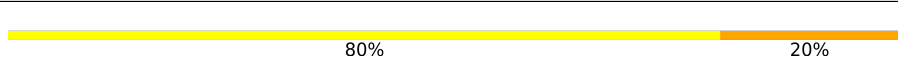
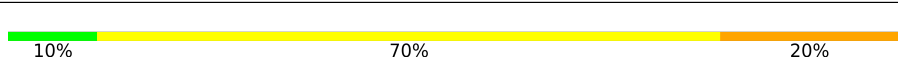
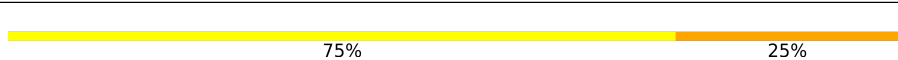
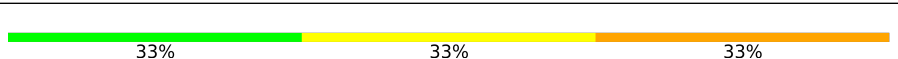
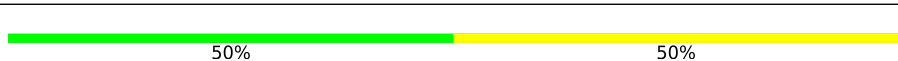
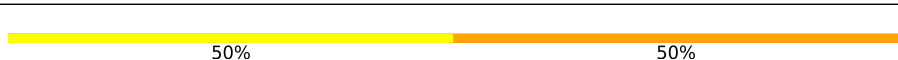
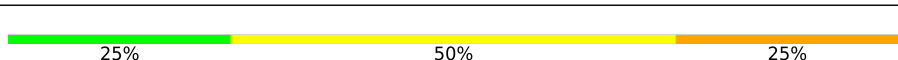
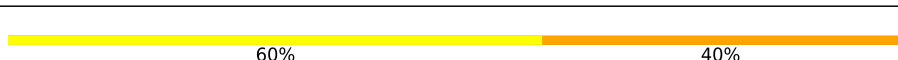
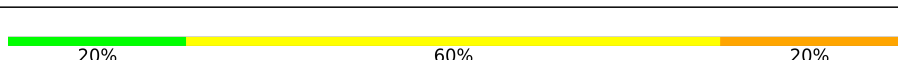
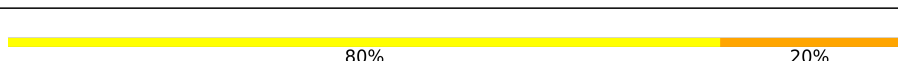
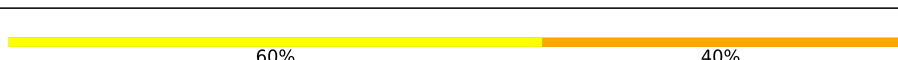
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	70%24%• 5%
1	C	1137	% 58%19%• 22%
1	E	1137	% 54%22%• 22%
1	G	1137	% 57%18%• 22%
2	B	727	% 74%18%• 7%

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Mol	Chain	Length	Quality of chain
2	D	727	
2	F	727	
2	H	727	
3	I	5	
4	J	10	
5	K	4	
5	T	4	
5	X	4	
6	L	3	
7	M	2	
8	N	4	
8	S	4	
9	O	7	
10	P	5	
11	Q	5	
11	U	5	
11	V	5	
12	R	6	
13	W	7	
14	Y	5	

2 Entry composition

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

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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

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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

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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

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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

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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

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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

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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

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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

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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

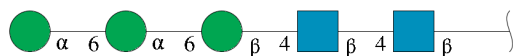
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Chain	Residue	Modelled	Actual	Comment	Reference
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H	688	LYS	-	expression tag	UNP P05107
H	689	ASN	-	expression tag	UNP P05107
H	690	ALA	-	expression tag	UNP P05107
H	691	GLN	-	expression tag	UNP P05107
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

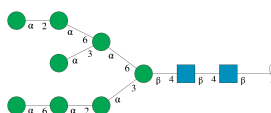
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran

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



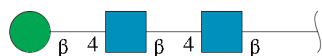
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-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
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-beta-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.



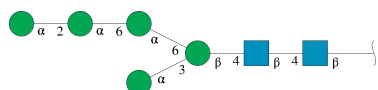
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



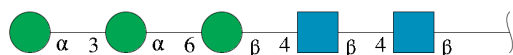
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
8	S	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



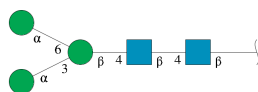
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



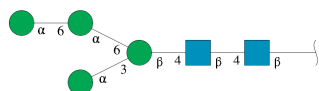
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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.



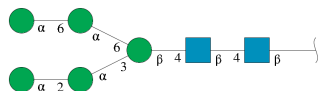
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			
11	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
11	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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.



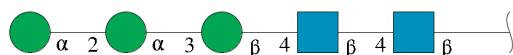
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	R	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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	0	0	0
			83	46	2	35			

- 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	0	0	0
			61	34	2	25			

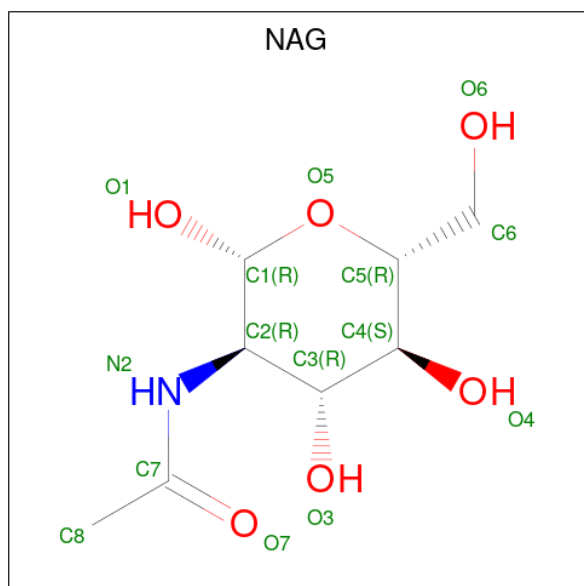
- Molecule 15 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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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	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		

- Molecule 18 is water.

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

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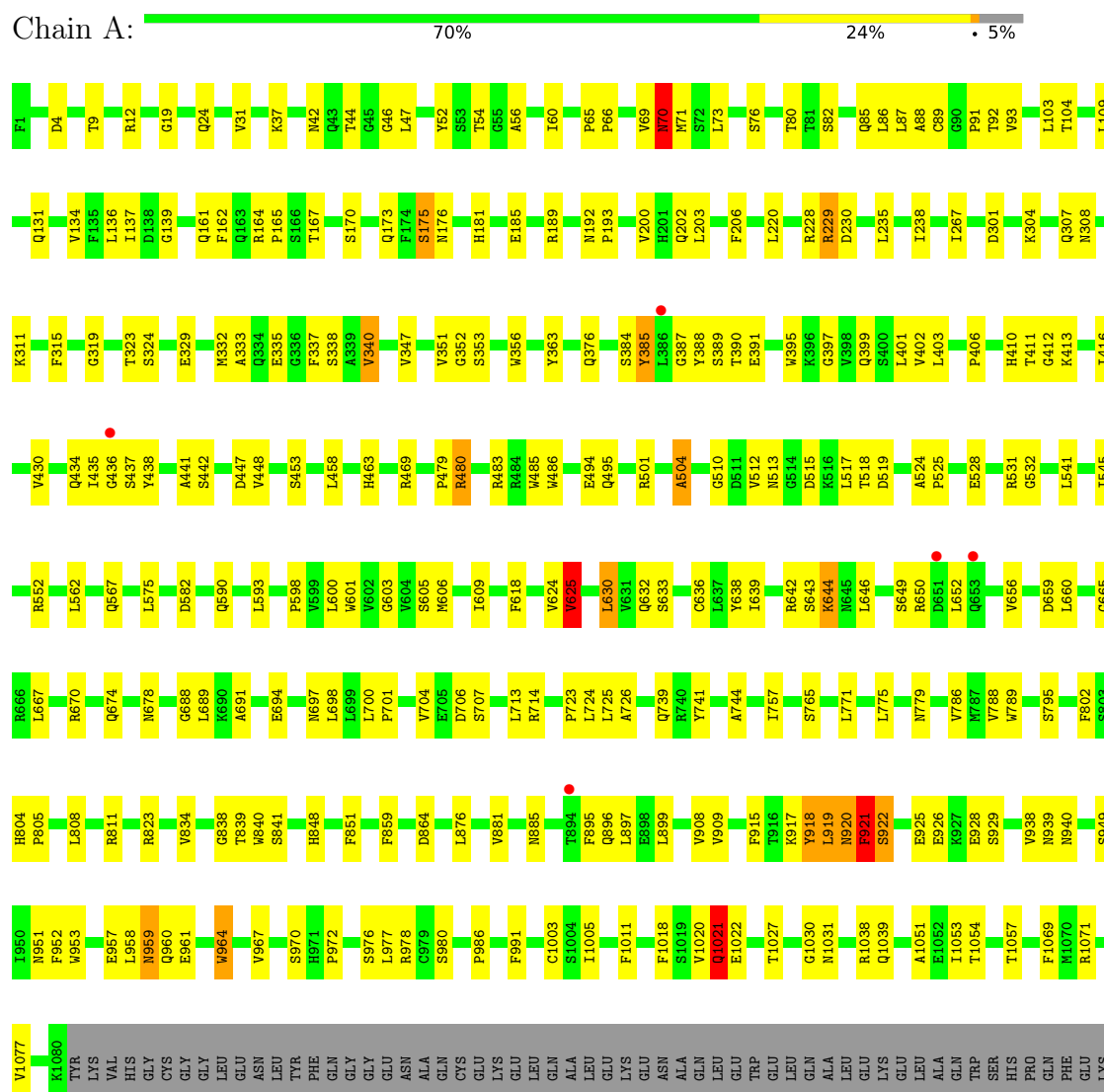
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	4	Total 4	O 4	0	0
18	C	7	Total 7	O 7	0	0
18	D	3	Total 3	O 3	0	0
18	E	10	Total 10	O 10	0	0
18	F	2	Total 2	O 2	0	0
18	G	10	Total 10	O 10	0	0
18	H	2	Total 2	O 2	0	0

3 Residue-property plots

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.

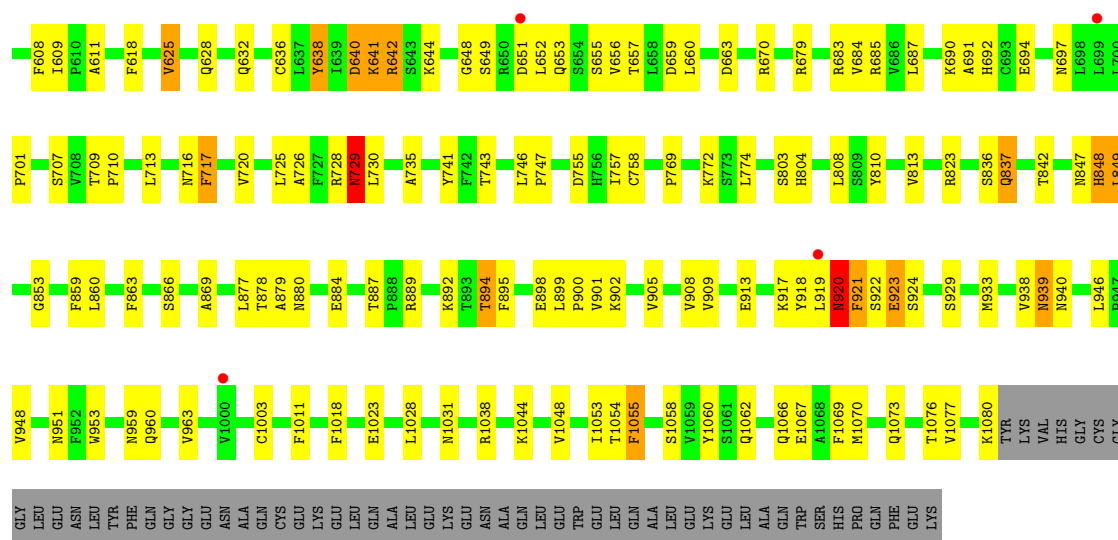
• Molecule 1: Integrin alpha-X



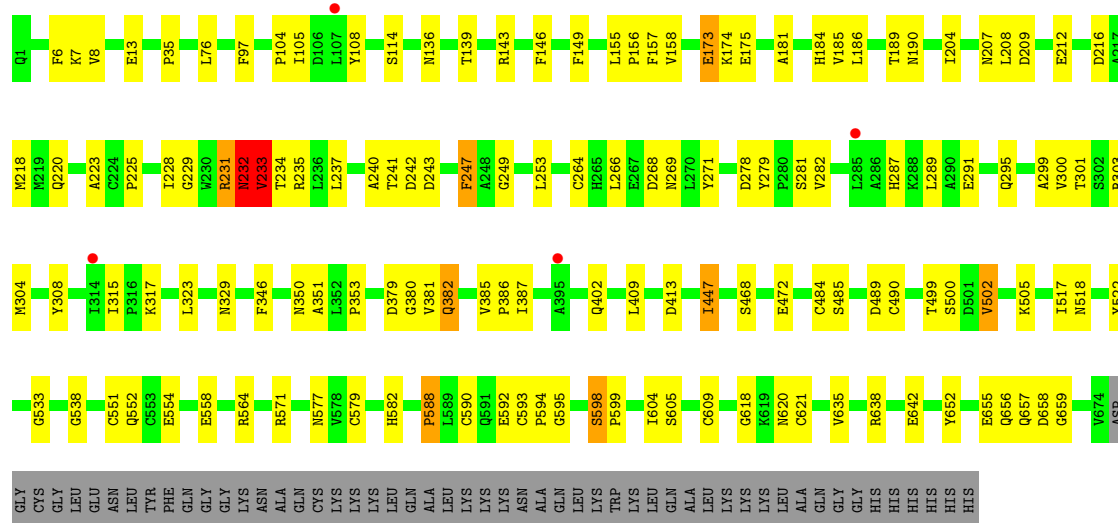
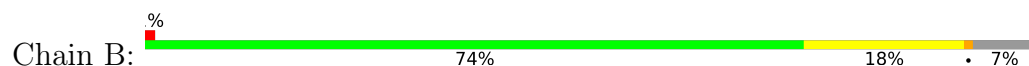
• Molecule 1: Integrin alpha-X



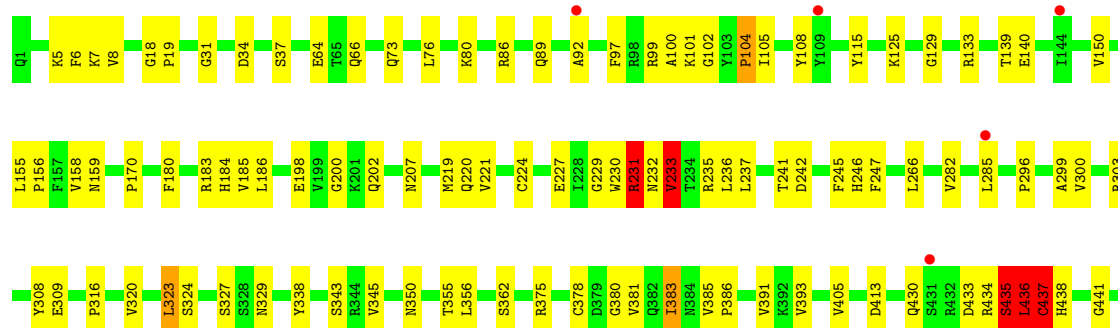


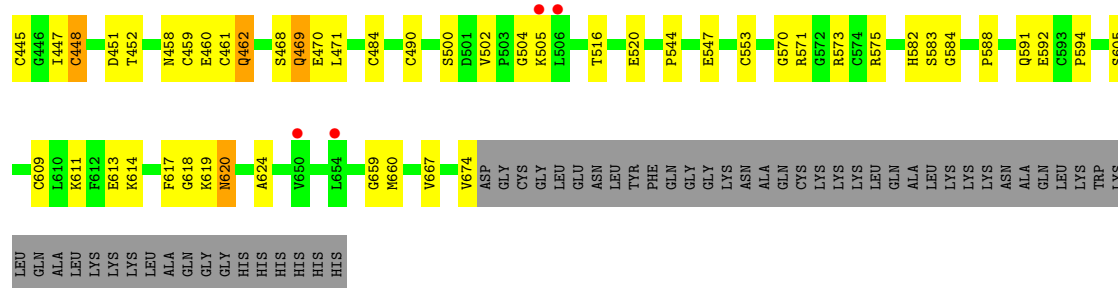


• Molecule 2: Integrin beta-2

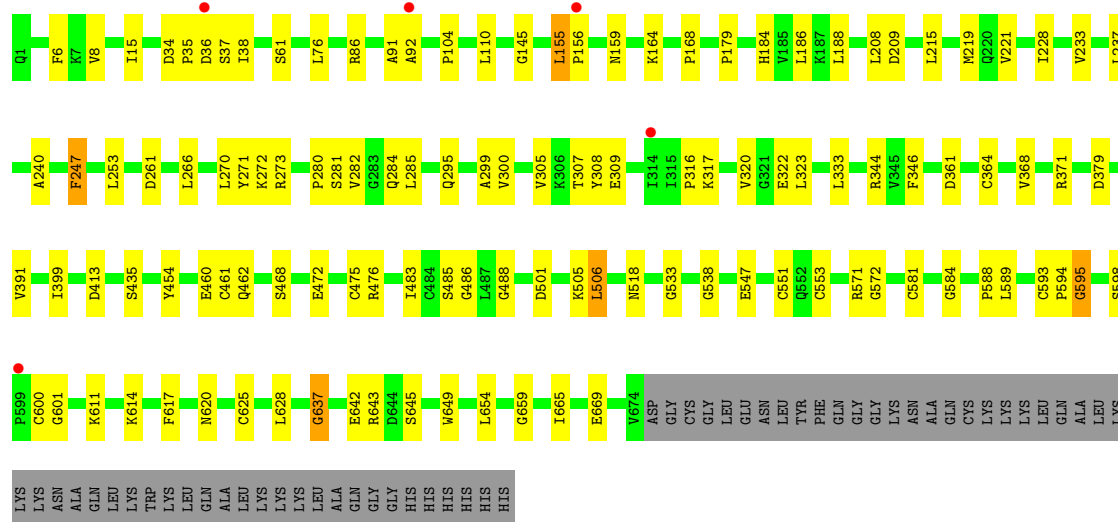
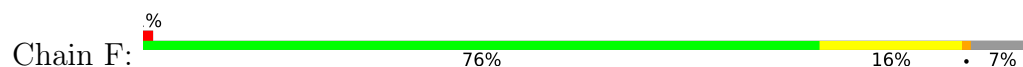


• Molecule 2: Integrin beta-2

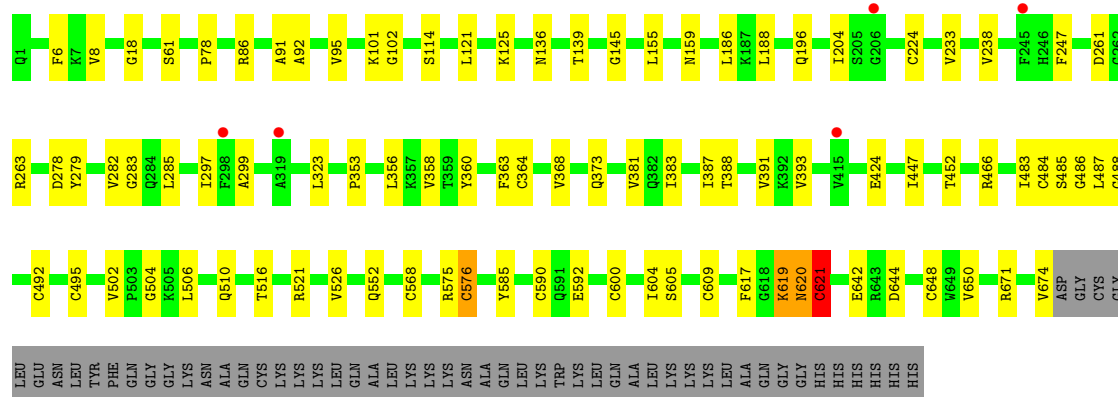
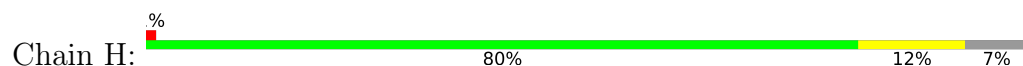




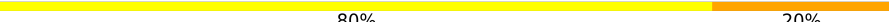
• Molecule 2: Integrin beta-2



• Molecule 2: Integrin beta-2



• 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-glucopyranose

Chain I:  80% 20%

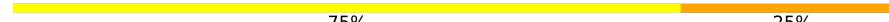


- Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  10% 70% 20%



- 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:  75% 25%



- 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:  25% 75%



- 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:  25% 75%



- 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:  33% 33% 33%



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

Chain M:  50% 50%



- 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



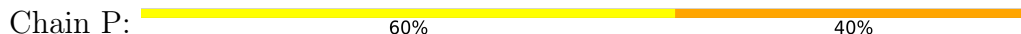
- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



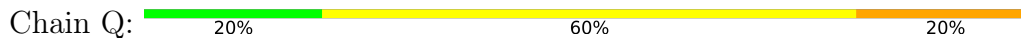
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



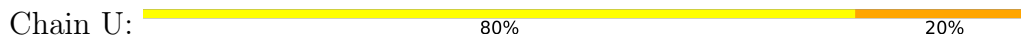
- Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



- 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





• 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



• 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



• 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



• 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



4 Data and refinement statistics

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 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.51-3.30) 99.8 (49.51-3.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.257 , 0.307 0.260 , 0.308	Depositor DCC
R_{free} test set	2041 reflections (1.01%)	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)	0.34 , 218.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, BMA, MAN, CA, NAG

