



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:47 PM EDT

PDB ID : 6M6T / pdb_00006m6t
Title : Amylomaltase from Streptococcus agalactiae in complex with acarbose
Authors : Wangkanont, K.; Tumhom, S.; Pongsawasdi, P.
Deposited on : 2020-03-16
Resolution : 2.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

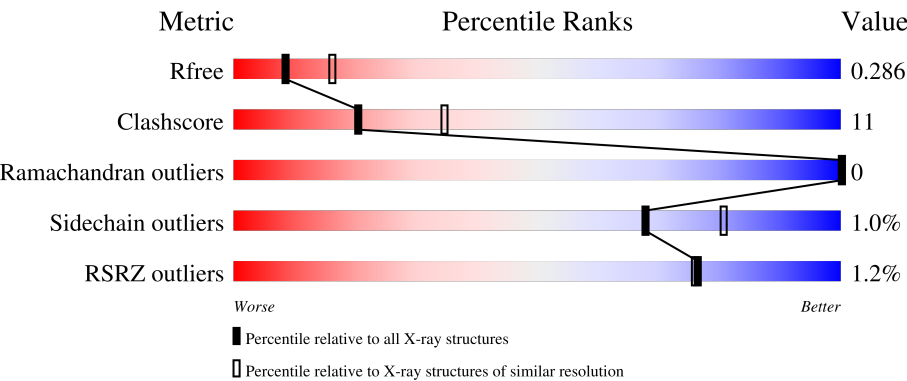
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.75 Å.

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



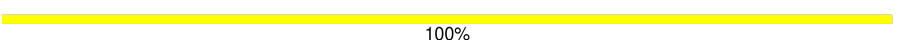
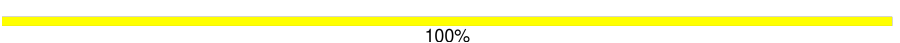
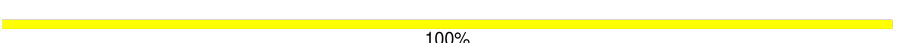
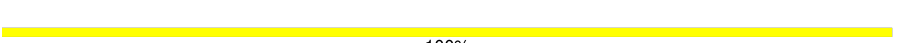
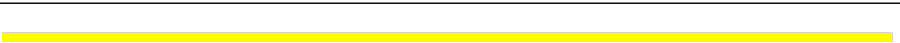
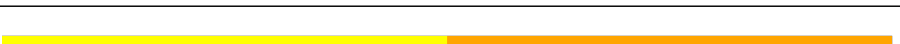
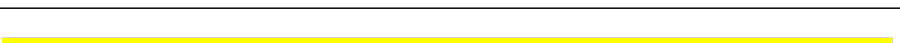
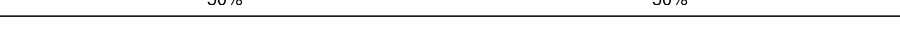
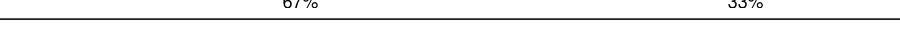
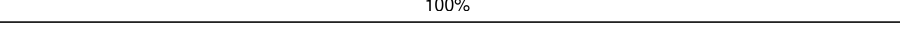
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	507	% 67% 30% .
1	B	507	% 68% 30% .
1	C	507	% 76% 22% .
1	D	507	74% 23% ..
1	E	507	76% 22% .

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Mol	Chain	Length	Quality of chain
1	F	507	
1	G	507	
1	H	507	
2	I	2	
2	K	2	
2	M	2	
2	O	2	
2	Q	2	
2	S	2	
2	W	2	
3	J	2	
3	L	2	
3	P	2	
3	T	2	
3	V	2	
3	X	2	
4	N	3	
4	R	3	
4	U	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33396 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 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			4067	2609	668	776	14			
1	B	497	Total	C	N	O	S	0	0	0
			4072	2612	669	777	14			
1	C	499	Total	C	N	O	S	0	1	0
			4100	2630	676	780	14			
1	D	496	Total	C	N	O	S	0	0	0
			4067	2609	668	776	14			
1	E	497	Total	C	N	O	S	0	0	0
			4075	2615	669	777	14			
1	F	496	Total	C	N	O	S	0	0	0
			4067	2609	668	776	14			
1	G	498	Total	C	N	O	S	0	0	0
			4084	2621	671	778	14			
1	H	495	Total	C	N	O	S	0	0	0
			4058	2603	666	775	14			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
A	1	ALA	-	expression tag	UNP A0A0E1EIJ0
A	499	LEU	-	expression tag	UNP A0A0E1EIJ0
A	500	GLU	-	expression tag	UNP A0A0E1EIJ0
A	501	HIS	-	expression tag	UNP A0A0E1EIJ0
A	502	HIS	-	expression tag	UNP A0A0E1EIJ0
A	503	HIS	-	expression tag	UNP A0A0E1EIJ0
A	504	HIS	-	expression tag	UNP A0A0E1EIJ0
A	505	HIS	-	expression tag	UNP A0A0E1EIJ0
A	506	HIS	-	expression tag	UNP A0A0E1EIJ0
B	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
B	1	ALA	-	expression tag	UNP A0A0E1EIJ0
B	499	LEU	-	expression tag	UNP A0A0E1EIJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	500	GLU	-	expression tag	UNP A0A0E1EIJ0
B	501	HIS	-	expression tag	UNP A0A0E1EIJ0
B	502	HIS	-	expression tag	UNP A0A0E1EIJ0
B	503	HIS	-	expression tag	UNP A0A0E1EIJ0
B	504	HIS	-	expression tag	UNP A0A0E1EIJ0
B	505	HIS	-	expression tag	UNP A0A0E1EIJ0
B	506	HIS	-	expression tag	UNP A0A0E1EIJ0
C	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
C	1	ALA	-	expression tag	UNP A0A0E1EIJ0
C	499	LEU	-	expression tag	UNP A0A0E1EIJ0
C	500	GLU	-	expression tag	UNP A0A0E1EIJ0
C	501	HIS	-	expression tag	UNP A0A0E1EIJ0
C	502	HIS	-	expression tag	UNP A0A0E1EIJ0
C	503	HIS	-	expression tag	UNP A0A0E1EIJ0
C	504	HIS	-	expression tag	UNP A0A0E1EIJ0
C	505	HIS	-	expression tag	UNP A0A0E1EIJ0
C	506	HIS	-	expression tag	UNP A0A0E1EIJ0
D	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
D	1	ALA	-	expression tag	UNP A0A0E1EIJ0
D	499	LEU	-	expression tag	UNP A0A0E1EIJ0
D	500	GLU	-	expression tag	UNP A0A0E1EIJ0
D	501	HIS	-	expression tag	UNP A0A0E1EIJ0
D	502	HIS	-	expression tag	UNP A0A0E1EIJ0
D	503	HIS	-	expression tag	UNP A0A0E1EIJ0
D	504	HIS	-	expression tag	UNP A0A0E1EIJ0
D	505	HIS	-	expression tag	UNP A0A0E1EIJ0
D	506	HIS	-	expression tag	UNP A0A0E1EIJ0
E	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
E	1	ALA	-	expression tag	UNP A0A0E1EIJ0
E	499	LEU	-	expression tag	UNP A0A0E1EIJ0
E	500	GLU	-	expression tag	UNP A0A0E1EIJ0
E	501	HIS	-	expression tag	UNP A0A0E1EIJ0
E	502	HIS	-	expression tag	UNP A0A0E1EIJ0
E	503	HIS	-	expression tag	UNP A0A0E1EIJ0
E	504	HIS	-	expression tag	UNP A0A0E1EIJ0
E	505	HIS	-	expression tag	UNP A0A0E1EIJ0
E	506	HIS	-	expression tag	UNP A0A0E1EIJ0
F	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
F	1	ALA	-	expression tag	UNP A0A0E1EIJ0
F	499	LEU	-	expression tag	UNP A0A0E1EIJ0
F	500	GLU	-	expression tag	UNP A0A0E1EIJ0
F	501	HIS	-	expression tag	UNP A0A0E1EIJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	502	HIS	-	expression tag	UNP A0A0E1EIJ0
F	503	HIS	-	expression tag	UNP A0A0E1EIJ0
F	504	HIS	-	expression tag	UNP A0A0E1EIJ0
F	505	HIS	-	expression tag	UNP A0A0E1EIJ0
F	506	HIS	-	expression tag	UNP A0A0E1EIJ0
G	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
G	1	ALA	-	expression tag	UNP A0A0E1EIJ0
G	499	LEU	-	expression tag	UNP A0A0E1EIJ0
G	500	GLU	-	expression tag	UNP A0A0E1EIJ0
G	501	HIS	-	expression tag	UNP A0A0E1EIJ0
G	502	HIS	-	expression tag	UNP A0A0E1EIJ0
G	503	HIS	-	expression tag	UNP A0A0E1EIJ0
G	504	HIS	-	expression tag	UNP A0A0E1EIJ0
G	505	HIS	-	expression tag	UNP A0A0E1EIJ0
G	506	HIS	-	expression tag	UNP A0A0E1EIJ0
H	0	MET	-	initiating methionine	UNP A0A0E1EIJ0
H	1	ALA	-	expression tag	UNP A0A0E1EIJ0
H	499	LEU	-	expression tag	UNP A0A0E1EIJ0
H	500	GLU	-	expression tag	UNP A0A0E1EIJ0
H	501	HIS	-	expression tag	UNP A0A0E1EIJ0
H	502	HIS	-	expression tag	UNP A0A0E1EIJ0
H	503	HIS	-	expression tag	UNP A0A0E1EIJ0
H	504	HIS	-	expression tag	UNP A0A0E1EIJ0
H	505	HIS	-	expression tag	UNP A0A0E1EIJ0
H	506	HIS	-	expression tag	UNP A0A0E1EIJ0

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			32	19	1	12			
2	K	2	Total	C	N	O	0	0	0
			32	19	1	12			
2	M	2	Total	C	N	O	0	0	0
			32	19	1	12			
2	O	2	Total	C	N	O	0	0	0
			32	19	1	12			
2	Q	2	Total	C	N	O	0	0	0
			32	19	1	12			
2	S	2	Total	C	N	O	0	0	0
			32	19	1	12			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	2	Total	C	N	O	0	0	0
			32	19	1	12			

- Molecule 3 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	2	Total	C	N	O	0	0	0
			33	19	1	13			
3	L	2	Total	C	N	O	0	0	0
			33	19	1	13			
3	P	2	Total	C	N	O	0	0	0
			33	19	1	13			
3	T	2	Total	C	N	O	0	0	0
			33	19	1	13			
3	V	2	Total	C	N	O	0	0	0
			33	19	1	13			
3	X	2	Total	C	N	O	0	0	0
			33	19	1	13			

- Molecule 4 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos e-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	3	Total	C	N	O	0	0	0
			44	25	1	18			
4	R	3	Total	C	N	O	0	0	0
			44	25	1	18			
4	U	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	26	Total	O	0	0
			26	26		
5	C	39	Total	O	0	0
			39	39		

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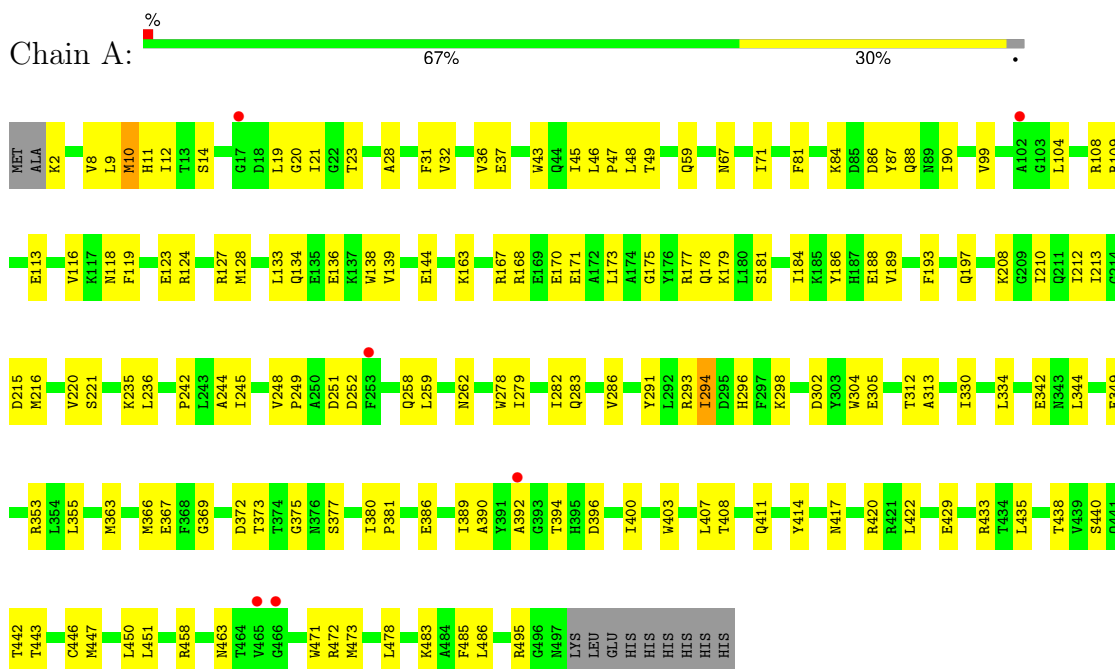
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	23	Total 23	O 23	0	0
5	E	48	Total 48	O 48	0	0
5	F	33	Total 33	O 33	0	0
5	G	25	Total 25	O 25	0	0
5	H	28	Total 28	O 28	0	0

3 Residue-property plots

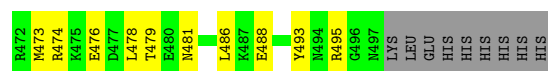
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-alpha-glucanotransferase

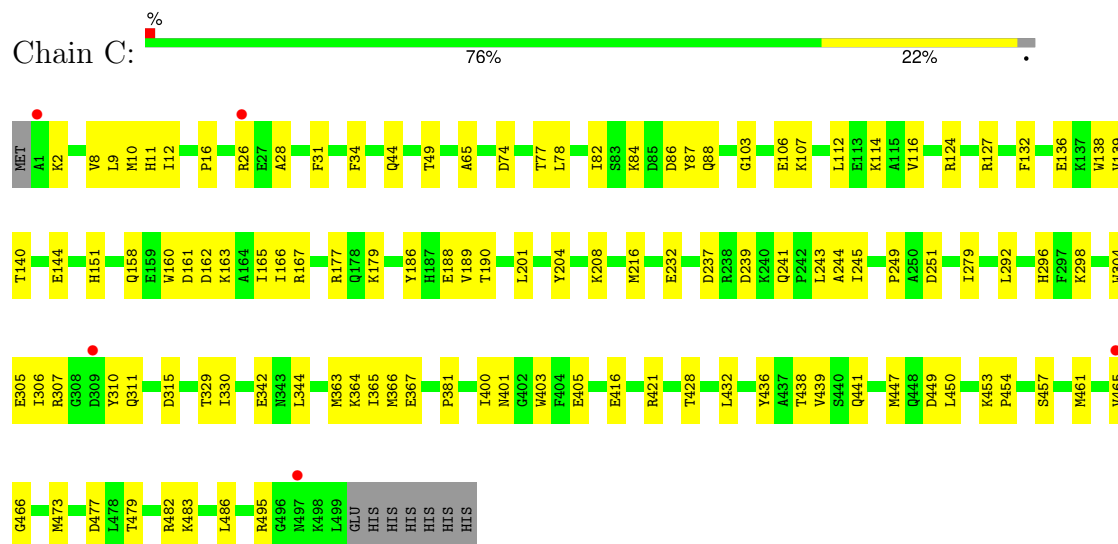


• Molecule 1: 4-alpha-glucanotransferase

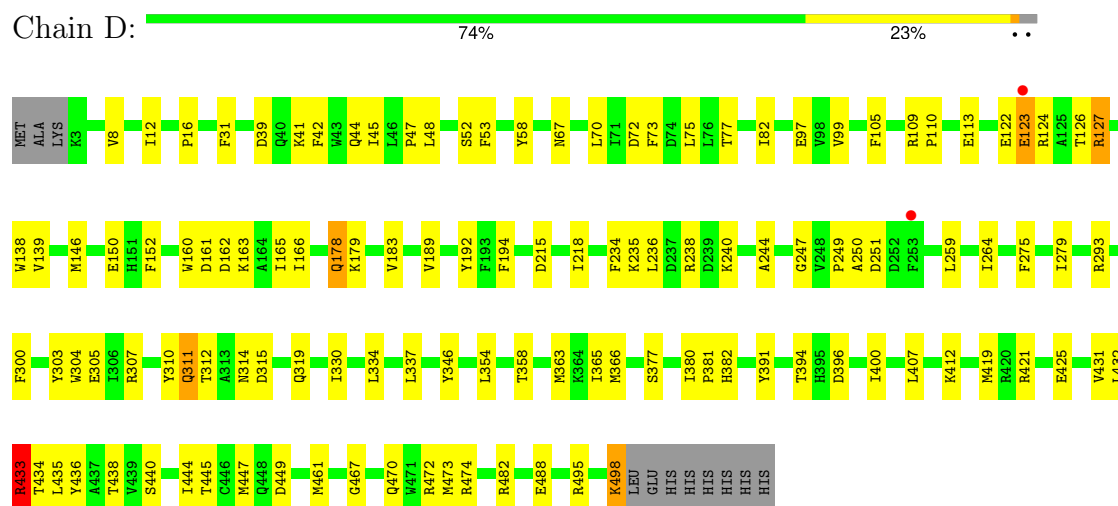




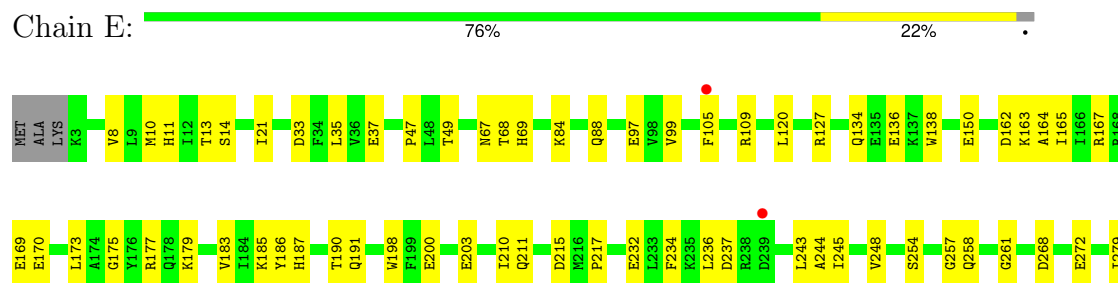
• Molecule 1: 4-alpha-glucanotransferase

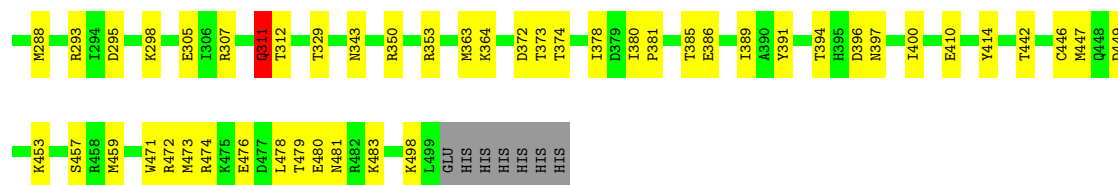


• Molecule 1: 4-alpha-glucanotransferase



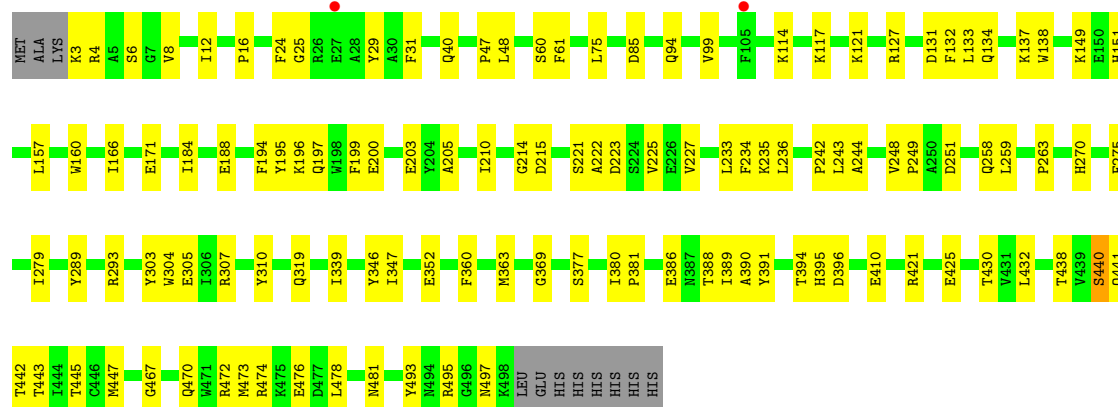
• Molecule 1: 4-alpha-glucanotransferase





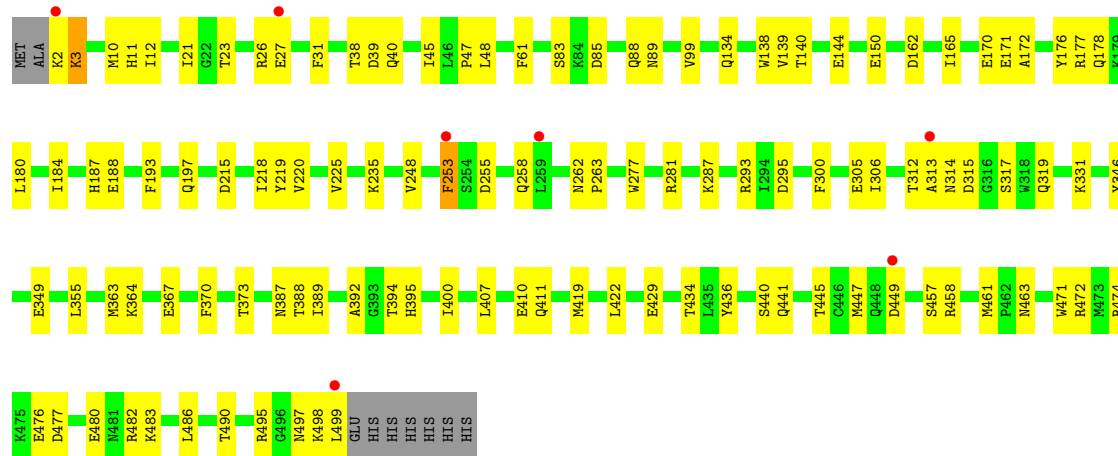
• Molecule 1: 4-alpha-glucanotransferase

Chain F: 75% 23% .



• Molecule 1: 4-alpha-glucanotransferase

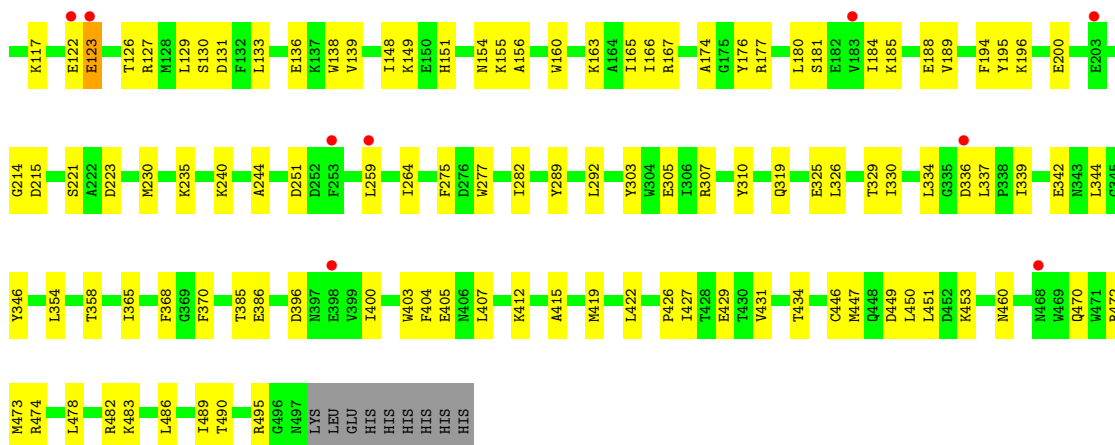
Chain G: 76% 22% .



• Molecule 1: 4-alpha-glucanotransferase

Chain H: 70% 27% .





- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain I: 50%

AS01
AC12

- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain K: 100%

AS01
AC12

- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain M: 100%

AS01
AC12

- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain O: 100%

AS01
AC12

- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain Q: 50%



- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain S:  50% 50%



- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain W:  100%



- Molecule 3: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  50% 50%

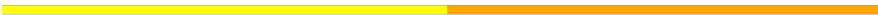


- Molecule 3: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  100%



- Molecule 3: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:  50% 50%



- Molecule 3: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain T:  100%



- Molecule 3: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain V:  50% 50%

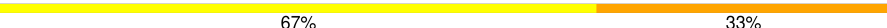
GLC1
GLC2
ACT12

- Molecule 3: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain X:  50% 50%

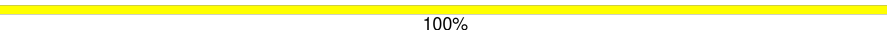
GLC1
GLC2
ACT12

- Molecule 4: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain N:  67% 33%

GLC1
GLC2
GLC3
ACT13

- Molecule 4: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain R:  100%

GLC1
GLC2
GLC3
ACT13

- Molecule 4: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain U:  33% 67%

GLC1
GLC2
GLC3
ACT13

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.75Å 216.07Å 224.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.75 29.82 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.82-2.75) 98.5 (29.82-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.205 , 0.287 0.205 , 0.286	Depositor DCC
R_{free} test set	6497 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33396	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7782e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, AC1, ASO

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	0.42	0/4176	0.63	1/5661 (0.0%)
1	B	0.45	0/4181	0.67	1/5668 (0.0%)
1	C	0.45	0/4209	0.65	0/5704
1	D	0.47	1/4176 (0.0%)	0.69	2/5661 (0.0%)
1	E	0.47	0/4184	0.67	1/5672 (0.0%)
1	F	0.44	0/4176	0.62	0/5661
1	G	0.45	0/4193	0.64	1/5683 (0.0%)
1	H	0.41	0/4167	0.63	0/5650
All	All	0.45	1/33462 (0.0%)	0.65	6/45360 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	433	ARG	C-O	-5.36	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	GLN	N-CA-C	-6.66	106.11	114.56
1	E	311	GLN	N-CA-C	-5.98	106.60	114.31
1	G	3	LYS	N-CA-C	-5.54	106.68	113.50
1	D	314	ASN	N-CA-C	-5.44	106.31	113.17
1	A	178	GLN	N-CA-C	-5.16	106.67	113.12
1	B	124	ARG	N-CA-C	-5.00	106.96	113.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4067	0	3886	119	0
1	B	4072	0	3894	106	0
1	C	4100	0	3930	80	0
1	D	4067	0	3886	88	0
1	E	4075	0	3897	85	0
1	F	4067	0	3886	82	0
1	G	4084	0	3910	88	0
1	H	4058	0	3873	98	0
2	I	32	0	20	4	0
2	K	32	0	20	0	0
2	M	32	0	20	0	0
2	O	32	0	20	0	0
2	Q	32	0	20	0	0
2	S	32	0	20	1	0
2	W	32	0	20	0	0
3	J	33	0	21	2	0
3	L	33	0	21	0	0
3	P	33	0	21	1	0
3	T	33	0	21	0	0
3	V	33	0	21	2	0
3	X	33	0	21	1	0
4	N	44	0	30	1	0
4	R	44	0	30	0	0
4	U	44	0	30	5	0
5	A	30	0	0	3	0
5	B	26	0	0	3	0
5	C	39	0	0	0	0
5	D	23	0	0	1	0
5	E	48	0	0	4	0
5	F	33	0	0	3	0
5	G	25	0	0	2	0
5	H	28	0	0	1	0
All	All	33396	0	31518	724	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 11.

