



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 08:39 AM EDT

PDB ID : 3RG1  
Title : Crystal structure of the RP105/MD-1 complex  
Authors : Yoon, S.I.; Hong, M.; Wilson, I.A.  
Deposited on : 2011-04-07  
Resolution : 2.91 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](mailto: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>.

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

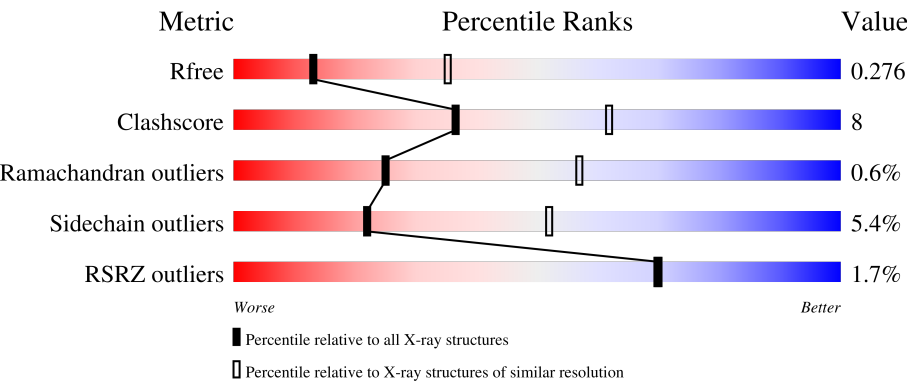
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 2.91 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 <sub>free</sub>	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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  $\geq 3$ , 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	612	<div><div>2%</div><div></div><div>79%</div><div>16%</div><div>..</div></div>
1	B	612	<div><div>%</div><div></div><div>79%</div><div>17%</div><div>..</div></div>
1	E	612	<div><div>2%</div><div></div><div>78%</div><div>17%</div><div>..</div></div>
1	F	612	<div><div>2%</div><div></div><div>79%</div><div>17%</div><div>..</div></div>
1	I	612	<div><div>2%</div><div></div><div>55%</div><div>9%</div><div>35%</div></div>

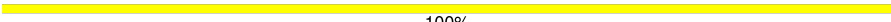
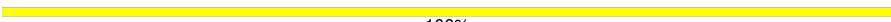
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Mol	Chain	Length	Quality of chain
1	J	612	 3% 79% 17% ..
1	M	612	 % 76% 19% ..
1	N	612	 % 77% 19% ..
2	C	147	 % 78% 15% • 6%
2	D	147	 % 76% 16% • 7%
2	G	147	 % 79% 14% .. 6%
2	H	147	 % 78% 15% • 6%
2	K	147	 3% 79% 12% • 7%
2	L	147	 % 80% 12% • 6%
2	O	147	 % 77% 14% .. 6%
2	P	147	 3% 80% 12% 8%
3	Q	3	 67% 33%
3	S	3	 67% 33%
3	U	3	 67% 33%
3	W	3	 67% 33%
3	Y	3	 33% 67%
3	a	3	 100%
3	c	3	 100%
3	e	3	 100%
4	R	8	 12% 88%
4	T	8	 75% 25%
4	V	8	 62% 38%
4	X	8	 88% 12%
4	Z	8	 88% 12%
4	b	8	 100%

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Mol	Chain	Length	Quality of chain
4	d	8	 100%
4	f	8	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PGT	H	201	-	-	-	X
5	PGT	L	201	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43795 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 CD180 molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4450	2805	766	860	19			
1	E	592	Total	C	N	O	S	0	0	0
			4381	2763	750	849	19			
1	I	397	Total	C	N	O	S	0	0	0
			2931	1862	489	570	10			
1	M	593	Total	C	N	O	S	0	0	0
			4447	2806	763	859	19			
1	B	599	Total	C	N	O	S	0	0	0
			4616	2921	788	885	22			
1	F	599	Total	C	N	O	S	0	0	0
			4493	2833	768	870	22			
1	J	599	Total	C	N	O	S	0	0	0
			4458	2816	756	865	21			
1	N	599	Total	C	N	O	S	0	0	0
			4591	2909	783	877	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A6QNK7
A	23	GLY	-	expression tag	UNP A6QNK7
A	627	THR	-	expression tag	UNP A6QNK7
A	628	HIS	-	expression tag	UNP A6QNK7
A	629	MET	-	expression tag	UNP A6QNK7
A	630	LEU	-	expression tag	UNP A6QNK7
A	631	VAL	-	expression tag	UNP A6QNK7
A	632	PRO	-	expression tag	UNP A6QNK7
A	633	ARG	-	expression tag	UNP A6QNK7
E	22	ALA	-	expression tag	UNP A6QNK7
E	23	GLY	-	expression tag	UNP A6QNK7
E	627	THR	-	expression tag	UNP A6QNK7
E	628	HIS	-	expression tag	UNP A6QNK7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	629	MET	-	expression tag	UNP A6QNK7
E	630	LEU	-	expression tag	UNP A6QNK7
E	631	VAL	-	expression tag	UNP A6QNK7
E	632	PRO	-	expression tag	UNP A6QNK7
E	633	ARG	-	expression tag	UNP A6QNK7
I	22	ALA	-	expression tag	UNP A6QNK7
I	23	GLY	-	expression tag	UNP A6QNK7
I	627	THR	-	expression tag	UNP A6QNK7
I	628	HIS	-	expression tag	UNP A6QNK7
I	629	MET	-	expression tag	UNP A6QNK7
I	630	LEU	-	expression tag	UNP A6QNK7
I	631	VAL	-	expression tag	UNP A6QNK7
I	632	PRO	-	expression tag	UNP A6QNK7
I	633	ARG	-	expression tag	UNP A6QNK7
M	22	ALA	-	expression tag	UNP A6QNK7
M	23	GLY	-	expression tag	UNP A6QNK7
M	627	THR	-	expression tag	UNP A6QNK7
M	628	HIS	-	expression tag	UNP A6QNK7
M	629	MET	-	expression tag	UNP A6QNK7
M	630	LEU	-	expression tag	UNP A6QNK7
M	631	VAL	-	expression tag	UNP A6QNK7
M	632	PRO	-	expression tag	UNP A6QNK7
M	633	ARG	-	expression tag	UNP A6QNK7
B	22	ALA	-	expression tag	UNP A6QNK7
B	23	GLY	-	expression tag	UNP A6QNK7
B	627	THR	-	expression tag	UNP A6QNK7
B	628	HIS	-	expression tag	UNP A6QNK7
B	629	MET	-	expression tag	UNP A6QNK7
B	630	LEU	-	expression tag	UNP A6QNK7
B	631	VAL	-	expression tag	UNP A6QNK7
B	632	PRO	-	expression tag	UNP A6QNK7
B	633	ARG	-	expression tag	UNP A6QNK7
F	22	ALA	-	expression tag	UNP A6QNK7
F	23	GLY	-	expression tag	UNP A6QNK7
F	627	THR	-	expression tag	UNP A6QNK7
F	628	HIS	-	expression tag	UNP A6QNK7
F	629	MET	-	expression tag	UNP A6QNK7
F	630	LEU	-	expression tag	UNP A6QNK7
F	631	VAL	-	expression tag	UNP A6QNK7
F	632	PRO	-	expression tag	UNP A6QNK7
F	633	ARG	-	expression tag	UNP A6QNK7
J	22	ALA	-	expression tag	UNP A6QNK7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	23	GLY	-	expression tag	UNP A6QNK7
J	627	THR	-	expression tag	UNP A6QNK7
J	628	HIS	-	expression tag	UNP A6QNK7
J	629	MET	-	expression tag	UNP A6QNK7
J	630	LEU	-	expression tag	UNP A6QNK7
J	631	VAL	-	expression tag	UNP A6QNK7
J	632	PRO	-	expression tag	UNP A6QNK7
J	633	ARG	-	expression tag	UNP A6QNK7
N	22	ALA	-	expression tag	UNP A6QNK7
N	23	GLY	-	expression tag	UNP A6QNK7
N	627	THR	-	expression tag	UNP A6QNK7
N	628	HIS	-	expression tag	UNP A6QNK7
N	629	MET	-	expression tag	UNP A6QNK7
N	630	LEU	-	expression tag	UNP A6QNK7
N	631	VAL	-	expression tag	UNP A6QNK7
N	632	PRO	-	expression tag	UNP A6QNK7
N	633	ARG	-	expression tag	UNP A6QNK7

- Molecule 2 is a protein called LY86 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	0	0
			1026	656	170	193	7			
2	D	136	Total	C	N	O	S	0	0	0
			1022	656	167	192	7			
2	G	138	Total	C	N	O	S	0	0	0
			1031	664	170	190	7			
2	H	138	Total	C	N	O	S	0	0	0
			1046	667	176	196	7			
2	K	136	Total	C	N	O	S	0	0	0
			1003	640	167	189	7			
2	L	138	Total	C	N	O	S	0	0	0
			1046	667	172	200	7			
2	O	138	Total	C	N	O	S	0	0	0
			1028	658	169	194	7			
2	P	135	Total	C	N	O	S	0	0	0
			1001	640	166	188	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	expression tag	UNP A4IFT3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	160	ALA	-	expression tag	UNP A4IFT3
C	161	ARG	-	expression tag	UNP A4IFT3
C	162	GLY	-	expression tag	UNP A4IFT3
C	163	LEU	-	expression tag	UNP A4IFT3
C	164	VAL	-	expression tag	UNP A4IFT3
C	165	PRO	-	expression tag	UNP A4IFT3
C	166	ARG	-	expression tag	UNP A4IFT3
D	20	ALA	-	expression tag	UNP A4IFT3
D	160	ALA	-	expression tag	UNP A4IFT3
D	161	ARG	-	expression tag	UNP A4IFT3
D	162	GLY	-	expression tag	UNP A4IFT3
D	163	LEU	-	expression tag	UNP A4IFT3
D	164	VAL	-	expression tag	UNP A4IFT3
D	165	PRO	-	expression tag	UNP A4IFT3
D	166	ARG	-	expression tag	UNP A4IFT3
G	20	ALA	-	expression tag	UNP A4IFT3
G	160	ALA	-	expression tag	UNP A4IFT3
G	161	ARG	-	expression tag	UNP A4IFT3
G	162	GLY	-	expression tag	UNP A4IFT3
G	163	LEU	-	expression tag	UNP A4IFT3
G	164	VAL	-	expression tag	UNP A4IFT3
G	165	PRO	-	expression tag	UNP A4IFT3
G	166	ARG	-	expression tag	UNP A4IFT3
H	20	ALA	-	expression tag	UNP A4IFT3
H	160	ALA	-	expression tag	UNP A4IFT3
H	161	ARG	-	expression tag	UNP A4IFT3
H	162	GLY	-	expression tag	UNP A4IFT3
H	163	LEU	-	expression tag	UNP A4IFT3
H	164	VAL	-	expression tag	UNP A4IFT3
H	165	PRO	-	expression tag	UNP A4IFT3
H	166	ARG	-	expression tag	UNP A4IFT3
K	20	ALA	-	expression tag	UNP A4IFT3
K	160	ALA	-	expression tag	UNP A4IFT3
K	161	ARG	-	expression tag	UNP A4IFT3
K	162	GLY	-	expression tag	UNP A4IFT3
K	163	LEU	-	expression tag	UNP A4IFT3
K	164	VAL	-	expression tag	UNP A4IFT3
K	165	PRO	-	expression tag	UNP A4IFT3
K	166	ARG	-	expression tag	UNP A4IFT3
L	20	ALA	-	expression tag	UNP A4IFT3
L	160	ALA	-	expression tag	UNP A4IFT3
L	161	ARG	-	expression tag	UNP A4IFT3

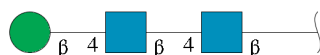
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Chain	Residue	Modelled	Actual	Comment	Reference
L	162	GLY	-	expression tag	UNP A4IFT3
L	163	LEU	-	expression tag	UNP A4IFT3
L	164	VAL	-	expression tag	UNP A4IFT3
L	165	PRO	-	expression tag	UNP A4IFT3
L	166	ARG	-	expression tag	UNP A4IFT3
O	20	ALA	-	expression tag	UNP A4IFT3
O	160	ALA	-	expression tag	UNP A4IFT3
O	161	ARG	-	expression tag	UNP A4IFT3
O	162	GLY	-	expression tag	UNP A4IFT3
O	163	LEU	-	expression tag	UNP A4IFT3
O	164	VAL	-	expression tag	UNP A4IFT3
O	165	PRO	-	expression tag	UNP A4IFT3
O	166	ARG	-	expression tag	UNP A4IFT3
P	20	ALA	-	expression tag	UNP A4IFT3
P	160	ALA	-	expression tag	UNP A4IFT3
P	161	ARG	-	expression tag	UNP A4IFT3
P	162	GLY	-	expression tag	UNP A4IFT3
P	163	LEU	-	expression tag	UNP A4IFT3
P	164	VAL	-	expression tag	UNP A4IFT3
P	165	PRO	-	expression tag	UNP A4IFT3
P	166	ARG	-	expression tag	UNP A4IFT3

- Molecule 3 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.



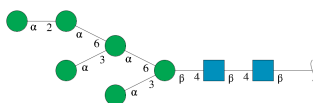
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	S	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	a	3	Total	C	N	O	0	0	0
			39	22	2	15			

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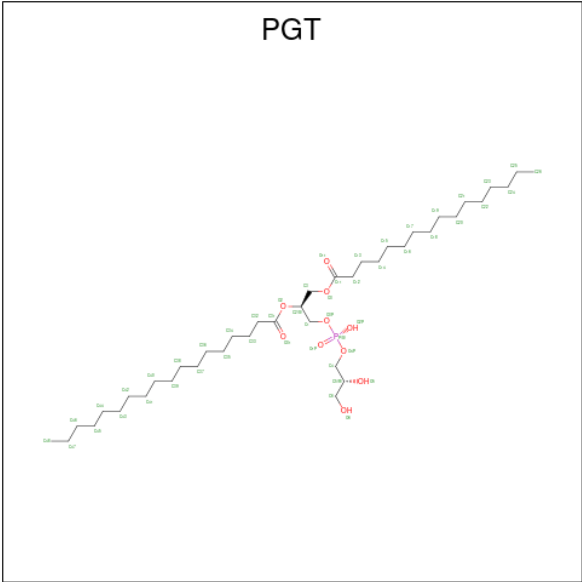
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
4	R	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	T	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	V	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	X	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	Z	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	b	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	d	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	f	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			31	27	4		
5	H	1	Total	C	O	0	0
			31	27	4		
5	L	1	Total	C	O	0	0
			31	27	4		
5	P	1	Total	C	O	0	0
			31	27	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	E	2	Total	O	0	0
			2	2		
6	I	1	Total	O	0	0
			1	1		
6	M	5	Total	O	0	0
			5	5		
6	B	9	Total	O	0	0
			9	9		
6	F	1	Total	O	0	0
			1	1		
6	J	1	Total	O	0	0
			1	1		
6	N	6	Total	O	0	0
			6	6		

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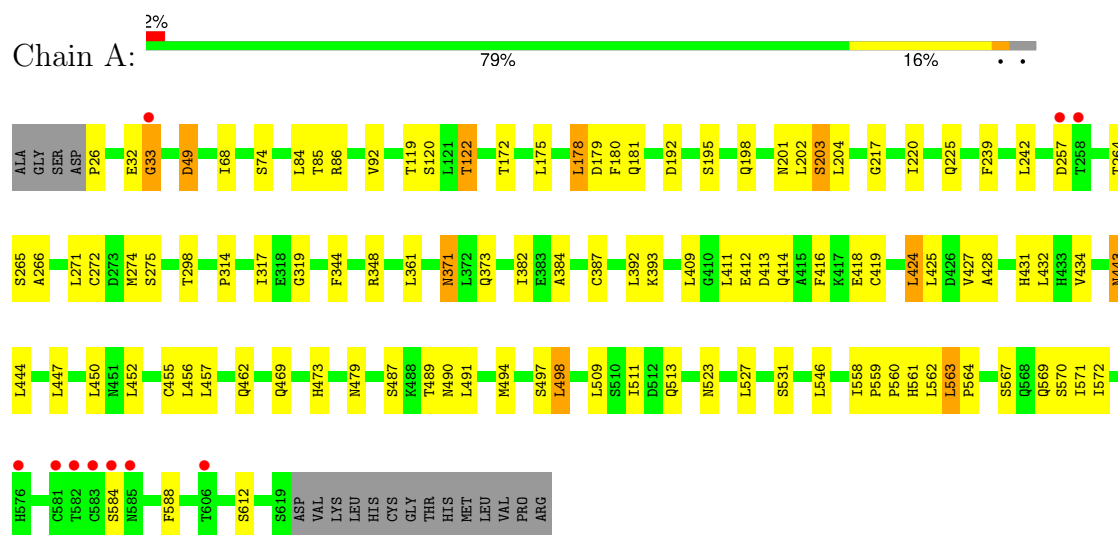
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	O 1	0	0
6	D	3	Total 3	O 3	0	0
6	G	1	Total 1	O 1	0	0
6	L	1	Total 1	O 1	0	0

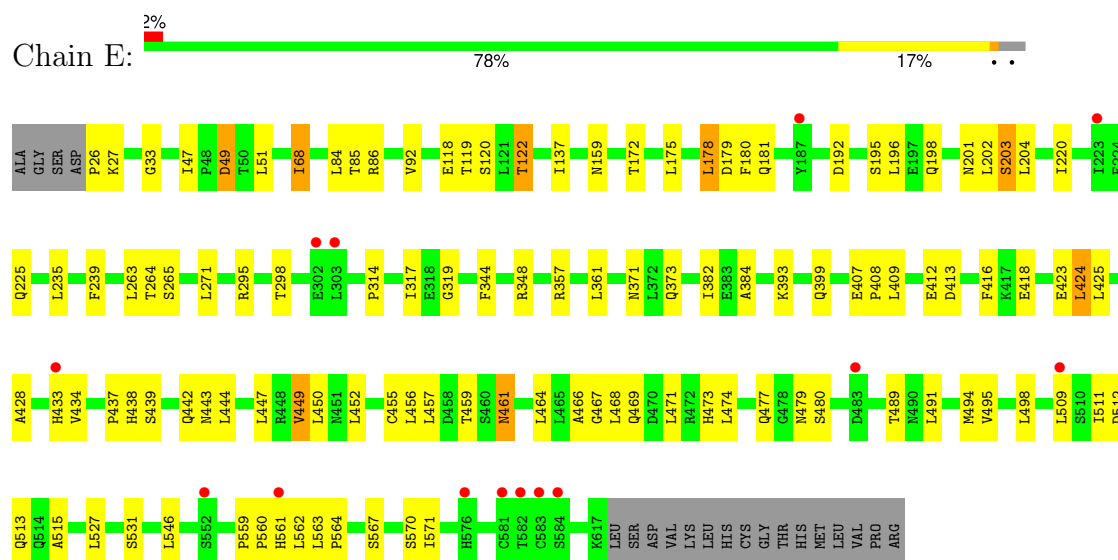
### 3 Residue-property plots

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: CD180 molecule

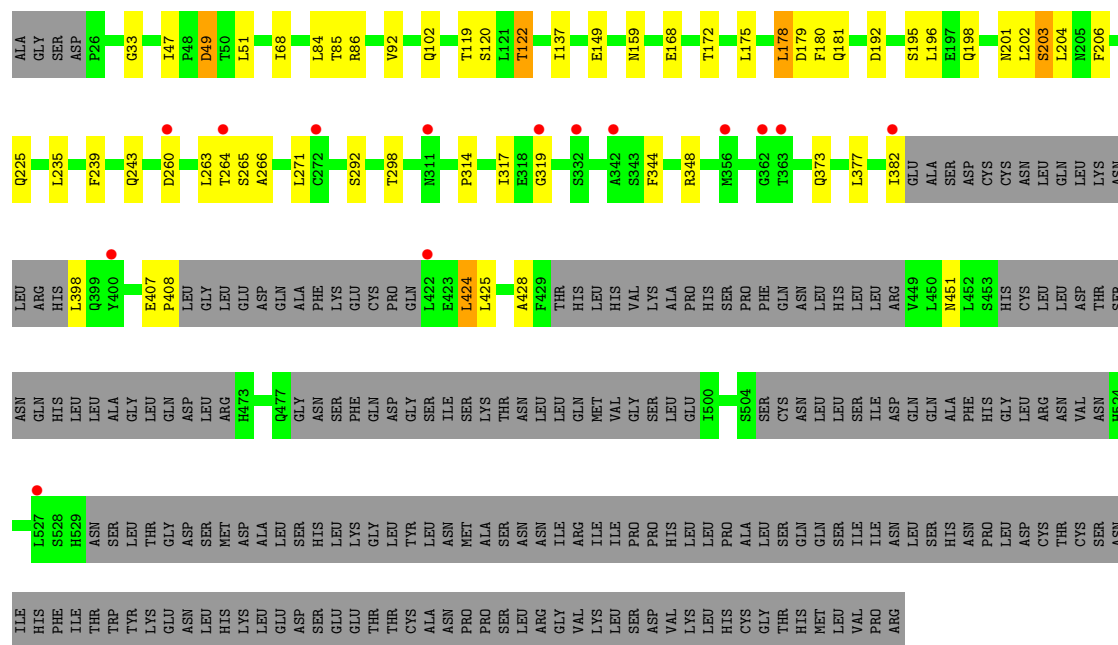


#### • Molecule 1: CD180 molecule

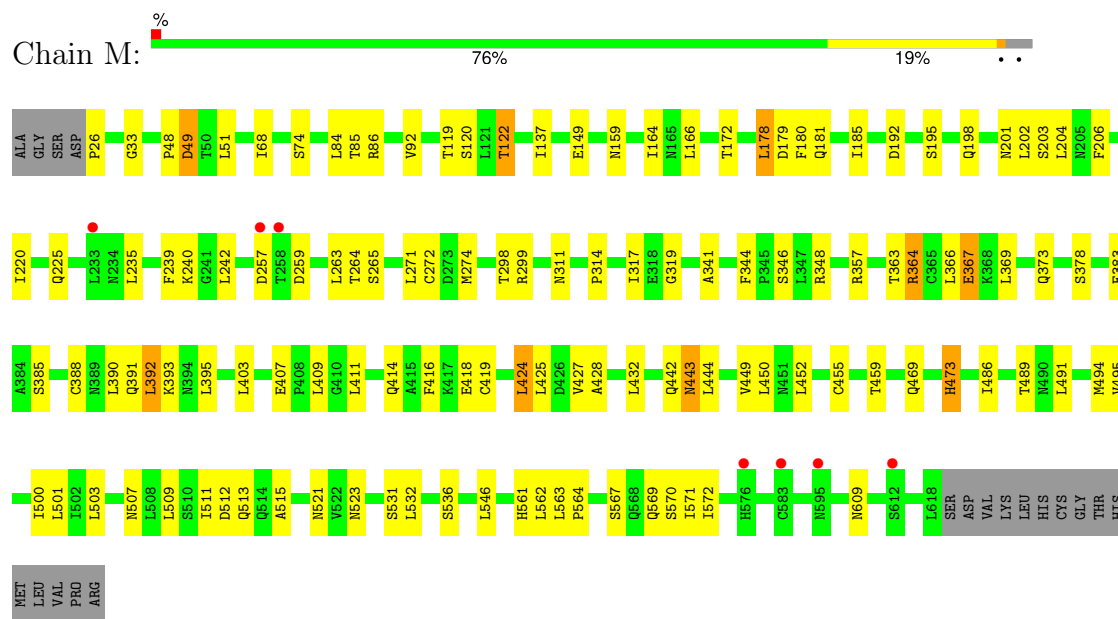


#### • Molecule 1: CD180 molecule

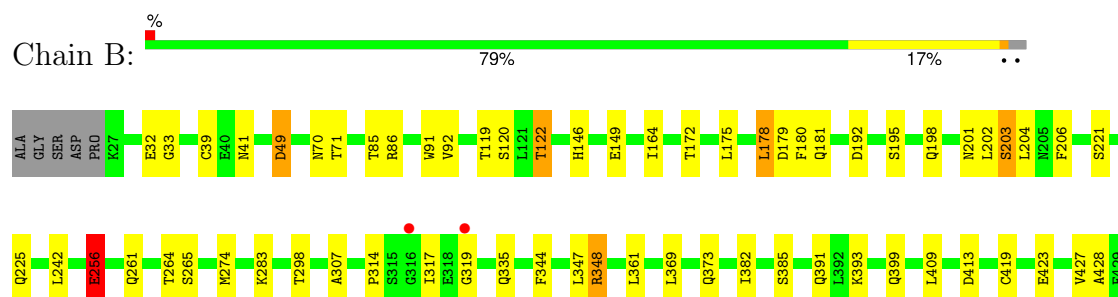


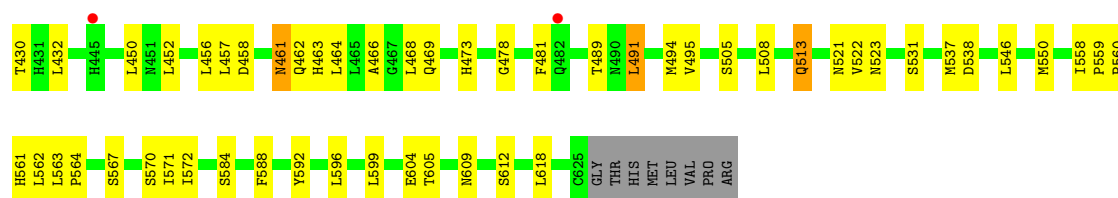


• Molecule 1: CD180 molecule

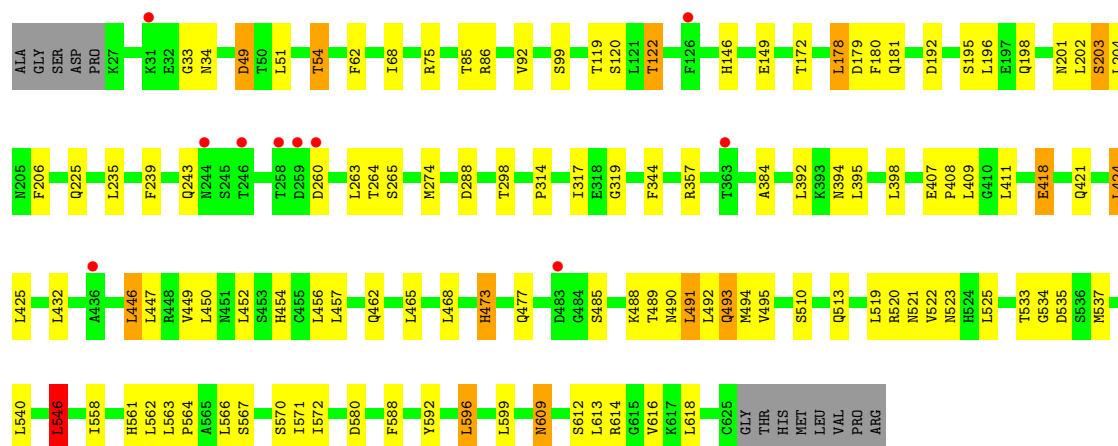
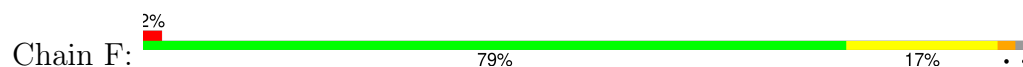


• Molecule 1: CD180 molecule

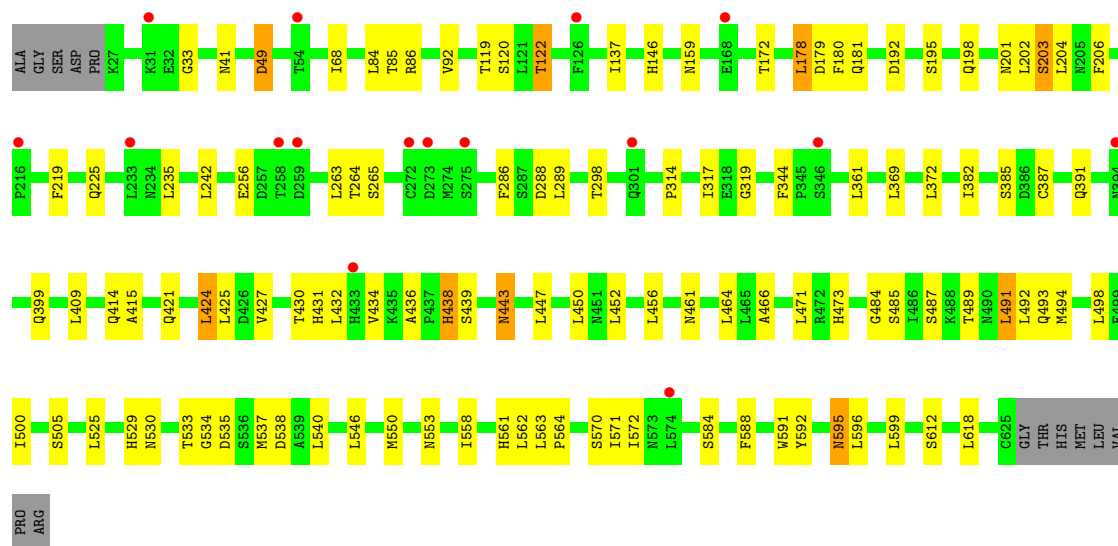
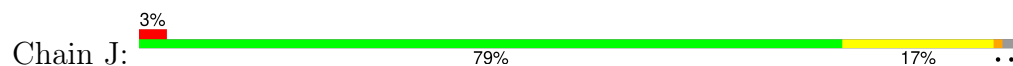




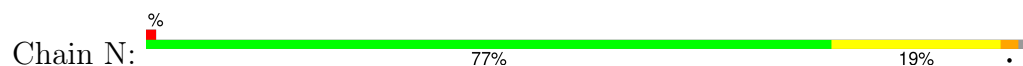
• Molecule 1: CD180 molecule

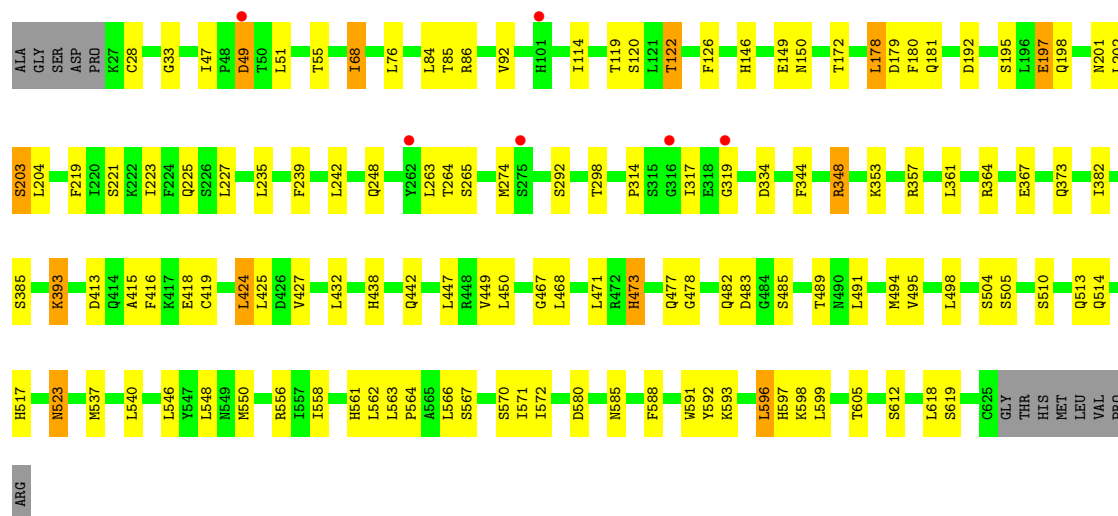


• Molecule 1: CD180 molecule

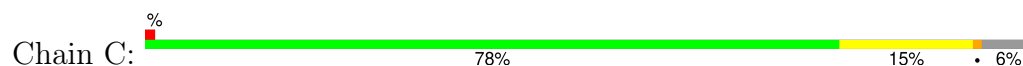


• Molecule 1: CD180 molecule

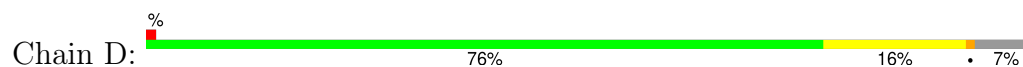




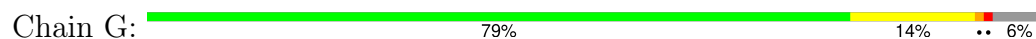
• Molecule 2: LY86 protein



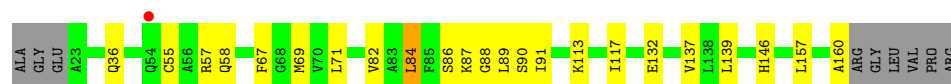
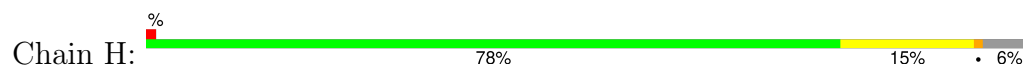
• Molecule 2: LY86 protein



