



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:13 PM UTC

PDB ID : 5UTY / pdb_00005uty
Title : Crystal Structure of a Stabilized DS-SOSIP.mut4 BG505 gp140 HIV-1 Env Trimer, Containing Mutations I201C-P433C (DS), L154M, N300M, N302M, T320L in Complex with Human Antibodies PGT122 and 35O22 at 4.1 Angstrom
Authors : Xu, K.; Chuang, G.-Y.; Pancera, M.; Kwong, P.D.
Deposited on : 2017-02-15
Resolution : 3.41 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

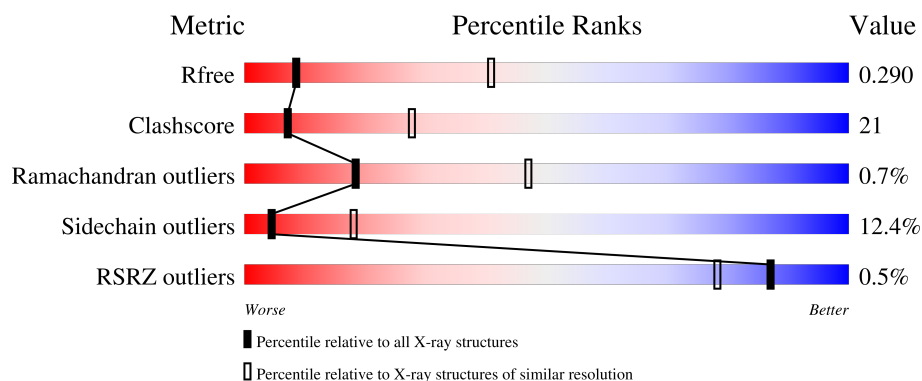
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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.



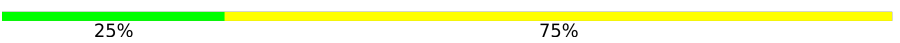
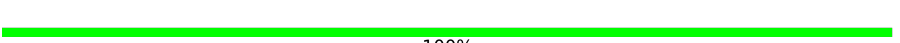
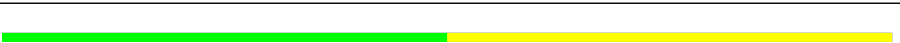
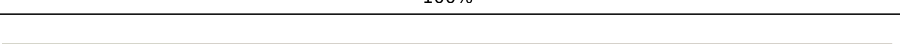
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	B	153	
2	D	243	
3	E	216	
4	G	505	

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Mol	Chain	Length	Quality of chain
5	H	235	
6	L	208	
7	A	6	
8	C	4	
9	F	5	
10	I	2	
10	J	2	
10	K	2	
10	N	2	
10	O	2	
10	Q	2	
10	R	2	
10	S	2	
10	T	2	
11	M	6	
12	P	10	

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
12	NAG	P	1	-	-	X	-
12	NAG	P	2	-	-	X	-
12	MAN	P	5	-	-	X	-
12	MAN	P	6	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 12020 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 HIV-1 BG505 strain Env gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	122	Total	C	N	O	S	0	0	0
			969	611	168	184	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	242	Total	C	N	O	S	0	0	0
			1820	1156	303	353	8			

- Molecule 3 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called HIV-1 BG505 strain Env gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	449	Total	C	N	O	S	0	0	0
			3542	2224	623	662	33			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	7	MET	-	initiating methionine	UNP Q2N0S6
G	8	PRO	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	9	MET	-	expression tag	UNP Q2N0S6
G	10	GLY	-	expression tag	UNP Q2N0S6
G	11	SER	-	expression tag	UNP Q2N0S6
G	12	LEU	-	expression tag	UNP Q2N0S6
G	13	GLN	-	expression tag	UNP Q2N0S6
G	14	PRO	-	expression tag	UNP Q2N0S6
G	15	LEU	-	expression tag	UNP Q2N0S6
G	16	ALA	-	expression tag	UNP Q2N0S6
G	17	THR	-	expression tag	UNP Q2N0S6
G	18	LEU	-	expression tag	UNP Q2N0S6
G	19	TYR	-	expression tag	UNP Q2N0S6
G	20	LEU	-	expression tag	UNP Q2N0S6
G	21	LEU	-	expression tag	UNP Q2N0S6
G	22	GLY	-	expression tag	UNP Q2N0S6
G	23	MET	-	expression tag	UNP Q2N0S6
G	24	LEU	-	expression tag	UNP Q2N0S6
G	25	VAL	-	expression tag	UNP Q2N0S6
G	26	ALA	-	expression tag	UNP Q2N0S6
G	27	SER	-	expression tag	UNP Q2N0S6
G	28	VAL	-	expression tag	UNP Q2N0S6
G	29	LEU	-	expression tag	UNP Q2N0S6
G	154	MET	LEU	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6
G	300	MET	ASN	engineered mutation	UNP Q2N0S6
G	302	MET	ASN	engineered mutation	UNP Q2N0S6
G	320	LEU	THR	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	insertion	UNP Q2N0S6
G	510	ARG	-	insertion	UNP Q2N0S6
G	511	ARG	-	insertion	UNP Q2N0S6
G	512	ARG	-	insertion	UNP Q2N0S6
G	513	ARG	-	insertion	UNP Q2N0S6

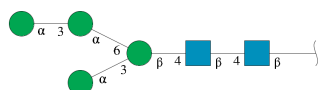
- Molecule 5 is a protein called PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	232	Total	C	N	O	S	0	0	0
			1762	1121	299	337	5			

- Molecule 6 is a protein called PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



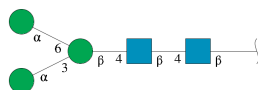
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



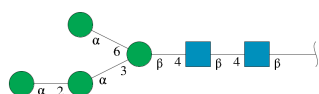
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



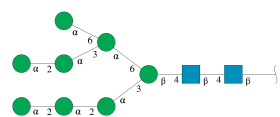
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called 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.



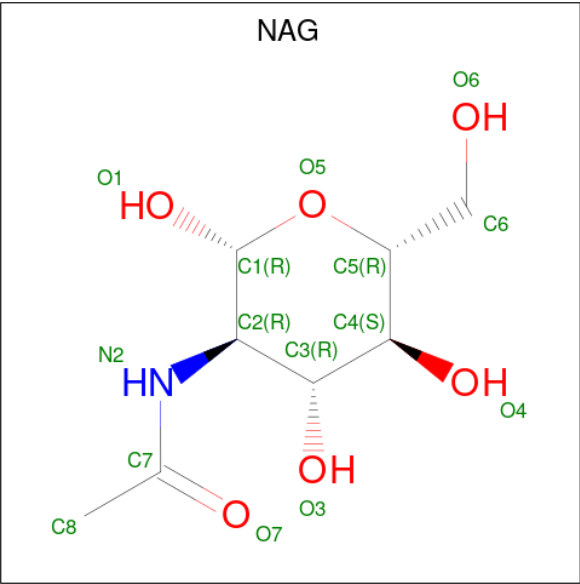
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 12 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)]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
12	P	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

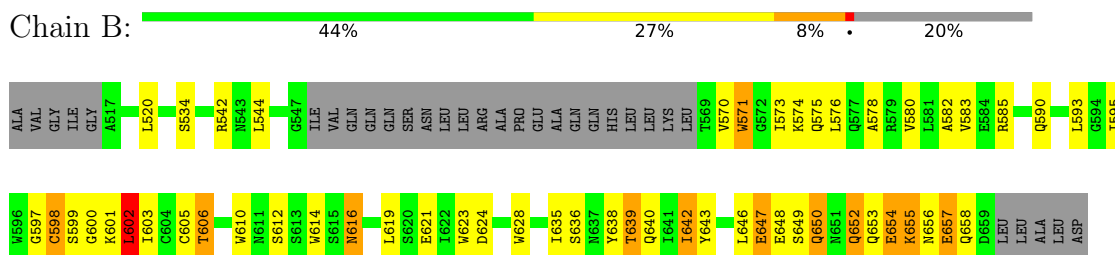


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	H	1	Total	C	N	O	0	0
			14	8	1	5		

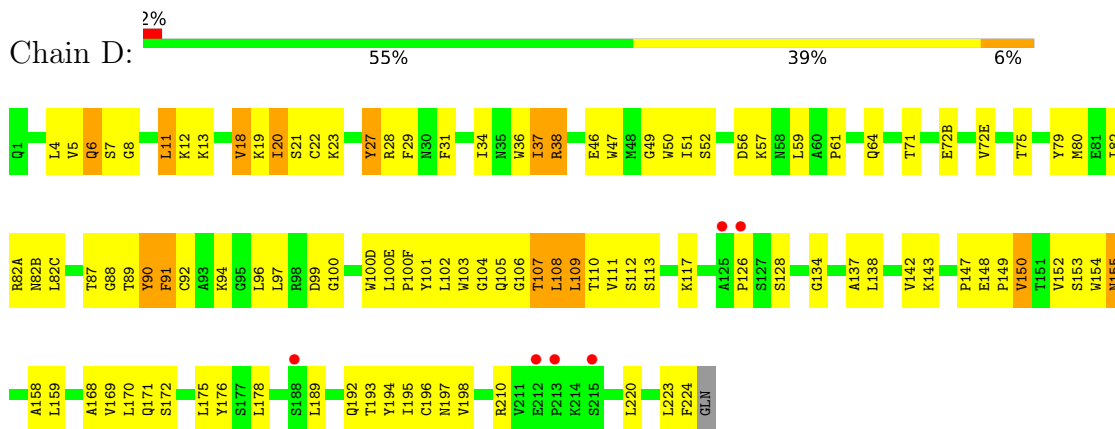
3 Residue-property plots

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

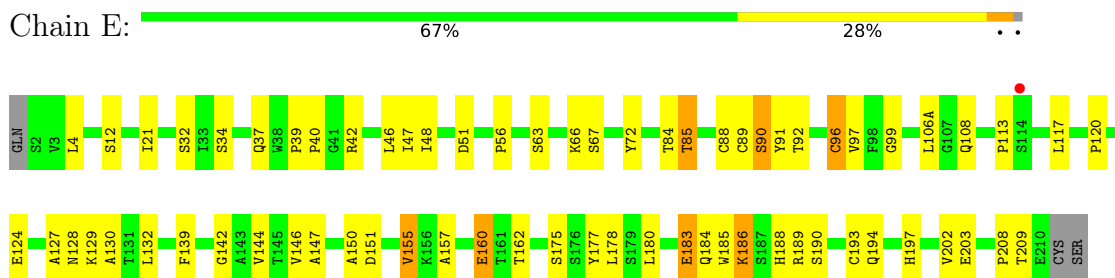
- Molecule 1: HIV-1 BG505 strain Env gp41



- Molecule 2: 35O22 Fab heavy chain

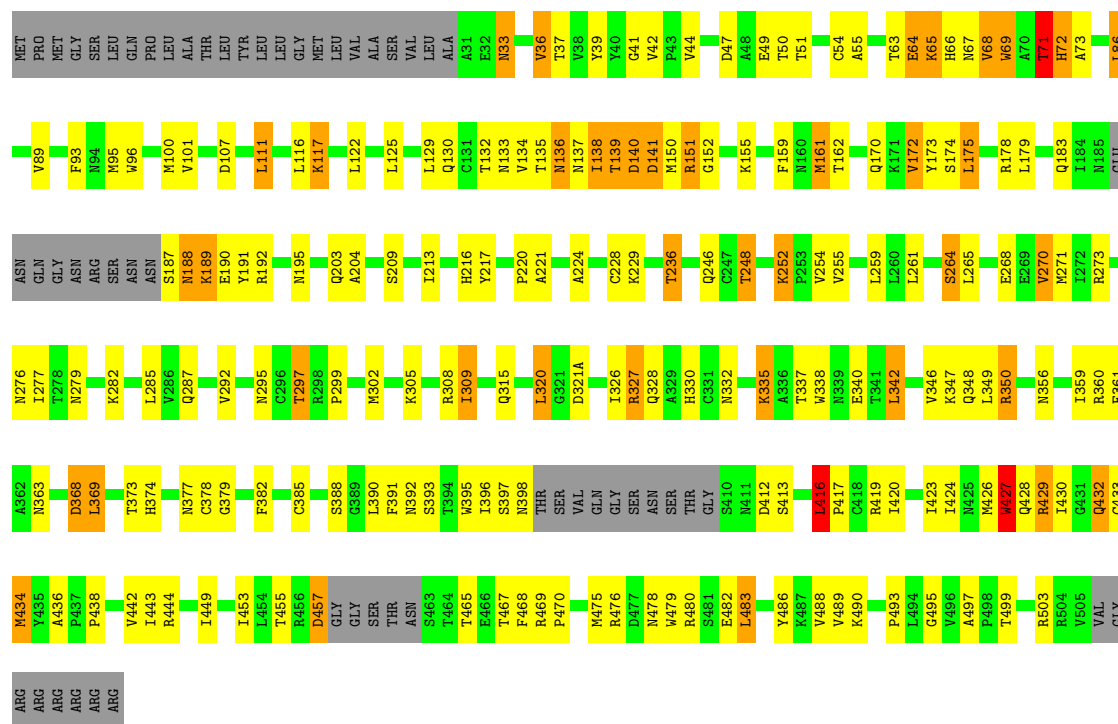


- Molecule 3: 35O22 Fab light chain



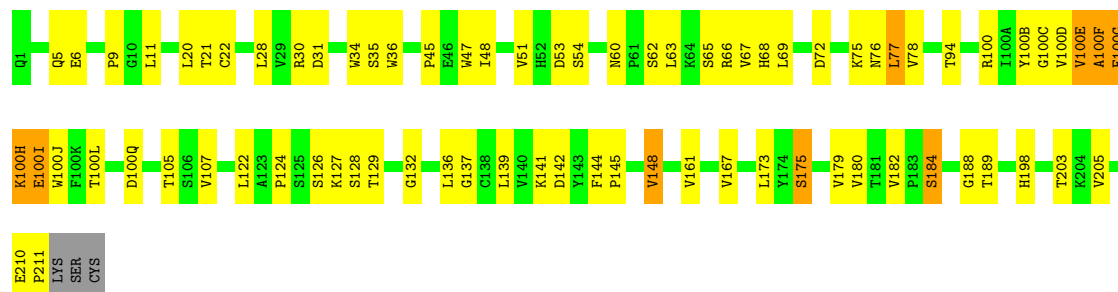
- Molecule 4: HIV-1 BG505 strain Env gp120





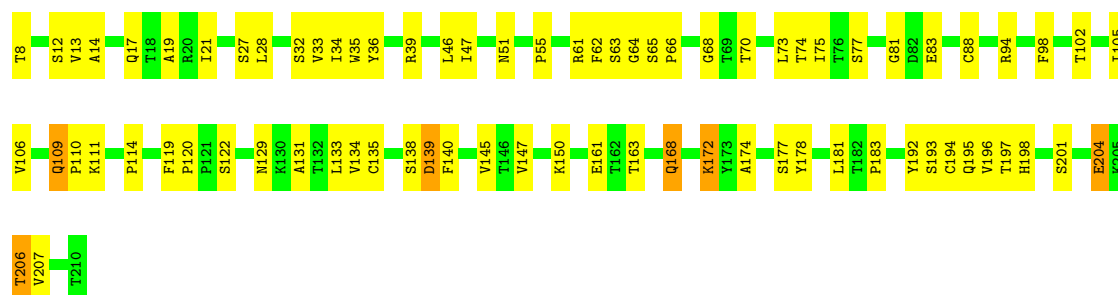
• Molecule 5: PGT122 Fab heavy chain

Chain H: 66% 29%



• Molecule 6: PGT122 Fab light chain

Chain L: 63% 34%



• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam

ido-2-deoxy-beta-D-glucopyranose

Chain A:  50% 50%

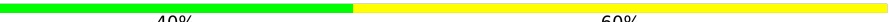


- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  25% 75%



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

Chain F:  40% 60%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



- Molecule 11: 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

Chain M:  100%



- Molecule 12: 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)] 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 P:  20% 80%