All (724) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG12	1:A:258:GLN:HB2	1.47	0.96
1:D:234:PHE:HB2	1:D:236:LEU:HD11	1.49	0.93
1:A:366:MET:HE1	1:A:435:LEU:HB2	1.51	0.89
1:F:425:GLU:OE2	1:F:430:THR:HG22	1.75	0.86
1:H:11:HIS:HB2	1:H:46:LEU:HD13	1.58	0.85
1:F:293:ARG:HH11	1:F:363:MET:HE1	1.43	0.83
1:A:21:ILE:HD12	1:A:99:VAL:HG11	1.61	0.81
1:A:59:GLN:HE22	2:I:2:AC1:HC61	1.46	0.81
1:B:9:LEU:HD13	1:B:44:GLN:HG2	1.63	0.80
1:A:216:MET:HE2	1:A:294:ILE:HD13	1.65	0.79
1:D:16:PRO:HD3	1:D:473:MET:HE2	1.66	0.78
1:H:336:ASP:O	1:H:337:LEU:HD22	1.84	0.78
1:H:447:MET:HE3	1:H:451:LEU:HD11	1.68	0.76
1:A:422:LEU:HD23	1:B:423:PRO:HD3	1.67	0.76
1:E:311:GLN:HA	1:E:311:GLN:OE1	1.85	0.76
1:B:23:THR:HG22	1:B:70:LEU:HA	1.68	0.75
1:A:87:TYR:HA	1:A:90:ILE:HG13	1.68	0.75
1:F:495:ARG:HG2	1:F:495:ARG:HH21	1.52	0.75
1:E:237:ASP:HB3	1:E:243:LEU:HD21	1.69	0.75
1:C:342:GLU:HA	1:C:363:MET:HG3	1.68	0.74
1:E:380:ILE:HG13	1:E:381:PRO:HD2	1.69	0.74
1:F:421:ARG:HG3	1:F:430:THR:HG21	1.67	0.74
1:D:482:ARG:HE	1:D:482:ARG:HA	1.52	0.74
1:F:425:GLU:CD	1:F:430:THR:HG22	2.13	0.73
1:B:385:THR:HG22	1:B:387:ASN:H	1.52	0.73
1:C:237:ASP:HB3	1:C:243:LEU:HD21	1.68	0.73
1:F:474:ARG:HB3	1:F:476:GLU:HG2	1.70	0.73
1:B:327:PHE:HA	1:B:330:ILE:HG22	1.71	0.73
1:A:181:SER:HB2	1:D:307:ARG:HH12	1.55	0.71
1:B:250:ALA:HB2	1:B:314:ASN:HD21	1.53	0.71
1:A:181:SER:CB	1:D:307:ARG:HH12	2.02	0.71
1:F:151:HIS:ND1	5:F:703:HOH:O	2.22	0.71
1:A:417:ASN:ND2	5:A:701:HOH:O	2.23	0.70
1:A:173:LEU:O	1:A:177:ARG:HG3	1.91	0.70
1:E:293:ARG:HD2	1:E:363:MET:HE3	1.74	0.70
1:E:97:GLU:CD	1:E:474:ARG:HH22	1.99	0.70
1:B:312:THR:HG23	1:B:314:ASN:H	1.57	0.70
1:G:436:TYR:O	1:G:495:ARG:NH1	2.24	0.69
1:H:478:LEU:HG	1:H:483:LYS:HE3	1.73	0.69
1:E:163:LYS:C	1:E:167:ARG:HH12	2.00	0.69
1:E:298:LYS:NZ	5:E:701:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG22	1:A:472:ARG:HD2	1.75	0.68
1:D:123:GLU:HG3	1:D:124:ARG:N	2.08	0.68
1:E:68:THR:HG21	1:E:190:THR:HG23	1.76	0.68
1:G:47:PRO:HG3	1:G:215:ASP:HB3	1.76	0.68
1:D:482:ARG:HA	1:D:482:ARG:NE	2.09	0.67
1:A:403:TRP:O	1:A:407:LEU:HD13	1.95	0.67
1:C:249:PRO:HG3	1:C:304:TRP:CD2	2.29	0.67
1:G:436:TYR:CE2	1:G:490:THR:HG22	2.29	0.67
1:F:8:VAL:HG11	1:F:447:MET:HE2	1.77	0.67
1:C:160:TRP:HB2	1:C:166:ILE:HD11	1.77	0.66
1:F:495:ARG:HG2	1:F:495:ARG:NH2	2.11	0.66
1:C:279:ILE:HD11	1:C:329:THR:HG22	1.78	0.66
1:H:426:PRO:HD2	1:H:429:GLU:OE1	1.95	0.66
1:E:69:HIS:HE1	1:E:105:PHE:HB3	1.60	0.66
1:E:363:MET:HE2	1:E:391:TYR:CE1	2.30	0.66
1:F:16:PRO:HD3	1:F:473:MET:HE2	1.78	0.66
1:F:12:ILE:HD12	1:F:48:LEU:HD21	1.77	0.66
1:F:12:ILE:HD13	1:F:24:PHE:HE1	1.60	0.65
1:G:39:ASP:HB3	1:G:497:ASN:H	1.62	0.65
1:C:16:PRO:HD3	1:C:473:MET:HE2	1.78	0.65
1:H:149:LYS:HG2	1:H:154:ASN:HA	1.76	0.65
1:C:245:ILE:HG13	1:C:306:ILE:HB	1.77	0.65
1:D:39:ASP:OD1	1:D:498:LYS:HG3	1.96	0.65
1:C:416:GLU:OE2	1:C:421:ARG:NH1	2.26	0.65
1:A:134:GLN:HG2	1:D:346:TYR:HD2	1.61	0.65
1:B:121:LYS:NZ	5:B:701:HOH:O	2.28	0.65
1:D:421:ARG:NH2	1:D:425:GLU:O	2.30	0.65
1:G:474:ARG:HB3	1:G:476:GLU:HG2	1.79	0.64
1:B:129:LEU:O	1:B:132:PHE:N	2.29	0.64
1:B:293:ARG:HH11	1:B:363:MET:HE1	1.62	0.64
1:H:370:PHE:CZ	1:H:419:MET:HE2	2.31	0.64
1:G:293:ARG:HH11	1:G:363:MET:HE1	1.62	0.64
1:C:296:HIS:CE1	1:C:298:LYS:HE3	2.33	0.64
1:C:416:GLU:HG2	1:C:421:ARG:HD2	1.79	0.64
1:F:432:LEU:HD22	1:F:445:THR:HG22	1.80	0.64
1:E:163:LYS:O	1:E:167:ARG:NH1	2.31	0.64
1:A:144:GLU:HG2	1:A:184:ILE:HD13	1.80	0.63
1:G:248:VAL:HG22	1:G:346:TYR:CZ	2.33	0.63
1:H:342:GLU:HG2	1:H:344:LEU:HD23	1.80	0.63
1:D:47:PRO:HG3	1:D:215:ASP:HB3	1.81	0.63
1:G:373:THR:HG21	1:G:410:GLU:CD	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:GLU:HG3	1:H:138:TRP:HE1	1.64	0.63
1:C:140:THR:HG22	1:C:188:GLU:OE2	1.98	0.63
1:E:68:THR:CG2	1:E:190:THR:HG23	2.29	0.63
1:F:244:ALA:HB1	1:F:305:GLU:HG3	1.81	0.63
1:G:436:TYR:HE2	1:G:490:THR:HG22	1.64	0.62
1:H:160:TRP:HB2	1:H:166:ILE:HD11	1.81	0.62
1:E:389:ILE:HG13	1:E:442:THR:HB	1.82	0.62
1:E:14:SER:OG	1:E:459:MET:HE1	2.00	0.62
1:G:317:SER:HB2	1:G:319:GLN:HE21	1.65	0.62
1:H:404:PHE:CE1	1:H:412:LYS:HG2	2.34	0.62
1:E:10:MET:HE2	1:E:473:MET:HE3	1.82	0.62
1:E:394:THR:HG23	1:E:396:ASP:H	1.65	0.62
1:C:436:TYR:CD2	1:C:495:ARG:HD2	2.35	0.61
1:D:8:VAL:HG11	1:D:447:MET:HE2	1.81	0.61
1:G:295:ASP:OD1	4:U:1:GLC:H1	2.01	0.61
1:B:11:HIS:CD2	1:B:13:THR:HG23	2.36	0.61
1:B:4:ARG:NH2	1:B:493:TYR:O	2.31	0.61
3:J:2:AC1:O6B	3:J:2:AC1:O4	2.19	0.61
1:B:419:MET:HG2	1:B:434:THR:HG21	1.81	0.61
1:D:31:PHE:HE1	1:D:447:MET:HE3	1.66	0.61
1:E:245:ILE:HD12	1:E:261:GLY:HA2	1.81	0.61
1:A:296:HIS:ND1	3:J:2:AC1:O3B	2.28	0.61
1:F:390:ALA:HB3	1:F:443:THR:HG22	1.82	0.61
1:A:440:SER:O	1:A:495:ARG:NH2	2.28	0.61
1:E:293:ARG:NH1	1:E:363:MET:HE1	2.16	0.61
1:G:39:ASP:OD1	1:G:498:LYS:HE3	1.99	0.61
1:C:249:PRO:HG3	1:C:304:TRP:CE2	2.36	0.60
1:C:400:ILE:HD12	1:C:449:ASP:HB3	1.83	0.60
1:D:264:ILE:HG13	1:D:305:GLU:HG3	1.83	0.60
1:C:77:THR:HG22	1:C:82:ILE:HG13	1.83	0.60
1:D:366:MET:HE3	1:D:431:VAL:HG13	1.82	0.60
1:F:394:THR:HG23	1:F:396:ASP:H	1.66	0.60
1:H:123:GLU:OE1	1:H:123:GLU:HA	2.01	0.60
1:F:293:ARG:NH1	1:F:363:MET:HE1	2.15	0.60
1:E:127:ARG:NH1	1:H:251:ASP:O	2.35	0.59
1:G:457:SER:HB2	1:G:471:TRP:CD1	2.36	0.59
1:D:99:VAL:HG23	1:D:472:ARG:HD2	1.84	0.59
1:G:367:GLU:HG3	1:G:392:ALA:O	2.02	0.59
1:B:144:GLU:O	1:B:148:ILE:HG13	2.01	0.59
1:F:293:ARG:HD2	1:F:363:MET:HE3	1.84	0.59
1:E:198:TRP:CD1	1:E:288:MET:HE3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:VAL:HG22	1:B:258:GLN:HB2	1.83	0.59
1:B:144:GLU:OE2	1:B:177:ARG:HD3	2.02	0.59
1:E:364:LYS:NZ	1:E:378:ILE:O	2.33	0.59
1:A:31:PHE:HE1	1:A:447:MET:HE3	1.68	0.58
1:F:248:VAL:HG22	1:F:258:GLN:HB2	1.85	0.58
1:H:165:ILE:HG21	1:H:176:TYR:CD1	2.38	0.58
1:A:45:ILE:HD12	1:A:48:LEU:HD21	1.85	0.58
1:B:419:MET:HE3	1:B:430:THR:HG22	1.85	0.58
1:H:275:PHE:CD1	1:H:326:LEU:HD12	2.39	0.58
1:H:415:ALA:HB1	1:H:419:MET:HE3	1.85	0.58
1:E:68:THR:HG21	1:E:190:THR:CG2	2.33	0.58
1:B:257:GLY:HA3	1:B:313:ALA:HB3	1.84	0.58
1:B:389:ILE:HD13	1:B:442:THR:HB	1.86	0.58
1:D:123:GLU:CG	1:D:124:ARG:N	2.64	0.58
1:D:433:ARG:NH2	1:D:488:GLU:OE1	2.36	0.58
1:E:169:GLU:OE2	1:E:169:GLU:HA	2.02	0.58
1:E:248:VAL:HG12	1:E:258:GLN:HB2	1.85	0.58
1:B:458:ARG:NH1	1:B:461:MET:SD	2.76	0.57
1:B:479:THR:HG22	1:B:481:ASN:H	1.68	0.57
1:D:467:GLY:HA2	1:D:470:GLN:NE2	2.18	0.57
1:G:47:PRO:HA	5:G:701:HOH:O	2.03	0.57
1:G:295:ASP:CG	4:U:1:GLC:H1	2.30	0.57
1:G:499:LEU:N	1:G:499:LEU:HD23	2.19	0.57
1:E:167:ARG:CZ	1:E:167:ARG:HB2	2.34	0.57
1:H:174:ALA:HA	1:H:177:ARG:HD2	1.87	0.57
1:B:131:ASP:HA	1:B:134:GLN:HB2	1.86	0.57
1:G:31:PHE:HE1	1:G:447:MET:HE2	1.67	0.57
1:G:486:LEU:O	1:G:490:THR:HG23	2.04	0.57
1:A:471:TRP:CH2	1:A:473:MET:HB2	2.40	0.57
1:F:377:SER:O	1:F:380:ILE:HG22	2.05	0.57
1:G:480:GLU:HA	1:G:483:LYS:HD3	1.86	0.57
1:A:37:GLU:OE2	1:A:483:LYS:NZ	2.38	0.57
1:B:10:MET:SD	1:B:447:MET:HG3	2.44	0.57
1:E:400:ILE:HD12	1:E:449:ASP:HB3	1.86	0.56
1:C:381:PRO:HB3	1:C:438:THR:HG22	1.88	0.56
1:E:164:ALA:HA	1:E:167:ARG:NH2	2.20	0.56
1:E:478:LEU:HG	1:E:483:LYS:HE2	1.87	0.56
1:E:479:THR:HG22	1:E:481:ASN:H	1.70	0.56
1:A:312:THR:HG22	1:A:313:ALA:H	1.68	0.56
1:C:106:GLU:OE1	1:C:106:GLU:N	2.37	0.56
1:D:293:ARG:HH22	1:D:394:THR:HG21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:ARG:NH2	1:F:493:TYR:O	2.21	0.56
1:H:3:LYS:HE3	1:H:386:GLU:OE1	2.06	0.56
1:C:367:GLU:HG2	1:C:403:TRP:CG	2.41	0.56
1:H:230:MET:HE1	1:H:277:TRP:HE1	1.70	0.56
1:B:10:MET:HE1	1:B:473:MET:HB2	1.88	0.56
1:B:342:GLU:HA	1:B:363:MET:HG3	1.88	0.56
1:E:97:GLU:HG3	1:E:474:ARG:NH2	2.21	0.56
1:A:450:LEU:HD11	1:A:486:LEU:HB2	1.88	0.56
1:G:440:SER:O	1:G:495:ARG:NH2	2.39	0.56
1:A:31:PHE:CE1	1:A:447:MET:HE3	2.40	0.55
1:H:405:GLU:OE2	1:H:405:GLU:N	2.39	0.55
1:C:465:VAL:HG13	1:C:466:GLY:H	1.72	0.55
1:D:77:THR:HG22	1:D:82:ILE:HG13	1.87	0.55
1:F:307:ARG:HD2	1:G:178:GLN:HG2	1.89	0.55
1:E:84:LYS:O	1:E:88:GLN:HB2	2.07	0.55
1:F:467:GLY:HA2	1:F:470:GLN:NE2	2.21	0.55
1:A:47:PRO:HG3	1:A:215:ASP:HB3	1.86	0.55
1:A:215:ASP:OD1	1:A:293:ARG:HD3	2.06	0.55
1:G:287:LYS:NZ	5:G:702:HOH:O	2.38	0.55
1:H:64:VAL:HG12	1:H:195:TYR:OH	2.06	0.55
1:H:451:LEU:HD23	1:H:453:LYS:NZ	2.22	0.55
1:A:390:ALA:HB3	1:A:443:THR:HG22	1.89	0.55
1:B:168:ARG:HB3	1:B:173:LEU:HD11	1.89	0.55
1:D:407:LEU:HB2	1:D:412:LYS:HG3	1.89	0.55
1:A:49:THR:O	1:A:67:ASN:HB2	2.07	0.55
1:B:403:TRP:CZ2	1:B:407:LEU:HD11	2.41	0.55
1:D:178:GLN:HG2	1:D:179:LYS:N	2.18	0.55
1:D:109:ARG:O	1:D:113:GLU:HG3	2.07	0.55
1:H:127:ARG:NH2	1:H:131:ASP:OD2	2.37	0.55
1:F:275:PHE:O	1:F:279:ILE:HG12	2.07	0.54
1:G:392:ALA:HB1	1:G:400:ILE:HD11	1.89	0.54
1:A:10:MET:HE2	1:A:14:SER:HB2	1.89	0.54
1:A:134:GLN:HG2	1:D:346:TYR:CD2	2.42	0.54
1:G:140:THR:HG22	1:G:188:GLU:OE2	2.07	0.54
1:H:151:HIS:CD2	1:H:180:LEU:HD21	2.42	0.54
1:D:146:MET:O	1:D:150:GLU:HG3	2.08	0.54
1:E:11:HIS:CD2	1:E:13:THR:HG23	2.42	0.54
1:A:380:ILE:HG13	1:A:381:PRO:HD2	1.89	0.54
1:H:163:LYS:HE2	1:H:167:ARG:HD3	1.90	0.54
1:A:173:LEU:HD22	1:A:177:ARG:NH2	2.23	0.54
1:B:13:THR:HG22	1:B:70:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ASP:HB2	3:P:2:AC1:O2	2.07	0.54
1:D:482:ARG:HE	1:D:482:ARG:CA	2.19	0.54
1:G:419:MET:HG2	1:G:434:THR:HG21	1.90	0.54
1:H:97:GLU:OE1	1:H:474:ARG:HD2	2.07	0.54
2:I:2:AC1:O6B	2:I:2:AC1:O4	2.19	0.54
1:C:74:ASP:OD1	1:C:87:TYR:OH	2.23	0.54
1:B:410:GLU:HG2	1:G:89:ASN:OD1	2.07	0.54
1:E:474:ARG:HG2	1:E:476:GLU:HG2	1.89	0.54
1:D:67:ASN:HB3	1:D:70:LEU:HG	1.90	0.53
1:D:234:PHE:HB2	1:D:236:LEU:CD1	2.31	0.53
1:D:381:PRO:HB3	1:D:438:THR:HG22	1.90	0.53
1:F:293:ARG:HD2	1:F:363:MET:CE	2.38	0.53
1:F:12:ILE:HD13	1:F:24:PHE:CE1	2.43	0.53
1:H:52:SER:OG	1:H:53:PHE:N	2.41	0.53
1:F:440:SER:O	1:F:495:ARG:NH1	2.23	0.53
1:D:432:LEU:HD22	1:D:445:THR:HG22	1.90	0.53
1:B:390:ALA:HB3	1:B:443:THR:HG22	1.90	0.53
1:H:307:ARG:NH2	5:H:707:HOH:O	2.40	0.53
1:D:44:GLN:HE22	1:D:391:TYR:HE2	1.55	0.53
1:H:138:TRP:CD1	1:H:138:TRP:H	2.25	0.53
1:H:45:ILE:HD12	1:H:46:LEU:O	2.09	0.53
1:H:244:ALA:HB1	1:H:305:GLU:HG3	1.89	0.53
1:E:21:ILE:HD12	1:E:99:VAL:HG11	1.91	0.53
1:H:184:ILE:O	1:H:188:GLU:HG3	2.09	0.53
1:H:196:LYS:O	1:H:200:GLU:HG2	2.08	0.53
1:G:45:ILE:HD12	1:G:48:LEU:HD21	1.91	0.53
1:H:450:LEU:HD11	1:H:486:LEU:HB2	1.89	0.53
1:A:171:GLU:HG2	5:A:730:HOH:O	2.09	0.53
1:A:181:SER:CB	1:D:307:ARG:NH1	2.72	0.53
1:C:82:ILE:HG22	1:C:114:LYS:HG2	1.92	0.53
1:C:453:LYS:HD2	1:C:454:PRO:HD3	1.91	0.53
1:B:454:PRO:O	1:B:457:SER:OG	2.27	0.52
1:D:330:ILE:HG22	1:D:337:LEU:HD11	1.91	0.52
1:E:211:GLN:NE2	5:E:705:HOH:O	2.39	0.52
1:F:363:MET:HE2	1:F:391:TYR:CE1	2.44	0.52
1:G:248:VAL:HG12	1:G:258:GLN:HB2	1.91	0.52
1:G:370:PHE:CZ	1:G:419:MET:HE2	2.44	0.52
1:D:160:TRP:HB2	1:D:166:ILE:HD11	1.91	0.52
1:H:47:PRO:HG3	1:H:215:ASP:HB3	1.92	0.52
1:E:162:ASP:O	1:E:165:ILE:HG22	2.09	0.52
1:F:395:HIS:NE2	2:S:1:ASO:O2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PHE:CD1	1:B:326:LEU:HD12	2.45	0.52
1:C:216:MET:HE3	1:C:292:LEU:HD21	1.90	0.52
1:D:380:ILE:HG13	1:D:381:PRO:HD2	1.92	0.52
1:A:28:ALA:O	1:A:32:VAL:HG23	2.09	0.52
1:H:354:LEU:O	1:H:358:THR:HG23	2.10	0.52
1:C:307:ARG:HG2	1:C:315:ASP:O	2.09	0.52
1:D:73:PHE:O	1:D:77:THR:HG23	2.09	0.52
1:D:259:LEU:HD11	1:D:310:TYR:CE2	2.45	0.52
1:A:8:VAL:HG11	1:A:447:MET:HE2	1.92	0.52
1:E:47:PRO:HG3	1:E:215:ASP:HB3	1.92	0.52
1:F:389:ILE:HD12	1:F:442:THR:HB	1.91	0.52
1:G:312:THR:HG22	1:G:314:ASN:H	1.74	0.52
1:A:11:HIS:CE1	1:A:46:LEU:HB2	2.45	0.52
1:B:47:PRO:HG3	1:B:215:ASP:HB3	1.92	0.52
1:B:307:ARG:HD2	1:C:177:ARG:HB3	1.91	0.52
1:B:367:GLU:HG2	1:B:403:TRP:CG	2.45	0.52
1:D:440:SER:O	1:D:495:ARG:NH1	2.30	0.51
1:G:220:VAL:O	1:G:262:ASN:HB3	2.10	0.51
1:G:235:LYS:NZ	1:G:305:GLU:OE1	2.39	0.51
1:H:133:LEU:HD22	1:H:139:VAL:HB	1.92	0.51
1:E:97:GLU:CG	1:E:474:ARG:NH2	2.73	0.51
1:E:183:VAL:O	1:E:186:TYR:HB3	2.10	0.51
1:F:227:VAL:HG13	1:F:236:LEU:HD11	1.91	0.51
1:A:249:PRO:HG3	1:A:304:TRP:CE3	2.44	0.51
1:D:162:ASP:HB3	1:D:165:ILE:HG22	1.92	0.51
1:D:363:MET:HE3	1:D:365:ILE:HD11	1.93	0.51
1:F:114:LYS:HD3	1:F:114:LYS:N	2.26	0.51
1:F:234:PHE:HB2	1:F:236:LEU:HG	1.91	0.51
1:F:236:LEU:HD23	1:F:242:PRO:HA	1.91	0.51
1:B:205:ALA:HB1	1:B:210:ILE:HB	1.93	0.51
1:B:355:LEU:HD11	1:B:360:PHE:HB2	1.92	0.51
1:G:373:THR:HG21	1:G:410:GLU:OE1	2.10	0.51
1:C:232:GLU:CD	1:C:232:GLU:H	2.17	0.51
1:C:477:ASP:O	1:C:479:THR:HG23	2.11	0.51
1:D:31:PHE:CE1	1:D:447:MET:HE3	2.45	0.51
1:D:105:PHE:CZ	1:D:109:ARG:HD3	2.45	0.51
1:C:279:ILE:HG12	1:C:330:ILE:HD13	1.92	0.51
1:H:79:GLU:OE1	1:H:196:LYS:HE3	2.11	0.51
1:D:124:ARG:O	1:D:127:ARG:N	2.44	0.51
1:H:10:MET:HE3	1:H:15:LEU:HD23	1.93	0.51
1:A:163:LYS:HB3	1:A:167:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLN:HG2	1:B:135:GLU:HG3	1.93	0.51
1:F:6:SER:OG	1:F:40:GLN:OE1	2.22	0.50
1:H:450:LEU:HD23	1:H:451:LEU:HD12	1.92	0.50
1:C:132:PHE:CE1	1:C:136:GLU:HG3	2.46	0.50
1:F:157:LEU:N	1:F:223:ASP:OD1	2.31	0.50
1:D:436:TYR:HE1	1:D:445:THR:HG23	1.75	0.50
1:E:453:LYS:HB3	1:E:457:SER:OG	2.12	0.50
1:A:119:PHE:HE1	1:A:128:MET:HE2	1.77	0.50
1:A:373:THR:HG22	1:A:414:TYR:CG	2.46	0.50
1:F:31:PHE:HE1	1:F:447:MET:HE3	1.77	0.50
1:E:479:THR:O	1:E:483:LYS:HG3	2.11	0.50
1:F:259:LEU:HD21	1:F:310:TYR:CZ	2.47	0.50
1:E:363:MET:HE2	1:E:391:TYR:CZ	2.47	0.50
1:B:244:ALA:HB1	1:B:305:GLU:HG3	1.94	0.50
1:A:124:ARG:O	1:A:128:MET:HG3	2.12	0.50
1:A:138:TRP:CE3	1:A:139:VAL:HA	2.46	0.50
1:B:2:LYS:HG2	1:B:3:LYS:H	1.77	0.50
1:G:258:GLN:HG2	1:G:463:ASN:HB2	1.93	0.50
1:B:394:THR:HG23	1:B:396:ASP:H	1.76	0.50
1:G:295:ASP:OD2	4:U:1:GLC:H1	2.12	0.50
1:H:400:ILE:HD13	1:H:431:VAL:HB	1.92	0.50
1:F:117:LYS:O	1:F:121:LYS:HG3	2.11	0.49
1:A:298:LYS:HE2	1:A:302:ASP:HB2	1.94	0.49
1:C:311:GLN:N	1:C:315:ASP:OD2	2.42	0.49
1:B:388:THR:HG1	1:B:440:SER:HG	1.57	0.49
1:H:16:PRO:HD3	1:H:473:MET:CE	2.42	0.49
1:A:342:GLU:OE1	1:A:344:LEU:HD12	2.12	0.49
1:D:183:VAL:HG21	5:D:711:HOH:O	2.12	0.49
1:H:307:ARG:O	1:H:310:TYR:HB3	2.12	0.49
1:F:495:ARG:HH21	1:F:495:ARG:CG	2.21	0.49
1:G:83:SER:HB2	1:G:85:ASP:OD1	2.13	0.49
1:H:396:ASP:OD1	1:H:460:ASN:ND2	2.41	0.49
1:A:71:ILE:O	1:A:108:ARG:NH2	2.45	0.49
1:F:195:TYR:HD2	1:F:199:PHE:HE2	1.60	0.49
1:H:214:GLY:HA3	1:H:289:TYR:CD2	2.48	0.49
1:A:392:ALA:HB1	1:A:400:ILE:HD11	1.95	0.49
1:E:200:GLU:HA	1:E:203:GLU:HG2	1.93	0.49
1:F:61:PHE:CE1	1:F:149:LYS:HE3	2.48	0.49
1:B:291:TYR:CD2	1:B:338:PRO:HB2	2.47	0.48
1:E:69:HIS:CE1	1:E:105:PHE:HB3	2.45	0.48
1:A:216:MET:HE3	1:A:278:TRP:HZ3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HD23	1:A:242:PRO:HA	1.93	0.48
1:B:41:LYS:HG2	1:B:42:PHE:CE2	2.48	0.48
1:B:133:LEU:HD13	1:B:139:VAL:HB	1.94	0.48
1:B:202:LYS:NZ	1:B:290:ASP:OD1	2.46	0.48
1:E:471:TRP:CH2	1:E:473:MET:HB2	2.47	0.48
1:C:10:MET:HG2	1:C:31:PHE:CZ	2.49	0.48
1:G:218:ILE:HG23	1:G:219:TYR:N	2.28	0.48
1:D:354:LEU:O	1:D:358:THR:HG23	2.13	0.48
1:G:458:ARG:HH11	1:G:461:MET:HE2	1.77	0.48
1:H:325:GLU:O	1:H:329:THR:HG23	2.13	0.48
1:H:344:LEU:HD11	1:H:365:ILE:HG13	1.96	0.48
1:D:44:GLN:HE21	1:D:444:ILE:HG21	1.77	0.48
1:F:94:GLN:N	5:F:707:HOH:O	2.47	0.48
1:F:251:ASP:OD1	1:F:251:ASP:N	2.45	0.48
1:A:258:GLN:HG2	1:A:463:ASN:HB2	1.96	0.48
1:D:400:ILE:HD12	1:D:449:ASP:HB3	1.95	0.48
1:F:410:GLU:CD	1:F:410:GLU:H	2.22	0.48
1:B:353:ARG:HD3	5:B:716:HOH:O	2.14	0.48
1:H:259:LEU:HD21	1:H:310:TYR:CZ	2.48	0.48
1:B:124:ARG:O	1:B:124:ARG:HG3	2.10	0.48
1:B:220:VAL:O	1:B:263:PRO:HD2	2.13	0.48
1:C:436:TYR:HD2	1:C:495:ARG:HD2	1.79	0.48
1:D:275:PHE:O	1:D:279:ILE:HG12	2.14	0.48
1:H:68:THR:HG23	1:H:112:LEU:HD13	1.96	0.48
1:B:193:PHE:O	1:B:197:GLN:HG3	2.13	0.48
1:B:217:PRO:O	1:B:281:ARG:NH2	2.39	0.48
1:H:133:LEU:HD11	1:H:188:GLU:OE2	2.13	0.48
1:H:495:ARG:HG2	1:H:495:ARG:NH2	2.29	0.48
1:C:479:THR:OG1	1:C:482:ARG:HG3	2.14	0.47
1:D:381:PRO:HB3	1:D:438:THR:CG2	2.44	0.47
1:E:8:VAL:HG11	1:E:447:MET:HE2	1.97	0.47
1:A:116:VAL:HG11	1:A:186:TYR:HA	1.96	0.47
1:A:123:GLU:OE2	1:A:124:ARG:NH2	2.47	0.47
1:A:355:LEU:HD12	1:A:355:LEU:HA	1.69	0.47
1:B:448:GLN:HG2	1:B:457:SER:HB2	1.96	0.47
1:C:158:GLN:HG2	1:C:241:GLN:HG2	1.95	0.47
1:D:247:GLY:O	1:D:304:TRP:HB3	2.14	0.47
1:D:419:MET:HG2	1:D:434:THR:HG21	1.95	0.47
1:D:249:PRO:HD3	1:D:304:TRP:CG	2.49	0.47
1:A:163:LYS:HB3	1:A:167:ARG:HH22	1.80	0.47
1:A:181:SER:HB3	1:D:307:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:LEU:HD11	1:D:310:TYR:HE2	1.79	0.47
1:E:120:LEU:HD11	1:E:185:LYS:HG2	1.96	0.47
1:A:11:HIS:HB2	1:A:46:LEU:HG	1.97	0.47
1:A:168:ARG:HB3	1:A:173:LEU:HD11	1.95	0.47
1:B:136:GLU:O	1:B:138:TRP:N	2.48	0.47
1:E:109:ARG:HH12	1:E:150:GLU:CD	2.22	0.47
1:E:170:GLU:HG2	1:H:235:LYS:HD3	1.97	0.47
1:E:175:GLY:O	1:E:179:LYS:HG3	2.15	0.47
1:F:47:PRO:HG3	1:F:215:ASP:HB3	1.96	0.47
1:G:38:THR:OG1	1:G:40:GLN:HG2	2.14	0.47
1:G:172:ALA:O	1:G:176:TYR:HD1	1.97	0.47
1:G:370:PHE:CE2	1:G:419:MET:HE2	2.50	0.47
1:A:433:ARG:HD2	1:B:420:ARG:CZ	2.45	0.47
1:D:377:SER:O	1:D:380:ILE:HG22	2.15	0.47
1:G:258:GLN:HE22	3:V:2:AC1:HC7	1.80	0.47
1:C:144:GLU:CD	1:C:177:ARG:HE	2.22	0.47
1:D:236:LEU:O	1:D:238:ARG:NH1	2.47	0.47
1:E:136:GLU:HB3	1:E:138:TRP:NE1	2.30	0.47
1:F:347:ILE:HG22	1:F:352:GLU:HG2	1.96	0.47
1:G:312:THR:O	1:G:315:ASP:HB2	2.15	0.47
1:H:99:VAL:HG22	1:H:472:ARG:HD2	1.96	0.47
1:F:303:TYR:CZ	1:F:319:GLN:HB2	2.50	0.47
1:B:366:MET:CE	1:B:381:PRO:HG3	2.45	0.46
1:D:44:GLN:NE2	1:D:444:ILE:HG21	2.31	0.46
1:E:99:VAL:HG22	1:E:472:ARG:HD2	1.96	0.46
1:F:222:ALA:HB2	1:F:263:PRO:HD3	1.97	0.46
1:F:249:PRO:HD3	1:F:304:TRP:CG	2.50	0.46
1:F:381:PRO:HB3	1:F:438:THR:HG22	1.97	0.46
1:C:244:ALA:HB1	1:C:305:GLU:HG3	1.97	0.46
1:B:211:GLN:HG2	1:B:290:ASP:OD2	2.15	0.46
1:C:9:LEU:HD12	1:C:44:GLN:O	2.15	0.46
1:C:400:ILE:HG21	1:C:428:THR:HA	1.97	0.46
1:E:353:ARG:NH2	5:E:710:HOH:O	2.48	0.46
1:F:138:TRP:CD1	1:F:138:TRP:H	2.30	0.46
1:C:11:HIS:CD2	1:C:12:ILE:H	2.34	0.46
1:H:117:LYS:HD2	1:H:117:LYS:HA	1.76	0.46
1:A:81:PHE:O	1:A:118:ASN:ND2	2.48	0.46
1:A:279:ILE:HD13	1:A:330:ILE:HG12	1.97	0.46
1:B:216:MET:HB2	1:B:292:LEU:HD11	1.98	0.46
1:E:373:THR:HA	1:E:414:TYR:CE2	2.51	0.46
1:F:248:VAL:CG2	1:F:258:GLN:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:TYR:HB3	1:G:134:GLN:NE2	2.30	0.46
1:C:366:MET:HE2	1:C:366:MET:HB3	1.73	0.46
1:F:205:ALA:HB1	1:F:210:ILE:HB	1.96	0.46
1:G:458:ARG:NH1	1:G:461:MET:HE2	2.30	0.46
1:B:254:SER:HB3	1:B:257:GLY:O	2.16	0.46
1:G:10:MET:HE2	1:G:447:MET:HE2	1.97	0.46
1:G:193:PHE:O	1:G:197:GLN:HG3	2.16	0.46
1:G:306:ILE:HD13	1:G:313:ALA:HA	1.97	0.46
1:A:133:LEU:HD21	1:A:188:GLU:HG2	1.97	0.46
1:B:3:LYS:HD2	1:B:3:LYS:HA	1.61	0.46
1:F:171:GLU:CD	1:F:171:GLU:H	2.24	0.46
1:F:199:PHE:O	1:F:203:GLU:HG2	2.16	0.46
1:A:43:TRP:HB3	1:A:212:ILE:HD13	1.97	0.46
1:B:75:LEU:HA	1:B:78:LEU:HG	1.97	0.46
1:B:275:PHE:O	1:B:279:ILE:HG12	2.16	0.46
1:D:363:MET:HG2	1:D:391:TYR:HE1	1.81	0.46
1:F:243:LEU:HD11	1:G:171:GLU:HG2	1.98	0.46
1:G:99:VAL:HG22	1:G:472:ARG:HD2	1.98	0.46
1:A:36:VAL:HG11	1:A:208:LYS:HB3	1.97	0.45
1:A:282:ILE:O	1:A:286:VAL:HG13	2.16	0.45
1:E:14:SER:OG	1:E:471:TRP:O	2.31	0.45
1:H:303:TYR:CZ	1:H:319:GLN:HB2	2.51	0.45
1:A:408:THR:HB	1:A:411:GLN:HB2	1.98	0.45
1:B:16:PRO:HG3	1:B:473:MET:HE2	1.98	0.45
1:D:394:THR:HG22	1:D:396:ASP:H	1.81	0.45
1:E:254:SER:HB2	1:E:257:GLY:H	1.81	0.45
1:F:160:TRP:HB2	1:F:166:ILE:HD11	1.98	0.45
1:C:453:LYS:HB3	1:C:457:SER:OG	2.15	0.45
1:D:52:SER:OG	1:D:53:PHE:N	2.47	0.45
1:D:461:MET:HE3	1:D:461:MET:HB2	1.76	0.45
1:F:99:VAL:HG22	1:F:472:ARG:HD2	1.98	0.45
1:G:138:TRP:H	1:G:138:TRP:CD1	2.33	0.45
1:C:296:HIS:HE1	1:C:298:LYS:HE3	1.76	0.45
1:G:277:TRP:CZ2	1:G:281:ARG:HD2	2.51	0.45
1:A:84:LYS:HA	1:A:87:TYR:CE1	2.52	0.45
1:G:138:TRP:CE3	1:G:139:VAL:HA	2.52	0.45
1:H:98:VAL:HG13	1:H:470:GLN:HB3	1.99	0.45
1:A:369:GLY:HA2	1:A:377:SER:OG	2.17	0.45
1:B:367:GLU:HG2	1:B:403:TRP:CD1	2.52	0.45
1:C:114:LYS:HE2	1:C:114:LYS:HB2	1.68	0.45
1:E:244:ALA:HB1	1:E:305:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:481:ASN:OD1	5:F:701:HOH:O	2.21	0.45
1:G:11:HIS:ND1	1:G:12:ILE:N	2.64	0.45
1:A:127:ARG:HG3	1:D:250:ALA:HB1	1.99	0.45
1:B:56:SER:HB2	1:B:469:TRP:CZ2	2.52	0.45
1:B:133:LEU:CD1	1:B:137:LYS:HA	2.47	0.45
1:B:334:LEU:HD23	1:B:337:LEU:HD21	1.98	0.45
1:B:459:MET:HE1	1:B:471:TRP:HB3	1.99	0.45
1:F:235:LYS:HG2	1:G:170:GLU:HG2	1.97	0.45
1:G:162:ASP:O	1:G:165:ILE:HG22	2.17	0.45
1:G:317:SER:HB2	1:G:319:GLN:NE2	2.31	0.45
1:H:185:LYS:O	1:H:189:VAL:HG23	2.16	0.45
1:A:45:ILE:CD1	1:A:48:LEU:HD21	2.47	0.44
1:A:59:GLN:CG	1:A:221:SER:HB2	2.47	0.44
1:G:220:VAL:O	1:G:263:PRO:HD2	2.17	0.44
1:A:20:GLY:O	1:A:99:VAL:HG13	2.17	0.44
1:B:230:MET:HE1	5:B:708:HOH:O	2.18	0.44
1:D:307:ARG:NH2	1:D:315:ASP:OD1	2.50	0.44
1:G:331:LYS:HB2	1:G:331:LYS:HE3	1.75	0.44
1:H:103:GLY:O	1:H:107:LYS:HD2	2.17	0.44
1:B:133:LEU:HD12	1:B:136:GLU:O	2.17	0.44
1:C:136:GLU:O	1:C:139:VAL:HG23	2.17	0.44
1:E:234:PHE:HB2	1:E:236:LEU:HG	1.98	0.44
1:H:156:ALA:HB1	1:H:223:ASP:HB2	1.99	0.44
1:A:123:GLU:OE1	1:A:124:ARG:HG2	2.17	0.44
1:A:372:ASP:OD1	1:A:372:ASP:C	2.61	0.44
1:A:435:LEU:O	1:A:438:THR:HG23	2.17	0.44
1:B:343:ASN:OD1	1:B:343:ASN:N	2.50	0.44
1:D:12:ILE:HD11	1:D:45:ILE:HG21	1.99	0.44
1:E:187:HIS:O	1:E:191:GLN:HG2	2.18	0.44
1:E:293:ARG:HH11	1:E:363:MET:HE1	1.81	0.44
1:F:60:SER:O	1:F:221:SER:HB3	2.17	0.44
1:G:39:ASP:CG	1:G:498:LYS:HE3	2.42	0.44
1:B:23:THR:HB	1:B:70:LEU:O	2.18	0.44
1:B:349:GLU:H	1:B:349:GLU:CD	2.26	0.44
1:G:355:LEU:HD12	1:G:355:LEU:HA	1.70	0.44
1:H:334:LEU:HB2	1:H:337:LEU:HD21	2.00	0.44
1:A:451:LEU:HD21	1:A:478:LEU:HD13	2.00	0.44
1:B:288:MET:HE3	1:B:288:MET:HB3	1.85	0.44
1:E:97:GLU:HG3	1:E:474:ARG:HH21	1.82	0.44
1:H:282:ILE:HD12	1:H:330:ILE:HD13	1.99	0.44
4:U:1:GLC:H3	3:V:2:AC1:O6B	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ALA:HB1	1:A:305:GLU:HG2	1.99	0.44
1:B:265:TYR:HE2	1:B:278:TRP:HZ2	1.66	0.44
1:C:116:VAL:HG22	1:C:189:VAL:HG12	2.00	0.44
1:C:251:ASP:OD1	4:N:3:AC1:O3	2.36	0.44
1:D:152:PHE:CE1	1:D:161:ASP:HB2	2.52	0.44
1:F:25:GLY:O	1:F:29:TYR:HD1	2.00	0.44
1:D:482:ARG:NE	1:D:482:ARG:CA	2.80	0.44
1:G:253:PHE:HD1	1:G:253:PHE:O	2.01	0.44
1:H:165:ILE:HG21	1:H:176:TYR:CE1	2.53	0.44
1:D:72:ASP:OD2	1:D:75:LEU:HG	2.18	0.44
1:H:127:ARG:HA	1:H:130:SER:HB3	2.00	0.44
1:B:272:GLU:OE2	1:B:272:GLU:HA	2.18	0.43
1:B:436:TYR:CD2	1:B:495:ARG:HD2	2.53	0.43
1:G:373:THR:HG21	1:G:410:GLU:OE2	2.18	0.43
1:A:330:ILE:HG23	1:A:334:LEU:HD12	2.00	0.43
1:B:366:MET:HE1	1:B:381:PRO:HG3	2.00	0.43
1:B:404:PHE:HA	1:B:407:LEU:HD12	1.99	0.43
1:E:394:THR:HG22	1:E:397:ASN:OD1	2.17	0.43
1:H:71:ILE:HD11	1:H:194:PHE:HB2	1.99	0.43
1:H:473:MET:HE2	1:H:473:MET:HB3	1.94	0.43
1:E:232:GLU:H	1:E:232:GLU:CD	2.25	0.43
1:G:150:GLU:OE2	1:G:187:HIS:CE1	2.70	0.43
1:H:342:GLU:OE2	1:H:344:LEU:HB2	2.18	0.43
1:E:279:ILE:HD11	1:E:329:THR:HG22	2.00	0.43
1:E:410:GLU:OE1	1:E:410:GLU:N	2.49	0.43
1:F:48:LEU:HB3	1:F:194:PHE:HZ	1.83	0.43
1:G:388:THR:O	1:G:389:ILE:HD13	2.18	0.43
1:H:34:PHE:HD1	1:H:483:LYS:HD3	1.82	0.43
1:H:151:HIS:CG	1:H:180:LEU:HD11	2.53	0.43
1:B:355:LEU:HD12	1:B:355:LEU:HA	1.76	0.43
1:G:392:ALA:CB	1:G:400:ILE:HD11	2.47	0.43
1:H:73:PHE:O	1:H:77:THR:HG23	2.19	0.43
1:A:116:VAL:HG22	1:A:189:VAL:HG12	1.99	0.43
1:A:342:GLU:HA	1:A:363:MET:HG3	2.01	0.43
1:B:7:GLY:HA3	1:B:42:PHE:HB2	2.00	0.43
1:B:52:SER:OG	1:B:53:PHE:N	2.49	0.43
1:B:148:ILE:HD13	1:B:165:ILE:HG12	1.99	0.43
1:B:265:TYR:CE2	1:B:278:TRP:HZ2	2.37	0.43
1:E:49:THR:O	1:E:67:ASN:HB2	2.19	0.43
1:F:3:LYS:HE3	1:F:386:GLU:OE2	2.19	0.43
1:G:218:ILE:HD12	1:G:300:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:LEU:O	1:H:339:ILE:HA	2.19	0.43
1:C:8:VAL:HG11	1:C:447:MET:HE2	2.01	0.43
1:C:401:ASN:O	1:C:405:GLU:HG3	2.19	0.43
1:H:59:GLN:HG2	1:H:221:SER:OG	2.19	0.43
1:H:419:MET:HB3	1:H:434:THR:OG1	2.18	0.43
1:H:450:LEU:O	1:H:482:ARG:HD3	2.19	0.43
1:B:355:LEU:O	1:B:355:LEU:HG	2.18	0.43
1:E:33:ASP:O	1:E:37:GLU:HG3	2.18	0.43
1:A:59:GLN:NE2	2:I:2:AC1:HC61	2.24	0.43
1:A:259:LEU:O	2:I:2:AC1:O3B	2.36	0.43
1:B:446:CYS:HB2	1:B:449:ASP:OD2	2.19	0.43
1:F:184:ILE:O	1:F:188:GLU:HG3	2.19	0.43
1:G:293:ARG:NH1	1:G:363:MET:HE1	2.30	0.43
1:B:113:GLU:O	1:B:117:LYS:HE2	2.19	0.43
1:C:84:LYS:HG2	1:C:88:GLN:HB3	2.01	0.43
1:C:103:GLY:O	1:C:107:LYS:HG3	2.17	0.43
1:C:439:VAL:HG12	1:D:382:HIS:O	2.18	0.43
1:D:109:ARG:HB3	1:D:110:PRO:HD3	2.00	0.43
1:E:134:GLN:HG2	1:H:346:TYR:CD2	2.53	0.43
1:F:478:LEU:HA	1:F:478:LEU:HD12	1.67	0.43
1:G:88:GLN:HG3	1:G:88:GLN:O	2.19	0.43
1:B:12:ILE:HG21	1:B:24:PHE:CE1	2.54	0.42
1:C:186:TYR:O	1:C:190:THR:HG23	2.18	0.42
1:D:163:LYS:HE3	1:D:163:LYS:HB3	1.73	0.42
1:E:164:ALA:HA	1:E:167:ARG:HH22	1.82	0.42
1:F:75:LEU:HB2	1:F:197:GLN:NE2	2.34	0.42
1:G:436:TYR:HE1	1:G:445:THR:CG2	2.32	0.42
1:A:210:ILE:HD13	1:A:210:ILE:HA	1.80	0.42
1:A:433:ARG:HD2	1:B:420:ARG:NE	2.33	0.42
1:B:77:THR:HG21	1:B:84:LYS:HG2	2.00	0.42
1:C:151:HIS:NE2	1:C:179:LYS:HE2	2.34	0.42
1:E:372:ASP:OD1	1:E:374:THR:HB	2.19	0.42
1:E:385:THR:OG1	1:E:386:GLU:N	2.52	0.42
1:F:432:LEU:HD23	1:F:432:LEU:HA	1.79	0.42
1:H:166:ILE:O	1:H:240:LYS:NZ	2.48	0.42
1:H:489:ILE:HG13	1:H:490:THR:N	2.34	0.42
1:A:9:LEU:HD23	1:A:446:CYS:SG	2.59	0.42
1:E:272:GLU:O	1:E:272:GLU:HG3	2.19	0.42
1:E:350:ARG:HD3	5:E:739:HOH:O	2.19	0.42
1:F:214:GLY:HA3	1:F:289:TYR:CG	2.54	0.42
1:F:233:LEU:HD22	1:F:270:HIS:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:404:PHE:O	1:H:407:LEU:HB2	2.20	0.42
1:A:84:LYS:C	1:A:86:ASP:H	2.27	0.42
1:A:104:LEU:O	1:A:108:ARG:HG3	2.19	0.42
1:C:28:ALA:HB1	1:C:201:LEU:HD21	2.01	0.42
1:D:189:VAL:O	1:D:192:TYR:HB3	2.19	0.42
1:D:249:PRO:HD3	1:D:304:TRP:CD1	2.54	0.42
1:G:31:PHE:CE1	1:G:447:MET:HE2	2.52	0.42
1:G:144:GLU:CD	1:G:177:ARG:HE	2.27	0.42
1:A:193:PHE:O	1:A:197:GLN:HG3	2.19	0.42
1:A:394:THR:HG23	1:A:396:ASP:H	1.85	0.42
1:H:53:PHE:C	1:H:55:ASP:H	2.28	0.42
1:A:429:GLU:HG2	1:A:485:PHE:CE1	2.54	0.42
1:C:112:LEU:O	1:C:116:VAL:HG23	2.19	0.42
1:C:461:MET:HE3	1:C:461:MET:HB2	1.75	0.42
1:C:465:VAL:HG13	1:C:466:GLY:N	2.34	0.42
1:H:403:TRP:CZ2	1:H:407:LEU:HD11	2.55	0.42
1:A:375:GLY:HA2	1:A:380:ILE:HD13	2.00	0.42
1:C:307:ARG:O	1:C:310:TYR:HB3	2.19	0.42
1:G:364:LYS:HD3	1:G:364:LYS:HA	1.63	0.42
1:H:155:LYS:HD2	1:H:155:LYS:HA	1.70	0.42
1:A:170:GLU:HG3	1:D:235:LYS:HG2	2.02	0.42
1:A:420:ARG:HD3	1:B:433:ARG:HD3	2.02	0.42
1:B:325:GLU:OE1	1:B:325:GLU:N	2.49	0.42
1:C:292:LEU:HA	1:C:292:LEU:HD12	1.68	0.42
1:F:61:PHE:O	1:F:225:VAL:HG12	2.18	0.42
1:F:134:GLN:O	1:F:137:LYS:HE2	2.20	0.42
1:H:163:LYS:HE2	1:H:167:ARG:CG	2.50	0.42
1:A:349:GLU:O	1:A:353:ARG:HG3	2.20	0.42
1:C:363:MET:HE3	1:C:363:MET:HB3	1.80	0.42
1:C:447:MET:HE2	1:C:447:MET:HB2	1.83	0.42
1:D:244:ALA:HB1	1:D:305:GLU:HG2	2.01	0.42
1:H:19:LEU:HA	1:H:92:PHE:CD2	2.54	0.42
1:A:19:LEU:HD12	1:A:23:THR:HG21	2.01	0.42
1:A:422:LEU:HD23	1:B:422:LEU:HA	2.02	0.42
1:B:7:GLY:O	1:B:444:ILE:HA	2.20	0.42
1:B:447:MET:HE1	1:B:478:LEU:HD13	2.02	0.42
1:H:447:MET:O	1:H:451:LEU:HD13	2.19	0.42
1:A:84:LYS:O	1:A:88:GLN:HB2	2.20	0.41
1:B:433:ARG:NH2	1:B:488:GLU:OE2	2.52	0.41
1:C:344:LEU:HD21	1:C:365:ILE:HD12	2.02	0.41
1:D:48:LEU:HB3	1:D:194:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ILE:HG23	1:D:334:LEU:HD12	2.01	0.41
1:E:35:LEU:HD12	1:E:210:ILE:HG21	2.02	0.41
1:E:479:THR:HG22	1:E:480:GLU:N	2.35	0.41
1:H:10:MET:HG2	1:H:31:PHE:CZ	2.55	0.41
1:A:2:LYS:HE2	1:A:386:GLU:OE1	2.20	0.41
1:A:144:GLU:HG2	1:A:184:ILE:CD1	2.49	0.41
1:A:286:VAL:HB	5:A:708:HOH:O	2.20	0.41
1:C:8:VAL:HG11	1:C:447:MET:CE	2.50	0.41
1:C:74:ASP:O	1:C:78:LEU:HD13	2.20	0.41
1:C:364:LYS:HA	1:C:364:LYS:HD3	1.66	0.41
1:C:367:GLU:HG2	1:C:403:TRP:CD1	2.55	0.41
1:E:343:ASN:OD1	1:E:343:ASN:N	2.54	0.41
1:F:127:ARG:NH1	1:F:131:ASP:OD1	2.53	0.41
1:G:474:ARG:HB2	1:G:477:ASP:OD1	2.20	0.41
1:H:45:ILE:HD11	1:H:289:TYR:CE1	2.55	0.41
1:H:177:ARG:O	1:H:181:SER:HB3	2.19	0.41
1:H:264:ILE:HD13	1:H:264:ILE:HA	1.86	0.41
1:H:427:ILE:HD12	1:H:427:ILE:HA	1.90	0.41
1:A:175:GLY:O	1:A:179:LYS:HB3	2.21	0.41
1:C:161:ASP:OD1	1:C:161:ASP:N	2.53	0.41
1:D:366:MET:HE1	1:D:435:LEU:HB2	2.01	0.41
1:A:213:ILE:HA	1:A:291:TYR:O	2.20	0.41
1:B:32:VAL:HG21	1:B:205:ALA:HB2	2.01	0.41
1:C:86:ASP:N	1:C:86:ASP:OD1	2.53	0.41
1:D:166:ILE:O	1:D:240:LYS:NZ	2.52	0.41
1:G:26:ARG:HG3	1:G:27:GLU:OE1	2.20	0.41
1:G:61:PHE:O	1:G:225:VAL:HG12	2.21	0.41
1:G:400:ILE:H	1:G:449:ASP:CG	2.28	0.41
1:H:129:LEU:HD13	1:H:189:VAL:HG22	2.02	0.41
1:A:12:ILE:H	1:A:12:ILE:HG12	1.54	0.41
1:C:204:TYR:CZ	1:C:208:LYS:HE3	2.55	0.41
1:E:217:PRO:HA	1:E:295:ASP:HB3	2.01	0.41
1:A:366:MET:HE2	1:A:366:MET:HB2	1.75	0.41
1:E:173:LEU:HD13	1:E:177:ARG:NH2	2.36	0.41
1:E:268:ASP:OD1	1:E:268:ASP:N	2.53	0.41
1:F:369:GLY:HA2	1:F:377:SER:OG	2.20	0.41
1:A:245:ILE:HD11	1:A:259:LEU:HD11	2.03	0.41
1:B:317:SER:HB2	1:C:140:THR:CB	2.50	0.41
1:E:446:CYS:HB2	1:E:449:ASP:OD2	2.21	0.41
1:G:407:LEU:HB3	1:G:411:GLN:HB3	2.01	0.41
1:G:422:LEU:CD1	1:H:422:LEU:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:251:ASP:HB2	3:X:2:AC1:O2	2.20	0.41
1:H:407:LEU:O	1:H:412:LYS:HE2	2.21	0.41
1:A:389:ILE:HD12	1:A:442:THR:HB	2.02	0.41
1:B:96:PRO:HG2	1:B:474:ARG:NH2	2.35	0.41
1:C:163:LYS:O	1:C:167:ARG:HG3	2.21	0.41
1:C:204:TYR:OH	1:C:208:LYS:HE3	2.20	0.41
1:H:148:ILE:HD13	1:H:165:ILE:HD12	2.02	0.41
4:U:3:AC1:O6B	4:U:3:AC1:O4	2.28	0.41
1:A:220:VAL:O	1:A:262:ASN:HB3	2.21	0.41
1:A:367:GLU:HG2	1:A:403:TRP:CG	2.55	0.41
1:A:429:GLU:HG2	1:A:485:PHE:CZ	2.55	0.41
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.79	0.41
1:C:2:LYS:HD3	1:C:441:GLN:NE2	2.36	0.41
1:C:34:PHE:HD1	1:C:483:LYS:HE3	1.86	0.41
1:C:49:THR:HA	1:C:65:ALA:O	2.20	0.41
1:C:450:LEU:HD22	1:C:486:LEU:HD22	2.03	0.41
1:D:41:LYS:HD3	1:D:42:PHE:CE2	2.56	0.41
1:D:303:TYR:CZ	1:D:319:GLN:HB2	2.56	0.41
1:F:196:LYS:HE2	1:F:200:GLU:OE1	2.21	0.41
1:G:255:ASP:OD1	1:G:255:ASP:N	2.29	0.41
1:H:112:LEU:HD23	1:H:112:LEU:HA	1.93	0.41
1:E:173:LEU:O	1:E:177:ARG:HG3	2.21	0.41
1:F:386:GLU:O	1:F:441:GLN:HB3	2.21	0.41
1:G:394:THR:OG1	1:G:395:HIS:N	2.52	0.41
1:H:446:CYS:HB2	1:H:449:ASP:OD2	2.21	0.41
1:A:109:ARG:NE	1:A:113:GLU:OE2	2.54	0.40
1:A:251:ASP:OD1	1:A:252:ASP:N	2.50	0.40
1:A:283:GLN:HE21	1:A:334:LEU:HD21	1.86	0.40
1:B:73:PHE:HB3	1:B:87:TYR:CE2	2.57	0.40
1:B:252:ASP:HB3	1:C:127:ARG:HH12	1.86	0.40
1:B:478:LEU:HD12	1:B:478:LEU:HA	1.82	0.40
1:D:97:GLU:HG2	1:D:474:ARG:HG3	2.03	0.40
1:E:254:SER:HB2	1:E:257:GLY:N	2.36	0.40
1:F:132:PHE:CD2	1:F:133:LEU:HD23	2.57	0.40
1:H:385:THR:HG22	1:H:386:GLU:H	1.86	0.40
1:A:136:GLU:O	1:A:139:VAL:HG23	2.21	0.40
1:A:293:ARG:HE	1:A:363:MET:HE1	1.86	0.40
1:A:312:THR:HG22	1:A:313:ALA:N	2.35	0.40
1:C:138:TRP:CD1	1:C:138:TRP:H	2.38	0.40
1:D:44:GLN:NE2	1:D:391:TYR:HE2	2.17	0.40
1:D:218:ILE:HG13	1:D:300:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:PHE:H	1:E:105:PHE:HD1	1.68	0.40
1:F:85:ASP:OD1	1:F:85:ASP:N	2.54	0.40
1:G:180:LEU:O	1:G:184:ILE:HG13	2.20	0.40
1:G:387:ASN:HA	1:G:441:GLN:OE1	2.21	0.40
1:G:429:GLU:OE1	1:G:482:ARG:NH2	2.47	0.40
1:H:113:GLU:O	1:H:113:GLU:HG3	2.20	0.40
1:A:90:ILE:HG22	1:A:90:ILE:O	2.21	0.40
1:A:396:ASP:O	1:A:458:ARG:NH2	2.43	0.40
1:A:408:THR:O	1:A:411:GLN:N	2.54	0.40
1:B:340:ILE:HD13	1:B:389:ILE:HG13	2.04	0.40
1:D:58:TYR:OH	1:D:215:ASP:OD2	2.37	0.40
1:D:138:TRP:CE3	1:D:139:VAL:HA	2.57	0.40
1:E:164:ALA:HA	1:E:167:ARG:CZ	2.51	0.40
1:G:21:ILE:O	1:G:23:THR:HG23	2.20	0.40
1:A:408:THR:HB	1:A:411:GLN:H	1.86	0.40
1:B:31:PHE:O	1:B:35:LEU:HG	2.22	0.40
1:B:476:GLU:H	1:B:476:GLU:HG3	1.71	0.40
1:C:163:LYS:HE2	1:C:239:ASP:CG	2.47	0.40
1:E:389:ILE:HG22	1:E:391:TYR:CE1	2.57	0.40
1:F:339:ILE:HD12	1:F:360:PHE:CZ	2.56	0.40
1:G:248:VAL:HG22	1:G:346:TYR:OH	2.20	0.40
1:A:235:LYS:NZ	1:A:305:GLU:OE2	2.39	0.40
1:B:133:LEU:O	1:B:133:LEU:HG	2.21	0.40
1:C:162:ASP:O	1:C:165:ILE:HG22	2.21	0.40
1:F:233:LEU:HB2	1:F:234:PHE:CE2	2.56	0.40
1:G:248:VAL:CG2	1:G:346:TYR:CE2	3.04	0.40
1:H:365:ILE:HB	1:H:368:PHE:CD2	2.57	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	494/507 (97%)	463 (94%)	31 (6%)	0	100	100
1	B	495/507 (98%)	466 (94%)	29 (6%)	0	100	100
1	C	498/507 (98%)	472 (95%)	26 (5%)	0	100	100
1	D	494/507 (97%)	462 (94%)	32 (6%)	0	100	100
1	E	495/507 (98%)	471 (95%)	24 (5%)	0	100	100
1	F	494/507 (97%)	467 (94%)	27 (6%)	0	100	100
1	G	496/507 (98%)	471 (95%)	25 (5%)	0	100	100
1	H	493/507 (97%)	459 (93%)	34 (7%)	0	100	100
All	All	3959/4056 (98%)	3731 (94%)	228 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	430/440 (98%)	428 (100%)	2 (0%)	81	89
1	B	430/440 (98%)	425 (99%)	5 (1%)	63	78
1	C	433/440 (98%)	429 (99%)	4 (1%)	70	82
1	D	430/440 (98%)	421 (98%)	9 (2%)	47	67
1	E	431/440 (98%)	427 (99%)	4 (1%)	70	82
1	F	430/440 (98%)	427 (99%)	3 (1%)	76	86
1	G	432/440 (98%)	428 (99%)	4 (1%)	70	82
1	H	429/440 (98%)	425 (99%)	4 (1%)	70	82
All	All	3445/3520 (98%)	3410 (99%)	35 (1%)	68	81

