



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:32 PM UTC

PDB ID : 4NCO / pdb_00004nco
Title : Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with the Broadly Neutralizing Fab PGT122
Authors : Julien, J.-P.; Stanfield, R.L.; Lyumkis, D.; Ward, A.B.; Wilson, I.A.
Deposited on : 2013-10-24
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

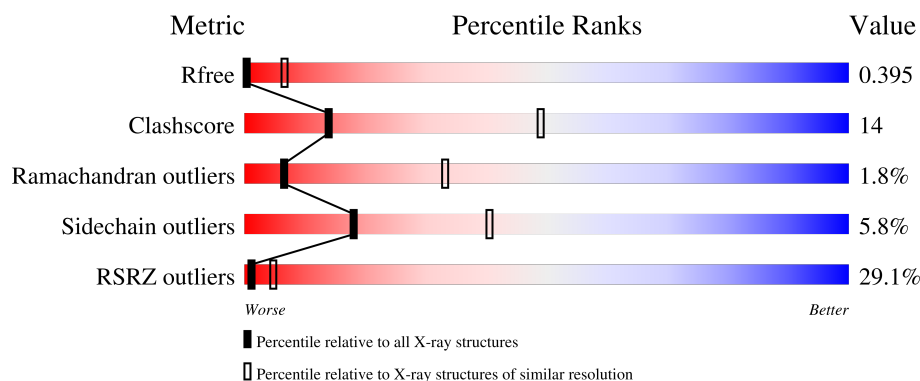
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.70 Å.

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



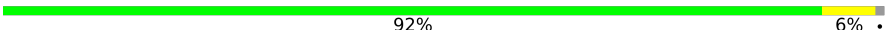
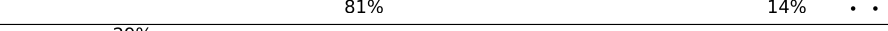
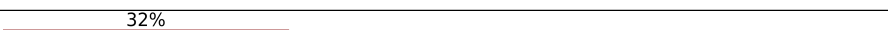
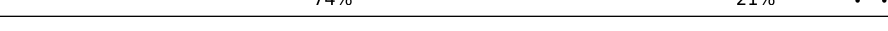
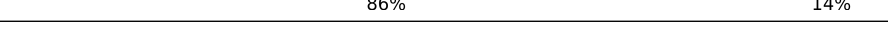
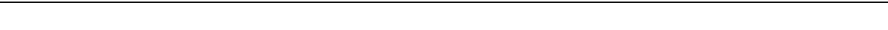
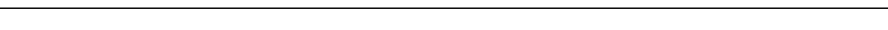
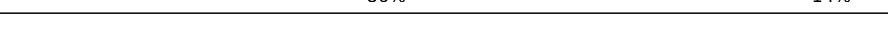
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1020 (5.48-3.92)
Clashscore	190562	1005 (5.40-3.96)
Ramachandran outliers	187476	1095 (5.50-3.90)
Sidechain outliers	187428	1077 (5.50-3.90)
RSRZ outliers	180081	1015 (5.48-3.92)

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

Mol	Chain	Length	Quality of chain
1	A	475	25% 48% 33% 7% 12%
1	E	475	24% 48% 34% 6% 12%
1	I	475	27% 48% 34% 6% 12%
2	B	78	95% ..
2	F	78	95% ..

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Mol	Chain	Length	Quality of chain
2	J	78	
3	C	211	
3	G	211	
3	K	211	
4	D	235	
4	H	235	
4	L	235	
5	M	7	
5	N	7	
5	O	7	
5	P	7	
5	S	7	
5	T	7	
5	U	7	
5	V	7	
5	Y	7	
5	Z	7	
5	a	7	
5	b	7	
6	Q	9	
6	W	9	
6	c	9	
7	R	2	
7	X	2	
7	d	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	O	1	-	-	-	X
7	MAN	R	1	-	-	-	X
7	MAN	R	2	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22014 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 BG505 SOSIP gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			
1	E	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			
1	I	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
I	332	ASN	THR	engineered mutation	UNP Q2N0S6
I	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	0	0	0
			385	231	77	77			
2	F	77	Total	C	N	O	0	0	0
			385	231	77	77			
2	J	77	Total	C	N	O	0	0	0
			385	231	77	77			

- Molecule 3 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			

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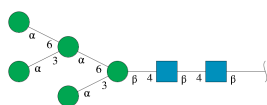
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			
3	K	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			

- Molecule 4 is a protein called PGT122 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			
4	H	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			
4	L	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



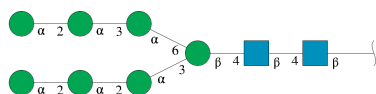
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	N	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	O	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	P	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	S	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	U	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	V	7	Total	C	N	O	0	0	0
			83	46	2	35			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	Z	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	a	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	b	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Q	9	Total	C	N	O	0	0	0
			105	58	2	45			
6	W	9	Total	C	N	O	0	0	0
			105	58	2	45			
6	c	9	Total	C	N	O	0	0	0
			105	58	2	45			

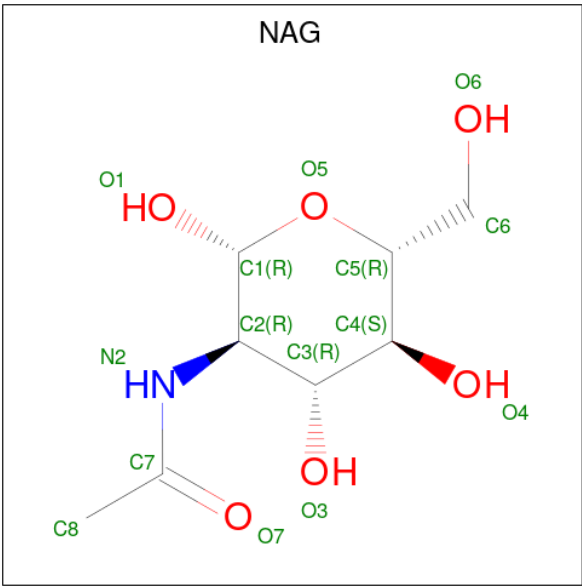
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
7	R	2	Total	C	O	0	0	0
			22	12	10			
7	X	2	Total	C	O	0	0	0
			22	12	10			
7	d	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

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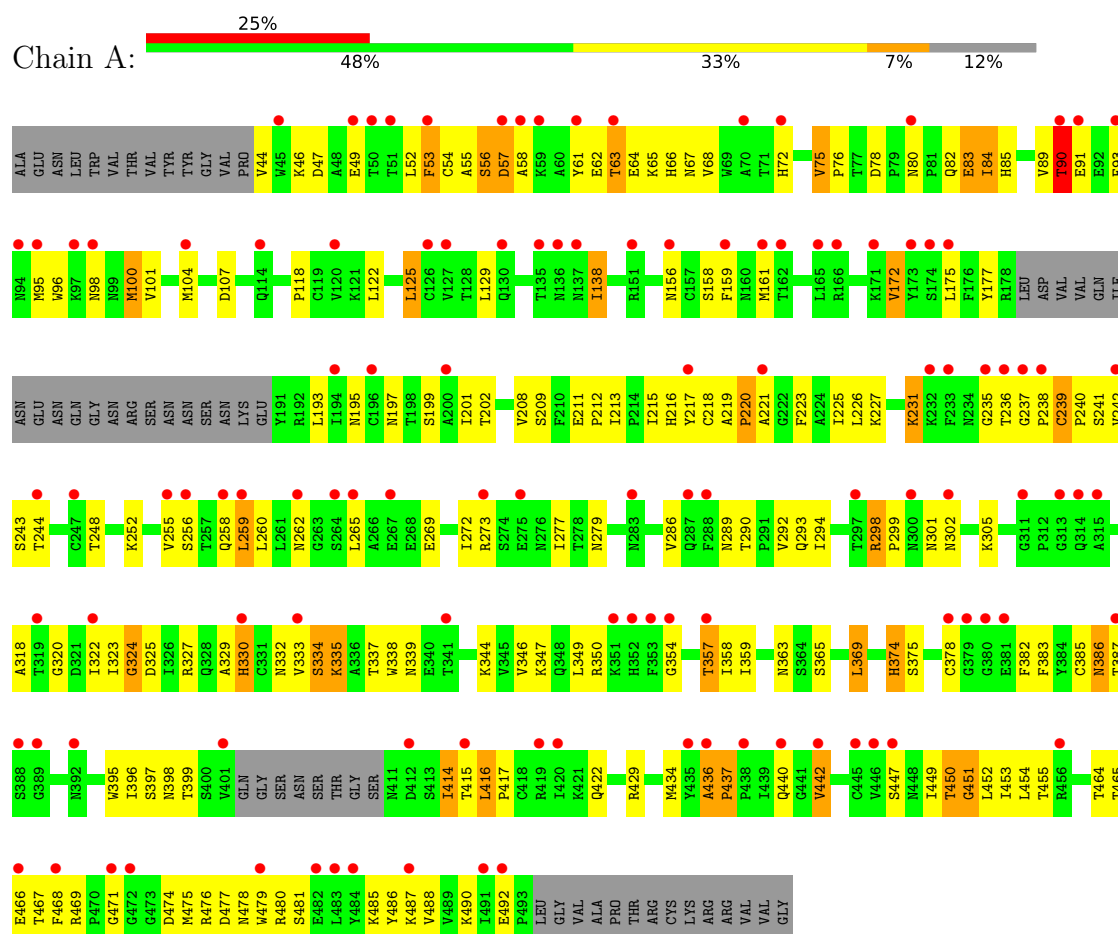
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		

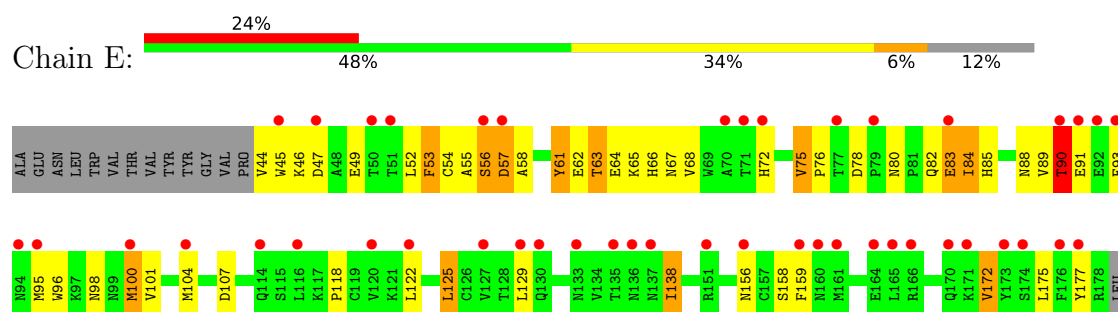
3 Residue-property plots [i](#)

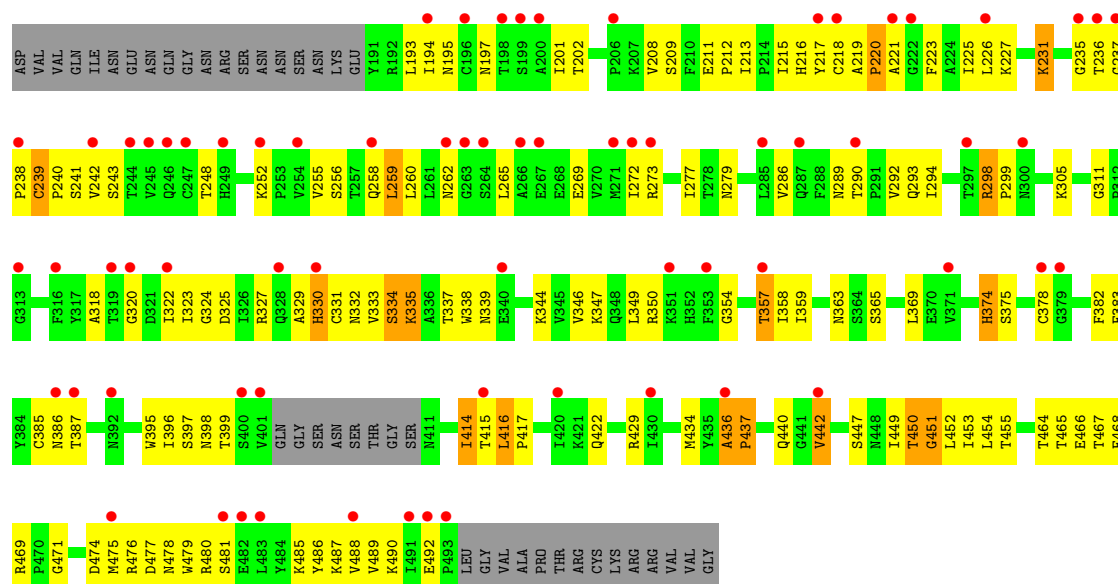
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BG505 SOSIP gp120

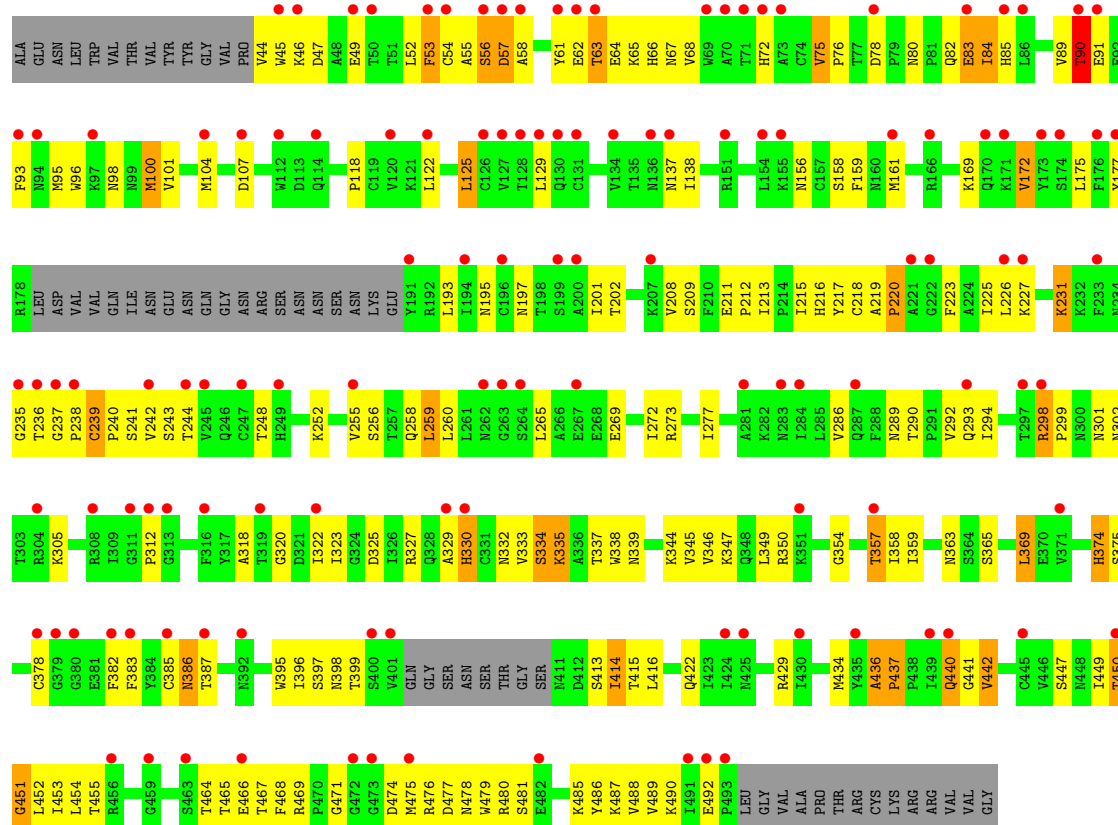


• Molecule 1: BG505 SOSIP gp120



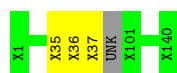


• Molecule 1: BG505 SOSIP gp120



• Molecule 2: BG505 SOSIP gp41





- Molecule 2: BG505 SOSIP gp41

Chain F: 95%



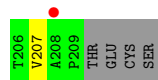
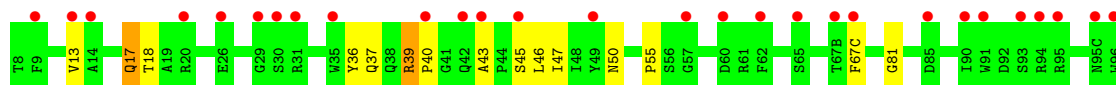
- Molecule 2: BG505 SOSIP gp41

Chain J: 92%



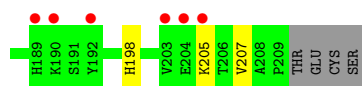
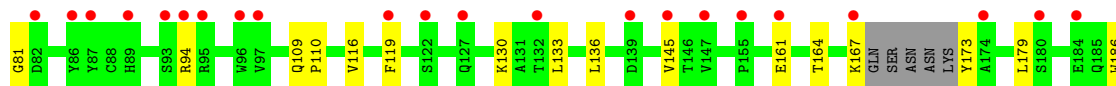
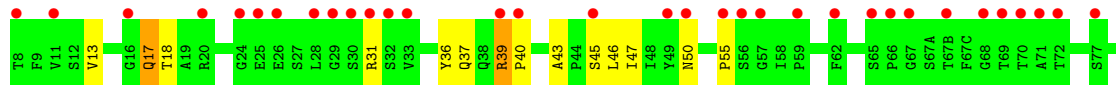
- Molecule 3: PGT122 light chain

Chain C: 24% 81% 14%



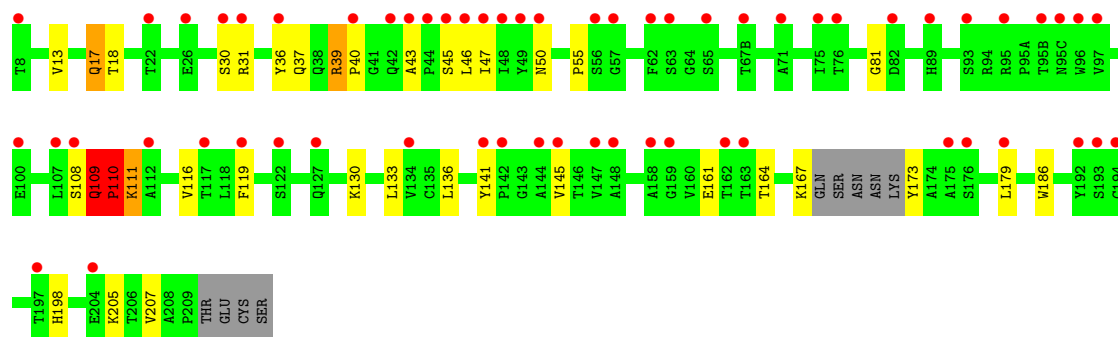
- Molecule 3: PGT122 light chain

Chain G: 29% 80% 15%

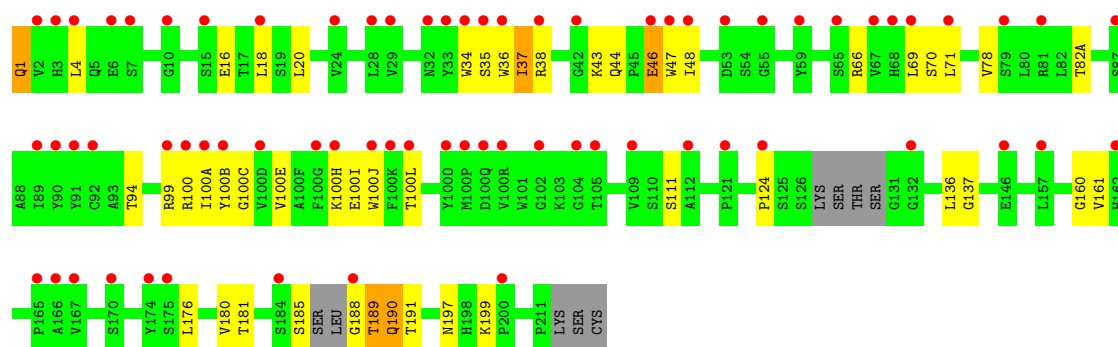
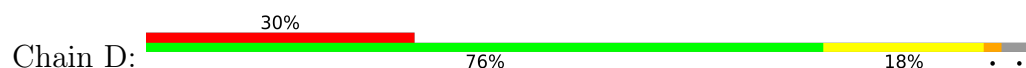


- Molecule 3: PGT122 light chain

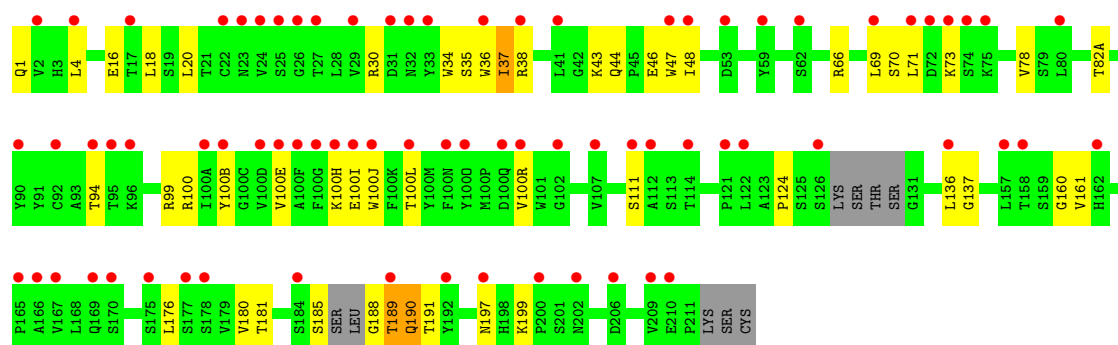
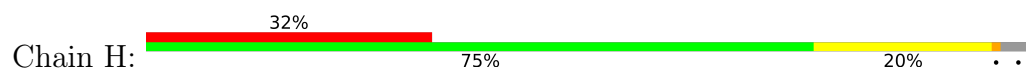
Chain K: 28% 79% 15%



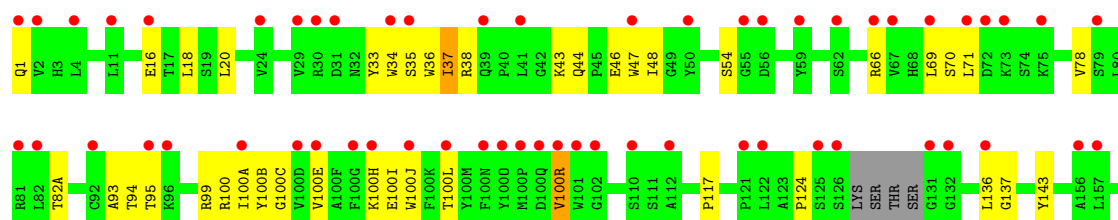
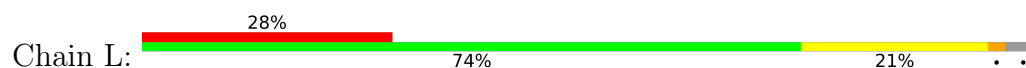
• Molecule 4: PGT122 heavy chain



• Molecule 4: PGT122 heavy chain



• Molecule 4: PGT122 heavy chain





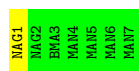
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 57% 29% 14%



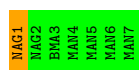
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 86% 14%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 86% 14%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 86% 14%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 71% 14% 14%

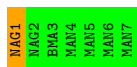


- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-

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

Chain T:  86% 14%

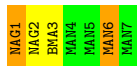
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  86% 14%

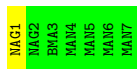
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  86% 14%

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  43% 29% 29%

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  86% 14%

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  86% 14%

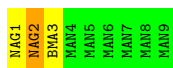
- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain b:  86% 14%



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

Chain Q:  67% 22% 11%



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

Chain W:  78% 22%



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

Chain c:  56% 22% 22%

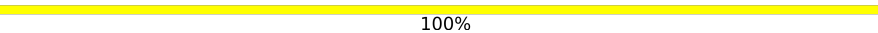


- Molecule 7: α -D-mannopyranose-(1-2)- α -D-mannopyranose

Chain R:  50% 50%



- Molecule 7: α -D-mannopyranose-(1-2)- α -D-mannopyranose

Chain X:  100%

MAN1
MAN2

- Molecule 7: α -D-mannopyranose-(1-2)- α -D-mannopyranose

Chain d:

50%

50%

MAN1
MAN2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.20Å 260.72Å 283.18Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	39.89 – 4.70 39.89 – 4.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (39.89-4.70) 88.9 (39.89-4.70)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 4.63Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.375 , 0.389 0.377 , 0.395	Depositor DCC
R_{free} test set	2621 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	136.6	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 597.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	22014	wwPDB-VP
Average B, all atoms (Å ²)	262.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.45	0/3161	1.24	33/4306 (0.8%)
1	E	0.47	0/3161	1.25	36/4306 (0.8%)
1	I	0.45	0/3161	1.23	31/4306 (0.7%)
3	C	0.35	0/1571	0.84	4/2151 (0.2%)
3	G	0.36	0/1571	0.84	4/2151 (0.2%)
3	K	0.36	0/1571	0.91	9/2151 (0.4%)
4	D	0.39	1/1774 (0.1%)	0.84	6/2421 (0.2%)
4	H	0.46	1/1774 (0.1%)	0.83	6/2421 (0.2%)
4	L	0.67	1/1774 (0.1%)	0.86	9/2421 (0.4%)
All	All	0.45	3/19518 (0.0%)	1.06	138/26634 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	E	0	3
1	I	0	3
3	C	0	1
3	G	0	1
3	K	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	100(R)	VAL	C-N	22.47	1.66	1.33
4	H	100(R)	VAL	C-N	10.38	1.48	1.33
4	D	46	GLU	C-N	-5.00	1.26	1.33

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	335	LYS	N-CA-C	13.96	127.77	111.71
1	A	335	LYS	N-CA-C	13.68	127.69	111.82
1	I	335	LYS	N-CA-C	13.50	127.48	111.82
1	I	239	CYS	CA-C-N	13.47	133.47	119.19
1	I	239	CYS	C-N-CA	13.47	133.47	119.19
1	E	239	CYS	CA-C-N	13.39	133.39	119.19
1	E	239	CYS	C-N-CA	13.39	133.39	119.19
1	A	239	CYS	CA-C-N	13.39	133.38	119.19
1	A	239	CYS	C-N-CA	13.39	133.38	119.19
1	E	334	SER	CA-C-N	10.80	135.84	120.28
1	E	334	SER	C-N-CA	10.80	135.84	120.28
1	A	334	SER	CA-C-N	9.98	135.48	120.31
1	A	334	SER	C-N-CA	9.98	135.48	120.31
1	I	334	SER	CA-C-N	9.66	134.99	120.31
1	I	334	SER	C-N-CA	9.66	134.99	120.31
1	E	237	GLY	CA-C-N	9.46	131.66	119.84
1	E	237	GLY	C-N-CA	9.46	131.66	119.84
1	A	237	GLY	CA-C-N	9.42	131.62	119.84
1	A	237	GLY	C-N-CA	9.42	131.62	119.84
1	I	237	GLY	CA-C-N	9.37	131.55	119.84
1	I	237	GLY	C-N-CA	9.37	131.55	119.84
1	A	78	ASP	CA-C-N	-9.12	112.44	121.65
1	A	78	ASP	C-N-CA	-9.12	112.44	121.65
1	E	78	ASP	CA-C-N	-9.05	112.50	121.65
1	E	78	ASP	C-N-CA	-9.05	112.50	121.65
1	I	78	ASP	CA-C-N	-9.05	112.51	121.65
1	I	78	ASP	C-N-CA	-9.05	112.51	121.65
1	E	324	GLY	N-CA-C	-8.72	104.10	114.48
1	A	259	LEU	CA-C-N	-8.72	109.19	122.09
1	A	259	LEU	C-N-CA	-8.72	109.19	122.09
1	E	259	LEU	CA-C-N	-8.68	109.25	122.09
1	E	259	LEU	C-N-CA	-8.68	109.25	122.09
1	I	259	LEU	CA-C-N	-8.64	109.30	122.09
1	I	259	LEU	C-N-CA	-8.64	109.30	122.09
4	L	100(R)	VAL	O-C-N	8.49	132.37	123.20
3	K	109	GLN	CA-C-N	8.27	128.90	120.14
3	K	109	GLN	C-N-CA	8.27	128.90	120.14
1	I	416	LEU	CA-C-N	8.11	130.20	120.23
1	I	416	LEU	C-N-CA	8.11	130.20	120.23
1	E	416	LEU	CA-C-N	8.07	130.16	120.23
1	E	416	LEU	C-N-CA	8.07	130.16	120.23
1	A	416	LEU	CA-C-N	8.02	130.09	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	LEU	C-N-CA	8.02	130.09	120.23
1	E	436	ALA	CA-C-N	-8.01	112.13	120.38
1	E	436	ALA	C-N-CA	-8.01	112.13	120.38
1	I	436	ALA	CA-C-N	-7.99	112.15	120.38
1	I	436	ALA	C-N-CA	-7.99	112.15	120.38
1	A	436	ALA	CA-C-N	-7.99	112.15	120.38
1	A	436	ALA	C-N-CA	-7.99	112.15	120.38
4	L	160	GLY	N-CA-C	-7.79	105.09	115.21
1	A	193	LEU	CB-CA-C	-7.37	108.08	116.63
1	I	193	LEU	CB-CA-C	-7.34	108.11	116.63
1	E	193	LEU	CB-CA-C	-7.34	108.12	116.63
1	I	450	THR	CA-C-N	-7.29	109.59	121.04
1	I	450	THR	C-N-CA	-7.29	109.59	121.04
1	E	450	THR	CA-C-N	-7.20	109.73	121.04
1	E	450	THR	C-N-CA	-7.20	109.73	121.04
1	A	450	THR	CA-C-N	-7.19	109.75	121.04
1	A	450	THR	C-N-CA	-7.19	109.75	121.04
1	E	451	GLY	N-CA-C	7.16	121.02	110.63
1	I	451	GLY	N-CA-C	7.14	120.98	110.63
1	A	451	GLY	N-CA-C	7.12	120.96	110.63
3	K	111	LYS	N-CA-C	6.42	126.14	113.29
1	E	337	THR	N-CA-C	-6.34	104.29	111.07
1	A	337	THR	N-CA-C	-6.32	104.30	111.07
1	I	337	THR	N-CA-C	-6.32	104.31	111.07
1	A	138	ILE	N-CA-C	6.16	117.23	108.42
1	A	386	ASN	N-CA-C	-6.13	100.96	110.10
1	E	138	ILE	N-CA-C	6.01	117.01	108.42
1	I	386	ASN	N-CA-C	-5.97	101.21	110.10
1	E	386	ASN	N-CA-C	-5.95	101.23	110.10
1	A	324	GLY	N-CA-C	-5.93	106.84	114.85
1	E	90	THR	N-CA-C	5.93	123.43	110.80
1	E	88	ASN	CB-CA-C	-5.92	109.18	117.23
3	K	108	SER	N-CA-C	5.92	119.69	112.23
1	I	90	THR	N-CA-C	5.91	123.39	110.80
1	A	90	THR	N-CA-C	5.86	123.29	110.80
4	L	100(R)	VAL	CA-C-N	-5.83	113.67	122.81
4	L	100(R)	VAL	C-N-CA	-5.83	113.67	122.81
1	I	334	SER	O-C-N	5.68	129.66	123.13
1	I	172	VAL	N-CA-C	5.64	116.87	108.46
3	C	43	ALA	CA-C-N	-5.62	113.99	119.78
3	C	43	ALA	C-N-CA	-5.62	113.99	119.78
1	E	334	SER	O-C-N	5.60	129.57	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	SER	O-C-N	5.60	129.57	123.13
1	A	172	VAL	N-CA-C	5.55	116.73	108.46
3	G	43	ALA	CA-C-N	-5.54	114.07	119.78
3	G	43	ALA	C-N-CA	-5.54	114.07	119.78
3	K	43	ALA	CA-C-N	-5.54	114.07	119.78
3	K	43	ALA	C-N-CA	-5.54	114.07	119.78
1	A	95	MET	N-CA-C	5.48	118.77	111.75
1	E	95	MET	N-CA-C	5.46	118.74	111.75
1	I	95	MET	N-CA-C	5.46	118.74	111.75
1	E	90	THR	CA-C-N	5.41	131.15	121.15
1	E	90	THR	C-N-CA	5.41	131.15	121.15
1	A	90	THR	CA-C-N	5.39	131.12	121.15
1	A	90	THR	C-N-CA	5.39	131.12	121.15
1	E	172	VAL	N-CA-C	5.38	116.48	108.46
3	K	119	PHE	CA-C-N	5.38	125.92	120.38
3	K	119	PHE	C-N-CA	5.38	125.92	120.38
1	I	90	THR	CA-C-N	5.37	131.08	121.15
1	I	90	THR	C-N-CA	5.37	131.08	121.15
3	K	110	PRO	N-CA-C	5.36	120.64	111.68
3	G	119	PHE	CA-C-N	5.36	125.90	120.38
3	G	119	PHE	C-N-CA	5.36	125.90	120.38
4	D	160	GLY	N-CA-C	-5.32	108.29	115.21
4	H	160	GLY	N-CA-C	-5.32	108.30	115.21
4	D	37	ILE	CA-C-N	-5.31	114.33	122.62
4	D	37	ILE	C-N-CA	-5.31	114.33	122.62
3	C	119	PHE	CA-C-N	5.30	125.83	120.38
3	C	119	PHE	C-N-CA	5.30	125.83	120.38
4	H	37	ILE	CA-C-N	-5.29	114.36	122.62
4	H	37	ILE	C-N-CA	-5.29	114.36	122.62
4	L	37	ILE	CA-C-N	-5.28	114.38	122.62
4	L	37	ILE	C-N-CA	-5.28	114.38	122.62
4	D	44	GLN	CA-C-N	-5.24	114.38	119.78
4	D	44	GLN	C-N-CA	-5.24	114.38	119.78
4	H	44	GLN	CA-C-N	-5.24	114.38	119.78
4	H	44	GLN	C-N-CA	-5.24	114.38	119.78
4	D	137	GLY	N-CA-C	5.20	119.95	111.27
4	L	137	GLY	N-CA-C	5.19	119.94	111.27
4	L	44	GLN	CA-C-N	-5.19	114.44	119.78
4	L	44	GLN	C-N-CA	-5.19	114.44	119.78
1	A	290	THR	CA-C-N	5.18	125.59	119.99
1	A	290	THR	C-N-CA	5.18	125.59	119.99
1	I	290	THR	CA-C-N	5.17	125.58	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	290	THR	C-N-CA	5.17	125.58	119.99
4	H	137	GLY	N-CA-C	5.16	119.89	111.27
1	E	290	THR	CA-C-N	5.15	125.55	119.99
1	E	290	THR	C-N-CA	5.15	125.55	119.99
1	E	440	GLN	CB-CA-C	-5.12	109.14	115.89
1	I	440	GLN	CB-CA-C	-5.11	109.14	115.89
1	A	440	GLN	CB-CA-C	-5.09	109.17	115.89
1	E	125	LEU	N-CA-C	5.07	118.56	112.38
1	E	311	GLY	CA-C-N	5.05	124.23	118.97
1	E	311	GLY	C-N-CA	5.05	124.23	118.97
1	A	125	LEU	N-CA-C	5.04	118.53	112.38
1	I	125	LEU	N-CA-C	5.01	118.50	112.38

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
1	A	56	SER	Peptide
1	A	80	ASN	Peptide
3	C	110	PRO	Peptide
1	E	236	THR	Peptide
1	E	56	SER	Peptide
1	E	80	ASN	Peptide
3	G	110	PRO	Peptide
1	I	236	THR	Peptide
1	I	56	SER	Peptide
1	I	80	ASN	Peptide
3	K	110	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	2821	146	0
1	E	3096	0	2821	145	0
1	I	3096	0	2821	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	385	0	82	2	0
2	F	385	0	82	2	0
2	J	385	0	82	3	0
3	C	1530	0	1472	21	0
3	G	1530	0	1472	19	0
3	K	1530	0	1472	23	0
4	D	1728	0	1699	37	0
4	H	1728	0	1699	33	0
4	L	1728	0	1699	46	0
5	M	83	0	70	1	0
5	N	83	0	70	0	0
5	O	83	0	70	6	0
5	P	83	0	70	0	0
5	S	83	0	70	1	0
5	T	83	0	70	0	0
5	U	83	0	70	6	0
5	V	83	0	70	0	0
5	Y	83	0	70	3	0
5	Z	83	0	70	0	0
5	a	83	0	70	4	0
5	b	83	0	70	0	0
6	Q	105	0	88	2	0
6	W	105	0	88	0	0
6	c	105	0	88	4	0
7	R	22	0	19	3	0
7	X	22	0	19	1	0
7	d	22	0	19	2	0
8	A	140	0	130	3	0
8	E	140	0	130	3	0
8	I	140	0	130	2	0
All	All	22014	0	19773	603	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 14.