• Molecule 2: LY86 protein

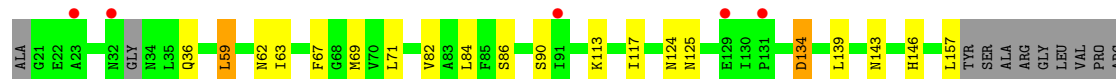
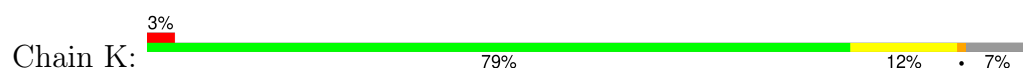


• Molecule 2: LY86 protein

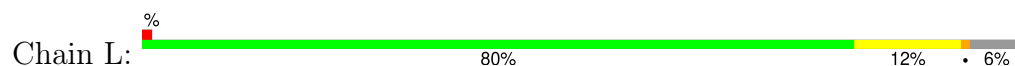


• Molecule 2: LY86 protein

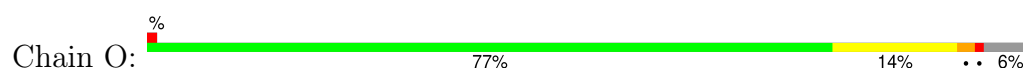




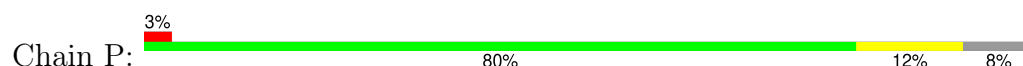
- Molecule 2: LY86 protein



- Molecule 2: LY86 protein



- Molecule 2: LY86 protein



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



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



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



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

Chain W:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain Y:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain a:  100%

MAG1  
MAG2  
BMA3

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

Chain c:  100%

MAG1  
MAG2  
BMA3

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

Chain e:  100%

MAG1  
MAG2  
BMA3

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

Chain R:  12% 88%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

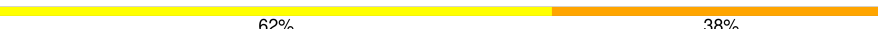
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1

-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  75% 25%

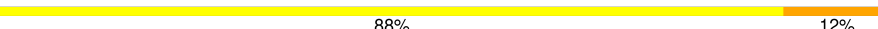


● Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  62% 38%

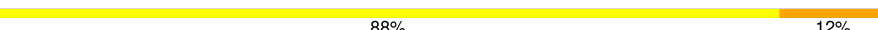


● Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  88% 12%



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

Chain Z:  88% 12%



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

Chain b:  100%



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

Chain d:

100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

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

Chain f:

100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.51Å 141.58Å 141.95Å 94.00° 91.66° 91.37°	Depositor
Resolution (Å)	20.00 – 2.91 20.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-2.91) 92.5 (20.00-2.91)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.238 , 0.276 0.240 , 0.276	Depositor DCC
$R_{free}$ test set	8030 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.8	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l 0.013 for -h,l,k 0.022 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	43795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.63	0/4537	0.67	0/6190
1	B	0.70	3/4708 (0.1%)	0.74	0/6409
1	E	0.50	0/4467	0.60	0/6104
1	F	0.50	0/4581	0.62	1/6256 (0.0%)
1	I	0.49	0/2980	0.58	0/4064
1	J	0.50	0/4546	0.62	0/6213
1	M	0.63	1/4534 (0.0%)	0.68	0/6189
1	N	0.65	1/4682 (0.0%)	0.69	1/6377 (0.0%)
2	C	0.70	1/1051 (0.1%)	0.69	1/1436 (0.1%)
2	D	0.73	0/1048	0.73	2/1432 (0.1%)
2	G	0.61	0/1057	0.69	1/1443 (0.1%)
2	H	0.68	0/1072	0.71	0/1463
2	K	0.52	0/1026	0.63	1/1401 (0.1%)
2	L	0.63	0/1072	0.67	0/1464
2	O	0.71	0/1054	0.70	1/1440 (0.1%)
2	P	0.70	0/1026	0.71	1/1402 (0.1%)
All	All	0.60	6/43441 (0.0%)	0.66	9/59283 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	28	CYS	CB-SG	5.89	1.92	1.82
1	B	256	GLU	CG-CD	5.68	1.60	1.51
1	B	39	CYS	CB-SG	-5.64	1.72	1.81
1	M	419	CYS	CB-SG	-5.39	1.73	1.81
2	C	30	CYS	CB-SG	-5.21	1.73	1.81
1	B	419	CYS	CB-SG	-5.13	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	111	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	G	92	LEU	CA-CB-CG	6.03	129.17	115.30
2	K	59	LEU	CA-CB-CG	5.48	127.91	115.30
2	D	111	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	C	55	CYS	CA-CB-SG	-5.29	104.48	114.00
1	N	556	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	D	55	CYS	CA-CB-SG	-5.08	104.86	114.00
2	O	55	CYS	CA-CB-SG	-5.05	104.91	114.00
1	F	546	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4450	0	4175	61	0
1	B	4616	0	4440	75	0
1	E	4381	0	4045	84	0
1	F	4493	0	4211	73	0
1	I	2931	0	2684	37	0
1	J	4458	0	4137	70	0
1	M	4447	0	4175	73	0
1	N	4591	0	4415	82	0
2	C	1026	0	929	17	0
2	D	1022	0	927	16	0
2	G	1031	0	946	13	0
2	H	1046	0	953	13	0
2	K	1003	0	895	9	0
2	L	1046	0	947	11	0
2	O	1028	0	923	15	0
2	P	1001	0	898	9	0
3	Q	39	0	34	1	0
3	S	39	0	34	1	0
3	U	39	0	34	3	0
3	W	39	0	34	1	0
3	Y	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	a	39	0	34	0	0
3	c	39	0	34	0	0
3	e	39	0	34	0	0
4	R	94	0	79	0	0
4	T	94	0	79	1	0
4	V	94	0	79	2	0
4	X	94	0	79	1	0
4	Z	94	0	79	1	0
4	b	94	0	79	0	0
4	d	94	0	79	0	0
4	f	94	0	79	0	0
5	D	31	0	44	1	0
5	H	31	0	44	1	0
5	L	31	0	44	1	0
5	P	31	0	44	1	0
6	A	6	0	0	0	0
6	B	9	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
6	M	5	0	0	0	0
6	N	6	0	0	0	0
All	All	43795	0	40780	658	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (658) 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:J:450:LEU:HD11	1:J:452:LEU:HD21	1.48	0.95
2:H:82:VAL:HG22	2:H:139:LEU:HD23	1.49	0.93
1:M:242:LEU:HB2	1:M:274:MET:HE1	1.52	0.92
1:N:523:ASN:HD22	1:N:523:ASN:C	1.75	0.90
2:D:62:ASN:HD22	2:D:124:ASN:HA	1.38	0.89
1:E:468:LEU:O	1:E:495:VAL:HG12	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:ALA:HB3	1:E:409:LEU:CD2	2.06	0.85
1:F:558:ILE:HD12	1:F:588:PHE:CE1	2.11	0.85
2:P:82:VAL:HG22	2:P:139:LEU:HD23	1.58	0.84
2:L:82:VAL:HG22	2:L:139:LEU:HD23	1.59	0.84
2:C:82:VAL:HG22	2:C:139:LEU:HD23	1.61	0.83
1:N:348:ARG:HG3	1:N:373:GLN:HE21	1.42	0.82
1:E:384:ALA:HB3	1:E:409:LEU:HD23	1.60	0.82
1:F:558:ILE:HD12	1:F:588:PHE:CD1	2.15	0.82
2:G:82:VAL:HG22	2:G:139:LEU:HD23	1.60	0.81
1:F:488:LYS:O	1:F:493:GLN:NE2	2.14	0.81
2:K:82:VAL:HG22	2:K:139:LEU:HD23	1.63	0.80
1:E:461:ASN:HD22	1:E:464:LEU:HD12	1.45	0.79
2:O:82:VAL:HG22	2:O:139:LEU:HD23	1.66	0.78
1:B:348:ARG:HG3	1:B:373:GLN:HE21	1.49	0.77
1:F:447:LEU:HD21	1:F:450:LEU:HD13	1.67	0.77
2:D:82:VAL:HG22	2:D:139:LEU:HD23	1.66	0.77
1:A:178:LEU:HD22	1:A:180:PHE:CE2	2.21	0.76
1:E:416:PHE:HB2	1:E:444:LEU:HD21	1.68	0.76
2:C:84:LEU:HD23	2:C:91:ILE:HG13	1.67	0.76
1:E:434:VAL:HG21	1:E:464:LEU:HD11	1.66	0.76
1:J:592:TYR:CE1	1:J:599:LEU:HD13	2.21	0.76
1:F:452:LEU:HD13	1:F:457:LEU:HD11	1.67	0.75
2:L:71:LEU:HD11	2:L:117:ILE:HD11	1.68	0.75
1:E:361:LEU:HD21	1:E:382:ILE:HD13	1.68	0.75
1:A:561:HIS:NE2	1:A:562:LEU:HD23	2.02	0.74
2:D:71:LEU:HD11	2:D:117:ILE:HD11	1.70	0.74
2:K:71:LEU:HD11	2:K:117:ILE:HD11	1.69	0.74
2:D:62:ASN:ND2	2:D:124:ASN:HA	2.03	0.73
2:G:84:LEU:HD23	2:G:91:ILE:HB	1.70	0.73
1:A:432:LEU:HD12	1:A:455:CYS:HB3	1.69	0.73
1:E:450:LEU:HG	1:E:452:LEU:HD11	1.70	0.73
1:J:178:LEU:HD22	1:J:180:PHE:CE2	2.24	0.73
2:O:86:SER:HB3	2:O:91:ILE:HD11	1.70	0.72
2:G:71:LEU:HD11	2:G:117:ILE:HD11	1.70	0.72
2:H:84:LEU:HD23	2:H:91:ILE:HB	1.69	0.72
1:B:592:TYR:CE1	1:B:599:LEU:HD13	2.24	0.72
1:F:384:ALA:HB3	1:F:409:LEU:HD23	1.72	0.72
1:N:178:LEU:HD22	1:N:180:PHE:CE2	2.25	0.72
1:B:452:LEU:HD12	1:B:457:LEU:HD11	1.72	0.71
1:I:348:ARG:HG3	1:I:373:GLN:HE21	1.54	0.71
1:J:558:ILE:HD12	1:J:588:PHE:CD1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:179:ASP:CG	1:N:181:GLN:HE21	1.94	0.71
1:E:457:LEU:HD22	1:E:464:LEU:HD21	1.71	0.71
1:F:570:SER:O	1:F:571:ILE:HD13	1.90	0.71
1:B:452:LEU:CD1	1:B:457:LEU:HD11	2.20	0.70
2:P:71:LEU:HD11	2:P:117:ILE:HD11	1.71	0.70
1:E:561:HIS:NE2	1:E:562:LEU:HD23	2.06	0.70
1:F:519:LEU:HB3	1:F:522:VAL:HG23	1.73	0.70
1:J:558:ILE:HD12	1:J:588:PHE:CE1	2.27	0.70
1:B:179:ASP:CG	1:B:181:GLN:HE21	1.95	0.69
2:O:84:LEU:HD23	2:O:91:ILE:HB	1.74	0.69
1:J:450:LEU:HD11	1:J:452:LEU:CD2	2.22	0.69
1:N:605:THR:HG22	1:N:618:LEU:HD13	1.74	0.69
1:A:179:ASP:CG	1:A:181:GLN:HE21	1.96	0.68
1:N:523:ASN:C	1:N:523:ASN:ND2	2.46	0.68
1:M:393:LYS:HA	1:M:418:GLU:HG2	1.74	0.68
1:A:371:ASN:N	1:A:371:ASN:HD22	1.92	0.68
1:F:537:MET:HE2	1:F:566:LEU:HD21	1.75	0.68
2:D:59:LEU:HD23	2:D:128:PHE:CZ	2.28	0.68
1:B:537:MET:CE	1:B:550:MET:HE3	2.24	0.67
1:A:384:ALA:HB3	1:A:409:LEU:HD22	1.77	0.67
1:E:179:ASP:CG	1:E:181:GLN:HE21	1.98	0.67
1:J:561:HIS:NE2	1:J:562:LEU:HD23	2.08	0.67
1:A:570:SER:O	1:A:571:ILE:HD13	1.94	0.67
1:E:178:LEU:HD22	1:E:180:PHE:CE2	2.31	0.66
2:O:125:ASN:ND2	2:O:126:PRO:O	2.28	0.66
1:J:570:SER:O	1:J:571:ILE:HD13	1.96	0.66
1:F:178:LEU:HD22	1:F:180:PHE:CE2	2.30	0.66
1:M:178:LEU:HD22	1:M:180:PHE:CE2	2.30	0.66
1:M:561:HIS:NE2	1:M:562:LEU:HD23	2.10	0.66
1:N:561:HIS:NE2	1:N:562:LEU:HD23	2.11	0.66
1:N:592:TYR:CE1	1:N:599:LEU:HD13	2.31	0.65
1:B:558:ILE:HD12	1:B:588:PHE:CD1	2.32	0.65
1:I:179:ASP:CG	1:I:181:GLN:HE21	1.98	0.65
1:I:92:VAL:HG12	1:I:120:SER:HB2	1.80	0.64
1:F:561:HIS:NE2	1:F:562:LEU:HD23	2.11	0.64
2:O:71:LEU:HD11	2:O:117:ILE:HD11	1.79	0.64
1:B:558:ILE:HD12	1:B:588:PHE:CE1	2.33	0.64
1:M:179:ASP:CG	1:M:181:GLN:HE21	2.00	0.64
1:N:468:LEU:HB2	1:N:495:VAL:HG12	1.79	0.63
1:F:179:ASP:CG	1:F:181:GLN:HE21	2.02	0.63
1:F:34:ASN:O	1:F:54:THR:OG1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:LEU:HD12	1:F:432:LEU:HD13	1.80	0.63
1:B:561:HIS:NE2	1:B:562:LEU:HD23	2.14	0.63
1:F:446:LEU:O	1:F:446:LEU:HD13	1.97	0.63
1:B:178:LEU:HD22	1:B:180:PHE:CE2	2.34	0.63
2:C:71:LEU:HD11	2:C:117:ILE:HD11	1.81	0.63
1:F:462:GLN:HE22	1:F:490:ASN:HA	1.63	0.62
1:E:450:LEU:HG	1:E:452:LEU:CD1	2.28	0.62
1:I:239:PHE:CE1	1:I:271:LEU:HD13	2.34	0.62
2:H:71:LEU:HD11	2:H:117:ILE:HD11	1.80	0.61
1:E:393:LYS:HA	1:E:418:GLU:HG2	1.82	0.61
1:M:383:GLU:OE2	1:M:407:GLU:HB3	2.01	0.61
1:N:572:ILE:HD12	1:N:572:ILE:N	2.15	0.61
1:E:26:PRO:O	1:E:27:LYS:HG2	2.01	0.61
1:E:416:PHE:CB	1:E:444:LEU:HD21	2.31	0.61
1:A:411:LEU:CD1	1:A:432:LEU:HD22	2.30	0.61
1:E:424:LEU:HD13	1:E:449:VAL:HB	1.83	0.61
1:I:178:LEU:HD22	1:I:180:PHE:CE2	2.36	0.61
2:G:67:PHE:HE2	2:G:69:MET:HE2	1.65	0.61
2:P:59:LEU:HD22	2:P:128:PHE:CZ	2.36	0.61
1:B:537:MET:CE	1:B:550:MET:CE	2.80	0.60
1:A:447:LEU:HD21	1:A:450:LEU:HD13	1.83	0.60
1:F:92:VAL:HG12	1:F:120:SER:HB2	1.83	0.60
1:J:92:VAL:HG12	1:J:120:SER:HB2	1.84	0.60
1:N:92:VAL:HG12	1:N:120:SER:HB2	1.83	0.60
1:F:317:ILE:HG22	1:F:319:GLY:H	1.67	0.59
2:G:92:LEU:HD11	2:G:94:PHE:HD1	1.67	0.59
1:M:569:GLN:HB2	1:M:572:ILE:HD11	1.83	0.59
1:N:570:SER:O	1:N:571:ILE:HD13	2.03	0.59
1:B:570:SER:O	1:B:571:ILE:HD13	2.03	0.59
1:E:348:ARG:HG3	1:E:373:GLN:HE21	1.68	0.59
1:M:92:VAL:HG12	1:M:120:SER:HB2	1.83	0.59
1:B:537:MET:HG3	1:B:550:MET:HE1	1.83	0.59
2:G:92:LEU:HD11	2:G:94:PHE:CD1	2.38	0.59
1:E:570:SER:O	1:E:571:ILE:HD13	2.02	0.59
1:I:428:ALA:HB3	3:U:1:NAG:H82	1.83	0.59
1:A:424:LEU:HD12	1:A:425:LEU:N	2.18	0.58
1:M:119:THR:HA	1:M:122:THR:HG23	1.85	0.58
1:M:450:LEU:HD11	1:M:452:LEU:HD21	1.85	0.58
1:B:391:GLN:OE1	1:B:391:GLN:N	2.34	0.58
1:N:597:HIS:CE1	1:N:598:LYS:HG3	2.38	0.58
5:D:201:PGT:H322	5:D:201:PGT:H122	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:ASN:HD22	1:E:464:LEU:CD1	2.14	0.58
1:B:202:LEU:HG	1:B:204:LEU:CD1	2.33	0.58
1:B:427:VAL:HG21	1:B:432:LEU:HD11	1.85	0.58
1:B:537:MET:HE3	1:B:550:MET:HE3	1.85	0.58
1:E:92:VAL:HG12	1:E:120:SER:HB2	1.85	0.58
1:B:495:VAL:HG23	1:B:495:VAL:O	2.03	0.58
2:D:67:PHE:HE2	2:D:69:MET:HE2	1.68	0.58
2:D:84:LEU:HD23	2:D:91:ILE:HD12	1.86	0.58
1:M:348:ARG:HG3	1:M:373:GLN:HE21	1.68	0.58
1:F:609:ASN:OD1	1:F:609:ASN:N	2.36	0.58
1:A:314:PRO:HG2	1:A:317:ILE:HD11	1.86	0.58
1:B:348:ARG:CG	1:B:373:GLN:HE21	2.15	0.58
1:B:314:PRO:HG2	1:B:317:ILE:HD11	1.86	0.57
1:F:519:LEU:HB3	1:F:522:VAL:CG2	2.34	0.57
1:N:537:MET:HG3	1:N:550:MET:HE1	1.86	0.57
2:K:63:ILE:HG22	2:K:125:ASN:OD1	2.04	0.57
1:E:459:THR:CB	1:E:491:LEU:HD11	2.34	0.57
2:P:59:LEU:HD22	2:P:128:PHE:CE2	2.39	0.57
1:M:570:SER:O	1:M:571:ILE:HD13	2.03	0.57
2:L:67:PHE:HE2	2:L:69:MET:HE2	1.68	0.57
1:B:361:LEU:HD21	1:B:382:ILE:HD13	1.86	0.57
1:J:202:LEU:HG	1:J:204:LEU:CD1	2.34	0.57
1:E:434:VAL:HG11	1:E:464:LEU:HD12	1.86	0.57
1:B:537:MET:HE2	1:B:550:MET:CE	2.34	0.57
1:N:558:ILE:HD12	1:N:588:PHE:CD1	2.40	0.56
2:P:67:PHE:HE2	2:P:69:MET:HE2	1.70	0.56
1:F:202:LEU:HG	1:F:204:LEU:CD1	2.36	0.56
1:J:179:ASP:CG	1:J:181:GLN:HE21	2.07	0.56
2:C:84:LEU:HD23	2:C:91:ILE:CG1	2.33	0.56
2:C:84:LEU:CD2	2:C:91:ILE:HD12	2.36	0.56
2:H:67:PHE:HE2	2:H:69:MET:HE2	1.71	0.56
2:P:59:LEU:CD2	2:P:128:PHE:CZ	2.89	0.56
1:B:537:MET:HE2	1:B:550:MET:HE3	1.87	0.56
1:J:436:ALA:HB2	1:J:461:ASN:HB2	1.87	0.56
1:E:202:LEU:HG	1:E:204:LEU:CD1	2.35	0.56
1:M:563:LEU:N	1:M:564:PRO:HD2	2.21	0.56
1:A:92:VAL:HG12	1:A:120:SER:HB2	1.86	0.56
1:E:467:GLY:C	1:E:469:GLN:HE22	2.07	0.56
1:J:439:SER:CB	1:J:466:ALA:HB3	2.35	0.56
1:M:202:LEU:HG	1:M:204:LEU:CD1	2.36	0.56
1:E:434:VAL:HG11	1:E:464:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:ILE:HG22	1:F:319:GLY:N	2.21	0.55
1:J:41:ASN:OD1	2:L:72:ARG:NH1	2.39	0.55
1:M:459:THR:HG22	1:M:491:LEU:CD2	2.36	0.55
1:I:85:THR:HG22	1:I:86:ARG:HB2	1.87	0.55
1:N:179:ASP:OD1	1:N:181:GLN:NE2	2.38	0.55
1:A:257:ASP:HB3	2:C:119:TYR:OH	2.07	0.55
1:E:450:LEU:CG	1:E:452:LEU:HD11	2.36	0.55
1:M:411:LEU:HD11	1:M:432:LEU:HD22	1.89	0.55
1:N:537:MET:HE2	1:N:566:LEU:HD21	1.89	0.55
2:H:36:GLN:HE21	2:H:157:LEU:HD12	1.72	0.55
1:A:424:LEU:HD12	1:A:424:LEU:C	2.26	0.55
1:J:85:THR:HG22	1:J:86:ARG:HB2	1.88	0.55
1:F:537:MET:HE1	1:F:566:LEU:HD11	1.89	0.55
2:G:67:PHE:CE2	2:G:69:MET:HE2	2.41	0.55
1:N:202:LEU:HG	1:N:204:LEU:CD1	2.37	0.55
2:K:67:PHE:HE2	2:K:69:MET:HE2	1.72	0.55
1:E:409:LEU:O	1:E:433:HIS:N	2.39	0.55
1:E:459:THR:HB	1:E:491:LEU:HD11	1.87	0.55
1:B:452:LEU:HD13	1:B:457:LEU:HD21	1.89	0.55
1:N:317:ILE:HG22	1:N:319:GLY:H	1.72	0.55
1:E:449:VAL:HG13	1:E:473:HIS:HB3	1.89	0.55
1:B:572:ILE:HB	1:B:599:LEU:HD23	1.89	0.55
1:N:537:MET:CE	1:N:550:MET:HE2	2.37	0.55
1:B:537:MET:CG	1:B:550:MET:HE1	2.37	0.54
1:N:558:ILE:HD12	1:N:588:PHE:CE1	2.43	0.54
5:H:201:PGT:H322	5:H:201:PGT:H122	1.88	0.54
2:G:86:SER:HB3	2:G:91:ILE:HD11	1.88	0.54
1:B:179:ASP:OD1	1:B:181:GLN:NE2	2.40	0.54
1:E:459:THR:HA	1:E:491:LEU:HD21	1.90	0.54
1:J:537:MET:HB2	1:J:562:LEU:HD13	1.88	0.54
1:A:563:LEU:N	1:A:564:PRO:HD2	2.22	0.54
1:M:264:THR:HG22	1:M:265:SER:N	2.23	0.54
5:P:201:PGT:H322	5:P:201:PGT:H122	1.89	0.54
1:B:592:TYR:CZ	1:B:599:LEU:HD13	2.43	0.53
2:P:36:GLN:HE21	2:P:157:LEU:HD12	1.73	0.53
1:I:202:LEU:HG	1:I:204:LEU:CD1	2.38	0.53
1:A:348:ARG:HG3	1:A:373:GLN:HE21	1.73	0.53
1:J:533:THR:O	1:J:535:ASP:N	2.42	0.53
1:N:334:ASP:OD2	1:N:357:ARG:HD2	2.08	0.53
2:G:36:GLN:HE21	2:G:157:LEU:HD12	1.73	0.53
1:A:414:GLN:HB3	1:A:443:ASN:HD21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:HG	1:A:479:ASN:OD1	2.08	0.53
1:I:196:LEU:HD13	1:I:202:LEU:HD21	1.90	0.53
1:M:317:ILE:HG22	1:M:319:GLY:H	1.74	0.53
1:M:424:LEU:HD12	1:M:425:LEU:N	2.24	0.53
1:A:411:LEU:HD11	1:A:432:LEU:HD22	1.91	0.53
1:A:511:ILE:HD11	1:A:527:LEU:HD22	1.90	0.53
1:I:377:LEU:HB3	1:I:382:ILE:CD1	2.38	0.53
1:B:92:VAL:HG12	1:B:120:SER:HB2	1.91	0.53
1:F:492:LEU:C	1:F:494:MET:H	2.10	0.53
1:J:439:SER:HB3	1:J:466:ALA:HB3	1.91	0.53
1:I:317:ILE:HG22	1:I:319:GLY:H	1.74	0.53
1:B:466:ALA:HA	1:B:494:MET:CG	2.39	0.53
1:J:525:LEU:HD23	1:J:540:LEU:HD21	1.91	0.53
1:N:317:ILE:HG22	1:N:319:GLY:N	2.24	0.53
1:B:605:THR:HG22	1:B:618:LEU:HD13	1.90	0.53
5:L:201:PGT:H122	5:L:201:PGT:H322	1.91	0.53
1:N:537:MET:HG3	1:N:550:MET:CE	2.39	0.53
2:D:67:PHE:CE2	2:D:69:MET:HE2	2.44	0.53
1:A:264:THR:HG22	1:A:265:SER:N	2.24	0.52
1:I:373:GLN:C	1:I:398:LEU:HD12	2.29	0.52
1:M:314:PRO:HG2	1:M:317:ILE:HD11	1.92	0.52
1:B:203:SER:C	1:B:204:LEU:HD12	2.29	0.52
1:A:317:ILE:HG22	1:A:319:GLY:H	1.74	0.52
1:J:414:GLN:HB3	1:J:443:ASN:ND2	2.24	0.52
1:E:179:ASP:OD1	1:E:181:GLN:NE2	2.42	0.52
1:N:264:THR:HG22	1:N:265:SER:N	2.24	0.52
1:N:197:GLU:OE2	1:N:221:SER:OG	2.27	0.52
2:O:67:PHE:HE2	2:O:69:MET:HE2	1.75	0.52
1:A:202:LEU:HG	1:A:204:LEU:CD1	2.40	0.52
1:E:563:LEU:N	1:E:564:PRO:HD2	2.25	0.52
1:I:317:ILE:HG22	1:I:319:GLY:N	2.25	0.52
1:J:201:ASN:HD22	1:J:225:GLN:HB2	1.75	0.52
1:M:364:ARG:O	1:M:367:GLU:HB3	2.10	0.52
1:M:366:LEU:HB3	1:M:369:LEU:HD12	1.91	0.52
1:N:314:PRO:HG2	1:N:317:ILE:HD11	1.91	0.52
2:C:36:GLN:HE21	2:C:157:LEU:HD12	1.74	0.52
2:O:36:GLN:HE21	2:O:157:LEU:HD12	1.75	0.52
2:C:67:PHE:HE2	2:C:69:MET:HE2	1.75	0.52
1:B:466:ALA:HA	1:B:494:MET:HG2	1.90	0.51
1:F:411:LEU:CD1	1:F:432:LEU:HD13	2.39	0.51
1:A:203:SER:C	1:A:204:LEU:HD12	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD12	1:B:430:THR:HG21	1.93	0.51
1:A:239:PHE:CE1	1:A:271:LEU:HD13	2.45	0.51
1:E:424:LEU:HD12	1:E:425:LEU:N	2.25	0.51
1:N:471:LEU:O	1:N:498:LEU:HD23	2.10	0.51
1:E:442:GLN:HA	1:E:467:GLY:HA3	1.92	0.51
1:M:317:ILE:HG22	1:M:319:GLY:N	2.25	0.51
1:J:203:SER:C	1:J:204:LEU:HD12	2.30	0.51
1:A:317:ILE:HG22	1:A:319:GLY:N	2.25	0.51
2:K:36:GLN:HE21	2:K:157:LEU:HD12	1.75	0.51
1:A:119:THR:HA	1:A:122:THR:HG23	1.93	0.51
1:E:428:ALA:HB3	3:S:1:NAG:H82	1.92	0.51
1:E:314:PRO:HG2	1:E:317:ILE:HD11	1.92	0.51
1:B:85:THR:HG22	1:B:86:ARG:HB2	1.92	0.51
1:J:317:ILE:HG22	1:J:319:GLY:H	1.76	0.51
1:N:393:LYS:HA	1:N:418:GLU:HG2	1.93	0.51
1:F:85:THR:HG22	1:F:86:ARG:HB2	1.93	0.51
2:O:127:GLY:O	2:O:128:PHE:HB3	2.11	0.51
1:I:119:THR:HA	1:I:122:THR:HG23	1.92	0.51
1:B:317:ILE:HG22	1:B:319:GLY:N	2.26	0.51
1:J:119:THR:HA	1:J:122:THR:HG23	1.92	0.51
1:N:477:GLN:HG3	1:N:504:SER:OG	2.11	0.51
1:A:201:ASN:HD22	1:A:225:GLN:HB2	1.74	0.51
1:B:122:THR:HG21	1:B:146:HIS:CD2	2.46	0.51
1:F:525:LEU:HD23	1:F:540:LEU:HD21	1.93	0.51
1:J:563:LEU:N	1:J:564:PRO:HD2	2.26	0.51
1:I:373:GLN:HA	1:I:398:LEU:HA	1.93	0.50
1:N:585:ASN:OD1	1:N:588:PHE:HB3	2.11	0.50
1:J:427:VAL:HG21	1:J:432:LEU:HD11	1.93	0.50
1:J:447:LEU:HD21	1:J:450:LEU:HB2	1.93	0.50
2:P:67:PHE:CE2	2:P:69:MET:HE2	2.46	0.50
1:F:314:PRO:HG2	1:F:317:ILE:HD11	1.94	0.50
1:N:563:LEU:N	1:N:564:PRO:HD2	2.27	0.50
1:A:371:ASN:N	1:A:371:ASN:ND2	2.59	0.50
1:M:311:ASN:HD22	2:H:160:ALA:H	1.59	0.50
1:N:596:LEU:HA	1:N:599:LEU:HD12	1.94	0.50
2:H:82:VAL:HG22	2:H:139:LEU:CD2	2.33	0.50
1:A:192:ASP:O	1:A:195:SER:HB3	2.11	0.50
1:E:511:ILE:HG22	1:E:512:ASP:O	2.11	0.50
1:N:192:ASP:O	1:N:195:SER:HB3	2.12	0.50
2:C:84:LEU:HD21	2:C:91:ILE:HD12	1.93	0.50
1:E:317:ILE:HG22	1:E:319:GLY:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:THR:HG21	1:F:146:HIS:CD2	2.46	0.50
1:J:409:LEU:CD1	1:J:430:THR:HG21	2.42	0.50
1:J:537:MET:HG2	1:J:550:MET:HE2	1.94	0.50
1:J:595:ASN:N	1:J:595:ASN:OD1	2.43	0.50
1:B:428:ALA:HB3	3:Y:1:NAG:H82	1.93	0.50
1:N:85:THR:HG22	1:N:86:ARG:HB2	1.92	0.50
1:F:392:LEU:HB3	1:F:395:LEU:HD12	1.94	0.50
1:N:427:VAL:HG21	1:N:432:LEU:HD11	1.94	0.50
1:F:119:THR:HA	1:F:122:THR:HG23	1.93	0.49
1:F:563:LEU:N	1:F:564:PRO:HD2	2.27	0.49
1:M:85:THR:HG22	1:M:86:ARG:HB2	1.92	0.49
1:E:447:LEU:HD23	1:E:471:LEU:HD13	1.93	0.49
1:I:314:PRO:HG2	1:I:317:ILE:HD11	1.93	0.49
1:E:85:THR:HG22	1:E:86:ARG:HB2	1.93	0.49
1:J:314:PRO:HG2	1:J:317:ILE:HD11	1.93	0.49
1:M:424:LEU:HD12	1:M:424:LEU:C	2.33	0.49
1:M:532:LEU:HD22	1:M:536:SER:OG	2.13	0.49
1:M:512:ASP:OD2	1:M:513:GLN:N	2.45	0.49
1:J:592:TYR:CZ	1:J:599:LEU:HD13	2.47	0.49
1:N:119:THR:HA	1:N:122:THR:HG23	1.94	0.49
1:E:413:ASP:HB2	1:E:438:HIS:CD2	2.48	0.49
1:M:363:THR:HG22	1:M:390:LEU:HB3	1.94	0.49
1:N:514:GLN:HG2	1:N:517:HIS:CE1	2.48	0.49
1:N:580:ASP:HB3	1:N:585:ASN:HD22	1.78	0.49
1:E:317:ILE:HG22	1:E:319:GLY:H	1.78	0.49
1:N:114:ILE:HA	2:O:116:GLN:NE2	2.28	0.48
1:N:203:SER:C	1:N:204:LEU:HD12	2.33	0.48
1:A:85:THR:HG22	1:A:86:ARG:HB2	1.94	0.48
1:A:179:ASP:OD1	1:A:181:GLN:NE2	2.45	0.48
1:M:201:ASN:HD22	1:M:225:GLN:HB2	1.76	0.48
1:J:286:PHE:CD1	1:J:289:LEU:HD13	2.47	0.48
1:M:414:GLN:OE1	1:M:443:ASN:ND2	2.47	0.48
1:J:471:LEU:HD23	1:J:498:LEU:HD21	1.95	0.48
1:A:393:LYS:HA	1:A:418:GLU:HG2	1.94	0.48
1:M:388:CYS:HB3	1:M:392:LEU:CD1	2.43	0.48
2:D:86:SER:CB	2:D:91:ILE:HD11	2.44	0.48
2:D:132:GLU:HG3	2:D:158:TYR:CB	2.43	0.48
1:M:486:ILE:HB	1:M:511:ILE:HG23	1.94	0.48
1:N:540:LEU:HD13	1:N:548:LEU:HD13	1.95	0.48
1:E:49:ASP:OD1	1:E:49:ASP:N	2.46	0.48
1:E:264:THR:HG22	1:E:265:SER:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:451:ASN:CB	3:U:1:NAG:C1	2.92	0.48
2:L:36:GLN:HE21	2:L:157:LEU:HD12	1.78	0.48
1:A:569:GLN:HB2	1:A:572:ILE:HD11	1.94	0.48
1:F:398:LEU:O	1:F:421:GLN:CB	2.62	0.48
1:F:424:LEU:HD12	1:F:425:LEU:N	2.28	0.48
1:M:392:LEU:HB3	1:M:395:LEU:HD12	1.96	0.48
1:F:51:LEU:O	1:F:75:ARG:NE	2.46	0.48
3:Y:2:NAG:HO6	4:Z:1:NAG:HO3	1.61	0.48
1:E:119:THR:HA	1:E:122:THR:HG23	1.94	0.47
1:B:119:THR:HA	1:B:122:THR:HG23	1.95	0.47
1:B:458:ASP:OD2	1:B:458:ASP:C	2.51	0.47
1:E:469:GLN:CD	1:E:469:GLN:N	2.67	0.47
1:B:49:ASP:OD1	1:B:49:ASP:N	2.46	0.47
1:F:179:ASP:OD1	1:F:181:GLN:NE2	2.47	0.47
1:F:447:LEU:CD2	1:F:450:LEU:HD13	2.42	0.47
1:N:442:GLN:HA	1:N:467:GLY:HA3	1.96	0.47
2:K:62:ASN:HD22	2:K:124:ASN:HA	1.78	0.47
2:K:67:PHE:CE2	2:K:69:MET:HE2	2.50	0.47
1:A:509:LEU:HD23	1:A:531:SER:HB2	1.95	0.47
1:E:452:LEU:HA	1:E:455:CYS:SG	2.54	0.47
1:I:424:LEU:HD12	1:I:425:LEU:N	2.30	0.47
1:M:311:ASN:ND2	2:H:160:ALA:H	2.12	0.47
1:J:317:ILE:HG22	1:J:319:GLY:N	2.28	0.47
1:J:434:VAL:HG13	1:J:438:HIS:HB2	1.97	0.47
2:G:92:LEU:HD13	2:G:92:LEU:C	2.35	0.47
1:J:202:LEU:HG	1:J:204:LEU:HD11	1.96	0.47
1:M:495:VAL:O	1:M:495:VAL:HG23	2.13	0.47
1:J:447:LEU:HD23	1:J:471:LEU:CD1	2.45	0.47
1:N:225:GLN:HG3	1:N:248:GLN:HE21	1.80	0.47
1:N:424:LEU:HD12	1:N:425:LEU:N	2.29	0.47
1:N:537:MET:CE	1:N:550:MET:CE	2.92	0.47
1:B:563:LEU:N	1:B:564:PRO:HD2	2.30	0.47
1:N:495:VAL:HG23	1:N:495:VAL:O	2.14	0.47
1:M:179:ASP:OD1	1:M:181:GLN:NE2	2.48	0.47
1:B:256:GLU:HG2	1:B:283:LYS:NZ	2.30	0.47
1:B:283:LYS:HA	1:B:307:ALA:O	2.15	0.47
1:N:364:ARG:O	1:N:367:GLU:HB3	2.15	0.47
1:N:415:ALA:HB3	1:N:416:PHE:CD1	2.50	0.47
2:D:36:GLN:HE21	2:D:157:LEU:HD12	1.79	0.47
1:E:399:GLN:NE2	1:E:423:GLU:OE2	2.46	0.47
1:N:201:ASN:HD22	1:N:225:GLN:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:179:ASP:OD1	1:I:181:GLN:NE2	2.47	0.46
2:L:67:PHE:CE2	2:L:69:MET:HE2	2.48	0.46
1:E:459:THR:HG22	1:E:491:LEU:HD11	1.96	0.46
1:M:391:GLN:OE1	1:M:391:GLN:N	2.43	0.46
1:B:317:ILE:HG22	1:B:319:GLY:H	1.79	0.46
1:F:592:TYR:CE1	1:F:599:LEU:HD13	2.50	0.46
2:L:63:ILE:HG22	2:L:125:ASN:OD1	2.16	0.46
1:F:462:GLN:O	1:F:494:MET:HE2	2.16	0.46
1:N:225:GLN:CG	1:N:248:GLN:HE21	2.28	0.46
1:N:537:MET:HE2	1:N:550:MET:HE2	1.96	0.46
1:N:563:LEU:HD21	1:N:591:TRP:HB2	1.96	0.46
1:E:192:ASP:O	1:E:195:SER:HB3	2.15	0.46
1:B:41:ASN:OD1	2:D:72:ARG:NH1	2.48	0.46
1:B:201:ASN:HD22	1:B:225:GLN:HB2	1.79	0.46
1:F:537:MET:HA	1:F:540:LEU:HD12	1.98	0.46
2:C:135:TYR:HB2	2:C:156:VAL:HB	1.97	0.46
1:J:592:TYR:CD1	1:J:599:LEU:HD13	2.51	0.46
1:N:235:LEU:HD12	1:N:263:LEU:HD21	1.98	0.46
1:E:201:ASN:HD22	1:E:225:GLN:HB2	1.80	0.46
1:I:68:ILE:HD11	1:I:84:LEU:HD13	1.97	0.46
1:F:264:THR:HG22	1:F:265:SER:N	2.30	0.46
1:N:564:PRO:HA	1:N:567:SER:OG	2.16	0.46
2:C:67:PHE:CE2	2:C:69:MET:HE2	2.51	0.46
2:C:84:LEU:CD2	2:C:91:ILE:CD1	2.94	0.46
1:I:264:THR:HG22	1:I:265:SER:N	2.31	0.46
1:F:491:LEU:HD12	1:F:492:LEU:N	2.30	0.46
1:J:192:ASP:O	1:J:195:SER:HB3	2.16	0.46
2:L:84:LEU:HD12	2:L:137:VAL:HG22	1.98	0.46
1:F:201:ASN:HD22	1:F:225:GLN:HB2	1.81	0.46
1:J:491:LEU:HD13	1:J:492:LEU:HD23	1.98	0.46
1:A:431:HIS:CE1	1:A:456:LEU:HD22	2.51	0.46
1:M:257:ASP:OD2	1:M:257:ASP:N	2.49	0.46
1:F:572:ILE:N	1:F:572:ILE:HD12	2.31	0.46
1:N:172:THR:OG1	1:N:198:GLN:HB2	2.16	0.46
1:N:202:LEU:HG	1:N:204:LEU:HD11	1.98	0.46
1:B:192:ASP:O	1:B:195:SER:HB3	2.16	0.46
1:N:592:TYR:CZ	1:N:599:LEU:HD13	2.51	0.45
2:L:84:LEU:HD23	2:L:91:ILE:HB	1.98	0.45
4:T:5:MAN:C1	4:T:6:MAN:O2	2.64	0.45
1:B:202:LEU:HG	1:B:204:LEU:HD11	1.97	0.45
2:C:63:ILE:HG22	2:C:125:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:THR:HG22	1:B:265:SER:N	2.32	0.45
1:N:485:SER:HB2	1:N:510:SER:OG	2.17	0.45
1:A:68:ILE:HD11	1:A:84:LEU:HD13	1.98	0.45
1:E:469:GLN:H	1:E:469:GLN:NE2	2.14	0.45
1:E:511:ILE:HD11	1:E:527:LEU:HD13	1.99	0.45
1:B:450:LEU:HD11	1:B:452:LEU:HD21	1.99	0.45
1:F:537:MET:HB2	1:F:562:LEU:HD13	1.99	0.45
1:F:533:THR:O	1:F:534:GLY:C	2.54	0.45
1:J:450:LEU:CD1	1:J:452:LEU:HD21	2.31	0.45
2:C:84:LEU:HD23	2:C:91:ILE:CD1	2.46	0.45
1:A:257:ASP:OD2	1:A:257:ASP:N	2.46	0.45
1:E:203:SER:C	1:E:204:LEU:HD12	2.37	0.45
1:M:459:THR:HG22	1:M:491:LEU:HD21	1.98	0.45
1:N:68:ILE:HD11	1:N:84:LEU:HD13	1.99	0.45
1:N:122:THR:HG21	1:N:146:HIS:CD2	2.52	0.45
1:M:68:ILE:HD11	1:M:84:LEU:HD13	1.98	0.45
1:M:571:ILE:C	1:M:572:ILE:HD12	2.36	0.45
1:F:204:LEU:HD23	1:F:206:PHE:CZ	2.52	0.45
1:J:172:THR:OG1	1:J:198:GLN:HB2	2.16	0.45
1:J:447:LEU:HD23	1:J:471:LEU:HD13	1.99	0.45
2:H:87:LYS:O	2:H:89:LEU:N	2.46	0.45
2:H:67:PHE:CE2	2:H:69:MET:HE2	2.50	0.45
1:F:613:LEU:O	1:F:616:VAL:HG23	2.16	0.45
1:J:387:CYS:O	1:J:415:ALA:HB1	2.15	0.45
1:J:439:SER:OG	1:J:466:ALA:HB3	2.16	0.45
1:N:239:PHE:O	1:N:274:MET:HE1	2.17	0.45
2:D:84:LEU:HD12	2:D:137:VAL:HG22	1.99	0.45
1:N:537:MET:CG	1:N:550:MET:HE1	2.46	0.45
2:P:64:ASN:HD22	2:P:122:PRO:HA	1.82	0.45
1:A:427:VAL:HG22	1:A:452:LEU:HD23	2.00	0.44
1:I:49:ASP:OD1	1:I:49:ASP:N	2.47	0.44
1:B:347:LEU:HB3	1:B:369:LEU:HD22	1.99	0.44
1:F:580:ASP:OD2	1:F:609:ASN:ND2	2.51	0.44
1:J:530:ASN:O	1:J:553:ASN:HA	2.17	0.44
1:M:192:ASP:O	1:M:195:SER:HB3	2.18	0.44
1:B:172:THR:OG1	1:B:198:GLN:HB2	2.17	0.44
1:B:513:GLN:HG3	1:B:538:ASP:OD2	2.17	0.44
1:B:537:MET:CG	1:B:550:MET:CE	2.96	0.44
1:N:413:ASP:HB2	1:N:438:HIS:CD2	2.52	0.44
1:M:242:LEU:HB2	1:M:274:MET:CE	2.34	0.44
1:N:593:LYS:HE2	1:N:619:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:LEU:HD12	1:I:175:LEU:HA	1.85	0.44
1:M:428:ALA:HB3	3:W:1:NAG:H82	1.99	0.44
1:F:49:ASP:OD1	1:F:49:ASP:N	2.50	0.44
1:N:122:THR:CG2	1:N:146:HIS:CD2	3.01	0.44
1:N:540:LEU:HD13	1:N:548:LEU:CD1	2.47	0.44
1:A:202:LEU:HG	1:A:204:LEU:HD11	1.99	0.44
1:A:416:PHE:HB2	1:A:444:LEU:HD21	2.00	0.44
1:J:137:ILE:O	1:J:159:ASN:HB3	2.18	0.44
2:K:134:ASP:OD1	2:K:134:ASP:N	2.49	0.44
1:F:452:LEU:CD1	1:F:457:LEU:HD11	2.42	0.44
1:N:424:LEU:HD12	1:N:424:LEU:C	2.38	0.44
1:A:348:ARG:CG	1:A:373:GLN:HE21	2.31	0.44
1:E:196:LEU:N	1:E:196:LEU:HD23	2.32	0.44
1:E:437:PRO:HA	1:E:461:ASN:OD1	2.18	0.44
1:M:427:VAL:HG23	1:M:455:CYS:SG	2.58	0.44
1:B:452:LEU:HD13	1:B:457:LEU:HD11	1.99	0.44
1:A:32:GLU:HG3	1:A:33:GLY:N	2.33	0.43
2:G:62:ASN:HD22	2:G:124:ASN:HA	1.83	0.43
1:A:172:THR:OG1	1:A:198:GLN:HB2	2.18	0.43
1:A:563:LEU:HD21	1:A:588:PHE:HA	2.00	0.43
1:E:202:LEU:HG	1:E:204:LEU:HD11	1.99	0.43
1:E:235:LEU:HD12	1:E:263:LEU:HD21	2.00	0.43
1:M:348:ARG:CG	1:M:373:GLN:HE21	2.32	0.43
1:F:122:THR:CG2	1:F:146:HIS:CD2	3.00	0.43
1:F:468:LEU:HB2	1:F:495:VAL:HG12	2.00	0.43
1:N:55:THR:HB	1:N:76:LEU:HD22	2.00	0.43
1:M:459:THR:HB	1:M:491:LEU:HD23	2.00	0.43
1:F:465:LEU:HB3	1:F:495:VAL:HG13	1.99	0.43
1:J:505:SER:HA	1:J:529:HIS:O	2.18	0.43
3:U:1:NAG:O4	4:V:1:NAG:H83	2.18	0.43
4:V:5:MAN:C1	4:V:6:MAN:O2	2.66	0.43
1:A:428:ALA:HB3	3:Q:1:NAG:H82	2.00	0.43
1:E:424:LEU:HD12	1:E:424:LEU:C	2.38	0.43
1:M:491:LEU:C	1:M:491:LEU:HD12	2.39	0.43
1:B:461:ASN:O	1:B:463:HIS:N	2.51	0.43
1:F:454:HIS:CE1	1:F:477:GLN:HG2	2.52	0.43
1:A:217:GLY:O	1:A:220:ILE:HG13	2.18	0.43
1:F:172:THR:OG1	1:F:198:GLN:HB2	2.18	0.43
1:J:49:ASP:OD1	1:J:49:ASP:N	2.51	0.43
1:N:242:LEU:HB2	1:N:274:MET:HE1	1.99	0.43
1:N:571:ILE:C	1:N:572:ILE:HD12	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:THR:CG2	1:E:491:LEU:HD11	2.48	0.43
1:I:203:SER:C	1:I:204:LEU:HD12	2.39	0.43
1:I:348:ARG:CG	1:I:373:GLN:HE21	2.26	0.43
1:N:49:ASP:OD1	1:N:49:ASP:N	2.51	0.43
1:E:137:ILE:O	1:E:159:ASN:HB3	2.19	0.43
1:E:434:VAL:CG2	1:E:464:LEU:HD11	2.42	0.43
1:B:204:LEU:HD23	1:B:206:PHE:CZ	2.53	0.43
1:F:394:ASN:H	1:F:418:GLU:HG2	1.84	0.43
1:A:559:PRO:HA	1:A:560:PRO:HD3	1.93	0.43
1:I:172:THR:OG1	1:I:198:GLN:HB2	2.19	0.43
1:F:62:PHE:CE2	1:F:86:ARG:HG2	2.54	0.43
1:F:519:LEU:O	1:F:521:ASN:N	2.52	0.43
1:J:385:SER:O	1:J:387:CYS:N	2.44	0.43
1:N:68:ILE:HG21	1:N:68:ILE:HD13	1.71	0.43
1:I:204:LEU:HD23	1:I:206:PHE:CZ	2.53	0.43
1:J:179:ASP:OD1	1:J:181:GLN:NE2	2.52	0.43
2:D:59:LEU:HD23	2:D:128:PHE:CE2	2.54	0.43
1:E:461:ASN:ND2	1:E:464:LEU:HD12	2.23	0.42
1:I:47:ILE:HG23	1:I:51:LEU:HD12	2.00	0.42
1:I:192:ASP:O	1:I:195:SER:HB3	2.18	0.42
1:F:192:ASP:O	1:F:195:SER:HB3	2.19	0.42
1:A:427:VAL:HG23	1:A:455:CYS:SG	2.59	0.42
1:E:450:LEU:HB3	1:E:471:LEU:HD21	2.00	0.42
1:A:558:ILE:HG22	1:A:563:LEU:HD13	2.02	0.42
1:E:495:VAL:HG23	1:E:495:VAL:O	2.19	0.42
1:A:264:THR:HG22	1:A:266:ALA:H	1.82	0.42
1:M:203:SER:C	1:M:204:LEU:HD12	2.40	0.42
1:M:388:CYS:HB3	1:M:392:LEU:HD12	2.01	0.42
1:B:91:TRP:CH2	2:C:48:PHE:HA	2.55	0.42
1:B:122:THR:HG22	1:B:146:HIS:HB3	2.02	0.42
1:A:413:ASP:O	1:A:414:GLN:C	2.58	0.42
1:A:462:GLN:OE1	1:A:490:ASN:C	2.57	0.42
1:M:119:THR:CA	1:M:122:THR:HG23	2.48	0.42
1:M:164:ILE:CG2	1:M:185:ILE:HD13	2.50	0.42
1:M:311:ASN:CB	2:H:132:GLU:HB3	2.50	0.42
1:N:537:MET:HE3	1:N:550:MET:HE2	2.01	0.42
2:H:57:ARG:NE	2:H:132:GLU:HG3	2.35	0.42
1:I:235:LEU:HD12	1:I:263:LEU:HD21	2.01	0.42
1:M:403:LEU:HD13	1:M:409:LEU:HD11	2.01	0.42
1:M:473:HIS:CD2	1:M:500:ILE:HD12	2.55	0.42
1:M:501:LEU:HD21	1:M:503:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:PRO:HA	1:B:567:SER:OG	2.20	0.42
2:H:84:LEU:HD12	2:H:137:VAL:HG22	2.01	0.42
1:A:497:SER:O	1:A:498:LEU:C	2.58	0.42
1:E:172:THR:OG1	1:E:198:GLN:HB2	2.18	0.42
1:A:564:PRO:HA	1:A:567:SER:OG	2.20	0.42
1:M:49:ASP:OD1	1:M:49:ASP:N	2.51	0.42
1:J:264:THR:HG22	1:J:265:SER:N	2.34	0.42
1:J:473:HIS:CD2	1:J:500:ILE:HD12	2.55	0.42
1:E:512:ASP:OD1	1:E:513:GLN:N	2.52	0.42
1:I:68:ILE:HD13	1:I:68:ILE:HG21	1.77	0.42
1:M:202:LEU:HG	1:M:204:LEU:HD11	2.02	0.42
1:B:537:MET:HB2	1:B:562:LEU:HD13	2.02	0.42
1:J:122:THR:HG21	1:J:146:HIS:CD2	2.54	0.42
2:K:143:ASN:OD1	2:K:143:ASN:C	2.58	0.42
1:A:49:ASP:OD1	1:A:49:ASP:N	2.53	0.42
1:E:474:LEU:HB2	1:E:498:LEU:HD21	2.01	0.42
1:M:137:ILE:O	1:M:159:ASN:HB3	2.20	0.42
1:B:559:PRO:HA	1:B:560:PRO:HD3	1.93	0.42
1:J:204:LEU:HD23	1:J:206:PHE:CZ	2.55	0.42
1:F:449:VAL:HG22	1:F:473:HIS:HB3	2.02	0.41
1:N:126:PHE:HA	1:N:150:ASN:HD22	1.85	0.41
2:O:59:LEU:HA	2:O:59:LEU:HD12	1.84	0.41
2:O:64:ASN:HD22	2:O:122:PRO:HA	1.85	0.41
1:E:47:ILE:HG23	1:E:51:LEU:HD12	2.02	0.41
1:E:459:THR:OG1	1:E:480:SER:O	2.28	0.41
1:I:201:ASN:HD22	1:I:225:GLN:HB2	1.85	0.41
1:M:48:PRO:HD2	1:M:51:LEU:HD12	2.02	0.41
1:B:399:GLN:NE2	1:B:423:GLU:OE2	2.52	0.41
1:J:391:GLN:OE1	1:J:391:GLN:N	2.51	0.41
1:N:449:VAL:HG22	1:N:473:HIS:HB3	2.01	0.41
2:D:84:LEU:HD23	2:D:91:ILE:CD1	2.50	0.41
1:A:392:LEU:HD13	1:A:419:CYS:SG	2.60	0.41
1:M:564:PRO:HA	1:M:567:SER:OG	2.20	0.41
1:F:394:ASN:N	1:F:418:GLU:HG2	2.34	0.41
1:J:424:LEU:HD12	1:J:425:LEU:N	2.34	0.41
1:J:431:HIS:CD2	1:J:456:LEU:HD13	2.55	0.41
1:J:591:TRP:NE1	1:J:595:ASN:ND2	2.69	0.41
1:N:447:LEU:HD21	1:N:450:LEU:HD13	2.01	0.41
1:E:235:LEU:HD12	1:E:263:LEU:CD2	2.50	0.41
1:E:384:ALA:HB3	1:E:409:LEU:HD21	1.98	0.41
1:E:511:ILE:CG2	1:E:515:ALA:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:204:LEU:HD23	1:M:206:PHE:CZ	2.56	0.41
1:J:235:LEU:HD12	1:J:263:LEU:HD21	2.02	0.41
1:J:473:HIS:CD2	1:J:500:ILE:CD1	3.04	0.41
2:O:86:SER:CB	2:O:91:ILE:HD11	2.47	0.41
1:E:175:LEU:HD12	1:E:175:LEU:HA	1.85	0.41
1:E:477:GLN:O	1:E:479:ASN:ND2	2.54	0.41
1:E:564:PRO:HA	1:E:567:SER:OG	2.21	0.41
1:B:481:PHE:CD1	1:B:508:LEU:HD21	2.55	0.41
1:F:407:GLU:HB3	1:F:408:PRO:HD2	2.03	0.41
1:I:202:LEU:HG	1:I:204:LEU:HD11	2.02	0.41
1:B:466:ALA:CA	1:B:494:MET:HG2	2.51	0.41
1:F:203:SER:C	1:F:204:LEU:HD12	2.41	0.41
1:J:443:ASN:OD1	1:J:443:ASN:N	2.54	0.41
1:J:537:MET:HG2	1:J:550:MET:CE	2.50	0.41
1:N:47:ILE:HG23	1:N:51:LEU:HD12	2.03	0.41
1:M:341:ALA:HB1	1:M:369:LEU:HD21	2.03	0.41
1:M:449:VAL:HG22	1:M:473:HIS:HB3	2.01	0.41
1:B:468:LEU:HB2	1:B:495:VAL:HG12	2.02	0.41
1:F:523:ASN:HA	1:F:546:LEU:HB3	2.03	0.41
1:M:572:ILE:HD12	1:M:572:ILE:N	2.36	0.41
1:F:537:MET:CE	1:F:566:LEU:HD11	2.50	0.41
1:F:537:MET:CE	1:F:566:LEU:HD21	2.47	0.41
1:F:596:LEU:HA	1:F:599:LEU:HD12	2.02	0.41
1:A:175:LEU:HD12	1:A:175:LEU:HA	1.90	0.41
1:A:361:LEU:HD21	1:A:382:ILE:HD13	2.02	0.41
1:E:509:LEU:HD23	1:E:531:SER:HB2	2.03	0.41
1:M:511:ILE:HG22	1:M:515:ALA:HB3	2.02	0.41
1:B:122:THR:CG2	1:B:146:HIS:CD2	3.04	0.41
1:B:464:LEU:HD23	1:B:491:LEU:HD23	2.03	0.41
1:B:478:GLY:HA2	1:B:505:SER:O	2.21	0.41
1:F:235:LEU:HD12	1:F:263:LEU:HD21	2.03	0.41
1:J:68:ILE:HD11	1:J:84:LEU:HD13	2.02	0.41
1:J:572:ILE:HB	1:J:599:LEU:HD23	2.03	0.41
1:N:514:GLN:HA	1:N:517:HIS:CD2	2.56	0.41
2:C:69:MET:HE2	2:C:69:MET:HB3	1.94	0.41
2:D:86:SER:HB2	2:D:91:ILE:HD11	2.02	0.41
2:L:84:LEU:HD23	2:L:91:ILE:CG2	2.50	0.41
1:I:137:ILE:O	1:I:159:ASN:HB3	2.21	0.41
1:I:264:THR:HG22	1:I:266:ALA:H	1.86	0.41
1:M:416:PHE:HB2	1:M:444:LEU:HD21	2.03	0.41
1:J:369:LEU:HD13	1:J:372:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:84:LEU:HD12	2:G:137:VAL:HG22	2.03	0.41
1:A:242:LEU:HB2	1:A:274:MET:CE	2.51	0.40
1:E:239:PHE:CE1	1:E:271:LEU:HD13	2.56	0.40
1:E:407:GLU:HB3	1:E:408:PRO:HD2	2.03	0.40
1:M:166:LEU:HB2	1:M:195:SER:OG	2.20	0.40
1:M:172:THR:OG1	1:M:198:GLN:HB2	2.21	0.40
1:B:242:LEU:HB2	1:B:274:MET:HE1	2.03	0.40
1:F:68:ILE:HD13	1:F:68:ILE:HG21	1.75	0.40
2:O:67:PHE:CE2	2:O:69:MET:HE2	2.55	0.40
1:A:572:ILE:N	1:A:572:ILE:HD12	2.37	0.40
1:M:378:SER:HB2	4:X:1:NAG:H62	2.04	0.40
1:J:464:LEU:HA	1:J:464:LEU:HD12	1.60	0.40
1:E:68:ILE:HD11	1:E:84:LEU:HD13	2.02	0.40
1:I:235:LEU:HD12	1:I:263:LEU:CD2	2.51	0.40
1:I:407:GLU:HB3	1:I:408:PRO:HD2	2.04	0.40
1:B:164:ILE:HG21	1:B:206:PHE:HE1	1.87	0.40
1:B:537:MET:HG2	1:B:550:MET:CE	2.51	0.40
1:F:239:PHE:HA	1:F:274:MET:HE1	2.02	0.40
1:F:564:PRO:HA	1:F:567:SER:OG	2.21	0.40
1:N:361:LEU:HD21	1:N:382:ILE:HD13	2.02	0.40
1:N:478:GLY:HA2	1:N:505:SER:O	2.21	0.40
2:O:84:LEU:HD12	2:O:137:VAL:HG22	2.02	0.40
1:E:371:ASN:N	1:E:371:ASN:ND2	2.69	0.40
1:E:439:SER:HB3	1:E:466:ALA:HB3	2.03	0.40
1:B:70:ASN:OD1	1:B:71:THR:HG23	2.21	0.40
1:B:175:LEU:HD12	1:B:175:LEU:HA	1.92	0.40
1:J:219:PHE:CD1	1:J:242:LEU:HD23	2.56	0.40
1:J:361:LEU:HD21	1:J:382:ILE:HD13	2.03	0.40
2:G:82:VAL:HG22	2:G:139:LEU:CD2	2.43	0.40
2:L:82:VAL:HG22	2:L:139:LEU:CD2	2.43	0.40
1:E:559:PRO:HA	1:E:560:PRO:HD3	1.93	0.40
1:M:235:LEU:HD12	1:M:263:LEU:HD21	2.03	0.40
1:M:239:PHE:CE1	1:M:271:LEU:HD13	2.56	0.40
1:F:424:LEU:HD12	1:F:424:LEU:C	2.40	0.40
1:N:219:PHE:CD2	1:N:227:LEU:HD11	2.57	0.40
2:C:143:ASN:OD1	2:C:143:ASN:C	2.60	0.40
2:O:27:HIS:HB2	2:O:39:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.



