Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 08:42 PM JST

PDB ID	:	6M6T
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 (i) 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 (i)) were used in the production of this report:

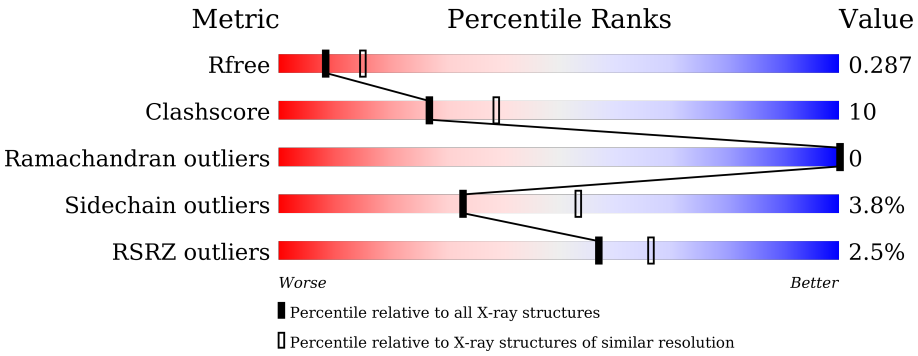
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	507	2% 67% 30%
1	B	507	3% 67% 31%
1	C	507	% 77% 21%
1	D	507	2% 74% 23%
1	E	507	% 76% 21%
1	F	507	2% 74% 23%

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Mol	Chain	Length	Quality of chain
1	G	507	2% 75% 22%
1	H	507	6% 69% 27%
2	I	2	50% 50%
2	K	2	100%
2	M	2	100%
2	O	2	100%
2	Q	2	50% 50%
2	S	2	100%
2	W	2	100%
3	J	2	50% 50%
3	L	2	100%
3	P	2	50% 50%
3	T	2	100%
3	V	2	50% 50%
3	X	2	50% 50%
4	N	3	67% 33%
4	R	3	100%
4	U	3	33% 67%

2 Entry composition (i)

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 32 19 1 12	0	0	0

- 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-glucopyranose.

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

- 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-glucopyranose-(1-4)-alpha-D-glucopyranose.

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

- Molecule 5 is water.

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

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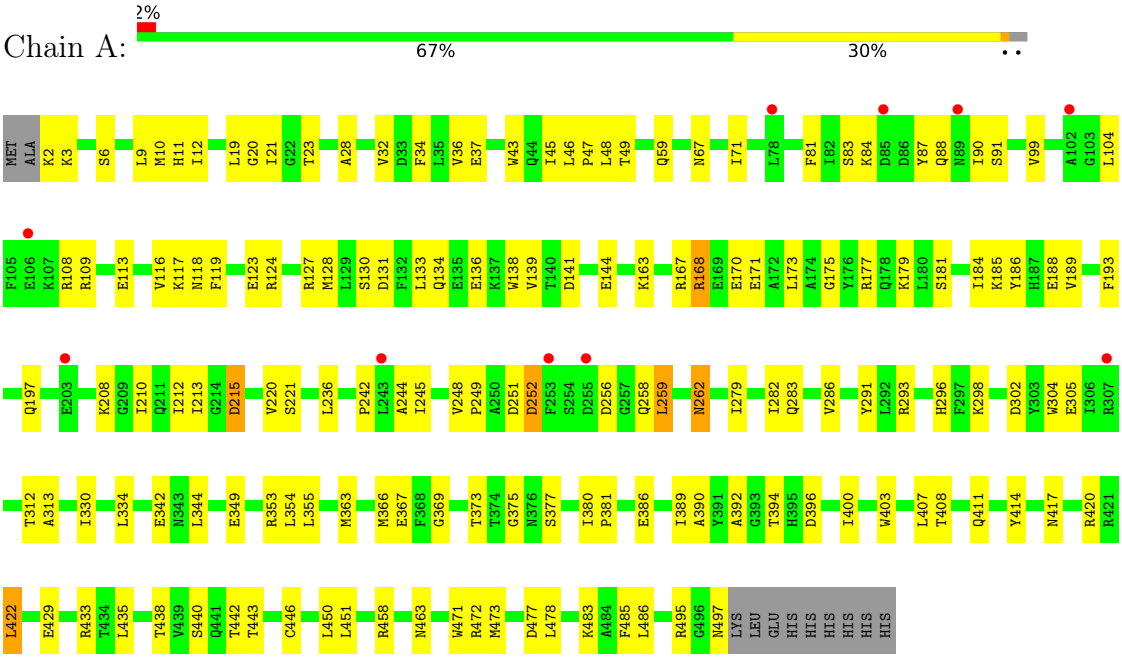
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	23	Total O 23 23	0	0
5	E	48	Total O 48 48	0	0
5	F	33	Total O 33 33	0	0
5	G	25	Total O 25 25	0	0
5	H	28	Total O 28 28	0	0

3 Residue-property plots (i)

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

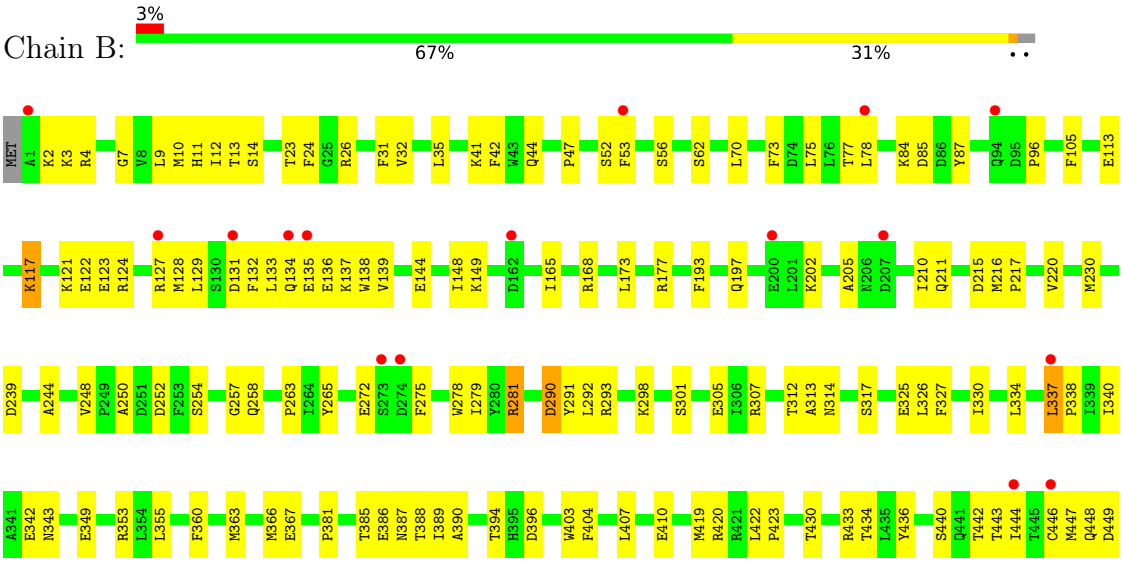
• Molecule 1: 4-alpha-glucanotransferase

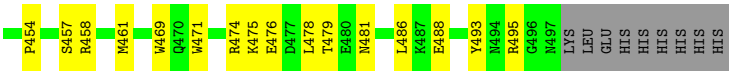
Chain A:



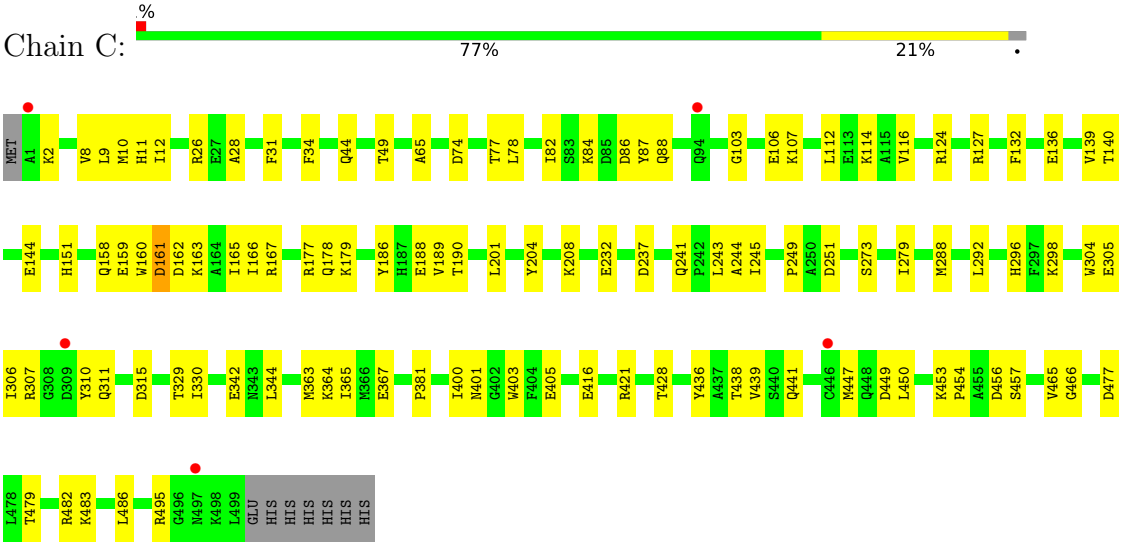
• Molecule 1: 4-alpha-glucanotransferase

Chain B:

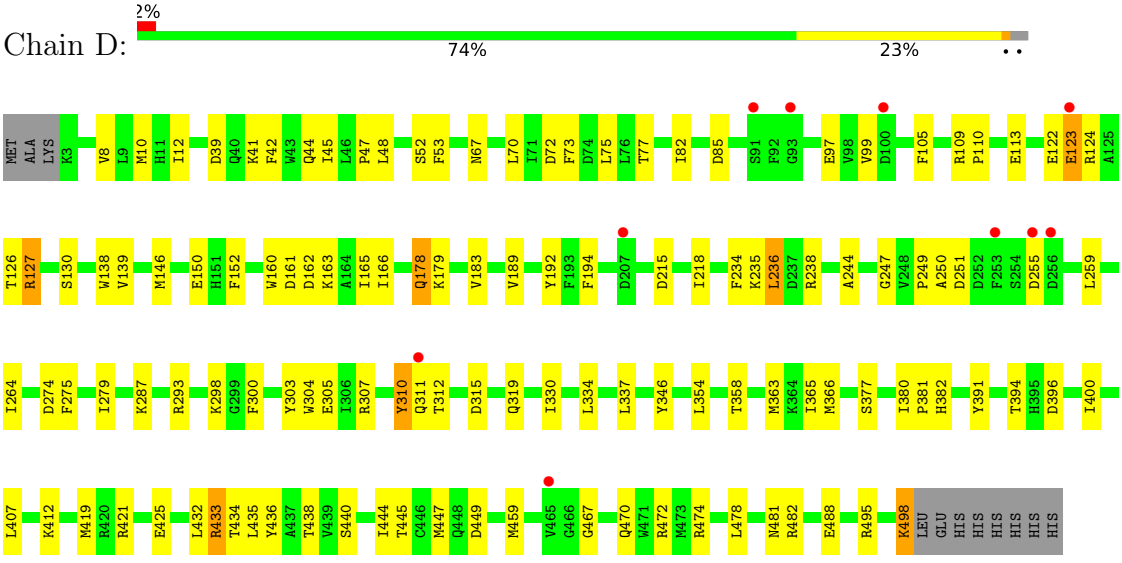




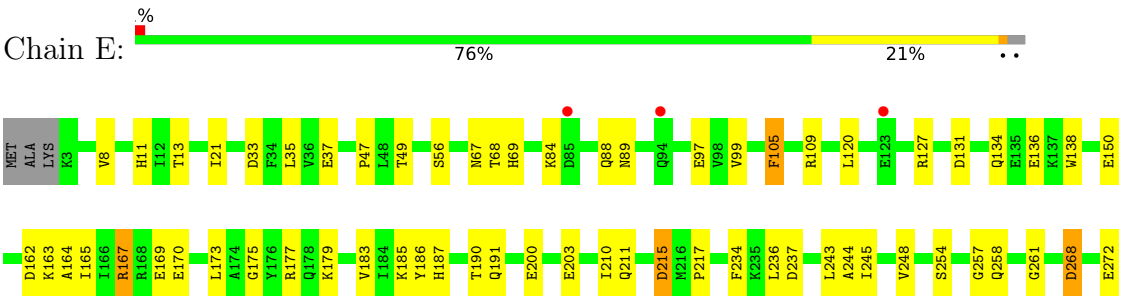
• Molecule 1: 4-alpha-glucanotransferase

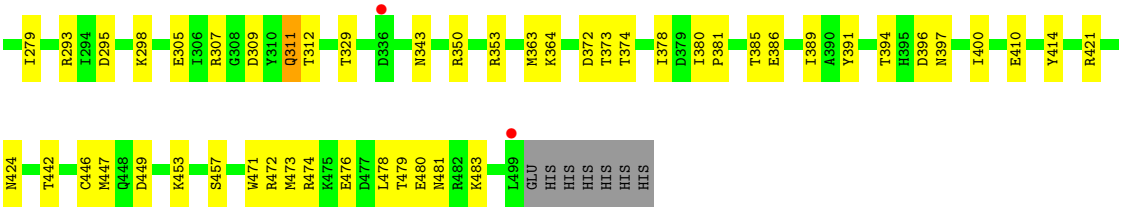


• Molecule 1: 4-alpha-glucanotransferase



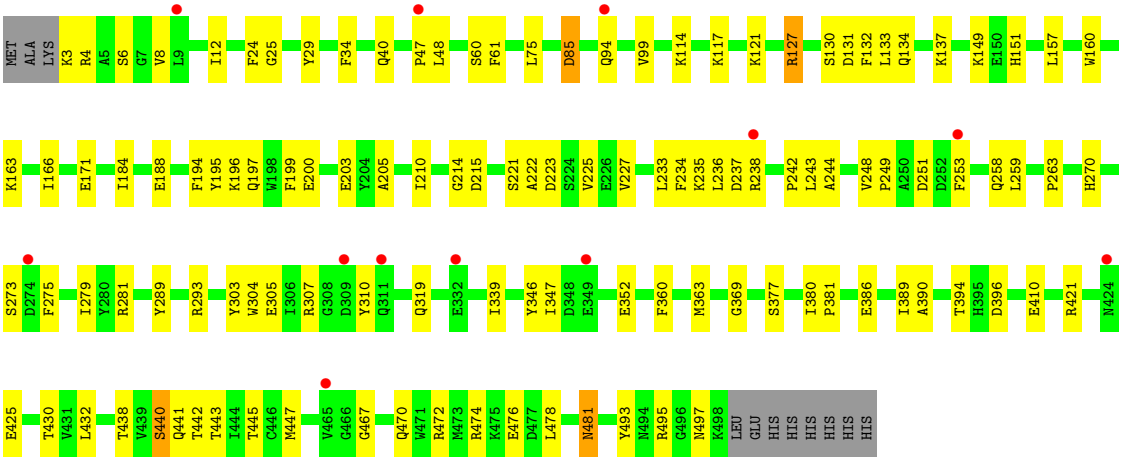
• Molecule 1: 4-alpha-glucanotransferase





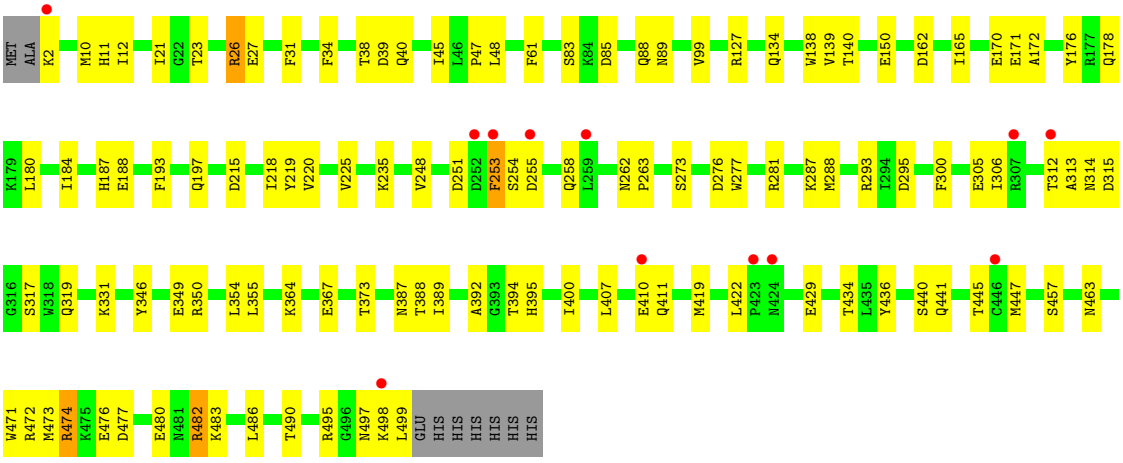
• Molecule 1: 4-alpha-glucanotransferase

Chain F:



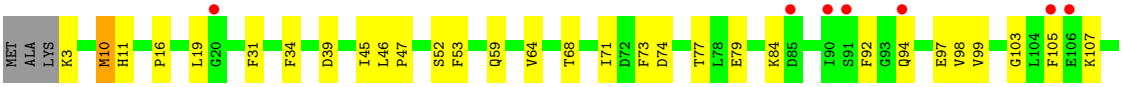
• Molecule 1: 4-alpha-glucanotransferase