All (603) 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:I:293:GLN:HB2	1:I:334:SER:HB3	1.33	1.11
1:E:293:GLN:HB2	1:E:334:SER:HB3	1.33	1.09
1:A:293:GLN:HB2	1:A:334:SER:HB3	1.33	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:GLU:HA	1:I:239:CYS:O	1.74	0.88
1:E:91:GLU:HA	1:E:239:CYS:O	1.74	0.86
1:A:91:GLU:HA	1:A:239:CYS:O	1.74	0.86
1:I:358:ILE:HB	1:I:465:THR:HG22	1.58	0.84
1:E:358:ILE:HB	1:E:465:THR:HG22	1.58	0.84
1:A:358:ILE:HB	1:A:465:THR:HG22	1.58	0.84
1:A:260:LEU:HB2	1:A:450:THR:O	1.78	0.83
1:I:260:LEU:HB2	1:I:450:THR:O	1.79	0.83
4:D:38:ARG:N	4:D:46:GLU:O	2.12	0.83
4:H:38:ARG:N	4:H:46:GLU:O	2.12	0.82
4:L:38:ARG:N	4:L:46:GLU:O	2.12	0.81
1:E:260:LEU:HB2	1:E:450:THR:O	1.79	0.81
4:H:38:ARG:O	4:H:46:GLU:N	2.15	0.79
4:D:38:ARG:O	4:D:46:GLU:N	2.15	0.78
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.48	0.78
1:I:269:GLU:HA	1:I:289:ASN:HD22	1.48	0.78
1:E:269:GLU:HA	1:E:289:ASN:HD22	1.48	0.77
4:L:38:ARG:O	4:L:46:GLU:N	2.15	0.76
1:E:335:LYS:HD3	1:E:414:ILE:HD11	1.67	0.76
4:D:99:ARG:HG2	4:D:100(L):THR:HG22	1.68	0.76
1:I:335:LYS:HD3	1:I:414:ILE:HD11	1.68	0.75
1:A:335:LYS:HD3	1:A:414:ILE:HD11	1.67	0.75
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.69	0.75
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.68	0.75
4:L:35:SER:HB3	4:L:47:TRP:HE1	1.51	0.74
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.69	0.74
1:E:101:VAL:HG13	1:E:479:TRP:HB2	1.69	0.74
1:E:55:ALA:HB3	1:E:216:HIS:HB2	1.68	0.74
4:H:99:ARG:HG2	4:H:100(L):THR:HG22	1.68	0.74
4:L:99:ARG:HG2	4:L:100(L):THR:HG22	1.68	0.74
1:I:55:ALA:HB3	1:I:216:HIS:HB2	1.68	0.74
1:A:436:ALA:HB3	1:A:437:PRO:HD3	1.70	0.73
1:I:436:ALA:HB3	1:I:437:PRO:HD3	1.69	0.73
1:E:436:ALA:HB3	1:E:437:PRO:HD3	1.70	0.73
1:A:327:ARG:HA	4:D:100(H):LYS:HD2	1.71	0.72
1:E:327:ARG:HA	4:H:100(H):LYS:HD2	1.70	0.72
1:E:227:LYS:HE3	1:E:485:LYS:HD2	1.75	0.69
1:I:227:LYS:HE3	1:I:485:LYS:HD2	1.75	0.69
4:D:100(C):GLY:HA3	6:Q:2:NAG:H4	1.74	0.69
1:A:227:LYS:HE3	1:A:485:LYS:HD2	1.75	0.69
4:L:37:ILE:HG23	4:L:47:TRP:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:ILE:HG23	4:D:47:TRP:HA	1.76	0.68
4:H:38:ARG:O	4:H:46:GLU:O	2.12	0.68
1:E:294:ILE:HG23	1:E:447:SER:HB2	1.76	0.68
4:H:37:ILE:HG23	4:H:47:TRP:HA	1.76	0.67
1:A:294:ILE:HG23	1:A:447:SER:HB2	1.76	0.67
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.27	0.67
1:I:477:ASP:OD1	1:I:480:ARG:NH1	2.27	0.67
4:D:38:ARG:O	4:D:46:GLU:O	2.12	0.67
2:F:35:UNK:O	2:F:37:UNK:O	2.12	0.67
2:B:35:UNK:O	2:B:37:UNK:O	2.12	0.67
3:G:39:ARG:HG3	3:G:40:PRO:HD2	1.77	0.67
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.27	0.67
2:J:35:UNK:O	2:J:37:UNK:O	2.12	0.67
4:L:38:ARG:O	4:L:46:GLU:O	2.12	0.67
3:K:39:ARG:HG3	3:K:40:PRO:HD2	1.77	0.66
1:I:294:ILE:HG23	1:I:447:SER:HB2	1.78	0.66
3:C:39:ARG:HG3	3:C:40:PRO:HD2	1.77	0.66
1:A:350:ARG:NH2	1:A:397:SER:O	2.29	0.66
4:D:35:SER:HB3	4:D:47:TRP:HE1	1.62	0.65
1:I:350:ARG:NH2	1:I:397:SER:O	2.29	0.65
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.79	0.65
1:I:327:ARG:HA	4:L:100(H):LYS:HD2	1.78	0.65
1:I:101:VAL:HG21	1:I:480:ARG:HG2	1.79	0.65
4:L:100(A):ILE:HB	7:d:1:MAN:H3	1.78	0.65
1:E:350:ARG:NH2	1:E:397:SER:O	2.29	0.64
3:K:37:GLN:N	3:K:45:SER:O	2.31	0.64
1:E:359:ILE:HD12	1:E:468:PHE:HE1	1.63	0.64
1:A:68:VAL:O	1:A:72:HIS:ND1	2.31	0.63
1:A:359:ILE:HD12	1:A:468:PHE:HE1	1.63	0.63
1:E:330:HIS:HE1	1:E:415:THR:HG21	1.63	0.63
1:E:68:VAL:O	1:E:72:HIS:ND1	2.31	0.63
1:E:91:GLU:O	1:E:238:PRO:HA	1.99	0.63
1:I:91:GLU:O	1:I:238:PRO:HA	1.99	0.63
1:E:101:VAL:HG21	1:E:480:ARG:HG2	1.79	0.63
4:H:34:TRP:CZ3	4:H:94:THR:HG22	2.34	0.63
1:I:359:ILE:HD12	1:I:468:PHE:HE1	1.63	0.63
3:C:37:GLN:N	3:C:45:SER:O	2.31	0.62
1:E:100:MET:HE2	1:E:488:VAL:H	1.64	0.62
3:G:37:GLN:N	3:G:45:SER:O	2.31	0.62
1:I:100:MET:HE2	1:I:488:VAL:H	1.64	0.62
1:A:100:MET:HE2	1:A:488:VAL:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:HIS:CG	4:H:100(E):VAL:HG23	2.34	0.62
1:A:91:GLU:O	1:A:238:PRO:HA	1.99	0.62
1:A:83:GLU:HG3	1:A:84:ILE:H	1.65	0.62
1:I:68:VAL:O	1:I:72:HIS:ND1	2.31	0.62
1:A:363:ASN:O	1:A:469:ARG:NH1	2.33	0.62
1:I:363:ASN:O	1:I:469:ARG:NH1	2.33	0.62
1:A:100:MET:N	1:A:100:MET:SD	2.73	0.61
1:E:330:HIS:CB	4:H:100(E):VAL:HG23	2.30	0.61
1:I:100:MET:SD	1:I:100:MET:N	2.73	0.61
1:E:226:LEU:HD11	1:E:487:LYS:HB3	1.82	0.61
1:I:83:GLU:HG3	1:I:84:ILE:H	1.65	0.61
1:E:358:ILE:HG13	1:E:397:SER:H	1.66	0.61
1:A:332:ASN:HB3	8:A:1295:NAG:H82	1.82	0.61
1:E:330:HIS:CE1	1:E:415:THR:CG2	2.84	0.61
1:E:363:ASN:O	1:E:469:ARG:NH1	2.33	0.61
1:A:177:TYR:HE2	1:A:422:GLN:HE21	1.49	0.60
1:I:226:LEU:HD11	1:I:487:LYS:HB3	1.83	0.60
1:A:330:HIS:ND1	4:D:100(E):VAL:HG23	2.16	0.60
1:E:332:ASN:HB3	8:E:1295:NAG:H82	1.83	0.60
4:H:37:ILE:HG13	4:H:47:TRP:HD1	1.67	0.60
1:I:358:ILE:HG13	1:I:397:SER:H	1.66	0.60
4:L:34:TRP:CZ3	4:L:94:THR:HG22	2.37	0.60
1:E:83:GLU:HG3	1:E:84:ILE:H	1.65	0.60
1:I:177:TYR:HE2	1:I:422:GLN:HE21	1.49	0.60
4:L:100(C):GLY:CA	6:c:2:NAG:H4	2.31	0.60
1:E:226:LEU:HD11	1:E:487:LYS:HD3	1.82	0.60
3:G:37:GLN:O	3:G:45:SER:O	2.20	0.60
1:E:100:MET:SD	1:E:100:MET:N	2.73	0.59
1:I:226:LEU:HD11	1:I:487:LYS:HD3	1.82	0.59
1:A:226:LEU:HD11	1:A:487:LYS:HD3	1.82	0.59
1:A:358:ILE:HG13	1:A:397:SER:H	1.66	0.59
1:E:52:LEU:HB3	1:E:217:TYR:HD2	1.67	0.59
1:A:226:LEU:HD11	1:A:487:LYS:HB3	1.83	0.59
1:I:52:LEU:HB3	1:I:217:TYR:HD2	1.68	0.59
3:C:37:GLN:O	3:C:45:SER:O	2.20	0.59
3:K:31:ARG:O	4:L:100:ARG:NH1	2.34	0.59
3:K:37:GLN:O	3:K:45:SER:O	2.20	0.59
4:L:54:SER:HB2	5:Y:6:MAN:O4	2.03	0.59
1:E:256:SER:HB2	1:E:374:HIS:HE1	1.68	0.59
4:L:37:ILE:HG13	4:L:47:TRP:HD1	1.66	0.59
1:E:177:TYR:HE2	1:E:422:GLN:HE21	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:LEU:CD1	1:I:487:LYS:HB3	2.33	0.59
1:I:258:GLN:O	1:I:452:LEU:HA	2.03	0.59
1:I:476:ARG:HA	1:I:479:TRP:CD1	2.38	0.59
4:D:37:ILE:HG13	4:D:47:TRP:HD1	1.67	0.58
1:E:258:GLN:O	1:E:452:LEU:HA	2.03	0.58
1:I:256:SER:HB2	1:I:374:HIS:HE1	1.68	0.58
1:E:226:LEU:CD1	1:E:487:LYS:HB3	2.33	0.58
1:E:476:ARG:HA	1:E:479:TRP:CD1	2.38	0.58
1:A:256:SER:HB2	1:A:374:HIS:HE1	1.68	0.58
4:L:33:TYR:HB2	4:L:95:THR:O	2.03	0.58
1:A:325:ASP:O	4:D:100(I):GLU:OE2	2.22	0.58
1:A:258:GLN:O	1:A:452:LEU:HA	2.03	0.58
3:K:36:TYR:HA	3:K:46:LEU:HA	1.85	0.58
4:D:4:LEU:HD11	4:D:94:THR:HG23	1.85	0.58
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.38	0.57
1:E:122:LEU:HA	1:E:201:ILE:HA	1.86	0.57
3:G:36:TYR:HA	3:G:46:LEU:HA	1.85	0.57
1:A:98:ASN:HB3	1:A:100:MET:HG2	1.87	0.57
1:I:332:ASN:HB3	8:I:1295:NAG:H82	1.85	0.57
3:C:36:TYR:HA	3:C:46:LEU:HA	1.85	0.57
1:A:122:LEU:HA	1:A:201:ILE:HA	1.86	0.57
1:A:226:LEU:CD1	1:A:487:LYS:HB3	2.33	0.57
1:A:422:GLN:O	1:A:434:MET:HA	2.05	0.57
3:C:145:VAL:HG12	3:C:198:HIS:HB2	1.86	0.57
1:I:98:ASN:HB3	1:I:100:MET:HG2	1.87	0.57
1:A:52:LEU:HB3	1:A:217:TYR:HD2	1.68	0.57
1:A:53:PHE:HB3	1:A:218:CYS:HB2	1.87	0.57
1:I:53:PHE:HB3	1:I:218:CYS:HB2	1.87	0.57
3:G:145:VAL:HG12	3:G:198:HIS:HB2	1.86	0.57
1:A:259:LEU:HB3	1:A:449:ILE:HG23	1.85	0.57
1:I:122:LEU:HA	1:I:201:ILE:HA	1.86	0.57
1:I:422:GLN:O	1:I:434:MET:HA	2.05	0.57
1:E:325:ASP:O	4:H:100(I):GLU:OE2	2.23	0.57
4:L:161:VAL:HG22	4:L:180:VAL:HG12	1.87	0.57
1:E:53:PHE:HB3	1:E:218:CYS:HB2	1.86	0.56
1:I:259:LEU:HB3	1:I:449:ILE:HG23	1.86	0.56
1:E:259:LEU:HB3	1:E:449:ILE:HG23	1.86	0.56
1:E:422:GLN:O	1:E:434:MET:HA	2.05	0.56
3:K:110:PRO:HB2	3:K:111:LYS:HB2	1.87	0.56
4:D:161:VAL:HG22	4:D:180:VAL:HG12	1.88	0.56
3:K:145:VAL:HG12	3:K:198:HIS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ASN:HB3	1:E:100:MET:HG2	1.86	0.56
1:E:330:HIS:HE1	1:E:415:THR:CG2	2.19	0.56
4:D:37:ILE:HG13	4:D:47:TRP:CD1	2.41	0.56
1:E:82:GLN:O	1:E:84:ILE:HG13	2.06	0.56
4:D:37:ILE:HA	4:D:47:TRP:HA	1.88	0.56
1:I:82:GLN:O	1:I:84:ILE:HG13	2.06	0.56
4:L:37:ILE:HG13	4:L:47:TRP:CD1	2.41	0.56
1:A:199:SER:HA	1:I:312:PRO:HB3	1.86	0.55
4:H:37:ILE:HA	4:H:47:TRP:HA	1.88	0.55
1:A:347:LYS:O	1:A:350:ARG:HG2	2.06	0.55
1:I:217:TYR:O	1:I:248:THR:HG23	2.07	0.55
4:H:37:ILE:HG13	4:H:47:TRP:CD1	2.41	0.55
3:C:50:ASN:OD1	4:D:100:ARG:NH2	2.36	0.55
1:I:347:LYS:O	1:I:350:ARG:HG2	2.06	0.55
1:E:217:TYR:O	1:E:248:THR:HG23	2.07	0.55
4:D:100(A):ILE:HB	7:R:1:MAN:H3	1.88	0.55
1:E:347:LYS:O	1:E:350:ARG:HG2	2.06	0.55
4:H:161:VAL:HG22	4:H:180:VAL:HG12	1.88	0.55
1:A:82:GLN:O	1:A:84:ILE:HG13	2.06	0.54
1:E:451:GLY:O	1:E:452:LEU:HD23	2.08	0.54
1:I:93:PHE:CE1	1:I:226:LEU:HD13	2.42	0.54
1:A:93:PHE:CE1	1:A:226:LEU:HD13	2.42	0.54
3:C:39:ARG:NH1	3:C:81:GLY:O	2.40	0.54
1:E:93:PHE:CE1	1:E:226:LEU:HD13	2.42	0.54
1:A:217:TYR:O	1:A:248:THR:HG23	2.07	0.54
1:A:346:VAL:HG21	1:A:395:TRP:CD1	2.43	0.54
1:E:478:ASN:O	1:E:481:SER:OG	2.20	0.54
3:K:39:ARG:NH1	3:K:81:GLY:O	2.40	0.54
1:A:396:ILE:HG22	1:A:398:ASN:H	1.73	0.54
1:E:396:ILE:HG22	1:E:398:ASN:H	1.73	0.54
4:D:34:TRP:CZ3	4:D:94:THR:HG22	2.43	0.54
1:E:64:GLU:HB2	1:E:209:SER:HB3	1.90	0.54
1:E:344:LYS:HA	1:E:347:LYS:HE2	1.90	0.54
3:G:50:ASN:ND2	7:X:2:MAN:O2	2.38	0.54
1:I:63:THR:OG1	1:I:64:GLU:N	2.40	0.54
1:I:344:LYS:HA	1:I:347:LYS:HE2	1.90	0.54
1:E:346:VAL:HG21	1:E:395:TRP:CD1	2.43	0.54
1:I:64:GLU:HB2	1:I:209:SER:HB3	1.90	0.54
1:I:82:GLN:O	1:I:84:ILE:N	2.41	0.54
4:H:4:LEU:HD11	4:H:94:THR:HG23	1.90	0.54
4:L:37:ILE:HA	4:L:47:TRP:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HB2	1:A:209:SER:HB3	1.90	0.53
1:I:451:GLY:O	1:I:452:LEU:HD23	2.07	0.53
4:L:54:SER:HB2	5:Y:6:MAN:HO4	1.72	0.53
1:A:451:GLY:O	1:A:452:LEU:HD23	2.07	0.53
1:E:55:ALA:O	1:E:216:HIS:ND1	2.42	0.53
1:E:63:THR:OG1	1:E:64:GLU:N	2.40	0.53
1:A:265:LEU:HD23	1:A:450:THR:HG23	1.91	0.53
1:A:298:ARG:HG2	1:A:383:PHE:CZ	2.43	0.53
3:G:37:GLN:HB2	3:G:47:ILE:HG12	1.90	0.53
1:I:55:ALA:O	1:I:216:HIS:ND1	2.42	0.53
1:I:346:VAL:HG21	1:I:395:TRP:CD1	2.43	0.53
3:K:37:GLN:HB2	3:K:47:ILE:HG12	1.91	0.53
3:K:109:GLN:HB3	3:K:141:TYR:HE2	1.73	0.53
1:A:82:GLN:O	1:A:84:ILE:N	2.41	0.53
1:I:265:LEU:HD23	1:I:450:THR:HG23	1.90	0.53
1:A:63:THR:OG1	1:A:64:GLU:N	2.40	0.53
1:A:344:LYS:HA	1:A:347:LYS:HE2	1.90	0.53
1:E:82:GLN:O	1:E:84:ILE:N	2.41	0.53
1:I:46:LYS:HB3	1:I:490:LYS:HG3	1.90	0.53
1:A:299:PRO:HA	1:A:442:VAL:HA	1.91	0.53
1:A:378:CYS:HB2	1:A:383:PHE:CE1	2.44	0.53
3:C:37:GLN:HB2	3:C:47:ILE:HG12	1.91	0.53
1:E:46:LYS:HB3	1:E:490:LYS:HG3	1.91	0.53
1:I:252:LYS:HD3	5:a:1:NAG:H81	1.89	0.53
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.90	0.53
4:L:35:SER:OG	4:L:95:THR:OG1	2.19	0.53
4:D:100(C):GLY:CA	6:Q:2:NAG:H4	2.37	0.53
1:E:265:LEU:HD23	1:E:450:THR:HG23	1.91	0.53
1:A:305:LYS:O	1:A:318:ALA:N	2.42	0.53
1:E:66:HIS:HB3	1:E:213:ILE:HG12	1.90	0.53
1:E:378:CYS:HB2	1:E:383:PHE:CE1	2.44	0.53
1:I:305:LYS:O	1:I:318:ALA:N	2.42	0.53
1:I:298:ARG:HG2	1:I:383:PHE:CZ	2.43	0.52
1:E:298:ARG:HG2	1:E:383:PHE:CZ	2.43	0.52
1:I:66:HIS:HB3	1:I:213:ILE:HG12	1.91	0.52
4:L:189:THR:OG1	4:L:190:GLN:N	2.42	0.52
1:E:305:LYS:O	1:E:318:ALA:N	2.42	0.52
1:I:299:PRO:HA	1:I:442:VAL:HA	1.91	0.52
3:K:133:LEU:HD12	3:K:179:LEU:HD23	1.92	0.52
1:A:55:ALA:O	1:A:216:HIS:ND1	2.42	0.52
1:E:93:PHE:HE1	1:E:226:LEU:HD13	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396:ILE:HG22	1:I:398:ASN:H	1.73	0.52
1:A:93:PHE:HE1	1:A:226:LEU:HD13	1.75	0.52
3:C:133:LEU:HD12	3:C:179:LEU:HD23	1.92	0.52
4:H:189:THR:OG1	4:H:190:GLN:N	2.42	0.52
1:I:346:VAL:HA	1:I:349:LEU:HD12	1.92	0.52
3:K:17:GLN:CD	3:K:18:THR:H	2.18	0.52
3:K:109:GLN:HB3	3:K:141:TYR:CE2	2.45	0.52
3:G:17:GLN:CD	3:G:18:THR:H	2.18	0.52
1:I:378:CYS:HB2	1:I:383:PHE:CE1	2.44	0.52
1:I:330:HIS:ND1	4:L:100(E):VAL:HA	2.25	0.52
4:H:185:SER:O	4:H:188:GLY:N	2.44	0.51
1:E:159:PHE:HB2	1:E:172:VAL:HG23	1.93	0.51
3:G:39:ARG:NH1	3:G:81:GLY:O	2.40	0.51
1:E:299:PRO:HA	1:E:442:VAL:HA	1.91	0.51
1:E:346:VAL:HA	1:E:349:LEU:HD12	1.92	0.51
1:I:478:ASN:O	1:I:481:SER:OG	2.20	0.51
3:C:17:GLN:CD	3:C:18:THR:H	2.18	0.51
3:C:50:ASN:ND2	7:R:2:MAN:O2	2.38	0.51
4:D:185:SER:O	4:D:188:GLY:N	2.44	0.51
1:E:252:LYS:HD3	5:U:1:NAG:H81	1.93	0.51
4:L:185:SER:O	4:L:188:GLY:N	2.44	0.51
1:A:334:SER:HB2	8:A:1295:NAG:H83	1.93	0.51
1:A:346:VAL:HA	1:A:349:LEU:HD12	1.92	0.51
1:E:90:THR:HG22	1:E:91:GLU:H	1.76	0.51
1:I:64:GLU:HA	1:I:209:SER:N	2.26	0.51
1:I:90:THR:HG22	1:I:91:GLU:H	1.76	0.51
3:G:133:LEU:HD12	3:G:179:LEU:HD23	1.92	0.50
4:H:35:SER:HB3	4:H:47:TRP:HE1	1.76	0.50
1:I:248:THR:HG22	1:I:486:TYR:CE1	2.46	0.50
1:A:64:GLU:HA	1:A:209:SER:N	2.26	0.50
1:A:335:LYS:HG3	1:A:339:ASN:OD1	2.11	0.50
1:I:286:VAL:HB	1:I:452:LEU:HB2	1.94	0.50
1:I:325:ASP:O	4:L:100(I):GLU:OE2	2.29	0.50
1:A:212:PRO:HB2	5:O:1:NAG:C8	2.42	0.50
1:I:335:LYS:HG3	1:I:339:ASN:OD1	2.12	0.50
1:A:65:LYS:HZ2	1:A:208:VAL:HG11	1.76	0.50
1:A:159:PHE:HB2	1:A:172:VAL:HG23	1.92	0.50
1:A:248:THR:HG22	1:A:486:TYR:CE1	2.46	0.50
1:E:64:GLU:HA	1:E:209:SER:N	2.26	0.50
1:E:332:ASN:OD1	1:E:415:THR:HG23	2.11	0.50
1:I:159:PHE:HB2	1:I:172:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HD3	5:O:1:NAG:H81	1.93	0.50
1:A:327:ARG:CA	4:D:100(H):LYS:HD2	2.41	0.50
1:A:158:SER:O	1:A:159:PHE:HD1	1.94	0.49
1:A:330:HIS:CE1	4:D:100(E):VAL:HA	2.46	0.49
1:E:96:TRP:HZ2	1:E:273:ARG:HB3	1.77	0.49
1:I:93:PHE:HE1	1:I:226:LEU:HD13	1.75	0.49
1:A:90:THR:HG22	1:A:91:GLU:H	1.76	0.49
1:A:226:LEU:HA	1:A:243:SER:O	2.12	0.49
1:E:129:LEU:HA	1:E:159:PHE:CE1	2.47	0.49
1:E:474:ASP:HB3	1:E:476:ARG:HG2	1.94	0.49
1:E:212:PRO:HB2	5:U:1:NAG:C8	2.42	0.49
3:G:37:GLN:HB2	3:G:47:ILE:CG1	2.42	0.49
1:A:96:TRP:HZ2	1:A:273:ARG:HB3	1.76	0.49
1:E:335:LYS:HG3	1:E:339:ASN:OD1	2.12	0.49
1:E:226:LEU:HA	1:E:243:SER:O	2.12	0.49
1:E:248:THR:HG22	1:E:486:TYR:CE1	2.46	0.49
1:I:96:TRP:HZ2	1:I:273:ARG:HB3	1.77	0.49
3:K:37:GLN:HB2	3:K:47:ILE:CG1	2.42	0.49
1:E:202:THR:HA	1:E:434:MET:HB2	1.95	0.49
1:I:226:LEU:HA	1:I:243:SER:O	2.12	0.49
3:K:37:GLN:O	3:K:45:SER:C	2.56	0.49
1:A:474:ASP:HB3	1:A:476:ARG:HG2	1.94	0.49
1:E:286:VAL:HB	1:E:452:LEU:HB2	1.94	0.49
1:E:158:SER:O	1:E:159:PHE:HD1	1.94	0.49
1:E:334:SER:HB2	8:E:1295:NAG:H83	1.94	0.48
3:G:37:GLN:O	3:G:45:SER:C	2.56	0.48
1:I:202:THR:HA	1:I:434:MET:HB2	1.95	0.48
1:A:138:ILE:C	5:M:1:NAG:HN2	2.21	0.48
3:C:37:GLN:O	3:C:45:SER:C	2.56	0.48
4:D:100(A):ILE:HB	7:R:1:MAN:C3	2.42	0.48
4:L:100(C):GLY:HA3	6:c:2:NAG:H4	1.95	0.48
1:I:129:LEU:HA	1:I:159:PHE:CE1	2.48	0.48
1:I:158:SER:O	1:I:159:PHE:HD1	1.95	0.48
4:L:35:SER:CB	4:L:95:THR:OG1	2.61	0.48
1:E:129:LEU:HG	1:E:159:PHE:CZ	2.48	0.48
1:A:85:HIS:CE1	1:A:241:SER:HA	2.49	0.48
1:A:455:THR:HG23	1:A:471:GLY:HA3	1.95	0.48
4:D:189:THR:OG1	4:D:190:GLN:N	2.42	0.48
1:A:46:LYS:HB3	1:A:490:LYS:HG3	1.94	0.48
1:E:129:LEU:HA	1:E:159:PHE:HE1	1.79	0.48
1:A:129:LEU:HA	1:A:159:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HA	1:A:159:PHE:HE1	1.79	0.48
1:I:474:ASP:HB3	1:I:476:ARG:HG2	1.94	0.48
4:L:38:ARG:O	4:L:46:GLU:C	2.57	0.48
1:A:212:PRO:HB2	5:O:1:NAG:H83	1.96	0.48
1:A:478:ASN:O	1:A:481:SER:OG	2.20	0.48
3:C:37:GLN:O	3:C:45:SER:OG	2.21	0.48
3:C:37:GLN:HB2	3:C:47:ILE:CG1	2.42	0.48
3:C:36:TYR:HB3	3:C:45:SER:O	2.14	0.48
1:E:455:THR:HG23	1:E:471:GLY:HA3	1.95	0.48
1:I:85:HIS:CE1	1:I:241:SER:HA	2.49	0.48
1:I:455:THR:HG23	1:I:471:GLY:HA3	1.95	0.48
1:I:375:SER:HA	1:I:383:PHE:O	2.14	0.47
3:K:36:TYR:HB3	3:K:45:SER:O	2.14	0.47
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.94	0.47
1:A:375:SER:HA	1:A:383:PHE:O	2.14	0.47
1:I:365:SER:HB2	1:I:469:ARG:HD3	1.96	0.47
1:A:365:SER:HB2	1:A:469:ARG:HD3	1.96	0.47
4:D:38:ARG:O	4:D:46:GLU:C	2.57	0.47
3:G:36:TYR:HB3	3:G:45:SER:O	2.14	0.47
1:I:259:LEU:HD13	1:I:449:ILE:HD13	1.96	0.47
3:K:30:SER:HB2	4:L:100(B):TYR:OH	2.15	0.47
1:A:64:GLU:OE2	1:A:211:GLU:N	2.48	0.47
1:A:65:LYS:HG3	1:A:208:VAL:HB	1.96	0.47
1:E:85:HIS:CE1	1:E:241:SER:HA	2.49	0.47
1:E:85:HIS:ND1	1:E:242:VAL:O	2.36	0.47
1:I:55:ALA:HB3	1:I:216:HIS:CB	2.42	0.47
4:D:43:LYS:HE3	4:D:43:LYS:HB3	1.65	0.47
1:E:212:PRO:HB2	5:U:1:NAG:H83	1.96	0.47
1:E:354:GLY:O	1:E:357:THR:OG1	2.33	0.47
1:E:365:SER:HB2	1:E:469:ARG:HD3	1.97	0.47
1:I:64:GLU:OE2	1:I:211:GLU:N	2.48	0.47
1:I:129:LEU:HG	1:I:159:PHE:CZ	2.49	0.47
1:I:330:HIS:CE1	1:I:415:THR:CG2	2.98	0.47
1:I:333:VAL:HG13	1:I:414:ILE:HD12	1.97	0.47
4:L:124:PRO:HG3	4:L:136:LEU:HG	1.97	0.47
1:A:75:VAL:HG22	1:A:76:PRO:HD2	1.97	0.47
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.65	0.47
2:B:35:UNK:O	2:B:36:UNK:C	2.63	0.47
1:E:64:GLU:OE2	1:E:211:GLU:N	2.48	0.47
1:E:65:LYS:HG3	1:E:208:VAL:HB	1.96	0.47
1:E:175:LEU:HD21	1:E:320:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:SER:HA	1:E:383:PHE:O	2.15	0.47
4:H:38:ARG:O	4:H:46:GLU:C	2.57	0.47
1:A:129:LEU:HG	1:A:159:PHE:CZ	2.49	0.47
1:E:298:ARG:HB3	1:E:329:ALA:HB1	1.97	0.47
1:I:65:LYS:HG3	1:I:208:VAL:HB	1.96	0.47
1:I:75:VAL:HG22	1:I:76:PRO:HD2	1.97	0.47
1:I:252:LYS:HD3	5:a:1:NAG:C8	2.45	0.47
1:I:332:ASN:OD1	1:I:415:THR:HG23	2.15	0.47
4:L:35:SER:HG	4:L:95:THR:CB	2.25	0.47
1:I:298:ARG:H	1:I:298:ARG:HG3	1.60	0.47
1:I:330:HIS:CE1	4:L:100(E):VAL:HA	2.50	0.47
4:L:36:TRP:HE1	4:L:78:VAL:HG12	1.80	0.47
1:A:202:THR:HA	1:A:434:MET:HB2	1.96	0.46
1:A:333:VAL:HG13	1:A:414:ILE:HD12	1.97	0.46
1:E:259:LEU:HD13	1:E:449:ILE:HD13	1.97	0.46
1:E:64:GLU:HG2	1:E:67:ASN:H	1.80	0.46
1:E:138:ILE:C	5:S:1:NAG:HN2	2.23	0.46
1:A:64:GLU:HG2	1:A:67:ASN:H	1.80	0.46
1:A:85:HIS:CE1	1:A:242:VAL:H	2.34	0.46
1:A:324:GLY:HA2	3:C:67(C):PHE:CZ	2.50	0.46
4:H:36:TRP:HE1	4:H:78:VAL:HG12	1.80	0.46
4:H:124:PRO:HG3	4:H:136:LEU:HG	1.98	0.46
1:I:413:SER:O	6:c:1:NAG:O6	2.34	0.46
1:E:55:ALA:HB3	1:E:216:HIS:CB	2.42	0.46
1:E:75:VAL:HG22	1:E:76:PRO:HD2	1.97	0.46
1:I:272:ILE:HG22	1:I:286:VAL:HG13	1.98	0.46
1:A:85:HIS:ND1	1:A:242:VAL:O	2.36	0.46
1:E:252:LYS:HD3	5:U:1:NAG:C8	2.44	0.46
1:I:64:GLU:HG2	1:I:67:ASN:H	1.80	0.46
1:A:252:LYS:HD3	5:O:1:NAG:C8	2.45	0.46
1:I:175:LEU:HD21	1:I:320:GLY:HA3	1.98	0.46
1:I:212:PRO:HB2	5:a:1:NAG:C8	2.46	0.46
3:K:50:ASN:ND2	7:d:2:MAN:H4	2.31	0.46
1:A:49:GLU:HG3	1:A:223:PHE:HE2	1.79	0.46
1:A:55:ALA:HB3	1:A:216:HIS:CB	2.42	0.46
1:A:259:LEU:HD13	1:A:449:ILE:HD13	1.97	0.46
1:I:129:LEU:HA	1:I:159:PHE:HE1	1.81	0.46
1:A:332:ASN:OD1	1:A:415:THR:HG23	2.16	0.46
1:A:96:TRP:CH2	1:A:235:GLY:HA3	2.51	0.45
4:D:36:TRP:HE1	4:D:78:VAL:HG12	1.80	0.45
2:F:35:UNK:O	2:F:36:UNK:C	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:HIS:CE1	1:I:242:VAL:H	2.34	0.45
1:I:330:HIS:CE1	1:I:415:THR:HG21	2.51	0.45
1:A:57:ASP:OD1	1:A:58:ALA:N	2.49	0.45
1:A:298:ARG:HB3	1:A:329:ALA:HB1	1.98	0.45
1:A:354:GLY:O	1:A:357:THR:OG1	2.34	0.45
4:D:47:TRP:O	4:D:48:ILE:HG13	2.16	0.45
1:E:85:HIS:CE1	1:E:242:VAL:H	2.34	0.45
1:E:298:ARG:HG2	1:E:383:PHE:HZ	1.82	0.45
3:G:31:ARG:O	4:H:100:ARG:NH1	2.45	0.45
4:H:47:TRP:O	4:H:48:ILE:HG13	2.16	0.45
1:A:175:LEU:HD21	1:A:320:GLY:HA3	1.97	0.45
1:A:272:ILE:HG22	1:A:286:VAL:HG13	1.98	0.45
1:E:49:GLU:HG3	1:E:223:PHE:HE2	1.81	0.45
1:E:57:ASP:OD1	1:E:58:ALA:N	2.48	0.45
1:E:96:TRP:CH2	1:E:235:GLY:HA3	2.51	0.45
1:E:223:PHE:CE2	1:E:490:LYS:HB3	2.52	0.45
1:A:298:ARG:HG2	1:A:383:PHE:HZ	1.82	0.45
1:I:298:ARG:HG2	1:I:383:PHE:HZ	1.82	0.45
2:J:35:UNK:O	2:J:36:UNK:C	2.63	0.45
1:I:49:GLU:HG3	1:I:223:PHE:HE2	1.80	0.45
4:D:124:PRO:HG3	4:D:136:LEU:HG	1.97	0.45
1:E:272:ILE:HG22	1:E:286:VAL:HG13	1.98	0.45
1:I:96:TRP:CH2	1:I:235:GLY:HA3	2.52	0.45
1:I:65:LYS:NZ	1:I:208:VAL:HG11	2.32	0.45
1:A:65:LYS:NZ	1:A:208:VAL:HG11	2.32	0.45
1:E:44:VAL:HB	1:E:492:GLU:HB2	1.99	0.45
1:A:252:LYS:HB3	5:O:1:NAG:H81	1.98	0.45
3:C:46:LEU:HD23	3:C:55:PRO:HG3	1.99	0.45
3:G:116:VAL:HG23	3:G:205:LYS:HD2	1.99	0.45
1:I:138:ILE:C	5:Y:1:NAG:HN2	2.25	0.45
1:I:220:PRO:HG2	1:I:223:PHE:CD1	2.52	0.45
1:I:298:ARG:HB3	1:I:329:ALA:HB1	1.99	0.45
1:E:422:GLN:OE1	1:E:436:ALA:HA	2.17	0.44
4:L:66:ARG:HD2	4:L:82(A):THR:O	2.17	0.44
4:D:66:ARG:HD2	4:D:82(A):THR:O	2.17	0.44
1:I:354:GLY:O	1:I:357:THR:OG1	2.34	0.44
1:E:62:GLU:O	1:E:63:THR:OG1	2.35	0.44
1:E:219:ALA:HB2	1:E:225:ILE:HG13	2.00	0.44
1:E:220:PRO:HG2	1:E:223:PHE:CD1	2.52	0.44
4:H:66:ARG:HD2	4:H:82(A):THR:O	2.17	0.44
1:I:85:HIS:ND1	1:I:242:VAL:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:47:TRP:O	4:L:48:ILE:HG13	2.16	0.44
3:C:167:LYS:HE3	3:C:173:TYR:CE1	2.52	0.44
1:E:65:LYS:NZ	1:E:208:VAL:HG11	2.32	0.44
1:I:259:LEU:HA	1:I:451:GLY:O	2.18	0.44
1:I:327:ARG:CA	4:L:100(H):LYS:HD2	2.44	0.44
3:K:46:LEU:HD23	3:K:55:PRO:HG3	1.99	0.44
4:L:34:TRP:CZ3	4:L:94:THR:CG2	3.01	0.44
1:A:259:LEU:HA	1:A:451:GLY:O	2.18	0.44
1:A:260:LEU:HD21	1:A:481:SER:OG	2.18	0.44
1:A:369:LEU:H	1:A:369:LEU:HG	1.58	0.44
1:I:260:LEU:HD21	1:I:481:SER:OG	2.17	0.44
1:I:440:GLN:HB3	1:I:441:GLY:H	1.53	0.44
4:L:100(C):GLY:HA2	6:c:2:NAG:H4	1.98	0.44
1:A:219:ALA:HB2	1:A:225:ILE:HG13	2.00	0.44
1:E:255:VAL:HG13	1:E:475:MET:SD	2.58	0.44
1:I:223:PHE:CD2	1:I:490:LYS:HB3	2.51	0.44
3:K:186:TRP:HH2	3:K:207:VAL:HG22	1.83	0.44
1:E:333:VAL:HG13	1:E:414:ILE:HD12	1.98	0.44
3:G:186:TRP:HH2	3:G:207:VAL:HG22	1.83	0.44
3:K:116:VAL:HG23	3:K:205:LYS:HD2	1.99	0.44
3:C:186:TRP:HH2	3:C:207:VAL:HG22	1.83	0.44
1:E:279:ASN:HB2	8:E:1276:NAG:O5	2.18	0.44
1:E:63:THR:O	1:E:208:VAL:HA	2.18	0.43
1:E:298:ARG:H	1:E:298:ARG:HG3	1.59	0.43
3:G:167:LYS:HE3	3:G:173:TYR:CE1	2.53	0.43
4:L:18:LEU:HD11	4:L:20:LEU:HD21	2.00	0.43
3:C:47:ILE:HD13	3:C:47:ILE:HA	1.87	0.43
1:I:255:VAL:HG13	1:I:475:MET:SD	2.58	0.43
1:I:369:LEU:H	1:I:369:LEU:HG	1.58	0.43
4:L:93:ALA:HA	4:L:100(R):VAL:O	2.18	0.43
1:A:54:CYS:SG	1:A:215:ILE:HG23	2.58	0.43
1:I:57:ASP:OD1	1:I:58:ALA:N	2.52	0.43
1:I:422:GLN:OE1	1:I:436:ALA:HA	2.17	0.43
1:A:422:GLN:OE1	1:A:436:ALA:HA	2.17	0.43
1:E:416:LEU:HA	1:E:417:PRO:HD3	1.65	0.43
4:H:43:LYS:HE3	4:H:43:LYS:HB3	1.65	0.43
1:A:255:VAL:HG13	1:A:475:MET:SD	2.58	0.43
3:C:116:VAL:HG23	3:C:205:LYS:HD2	2.00	0.43
1:E:259:LEU:HA	1:E:451:GLY:O	2.18	0.43
1:I:219:ALA:HB2	1:I:225:ILE:HG13	2.00	0.43
1:A:330:HIS:CE1	1:A:415:THR:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:TYR:HB3	1:E:62:GLU:H	1.53	0.43
1:I:54:CYS:SG	1:I:215:ILE:HG23	2.59	0.43
3:K:167:LYS:HE3	3:K:173:TYR:CE1	2.53	0.43
1:A:63:THR:O	1:A:208:VAL:HA	2.18	0.43
1:E:129:LEU:HG	1:E:159:PHE:HZ	1.83	0.43
1:E:239:CYS:HA	1:E:240:PRO:HD3	1.46	0.43
4:D:111:SER:O	4:D:111:SER:OG	2.32	0.43
3:G:46:LEU:HD23	3:G:55:PRO:HG3	1.99	0.43
1:I:63:THR:O	1:I:208:VAL:HA	2.18	0.43
1:I:104:MET:HG3	1:I:217:TYR:OH	2.19	0.43
1:A:220:PRO:HG2	1:A:223:PHE:CD1	2.53	0.43
1:E:252:LYS:HB3	5:U:1:NAG:H81	2.01	0.43
3:K:47:ILE:HD12	3:K:47:ILE:HG23	1.80	0.43
1:E:93:PHE:HD2	1:E:239:CYS:HB3	1.84	0.43
1:I:212:PRO:HB2	5:a:1:NAG:H83	2.00	0.43
4:L:43:LYS:HB3	4:L:43:LYS:HE3	1.65	0.43
1:A:292:VAL:HB	1:A:449:ILE:HB	2.01	0.42
1:E:54:CYS:SG	1:E:215:ILE:HG23	2.58	0.42
1:E:260:LEU:HD21	1:E:481:SER:OG	2.18	0.42
1:I:301:ASN:O	1:I:302:ASN:ND2	2.52	0.42
1:A:298:ARG:H	1:A:298:ARG:HG3	1.58	0.42
1:A:453:ILE:O	1:A:454:LEU:HD23	2.19	0.42
1:I:335:LYS:HA	1:I:338:TRP:HB3	2.02	0.42
1:A:93:PHE:HD2	1:A:239:CYS:HB3	1.84	0.42
1:I:44:VAL:HB	1:I:492:GLU:HB2	2.00	0.42
1:A:104:MET:HG3	1:A:217:TYR:OH	2.19	0.42
1:A:129:LEU:HG	1:A:159:PHE:HZ	1.84	0.42
1:I:129:LEU:HG	1:I:159:PHE:HZ	1.85	0.42
1:I:239:CYS:HA	1:I:240:PRO:HD3	1.46	0.42
1:I:359:ILE:HD13	1:I:466:GLU:HB2	2.02	0.42
1:A:223:PHE:CE2	1:A:490:LYS:HB3	2.54	0.42
1:E:292:VAL:HB	1:E:449:ILE:HB	2.01	0.42
1:E:453:ILE:O	1:E:454:LEU:HD23	2.19	0.42
1:E:223:PHE:CD2	1:E:490:LYS:HB3	2.55	0.42
1:I:161:MET:SD	1:I:172:VAL:HG21	2.60	0.42
1:I:453:ILE:O	1:I:454:LEU:HD23	2.19	0.42
1:I:161:MET:O	1:I:169:LYS:HA	2.20	0.42
1:E:104:MET:HG3	1:E:217:TYR:OH	2.19	0.42
4:H:18:LEU:HD11	4:H:20:LEU:HD21	2.01	0.42
4:H:111:SER:O	4:H:111:SER:OG	2.33	0.42
1:A:359:ILE:HD13	1:A:466:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:CYS:HA	1:E:216:HIS:O	2.20	0.42
1:I:45:TRP:HB3	1:I:489:VAL:HG21	2.02	0.42
1:A:330:HIS:CE1	1:A:415:THR:CG2	3.03	0.41
4:D:18:LEU:HD11	4:D:20:LEU:HD21	2.01	0.41
1:I:54:CYS:HA	1:I:216:HIS:O	2.20	0.41
1:E:335:LYS:O	1:E:339:ASN:N	2.48	0.41
1:E:335:LYS:HA	1:E:338:TRP:HB3	2.03	0.41
1:A:54:CYS:HA	1:A:216:HIS:O	2.20	0.41
4:D:197:ASN:OD1	4:D:199:LYS:HG3	2.21	0.41
1:E:436:ALA:CB	1:E:437:PRO:HD3	2.46	0.41
4:H:197:ASN:OD1	4:H:199:LYS:HG3	2.21	0.41
1:E:220:PRO:HB2	1:E:221:ALA:H	1.76	0.41
1:I:93:PHE:HD2	1:I:239:CYS:HB3	1.84	0.41
1:A:335:LYS:O	1:A:339:ASN:N	2.48	0.41
4:L:38:ARG:HB3	4:L:48:ILE:HD11	2.03	0.41
1:A:62:GLU:O	1:A:63:THR:OG1	2.35	0.41
1:A:262:ASN:CG	5:O:1:NAG:H82	2.46	0.41
1:A:301:ASN:O	1:A:302:ASN:ND2	2.54	0.41
1:A:385:CYS:O	1:A:387:THR:HG23	2.21	0.41
1:E:325:ASP:CB	3:G:94:ARG:HH11	2.33	0.41
1:A:44:VAL:HB	1:A:492:GLU:HB2	2.01	0.41
1:A:231:LYS:H	1:A:231:LYS:HD3	1.85	0.41
1:A:279:ASN:HB2	8:A:1276:NAG:O5	2.21	0.41
1:E:231:LYS:H	1:E:231:LYS:HD3	1.85	0.41
4:H:38:ARG:HB3	4:H:48:ILE:HD11	2.03	0.41
4:D:36:TRP:O	4:D:48:ILE:HB	2.21	0.41
1:E:262:ASN:CG	5:U:1:NAG:H82	2.46	0.41
1:E:359:ILE:HD13	1:E:466:GLU:HB2	2.02	0.41
4:H:36:TRP:O	4:H:48:ILE:HB	2.21	0.41
4:H:46:GLU:O	4:H:47:TRP:O	2.39	0.41
1:I:334:SER:HB2	8:I:1295:NAG:H83	2.02	0.41
1:I:335:LYS:HE2	1:I:339:ASN:ND2	2.36	0.41
1:I:385:CYS:O	1:I:387:THR:HG23	2.21	0.41
4:L:197:ASN:OD1	4:L:199:LYS:HG3	2.20	0.41
1:A:83:GLU:HA	1:A:244:THR:O	2.21	0.41
1:A:231:LYS:HB2	1:A:231:LYS:NZ	2.36	0.41
1:E:385:CYS:O	1:E:387:THR:HG23	2.21	0.41
1:I:62:GLU:HB3	1:I:63:THR:H	1.67	0.41
1:I:231:LYS:H	1:I:231:LYS:HD3	1.85	0.41
1:I:231:LYS:NZ	1:I:231:LYS:HB2	2.36	0.41
1:E:292:VAL:HG11	1:E:338:TRP:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:GLU:HA	1:I:244:THR:O	2.21	0.41
1:I:292:VAL:HB	1:I:449:ILE:HB	2.02	0.40
4:L:100(B):TYR:H	4:L:100(J):TRP:NE1	2.19	0.40
1:A:220:PRO:HB2	1:A:221:ALA:H	1.76	0.40
4:D:46:GLU:O	4:D:47:TRP:O	2.39	0.40
1:E:45:TRP:HB3	1:E:489:VAL:HG21	2.02	0.40
1:E:335:LYS:HE2	1:E:339:ASN:ND2	2.36	0.40
1:I:330:HIS:HB3	4:L:100(E):VAL:HG23	2.03	0.40
1:A:239:CYS:HA	1:A:240:PRO:HD3	1.46	0.40
1:E:331:CYS:SG	1:E:332:ASN:N	2.95	0.40
4:L:35:SER:HB2	4:L:95:THR:OG1	2.21	0.40
4:L:36:TRP:O	4:L:48:ILE:HB	2.21	0.40
4:L:117:PRO:HB3	4:L:143:TYR:HB3	2.04	0.40
4:D:100(B):TYR:H	4:D:100(J):TRP:NE1	2.19	0.40
4:H:30:ARG:HD3	4:H:73:LYS:HD3	2.04	0.40
1:I:223:PHE:CE2	1:I:490:LYS:HB3	2.57	0.40
1:I:345:VAL:O	1:I:349:LEU:HG	2.22	0.40
1:I:359:ILE:HD12	1:I:468:PHE:CE1	2.50	0.40
2:J:9:UNK:O	2:J:10:UNK:C	2.69	0.40
1:A:161:MET:SD	1:A:172:VAL:HG21	2.61	0.40
1:A:335:LYS:HE2	1:A:339:ASN:ND2	2.36	0.40
1:A:335:LYS:HA	1:A:338:TRP:HB3	2.03	0.40
4:D:1:GLN:OE1	4:D:1:GLN:N	2.53	0.40
4:H:100(B):TYR:H	4:H:100(J):TRP:NE1	2.19	0.40
1:I:65:LYS:HZ2	1:I:208:VAL:HG11	1.87	0.40
1:I:292:VAL:HG11	1:I:338:TRP:HE3	1.86	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	414/475 (87%)	349 (84%)	51 (12%)	14 (3%)	3	20
1	E	414/475 (87%)	348 (84%)	51 (12%)	15 (4%)	2	20
1	I	414/475 (87%)	348 (84%)	52 (13%)	14 (3%)	3	20
3	C	198/211 (94%)	191 (96%)	7 (4%)	0	100	100
3	G	198/211 (94%)	191 (96%)	7 (4%)	0	100	100
3	K	198/211 (94%)	192 (97%)	6 (3%)	0	100	100
4	D	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	24	63
4	H	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	24	63
4	L	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	24	63
All	All	2496/2763 (90%)	2258 (90%)	192 (8%)	46 (2%)	6	33