NAG1	NAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	131.45Å 131.45Å 312.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.48 – 3.41 41.48 – 3.41	Depositor EDS
% Data completeness (in resolution range)	58.0 (41.48-3.41) 58.0 (41.48-3.41)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.241 , 0.288 0.245 , 0.290	Depositor DCC
R_{free} test set	1269 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.138 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12020	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.57	0/987	0.72	2/1338 (0.1%)
2	D	0.26	0/1867	0.49	1/2544 (0.0%)
3	E	0.13	0/1659	0.38	0/2269
4	G	0.33	1/3615 (0.0%)	0.59	3/4903 (0.1%)
5	H	0.42	3/1810 (0.2%)	0.48	0/2474
6	L	0.13	0/1619	0.44	0/2217
All	All	0.32	4/11557 (0.0%)	0.52	6/15745 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	1
5	H	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	100(I)	GLU	CD-OE1	-5.96	1.14	1.25
5	H	100(F)	ALA	CA-C	-5.43	1.45	1.52
5	H	100(I)	GLU	CD-OE2	5.17	1.35	1.25
4	G	427	TRP	CA-C	-5.10	1.46	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	416	LEU	C-N-CD	-11.71	77.00	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	71	THR	N-CA-C	10.77	123.02	111.28
4	G	136	ASN	N-CA-C	6.49	118.07	108.60
2	D	91	PHE	N-CA-C	6.32	118.37	108.96
1	B	646	LEU	O-C-N	-6.06	115.30	122.20
1	B	600	GLY	N-CA-C	-5.63	99.84	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	416	LEU	Mainchain
5	H	100(G)	PHE	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	B	969	0	938	45	2
2	D	1820	0	1788	129	0
3	E	1615	0	1542	44	0
4	G	3542	0	3475	146	0
5	H	1762	0	1724	83	0
6	L	1577	0	1518	50	0
7	A	72	0	61	7	0
8	C	50	0	43	3	0
9	F	61	0	52	1	0
10	I	28	0	25	2	0
10	J	28	0	25	0	0
10	K	28	0	25	2	0
10	N	28	0	25	1	0
10	O	28	0	25	0	0
10	Q	28	0	25	0	0
10	R	28	0	25	0	0
10	S	28	0	25	2	0
10	T	28	0	25	0	0
11	M	72	0	61	3	0
12	P	116	0	97	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	42	0	39	0	0
13	G	56	0	52	1	0
13	H	14	0	13	1	0
All	All	12020	0	11628	491	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (491) 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)
2:D:109:LEU:HD12	2:D:110:THR:N	1.29	1.48
5:H:100(D):VAL:HA	12:P:2:NAG:H2	1.29	1.11
2:D:8:GLY:HA2	2:D:107:THR:HG23	1.19	1.10
2:D:7:SER:O	2:D:107:THR:HG21	1.52	1.10
1:B:590:GLN:HE22	1:B:601:LYS:HE2	1.09	1.09
1:B:590:GLN:NE2	1:B:601:LYS:HE2	1.68	1.07
2:D:109:LEU:HD12	2:D:110:THR:CA	1.86	1.05
2:D:109:LEU:CD1	2:D:110:THR:N	2.20	1.04
11:M:1:NAG:H61	11:M:2:NAG:HN2	1.23	1.03
4:G:136:ASN:OD1	4:G:137:ASN:N	1.95	0.98
2:D:7:SER:O	2:D:107:THR:CG2	2.12	0.95
4:G:71:THR:O	4:G:73:ALA:N	1.98	0.95
2:D:109:LEU:HD12	2:D:110:THR:C	1.90	0.94
2:D:109:LEU:CD1	2:D:110:THR:C	2.41	0.93
2:D:108:LEU:HD13	2:D:149:PRO:HG3	1.48	0.93
2:D:8:GLY:HA2	2:D:107:THR:CG2	2.00	0.92
2:D:108:LEU:HD13	2:D:149:PRO:CG	2.00	0.91
2:D:109:LEU:HD12	2:D:110:THR:H	1.28	0.91
2:D:8:GLY:CA	2:D:107:THR:HG23	1.99	0.91
5:H:100(B):TYR:H	5:H:100(B):TYR:HD2	1.19	0.90
5:H:100(D):VAL:HA	12:P:2:NAG:C2	2.03	0.89
5:H:100(D):VAL:HG22	5:H:100(I):GLU:OE2	1.72	0.89
4:G:100:MET:HB2	4:G:483:LEU:HD11	1.54	0.87
6:L:120:PRO:HG3	6:L:207:VAL:HG21	1.56	0.87
2:D:109:LEU:HD11	2:D:111:VAL:N	1.89	0.87
4:G:138:ILE:HD11	4:G:140:ASP:HA	1.57	0.86
5:H:100(D):VAL:HG23	5:H:100(F):ALA:H	1.39	0.86
12:P:8:MAN:O3	12:P:9:MAN:O5	1.93	0.86
2:D:90:TYR:HE2	2:D:109:LEU:HB3	1.41	0.85
2:D:126:PRO:HA	2:D:137:ALA:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLN:HE22	2:D:92:CYS:N	1.75	0.84
2:D:109:LEU:HD21	2:D:111:VAL:HG22	1.59	0.84
2:D:11:LEU:HB3	2:D:147:PRO:HG3	1.60	0.83
6:L:195:GLN:HG2	6:L:204:GLU:HB2	1.63	0.80
1:B:652:GLN:HE21	1:B:653:GLN:N	1.80	0.79
2:D:108:LEU:HD11	2:D:148:GLU:HB3	1.64	0.79
4:G:204:ALA:HB2	4:G:434:MET:HE2	1.65	0.79
6:L:131:ALA:HB3	6:L:181:LEU:O	1.82	0.79
2:D:89:THR:HG22	2:D:91:PHE:CE1	2.18	0.79
4:G:138:ILE:CD1	4:G:140:ASP:HA	2.13	0.79
4:G:138:ILE:HD12	4:G:139:THR:C	2.09	0.78
2:D:108:LEU:HD22	2:D:149:PRO:HD3	1.66	0.78
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.63	0.78
4:G:68:VAL:HG12	4:G:209:SER:HB3	1.67	0.77
2:D:6:GLN:NE2	2:D:92:CYS:HB2	2.00	0.77
5:H:167:VAL:HB	6:L:163:THR:HG22	1.67	0.77
2:D:6:GLN:HE22	2:D:92:CYS:H	1.32	0.77
2:D:6:GLN:HG3	2:D:105:GLN:H	1.49	0.75
1:B:652:GLN:HE21	1:B:652:GLN:C	1.96	0.74
5:H:22:CYS:HB3	5:H:78:VAL:HB	1.70	0.73
2:D:128:SER:HB2	2:D:220:LEU:HB2	1.67	0.73
4:G:429:ARG:O	4:G:429:ARG:NH2	2.15	0.73
1:B:602:LEU:HD23	1:B:602:LEU:N	2.03	0.72
1:B:653:GLN:O	1:B:657:GLU:HB3	1.88	0.72
5:H:75:LYS:HB3	5:H:77:LEU:HD12	1.71	0.72
3:E:47:ILE:HG22	3:E:48:ILE:HG12	1.72	0.72
4:G:71:THR:O	4:G:72:HIS:C	2.32	0.72
5:H:51:VAL:HB	5:H:69:LEU:HD13	1.72	0.72
2:D:90:TYR:CE2	2:D:109:LEU:HB3	2.24	0.72
3:E:183:GLU:HA	3:E:186:LYS:HB3	1.71	0.72
5:H:100(C):GLY:O	12:P:2:NAG:H2	1.89	0.71
2:D:109:LEU:CD1	2:D:111:VAL:N	2.53	0.71
2:D:108:LEU:C	2:D:108:LEU:HD23	2.16	0.71
6:L:150:LYS:HB2	6:L:193:SER:HB2	1.71	0.70
4:G:297:THR:HB	4:G:444:ARG:HG2	1.72	0.70
5:H:28:LEU:HD12	5:H:30:ARG:HB3	1.73	0.69
4:G:427:TRP:O	4:G:428:GLN:C	2.32	0.69
4:G:187:SER:OG	4:G:188:ASN:N	2.26	0.69
6:L:33:VAL:N	6:L:51:ASN:OD1	2.25	0.69
4:G:138:ILE:HD12	4:G:138:ILE:C	2.18	0.69
4:G:190:GLU:O	4:G:191:TYR:CD1	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:100(G):PHE:O	5:H:100(H):LYS:HG2	1.93	0.68
2:D:152:VAL:HG22	2:D:198:VAL:HG22	1.74	0.68
4:G:270:VAL:HG23	4:G:348:GLN:HG3	1.76	0.68
6:L:83:GLU:HG3	6:L:106:VAL:HG23	1.75	0.68
3:E:37:GLN:HB2	3:E:47:ILE:HD11	1.76	0.68
3:E:91:TYR:HB3	3:E:96:CYS:HB2	1.76	0.68
2:D:108:LEU:HD11	2:D:148:GLU:CB	2.23	0.67
2:D:108:LEU:HD21	2:D:148:GLU:O	1.94	0.67
4:G:170:GLN:HG3	4:G:172:VAL:HG22	1.75	0.67
4:G:292:VAL:HG12	4:G:449:ILE:HB	1.76	0.67
5:H:100(D):VAL:HG12	12:P:1:NAG:O4	1.95	0.67
1:B:605:CYS:HA	4:G:37:THR:HG22	1.77	0.66
2:D:109:LEU:HD11	2:D:110:THR:C	2.16	0.66
3:E:151:ASP:HB2	3:E:188:HIS:HB3	1.78	0.66
2:D:36:TRP:C	2:D:37:ILE:HG13	2.20	0.66
2:D:108:LEU:HD13	2:D:149:PRO:CD	2.24	0.66
4:G:426:MET:O	4:G:427:TRP:HB2	1.96	0.66
4:G:65:LYS:HB3	4:G:68:VAL:HG13	1.78	0.66
6:L:14:ALA:HB3	6:L:17:GLN:HG3	1.78	0.66
5:H:141:LYS:HA	5:H:175:SER:HB3	1.78	0.65
2:D:109:LEU:HD21	2:D:111:VAL:CG2	2.26	0.65
3:E:160:GLU:HG3	3:E:177:TYR:HB2	1.79	0.65
4:G:141:ASP:OD2	4:G:141:ASP:N	2.27	0.65
5:H:100(D):VAL:HG23	5:H:100(F):ALA:CB	2.26	0.65
2:D:109:LEU:CD1	2:D:110:THR:H	2.00	0.65
1:B:616:ASN:OD1	1:B:616:ASN:N	2.30	0.65
4:G:368:ASP:OD1	4:G:368:ASP:N	2.24	0.65
5:H:100(C):GLY:O	12:P:2:NAG:H4	1.97	0.64
4:G:342:LEU:HD13	4:G:395:TRP:HE1	1.63	0.64
5:H:100(G):PHE:HD1	5:H:100(I):GLU:CA	2.11	0.64
3:E:120:PRO:HB3	3:E:130:ALA:HA	1.79	0.64
3:E:4:LEU:HB3	3:E:99:GLY:HA2	1.80	0.64
7:A:2:NAG:H3	7:A:2:NAG:H83	1.79	0.64
2:D:108:LEU:HD23	2:D:108:LEU:O	1.98	0.63
1:B:590:GLN:NE2	1:B:601:LYS:CE	2.53	0.63
4:G:332:ASN:HD22	12:P:1:NAG:H83	1.62	0.63
2:D:6:GLN:NE2	2:D:92:CYS:H	1.96	0.63
3:E:32:SER:O	3:E:90:SER:HA	1.99	0.62
2:D:90:TYR:HE2	2:D:109:LEU:CB	2.11	0.62
4:G:379:GLY:HA3	4:G:443:ILE:HD11	1.82	0.62
12:P:7:MAN:O4	12:P:8:MAN:H2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:179:LEU:HD11	4:G:419:ARG:HB3	1.82	0.62
2:D:109:LEU:HD12	2:D:109:LEU:C	2.18	0.62
4:G:374:HIS:HB3	4:G:385:CYS:HB2	1.80	0.62
6:L:39:ARG:NH1	6:L:81:GLY:O	2.33	0.61
1:B:610:TRP:HE3	4:G:36:VAL:HG12	1.65	0.61
4:G:188:ASN:HD22	4:G:189:LYS:N	1.99	0.61
11:M:2:NAG:O7	11:M:2:NAG:O3	2.17	0.61
2:D:91:PHE:CE2	2:D:106:GLY:HA2	2.36	0.61
3:E:146:VAL:HA	3:E:194:GLN:O	2.01	0.61
4:G:189:LYS:O	4:G:190:GLU:HG3	2.01	0.61
2:D:6:GLN:OE1	2:D:104:GLY:HA3	2.00	0.61
4:G:33:ASN:N	4:G:33:ASN:OD1	2.32	0.61
3:E:127:ALA:H	3:E:128:ASN:HA	1.64	0.61
4:G:138:ILE:HD12	4:G:140:ASP:N	2.16	0.61
5:H:77:LEU:HD11	13:H:301:NAG:H2	1.83	0.61
5:H:100(C):GLY:HA3	5:H:100(I):GLU:OE1	2.01	0.61
4:G:360:ARG:HB3	4:G:467:THR:HG22	1.84	0.60
1:B:597:GLY:HA3	1:B:650:GLN:HE21	1.66	0.60
2:D:100(D):TRP:HH2	3:E:96:CYS:HB3	1.66	0.60
4:G:41:GLY:H	4:G:493:PRO:HB2	1.67	0.60
4:G:190:GLU:O	4:G:191:TYR:CG	2.55	0.60
2:D:155:ASN:ND2	2:D:192:GLN:OE1	2.35	0.60
2:D:90:TYR:CE2	2:D:109:LEU:CB	2.85	0.59
2:D:50:TRP:O	2:D:57:LYS:HA	2.02	0.59
4:G:188:ASN:O	4:G:189:LYS:HE3	2.01	0.59
12:P:5:MAN:C2	12:P:6:MAN:H5	2.32	0.59
2:D:171:GLN:HG2	2:D:172:SER:H	1.67	0.59
3:E:117:LEU:HD11	3:E:132:LEU:HB3	1.84	0.59
2:D:89:THR:CG2	2:D:91:PHE:CZ	2.85	0.59
4:G:188:ASN:ND2	4:G:189:LYS:H	2.00	0.59
4:G:101:VAL:HG23	4:G:483:LEU:HD12	1.84	0.59
5:H:100(D):VAL:HG12	12:P:1:NAG:C3	2.32	0.59
12:P:5:MAN:H2	12:P:6:MAN:C5	2.32	0.59
2:D:6:GLN:NE2	2:D:92:CYS:CB	2.66	0.59
5:H:161:VAL:HG22	5:H:180:VAL:HG12	1.85	0.59
2:D:155:ASN:HB2	2:D:158:ALA:HB3	1.85	0.59
2:D:91:PHE:CE2	2:D:106:GLY:CA	2.85	0.58
3:E:180:LEU:HD13	3:E:184:GLN:HG2	1.83	0.58
4:G:130:GLN:NE2	10:I:1:NAG:O7	2.36	0.58
4:G:173:TYR:OH	4:G:305:LYS:NZ	2.36	0.58
6:L:110:PRO:HG2	6:L:111:LYS:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:PHE:HA	7:A:1:NAG:H62	1.86	0.58
12:P:5:MAN:H2	12:P:6:MAN:H5	1.86	0.58
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.84	0.58
6:L:135:CYS:HB3	6:L:177:SER:HB3	1.86	0.58
4:G:122:LEU:HD21	4:G:203:GLN:HB2	1.85	0.58
1:B:601:LYS:O	1:B:602:LEU:HG	2.04	0.57
4:G:159:PHE:CE2	4:G:161:MET:HG2	2.39	0.57
2:D:13:LYS:HG2	2:D:113:SER:HA	1.86	0.57
4:G:39:TYR:HB2	4:G:495:GLY:O	2.02	0.57
5:H:100(D):VAL:CG1	12:P:1:NAG:H3	2.34	0.57
10:I:2:NAG:H3	10:I:2:NAG:H83	1.85	0.57
5:H:22:CYS:HB2	5:H:36:TRP:CZ2	2.40	0.57
2:D:5:VAL:HB	2:D:23:LYS:HB2	1.87	0.57
13:G:629:NAG:H83	13:G:629:NAG:H3	1.87	0.57
6:L:13:VAL:HG21	6:L:19:ALA:HB2	1.86	0.57
2:D:8:GLY:CA	2:D:107:THR:CG2	2.73	0.57
4:G:254:VAL:HG11	4:G:261:LEU:HB2	1.87	0.57
3:E:178:LEU:HD21	3:E:180:LEU:HD12	1.87	0.56
3:E:12:SER:HB2	3:E:106(A):LEU:HG	1.87	0.56
4:G:138:ILE:CD1	4:G:140:ASP:CA	2.83	0.56
5:H:34:TRP:HZ3	5:H:94:THR:HG22	1.71	0.56
5:H:100(G):PHE:CD1	5:H:100(I):GLU:N	2.73	0.56
6:L:63:SER:HB3	6:L:74:THR:HB	1.87	0.56
5:H:100(I):GLU:HG3	5:H:100(I):GLU:O	2.05	0.56
4:G:101:VAL:HG21	4:G:480:ARG:HG3	1.88	0.56
5:H:100(B):TYR:CE2	5:H:100(I):GLU:C	2.84	0.56
2:D:11:LEU:HD23	2:D:147:PRO:HD3	1.88	0.56
4:G:138:ILE:HD11	4:G:140:ASP:CA	2.33	0.56
5:H:36:TRP:HB3	5:H:48:ILE:HD12	1.87	0.56
5:H:100(D):VAL:HG23	5:H:100(F):ALA:N	2.18	0.55
2:D:89:THR:HG22	2:D:91:PHE:CZ	2.40	0.55
2:D:90:TYR:C	2:D:91:PHE:CD1	2.84	0.55
4:G:195:ASN:HB3	4:G:423:ILE:HG21	1.88	0.55
4:G:321(A):ASP:OD1	4:G:321(A):ASP:N	2.37	0.55
5:H:100(G):PHE:HB3	5:H:100(I):GLU:H	1.71	0.55
5:H:100(B):TYR:HE2	5:H:100(I):GLU:C	2.14	0.55
6:L:133:LEU:O	6:L:178:TYR:HA	2.06	0.55
3:E:139:PHE:HE2	3:E:142:GLY:HA2	1.70	0.55
4:G:137:ASN:OD1	8:C:1:NAG:O5	2.25	0.55
5:H:28:LEU:HD23	5:H:28:LEU:H	1.71	0.55
12:P:5:MAN:C2	12:P:6:MAN:C5	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:100(D):VAL:O	5:H:100(E):VAL:HB	2.07	0.54
1:B:574:LYS:HG3	4:G:51:THR:HG22	1.90	0.54
5:H:100(G):PHE:CD1	5:H:100(H):LYS:C	2.85	0.54
4:G:327:ARG:HD2	5:H:100(I):GLU:OE1	2.08	0.54
2:D:134:GLY:HA2	2:D:223:LEU:HD13	1.89	0.54
5:H:100(G):PHE:HB3	5:H:100(I):GLU:N	2.23	0.54
5:H:126:SER:O	5:H:128:SER:N	2.41	0.54
4:G:150:MET:HG3	4:G:152:GLY:H	1.72	0.53
2:D:96:LEU:HD23	2:D:100(E):LEU:HB3	1.90	0.53
4:G:107:ASP:OD2	4:G:217:TYR:OH	2.22	0.53
4:G:189:LYS:C	4:G:190:GLU:HG3	2.33	0.53
5:H:35:SER:HB3	5:H:47:TRP:HE1	1.72	0.53
6:L:66:PRO:CB	12:P:6:MAN:H62	2.38	0.53
2:D:99:ASP:OD1	2:D:100:GLY:N	2.42	0.53
4:G:138:ILE:CD1	4:G:140:ASP:N	2.72	0.53
4:G:129:LEU:HD23	4:G:159:PHE:HD1	1.73	0.53
4:G:151:ARG:HB2	4:G:178:ARG:HH12	1.74	0.53
5:H:124:PRO:HG3	5:H:136:LEU:HD12	1.90	0.53
4:G:292:VAL:HG21	4:G:338:TRP:HD1	1.74	0.53
4:G:299:PRO:HD2	4:G:327:ARG:O	2.09	0.53
6:L:36:TYR:HD1	6:L:46:LEU:HA	1.74	0.53
5:H:100(D):VAL:HG11	12:P:1:NAG:H3	1.90	0.53
6:L:36:TYR:CD1	6:L:46:LEU:HA	2.44	0.53
2:D:7:SER:O	2:D:107:THR:HG23	2.05	0.53
4:G:264:SER:N	4:G:482:GLU:OE2	2.42	0.53
4:G:457:ASP:N	4:G:457:ASP:OD1	2.40	0.53
2:D:126:PRO:HG3	2:D:138:LEU:HB3	1.91	0.52