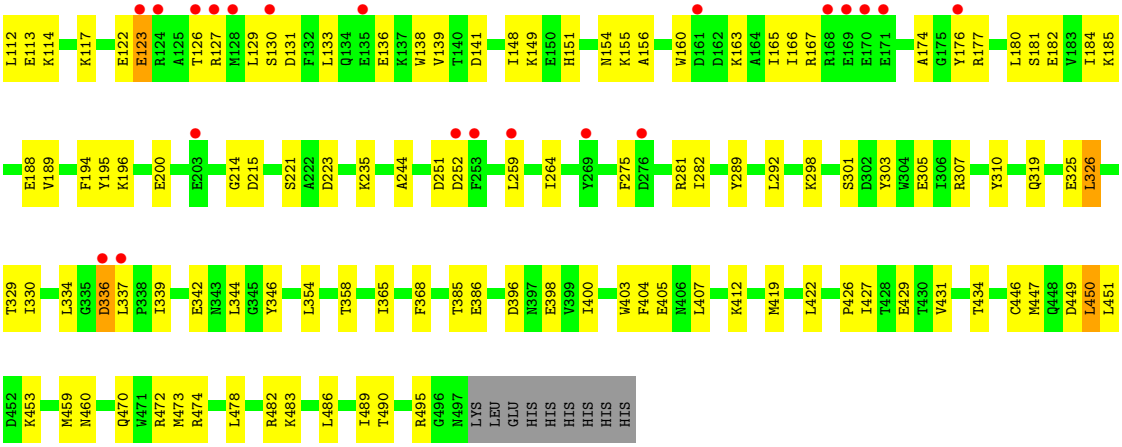
Chain G:



• Molecule 1: 4-alpha-glucanotransferase

Chain H:



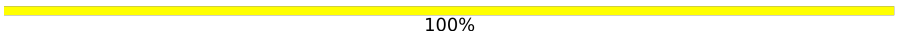


• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain I:

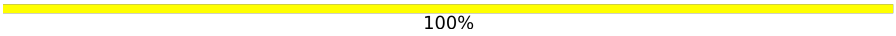
• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain K:



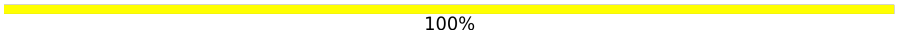
• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain M:



• 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:

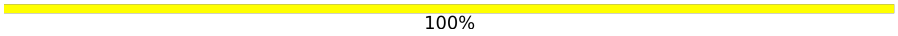


• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain Q:

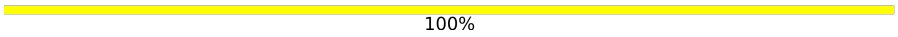
• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol

Chain S:



• 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:

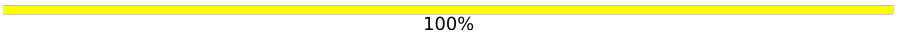


• Molecule 3: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:

• 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:

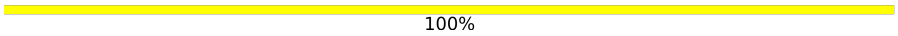


• Molecule 3: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:

• 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:



• 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

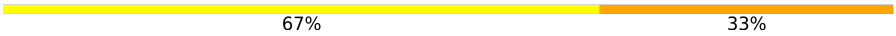
Chain V:

• 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 X:

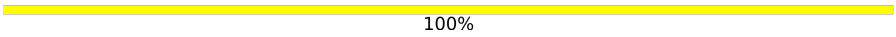
• Molecule 4: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:



• Molecule 4: 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-(1-4)-alpha-D-glucopyranose

Chain R:



• Molecule 4: 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-(1-4)-alpha-D-glucopyranose

Chain U:

4 Data and refinement statistics (i)

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) 98.6 (29.82-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.205 , 0.287 0.205 , 0.287	Depositor DCC
R_{free} test set	6483 reflections (5.00%)	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 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	0/4176	0.61	0/5661
1	B	0.51	0/4181	0.63	0/5668
1	C	0.53	0/4209	0.64	0/5704
1	D	0.50	0/4176	0.62	1/5661 (0.0%)
1	E	0.52	0/4184	0.63	0/5672
1	F	0.51	0/4176	0.61	0/5661
1	G	0.50	0/4193	0.62	0/5683
1	H	0.47	0/4167	0.61	0/5650
All	All	0.50	0/33462	0.62	1/45360 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	310	TYR	CB-CA-C	-5.00	100.39	110.40

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	108	0
1	B	4072	0	3894	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4100	0	3930	72	0
1	D	4067	0	3886	81	0
1	E	4075	0	3897	80	0
1	F	4067	0	3886	75	0
1	G	4084	0	3910	78	0
1	H	4058	0	3873	89	0
2	I	32	0	20	3	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	0	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	2	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	662	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 10.

All (662) 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:F:293:ARG:HD2	1:F:363:MET:HE3	1.46	0.94
1:D:234:PHE:HB2	1:D:236:LEU:HD11	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:HE1	1:A:435:LEU:HB2	1.50	0.90
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: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:H:336:ASP:O	1:H:337:LEU:HD22	1.84	0.78
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: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: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:F:425:GLU:CD	1:F:430:THR:HG22	2.13	0.69
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:D:8:VAL:HG11	1:D:447:MET:HE2	1.76	0.67
1:G:436:TYR:CE2	1:G:490:THR:HG22	2.29	0.67
1:C:160:TRP:HB2	1:C:166:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:97:GLU:CD	1:E:474:ARG:HH22	1.99	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:E:163:LYS:C	1:E:167:ARG:HH12	2.00	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:F:8:VAL:HG11	1:F:447:MET:HE1	1.79	0.64
1:G:31:PHE:HE1	1:G:447:MET:HE2	1.61	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: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:E:298:LYS:NZ	5:E:701:HOH:O	2.25	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: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: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:E:293:ARG:NH1	1:E:363:MET:HE1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:419:MET:HG2	1:B:434:THR:HG21	1.81	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: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: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: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:D:178:GLN:HG2	1:D:179:LYS:N	2.18	0.59
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: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:H:275:PHE:CD1	1:H:326:LEU:HD12	2.39	0.58
1:E:68:THR:HG21	1:E:190:THR:CG2	2.33	0.58
1:G:373:THR:HG21	1:G:410:GLU:CD	2.23	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:499:LEU:N	1:G:499:LEU:HD23	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:J:2:AC1:O6B	3:J:2:AC1:O4	2.19	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:D:363:MET:HE3	1:D:365:ILE:HD11	1.87	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
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: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:C:8:VAL:HG11	1:C:447:MET:HE2	1.89	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:E:8:VAL:HG11	1:E:447:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:G:31:PHE:CE1	1:G:447:MET:HE2	2.41	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: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: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:G:295:ASP:CG	4:U:1:GLC:H1	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:248:VAL:HG12	1:G:258:GLN:HB2	1.91	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:B:275:PHE:CD1	1:B:326:LEU:HD12	2.45	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: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: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:G:235:LYS:NZ	1:G:305:GLU:OE1	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASP:O	1:C:479:THR:HG23	2.11	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:G:287:LYS:NZ	5:G:702:HOH:O	2.38	0.51
1:A:163:LYS:HB3	1:A:167:ARG:NH2	2.26	0.51
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:B:293:ARG:HD3	1:B:363:MET:HE3	1.93	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:373:THR:HG22	1:A:414:TYR:CG	2.46	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:B:419:MET:HE3	1:B:430:THR:HG22	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:293:ARG:HH11	1:E:363:MET:HE1	1.76	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:232:GLU:CD	1:C:232:GLU:H	2.17	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: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:119:PHE:HE1	1:A:128:MET:HE2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:VAL:CG2	1:F:258:GLN:HB2	2.45	0.46
1:F:346:TYR:HB3	1:G:134:GLN:NE2	2.30	0.46
1:F:205:ALA:HB1	1:F:210:ILE:HB	1.96	0.46
1:B:10:MET:HE2	1:B:471:TRP:HZ3	1.80	0.46
1:B:254:SER:HB3	1:B:257:GLY:O	2.16	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: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: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: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:F:99:VAL:HG22	1:F:472:ARG:HD2	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:52:SER:OG	1:B:53:PHE:N	2.49	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: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:F:60:SER:O	1:F:221:SER:HB3	2.17	0.44
1:B:23:THR:HB	1:B:70:LEU:O	2.18	0.44
1:D:366:MET:HE2	1:D:435:LEU:HB2	1.98	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:HE2	1:A:366:MET:HB2	1.72	0.43
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: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:E:293:ARG:HD2	1:E:363:MET:CE	2.48	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:F:410:GLU:CD	1:F:410:GLU:H	2.22	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: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:E:293:ARG:HD2	1:E:363:MET:HE1	2.00	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
1:H:292:LEU:O	1:H:339:ILE:HA	2.19	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: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:B:113:GLU:O	1:B:117:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:394:THR:OG1	1:G:395:HIS:N	2.52	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: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
1:H:404:PHE:O	1:H:407:LEU:HB2	2.20	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:E:109:ARG:HH12	1:E:150:GLU:CD	2.22	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: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: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:144:GLU:CD	1:C:177:ARG:HE	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:244:ALA:HB1	1:D:305:GLU:HG2	2.01	0.42
1:F:293:ARG:HH11	1:F:363:MET:CE	2.33	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: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:161:ASP:N	1:C:161:ASP:OD1	2.53	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:366:MET:HE1	1:B:381:PRO:HG3	2.03	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:C:8:VAL:HG11	1:C:447:MET:CE	2.50	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
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:F:171:GLU:CD	1:F:171:GLU:H	2.24	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:E:309:ASP:N	1:E:309:ASP:OD1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:MET:HE3	1:G:473:MET:SD	2.61	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: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:312:THR:HG22	1:A:313:ALA:N	2.35	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
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:230:MET:HB2	1:B:230:MET:HE3	1.84	0.40
1:B:340:ILE:HD13	1:B:389:ILE:HG13	2.04	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: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: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

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

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/440 (98%)	409 (95%)	21 (5%)	25	43
1	B	430/440 (98%)	410 (95%)	20 (5%)	26	45
1	C	433/440 (98%)	424 (98%)	9 (2%)	53	71
1	D	430/440 (98%)	410 (95%)	20 (5%)	26	45
1	E	431/440 (98%)	419 (97%)	12 (3%)	43	63
1	F	430/440 (98%)	417 (97%)	13 (3%)	41	61
1	G	432/440 (98%)	415 (96%)	17 (4%)	32	52
1	H	429/440 (98%)	408 (95%)	21 (5%)	25	43
All	All	3445/3520 (98%)	3312 (96%)	133 (4%)	33	52

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6	SER
1	A	10	MET
1	A	34	PHE
1	A	83	SER
1	A	91	SER
1	A	117	LYS
1	A	130	SER
1	A	131	ASP
1	A	141	ASP
1	A	168	ARG
1	A	185	LYS
1	A	215	ASP
1	A	252	ASP
1	A	256	ASP
1	A	259	LEU
1	A	262	ASN
1	A	354	LEU
1	A	422	LEU
1	A	477	ASP
1	A	497	ASN
1	B	14	SER
1	B	26	ARG
1	B	62	SER
1	B	85	ASP
1	B	105	PHE
1	B	117	LYS

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Mol	Chain	Res	Type
1	B	122	GLU
1	B	123	GLU
1	B	127	ARG
1	B	128	MET
1	B	149	LYS
1	B	239	ASP
1	B	281	ARG
1	B	290	ASP
1	B	298	LYS
1	B	301	SER
1	B	337	LEU
1	B	349	GLU
1	B	386	GLU
1	B	475	LYS
1	C	26[A]	ARG
1	C	26[B]	ARG
1	C	124	ARG
1	C	159	GLU
1	C	161	ASP
1	C	178	GLN
1	C	273	SER
1	C	288	MET
1	C	456	ASP
1	D	10	MET
1	D	85	ASP
1	D	122	GLU
1	D	123	GLU
1	D	126	THR
1	D	127	ARG
1	D	130	SER
1	D	178	GLN
1	D	236	LEU
1	D	255	ASP
1	D	274	ASP
1	D	287	LYS
1	D	298	LYS
1	D	311	GLN
1	D	312	THR
1	D	433	ARG
1	D	459	MET
1	D	478	LEU
1	D	481	ASN

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Mol	Chain	Res	Type
1	D	498	LYS
1	E	56	SER
1	E	89	ASN
1	E	105	PHE
1	E	131	ASP
1	E	167	ARG
1	E	215	ASP
1	E	268	ASP
1	E	307	ARG
1	E	311	GLN
1	E	312	THR
1	E	421	ARG
1	E	424	ASN
1	F	34	PHE
1	F	85	ASP
1	F	127	ARG
1	F	130	SER
1	F	163	LYS
1	F	237	ASP
1	F	238	ARG
1	F	253	PHE
1	F	273	SER
1	F	281	ARG
1	F	440	SER
1	F	481	ASN
1	F	497	ASN
1	G	2	LYS
1	G	10	MET
1	G	26	ARG
1	G	34	PHE
1	G	127	ARG
1	G	251	ASP
1	G	253	PHE
1	G	254	SER
1	G	273	SER
1	G	276	ASP
1	G	288	MET
1	G	293	ARG
1	G	349	GLU
1	G	350	ARG
1	G	354	LEU
1	G	474	ARG

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Mol	Chain	Res	Type
1	G	482	ARG
1	H	10	MET
1	H	39	ASP
1	H	74	ASP
1	H	84	LYS
1	H	94	GLN
1	H	105	PHE
1	H	114	LYS
1	H	122	GLU
1	H	123	GLU
1	H	126	THR
1	H	141	ASP
1	H	182	GLU
1	H	252	ASP
1	H	281	ARG
1	H	298	LYS
1	H	301	SER
1	H	326	LEU
1	H	336	ASP
1	H	398	GLU
1	H	450	LEU
1	H	459	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	283	GLN
1	B	88	GLN
1	C	11	HIS
1	C	44	GLN
1	C	89	ASN
1	C	258	GLN
1	C	311	GLN
1	C	481	ASN
1	E	40	GLN
1	E	69	HIS
1	E	424	ASN
1	E	481	ASN
1	F	94	GLN
1	F	296	HIS
1	G	270	HIS