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	83	GLU
1	A	323	ILE
1	A	429	ARG
1	E	57	ASP
1	E	83	GLU
1	E	323	ILE
1	E	429	ARG
1	I	57	ASP
1	I	83	GLU
1	I	323	ILE
1	I	429	ARG
1	A	195	ASN
1	A	322	ILE
4	D	189	THR
1	E	195	ASN
1	E	322	ILE
4	H	189	THR
1	I	195	ASN
1	I	322	ILE
4	L	189	THR
1	A	56	SER
1	E	56	SER
1	I	56	SER
1	A	63	THR
1	A	220	PRO

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Mol	Chain	Res	Type
1	E	63	THR
1	E	220	PRO
1	I	63	THR
1	I	220	PRO
1	A	84	ILE
1	A	118	PRO
1	E	84	ILE
1	E	118	PRO
1	I	84	ILE
1	I	89	VAL
1	I	118	PRO
1	A	89	VAL
1	A	437	PRO
1	E	89	VAL
1	E	437	PRO
1	I	437	PRO
1	A	442	VAL
1	E	442	VAL
1	I	442	VAL
1	E	194	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/422 (75%)	294 (93%)	23 (7%)	13	34
1	E	317/422 (75%)	295 (93%)	22 (7%)	14	37
1	I	317/422 (75%)	293 (92%)	24 (8%)	12	33
3	C	171/180 (95%)	163 (95%)	8 (5%)	23	45
3	G	171/180 (95%)	163 (95%)	8 (5%)	23	45
3	K	171/180 (95%)	163 (95%)	8 (5%)	23	45
4	D	196/205 (96%)	187 (95%)	9 (5%)	24	46
4	H	196/205 (96%)	187 (95%)	9 (5%)	24	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	196/205 (96%)	187 (95%)	9 (5%)	24	46
All	All	2052/2421 (85%)	1932 (94%)	120 (6%)	18	40

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	53	PHE
1	A	61	TYR
1	A	75	VAL
1	A	90	THR
1	A	100	MET
1	A	107	ASP
1	A	125	LEU
1	A	156	ASN
1	A	197	ASN
1	A	231	LYS
1	A	277	ILE
1	A	298	ARG
1	A	330	HIS
1	A	357	THR
1	A	369	LEU
1	A	374	HIS
1	A	382	PHE
1	A	386	ASN
1	A	399	THR
1	A	414	ILE
1	A	464	THR
1	A	467	THR
3	C	13	VAL
3	C	17	GLN
3	C	39	ARG
3	C	109	GLN
3	C	130	LYS
3	C	136	LEU
3	C	161	GLU
3	C	164	THR
4	D	1	GLN
4	D	16	GLU
4	D	69	LEU
4	D	70	SER
4	D	71	LEU

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Mol	Chain	Res	Type
4	D	176	LEU
4	D	181	THR
4	D	190	GLN
4	D	191	THR
1	E	47	ASP
1	E	53	PHE
1	E	61	TYR
1	E	75	VAL
1	E	90	THR
1	E	100	MET
1	E	107	ASP
1	E	125	LEU
1	E	156	ASN
1	E	197	ASN
1	E	231	LYS
1	E	277	ILE
1	E	298	ARG
1	E	330	HIS
1	E	357	THR
1	E	369	LEU
1	E	374	HIS
1	E	382	PHE
1	E	399	THR
1	E	414	ILE
1	E	464	THR
1	E	467	THR
3	G	13	VAL
3	G	17	GLN
3	G	39	ARG
3	G	109	GLN
3	G	130	LYS
3	G	136	LEU
3	G	161	GLU
3	G	164	THR
4	H	1	GLN
4	H	16	GLU
4	H	69	LEU
4	H	70	SER
4	H	71	LEU
4	H	176	LEU
4	H	181	THR
4	H	190	GLN

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Mol	Chain	Res	Type
4	H	191	THR
1	I	47	ASP
1	I	53	PHE
1	I	61	TYR
1	I	75	VAL
1	I	90	THR
1	I	100	MET
1	I	107	ASP
1	I	125	LEU
1	I	137	ASN
1	I	156	ASN
1	I	197	ASN
1	I	231	LYS
1	I	277	ILE
1	I	298	ARG
1	I	330	HIS
1	I	357	THR
1	I	369	LEU
1	I	374	HIS
1	I	382	PHE
1	I	386	ASN
1	I	399	THR
1	I	414	ILE
1	I	464	THR
1	I	467	THR
3	K	13	VAL
3	K	17	GLN
3	K	39	ARG
3	K	109	GLN
3	K	130	LYS
3	K	136	LEU
3	K	161	GLU
3	K	164	THR
4	L	1	GLN
4	L	16	GLU
4	L	69	LEU
4	L	70	SER
4	L	71	LEU
4	L	176	LEU
4	L	181	THR
4	L	190	GLN
4	L	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	330	HIS
1	A	374	HIS
3	C	17	GLN
3	C	198	HIS
1	E	130	GLN
1	E	330	HIS
1	E	374	HIS
1	E	398	ASN
3	G	50	ASN
1	I	330	HIS
1	I	374	HIS
3	K	17	GLN
3	K	109	GLN
3	K	198	HIS
4	L	169	GLN

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](#)