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	0.23	0/8557	0.58	1/11623 (0.0%)
1	C	0.27	1/6997 (0.0%)	0.61	4/9516 (0.0%)
1	E	0.23	0/7004	0.59	1/9526 (0.0%)
1	G	0.24	0/6941	0.58	0/9447
2	B	0.23	0/5291	0.59	5/7144 (0.1%)
2	D	0.23	0/5274	0.59	2/7122 (0.0%)
2	F	0.18	0/5288	0.54	1/7140 (0.0%)
2	H	0.20	0/5280	0.56	0/7129
All	All	0.23	1/50632 (0.0%)	0.58	14/68647 (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	9.26	1.55	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	448	CYS	CA-CB-SG	7.15	130.84	114.40
2	F	637	GLY	N-CA-C	6.80	121.69	111.42
1	C	716	ASN	CA-CB-CG	5.98	118.58	112.60
2	D	437	CYS	N-CA-C	-5.81	103.38	111.52
1	E	16	ALA	CB-CA-C	-5.54	109.69	117.23
2	B	232	ASN	CA-C-N	5.34	131.59	121.97
2	B	232	ASN	C-N-CA	5.34	131.59	121.97
1	C	920	ASN	CA-C-N	5.34	131.74	121.54
1	C	920	ASN	C-N-CA	5.34	131.74	121.54
1	A	921	PHE	N-CA-C	-5.31	99.49	110.80
1	C	481	GLY	N-CA-C	-5.22	100.85	110.83
2	B	35	PRO	CA-C-N	5.20	127.97	120.38
2	B	35	PRO	C-N-CA	5.20	127.97	120.38
2	B	233	VAL	N-CA-C	-5.11	98.72	109.34

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
1	G	82	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8371	0	8200	211	1
1	C	6834	0	6700	175	0
1	E	6838	0	6699	199	0
1	G	6787	0	6617	158	0
2	B	5191	0	4979	91	0
2	D	5178	0	4963	121	1
2	F	5189	0	4987	77	0
2	H	5184	0	4971	54	0
3	I	61	0	52	3	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	28	0	26	2	0
17	E	56	0	52	2	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	1041	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 (1041) 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:332:MET:HE1	2:F:208:LEU:HD13	1.72	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
1:A:395:TRP:CD1	1:A:453:SER:HG	2.10	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:917:LYS:HZ3	2:F:642:GLU:HB2	1.58	0.68
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:71:MET:HE2	1:G:73:LEU:HB3	1.81	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
3:I:1:NAG:O7	3:I:1:NAG:O3	2.17	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:A:659:ASP:CG	5:K:1:NAG:H82	2.26	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:A:961:GLU:HG3	1:A:1039:GLN:CD	2.25	0.60
1:E:1069:PHE:CE2	2:F:584:GLY:HA3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:750:LYS:HE3	1:E:796:TYR:HB2	1.83	0.60
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:E:1071[B]:ARG:HH22	1:G:755:ASP:C	2.09	0.60
1:G:9:THR:HB	1:G:593:LEU:HB3	1.84	0.60
1:A:71:MET:HE2	1:A:73:LEU:HB3	1.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:469:GLN:C	2:D:471:LEU:H	2.12	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:D:343:SER:HG	2:D:380:GLY:H	1.50	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:788:VAL:HG21	1:A:881:VAL:HG21	1.88	0.56
1:E:47:LEU:HB3	1:E:60:ILE:HD12	1.88	0.56
1:E:1052:GLU:CD	1:E:1071[B]:ARG:NH1	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:3920:NAG:O4	2:H:674:VAL:HG13	2.07	0.54
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
2:B:618:GLY:C	2:B:620:ASN:H	2.15	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
1:G:920:ASN:C	1:G:920:ASN:OD1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:424:GLU:CD	2:H:424:GLU:H	2.18	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
1:E:1056:ASP:OD1	1:E:1058:SER:OG	2.28	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: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
1:A:1020:VAL:C	1:A:1022:GLU:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:913:GLU:H	1:G:913:GLU:CD	2.20	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:C:650:ARG:C	1:C:652:LEU:H	2.20	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
1:C:480:ARG:HD3	1:C:480:ARG:C	2.36	0.50
2:D:356:LEU:HD11	2:D:393:VAL:HG13	1.94	0.50
1:E:917:LYS:NZ	2:F:642:GLU:HB2	2.26	0.50
2:F:309:GLU:HA	2:F:320:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:D:571:ARG:HG3	2:D:660:MET:HE3	1.94	0.49
1:E:407:ARG:O	1:E:408:TYR:C	2.56	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:B:303:ARG:NH1	2:B:304:MET:HE2	2.27	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
1:A:940:ASN:CG	1:A:1020:VAL:HA	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:483:ILE:C	2:H:485:SER:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:1066:GLN:CD	1:G:1066:GLN:H	2.23	0.47
2:D:447:ILE:HG12	2:D:448:CYS:O	2.14	0.47
1:E:1052:GLU:CD	1:E:1071[B]:ARG:HH11	2.23	0.47
1:G:4:ASP:C	1:G:4:ASP:OD1	2.56	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
2:D:343:SER:HG	2:D:380:GLY:N	2.12	0.47
1:E:876:LEU:HD13	1:E:898:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:998:ASN:C	1:C:1000:VAL:H	2.22	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:430:GLN:H	2:D:430:GLN:CD	2.23	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:920:ASN:OD1	1:A:920:ASN:C	2.59	0.46
1:C:47:LEU:HB3	1:C:60:ILE:HD12	1.96	0.46
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:726:ALA:C	1:G:728:ARG:H	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:469:GLN:C	2:D:471:LEU:N	2.74	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
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: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:E:998:ASN:C	1:E:1000:VAL:H	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:532:GLY:HA3	1:G:565:PHE:HB3	1.97	0.45
1:A:332:MET:HE2	1:A:332:MET:HB3	1.86	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
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
2:D:129:GLY:C	2:D:133:ARG:HH11	2.25	0.45
1:G:67:GLU:HB3	1:G:123:ARG:HD3	1.99	0.45
1:G:365:PRO:O	1:G:367:MET:HE3	2.16	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: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:E:929:SER:OG	17:E:3031:NAG:O7	2.32	0.44
1:A:513:ASN:OD1	1:A:515:ASP:CG	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:129:GLY:C	2:D:133:ARG:NH1	2.76	0.44
1:E:351:VAL:HG11	2:F:253:LEU:HD21	2.00	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
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
2:B:243:ASP:HA	2:B:304:MET:HE3	2.00	0.44
1:C:394:LEU:HD23	1:C:394:LEU:HA	1.59	0.44
1:E:519:ASP:CG	1:E:538:HIS:HD1	2.22	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
11:V:2:NAG:HO3	11:V:2:NAG:C7	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PHE:C	2:B:279:TYR:HB2	2.43	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
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
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:101:MET:HE3	1:G:101:MET:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:727:PHE:O	1:C:728:ARG:C	2.62	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
1:E:830:ASP:OD1	1:E:830:ASP:N	2.50	0.43
1:E:976:SER:C	1:E:978:ARG:H	2.27	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
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: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:192:ASN:O	1:A:193:PRO:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:652:LEU:HD23	1:C:652:LEU:HA	1.88	0.42
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
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:HA	1:C:1077:VAL:O	2.19	0.42
1:C:918:TYR:CZ	1:C:1079:GLU:HB3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:447:ASP:O	1:A:518:THR:OG1	2.33	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:218:MET:HE2	2:B:289:LEU:HD11	2.01	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
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:438:TYR:OH	2:B:249:GLY:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:7:LYS:O	2:B:13:GLU:HB3	2.20	0.41
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: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:729:ASN:HD22	1:G:729:ASN:H	1.67	0.41
2:H:447:ILE:HD13	2:H:447:ILE:HA	1.93	0.41
1:A:92:THR:C	1:A:103:LEU:HD22	2.46	0.41
1:A:438:TYR:HH	2:B:249:GLY:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:34:ALA:O	1:G:35:PRO:C	2.64	0.41
1:G:512:VAL:HG22	1:G:519:ASP:OD2	2.20	0.41
1:C:101:MET:HE3	1:C:101:MET:HB3	1.93	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:640:ASP:C	1:G:641:LYS:O	2.62	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
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
1:A:639:ILE:HG23	1:A:639:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:642:ARG:O	1:C:643:SER:HB3	2.20	0.41
1:C:676:THR:C	1:C:678:ASN:H	2.29	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:623:GLN:O	1:C:624:VAL:C	2.64	0.41
1:C:1020:VAL:HG12	1:C:1021:GLN:HG2	2.02	0.41
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:71:MET:O	1:C:92:THR:OG1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:963:VAL:HG13	1:E:1036:TRP:NE1	2.35	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: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
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

5.3.1 Protein backbone

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%)	6	27
1	C	883/1137 (78%)	792 (90%)	68 (8%)	23 (3%)	4	23
1	E	884/1137 (78%)	791 (90%)	73 (8%)	20 (2%)	5	25
1	G	880/1137 (77%)	788 (90%)	71 (8%)	21 (2%)	4	24
2	B	673/727 (93%)	596 (89%)	71 (10%)	6 (1%)	14	43
2	D	672/727 (92%)	616 (92%)	47 (7%)	9 (1%)	9	35
2	F	673/727 (93%)	605 (90%)	60 (9%)	8 (1%)	10	37
2	H	672/727 (92%)	615 (92%)	47 (7%)	10 (2%)	8	32
All	All	6415/7456 (86%)	5761 (90%)	535 (8%)	119 (2%)	6	28

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	909 (99%)	13 (1%)	59	73
1	C	756/969 (78%)	749 (99%)	7 (1%)	70	78
1	E	756/969 (78%)	737 (98%)	19 (2%)	42	64
1	G	748/969 (77%)	733 (98%)	15 (2%)	48	68
2	B	584/625 (93%)	577 (99%)	7 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	582/625 (93%)	572 (98%)	10 (2%)	53	71
2	F	584/625 (93%)	581 (100%)	3 (0%)	81	83
2	H	583/625 (93%)	579 (99%)	4 (1%)	76	80
All	All	5515/6376 (86%)	5437 (99%)	78 (1%)	59	73

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	625	VAL
1	A	630	LEU
1	A	656	VAL
1	A	700	LEU
1	A	771	LEU
1	A	808	LEU
1	A	834	VAL
1	A	899	LEU
1	A	919	LEU
1	A	959	ASN
1	A	964	TRP
1	A	1021	GLN
2	B	232	ASN
2	B	247	PHE
2	B	266	LEU
2	B	268	ASP
2	B	447	ILE
2	B	502	VAL
2	B	598	SER
1	C	394	LEU
1	C	480	ARG
1	C	601	TRP
1	C	625	VAL
1	C	638	TYR
1	C	690	LYS
1	C	716	ASN
2	D	231	ARG
2	D	233	VAL
2	D	323	LEU
2	D	383	ILE
2	D	435	SER
2	D	436	LEU

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Mol	Chain	Res	Type
2	D	437	CYS
2	D	445	CYS
2	D	462	GLN
2	D	469	GLN
1	E	70	ASN
1	E	73	LEU
1	E	86	LEU
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
1	E	774	LEU
1	E	899	LEU
1	E	919	LEU
1	E	946	LEU
1	E	964	TRP
1	E	1031	ASN
1	E	1055	PHE
2	F	110	LEU
2	F	155	LEU
2	F	247	PHE
1	G	4	ASP
1	G	8	LEU
1	G	73	LEU
1	G	115	LEU
1	G	638	TYR
1	G	717	PHE
1	G	729	ASN
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

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Mol	Chain	Res	Type
2	H	492	CYS
2	H	506	LEU
2	H	621	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) 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	201	HIS
1	A	697	ASN
1	A	751	ASN
1	A	779	ASN
1	A	826	HIS
1	A	1039	GLN
2	B	28	ASN
2	B	45	GLN
2	B	167	ASN
2	B	287	HIS
2	B	657	GLN
1	C	24	GLN
1	C	43	GLN
1	C	95	HIS
1	C	463	HIS
1	C	472	GLN
1	C	590	GLN
1	C	628	GLN
1	C	653	GLN
1	C	930	HIS
1	C	939	ASN
1	C	1021	GLN
2	D	75	GLN
2	D	89	GLN
2	D	220	GLN
2	D	384	ASN
2	D	438	HIS
1	E	124	GLN
1	E	376	GLN
1	E	410	HIS

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Mol	Chain	Res	Type
1	E	463	HIS
1	E	628	GLN
1	E	653	GLN
1	E	697	ASN
1	E	779	ASN
1	E	971	HIS
1	E	998	ASN
2	F	45	GLN
2	F	332	GLN
2	F	438	HIS
2	F	577	ASN
1	G	27	ASN
1	G	85	GLN
1	G	117	GLN
1	G	419	GLN
1	G	573	GLN
1	G	674	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	1073	GLN
2	H	45	GLN
2	H	159	ASN
2	H	295	GLN
2	H	464	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.30	0	17,19,21	0.69	0
3	NAG	I	2	3	14,14,15	0.41	0	17,19,21	1.67	6 (35%)
3	BMA	I	3	3	11,11,12	1.82	3 (27%)	15,15,17	2.68	4 (26%)
3	MAN	I	4	3	11,11,12	0.72	0	15,15,17	1.52	2 (13%)
3	MAN	I	5	3	11,11,12	0.63	0	15,15,17	1.01	1 (6%)
4	NAG	J	1	1,4	14,14,15	0.47	0	17,19,21	0.72	0
4	MAN	J	10	4	11,11,12	1.08	1 (9%)	15,15,17	1.88	3 (20%)
4	NAG	J	2	4	14,14,15	1.05	1 (7%)	17,19,21	0.90	0
4	BMA	J	3	4	11,11,12	1.97	2 (18%)	15,15,17	2.24	3 (20%)
4	MAN	J	4	4	11,11,12	1.42	2 (18%)	15,15,17	0.96	1 (6%)
4	MAN	J	5	4	11,11,12	0.73	0	15,15,17	1.19	1 (6%)
4	MAN	J	6	4	11,11,12	0.93	1 (9%)	15,15,17	1.71	4 (26%)
4	MAN	J	7	4	11,11,12	1.76	3 (27%)	15,15,17	1.50	2 (13%)
4	MAN	J	8	4	11,11,12	1.02	1 (9%)	15,15,17	0.99	1 (6%)
4	MAN	J	9	4	11,11,12	0.73	0	15,15,17	0.94	2 (13%)
5	NAG	K	1	1,5	14,14,15	0.50	0	17,19,21	0.85	1 (5%)
5	NAG	K	2	5	14,14,15	0.45	0	17,19,21	0.72	0
5	BMA	K	3	5	11,11,12	1.50	3 (27%)	15,15,17	2.62	3 (20%)
5	MAN	K	4	5	11,11,12	0.75	0	15,15,17	1.63	2 (13%)
6	NAG	L	1	1,6	14,14,15	0.62	1 (7%)	17,19,21	0.97	2 (11%)
6	NAG	L	2	6	14,14,15	0.43	0	17,19,21	0.51	0
6	BMA	L	3	6	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
7	NAG	M	1	7,2	14,14,15	1.27	1 (7%)	17,19,21	1.79	5 (29%)
7	NAG	M	2	7	14,14,15	0.22	0	17,19,21	0.36	0
8	NAG	N	1	1,8	14,14,15	1.12	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	N	2	8	14,14,15	0.82	1 (7%)	17,19,21	1.54	5 (29%)
8	BMA	N	3	8	11,11,12	2.65	3 (27%)	15,15,17	1.70	4 (26%)
8	MAN	N	4	8	11,11,12	0.80	0	15,15,17	1.05	2 (13%)
9	NAG	O	1	9,1	14,14,15	0.76	1 (7%)	17,19,21	0.75	0
9	NAG	O	2	9	14,14,15	0.67	0	17,19,21	2.02	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BMA	O	3	9	11,11,12	2.19	4 (36%)	15,15,17	1.79	3 (20%)
9	MAN	O	4	9	11,11,12	0.81	1 (9%)	15,15,17	0.97	2 (13%)
9	MAN	O	5	9	11,11,12	1.93	4 (36%)	15,15,17	1.34	2 (13%)
9	MAN	O	6	9	11,11,12	1.11	1 (9%)	15,15,17	1.44	2 (13%)
9	MAN	O	7	9	11,11,12	1.14	2 (18%)	15,15,17	1.30	2 (13%)
10	NAG	P	1	1,10	14,14,15	0.78	1 (7%)	17,19,21	0.89	1 (5%)
10	NAG	P	2	10	14,14,15	0.48	0	17,19,21	1.41	2 (11%)
10	BMA	P	3	10	11,11,12	0.70	0	15,15,17	1.09	2 (13%)
10	MAN	P	4	10	11,11,12	1.23	1 (9%)	15,15,17	1.55	2 (13%)
10	MAN	P	5	10	11,11,12	1.41	2 (18%)	15,15,17	0.92	1 (6%)
11	NAG	Q	1	1,11	14,14,15	0.50	0	17,19,21	1.22	1 (5%)
11	NAG	Q	2	11	14,14,15	0.55	0	17,19,21	0.54	0
11	BMA	Q	3	11	11,11,12	1.20	1 (9%)	15,15,17	0.96	1 (6%)
11	MAN	Q	4	11	11,11,12	1.76	4 (36%)	15,15,17	1.92	3 (20%)
11	MAN	Q	5	11	11,11,12	0.59	0	15,15,17	2.11	2 (13%)
12	NAG	R	1	1,12	14,14,15	0.80	0	17,19,21	0.82	1 (5%)
12	NAG	R	2	12	14,14,15	1.13	2 (14%)	17,19,21	1.04	1 (5%)
12	BMA	R	3	12	11,11,12	2.26	6 (54%)	15,15,17	1.98	5 (33%)
12	MAN	R	4	12	11,11,12	2.72	6 (54%)	15,15,17	1.31	1 (6%)
12	MAN	R	5	12	11,11,12	0.79	0	15,15,17	0.96	1 (6%)
12	MAN	R	6	12	11,11,12	0.74	0	15,15,17	1.02	2 (13%)
8	NAG	S	1	1,8	14,14,15	0.70	0	17,19,21	0.79	1 (5%)
8	NAG	S	2	8	14,14,15	0.32	0	17,19,21	0.46	0
8	BMA	S	3	8	11,11,12	0.95	1 (9%)	15,15,17	1.19	2 (13%)
8	MAN	S	4	8	11,11,12	0.66	0	15,15,17	1.51	2 (13%)
5	NAG	T	1	1,5	14,14,15	0.88	1 (7%)	17,19,21	0.90	0
5	NAG	T	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.76	0
5	BMA	T	3	5	11,11,12	0.96	1 (9%)	15,15,17	1.61	2 (13%)
5	MAN	T	4	5	11,11,12	0.92	1 (9%)	15,15,17	0.87	1 (6%)
11	NAG	U	1	1,11	14,14,15	1.11	1 (7%)	17,19,21	2.19	3 (17%)
11	NAG	U	2	11	14,14,15	0.67	1 (7%)	17,19,21	0.97	1 (5%)
11	BMA	U	3	11	11,11,12	1.79	3 (27%)	15,15,17	1.68	2 (13%)
11	MAN	U	4	11	11,11,12	0.76	0	15,15,17	1.09	2 (13%)
11	MAN	U	5	11	11,11,12	2.40	2 (18%)	15,15,17	1.98	2 (13%)
11	NAG	V	1	1,11	14,14,15	0.54	0	17,19,21	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	V	2	11	14,14,15	0.53	0	17,19,21	0.88	0
11	BMA	V	3	11	11,11,12	0.79	0	15,15,17	1.12	1 (6%)
11	MAN	V	4	11	11,11,12	0.99	1 (9%)	15,15,17	2.15	4 (26%)
11	MAN	V	5	11	11,11,12	0.98	0	15,15,17	1.80	2 (13%)
13	NAG	W	1	13,1	14,14,15	1.59	1 (7%)	17,19,21	0.94	1 (5%)
13	NAG	W	2	13	14,14,15	0.67	0	17,19,21	1.30	4 (23%)
13	BMA	W	3	13	11,11,12	1.48	3 (27%)	15,15,17	1.93	6 (40%)
13	MAN	W	4	13	11,11,12	1.65	3 (27%)	15,15,17	1.40	1 (6%)
13	MAN	W	5	13	11,11,12	0.78	0	15,15,17	1.29	1 (6%)
13	MAN	W	6	13	11,11,12	0.94	1 (9%)	15,15,17	1.15	2 (13%)
13	MAN	W	7	13	11,11,12	0.70	0	15,15,17	1.37	3 (20%)
5	NAG	X	1	1,5	14,14,15	0.55	0	17,19,21	1.14	2 (11%)
5	NAG	X	2	5	14,14,15	0.78	1 (7%)	17,19,21	1.19	1 (5%)
5	BMA	X	3	5	11,11,12	1.11	0	15,15,17	1.31	1 (6%)
5	MAN	X	4	5	11,11,12	1.01	1 (9%)	15,15,17	0.91	1 (6%)
14	NAG	Y	1	1,14	14,14,15	1.12	1 (7%)	17,19,21	1.20	2 (11%)
14	NAG	Y	2	14	14,14,15	0.74	1 (7%)	17,19,21	2.23	2 (11%)
14	BMA	Y	3	14	11,11,12	1.17	1 (9%)	15,15,17	0.92	1 (6%)
14	MAN	Y	4	14	11,11,12	0.88	1 (9%)	15,15,17	1.78	1 (6%)
14	MAN	Y	5	14	11,11,12	1.33	1 (9%)	15,15,17	1.58	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,5	-	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	1,6	-	1/6/23/26	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	-	2/6/23/26	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	-	2/6/23/26	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	1,10	-	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	1,11	-	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	1,12	-	4/6/23/26	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,5	-	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	1,11	-	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	1,11	-	3/6/23/26	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	1,5	-	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	1,14	-	2/6/23/26	0/1/1/1
14	NAG	Y	2	14	-	5/6/23/26	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
14	MAN	Y	5	14	-	0/2/19/22	0/1/1/1