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	294	ILE

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Mol	Chain	Res	Type
1	B	26	ARG
1	B	122	GLU
1	B	123	GLU
1	B	127	ARG
1	B	128	MET
1	C	26[A]	ARG
1	C	26[B]	ARG
1	C	124	ARG
1	C	432	LEU
1	D	122	GLU
1	D	123	GLU
1	D	126	THR
1	D	127	ARG
1	D	178	GLN
1	D	311	GLN
1	D	312	THR
1	D	433	ARG
1	D	498	LYS
1	E	307	ARG
1	E	311	GLN
1	E	312	THR
1	E	498	LYS
1	F	388	THR
1	F	440	SER
1	F	497	ASN
1	G	2	LYS
1	G	3	LYS
1	G	253	PHE
1	G	349	GLU
1	H	84	LYS
1	H	122	GLU
1	H	123	GLU
1	H	126	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	94	GLN
1	A	154	ASN
1	A	283	GLN
1	A	319	GLN

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Mol	Chain	Res	Type
1	A	383	ASN
1	A	481	ASN
1	B	88	GLN
1	B	94	GLN
1	B	319	GLN
1	B	441	GLN
1	B	460	ASN
1	C	11	HIS
1	C	40	GLN
1	C	89	ASN
1	C	154	ASN
1	C	258	GLN
1	C	481	ASN
1	D	44	GLN
1	D	69	HIS
1	D	118	ASN
1	D	151	HIS
1	D	258	GLN
1	D	283	GLN
1	D	470	GLN
1	D	481	ASN
1	E	40	GLN
1	E	69	HIS
1	E	134	GLN
1	E	206	ASN
1	E	319	GLN
1	E	382	HIS
1	E	417	ASN
1	E	424	ASN
1	E	463	ASN
1	E	481	ASN
1	F	44	GLN
1	F	94	GLN
1	F	118	ASN
1	F	151	HIS
1	F	283	GLN
1	F	296	HIS
1	G	154	ASN
1	G	270	HIS
1	G	311	GLN
1	G	319	GLN
1	G	417	ASN

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Mol	Chain	Res	Type
1	G	448	GLN
1	H	206	ASN
1	H	417	ASN
1	H	441	GLN
1	H	494	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 ⓘ

35 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	$\# Z > 2$
2	ASO	I	1	2	11,11,11	0.90	0	15,15,15	1.14	1 (6%)
2	AC1	I	2	2	21,22,23	3.49	4 (19%)	22,32,34	1.21	3 (13%)
3	GLC	J	1	3	12,12,12	1.43	4 (33%)	17,17,17	1.86	5 (29%)
3	AC1	J	2	3	21,22,23	3.72	6 (28%)	22,32,34	1.39	2 (9%)
2	ASO	K	1	2	11,11,11	0.76	1 (9%)	15,15,15	1.02	1 (6%)
2	AC1	K	2	2	21,22,23	3.52	5 (23%)	22,32,34	1.09	2 (9%)
3	GLC	L	1	3	12,12,12	1.03	0	17,17,17	1.24	2 (11%)
3	AC1	L	2	3	21,22,23	3.84	3 (14%)	22,32,34	1.23	2 (9%)
2	ASO	M	1	2	11,11,11	1.02	0	15,15,15	1.05	1 (6%)
2	AC1	M	2	2	21,22,23	3.36	4 (19%)	22,32,34	1.40	1 (4%)
4	GLC	N	1	4	12,12,12	1.34	1 (8%)	17,17,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLC	N	2	4	11,11,12	0.72	0	15,15,17	1.45	2 (13%)
4	AC1	N	3	4	21,22,23	3.60	3 (14%)	22,32,34	1.25	3 (13%)
2	ASO	O	1	2	11,11,11	0.77	0	15,15,15	1.24	2 (13%)
2	AC1	O	2	2	21,22,23	3.27	3 (14%)	22,32,34	0.86	1 (4%)
3	GLC	P	1	3	12,12,12	1.17	1 (8%)	17,17,17	0.62	0
3	AC1	P	2	3	21,22,23	3.49	3 (14%)	22,32,34	1.04	1 (4%)
2	ASO	Q	1	2	11,11,11	0.87	0	15,15,15	0.99	0
2	AC1	Q	2	2	21,22,23	3.47	4 (19%)	22,32,34	1.31	3 (13%)
4	GLC	R	1	4	12,12,12	1.47	2 (16%)	17,17,17	1.40	3 (17%)
4	GLC	R	2	4	11,11,12	1.15	0	15,15,17	1.07	2 (13%)
4	AC1	R	3	4	21,22,23	3.38	4 (19%)	22,32,34	0.92	1 (4%)
2	ASO	S	1	2	11,11,11	0.90	1 (9%)	15,15,15	1.10	1 (6%)
2	AC1	S	2	2	21,22,23	3.72	4 (19%)	22,32,34	1.44	2 (9%)
3	GLC	T	1	3	12,12,12	1.60	2 (16%)	17,17,17	0.94	0
3	AC1	T	2	3	21,22,23	3.33	4 (19%)	22,32,34	1.17	2 (9%)
4	GLC	U	1	4	12,12,12	1.15	2 (16%)	17,17,17	1.19	2 (11%)
4	GLC	U	2	4	11,11,12	0.79	0	15,15,17	1.39	2 (13%)
4	AC1	U	3	4	21,22,23	3.62	4 (19%)	22,32,34	1.02	2 (9%)
3	GLC	V	1	3	12,12,12	0.88	1 (8%)	17,17,17	0.76	0
3	AC1	V	2	3	21,22,23	3.51	4 (19%)	22,32,34	1.46	3 (13%)
2	ASO	W	1	2	11,11,11	1.36	1 (9%)	15,15,15	0.99	1 (6%)
2	AC1	W	2	2	21,22,23	3.24	3 (14%)	22,32,34	1.08	1 (4%)
3	GLC	X	1	3	12,12,12	1.12	1 (8%)	17,17,17	1.02	1 (5%)
3	AC1	X	2	3	21,22,23	3.27	4 (19%)	22,32,34	1.04	2 (9%)