## 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	592/612 (97%)	552 (93%)	36 (6%)	4 (1%)	22	53
1	B	597/612 (98%)	556 (93%)	38 (6%)	3 (0%)	29	60
1	E	590/612 (96%)	544 (92%)	43 (7%)	3 (0%)	29	60
1	F	597/612 (98%)	557 (93%)	37 (6%)	3 (0%)	29	60
1	I	383/612 (63%)	361 (94%)	21 (6%)	1 (0%)	41	70
1	J	597/612 (98%)	553 (93%)	39 (6%)	5 (1%)	19	49
1	M	591/612 (97%)	546 (92%)	43 (7%)	2 (0%)	41	70
1	N	597/612 (98%)	560 (94%)	35 (6%)	2 (0%)	41	70
2	C	136/147 (92%)	125 (92%)	8 (6%)	3 (2%)	6	23
2	D	134/147 (91%)	125 (93%)	8 (6%)	1 (1%)	22	53
2	G	136/147 (92%)	127 (93%)	6 (4%)	3 (2%)	6	23
2	H	136/147 (92%)	126 (93%)	9 (7%)	1 (1%)	22	53
2	K	132/147 (90%)	125 (95%)	6 (4%)	1 (1%)	19	49
2	L	136/147 (92%)	127 (93%)	8 (6%)	1 (1%)	22	53
2	O	136/147 (92%)	129 (95%)	6 (4%)	1 (1%)	22	53
2	P	133/147 (90%)	123 (92%)	9 (7%)	1 (1%)	19	49
All	All	5623/6072 (93%)	5236 (93%)	352 (6%)	35 (1%)	25	57

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	494	MET
1	J	438	HIS
1	J	534	GLY
1	N	494	MET
2	C	128	PHE
2	O	128	PHE

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Mol	Chain	Res	Type
1	A	494	MET
1	A	498	LEU
1	J	484	GLY
2	G	88	GLY
1	A	33	GLY
1	E	461	ASN
1	B	461	ASN
1	B	462	GLN
1	J	493	GLN
1	A	412	GLU
1	E	412	GLU
1	B	33	GLY
1	F	520	ARG
2	D	91	ILE
2	G	23	ALA
1	F	493	GLN
1	J	33	GLY
2	C	86	SER
2	G	89	LEU
2	K	86	SER
2	L	91	ILE
1	E	33	GLY
1	I	33	GLY
1	M	33	GLY
2	C	126	PRO
2	P	130	ILE
1	F	33	GLY
1	N	33	GLY
2	H	88	GLY

### 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	481/561 (86%)	455 (95%)	26 (5%)	22	52
1	B	516/561 (92%)	484 (94%)	32 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	463/561 (82%)	445 (96%)	18 (4%)	32	64
1	F	488/561 (87%)	457 (94%)	31 (6%)	17	44
1	I	304/561 (54%)	291 (96%)	13 (4%)	29	61
1	J	478/561 (85%)	454 (95%)	24 (5%)	24	55
1	M	481/561 (86%)	449 (93%)	32 (7%)	16	41
1	N	511/561 (91%)	484 (95%)	27 (5%)	22	53
2	C	102/125 (82%)	98 (96%)	4 (4%)	32	64
2	D	103/125 (82%)	98 (95%)	5 (5%)	25	56
2	G	103/125 (82%)	98 (95%)	5 (5%)	25	56
2	H	105/125 (84%)	98 (93%)	7 (7%)	16	41
2	K	98/125 (78%)	92 (94%)	6 (6%)	18	46
2	L	106/125 (85%)	99 (93%)	7 (7%)	16	42
2	O	102/125 (82%)	96 (94%)	6 (6%)	19	48
2	P	99/125 (79%)	96 (97%)	3 (3%)	41	73
All	All	4540/5488 (83%)	4294 (95%)	246 (5%)	22	52