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	3	BMA	O5-C1	-6.59	1.32	1.43
11	U	5	MAN	O5-C5	6.54	1.56	1.43
13	W	1	NAG	O5-C1	-5.72	1.34	1.43
4	J	3	BMA	O5-C1	-5.23	1.34	1.43
3	I	3	BMA	O5-C1	-4.60	1.36	1.43
12	R	4	MAN	C1-C2	4.52	1.63	1.52
12	R	4	MAN	C2-C3	4.42	1.59	1.52
4	J	7	MAN	O5-C1	-4.37	1.36	1.43
9	O	3	BMA	C1-C2	4.20	1.62	1.52
9	O	5	MAN	O2-C2	4.18	1.52	1.43
8	N	3	BMA	C1-C2	4.08	1.62	1.52
12	R	3	BMA	O5-C1	-4.02	1.36	1.43
14	Y	1	NAG	O5-C1	-3.86	1.37	1.43
12	R	4	MAN	O2-C2	3.79	1.51	1.43
4	J	2	NAG	O5-C1	-3.77	1.37	1.43
7	M	1	NAG	C1-C2	3.73	1.57	1.52
5	K	3	BMA	O5-C1	-3.68	1.37	1.43
12	R	4	MAN	O5-C1	-3.64	1.37	1.43
11	U	1	NAG	O5-C1	-3.63	1.37	1.43
4	J	4	MAN	C2-C3	3.59	1.58	1.52
11	U	5	MAN	O5-C1	3.59	1.49	1.43
8	N	1	NAG	O5-C1	-3.46	1.37	1.43
9	O	5	MAN	C2-C3	3.42	1.57	1.52
11	Q	4	MAN	O5-C5	3.39	1.50	1.43
5	T	1	NAG	O5-C1	-3.25	1.38	1.43
13	W	4	MAN	C1-C2	3.23	1.59	1.52
9	O	3	BMA	O3-C3	3.21	1.50	1.43
9	O	3	BMA	O5-C1	-3.16	1.38	1.43
12	R	3	BMA	O5-C5	-3.07	1.37	1.43
11	U	3	BMA	C6-C5	3.02	1.61	1.51
13	W	4	MAN	C2-C3	2.96	1.57	1.52
9	O	6	MAN	O5-C5	2.96	1.49	1.43
4	J	10	MAN	C1-C2	2.95	1.59	1.52
14	Y	5	MAN	C1-C2	2.90	1.59	1.52
8	N	2	NAG	O5-C1	-2.89	1.38	1.43
12	R	2	NAG	C1-C2	-2.88	1.48	1.52
12	R	3	BMA	C6-C5	-2.85	1.42	1.51
14	Y	3	BMA	O5-C1	-2.84	1.38	1.43
11	Q	3	BMA	C4-C3	2.80	1.59	1.52
11	Q	4	MAN	C1-C2	2.78	1.58	1.52
12	R	4	MAN	O5-C5	2.78	1.48	1.43
10	P	1	NAG	C1-C2	2.77	1.56	1.52
9	O	3	BMA	C2-C3	2.76	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	3	BMA	C4-C3	2.74	1.59	1.52
3	I	3	BMA	C4-C5	2.71	1.58	1.53
11	Q	4	MAN	O5-C1	2.69	1.48	1.43
5	X	4	MAN	O5-C1	-2.68	1.39	1.43
9	O	1	NAG	O5-C1	-2.61	1.39	1.43
11	U	3	BMA	C1-C2	2.60	1.58	1.52
10	P	4	MAN	O3-C3	2.60	1.49	1.43
13	W	3	BMA	C4-C3	2.59	1.59	1.52
3	I	3	BMA	C4-C3	2.58	1.59	1.52
11	U	3	BMA	O6-C6	2.54	1.53	1.42
14	Y	4	MAN	O5-C5	2.54	1.48	1.43
4	J	6	MAN	C1-C2	2.53	1.58	1.52
13	W	3	BMA	O4-C4	-2.53	1.36	1.43
5	T	2	NAG	O5-C1	-2.48	1.39	1.43
9	O	7	MAN	O5-C5	2.47	1.48	1.43
4	J	3	BMA	C2-C3	2.46	1.56	1.52
9	O	7	MAN	C1-C2	2.46	1.58	1.52
4	J	7	MAN	C4-C3	2.45	1.58	1.52
13	W	6	MAN	O5-C1	-2.45	1.39	1.43
5	K	3	BMA	C4-C3	2.43	1.58	1.52
12	R	3	BMA	C4-C5	2.42	1.58	1.53
5	T	4	MAN	O5-C1	-2.41	1.39	1.43
4	J	8	MAN	O5-C1	-2.41	1.39	1.43
5	T	3	BMA	C1-C2	2.38	1.57	1.52
11	U	2	NAG	O5-C1	-2.37	1.39	1.43
12	R	3	BMA	C2-C3	2.35	1.56	1.52
10	P	5	MAN	C1-C2	2.35	1.57	1.52
13	W	3	BMA	C1-C2	2.33	1.57	1.52
5	X	2	NAG	O5-C1	-2.33	1.39	1.43
11	V	4	MAN	C1-C2	2.29	1.57	1.52
12	R	2	NAG	O5-C1	-2.28	1.39	1.43
9	O	4	MAN	O5-C1	-2.25	1.39	1.43
9	O	5	MAN	C4-C3	2.25	1.58	1.52
10	P	5	MAN	O5-C5	2.22	1.47	1.43
13	W	4	MAN	O2-C2	2.17	1.47	1.43
6	L	1	NAG	O5-C1	-2.13	1.40	1.43
11	Q	4	MAN	C2-C3	2.12	1.55	1.52
9	O	5	MAN	C1-C2	2.12	1.57	1.52
14	Y	2	NAG	O5-C1	-2.10	1.40	1.43
4	J	4	MAN	C1-C2	2.09	1.57	1.52
12	R	3	BMA	O3-C3	2.06	1.48	1.43
8	S	3	BMA	O5-C1	-2.04	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	7	MAN	C1-C2	2.02	1.57	1.52
12	R	4	MAN	C4-C3	2.01	1.57	1.52
5	K	3	BMA	C4-C5	2.00	1.57	1.53

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	BMA	C1-C2-C3	-7.54	98.66	109.64
14	Y	2	NAG	C2-N2-C7	7.16	132.50	122.90
11	U	1	NAG	C2-N2-C7	7.11	132.42	122.90
11	Q	5	MAN	C1-O5-C5	7.02	121.59	112.19
11	V	4	MAN	C1-O5-C5	6.83	121.34	112.19
5	K	3	BMA	C1-O5-C5	-6.69	103.22	112.19
11	U	5	MAN	C1-O5-C5	6.43	120.80	112.19
5	K	3	BMA	C1-C2-C3	-6.34	100.41	109.64
11	Q	4	MAN	C1-O5-C5	6.09	120.34	112.19
4	J	3	BMA	C1-O5-C5	6.07	120.32	112.19
14	Y	4	MAN	C1-O5-C5	6.02	120.25	112.19
11	V	5	MAN	C1-O5-C5	5.94	120.15	112.19
3	I	3	BMA	C1-O5-C5	-5.77	104.46	112.19
4	J	10	MAN	C1-O5-C5	5.45	119.50	112.19
5	K	4	MAN	C1-O5-C5	5.07	118.98	112.19
4	J	6	MAN	C1-O5-C5	4.86	118.71	112.19
10	P	2	NAG	C2-N2-C7	4.68	129.18	122.90
12	R	3	BMA	O3-C3-C2	4.64	119.52	110.05
4	J	3	BMA	O5-C5-C6	-4.61	98.70	107.66
9	O	3	BMA	O3-C3-C2	4.56	119.36	110.05
11	Q	1	NAG	C2-N2-C7	4.44	128.85	122.90
9	O	2	NAG	C2-N2-C7	4.41	128.81	122.90
9	O	6	MAN	C1-O5-C5	4.32	117.98	112.19
14	Y	5	MAN	C1-O5-C5	4.25	117.89	112.19
11	U	3	BMA	O5-C5-C6	4.25	115.93	107.66
8	S	4	MAN	C1-O5-C5	4.24	117.87	112.19
14	Y	2	NAG	C1-C2-N2	4.24	117.11	110.43
13	W	4	MAN	O3-C3-C2	4.10	118.42	110.05
9	O	2	NAG	C1-C2-N2	4.08	116.86	110.43
10	P	4	MAN	C1-O5-C5	4.06	117.63	112.19
7	M	1	NAG	C2-N2-C7	-4.01	117.53	122.90
5	T	3	BMA	C1-O5-C5	3.90	117.41	112.19
3	I	4	MAN	C1-O5-C5	3.87	117.37	112.19
5	X	2	NAG	C2-N2-C7	3.72	127.88	122.90
5	X	3	BMA	O2-C2-C3	-3.66	102.57	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W	5	MAN	C1-O5-C5	3.63	117.05	112.19
8	N	2	NAG	C2-N2-C7	3.56	127.68	122.90
9	O	7	MAN	C1-O5-C5	3.56	116.96	112.19
13	W	6	MAN	C1-O5-C5	3.52	116.90	112.19
9	O	3	BMA	C2-C3-C4	-3.48	104.74	110.86
8	N	3	BMA	O2-C2-C3	-3.47	102.95	110.15
12	R	4	MAN	O2-C2-C3	-3.34	103.23	110.15
4	J	7	MAN	O2-C2-C3	-3.33	103.24	110.15
13	W	7	MAN	C1-O5-C5	3.31	116.62	112.19
5	X	1	NAG	C1-O5-C5	3.30	116.61	112.19
10	P	4	MAN	O3-C3-C2	3.23	116.65	110.05
4	J	5	MAN	C1-O5-C5	3.20	116.48	112.19
13	W	3	BMA	O4-C4-C5	-3.19	101.47	109.32
11	U	1	NAG	C1-C2-N2	3.18	115.45	110.43
11	U	4	MAN	C1-O5-C5	3.06	116.28	112.19
11	Q	5	MAN	O5-C1-C2	3.05	118.06	110.79
12	R	3	BMA	C3-C4-C5	2.97	115.62	110.23
3	I	2	NAG	C1-C2-N2	2.95	115.08	110.43
9	O	5	MAN	C1-O5-C5	2.94	116.13	112.19
8	S	3	BMA	C1-O5-C5	2.93	116.11	112.19
11	U	3	BMA	O2-C2-C3	-2.92	104.11	110.15
9	O	2	NAG	O3-C3-C4	2.91	117.23	110.38
4	J	10	MAN	C1-C2-C3	2.90	113.87	109.64
5	T	3	BMA	O2-C2-C3	-2.90	104.15	110.15
14	Y	1	NAG	C2-N2-C7	2.89	126.77	122.90
10	P	3	BMA	C1-O5-C5	2.88	116.04	112.19
14	Y	5	MAN	O2-C2-C3	-2.87	104.21	110.15
6	L	1	NAG	C1-O5-C5	-2.85	108.36	112.19
13	W	3	BMA	C2-C3-C4	-2.83	105.88	110.86
13	W	7	MAN	O2-C2-C3	-2.81	104.33	110.15
12	R	6	MAN	C1-O5-C5	2.81	115.95	112.19
3	I	4	MAN	O2-C2-C3	-2.80	104.34	110.15
3	I	2	NAG	C1-O5-C5	2.79	115.92	112.19
9	O	6	MAN	O2-C2-C3	-2.78	104.39	110.15
13	W	3	BMA	O5-C5-C6	2.76	113.04	107.66
13	W	2	NAG	O3-C3-C4	2.75	116.87	110.38
7	M	1	NAG	C1-C2-N2	2.74	114.76	110.43
12	R	3	BMA	C1-O5-C5	-2.73	108.53	112.19
4	J	7	MAN	C1-C2-C3	2.71	113.60	109.64
12	R	3	BMA	O5-C5-C6	-2.71	102.40	107.66
7	M	1	NAG	O4-C4-C3	-2.69	104.02	110.38
11	U	2	NAG	C2-N2-C7	2.69	126.50	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	4	MAN	O2-C2-C3	-2.68	104.59	110.15
13	W	3	BMA	C1-O5-C5	-2.68	108.59	112.19
3	I	2	NAG	C4-C3-C2	-2.68	107.09	111.02
9	O	5	MAN	O2-C2-C1	2.68	115.36	109.22
3	I	2	NAG	O4-C4-C3	2.67	116.68	110.38
7	M	1	NAG	C1-O5-C5	-2.65	108.64	112.19
8	N	3	BMA	C1-O5-C5	-2.64	108.65	112.19
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
4	J	8	MAN	O2-C2-C3	-2.54	104.90	110.15
4	J	10	MAN	O2-C2-C3	-2.53	104.90	110.15
8	N	2	NAG	O3-C3-C2	-2.53	104.15	109.40
5	X	1	NAG	C1-C2-N2	2.50	114.38	110.43
4	J	6	MAN	C1-C2-C3	2.50	113.28	109.64
8	S	4	MAN	O2-C2-C3	-2.47	105.03	110.15
11	V	4	MAN	O2-C2-C3	-2.47	105.03	110.15
3	I	5	MAN	C1-O5-C5	2.47	115.49	112.19
8	N	3	BMA	O6-C6-C5	-2.46	102.94	111.33
11	U	1	NAG	O4-C4-C3	-2.46	104.57	110.38
11	Q	4	MAN	C1-C2-C3	2.44	113.20	109.64
12	R	1	NAG	O4-C4-C3	2.41	116.06	110.38
12	R	2	NAG	O3-C3-C2	-2.38	104.45	109.40
11	V	4	MAN	O5-C1-C2	2.37	116.43	110.79
11	U	4	MAN	O2-C2-C3	-2.36	105.27	110.15
4	J	3	BMA	O6-C6-C5	-2.35	103.33	111.33
12	R	5	MAN	O2-C2-C3	-2.35	105.29	110.15
4	J	6	MAN	O2-C2-C3	-2.34	105.31	110.15
9	O	3	BMA	C1-C2-C3	-2.32	106.26	109.64
3	I	2	NAG	O3-C3-C4	2.32	115.83	110.38
11	Q	3	BMA	O2-C2-C3	-2.31	105.36	110.15
11	V	4	MAN	C1-C2-C3	2.30	112.99	109.64
8	N	3	BMA	O5-C5-C6	2.29	112.12	107.66
4	J	9	MAN	O2-C2-C3	-2.29	105.40	110.15
11	V	3	BMA	O2-C2-C3	-2.29	105.41	110.15
13	W	2	NAG	C4-C3-C2	-2.29	107.66	111.02
10	P	3	BMA	O2-C2-C3	-2.28	105.42	110.15
13	W	3	BMA	C1-C2-C3	-2.28	106.33	109.64
8	S	1	NAG	C2-N2-C7	2.27	125.95	122.90
9	O	4	MAN	C1-O5-C5	2.27	115.23	112.19
3	I	3	BMA	O2-C2-C1	2.25	114.37	109.22
8	N	2	NAG	C1-C2-N2	2.24	113.96	110.43
13	W	2	NAG	C1-C2-N2	2.23	113.94	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	5	MAN	O2-C2-C3	-2.23	105.54	110.15
4	J	6	MAN	O5-C1-C2	2.23	116.10	110.79
5	K	4	MAN	O2-C2-C3	-2.23	105.54	110.15
12	R	6	MAN	O2-C2-C3	-2.22	105.55	110.15
11	Q	4	MAN	O2-C2-C3	-2.22	105.56	110.15
8	N	4	MAN	C1-O5-C5	2.22	115.16	112.19
14	Y	1	NAG	C1-C2-N2	2.21	113.92	110.43
5	K	1	NAG	C1-C2-N2	2.19	113.88	110.43
9	O	4	MAN	O2-C2-C3	-2.19	105.62	110.15
10	P	5	MAN	O2-C2-C3	-2.19	105.62	110.15
9	O	2	NAG	C3-C4-C5	-2.17	106.29	110.23
8	S	3	BMA	O2-C2-C3	-2.17	105.66	110.15
5	X	4	MAN	O2-C2-C3	-2.17	105.66	110.15
5	K	3	BMA	O2-C2-C3	-2.16	105.68	110.15
4	J	9	MAN	C1-O5-C5	2.16	115.08	112.19
5	T	4	MAN	O2-C2-C3	-2.16	105.68	110.15
9	O	2	NAG	C1-O5-C5	2.15	115.07	112.19
3	I	3	BMA	O3-C3-C2	2.14	114.43	110.05
13	W	3	BMA	O2-C2-C3	-2.13	105.73	110.15
3	I	2	NAG	C3-C4-C5	-2.12	106.38	110.23
13	W	6	MAN	O2-C2-C3	-2.10	105.80	110.15
9	O	7	MAN	C1-C2-C3	2.10	112.70	109.64
13	W	1	NAG	O3-C3-C2	-2.10	105.04	109.40
10	P	1	NAG	C2-N2-C7	2.09	125.70	122.90
11	V	5	MAN	O5-C1-C2	2.08	115.76	110.79
10	P	2	NAG	C1-O5-C5	2.07	114.96	112.19
13	W	7	MAN	O6-C6-C5	-2.07	104.30	111.33
12	R	3	BMA	O3-C3-C4	-2.05	105.54	110.38
8	N	2	NAG	O4-C4-C3	-2.05	105.54	110.38
14	Y	3	BMA	O2-C2-C3	-2.04	105.92	110.15
13	W	2	NAG	O3-C3-C2	-2.04	105.16	109.40
8	N	2	NAG	C4-C3-C2	2.04	114.01	111.02
4	J	4	MAN	O5-C5-C4	-2.04	105.87	110.83
8	N	1	NAG	C1-O5-C5	-2.04	109.46	112.19
6	L	1	NAG	C2-N2-C7	2.03	125.62	122.90
6	L	3	BMA	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	2	NAG	C3-C2-N2-C7

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

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

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

There are no ring outliers.

40 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Q	1	NAG	1	0
5	X	1	NAG	3	0
12	R	1	NAG	1	0
14	Y	5	MAN	1	0
13	W	6	MAN	1	0
5	T	4	MAN	0	1
5	T	2	NAG	3	0
9	O	2	NAG	2	0
6	L	1	NAG	2	0
5	K	1	NAG	2	0
13	W	7	MAN	2	0
12	R	4	MAN	1	0

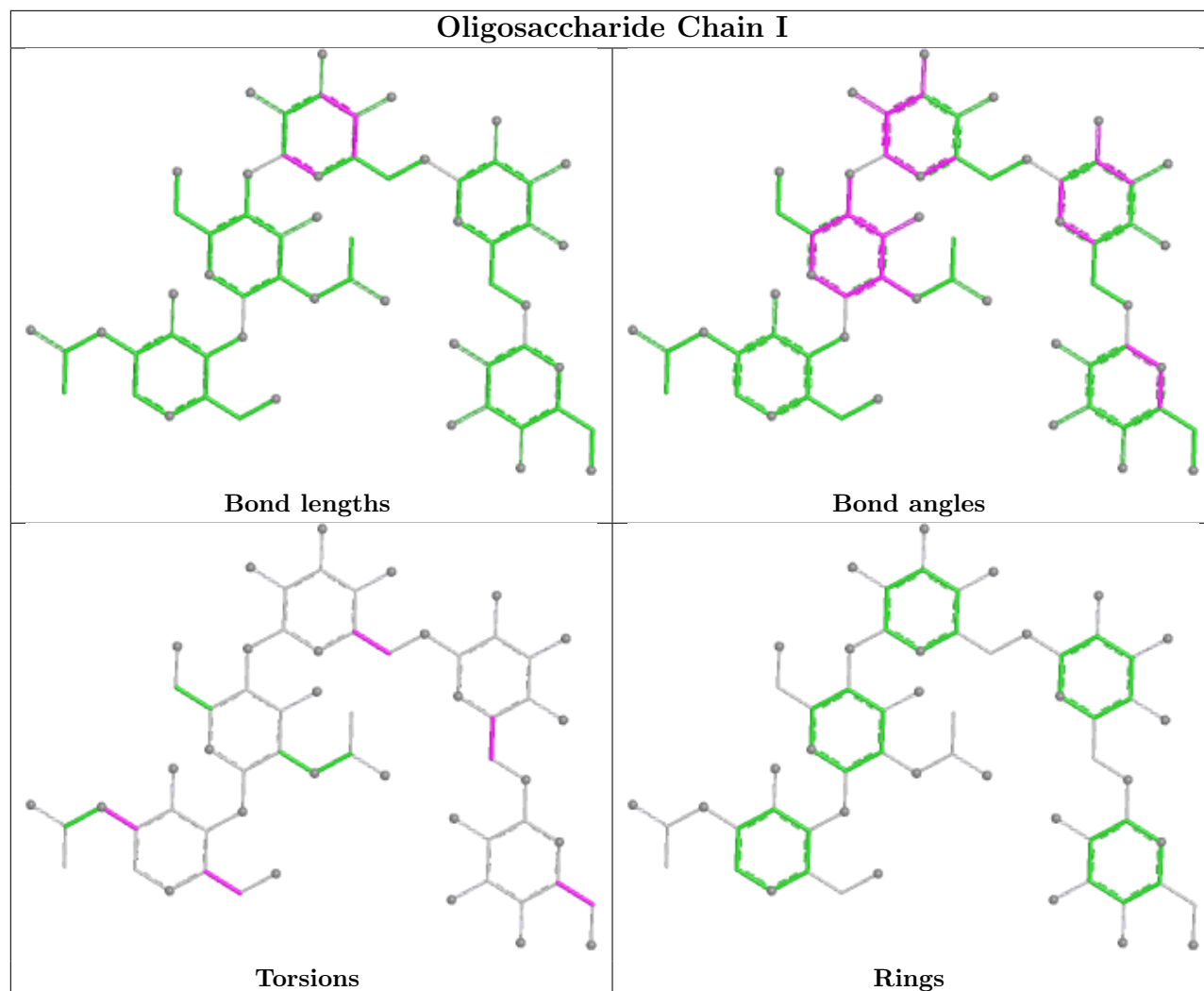
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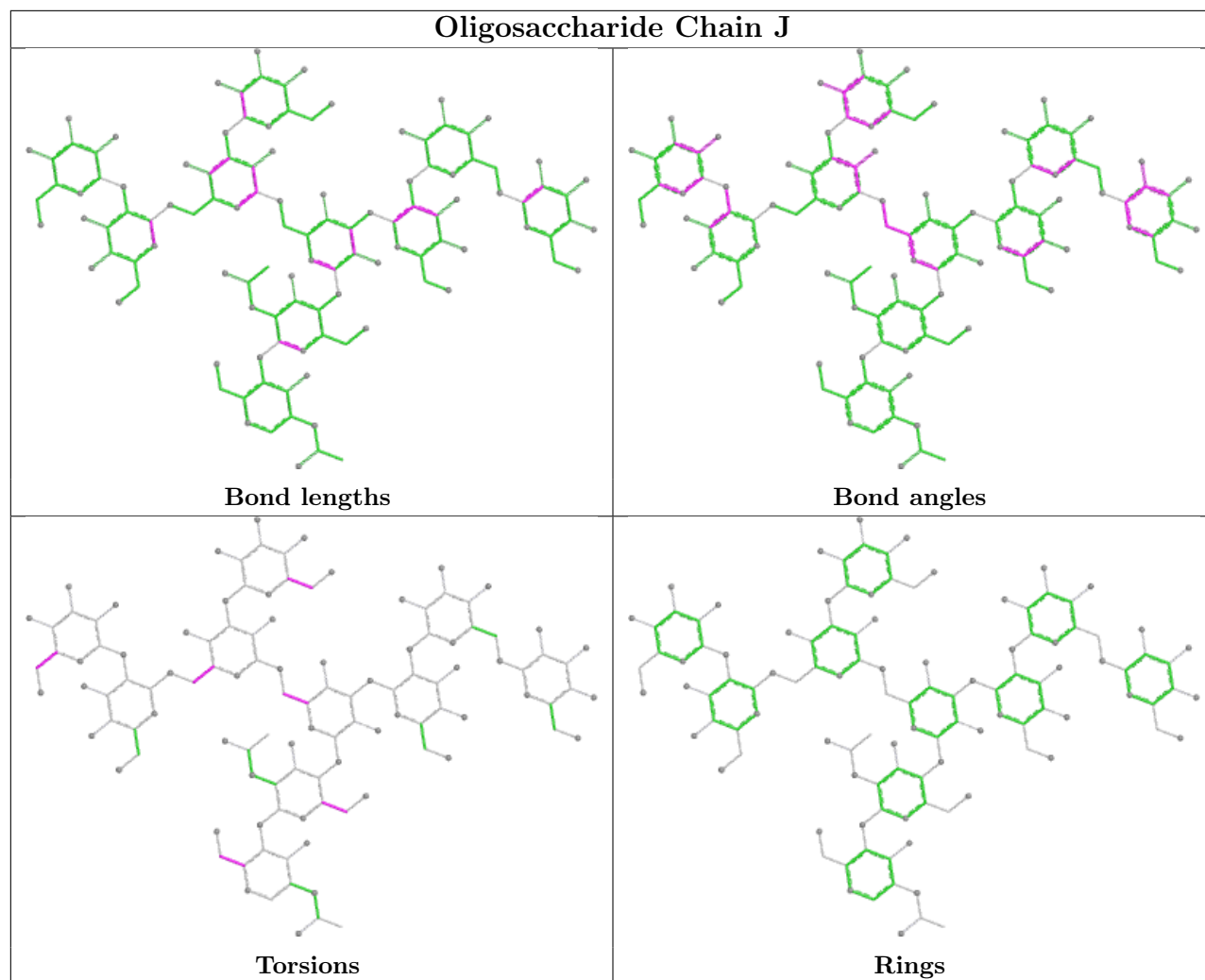
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	S	1	NAG	4	0
3	I	1	NAG	3	0
5	K	2	NAG	2	0
5	X	4	MAN	1	0
5	X	3	BMA	1	0
11	V	2	NAG	2	0
14	Y	1	NAG	2	0
14	Y	4	MAN	1	0
10	P	1	NAG	3	0
14	Y	3	BMA	1	0
5	T	3	BMA	2	0
13	W	4	MAN	2	0
11	V	5	MAN	2	0
12	R	3	BMA	1	0
8	N	1	NAG	3	0
11	V	1	NAG	5	0
11	U	1	NAG	1	0
9	O	1	NAG	3	0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