117 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	$\# Z > 2$
5	NAG	M	1	5,1	14,14,15	0.57	0	17,19,21	1.35	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	2	5	14,14,15	0.54	0	17,19,21	0.82	0
5	BMA	M	3	5	11,11,12	0.68	0	15,15,17	0.77	1 (6%)
5	MAN	M	4	5	11,11,12	0.69	0	15,15,17	0.76	0
5	MAN	M	5	5	11,11,12	0.62	0	15,15,17	0.56	0
5	MAN	M	6	5	11,11,12	0.64	0	15,15,17	1.02	1 (6%)
5	MAN	M	7	5	11,11,12	0.58	0	15,15,17	0.56	0
5	NAG	N	1	5,1	14,14,15	0.59	0	17,19,21	1.42	3 (17%)
5	NAG	N	2	5	14,14,15	0.55	0	17,19,21	0.88	0
5	BMA	N	3	5	11,11,12	0.75	0	15,15,17	0.77	0
5	MAN	N	4	5	11,11,12	0.71	0	15,15,17	0.99	0
5	MAN	N	5	5	11,11,12	0.62	0	15,15,17	0.56	0
5	MAN	N	6	5	11,11,12	0.69	0	15,15,17	0.69	0
5	MAN	N	7	5	11,11,12	0.57	0	15,15,17	0.60	0
5	NAG	O	1	5,1	14,14,15	0.74	0	17,19,21	1.45	3 (17%)
5	NAG	O	2	5	14,14,15	0.55	0	17,19,21	0.74	0
5	BMA	O	3	5	11,11,12	0.73	0	15,15,17	0.65	0
5	MAN	O	4	5	11,11,12	0.68	0	15,15,17	0.81	0
5	MAN	O	5	5	11,11,12	0.62	0	15,15,17	0.54	0
5	MAN	O	6	5	11,11,12	0.69	0	15,15,17	0.69	0
5	MAN	O	7	5	11,11,12	0.58	0	15,15,17	0.58	0
5	NAG	P	1	5,1	14,14,15	0.60	0	17,19,21	1.16	1 (5%)
5	NAG	P	2	5	14,14,15	0.57	0	17,19,21	0.77	0
5	BMA	P	3	5	11,11,12	0.71	0	15,15,17	0.71	0
5	MAN	P	4	5	11,11,12	0.69	0	15,15,17	0.81	0
5	MAN	P	5	5	11,11,12	0.61	0	15,15,17	0.54	0
5	MAN	P	6	5	11,11,12	0.67	0	15,15,17	0.70	0
5	MAN	P	7	5	11,11,12	0.57	0	15,15,17	0.56	0
6	NAG	Q	1	1,6	14,14,15	0.61	0	17,19,21	1.50	3 (17%)
6	NAG	Q	2	6	14,14,15	0.52	0	17,19,21	1.09	1 (5%)
6	BMA	Q	3	6	11,11,12	0.69	0	15,15,17	1.24	1 (6%)
6	MAN	Q	4	6	11,11,12	0.52	0	15,15,17	0.73	0
6	MAN	Q	5	6	11,11,12	0.59	0	15,15,17	0.73	0
6	MAN	Q	6	6	11,11,12	0.64	0	15,15,17	0.56	0
6	MAN	Q	7	6	11,11,12	0.65	0	15,15,17	0.95	0
6	MAN	Q	8	6	11,11,12	0.60	0	15,15,17	0.57	0
6	MAN	Q	9	6	11,11,12	0.61	0	15,15,17	0.50	0
7	MAN	R	1	7	11,11,12	0.70	0	15,15,17	1.08	1 (6%)
7	MAN	R	2	7	11,11,12	0.68	0	15,15,17	0.58	0
5	NAG	S	1	5,1	14,14,15	0.57	0	17,19,21	1.35	1 (5%)
5	NAG	S	2	5	14,14,15	0.53	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	S	3	5	11,11,12	0.68	0	15,15,17	0.77	1 (6%)
5	MAN	S	4	5	11,11,12	0.69	0	15,15,17	0.75	0
5	MAN	S	5	5	11,11,12	0.61	0	15,15,17	0.56	0
5	MAN	S	6	5	11,11,12	0.67	0	15,15,17	0.73	0
5	MAN	S	7	5	11,11,12	0.59	0	15,15,17	0.55	0
5	NAG	T	1	5,1	14,14,15	0.59	0	17,19,21	1.41	3 (17%)
5	NAG	T	2	5	14,14,15	0.54	0	17,19,21	0.89	0
5	BMA	T	3	5	11,11,12	0.76	0	15,15,17	0.78	0
5	MAN	T	4	5	11,11,12	0.72	0	15,15,17	0.98	0
5	MAN	T	5	5	11,11,12	0.61	0	15,15,17	0.56	0
5	MAN	T	6	5	11,11,12	0.69	0	15,15,17	0.69	0
5	MAN	T	7	5	11,11,12	0.57	0	15,15,17	0.60	0
5	NAG	U	1	5,1	14,14,15	0.73	0	17,19,21	1.43	3 (17%)
5	NAG	U	2	5	14,14,15	0.54	0	17,19,21	0.72	0
5	BMA	U	3	5	11,11,12	0.73	0	15,15,17	0.66	0
5	MAN	U	4	5	11,11,12	0.68	0	15,15,17	0.80	0
5	MAN	U	5	5	11,11,12	0.62	0	15,15,17	0.54	0
5	MAN	U	6	5	11,11,12	0.68	0	15,15,17	0.70	0
5	MAN	U	7	5	11,11,12	0.58	0	15,15,17	0.59	0
5	NAG	V	1	5,1	14,14,15	0.60	0	17,19,21	1.10	1 (5%)
5	NAG	V	2	5	14,14,15	0.56	0	17,19,21	0.77	0
5	BMA	V	3	5	11,11,12	0.70	0	15,15,17	0.73	0
5	MAN	V	4	5	11,11,12	0.69	0	15,15,17	0.81	0
5	MAN	V	5	5	11,11,12	0.63	0	15,15,17	0.54	0
5	MAN	V	6	5	11,11,12	0.68	0	15,15,17	0.69	0
5	MAN	V	7	5	11,11,12	0.59	0	15,15,17	0.56	0
6	NAG	W	1	1,6	14,14,15	0.62	0	17,19,21	1.54	3 (17%)
6	NAG	W	2	6	14,14,15	0.56	0	17,19,21	0.76	0
6	BMA	W	3	6	11,11,12	0.74	0	15,15,17	0.89	1 (6%)
6	MAN	W	4	6	11,11,12	0.52	0	15,15,17	0.70	0
6	MAN	W	5	6	11,11,12	0.58	0	15,15,17	0.74	0
6	MAN	W	6	6	11,11,12	0.65	0	15,15,17	0.56	0
6	MAN	W	7	6	11,11,12	0.65	0	15,15,17	0.95	0
6	MAN	W	8	6	11,11,12	0.61	0	15,15,17	0.56	0
6	MAN	W	9	6	11,11,12	0.62	0	15,15,17	0.51	0
7	MAN	X	1	7	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
7	MAN	X	2	7	11,11,12	0.64	0	15,15,17	0.71	0
5	NAG	Y	1	5,1	14,14,15	0.57	0	17,19,21	1.42	1 (5%)
5	NAG	Y	2	5	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
5	BMA	Y	3	5	11,11,12	0.66	0	15,15,17	0.82	1 (6%)
5	MAN	Y	4	5	11,11,12	0.68	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	Y	5	5	11,11,12	0.63	0	15,15,17	0.54	0
5	MAN	Y	6	5	11,11,12	0.67	0	15,15,17	1.04	1 (6%)
5	MAN	Y	7	5	11,11,12	0.58	0	15,15,17	0.55	0
5	NAG	Z	1	5,1	14,14,15	0.61	0	17,19,21	1.46	2 (11%)
5	NAG	Z	2	5	14,14,15	0.57	0	17,19,21	0.89	0
5	BMA	Z	3	5	11,11,12	0.75	0	15,15,17	0.78	0
5	MAN	Z	4	5	11,11,12	0.72	0	15,15,17	1.00	0
5	MAN	Z	5	5	11,11,12	0.62	0	15,15,17	0.56	0
5	MAN	Z	6	5	11,11,12	0.67	0	15,15,17	0.69	0
5	MAN	Z	7	5	11,11,12	0.55	0	15,15,17	0.61	0
5	NAG	a	1	5,1	14,14,15	0.71	0	17,19,21	1.47	3 (17%)
5	NAG	a	2	5	14,14,15	0.55	0	17,19,21	0.74	0
5	BMA	a	3	5	11,11,12	0.73	0	15,15,17	0.66	0
5	MAN	a	4	5	11,11,12	0.68	0	15,15,17	0.81	0
5	MAN	a	5	5	11,11,12	0.62	0	15,15,17	0.54	0
5	MAN	a	6	5	11,11,12	0.69	0	15,15,17	0.70	0
5	MAN	a	7	5	11,11,12	0.58	0	15,15,17	0.58	0
5	NAG	b	1	5,1	14,14,15	0.67	0	17,19,21	1.15	1 (5%)
5	NAG	b	2	5	14,14,15	0.57	0	17,19,21	0.79	0
5	BMA	b	3	5	11,11,12	0.72	0	15,15,17	0.71	0
5	MAN	b	4	5	11,11,12	0.69	0	15,15,17	0.81	0
5	MAN	b	5	5	11,11,12	0.62	0	15,15,17	0.54	0
5	MAN	b	6	5	11,11,12	0.69	0	15,15,17	0.69	0
5	MAN	b	7	5	11,11,12	0.58	0	15,15,17	0.57	0
6	NAG	c	1	1,6	14,14,15	0.55	0	17,19,21	1.56	3 (17%)
6	NAG	c	2	6	14,14,15	0.57	0	17,19,21	1.13	1 (5%)
6	BMA	c	3	6	11,11,12	0.70	0	15,15,17	1.30	1 (6%)
6	MAN	c	4	6	11,11,12	0.51	0	15,15,17	0.74	0
6	MAN	c	5	6	11,11,12	0.58	0	15,15,17	0.74	0
6	MAN	c	6	6	11,11,12	0.66	0	15,15,17	0.56	0
6	MAN	c	7	6	11,11,12	0.65	0	15,15,17	1.03	1 (6%)
6	MAN	c	8	6	11,11,12	0.61	0	15,15,17	0.56	0
6	MAN	c	9	6	11,11,12	0.62	0	15,15,17	0.50	0
7	MAN	d	1	7	11,11,12	0.71	0	15,15,17	1.03	1 (6%)
7	MAN	d	2	7	11,11,12	0.73	0	15,15,17	0.68	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	MAN	S	4	5	-	0/2/19/22	0/1/1/1
5	MAN	S	5	5	-	0/2/19/22	0/1/1/1
5	MAN	S	6	5	-	0/2/19/22	0/1/1/1
5	MAN	S	7	5	-	0/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
5	MAN	T	4	5	-	1/2/19/22	0/1/1/1
5	MAN	T	5	5	-	0/2/19/22	0/1/1/1
5	MAN	T	6	5	-	0/2/19/22	0/1/1/1
5	MAN	T	7	5	-	0/2/19/22	0/1/1/1
5	NAG	U	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	BMA	U	3	5	-	0/2/19/22	0/1/1/1
5	MAN	U	4	5	-	2/2/19/22	0/1/1/1
5	MAN	U	5	5	-	0/2/19/22	0/1/1/1
5	MAN	U	6	5	-	0/2/19/22	0/1/1/1
5	MAN	U	7	5	-	0/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
5	BMA	V	3	5	-	0/2/19/22	0/1/1/1
5	MAN	V	4	5	-	2/2/19/22	0/1/1/1
5	MAN	V	5	5	-	0/2/19/22	0/1/1/1
5	MAN	V	6	5	-	0/2/19/22	0/1/1/1
5	MAN	V	7	5	-	0/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	1/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	MAN	W	4	6	-	0/2/19/22	0/1/1/1
6	MAN	W	5	6	-	2/2/19/22	0/1/1/1
6	MAN	W	6	6	-	0/2/19/22	0/1/1/1
6	MAN	W	7	6	-	2/2/19/22	0/1/1/1
6	MAN	W	8	6	-	0/2/19/22	0/1/1/1
6	MAN	W	9	6	-	0/2/19/22	0/1/1/1
7	MAN	X	1	7	-	2/2/19/22	1/1/1/1
7	MAN	X	2	7	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	Y	5	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	6	5	-	2/2/19/22	0/1/1/1
5	MAN	Y	7	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Z	4	5	-	1/2/19/22	0/1/1/1
5	MAN	Z	5	5	-	0/2/19/22	0/1/1/1
5	MAN	Z	6	5	-	0/2/19/22	0/1/1/1
5	MAN	Z	7	5	-	0/2/19/22	0/1/1/1
5	NAG	a	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	MAN	a	4	5	-	2/2/19/22	0/1/1/1
5	MAN	a	5	5	-	0/2/19/22	0/1/1/1
5	MAN	a	6	5	-	0/2/19/22	0/1/1/1
5	MAN	a	7	5	-	0/2/19/22	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	MAN	b	4	5	-	2/2/19/22	0/1/1/1
5	MAN	b	5	5	-	0/2/19/22	0/1/1/1
5	MAN	b	6	5	-	0/2/19/22	0/1/1/1
5	MAN	b	7	5	-	0/2/19/22	0/1/1/1
6	NAG	c	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	MAN	c	4	6	-	0/2/19/22	0/1/1/1
6	MAN	c	5	6	-	2/2/19/22	0/1/1/1
6	MAN	c	6	6	-	0/2/19/22	0/1/1/1
6	MAN	c	7	6	-	2/2/19/22	0/1/1/1
6	MAN	c	8	6	-	0/2/19/22	0/1/1/1
6	MAN	c	9	6	-	0/2/19/22	0/1/1/1
7	MAN	d	1	7	-	2/2/19/22	0/1/1/1
7	MAN	d	2	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	1	NAG	C4-C3-C2	4.11	117.05	111.02
5	S	1	NAG	C4-C3-C2	3.87	116.69	111.02
5	M	1	NAG	C4-C3-C2	3.84	116.65	111.02
6	c	3	BMA	C1-C2-C3	3.69	115.01	109.64
6	c	1	NAG	O5-C1-C2	-3.53	105.83	111.29
6	Q	3	BMA	C1-C2-C3	3.51	114.75	109.64
6	W	1	NAG	C3-C4-C5	3.48	116.53	110.23
6	c	1	NAG	C3-C4-C5	3.47	116.52	110.23
5	O	1	NAG	C3-C4-C5	3.44	116.47	110.23
5	a	1	NAG	C3-C4-C5	3.44	116.47	110.23
6	Q	1	NAG	C3-C4-C5	3.38	116.36	110.23
6	W	1	NAG	O5-C1-C2	-3.37	106.08	111.29
5	U	1	NAG	C3-C4-C5	3.34	116.28	110.23
5	Z	1	NAG	C3-C4-C5	3.33	116.27	110.23
5	T	1	NAG	O5-C1-C2	-3.28	106.22	111.29
6	Q	1	NAG	O5-C1-C2	-3.27	106.23	111.29
5	Z	1	NAG	O5-C1-C2	-3.23	106.29	111.29
5	N	1	NAG	O5-C1-C2	-3.22	106.31	111.29
5	N	1	NAG	C3-C4-C5	2.92	115.53	110.23
5	U	1	NAG	C4-C3-C2	2.89	115.26	111.02
5	O	1	NAG	C4-C3-C2	2.84	115.18	111.02
5	a	1	NAG	C4-C3-C2	2.81	115.14	111.02
5	T	1	NAG	C3-C4-C5	2.77	115.26	110.23
5	b	1	NAG	C4-C3-C2	2.60	114.83	111.02
5	V	1	NAG	C4-C3-C2	2.59	114.81	111.02
5	P	1	NAG	C4-C3-C2	2.50	114.68	111.02
6	c	2	NAG	C3-C4-C5	2.42	114.61	110.23
6	Q	1	NAG	C4-C3-C2	2.41	114.55	111.02
6	c	1	NAG	C4-C3-C2	2.39	114.52	111.02
5	Y	6	MAN	C2-C3-C4	-2.37	106.69	110.86
5	a	1	NAG	O5-C1-C2	-2.36	107.64	111.29
6	W	3	BMA	C1-C2-C3	2.36	113.08	109.64
7	d	1	MAN	O5-C1-C2	2.35	116.40	110.79
7	X	1	MAN	O5-C1-C2	2.34	116.37	110.79
5	Y	3	BMA	C1-C2-C3	2.34	113.05	109.64
5	U	1	NAG	O5-C1-C2	-2.30	107.73	111.29
6	W	1	NAG	C4-C3-C2	2.29	114.38	111.02
6	Q	2	NAG	C3-C4-C5	2.24	114.29	110.23
7	R	1	MAN	O5-C1-C2	2.23	116.10	110.79
5	O	1	NAG	O5-C1-C2	-2.23	107.85	111.29
6	c	7	MAN	O5-C5-C6	2.16	111.87	107.66
5	T	1	NAG	C4-C3-C2	2.10	114.10	111.02
5	M	6	MAN	C2-C3-C4	-2.10	107.17	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	2	NAG	O5-C1-C2	-2.08	108.08	111.29
5	S	3	BMA	C1-C2-C3	2.05	112.63	109.64
5	N	1	NAG	C4-C3-C2	2.03	113.99	111.02
5	M	3	BMA	C1-C2-C3	2.02	112.58	109.64

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C1-C2-N2-C7
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	S	1	NAG	C1-C2-N2-C7
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	a	1	NAG	C8-C7-N2-C2
5	a	1	NAG	O7-C7-N2-C2
7	X	1	MAN	O5-C5-C6-O6
7	d	1	MAN	O5-C5-C6-O6
7	R	1	MAN	O5-C5-C6-O6
6	Q	5	MAN	O5-C5-C6-O6
6	W	5	MAN	O5-C5-C6-O6
6	c	5	MAN	O5-C5-C6-O6
6	W	7	MAN	C4-C5-C6-O6
7	X	1	MAN	C4-C5-C6-O6
6	Q	7	MAN	C4-C5-C6-O6
6	c	7	MAN	C4-C5-C6-O6
7	R	1	MAN	C4-C5-C6-O6
5	M	1	NAG	C8-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	Y	1	NAG	C8-C7-N2-C2
7	d	1	MAN	C4-C5-C6-O6
5	M	1	NAG	O7-C7-N2-C2
6	Q	7	MAN	O5-C5-C6-O6
6	W	7	MAN	O5-C5-C6-O6
6	c	7	MAN	O5-C5-C6-O6
5	S	1	NAG	O7-C7-N2-C2
5	Y	1	NAG	O7-C7-N2-C2
5	O	4	MAN	O5-C5-C6-O6
5	U	4	MAN	O5-C5-C6-O6
5	a	4	MAN	O5-C5-C6-O6
6	Q	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	P	4	MAN	O5-C5-C6-O6
5	V	4	MAN	O5-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
6	W	5	MAN	C4-C5-C6-O6
6	c	5	MAN	C4-C5-C6-O6
5	Y	6	MAN	C4-C5-C6-O6
5	Y	6	MAN	O5-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6
5	T	4	MAN	O5-C5-C6-O6
5	Z	4	MAN	O5-C5-C6-O6
5	Y	1	NAG	C1-C2-N2-C7
6	c	2	NAG	C4-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
5	Y	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C4-C5-C6-O6
5	O	4	MAN	C4-C5-C6-O6
5	U	4	MAN	C4-C5-C6-O6
5	a	4	MAN	C4-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
5	V	4	MAN	C4-C5-C6-O6
5	b	4	MAN	C4-C5-C6-O6
5	P	4	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	1	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 33 short contacts:

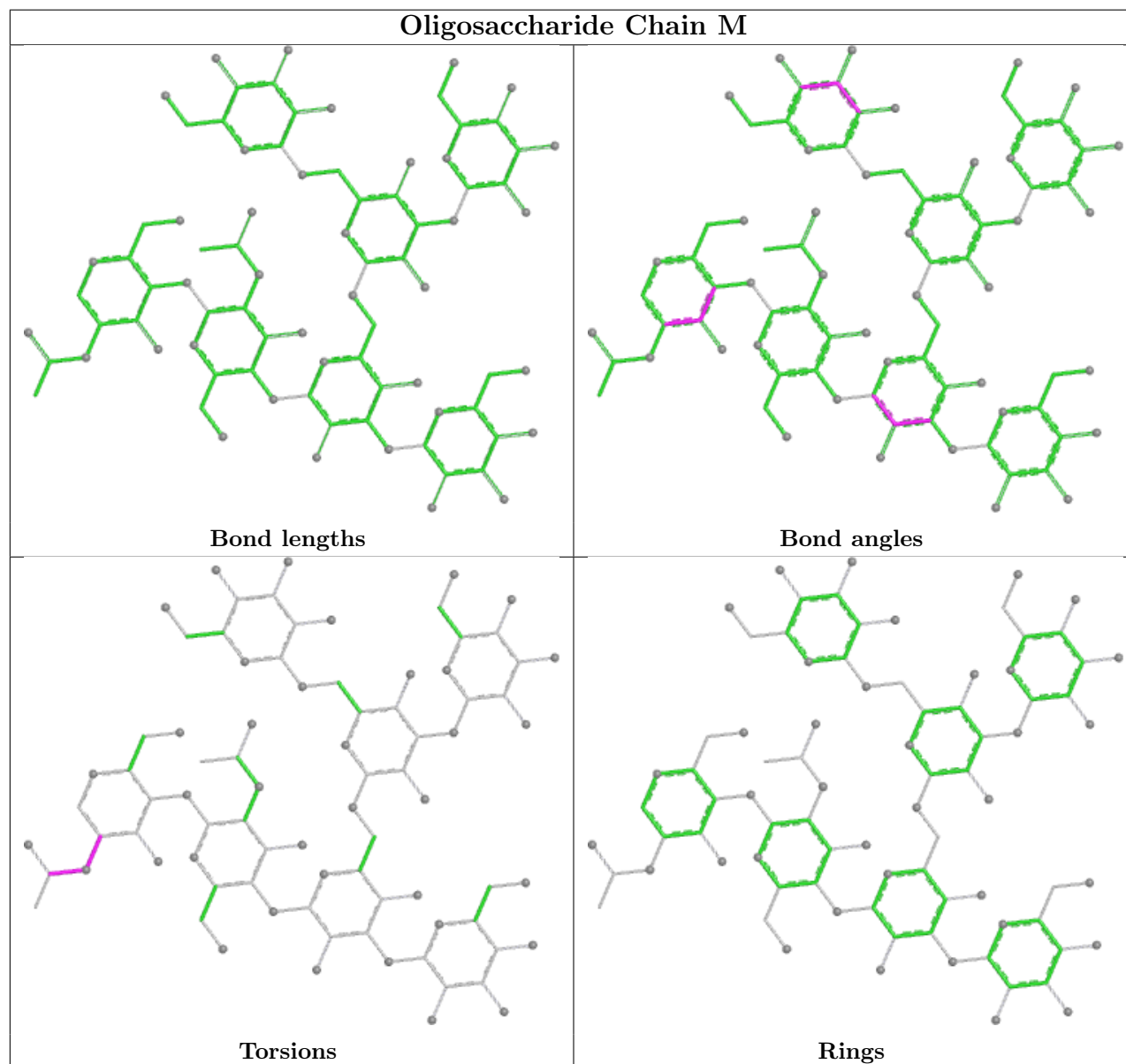
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	1	NAG	6	0
5	O	1	NAG	6	0
5	Y	1	NAG	1	0
5	a	1	NAG	4	0
5	S	1	NAG	1	0
6	c	2	NAG	3	0
7	R	1	MAN	2	0
6	Q	2	NAG	2	0
7	R	2	MAN	1	0
5	Y	6	MAN	2	0
7	d	2	MAN	1	0

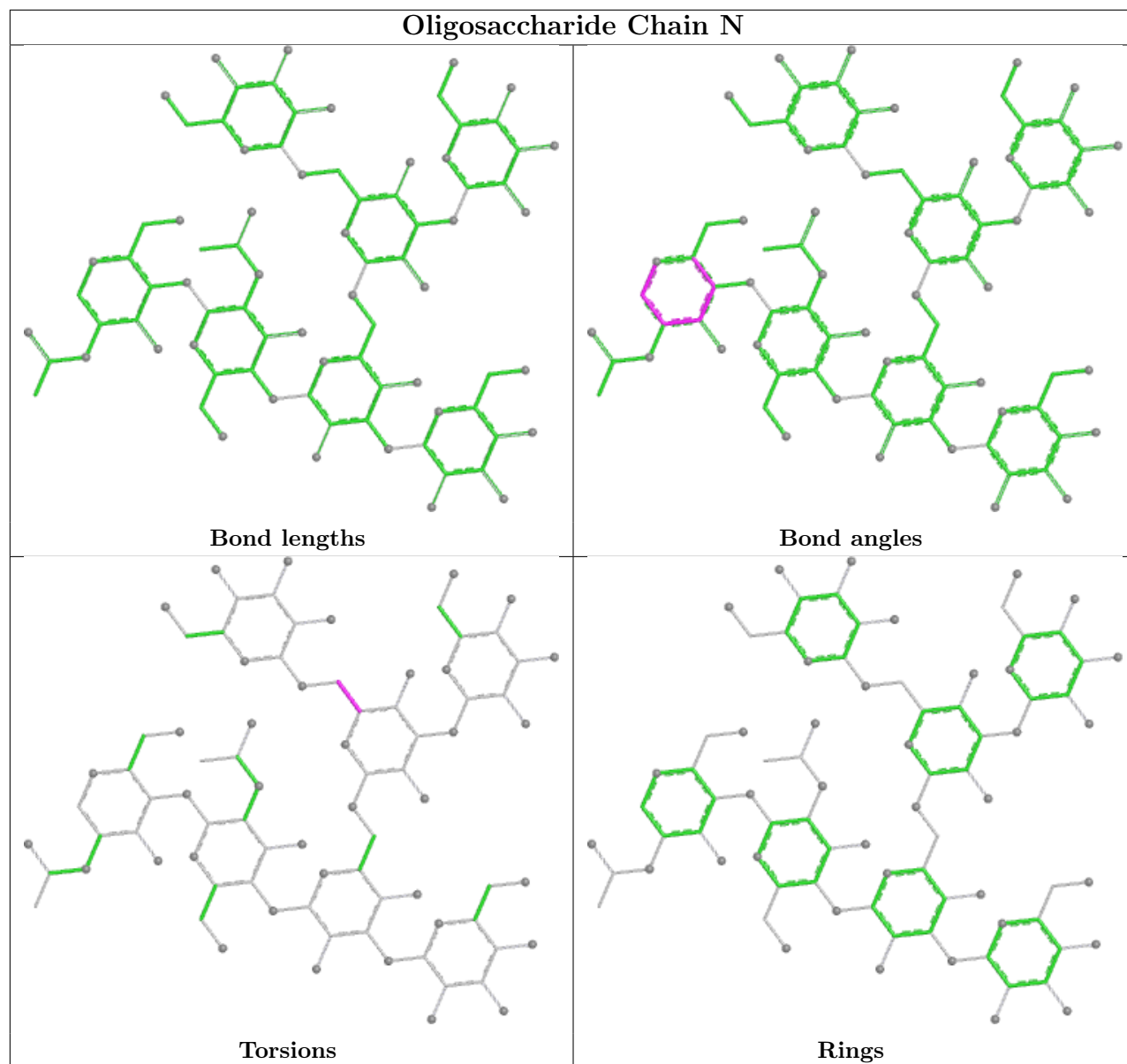
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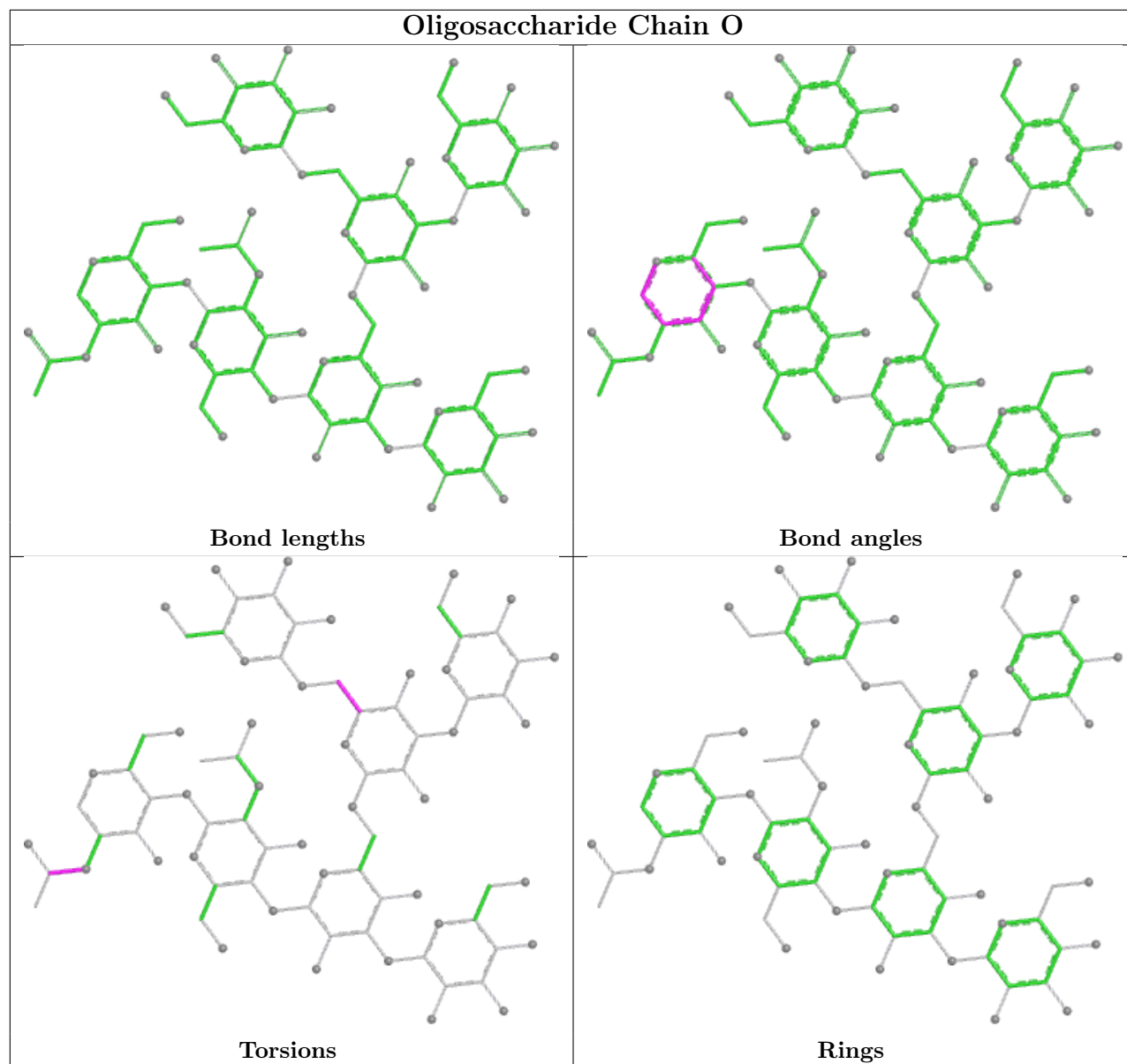
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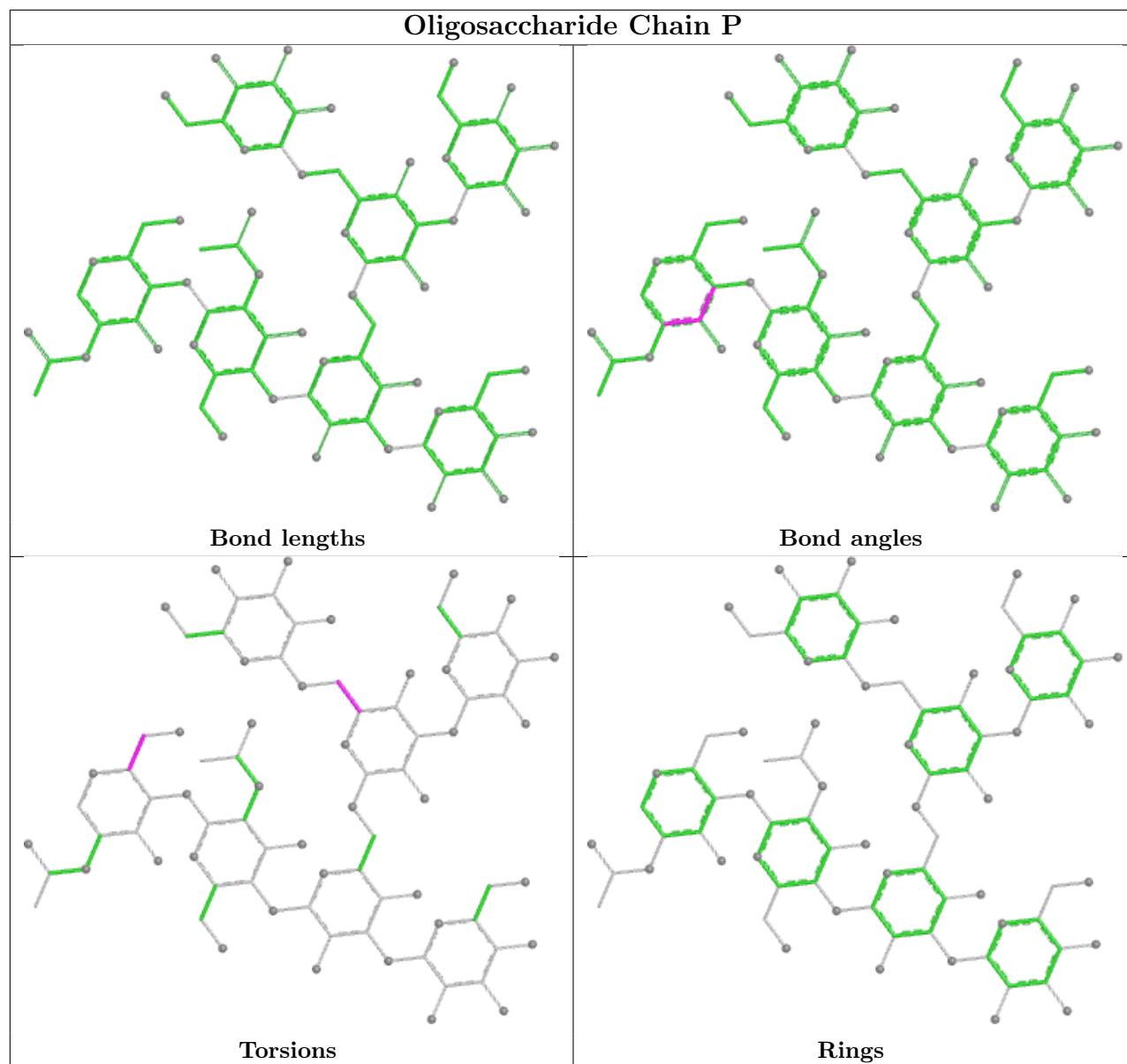
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	c	1	NAG	1	0
5	M	1	NAG	1	0
7	d	1	MAN	1	0
7	X	2	MAN	1	0

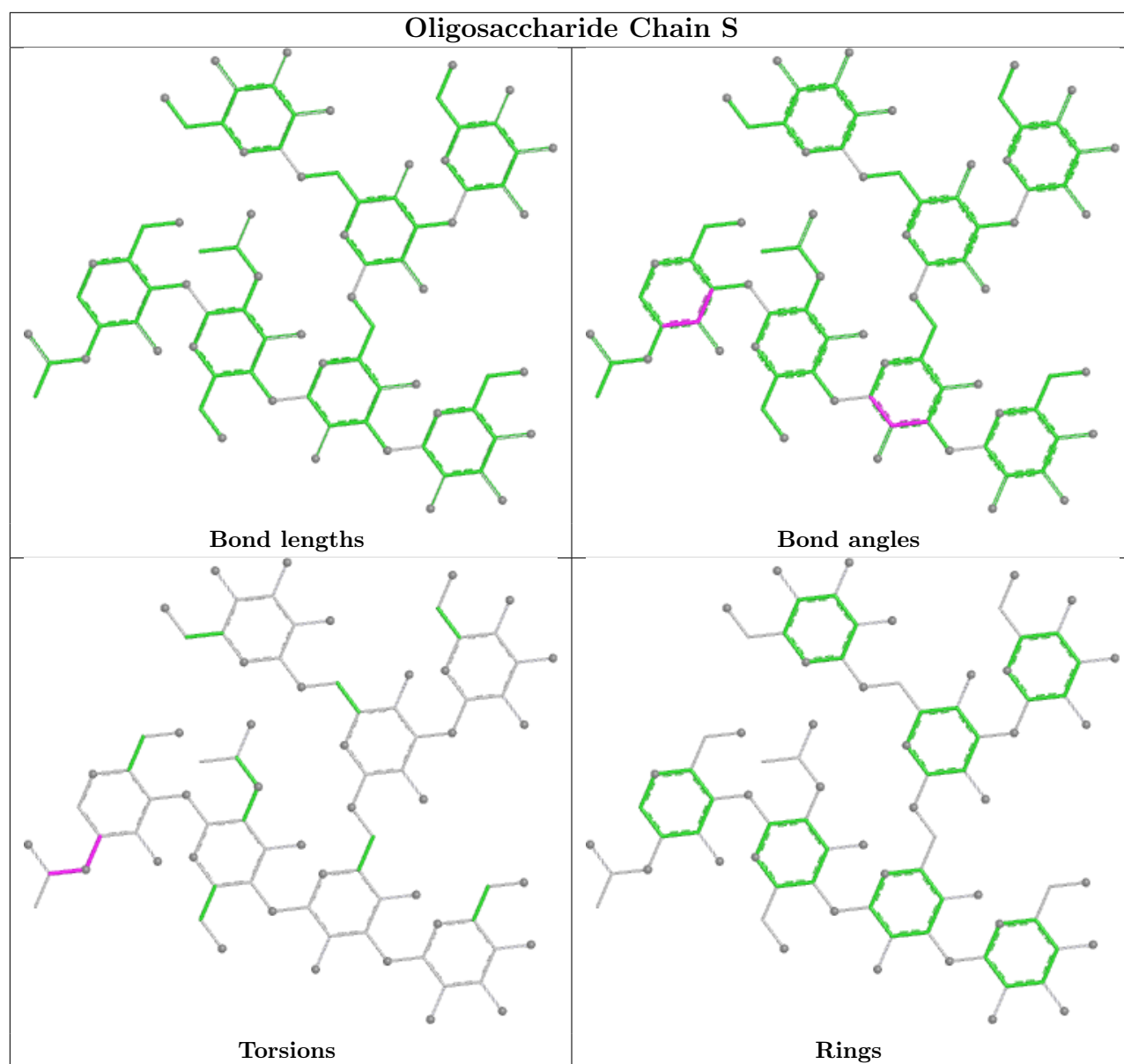
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