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	A	49	ASP
1	A	74	SER
1	A	122	THR
1	A	178	LEU
1	A	203	SER
1	A	272	CYS
1	A	275	SER
1	A	298	THR
1	A	344	PHE
1	A	371	ASN
1	A	387	CYS
1	A	424	LEU
1	A	434	VAL
1	A	443	ASN
1	A	469	GLN
1	A	473	HIS
1	A	487	SER

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Mol	Chain	Res	Type
1	A	489	THR
1	A	491	LEU
1	A	513	GLN
1	A	523	ASN
1	A	546	LEU
1	A	563	LEU
1	A	584	SER
1	A	612	SER
1	E	49	ASP
1	E	68	ILE
1	E	118	GLU
1	E	122	THR
1	E	178	LEU
1	E	203	SER
1	E	220	ILE
1	E	295	ARG
1	E	298	THR
1	E	344	PHE
1	E	357	ARG
1	E	424	LEU
1	E	443	ASN
1	E	449	VAL
1	E	456	LEU
1	E	489	THR
1	E	494	MET
1	E	546	LEU
1	I	49	ASP
1	I	102	GLN
1	I	122	THR
1	I	149	GLU
1	I	168	GLU
1	I	178	LEU
1	I	203	SER
1	I	243	GLN
1	I	260	ASP
1	I	292	SER
1	I	298	THR
1	I	344	PHE
1	I	424	LEU
1	M	26	PRO
1	M	49	ASP
1	M	74	SER

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Mol	Chain	Res	Type
1	M	122	THR
1	M	149	GLU
1	M	178	LEU
1	M	220	ILE
1	M	240	LYS
1	M	259	ASP
1	M	272	CYS
1	M	298	THR
1	M	299	ARG
1	M	344	PHE
1	M	346	SER
1	M	357	ARG
1	M	364	ARG
1	M	367	GLU
1	M	385	SER
1	M	392	LEU
1	M	424	LEU
1	M	442	GLN
1	M	443	ASN
1	M	469	GLN
1	M	473	HIS
1	M	489	THR
1	M	507	ASN
1	M	509	LEU
1	M	521	ASN
1	M	523	ASN
1	M	531	SER
1	M	546	LEU
1	M	609	ASN
1	B	32	GLU
1	B	49	ASP
1	B	122	THR
1	B	149	GLU
1	B	178	LEU
1	B	203	SER
1	B	221	SER
1	B	256	GLU
1	B	261	GLN
1	B	298	THR
1	B	335	GLN
1	B	344	PHE
1	B	348	ARG

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Mol	Chain	Res	Type
1	B	385	SER
1	B	393	LYS
1	B	413	ASP
1	B	456	LEU
1	B	469	GLN
1	B	473	HIS
1	B	489	THR
1	B	491	LEU
1	B	513	GLN
1	B	521	ASN
1	B	522	VAL
1	B	523	ASN
1	B	531	SER
1	B	546	LEU
1	B	584	SER
1	B	596	LEU
1	B	604	GLU
1	B	609	ASN
1	B	612	SER
1	F	49	ASP
1	F	54	THR
1	F	99	SER
1	F	122	THR
1	F	149	GLU
1	F	178	LEU
1	F	196	LEU
1	F	203	SER
1	F	243	GLN
1	F	260	ASP
1	F	288	ASP
1	F	298	THR
1	F	344	PHE
1	F	357	ARG
1	F	418	GLU
1	F	424	LEU
1	F	446	LEU
1	F	456	LEU
1	F	473	HIS
1	F	485	SER
1	F	489	THR
1	F	491	LEU
1	F	510	SER

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Mol	Chain	Res	Type
1	F	513	GLN
1	F	535	ASP
1	F	546	LEU
1	F	596	LEU
1	F	609	ASN
1	F	612	SER
1	F	614	ARG
1	F	618	LEU
1	J	49	ASP
1	J	122	THR
1	J	178	LEU
1	J	203	SER
1	J	256	GLU
1	J	288	ASP
1	J	298	THR
1	J	344	PHE
1	J	399	GLN
1	J	421	GLN
1	J	424	LEU
1	J	443	ASN
1	J	485	SER
1	J	487	SER
1	J	489	THR
1	J	491	LEU
1	J	494	MET
1	J	538	ASP
1	J	546	LEU
1	J	584	SER
1	J	595	ASN
1	J	596	LEU
1	J	612	SER
1	J	618	LEU
1	N	49	ASP
1	N	68	ILE
1	N	122	THR
1	N	149	GLU
1	N	178	LEU
1	N	197	GLU
1	N	203	SER
1	N	223	ILE
1	N	292	SER
1	N	298	THR

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Mol	Chain	Res	Type
1	N	344	PHE
1	N	348	ARG
1	N	353	LYS
1	N	385	SER
1	N	393	LYS
1	N	419	CYS
1	N	424	LEU
1	N	473	HIS
1	N	482	GLN
1	N	483	ASP
1	N	489	THR
1	N	491	LEU
1	N	513	GLN
1	N	523	ASN
1	N	546	LEU
1	N	596	LEU
1	N	612	SER
2	C	84	LEU
2	C	91	ILE
2	C	113	LYS
2	C	146	HIS
2	D	84	LEU
2	D	90	SER
2	D	113	LYS
2	D	130	ILE
2	D	146	HIS
2	G	42	CYS
2	G	84	LEU
2	G	92	LEU
2	G	113	LYS
2	G	146	HIS
2	H	55	CYS
2	H	58	GLN
2	H	84	LEU
2	H	86	SER
2	H	90	SER
2	H	113	LYS
2	H	146	HIS
2	K	59	LEU
2	K	84	LEU
2	K	90	SER
2	K	113	LYS

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Mol	Chain	Res	Type
2	K	134	ASP
2	K	146	HIS
2	L	42	CYS
2	L	55	CYS
2	L	62	ASN
2	L	84	LEU
2	L	90	SER
2	L	113	LYS
2	L	146	HIS
2	O	59	LEU
2	O	84	LEU
2	O	113	LYS
2	O	125	ASN
2	O	128	PHE
2	O	146	HIS
2	P	84	LEU
2	P	113	LYS
2	P	146	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	102	GLN
1	A	104	ASN
1	A	181	GLN
1	A	201	ASN
1	A	225	GLN
1	A	311	ASN
1	A	371	ASN
1	A	373	GLN
1	A	431	HIS
1	A	443	ASN
1	A	469	GLN
1	A	482	GLN
1	A	523	ASN
1	E	34	ASN
1	E	104	ASN
1	E	181	GLN
1	E	201	ASN
1	E	225	GLN
1	E	248	GLN

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Mol	Chain	Res	Type
1	E	311	ASN
1	E	371	ASN
1	E	373	GLN
1	E	433	HIS
1	E	438	HIS
1	E	461	ASN
1	E	469	GLN
1	E	477	GLN
1	I	102	GLN
1	I	104	ASN
1	I	146	HIS
1	I	181	GLN
1	I	201	ASN
1	I	225	GLN
1	I	243	GLN
1	I	311	ASN
1	I	373	GLN
1	M	101	HIS
1	M	104	ASN
1	M	181	GLN
1	M	201	ASN
1	M	225	GLN
1	M	311	ASN
1	M	371	ASN
1	M	373	GLN
1	M	414	GLN
1	M	421	GLN
1	M	443	ASN
1	M	517	HIS
1	M	523	ASN
1	M	529	HIS
1	B	104	ASN
1	B	146	HIS
1	B	150	ASN
1	B	181	GLN
1	B	201	ASN
1	B	225	GLN
1	B	261	GLN
1	B	311	ASN
1	B	373	GLN
1	B	445	HIS
1	B	469	GLN

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Mol	Chain	Res	Type
1	B	514	GLN
1	B	517	HIS
1	B	523	ASN
1	B	609	ASN
1	F	104	ASN
1	F	146	HIS
1	F	150	ASN
1	F	181	GLN
1	F	201	ASN
1	F	225	GLN
1	F	311	ASN
1	F	462	GLN
1	F	477	GLN
1	F	493	GLN
1	F	568	GLN
1	F	597	HIS
1	J	104	ASN
1	J	146	HIS
1	J	150	ASN
1	J	181	GLN
1	J	201	ASN
1	J	225	GLN
1	J	311	ASN
1	J	462	GLN
1	J	477	GLN
1	J	597	HIS
1	J	609	ASN
1	N	104	ASN
1	N	146	HIS
1	N	150	ASN
1	N	181	GLN
1	N	186	HIS
1	N	201	ASN
1	N	225	GLN
1	N	248	GLN
1	N	261	GLN
1	N	311	ASN
1	N	373	GLN
1	N	477	GLN
1	N	493	GLN
1	N	517	HIS
1	N	523	ASN

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Mol	Chain	Res	Type
2	C	62	ASN
2	C	64	ASN
2	D	36	GLN
2	D	62	ASN
2	D	64	ASN
2	G	36	GLN
2	G	62	ASN
2	G	64	ASN
2	H	62	ASN
2	H	64	ASN
2	K	36	GLN
2	K	62	ASN
2	K	64	ASN
2	L	36	GLN
2	L	62	ASN
2	L	64	ASN
2	L	124	ASN
2	O	36	GLN
2	O	62	ASN
2	O	64	ASN
2	P	36	GLN
2	P	64	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

88 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	Q	1	1,3	14,14,15	0.79	0	17,19,21	1.20	2 (11%)
3	NAG	Q	2	3	14,14,15	0.77	0	17,19,21	1.71	4 (23%)
3	BMA	Q	3	3	11,11,12	1.03	0	15,15,17	1.16	1 (6%)
4	NAG	R	1	1,4	14,14,15	0.52	0	17,19,21	1.47	3 (17%)
4	NAG	R	2	4	14,14,15	0.67	0	17,19,21	1.13	1 (5%)
4	BMA	R	3	4	11,11,12	0.76	0	15,15,17	1.39	2 (13%)
4	MAN	R	4	4	11,11,12	0.73	0	15,15,17	1.14	3 (20%)
4	MAN	R	5	4	11,11,12	0.67	0	15,15,17	2.01	4 (26%)
4	MAN	R	6	4	11,11,12	0.79	0	15,15,17	2.76	5 (33%)
4	MAN	R	7	4	11,11,12	0.76	0	15,15,17	0.93	0
4	MAN	R	8	4	11,11,12	0.84	0	15,15,17	2.18	6 (40%)
3	NAG	S	1	1,3	14,14,15	0.81	0	17,19,21	1.13	2 (11%)
3	NAG	S	2	3	14,14,15	0.76	0	17,19,21	1.69	5 (29%)
3	BMA	S	3	3	11,11,12	1.34	0	15,15,17	1.17	1 (6%)
4	NAG	T	1	1,4	14,14,15	0.58	0	17,19,21	1.20	2 (11%)
4	NAG	T	2	4	14,14,15	0.90	0	17,19,21	1.35	2 (11%)
4	BMA	T	3	4	11,11,12	1.20	2 (18%)	15,15,17	1.10	1 (6%)
4	MAN	T	4	4	11,11,12	0.56	0	15,15,17	0.96	1 (6%)
4	MAN	T	5	4	11,11,12	0.67	0	15,15,17	2.34	4 (26%)
4	MAN	T	6	4	11,11,12	0.65	0	15,15,17	2.52	7 (46%)
4	MAN	T	7	4	11,11,12	0.89	0	15,15,17	1.20	1 (6%)
4	MAN	T	8	4	11,11,12	0.86	0	15,15,17	2.22	7 (46%)
3	NAG	U	1	3	14,14,15	0.77	0	17,19,21	1.59	3 (17%)
3	NAG	U	2	3	14,14,15	0.45	0	17,19,21	1.89	4 (23%)
3	BMA	U	3	3	11,11,12	1.25	0	15,15,17	0.92	1 (6%)
4	NAG	V	1	1,4	14,14,15	0.72	0	17,19,21	1.19	3 (17%)
4	NAG	V	2	4	14,14,15	0.68	0	17,19,21	1.39	1 (5%)
4	BMA	V	3	4	11,11,12	1.16	1 (9%)	15,15,17	1.19	2 (13%)
4	MAN	V	4	4	11,11,12	0.63	0	15,15,17	1.32	1 (6%)
4	MAN	V	5	4	11,11,12	0.86	1 (9%)	15,15,17	2.43	6 (40%)
4	MAN	V	6	4	11,11,12	0.75	0	15,15,17	2.49	4 (26%)
4	MAN	V	7	4	11,11,12	0.82	0	15,15,17	1.15	1 (6%)
4	MAN	V	8	4	11,11,12	0.64	0	15,15,17	2.01	5 (33%)
3	NAG	W	1	1,3	14,14,15	0.86	1 (7%)	17,19,21	1.32	3 (17%)
3	NAG	W	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.54	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	W	3	3	11,11,12	1.02	0	15,15,17	1.07	1 (6%)
4	NAG	X	1	1,4	14,14,15	0.54	0	17,19,21	1.53	3 (17%)
4	NAG	X	2	4	14,14,15	0.79	0	17,19,21	1.38	4 (23%)
4	BMA	X	3	4	11,11,12	0.79	0	15,15,17	1.09	1 (6%)
4	MAN	X	4	4	11,11,12	0.88	0	15,15,17	1.03	1 (6%)
4	MAN	X	5	4	11,11,12	0.63	0	15,15,17	1.94	3 (20%)
4	MAN	X	6	4	11,11,12	0.77	0	15,15,17	2.51	5 (33%)
4	MAN	X	7	4	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
4	MAN	X	8	4	11,11,12	0.83	0	15,15,17	1.96	6 (40%)
3	NAG	Y	1	1,3	14,14,15	1.15	2 (14%)	17,19,21	1.72	3 (17%)
3	NAG	Y	2	3	14,14,15	0.86	0	17,19,21	1.47	3 (17%)
3	BMA	Y	3	3	11,11,12	0.90	0	15,15,17	1.16	1 (6%)
4	NAG	Z	1	1,4	14,14,15	0.96	1 (7%)	17,19,21	1.44	3 (17%)
4	NAG	Z	2	4	14,14,15	1.08	1 (7%)	17,19,21	1.50	4 (23%)
4	BMA	Z	3	4	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
4	MAN	Z	4	4	11,11,12	1.08	1 (9%)	15,15,17	1.42	2 (13%)
4	MAN	Z	5	4	11,11,12	1.21	1 (9%)	15,15,17	2.21	5 (33%)
4	MAN	Z	6	4	11,11,12	1.11	2 (18%)	15,15,17	2.41	6 (40%)
4	MAN	Z	7	4	11,11,12	1.25	1 (9%)	15,15,17	1.44	4 (26%)
4	MAN	Z	8	4	11,11,12	0.77	0	15,15,17	1.99	7 (46%)
3	NAG	a	1	1,3	14,14,15	0.60	0	17,19,21	1.65	2 (11%)
3	NAG	a	2	3	14,14,15	0.61	0	17,19,21	2.06	3 (17%)
3	BMA	a	3	3	11,11,12	1.13	0	15,15,17	1.07	1 (6%)
4	NAG	b	1	1,4	14,14,15	0.53	0	17,19,21	1.03	2 (11%)
4	NAG	b	2	4	14,14,15	0.66	0	17,19,21	1.11	1 (5%)
4	BMA	b	3	4	11,11,12	0.81	0	15,15,17	1.12	2 (13%)
4	MAN	b	4	4	11,11,12	0.53	0	15,15,17	1.07	1 (6%)
4	MAN	b	5	4	11,11,12	0.89	0	15,15,17	2.15	5 (33%)
4	MAN	b	6	4	11,11,12	0.82	0	15,15,17	2.56	6 (40%)
4	MAN	b	7	4	11,11,12	0.82	0	15,15,17	1.09	1 (6%)
4	MAN	b	8	4	11,11,12	0.93	0	15,15,17	2.20	6 (40%)
3	NAG	c	1	1,3	14,14,15	0.75	0	17,19,21	1.67	2 (11%)
3	NAG	c	2	3	14,14,15	0.59	0	17,19,21	1.98	4 (23%)
3	BMA	c	3	3	11,11,12	1.11	0	15,15,17	1.10	1 (6%)
4	NAG	d	1	1,4	14,14,15	0.35	0	17,19,21	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	d	2	4	14,14,15	0.83	0	17,19,21	1.20	2 (11%)
4	BMA	d	3	4	11,11,12	0.84	0	15,15,17	1.24	2 (13%)
4	MAN	d	4	4	11,11,12	0.65	0	15,15,17	0.92	1 (6%)
4	MAN	d	5	4	11,11,12	0.94	0	15,15,17	2.19	5 (33%)
4	MAN	d	6	4	11,11,12	0.66	0	15,15,17	2.55	5 (33%)
4	MAN	d	7	4	11,11,12	0.89	1 (9%)	15,15,17	1.12	0
4	MAN	d	8	4	11,11,12	0.86	0	15,15,17	1.83	4 (26%)
3	NAG	e	1	1,3	14,14,15	0.85	1 (7%)	17,19,21	1.64	3 (17%)
3	NAG	e	2	3	14,14,15	0.75	0	17,19,21	1.44	5 (29%)
3	BMA	e	3	3	11,11,12	1.07	0	15,15,17	1.04	1 (6%)
4	NAG	f	1	1,4	14,14,15	0.69	0	17,19,21	1.52	4 (23%)
4	NAG	f	2	4	14,14,15	0.86	1 (7%)	17,19,21	1.49	3 (17%)
4	BMA	f	3	4	11,11,12	0.71	0	15,15,17	1.29	2 (13%)
4	MAN	f	4	4	11,11,12	0.77	0	15,15,17	1.19	1 (6%)
4	MAN	f	5	4	11,11,12	0.95	0	15,15,17	2.04	2 (13%)
4	MAN	f	6	4	11,11,12	0.98	0	15,15,17	2.63	5 (33%)
4	MAN	f	7	4	11,11,12	1.14	1 (9%)	15,15,17	1.29	1 (6%)
4	MAN	f	8	4	11,11,12	0.67	0	15,15,17	2.03	6 (40%)

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	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
4	MAN	R	4	4	-	0/2/19/22	0/1/1/1
4	MAN	R	5	4	-	0/2/19/22	0/1/1/1
4	MAN	R	6	4	-	2/2/19/22	1/1/1/1
4	MAN	R	7	4	-	2/2/19/22	0/1/1/1
4	MAN	R	8	4	-	2/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	Z	5	4	-	0/2/19/22	0/1/1/1
4	MAN	Z	6	4	-	2/2/19/22	1/1/1/1
4	MAN	Z	7	4	-	2/2/19/22	0/1/1/1
4	MAN	Z	8	4	-	2/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	BMA	a	3	3	-	0/2/19/22	0/1/1/1
4	NAG	b	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	BMA	b	3	4	-	0/2/19/22	0/1/1/1
4	MAN	b	4	4	-	0/2/19/22	0/1/1/1
4	MAN	b	5	4	-	0/2/19/22	0/1/1/1
4	MAN	b	6	4	-	2/2/19/22	1/1/1/1
4	MAN	b	7	4	-	2/2/19/22	0/1/1/1
4	MAN	b	8	4	-	2/2/19/22	0/1/1/1
3	NAG	c	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	0/2/19/22	0/1/1/1
4	NAG	d	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	BMA	d	3	4	-	0/2/19/22	0/1/1/1
4	MAN	d	4	4	-	0/2/19/22	0/1/1/1
4	MAN	d	5	4	-	1/2/19/22	0/1/1/1
4	MAN	d	6	4	-	2/2/19/22	1/1/1/1
4	MAN	d	7	4	-	2/2/19/22	0/1/1/1
4	MAN	d	8	4	-	2/2/19/22	0/1/1/1
3	NAG	e	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	BMA	e	3	3	-	0/2/19/22	0/1/1/1
4	NAG	f	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	0/1/1/1
4	BMA	f	3	4	-	0/2/19/22	0/1/1/1
4	MAN	f	4	4	-	0/2/19/22	0/1/1/1
4	MAN	f	5	4	-	0/2/19/22	0/1/1/1
4	MAN	f	6	4	-	2/2/19/22	1/1/1/1
4	MAN	f	7	4	-	2/2/19/22	0/1/1/1
4	MAN	f	8	4	-	2/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f	7	MAN	O5-C5	-3.13	1.37	1.43
3	Y	1	NAG	O5-C5	-2.90	1.37	1.43
4	Z	2	NAG	O5-C1	-2.65	1.39	1.43
4	Z	7	MAN	O5-C5	-2.64	1.38	1.43
3	Y	1	NAG	O5-C1	-2.55	1.39	1.43
4	Z	4	MAN	O5-C1	-2.54	1.39	1.43
4	Z	1	NAG	O5-C5	-2.48	1.38	1.43
4	f	2	NAG	O5-C1	-2.48	1.39	1.43
4	Z	6	MAN	O2-C2	-2.36	1.38	1.43
4	d	7	MAN	O5-C5	-2.20	1.39	1.43
4	T	3	BMA	O5-C1	2.17	1.47	1.43
3	W	1	NAG	C1-C2	2.16	1.55	1.52
4	Z	6	MAN	O5-C5	-2.15	1.39	1.43
4	Z	5	MAN	O4-C4	-2.14	1.37	1.43
4	V	5	MAN	C1-C2	2.13	1.57	1.52
3	e	1	NAG	O5-C5	-2.07	1.39	1.43
3	W	2	NAG	C2-N2	-2.05	1.42	1.46
4	V	3	BMA	C1-C2	2.03	1.57	1.52
4	T	3	BMA	C1-C2	2.01	1.57	1.52

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	5	MAN	O2-C2-C1	6.60	124.34	109.22
4	T	5	MAN	O2-C2-C1	6.47	124.04	109.22
3	a	2	NAG	C1-O5-C5	-6.41	103.59	112.19
4	Z	5	MAN	O2-C2-C1	5.91	122.75	109.22
4	X	6	MAN	C1-O5-C5	-5.90	104.28	112.19
4	f	5	MAN	O2-C2-C1	5.65	122.16	109.22
4	f	6	MAN	O2-C2-C3	-5.60	98.56	110.15
4	R	6	MAN	C1-O5-C5	-5.57	104.73	112.19
4	d	6	MAN	C1-O5-C5	-5.46	104.86	112.19
4	R	5	MAN	O2-C2-C1	5.43	121.67	109.22
4	b	5	MAN	O2-C2-C1	5.37	121.52	109.22
4	d	5	MAN	O2-C2-C1	5.33	121.42	109.22
4	V	6	MAN	C2-C3-C4	-5.30	101.54	110.86
4	T	6	MAN	C2-C3-C4	-5.24	101.64	110.86
3	c	2	NAG	C1-O5-C5	-5.23	105.18	112.19
3	Y	1	NAG	O5-C1-C2	-5.22	103.21	111.29
4	X	5	MAN	O2-C2-C1	5.12	120.96	109.22
3	e	1	NAG	O5-C1-C2	-5.00	103.56	111.29
4	T	6	MAN	C1-O5-C5	-4.98	105.52	112.19
4	V	6	MAN	C1-O5-C5	-4.94	105.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	6	MAN	C2-C3-C4	-4.85	102.33	110.86
4	Z	6	MAN	C2-C3-C4	-4.79	102.44	110.86
4	b	6	MAN	C1-O5-C5	-4.78	105.78	112.19
4	f	6	MAN	C1-O5-C5	-4.72	105.86	112.19
3	U	2	NAG	C1-O5-C5	-4.69	105.91	112.19
4	X	6	MAN	C2-C3-C4	-4.63	102.72	110.86
4	b	6	MAN	C2-C3-C4	-4.61	102.75	110.86
3	a	1	NAG	O5-C1-C2	-4.60	104.17	111.29
3	Q	2	NAG	C1-O5-C5	-4.60	106.02	112.19
4	d	8	MAN	C2-C3-C4	4.53	118.83	110.86
4	d	6	MAN	C2-C3-C4	-4.46	103.02	110.86
4	Z	4	MAN	C1-O5-C5	4.43	118.13	112.19
4	f	6	MAN	C2-C3-C4	-4.38	103.16	110.86
4	R	6	MAN	C3-C4-C5	-4.37	102.32	110.23
4	d	6	MAN	C3-C4-C5	-4.23	102.56	110.23
4	Z	6	MAN	C1-O5-C5	-4.19	106.57	112.19
3	U	1	NAG	O5-C1-C2	-4.11	104.93	111.29
3	U	2	NAG	C2-N2-C7	-4.10	117.41	122.90
4	R	6	MAN	O2-C2-C3	-4.09	101.68	110.15
4	f	8	MAN	C2-C3-C4	4.07	118.02	110.86
4	b	6	MAN	C3-C4-C5	-4.04	102.90	110.23
4	X	8	MAN	C2-C3-C4	4.00	117.90	110.86
4	b	6	MAN	O2-C2-C3	-3.93	102.00	110.15
4	Z	6	MAN	C3-C4-C5	-3.92	103.13	110.23
3	c	1	NAG	O5-C1-C2	-3.87	105.30	111.29
4	V	6	MAN	O2-C2-C3	-3.87	102.13	110.15
4	T	5	MAN	O2-C2-C3	-3.86	102.15	110.15
4	T	6	MAN	C3-C4-C5	-3.79	103.35	110.23
4	f	5	MAN	O2-C2-C3	-3.78	102.32	110.15
4	f	6	MAN	C3-C4-C5	-3.76	103.42	110.23
4	R	8	MAN	C1-O5-C5	-3.75	107.17	112.19
4	T	2	NAG	C1-C2-N2	-3.74	104.55	110.43
4	T	8	MAN	C1-O5-C5	-3.72	107.20	112.19
4	b	8	MAN	C2-C3-C4	3.69	117.36	110.86
4	Z	6	MAN	O2-C2-C3	-3.67	102.54	110.15
4	V	2	NAG	C1-C2-N2	-3.65	104.69	110.43
4	V	5	MAN	O2-C2-C3	-3.56	102.78	110.15
3	W	2	NAG	C1-O5-C5	-3.54	107.44	112.19
4	T	8	MAN	C2-C3-C4	3.53	117.07	110.86
4	V	8	MAN	C2-C3-C4	3.53	117.06	110.86
4	X	6	MAN	C3-C4-C5	-3.49	103.90	110.23
4	b	8	MAN	O3-C3-C2	-3.49	102.93	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	8	MAN	C2-C3-C4	3.48	116.99	110.86
4	b	5	MAN	O2-C2-C3	-3.48	102.95	110.15
4	V	8	MAN	C1-O5-C5	-3.47	107.54	112.19
3	Y	2	NAG	O5-C5-C6	3.46	114.41	107.66
4	X	5	MAN	O2-C2-C3	-3.44	103.02	110.15
4	Z	5	MAN	O5-C5-C4	-3.44	102.46	110.83
4	b	6	MAN	O5-C1-C2	-3.44	102.58	110.79
3	a	2	NAG	O5-C5-C6	3.41	114.30	107.66
3	Y	1	NAG	C1-O5-C5	3.40	116.74	112.19
4	R	3	BMA	C1-C2-C3	3.36	114.54	109.64
4	f	2	NAG	O5-C1-C2	-3.32	106.15	111.29
4	R	8	MAN	O2-C2-C1	3.30	116.78	109.22
4	Z	8	MAN	C2-C3-C4	3.30	116.66	110.86
4	R	5	MAN	O2-C2-C3	-3.27	103.38	110.15
3	S	2	NAG	C2-N2-C7	-3.26	118.54	122.90
3	S	2	NAG	C1-O5-C5	-3.25	107.83	112.19
3	a	1	NAG	O4-C4-C5	-3.25	101.33	109.32
4	V	6	MAN	C3-C4-C5	-3.23	104.37	110.23
4	T	3	BMA	C1-C2-C3	3.22	114.33	109.64
4	R	6	MAN	O5-C1-C2	-3.19	103.18	110.79
4	d	6	MAN	O5-C1-C2	-3.19	103.18	110.79
4	X	3	BMA	C1-C2-C3	3.19	114.29	109.64
4	f	3	BMA	C1-C2-C3	3.18	114.28	109.64
4	Z	2	NAG	O5-C1-C2	-3.16	106.40	111.29
4	Z	1	NAG	O5-C1-C2	-3.15	106.42	111.29
4	X	1	NAG	O5-C1-C2	-3.14	106.43	111.29
4	Z	3	BMA	O2-C2-C3	-3.14	103.66	110.15
3	Q	2	NAG	O5-C5-C6	3.11	113.72	107.66
3	a	2	NAG	C2-N2-C7	-3.11	118.73	122.90
4	b	5	MAN	C2-C3-C4	-3.10	105.41	110.86
4	f	2	NAG	C1-C2-N2	-3.08	105.58	110.43
3	c	1	NAG	O4-C4-C5	-3.07	101.76	109.32
4	f	3	BMA	O2-C2-C3	-3.07	103.79	110.15
3	W	1	NAG	O5-C1-C2	-3.07	106.55	111.29
4	d	5	MAN	O5-C5-C4	-3.06	103.37	110.83
3	c	2	NAG	O5-C1-C2	-3.06	106.55	111.29
4	R	3	BMA	O2-C2-C3	-3.06	103.81	110.15
4	R	8	MAN	O3-C3-C2	-3.06	103.81	110.05
4	T	8	MAN	C3-C4-C5	3.03	115.72	110.23
4	b	2	NAG	C4-C3-C2	3.03	115.45	111.02
4	T	5	MAN	O5-C5-C4	-3.03	103.47	110.83
4	X	6	MAN	O2-C2-C3	-3.02	103.89	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	6	MAN	O5-C1-C2	-3.02	103.59	110.79
4	R	1	NAG	O5-C1-C2	-3.00	106.65	111.29
3	S	2	NAG	O5-C5-C6	2.99	113.49	107.66
4	f	1	NAG	O7-C7-N2	2.96	127.21	121.98
4	f	8	MAN	O3-C3-C4	-2.95	103.42	110.38
4	V	8	MAN	O5-C5-C6	2.95	113.40	107.66
3	S	1	NAG	O5-C1-C2	-2.94	106.74	111.29
3	c	2	NAG	O5-C5-C6	2.94	113.38	107.66
3	W	1	NAG	O4-C4-C5	-2.93	102.10	109.32
4	d	5	MAN	C3-C4-C5	-2.93	104.92	110.23
3	U	1	NAG	O5-C5-C6	2.92	113.34	107.66
4	Z	5	MAN	O2-C2-C3	-2.91	104.12	110.15
4	R	2	NAG	C4-C3-C2	2.90	115.27	111.02
4	Z	8	MAN	C1-O5-C5	-2.90	108.30	112.19
4	V	3	BMA	C1-C2-C3	2.90	113.86	109.64
4	b	8	MAN	O2-C2-C1	2.89	115.83	109.22
4	T	1	NAG	O5-C1-C2	-2.88	106.83	111.29
4	X	2	NAG	C1-C2-N2	-2.87	105.90	110.43
4	d	6	MAN	O2-C2-C3	-2.87	104.20	110.15
4	T	8	MAN	O2-C2-C1	2.86	115.77	109.22
4	f	7	MAN	C1-C2-C3	-2.85	105.50	109.64
4	b	3	BMA	C1-C2-C3	2.84	113.78	109.64
3	e	2	NAG	O5-C5-C6	2.83	113.16	107.66
4	f	1	NAG	O7-C7-C8	-2.82	117.03	122.05
4	X	8	MAN	O3-C3-C4	-2.82	103.73	110.38
4	d	3	BMA	C1-C2-C3	2.82	113.75	109.64
4	Z	3	BMA	C1-C2-C3	2.82	113.74	109.64
4	V	5	MAN	O5-C5-C4	-2.81	104.00	110.83
3	Y	2	NAG	C2-N2-C7	-2.80	119.14	122.90
4	b	8	MAN	O2-C2-C3	-2.80	104.36	110.15
3	Q	1	NAG	O4-C4-C5	-2.77	102.51	109.32
4	T	6	MAN	O5-C1-C2	-2.76	104.20	110.79
4	Z	2	NAG	C1-C2-N2	-2.76	106.09	110.43
4	Z	2	NAG	O7-C7-C8	-2.73	117.19	122.05
4	f	8	MAN	O5-C5-C6	2.73	112.97	107.66
4	V	1	NAG	C1-C2-N2	-2.72	106.15	110.43
4	b	5	MAN	O5-C5-C4	-2.71	104.22	110.83
4	R	5	MAN	O5-C5-C4	-2.71	104.23	110.83
3	e	2	NAG	C1-O5-C5	-2.71	108.55	112.19
4	b	8	MAN	C3-C4-C5	2.71	115.14	110.23
4	X	6	MAN	O5-C1-C2	-2.71	104.33	110.79
4	T	8	MAN	O5-C5-C6	2.70	112.92	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	8	MAN	O5-C5-C4	-2.69	104.29	110.83
4	V	5	MAN	O3-C3-C4	-2.68	104.05	110.38
4	R	8	MAN	O5-C5-C6	2.67	112.87	107.66
4	R	8	MAN	C3-C4-C5	2.67	115.08	110.23
4	Z	8	MAN	O3-C3-C2	-2.67	104.61	110.05
4	X	8	MAN	C1-O5-C5	-2.66	108.62	112.19
3	W	2	NAG	O5-C5-C6	2.66	112.84	107.66
3	U	2	NAG	O5-C5-C6	2.66	112.83	107.66
4	Z	8	MAN	O5-C5-C6	2.64	112.80	107.66
4	Z	3	BMA	C1-O5-C5	2.62	115.70	112.19
4	d	3	BMA	O2-C2-C3	-2.62	104.72	110.15
3	Y	2	NAG	O4-C4-C3	-2.61	104.22	110.38
3	Y	1	NAG	O4-C4-C5	-2.60	102.93	109.32
3	Y	3	BMA	C3-C4-C5	2.60	114.94	110.23
4	Z	7	MAN	C1-C2-C3	-2.59	105.88	109.64
4	d	8	MAN	O5-C5-C6	2.59	112.70	107.66
4	d	5	MAN	O2-C2-C3	-2.59	104.80	110.15
4	T	1	NAG	C1-C2-N2	-2.58	106.37	110.43
4	V	4	MAN	O5-C5-C4	-2.58	104.56	110.83
3	Q	3	BMA	O3-C3-C4	2.57	116.44	110.38
4	Z	8	MAN	C3-C4-C5	2.57	114.89	110.23
3	e	1	NAG	O4-C4-C5	-2.57	103.00	109.32
4	f	1	NAG	C1-C2-N2	-2.54	106.42	110.43
3	c	2	NAG	C2-N2-C7	-2.54	119.50	122.90
4	Z	2	NAG	C4-C3-C2	2.53	114.72	111.02
4	X	8	MAN	O5-C5-C6	2.52	112.57	107.66
4	f	8	MAN	C1-O5-C5	-2.48	108.87	112.19
4	d	2	NAG	C4-C3-C2	2.46	114.63	111.02
3	e	2	NAG	C2-N2-C7	-2.45	119.62	122.90
4	b	7	MAN	C1-C2-C3	-2.44	106.09	109.64
4	d	2	NAG	O5-C1-C2	-2.40	107.58	111.29
4	b	1	NAG	C1-C2-N2	-2.39	106.66	110.43
4	X	1	NAG	O4-C4-C3	2.39	116.01	110.38
4	T	6	MAN	O2-C2-C3	-2.39	105.20	110.15
4	R	1	NAG	C1-C2-N2	-2.37	106.69	110.43
4	f	2	NAG	C4-C3-C2	2.37	114.49	111.02
3	W	2	NAG	O5-C1-C2	-2.37	107.63	111.29
4	d	5	MAN	O3-C3-C4	-2.36	104.81	110.38
4	Z	7	MAN	O5-C1-C2	-2.35	105.17	110.79
4	f	4	MAN	C1-O5-C5	2.34	115.32	112.19
3	Q	2	NAG	C2-N2-C7	-2.33	119.78	122.90
4	V	3	BMA	O2-C2-C3	-2.32	105.34	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	b	8	MAN	C1-O5-C5	-2.32	109.08	112.19
3	Q	1	NAG	O5-C1-C2	-2.32	107.71	111.29
3	e	2	NAG	O5-C1-C2	-2.31	107.72	111.29
4	Z	1	NAG	C1-C2-N2	-2.30	106.80	110.43
3	S	3	BMA	O2-C2-C1	2.30	114.50	109.22
4	X	8	MAN	C3-C4-C5	2.30	114.40	110.23
4	X	2	NAG	C4-C3-C2	2.30	114.38	111.02
4	R	1	NAG	O5-C5-C6	2.30	112.13	107.66
4	X	4	MAN	O5-C5-C4	-2.29	105.25	110.83
3	S	2	NAG	O5-C1-C2	-2.29	107.75	111.29
3	S	1	NAG	O4-C4-C5	-2.28	103.70	109.32
4	X	2	NAG	O5-C1-C2	-2.28	107.76	111.29
3	S	2	NAG	O4-C4-C3	-2.28	105.01	110.38
4	X	8	MAN	O2-C2-C1	2.27	114.42	109.22
3	U	2	NAG	O5-C1-C2	-2.27	107.78	111.29
4	V	8	MAN	C3-C4-C5	2.26	114.33	110.23
4	Z	7	MAN	O4-C4-C3	-2.26	105.05	110.38
4	b	6	MAN	O6-C6-C5	-2.25	103.66	111.33
3	U	1	NAG	O4-C4-C5	-2.25	103.79	109.32
4	R	4	MAN	O5-C5-C6	2.24	112.02	107.66
4	R	5	MAN	C1-C2-C3	-2.23	106.39	109.64
4	f	1	NAG	O5-C1-C2	-2.22	107.85	111.29
4	Z	8	MAN	O5-C5-C4	-2.22	105.42	110.83
3	W	1	NAG	O7-C7-C8	-2.22	118.10	122.05
4	Z	4	MAN	O5-C5-C6	2.21	111.97	107.66
4	X	1	NAG	C1-C2-N2	-2.21	106.95	110.43
4	f	8	MAN	O2-C2-C1	2.21	114.28	109.22
3	W	2	NAG	C2-N2-C7	-2.20	119.95	122.90
4	X	7	MAN	O5-C5-C4	-2.20	105.48	110.83
4	Z	6	MAN	O5-C1-C2	-2.20	105.55	110.79
4	R	4	MAN	C1-O5-C5	2.19	115.12	112.19
4	X	7	MAN	O5-C1-C2	-2.19	105.56	110.79
4	d	8	MAN	O2-C2-C1	2.19	114.24	109.22
4	b	3	BMA	O2-C2-C3	-2.19	105.62	110.15
4	X	2	NAG	O7-C7-C8	-2.17	118.19	122.05
4	d	8	MAN	O3-C3-C2	-2.17	105.63	110.05
4	Z	7	MAN	O5-C5-C4	-2.15	105.59	110.83
4	V	1	NAG	O5-C1-C2	-2.15	107.96	111.29
4	T	7	MAN	O4-C4-C5	-2.14	104.05	109.32
4	d	4	MAN	C1-O5-C5	2.13	115.04	112.19
4	T	4	MAN	C1-O5-C5	2.13	115.03	112.19
4	T	6	MAN	O4-C4-C5	2.12	114.55	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	2	NAG	C4-C3-C2	2.12	114.13	111.02
4	Z	1	NAG	C2-N2-C7	2.12	125.74	122.90
4	Z	5	MAN	C2-C3-C4	-2.11	107.14	110.86
4	b	4	MAN	C1-O5-C5	2.11	115.01	112.19
4	Z	5	MAN	C1-C2-C3	-2.11	106.58	109.64
3	e	3	BMA	C3-C4-C5	2.11	114.05	110.23
4	f	8	MAN	C3-C4-C5	2.10	114.04	110.23
4	b	5	MAN	C1-O5-C5	-2.10	109.38	112.19
4	T	6	MAN	O3-C3-C2	2.10	114.33	110.05
3	Q	2	NAG	O5-C1-C2	-2.09	108.06	111.29
3	c	3	BMA	C3-C4-C5	2.08	114.00	110.23
3	W	3	BMA	C3-C4-C5	2.08	114.00	110.23
4	d	1	NAG	O5-C1-C2	-2.08	108.08	111.29
3	e	2	NAG	O4-C4-C3	-2.08	105.48	110.38
4	T	8	MAN	O4-C4-C5	-2.06	104.25	109.32
4	T	5	MAN	C1-C2-C3	-2.06	106.64	109.64
4	Z	6	MAN	O6-C6-C5	-2.05	104.34	111.33
3	e	1	NAG	O5-C5-C6	2.05	111.66	107.66
4	b	1	NAG	O5-C1-C2	-2.05	108.12	111.29
3	U	3	BMA	C3-C4-C5	2.05	113.94	110.23
4	X	5	MAN	C3-C4-C5	-2.04	106.53	110.23
4	Z	8	MAN	O2-C2-C1	2.04	113.89	109.22
4	V	5	MAN	C1-C2-C3	-2.03	106.68	109.64
4	V	5	MAN	C3-C4-C5	-2.03	106.55	110.23
3	a	3	BMA	C3-C4-C5	2.03	113.91	110.23
4	V	8	MAN	O3-C3-C2	-2.03	105.92	110.05
4	V	1	NAG	O4-C4-C3	2.02	115.14	110.38
4	V	7	MAN	O2-C2-C1	2.02	113.84	109.22
4	R	4	MAN	C1-C2-C3	2.02	112.58	109.64
4	d	1	NAG	O5-C5-C6	2.01	111.58	107.66