3:E:162:THR:OG1	3:E:175:SER:N	2.39	0.52
2:D:49:GLY:HA3	2:D:59:LEU:HD23	1.90	0.52
4:G:248:THR:HB	4:G:486:TYR:CE1	2.44	0.52
4:G:259:LEU:HD12	4:G:374:HIS:CD2	2.44	0.52
4:G:356:ASN:HB3	4:G:398:ASN:OD1	2.09	0.52
6:L:145:VAL:HG12	6:L:198:HIS:HB2	1.92	0.52
12:P:1:NAG:O3	12:P:2:NAG:O5	2.27	0.52
1:B:571:TRP:CE3	1:B:571:TRP:HA	2.45	0.52
2:D:91:PHE:CD2	2:D:106:GLY:HA2	2.44	0.52
4:G:161:MET:HE3	4:G:162:THR:H	1.74	0.52
5:H:100(D):VAL:HG23	5:H:100(F):ALA:HB2	1.90	0.52
5:H:139:LEU:HD21	5:H:141:LYS:HB2	1.91	0.52
3:E:147:ALA:O	3:E:194:GLN:HB2	2.10	0.52
3:E:34:SER:O	3:E:88:CYS:HA	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:116:LEU:HD11	4:G:434:MET:HE3	1.91	0.51
5:H:100(G):PHE:HD1	5:H:100(I):GLU:HA	1.76	0.51
5:H:63:LEU:HD22	5:H:66:ARG:HH21	1.73	0.51
4:G:135:THR:OG1	9:F:1:NAG:O7	2.28	0.51
4:G:424:ILE:O	4:G:433:CYS:HA	2.10	0.51
5:H:22:CYS:HB2	5:H:36:TRP:HZ2	1.76	0.51
2:D:19:LYS:C	2:D:20:ILE:HG13	2.34	0.51
4:G:335:LYS:NZ	4:G:412:ASP:OD2	2.44	0.51
2:D:61:PRO:HA	2:D:64:GLN:HB2	1.93	0.51
2:D:117:LYS:HE3	2:D:175:LEU:HD13	1.92	0.50
6:L:131:ALA:HB3	6:L:181:LEU:C	2.37	0.50
4:G:138:ILE:HD12	4:G:139:THR:N	2.27	0.50
2:D:90:TYR:OH	2:D:109:LEU:HB2	2.11	0.50
4:G:391:PHE:CZ	4:G:470:PRO:HG3	2.46	0.50
3:E:127:ALA:N	3:E:128:ASN:HA	2.23	0.50
5:H:100:ARG:NH2	12:P:5:MAN:O4	2.44	0.50
1:B:602:LEU:N	1:B:602:LEU:CD2	2.73	0.50
2:D:143:LYS:NZ	3:E:124:GLU:OE2	2.44	0.50
5:H:142:ASP:HA	5:H:173:LEU:HB3	1.93	0.50
4:G:429:ARG:HD2	4:G:429:ARG:C	2.36	0.50
3:E:21:ILE:O	3:E:72:TYR:HA	2.12	0.49
7:A:1:NAG:H61	7:A:2:NAG:H82	1.93	0.49
1:B:602:LEU:O	1:B:603:ILE:C	2.54	0.49
1:B:655:LYS:HD2	1:B:655:LYS:C	2.36	0.49
2:D:142:VAL:HG11	2:D:150:VAL:HG11	1.93	0.49
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.47	0.49
2:D:50:TRP:CZ2	7:A:4:MAN:H62	2.47	0.49
2:D:37:ILE:HD13	2:D:103:TRP:CH2	2.47	0.49
4:G:67:ASN:O	4:G:67:ASN:ND2	2.46	0.49
6:L:34:ILE:O	6:L:88:CYS:HA	2.11	0.49
2:D:153:SER:OG	2:D:197:ASN:HB2	2.12	0.49
2:D:94:LYS:O	2:D:100(F):PRO:HA	2.12	0.49
5:H:28:LEU:HG	5:H:31:ASP:HB2	1.95	0.49
5:H:203:THR:HG22	5:H:205:VAL:HG23	1.95	0.49
10:N:1:NAG:H61	10:N:2:NAG:N2	2.27	0.49
2:D:108:LEU:C	2:D:108:LEU:CD2	2.85	0.49
4:G:71:THR:C	4:G:73:ALA:N	2.67	0.49
2:D:87:THR:HG23	2:D:110:THR:HA	1.95	0.49
2:D:168:ALA:HB2	2:D:178:LEU:HD23	1.95	0.49
12:P:2:NAG:O7	12:P:2:NAG:H3	2.12	0.49
4:G:187:SER:HG	4:G:188:ASN:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:100(J):TRP:CD1	5:H:100(J):TRP:C	2.88	0.48
4:G:161:MET:O	4:G:170:GLN:HG2	2.13	0.48
4:G:135:THR:HB	6:L:94:ARG:HH21	1.79	0.48
10:S:1:NAG:H61	10:S:2:NAG:N2	2.28	0.48
4:G:363:ASN:HB3	4:G:388:SER:HA	1.96	0.48
5:H:11:LEU:HD22	5:H:145:PRO:HG3	1.94	0.48
2:D:52:SER:OG	7:A:2:NAG:O7	2.21	0.48
1:B:655:LYS:C	1:B:655:LYS:CD	2.86	0.48
2:D:154:TRP:HZ3	2:D:194:TYR:HB3	1.79	0.48
1:B:636:SER:O	1:B:639:THR:OG1	2.31	0.48
5:H:9:PRO:HD2	5:H:20:LEU:HD23	1.95	0.48
4:G:151:ARG:HB2	4:G:178:ARG:NH1	2.28	0.47
4:G:188:ASN:HD22	4:G:189:LYS:H	1.58	0.47
4:G:129:LEU:HD12	4:G:192:ARG:HA	1.97	0.47
5:H:100(D):VAL:CG2	5:H:100(F):ALA:CB	2.92	0.47
2:D:6:GLN:HE22	2:D:92:CYS:CB	2.27	0.47
5:H:126:SER:O	5:H:129:THR:N	2.47	0.47
2:D:101:TYR:HD1	3:E:46:LEU:HD23	1.78	0.47
6:L:61:ARG:HE	6:L:77:SER:HB2	1.78	0.47
5:H:100(E):VAL:HG12	5:H:100(E):VAL:O	2.14	0.47
2:D:27:TYR:CE2	2:D:94:LYS:HD3	2.49	0.47
6:L:114:PRO:HB3	6:L:140:PHE:HB3	1.95	0.47
2:D:89:THR:HG21	2:D:91:PHE:CZ	2.50	0.47
4:G:236:THR:OG1	10:K:1:NAG:H82	2.15	0.47
1:B:578:ALA:HB1	4:G:220:PRO:HG3	1.96	0.47
4:G:36:VAL:HA	4:G:497:ALA:O	2.15	0.47
4:G:292:VAL:HG23	4:G:337:THR:HG22	1.96	0.46
5:H:5:GLN:NE2	5:H:6:GLU:O	2.43	0.46
4:G:188:ASN:ND2	4:G:189:LYS:N	2.60	0.46
4:G:346:VAL:HG23	4:G:349:LEU:HD12	1.97	0.46
4:G:382:PHE:HE2	4:G:436:ALA:HB2	1.80	0.46
6:L:168:GLN:OE1	6:L:174:ALA:HB2	2.15	0.46
1:B:654:GLU:OE1	1:B:654:GLU:HA	2.16	0.46
2:D:37:ILE:CD1	2:D:103:TRP:CH2	2.99	0.46
6:L:32:SER:HA	6:L:51:ASN:HD21	1.79	0.46
1:B:639:THR:HB	1:B:643:TYR:CE2	2.51	0.46
2:D:7:SER:OG	2:D:20:ILE:HG22	2.16	0.46
4:G:86:LEU:HB3	4:G:89:VAL:HG21	1.96	0.46
6:L:35:TRP:CD2	6:L:73:LEU:HD13	2.51	0.46
3:E:150:ALA:HB1	3:E:188:HIS:CD2	2.51	0.46
2:D:91:PHE:CE2	2:D:106:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:151:ARG:HD2	4:G:178:ARG:HH12	1.81	0.46
4:G:276:ASN:ND2	4:G:279:ASN:HB2	2.30	0.46
5:H:139:LEU:HD12	6:L:134:VAL:HG21	1.97	0.46
6:L:12:SER:HA	6:L:105:ILE:O	2.16	0.46
4:G:64:GLU:HG2	4:G:65:LYS:H	1.81	0.46
1:B:649:SER:O	1:B:650:GLN:C	2.56	0.46
4:G:224:ALA:HB3	4:G:489:VAL:HG23	1.97	0.46
4:G:350:ARG:NH1	4:G:397:SER:O	2.49	0.46
2:D:96:LEU:HD12	2:D:97:LEU:N	2.31	0.45
3:E:124:GLU:HG2	3:E:129:LYS:HB2	1.98	0.45
4:G:282:LYS:HA	4:G:282:LYS:HD3	1.71	0.45
5:H:188:GLY:HA3	5:H:189:THR:HA	1.61	0.45
1:B:601:LYS:C	1:B:602:LEU:CG	2.88	0.45
2:D:37:ILE:HD13	2:D:103:TRP:HH2	1.82	0.45
2:D:108:LEU:CD2	2:D:149:PRO:HD3	2.43	0.45
3:E:162:THR:HG1	3:E:175:SER:H	1.60	0.45
5:H:148:VAL:HG22	5:H:198:HIS:HB2	1.99	0.45
1:B:635:ILE:O	1:B:639:THR:HG23	2.16	0.45
2:D:169:VAL:HB	3:E:162:THR:CG2	2.47	0.45
3:E:84:THR:OG1	3:E:85:THR:N	2.49	0.45
3:E:139:PHE:CE2	3:E:142:GLY:HA2	2.50	0.45
5:H:100(L):THR:OG1	8:C:2:NAG:O6	2.33	0.45
6:L:192:TYR:O	6:L:206:THR:HA	2.16	0.45
1:B:610:TRP:CE3	4:G:36:VAL:HG12	2.47	0.45
6:L:21:ILE:HG23	6:L:102:THR:HG21	1.98	0.45
1:B:571:TRP:HA	1:B:571:TRP:HE3	1.80	0.45
5:H:20:LEU:HD11	5:H:107:VAL:HG21	1.99	0.45
6:L:32:SER:HA	6:L:51:ASN:ND2	2.32	0.45
11:M:2:NAG:HO3	11:M:2:NAG:C7	2.24	0.45
2:D:4:LEU:HG	2:D:23:LYS:O	2.16	0.45
3:E:39:PRO:HB2	3:E:42:ARG:HB2	1.98	0.45
5:H:100(J):TRP:CD1	5:H:100(J):TRP:O	2.70	0.45
6:L:109:GLN:N	6:L:110:PRO:HA	2.31	0.45
2:D:108:LEU:CD2	2:D:148:GLU:O	2.65	0.45
4:G:320:LEU:HG	4:G:438:PRO:HB3	1.99	0.45
5:H:53:ASP:O	5:H:54:SER:OG	2.27	0.45
12:P:2:NAG:O3	12:P:3:BMA:C1	2.65	0.45
3:E:155:VAL:HG13	3:E:157:ALA:H	1.82	0.45
5:H:137:GLY:HA3	5:H:179:VAL:HG12	1.99	0.45
1:B:621:GLU:CD	3:E:56:PRO:HG3	2.42	0.45
4:G:346:VAL:HG22	4:G:359:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:100(Q):ASP:HA	6:L:46:LEU:HD13	1.99	0.45
6:L:62:PHE:HE2	6:L:75:ILE:HG23	1.82	0.44
1:B:603:ILE:HG12	4:G:39:TYR:CD2	2.52	0.44
2:D:90:TYR:CE1	2:D:107:THR:O	2.70	0.44
5:H:132:GLY:HA2	5:H:184:SER:HB3	1.99	0.44
6:L:129:ASN:OD1	6:L:183:PRO:HG3	2.18	0.44
1:B:623:TRP:HH2	4:G:39:TYR:HH	1.63	0.44
4:G:93:PHE:CE1	4:G:228:CYS:HB2	2.52	0.44
4:G:320:LEU:H	4:G:320:LEU:HD12	1.82	0.44
5:H:100(B):TYR:CE2	5:H:100(I):GLU:O	2.70	0.44
1:B:614:TRP:CD2	1:B:642:ILE:HD11	2.53	0.44
2:D:88:GLY:O	2:D:90:TYR:CD2	2.70	0.44
5:H:48:ILE:O	5:H:60:ASN:HB2	2.16	0.44
10:S:1:NAG:H61	10:S:2:NAG:C7	2.48	0.44
4:G:369:LEU:O	4:G:373:THR:OG1	2.35	0.44
1:B:544:LEU:O	4:G:221:ALA:HB1	2.17	0.44
4:G:137:ASN:HD22	8:C:1:NAG:C7	2.30	0.44
4:G:259:LEU:HD13	4:G:449:ILE:HD13	2.00	0.44
5:H:47:TRP:O	5:H:60:ASN:ND2	2.50	0.44
2:D:38:ARG:NH2	2:D:46:GLU:OE1	2.41	0.44
5:H:100(D):VAL:CG1	12:P:1:NAG:C3	2.96	0.44
2:D:80:MET:HE3	2:D:80:MET:HB3	1.94	0.44
4:G:138:ILE:CD1	4:G:139:THR:C	2.86	0.44
4:G:276:ASN:HD22	4:G:279:ASN:HB2	1.83	0.44
2:D:29:PHE:HB3	2:D:72(B):GLU:OE2	2.18	0.43
2:D:171:GLN:HG2	2:D:172:SER:N	2.31	0.43
3:E:190:SER:HA	3:E:208:PRO:HD3	1.99	0.43
4:G:95:MET:SD	4:G:273:ARG:HD3	2.58	0.43
4:G:117:LYS:HD2	4:G:117:LYS:HA	1.70	0.43
6:L:13:VAL:HG21	6:L:19:ALA:CB	2.48	0.43
7:A:3:BMA:H61	7:A:4:MAN:H2	1.29	0.43
1:B:598:CYS:O	1:B:599:SER:HB3	2.17	0.43
4:G:155:LYS:O	4:G:175:LEU:HA	2.18	0.43
4:G:159:PHE:HE2	4:G:161:MET:HG2	1.83	0.43
4:G:69:TRP:CE3	4:G:111:LEU:HD21	2.53	0.43
2:D:51:ILE:HD13	2:D:71:THR:HG23	1.99	0.43
1:B:576:LEU:O	1:B:580:VAL:HG23	2.19	0.43
4:G:96:TRP:HA	4:G:480:ARG:HD3	2.00	0.43
4:G:252:LYS:H	4:G:252:LYS:HG2	1.56	0.43
2:D:194:TYR:H	2:D:210:ARG:NH1	2.16	0.43
4:G:490:LYS:HB2	4:G:490:LYS:HE3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:LEU:HD21	2:D:224:PHE:HE1	1.84	0.43
4:G:455:THR:OG1	4:G:469:ARG:O	2.35	0.43
6:L:147:VAL:HG22	6:L:196:VAL:HG22	1.99	0.43
2:D:38:ARG:HG3	2:D:38:ARG:O	2.19	0.42
2:D:171:GLN:HG3	3:E:160:GLU:OE2	2.19	0.42
4:G:330:HIS:HA	4:G:416:LEU:O	2.19	0.42
1:B:612:SER:OG	1:B:616:ASN:HB3	2.19	0.42
4:G:326:ILE:O	4:G:326:ILE:HG13	2.19	0.42
6:L:139:ASP:HA	6:L:172:LYS:HB2	2.01	0.42
2:D:6:GLN:HG3	2:D:105:GLN:N	2.25	0.42
2:D:21:SER:HB3	2:D:79:TYR:CD2	2.54	0.42
5:H:100(G):PHE:HB3	5:H:100(I):GLU:HB3	2.00	0.42
6:L:35:TRP:CG	6:L:73:LEU:HD13	2.54	0.42
2:D:6:GLN:NE2	2:D:22:CYS:SG	2.93	0.42
2:D:27:TYR:CZ	2:D:29:PHE:HA	2.54	0.42
3:E:185:TRP:CZ3	3:E:208:PRO:HB2	2.54	0.42
1:B:571:TRP:CZ2	4:G:54:CYS:HB3	2.54	0.42
1:B:574:LYS:NZ	4:G:107:ASP:OD1	2.38	0.42
2:D:47:TRP:HZ2	2:D:50:TRP:CD1	2.38	0.42
4:G:309:ILE:O	4:G:315:GLN:HB2	2.19	0.42
6:L:62:PHE:CE2	6:L:75:ILE:HG23	2.54	0.42
2:D:12:LYS:HE3	2:D:18:VAL:HB	2.02	0.42
2:D:31:PHE:HA	7:A:1:NAG:C6	2.50	0.42
2:D:96:LEU:CD2	2:D:100(E):LEU:HB3	2.49	0.42
1:B:624:ASP:HB3	2:D:99:ASP:O	2.20	0.42
2:D:193:THR:HG22	2:D:195:ILE:HG13	2.01	0.42
3:E:189:ARG:H	3:E:189:ARG:HD2	1.85	0.42
6:L:27:SER:OG	6:L:68:GLY:N	2.52	0.42
2:D:51:ILE:HA	2:D:56:ASP:O	2.20	0.42
4:G:350:ARG:H	4:G:350:ARG:HG2	1.53	0.42
2:D:34:ILE:O	2:D:50:TRP:HA	2.20	0.42
3:E:113:PRO:HG2	3:E:202:VAL:HG21	2.02	0.42
3:E:193:CYS:O	3:E:203:GLU:HA	2.19	0.42
6:L:168:GLN:OE1	6:L:172:LYS:HE2	2.20	0.42
1:B:597:GLY:CA	1:B:650:GLN:HE21	2.32	0.41
2:D:108:LEU:HD13	2:D:149:PRO:HD3	2.02	0.41
4:G:382:PHE:CE2	4:G:436:ALA:HB2	2.54	0.41
6:L:194:CYS:O	6:L:204:GLU:HA	2.21	0.41
3:E:151:ASP:HB2	3:E:188:HIS:CB	2.47	0.41
4:G:270:VAL:O	4:G:348:GLN:HG3	2.20	0.41
4:G:346:VAL:HA	4:G:349:LEU:HG	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:361:PHE:CD1	4:G:468:PHE:HB2	2.56	0.41
1:B:601:LYS:C	1:B:602:LEU:HD23	2.46	0.41
4:G:361:PHE:HE2	4:G:395:TRP:CD1	2.38	0.41
5:H:100(B):TYR:HE2	5:H:100(J):TRP:N	2.19	0.41
6:L:145:VAL:HA	6:L:197:THR:O	2.20	0.41
2:D:89:THR:HG22	2:D:90:TYR:N	2.35	0.41
2:D:168:ALA:HB1	2:D:176:TYR:HB3	2.02	0.41
2:D:194:TYR:O	2:D:210:ARG:HD2	2.20	0.41
4:G:302:MET:HE2	4:G:320:LEU:HD23	2.02	0.41
3:E:144:VAL:HG12	3:E:197:HIS:HB2	2.03	0.41
2:D:193:THR:HG23	2:D:210:ARG:NE	2.36	0.41
4:G:155:LYS:HE2	4:G:178:ARG:HD2	2.03	0.41
5:H:100(D):VAL:H	5:H:100(I):GLU:CD	2.29	0.41
1:B:640:GLN:HA	1:B:643:TYR:HD2	1.86	0.41
3:E:39:PRO:HA	3:E:40:PRO:HD3	1.98	0.41
3:E:66:LYS:HG2	3:E:67:SER:O	2.21	0.41
5:H:100(G):PHE:HD1	5:H:100(I):GLU:N	2.17	0.41
5:H:144:PHE:HA	5:H:145:PRO:HA	1.82	0.41
2:D:7:SER:C	2:D:107:THR:HG23	2.46	0.41
2:D:11:LEU:HD13	2:D:112:SER:OG	2.21	0.41
2:D:72(E):VAL:HA	10:K:2:NAG:H81	2.03	0.41
4:G:347:LYS:HA	4:G:350:ARG:HD2	2.02	0.41
4:G:360:ARG:HH21	4:G:467:THR:HG21	1.85	0.41
6:L:63:SER:OG	6:L:64:GLY:N	2.54	0.41
1:B:628:TRP:HB3	4:G:44:VAL:HG23	2.02	0.40
2:D:89:THR:CG2	2:D:90:TYR:N	2.84	0.40
4:G:86:LEU:HB3	4:G:89:VAL:CG2	2.51	0.40
5:H:45:PRO:O	6:L:98:PHE:HB2	2.22	0.40
5:H:100(D):VAL:CG2	5:H:100(F):ALA:HB3	2.51	0.40
5:H:124:PRO:HG2	5:H:211:PRO:HG3	2.03	0.40
1:B:606:THR:HG23	4:G:503:ARG:HH21	1.86	0.40
5:H:210:GLU:HA	5:H:211:PRO:HD3	1.87	0.40
1:B:652:GLN:NE2	1:B:653:GLN:N	2.60	0.40
4:G:42:VAL:HG11	4:G:495:GLY:HA3	2.03	0.40
4:G:412:ASP:OD1	4:G:413:SER:N	2.52	0.40
5:H:67:VAL:O	5:H:68:HIS:ND1	2.55	0.40
5:H:72:ASP:O	5:H:76:ASN:N	2.55	0.40
5:H:122:LEU:HD13	6:L:119:PHE:HD1	1.86	0.40
6:L:51:ASN:HB3	6:L:65:SER:O	2.21	0.40
2:D:90:TYR:OH	2:D:109:LEU:N	2.55	0.40
2:D:159:LEU:HD22	2:D:194:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:39:PRO:HA	3:E:84:THR:OG1	2.22	0.40
4:G:453:ILE:HD11	4:G:478:ASN:ND2	2.36	0.40
5:H:100(G):PHE:HB3	5:H:100(I):GLU:CB	2.52	0.40
2:D:47:TRP:HZ2	2:D:50:TRP:HD1	1.70	0.40
4:G:50:THR:OG1	4:G:51:THR:N	2.54	0.40
4:G:183:GLN:HB3	4:G:191:TYR:CE2	2.57	0.40
4:G:271:MET:HE3	4:G:271:MET:HB3	1.89	0.40
6:L:47:ILE:O	6:L:55:PRO:HD2	2.21	0.40
6:L:66:PRO:HG3	12:P:6:MAN:H62	2.03	0.40
12:P:5:MAN:O3	12:P:6:MAN:C1	2.70	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:ARG:CZ	1:B:647:GLU:OE2[3_845]	1.87	0.33
1:B:542:ARG:NE	1:B:647:GLU:OE2[3_845]	1.93	0.27