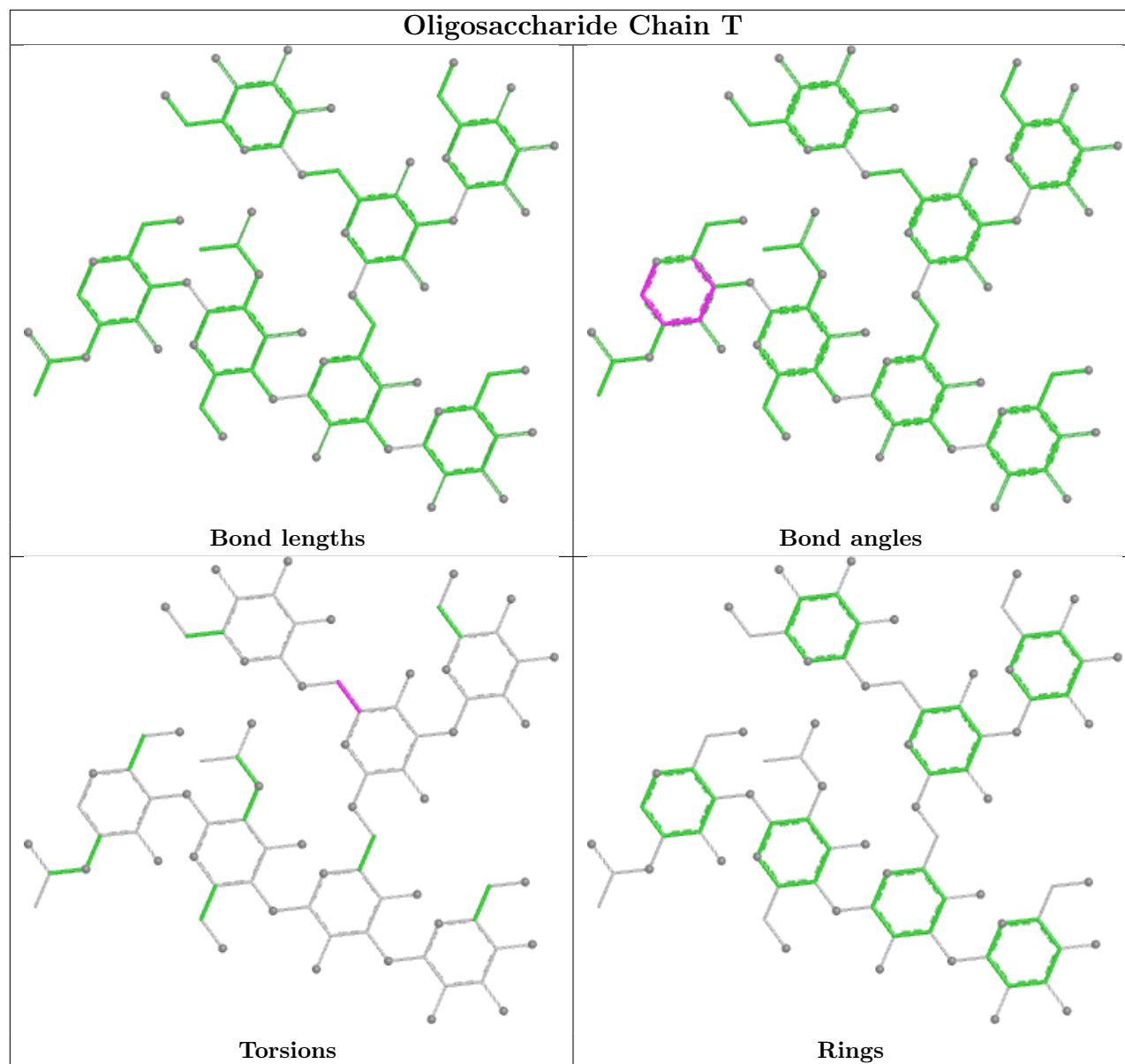


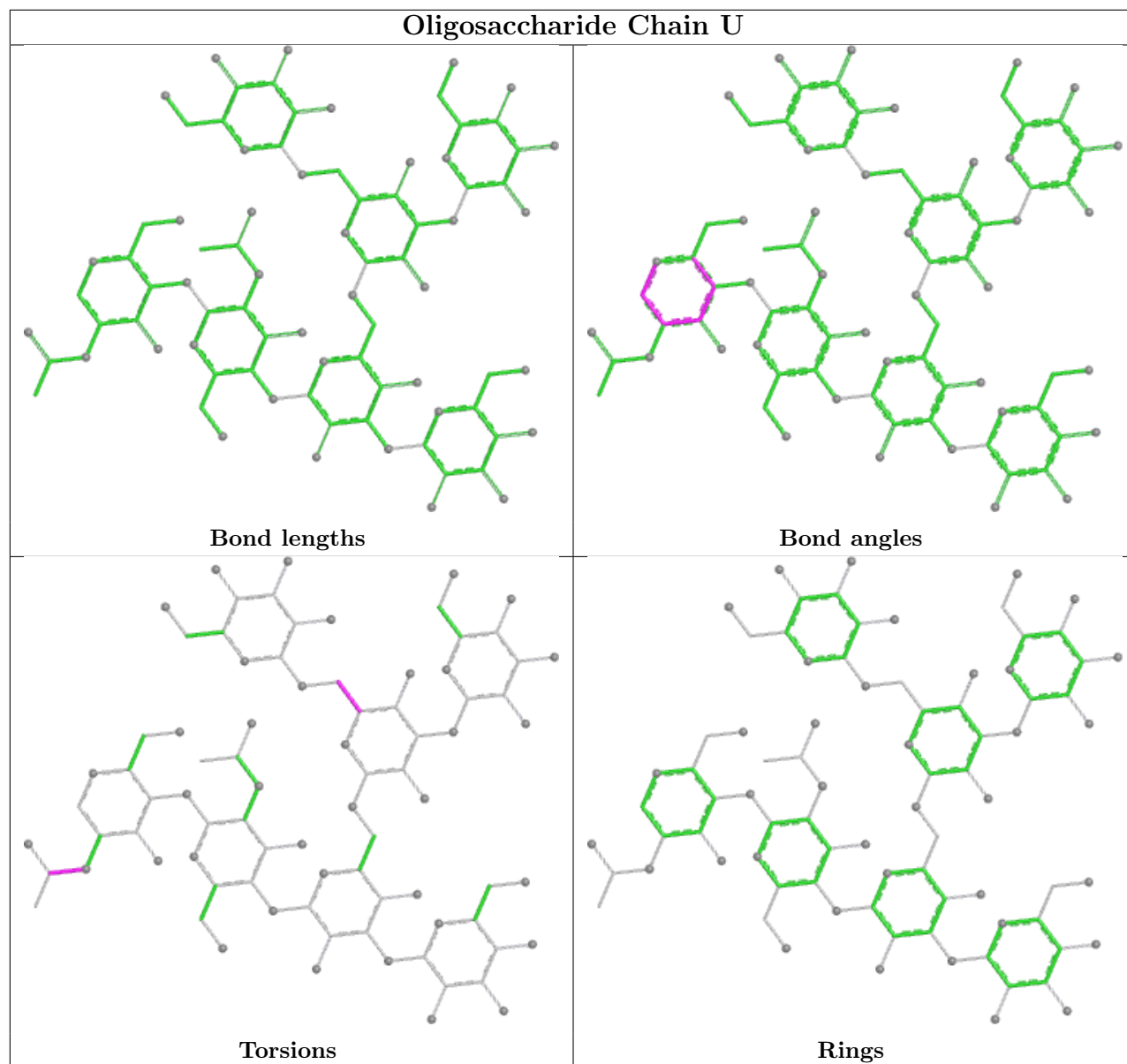


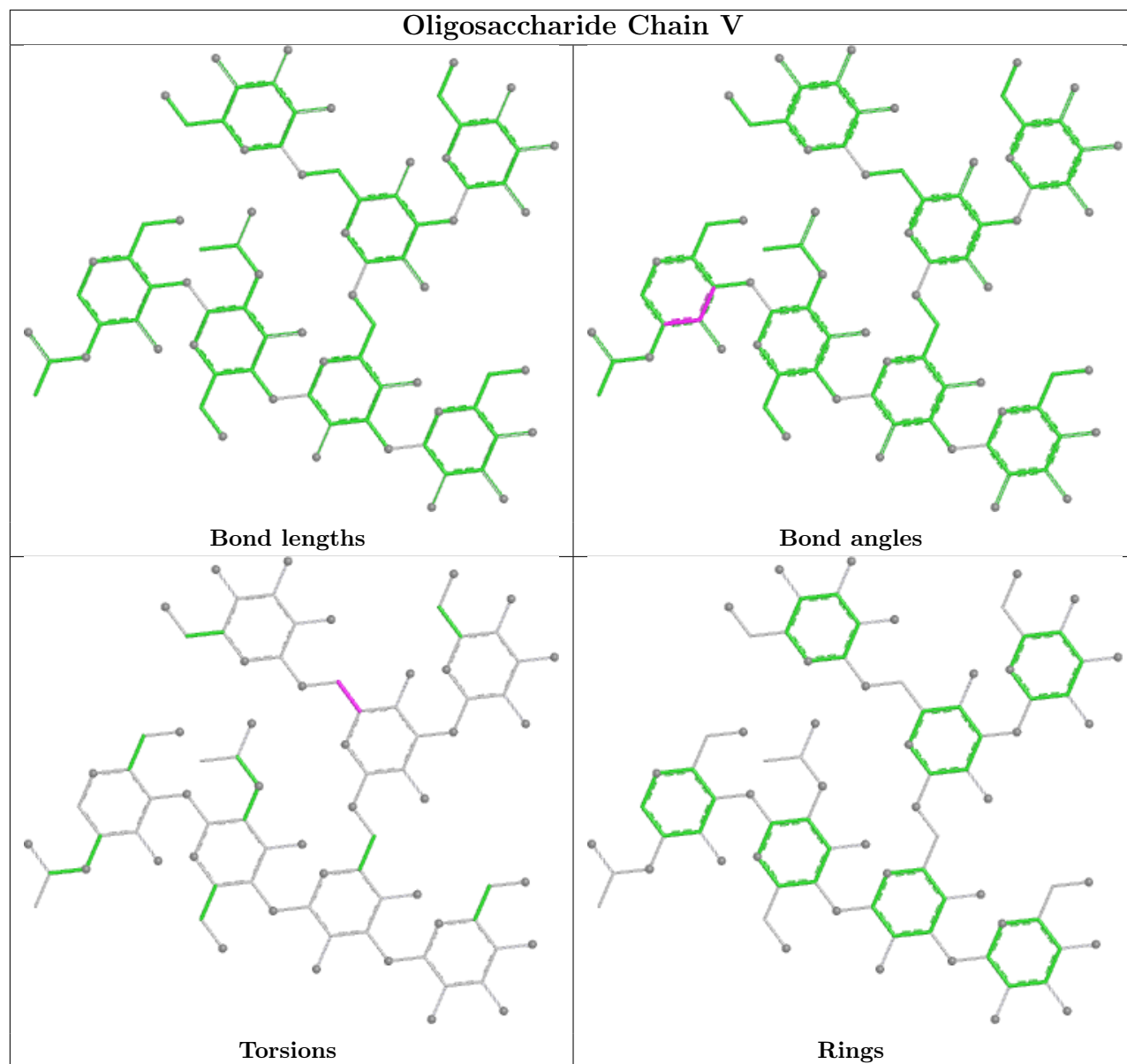


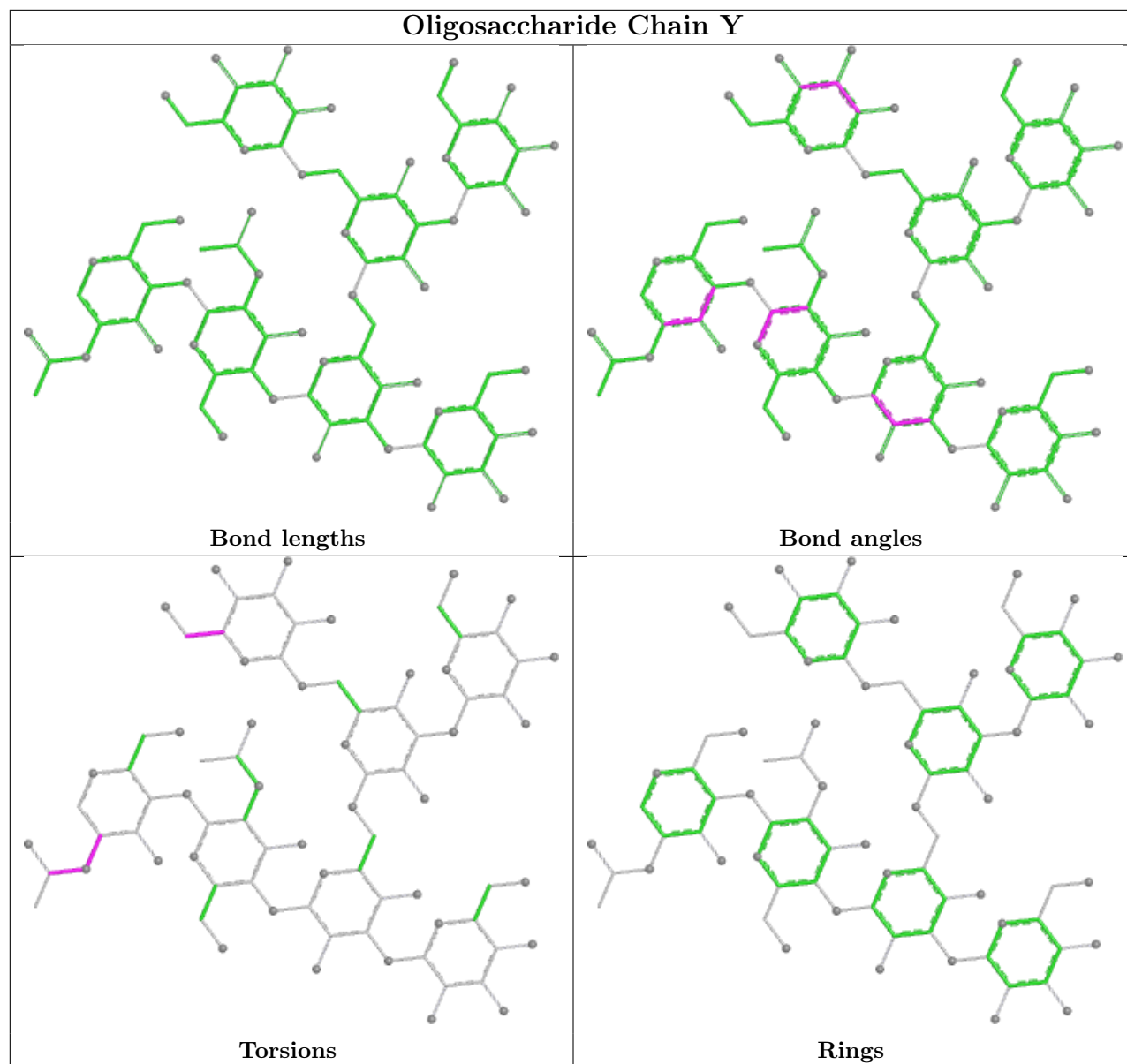


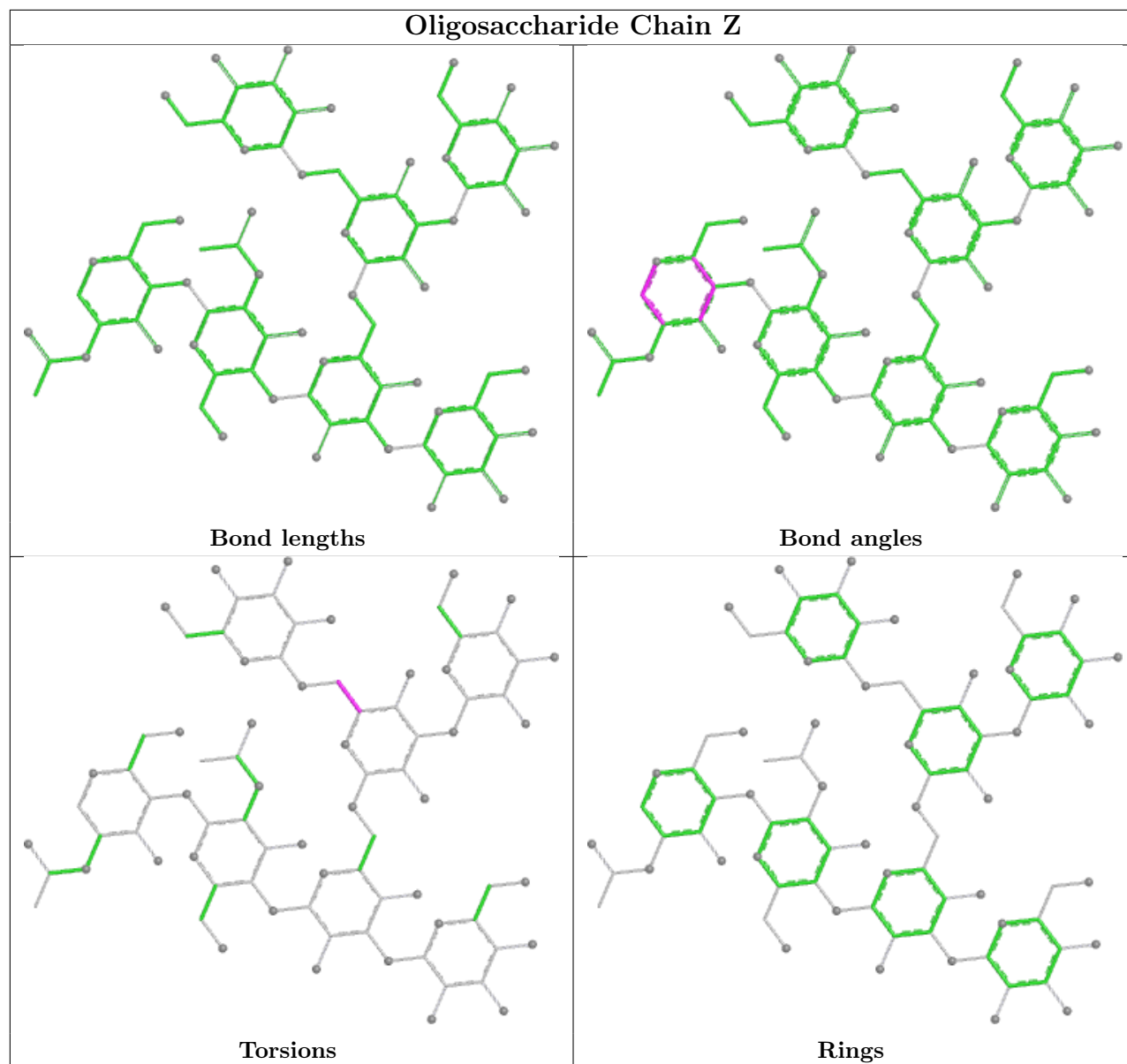


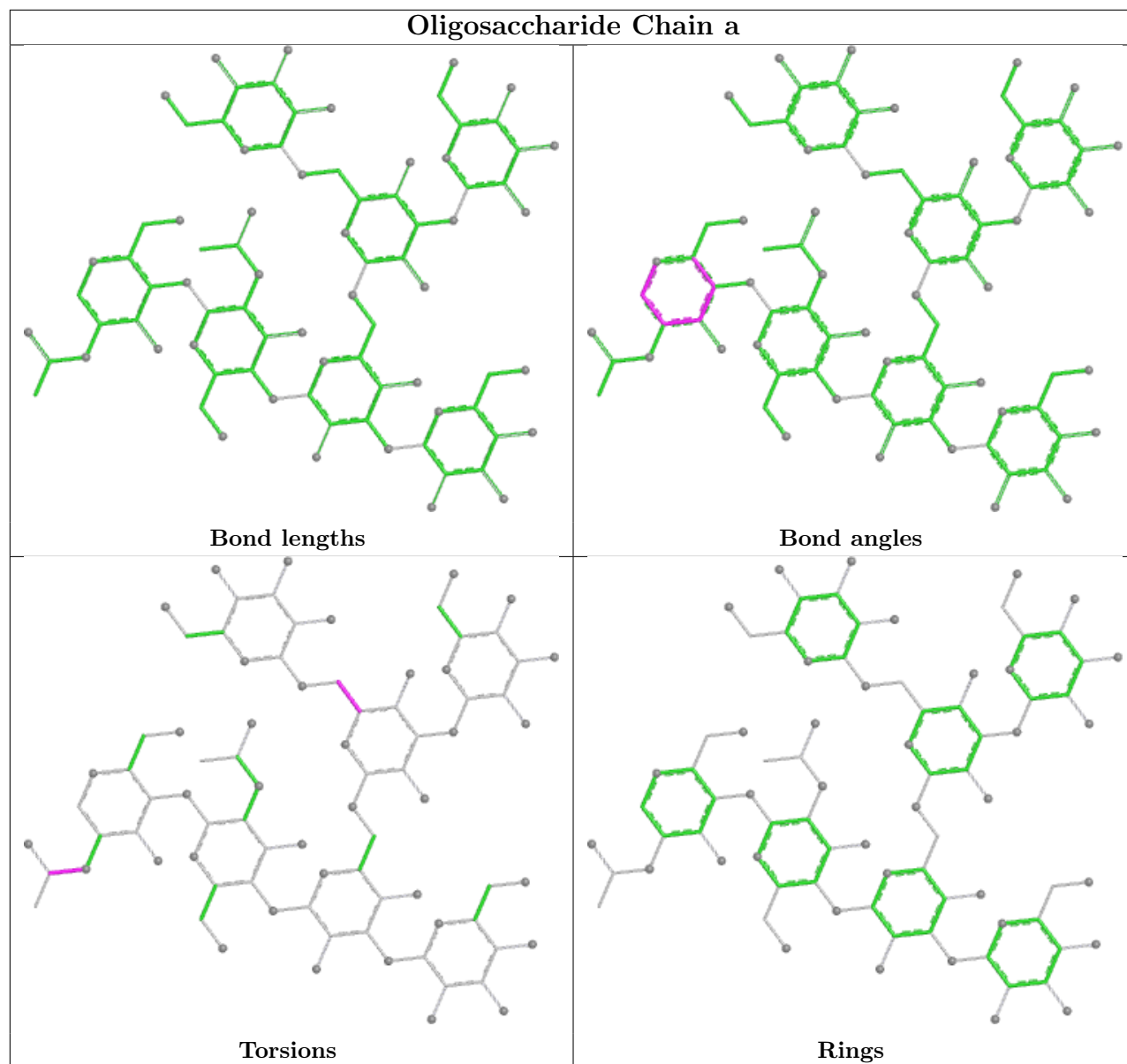


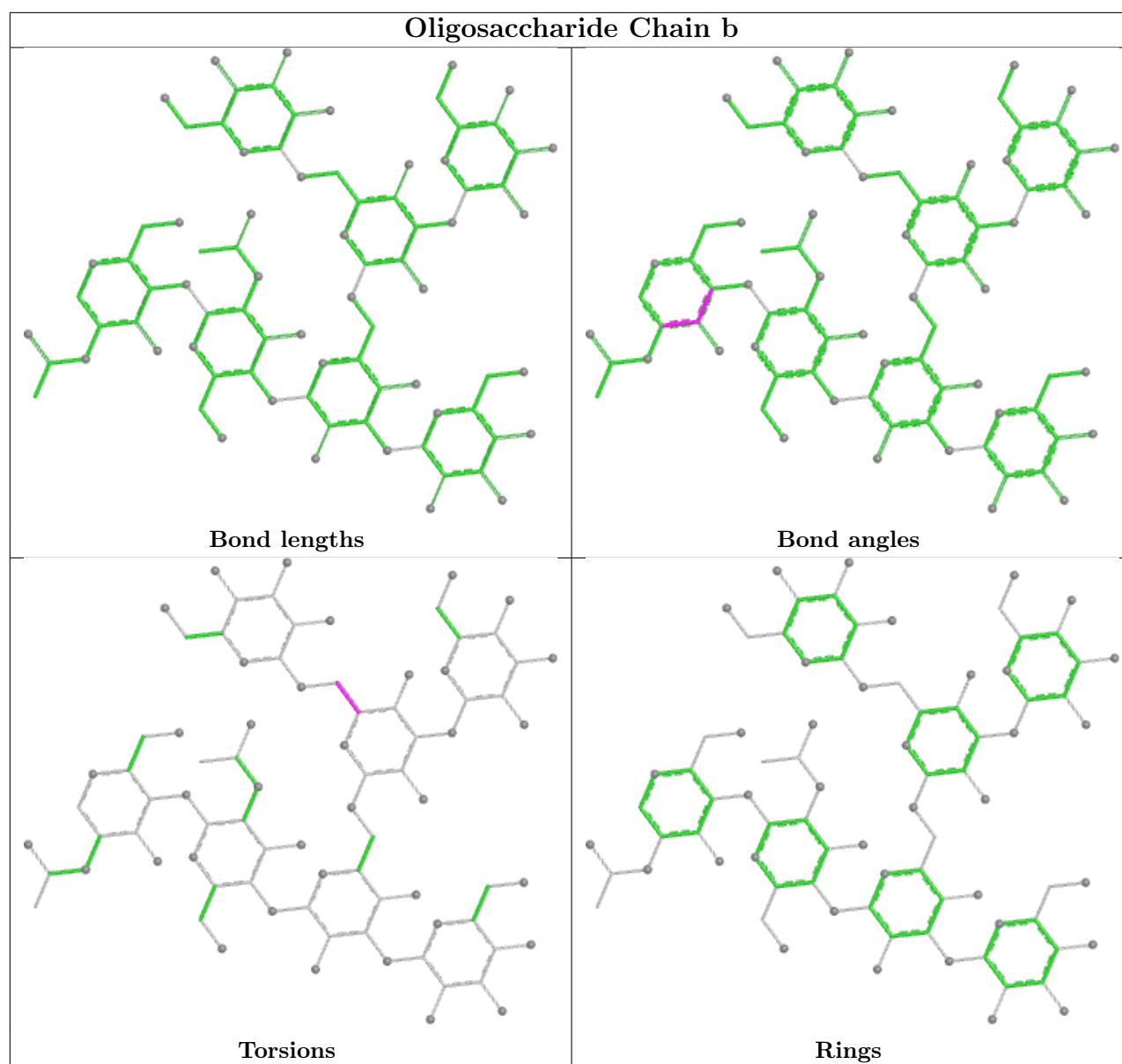


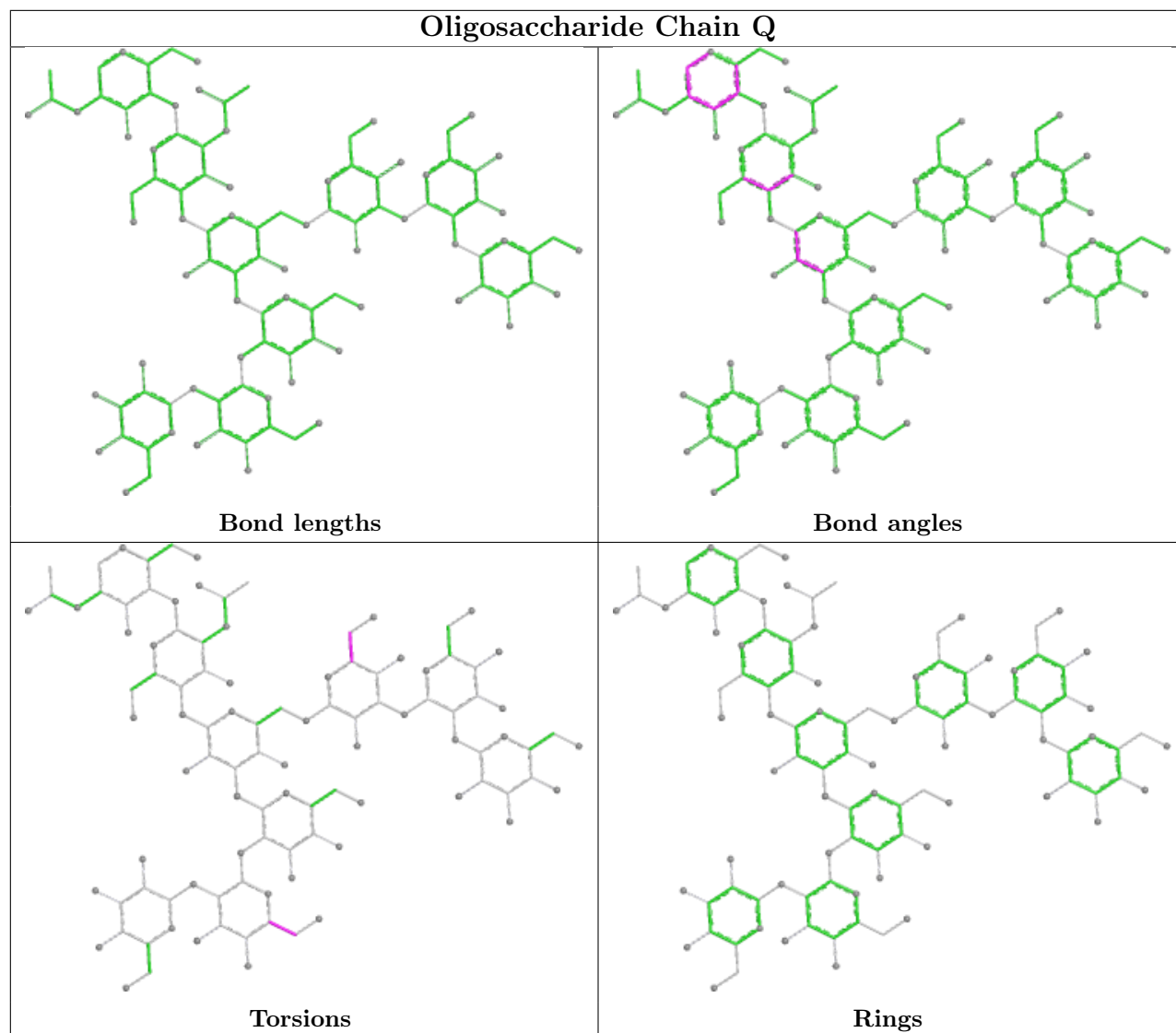


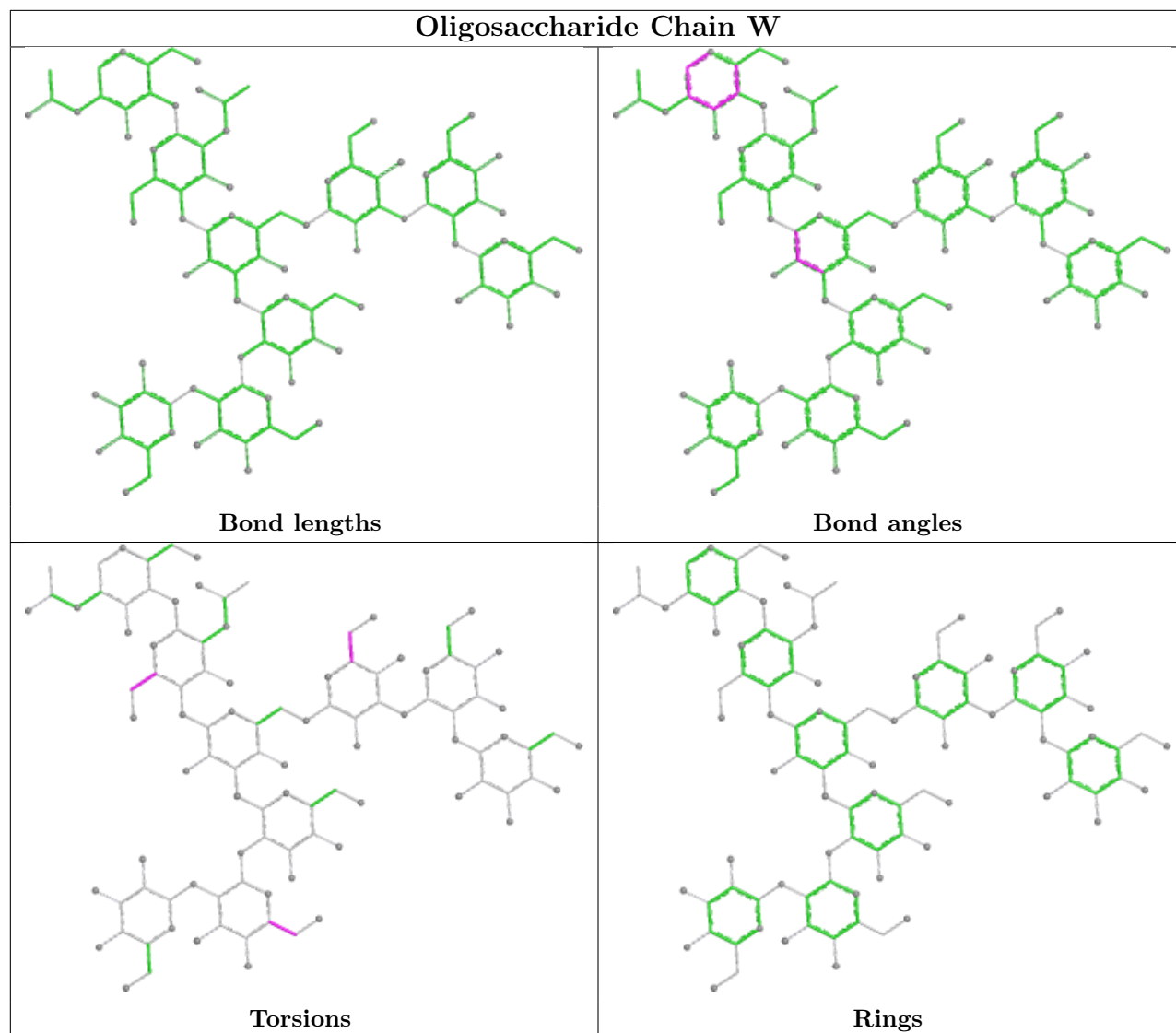


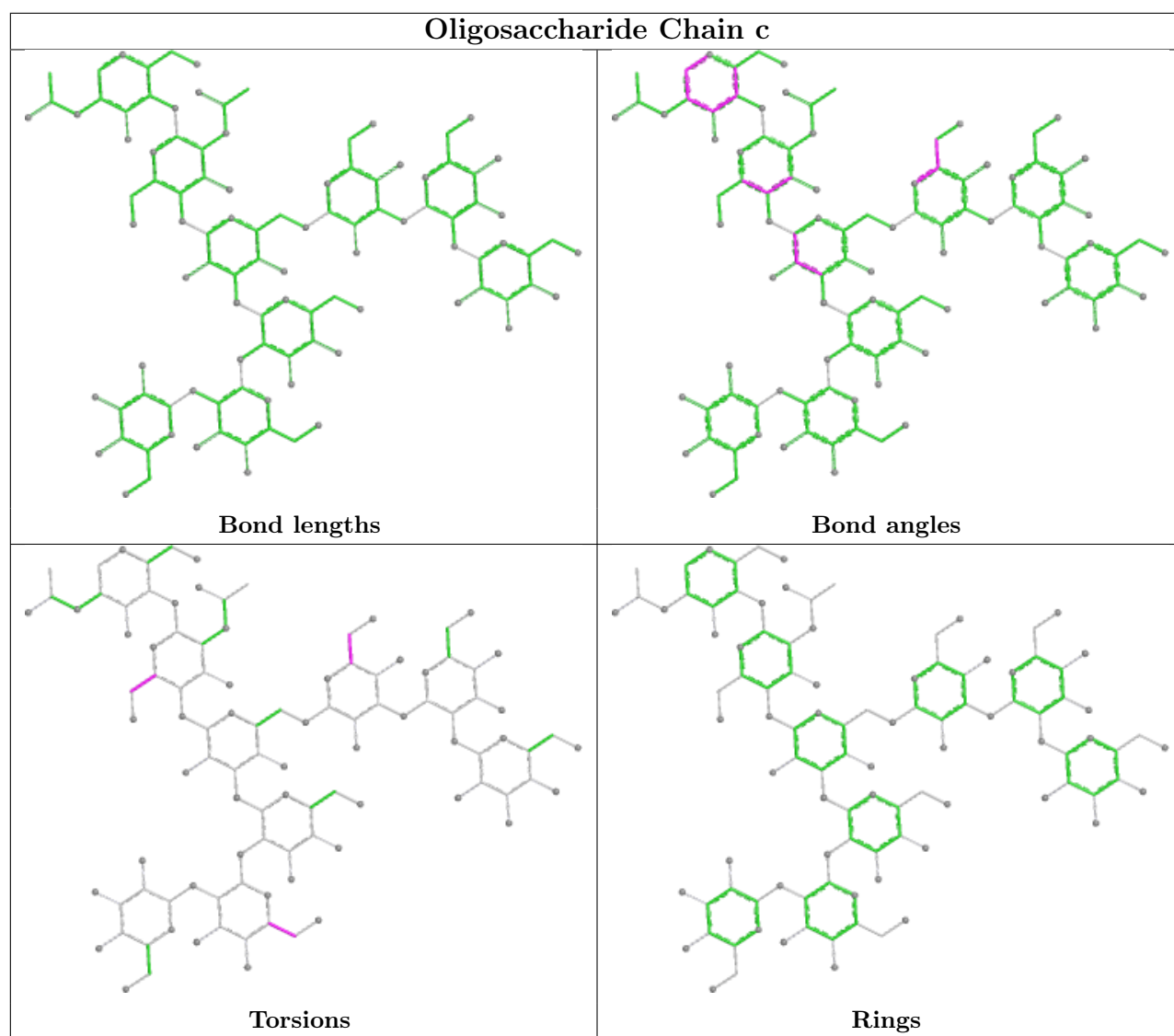


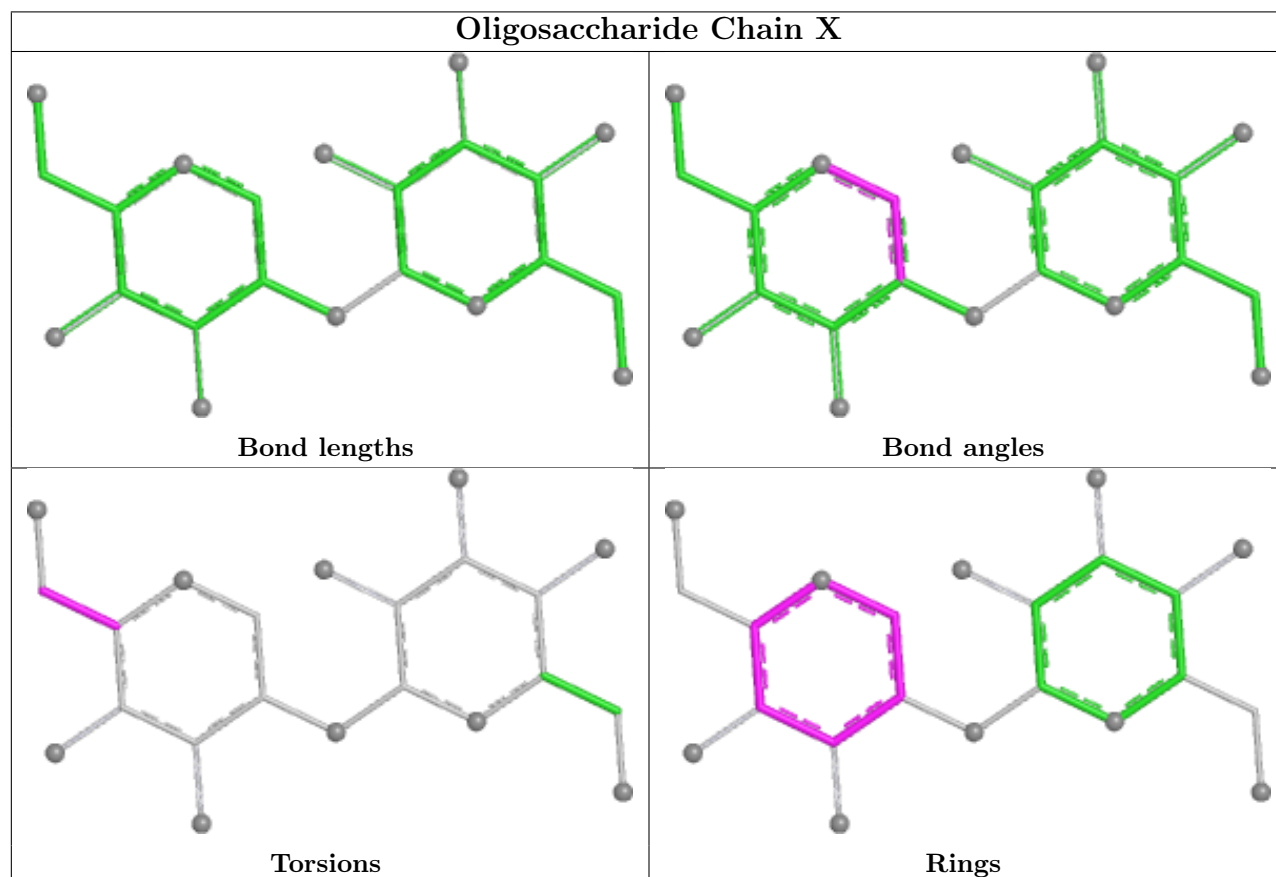
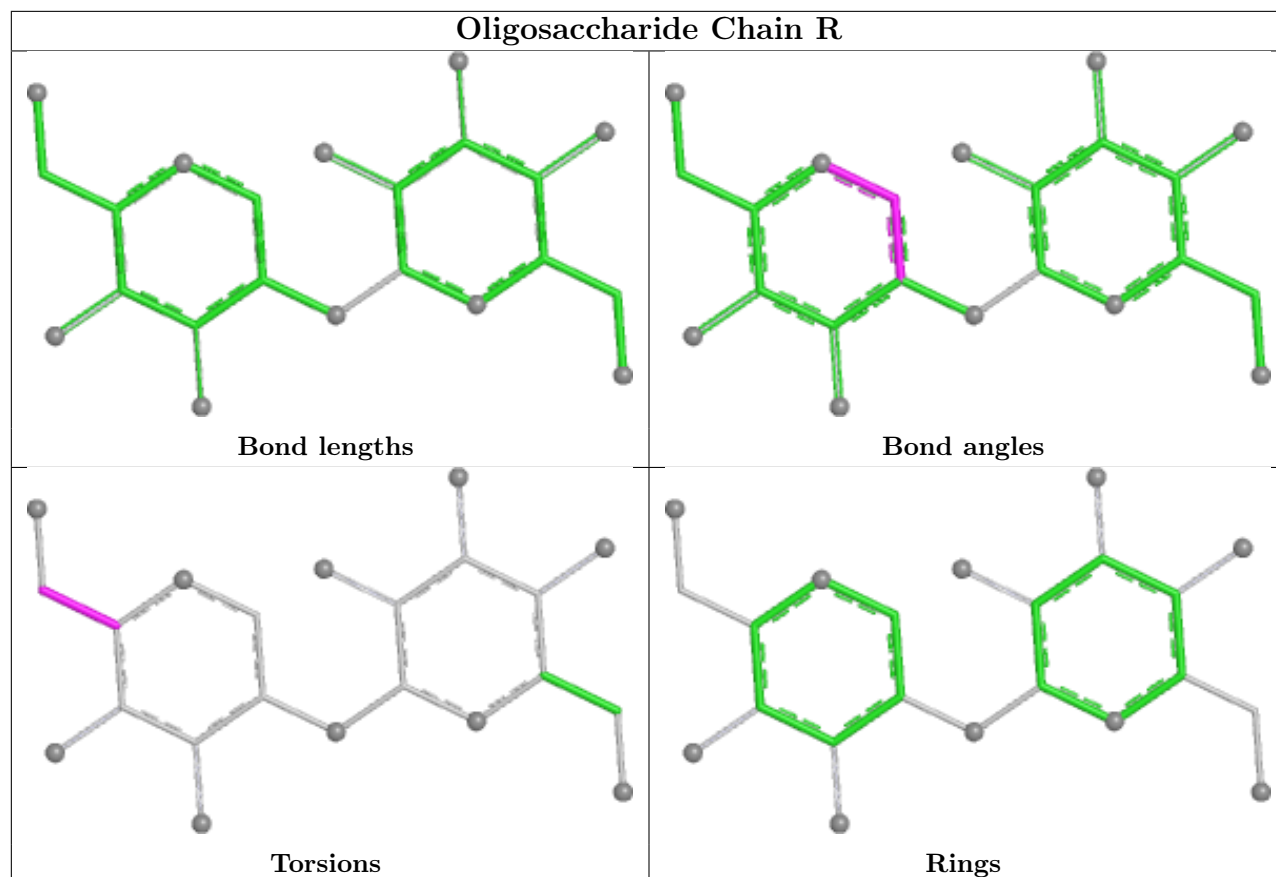


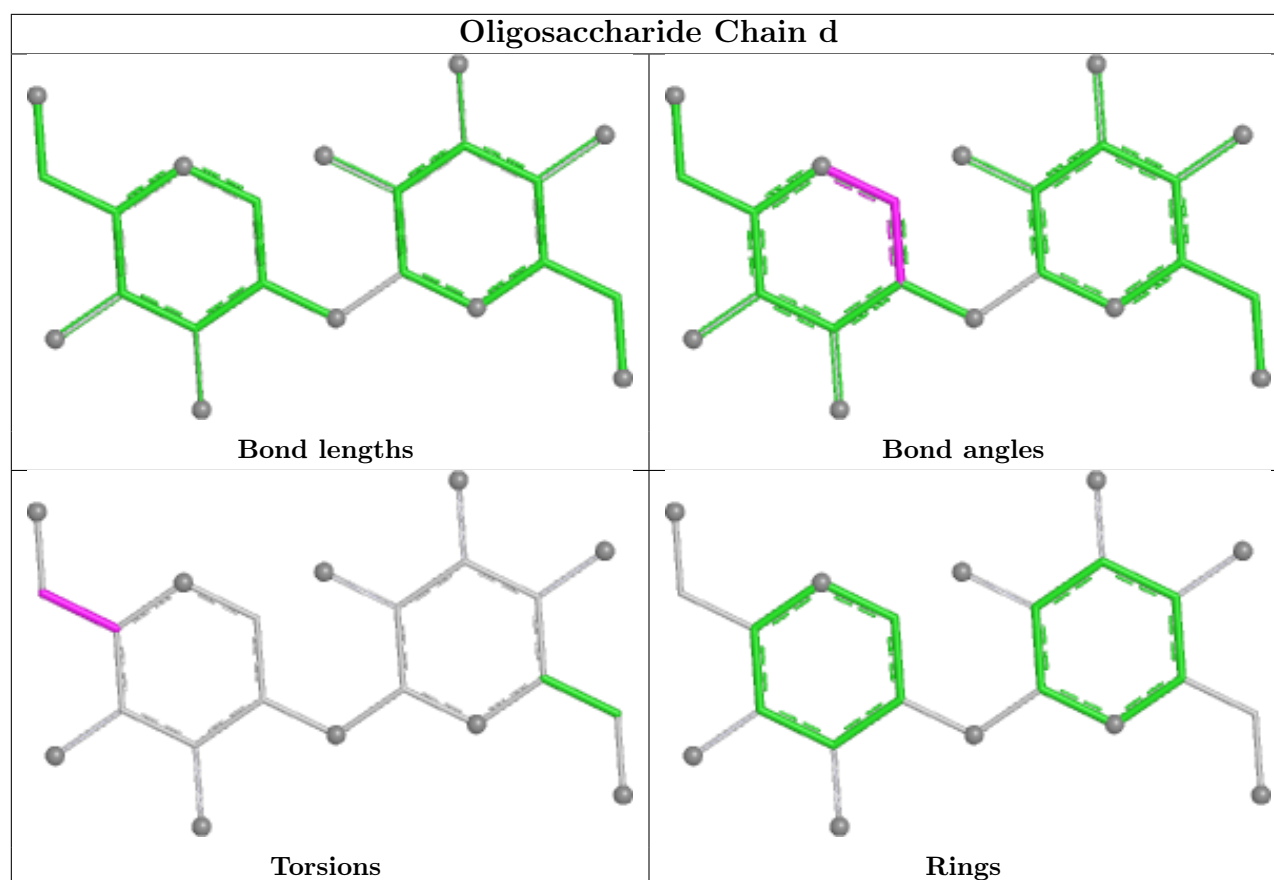












5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	A	1392	1	14,14,15	0.44	0	17,19,21	0.70	0
8	NAG	I	1276	1	14,14,15	0.45	0	17,19,21	1.03	1 (5%)
8	NAG	E	1088	1	14,14,15	0.55	0	17,19,21	0.73	0
8	NAG	E	1295	1	14,14,15	0.50	0	17,19,21	0.75	0
8	NAG	A	1197	1	14,14,15	0.45	0	17,19,21	0.88	1 (5%)
8	NAG	E	1197	1	14,14,15	0.45	0	17,19,21	0.80	0
8	NAG	I	1448	1	14,14,15	0.45	0	17,19,21	1.58	3 (17%)
8	NAG	E	1234	1	14,14,15	0.42	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	E	1392	1	14,14,15	0.47	0	17,19,21	0.67	0
8	NAG	A	1448	1	14,14,15	0.49	0	17,19,21	1.50	3 (17%)
8	NAG	I	1160	1	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
8	NAG	E	1448	1	14,14,15	0.48	0	17,19,21	1.56	3 (17%)
8	NAG	E	1355	1	14,14,15	0.49	0	17,19,21	0.71	0
8	NAG	I	1392	1	14,14,15	0.42	0	17,19,21	0.75	0
8	NAG	I	1088	1	14,14,15	0.50	0	17,19,21	0.86	1 (5%)
8	NAG	A	1160	1	14,14,15	0.48	0	17,19,21	0.75	0
8	NAG	A	1088	1	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
8	NAG	A	1295	1	14,14,15	0.53	0	17,19,21	0.71	0
8	NAG	I	1355	1	14,14,15	0.46	0	17,19,21	0.85	1 (5%)
8	NAG	A	1276	1	14,14,15	0.40	0	17,19,21	1.18	2 (11%)
8	NAG	E	1160	1	14,14,15	0.49	0	17,19,21	0.69	0
8	NAG	A	1234	1	14,14,15	0.43	0	17,19,21	1.19	2 (11%)
8	NAG	A	1355	1	14,14,15	0.49	0	17,19,21	0.74	0
8	NAG	E	1386	1	14,14,15	0.58	0	17,19,21	0.72	0
8	NAG	E	1276	1	14,14,15	0.44	0	17,19,21	1.25	3 (17%)
8	NAG	I	1234	1	14,14,15	0.45	0	17,19,21	1.18	2 (11%)
8	NAG	I	1295	1	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
8	NAG	I	1386	1	14,14,15	0.54	0	17,19,21	0.79	1 (5%)
8	NAG	I	1197	1	14,14,15	0.49	0	17,19,21	0.80	0
8	NAG	A	1386	1	14,14,15	0.58	0	17,19,21	0.75	1 (5%)

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
8	NAG	A	1392	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1276	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1088	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1295	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1197	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1197	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1448	1	-	4/6/23/26	0/1/1/1
8	NAG	E	1234	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1392	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1448	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	I	1160	1	-	2/6/23/26	0/1/1/1
8	NAG	E	1448	1	-	4/6/23/26	0/1/1/1
8	NAG	E	1355	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1392	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1088	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1160	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1088	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1295	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1355	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1276	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1160	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1234	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1386	1	-	1/6/23/26	0/1/1/1