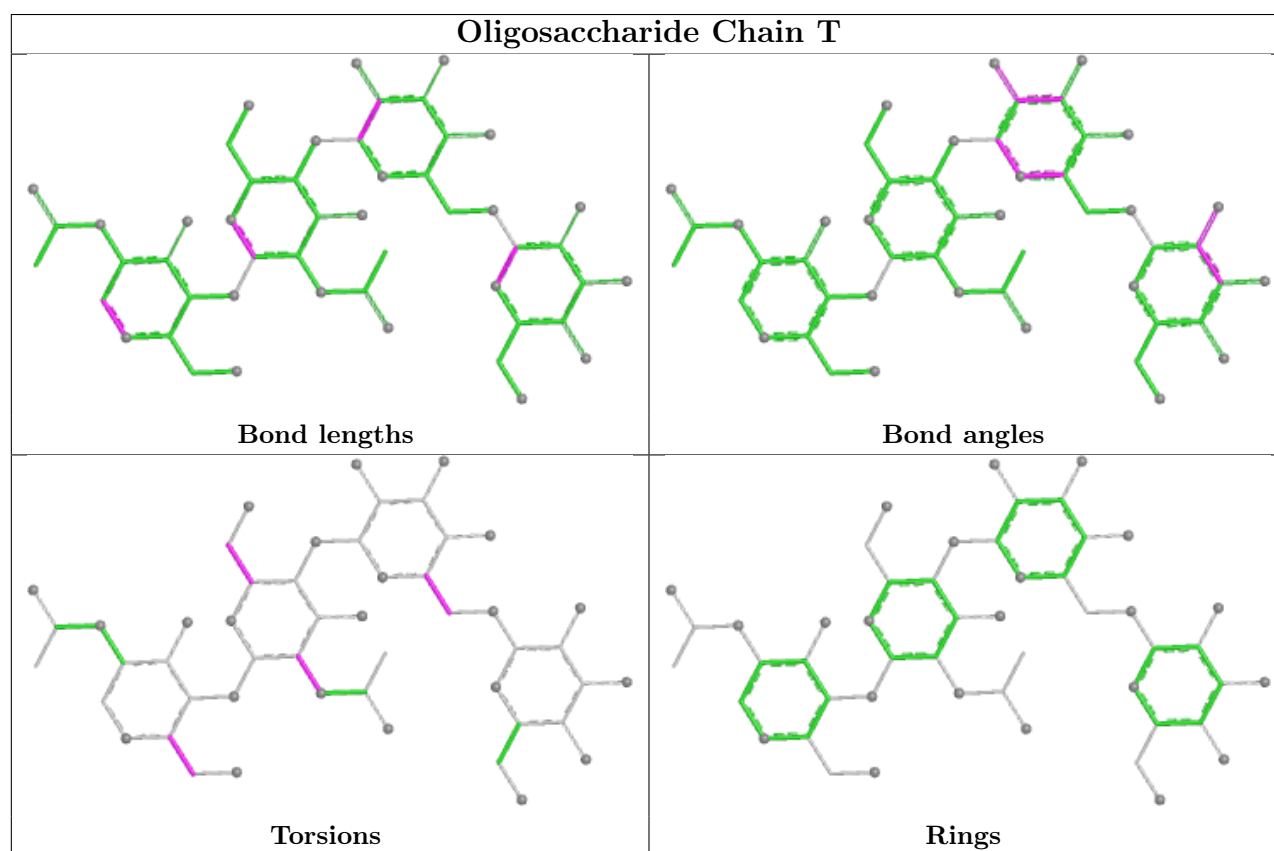
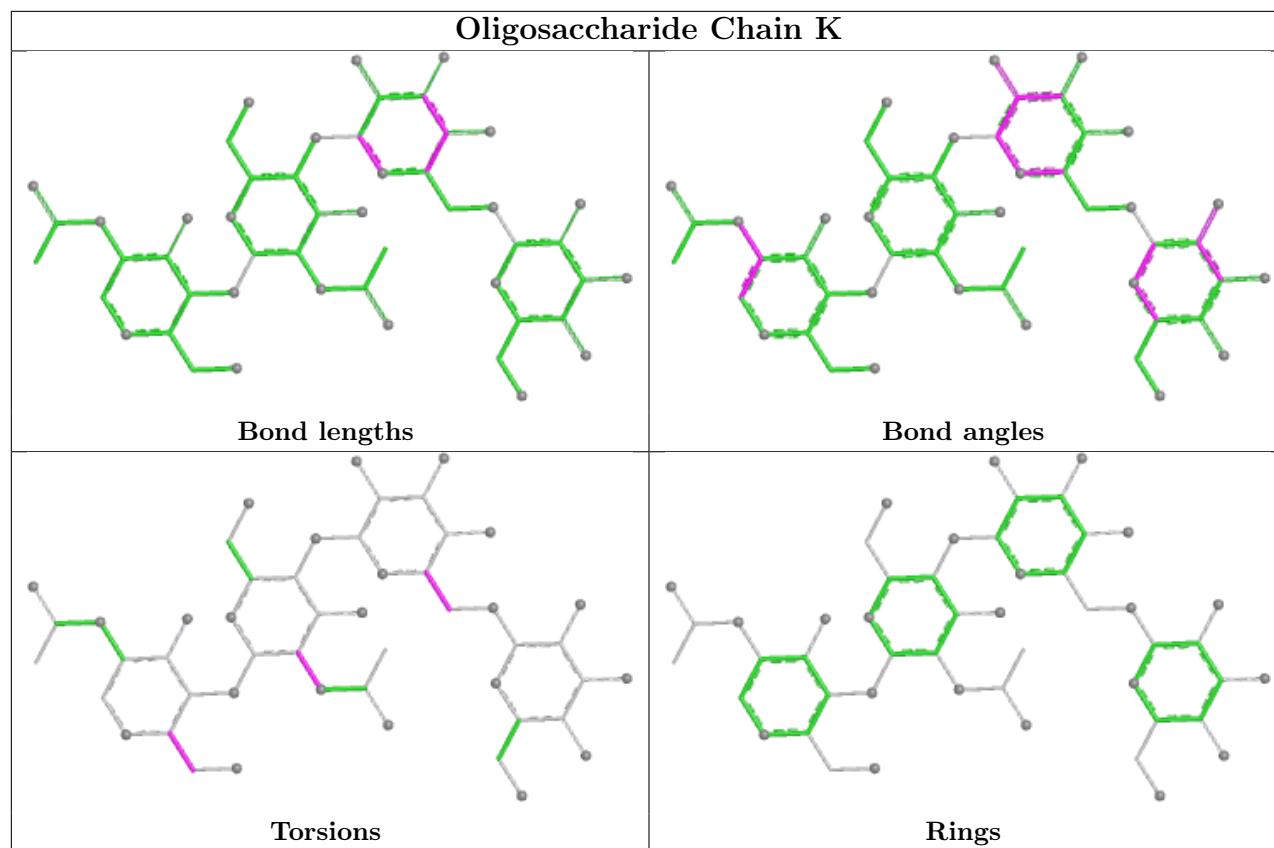
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

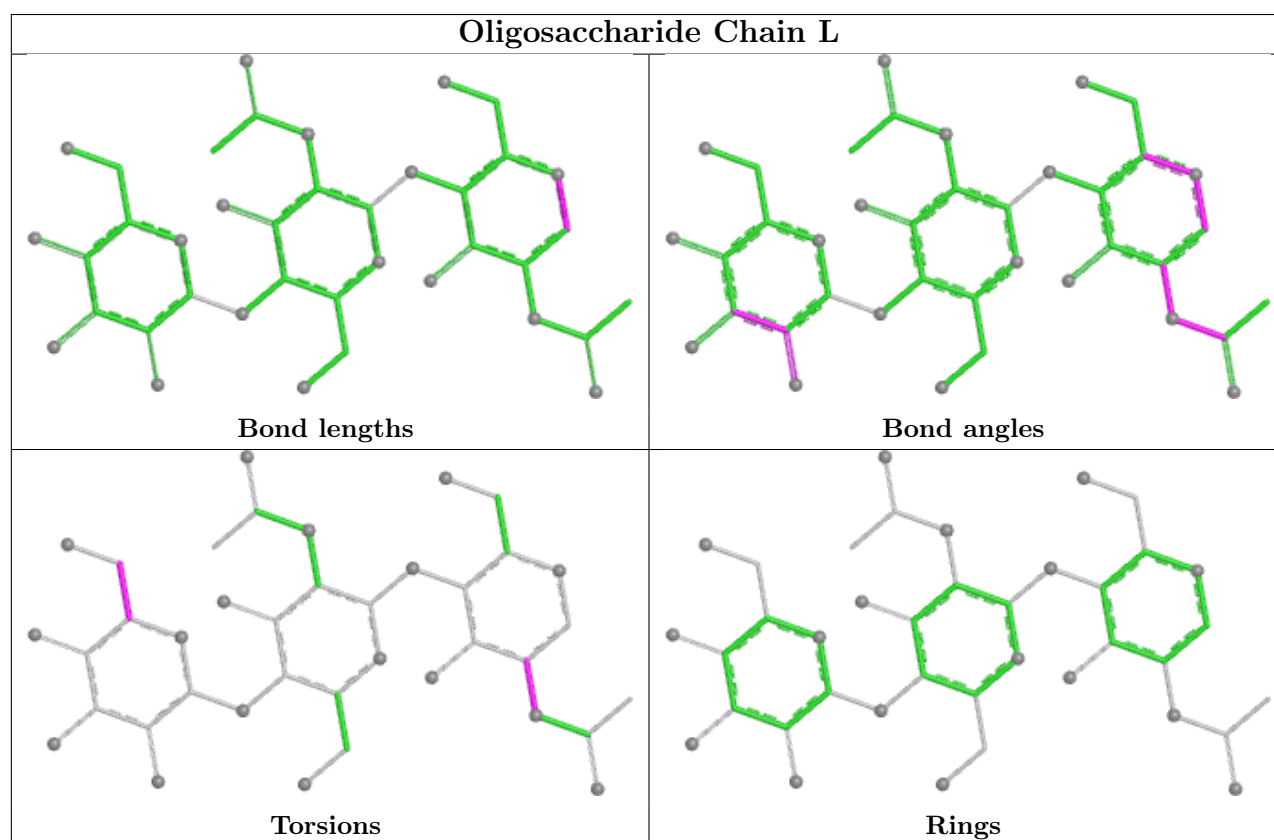
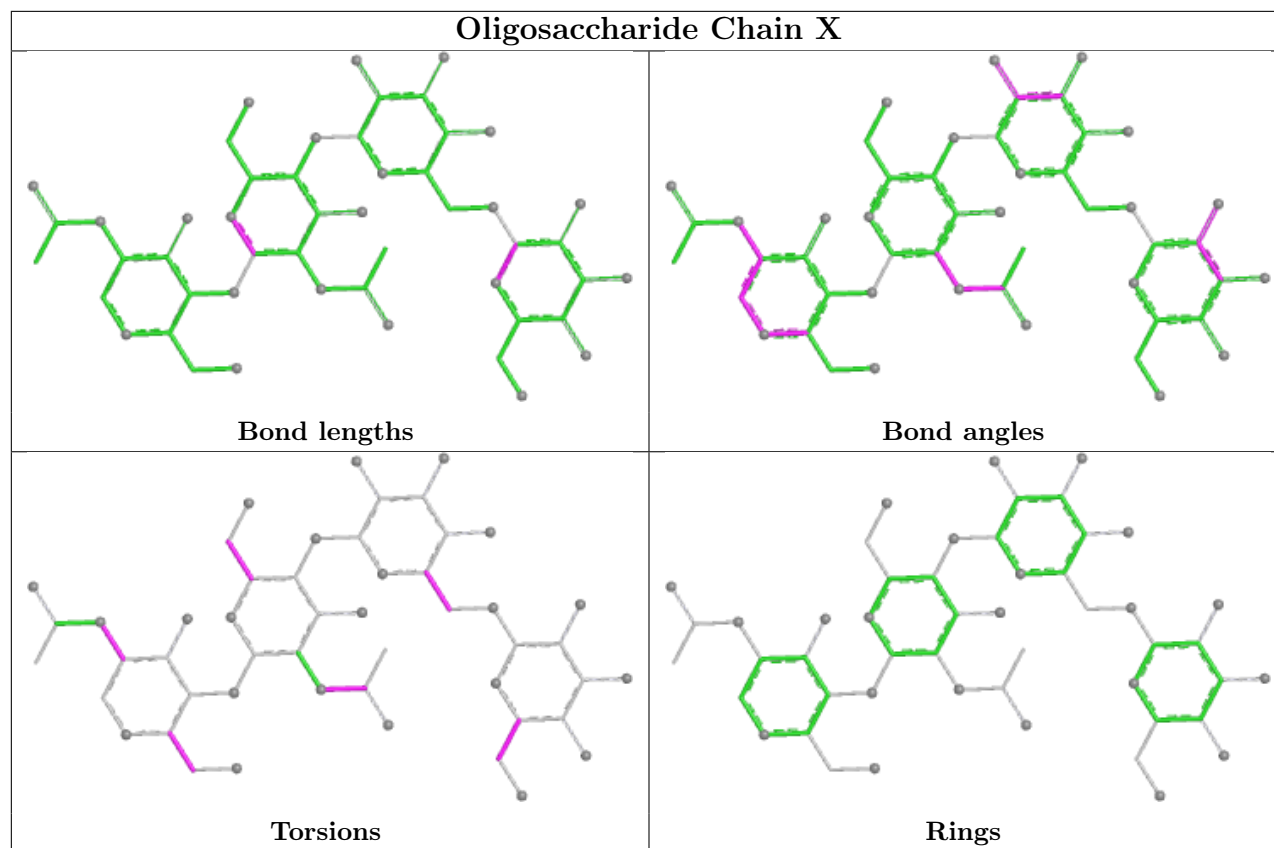
Oligosaccharide Chain I