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	118/153 (77%)	109 (92%)	7 (6%)	2 (2%)	7	27
2	D	240/243 (99%)	230 (96%)	10 (4%)	0	100	100
3	E	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
4	G	441/505 (87%)	404 (92%)	32 (7%)	5 (1%)	11	37
5	H	230/235 (98%)	214 (93%)	13 (6%)	3 (1%)	9	33
6	L	206/208 (99%)	190 (92%)	16 (8%)	0	100	100
All	All	1446/1560 (93%)	1353 (94%)	83 (6%)	10 (1%)	18	47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	72	HIS
5	H	100(E)	VAL
1	B	602	LEU
4	G	328	GLN
4	G	417	PRO
5	H	100(H)	LYS
4	G	427	TRP
4	G	432	GLN
5	H	127	LYS
1	B	598	CYS

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	B	104/129 (81%)	78 (75%)	26 (25%)	0	2
2	D	203/206 (98%)	181 (89%)	22 (11%)	6	22
3	E	186/189 (98%)	172 (92%)	14 (8%)	12	37
4	G	403/448 (90%)	329 (82%)	74 (18%)	1	7
5	H	198/205 (97%)	189 (96%)	9 (4%)	24	50
6	L	177/177 (100%)	164 (93%)	13 (7%)	13	37
All	All	1271/1354 (94%)	1113 (88%)	158 (12%)	4	18

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	520	LEU
1	B	534	SER
1	B	570	VAL
1	B	571	TRP
1	B	573	ILE
1	B	575	GLN
1	B	583	VAL

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Mol	Chain	Res	Type
1	B	585	ARG
1	B	593	LEU
1	B	595	ILE
1	B	602	LEU
1	B	606	THR
1	B	616	ASN
1	B	619	LEU
1	B	638	TYR
1	B	639	THR
1	B	642	ILE
1	B	647	GLU
1	B	648	GLU
1	B	650	GLN
1	B	652	GLN
1	B	654	GLU
1	B	655	LYS
1	B	656	ASN
1	B	657	GLU
1	B	658	GLN
2	D	6	GLN
2	D	11	LEU
2	D	18	VAL
2	D	20	ILE
2	D	27	TYR
2	D	28	ARG
2	D	37	ILE
2	D	38	ARG
2	D	75	THR
2	D	82	ILE
2	D	82(A)	ARG
2	D	82(B)	ASN
2	D	82(C)	LEU
2	D	90	TYR
2	D	102	LEU
2	D	107	THR
2	D	108	LEU
2	D	109	LEU
2	D	150	VAL
2	D	155	ASN
2	D	170	LEU
2	D	196	CYS
3	E	51	ASP

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Mol	Chain	Res	Type
3	E	63	SER
3	E	85	THR
3	E	89	CYS
3	E	90	SER
3	E	92	THR
3	E	96	CYS
3	E	97	VAL
3	E	108	GLN
3	E	155	VAL
3	E	160	GLU
3	E	183	GLU
3	E	186	LYS
3	E	209	THR
4	G	33	ASN
4	G	36	VAL
4	G	47	ASP
4	G	49	GLU
4	G	63	THR
4	G	64	GLU
4	G	65	LYS
4	G	66	HIS
4	G	68	VAL
4	G	69	TRP
4	G	71	THR
4	G	86	LEU
4	G	111	LEU
4	G	117	LYS
4	G	125	LEU
4	G	132	THR
4	G	133	ASN
4	G	134	VAL
4	G	138	ILE
4	G	139	THR
4	G	140	ASP
4	G	141	ASP
4	G	151	ARG
4	G	161	MET
4	G	172	VAL
4	G	174	SER
4	G	175	LEU
4	G	188	ASN
4	G	189	LYS

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Mol	Chain	Res	Type
4	G	213	ILE
4	G	229	LYS
4	G	236	THR
4	G	246	GLN
4	G	248	THR
4	G	252	LYS
4	G	255	VAL
4	G	264	SER
4	G	265	LEU
4	G	268	GLU
4	G	270	VAL
4	G	277	ILE
4	G	285	LEU
4	G	287	GLN
4	G	295	ASN
4	G	297	THR
4	G	308	ARG
4	G	309	ILE
4	G	320	LEU
4	G	327	ARG
4	G	335	LYS
4	G	340	GLU
4	G	342	LEU
4	G	350	ARG
4	G	368	ASP
4	G	369	LEU
4	G	377	ASN
4	G	378	CYS
4	G	390	LEU
4	G	392	ASN
4	G	393	SER
4	G	396	ILE
4	G	416	LEU
4	G	420	ILE
4	G	429	ARG
4	G	430	ILE
4	G	432	GLN
4	G	434	MET
4	G	442	VAL
4	G	457	ASP
4	G	465	THR
4	G	475	MET

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Mol	Chain	Res	Type
4	G	483	LEU
4	G	488	VAL
4	G	499	THR
5	H	21	THR
5	H	62	SER
5	H	65	SER
5	H	77	LEU
5	H	105	THR
5	H	148	VAL
5	H	175	SER
5	H	182	VAL
5	H	184	SER
6	L	8	THR
6	L	28	LEU
6	L	70	THR
6	L	109	GLN
6	L	122	SER
6	L	138	SER
6	L	139	ASP
6	L	161	GLU
6	L	168	GLN
6	L	172	LYS
6	L	201	SER
6	L	204	GLU
6	L	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	543	ASN
1	B	590	GLN
1	B	625	ASN
1	B	652	GLN
2	D	6	GLN
2	D	199	ASN
3	E	108	GLN
3	E	170	ASN
4	G	99	ASN
4	G	130	GLN
4	G	188	ASN
4	G	246	GLN
4	G	283	ASN

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Mol	Chain	Res	Type
5	H	162	HIS
6	L	168	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

49 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	$\# Z > 2$
7	NAG	A	1	7,4	14,14,15	0.37	0	17,19,21	0.46	0
7	NAG	A	2	7	14,14,15	0.47	0	17,19,21	1.28	1 (5%)
7	BMA	A	3	7	11,11,12	1.11	1 (9%)	15,15,17	0.85	0
7	MAN	A	4	7	11,11,12	1.33	1 (9%)	15,15,17	1.54	3 (20%)
7	MAN	A	5	7	11,11,12	1.17	1 (9%)	15,15,17	1.67	1 (6%)
7	MAN	A	6	7	11,11,12	0.76	1 (9%)	15,15,17	1.18	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.42	0	17,19,21	0.45	0
8	NAG	C	2	8	14,14,15	0.31	0	17,19,21	0.42	0
8	BMA	C	3	8	11,11,12	0.56	0	15,15,17	0.75	0
8	MAN	C	4	8	11,11,12	0.91	1 (9%)	15,15,17	1.25	2 (13%)
9	NAG	F	1	4,9	14,14,15	0.30	0	17,19,21	0.44	0
9	NAG	F	2	9	14,14,15	0.19	0	17,19,21	0.41	0
9	BMA	F	3	9	11,11,12	0.56	0	15,15,17	0.66	0
9	MAN	F	4	9	11,11,12	0.73	1 (9%)	15,15,17	1.13	2 (13%)
9	MAN	F	5	9	11,11,12	0.75	0	15,15,17	0.86	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	I	1	10,4	14,14,15	1.71	3 (21%)	17,19,21	1.16	2 (11%)
10	NAG	I	2	10	14,14,15	0.61	0	17,19,21	1.37	2 (11%)
10	NAG	J	1	10,4	14,14,15	0.21	0	17,19,21	0.62	1 (5%)
10	NAG	J	2	10	14,14,15	0.30	0	17,19,21	0.51	0
10	NAG	K	1	10,4	14,14,15	0.21	0	17,19,21	0.70	1 (5%)
10	NAG	K	2	10	14,14,15	0.23	0	17,19,21	0.42	0
11	NAG	M	1	11,4	14,14,15	0.33	0	17,19,21	0.60	0
11	NAG	M	2	11	14,14,15	0.49	0	17,19,21	0.71	0
11	BMA	M	3	11	11,11,12	1.40	3 (27%)	15,15,17	1.18	1 (6%)
11	MAN	M	4	11	11,11,12	1.36	3 (27%)	15,15,17	1.91	3 (20%)
11	MAN	M	5	11	11,11,12	0.76	0	15,15,17	1.11	2 (13%)
11	MAN	M	6	11	11,11,12	1.17	2 (18%)	15,15,17	1.67	2 (13%)
10	NAG	N	1	10,4	14,14,15	0.41	0	17,19,21	0.72	1 (5%)
10	NAG	N	2	10	14,14,15	0.29	0	17,19,21	0.51	0
10	NAG	O	1	10,4	14,14,15	0.22	0	17,19,21	0.49	0
10	NAG	O	2	10	14,14,15	0.24	0	17,19,21	0.45	0
12	NAG	P	1	12,4	14,14,15	0.97	0	17,19,21	1.74	3 (17%)
12	MAN	P	10	12	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
12	NAG	P	2	12	14,14,15	0.52	0	17,19,21	1.77	5 (29%)
12	BMA	P	3	12	11,11,12	0.53	0	15,15,17	1.49	4 (26%)
12	MAN	P	4	12	11,11,12	0.61	0	15,15,17	1.12	1 (6%)
12	MAN	P	5	12	11,11,12	0.94	0	15,15,17	2.05	4 (26%)
12	MAN	P	6	12	11,11,12	0.76	0	15,15,17	1.89	4 (26%)
12	MAN	P	7	12	11,11,12	0.88	0	15,15,17	1.76	4 (26%)
12	MAN	P	8	12	11,11,12	0.72	0	15,15,17	1.14	1 (6%)
12	MAN	P	9	12	11,11,12	0.46	0	15,15,17	2.04	2 (13%)
10	NAG	Q	1	10,4	14,14,15	0.20	0	17,19,21	0.40	0
10	NAG	Q	2	10	14,14,15	0.23	0	17,19,21	0.46	0
10	NAG	R	1	10,4	14,14,15	0.26	0	17,19,21	0.79	1 (5%)
10	NAG	R	2	10	14,14,15	0.30	0	17,19,21	0.49	0
10	NAG	S	1	10,4	14,14,15	0.94	1 (7%)	17,19,21	0.78	0
10	NAG	S	2	10	14,14,15	0.34	0	17,19,21	0.66	1 (5%)
10	NAG	T	1	10,4	14,14,15	0.23	0	17,19,21	0.56	0
10	NAG	T	2	10	14,14,15	0.24	0	17,19,21	0.40	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
7	NAG	A	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
8	BMA	C	3	8	-	1/2/19/22	0/1/1/1
8	MAN	C	4	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	1/6/23/26	0/1/1/1
9	BMA	F	3	9	-	0/2/19/22	0/1/1/1
9	MAN	F	4	9	-	1/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
10	NAG	I	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	I	2	10	-	4/6/23/26	0/1/1/1
10	NAG	J	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	NAG	K	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	1/6/23/26	0/1/1/1
11	NAG	M	1	11,4	-	2/6/23/26	0/1/1/1
11	NAG	M	2	11	-	3/6/23/26	0/1/1/1
11	BMA	M	3	11	-	2/2/19/22	0/1/1/1
11	MAN	M	4	11	-	0/2/19/22	0/1/1/1
11	MAN	M	5	11	-	1/2/19/22	1/1/1/1
11	MAN	M	6	11	-	1/2/19/22	0/1/1/1
10	NAG	N	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	0/6/23/26	0/1/1/1
10	NAG	O	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
12	NAG	P	1	12,4	-	2/6/23/26	0/1/1/1
12	MAN	P	10	12	-	0/2/19/22	0/1/1/1
12	NAG	P	2	12	-	4/6/23/26	0/1/1/1
12	BMA	P	3	12	-	0/2/19/22	0/1/1/1
12	MAN	P	4	12	-	0/2/19/22	0/1/1/1
12	MAN	P	5	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	P	6	12	-	2/2/19/22	0/1/1/1
12	MAN	P	7	12	-	2/2/19/22	0/1/1/1
12	MAN	P	8	12	-	0/2/19/22	0/1/1/1
12	MAN	P	9	12	-	0/2/19/22	0/1/1/1
10	NAG	Q	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	2/6/23/26	0/1/1/1
10	NAG	R	1	10,4	-	4/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	NAG	S	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
10	NAG	T	1	10,4	-	4/6/23/26	0/1/1/1
10	NAG	T	2	10	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	1	NAG	O5-C1	-5.00	1.35	1.43
7	A	4	MAN	C1-C2	3.78	1.61	1.52
10	S	1	NAG	O5-C1	-3.40	1.38	1.43
10	I	1	NAG	C1-C2	3.08	1.56	1.52
11	M	3	BMA	C4-C5	2.95	1.59	1.53
11	M	4	MAN	C4-C5	2.92	1.59	1.53
8	C	4	MAN	C1-C2	2.48	1.58	1.52
11	M	4	MAN	O5-C5	2.48	1.48	1.43
11	M	6	MAN	O5-C5	2.38	1.48	1.43
11	M	3	BMA	O5-C5	2.31	1.47	1.43
11	M	6	MAN	C1-C2	2.25	1.57	1.52
10	I	1	NAG	C3-C2	2.22	1.57	1.52
7	A	5	MAN	O5-C5	2.18	1.47	1.43
7	A	3	BMA	O5-C1	-2.16	1.40	1.43
11	M	3	BMA	C4-C3	2.11	1.57	1.52
7	A	6	MAN	C1-C2	2.10	1.57	1.52
9	F	4	MAN	C1-C2	2.02	1.57	1.52
11	M	4	MAN	C4-C3	2.02	1.57	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	9	MAN	C1-O5-C5	6.38	120.73	112.19
11	M	4	MAN	C1-O5-C5	5.39	119.41	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5	MAN	C1-O5-C5	5.09	119.00	112.19
12	P	5	MAN	O2-C2-C1	-4.92	97.96	109.22
10	I	2	NAG	C2-N2-C7	4.61	129.08	122.90
11	M	6	MAN	C1-O5-C5	4.47	118.18	112.19
12	P	6	MAN	O2-C2-C3	-4.43	100.97	110.15
7	A	2	NAG	C2-N2-C7	4.38	128.77	122.90
12	P	2	NAG	O5-C1-C2	-4.23	104.74	111.29
7	A	4	MAN	C1-O5-C5	4.09	117.67	112.19
12	P	1	NAG	C1-O5-C5	3.73	117.19	112.19
12	P	1	NAG	C3-C4-C5	-3.62	103.67	110.23
12	P	7	MAN	O5-C1-C2	-3.54	102.34	110.79
12	P	5	MAN	O5-C1-C2	-3.54	102.36	110.79
12	P	7	MAN	C1-C2-C3	-3.53	104.50	109.64
12	P	9	MAN	C2-C3-C4	3.51	117.03	110.86
10	I	1	NAG	C4-C3-C2	3.37	115.95	111.02
12	P	4	MAN	C1-O5-C5	3.31	116.62	112.19
7	A	6	MAN	C1-O5-C5	3.29	116.60	112.19
8	C	4	MAN	C1-O5-C5	3.22	116.51	112.19
11	M	4	MAN	C3-C4-C5	3.21	116.05	110.23
11	M	5	MAN	C1-O5-C5	3.11	116.36	112.19
12	P	6	MAN	O3-C3-C4	-3.09	103.08	110.38
9	F	4	MAN	C1-O5-C5	3.02	116.23	112.19
12	P	3	BMA	O5-C5-C6	2.97	113.44	107.66
7	A	4	MAN	C1-C2-C3	2.92	113.90	109.64
12	P	6	MAN	O5-C5-C4	-2.85	103.90	110.83
12	P	7	MAN	C1-O5-C5	2.84	116.00	112.19
12	P	8	MAN	O2-C2-C3	-2.72	104.52	110.15
12	P	2	NAG	O4-C4-C3	-2.66	104.10	110.38
12	P	2	NAG	O3-C3-C4	-2.65	104.14	110.38
12	P	3	BMA	C1-C2-C3	2.57	113.39	109.64
12	P	6	MAN	O3-C3-C2	-2.55	104.84	110.05
12	P	7	MAN	O4-C4-C3	-2.53	104.42	110.38
12	P	5	MAN	O3-C3-C4	-2.39	104.74	110.38
12	P	2	NAG	C3-C4-C5	-2.38	105.92	110.23
12	P	1	NAG	C1-C2-N2	-2.38	106.68	110.43
12	P	2	NAG	O3-C3-C2	2.37	114.32	109.40
10	R	1	NAG	C1-O5-C5	2.36	115.35	112.19
12	P	10	MAN	C1-O5-C5	2.31	115.28	112.19
10	N	1	NAG	C1-O5-C5	2.29	115.26	112.19
11	M	6	MAN	O2-C2-C3	-2.29	105.41	110.15
10	I	2	NAG	C1-C2-N2	2.22	113.93	110.43
11	M	3	BMA	C3-C4-C5	2.21	114.24	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S	2	NAG	C1-O5-C5	2.20	115.14	112.19
7	A	4	MAN	O2-C2-C3	-2.19	105.62	110.15
10	I	1	NAG	O5-C5-C4	-2.18	105.51	110.83
8	C	4	MAN	O2-C2-C3	-2.17	105.67	110.15
11	M	4	MAN	O2-C2-C3	-2.15	105.70	110.15
12	P	10	MAN	O2-C2-C3	-2.12	105.76	110.15
12	P	3	BMA	O5-C5-C4	-2.11	105.70	110.83
7	A	6	MAN	O2-C2-C3	-2.10	105.80	110.15
12	P	3	BMA	O2-C2-C1	-2.08	104.46	109.22
12	P	5	MAN	C6-C5-C4	-2.08	107.92	113.02
9	F	5	MAN	O2-C2-C3	-2.06	105.88	110.15
9	F	4	MAN	O2-C2-C3	-2.06	105.89	110.15
11	M	5	MAN	O2-C2-C3	-2.05	105.91	110.15
10	J	1	NAG	C1-O5-C5	2.04	114.92	112.19
10	K	1	NAG	C1-O5-C5	2.04	114.91	112.19