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
2	ASO	I	1	2	-	2/2/19/19	0/1/1/1
2	AC1	I	2	2	-	3/6/43/46	0/2/2/2
3	GLC	J	1	3	-	2/2/22/22	0/1/1/1
3	AC1	J	2	3	-	2/6/43/46	0/2/2/2
2	ASO	K	1	2	-	0/2/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AC1	K	2	2	-	4/6/43/46	0/2/2/2
3	GLC	L	1	3	-	1/2/22/22	0/1/1/1
3	AC1	L	2	3	-	2/6/43/46	0/2/2/2
2	ASO	M	1	2	-	0/2/19/19	0/1/1/1
2	AC1	M	2	2	-	5/6/43/46	0/2/2/2
4	GLC	N	1	4	-	1/2/22/22	0/1/1/1
4	GLC	N	2	4	-	2/2/19/22	0/1/1/1
4	AC1	N	3	4	-	3/6/43/46	0/2/2/2
2	ASO	O	1	2	-	0/2/19/19	0/1/1/1
2	AC1	O	2	2	-	2/6/43/46	0/2/2/2
3	GLC	P	1	3	-	2/2/22/22	0/1/1/1
3	AC1	P	2	3	-	1/6/43/46	0/2/2/2
2	ASO	Q	1	2	-	0/2/19/19	0/1/1/1
2	AC1	Q	2	2	-	4/6/43/46	0/2/2/2
4	GLC	R	1	4	-	2/2/22/22	0/1/1/1
4	GLC	R	2	4	-	2/2/19/22	0/1/1/1
4	AC1	R	3	4	-	3/6/43/46	0/2/2/2
2	ASO	S	1	2	-	1/2/19/19	0/1/1/1
2	AC1	S	2	2	-	2/6/43/46	0/2/2/2
3	GLC	T	1	3	-	1/2/22/22	0/1/1/1
3	AC1	T	2	3	-	1/6/43/46	0/2/2/2
4	GLC	U	1	4	-	2/2/22/22	0/1/1/1
4	GLC	U	2	4	-	2/2/19/22	0/1/1/1
4	AC1	U	3	4	-	3/6/43/46	0/2/2/2
3	GLC	V	1	3	-	0/2/22/22	0/1/1/1
3	AC1	V	2	3	-	3/6/43/46	0/2/2/2
2	ASO	W	1	2	-	2/2/19/19	0/1/1/1
2	AC1	W	2	2	-	3/6/43/46	0/2/2/2
3	GLC	X	1	3	-	2/2/22/22	0/1/1/1
3	AC1	X	2	3	-	1/6/43/46	0/2/2/2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	AC1	C4A-C5B	-14.44	1.39	1.51
2	S	2	AC1	C4A-C5B	-13.85	1.40	1.51
4	N	3	AC1	C4A-C5B	-13.25	1.40	1.51
4	U	3	AC1	C4A-C5B	-13.19	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	AC1	C4A-C5B	-12.90	1.40	1.51
3	P	2	AC1	C4A-C5B	-12.46	1.41	1.51
2	M	2	AC1	C4A-C5B	-12.31	1.41	1.51
2	I	2	AC1	C4A-C5B	-12.29	1.41	1.51
2	K	2	AC1	C4A-C5B	-12.15	1.41	1.51
3	V	2	AC1	C4A-C5B	-11.97	1.41	1.51
3	T	2	AC1	C4A-C5B	-11.77	1.41	1.51
2	Q	2	AC1	C4A-C5B	-11.53	1.42	1.51
4	R	3	AC1	C4A-C5B	-11.43	1.42	1.51
2	O	2	AC1	C4A-C5B	-11.20	1.42	1.51
3	X	2	AC1	C4A-C5B	-11.20	1.42	1.51
2	W	2	AC1	C4A-C5B	-10.99	1.42	1.51
3	V	2	AC1	C1B-C7B	-9.04	1.37	1.50
2	Q	2	AC1	C1B-C7B	-8.53	1.38	1.50
3	J	2	AC1	C1B-C7B	-7.93	1.39	1.50
2	K	2	AC1	C1B-C7B	-7.65	1.39	1.50
3	L	2	AC1	C1B-C7B	-7.57	1.39	1.50
4	N	3	AC1	C1B-C7B	-7.51	1.39	1.50
2	W	2	AC1	C1B-C7B	-7.18	1.40	1.50
4	R	3	AC1	C1B-C7B	-7.17	1.40	1.50
2	I	2	AC1	C7B-C5B	7.14	1.42	1.32
2	O	2	AC1	C1B-C7B	-7.09	1.40	1.50
3	P	2	AC1	C1B-C7B	-7.06	1.40	1.50
2	S	2	AC1	C1B-C7B	-7.03	1.40	1.50
3	X	2	AC1	C1B-C7B	-6.86	1.40	1.50
2	M	2	AC1	C1B-C7B	-6.76	1.41	1.50
4	U	3	AC1	C1B-C7B	-6.72	1.41	1.50
3	T	2	AC1	C1B-C7B	-6.45	1.41	1.50
2	I	2	AC1	C1B-C7B	-5.82	1.42	1.50
3	T	2	AC1	C7B-C5B	5.67	1.40	1.32
4	U	3	AC1	C7B-C5B	5.64	1.40	1.32
2	W	2	AC1	C7B-C5B	5.63	1.40	1.32
2	S	2	AC1	C7B-C5B	5.61	1.40	1.32
3	X	2	AC1	C7B-C5B	5.52	1.40	1.32
4	R	3	AC1	C7B-C5B	5.45	1.40	1.32
2	O	2	AC1	C7B-C5B	5.40	1.40	1.32
3	P	2	AC1	C7B-C5B	5.39	1.40	1.32
2	K	2	AC1	C7B-C5B	5.27	1.40	1.32
2	Q	2	AC1	C7B-C5B	5.23	1.40	1.32
3	J	2	AC1	C7B-C5B	5.08	1.40	1.32
2	M	2	AC1	C7B-C5B	4.95	1.39	1.32
4	N	3	AC1	C7B-C5B	4.79	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	AC1	C7B-C5B	4.72	1.39	1.32
3	V	2	AC1	C7B-C5B	4.08	1.38	1.32
3	T	1	GLC	O4-C4	3.61	1.51	1.43
2	W	1	ASO	C2-C3	-3.58	1.47	1.52
4	R	3	AC1	O5-C1	3.42	1.49	1.43
3	J	2	AC1	C3B-C4A	-3.36	1.48	1.53
3	J	2	AC1	O5-C1	3.10	1.48	1.43
4	R	1	GLC	O4-C4	2.85	1.50	1.43
3	X	2	AC1	C2-C3	2.61	1.56	1.52
4	R	1	GLC	O1-C1	2.43	1.47	1.39
2	K	2	AC1	C3B-C4A	-2.38	1.49	1.53
3	X	1	GLC	O4-C4	2.37	1.48	1.43
4	N	1	GLC	O4-C4	2.34	1.48	1.43
2	K	2	AC1	C2B-C1B	2.31	1.56	1.53
3	J	2	AC1	C2B-C1B	-2.30	1.50	1.53
4	U	3	AC1	O5-C1	2.29	1.47	1.43
3	T	2	AC1	C3B-C4A	2.28	1.56	1.53
4	U	1	GLC	C4-C3	2.23	1.58	1.52
3	J	1	GLC	C1-C2	2.20	1.57	1.52
3	T	1	GLC	O1-C1	2.19	1.46	1.39
2	Q	2	AC1	C2B-C1B	2.15	1.55	1.53
3	J	1	GLC	O5-C5	2.12	1.49	1.44
3	P	1	GLC	O4-C4	2.12	1.48	1.43
2	I	2	AC1	O4-C4A	2.11	1.46	1.42
2	K	1	ASO	C2-C3	-2.06	1.49	1.52
2	M	2	AC1	C2-C3	-2.06	1.49	1.52
2	S	1	ASO	C2-C3	2.05	1.55	1.52
3	J	1	GLC	O4-C4	2.04	1.48	1.43
3	V	2	AC1	C2B-C1B	-2.03	1.50	1.53
4	U	1	GLC	O5-C1	2.02	1.47	1.42
2	S	2	AC1	C3B-C4A	2.01	1.55	1.53
3	V	1	GLC	O1-C1	2.01	1.45	1.39
3	J	1	GLC	O5-C1	2.01	1.47	1.42

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	2	AC1	C7B-C1B-N4A	-4.64	103.84	110.68
3	J	1	GLC	C4-C3-C2	-4.54	102.86	110.83
2	M	2	AC1	C2B-C3B-C4A	-4.51	103.08	110.22
4	N	2	GLC	C2-C3-C4	-3.89	104.01	110.86
2	S	2	AC1	C7B-C1B-N4A	-3.82	105.05	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2	GLC	C2-C3-C4	-3.58	104.56	110.86
3	L	2	AC1	C6-C5-C4	-3.50	107.15	113.57
3	L	1	GLC	O5-C5-C6	3.39	114.83	106.44
2	W	2	AC1	C2B-C3B-C4A	-3.36	104.90	110.22
2	S	2	AC1	C2B-C3B-C4A	-3.34	104.93	110.22
4	U	3	AC1	C1-C2-C3	-3.32	104.81	109.64
2	Q	2	AC1	C7B-C1B-N4A	-3.27	105.86	110.68
3	V	2	AC1	C2B-C3B-C4A	-3.23	105.12	110.22
3	J	2	AC1	C6-C5-C4	-3.15	107.80	113.57
3	J	1	GLC	O4-C4-C5	3.14	117.06	109.32
4	N	3	AC1	C6-C5-C4	-3.08	107.93	113.57
2	Q	2	AC1	C2B-C3B-C4A	-2.93	105.58	110.22
3	L	2	AC1	C7B-C1B-N4A	-2.91	106.39	110.68
3	T	2	AC1	C2B-C3B-C4A	-2.91	105.62	110.22
2	K	2	AC1	C7B-C1B-N4A	-2.91	106.40	110.68
4	U	2	GLC	O5-C5-C6	-2.85	102.12	107.66
3	J	1	GLC	O5-C5-C6	2.76	113.29	106.44
2	W	1	ASO	O3-C3-C2	-2.75	104.44	110.05
3	X	2	AC1	C2B-C3B-C4A	-2.74	105.89	110.22
3	T	2	AC1	C6-C5-C4	-2.69	108.64	113.57
4	R	3	AC1	C1-C2-C3	-2.69	105.73	109.64
3	L	1	GLC	C6-C5-C4	-2.66	106.49	113.02
2	I	1	ASO	C1-O5-C5	2.63	115.71	112.19
3	J	1	GLC	O4-C4-C3	2.63	116.57	110.38
4	R	1	GLC	C4-C3-C2	-2.57	106.32	110.83
4	N	3	AC1	C2B-C3B-C4A	-2.46	106.33	110.22
3	P	2	AC1	C6-C5-C4	-2.43	109.11	113.57
2	K	2	AC1	C2B-C3B-C4A	-2.40	106.41	110.22
4	U	3	AC1	O3-C3-C4	2.37	114.30	109.58
4	N	2	GLC	C3-C4-C5	-2.30	106.06	110.23
3	J	1	GLC	C3-C4-C5	-2.29	106.07	110.23
2	I	2	AC1	O3-C3-C2	-2.29	105.38	110.05
2	M	1	ASO	C6-C5-C4	-2.28	107.41	113.02
4	R	1	GLC	O1-C1-O5	2.27	117.16	110.41
2	I	2	AC1	C6-C5-C4	-2.27	109.41	113.57
3	J	2	AC1	O5-C5-C6	2.27	112.32	107.40
2	I	2	AC1	C2B-C3B-C4A	-2.26	106.64	110.22
2	O	2	AC1	C2B-C3B-C4A	-2.26	106.64	110.22
2	O	1	ASO	C3-C4-C5	-2.23	106.18	110.23
4	U	1	GLC	O3-C3-C4	2.23	115.63	110.38
2	O	1	ASO	C6-C5-C4	-2.22	107.56	113.02
2	Q	2	AC1	O3-C3-C2	-2.21	105.55	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	1	GLC	C6-C5-C4	-2.18	107.66	113.02
3	X	2	AC1	C6-C5-C4	-2.18	109.57	113.57
4	U	1	GLC	C1-C2-C3	-2.18	105.91	110.36
4	R	2	GLC	O5-C5-C6	2.14	111.84	107.66
2	K	1	ASO	O2-C2-C3	-2.13	105.73	110.15
4	R	2	GLC	C1-O5-C5	2.04	114.92	112.19
3	X	1	GLC	C6-C5-C4	-2.04	108.02	113.02
3	V	2	AC1	C1-C2-C3	-2.03	106.69	109.64
2	S	1	ASO	O5-C5-C6	-2.01	103.75	107.66
4	N	3	AC1	C7B-C1B-N4A	-2.00	107.73	110.68

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	2	AC1	C4A-C5B-C6B-O6B
2	I	2	AC1	C7B-C5B-C6B-O6B
2	K	2	AC1	C5-C4-N4A-C1B
2	K	2	AC1	C4A-C5B-C6B-O6B
2	K	2	AC1	C7B-C5B-C6B-O6B
2	M	2	AC1	C5-C4-N4A-C1B
2	M	2	AC1	C4A-C5B-C6B-O6B
2	M	2	AC1	C7B-C5B-C6B-O6B
2	Q	2	AC1	C5-C4-N4A-C1B
2	Q	2	AC1	C4A-C5B-C6B-O6B
2	Q	2	AC1	C7B-C5B-C6B-O6B
2	S	2	AC1	C5-C4-N4A-C1B
2	W	2	AC1	C4A-C5B-C6B-O6B
2	W	2	AC1	C7B-C5B-C6B-O6B
3	L	2	AC1	C7B-C5B-C6B-O6B
3	T	2	AC1	C7B-C1B-N4A-C4
3	V	2	AC1	C7B-C1B-N4A-C4
3	V	2	AC1	C4A-C5B-C6B-O6B
4	N	3	AC1	C7B-C5B-C6B-O6B
4	R	3	AC1	C7B-C5B-C6B-O6B
4	U	3	AC1	C7B-C5B-C6B-O6B
4	R	1	GLC	O5-C5-C6-O6
4	U	1	GLC	O5-C5-C6-O6
3	X	1	GLC	C4-C5-C6-O6
4	R	1	GLC	C4-C5-C6-O6
3	X	1	GLC	O5-C5-C6-O6
4	U	1	GLC	C4-C5-C6-O6

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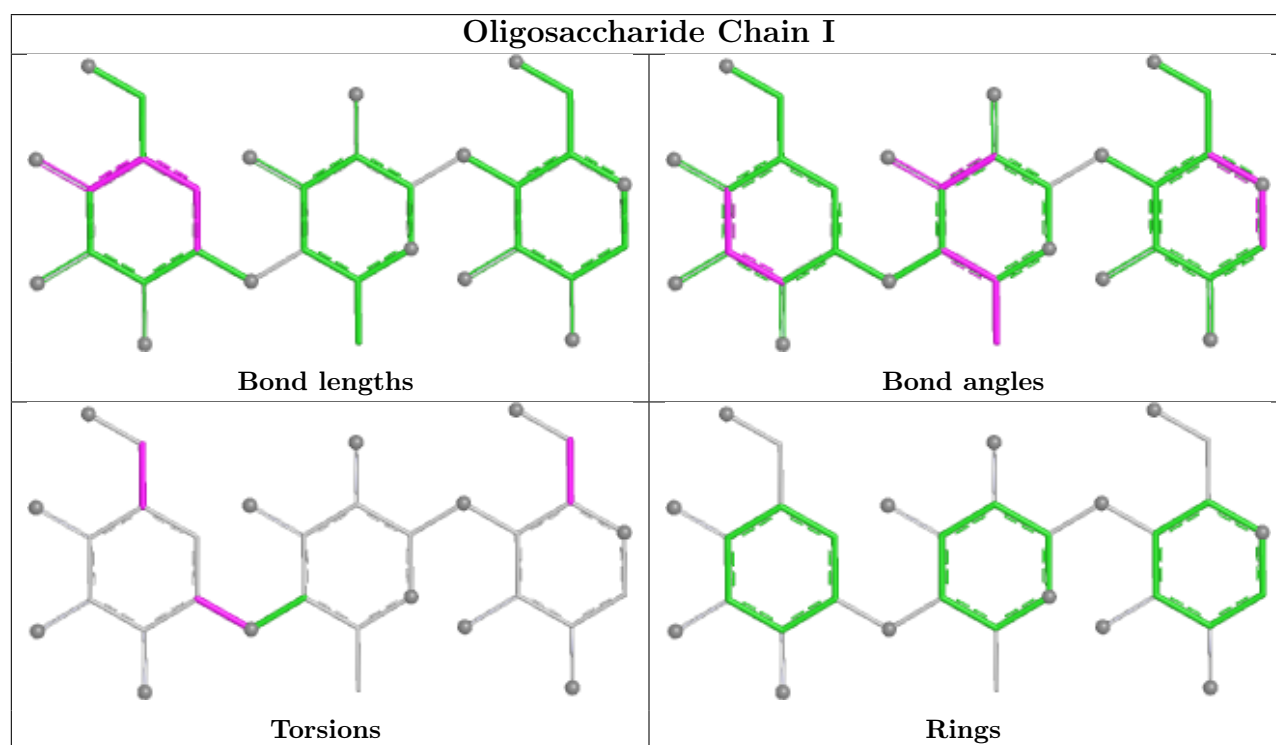
Mol	Chain	Res	Type	Atoms
3	J	1	GLC	C4-C5-C6-O6
2	I	1	ASO	O5-C5-C6-O6
4	R	2	GLC	O5-C5-C6-O6
2	I	1	ASO	C4-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
2	W	1	ASO	O5-C5-C6-O6
4	U	2	GLC	O5-C5-C6-O6
3	T	1	GLC	O5-C5-C6-O6
2	S	1	ASO	O5-C5-C6-O6
4	R	2	GLC	C4-C5-C6-O6
4	N	1	GLC	O5-C5-C6-O6
4	N	2	GLC	O5-C5-C6-O6
2	I	2	AC1	C2B-C1B-N4A-C4
2	K	2	AC1	C3-C4-N4A-C1B
2	M	2	AC1	C3-C4-N4A-C1B
2	O	2	AC1	C5-C4-N4A-C1B
2	Q	2	AC1	C3-C4-N4A-C1B
2	S	2	AC1	C3-C4-N4A-C1B
4	U	2	GLC	C4-C5-C6-O6
3	L	1	GLC	O5-C5-C6-O6
3	P	1	GLC	C4-C5-C6-O6
3	J	2	AC1	C4A-C5B-C6B-O6B
3	J	2	AC1	C7B-C5B-C6B-O6B
4	N	3	AC1	C4A-C5B-C6B-O6B
4	R	3	AC1	C4A-C5B-C6B-O6B
2	M	2	AC1	C7B-C1B-N4A-C4
3	L	2	AC1	C7B-C1B-N4A-C4
3	P	2	AC1	C7B-C1B-N4A-C4
3	X	2	AC1	C7B-C1B-N4A-C4
4	N	3	AC1	C7B-C1B-N4A-C4
4	R	3	AC1	C7B-C1B-N4A-C4
3	P	1	GLC	O5-C5-C6-O6
4	U	3	AC1	C2B-C1B-N4A-C4
2	W	2	AC1	C5-C4-N4A-C1B
2	W	1	ASO	C4-C5-C6-O6
3	V	2	AC1	C7B-C5B-C6B-O6B
4	U	3	AC1	C4A-C5B-C6B-O6B
4	N	2	GLC	C4-C5-C6-O6
2	O	2	AC1	C3-C4-N4A-C1B

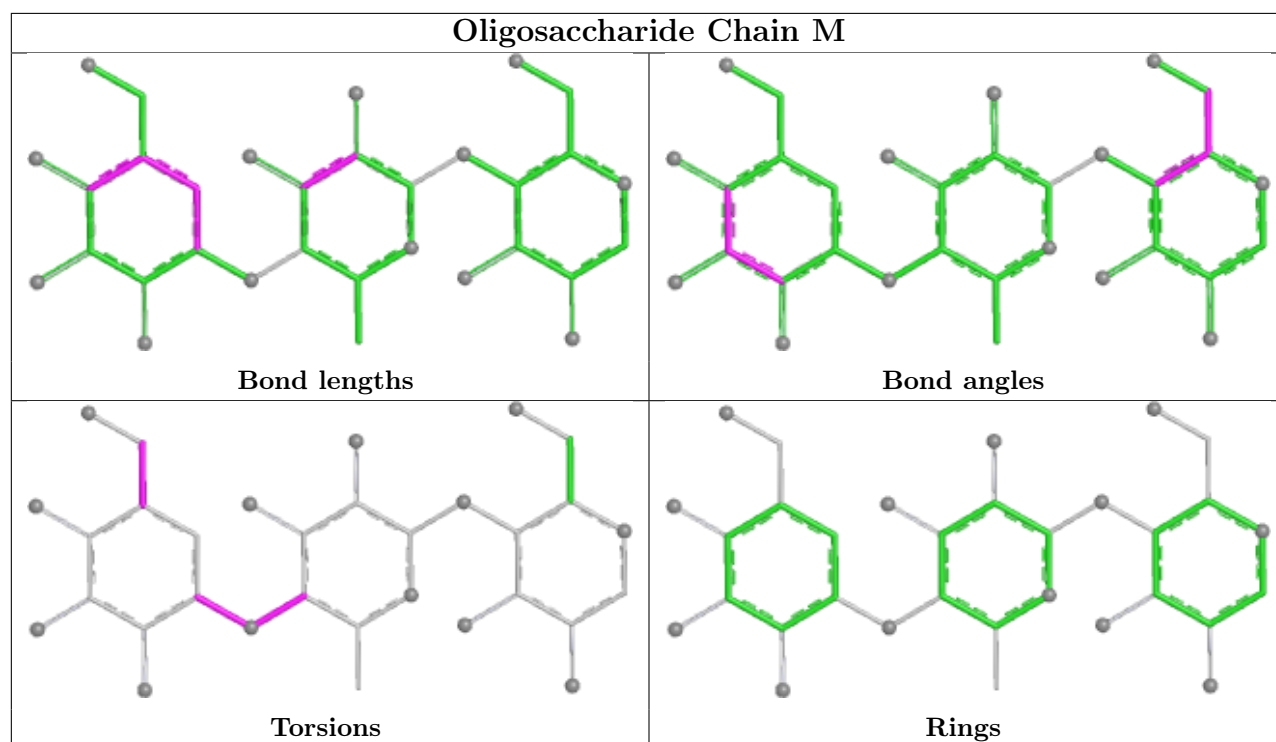
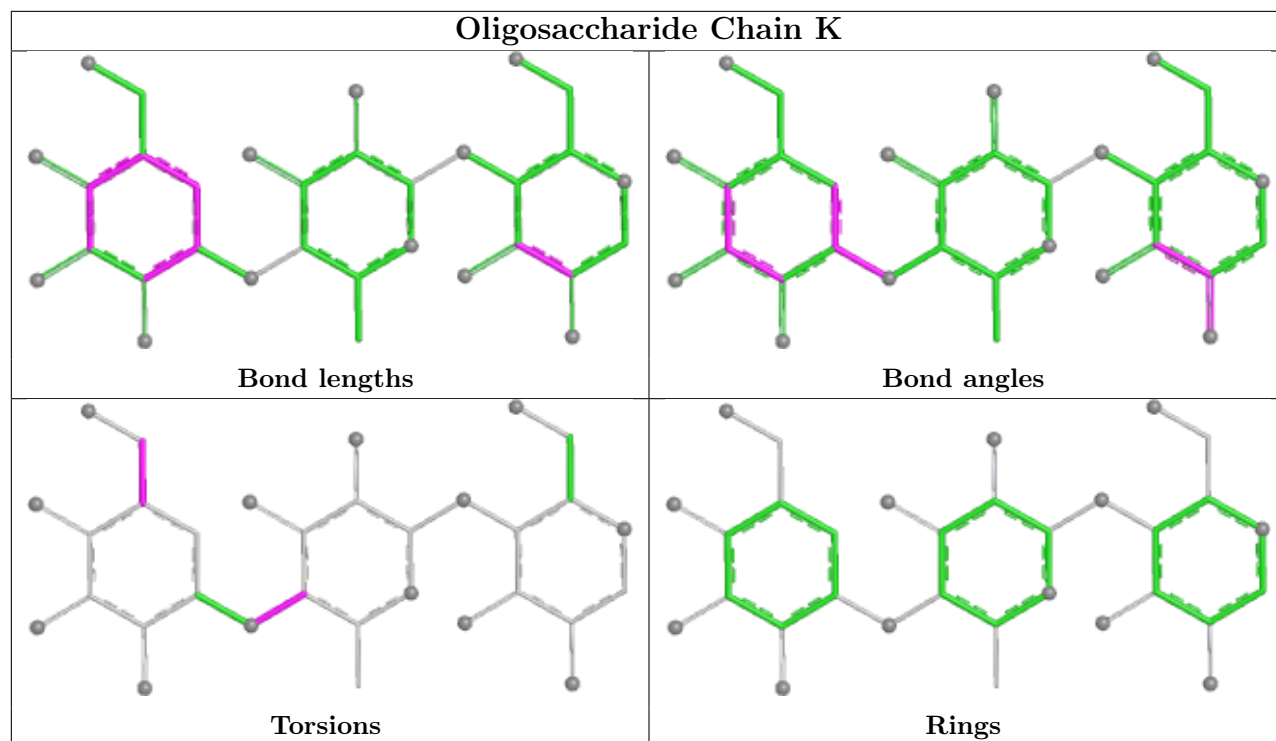
There are no ring outliers.