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	c	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
4	X	7	MAN	O5-C5-C6-O6
4	Z	6	MAN	O5-C5-C6-O6
4	b	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	Q	2	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
4	T	6	MAN	O5-C5-C6-O6
4	V	6	MAN	O5-C5-C6-O6
4	R	7	MAN	C4-C5-C6-O6
4	Z	7	MAN	C4-C5-C6-O6
4	V	7	MAN	O5-C5-C6-O6
4	R	6	MAN	O5-C5-C6-O6
4	X	6	MAN	O5-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
4	b	7	MAN	C4-C5-C6-O6
4	d	7	MAN	C4-C5-C6-O6
4	T	7	MAN	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
4	R	7	MAN	O5-C5-C6-O6
4	Z	7	MAN	O5-C5-C6-O6
4	b	7	MAN	O5-C5-C6-O6
4	d	6	MAN	O5-C5-C6-O6
4	d	7	MAN	O5-C5-C6-O6
4	f	6	MAN	O5-C5-C6-O6
4	f	7	MAN	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
4	f	7	MAN	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
4	b	8	MAN	O5-C5-C6-O6
4	V	7	MAN	C4-C5-C6-O6
4	d	6	MAN	C4-C5-C6-O6
4	f	6	MAN	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
4	X	8	MAN	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
4	T	7	MAN	C4-C5-C6-O6
4	R	8	MAN	O5-C5-C6-O6
4	V	8	MAN	O5-C5-C6-O6
4	d	8	MAN	O5-C5-C6-O6
4	X	6	MAN	C4-C5-C6-O6
4	T	8	MAN	O5-C5-C6-O6
4	f	8	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	R	6	MAN	C4-C5-C6-O6
4	Z	8	MAN	O5-C5-C6-O6
4	b	6	MAN	C4-C5-C6-O6
4	V	6	MAN	C4-C5-C6-O6
4	b	8	MAN	C4-C5-C6-O6
4	Z	6	MAN	C4-C5-C6-O6
4	T	6	MAN	C4-C5-C6-O6
4	V	8	MAN	C4-C5-C6-O6
4	X	8	MAN	C4-C5-C6-O6
4	T	8	MAN	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
4	d	8	MAN	C4-C5-C6-O6
4	R	8	MAN	C4-C5-C6-O6
4	X	7	MAN	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	Z	8	MAN	C4-C5-C6-O6
4	f	8	MAN	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
4	d	5	MAN	C4-C5-C6-O6

All (8) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	6	MAN	C1-C2-C3-C4-C5-O5
4	d	6	MAN	C1-C2-C3-C4-C5-O5
4	R	6	MAN	C1-C2-C3-C4-C5-O5
4	f	6	MAN	C1-C2-C3-C4-C5-O5
4	b	6	MAN	C1-C2-C3-C4-C5-O5
4	T	6	MAN	C1-C2-C3-C4-C5-O5
4	V	6	MAN	C1-C2-C3-C4-C5-O5

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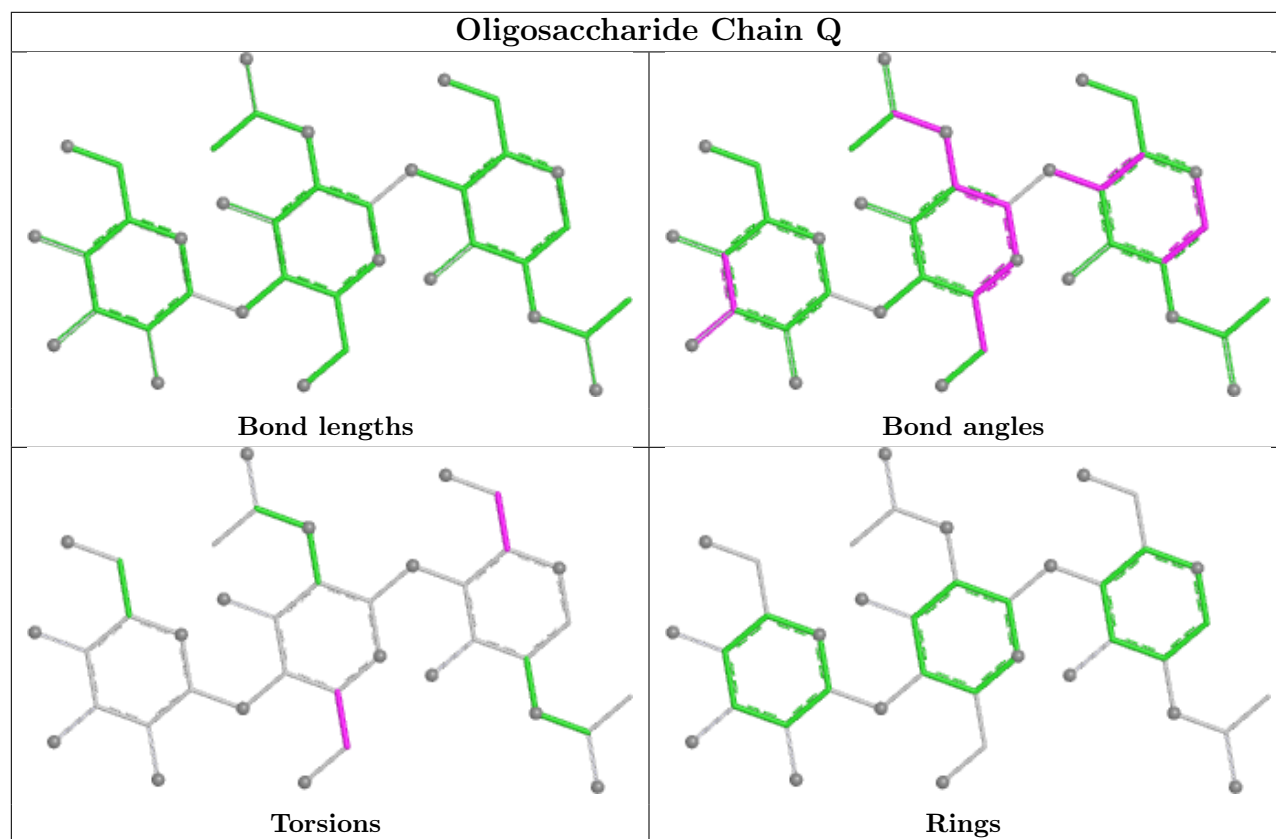
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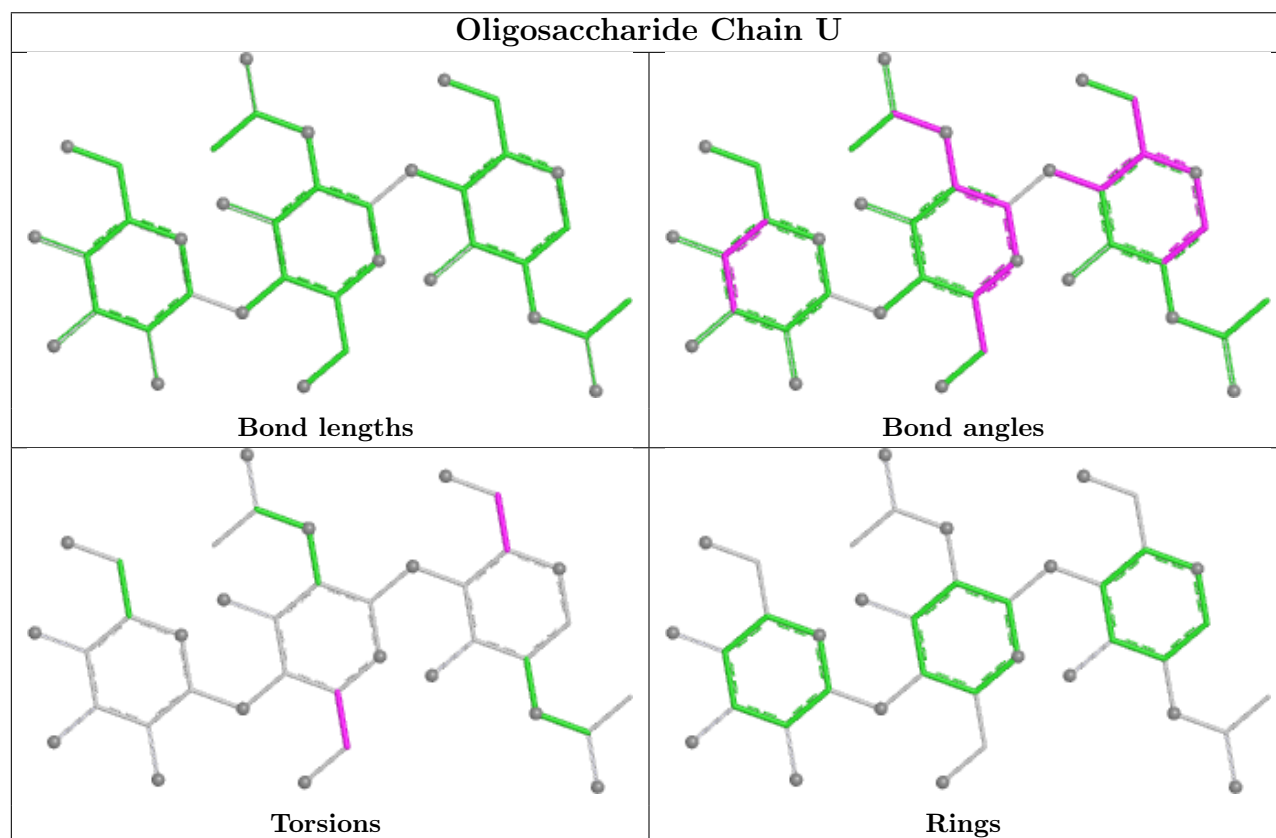
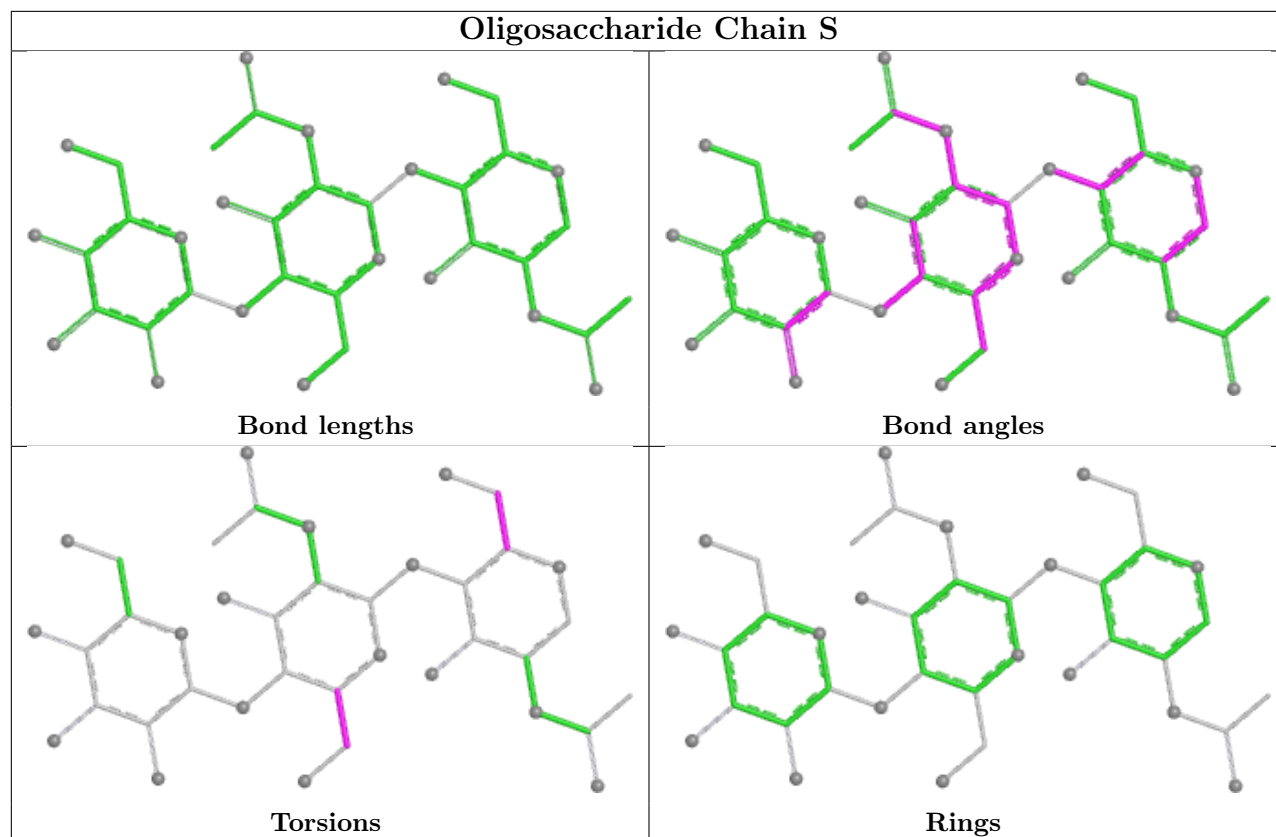
Mol	Chain	Res	Type	Atoms
4	Z	6	MAN	C1-C2-C3-C4-C5-O5

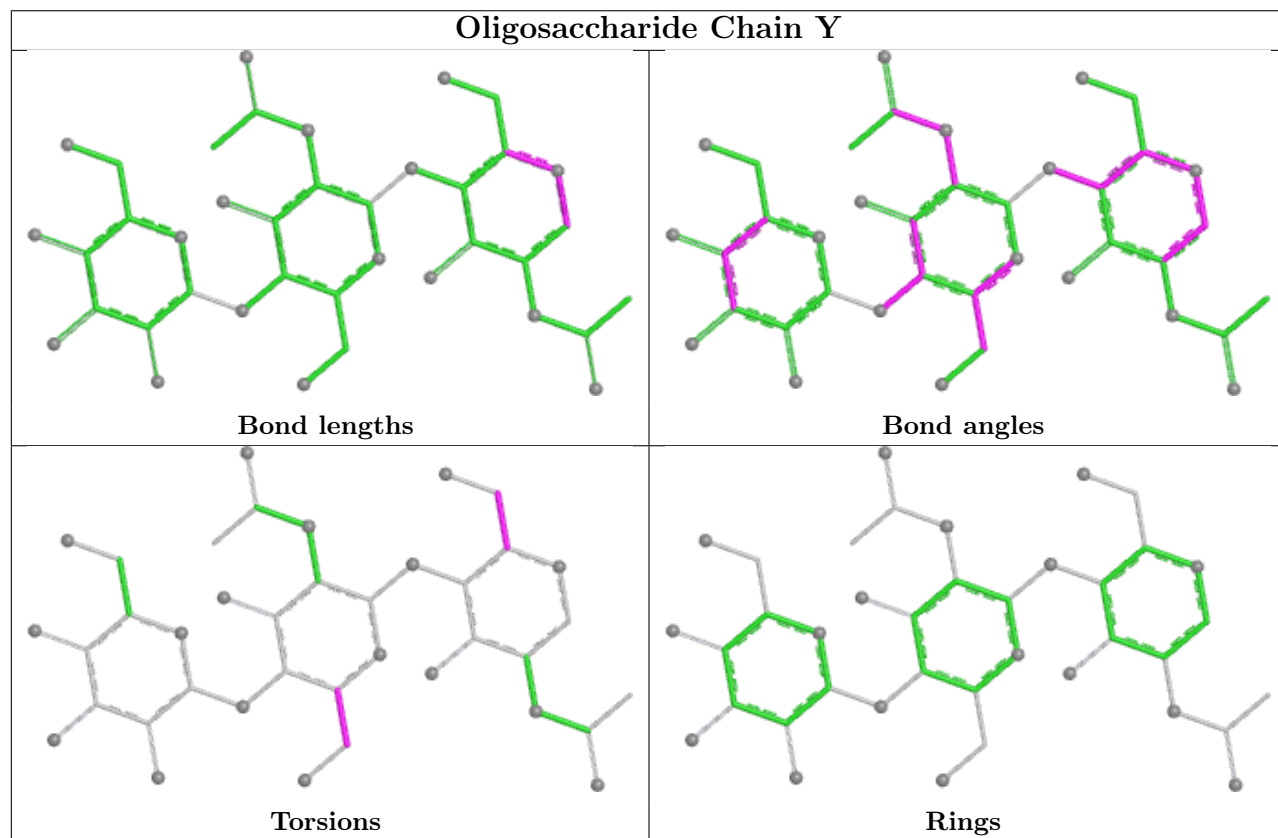
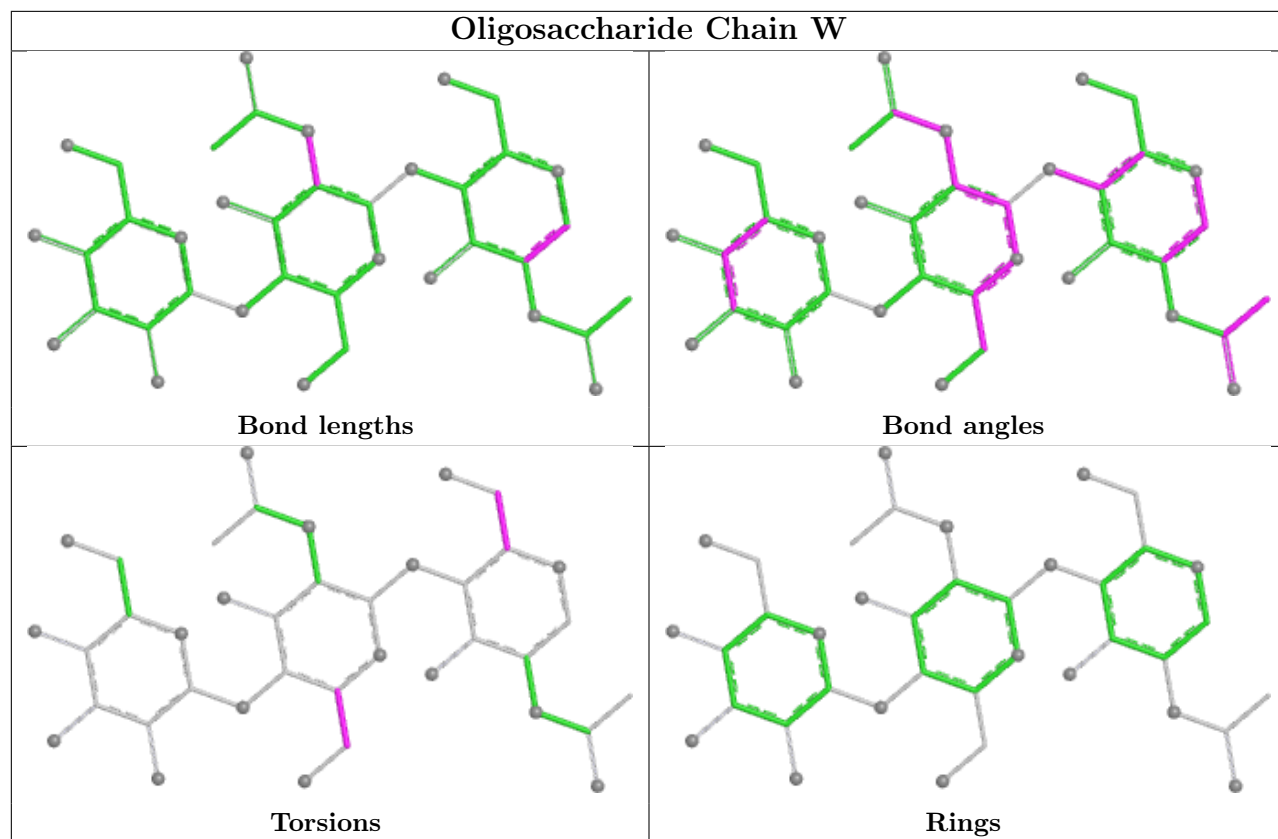
13 monomers are involved in 11 short contacts:

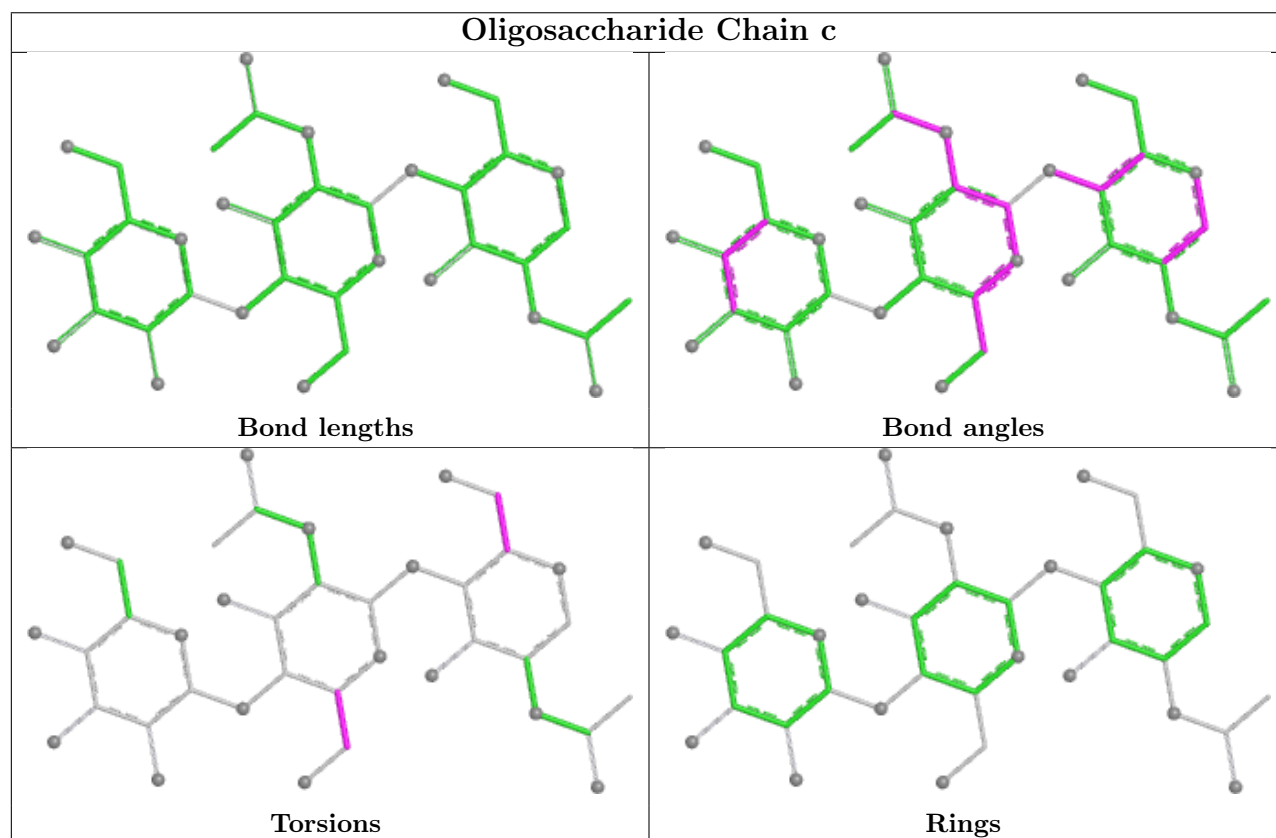
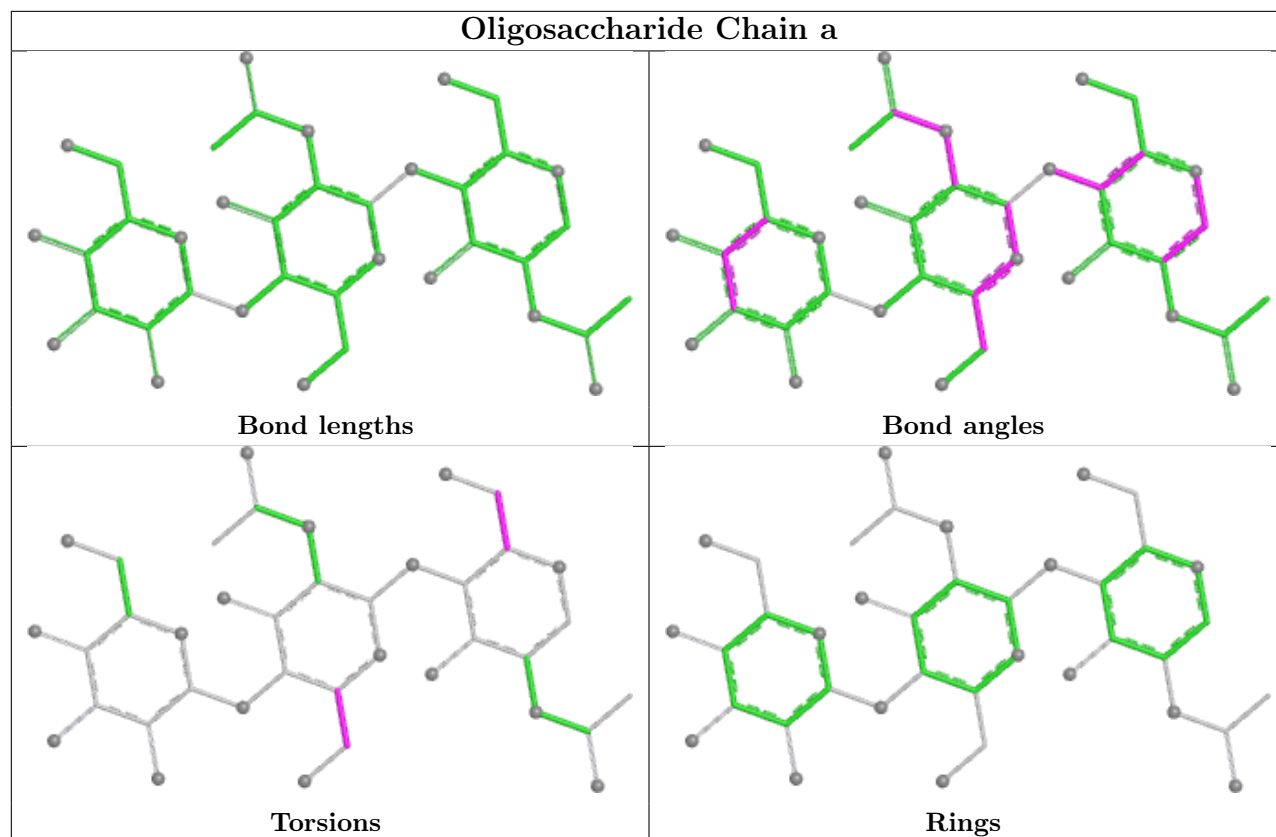
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	1	NAG	1	0
3	U	1	NAG	3	0
4	T	5	MAN	1	0
3	Y	2	NAG	1	0
3	W	1	NAG	1	0
4	V	6	MAN	1	0
3	S	1	NAG	1	0
4	X	1	NAG	1	0
4	V	5	MAN	1	0
3	Q	1	NAG	1	0
4	V	1	NAG	1	0
4	Z	1	NAG	1	0
4	T	6	MAN	1	0