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	P	2	NAG	C3-C2-N2-C7
10	S	1	NAG	O5-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
12	P	6	MAN	C4-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6
11	M	2	NAG	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
10	Q	2	NAG	O5-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
12	P	2	NAG	O5-C5-C6-O6
12	P	7	MAN	O5-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
11	M	3	BMA	O5-C5-C6-O6
10	Q	2	NAG	C4-C5-C6-O6
12	P	6	MAN	O5-C5-C6-O6
11	M	2	NAG	C4-C5-C6-O6
11	M	1	NAG	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
12	P	5	MAN	O5-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	O	2	NAG	C4-C5-C6-O6
11	M	1	NAG	C4-C5-C6-O6
10	S	2	NAG	O5-C5-C6-O6
12	P	2	NAG	C4-C5-C6-O6
10	R	1	NAG	C4-C5-C6-O6
10	O	1	NAG	C4-C5-C6-O6
12	P	7	MAN	C4-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
10	I	1	NAG	C8-C7-N2-C2
10	I	1	NAG	O7-C7-N2-C2
10	I	2	NAG	C8-C7-N2-C2
10	I	2	NAG	O7-C7-N2-C2
10	J	1	NAG	C8-C7-N2-C2
10	J	1	NAG	O7-C7-N2-C2
10	T	1	NAG	C8-C7-N2-C2
10	T	1	NAG	O7-C7-N2-C2
12	P	1	NAG	C8-C7-N2-C2
12	P	1	NAG	O7-C7-N2-C2
7	A	4	MAN	O5-C5-C6-O6
12	P	5	MAN	C4-C5-C6-O6
7	A	4	MAN	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
10	N	1	NAG	O5-C5-C6-O6
10	O	1	NAG	O5-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
8	C	3	BMA	O5-C5-C6-O6
11	M	5	MAN	O5-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
11	M	3	BMA	C4-C5-C6-O6
11	M	6	MAN	O5-C5-C6-O6
9	F	4	MAN	O5-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
10	R	1	NAG	C3-C2-N2-C7
11	M	2	NAG	C3-C2-N2-C7
10	K	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	2	NAG	C1-C2-N2-C7
10	I	2	NAG	C1-C2-N2-C7
10	R	1	NAG	C1-C2-N2-C7
12	P	2	NAG	C1-C2-N2-C7
10	I	2	NAG	C3-C2-N2-C7
7	A	5	MAN	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6

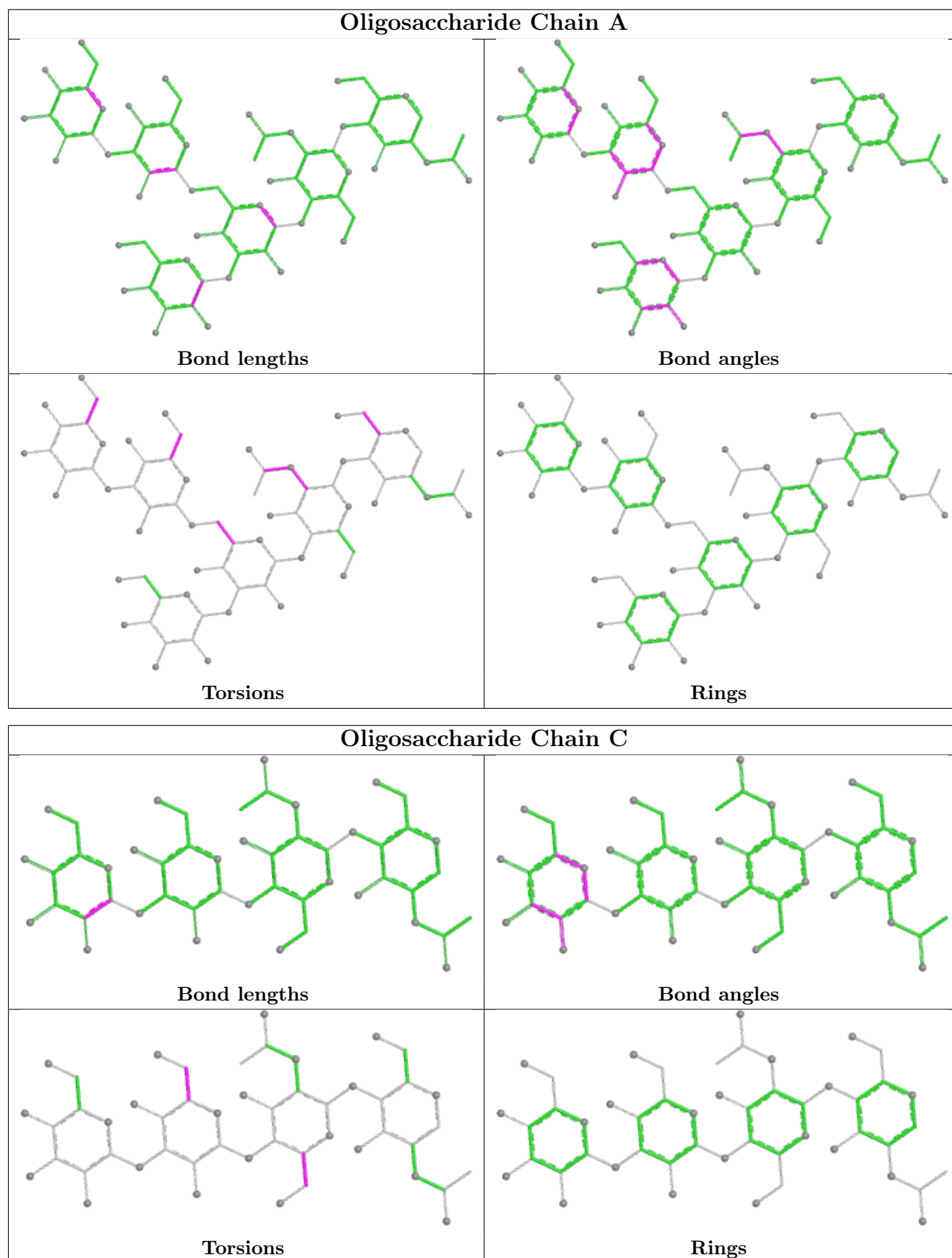
All (1) ring outliers are listed below:

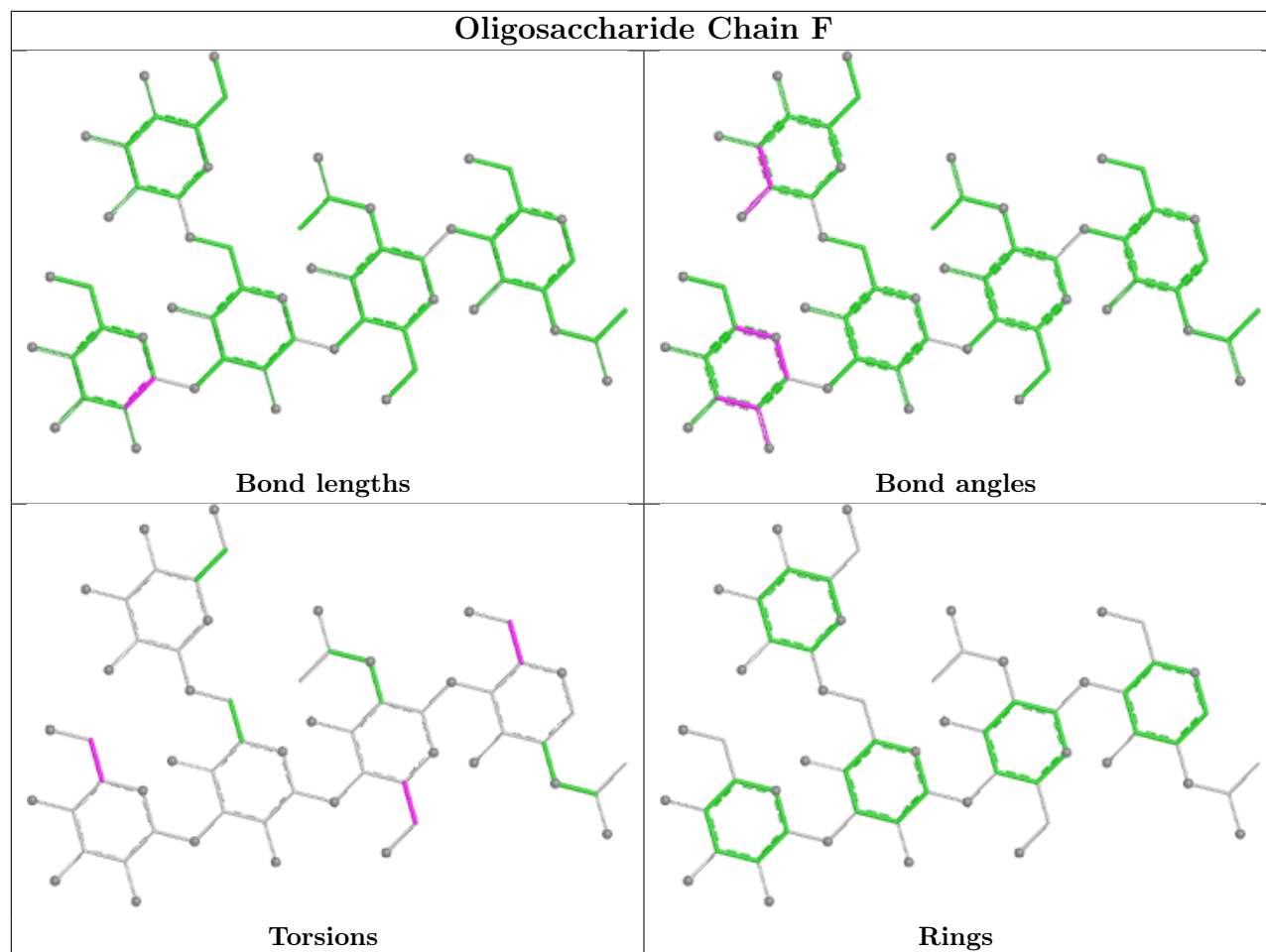
Mol	Chain	Res	Type	Atoms
11	M	5	MAN	C1-C2-C3-C4-C5-O5

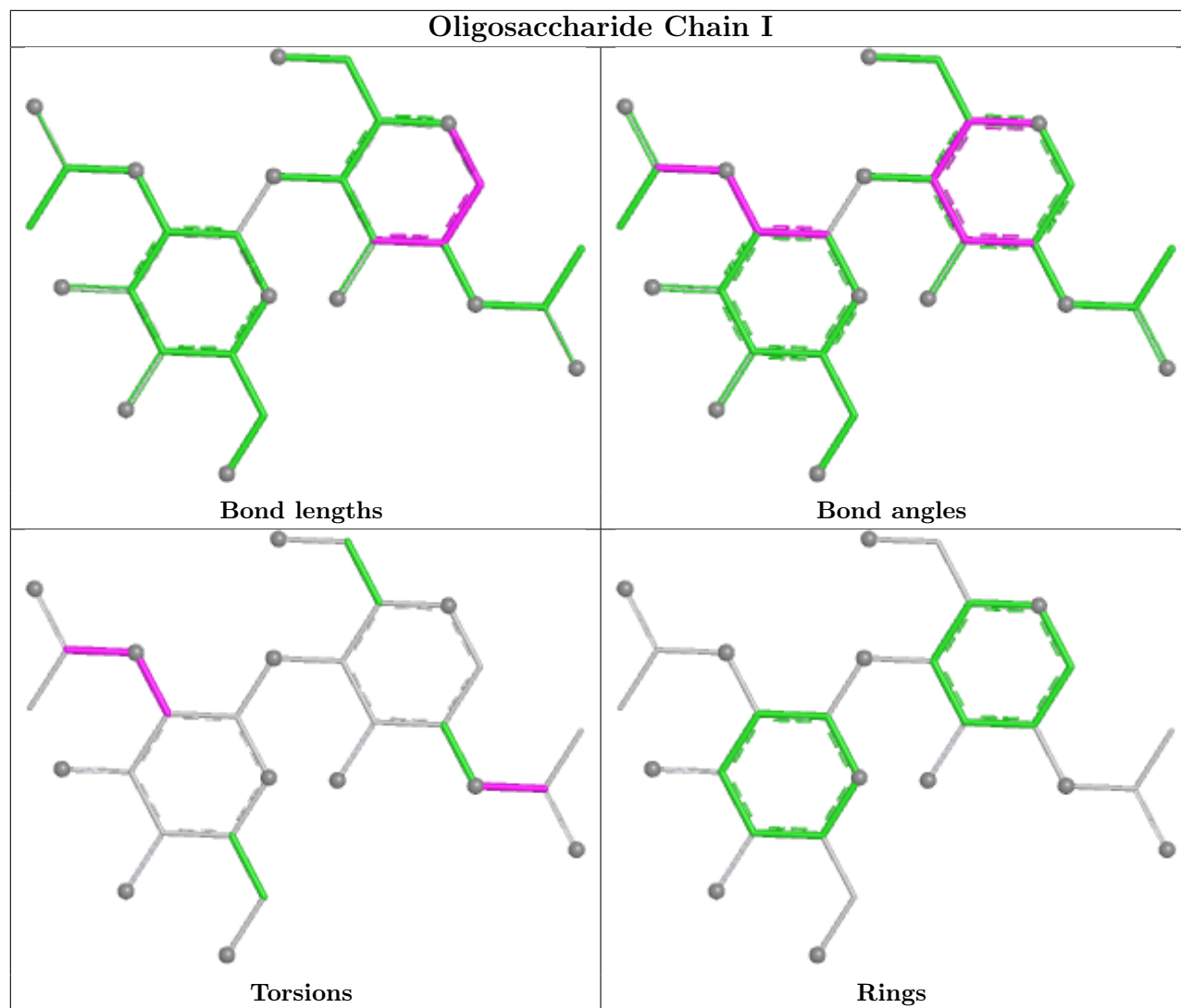
25 monomers are involved in 44 short contacts:

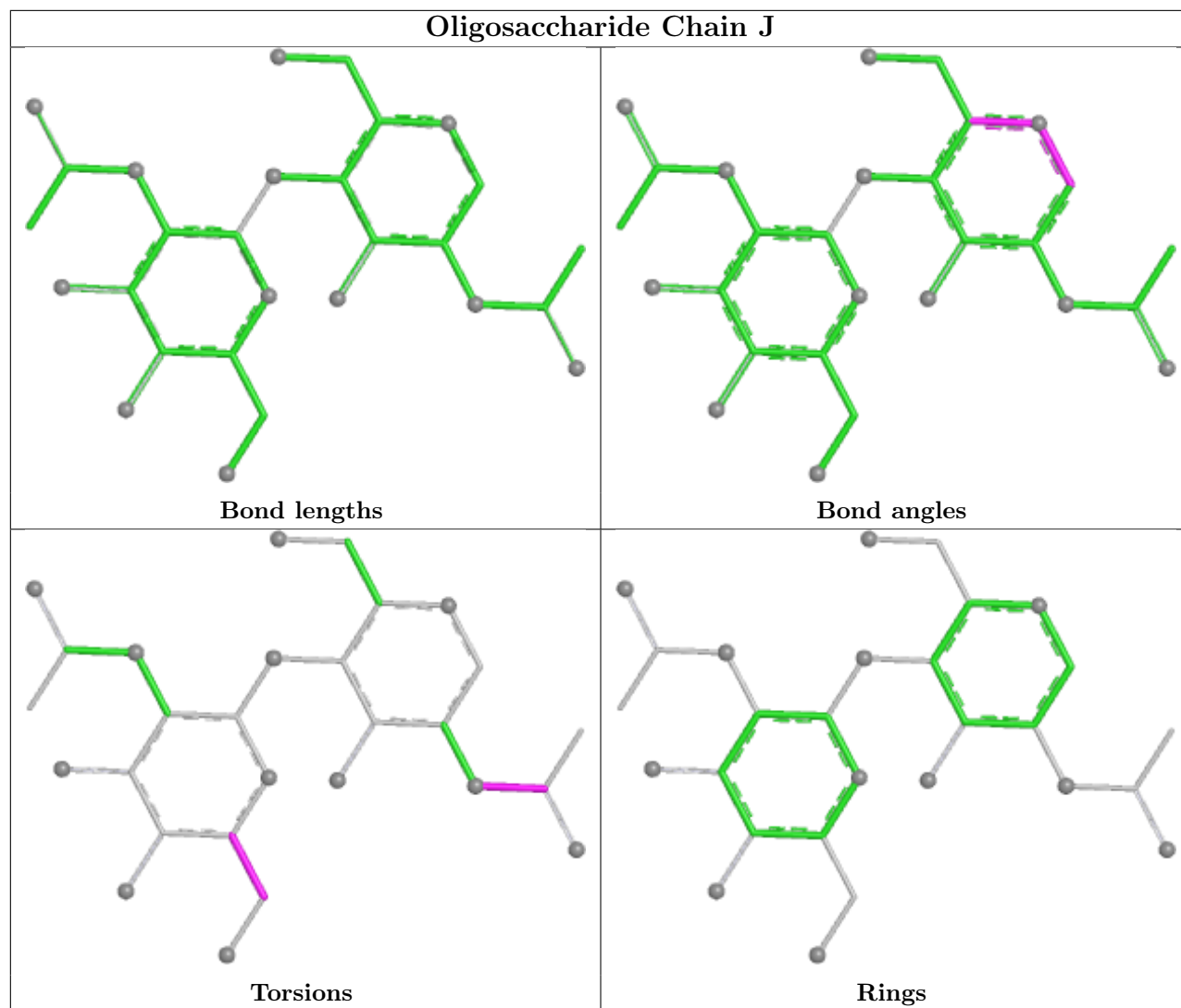
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	5	MAN	6	0
7	A	1	NAG	3	0
7	A	3	BMA	1	0
10	N	1	NAG	1	0
12	P	8	MAN	2	0
11	M	1	NAG	1	0
10	N	2	NAG	1	0
8	C	2	NAG	1	0
10	I	1	NAG	1	0
12	P	7	MAN	1	0
10	K	2	NAG	1	0
12	P	2	NAG	7	0
12	P	3	BMA	1	0
12	P	9	MAN	1	0
7	A	4	MAN	2	0
10	S	2	NAG	2	0
10	K	1	NAG	1	0
11	M	2	NAG	3	0
12	P	1	NAG	7	0
10	I	2	NAG	1	0
8	C	1	NAG	2	0
7	A	2	NAG	3	0
10	S	1	NAG	2	0
9	F	1	NAG	1	0
12	P	6	MAN	7	0

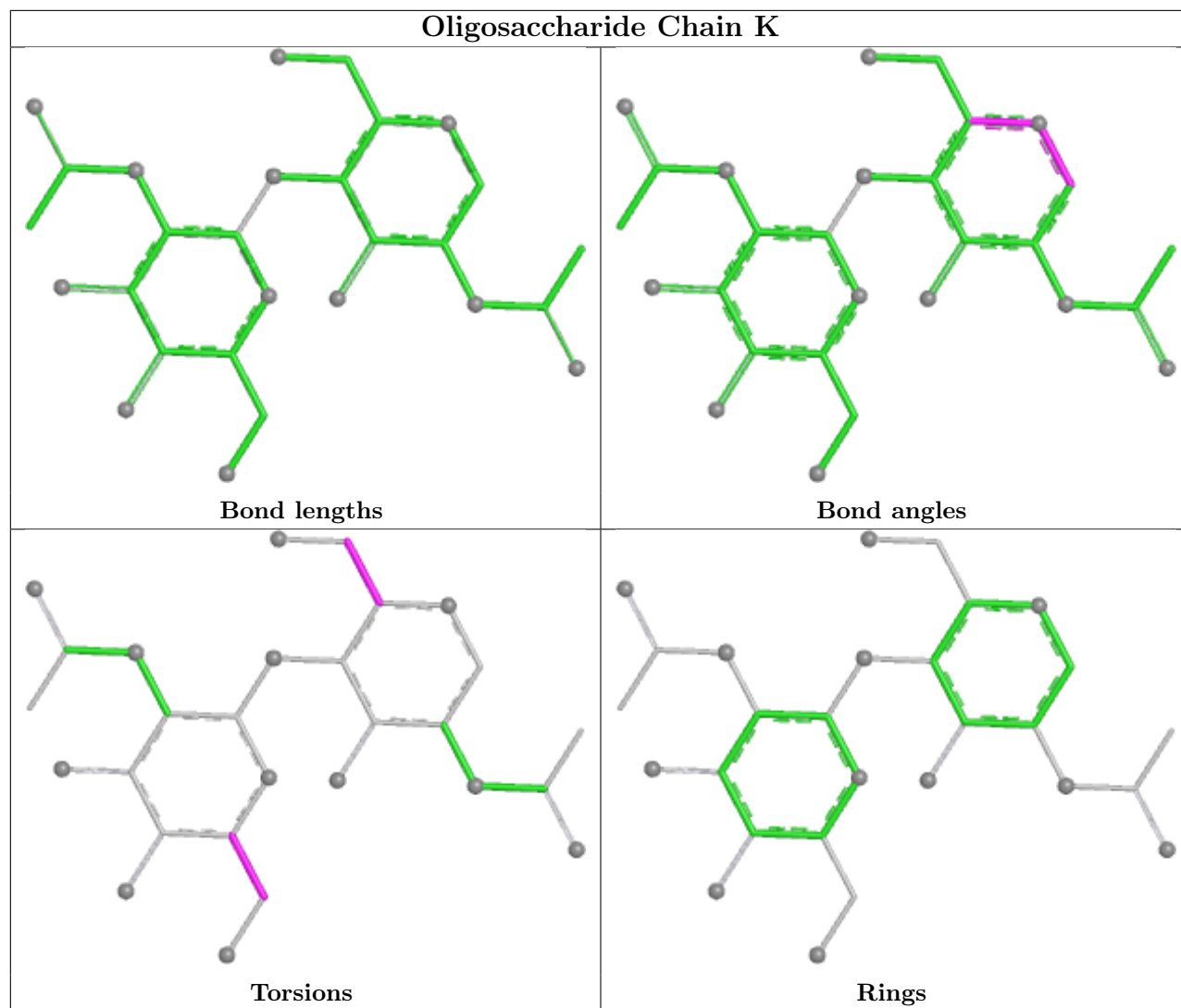
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