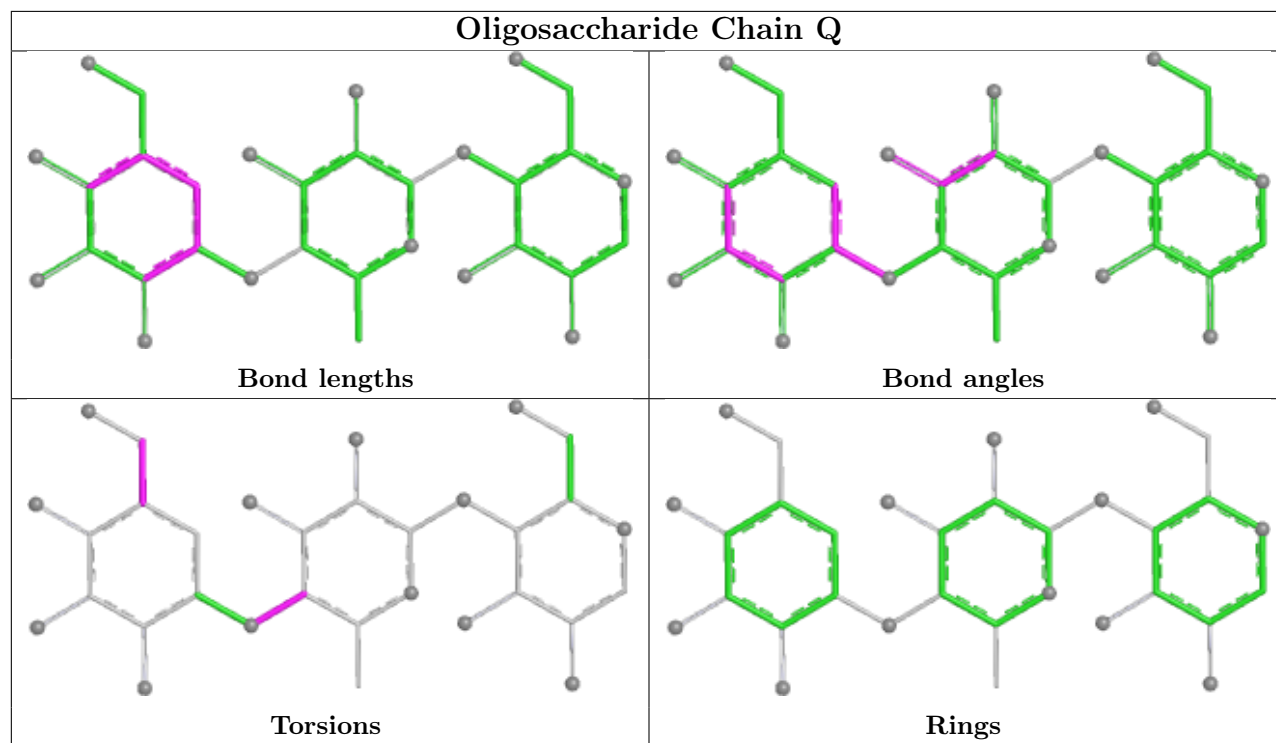
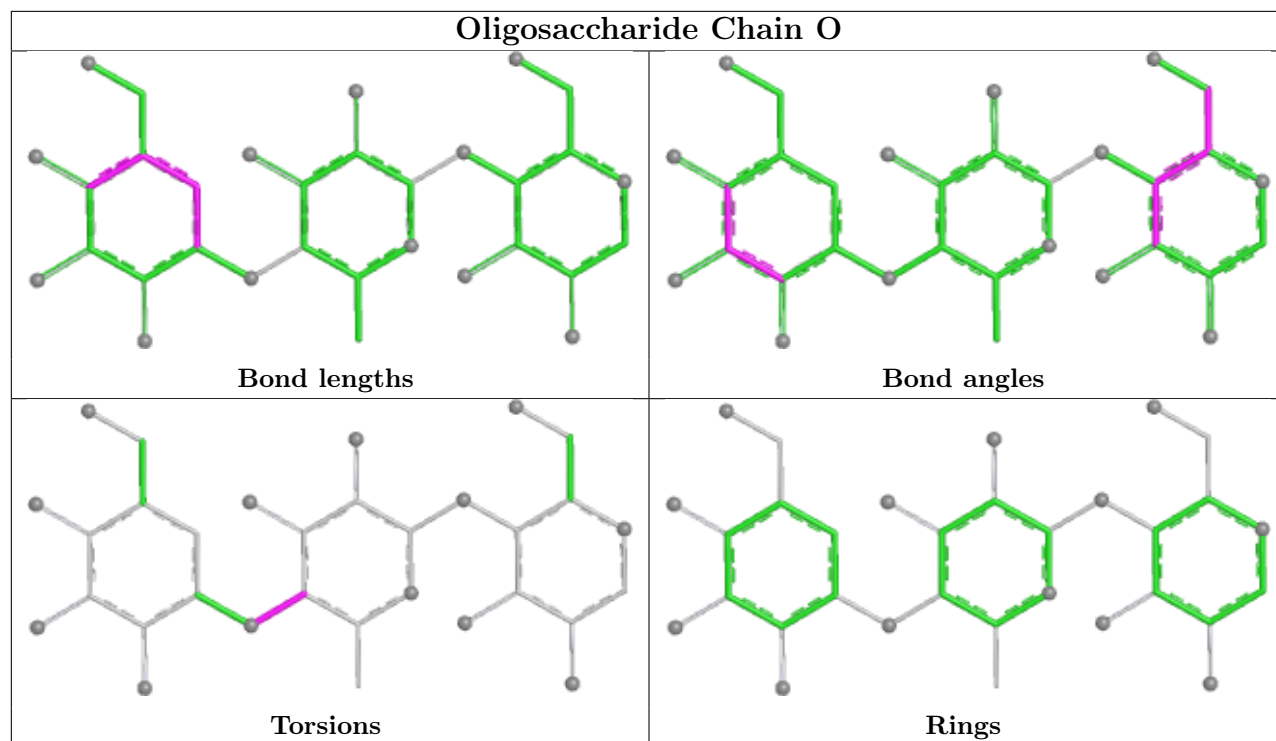
9 monomers are involved in 16 short contacts:

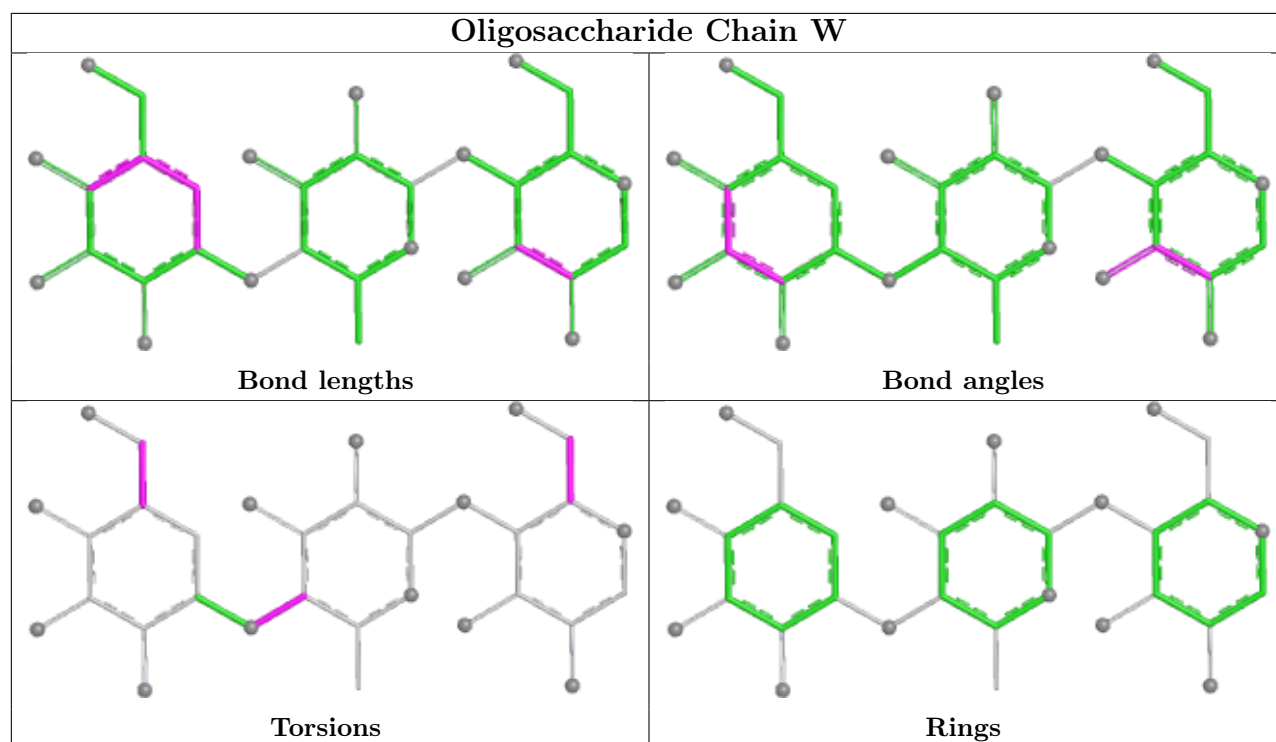
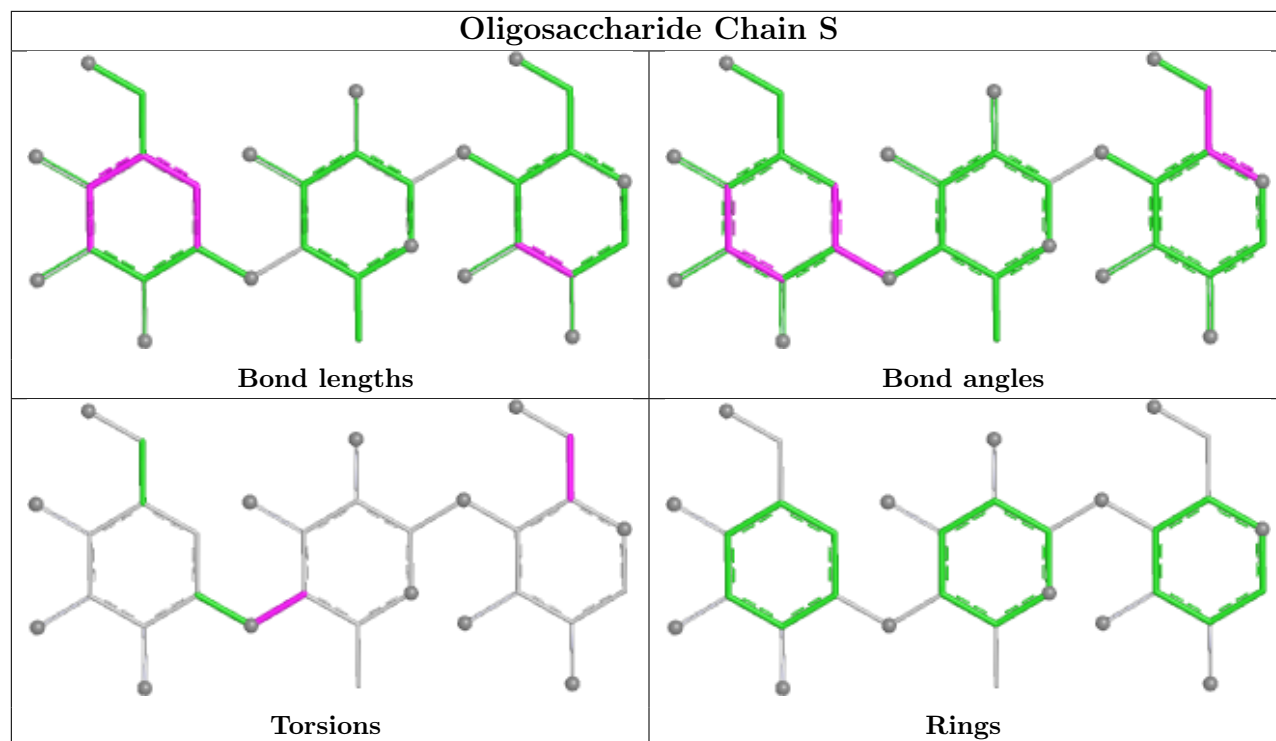
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	2	AC1	1	0
4	U	3	AC1	1	0
3	J	2	AC1	2	0
4	N	3	AC1	1	0
3	V	2	AC1	2	0
2	I	2	AC1	4	0
4	U	1	GLC	4	0
3	X	2	AC1	1	0
2	S	1	ASO	1	0