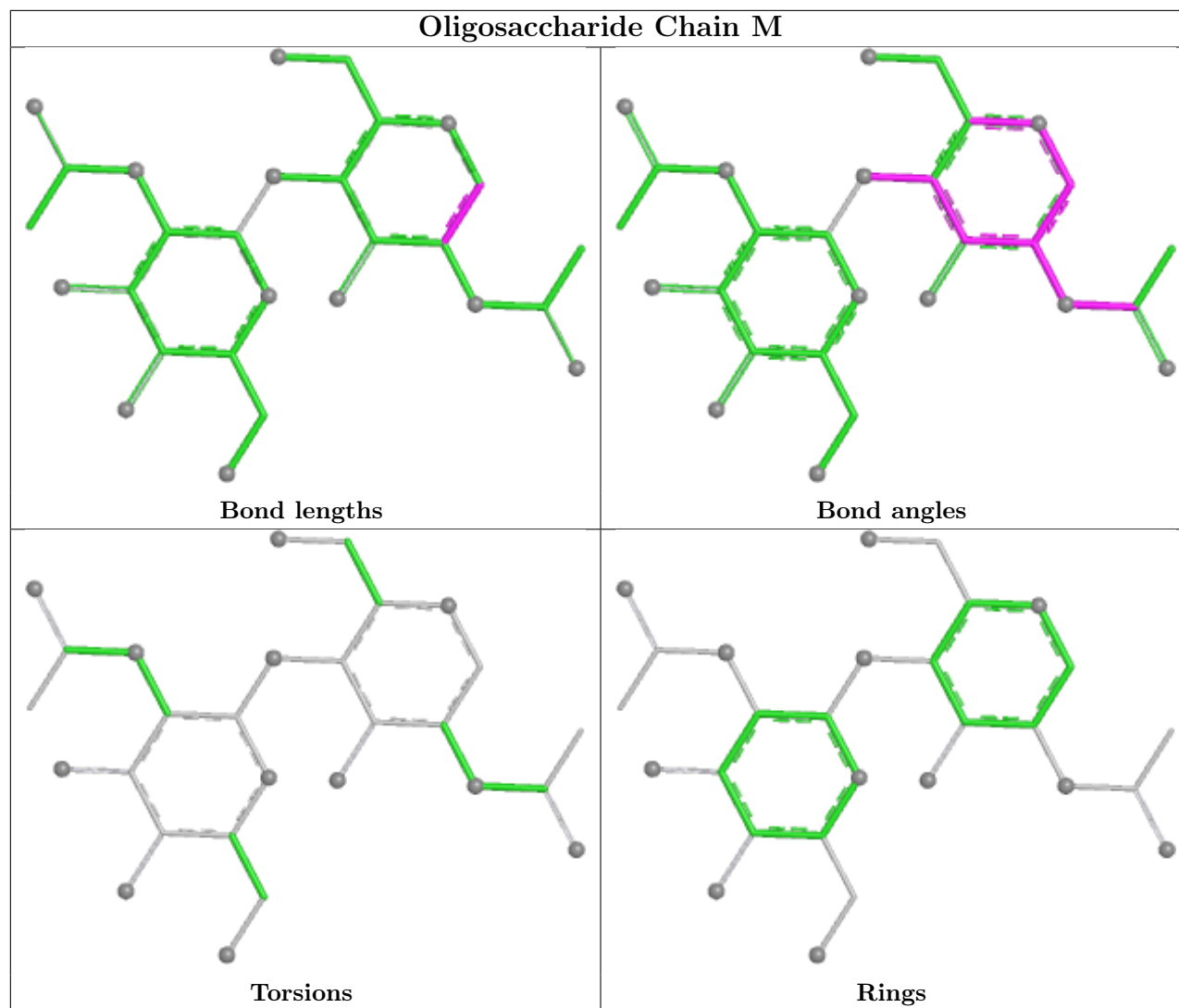


Oligosaccharide Chain J

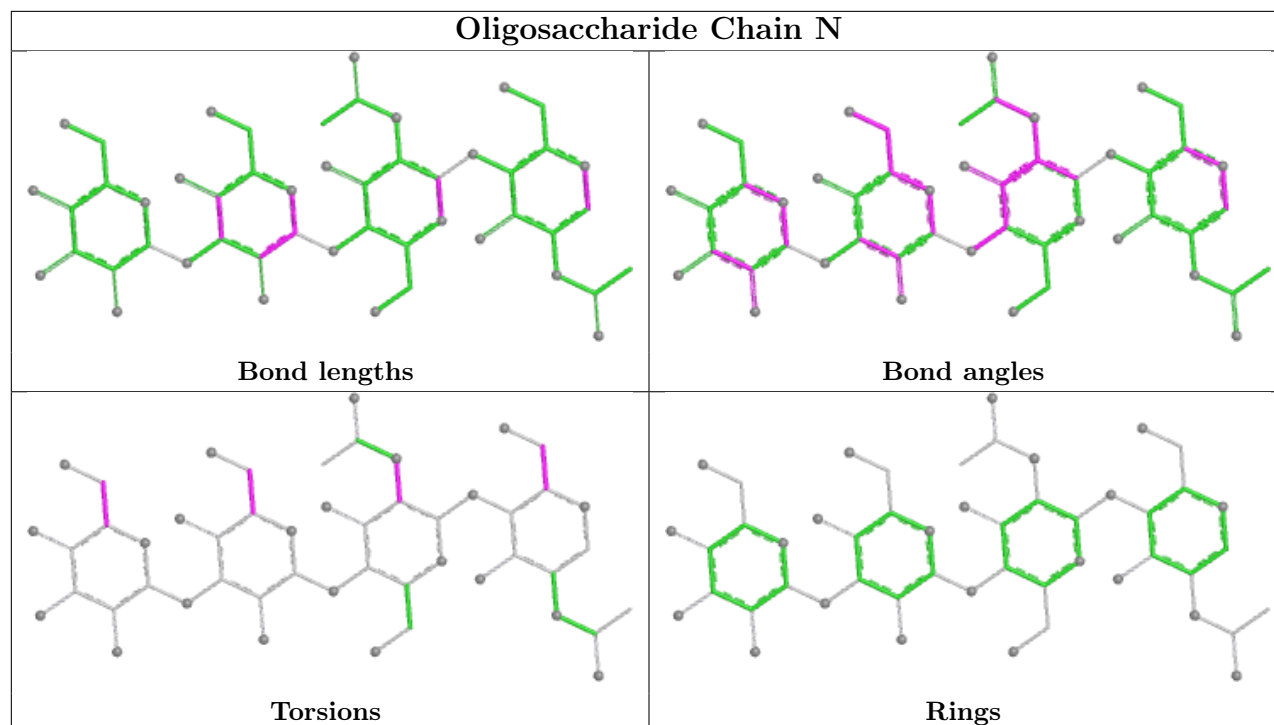




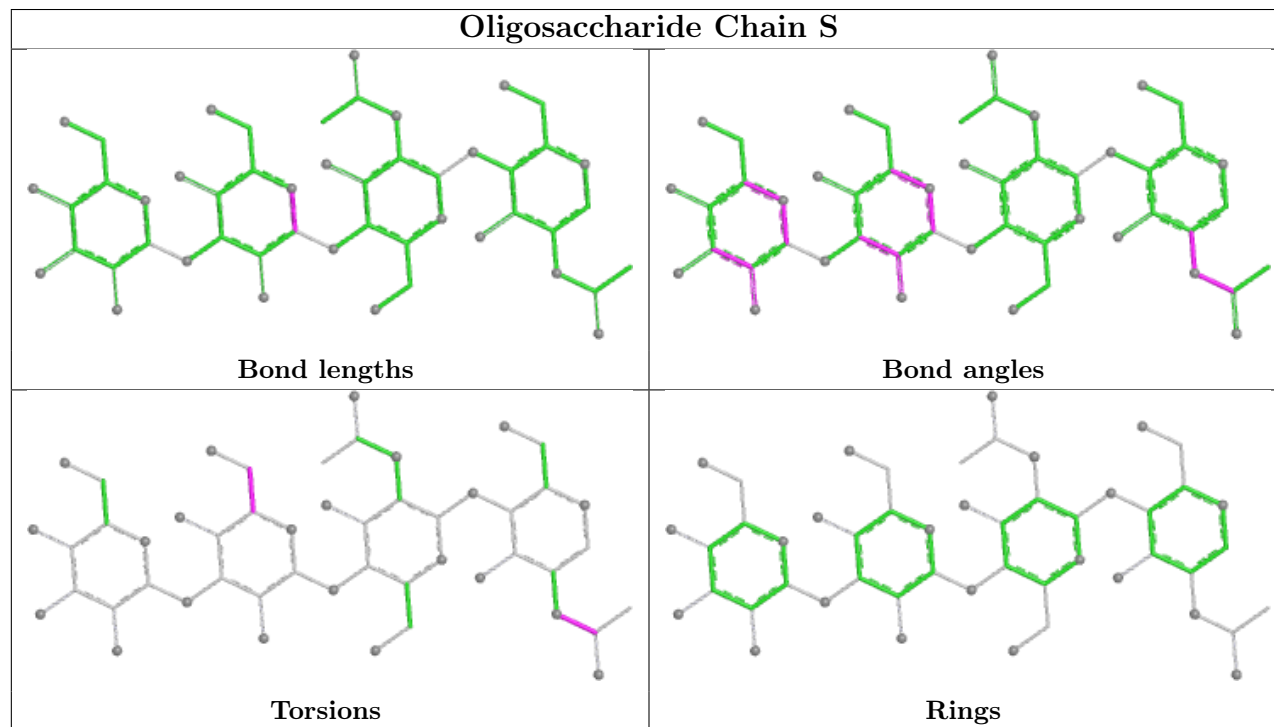


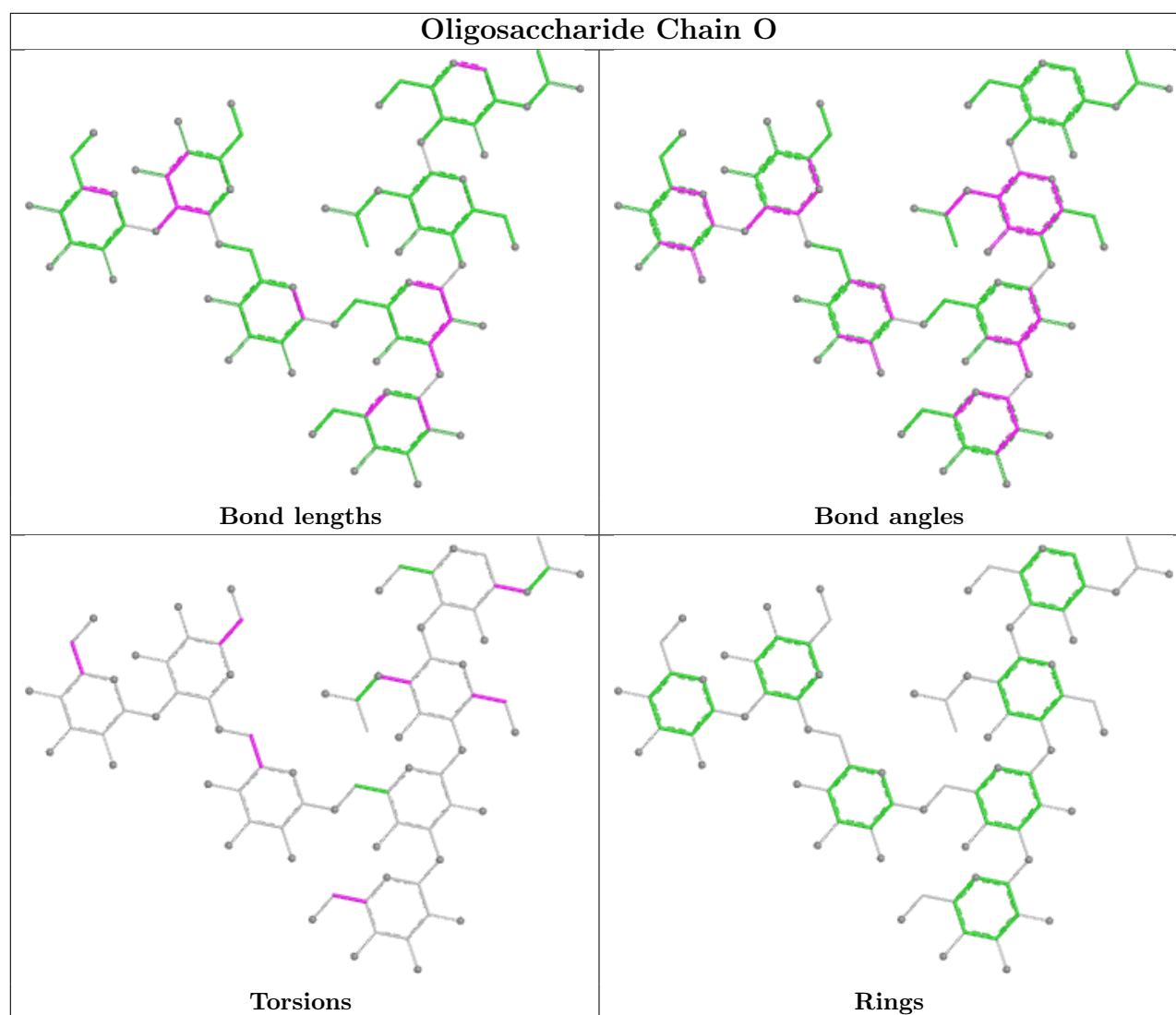


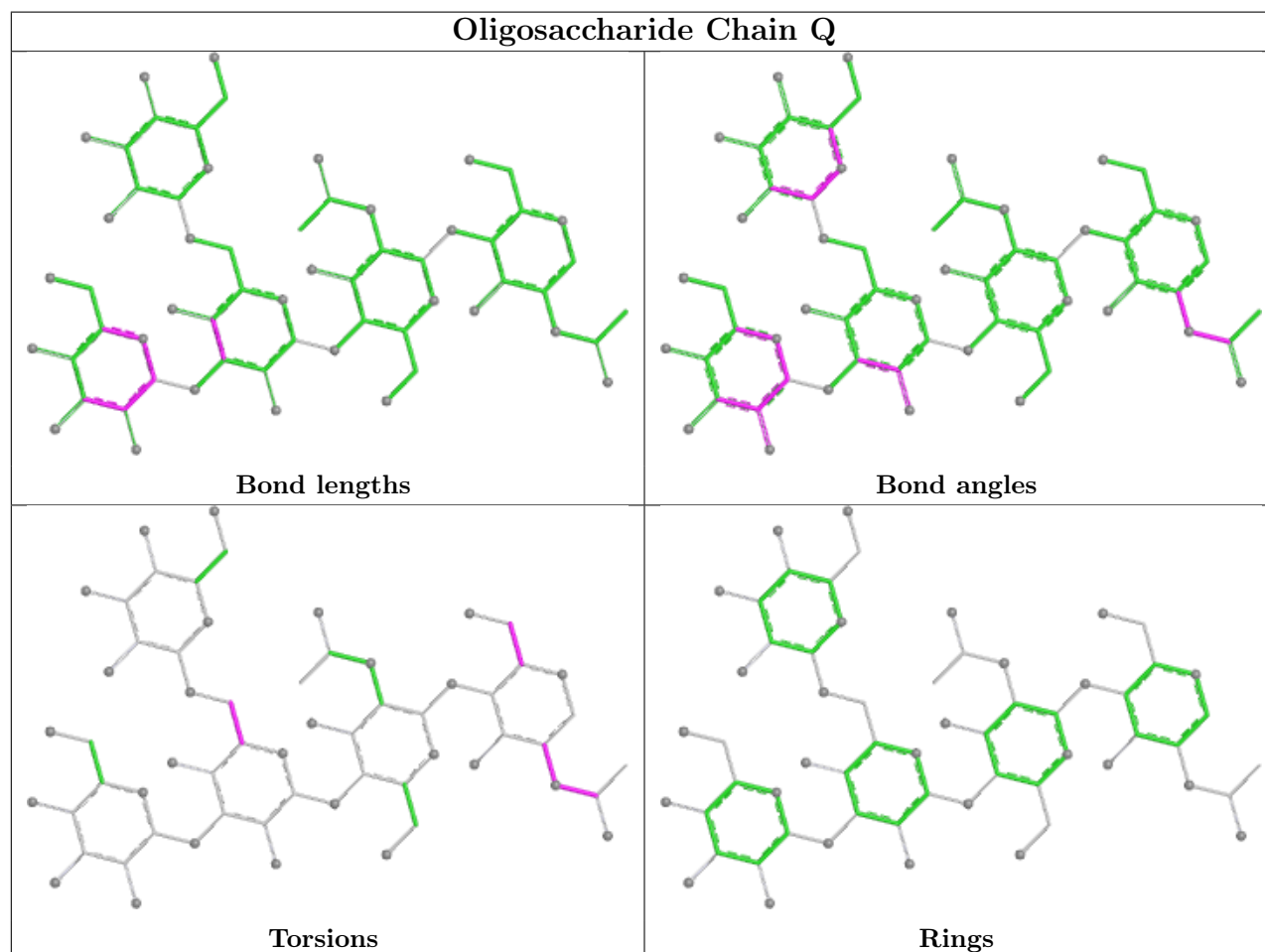
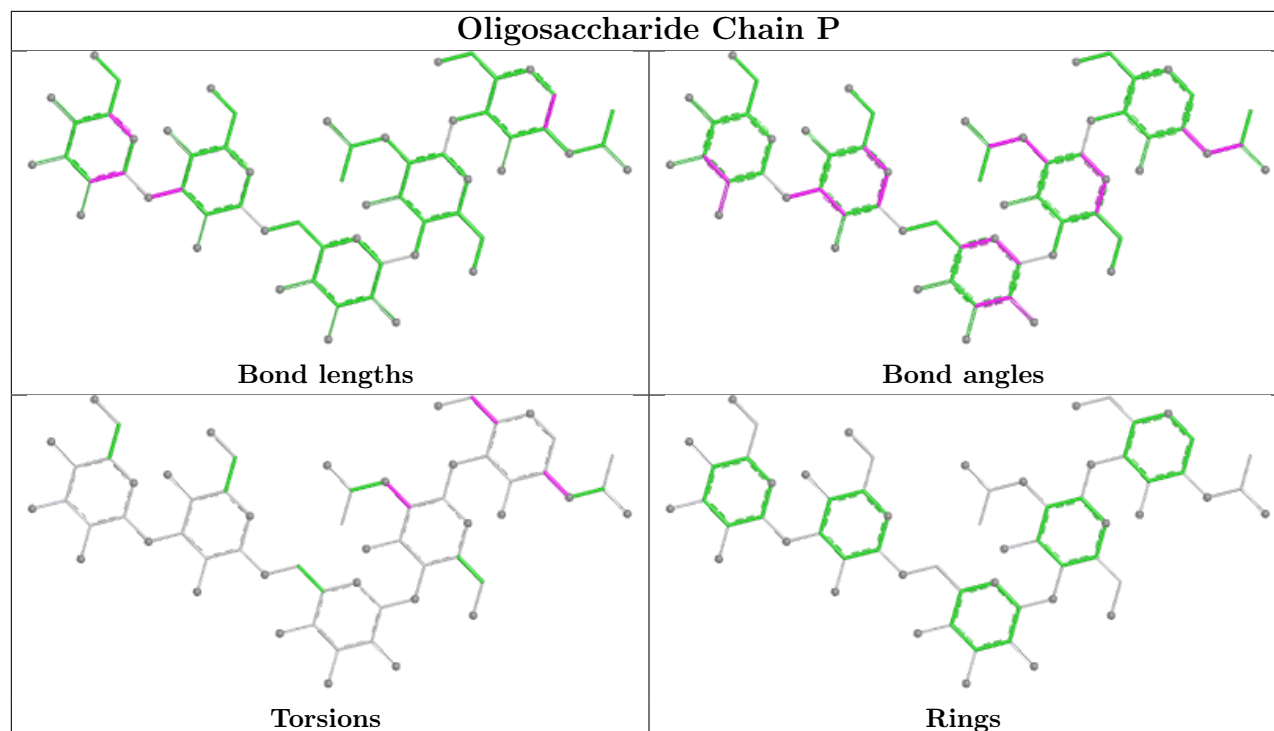
Oligosaccharide Chain N