8	NAG	E	1276	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1234	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1295	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1386	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1197	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1386	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1448	NAG	C1-O5-C5	3.37	116.71	112.19
8	E	1448	NAG	C1-O5-C5	3.35	116.68	112.19
8	A	1448	NAG	C1-O5-C5	3.13	116.38	112.19
8	A	1276	NAG	C1-O5-C5	3.03	116.25	112.19
8	E	1276	NAG	C1-O5-C5	3.01	116.21	112.19
8	I	1448	NAG	O5-C1-C2	-2.87	106.86	111.29
8	E	1448	NAG	O5-C1-C2	-2.85	106.87	111.29
8	A	1448	NAG	O5-C1-C2	-2.75	107.04	111.29
8	A	1234	NAG	C1-O5-C5	2.65	115.73	112.19
8	I	1276	NAG	C1-O5-C5	2.56	115.62	112.19
8	I	1448	NAG	C2-N2-C7	-2.53	119.50	122.90
8	A	1088	NAG	C1-O5-C5	2.45	115.47	112.19
8	I	1088	NAG	C1-O5-C5	2.44	115.46	112.19
8	E	1448	NAG	C2-N2-C7	-2.44	119.64	122.90
8	A	1448	NAG	C2-N2-C7	-2.38	119.71	122.90
8	I	1234	NAG	O5-C1-C2	-2.33	107.68	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	1234	NAG	O5-C1-C2	-2.29	107.74	111.29
8	A	1197	NAG	C1-O5-C5	2.28	115.25	112.19
8	I	1160	NAG	C1-O5-C5	2.26	115.21	112.19
8	E	1276	NAG	O5-C1-C2	-2.21	107.88	111.29
8	I	1234	NAG	C1-O5-C5	2.15	115.06	112.19
8	A	1234	NAG	O5-C1-C2	-2.13	107.99	111.29
8	E	1234	NAG	C1-O5-C5	2.10	115.00	112.19
8	A	1386	NAG	C1-O5-C5	2.09	114.99	112.19
8	E	1276	NAG	C2-N2-C7	-2.09	120.09	122.90
8	I	1355	NAG	C1-O5-C5	2.07	114.95	112.19
8	I	1386	NAG	C1-O5-C5	2.07	114.95	112.19
8	I	1295	NAG	C1-O5-C5	2.05	114.93	112.19
8	A	1276	NAG	C2-N2-C7	-2.00	120.22	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	1160	NAG	C8-C7-N2-C2
8	A	1448	NAG	O5-C5-C6-O6
8	E	1448	NAG	O5-C5-C6-O6
8	A	1160	NAG	C8-C7-N2-C2
8	E	1160	NAG	O7-C7-N2-C2
8	I	1160	NAG	C8-C7-N2-C2
8	I	1160	NAG	O7-C7-N2-C2
8	I	1448	NAG	O5-C5-C6-O6
8	I	1448	NAG	C8-C7-N2-C2
8	A	1160	NAG	O7-C7-N2-C2
8	A	1448	NAG	C8-C7-N2-C2
8	E	1448	NAG	C8-C7-N2-C2
8	I	1448	NAG	O7-C7-N2-C2
8	A	1448	NAG	O7-C7-N2-C2
8	A	1448	NAG	C4-C5-C6-O6
8	E	1448	NAG	O7-C7-N2-C2
8	E	1448	NAG	C4-C5-C6-O6
8	I	1448	NAG	C4-C5-C6-O6
8	E	1386	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1295	NAG	2	0
8	A	1295	NAG	2	0
8	A	1276	NAG	1	0
8	E	1276	NAG	1	0
8	I	1295	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	100(R):VAL	C	101:TRP	N	1.66

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	420/475 (88%)	1.31	117 (27%) 1 5	7, 227, 434, 596	0
1	E	420/475 (88%)	1.43	114 (27%) 1 5	16, 221, 423, 559	0
1	I	420/475 (88%)	1.50	126 (30%) 1 5	25, 216, 434, 550	0
2	B	0/78	-	-	-	-
2	F	0/78	-	-	-	-
2	J	0/78	-	-	-	-
3	C	202/211 (95%)	1.25	50 (24%) 2 5	74, 234, 422, 563	0
3	G	202/211 (95%)	1.52	61 (30%) 1 4	43, 229, 392, 572	0
3	K	202/211 (95%)	1.48	60 (29%) 1 5	47, 291, 454, 533	0
4	D	226/235 (96%)	1.48	70 (30%) 1 4	67, 232, 488, 582	0
4	H	226/235 (96%)	1.56	76 (33%) 1 4	56, 232, 421, 563	0
4	L	226/235 (96%)	1.49	66 (29%) 1 5	71, 287, 466, 582	0
All	All	2544/2997 (84%)	1.44	740 (29%) 1 5	7, 236, 440, 596	0

All (740) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	100(A)	ILE	13.8
4	H	100(A)	ILE	9.1
1	I	236	THR	8.7
1	E	313	GLY	8.6
4	H	72	ASP	7.9
3	G	71	ALA	7.5
3	G	67	GLY	7.2
1	I	491	ILE	7.2
1	E	236	THR	7.0
1	E	263	GLY	6.8
1	A	126	CYS	6.8
4	L	100(Q)	ASP	6.8