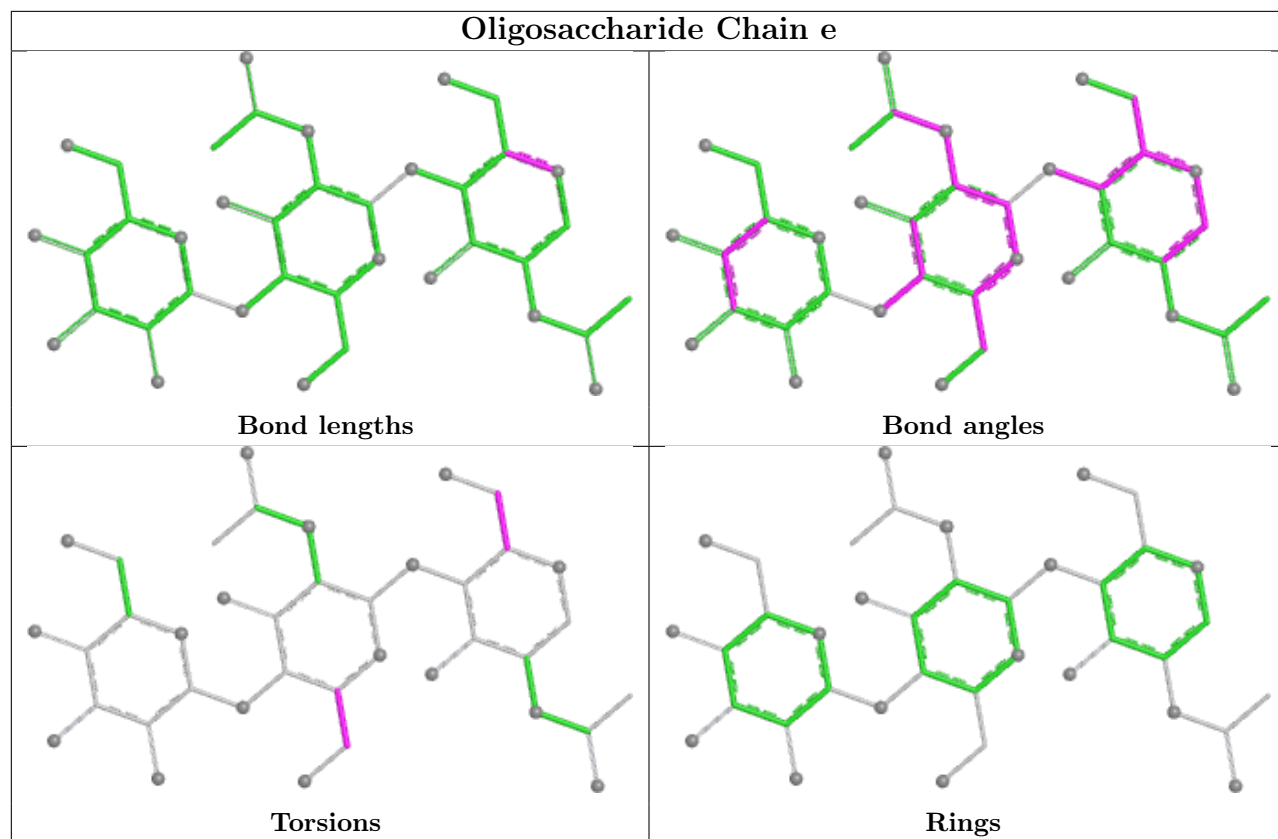
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

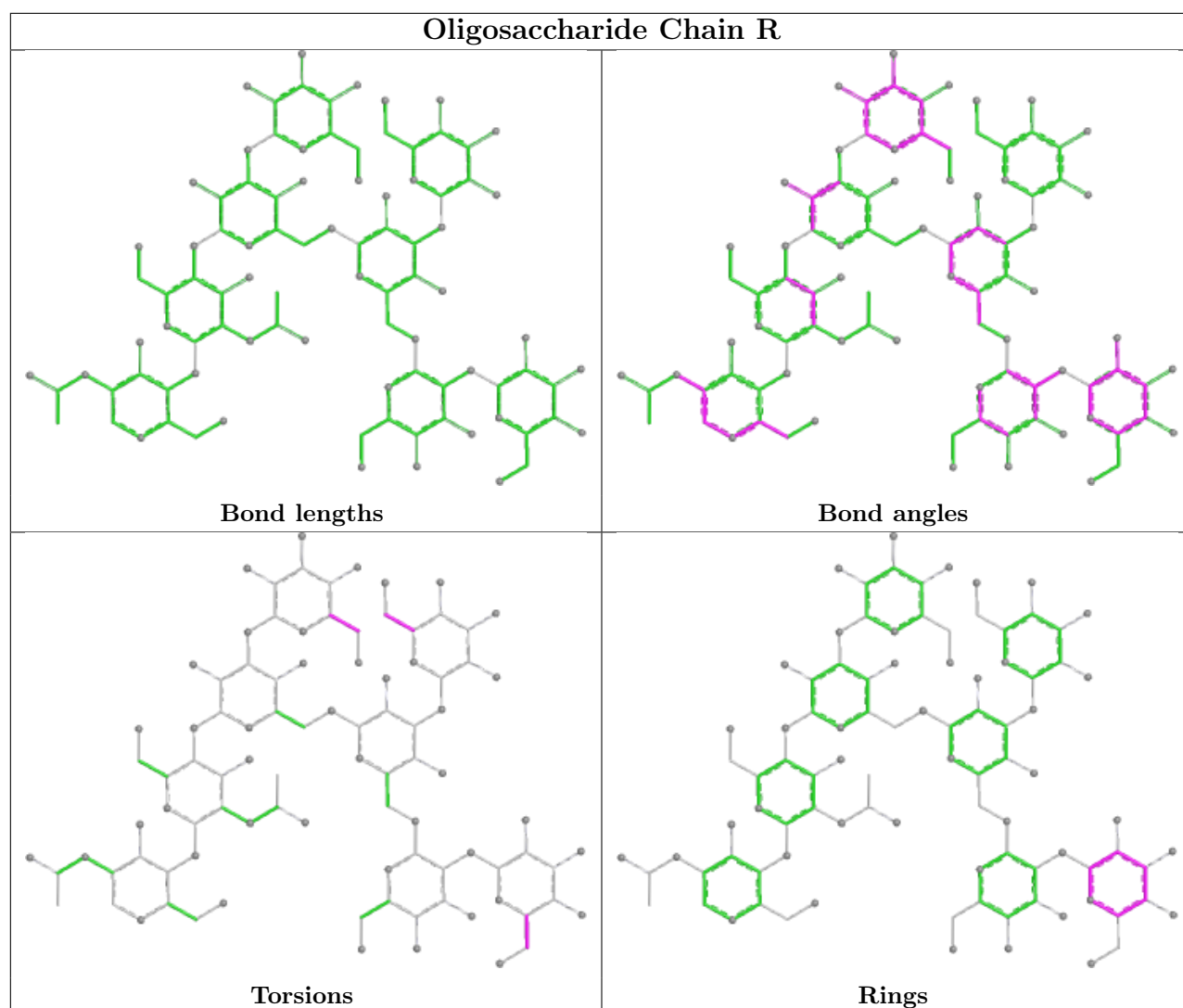




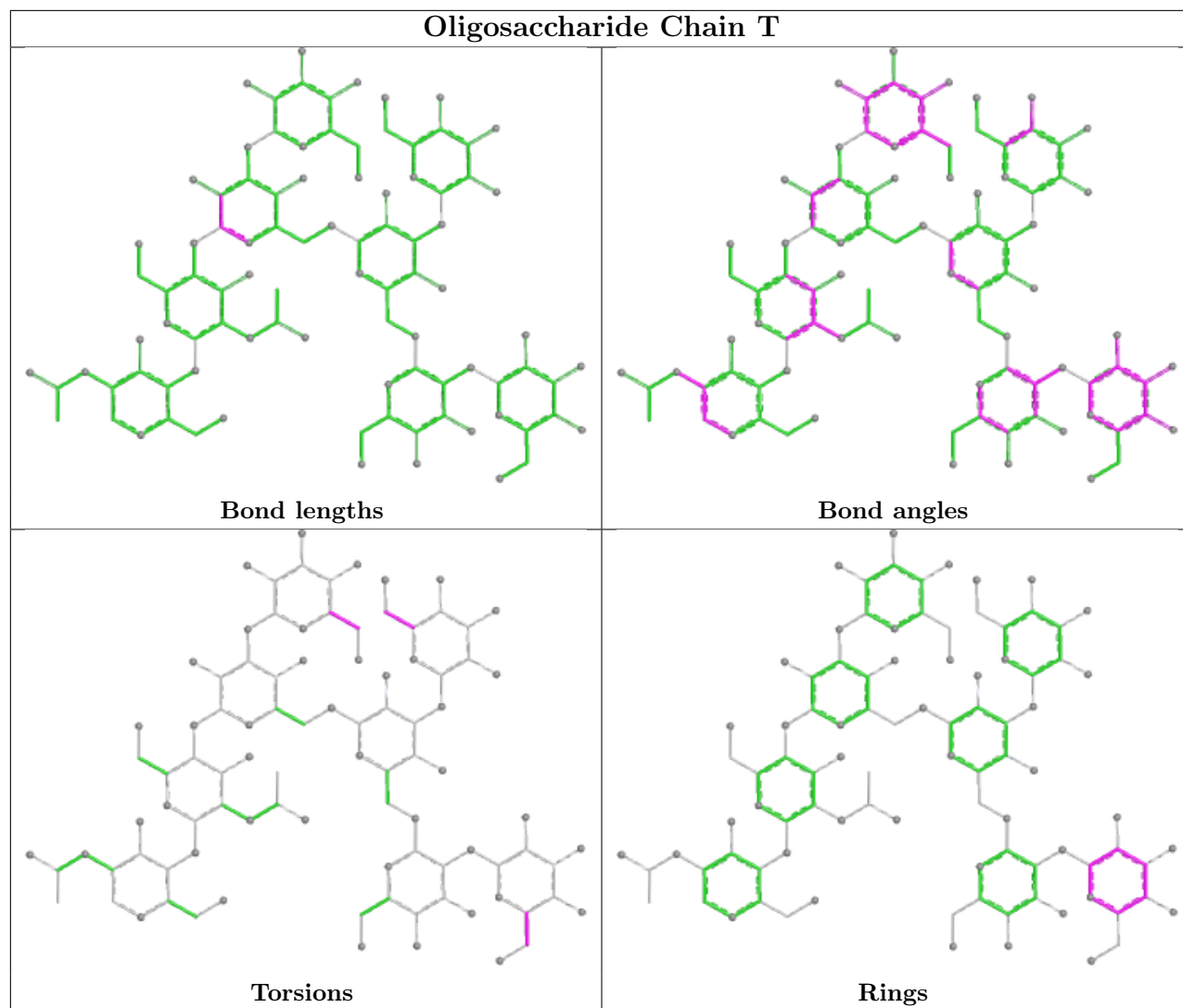


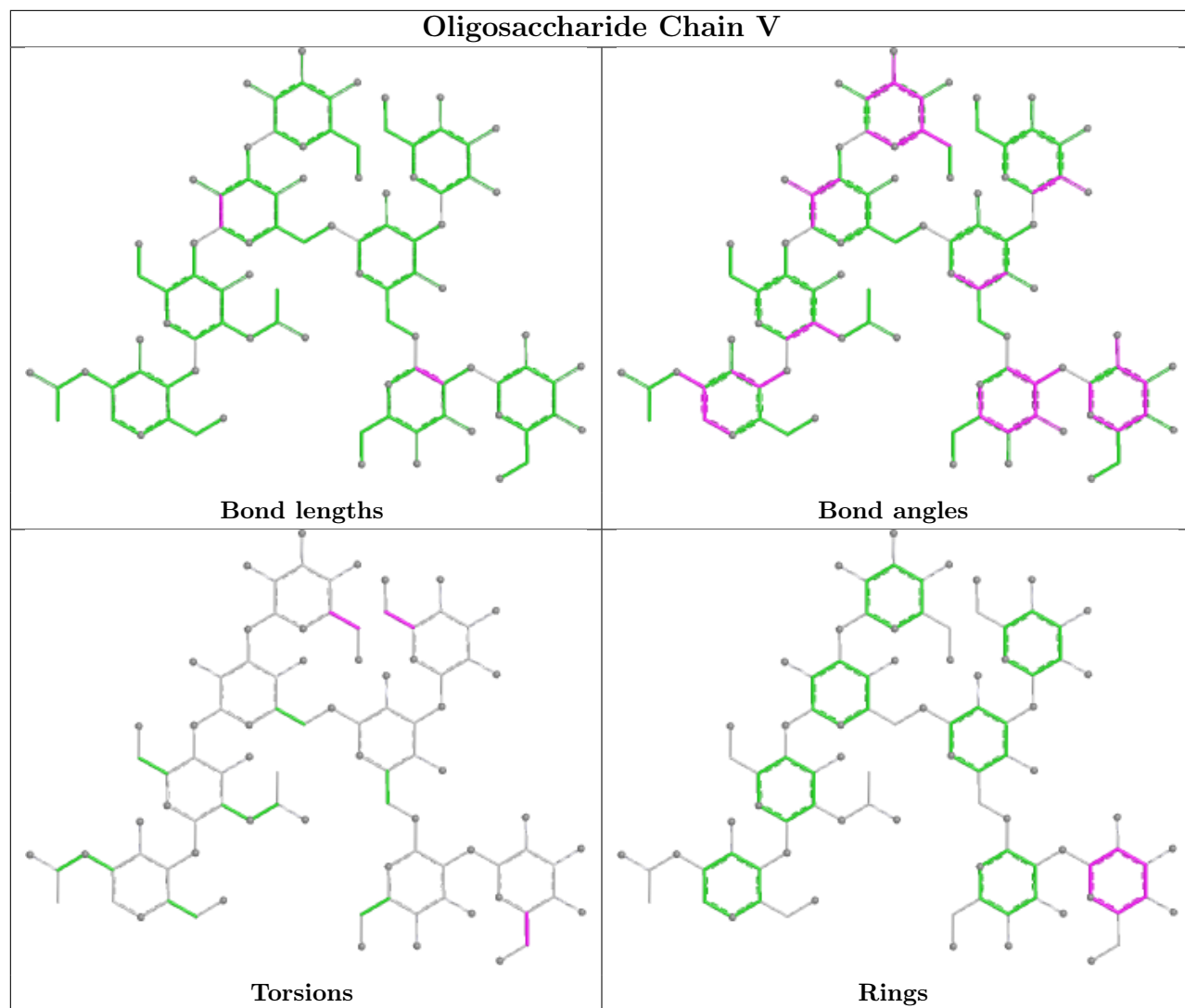


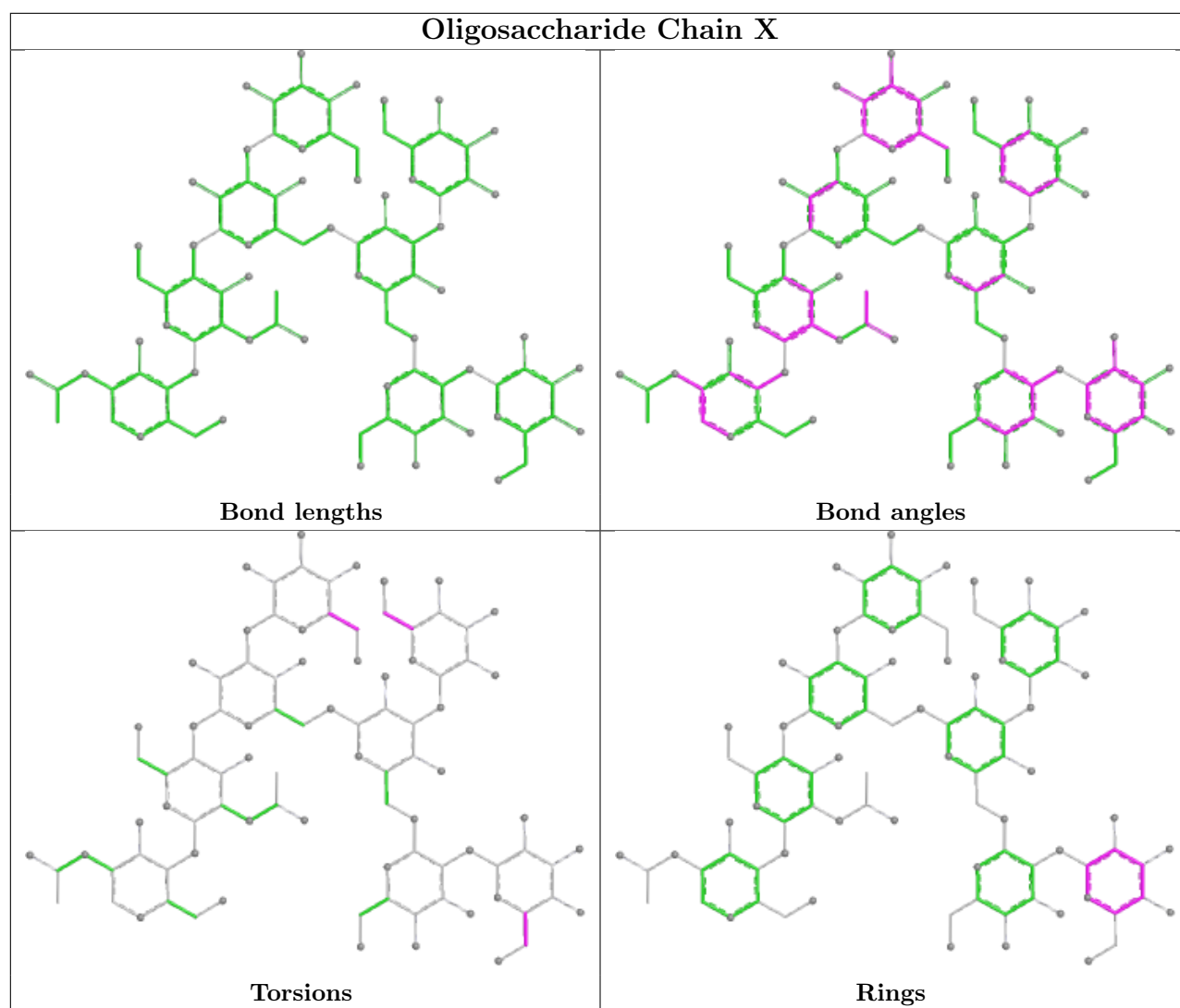


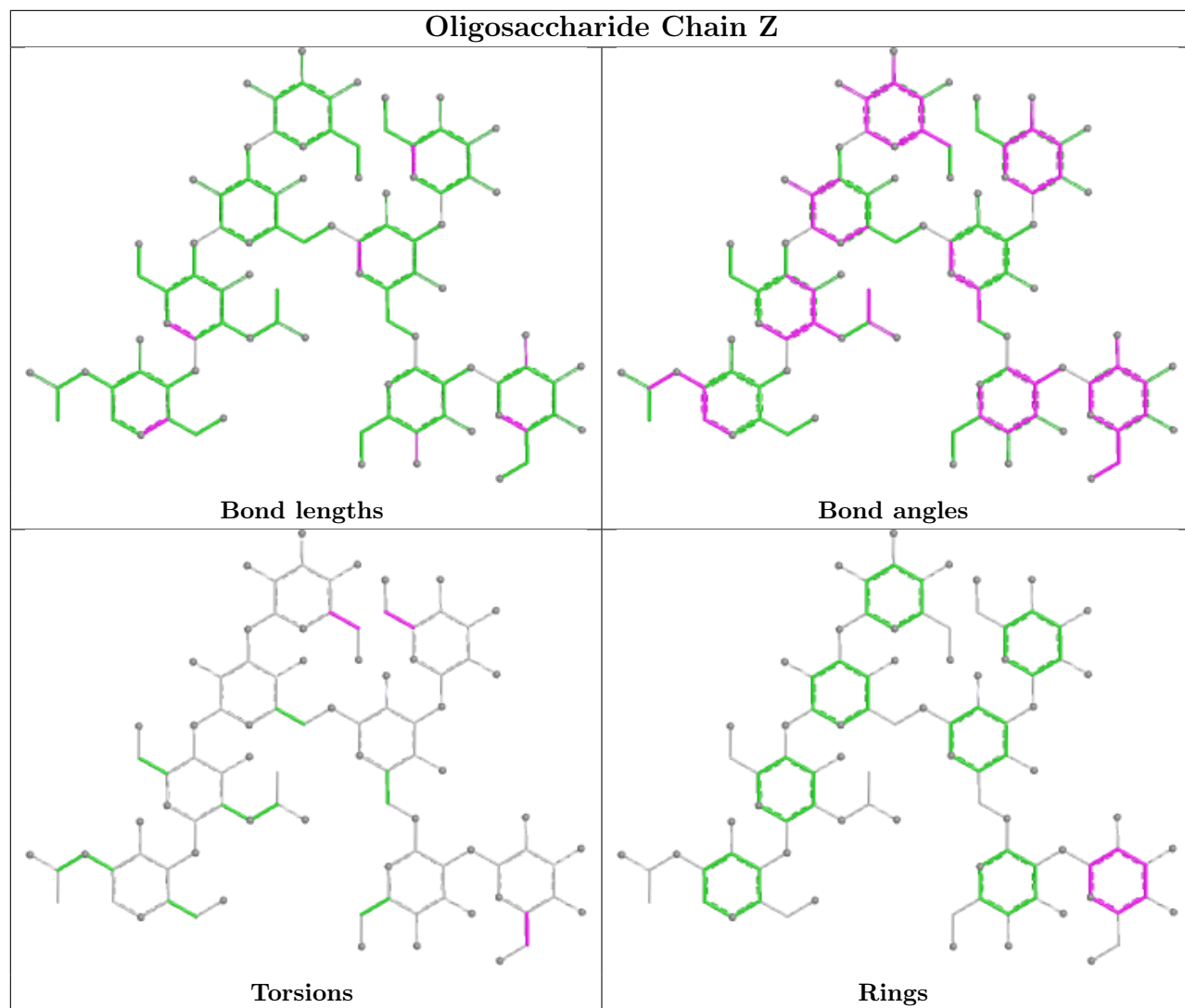


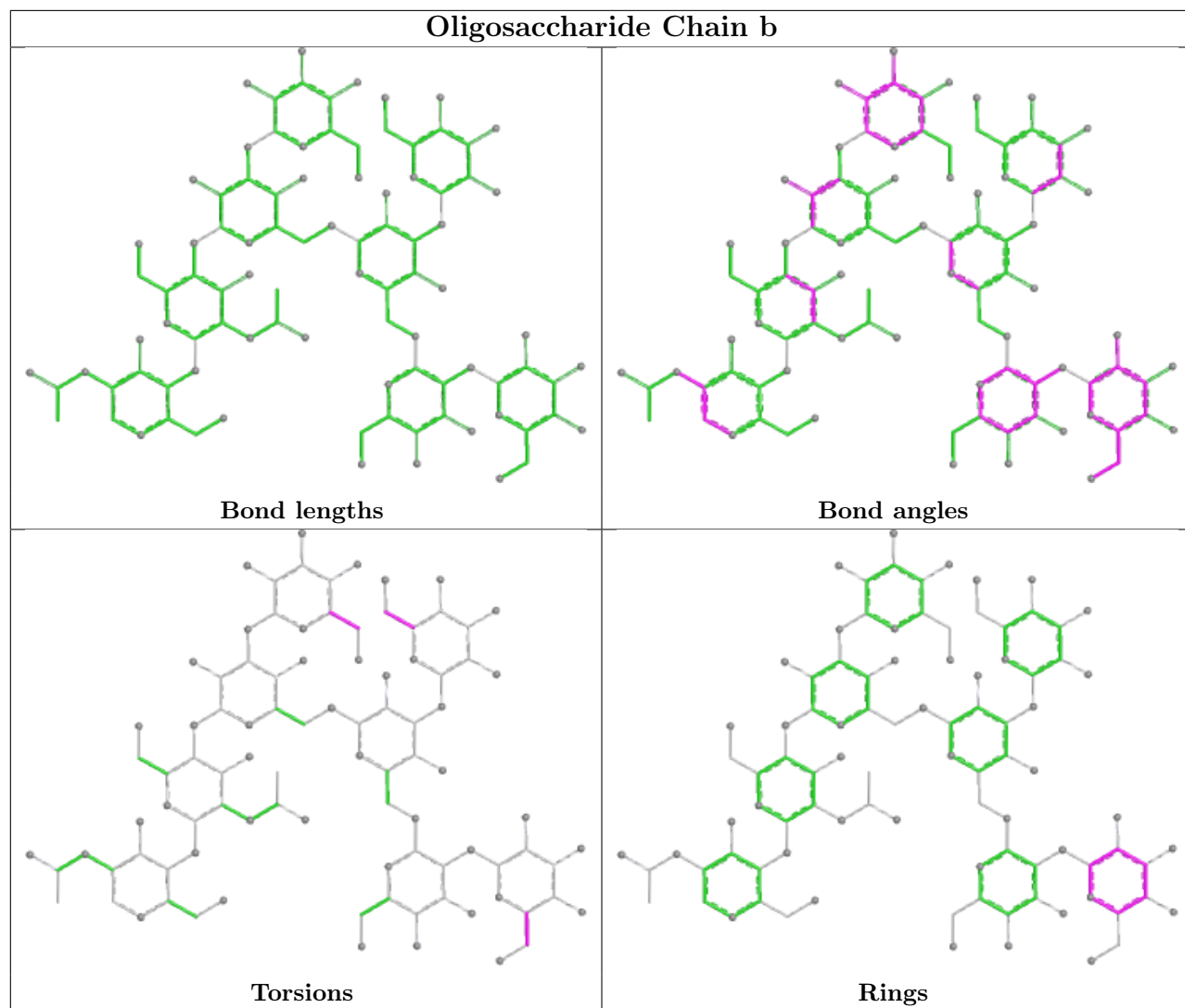




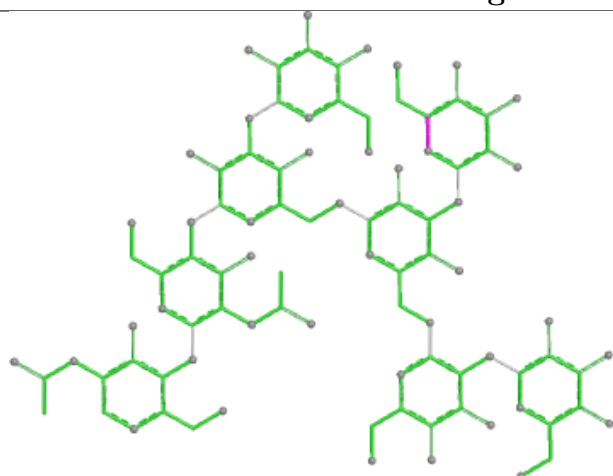




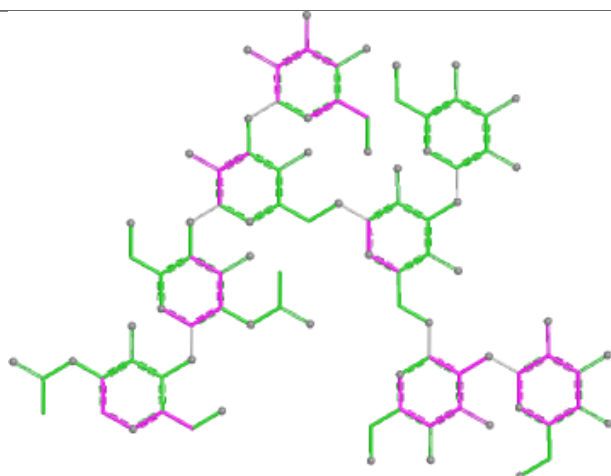




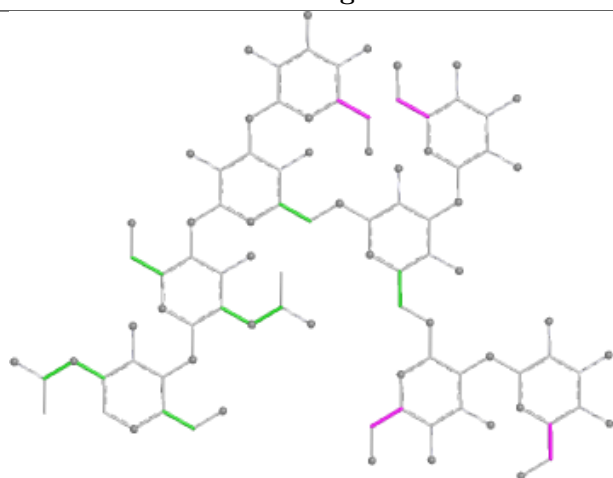
## Oligosaccharide Chain d



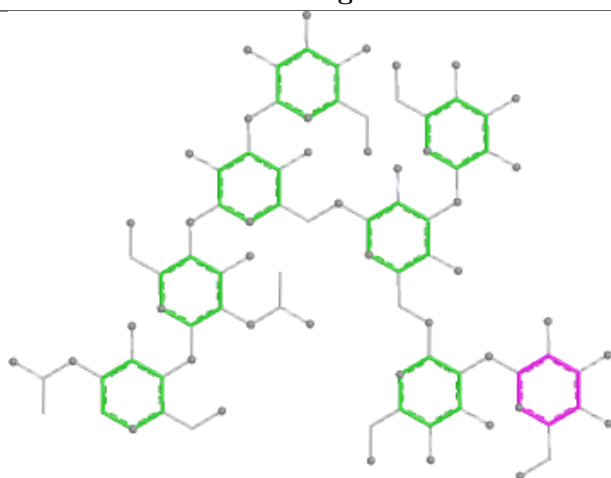
Bond lengths



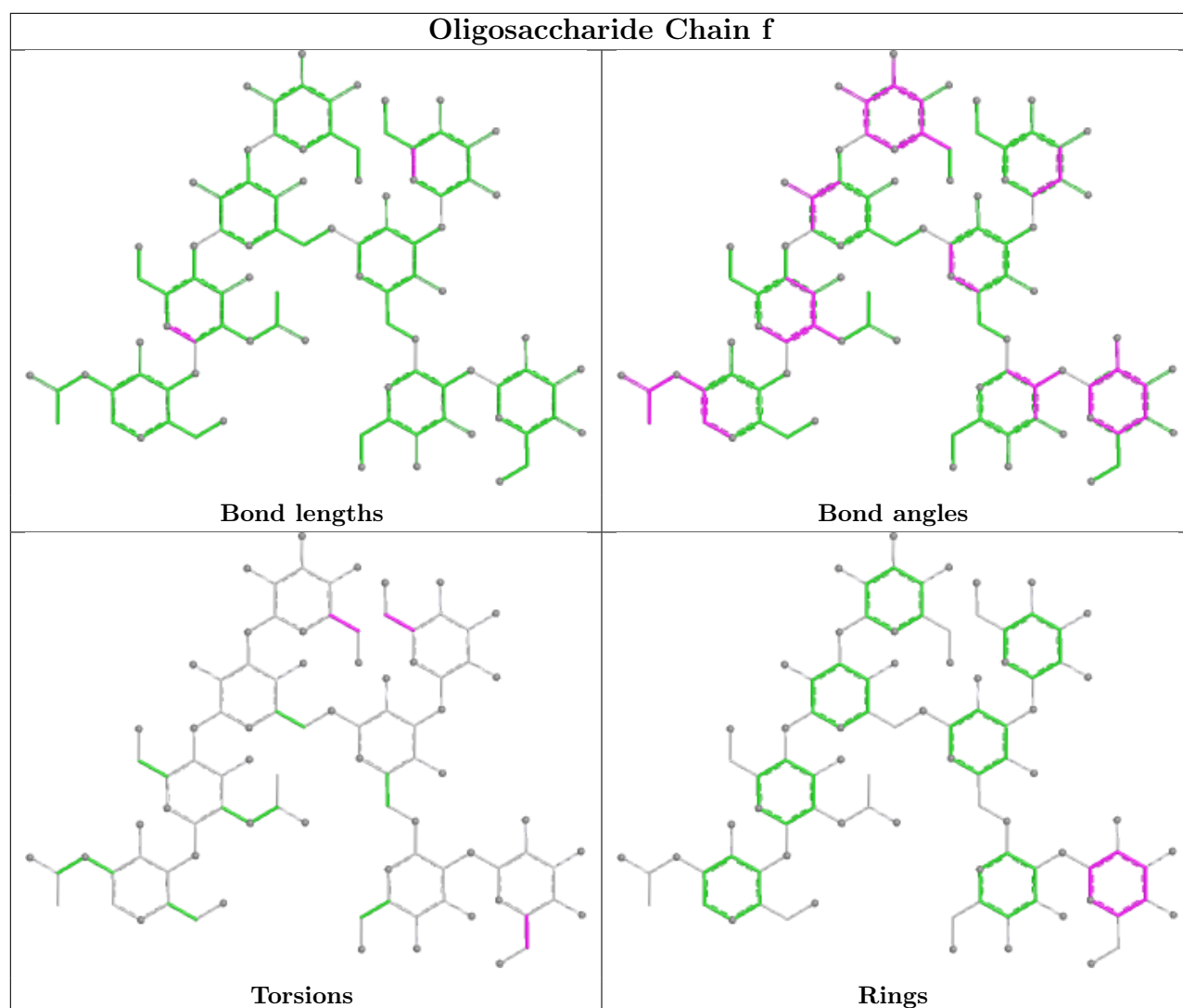
Bond angles



Torsions



Rings



## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	PGT	P	201	-	30,30,50	1.08	3 (10%)	31,31,56	1.17	4 (12%)
5	PGT	H	201	-	30,30,50	1.13	2 (6%)	31,31,56	1.17	3 (9%)
5	PGT	L	201	-	30,30,50	1.11	3 (10%)	31,31,56	1.05	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PGT	D	201	-	30,30,50	1.03	3 (10%)	31,31,56	1.12	4 (12%)