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Mol	Chain	Res	Type
1	G	311	GLN
1	G	319	GLN
1	H	118	ASN
1	H	206	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.94	0	15,15,15	1.23	2 (13%)
2	AC1	I	2	2	21,22,23	3.47	5 (23%)	22,32,34	1.20	2 (9%)
3	GLC	J	1	3	12,12,12	1.44	3 (25%)	17,17,17	1.87	5 (29%)
3	AC1	J	2	3	21,22,23	3.66	6 (28%)	22,32,34	1.30	2 (9%)
2	ASO	K	1	2	11,11,11	0.79	1 (9%)	15,15,15	1.11	1 (6%)
2	AC1	K	2	2	21,22,23	3.47	5 (23%)	22,32,34	1.16	2 (9%)
3	GLC	L	1	3	12,12,12	1.03	0	17,17,17	1.26	2 (11%)
3	AC1	L	2	3	21,22,23	3.77	3 (14%)	22,32,34	1.08	2 (9%)
2	ASO	M	1	2	11,11,11	1.04	0	15,15,15	1.08	1 (6%)
2	AC1	M	2	2	21,22,23	3.31	4 (19%)	22,32,34	1.40	2 (9%)
4	GLC	N	1	4	12,12,12	1.36	1 (8%)	17,17,17	0.65	0
4	GLC	N	2	4	11,11,12	0.75	0	15,15,17	1.52	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	AC1	N	3	4	21,22,23	3.53	3 (14%)	22,32,34	1.28	4 (18%)
2	ASO	O	1	2	11,11,11	0.80	0	15,15,15	1.31	2 (13%)
2	AC1	O	2	2	21,22,23	3.23	4 (19%)	22,32,34	0.88	1 (4%)
3	GLC	P	1	3	12,12,12	1.19	1 (8%)	17,17,17	0.63	0
3	AC1	P	2	3	21,22,23	3.45	3 (14%)	22,32,34	0.95	0
2	ASO	Q	1	2	11,11,11	0.91	0	15,15,15	1.04	0
2	AC1	Q	2	2	21,22,23	3.43	4 (19%)	22,32,34	1.32	3 (13%)
4	GLC	R	1	4	12,12,12	1.49	2 (16%)	17,17,17	1.41	3 (17%)
4	GLC	R	2	4	11,11,12	1.16	0	15,15,17	1.31	3 (20%)
4	AC1	R	3	4	21,22,23	3.34	4 (19%)	22,32,34	1.16	2 (9%)
2	ASO	S	1	2	11,11,11	0.94	1 (9%)	15,15,15	1.18	1 (6%)
2	AC1	S	2	2	21,22,23	3.66	3 (14%)	22,32,34	1.44	2 (9%)
3	GLC	T	1	3	12,12,12	1.64	2 (16%)	17,17,17	0.95	0
3	AC1	T	2	3	21,22,23	3.29	4 (19%)	22,32,34	1.10	2 (9%)
4	GLC	U	1	4	12,12,12	1.15	1 (8%)	17,17,17	1.19	2 (11%)
4	GLC	U	2	4	11,11,12	0.82	0	15,15,17	1.50	2 (13%)
4	AC1	U	3	4	21,22,23	3.57	4 (19%)	22,32,34	1.56	3 (13%)
3	GLC	V	1	3	12,12,12	0.89	0	17,17,17	0.76	0
3	AC1	V	2	3	21,22,23	3.44	3 (14%)	22,32,34	1.46	3 (13%)
2	ASO	W	1	2	11,11,11	1.41	1 (9%)	15,15,15	1.06	1 (6%)
2	AC1	W	2	2	21,22,23	3.20	3 (14%)	22,32,34	1.19	1 (4%)
3	GLC	X	1	3	12,12,12	1.13	1 (8%)	17,17,17	1.03	1 (5%)
3	AC1	X	2	3	21,22,23	3.24	4 (19%)	22,32,34	1.02	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/6/43/46	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 (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	AC1	C4A-C5B	-14.14	1.39	1.51
2	S	2	AC1	C4A-C5B	-13.56	1.40	1.51
4	N	3	AC1	C4A-C5B	-12.97	1.40	1.51
4	U	3	AC1	C4A-C5B	-12.91	1.40	1.51
3	J	2	AC1	C4A-C5B	-12.63	1.40	1.51
3	P	2	AC1	C4A-C5B	-12.19	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	2	AC1	C4A-C5B	-12.04	1.41	1.51
2	I	2	AC1	C4A-C5B	-12.03	1.41	1.51
2	K	2	AC1	C4A-C5B	-11.89	1.41	1.51
3	V	2	AC1	C4A-C5B	-11.72	1.41	1.51
3	T	2	AC1	C4A-C5B	-11.52	1.41	1.51
2	Q	2	AC1	C4A-C5B	-11.28	1.42	1.51
4	R	3	AC1	C4A-C5B	-11.18	1.42	1.51
2	O	2	AC1	C4A-C5B	-10.96	1.42	1.51
3	X	2	AC1	C4A-C5B	-10.95	1.42	1.51
2	W	2	AC1	C4A-C5B	-10.75	1.42	1.51
3	V	2	AC1	C1B-C7B	-8.83	1.37	1.50
2	Q	2	AC1	C1B-C7B	-8.33	1.38	1.50
3	J	2	AC1	C1B-C7B	-7.73	1.39	1.50
2	K	2	AC1	C1B-C7B	-7.46	1.39	1.50
3	L	2	AC1	C1B-C7B	-7.38	1.39	1.50
4	N	3	AC1	C1B-C7B	-7.33	1.39	1.50
2	I	2	AC1	C7B-C5B	7.25	1.42	1.32
2	W	2	AC1	C1B-C7B	-7.00	1.40	1.50
4	R	3	AC1	C1B-C7B	-6.99	1.40	1.50
2	O	2	AC1	C1B-C7B	-6.91	1.40	1.50
3	P	2	AC1	C1B-C7B	-6.88	1.40	1.50
2	S	2	AC1	C1B-C7B	-6.85	1.40	1.50
3	X	2	AC1	C1B-C7B	-6.69	1.40	1.50
2	M	2	AC1	C1B-C7B	-6.59	1.41	1.50
4	U	3	AC1	C1B-C7B	-6.55	1.41	1.50
3	T	2	AC1	C1B-C7B	-6.29	1.41	1.50
3	T	2	AC1	C7B-C5B	5.77	1.40	1.32
4	U	3	AC1	C7B-C5B	5.74	1.40	1.32
2	W	2	AC1	C7B-C5B	5.73	1.40	1.32
2	S	2	AC1	C7B-C5B	5.71	1.40	1.32
2	I	2	AC1	C1B-C7B	-5.67	1.42	1.50
3	X	2	AC1	C7B-C5B	5.62	1.40	1.32
4	R	3	AC1	C7B-C5B	5.55	1.40	1.32
2	O	2	AC1	C7B-C5B	5.51	1.40	1.32
3	P	2	AC1	C7B-C5B	5.49	1.40	1.32
2	K	2	AC1	C7B-C5B	5.38	1.40	1.32
2	Q	2	AC1	C7B-C5B	5.33	1.40	1.32
3	J	2	AC1	C7B-C5B	5.18	1.40	1.32
2	M	2	AC1	C7B-C5B	5.05	1.39	1.32
4	N	3	AC1	C7B-C5B	4.89	1.39	1.32
3	L	2	AC1	C7B-C5B	4.82	1.39	1.32
3	V	2	AC1	C7B-C5B	4.18	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	GLC	O4-C4	3.79	1.51	1.43
2	W	1	ASO	C2-C3	-3.75	1.47	1.52
4	R	3	AC1	O5-C1	3.58	1.49	1.43
3	J	2	AC1	O5-C1	3.24	1.48	1.43
3	J	2	AC1	C3B-C4A	-3.21	1.48	1.53
4	R	1	GLC	O4-C4	2.98	1.50	1.43
3	X	2	AC1	C2-C3	2.69	1.56	1.52
3	X	1	GLC	O4-C4	2.48	1.48	1.43
4	N	1	GLC	O4-C4	2.45	1.48	1.43
4	U	3	AC1	O5-C1	2.39	1.47	1.43
4	R	1	GLC	O1-C1	2.39	1.47	1.39
2	K	2	AC1	C2B-C1B	2.32	1.56	1.52
4	U	1	GLC	C4-C3	2.27	1.58	1.52
2	K	2	AC1	C3B-C4A	-2.26	1.49	1.53
3	P	1	GLC	O4-C4	2.22	1.48	1.43
3	T	2	AC1	C3B-C4A	2.19	1.56	1.53
2	O	2	AC1	C6B-C5B	2.18	1.55	1.50
2	Q	2	AC1	C2B-C1B	2.17	1.55	1.52
3	J	2	AC1	C2B-C1B	-2.16	1.50	1.52
2	K	1	ASO	C2-C3	-2.16	1.49	1.52
2	M	2	AC1	C2-C3	-2.16	1.49	1.52
3	T	1	GLC	O1-C1	2.15	1.46	1.39
3	J	1	GLC	O5-C5	2.15	1.49	1.44
3	J	1	GLC	C1-C2	2.14	1.57	1.52
3	J	1	GLC	O4-C4	2.13	1.48	1.43
2	S	1	ASO	C2-C3	2.11	1.55	1.52
2	I	2	AC1	O4-C4A	2.03	1.46	1.42
2	I	2	AC1	C6B-C5B	2.02	1.55	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	3	AC1	C2-C3-C4	-5.05	106.17	110.63
3	J	1	GLC	C4-C3-C2	-4.56	102.86	110.82
3	V	2	AC1	C7B-C1B-N4A	-4.56	103.84	110.68
2	M	2	AC1	C2B-C3B-C4A	-4.47	103.08	110.18
4	N	2	GLC	C2-C3-C4	-3.98	104.01	110.89
4	U	3	AC1	C1-C2-C3	-3.95	104.81	109.67
2	S	2	AC1	C7B-C1B-N4A	-3.75	105.05	110.68
4	U	2	GLC	C2-C3-C4	-3.66	104.56	110.89
3	L	1	GLC	O5-C5-C6	3.38	114.83	106.44
2	W	2	AC1	C2B-C3B-C4A	-3.32	104.90	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	2	AC1	C2B-C3B-C4A	-3.30	104.93	110.18
4	U	2	GLC	O5-C5-C6	-3.24	102.12	107.20
2	Q	2	AC1	C7B-C1B-N4A	-3.21	105.86	110.68
4	R	3	AC1	C1-C2-C3	-3.20	105.73	109.67
3	V	2	AC1	C2B-C3B-C4A	-3.19	105.12	110.18
3	J	1	GLC	O4-C4-C5	3.13	117.06	109.30
4	R	2	GLC	O5-C5-C6	2.95	111.84	107.20
2	W	1	ASO	O3-C3-C2	-2.90	104.44	109.99
2	Q	2	AC1	C2B-C3B-C4A	-2.90	105.58	110.18
3	T	2	AC1	C2B-C3B-C4A	-2.87	105.62	110.18
3	L	2	AC1	C7B-C1B-N4A	-2.86	106.39	110.68
2	K	2	AC1	C7B-C1B-N4A	-2.85	106.40	110.68
3	L	1	GLC	C6-C5-C4	-2.78	106.49	113.00
3	J	1	GLC	O5-C5-C6	2.76	113.29	106.44
4	N	3	AC1	C2-C3-C4	-2.72	108.23	110.63
4	R	3	AC1	C2-C3-C4	-2.71	108.24	110.63
3	X	2	AC1	C2B-C3B-C4A	-2.70	105.89	110.18
3	J	1	GLC	O4-C4-C3	2.69	116.57	110.35
4	R	2	GLC	O5-C1-C2	-2.65	106.68	110.77
2	I	1	ASO	C1-O5-C5	2.60	115.71	112.19
4	R	1	GLC	C4-C3-C2	-2.58	106.32	110.82
3	J	2	AC1	O6B-C6B-C5B	-2.50	106.52	112.50
4	N	3	AC1	C2B-C3B-C4A	-2.42	106.33	110.18
3	V	2	AC1	C1-C2-C3	-2.42	106.69	109.67
2	I	2	AC1	O3-C3-C2	-2.41	105.38	109.99
2	M	1	ASO	C6-C5-C4	-2.39	107.41	113.00
2	K	2	AC1	C2B-C3B-C4A	-2.37	106.41	110.18
4	N	2	GLC	C3-C4-C5	-2.34	106.06	110.24
3	J	1	GLC	C3-C4-C5	-2.34	106.07	110.24
2	O	1	ASO	C6-C5-C4	-2.32	107.56	113.00
2	Q	2	AC1	O3-C3-C2	-2.32	105.55	109.99
3	J	2	AC1	O5-C5-C6	2.32	112.32	107.33
4	U	3	AC1	O3-C3-C4	2.30	114.30	109.66
4	U	1	GLC	O3-C3-C4	2.29	115.63	110.35
4	R	1	GLC	C6-C5-C4	-2.28	107.66	113.00
2	O	1	ASO	C3-C4-C5	-2.27	106.18	110.24
4	R	1	GLC	O1-C1-O5	2.26	117.16	110.38
3	T	2	AC1	O5-C1-C2	-2.24	107.31	110.77
3	L	2	AC1	O5-C1-C2	-2.24	107.32	110.77
2	I	2	AC1	C2B-C3B-C4A	-2.23	106.64	110.18
2	O	2	AC1	C2B-C3B-C4A	-2.23	106.64	110.18
2	K	1	ASO	O2-C2-C3	-2.20	105.73	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	1	ASO	O5-C5-C6	-2.20	103.75	107.20
3	X	1	GLC	C6-C5-C4	-2.13	108.02	113.00
4	U	1	GLC	C1-C2-C3	-2.12	105.91	110.31
4	N	3	AC1	O6B-C6B-C5B	-2.11	107.45	112.50
4	N	2	GLC	C6-C5-C4	-2.07	108.16	113.00
3	X	2	AC1	O5-C1-C2	-2.02	107.65	110.77
2	I	1	ASO	O5-C5-C6	-2.02	104.04	107.20
4	R	2	GLC	C1-O5-C5	2.02	114.92	112.19
2	M	2	AC1	O6B-C6B-C5B	-2.01	107.70	112.50
4	N	3	AC1	C1-C2-C3	-2.00	107.20	109.67

There are no chirality outliers.

All (65) 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-C1B-N4A-C4
3	L	2	AC1	C7B-C5B-C6B-O6B
3	P	2	AC1	C7B-C1B-N4A-C4
3	T	2	AC1	C7B-C1B-N4A-C4
3	V	2	AC1	C7B-C1B-N4A-C4
3	V	2	AC1	C4A-C5B-C6B-O6B
3	X	2	AC1	C7B-C1B-N4A-C4
4	N	3	AC1	C7B-C1B-N4A-C4
4	N	3	AC1	C7B-C5B-C6B-O6B
4	R	3	AC1	C7B-C1B-N4A-C4
4	R	3	AC1	C7B-C5B-C6B-O6B
4	U	3	AC1	C7B-C5B-C6B-O6B
4	R	1	GLC	O5-C5-C6-O6

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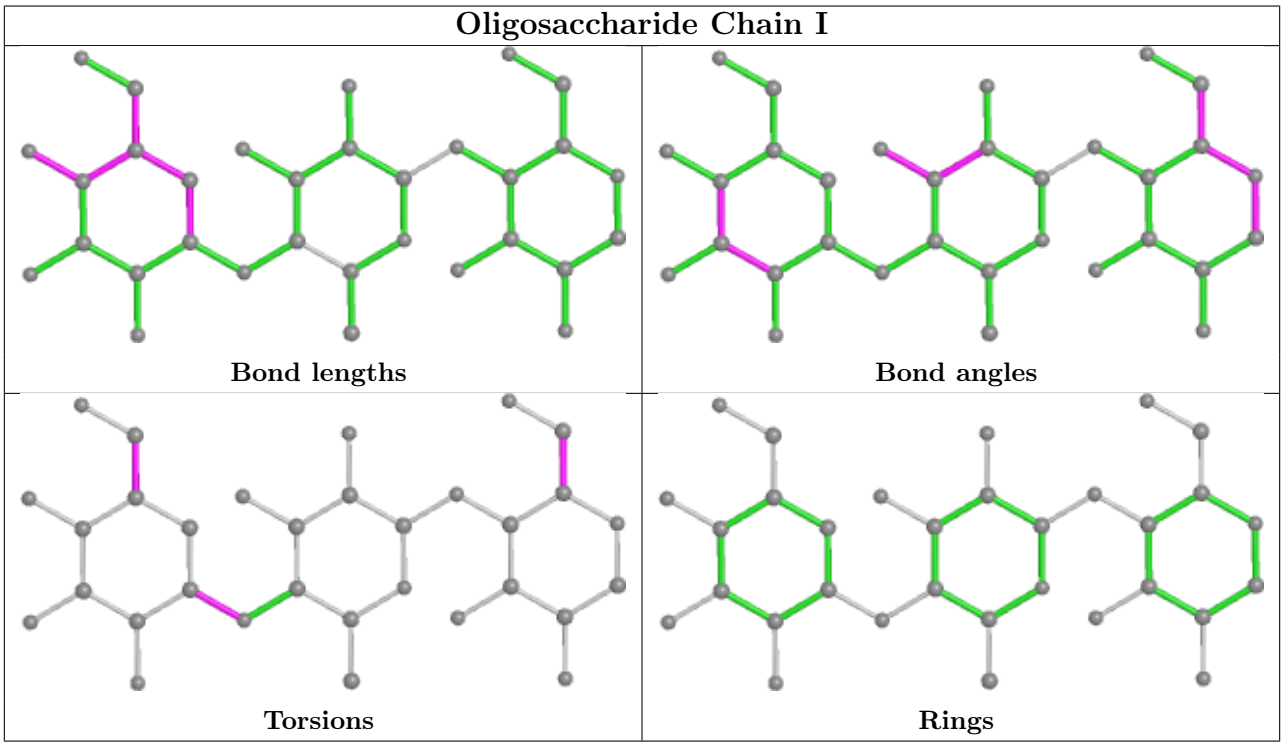
Mol	Chain	Res	Type	Atoms
4	U	1	GLC	O5-C5-C6-O6
3	X	1	GLC	C4-C5-C6-O6
4	R	1	GLC	C4-C5-C6-O6
3	X	1	GLC	O5-C5-C6-O6
3	J	1	GLC	C4-C5-C6-O6
4	U	1	GLC	C4-C5-C6-O6
2	I	1	ASO	O5-C5-C6-O6
4	R	2	GLC	O5-C5-C6-O6
2	I	1	ASO	C4-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
2	W	1	ASO	O5-C5-C6-O6
4	U	2	GLC	O5-C5-C6-O6
3	T	1	GLC	O5-C5-C6-O6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

There are no ring outliers.

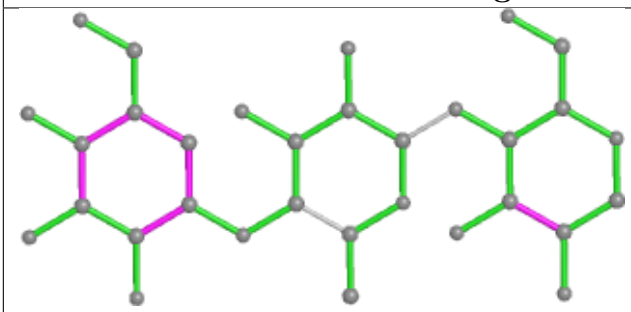
8 monomers are involved in 14 short contacts:

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

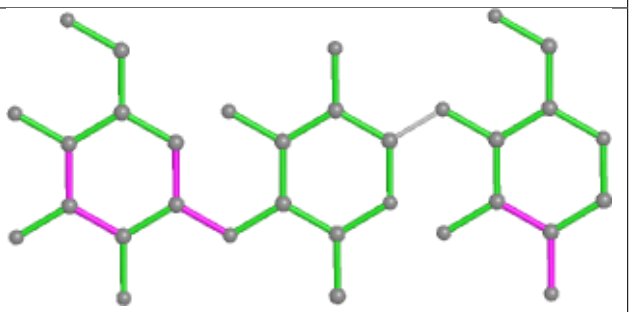
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