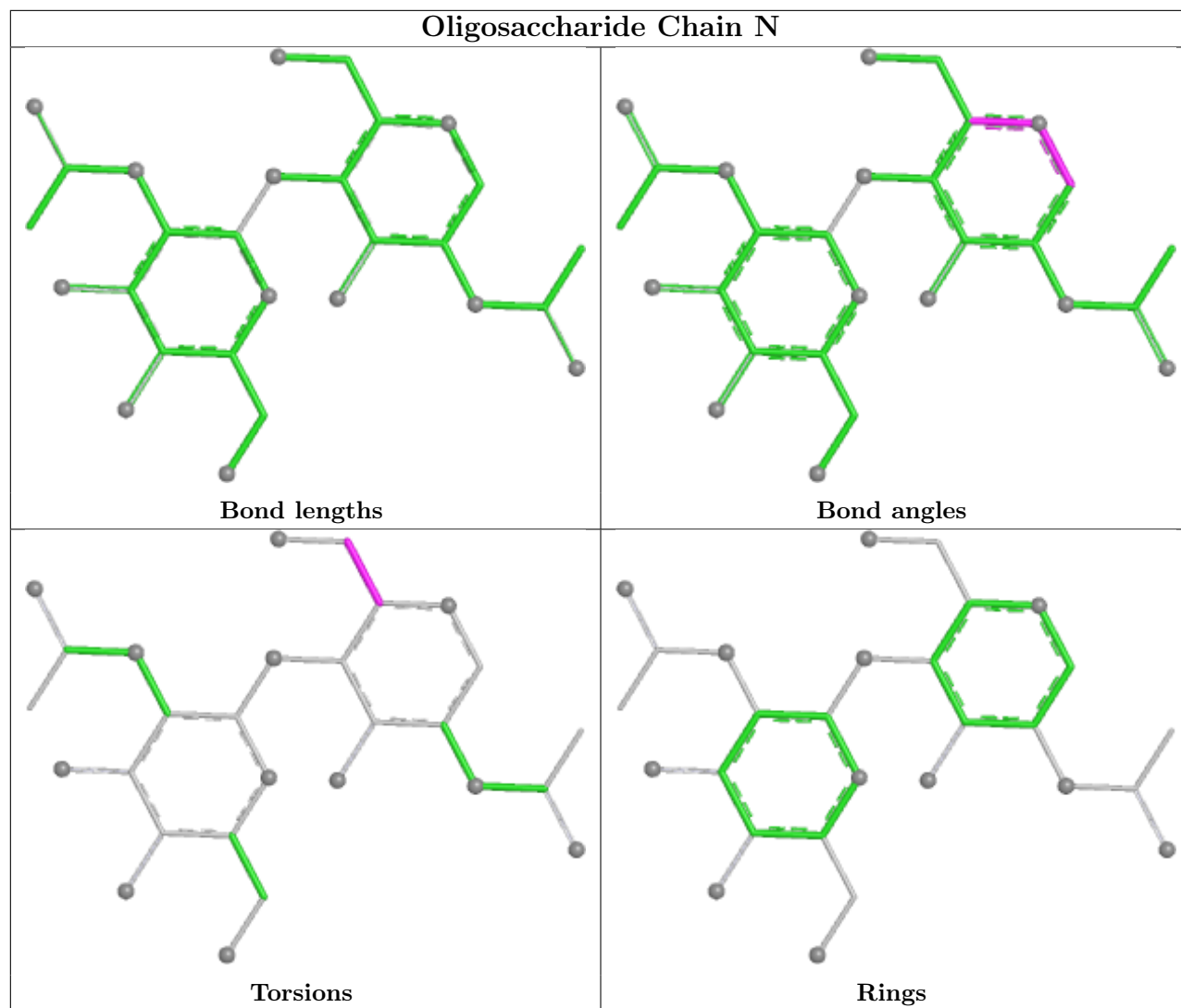


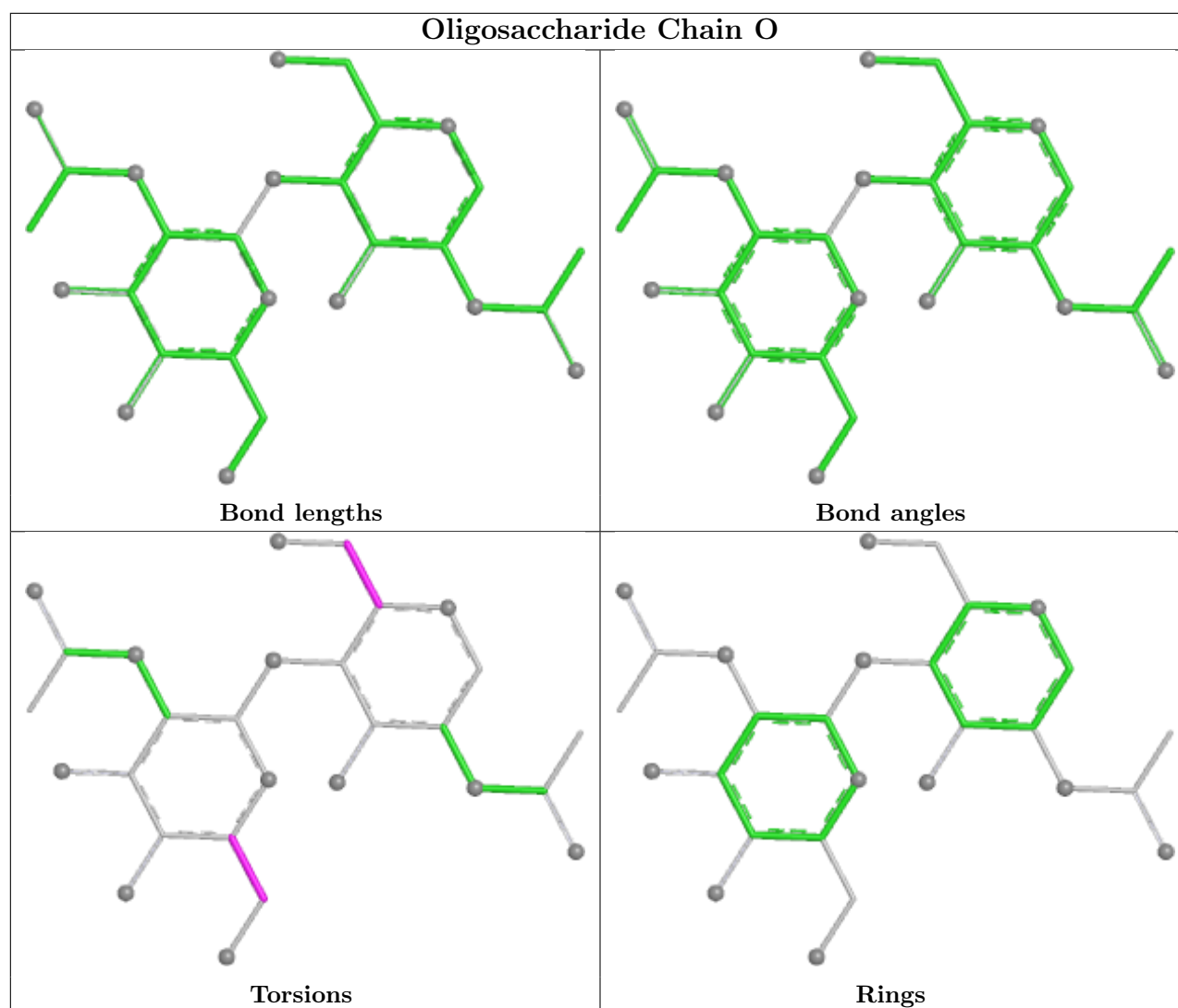


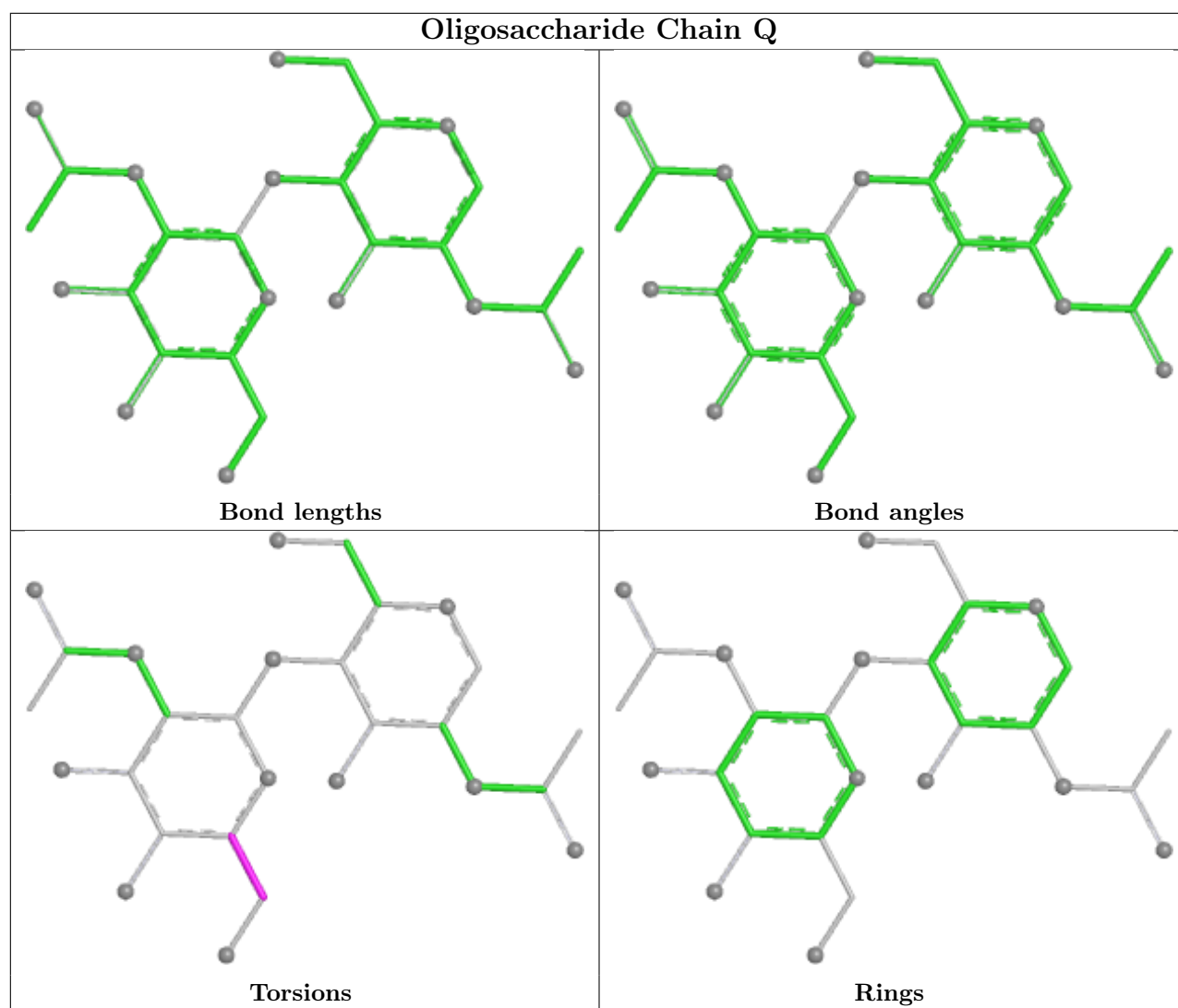


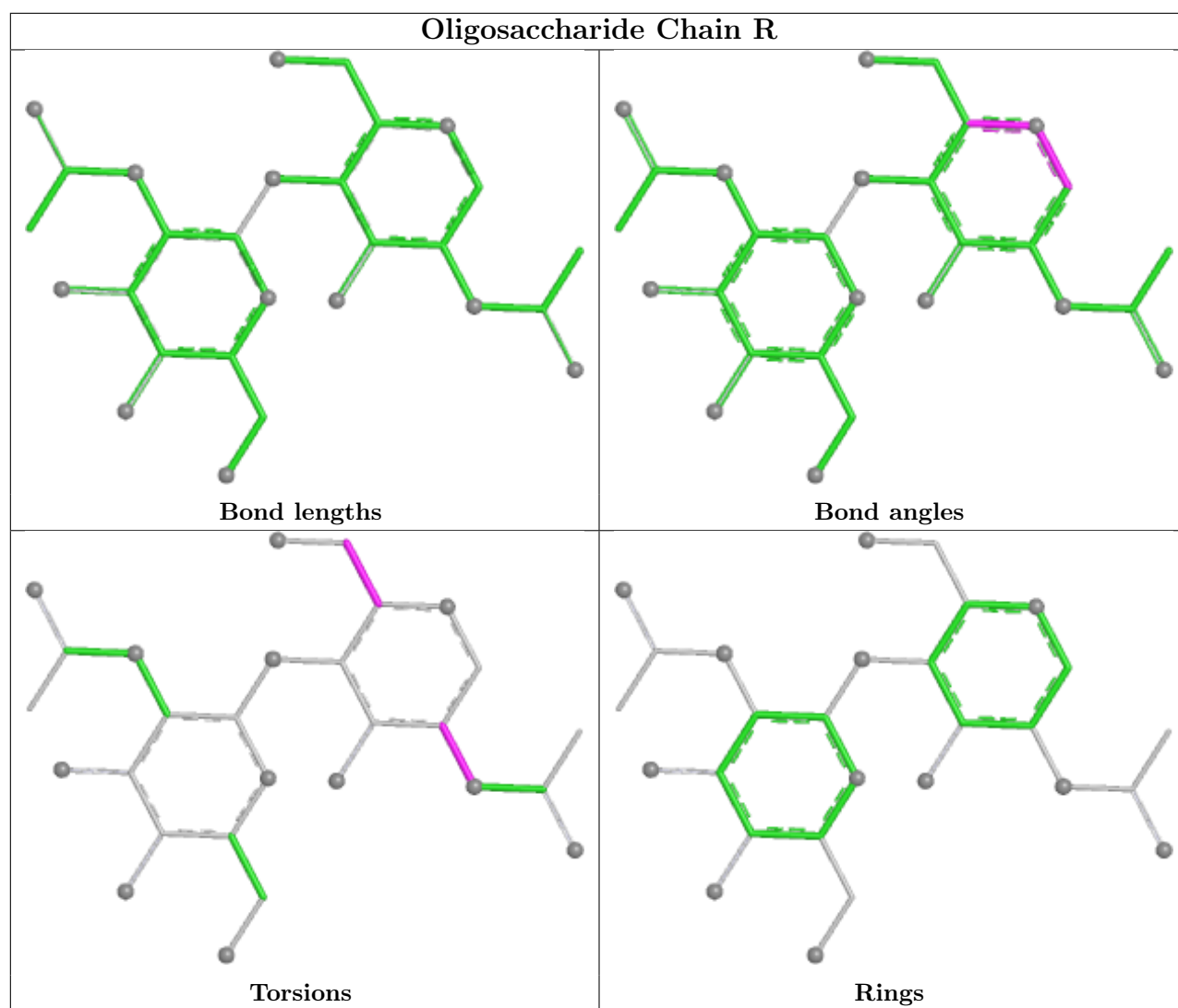


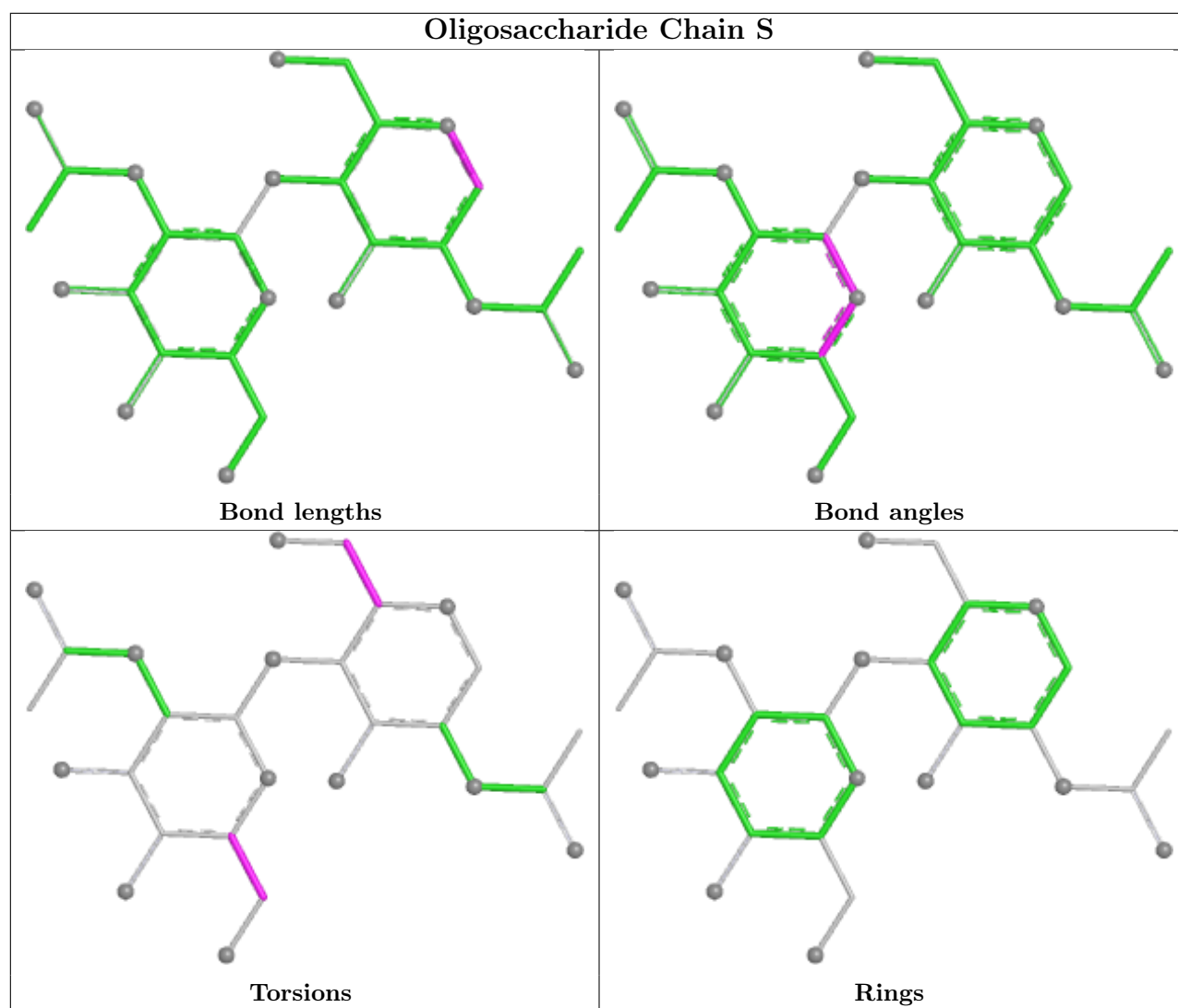


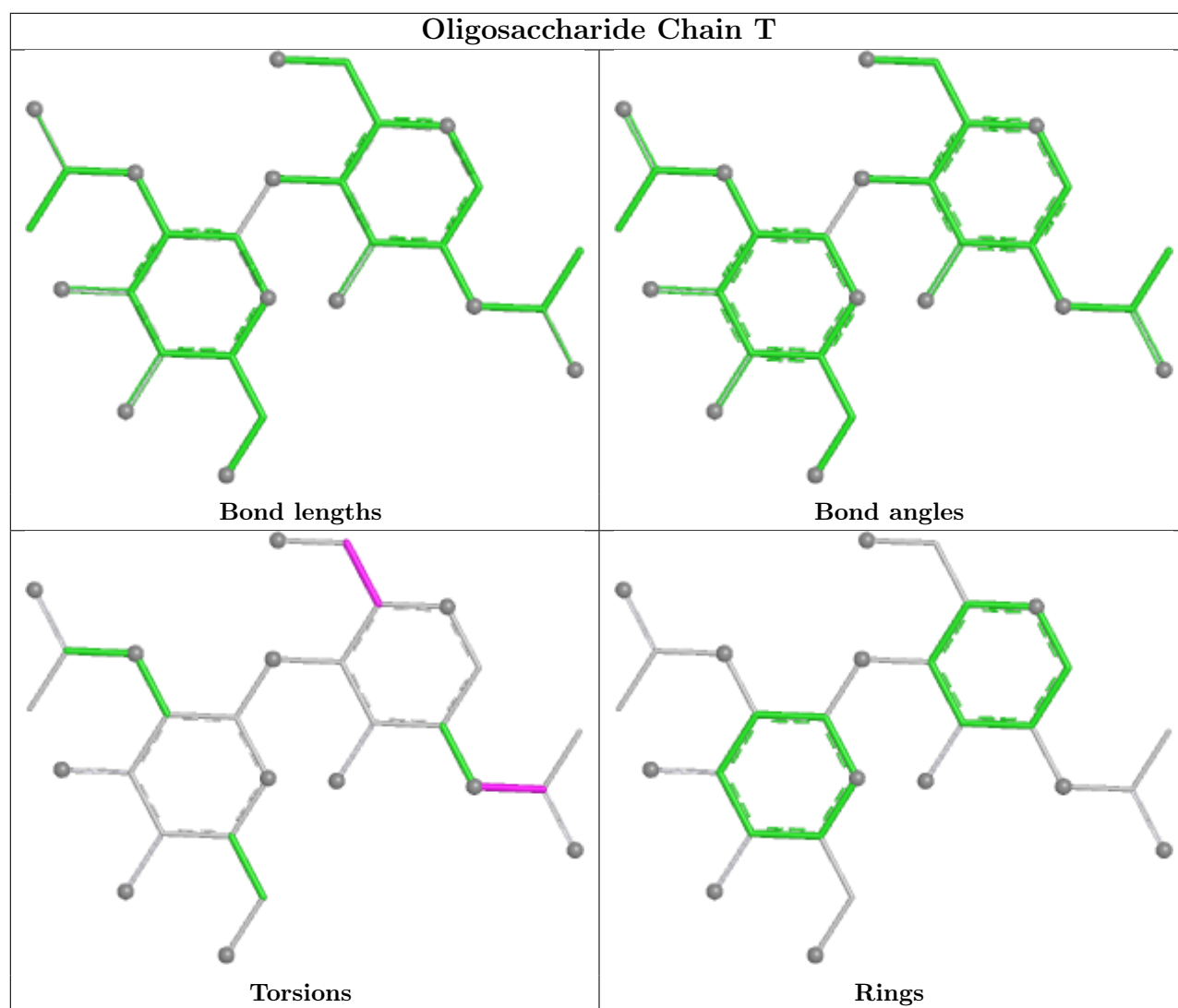




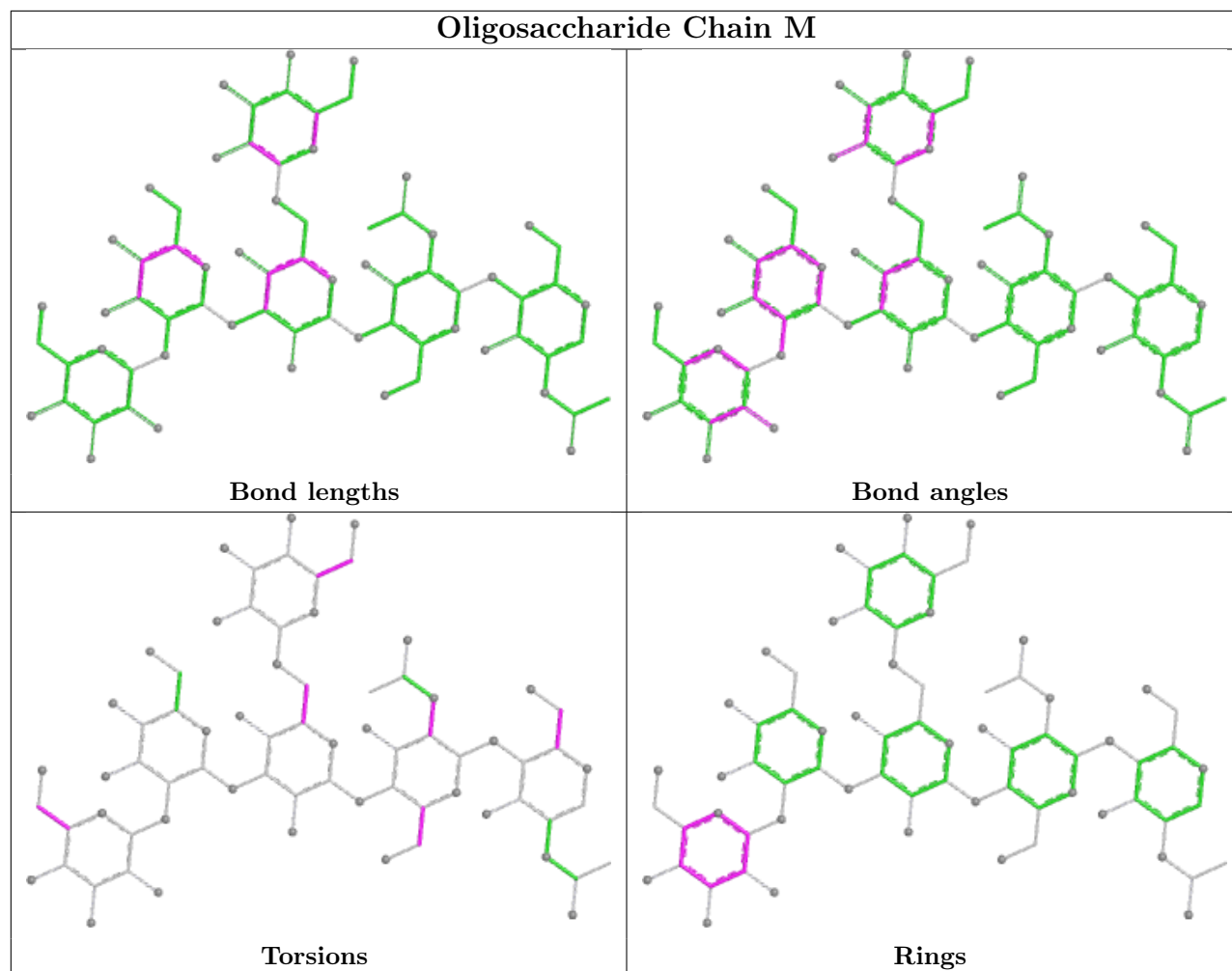


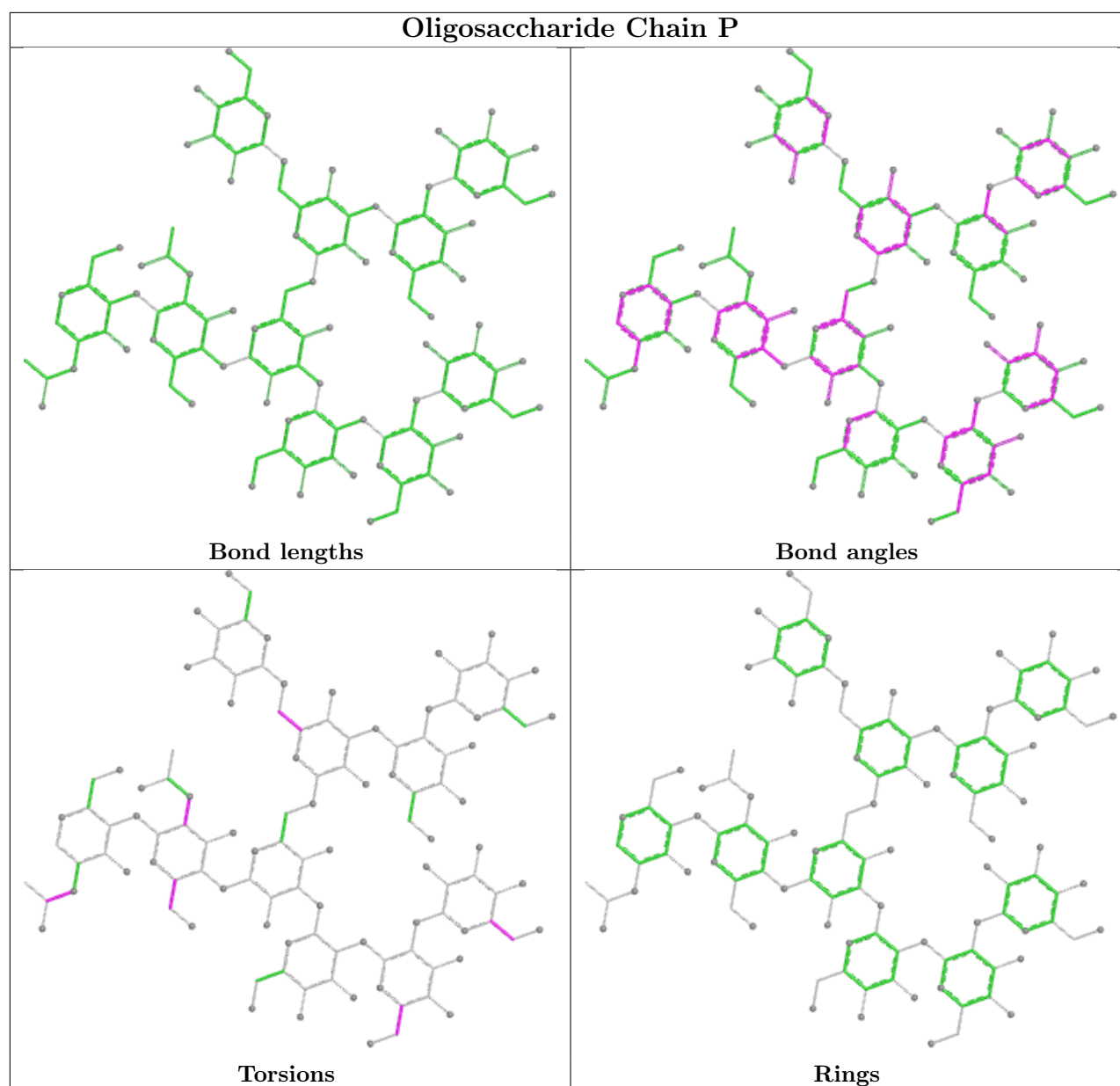






Oligosaccharide Chain M





5.6 Ligand geometry [i](#)

8 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
13	NAG	G	607	4	14,14,15	0.57	0	17,19,21	0.56	0
13	NAG	G	653	4	14,14,15	0.26	0	17,19,21	0.44	0
13	NAG	G	629	4	14,14,15	0.45	0	17,19,21	1.39	2 (11%)
13	NAG	G	644	4	14,14,15	0.37	0	17,19,21	0.58	0
13	NAG	B	701	1	14,14,15	0.50	0	17,19,21	0.45	0
13	NAG	B	702	1	14,14,15	0.24	0	17,19,21	0.53	0
13	NAG	B	703	1	14,14,15	0.27	0	17,19,21	0.49	0
13	NAG	H	301	5	14,14,15	0.18	0	17,19,21	0.67	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
13	NAG	G	607	4	-	3/6/23/26	0/1/1/1
13	NAG	G	653	4	-	2/6/23/26	0/1/1/1
13	NAG	G	629	4	-	6/6/23/26	0/1/1/1
13	NAG	G	644	4	-	4/6/23/26	0/1/1/1
13	NAG	B	701	1	-	2/6/23/26	0/1/1/1
13	NAG	B	702	1	-	3/6/23/26	0/1/1/1
13	NAG	B	703	1	-	2/6/23/26	0/1/1/1
13	NAG	H	301	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	629	NAG	C2-N2-C7	4.54	128.99	122.90
13	G	629	NAG	C1-C2-N2	2.10	113.74	110.43