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
5	PGT	P	201	-	-	17/30/30/55	-
5	PGT	H	201	-	-	17/30/30/55	-
5	PGT	L	201	-	-	16/30/30/55	-
5	PGT	D	201	-	-	17/30/30/55	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	201	PGT	C32-C31	2.29	1.57	1.50
5	H	201	PGT	O3-C11	2.28	1.40	1.33
5	P	201	PGT	O3-C11	2.26	1.39	1.33
5	H	201	PGT	C32-C31	2.24	1.57	1.50
5	P	201	PGT	C32-C31	2.20	1.57	1.50
5	L	201	PGT	C12-C11	2.16	1.57	1.50
5	D	201	PGT	C12-C11	2.13	1.56	1.50
5	L	201	PGT	O3-C11	2.12	1.39	1.33
5	P	201	PGT	C12-C11	2.09	1.56	1.50
5	D	201	PGT	C32-C31	2.06	1.56	1.50
5	D	201	PGT	O3-C11	2.05	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	PGT	O3-C11-C12	3.27	121.79	111.83
5	D	201	PGT	O2-C31-C32	3.12	121.36	111.83
5	P	201	PGT	O2-C31-C32	3.09	121.25	111.83
5	H	201	PGT	O2-C31-C32	3.02	121.06	111.83
5	P	201	PGT	O3-C11-C12	2.98	120.93	111.83
5	L	201	PGT	O2-C31-C32	2.90	120.67	111.83
5	L	201	PGT	O3-C11-C12	2.71	120.10	111.83
5	D	201	PGT	O3-C11-C12	2.68	120.01	111.83
5	D	201	PGT	O2-C31-O31	-2.56	117.22	123.63
5	P	201	PGT	O2-C31-O31	-2.52	117.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	PGT	O2-C31-O31	-2.43	117.55	123.63
5	L	201	PGT	O2-C31-O31	-2.18	118.17	123.63
5	P	201	PGT	O3-C11-O11	-2.04	118.52	123.63
5	D	201	PGT	O3-C3-C2	2.02	114.52	108.61

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	201	PGT	C12-C11-O3-C3
5	H	201	PGT	C12-C11-O3-C3
5	H	201	PGT	O11-C11-O3-C3
5	P	201	PGT	O11-C11-O3-C3
5	D	201	PGT	O11-C11-O3-C3
5	L	201	PGT	O11-C11-O3-C3
5	P	201	PGT	C12-C11-O3-C3
5	L	201	PGT	C12-C11-O3-C3
5	H	201	PGT	C31-C32-C33-C34
5	D	201	PGT	C31-C32-C33-C34
5	P	201	PGT	C31-C32-C33-C34
5	L	201	PGT	C31-C32-C33-C34
5	H	201	PGT	C32-C31-O2-C2
5	P	201	PGT	C32-C31-O2-C2
5	D	201	PGT	C32-C31-O2-C2
5	L	201	PGT	C32-C31-O2-C2
5	H	201	PGT	C35-C36-C37-C38
5	L	201	PGT	C35-C36-C37-C38
5	P	201	PGT	C35-C36-C37-C38
5	D	201	PGT	C35-C36-C37-C38
5	H	201	PGT	O31-C31-O2-C2
5	P	201	PGT	O31-C31-O2-C2
5	L	201	PGT	O31-C31-O2-C2
5	H	201	PGT	C33-C34-C35-C36
5	L	201	PGT	C39-C40-C41-C42
5	D	201	PGT	C33-C34-C35-C36
5	L	201	PGT	C33-C34-C35-C36
5	H	201	PGT	C39-C40-C41-C42
5	P	201	PGT	C39-C40-C41-C42
5	P	201	PGT	C33-C34-C35-C36
5	D	201	PGT	O31-C31-O2-C2
5	D	201	PGT	C39-C40-C41-C42
5	L	201	PGT	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
5	D	201	PGT	C18-C19-C20-C21
5	L	201	PGT	C34-C35-C36-C37
5	H	201	PGT	C34-C35-C36-C37
5	H	201	PGT	C18-C19-C20-C21
5	P	201	PGT	C18-C19-C20-C21
5	D	201	PGT	C34-C35-C36-C37
5	P	201	PGT	C34-C35-C36-C37
5	H	201	PGT	C17-C18-C19-C20
5	D	201	PGT	C17-C18-C19-C20
5	P	201	PGT	C17-C18-C19-C20
5	H	201	PGT	C32-C33-C34-C35
5	L	201	PGT	C17-C18-C19-C20
5	P	201	PGT	C32-C33-C34-C35
5	D	201	PGT	C32-C33-C34-C35
5	L	201	PGT	C32-C33-C34-C35
5	H	201	PGT	C14-C15-C16-C17
5	L	201	PGT	C14-C15-C16-C17
5	D	201	PGT	C14-C15-C16-C17
5	P	201	PGT	C14-C15-C16-C17
5	L	201	PGT	C38-C39-C40-C41
5	D	201	PGT	C38-C39-C40-C41
5	H	201	PGT	C38-C39-C40-C41
5	L	201	PGT	C15-C16-C17-C18
5	P	201	PGT	C15-C16-C17-C18
5	H	201	PGT	C15-C16-C17-C18
5	D	201	PGT	C15-C16-C17-C18
5	P	201	PGT	C38-C39-C40-C41
5	H	201	PGT	O2-C31-C32-C33
5	P	201	PGT	O2-C31-C32-C33
5	D	201	PGT	O2-C31-C32-C33
5	L	201	PGT	O2-C31-C32-C33
5	D	201	PGT	O31-C31-C32-C33
5	H	201	PGT	O31-C31-C32-C33
5	P	201	PGT	O31-C31-C32-C33

There are no ring outliers.

4 monomers are involved in 4 short contacts:

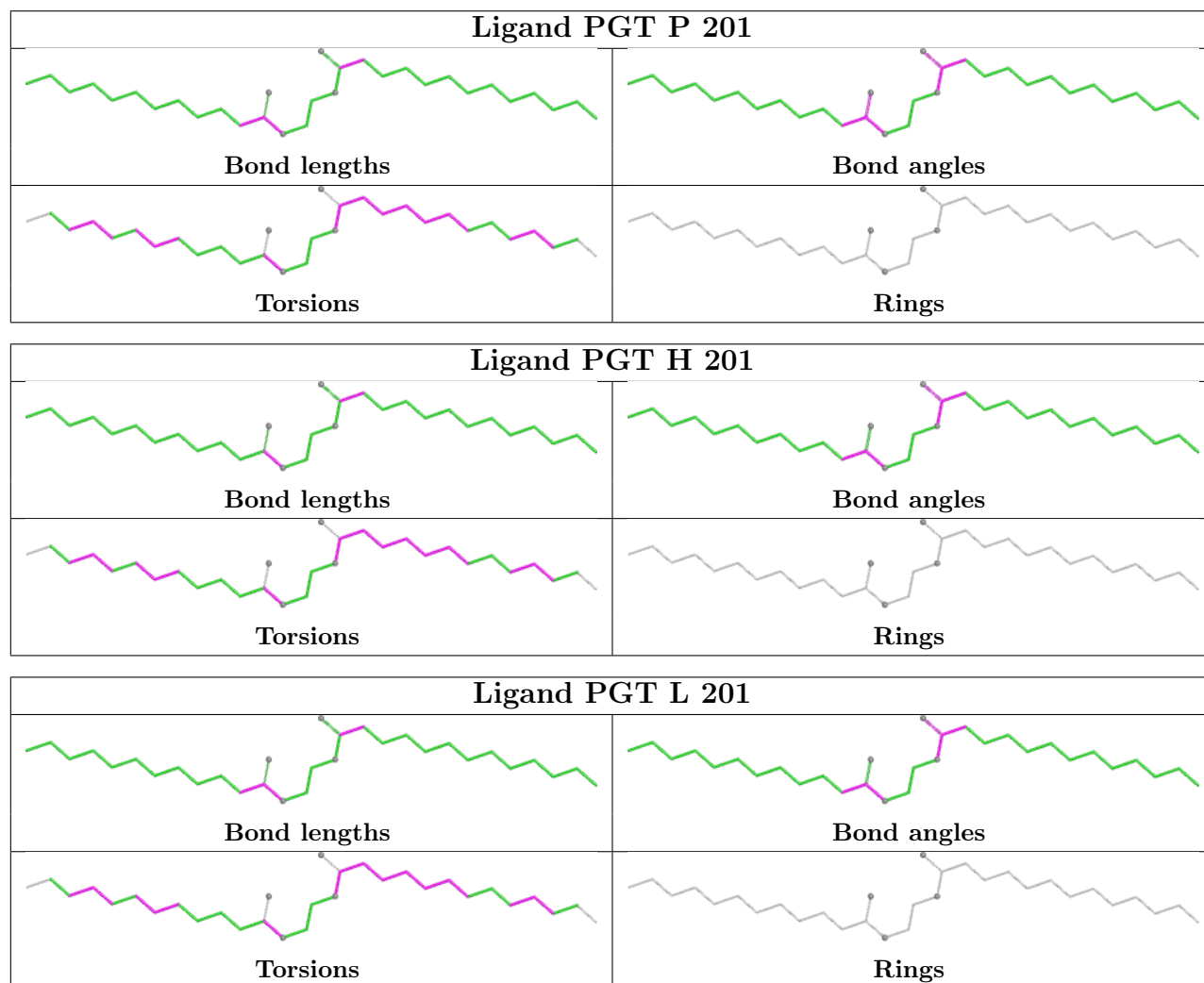
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	201	PGT	1	0
5	H	201	PGT	1	0
5	L	201	PGT	1	0

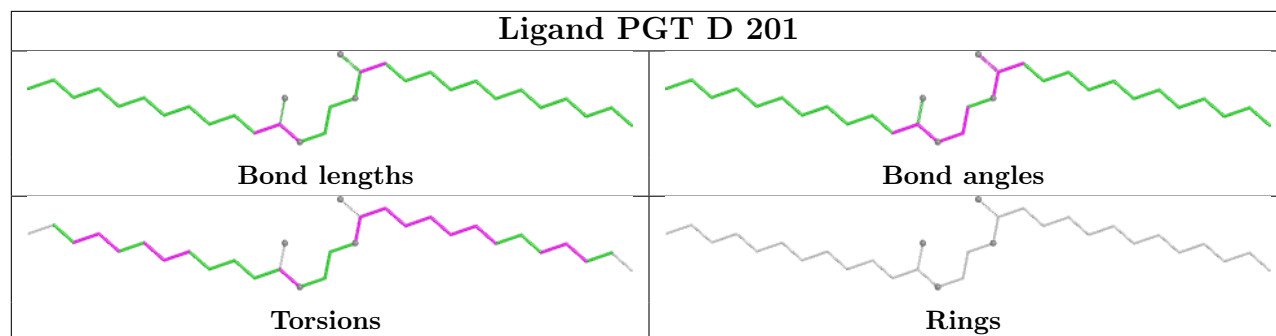
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	201	PGT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	594/612 (97%)	-0.08	10 (1%) 70 70	47, 67, 96, 120	0
1	B	599/612 (97%)	-0.23	4 (0%) 87 88	41, 59, 76, 85	0
1	E	592/612 (96%)	0.09	14 (2%) 59 57	55, 94, 128, 161	0
1	F	599/612 (97%)	-0.03	10 (1%) 70 70	57, 85, 118, 134	0
1	I	397/612 (64%)	0.12	14 (3%) 44 40	55, 94, 136, 151	0
1	J	599/612 (97%)	0.06	16 (2%) 54 51	65, 89, 114, 127	0
1	M	593/612 (96%)	-0.07	7 (1%) 79 79	47, 71, 98, 124	0
1	N	599/612 (97%)	-0.22	6 (1%) 82 82	46, 63, 88, 104	0
2	C	138/147 (93%)	-0.24	1 (0%) 87 88	46, 61, 98, 108	0
2	D	136/147 (92%)	-0.16	2 (1%) 73 73	43, 59, 108, 125	0
2	G	138/147 (93%)	-0.15	0 100 100	54, 72, 104, 112	0
2	H	138/147 (93%)	-0.21	1 (0%) 87 88	54, 65, 82, 86	0
2	K	136/147 (92%)	0.16	5 (3%) 41 38	59, 84, 139, 159	0
2	L	138/147 (93%)	-0.15	2 (1%) 75 76	57, 68, 85, 93	0
2	O	138/147 (93%)	-0.27	1 (0%) 87 88	45, 59, 100, 117	0
2	P	135/147 (91%)	-0.03	4 (2%) 50 46	45, 64, 112, 131	0
All	All	5669/6072 (93%)	-0.07	97 (1%) 70 70	41, 74, 116, 161	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	584	SER	4.8
1	I	311	ASN	4.7
1	E	552	SER	4.7
1	J	258	THR	4.5
1	E	583	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	M	576	HIS	4.1
2	L	54	GLN	4.1
1	F	126	PHE	4.0
1	A	583	CYS	4.0
1	J	394	ASN	4.0
1	J	273	ASP	3.9
1	J	31	LYS	3.7
1	J	233	LEU	3.7
2	P	31	ARG	3.6
1	J	275	SER	3.6
1	I	319	GLY	3.6
1	I	342	ALA	3.6
1	E	582	THR	3.5
2	P	23	ALA	3.5
1	J	259	ASP	3.4
2	D	34	ASN	3.4
1	B	319	GLY	3.3
1	N	316	GLY	3.3
2	H	54	GLN	3.3
1	E	483	ASP	3.3
2	P	32	ASN	3.3
1	M	258	THR	3.3
1	A	258	THR	3.3
1	F	259	ASP	3.2
2	L	55	CYS	3.1
1	J	433	HIS	3.0
1	I	363	THR	3.0
2	C	34	ASN	2.9
1	A	582	THR	2.9
2	K	131	PRO	2.8
1	A	585	ASN	2.8
1	I	332	SER	2.8
1	F	363	THR	2.7
1	M	583	CYS	2.7
1	E	576	HIS	2.7
1	N	319	GLY	2.6
1	B	316	GLY	2.6
1	A	576	HIS	2.6
1	J	346	SER	2.6
1	E	223	ILE	2.6
1	J	54	THR	2.6
1	I	362	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	55	CYS	2.5
1	E	433	HIS	2.5
1	A	581	CYS	2.5
1	A	606	THR	2.5
2	K	91	ILE	2.5
1	E	509	LEU	2.4
2	K	129	GLU	2.4
1	I	260	ASP	2.4
2	P	34	ASN	2.4
1	E	581	CYS	2.4
1	J	126	PHE	2.4
1	I	527	LEU	2.3
1	F	258	THR	2.3
1	I	264	THR	2.3
1	E	561	HIS	2.3
1	I	422	LEU	2.3
1	J	301	GLN	2.2
1	F	436	ALA	2.2
1	F	260	ASP	2.2
2	O	34	ASN	2.2
1	N	101	HIS	2.2
1	J	574	LEU	2.2
1	E	187	TYR	2.2
1	I	272	CYS	2.2
1	J	272	CYS	2.2
1	N	49	ASP	2.2
1	A	257	ASP	2.1
1	E	302	GLU	2.1
1	I	400	TYR	2.1
1	B	445	HIS	2.1
2	K	23	ALA	2.1
1	M	612	SER	2.1
1	N	275	SER	2.1
1	F	246	THR	2.1
1	N	262	TYR	2.1
1	M	257	ASP	2.1
1	A	33	GLY	2.1
1	F	483	ASP	2.1
1	I	382	ILE	2.1
1	M	595	ASN	2.1
1	A	584	SER	2.1
1	I	356	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	244	ASN	2.1
1	M	233	LEU	2.0
1	J	168	GLU	2.0
1	J	216	PRO	2.0
1	F	31	LYS	2.0
1	E	303	LEU	2.0
1	B	482	GLN	2.0
2	K	32	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
3	BMA	S	3	11/12	0.81	0.41	51,54,56,58	0
3	BMA	U	3	11/12	0.83	0.37	51,54,56,58	0
4	MAN	V	8	11/12	0.84	0.34	51,51,54,55	0
4	MAN	d	8	11/12	0.84	0.30	51,51,54,55	0
3	BMA	a	3	11/12	0.85	0.37	51,54,56,58	0
3	BMA	e	3	11/12	0.85	0.27	51,54,56,57	0
4	MAN	d	7	11/12	0.86	0.22	47,49,49,53	0
4	MAN	b	8	11/12	0.87	0.24	51,51,54,55	0
4	MAN	V	7	11/12	0.88	0.40	47,49,50,52	0
3	NAG	U	2	14/15	0.88	0.29	48,50,52,56	0
3	BMA	c	3	11/12	0.88	0.27	51,54,56,58	0
3	BMA	Y	3	11/12	0.88	0.29	51,54,56,58	0
4	NAG	T	2	14/15	0.88	0.31	47,48,50,51	0
3	BMA	W	3	11/12	0.89	0.42	52,54,56,58	0
4	MAN	R	8	11/12	0.89	0.28	51,51,54,55	0
3	NAG	Q	2	14/15	0.90	0.29	47,50,52,56	0
4	MAN	b	7	11/12	0.90	0.19	47,49,49,52	0
3	NAG	S	2	14/15	0.90	0.24	47,50,53,56	0
4	BMA	T	3	11/12	0.90	0.26	46,47,48,49	0
4	MAN	R	6	11/12	0.90	0.29	47,48,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	T	5	11/12	0.91	0.24	47,47,48,50	0
4	NAG	X	2	14/15	0.91	0.22	46,48,50,51	0
4	MAN	X	7	11/12	0.91	0.24	47,49,49,52	0
4	MAN	T	7	11/12	0.91	0.36	47,49,50,52	0
4	NAG	V	2	14/15	0.91	0.26	46,48,50,50	0
4	MAN	V	6	11/12	0.91	0.31	47,48,53,56	0
3	BMA	Q	3	11/12	0.91	0.40	51,54,56,58	0
4	MAN	f	8	11/12	0.91	0.29	51,51,54,55	0
4	MAN	X	8	11/12	0.92	0.34	51,51,54,55	0
4	MAN	Z	7	11/12	0.92	0.16	47,49,49,52	0
4	MAN	Z	8	11/12	0.92	0.22	51,51,54,55	0
3	NAG	c	2	14/15	0.92	0.25	47,50,52,56	0
3	NAG	U	1	14/15	0.92	0.15	44,46,50,51	0
4	MAN	T	8	11/12	0.92	0.38	51,51,54,55	0
4	MAN	R	7	11/12	0.92	0.18	47,49,50,52	0
4	BMA	V	3	11/12	0.92	0.21	46,47,48,49	0
3	NAG	W	2	14/15	0.93	0.26	47,50,52,56	0
4	NAG	b	1	14/15	0.93	0.15	45,48,51,52	0
4	MAN	b	6	11/12	0.93	0.21	47,48,53,56	0
4	NAG	V	1	14/15	0.93	0.14	45,48,51,52	0
4	NAG	T	1	14/15	0.93	0.17	45,48,51,52	0
4	NAG	d	1	14/15	0.93	0.17	45,48,51,52	0
4	MAN	d	6	11/12	0.93	0.20	47,48,53,56	0
4	MAN	T	6	11/12	0.93	0.18	47,48,53,56	0
4	MAN	V	4	11/12	0.93	0.28	46,47,48,49	0
4	NAG	f	1	14/15	0.93	0.19	45,47,51,52	0
4	MAN	f	7	11/12	0.93	0.15	47,49,49,52	0
3	NAG	a	2	14/15	0.93	0.25	47,50,52,56	0
4	BMA	Z	3	11/12	0.94	0.14	46,46,47,49	0
4	MAN	Z	6	11/12	0.94	0.17	46,48,53,56	0
4	BMA	d	3	11/12	0.94	0.20	46,47,48,49	0
4	MAN	d	5	11/12	0.94	0.15	46,47,49,49	0
3	NAG	c	1	14/15	0.94	0.14	43,46,49,51	0
4	MAN	X	6	11/12	0.94	0.29	47,48,53,56	0
4	BMA	R	3	11/12	0.94	0.22	46,47,48,49	0
4	BMA	b	3	11/12	0.94	0.14	46,47,48,49	0
4	MAN	f	6	11/12	0.94	0.16	47,48,53,56	0
4	MAN	V	5	11/12	0.94	0.36	46,47,49,50	0
4	NAG	Z	2	14/15	0.94	0.18	46,48,50,50	0
4	NAG	R	1	14/15	0.95	0.17	45,47,51,52	0
4	NAG	X	1	14/15	0.95	0.20	45,48,51,52	0
3	NAG	W	1	14/15	0.95	0.18	44,46,49,51	0

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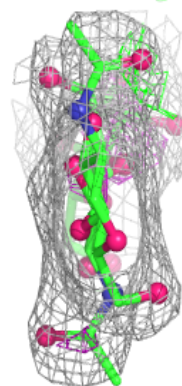
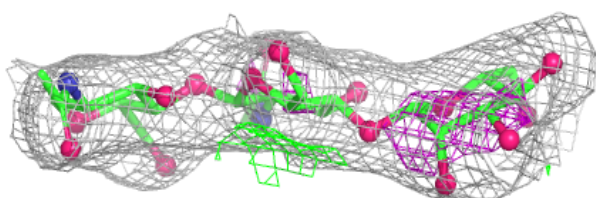
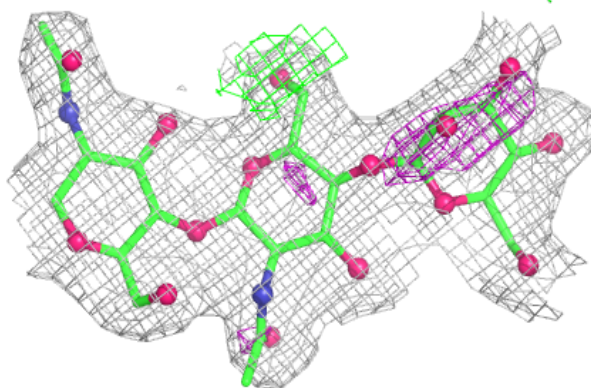
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	Z	4	11/12	0.95	0.15	46,46,48,48	0
4	BMA	X	3	11/12	0.95	0.20	46,47,47,49	0
4	BMA	f	3	11/12	0.95	0.13	46,46,47,49	0
4	MAN	R	5	11/12	0.95	0.23	46,47,48,49	0
4	NAG	d	2	14/15	0.95	0.25	47,48,50,50	0
3	NAG	S	1	14/15	0.95	0.15	44,46,50,51	0
3	NAG	Y	2	14/15	0.96	0.14	47,49,52,56	0
3	NAG	Q	1	14/15	0.96	0.13	44,46,50,51	0
3	NAG	a	1	14/15	0.96	0.13	44,46,50,51	0
4	MAN	b	4	11/12	0.96	0.11	46,47,48,49	0
4	MAN	b	5	11/12	0.96	0.17	46,47,48,49	0
4	MAN	R	4	11/12	0.96	0.17	46,47,48,49	0
4	NAG	f	2	14/15	0.96	0.17	46,47,50,50	0
3	NAG	Y	1	14/15	0.96	0.14	43,46,49,51	0
4	MAN	f	4	11/12	0.96	0.11	46,47,48,48	0
4	MAN	T	4	11/12	0.96	0.18	46,47,48,49	0
3	NAG	e	1	14/15	0.96	0.14	43,46,49,51	0
4	MAN	X	4	11/12	0.96	0.18	46,47,48,49	0
4	MAN	d	4	11/12	0.97	0.10	46,47,48,48	0
4	NAG	b	2	14/15	0.97	0.23	47,48,50,50	0
4	NAG	Z	1	14/15	0.97	0.18	45,47,51,52	0
4	MAN	f	5	11/12	0.97	0.17	46,47,48,49	0
3	NAG	e	2	14/15	0.97	0.13	47,49,52,56	0
4	NAG	R	2	14/15	0.97	0.14	47,48,50,50	0
4	MAN	X	5	11/12	0.97	0.22	46,47,48,49	0
4	MAN	Z	5	11/12	0.98	0.16	46,47,48,49	0

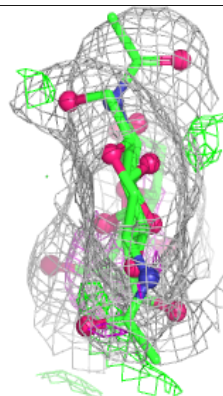
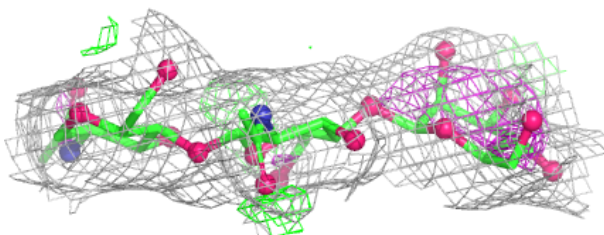
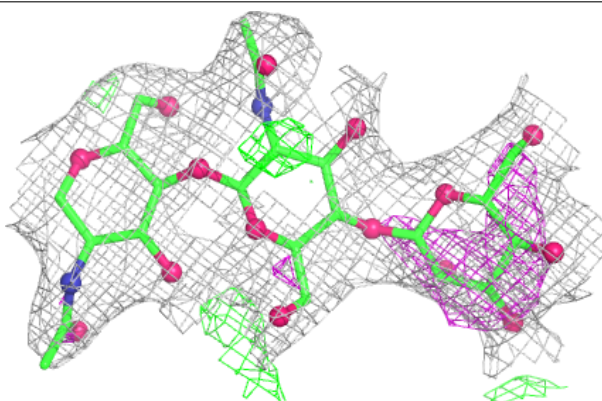
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain Q:**

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

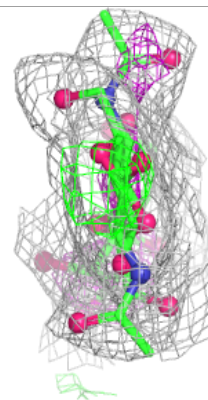
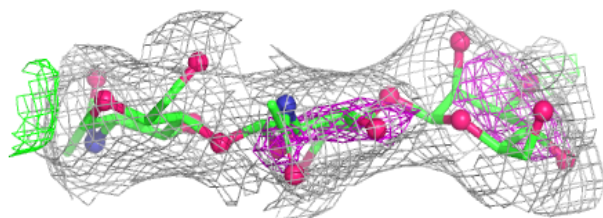
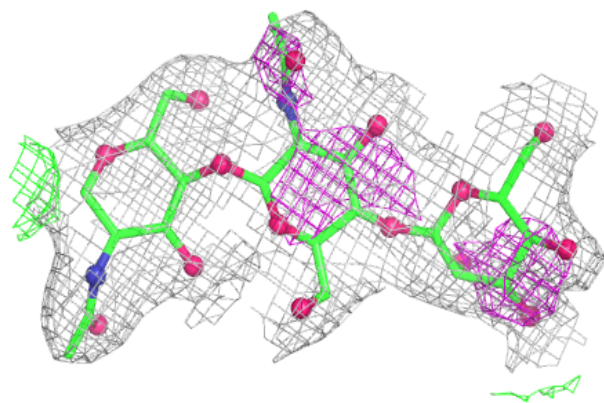
**Electron density around Chain S:**

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and green (positive)

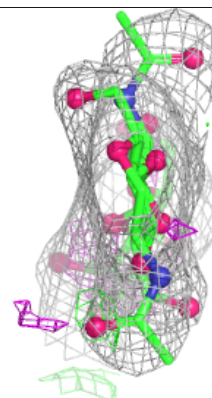
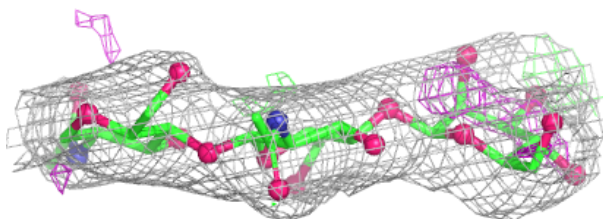
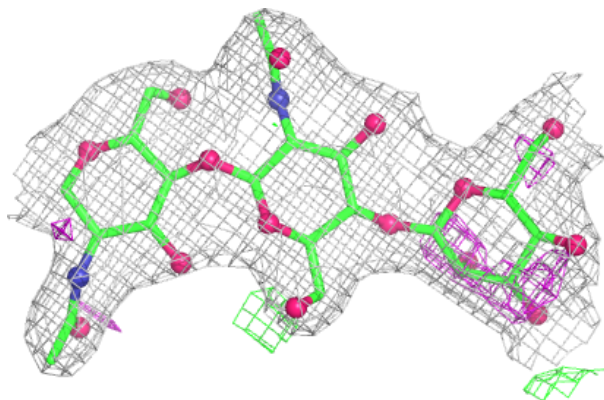