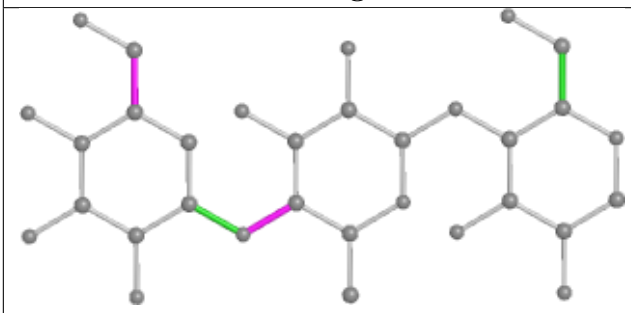
Oligosaccharide Chain K



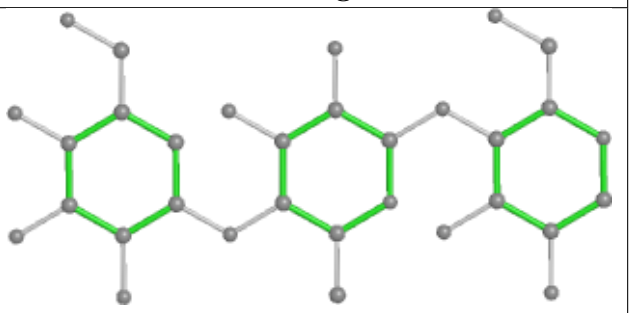
Bond lengths



Bond angles

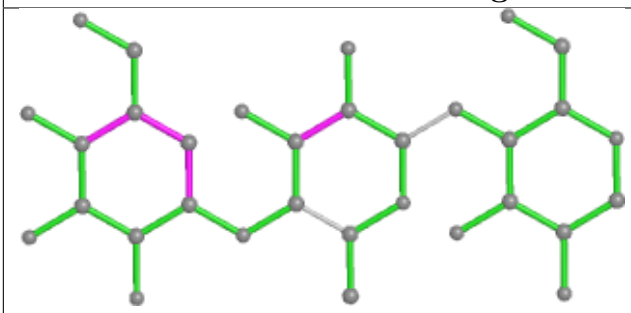


Torsions

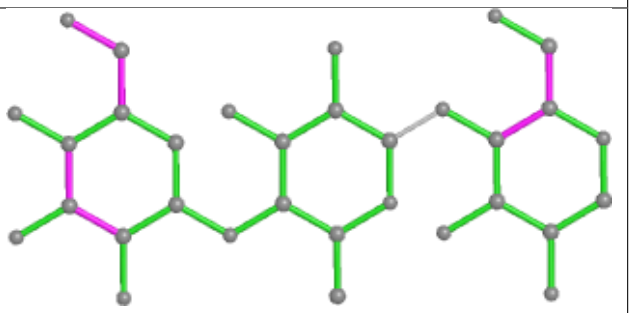


Rings

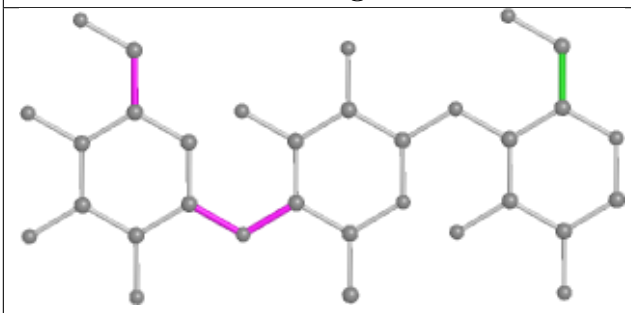
Oligosaccharide Chain M



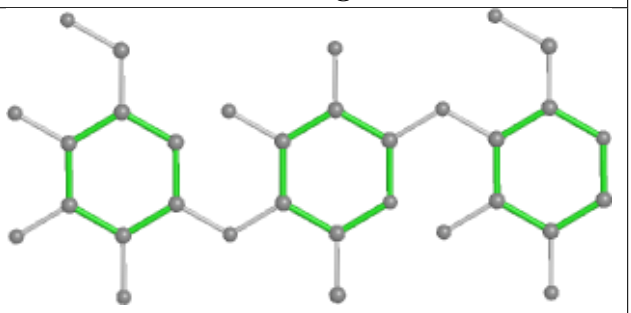
Bond lengths



Bond angles

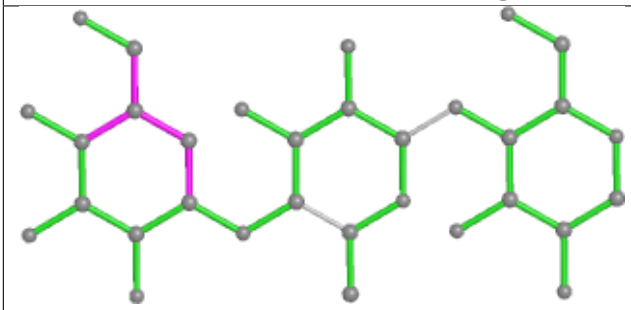


Torsions

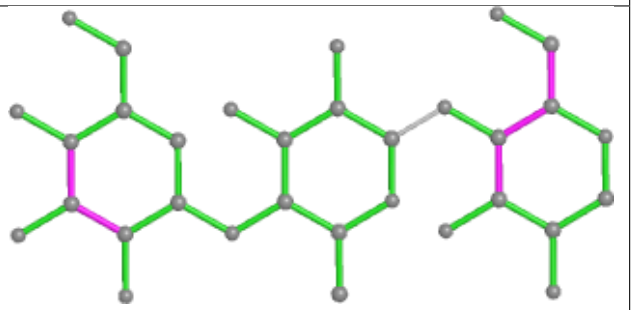


Rings

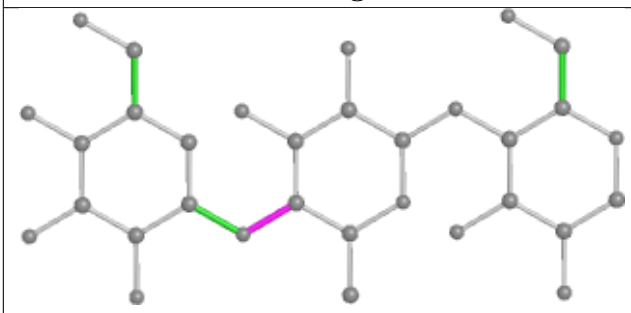
Oligosaccharide Chain O



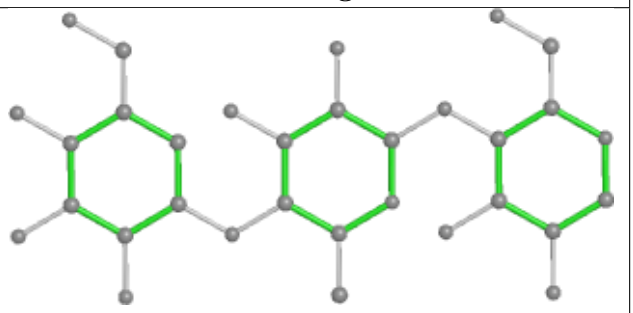
Bond lengths



Bond angles

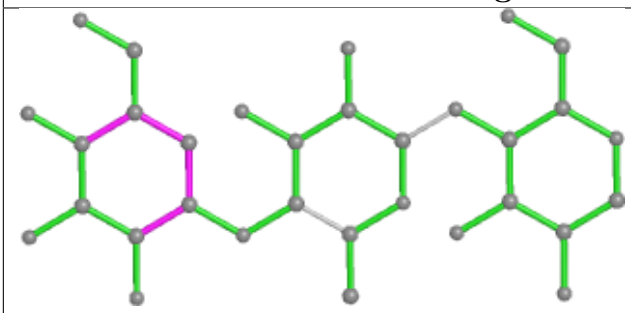


Torsions

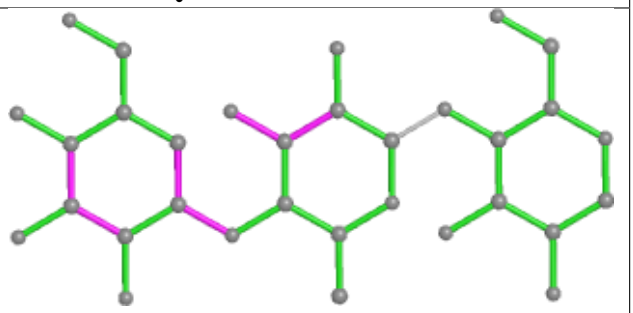


Rings

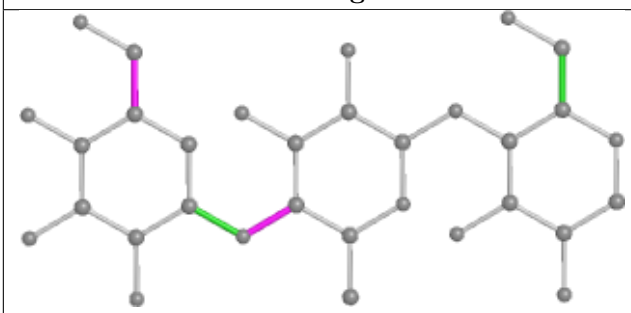
Oligosaccharide Chain Q



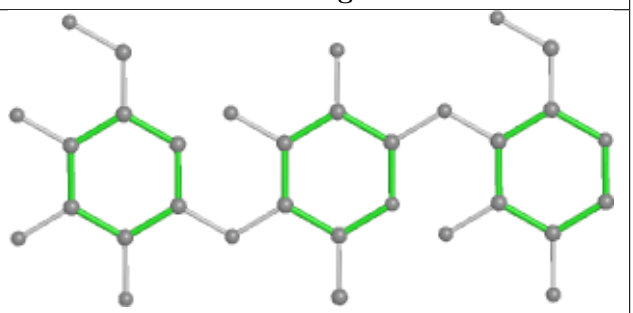
Bond lengths



Bond angles

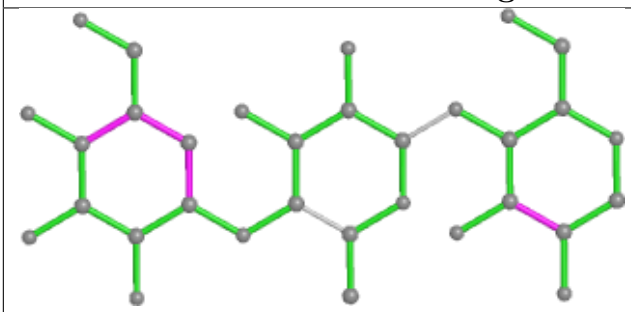


Torsions

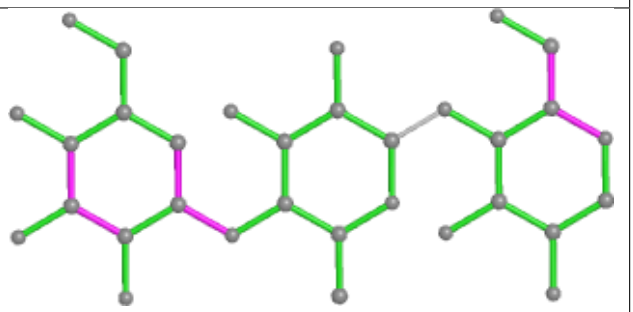


Rings

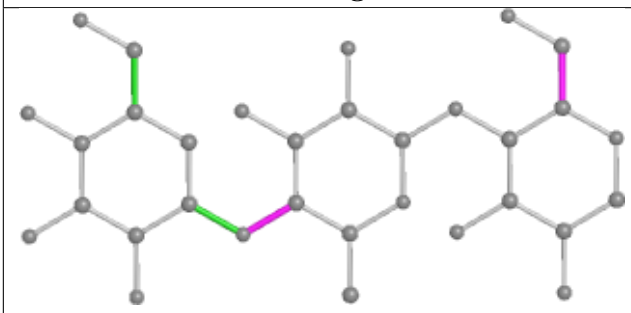
Oligosaccharide Chain S



Bond lengths



Bond angles



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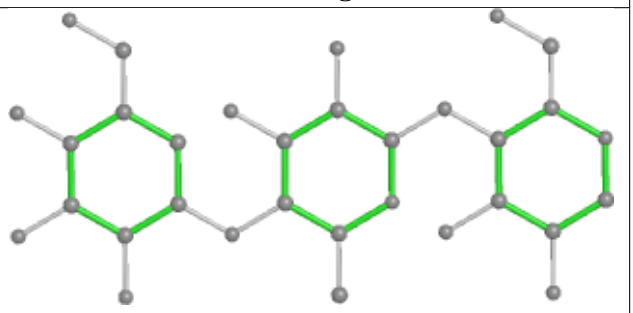
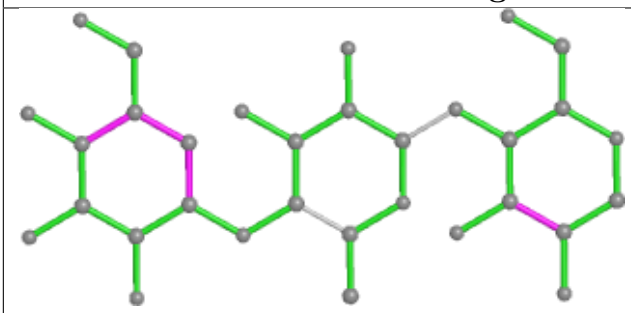
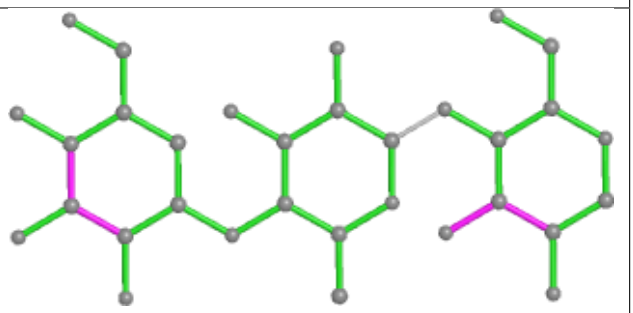


Rings

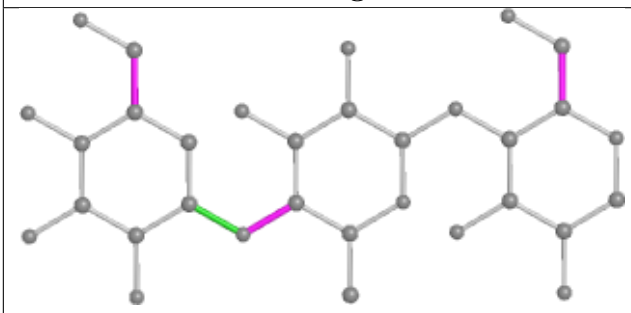
Oligosaccharide Chain W



Bond lengths



Bond angles



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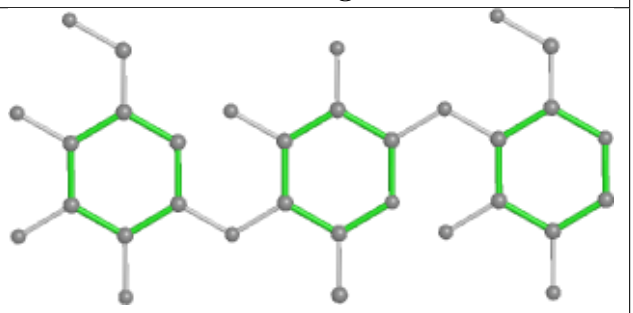
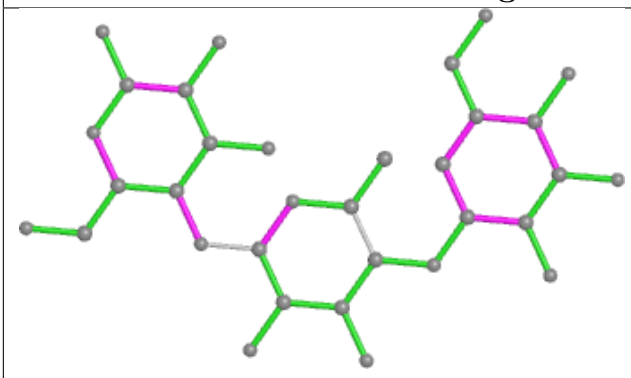
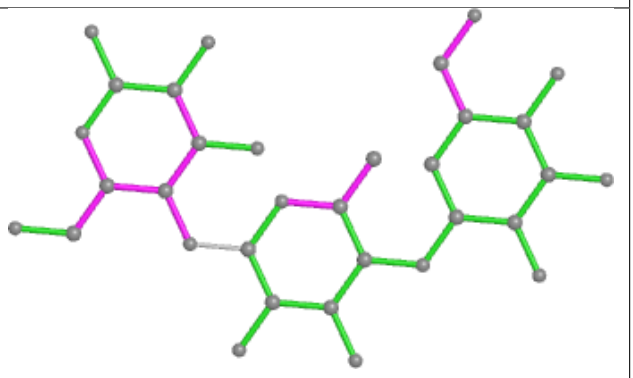


Rings

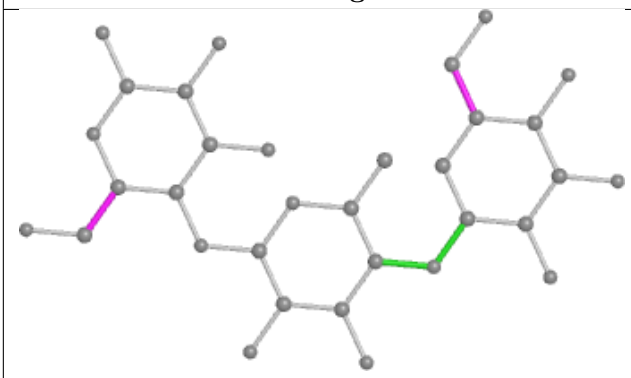
Oligosaccharide Chain J



Bond lengths



Bond angles



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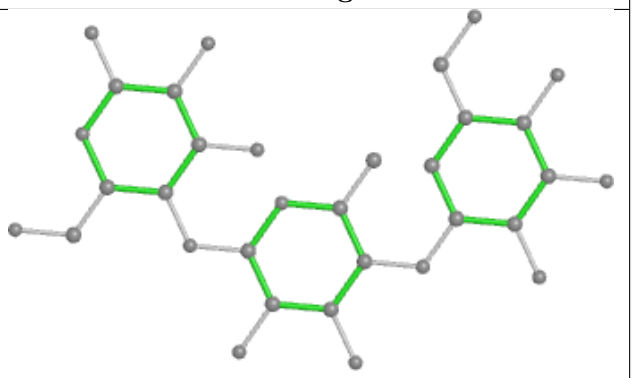
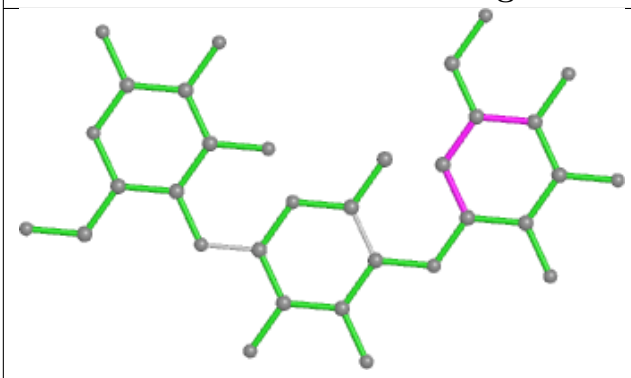
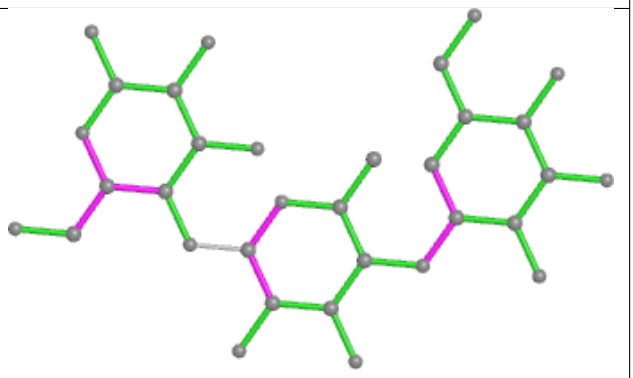