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

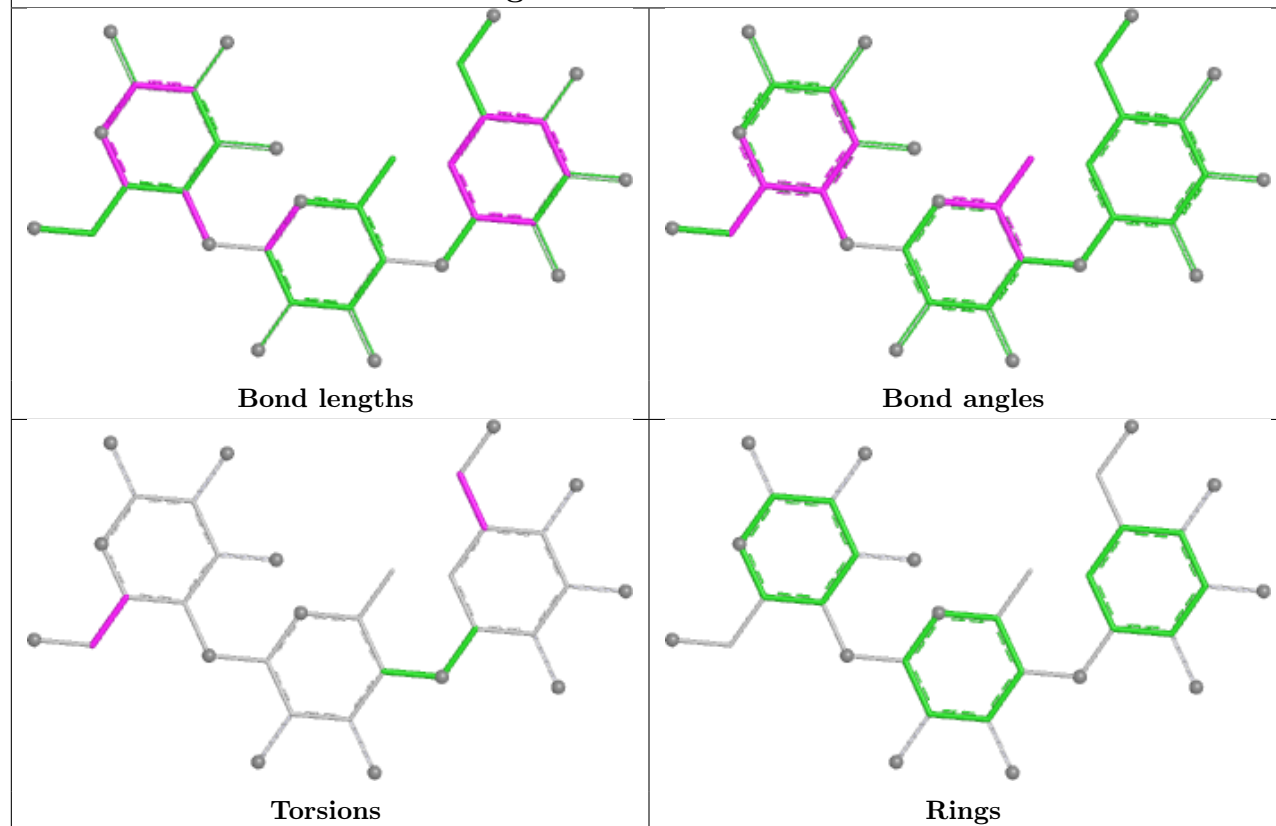




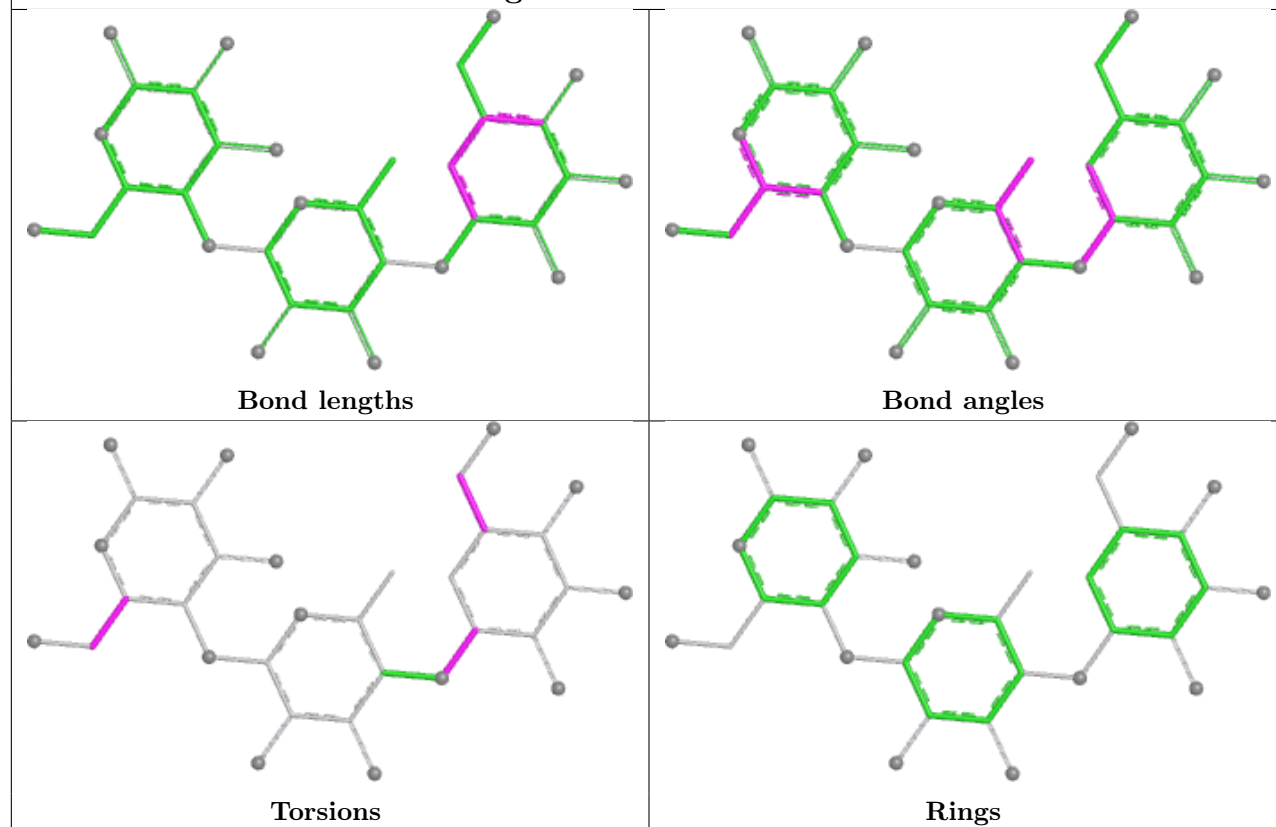




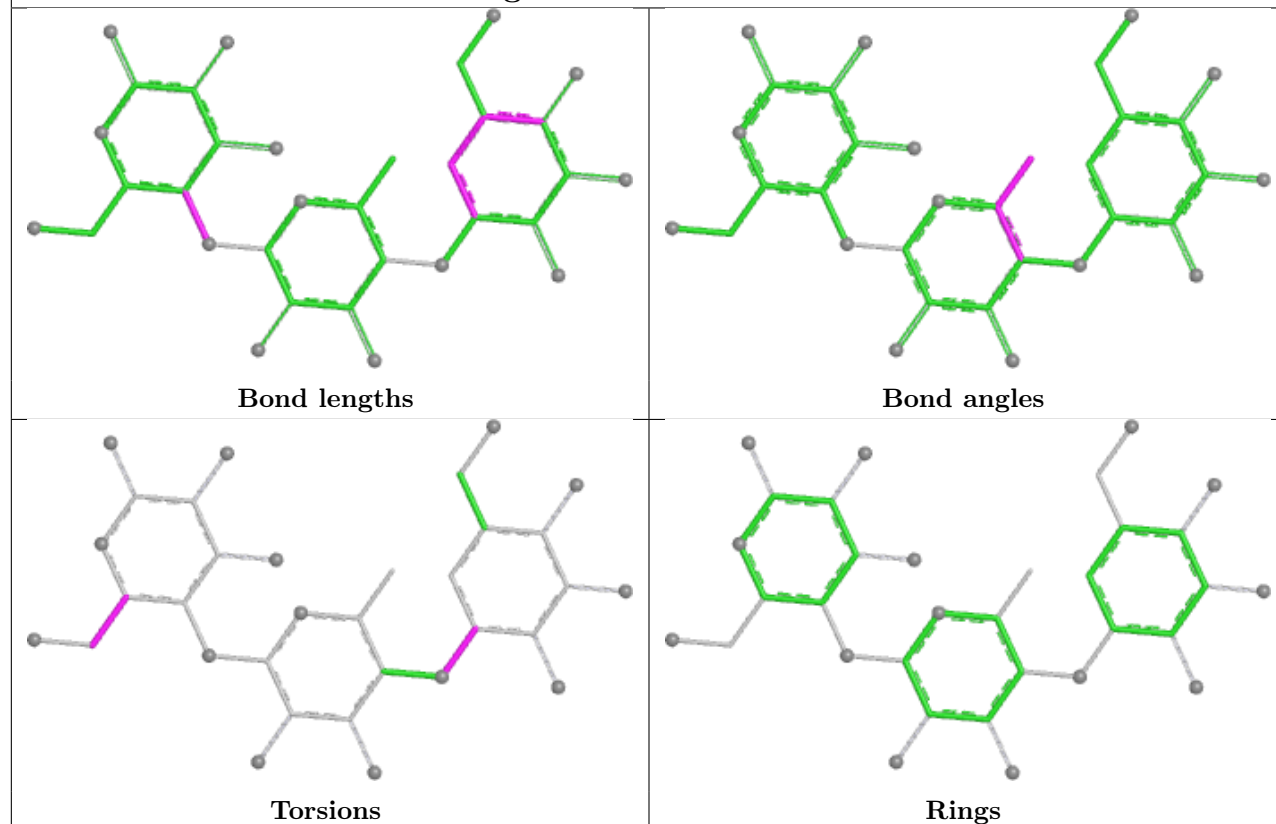
Oligosaccharide Chain J



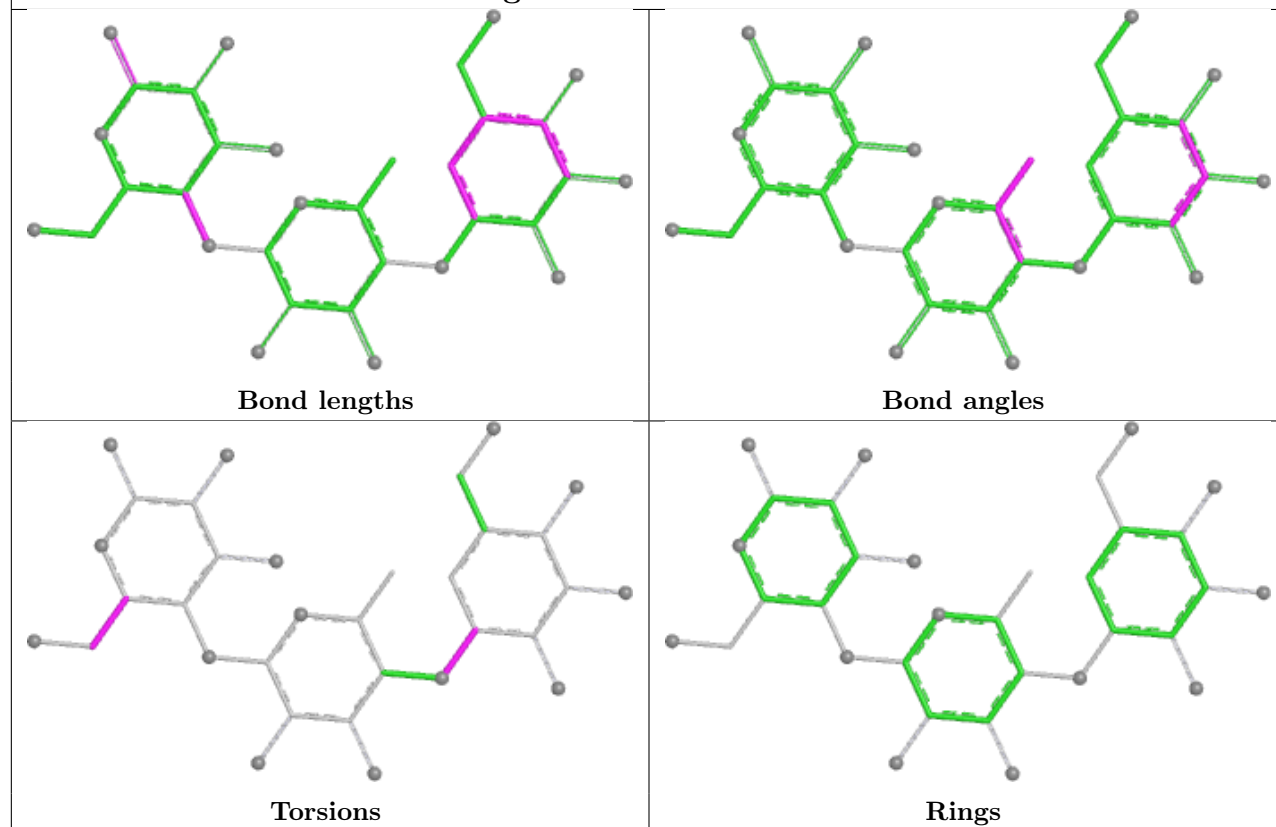
Oligosaccharide Chain L



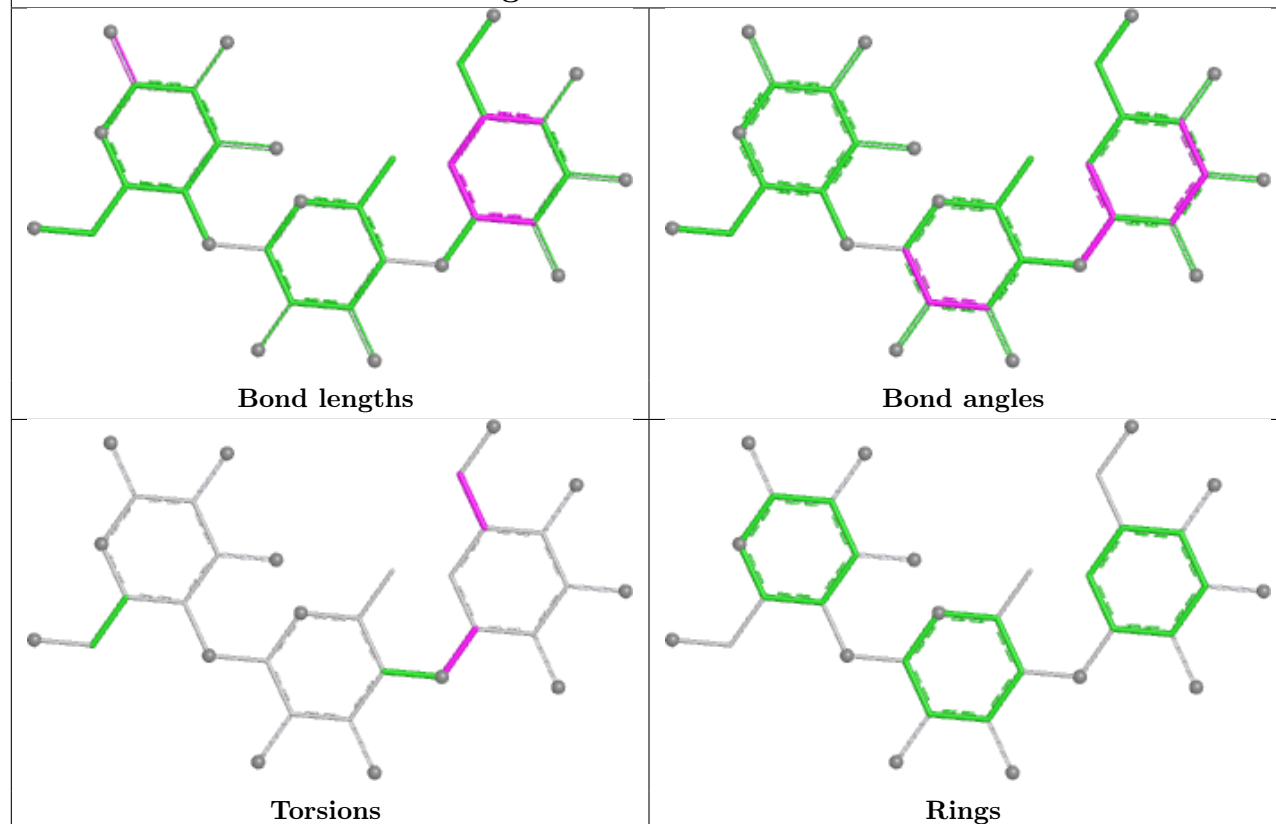
Oligosaccharide Chain P



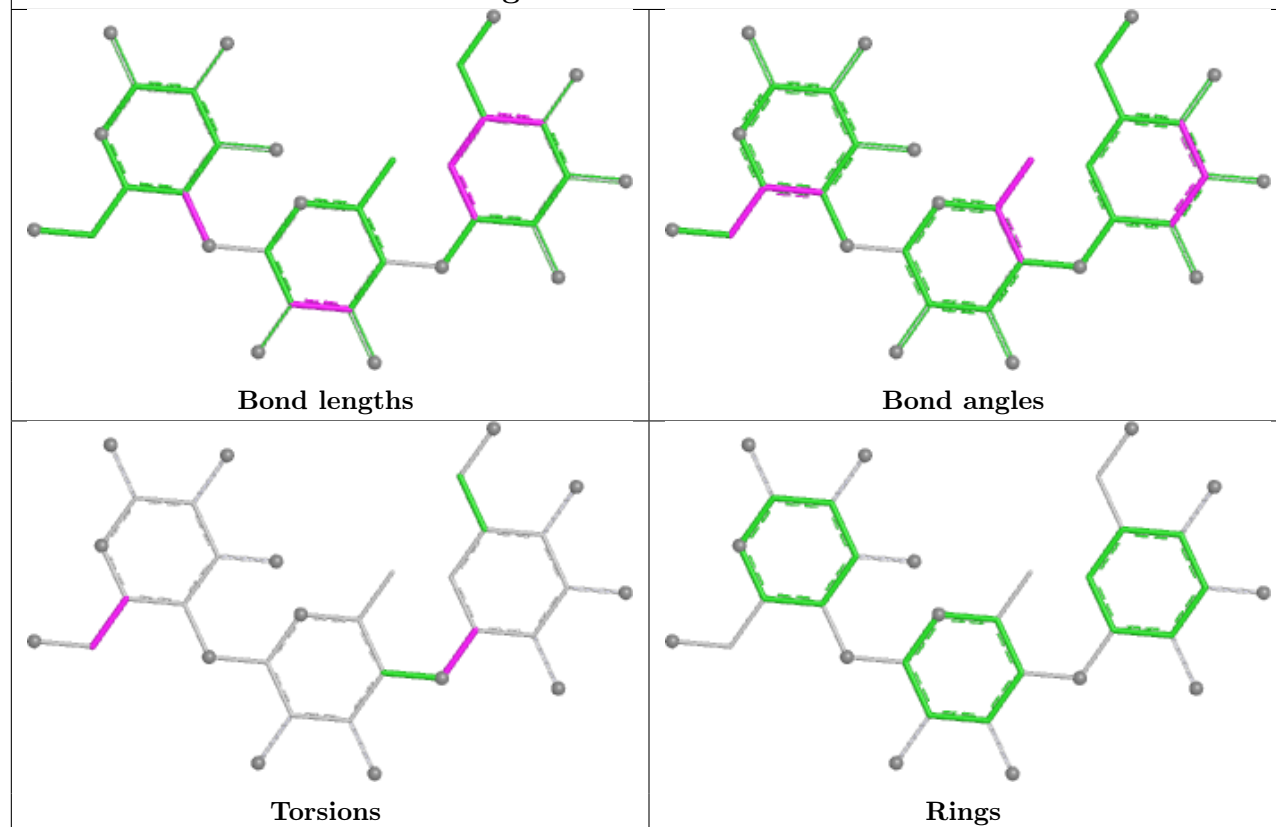
Oligosaccharide Chain T

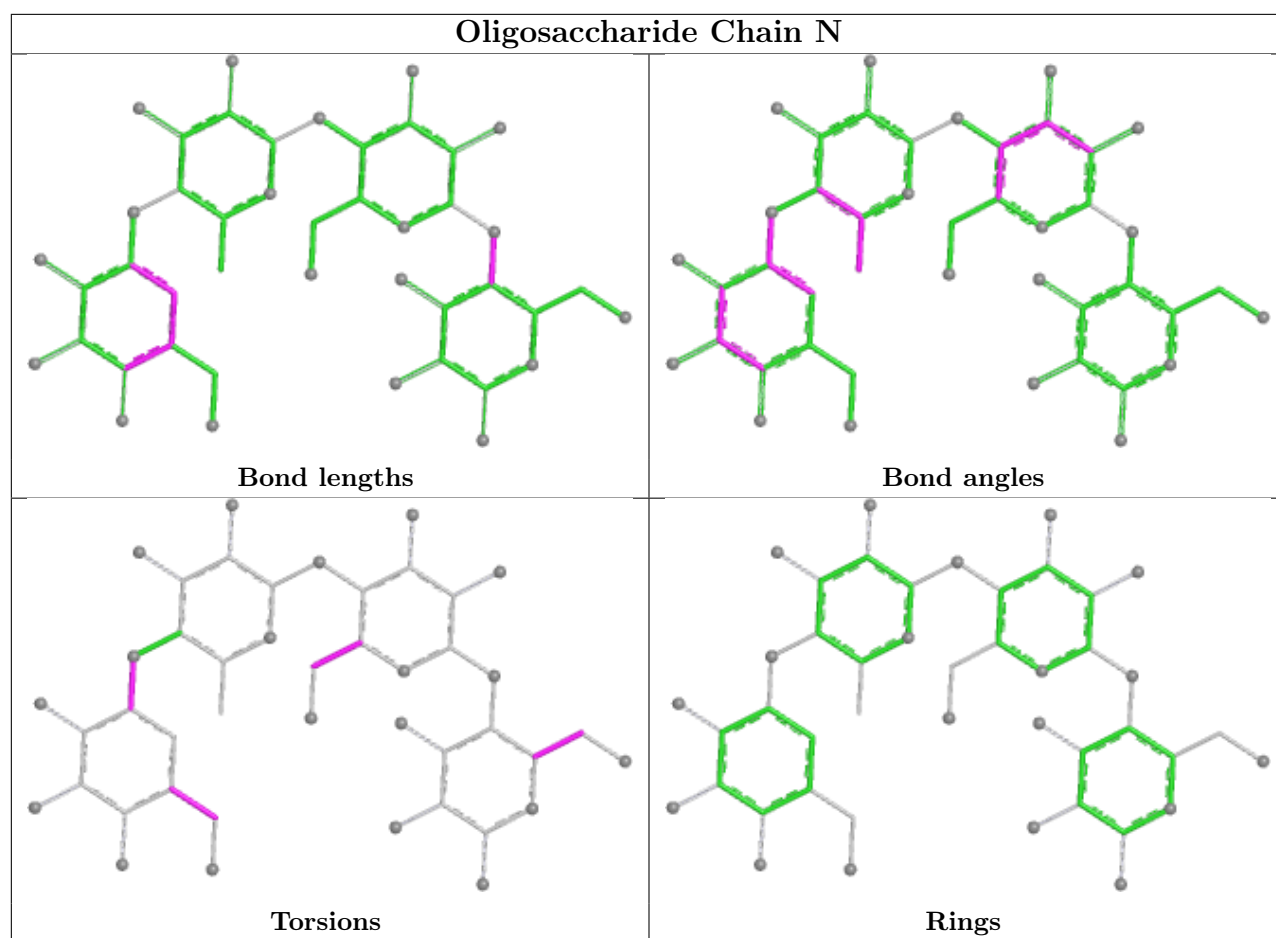


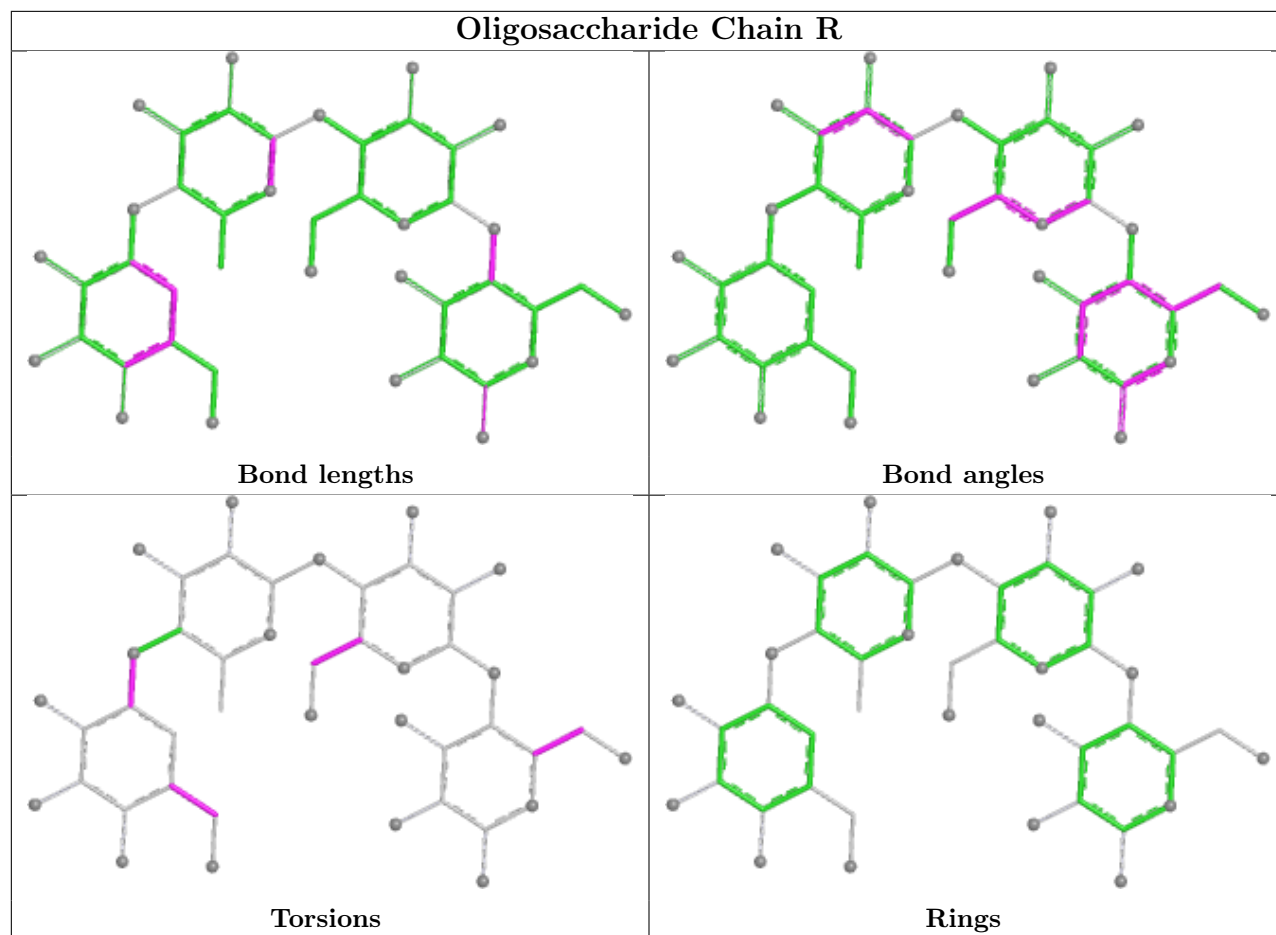
Oligosaccharide Chain V

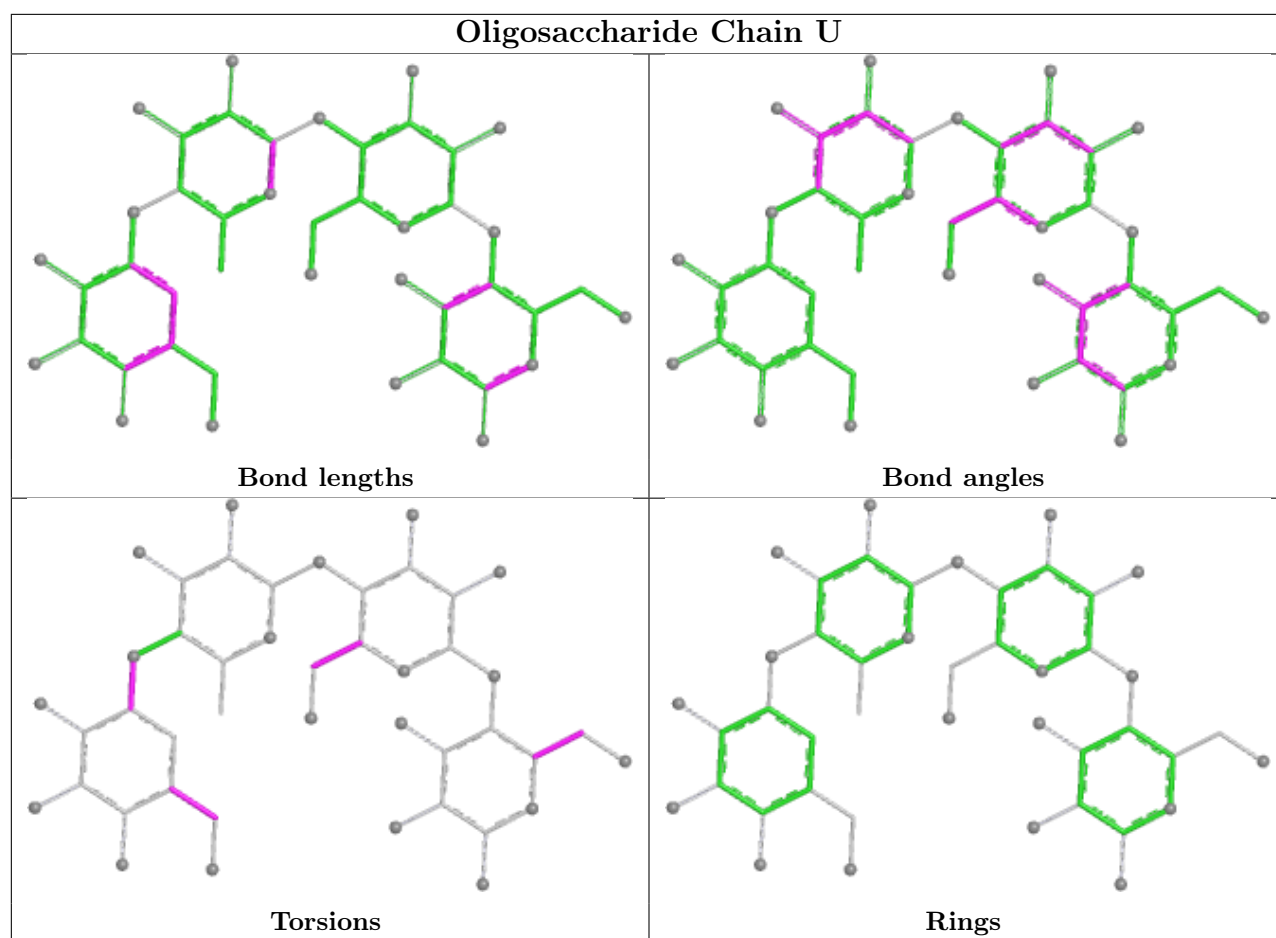


Oligosaccharide Chain X









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/507 (97%)	0.35	6 (1%) 76 76	34, 53, 75, 100	0
1	B	497/507 (98%)	0.38	6 (1%) 76 76	36, 51, 72, 86	0
1	C	499/507 (98%)	0.04	5 (1%) 79 79	29, 42, 62, 80	1 (0%)
1	D	496/507 (97%)	0.12	2 (0%) 88 89	30, 46, 68, 92	0
1	E	497/507 (98%)	0.03	2 (0%) 88 89	28, 41, 62, 88	0
1	F	496/507 (97%)	0.08	2 (0%) 88 89	28, 46, 68, 85	0
1	G	498/507 (98%)	0.22	7 (1%) 73 73	33, 49, 69, 100	0
1	H	495/507 (97%)	0.60	17 (3%) 48 46	36, 59, 84, 98	0
All	All	3974/4056 (97%)	0.23	47 (1%) 76 76	28, 49, 73, 100	1 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	105	PHE	3.7
1	C	26[A]	ARG	3.6
1	G	2	LYS	3.3
1	E	239	ASP	3.1
1	H	253	PHE	3.1
1	B	207	ASP	3.0
1	B	78	LEU	2.9
1	A	253	PHE	2.8
1	C	309	ASP	2.8
1	A	102	ALA	2.8
1	H	203	GLU	2.6
1	F	27	GLU	2.6
1	H	398	GLU	2.6
1	F	105	PHE	2.6
1	B	22	GLY	2.5
1	H	122	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	123	GLU	2.5
1	D	253	PHE	2.5
1	C	497	ASN	2.5
1	A	17	GLY	2.5
1	A	466	GLY	2.5
1	H	20	GLY	2.4
1	G	253	PHE	2.4
1	B	337	LEU	2.4
1	B	94	GLN	2.3
1	G	499	LEU	2.3
1	H	113	GLU	2.3
1	H	104	LEU	2.3
1	H	76	LEU	2.3
1	H	82	ILE	2.2
1	H	259	LEU	2.2
1	H	83	SER	2.2
1	G	313	ALA	2.2
1	G	27	GLU	2.2
1	G	449	ASP	2.2
1	G	259	LEU	2.1
1	C	465	VAL	2.1
1	E	105	PHE	2.1
1	D	123	GLU	2.1
1	H	468	ASN	2.1
1	A	465	VAL	2.1
1	H	183	VAL	2.1
1	H	336	ASP	2.1
1	B	125	ALA	2.1
1	C	1	ALA	2.1
1	A	392	ALA	2.1
1	H	103	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

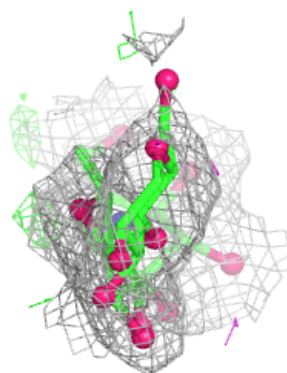
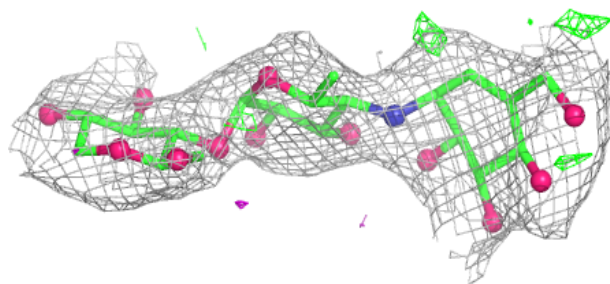
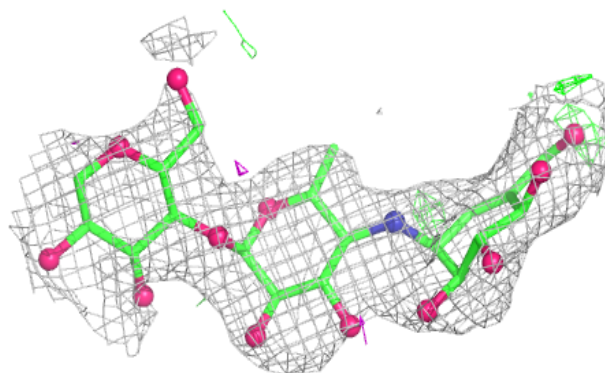
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	J	1	12/12	0.57	0.19	75,87,97,98	0
3	GLC	V	1	12/12	0.68	0.17	76,86,96,98	0
3	GLC	X	1	12/12	0.71	0.13	64,70,76,76	0
4	GLC	R	1	12/12	0.74	0.14	62,69,73,74	0
3	GLC	T	1	12/12	0.75	0.12	65,72,78,80	0
3	AC1	J	2	21/22	0.76	0.13	60,68,78,81	0
4	AC1	U	3	21/22	0.78	0.11	60,67,80,82	0
2	ASO	I	1	11/11	0.80	0.14	55,63,67,68	0
2	AC1	O	2	21/22	0.80	0.11	47,58,64,66	0
3	AC1	P	2	21/22	0.80	0.12	60,73,78,80	0
2	AC1	W	2	21/22	0.80	0.13	50,63,71,72	0
3	AC1	V	2	21/22	0.81	0.12	55,65,76,77	0
3	AC1	T	2	21/22	0.82	0.12	62,74,79,82	0
3	AC1	L	2	21/22	0.82	0.12	48,61,71,72	0
2	AC1	I	2	21/22	0.83	0.11	54,60,67,68	0
3	GLC	P	1	12/12	0.84	0.09	69,73,80,81	0
4	GLC	N	1	12/12	0.85	0.10	55,62,74,85	0
2	ASO	W	1	11/11	0.85	0.12	54,60,66,67	0
4	GLC	U	1	12/12	0.85	0.11	57,62,68,69	0
3	AC1	X	2	21/22	0.85	0.12	54,67,73,75	0
2	AC1	K	2	21/22	0.87	0.11	43,57,65,71	0
4	AC1	R	3	21/22	0.87	0.11	38,50,58,61	0
2	AC1	S	2	21/22	0.88	0.10	44,53,62,69	0
2	AC1	M	2	21/22	0.89	0.11	37,45,54,60	0
3	GLC	L	1	12/12	0.90	0.09	59,62,67,75	0
4	GLC	N	2	11/12	0.91	0.09	43,51,58,63	0
4	GLC	R	2	11/12	0.92	0.10	49,54,60,63	0
4	GLC	U	2	11/12	0.92	0.08	54,59,64,68	0
4	AC1	N	3	21/22	0.92	0.09	42,49,54,60	0
2	ASO	O	1	11/11	0.93	0.09	43,49,52,54	0
2	ASO	Q	1	11/11	0.93	0.09	32,37,42,51	0
2	AC1	Q	2	21/22	0.93	0.09	34,42,49,62	0
2	ASO	K	1	11/11	0.94	0.07	42,45,48,57	0
2	ASO	S	1	11/11	0.94	0.09	42,45,48,57	0
2	ASO	M	1	11/11	0.95	0.07	32,36,38,38	0