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Mol	Chain	Res	Type	RSRZ
1	E	70	ALA	6.6
3	G	66	PRO	6.5
4	D	121	PRO	6.5
4	H	100(H)	LYS	6.2
3	K	47	ILE	6.1
3	K	82	ASP	6.0
1	I	122	LEU	6.0
1	E	45	TRP	6.0
1	I	238	PRO	5.8
4	L	100(A)	ILE	5.8
3	G	122	SER	5.8
1	A	491	ILE	5.8
3	G	24	GLY	5.7
4	L	185	SER	5.7
3	C	30	SER	5.7
4	L	100(H)	LYS	5.7
1	E	262	ASN	5.6
3	G	45	SER	5.6
1	E	491	ILE	5.5
3	K	147	VAL	5.4
3	G	56	SER	5.4
1	A	392	ASN	5.4
1	E	160	ASN	5.4
1	I	287	GLN	5.3
1	A	483	LEU	5.3
1	E	200	ALA	5.2
4	D	100(Q)	ASP	5.2
1	A	127	VAL	5.2
1	A	63	THR	5.2
1	I	297	THR	5.2
4	H	69	LEU	5.1
1	E	401	VAL	5.1
1	I	330	HIS	5.1
1	A	238	PRO	5.1
4	H	100(B)	TYR	5.0
1	E	340	GLU	5.0
4	H	200	PRO	5.0
1	I	378	CYS	5.0
4	D	90	TYR	5.0
3	K	145	VAL	5.0
1	I	262	ASN	5.0
4	L	4	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	244	THR	4.9
1	E	287	GLN	4.9
3	G	25	GLU	4.9
4	D	170	SER	4.9
4	L	211	PRO	4.9
3	K	95(C)	ASN	4.8
1	I	492	GLU	4.8
1	I	72	HIS	4.8
3	C	13	VAL	4.7
4	H	100(Q)	ASP	4.7
4	D	109	VAL	4.7
1	E	387	THR	4.7
3	C	20	ARG	4.7
3	G	20	ARG	4.6
4	L	156	ALA	4.6
3	K	162	THR	4.6
3	C	95	ARG	4.6
3	K	62	PHE	4.6
1	I	244	THR	4.6
1	E	272	ILE	4.5
3	C	127	GLN	4.5
4	H	100(N)	PHE	4.5
1	I	379	GLY	4.5
1	I	71	THR	4.5
4	D	59	TYR	4.5
1	I	50	THR	4.5
4	D	34	TRP	4.5
1	E	173	TYR	4.4
1	I	200	ALA	4.4
1	I	174	SER	4.4
4	L	29	VAL	4.4
3	C	162	THR	4.4
4	L	96	LYS	4.4
4	H	73	LYS	4.4
1	I	196	CYS	4.3
4	H	4	LEU	4.3
3	C	93	SER	4.3
1	A	91	GLU	4.3
1	I	221	ALA	4.3
1	E	392	ASN	4.3
1	A	242	VAL	4.3
4	H	102	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	484	TYR	4.3
3	C	45	SER	4.2
3	C	204	GLU	4.2
4	H	112	ALA	4.2
1	A	378	CYS	4.2
4	D	4	LEU	4.2
1	A	415	THR	4.2
1	I	57	ASP	4.2
4	H	158	THR	4.1
1	I	493	PRO	4.1
1	E	122	LEU	4.1
1	E	482	GLU	4.1
1	I	237	GLY	4.1
1	I	83	GLU	4.1
1	A	137	ASN	4.1
1	E	238	PRO	4.0
1	I	127	VAL	4.0
1	A	264	SER	4.0
3	G	70	THR	4.0
1	E	127	VAL	4.0
4	D	10	GLY	4.0
1	A	136	ASN	4.0
3	C	147	VAL	4.0
1	E	114	GLN	4.0
3	C	26	GLU	3.9
4	H	75	LYS	3.9
1	A	156	ASN	3.9
1	I	151	ARG	3.9
4	D	100(R)	VAL	3.9
4	H	121	PRO	3.9
4	L	62	SER	3.9
4	L	102	GLY	3.9
4	L	92	CYS	3.9
1	I	445	CYS	3.8
4	H	31	ASP	3.8
4	H	100(O)	TYR	3.8
3	G	119	PHE	3.8
1	A	471	GLY	3.8
1	E	264	SER	3.8
4	L	71	LEU	3.8
3	C	145	VAL	3.8
1	A	388	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	298	ARG	3.8
3	C	122	SER	3.8
3	K	45	SER	3.8
1	I	53	PHE	3.8
1	I	73	ALA	3.8
1	E	330	HIS	3.8
3	G	68	GLY	3.7
4	D	100(H)	LYS	3.7
1	I	380	GLY	3.7
1	E	199	SER	3.7
3	K	141	TYR	3.7
4	L	59	TYR	3.7
1	A	161	MET	3.7
1	E	92	GLU	3.7
4	L	101	TRP	3.7
1	E	94	ASN	3.7
3	K	30	SER	3.7
4	D	105	THR	3.7
3	K	97	VAL	3.7
1	E	104	MET	3.7
1	E	492	GLU	3.7
1	I	114	GLN	3.7
4	H	100(J)	TRP	3.7
4	D	32	ASN	3.7
1	I	93	PHE	3.7
4	L	122	LEU	3.7
1	I	319	THR	3.6
4	L	157	LEU	3.6
3	K	26	GLU	3.6
1	E	196	CYS	3.6
4	H	59	TYR	3.6
1	I	313	GLY	3.6
1	E	93	PHE	3.6
1	A	114	GLN	3.6
4	H	95	THR	3.6
3	C	158	ALA	3.6
3	G	94	ARG	3.6
3	K	100	GLU	3.6
3	K	175	ALA	3.6
3	G	40	PRO	3.6
1	E	217	TYR	3.6
1	A	300	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
3	K	93	SER	3.6
3	G	204	GLU	3.6
1	I	207	LYS	3.6
4	D	157	LEU	3.5
1	E	51	THR	3.5
1	E	171	LYS	3.5
1	I	49	GLU	3.5
3	G	8	THR	3.5
3	K	57	GLY	3.5
1	I	126	CYS	3.5
3	K	65	SER	3.5
1	I	351	LYS	3.5
3	G	167	LYS	3.5
4	H	100(R)	VAL	3.5
1	E	237	GLY	3.5
3	C	163	THR	3.5
4	L	100(L)	THR	3.5
1	E	430	ILE	3.5
1	I	263	GLY	3.5
1	A	151	ARG	3.5
1	A	162	THR	3.5
3	G	72	THR	3.5
3	C	90	ILE	3.5
4	D	174	TYR	3.5
1	I	267	GLU	3.5
1	I	385	CYS	3.5
3	G	139	ASP	3.4
3	K	108	SER	3.4
4	H	126	SER	3.4
4	D	68	HIS	3.4
1	E	83	GLU	3.4
1	I	91	GLU	3.4
1	I	90	THR	3.4
1	I	387	THR	3.4
4	D	100(B)	TYR	3.4
1	A	466	GLU	3.4
4	L	112	ALA	3.4
1	A	440	GLN	3.4
1	A	98	ASN	3.4
4	L	100(G)	PHE	3.4
4	D	69	LEU	3.4
1	E	151	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	258	GLN	3.4
4	D	175	SER	3.4
1	I	439	ILE	3.4
1	A	275	GLU	3.3
1	I	382	PHE	3.3
3	G	180	SER	3.3
1	A	244	THR	3.3
4	L	121	PRO	3.3
3	K	204	GLU	3.3
4	L	24	VAL	3.3
4	D	55	GLY	3.3
1	I	329	ALA	3.3
3	K	163	THR	3.3
1	I	475	MET	3.3
1	A	267	GLU	3.3
1	A	258	GLN	3.3
1	E	246	GLN	3.3
1	E	56	SER	3.3
1	A	456	ARG	3.3
1	I	304	ARG	3.3
1	I	450	THR	3.3
4	H	17	THR	3.3
4	H	170	SER	3.3
3	G	86	TYR	3.3
1	I	227	LYS	3.3
1	A	273	ARG	3.3
1	E	290	THR	3.3
1	I	94	ASN	3.3
4	L	100(O)	TYR	3.3
1	E	91	GLU	3.3
4	D	6	GLU	3.3
1	A	53	PHE	3.3
1	E	174	SER	3.3
3	G	87	TYR	3.3
3	K	22	THR	3.3
4	L	50	TYR	3.3
4	L	210	GLU	3.2
1	A	95	MET	3.2
4	H	48	ILE	3.2
4	H	165	PRO	3.2
1	E	50	THR	3.2
1	E	297	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLY	3.2
1	I	473	GLY	3.2
1	I	440	GLN	3.2
1	A	45	TRP	3.2
4	L	2	VAL	3.2
1	I	45	TRP	3.2
4	H	26	GLY	3.2
1	E	271	MET	3.2
4	L	1	GLN	3.2
1	A	171	LYS	3.2
4	L	183	PRO	3.2
1	E	90	THR	3.2
3	G	31	ARG	3.2
4	D	79	SER	3.2
4	H	178	SER	3.2
3	C	31	ARG	3.2
1	E	493	PRO	3.2
4	L	194	CYS	3.2
3	G	95	ARG	3.2
1	I	430	ILE	3.2
1	A	357	THR	3.1
1	E	71	THR	3.1
1	I	400	SER	3.1
4	D	165	PRO	3.1
3	C	57	GLY	3.1
3	K	95(B)	THR	3.1
1	A	287	GLN	3.1
3	K	31	ARG	3.1
4	D	167	VAL	3.1
4	H	29	VAL	3.1
1	E	249	HIS	3.1
3	C	139	ASP	3.1
1	E	379	GLY	3.1
1	I	58	ALA	3.1
1	I	129	LEU	3.1
1	I	482	GLU	3.1
1	A	57	ASP	3.1
4	L	110	SER	3.1
4	H	24	VAL	3.1
4	H	202	ASN	3.1
1	A	419	ARG	3.1
1	I	308	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	61	TYR	3.1
4	D	100(L)	THR	3.1
4	D	146	GLU	3.1
1	A	166	ARG	3.1
1	E	254	VAL	3.1
1	A	492	GLU	3.1
4	D	104	GLY	3.0
3	K	56	SER	3.0
4	D	87	SER	3.0
1	A	49	GLU	3.0
4	D	2	VAL	3.0
1	A	379	GLY	3.0
3	K	122	SER	3.0
4	D	65	SER	3.0
4	L	100(J)	TRP	3.0
4	D	100(G)	PHE	3.0
1	A	97	LYS	3.0
1	I	401	VAL	3.0
4	D	92	CYS	3.0
3	G	205	LYS	3.0
3	C	94	ARG	3.0
3	K	95	ARG	3.0
1	A	420	ILE	3.0
1	E	137	ASN	3.0
1	I	173	TYR	3.0
3	C	96	TRP	3.0
1	A	256	SER	3.0
4	H	80	LEU	3.0
1	A	196	CYS	3.0
1	A	247	CYS	3.0
1	A	58	ALA	3.0
3	K	119	PHE	3.0
1	E	273	ARG	3.0
1	I	78	ASP	3.0
3	G	77	SER	3.0
1	I	171	LYS	3.0
4	D	112	ALA	3.0
4	D	100(O)	TYR	2.9
3	G	62	PHE	2.9
1	I	456	ARG	2.9
4	L	100(R)	VAL	2.9
4	H	169	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	351	LYS	2.9
1	I	472	GLY	2.9
4	H	100(L)	THR	2.9
4	D	46	GLU	2.9
4	L	69	LEU	2.9
1	A	479	TRP	2.9
4	H	157	LEU	2.9
1	I	136	ASN	2.9
1	I	69	TRP	2.9
1	A	438	PRO	2.9
1	I	312	PRO	2.9
1	E	165	LEU	2.9
1	E	415	THR	2.9
1	A	283	ASN	2.9
1	I	137	ASN	2.9
1	I	242	VAL	2.9
4	H	94	THR	2.9
4	H	114	THR	2.9
4	L	177	SER	2.9
1	I	392	ASN	2.9
1	I	222	GLY	2.9
4	L	188	GLY	2.9
1	E	436	ALA	2.9
1	A	50	THR	2.9
4	H	175	SER	2.9
1	A	159	PHE	2.9
3	G	127	GLN	2.9
1	E	129	LEU	2.9
3	C	95(C)	ASN	2.9
4	L	41	LEU	2.9
3	G	145	VAL	2.8
4	H	189	THR	2.8
1	I	62	GLU	2.8
4	D	102	GLY	2.8
4	H	23	ASN	2.8
1	I	70	ALA	2.8
3	K	40	PRO	2.8
1	I	85	HIS	2.8
1	A	135	THR	2.8
3	G	30	SER	2.8
4	H	22	CYS	2.8
1	A	104	MET	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	130	LYS	2.8
1	A	72	HIS	2.8
1	I	63	THR	2.8
3	K	48	ILE	2.8
4	D	29	VAL	2.8
4	H	74	SER	2.8
1	E	206	PRO	2.8
1	A	265	LEU	2.8
1	A	236	THR	2.8
1	I	264	SER	2.8
3	C	146	THR	2.8
1	E	328	GLN	2.8
4	H	53	ASP	2.8
1	A	70	ALA	2.8
1	E	221	ALA	2.8
1	I	283	ASN	2.8
1	E	161	MET	2.8
1	E	320	GLY	2.8
4	D	91	TYR	2.8
4	L	56	ASP	2.8
1	E	300	ASN	2.8
3	C	62	PHE	2.8
1	A	401	VAL	2.8
1	E	120	VAL	2.8
1	A	232	LYS	2.8
4	D	200	PRO	2.8
3	C	85	ASP	2.8
3	G	82	ASP	2.8
1	A	353	PHE	2.8
1	A	80	ASN	2.7
1	E	371	VAL	2.7
4	D	24	VAL	2.7
1	E	267	GLU	2.7
3	G	161	GLU	2.7
4	H	209	VAL	2.7
3	K	46	LEU	2.7
3	G	174	ALA	2.7
3	K	43	ALA	2.7
1	A	90	THR	2.7
4	D	67	VAL	2.7
4	D	188	GLY	2.7
4	D	81	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	33	TYR	2.7
4	H	47	TRP	2.7
1	A	442	VAL	2.7
4	L	126	SER	2.7
1	A	233	PHE	2.7
3	G	89	HIS	2.7
3	G	97	VAL	2.7
4	D	99	ARG	2.7
4	L	39	GLN	2.7
4	H	122	LEU	2.7
4	L	181	THR	2.7
4	D	15	SER	2.7
1	I	107	ASP	2.7
1	A	221	ALA	2.7
1	I	371	VAL	2.7
3	G	59	PRO	2.7
4	H	2	VAL	2.7
1	E	247	CYS	2.7
4	H	92	CYS	2.7
1	A	330	HIS	2.6
1	E	242	VAL	2.6
3	C	67(C)	PHE	2.6
1	I	46	LYS	2.6
1	E	442	VAL	2.6
3	G	192	TYR	2.6
4	L	34	TRP	2.6
4	L	100(P)	MET	2.6
1	A	262	ASN	2.6
4	H	25	SER	2.6
4	H	166	ALA	2.6
1	I	120	VAL	2.6
4	H	33	TYR	2.6
1	E	483	LEU	2.6
4	H	36	TRP	2.6
1	E	170	GLN	2.6
3	K	127	GLN	2.6
1	E	222	GLY	2.6
1	I	322	ILE	2.6
1	A	435	TYR	2.6
4	L	11	LEU	2.6
1	A	314	GLN	2.6
1	A	235	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	351	LYS	2.6
1	E	266	ALA	2.6
4	L	81	ARG	2.6
1	A	61	TYR	2.6
1	A	319	THR	2.6
1	A	315	ALA	2.6
1	I	86	LEU	2.6
3	G	33	VAL	2.6
3	G	147	VAL	2.6
4	H	100(E)	VAL	2.6
4	D	36	TRP	2.6
3	G	189	HIS	2.6
4	D	3	HIS	2.6
1	I	170	GLN	2.6
4	H	41	LEU	2.6
1	E	156	ASN	2.6
1	E	166	ARG	2.6
1	I	166	ARG	2.6
1	I	155	LYS	2.5
3	K	89	HIS	2.5
1	E	322	ILE	2.5
4	D	18	LEU	2.5
4	D	53	ASP	2.5
1	I	130	GLN	2.5
1	I	293	GLN	2.5
3	C	208	ALA	2.5
1	A	288	PHE	2.5
1	E	316	PHE	2.5
4	L	163	THR	2.5
1	E	235	GLY	2.5
3	G	29	GLY	2.5
3	C	14	ALA	2.5
3	C	42	GLN	2.5
3	G	155	PRO	2.5
4	D	124	PRO	2.5
4	L	75	LYS	2.5
1	I	424	ILE	2.5
4	D	38	ARG	2.5
1	A	482	GLU	2.5
3	C	60	ASP	2.5
1	A	217	TYR	2.5
1	I	131	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	333	VAL	2.5
1	I	245	VAL	2.5
3	C	35	TRP	2.5
1	E	95	MET	2.5
3	G	65	SER	2.5
4	H	162	HIS	2.5
4	H	210	GLU	2.5
1	I	177	TYR	2.5
3	C	203	VAL	2.5
3	K	96	TRP	2.5
4	L	100(D)	VAL	2.5
4	D	28	LEU	2.5
4	D	71	LEU	2.5
3	K	142	PRO	2.5
1	E	133	ASN	2.5
3	K	76	THR	2.5
3	K	117	THR	2.5
1	I	191	TYR	2.5
4	L	82	LEU	2.5
1	I	194	ILE	2.5
3	K	148	ALA	2.5
1	E	135	THR	2.4
3	C	91	TRP	2.4
1	A	173	TYR	2.4
1	E	378	CYS	2.4
3	K	194	CYS	2.4
4	L	125	SER	2.4
1	I	97	LYS	2.4
1	E	116	LEU	2.4
1	I	112	TRP	2.4
1	I	357	THR	2.4
3	G	39	ARG	2.4
1	A	259	LEU	2.4
1	E	57	ASP	2.4
1	E	159	PHE	2.4
1	E	194	ILE	2.4
3	K	50	ASN	2.4
4	H	32	ASN	2.4
4	H	167	VAL	2.4
1	A	130	GLN	2.4
3	G	26	GLU	2.4
3	K	67(B)	THR	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	47	TRP	2.4
1	I	284	ILE	2.4
3	C	65	SER	2.4
4	H	71	LEU	2.4
1	I	316	PHE	2.4
3	K	158	ALA	2.4
3	G	11	VAL	2.4
1	A	381	GLU	2.4
1	I	154	LEU	2.4
1	I	226	LEU	2.4
1	E	285	LEU	2.4
3	K	112	ALA	2.3
4	H	177	SER	2.3
1	I	161	MET	2.3
3	C	135	CYS	2.3
1	A	94	ASN	2.3
1	I	233	PHE	2.3
1	I	235	GLY	2.3
1	A	194	ILE	2.3
1	A	322	ILE	2.3
4	H	27	THR	2.3
1	A	446	VAL	2.3
4	L	35	SER	2.3
4	L	100(E)	VAL	2.3
1	A	412	ASP	2.3
1	A	200	ALA	2.3
4	D	166	ALA	2.3
1	A	341	THR	2.3
1	E	319	THR	2.3
4	D	184	SER	2.3
4	H	62	SER	2.3
1	I	435	TYR	2.3
1	A	93	PHE	2.3
1	E	420	ILE	2.3
1	I	281	ALA	2.3
1	A	302	ASN	2.3
1	I	425	ASN	2.3
4	L	30	ARG	2.3
1	E	198	THR	2.3
3	K	8	THR	2.3
3	K	63	SER	2.3
1	I	176	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	162	HIS	2.3
4	H	206	ASP	2.3
4	L	132	GLY	2.3
1	A	255	VAL	2.3
4	H	100(D)	VAL	2.3
3	K	179	LEU	2.3
3	G	67(B)	THR	2.3
3	G	132	THR	2.3
3	K	193	SER	2.3
4	H	192	TYR	2.3
1	A	472	GLY	2.3
3	K	42	GLN	2.3
4	L	66	ARG	2.3
4	H	100(I)	GLU	2.3
1	E	357	THR	2.3
1	A	297	THR	2.2
3	C	176	SER	2.2
1	A	352	HIS	2.2
3	G	184	GLU	2.2
3	K	49	TYR	2.2
3	K	75	ILE	2.2
1	E	226	LEU	2.2
1	A	120	VAL	2.2
1	E	481	SER	2.2
4	D	7	SER	2.2
4	H	107	VAL	2.2
4	L	79	SER	2.2
1	E	252	LYS	2.2
1	A	387	THR	2.2
1	I	459	GLY	2.2
3	G	69	THR	2.2
3	K	144	ALA	2.2
1	E	72	HIS	2.2
3	G	16	GLY	2.2
3	K	159	GLY	2.2
1	A	174	SER	2.2
1	E	400	SER	2.2
3	K	176	SER	2.2
1	A	175	LEU	2.2
3	G	49	TYR	2.2
3	K	192	TYR	2.2
1	A	389	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	43	ALA	2.2
3	C	67(B)	THR	2.2
1	A	468	PHE	2.2
1	A	165	LEU	2.2
1	I	54	CYS	2.2
4	H	38	ARG	2.2
3	G	57	GLY	2.2
1	E	386	ASN	2.2
1	E	353	PHE	2.2
3	C	9	PHE	2.2
4	D	48	ILE	2.2
4	L	100(N)	PHE	2.2
3	C	179	LEU	2.2
3	G	190	LYS	2.2
1	I	56	SER	2.2
4	D	35	SER	2.2
4	H	184	SER	2.2
1	E	130	GLN	2.2
1	I	466	GLU	2.2
1	I	383	PHE	2.1
3	G	203	VAL	2.1
4	D	100(D)	VAL	2.1
4	H	90	TYR	2.1
1	I	104	MET	2.1
1	A	237	GLY	2.1
3	C	155	PRO	2.1
1	A	51	THR	2.1
1	I	128	THR	2.1
3	C	196	VAL	2.1
1	E	100	MET	2.1
1	E	164	GLU	2.1
3	C	29	GLY	2.1
4	D	42	GLY	2.1
4	L	55	GLY	2.1
3	K	134	VAL	2.1
3	K	36	TYR	2.1
1	A	380	GLY	2.1
3	C	111	LYS	2.1
4	L	47	TRP	2.1
4	D	100(K)	PHE	2.1
1	E	47	ASP	2.1
1	E	218	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	247	CYS	2.1
1	E	136	ASN	2.1
1	E	177	TYR	2.1
1	I	249	HIS	2.1
4	L	95	THR	2.1
1	I	463	SER	2.1
4	H	100(G)	PHE	2.1
4	H	136	LEU	2.1
1	E	77	THR	2.1
3	G	50	ASN	2.1
4	H	197	ASN	2.1
4	D	132	GLY	2.1
1	E	488	VAL	2.1
1	I	255	VAL	2.1
1	E	475	MET	2.1
4	L	72	ASP	2.1
1	A	354	GLY	2.1
3	K	71	ALA	2.1
3	G	55	PRO	2.1
4	D	100(J)	TRP	2.1
4	H	111	SER	2.1
4	D	100	ARG	2.0
1	A	59	LYS	2.0
3	K	107	LEU	2.0
3	C	192	TYR	2.0
1	E	176	PHE	2.0
4	D	89	ILE	2.0
1	A	445	CYS	2.0
3	G	96	TRP	2.0
3	K	44	PRO	2.0
1	I	134	VAL	2.0
4	L	67	VAL	2.0
4	L	136	LEU	2.0
1	A	436	ALA	2.0
4	L	31	ASP	2.0
4	L	131	GLY	2.0
1	E	79	PRO	2.0
3	C	40	PRO	2.0
4	D	100(P)	MET	2.0
1	A	447	SER	2.0
1	I	199	SER	2.0
3	C	49	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	311	GLY	2.0
1	I	311	GLY	2.0
4	H	100(F)	ALA	2.0
1	E	245	VAL	2.0
3	C	195	GLN	2.0
1	A	487	LYS	2.0
3	C	132	THR	2.0
3	G	28	LEU	2.0
3	K	197	THR	2.0
4	H	96	LYS	2.0
4	L	16	GLU	2.0
4	L	73	LYS	2.0
3	G	32	SER	2.0
3	G	93	SER	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MAN	X	1	11/12	-0.42	0.34	427,427,427,427	0
5	MAN	Y	4	11/12	-0.34	0.21	550,550,550,550	0
7	MAN	R	1	11/12	-0.24	0.43	550,550,550,550	0
5	NAG	Y	1	14/15	-0.15	0.29	530,530,530,530	0
5	NAG	Y	2	14/15	-0.09	0.23	460,460,460,460	0
5	MAN	S	4	11/12	-0.05	0.15	550,550,550,550	0
5	MAN	M	4	11/12	-0.03	0.16	517,517,517,517	0
5	MAN	S	6	11/12	0.06	0.19	497,497,497,497	0
7	MAN	R	2	11/12	0.09	0.42	489,489,489,489	0
5	MAN	P	6	11/12	0.09	0.16	470,470,470,470	0
6	MAN	Q	9	11/12	0.13	0.17	303,303,303,303	0
5	MAN	U	6	11/12	0.15	0.17	515,515,515,515	0
5	MAN	Y	6	11/12	0.16	0.17	494,494,494,494	0
5	MAN	Z	7	11/12	0.16	0.34	550,550,550,550	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	Z	6	11/12	0.17	0.18	428,428,428,428	0
5	MAN	P	4	11/12	0.18	0.10	483,483,483,483	0
5	MAN	V	6	11/12	0.19	0.14	454,454,454,454	0
5	BMA	V	3	11/12	0.26	0.15	492,492,492,492	0
5	MAN	V	4	11/12	0.27	0.13	471,471,471,471	0
5	MAN	N	7	11/12	0.28	0.37	498,498,498,498	0
5	MAN	S	5	11/12	0.29	0.16	550,550,550,550	0
5	MAN	O	6	11/12	0.30	0.17	455,455,455,455	0
5	MAN	U	4	11/12	0.31	0.23	550,550,550,550	0
5	NAG	M	1	14/15	0.31	0.22	439,439,439,439	0
6	MAN	W	7	11/12	0.31	0.15	418,418,418,418	0
5	MAN	M	7	11/12	0.32	0.15	451,451,451,451	0
5	MAN	M	5	11/12	0.32	0.15	481,481,481,481	0
6	MAN	Q	7	11/12	0.33	0.12	309,309,309,309	0
5	NAG	S	1	14/15	0.33	0.28	550,550,550,550	0
5	BMA	S	3	11/12	0.34	0.16	500,500,500,500	0
6	MAN	Q	5	11/12	0.35	0.27	302,302,302,302	0
5	MAN	N	6	11/12	0.37	0.16	464,464,464,464	0
6	BMA	W	3	11/12	0.38	0.13	400,400,400,400	0
6	MAN	W	5	11/12	0.38	0.27	330,330,330,330	0
5	MAN	Y	5	11/12	0.39	0.19	477,477,477,477	0
5	MAN	Y	7	11/12	0.40	0.26	520,520,520,520	0
5	MAN	N	4	11/12	0.40	0.21	550,550,550,550	0
5	MAN	Z	4	11/12	0.41	0.14	550,550,550,550	0
6	MAN	W	6	11/12	0.41	0.31	452,452,452,452	0
5	MAN	S	7	11/12	0.43	0.19	518,518,518,518	0
5	MAN	M	6	11/12	0.46	0.16	434,434,434,434	0
5	BMA	Y	3	11/12	0.47	0.13	402,402,402,402	0
5	MAN	O	4	11/12	0.47	0.20	550,550,550,550	0
5	MAN	P	7	11/12	0.48	0.29	447,447,447,447	0
5	MAN	T	5	11/12	0.49	0.19	422,422,422,422	0
7	MAN	X	2	11/12	0.49	0.40	545,545,545,545	0
5	MAN	Z	5	11/12	0.50	0.18	410,410,410,410	0
5	BMA	O	3	11/12	0.50	0.15	506,506,506,506	0
5	MAN	T	7	11/12	0.52	0.32	542,542,542,542	0
5	MAN	T	6	11/12	0.53	0.16	446,446,446,446	0
6	MAN	W	9	11/12	0.53	0.09	335,335,335,335	0
5	BMA	P	3	11/12	0.55	0.13	455,455,455,455	0
5	NAG	U	1	14/15	0.55	0.38	408,408,408,408	0
5	MAN	U	5	11/12	0.57	0.19	550,550,550,550	0
5	MAN	T	4	11/12	0.57	0.15	550,550,550,550	0
5	BMA	U	3	11/12	0.58	0.12	340,340,340,340	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	O	5	11/12	0.58	0.18	468,468,468,468	0
5	MAN	V	5	11/12	0.59	0.21	495,495,495,495	0
5	BMA	Z	3	11/12	0.59	0.13	491,491,491,491	0
5	NAG	P	2	14/15	0.60	0.16	307,307,307,307	0
5	BMA	M	3	11/12	0.62	0.11	356,356,356,356	0
6	NAG	Q	1	14/15	0.65	0.32	366,366,366,366	0
5	BMA	N	3	11/12	0.66	0.10	483,483,483,483	0
6	MAN	W	4	11/12	0.66	0.34	550,550,550,550	0
5	MAN	N	5	11/12	0.67	0.14	329,329,329,329	0
5	NAG	O	1	14/15	0.70	0.40	423,423,423,423	0
5	BMA	T	3	11/12	0.71	0.10	466,466,466,466	0
6	MAN	Q	8	11/12	0.72	0.22	500,500,500,500	0
6	MAN	Q	4	11/12	0.72	0.30	550,550,550,550	0
5	NAG	V	2	14/15	0.73	0.16	335,335,335,335	0
5	NAG	a	1	14/15	-	-	437,437,437,437	0
5	NAG	a	2	14/15	-	-	231,231,231,231	0
5	BMA	a	3	11/12	-	-	297,297,297,297	0
5	MAN	a	4	11/12	-	-	545,545,545,545	0
5	MAN	a	5	11/12	-	-	507,507,507,507	0
5	MAN	a	6	11/12	-	-	532,532,532,532	0
5	MAN	a	7	11/12	-	-	197,197,197,197	0
5	NAG	b	1	14/15	-	-	276,276,276,276	0
5	NAG	b	2	14/15	-	-	382,382,382,382	0
5	BMA	b	3	11/12	-	-	474,474,474,474	0
5	MAN	b	4	11/12	-	-	467,467,467,467	0
5	MAN	b	5	11/12	-	-	482,482,482,482	0
5	MAN	b	6	11/12	-	-	474,474,474,474	0
5	MAN	b	7	11/12	-	-	330,330,330,330	0
6	NAG	W	1	14/15	0.73	0.24	302,302,302,302	0
6	NAG	W	2	14/15	0.74	0.24	388,388,388,388	0
5	NAG	M	2	14/15	0.75	0.18	519,519,519,519	0
6	MAN	Q	6	11/12	0.75	0.21	422,422,422,422	0
6	BMA	Q	3	11/12	0.75	0.10	292,292,292,292	0
5	NAG	P	1	14/15	0.75	0.21	202,202,202,202	0
6	MAN	W	8	11/12	0.75	0.23	491,491,491,491	0
5	MAN	V	7	11/12	0.76	0.18	377,377,377,377	0
5	NAG	U	2	14/15	0.77	0.29	310,310,310,310	0
5	MAN	P	5	11/12	0.78	0.18	418,418,418,418	0
5	NAG	S	2	14/15	0.79	0.15	488,488,488,488	0
5	NAG	T	1	14/15	0.82	0.22	186,186,186,186	0
6	NAG	Q	2	14/15	0.83	0.13	258,258,258,258	0
5	MAN	O	7	11/12	0.84	0.10	229,229,229,229	0

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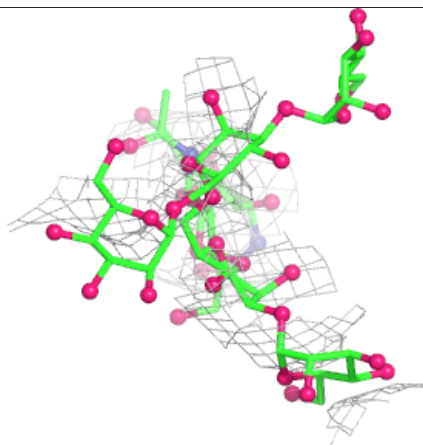
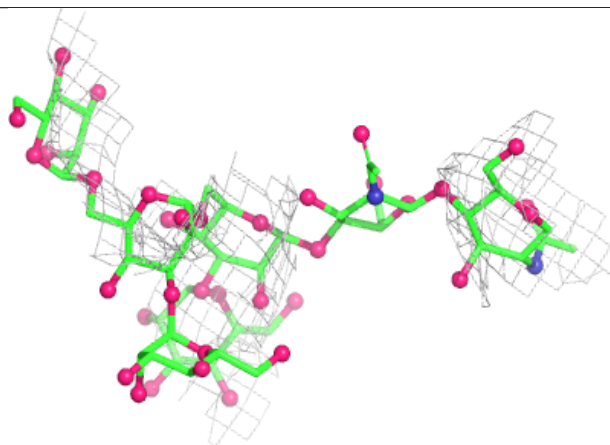
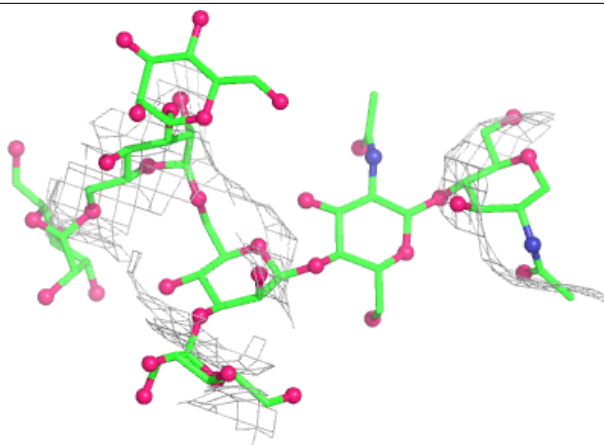
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	U	7	11/12	0.84	0.10	195,195,195,195	0
5	NAG	N	1	14/15	0.84	0.28	356,356,356,356	0
5	NAG	V	1	14/15	0.85	0.25	242,242,242,242	0
5	NAG	O	2	14/15	0.89	0.27	410,410,410,410	0
6	NAG	c	1	14/15	-	-	292,292,292,292	0
6	NAG	c	2	14/15	-	-	213,213,213,213	0
6	BMA	c	3	11/12	-	-	345,345,345,345	0
6	MAN	c	4	11/12	-	-	550,550,550,550	0
6	MAN	c	5	11/12	-	-	277,277,277,277	0
6	MAN	c	6	11/12	-	-	436,436,436,436	0
6	MAN	c	7	11/12	-	-	382,382,382,382	0
6	MAN	c	8	11/12	-	-	507,507,507,507	0
6	MAN	c	9	11/12	-	-	362,362,362,362	0
5	NAG	Z	2	14/15	0.90	0.14	375,375,375,375	0
5	NAG	Z	1	14/15	0.90	0.22	337,337,337,337	0
5	NAG	N	2	14/15	0.91	0.14	310,310,310,310	0
5	NAG	T	2	14/15	0.97	0.13	301,301,301,301	0
7	MAN	d	1	11/12	-	-	408,408,408,408	0
7	MAN	d	2	11/12	-	-	550,550,550,550	0

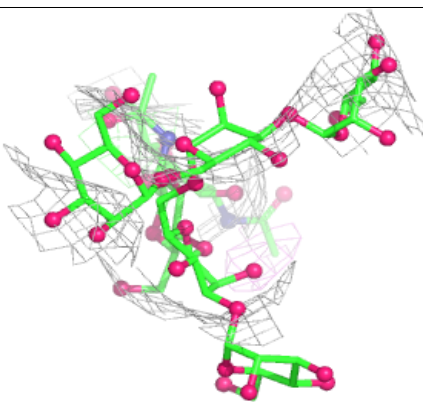
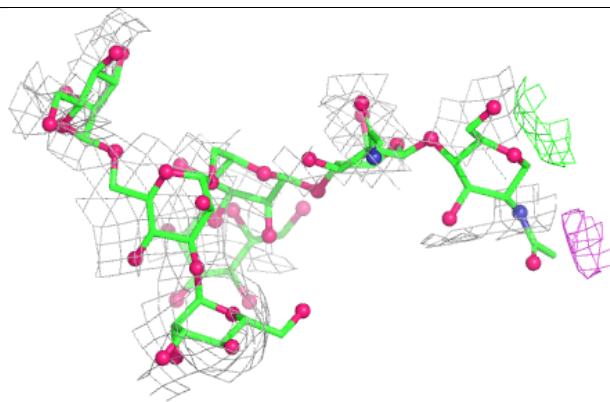
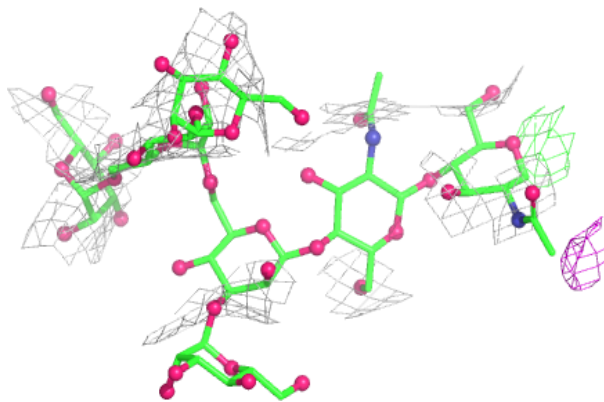
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

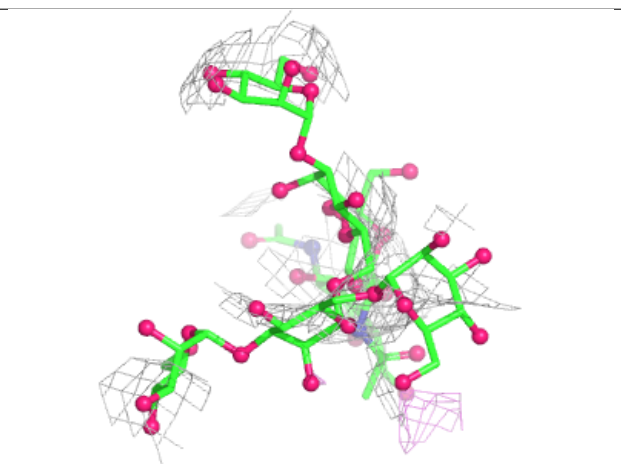
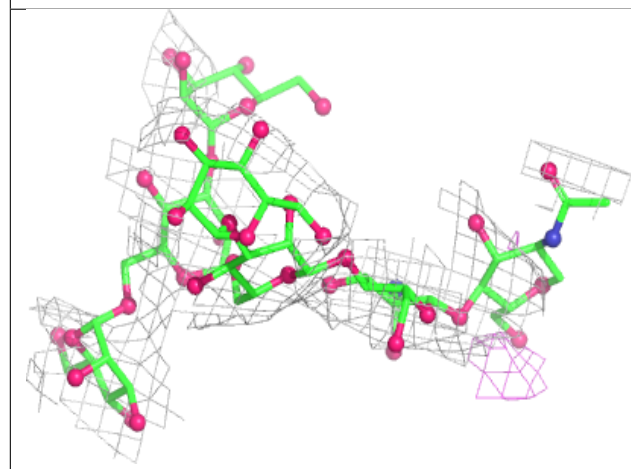
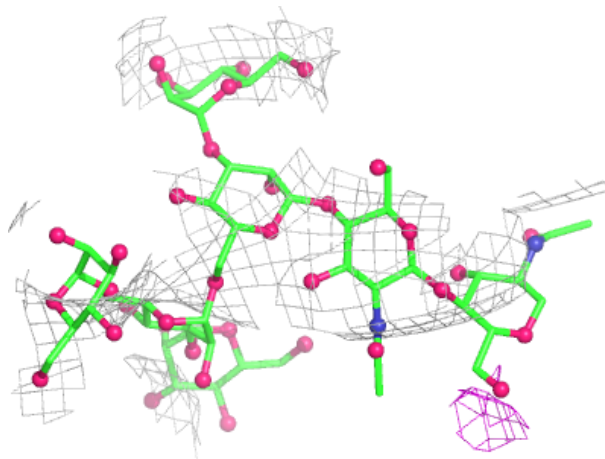
**Electron density around Chain N:**

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



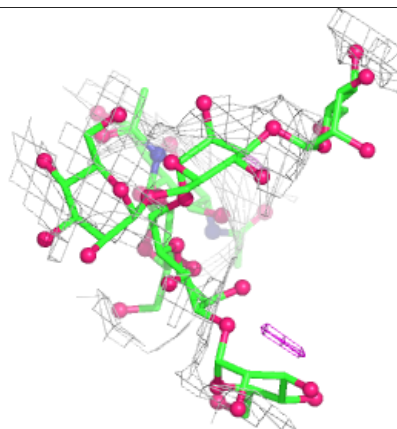
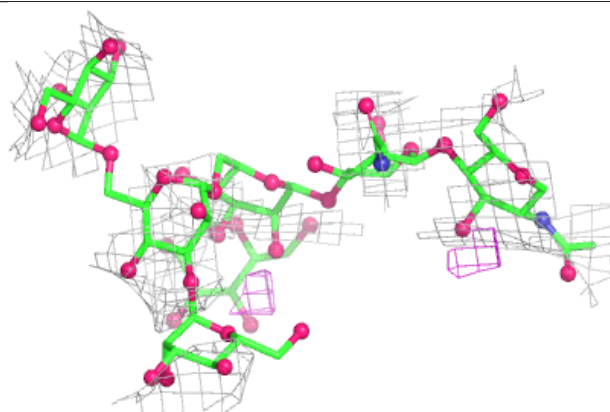
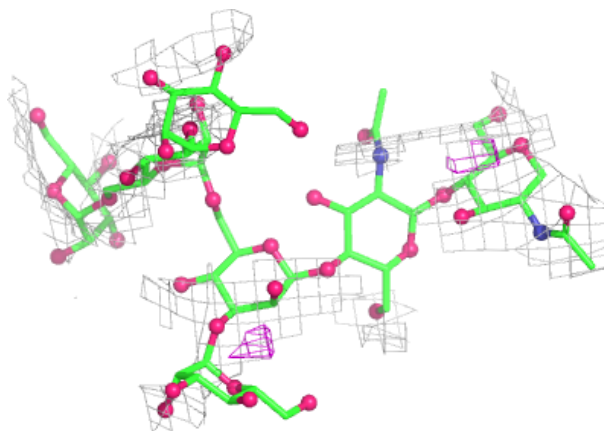
Electron density around Chain O:

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



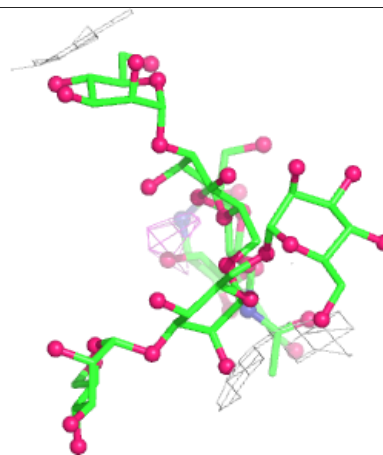
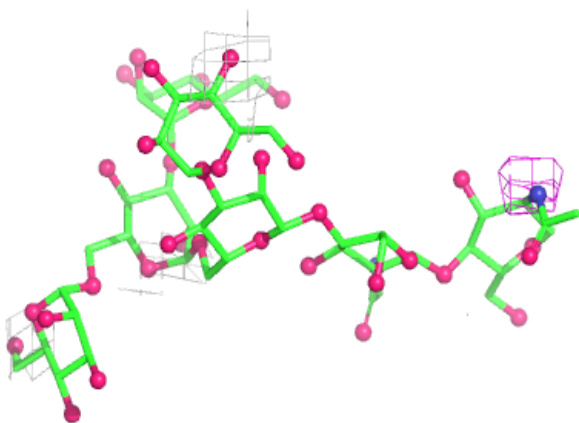
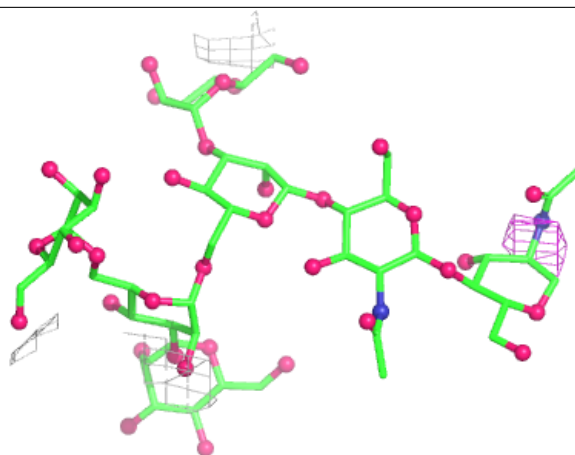
Electron density around Chain P:

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

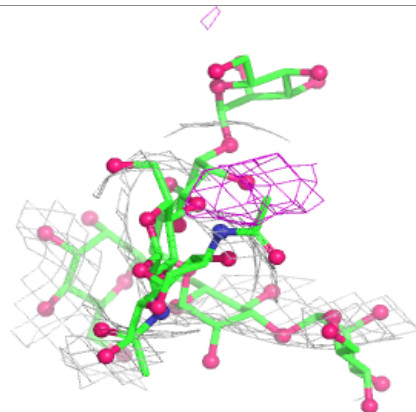
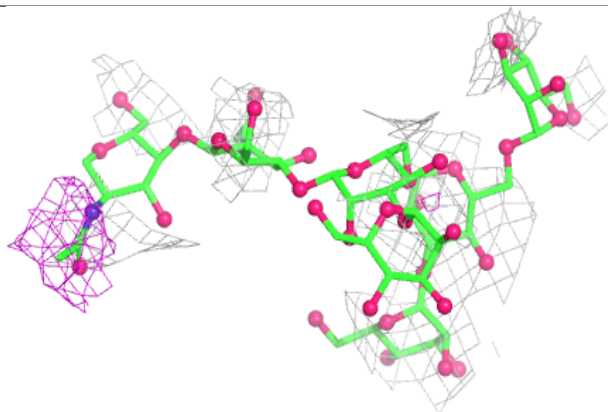
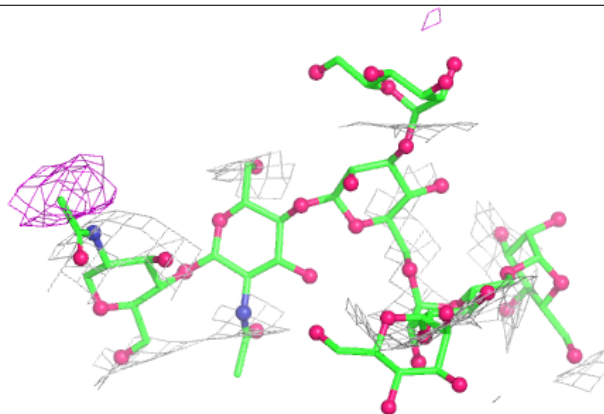


Electron density around Chain S:

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

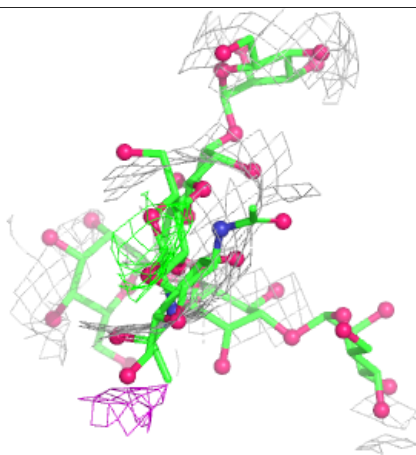
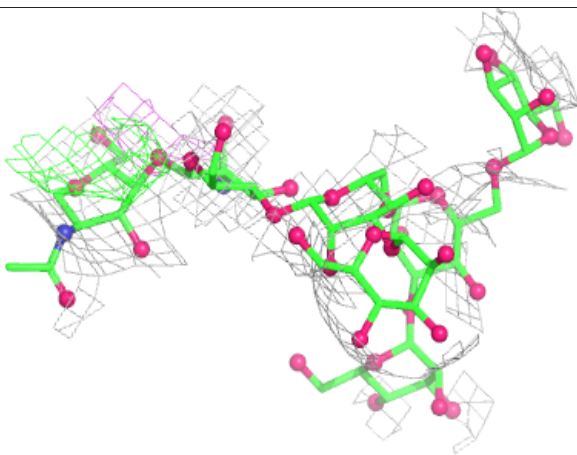
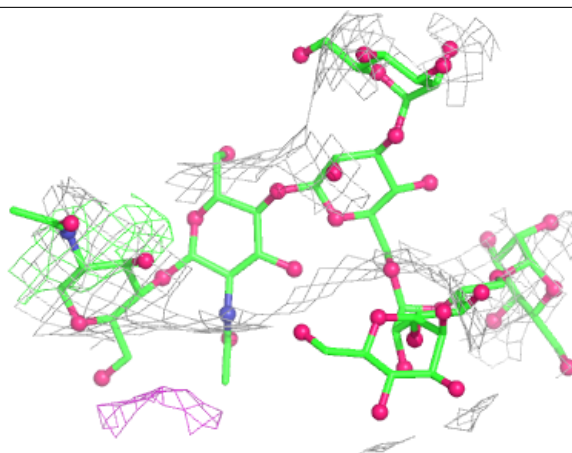
**Electron density around Chain T:**

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

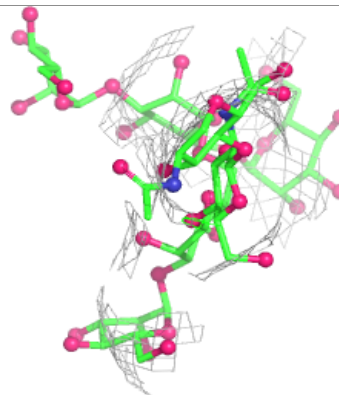
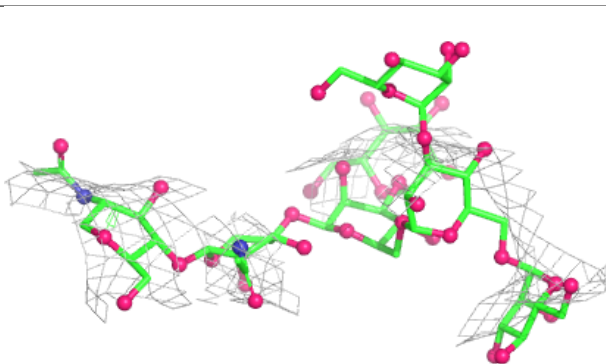
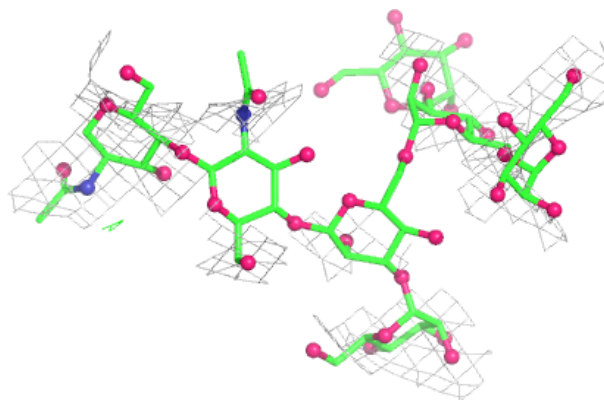


Electron density around Chain U:

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

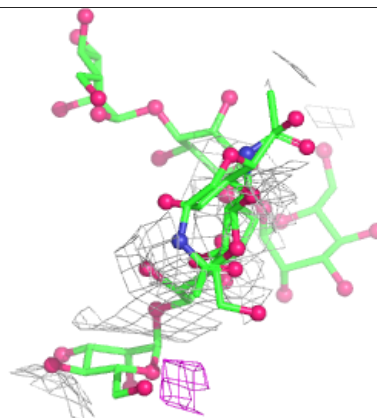
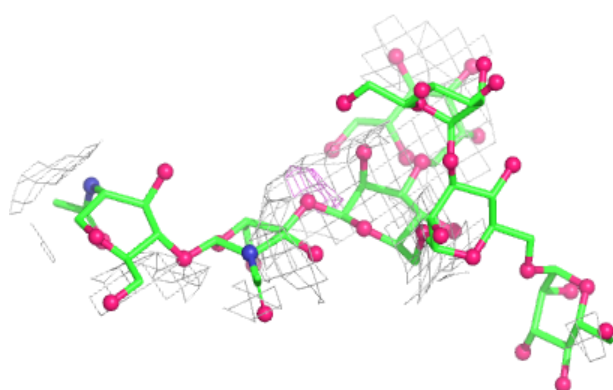
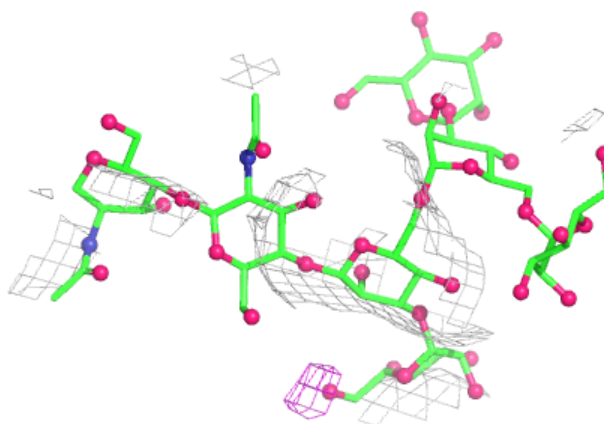
**Electron density around Chain V:**

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

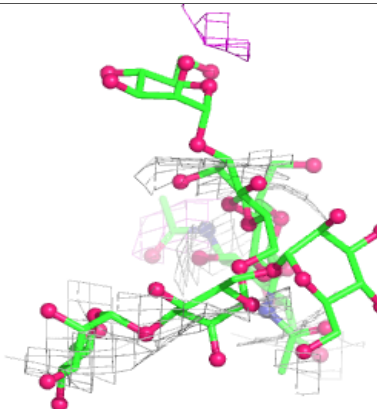
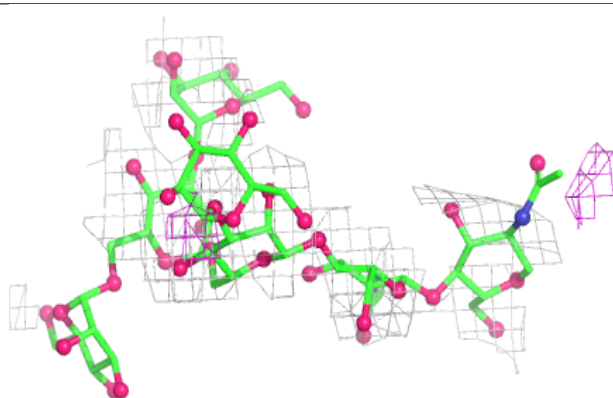
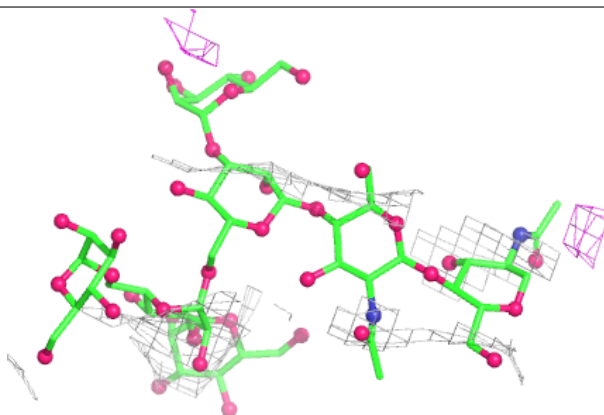


Electron density around Chain Y:

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

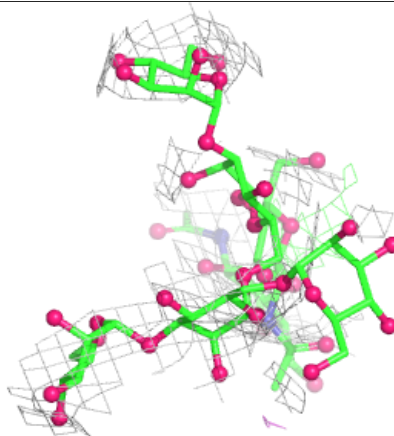
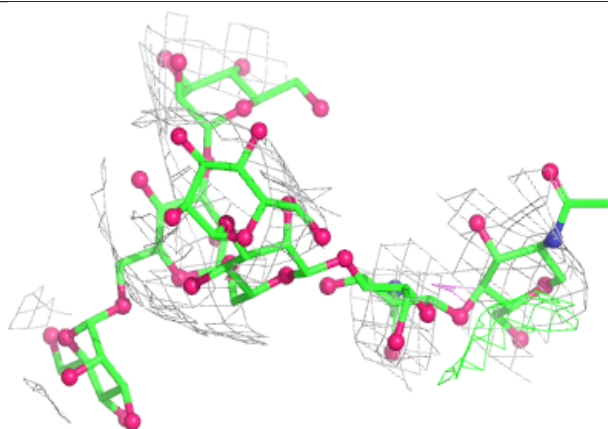
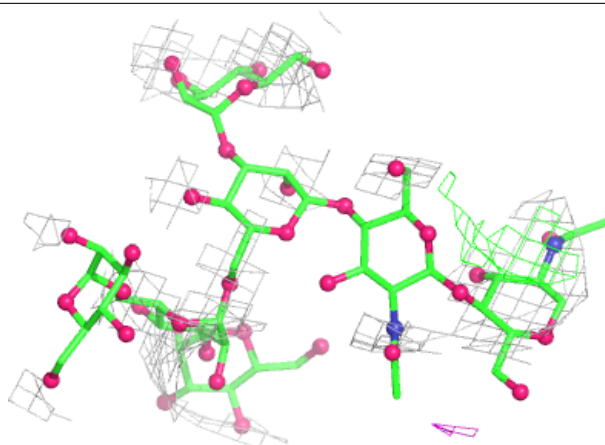
**Electron density around Chain Z:**

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

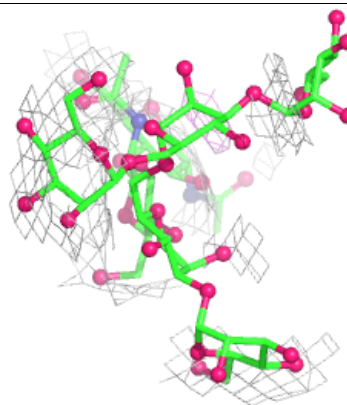
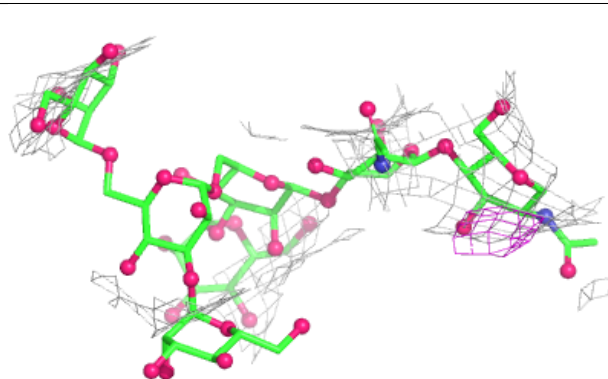
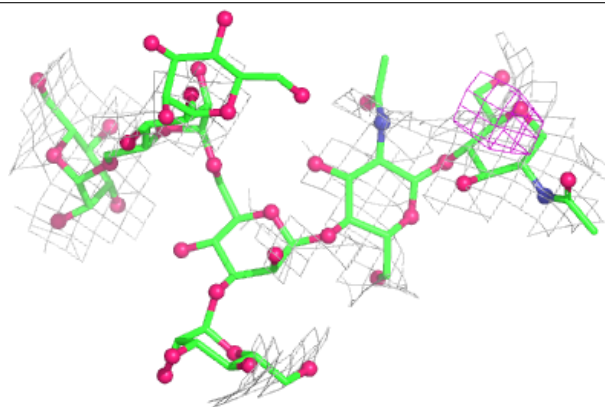


Electron density around Chain a:

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

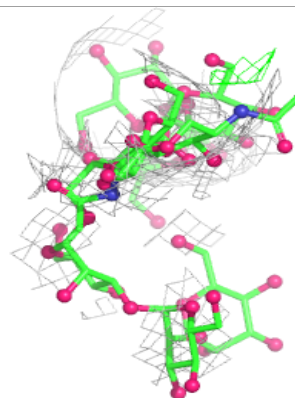
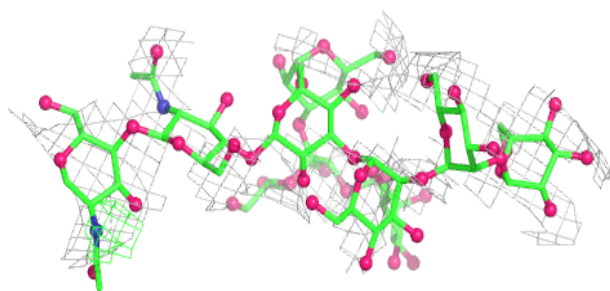
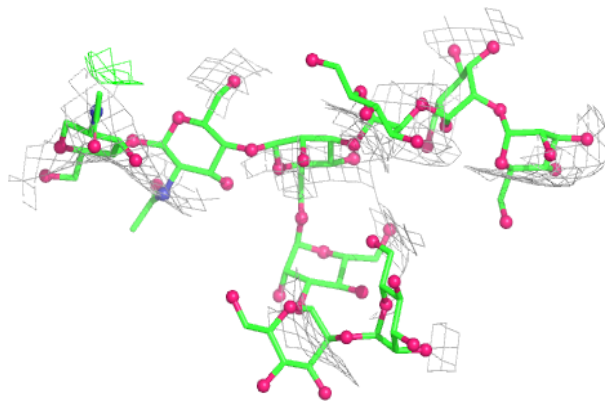
**Electron density around Chain b:**

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

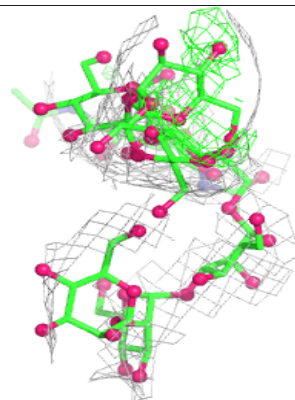
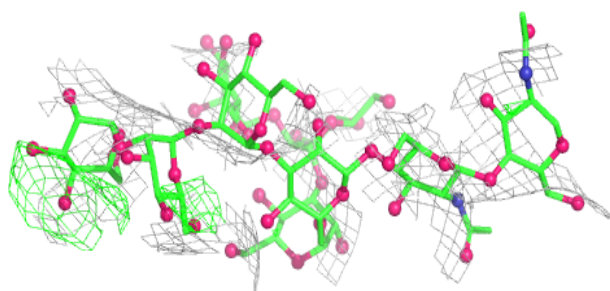
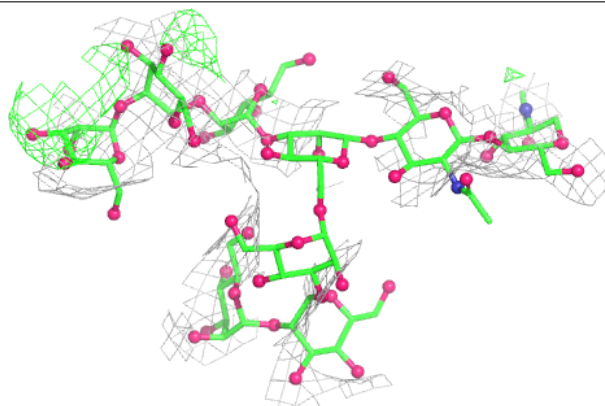


Electron density around Chain Q:

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

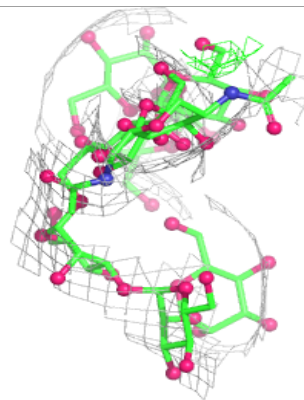
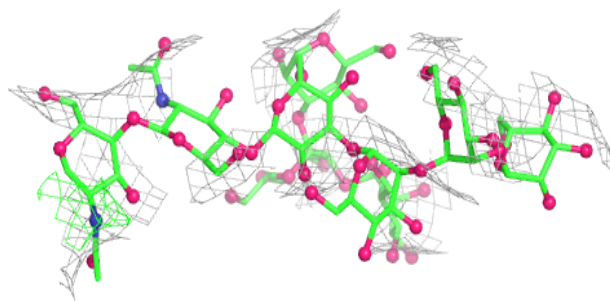
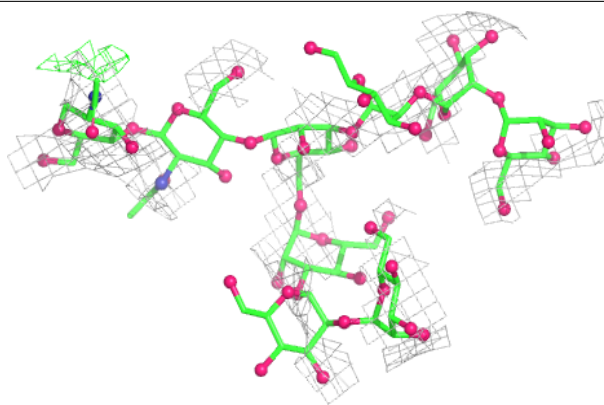
**Electron density around Chain W:**

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



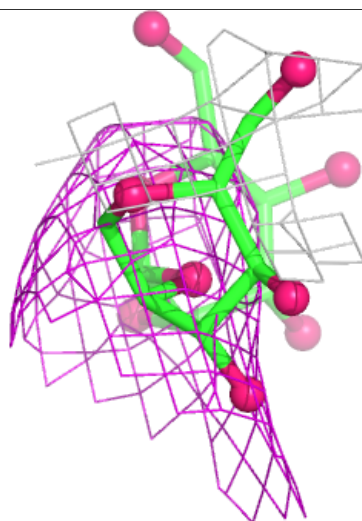
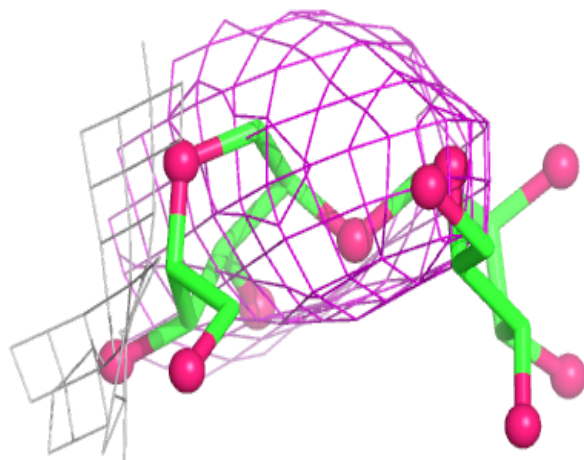
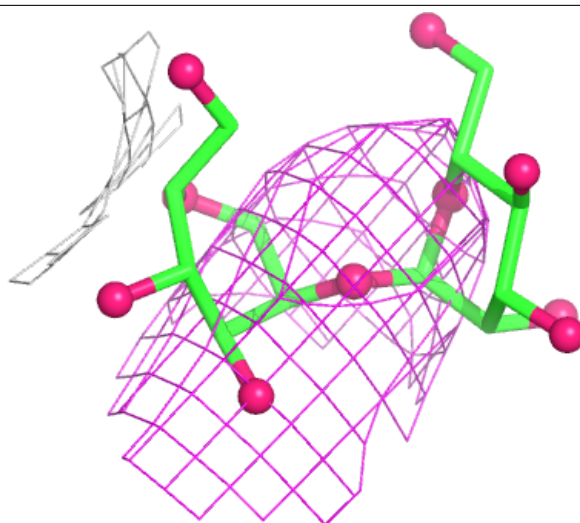
Electron density around Chain c:

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



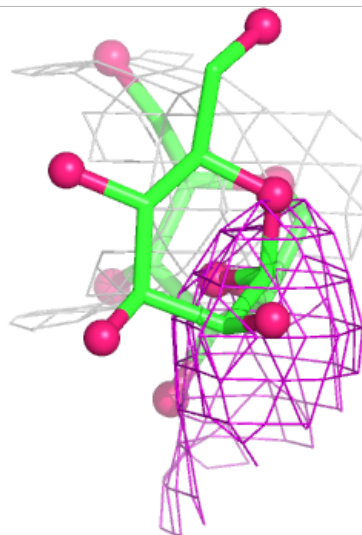
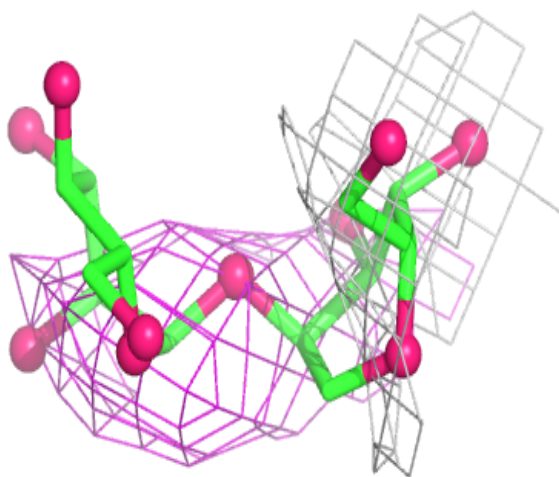
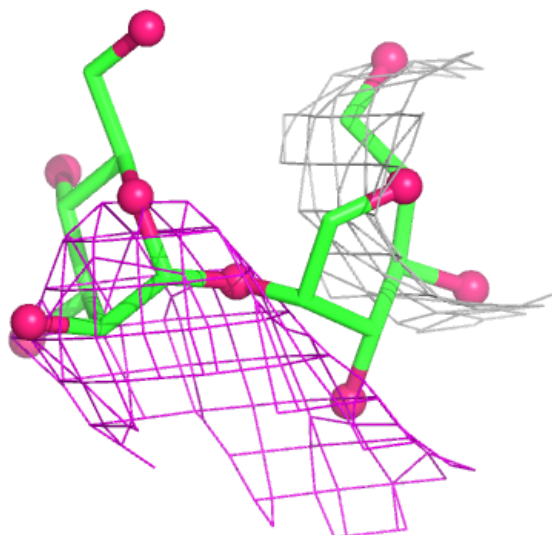
Electron density around Chain R:

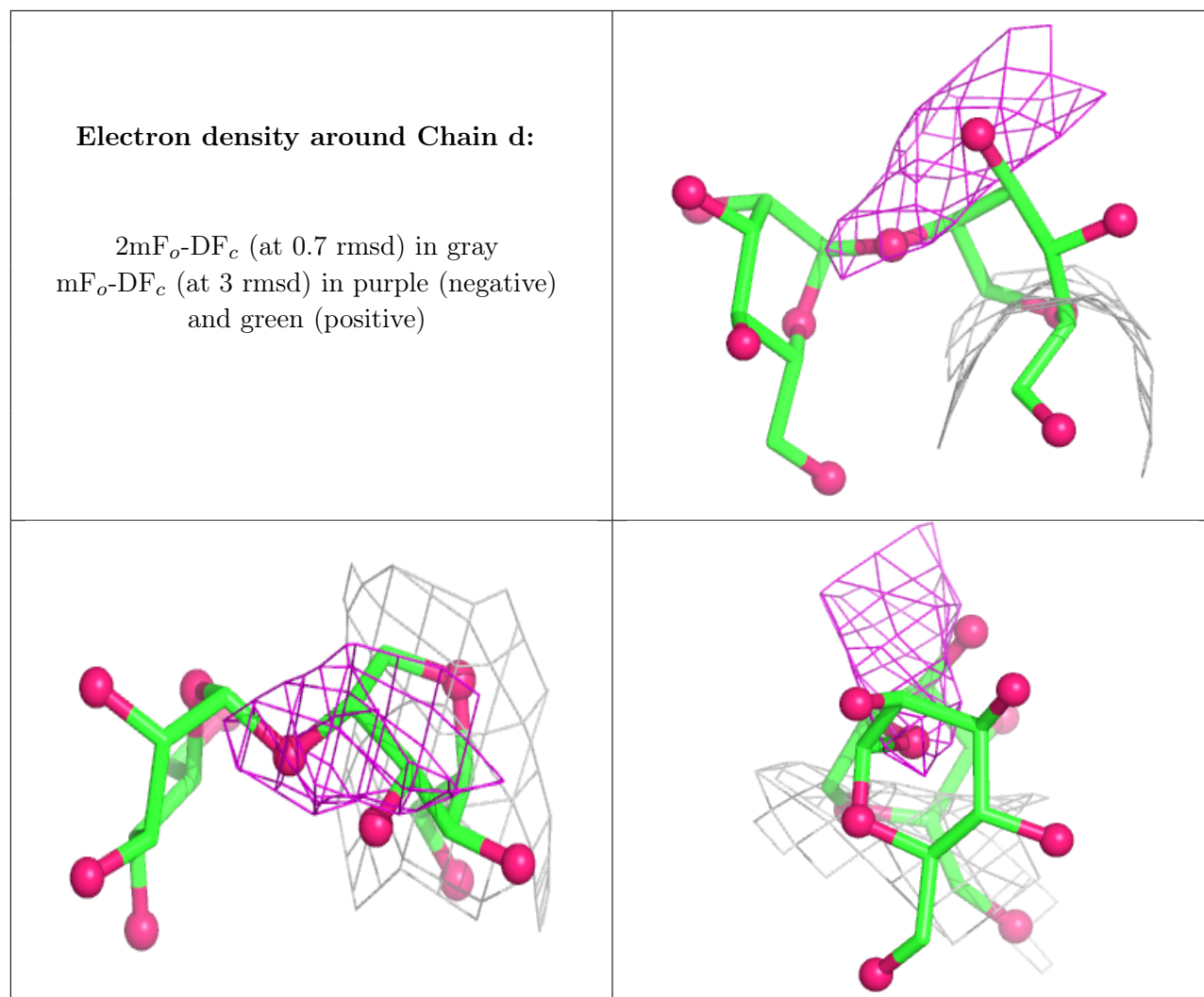
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain X:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	E	1355	14/15	0.15	0.21	411,411,411,411	0
8	NAG	E	1392	14/15	0.23	0.20	305,305,305,305	0
8	NAG	I	1355	14/15	0.23	0.13	266,266,266,266	0
8	NAG	A	1392	14/15	0.25	0.32	386,386,386,386	0
8	NAG	A	1355	14/15	0.37	0.13	238,238,238,238	0
8	NAG	A	1448	14/15	0.39	0.33	279,279,279,279	0
8	NAG	I	1160	14/15	0.45	0.22	362,362,362,362	0
8	NAG	E	1448	14/15	0.47	0.37	361,361,361,361	0
8	NAG	E	1088	14/15	0.49	0.14	486,486,486,486	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	I	1234	14/15	0.54	0.25	345,345,345,345	0
8	NAG	I	1392	14/15	0.55	0.22	345,345,345,345	0
8	NAG	I	1197	14/15	0.59	0.24	304,304,304,304	0
8	NAG	A	1088	14/15	0.60	0.15	474,474,474,474	0
8	NAG	E	1160	14/15	0.63	0.17	245,245,245,245	0
8	NAG	I	1088	14/15	0.64	0.20	503,503,503,503	0
8	NAG	E	1234	14/15	0.64	0.26	405,405,405,405	0
8	NAG	A	1160	14/15	0.66	0.15	267,267,267,267	0
8	NAG	I	1448	14/15	0.66	0.29	287,287,287,287	0
8	NAG	E	1276	14/15	0.67	0.17	313,313,313,313	0
8	NAG	A	1234	14/15	0.68	0.27	431,431,431,431	0
8	NAG	E	1197	14/15	0.72	0.26	288,288,288,288	0
8	NAG	E	1295	14/15	0.73	0.34	356,356,356,356	0
8	NAG	A	1386	14/15	0.75	0.31	356,356,356,356	0
8	NAG	A	1276	14/15	0.78	0.14	288,288,288,288	0
8	NAG	I	1276	14/15	0.80	0.14	281,281,281,281	0
8	NAG	I	1386	14/15	0.80	0.27	331,331,331,331	0
8	NAG	A	1295	14/15	0.82	0.32	330,330,330,330	0
8	NAG	I	1295	14/15	0.84	0.36	323,323,323,323	0
8	NAG	E	1386	14/15	0.85	0.25	427,427,427,427	0
8	NAG	A	1197	14/15	0.86	0.20	302,302,302,302	0

6.5 Other polymers

There are no such residues in this entry.