Rings

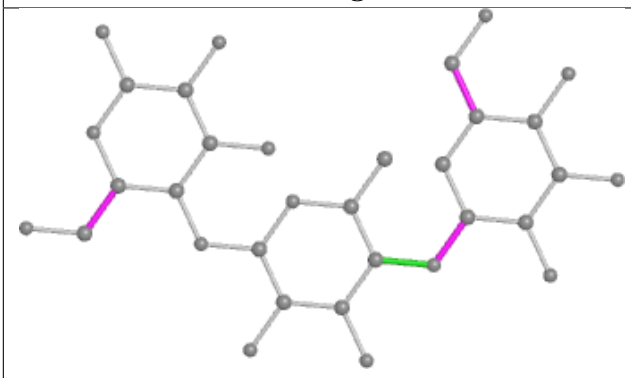
Oligosaccharide Chain L



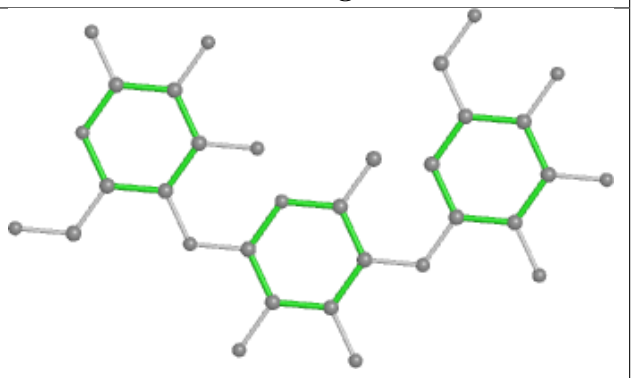
Bond lengths



Bond angles

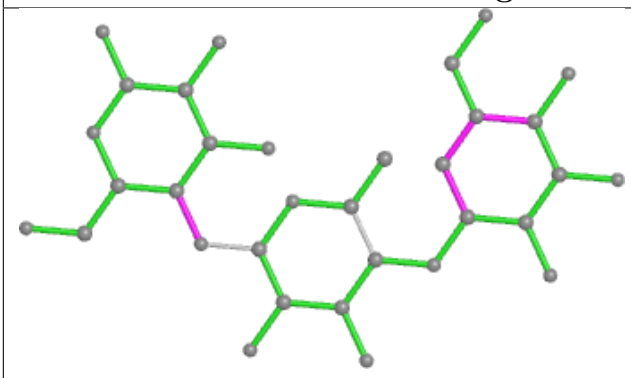


Torsions

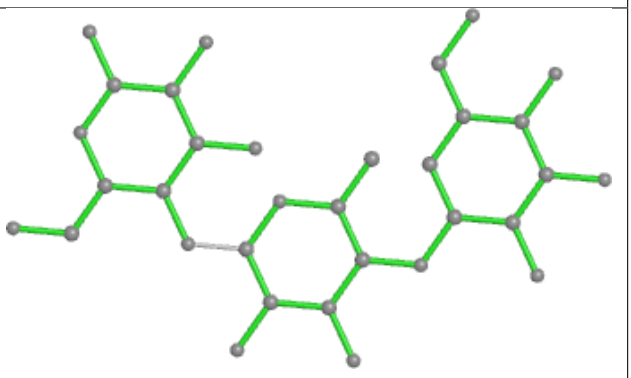


Rings

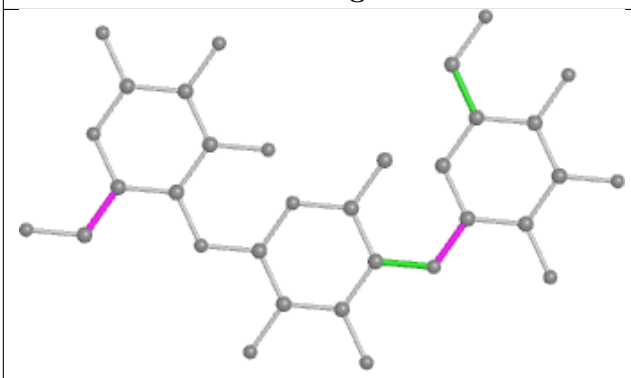
Oligosaccharide Chain P



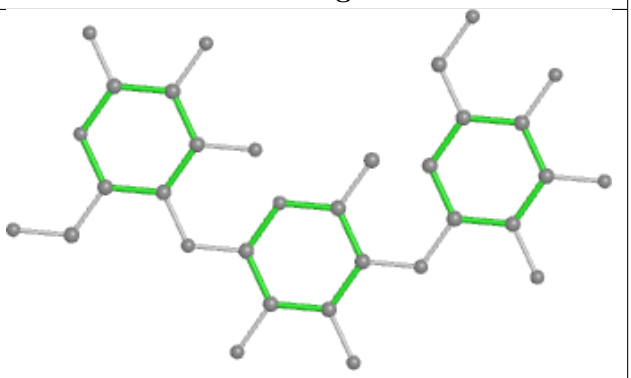
Bond lengths



Bond angles

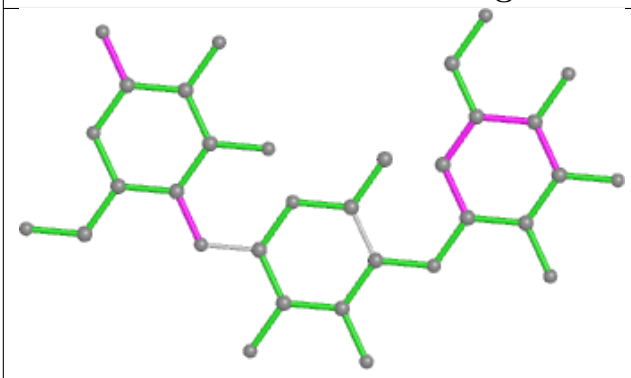


Torsions

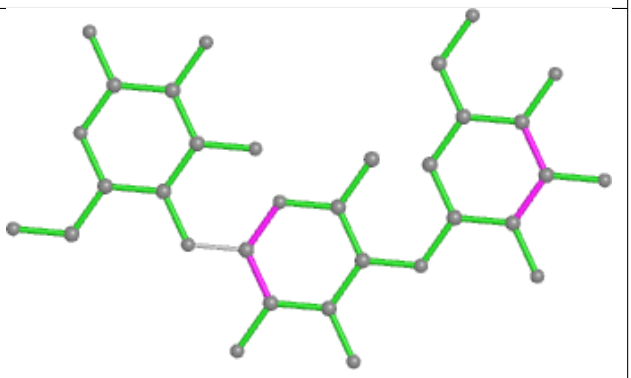


Rings

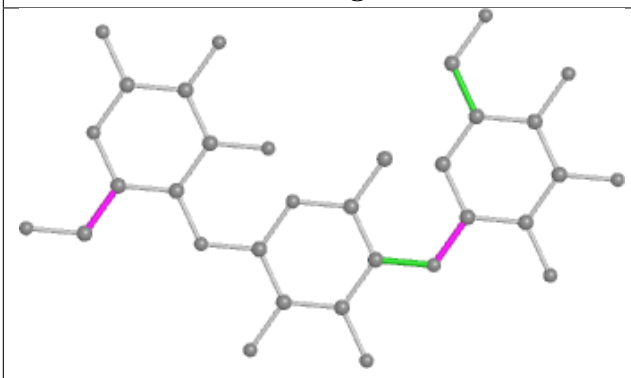
Oligosaccharide Chain T



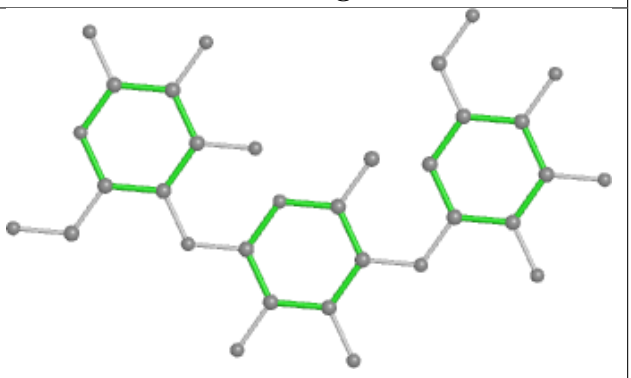
Bond lengths



Bond angles

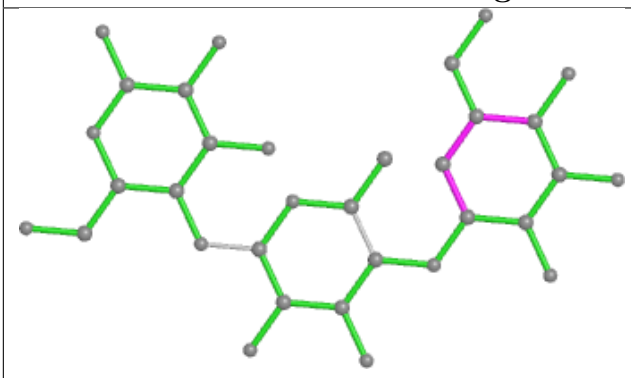


Torsions

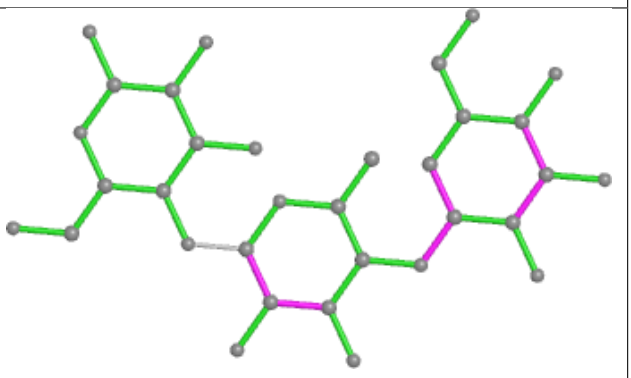


Rings

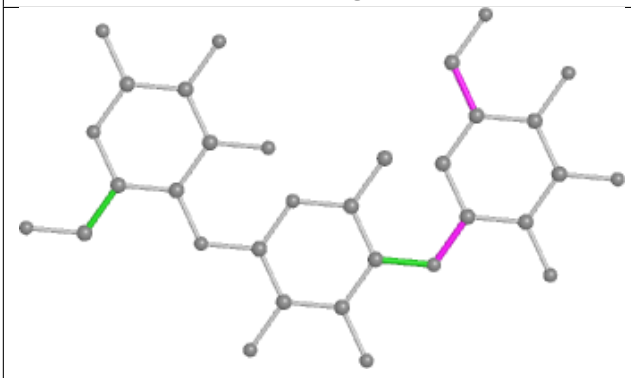
Oligosaccharide Chain V



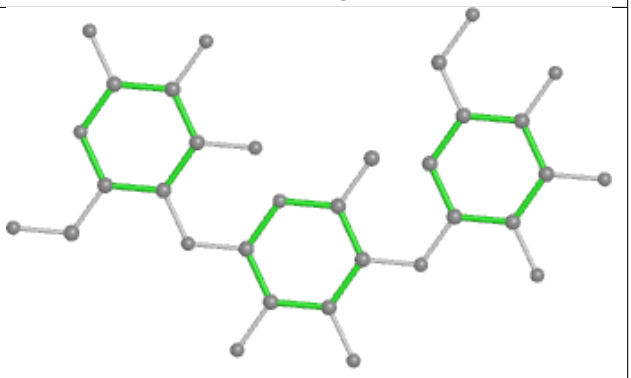
Bond lengths



Bond angles

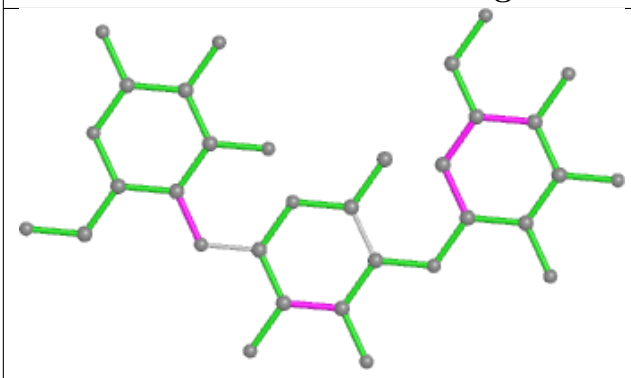


Torsions

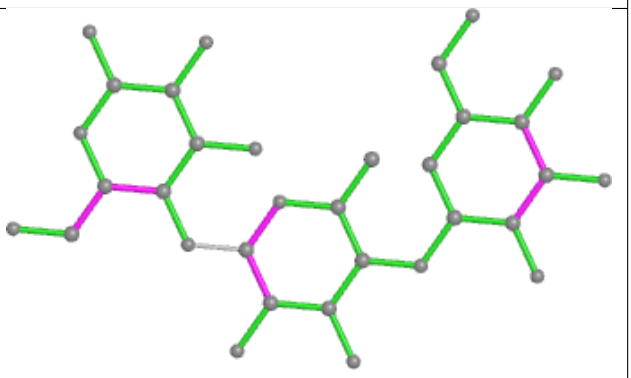


Rings

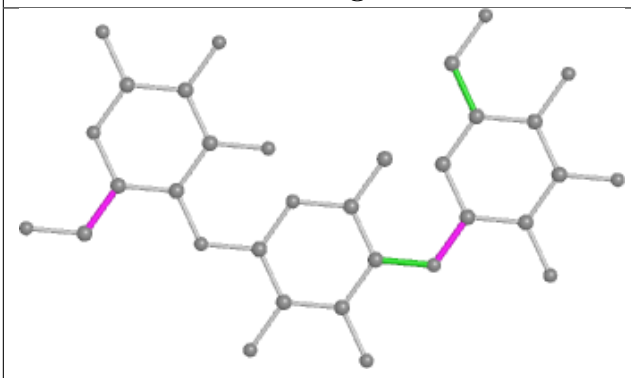
Oligosaccharide Chain X



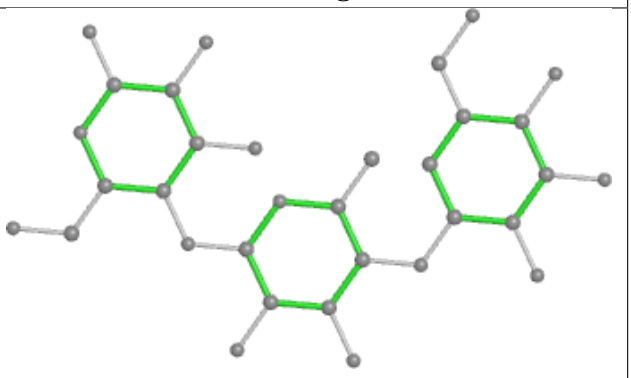
Bond lengths



Bond angles

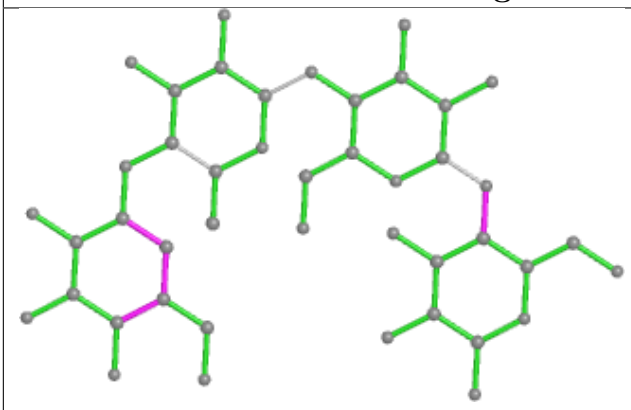


Torsions

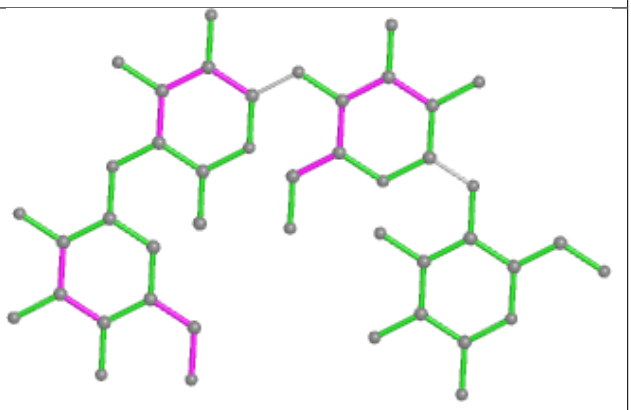


Rings

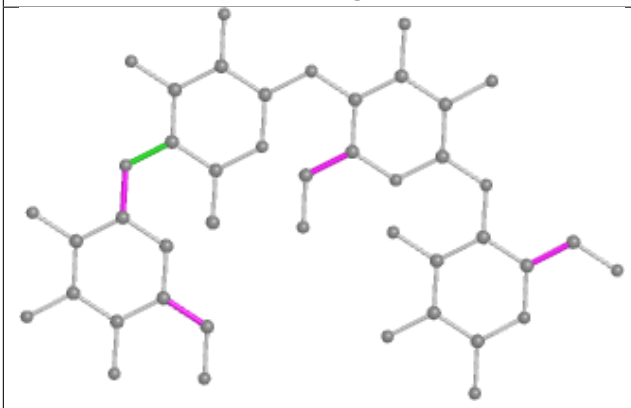
Oligosaccharide Chain N



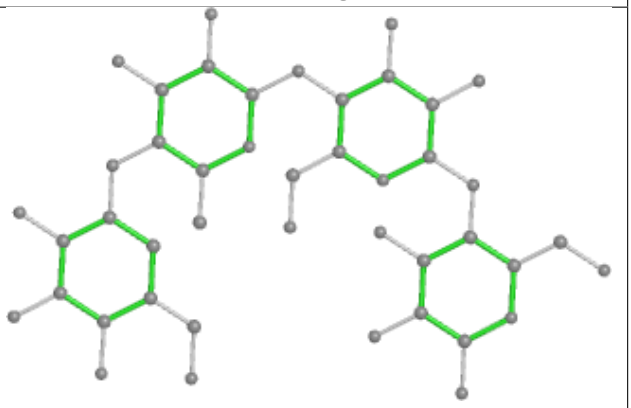
Bond lengths



Bond angles

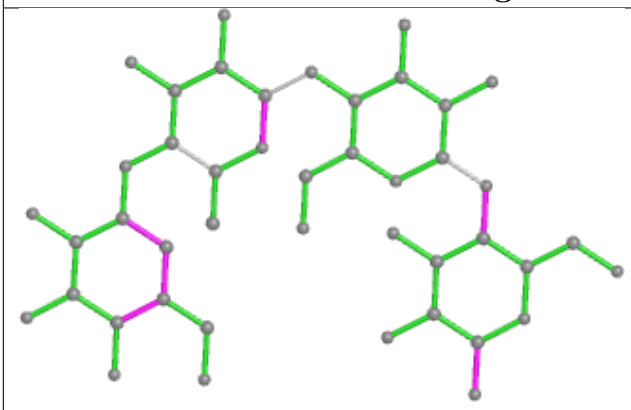


Torsions

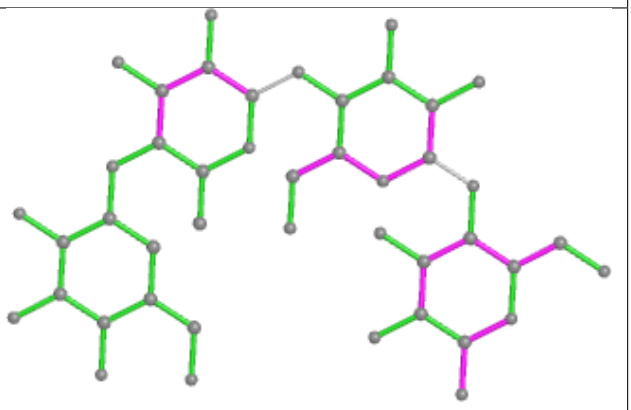


Rings

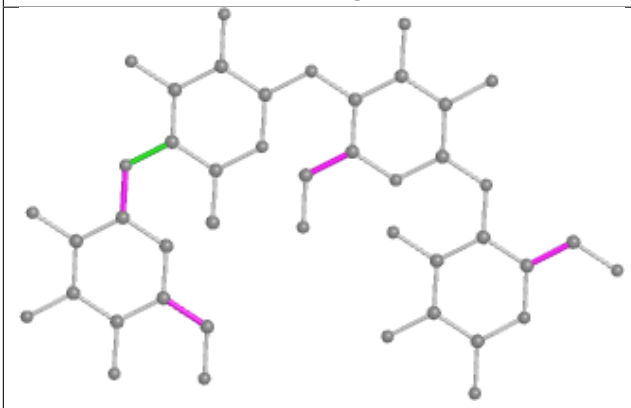
Oligosaccharide Chain R



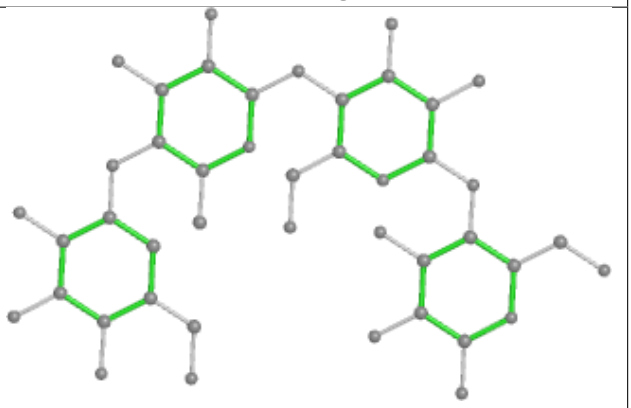
Bond lengths



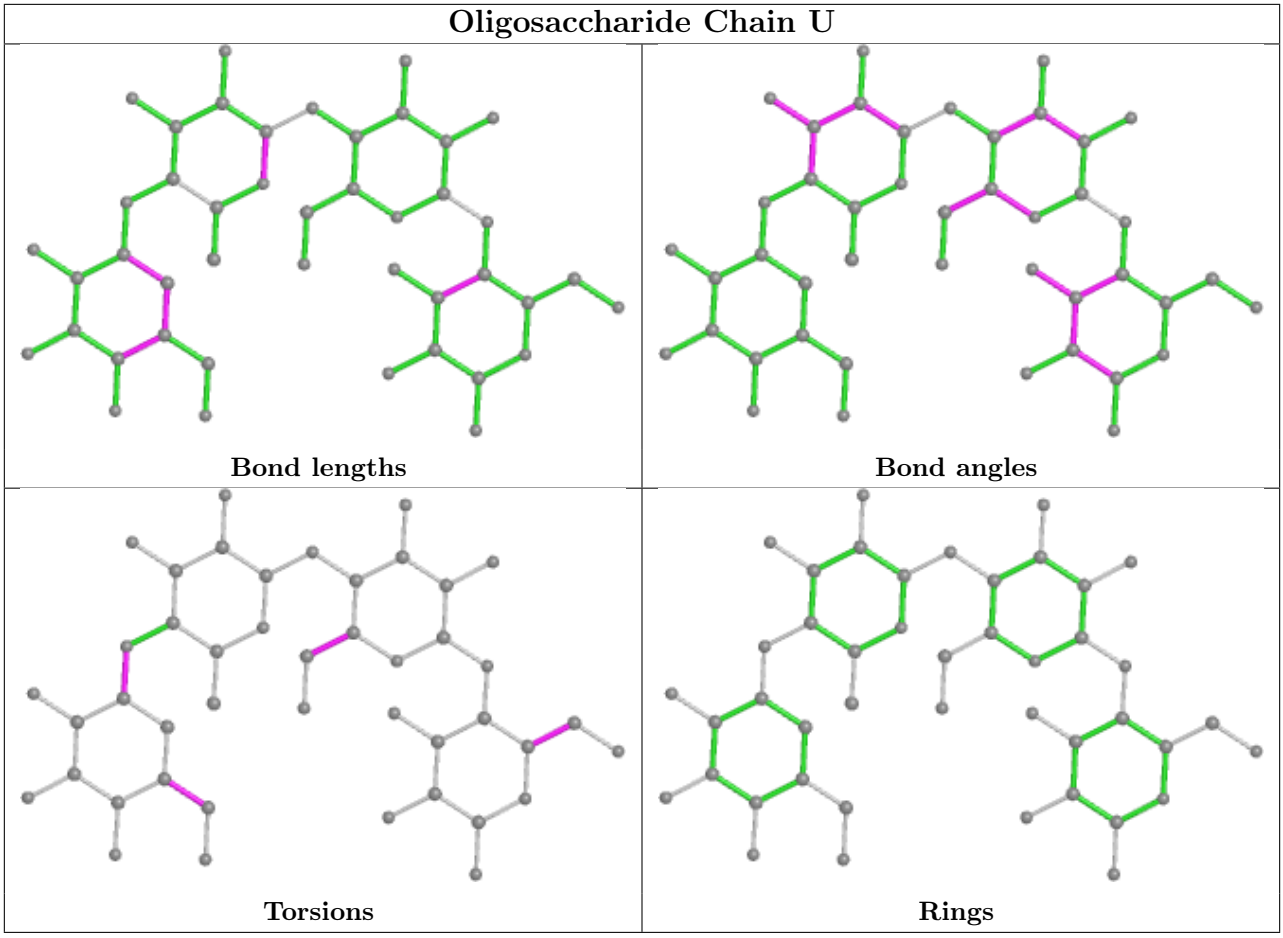
Bond angles



Torsions



Rings



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	496/507 (97%)	0.23	10 (2%)	65	73	34, 53, 75, 100	0
1	B	497/507 (98%)	0.27	16 (3%)	47	56	36, 51, 72, 86	0
1	C	499/507 (98%)	-0.04	5 (1%)	82	87	29, 42, 62, 80	0
1	D	496/507 (97%)	0.09	10 (2%)	65	73	30, 46, 68, 92	0
1	E	497/507 (98%)	-0.07	5 (1%)	82	87	28, 41, 62, 88	0
1	F	496/507 (97%)	0.08	12 (2%)	59	68	28, 46, 68, 85	0
1	G	498/507 (98%)	0.11	12 (2%)	59	68	33, 49, 69, 100	0
1	H	495/507 (97%)	0.39	28 (5%)	23	28	36, 59, 84, 98	0
All	All	3974/4056 (97%)	0.13	98 (2%)	57	66	28, 49, 73, 100	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	5.5
1	D	253	PHE	5.0
1	B	1	ALA	4.4
1	E	499	LEU	4.4
1	H	123	GLU	4.3
1	G	253	PHE	4.3
1	B	207	ASP	4.1
1	A	253	PHE	3.7
1	H	105	PHE	3.7
1	B	94	GLN	3.6
1	A	89	ASN	3.6
1	D	465	VAL	3.5
1	H	90	ILE	3.4
1	B	337	LEU	3.3
1	B	127	ARG	3.3
1	H	253	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	446	CYS	3.3
1	G	2	LYS	3.1
1	H	127	ARG	3.1
1	B	135	GLU	3.1
1	F	465	VAL	3.1
1	B	78	LEU	3.1
1	G	252	ASP	3.0
1	H	85	ASP	3.0
1	C	309	ASP	2.9
1	H	94	GLN	2.9
1	F	274	ASP	2.9
1	C	446	CYS	2.8
1	G	312	THR	2.8
1	B	274	ASP	2.8