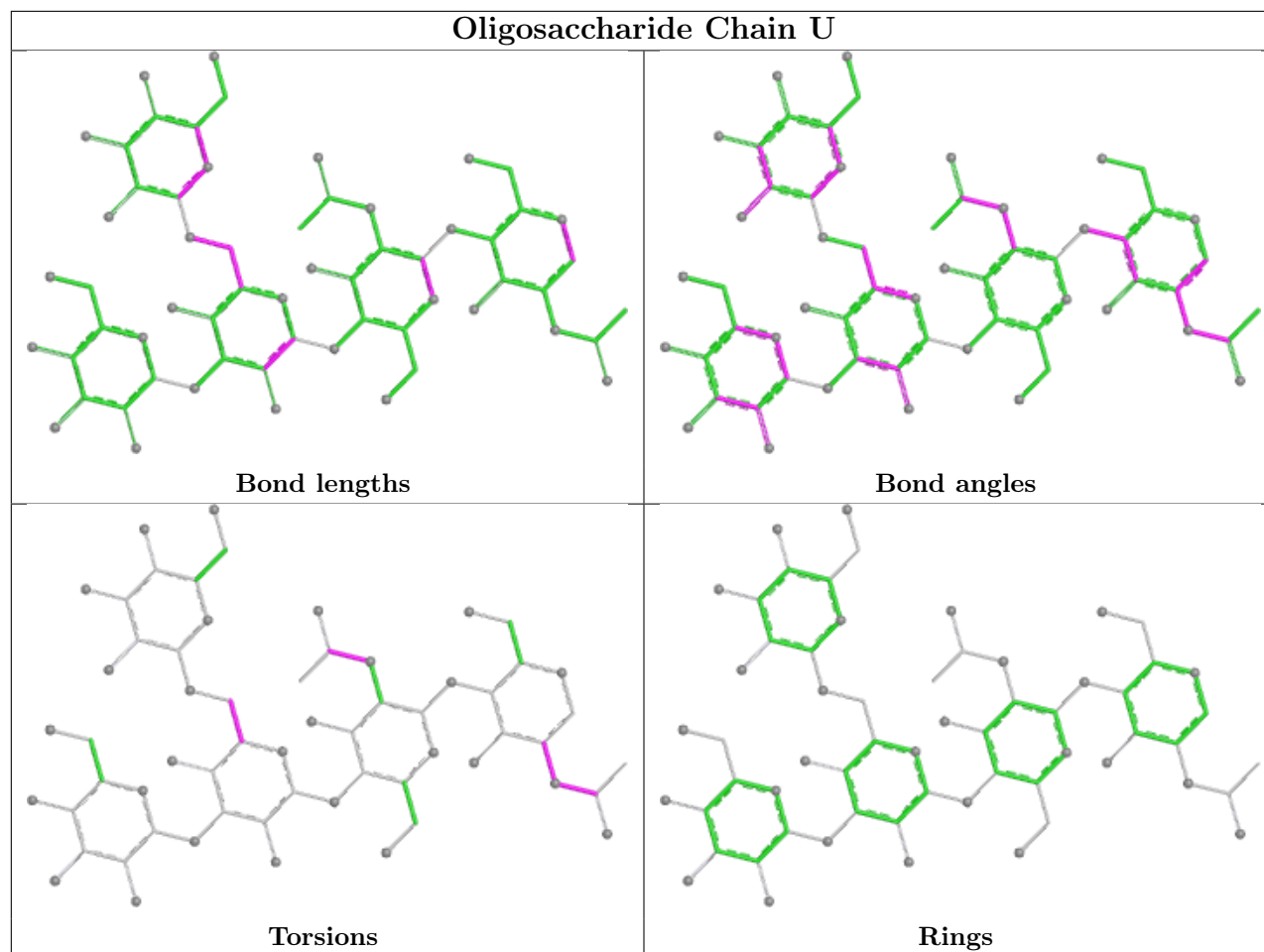


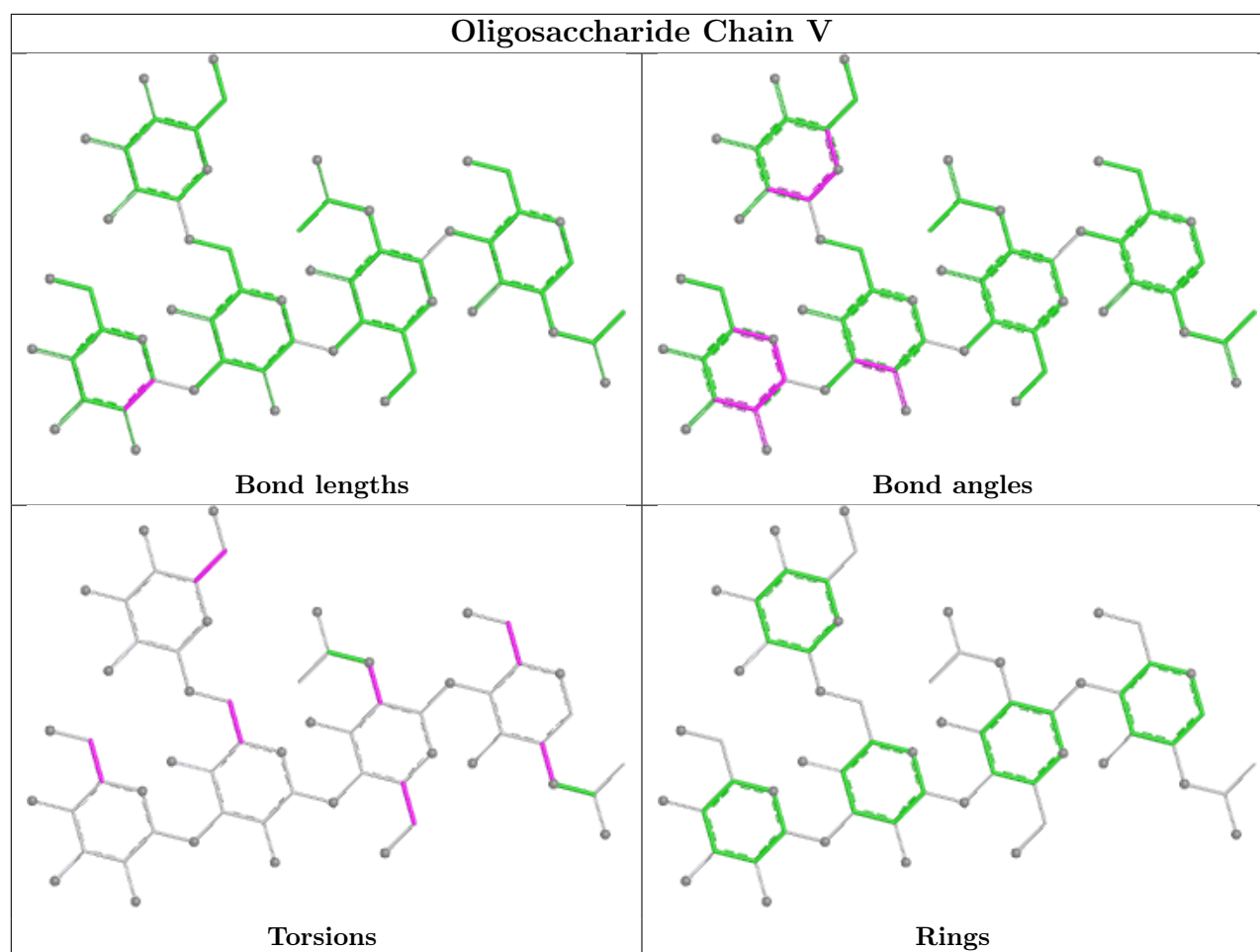
Oligosaccharide Chain S

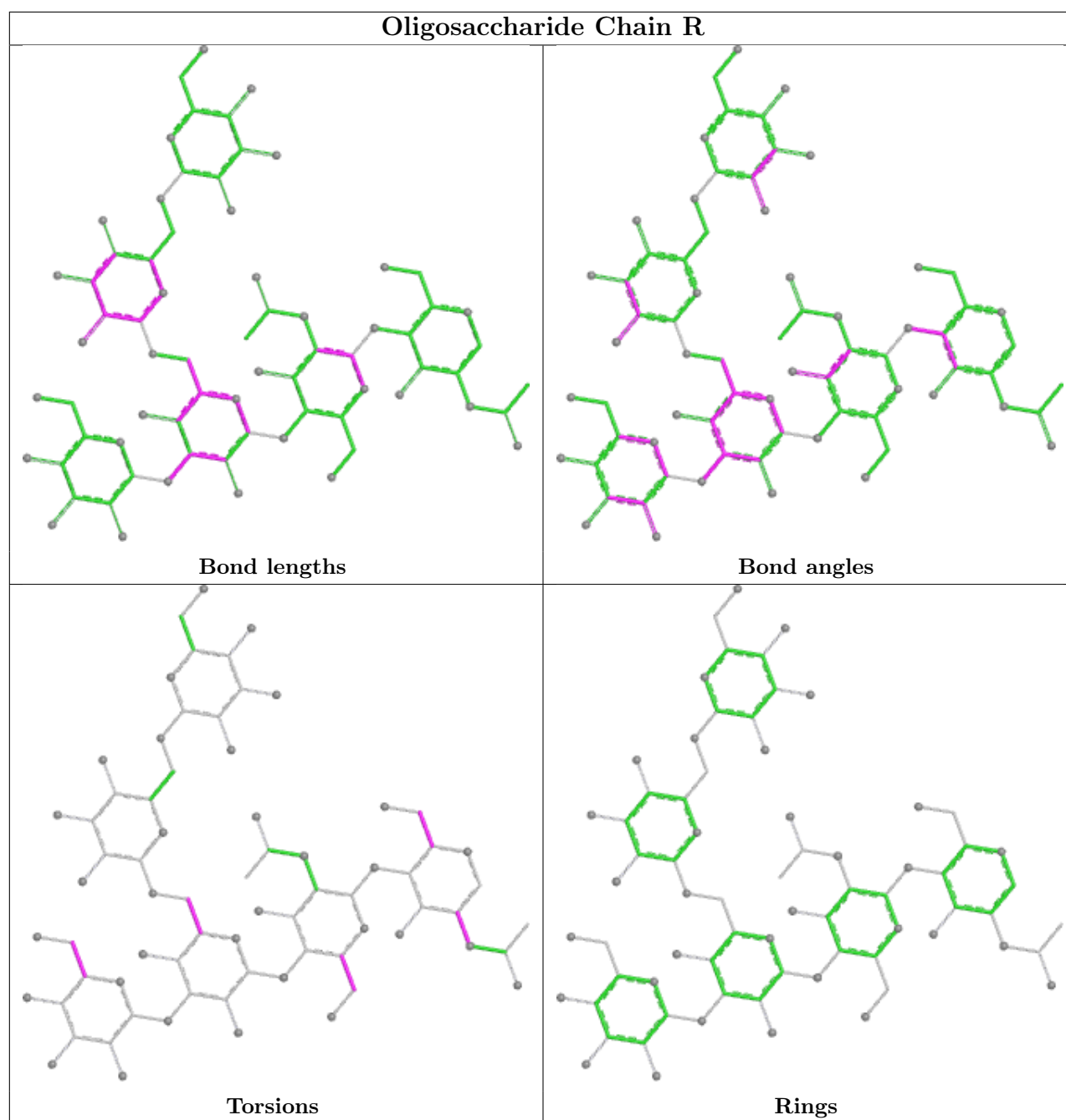


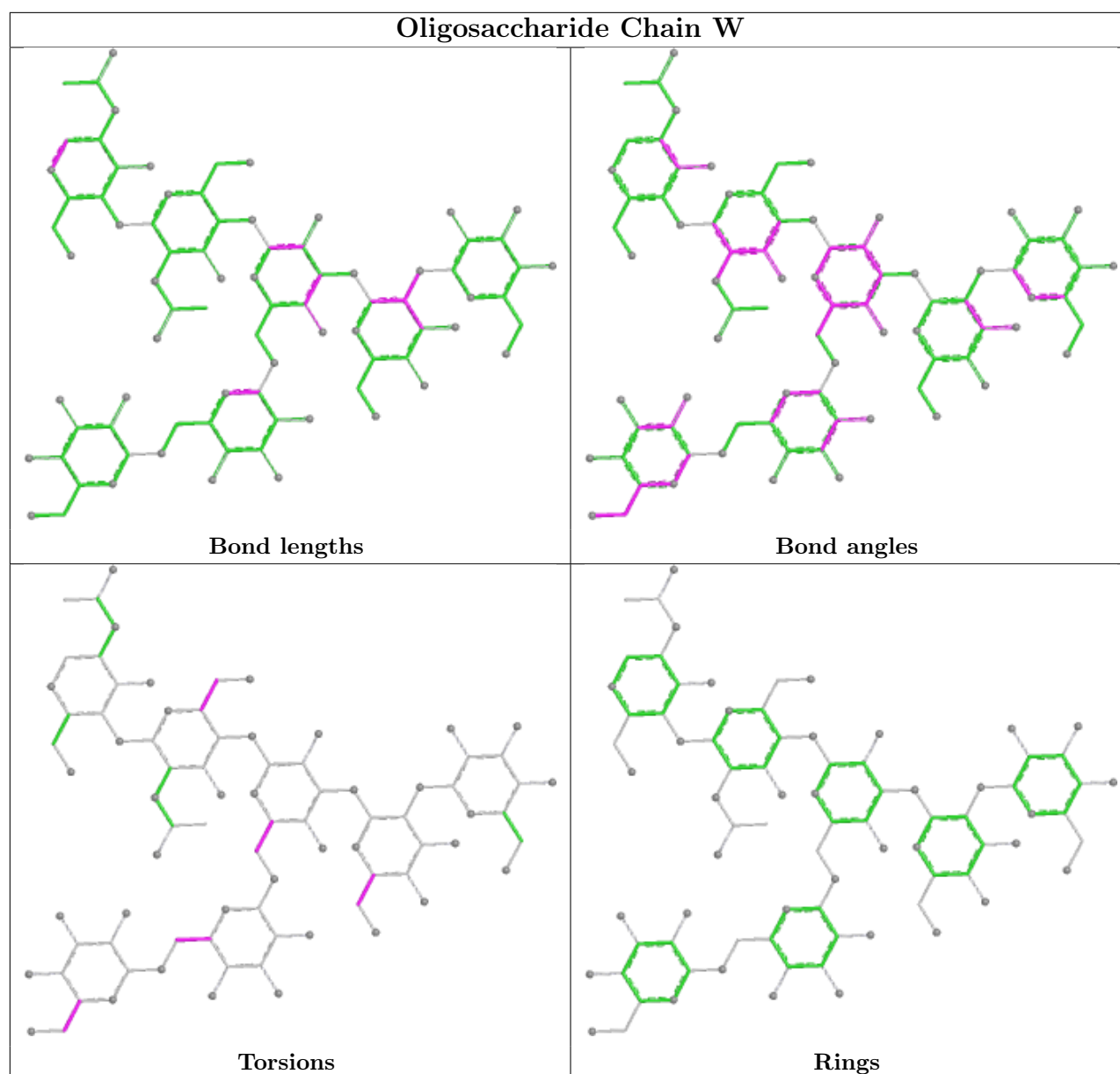


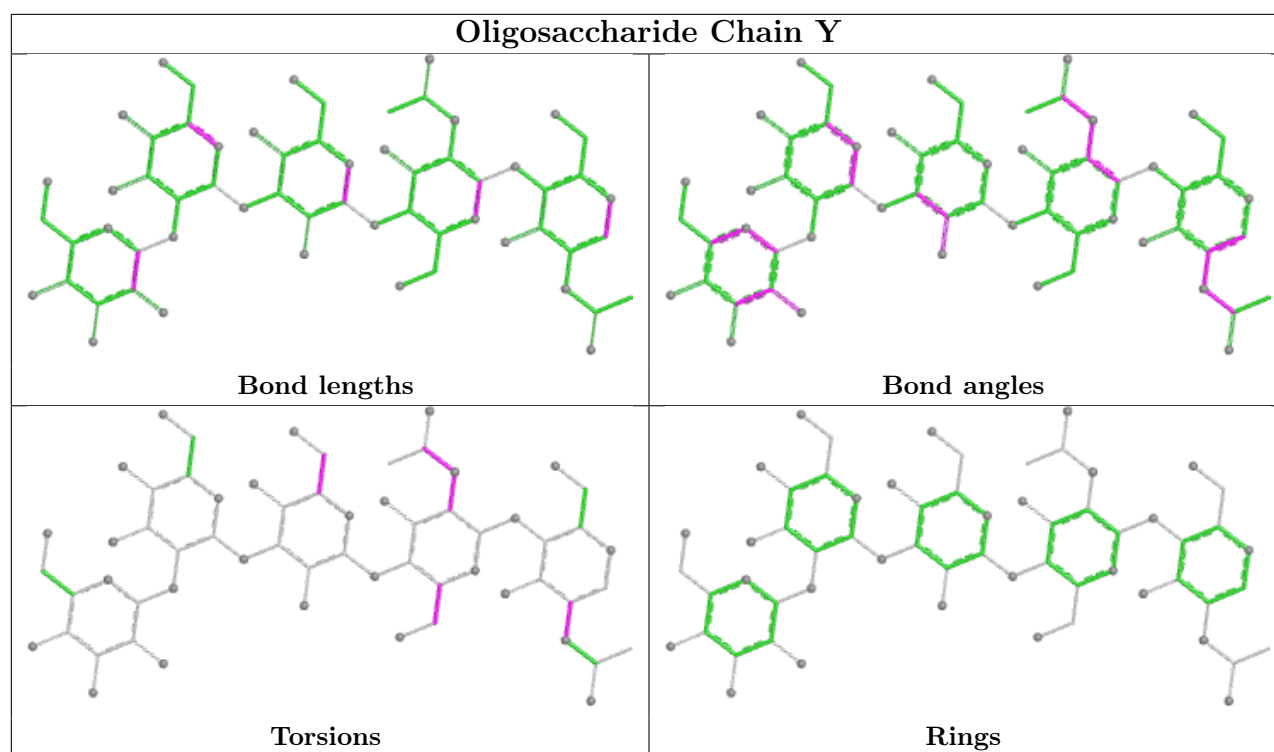












5.6 Ligand geometry [i](#)

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	F	3620	2	14,14,15	0.52	0	17,19,21	0.58	0
17	NAG	E	3042	1	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
17	NAG	A	3031	1	14,14,15	0.26	0	17,19,21	0.54	0
17	NAG	D	3620	2	14,14,15	0.39	0	17,19,21	0.42	0
17	NAG	G	3920	1	14,14,15	0.88	1 (7%)	17,19,21	0.63	0
17	NAG	H	3190	2	14,14,15	1.12	1 (7%)	17,19,21	0.93	1 (5%)
17	NAG	B	3620	2	14,14,15	0.41	0	17,19,21	0.51	0
17	NAG	C	3042	1	14,14,15	1.12	2 (14%)	17,19,21	0.49	0
17	NAG	A	3678	1	14,14,15	0.67	1 (7%)	17,19,21	0.65	0
17	NAG	F	3190	2	14,14,15	0.35	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	A	3042	1	14,14,15	0.73	1 (7%)	17,19,21	1.47	2 (11%)
17	NAG	C	3920	1	14,14,15	0.79	1 (7%)	17,19,21	0.81	0
17	NAG	H	3620	2	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
17	NAG	G	3042	1	14,14,15	0.86	1 (7%)	17,19,21	0.60	0
17	NAG	H	3094	2	14,14,15	0.54	0	17,19,21	0.43	0
17	NAG	A	3920	1	14,14,15	0.80	1 (7%)	17,19,21	0.53	0
17	NAG	E	3031	1	14,14,15	0.31	0	17,19,21	0.44	0
17	NAG	E	3920	1	14,14,15	0.74	1 (7%)	17,19,21	4.05	3 (17%)
17	NAG	G	3031	1	14,14,15	0.34	0	17,19,21	0.57	0
17	NAG	F	3094	2	14,14,15	0.46	0	17,19,21	0.61	0
17	NAG	D	3232	2	14,14,15	0.90	1 (7%)	17,19,21	0.85	1 (5%)
17	NAG	C	3678	1	14,14,15	0.84	1 (7%)	17,19,21	1.39	2 (11%)
17	NAG	E	3678	1	14,14,15	0.35	0	17,19,21	1.15	1 (5%)
17	NAG	C	3031	1	14,14,15	0.28	0	17,19,21	0.56	0
17	NAG	G	3678	1	14,14,15	0.70	1 (7%)	17,19,21	0.65	0
17	NAG	B	3232	2	14,14,15	1.00	1 (7%)	17,19,21	1.77	2 (11%)
17	NAG	H	3232	2	14,14,15	0.87	1 (7%)	17,19,21	2.60	3 (17%)

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	F	3620	2	-	2/6/23/26	0/1/1/1
17	NAG	E	3042	1	-	3/6/23/26	0/1/1/1
17	NAG	A	3031	1	-	2/6/23/26	0/1/1/1
17	NAG	D	3620	2	-	1/6/23/26	0/1/1/1
17	NAG	G	3920	1	-	2/6/23/26	0/1/1/1
17	NAG	H	3190	2	-	2/6/23/26	0/1/1/1
17	NAG	B	3620	2	-	2/6/23/26	0/1/1/1
17	NAG	C	3042	1	-	3/6/23/26	0/1/1/1
17	NAG	A	3678	1	-	3/6/23/26	0/1/1/1
17	NAG	F	3190	2	-	2/6/23/26	0/1/1/1
17	NAG	A	3042	1	-	1/6/23/26	0/1/1/1
17	NAG	C	3920	1	-	1/6/23/26	0/1/1/1
17	NAG	H	3620	2	-	2/6/23/26	0/1/1/1

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	3190	NAG	O5-C1	-4.00	1.37	1.43
17	C	3042	NAG	C1-C2	3.35	1.56	1.52
17	B	3232	NAG	O5-C1	-3.24	1.38	1.43
17	G	3042	NAG	C1-C2	3.09	1.56	1.52
17	D	3232	NAG	C1-C2	3.08	1.56	1.52
17	G	3920	NAG	O5-C1	-3.02	1.38	1.43
17	A	3920	NAG	C1-C2	2.63	1.55	1.52
17	H	3232	NAG	O5-C1	2.58	1.48	1.43
17	G	3678	NAG	O5-C1	-2.55	1.39	1.43
17	A	3678	NAG	O5-C1	-2.44	1.39	1.43
17	C	3920	NAG	C1-C2	2.35	1.55	1.52
17	C	3678	NAG	C1-C2	2.33	1.55	1.52
17	A	3042	NAG	O5-C1	2.30	1.47	1.43
17	C	3042	NAG	O5-C1	2.21	1.47	1.43
17	E	3920	NAG	O5-C1	2.20	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	3920	NAG	C1-O5-C5	11.12	127.09	112.19
17	E	3920	NAG	C2-N2-C7	10.42	136.87	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	3232	NAG	C2-N2-C7	7.84	133.41	122.90
17	E	3920	NAG	C1-C2-N2	5.68	119.39	110.43
17	B	3232	NAG	C1-O5-C5	-5.47	104.85	112.19
17	A	3042	NAG	C2-N2-C7	5.18	129.84	122.90
17	H	3232	NAG	C1-O5-C5	4.50	118.21	112.19
17	H	3232	NAG	C1-C2-N2	4.45	117.44	110.43
17	E	3678	NAG	C1-O5-C5	4.28	117.92	112.19
17	C	3678	NAG	C1-O5-C5	3.96	117.49	112.19
17	F	3190	NAG	C1-O5-C5	3.64	117.06	112.19
17	B	3232	NAG	C2-N2-C7	3.22	127.22	122.90
17	C	3678	NAG	C2-N2-C7	2.71	126.54	122.90
17	H	3620	NAG	C1-O5-C5	2.57	115.63	112.19
17	H	3190	NAG	C1-O5-C5	2.37	115.36	112.19
17	D	3232	NAG	C1-O5-C5	-2.20	109.24	112.19
17	E	3042	NAG	C1-O5-C5	2.12	115.03	112.19
17	A	3042	NAG	C1-C2-N2	2.04	113.64	110.43

There are no chirality outliers.

All (56) 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	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	A	3031	NAG	C4-C5-C6-O6
17	E	3678	NAG	C4-C5-C6-O6
17	C	3031	NAG	C4-C5-C6-O6
17	A	3678	NAG	O5-C5-C6-O6
17	H	3190	NAG	C4-C5-C6-O6
17	F	3190	NAG	O5-C5-C6-O6
17	H	3620	NAG	O5-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

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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	F	3094	NAG	C4-C5-C6-O6
17	H	3094	NAG	O5-C5-C6-O6
17	B	3620	NAG	O5-C5-C6-O6
17	G	3920	NAG	O5-C5-C6-O6
17	A	3678	NAG	C4-C5-C6-O6
17	F	3094	NAG	O5-C5-C6-O6
17	F	3190	NAG	C4-C5-C6-O6
17	H	3620	NAG	C4-C5-C6-O6
17	D	3620	NAG	O5-C5-C6-O6
17	C	3042	NAG	O5-C5-C6-O6
17	E	3042	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	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	B	3620	NAG	C4-C5-C6-O6
17	A	3678	NAG	C1-C2-N2-C7
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	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.

14 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	3031	NAG	1	0
17	D	3620	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	3920	NAG	2	0
17	C	3042	NAG	1	0
17	C	3920	NAG	5	0
17	G	3042	NAG	3	0
17	H	3094	NAG	1	0
17	A	3920	NAG	2	0
17	E	3031	NAG	1	0
17	E	3920	NAG	1	0
17	F	3094	NAG	1	0
17	D	3232	NAG	1	0
17	C	3031	NAG	1	0
17	H	3232	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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, 95th 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%)	-0.29	5 (0%)	87 76	86, 154, 246, 360	0
1	C	884/1137 (77%)	-0.18	9 (1%)	79 63	72, 184, 288, 417	3 (0%)
1	E	884/1137 (77%)	-0.24	10 (1%)	78 60	64, 163, 267, 405	3 (0%)
1	G	883/1137 (77%)	-0.26	8 (0%)	81 65	82, 148, 255, 387	1 (0%)
2	B	674/727 (92%)	-0.31	4 (0%)	85 73	92, 217, 318, 438	1 (0%)
2	D	674/727 (92%)	-0.21	9 (1%)	75 56	136, 266, 376, 453	0
2	F	674/727 (92%)	-0.32	5 (0%)	84 70	105, 213, 308, 375	1 (0%)
2	H	674/727 (92%)	-0.35	5 (0%)	84 70	101, 222, 327, 434	0
All	All	6427/7456 (86%)	-0.27	55 (0%)	81 65	64, 188, 313, 453	9 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	395[A]	TRP	6.5
2	H	298	PHE	5.8
1	E	643	SER	4.8
1	E	332	MET	4.2
2	D	431	SER	3.6
1	A	651	ASP	3.6
2	B	285	LEU	3.6
2	D	92	ALA	3.4
1	C	398	VAL	3.4
1	A	436	GLY	3.3
2	D	506	LEU	3.3
2	D	285	LEU	3.2
1	C	653	GLN	3.2
1	E	433	THR	3.1
1	E	777	GLY	3.0
1	G	651	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	92	ALA	2.9
1	E	339	ALA	2.8
1	C	919	LEU	2.7
1	G	919	LEU	2.6
1	C	690	LYS	2.6
2	D	650	VAL	2.5
1	E	651	ASP	2.5
1	G	1000	VAL	2.5
2	H	319	ALA	2.4
1	E	669	PRO	2.4
2	F	156	PRO	2.4
2	D	109	TYR	2.3
2	D	144	ILE	2.3
2	B	107	LEU	2.3
1	G	335	GLU	2.3
2	B	314	ILE	2.3
2	F	36[A]	ASP	2.3
1	A	653	GLN	2.3
1	E	398	VAL	2.3
2	H	206	GLY	2.2
1	G	478	LEU	2.2
1	A	894	THR	2.2
2	D	654	LEU	2.2
1	C	650	ARG	2.2
2	H	415	VAL	2.2
1	G	379	VAL	2.2
2	F	314	ILE	2.2
1	G	699	LEU	2.1
2	D	505	LYS	2.1
2	B	395	ALA	2.1
1	E	352	GLY	2.1
2	F	599	PRO	2.1
1	C	357	SER	2.1
1	C	729	ASN	2.1
1	C	724	LEU	2.1
1	A	386	LEU	2.1
1	C	850	ILE	2.1
1	E	674	GLN	2.0
2	H	245	PHE	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, 95th 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($\text{\AA}^2$)	Q<0.9
14	BMA	Y	3	11/12	-0.08	0.11	261,315,353,371	0
11	MAN	V	5	11/12	-0.03	0.08	237,293,323,332	0
8	MAN	S	4	11/12	-0.02	0.08	269,325,347,348	0
8	BMA	N	3	11/12	-0.01	0.08	297,334,341,350	0
9	MAN	O	6	11/12	0.03	0.10	274,292,298,299	0
10	BMA	P	3	11/12	0.04	0.08	305,318,338,338	0
11	NAG	Q	2	14/15	0.06	0.10	261,295,308,310	0
10	MAN	P	4	11/12	0.09	0.09	287,306,320,322	0
3	MAN	I	5	11/12	0.14	0.08	261,289,311,344	0
11	MAN	U	5	11/12	0.16	0.08	200,226,241,242	0
11	MAN	Q	5	11/12	0.19	0.12	249,281,295,299	0
5	NAG	X	2	14/15	0.19	0.09	260,287,322,339	0
4	MAN	J	10	11/12	0.21	0.06	280,311,318,330	0
11	BMA	U	3	11/12	0.23	0.07	260,320,325,331	0
6	BMA	L	3	11/12	0.24	0.07	252,306,330,335	0
8	MAN	N	4	11/12	0.24	0.06	251,320,334,336	0
7	NAG	M	2	14/15	0.24	0.06	273,334,340,343	0
4	MAN	J	9	11/12	0.26	0.09	263,300,333,333	0
8	NAG	N	2	14/15	0.30	0.10	219,269,303,323	0
12	BMA	R	3	11/12	0.32	0.07	274,304,315,326	0
12	MAN	R	6	11/12	0.33	0.08	230,277,297,301	0
9	NAG	O	2	14/15	0.33	0.09	229,298,329,346	0
9	MAN	O	5	11/12	0.34	0.08	273,287,297,298	0
11	BMA	V	3	11/12	0.37	0.07	310,323,330,334	0
13	MAN	W	7	11/12	0.38	0.08	230,289,305,305	0
9	MAN	O	7	11/12	0.38	0.07	317,336,352,359	0
14	NAG	Y	2	14/15	0.39	0.10	239,315,332,345	0
12	MAN	R	5	11/12	0.39	0.07	214,236,249,250	0
8	BMA	S	3	11/12	0.40	0.07	320,330,340,343	0
11	MAN	V	4	11/12	0.41	0.06	263,276,302,308	0
5	BMA	K	3	11/12	0.41	0.07	313,322,328,341	0
4	BMA	J	3	11/12	0.42	0.10	260,272,289,292	0