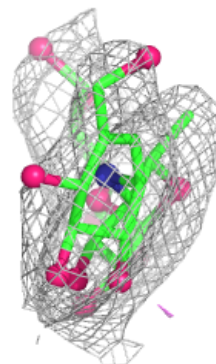
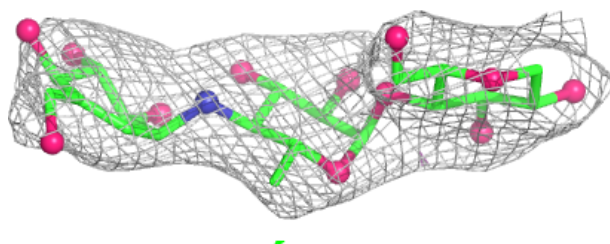
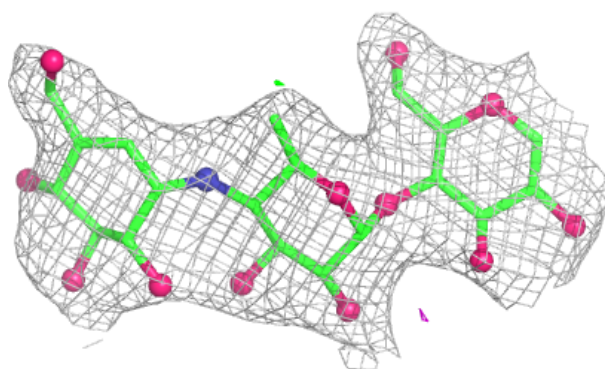
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

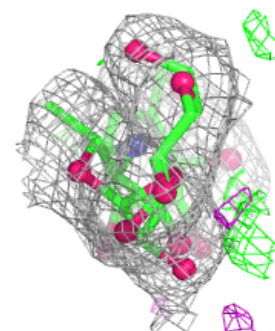
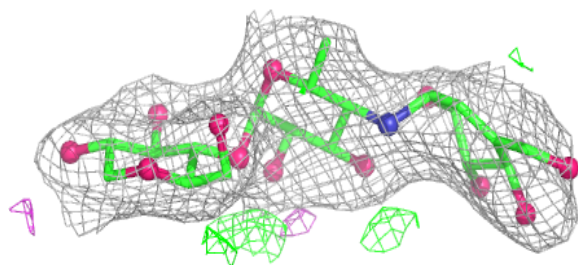
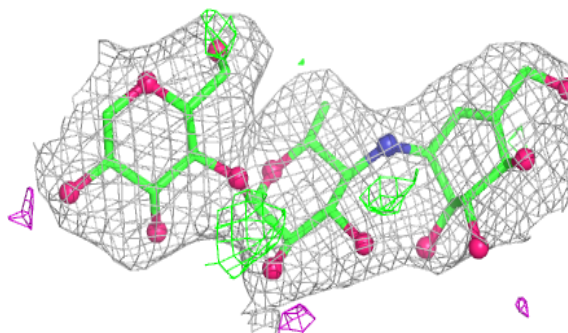
**Electron density around Chain K:**

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

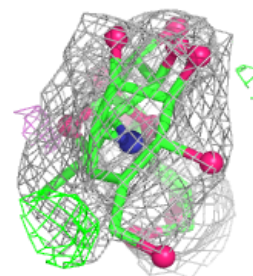
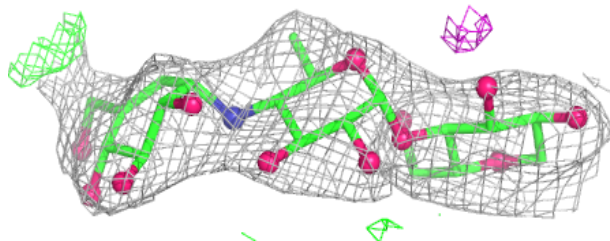
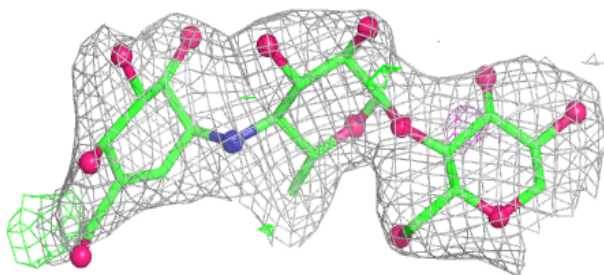


Electron density around Chain M:

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

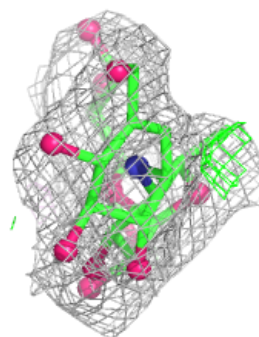
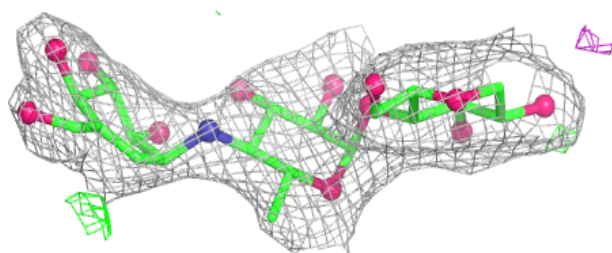
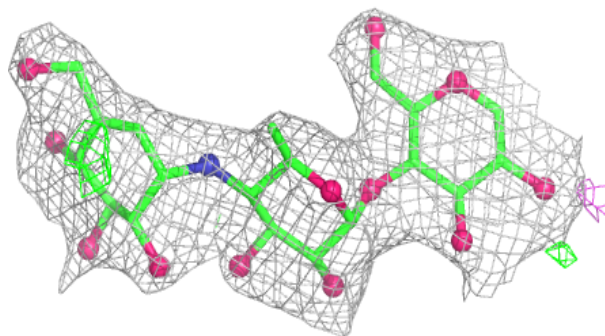
**Electron density around Chain O:**

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

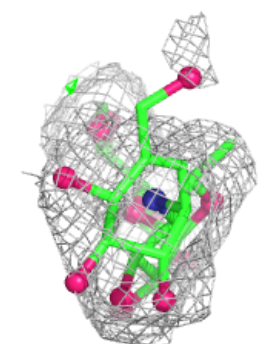
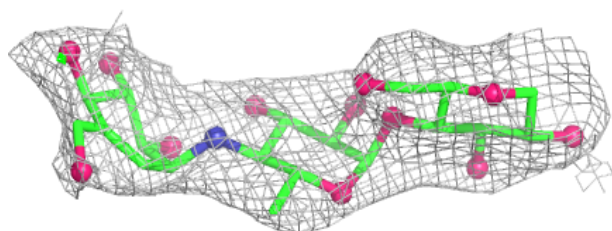
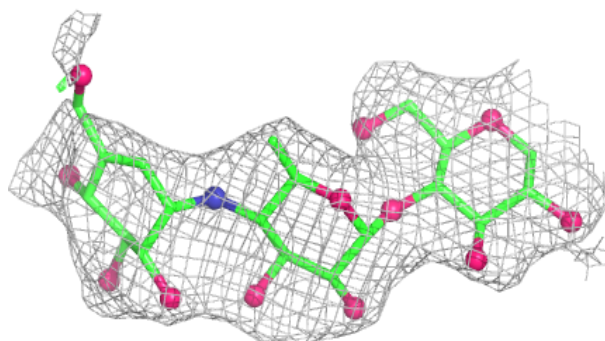


Electron density around Chain Q:

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

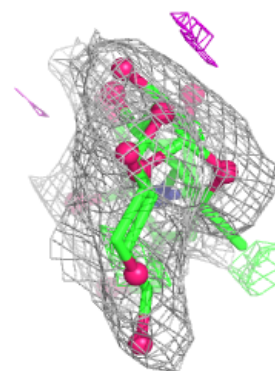
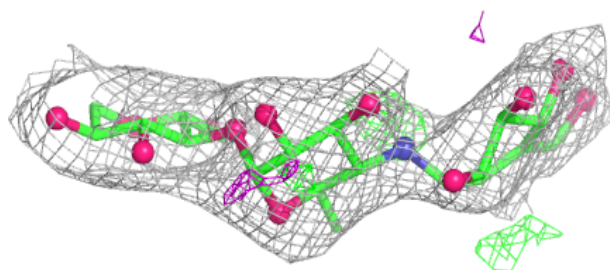
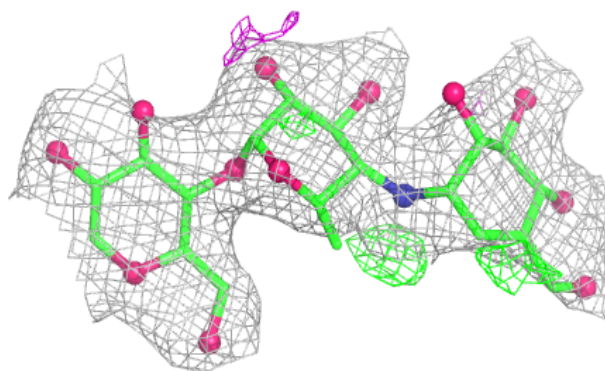
**Electron density around Chain S:**

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

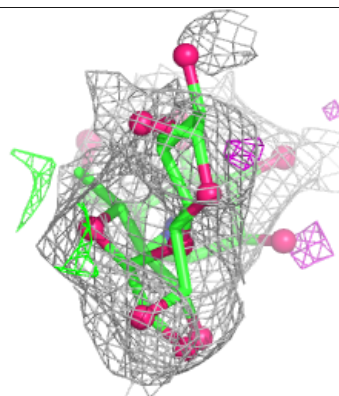
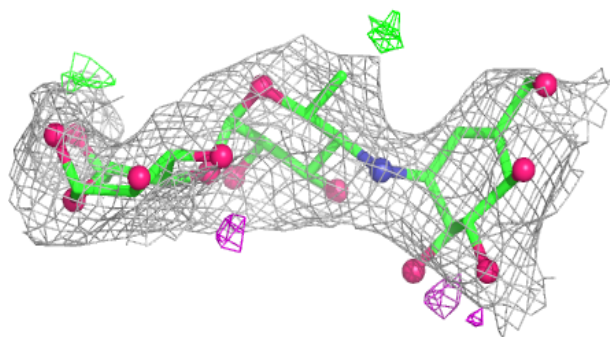
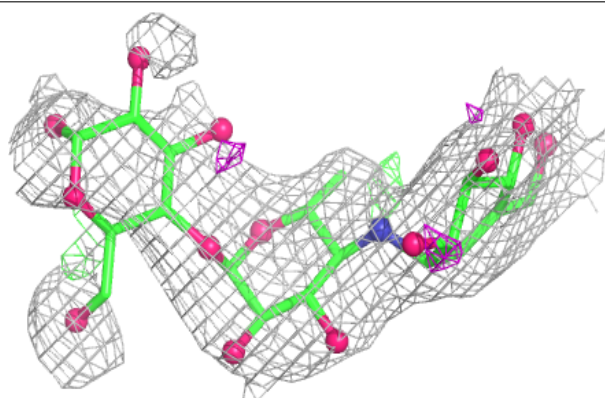


Electron density around Chain W:

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

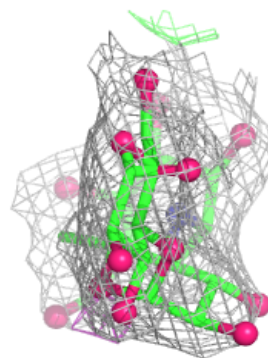
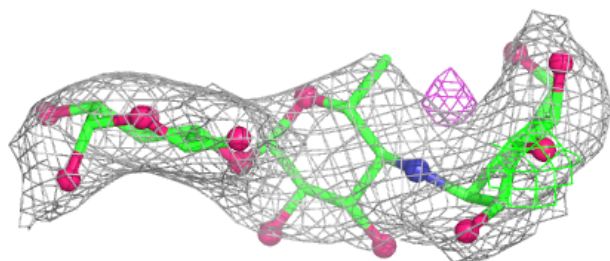
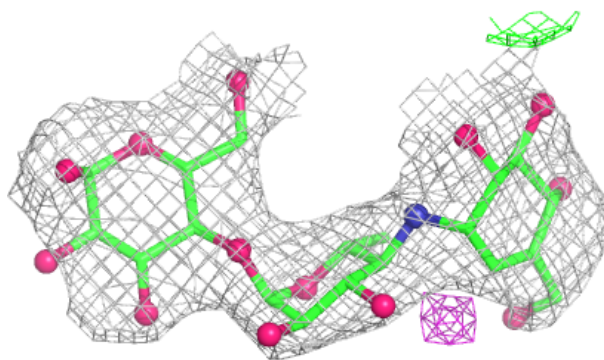
**Electron density around Chain J:**

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

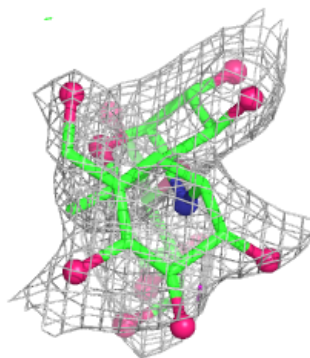
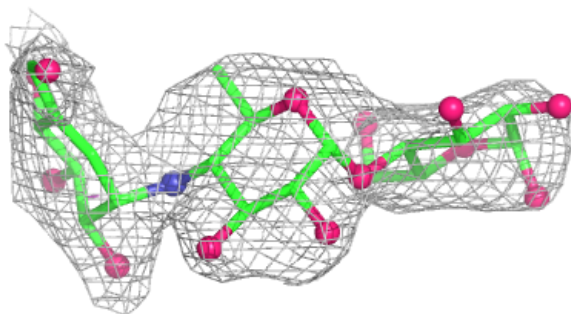
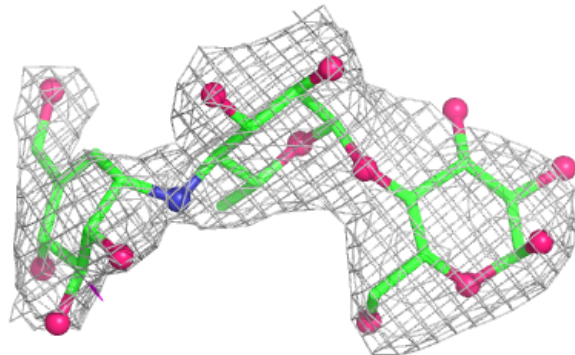


Electron density around Chain L:

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

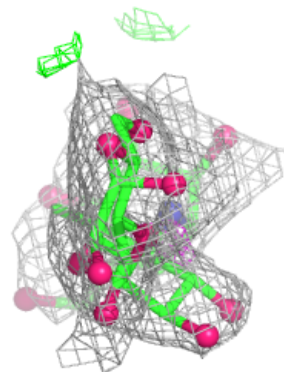
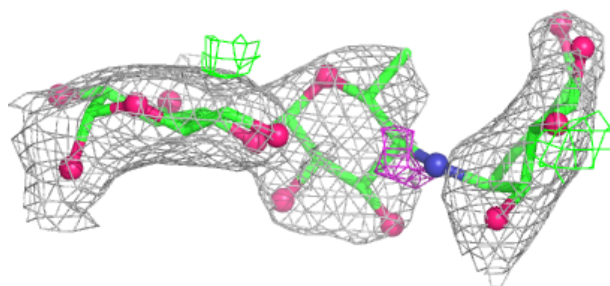
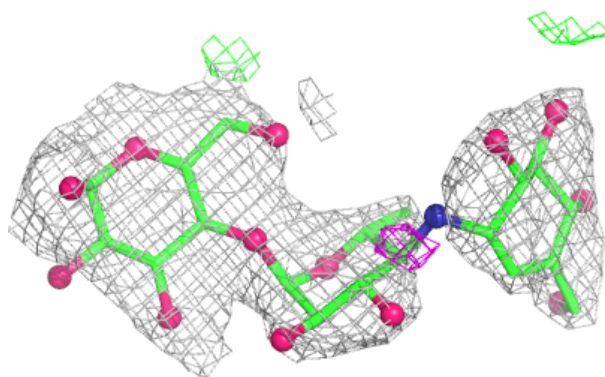
**Electron density around Chain P:**

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

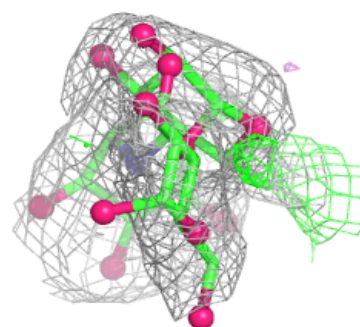
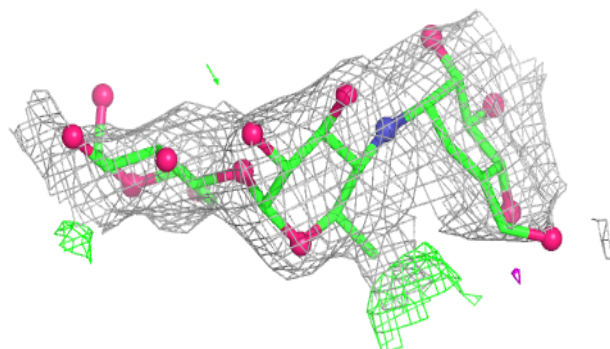
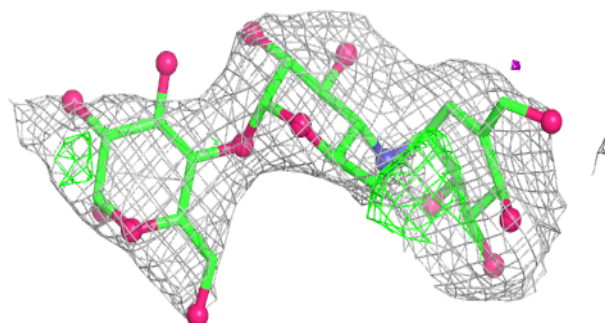


Electron density around Chain T:

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

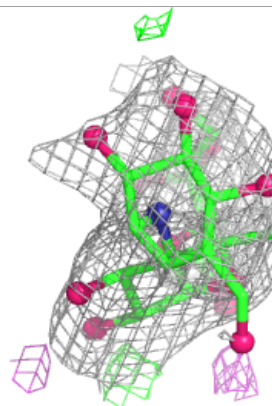
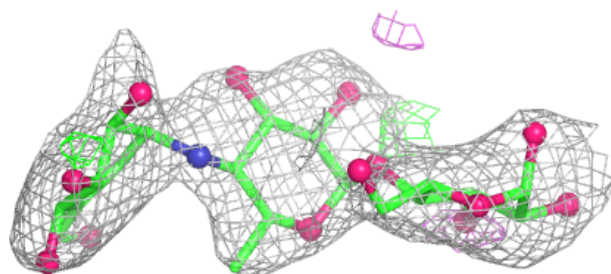
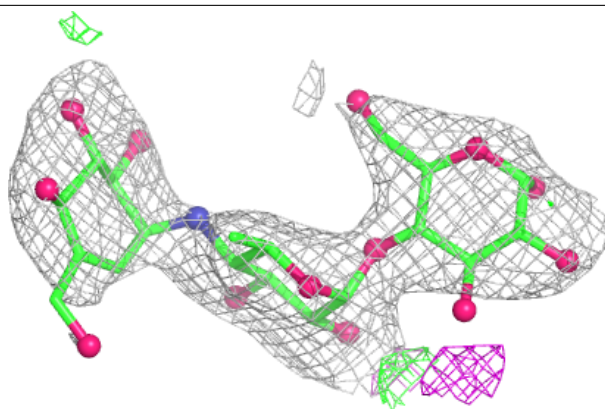
**Electron density around Chain V:**

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

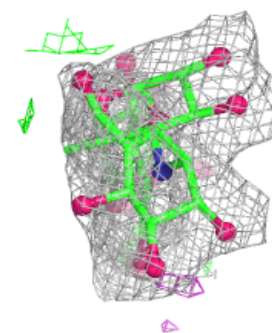
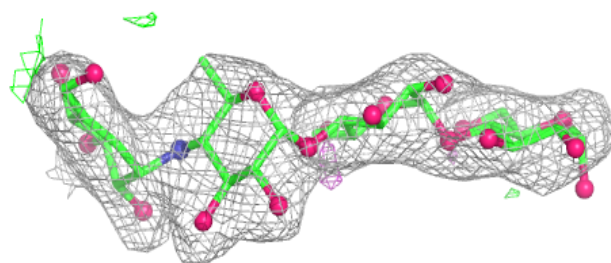
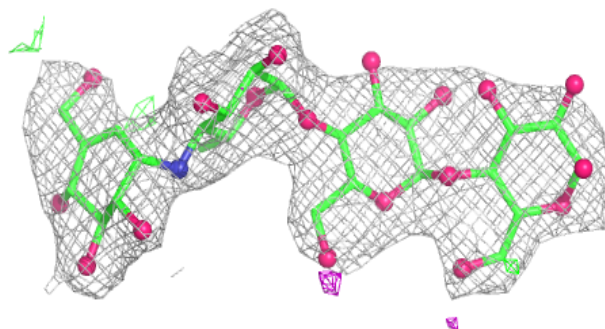


Electron density around Chain X:

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

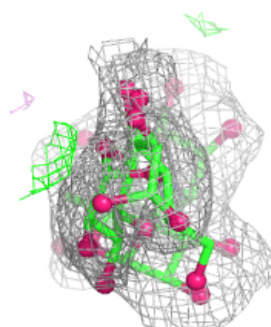
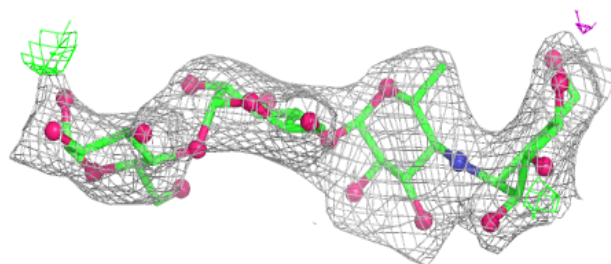
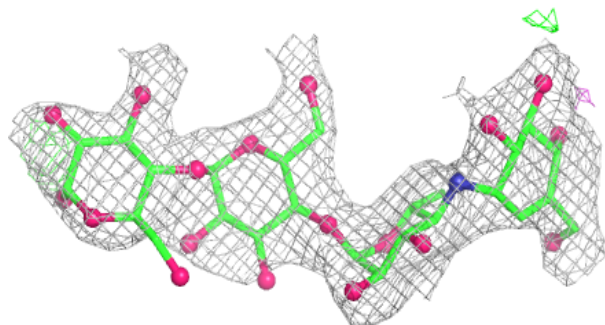
**Electron density around Chain N:**

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

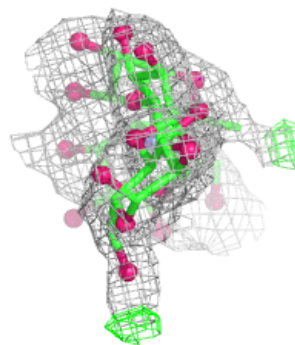
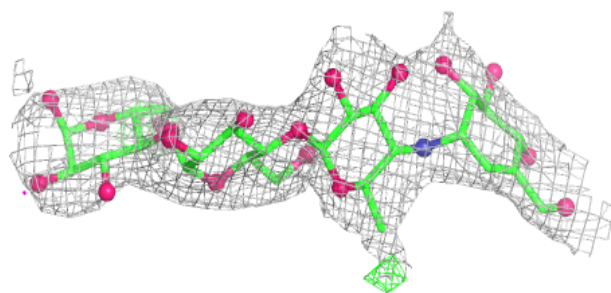
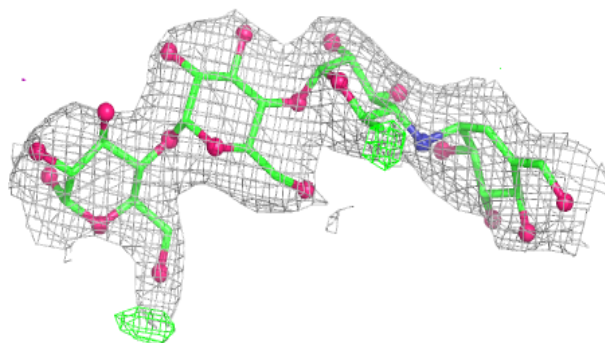


Electron density around Chain R:

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

**Electron density around Chain U:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.