1	B	162	ASP	2.7
1	D	91	SER	2.7
1	B	131	ASP	2.7
1	A	307	ARG	2.7
1	D	256	ASP	2.7
1	C	497	ASN	2.6
1	A	203	GLU	2.6
1	H	135	GLU	2.6
1	A	85	ASP	2.6
1	F	253	PHE	2.5
1	F	332	GLU	2.5
1	F	94	GLN	2.5
1	F	311	GLN	2.5
1	H	161	ASP	2.5
1	G	259	LEU	2.5
1	B	200	GLU	2.4
1	H	126	THR	2.4
1	H	124	ARG	2.4
1	D	123	GLU	2.4
1	F	349	GLU	2.4
1	B	444	ILE	2.4
1	E	336	ASP	2.4
1	B	134	GLN	2.3
1	A	243	LEU	2.3
1	B	53	PHE	2.3
1	H	106	GLU	2.3
1	B	446	CYS	2.3
1	E	123	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	203	GLU	2.3
1	H	168	ARG	2.3
1	E	85	ASP	2.3
1	C	94	GLN	2.2
1	H	337	LEU	2.2
1	G	255	ASP	2.2
1	H	336	ASP	2.2
1	F	424	ASN	2.2
1	H	91	SER	2.2
1	H	170	GLU	2.2
1	F	238	ARG	2.2
1	F	47	PRO	2.2
1	A	255	ASP	2.2
1	D	100	ASP	2.2
1	H	171	GLU	2.2
1	H	269	TYR	2.2
1	H	130	SER	2.2
1	H	259	LEU	2.2
1	H	276	ASP	2.2
1	A	78	LEU	2.1
1	D	207	ASP	2.1
1	H	176	TYR	2.1
1	E	94	GLN	2.1
1	H	128	MET	2.1
1	F	9	LEU	2.1
1	G	498	LYS	2.1
1	D	255	ASP	2.1
1	H	20	GLY	2.1
1	D	93	GLY	2.1
1	F	309	ASP	2.1
1	A	102	ALA	2.0
1	G	307	ARG	2.0
1	B	273	SER	2.0
1	D	311	GLN	2.0
1	G	423	PRO	2.0
1	H	169	GLU	2.0
1	G	424	ASN	2.0
1	H	252	ASP	2.0
1	A	106	GLU	2.0
1	G	410	GLU	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	J	1	12/12	0.60	0.30	75,87,97,98	0
3	GLC	T	1	12/12	0.81	0.29	65,72,78,80	0
3	AC1	T	2	21/22	0.82	0.32	62,74,79,82	0
3	GLC	V	1	12/12	0.82	0.34	76,86,96,98	0
4	GLC	R	1	12/12	0.83	0.36	62,69,73,74	0
3	AC1	L	2	21/22	0.84	0.23	48,61,71,72	0
3	AC1	V	2	21/22	0.86	0.20	55,65,76,77	0
3	GLC	X	1	12/12	0.86	0.21	64,70,76,76	0
3	AC1	P	2	21/22	0.86	0.28	60,73,78,80	0
2	ASO	I	1	11/11	0.87	0.23	55,63,67,68	0
2	AC1	O	2	21/22	0.87	0.22	47,58,64,66	0
3	AC1	X	2	21/22	0.87	0.23	54,67,73,75	0
2	AC1	W	2	21/22	0.87	0.23	50,63,71,72	0
4	AC1	U	3	21/22	0.87	0.22	60,67,80,82	0
2	AC1	S	2	21/22	0.88	0.20	44,53,62,69	0
3	AC1	J	2	21/22	0.88	0.20	60,68,78,81	0
4	GLC	N	1	12/12	0.90	0.23	55,62,74,85	0
2	AC1	K	2	21/22	0.90	0.18	43,57,65,71	0
2	AC1	I	2	21/22	0.90	0.17	54,60,67,68	0
4	AC1	R	3	21/22	0.91	0.17	38,50,58,61	0
2	ASO	W	1	11/11	0.91	0.20	54,60,66,67	0
3	GLC	P	1	12/12	0.92	0.28	69,73,80,81	0
4	GLC	U	1	12/12	0.92	0.20	57,62,68,69	0
2	AC1	Q	2	21/22	0.92	0.18	34,42,49,62	0
3	GLC	L	1	12/12	0.93	0.15	59,62,67,75	0
2	AC1	M	2	21/22	0.93	0.16	37,45,54,60	0
4	GLC	R	2	11/12	0.93	0.19	49,54,60,63	0
4	GLC	U	2	11/12	0.94	0.15	54,59,64,68	0
4	AC1	N	3	21/22	0.94	0.14	42,49,54,60	0
4	GLC	N	2	11/12	0.95	0.18	43,51,58,63	0
2	ASO	Q	1	11/11	0.95	0.17	32,37,42,51	0
2	ASO	O	1	11/11	0.96	0.16	43,49,52,54	0

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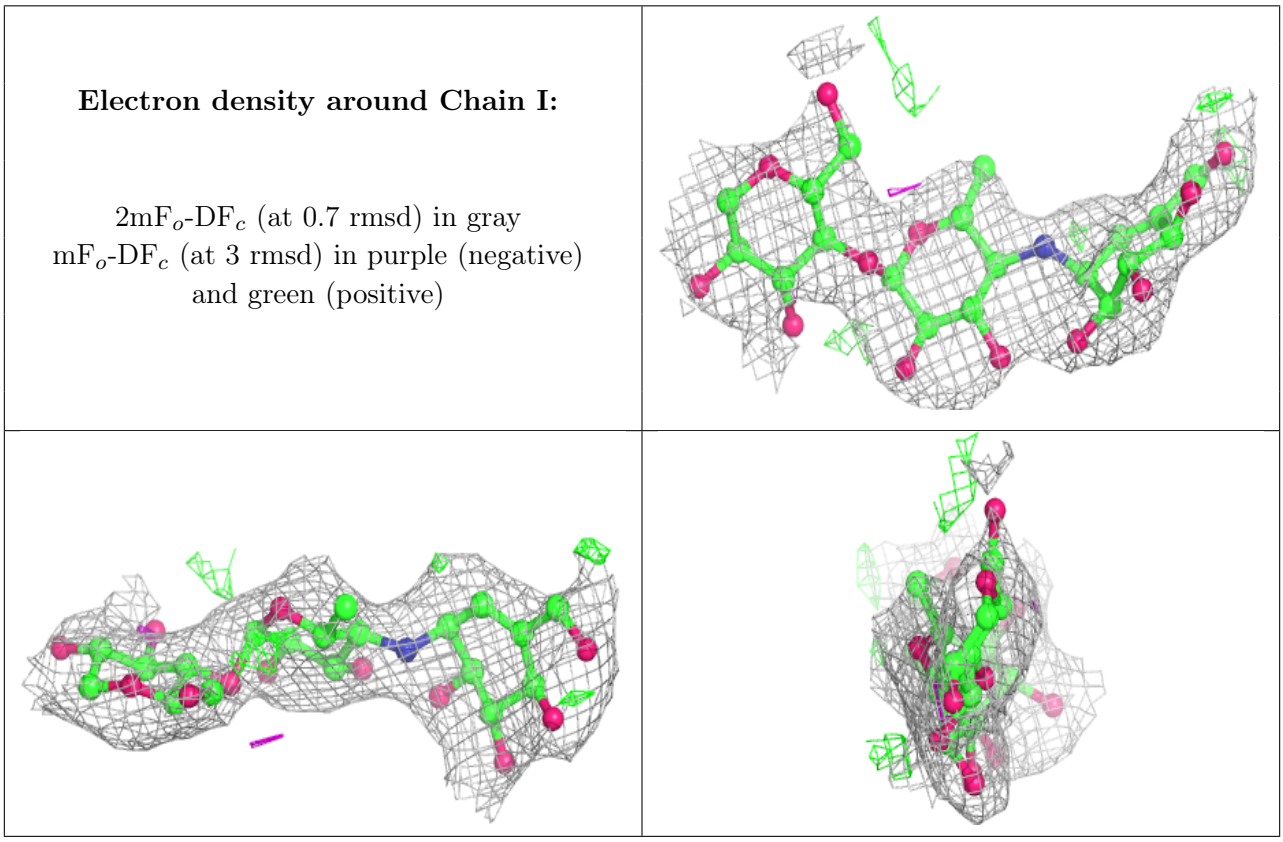
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ASO	K	1	11/11	0.96	0.17	42,45,48,57	0
2	ASO	S	1	11/11	0.96	0.18	42,45,48,57	0
2	ASO	M	1	11/11	0.98	0.11	32,36,38,38	0

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.