**Electron density around Chain U:**

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

**Electron density around Chain W:**

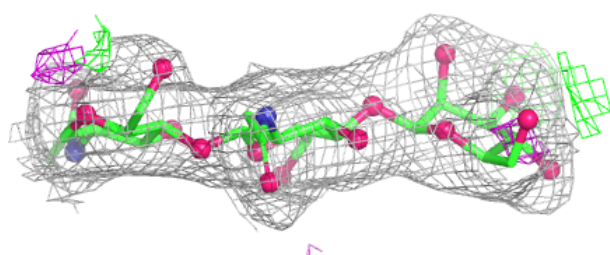
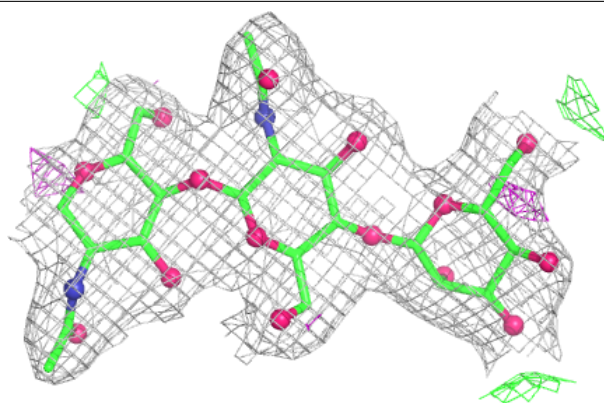
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



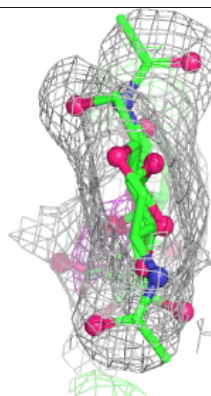
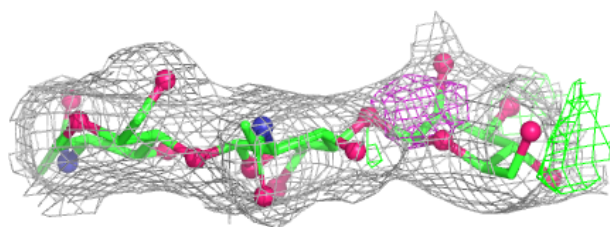
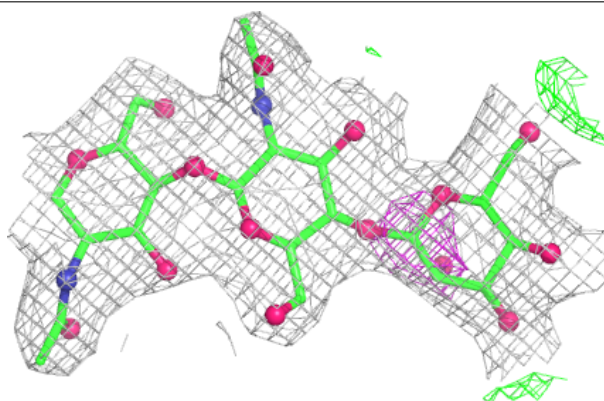


**Electron density around Chain Y:**

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

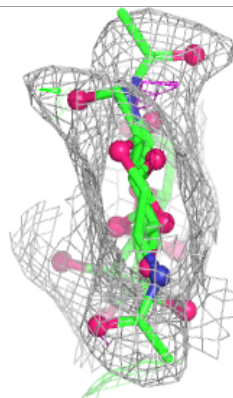
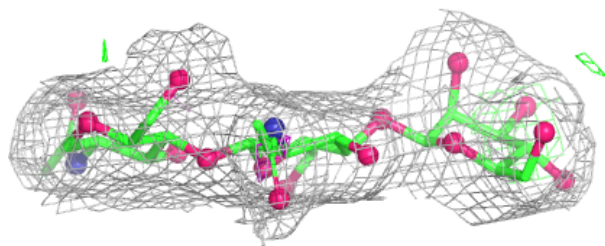
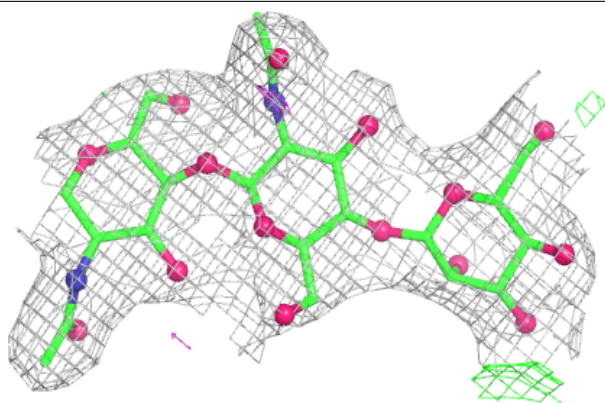
**Electron density around Chain a:**

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



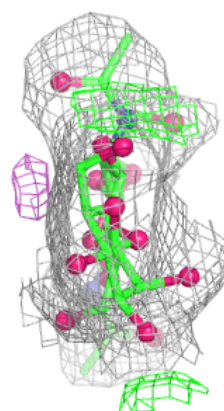
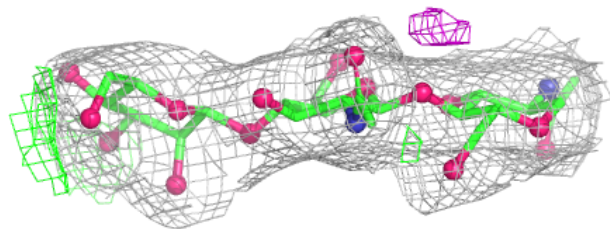
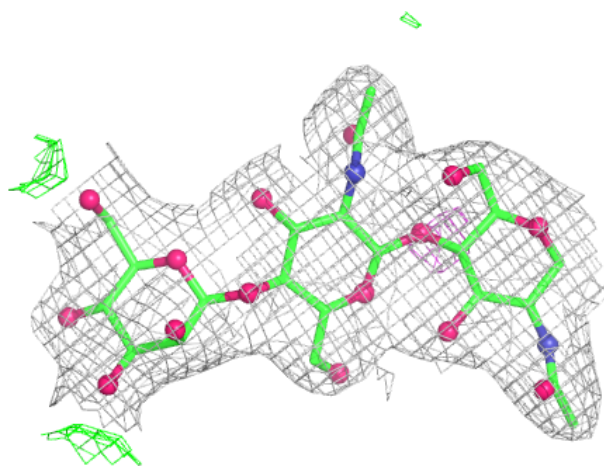
**Electron density around Chain c:**

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



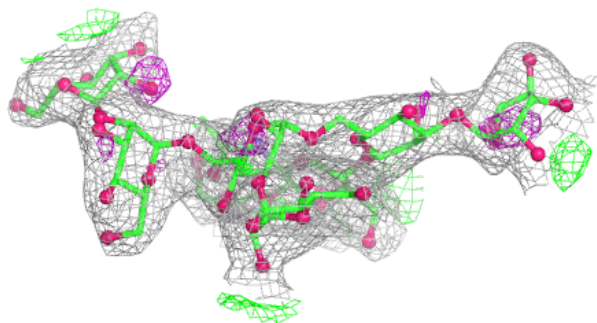
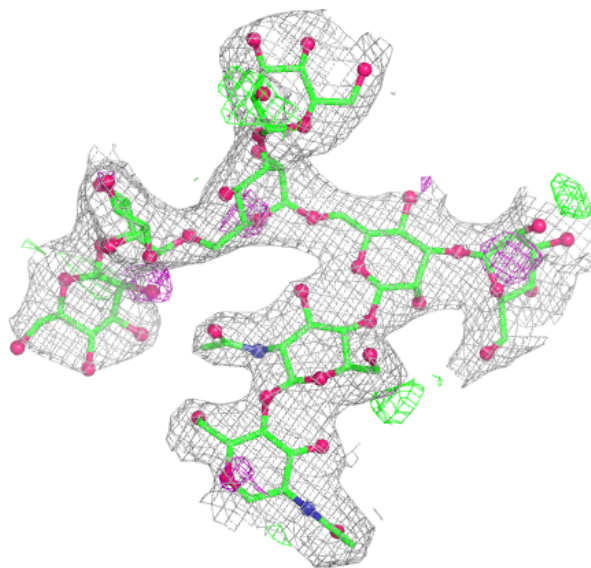
**Electron density around Chain e:**

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



**Electron density around Chain R:**

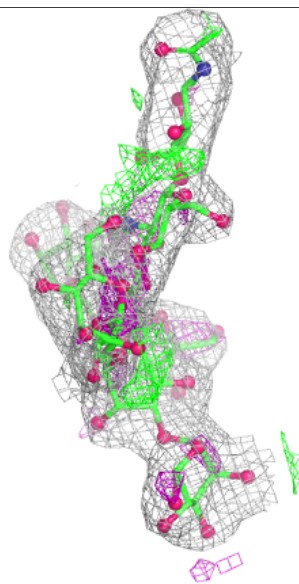
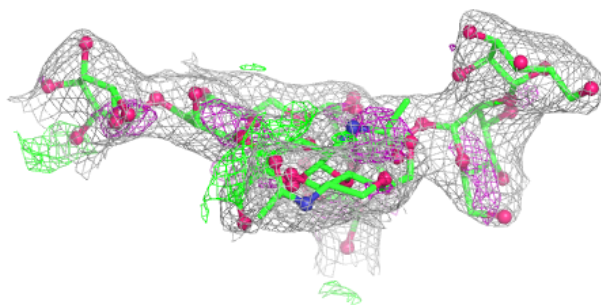
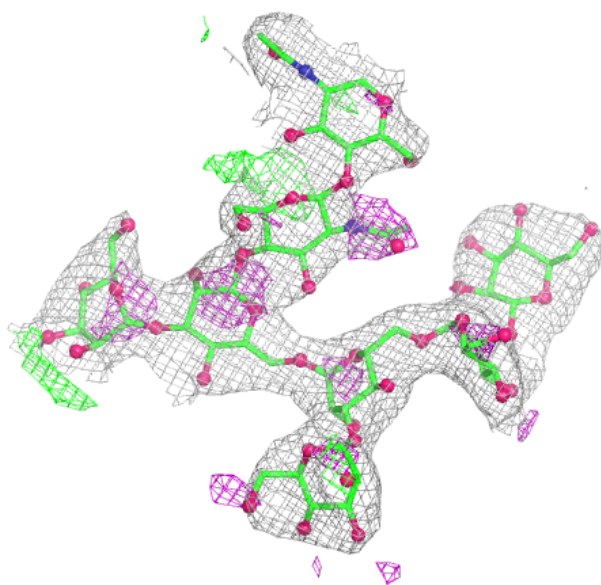
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





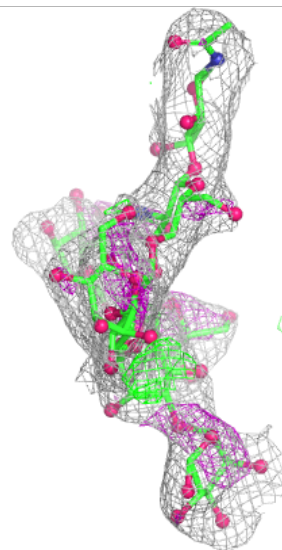
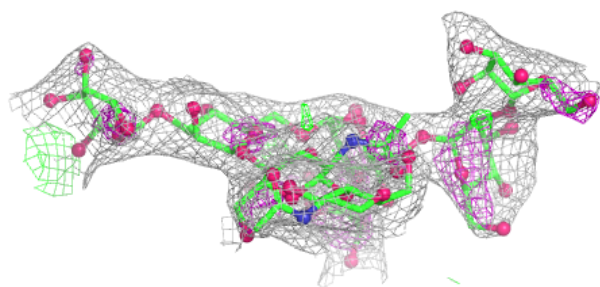
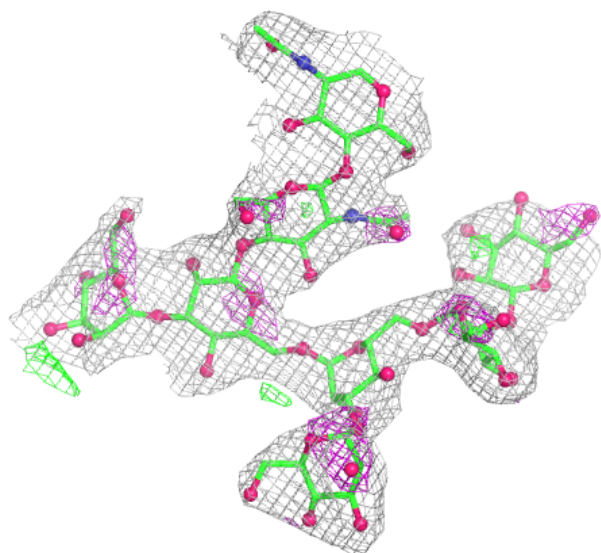
**Electron density around Chain T:**

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



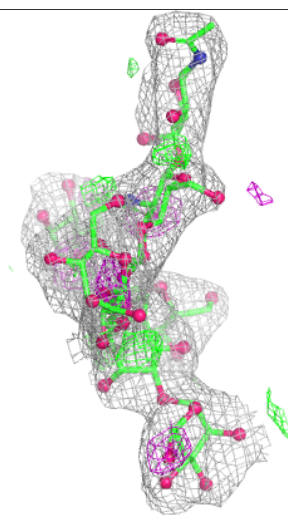
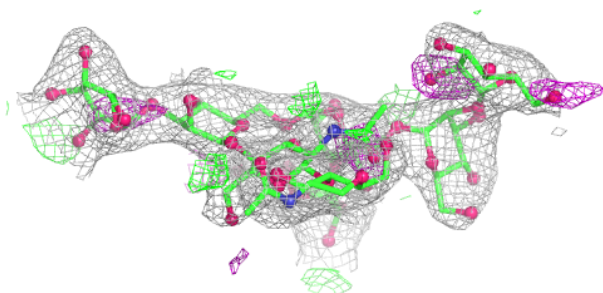
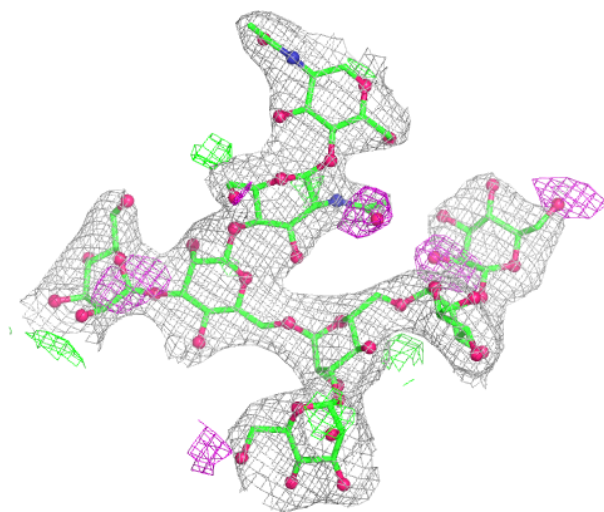
**Electron density around Chain V:**

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



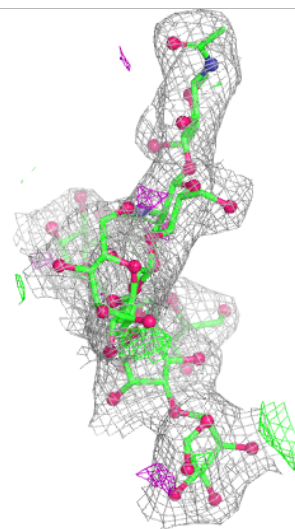
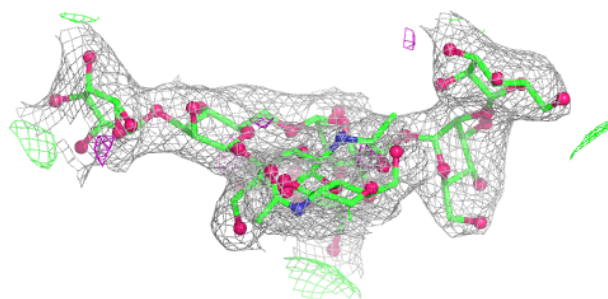
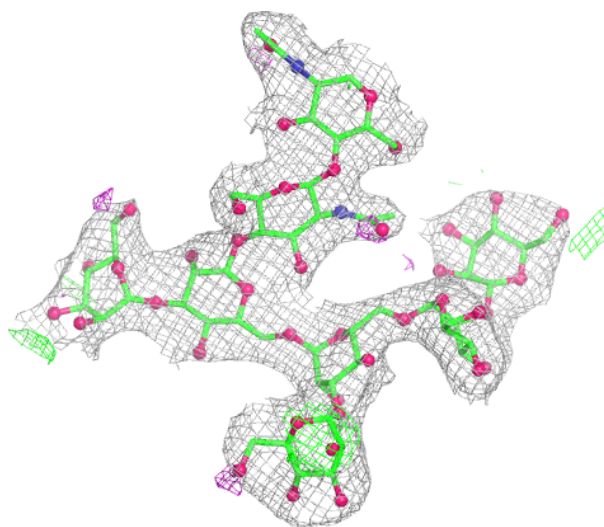
**Electron density around Chain X:**

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



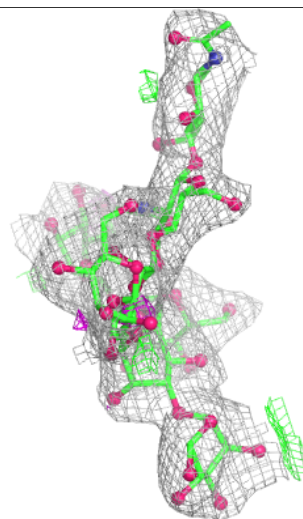
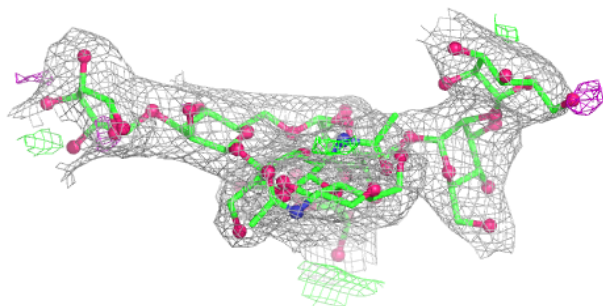
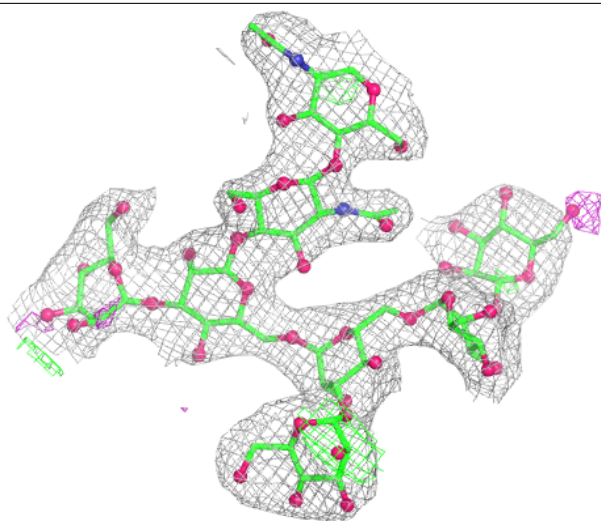
**Electron density around Chain Z:**

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



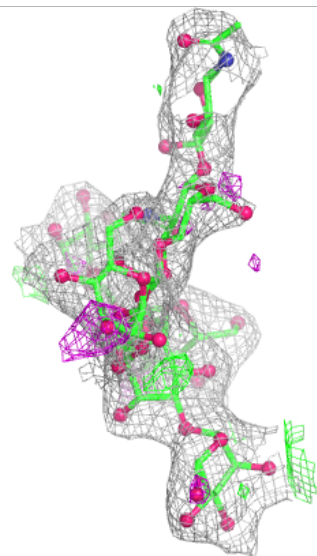
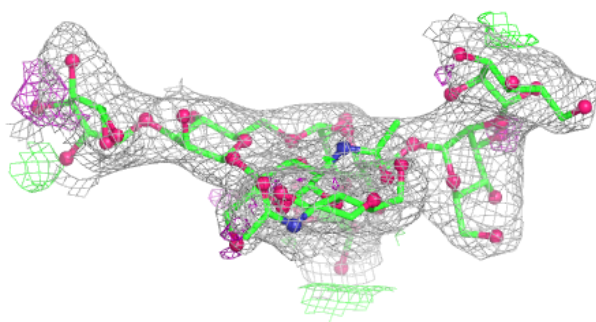
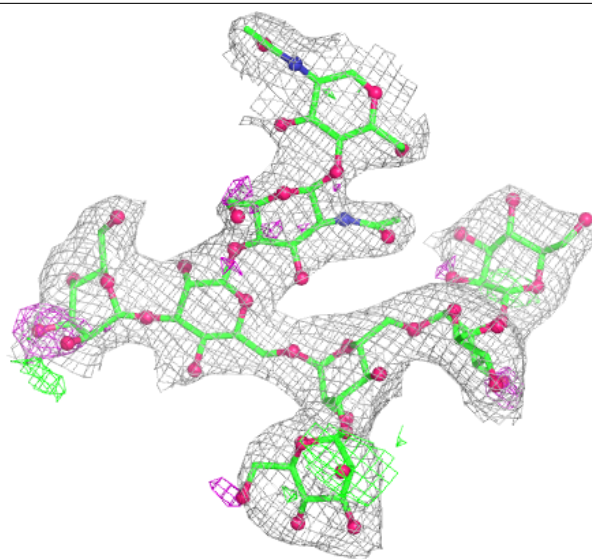
**Electron density around Chain b:**

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

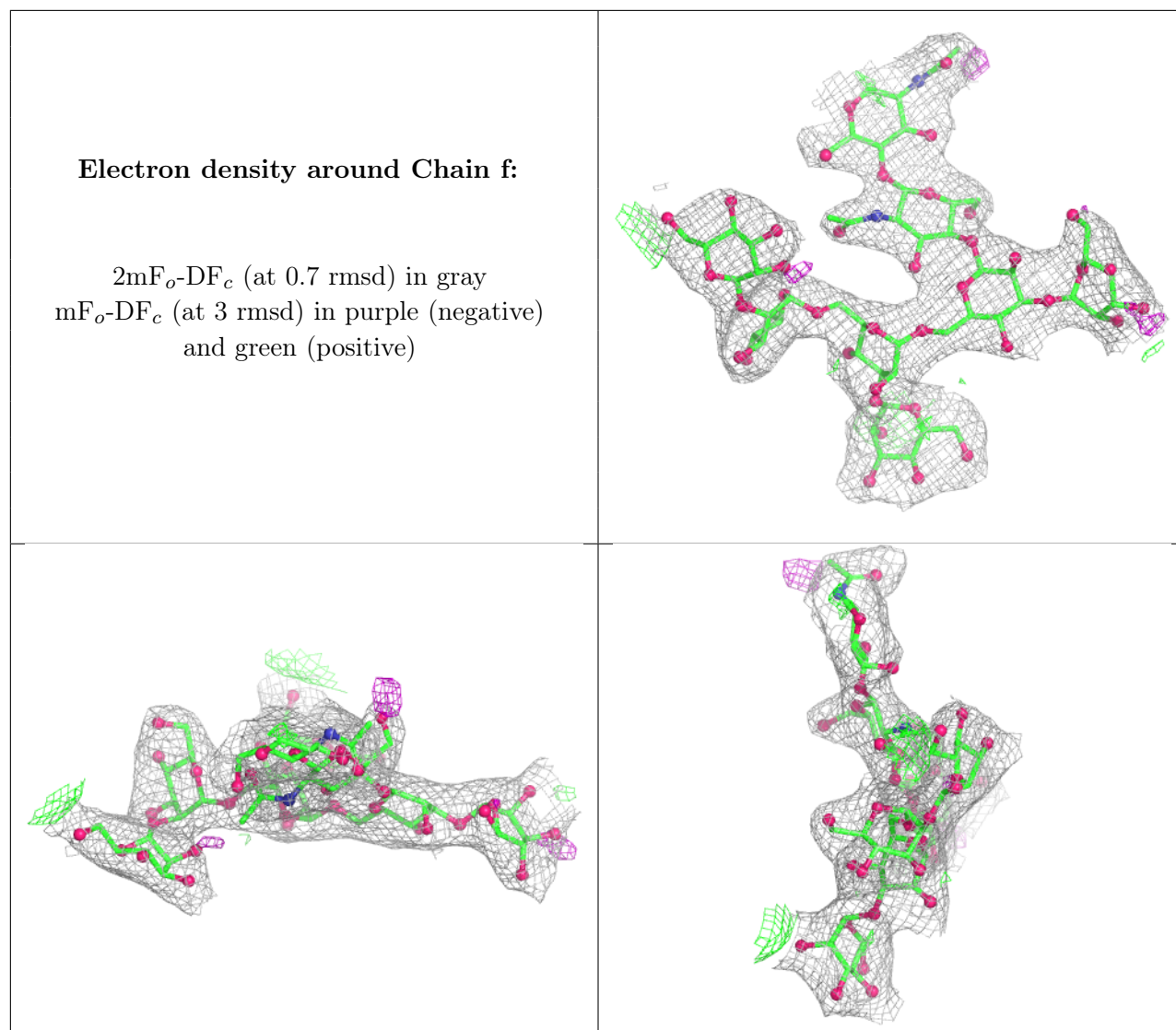


**Electron density around Chain d:**

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







## 6.4 Ligands ⓘ

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

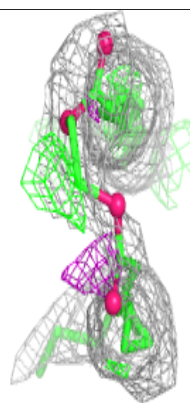
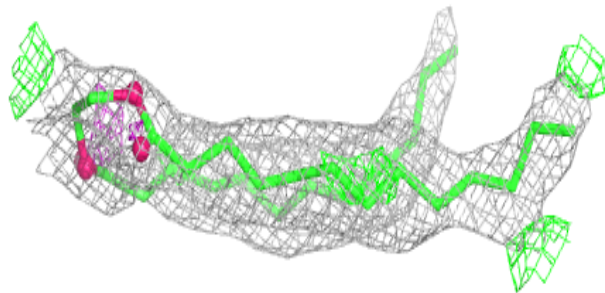
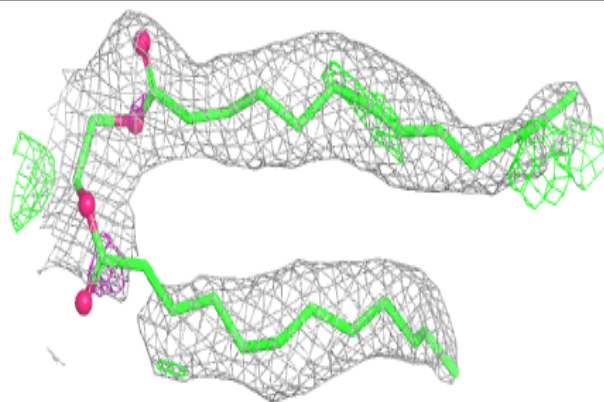
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PGT	L	201	31/51	0.55	0.48	71,78,92,93	0
5	PGT	H	201	31/51	0.62	0.42	71,79,92,93	0
5	PGT	D	201	31/51	0.70	0.39	71,78,92,93	0
5	PGT	P	201	31/51	0.74	0.34	71,78,92,93	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

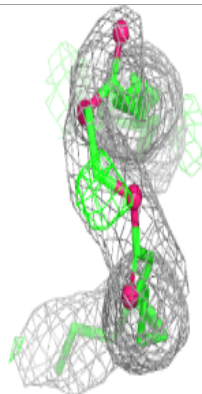
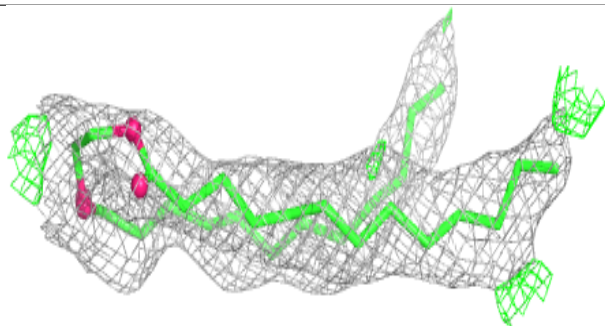
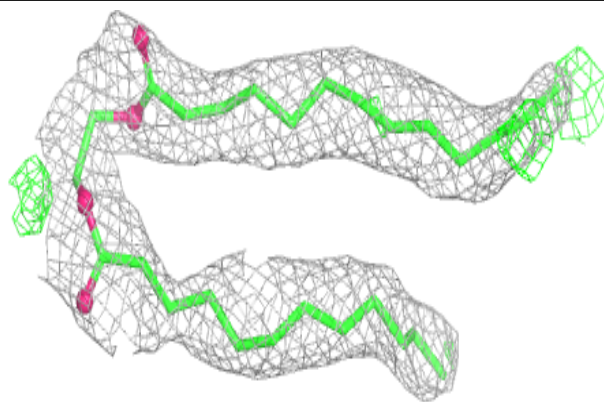
**Electron density around PGT L 201:**

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



**Electron density around PGT H 201:**

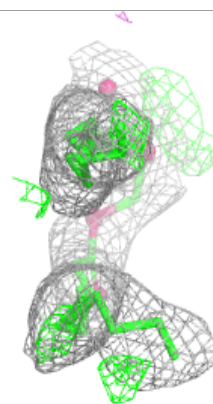
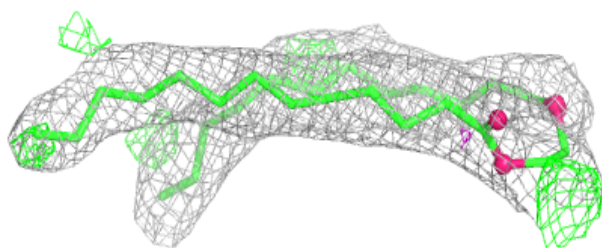
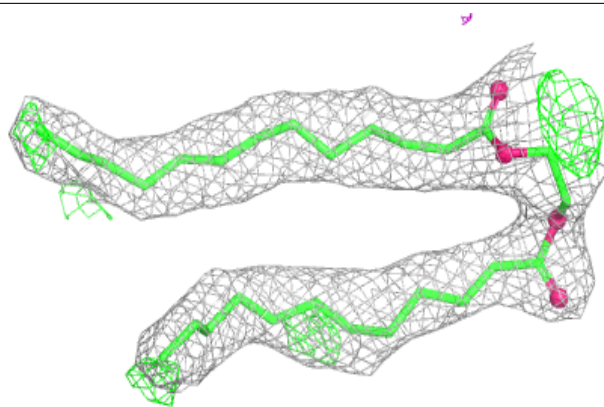
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



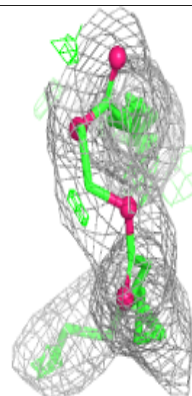
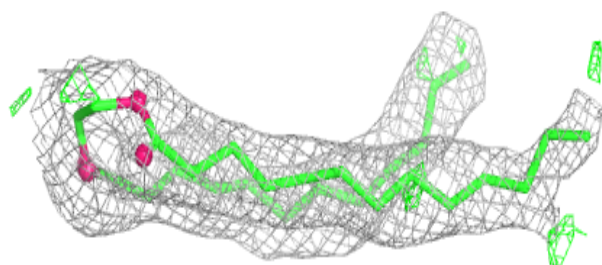
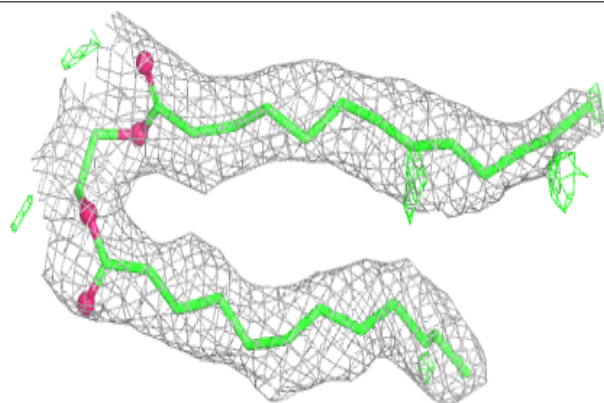


**Electron density around PGT D 201:**

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

**Electron density around PGT P 201:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.