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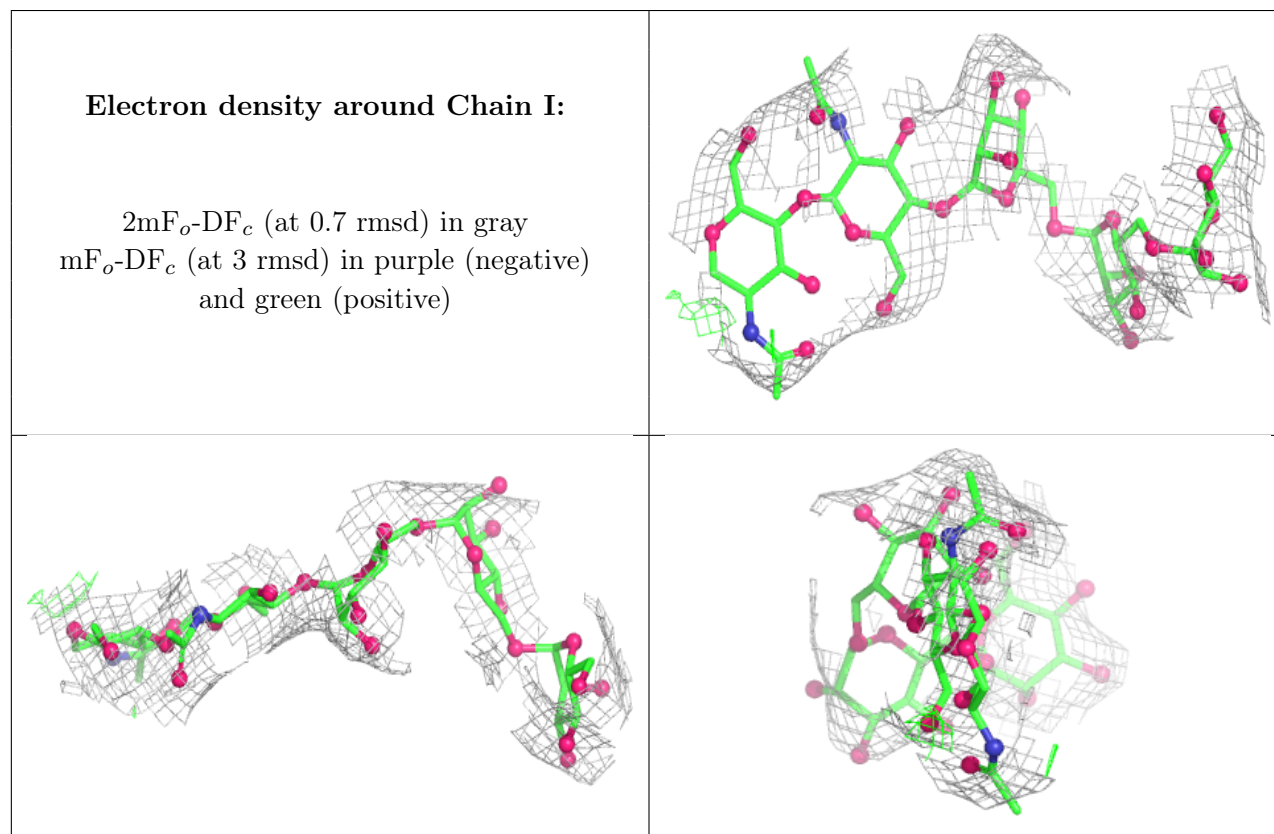
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	J	6	11/12	0.42	0.09	219,247,260,292	0
13	MAN	W	5	11/12	0.45	0.07	307,322,345,358	0
5	BMA	X	3	11/12	0.46	0.07	337,345,352,353	0
5	BMA	T	3	11/12	0.46	0.08	329,335,342,344	0
12	MAN	R	4	11/12	0.46	0.07	243,252,266,272	0
3	BMA	I	3	11/12	0.47	0.07	291,299,315,325	0
9	BMA	O	3	11/12	0.47	0.07	336,352,372,394	0
11	MAN	Q	4	11/12	0.48	0.08	205,224,243,264	0
13	BMA	W	3	11/12	0.48	0.07	328,334,347,350	0
11	BMA	Q	3	11/12	0.48	0.06	287,305,328,361	0
4	MAN	J	7	11/12	0.50	0.09	309,311,326,327	0
4	MAN	J	8	11/12	0.51	0.07	308,325,333,336	0
8	NAG	N	1	14/15	0.51	0.11	220,240,264,265	0
6	NAG	L	2	14/15	0.52	0.09	225,301,319,329	0
3	MAN	I	4	11/12	0.52	0.07	282,287,289,290	0
14	MAN	Y	4	11/12	0.53	0.07	217,278,294,299	0
9	NAG	O	1	14/15	0.54	0.12	257,282,326,328	0
9	MAN	O	4	11/12	0.54	0.10	288,304,311,317	0
5	MAN	K	4	11/12	0.56	0.06	265,290,297,302	0
13	MAN	W	6	11/12	0.60	0.07	309,319,344,347	0
10	MAN	P	5	11/12	0.65	0.07	186,218,245,252	0
11	NAG	U	2	14/15	0.65	0.11	285,304,339,371	0
12	NAG	R	2	14/15	0.66	0.09	219,262,289,297	0
11	MAN	U	4	11/12	0.67	0.08	246,284,314,321	0
5	NAG	K	2	14/15	0.68	0.07	271,296,314,323	0
4	MAN	J	5	11/12	0.69	0.10	269,291,305,306	0
7	NAG	M	1	14/15	0.69	0.09	252,275,300,325	0
5	MAN	X	4	11/12	0.70	0.06	270,309,322,327	0
8	NAG	S	2	14/15	0.71	0.07	233,292,313,337	0
13	MAN	W	4	11/12	0.71	0.07	346,370,378,391	0
14	MAN	Y	5	11/12	0.71	0.06	178,213,255,260	0
12	NAG	R	1	14/15	0.72	0.09	212,243,256,277	0
5	MAN	T	4	11/12	0.74	0.06	268,299,311,315	0
6	NAG	L	1	14/15	0.76	0.13	213,237,268,301	0
5	NAG	T	2	14/15	0.76	0.07	233,281,330,342	0
5	NAG	X	1	14/15	0.77	0.09	130,217,244,263	0
3	NAG	I	2	14/15	0.77	0.08	201,244,258,278	0
10	NAG	P	2	14/15	0.78	0.08	276,297,343,352	0
4	NAG	J	2	14/15	0.78	0.08	230,288,304,324	0
11	NAG	V	2	14/15	0.78	0.08	225,265,287,289	0
13	NAG	W	2	14/15	0.79	0.07	242,271,298,315	0
11	NAG	U	1	14/15	0.79	0.13	194,219,246,273	0

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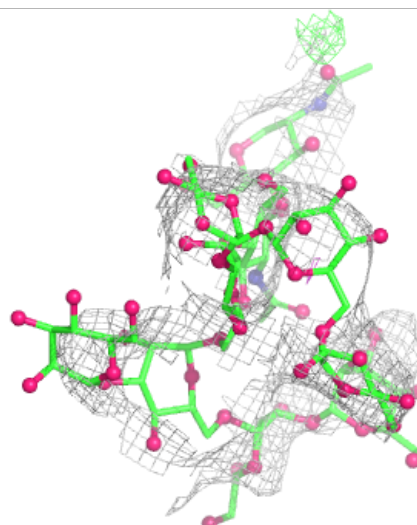
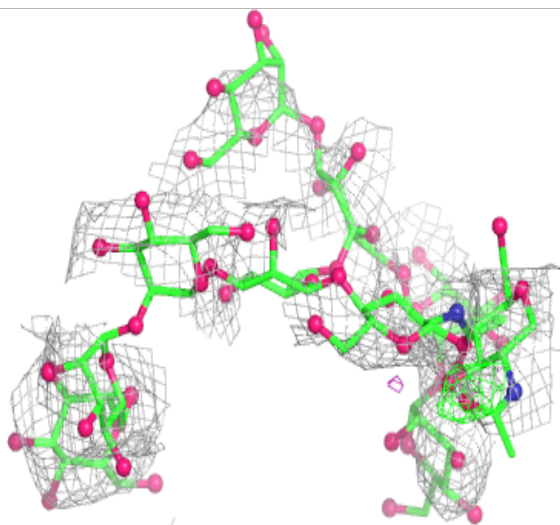
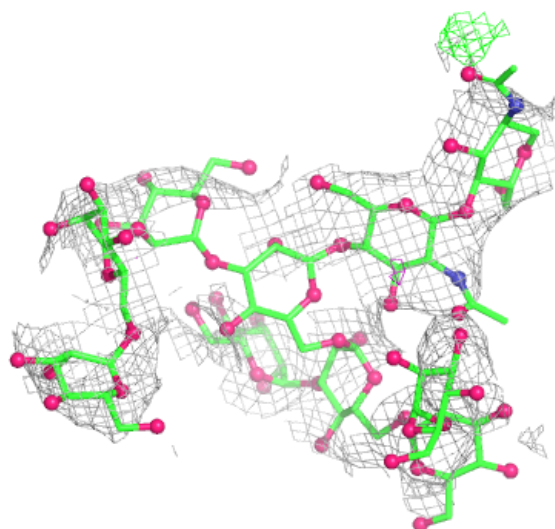
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	K	1	14/15	0.82	0.07	105,177,205,238	0
10	NAG	P	1	14/15	0.83	0.07	116,173,218,249	0
14	NAG	Y	1	14/15	0.83	0.14	162,214,255,297	0
11	NAG	Q	1	14/15	0.84	0.14	167,216,284,298	0
13	NAG	W	1	14/15	0.85	0.08	253,265,294,302	0
4	NAG	J	1	14/15	0.85	0.11	214,248,299,302	0
4	MAN	J	4	11/12	0.86	0.07	253,283,295,302	0
3	NAG	I	1	14/15	0.88	0.11	182,238,254,256	0
11	NAG	V	1	14/15	0.90	0.10	208,268,306,312	0
8	NAG	S	1	14/15	0.91	0.08	222,248,291,302	0
5	NAG	T	1	14/15	0.93	0.08	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.



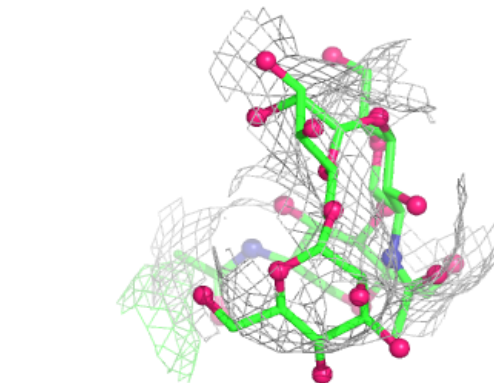
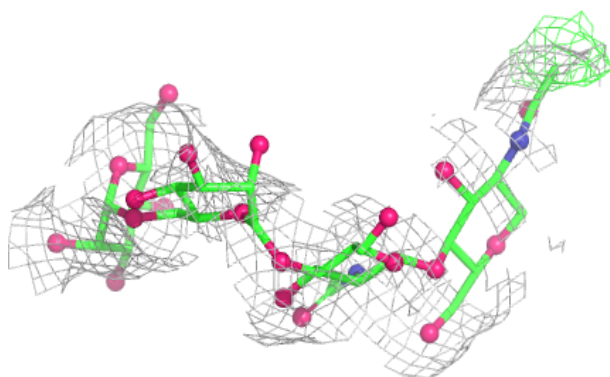
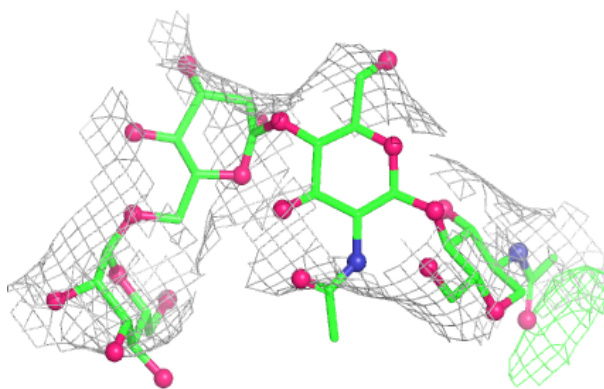
Electron density around Chain J:

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

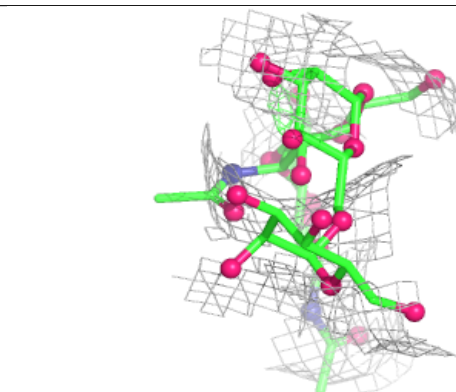
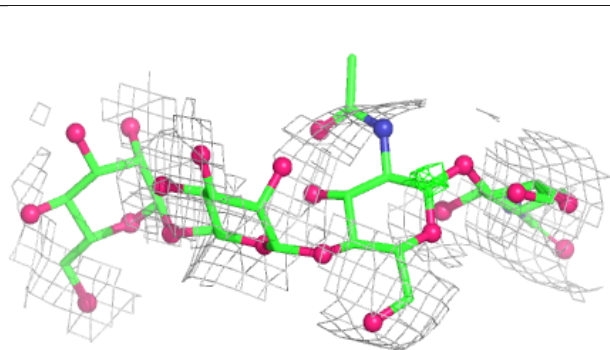
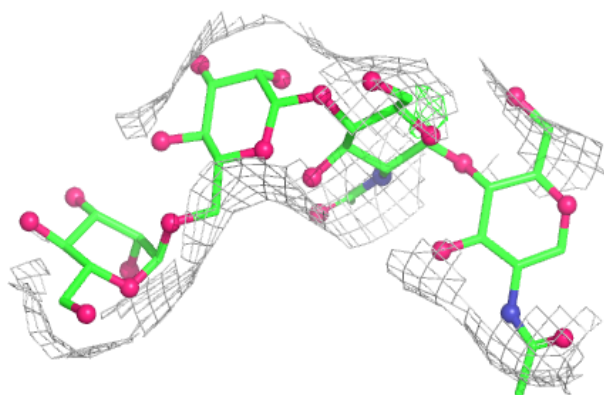


Electron density around Chain K:

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

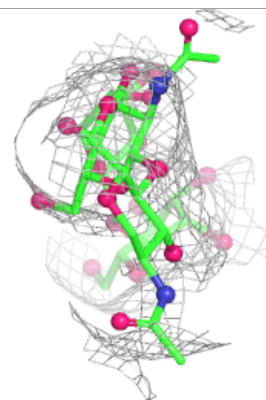
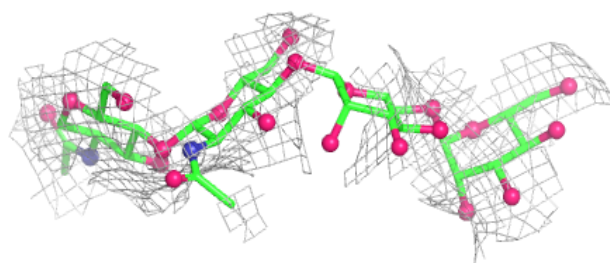
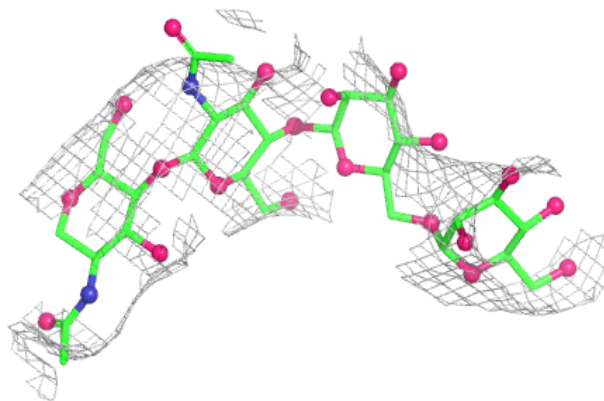
**Electron density around Chain T:**

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

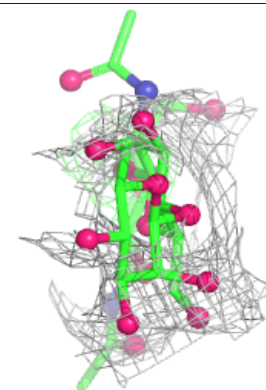
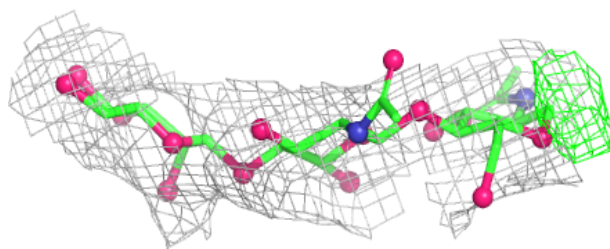
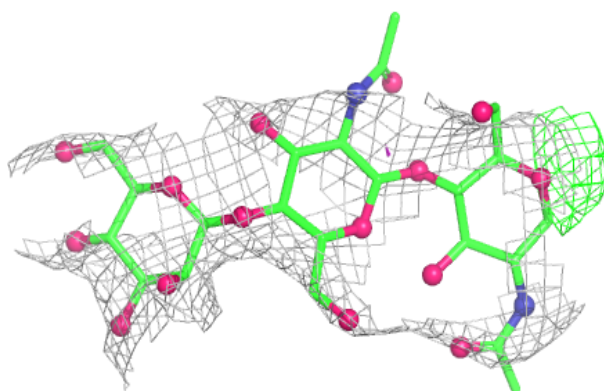


Electron density around Chain X:

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

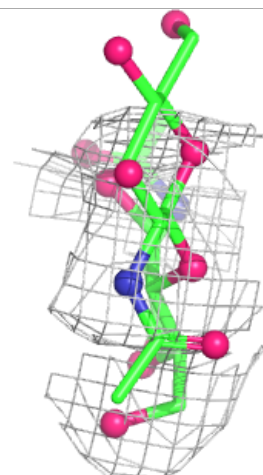
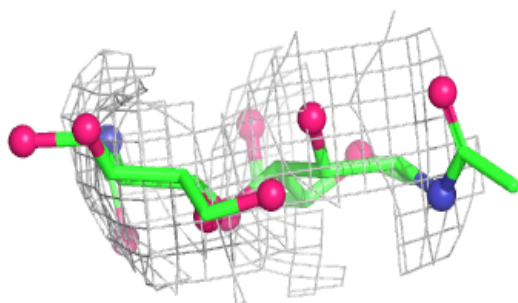
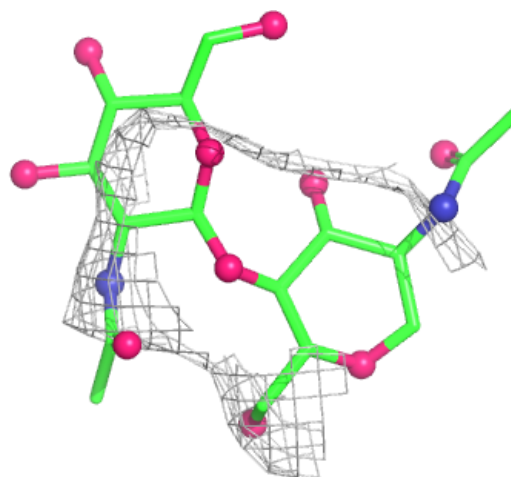
**Electron density around Chain L:**

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



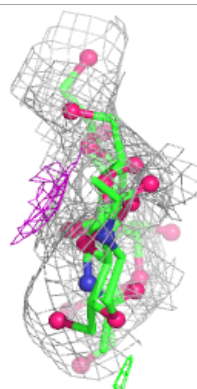
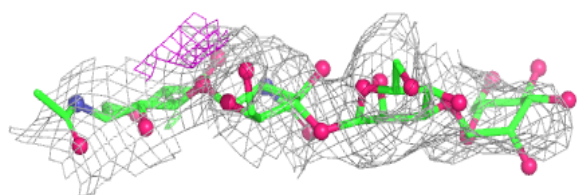
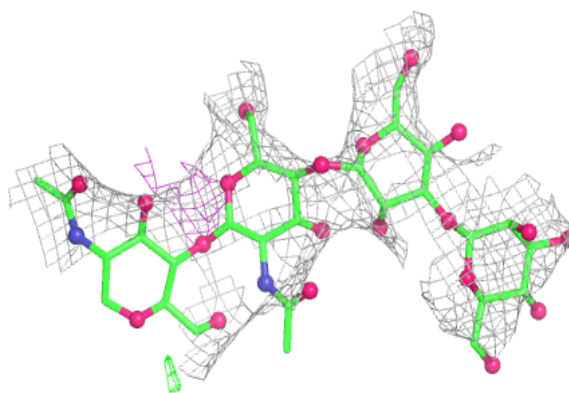
Electron density around Chain M:

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

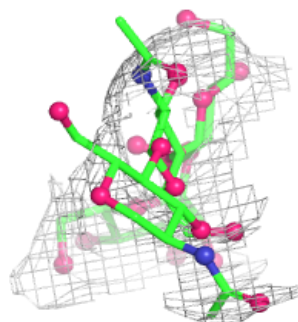
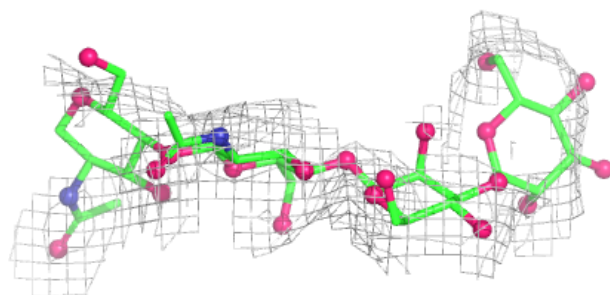
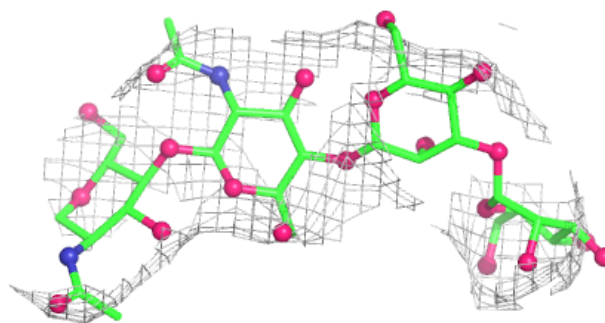


Electron density around Chain N:

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

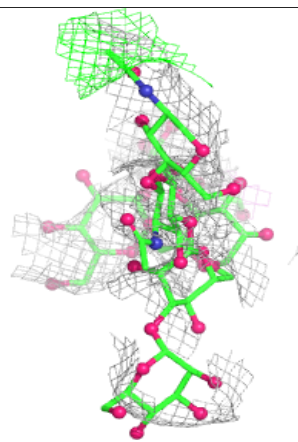
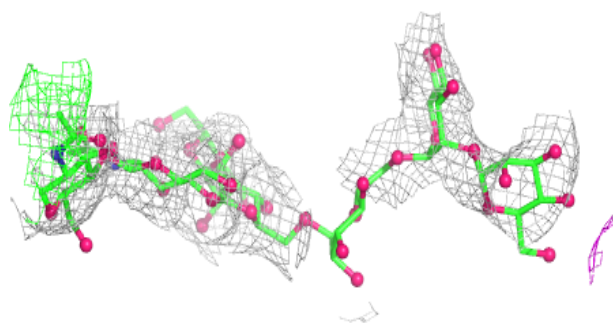
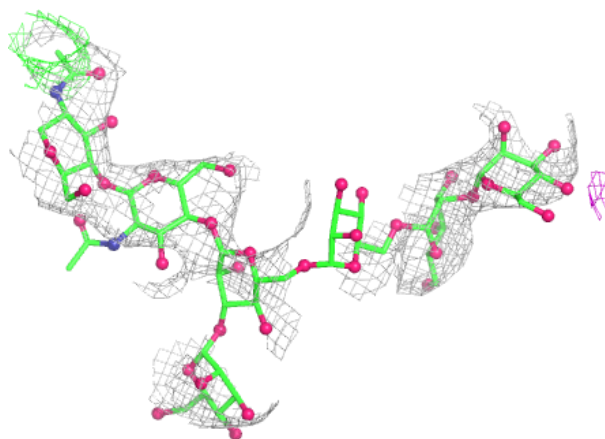
**Electron density around Chain S:**

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



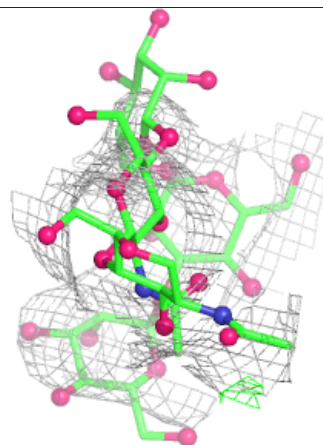
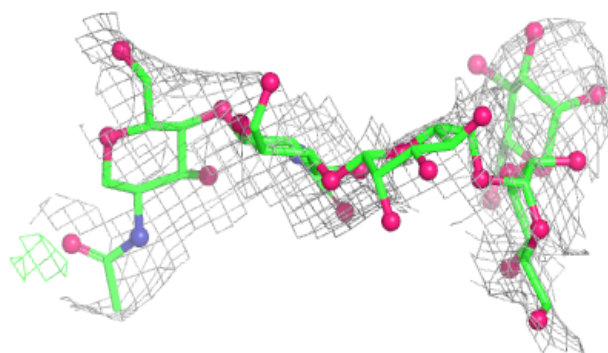
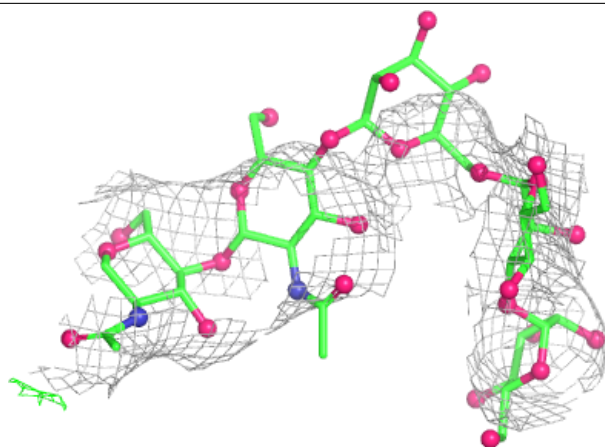
Electron density around Chain O:

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



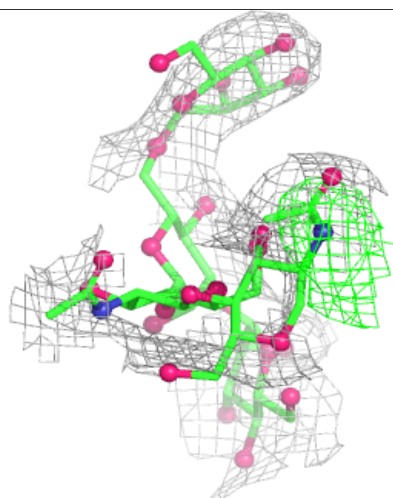
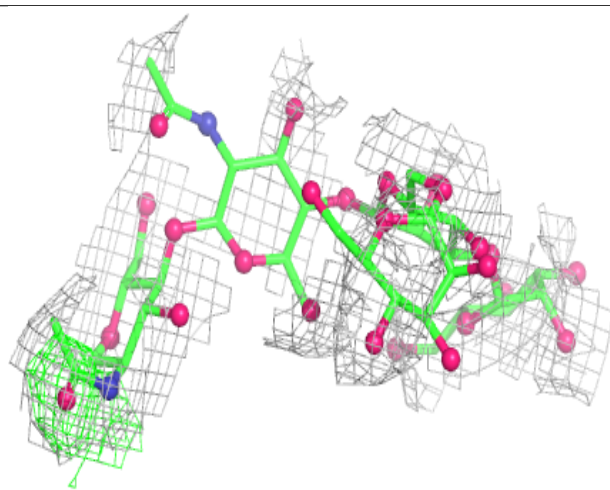
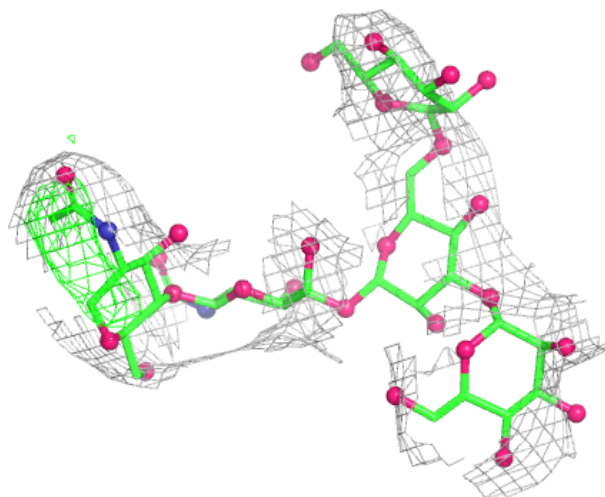
Electron density around Chain P:

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



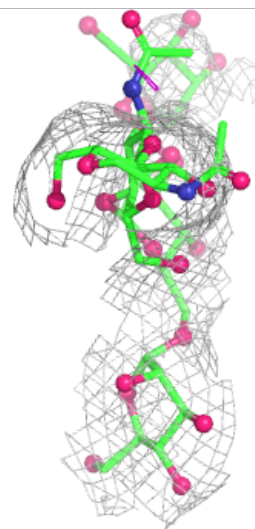
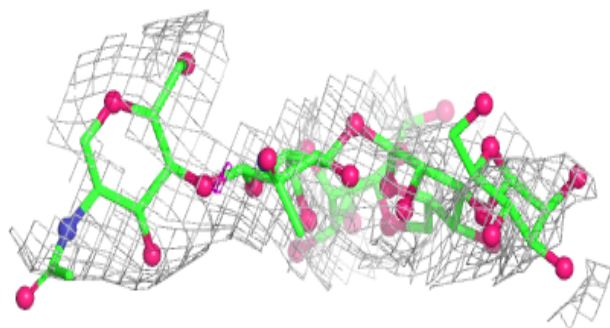
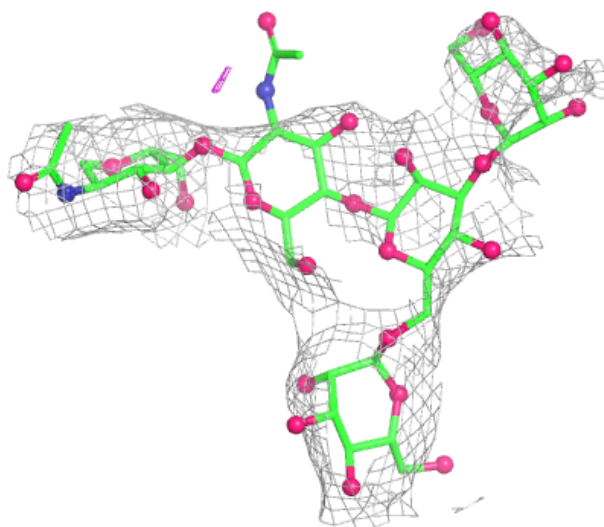
Electron density around Chain Q:

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



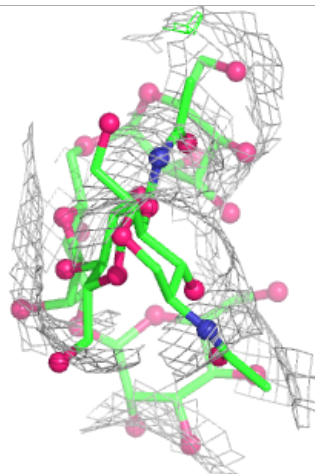
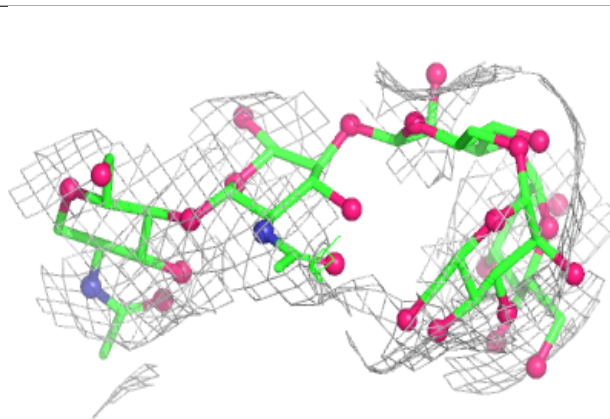
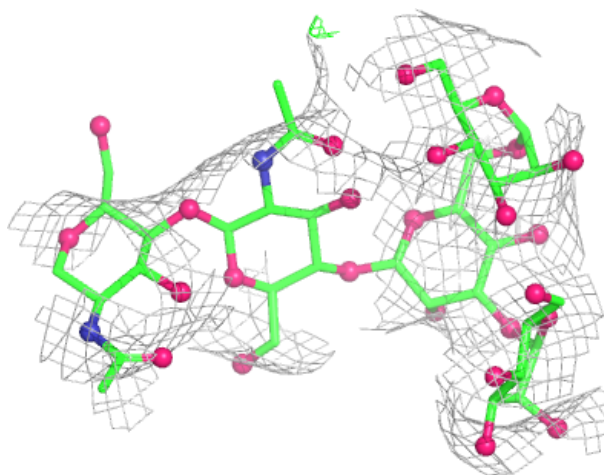
Electron density around Chain U:

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



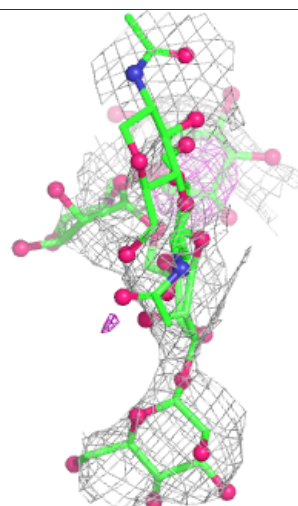
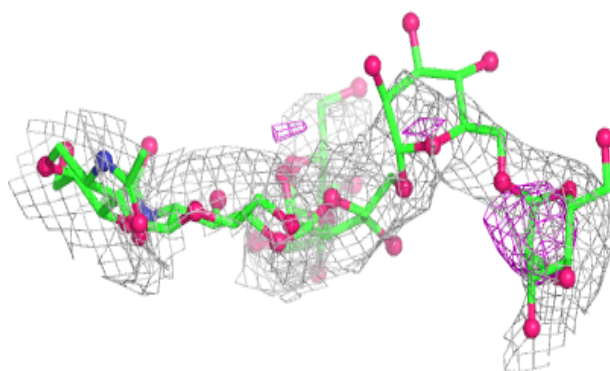
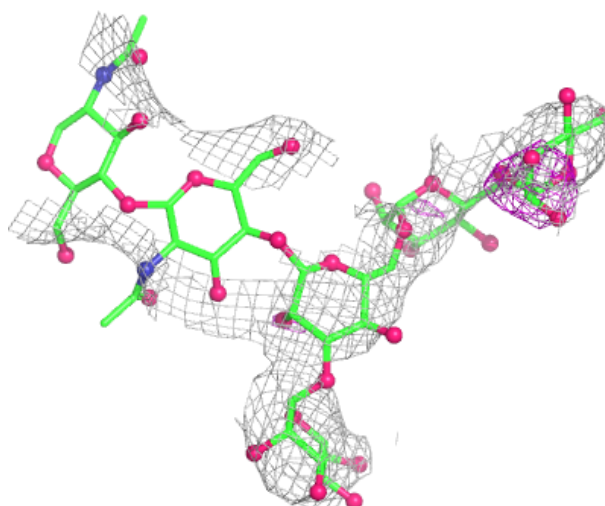
Electron density around Chain V:

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



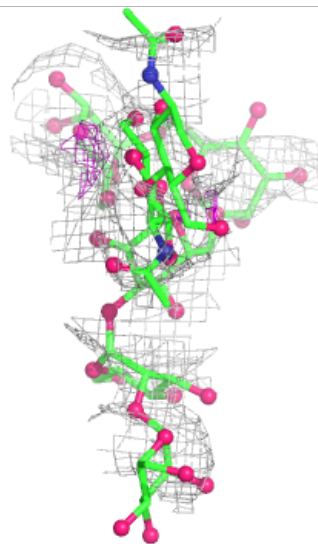
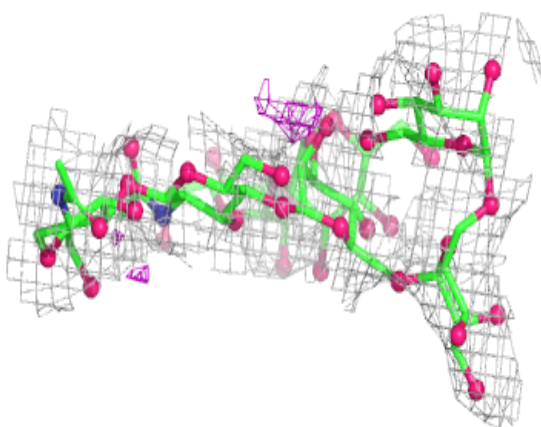
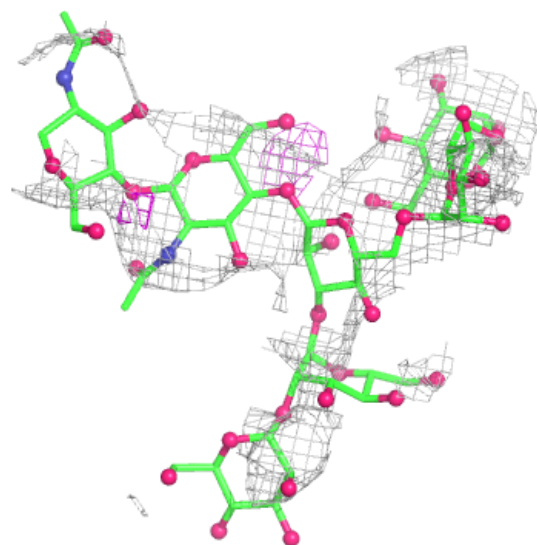
Electron density around Chain R:

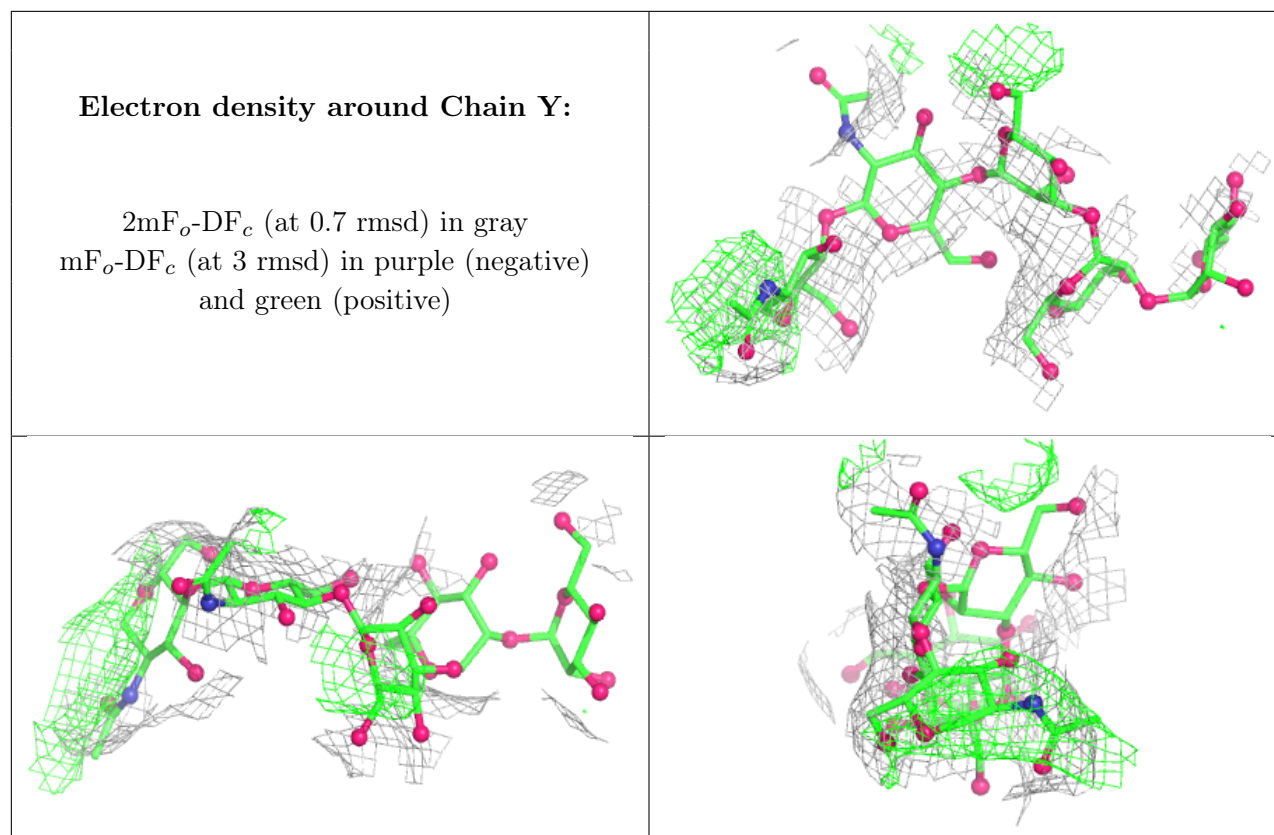
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [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, 95th 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($\text{\AA}^2$)	Q<0.9
17	NAG	F	3190	14/15	-0.01	0.08	235,263,275,278	0
17	NAG	B	3232	14/15	0.17	0.10	192,229,251,259	0
17	NAG	D	3620	14/15	0.19	0.09	259,279,292,296	0
17	NAG	H	3190	14/15	0.28	0.07	215,264,276,276	0
17	NAG	H	3094	14/15	0.39	0.10	239,260,312,313	0
17	NAG	A	3678	14/15	0.43	0.09	162,236,250,253	0
17	NAG	D	3232	14/15	0.45	0.08	220,239,242,244	0
15	CA	F	2002	1/1	0.49	0.08	505,505,505,505	0
15	CA	D	2002	1/1	0.49	0.11	715,715,715,715	0
17	NAG	H	3232	14/15	0.49	0.08	189,210,226,226	0
17	NAG	C	3920	14/15	0.50	0.11	261,304,317,320	0
17	NAG	C	3042	14/15	0.54	0.09	195,241,267,281	0
17	NAG	F	3620	14/15	0.55	0.07	281,300,312,313	0
17	NAG	G	3678	14/15	0.59	0.08	196,238,257,263	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	NAG	B	3620	14/15	0.59	0.08	221,253,270,280	0
17	NAG	C	3678	14/15	0.60	0.11	225,273,310,321	0
17	NAG	E	3920	14/15	0.60	0.09	230,286,310,319	0
17	NAG	A	3042	14/15	0.61	0.14	237,241,277,278	0
17	NAG	E	3042	14/15	0.63	0.08	205,258,290,292	0
17	NAG	F	3094	14/15	0.65	0.09	221,279,292,292	0
17	NAG	C	3031	14/15	0.71	0.07	200,248,281,285	0
17	NAG	G	3920	14/15	0.72	0.10	152,193,229,237	0
17	NAG	A	3920	14/15	0.74	0.07	165,310,345,346	0
17	NAG	E	3678	14/15	0.81	0.10	188,244,283,300	0
17	NAG	G	3042	14/15	0.83	0.08	206,259,269,270	0
15	CA	B	2002	1/1	0.83	0.06	457,457,457,457	0
17	NAG	A	3031	14/15	0.84	0.07	126,244,266,274	0
17	NAG	G	3031	14/15	0.85	0.10	139,227,255,259	0
17	NAG	E	3031	14/15	0.86	0.07	172,223,244,254	0
17	NAG	H	3620	14/15	0.87	0.10	203,255,288,311	0
16	MG	A	2009	1/1	0.93	0.05	370,370,370,370	0
15	CA	H	2002	1/1	0.93	0.04	448,448,448,448	0
15	CA	E	2006	1/1	0.94	0.04	242,242,242,242	0
15	CA	G	2006	1/1	0.95	0.04	214,214,214,214	0
15	CA	E	2007	1/1	0.95	0.04	246,246,246,246	0
15	CA	A	2006	1/1	0.96	0.04	234,234,234,234	0
15	CA	A	2005	1/1	0.96	0.05	282,282,282,282	0
15	CA	E	2005	1/1	0.97	0.06	276,276,276,276	0
15	CA	C	2005	1/1	0.97	0.08	236,236,236,236	0
15	CA	G	2005	1/1	0.98	0.03	240,240,240,240	0
15	CA	C	2007	1/1	0.98	0.04	311,311,311,311	0
15	CA	G	2007	1/1	0.98	0.04	189,189,189,189	0
15	CA	C	2006	1/1	0.98	0.03	232,232,232,232	0
15	CA	A	2007	1/1	0.99	0.05	238,238,238,238	0

6.5 Other polymers ⓘ

There are no such residues in this entry.