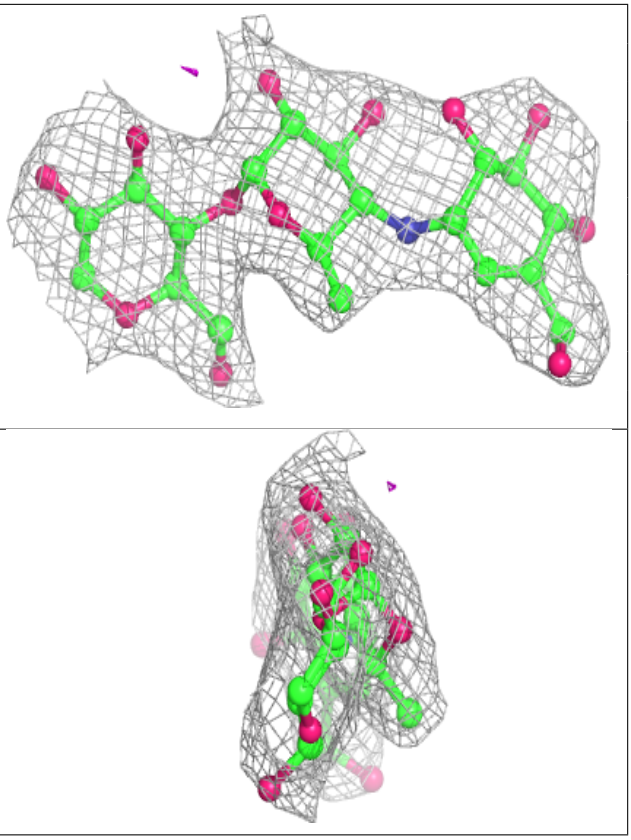
Electron density around Chain I:

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



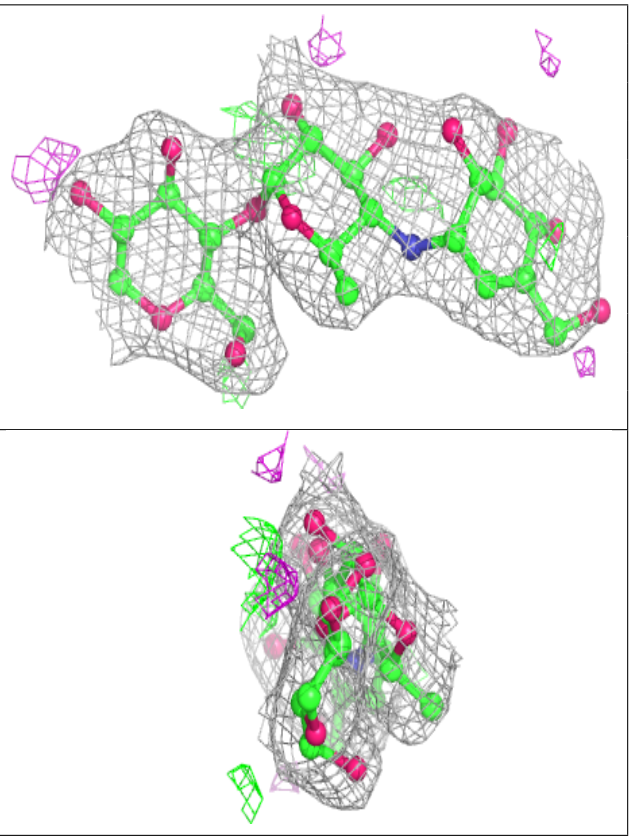
Electron density around Chain K:

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



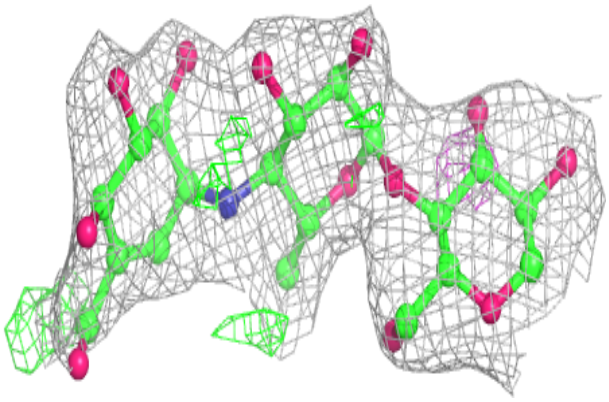
Electron density around Chain M:

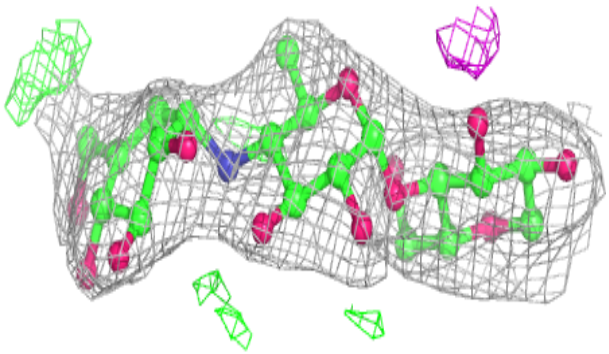
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

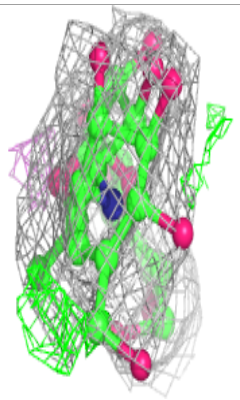


Electron density around Chain O:

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

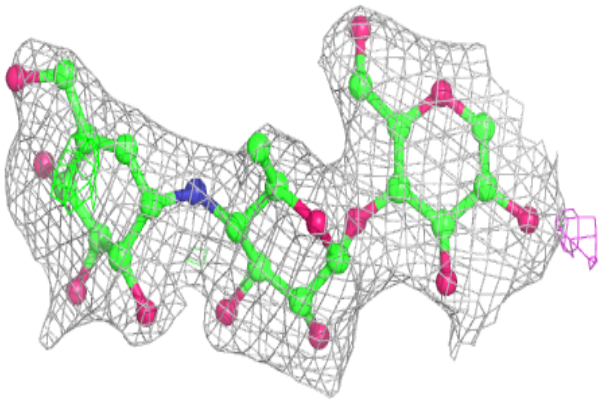


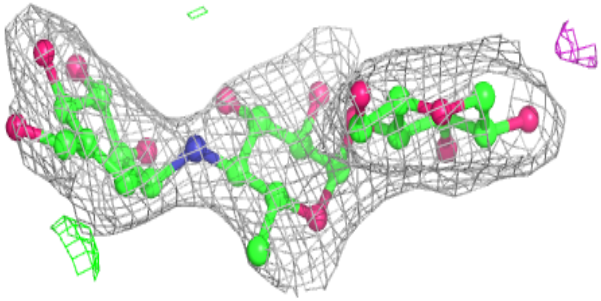


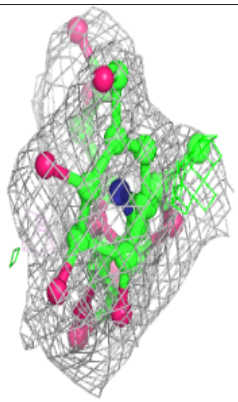


Electron density around Chain Q:

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

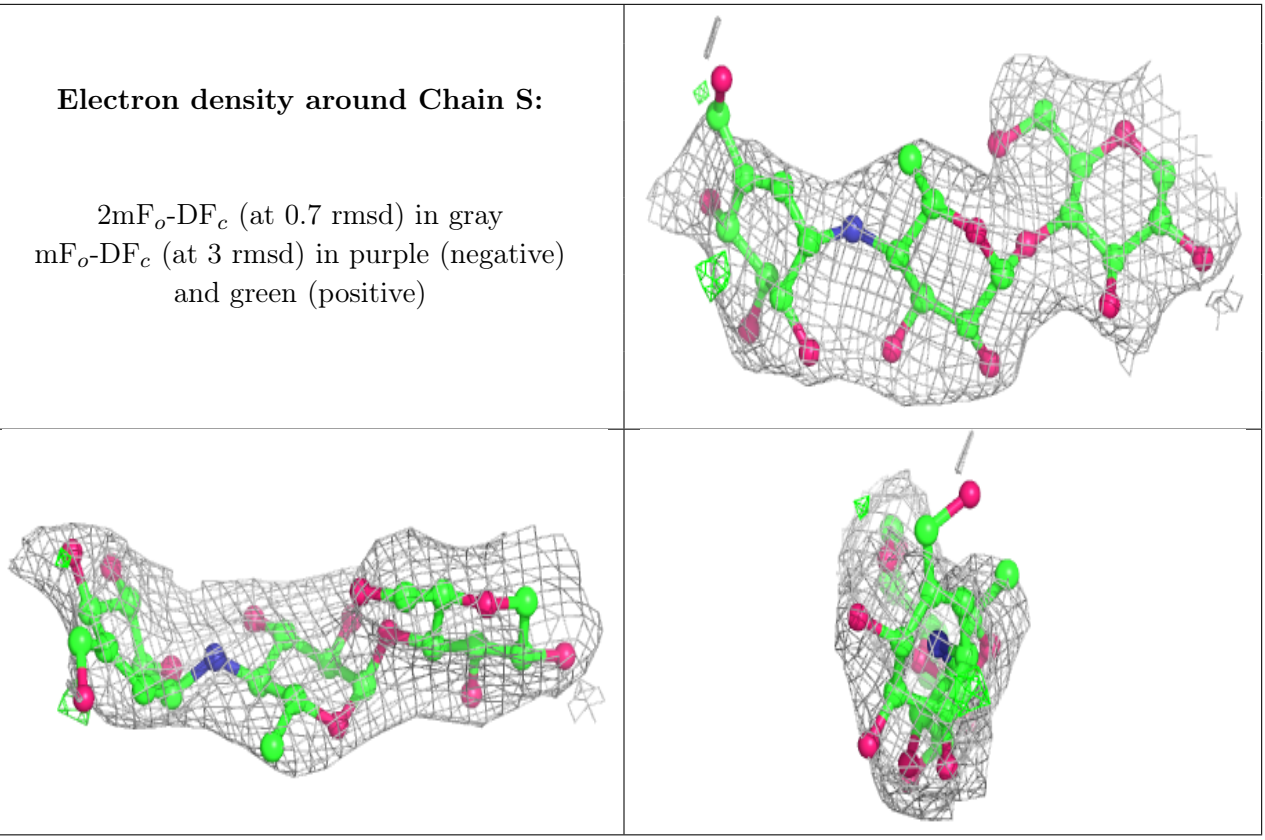






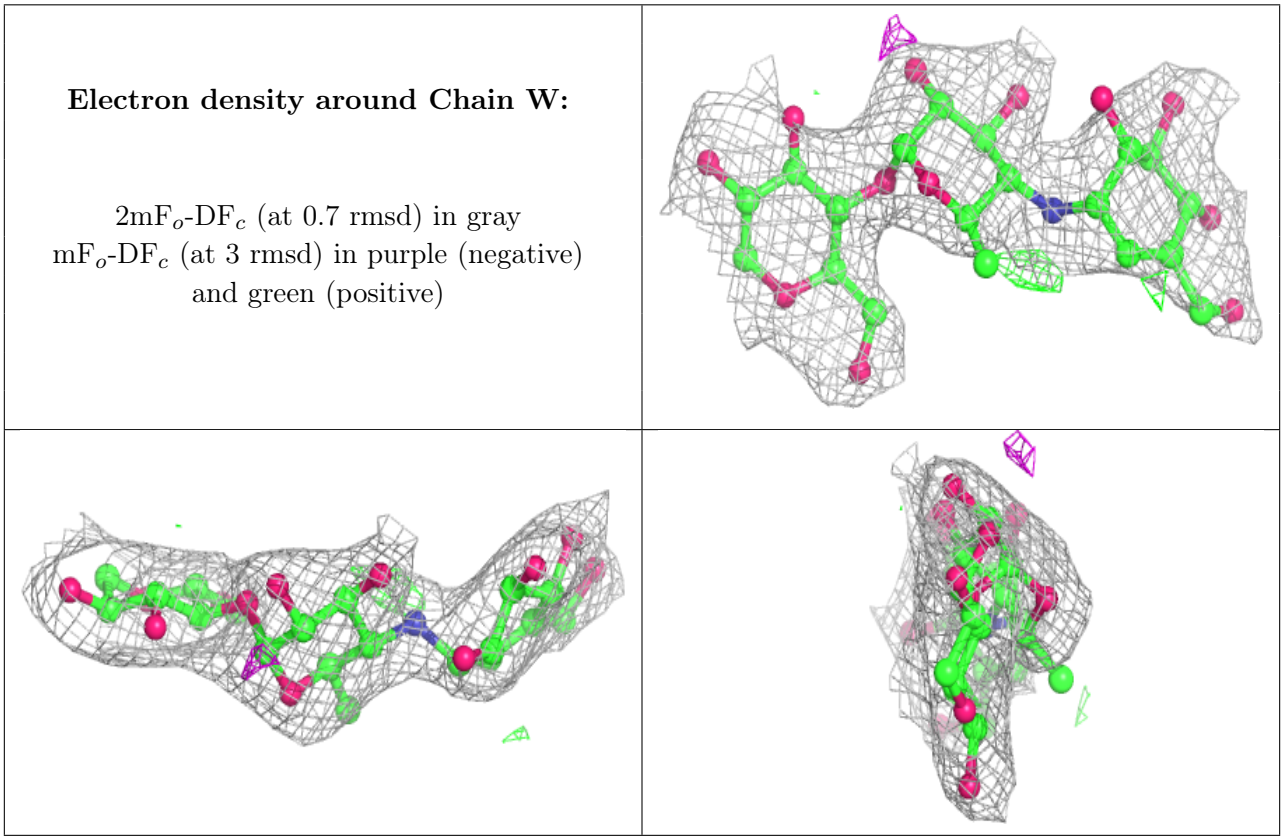
Electron density around Chain S:

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



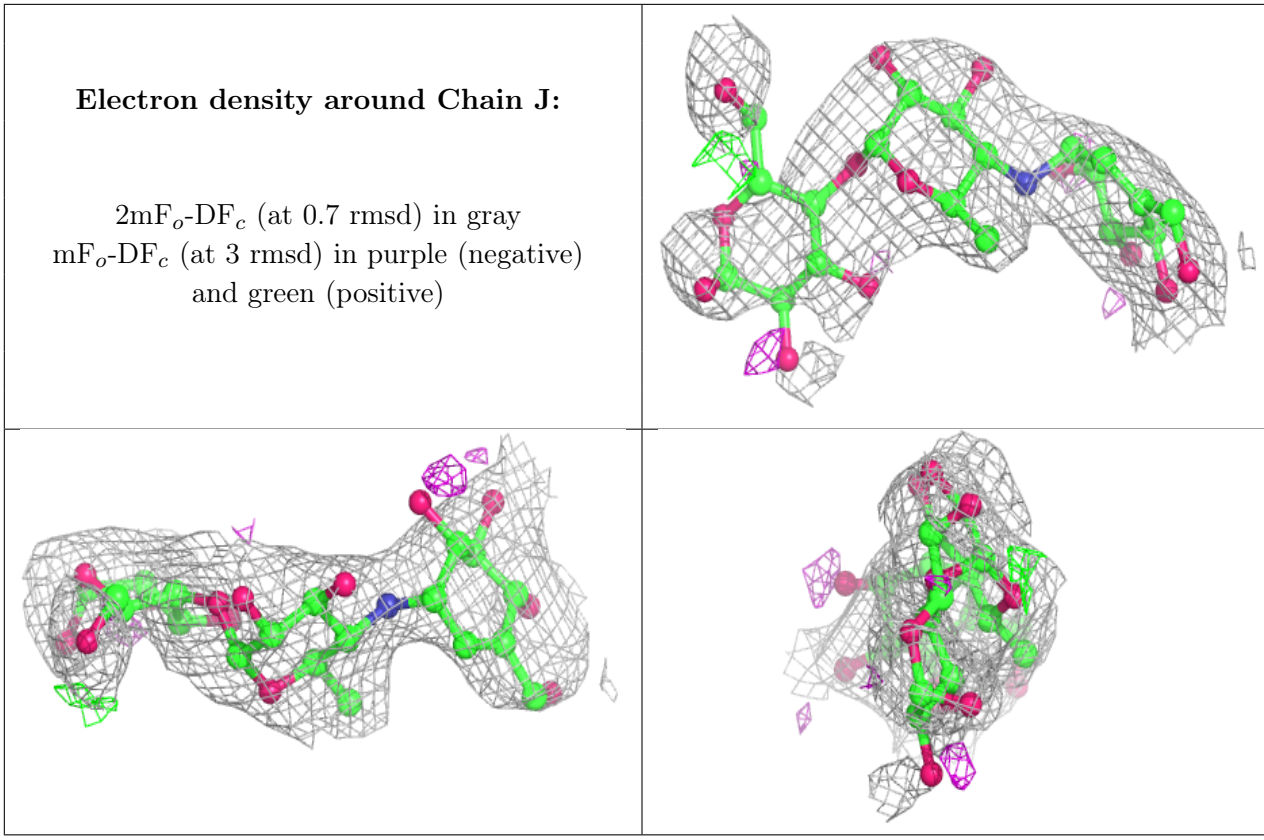
Electron density around Chain W:

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



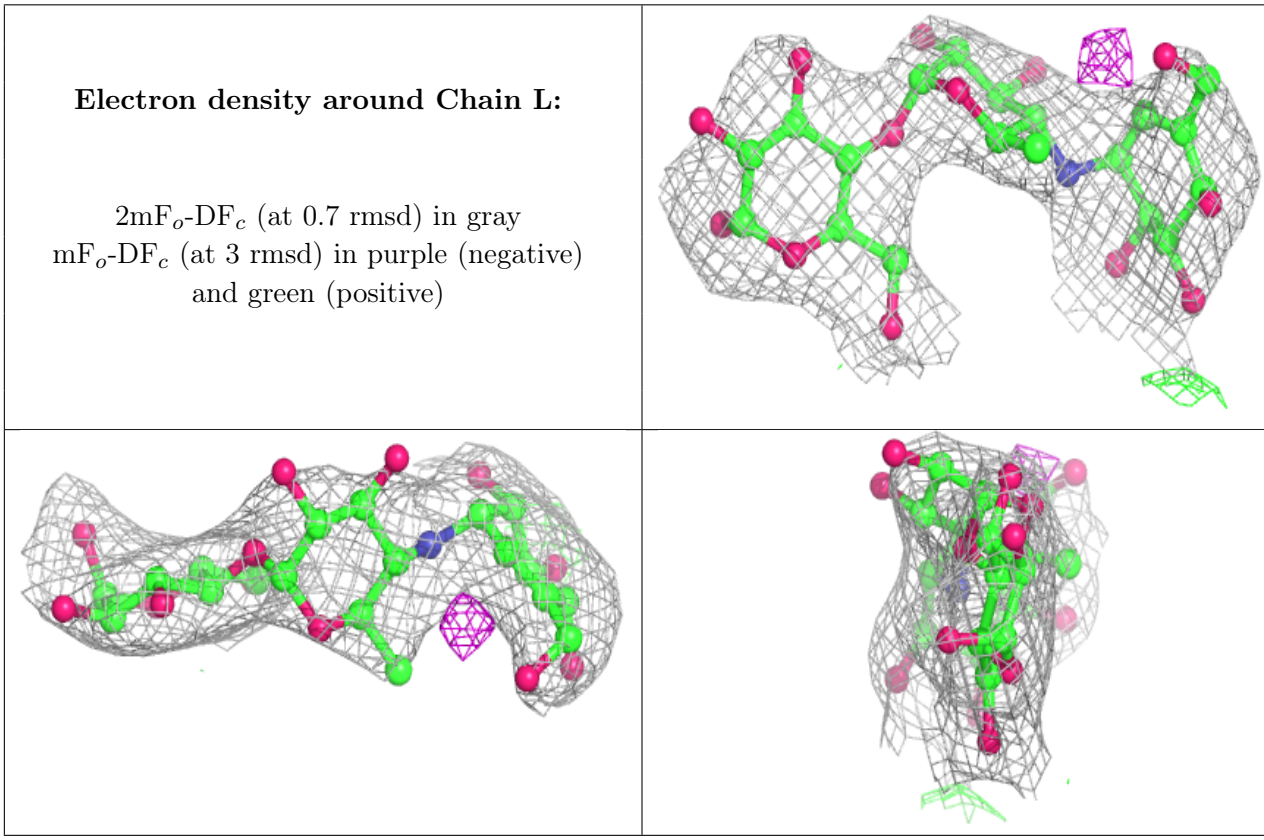
Electron density around Chain J:

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



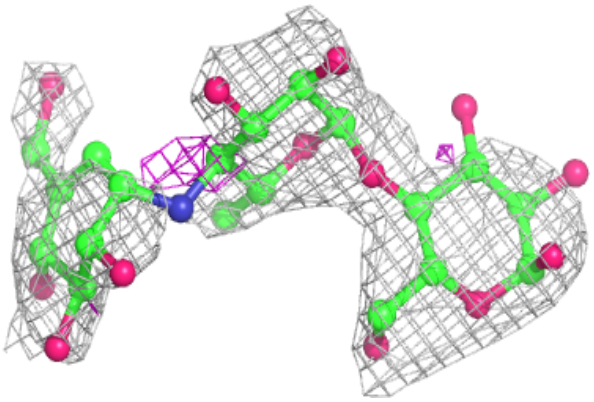
Electron density around Chain L:

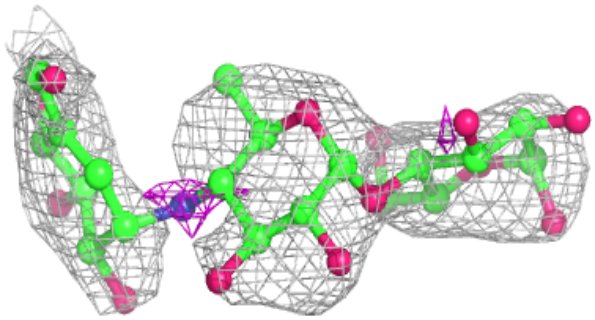
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

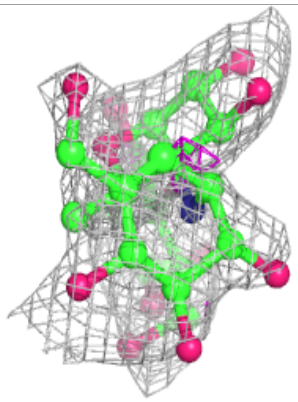


Electron density around Chain P:

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

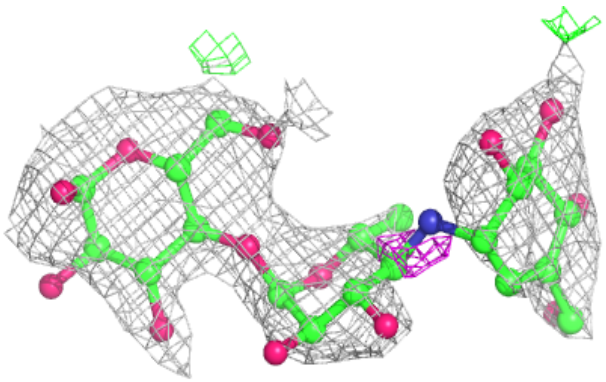


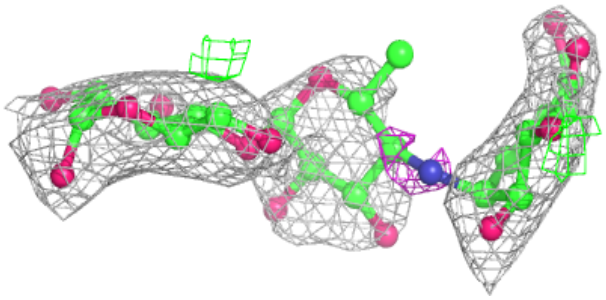


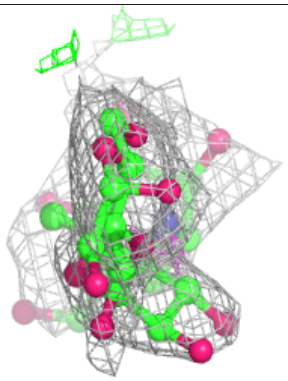


Electron density around Chain T:

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

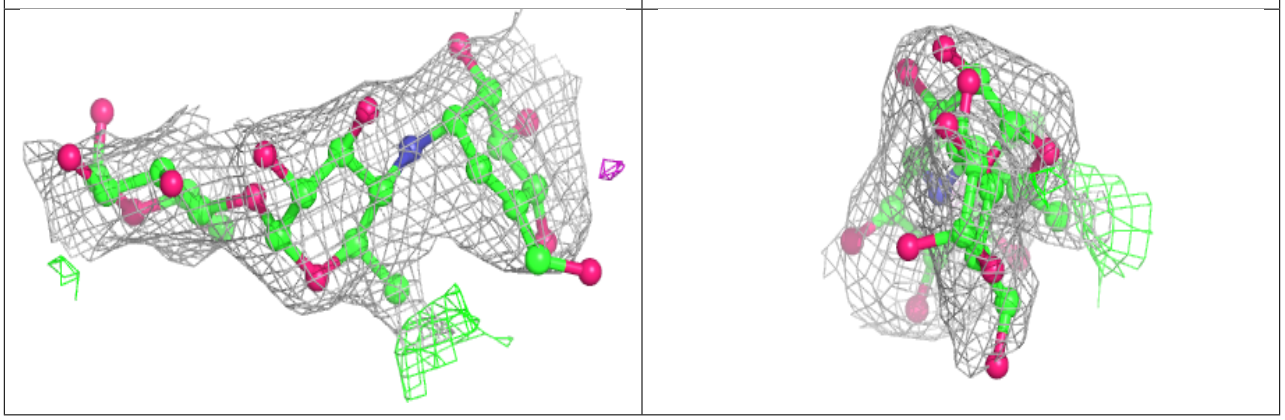






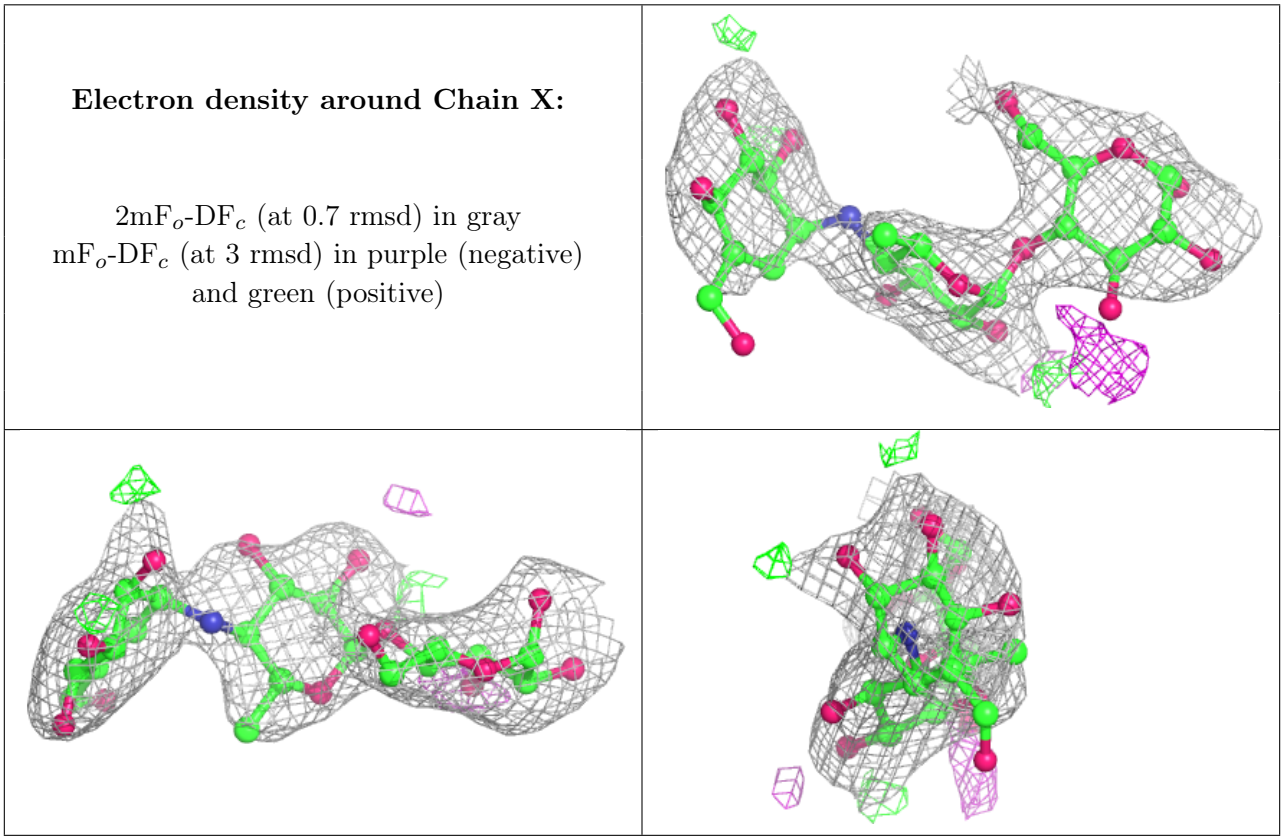
Electron density around Chain V:

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



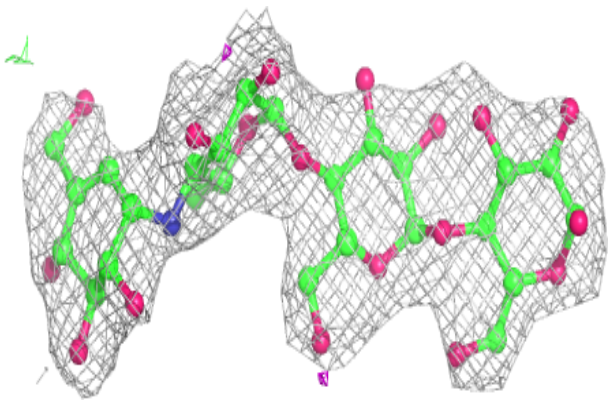
Electron density around Chain X:

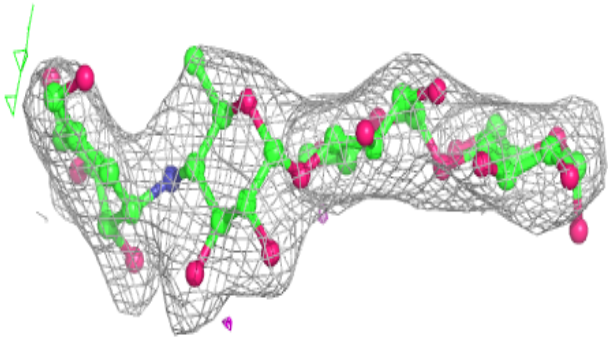
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

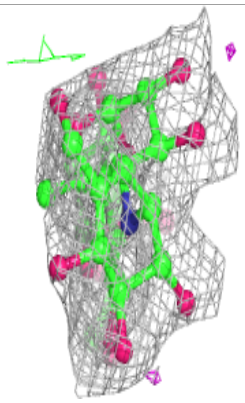


Electron density around Chain N:

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

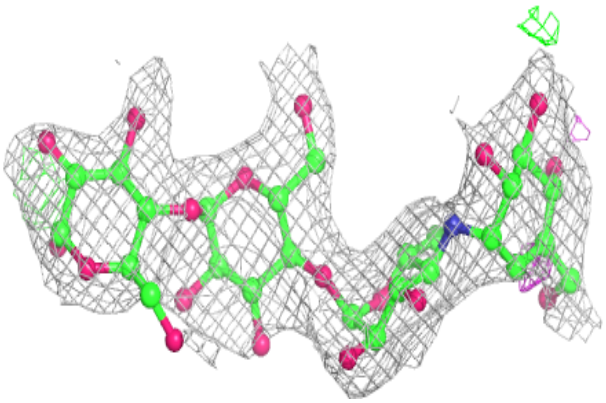


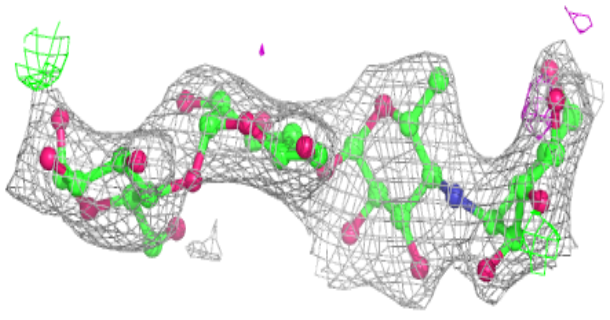


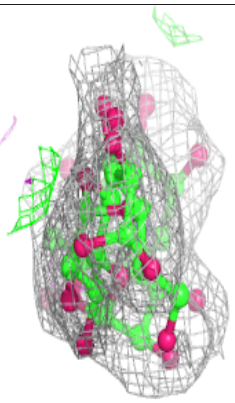


Electron density around Chain R:

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

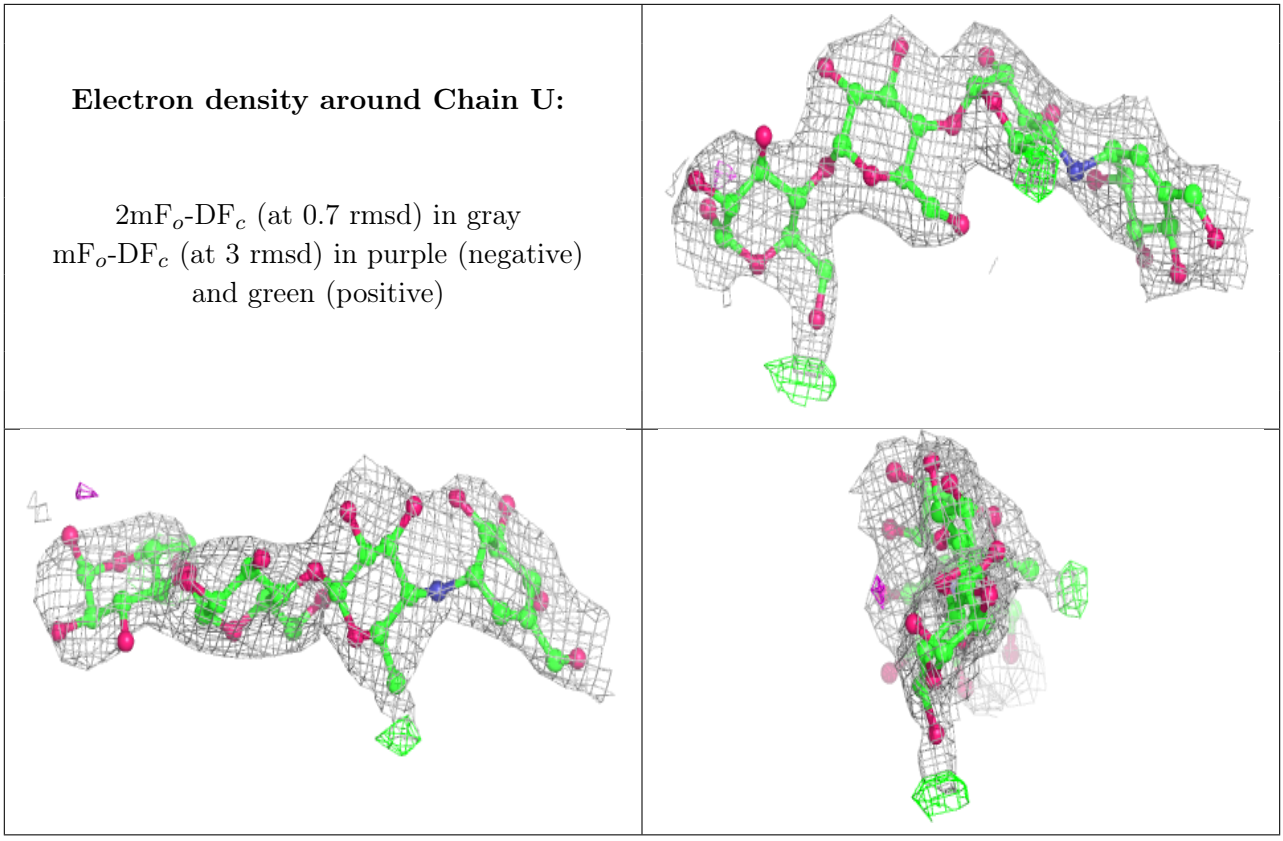






Electron density around Chain U:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.