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	H	301	NAG	C1-C2-N2-C7
13	G	629	NAG	O5-C5-C6-O6
13	G	629	NAG	C4-C5-C6-O6
13	G	653	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	B	701	NAG	O5-C5-C6-O6
13	G	644	NAG	O5-C5-C6-O6
13	G	607	NAG	C8-C7-N2-C2
13	G	607	NAG	O7-C7-N2-C2
13	G	629	NAG	C8-C7-N2-C2
13	G	629	NAG	O7-C7-N2-C2
13	G	644	NAG	C8-C7-N2-C2
13	G	644	NAG	O7-C7-N2-C2
13	H	301	NAG	C4-C5-C6-O6
13	H	301	NAG	O5-C5-C6-O6
13	G	653	NAG	C4-C5-C6-O6
13	B	703	NAG	O5-C5-C6-O6
13	G	607	NAG	O5-C5-C6-O6
13	G	644	NAG	C4-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6
13	B	702	NAG	C1-C2-N2-C7
13	B	701	NAG	C4-C5-C6-O6
13	G	629	NAG	C1-C2-N2-C7
13	B	703	NAG	C4-C5-C6-O6
13	B	702	NAG	C3-C2-N2-C7
13	G	629	NAG	C3-C2-N2-C7
13	H	301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	629	NAG	1	0
13	H	301	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	122/153 (79%)	-1.37	0	100 100	21, 77, 141, 229	0
2	D	242/243 (99%)	-0.98	6 (2%)	58 43	82, 179, 336, 392	0
3	E	213/216 (98%)	-1.20	1 (0%)	87 78	89, 186, 303, 337	0
4	G	449/505 (88%)	-1.39	0	100 100	28, 80, 170, 246	0
5	H	232/235 (98%)	-1.38	0	100 100	48, 104, 179, 228	0
6	L	208/208 (100%)	-1.49	0	100 100	35, 78, 142, 198	0
All	All	1466/1560 (93%)	-1.31	7 (0%)	87 78	21, 105, 266, 392	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	212	GLU	8.2
2	D	215	SER	7.8
2	D	126	PRO	3.5
2	D	188	SER	2.9
2	D	213	PRO	2.5
2	D	125	ALA	2.3
3	E	114	SER	2.1

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

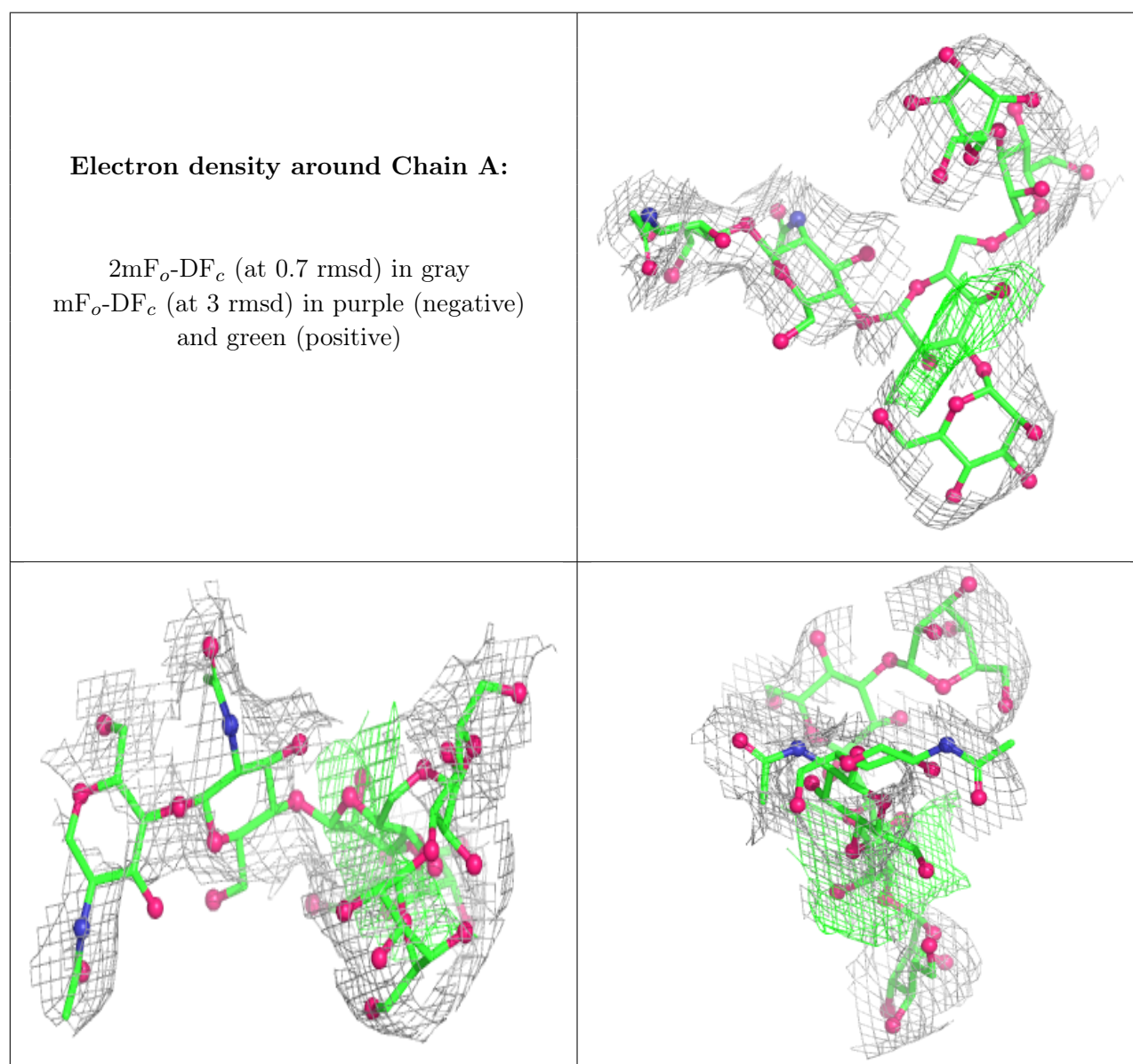
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	1	14/15	-	-	76,102,129,143	0
7	NAG	A	2	14/15	-	-	121,124,132,138	0
7	BMA	A	3	11/12	-	-	78,113,127,141	0
7	MAN	A	4	11/12	-	-	138,154,176,182	0
7	MAN	A	5	11/12	-	-	137,141,157,167	0
7	MAN	A	6	11/12	-	-	90,101,137,152	0
8	NAG	C	1	14/15	-	-	108,140,173,177	0
8	NAG	C	2	14/15	-	-	116,144,163,180	0
8	BMA	C	3	11/12	-	-	176,187,198,207	0
8	MAN	C	4	11/12	-	-	140,169,187,189	0
9	NAG	F	1	14/15	-	-	59,103,114,116	0
9	NAG	F	2	14/15	-	-	118,131,139,146	0
9	BMA	F	3	11/12	-	-	121,143,150,157	0
9	MAN	F	4	11/12	-	-	108,121,130,130	0
9	MAN	F	5	11/12	-	-	125,144,153,154	0
12	MAN	P	9	11/12	0.97	0.02	154,182,188,190	0
10	NAG	S	1	14/15	0.98	0.05	123,161,167,173	0
10	NAG	S	2	14/15	0.98	0.03	150,172,182,188	0
10	NAG	T	2	14/15	0.98	0.06	161,172,192,195	0
11	MAN	M	5	11/12	0.98	0.04	151,168,188,200	0
11	MAN	M	6	11/12	0.98	0.04	103,117,139,141	0
10	NAG	O	2	14/15	0.98	0.04	137,151,165,171	0
10	NAG	Q	1	14/15	0.99	0.03	106,122,146,148	0
10	NAG	Q	2	14/15	0.99	0.03	154,160,187,192	0
10	NAG	R	1	14/15	0.99	0.03	94,123,148,151	0
10	NAG	R	2	14/15	0.99	0.03	116,130,146,153	0
10	NAG	J	2	14/15	0.99	0.03	178,208,220,224	0
10	NAG	K	1	14/15	0.99	0.03	94,149,177,180	0
10	NAG	T	1	14/15	0.99	0.04	74,132,158,161	0
10	NAG	K	2	14/15	0.99	0.07	175,193,201,202	0
11	NAG	M	2	14/15	0.99	0.04	91,112,147,147	0
11	BMA	M	3	11/12	0.99	0.03	125,141,151,160	0
11	MAN	M	4	11/12	0.99	0.03	115,135,152,174	0
10	NAG	N	2	14/15	0.99	0.04	108,129,138,138	0
10	NAG	O	1	14/15	0.99	0.05	68,106,128,130	0
12	NAG	P	2	14/15	0.99	0.03	107,122,133,141	0
12	BMA	P	3	11/12	0.99	0.03	102,130,146,147	0
12	MAN	P	4	11/12	0.99	0.03	60,76,97,104	0
12	MAN	P	6	11/12	0.99	0.04	98,116,138,147	0
12	MAN	P	8	11/12	0.99	0.02	149,153,163,174	0
10	NAG	I	2	14/15	0.99	0.04	113,138,175,178	0
12	MAN	P	10	11/12	0.99	0.04	154,157,159,160	0

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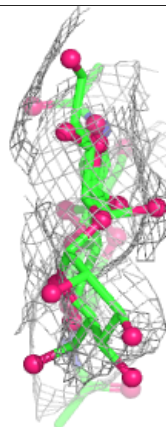
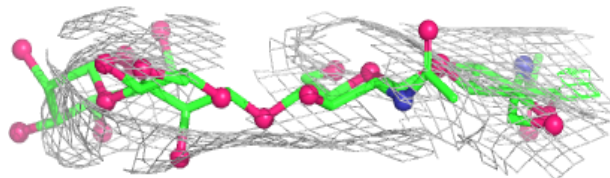
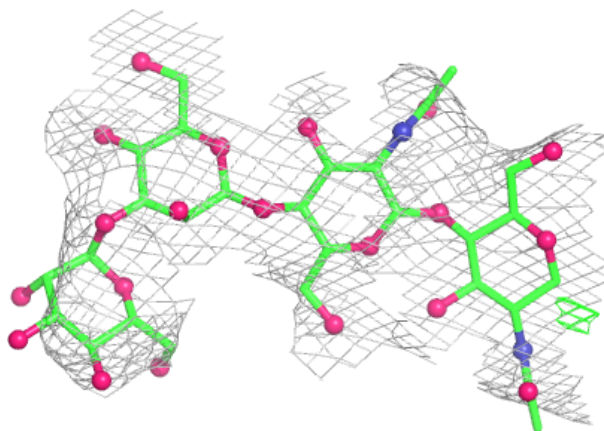
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	M	1	14/15	1.00	0.05	42,73,91,100	0
12	MAN	P	5	11/12	1.00	0.03	72,87,111,116	0
10	NAG	N	1	14/15	1.00	0.02	83,102,127,127	0
12	MAN	P	7	11/12	1.00	0.02	141,147,162,166	0
12	NAG	P	1	14/15	1.00	0.03	51,96,122,126	0
10	NAG	J	1	14/15	1.00	0.02	133,159,187,193	0
10	NAG	I	1	14/15	1.00	0.05	93,109,128,135	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.



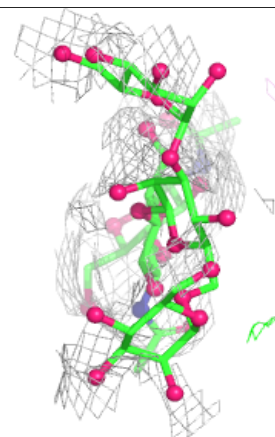
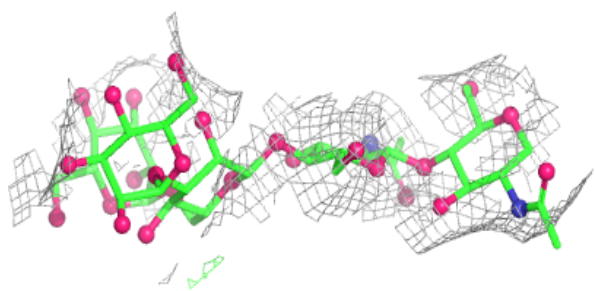
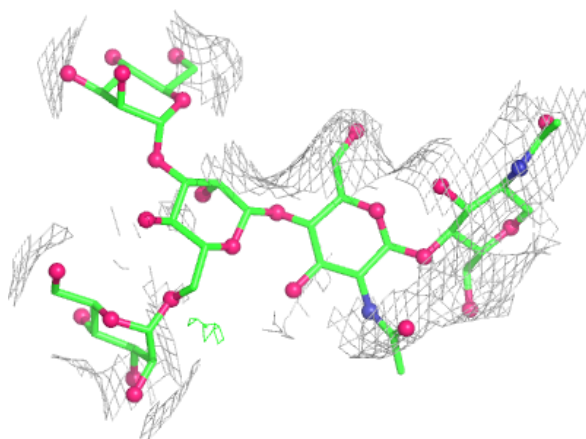
Electron density around Chain C:

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



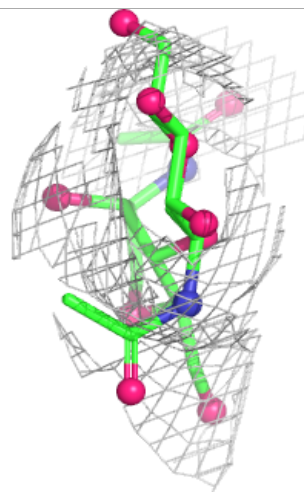
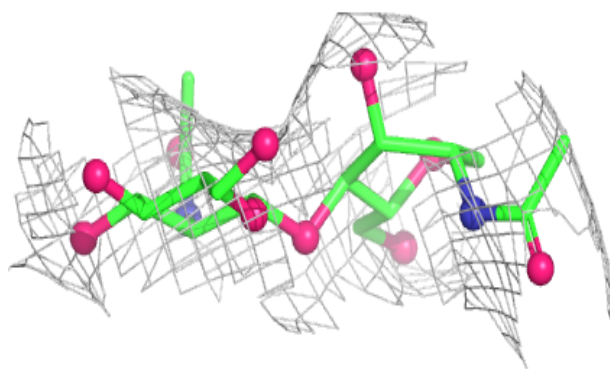
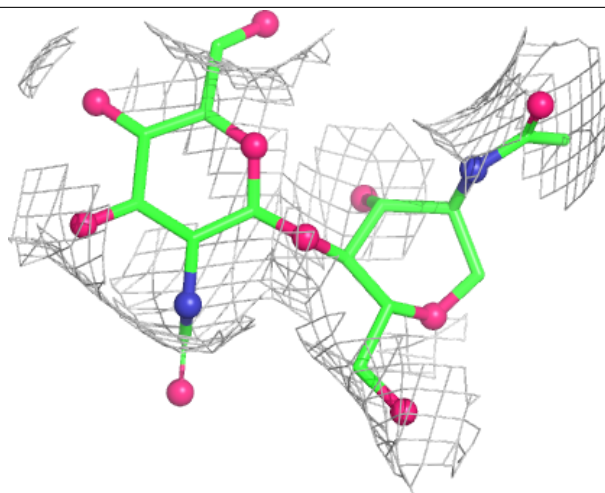
Electron density around Chain F:

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



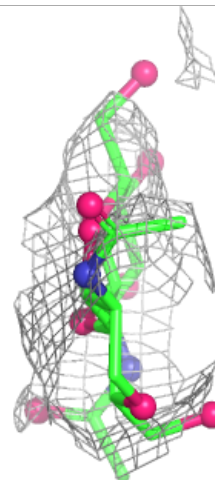
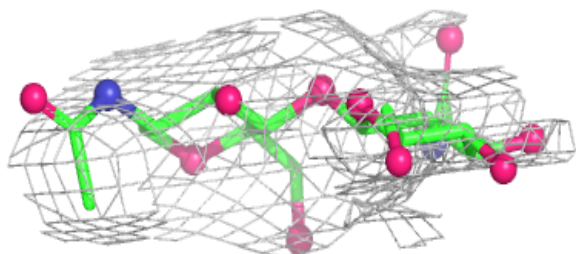
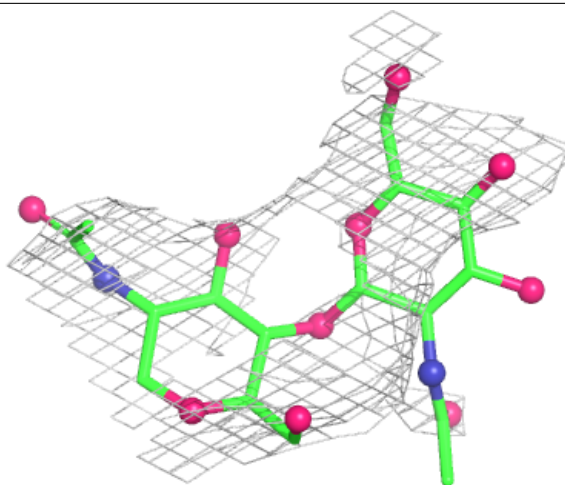
Electron density around Chain I:

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



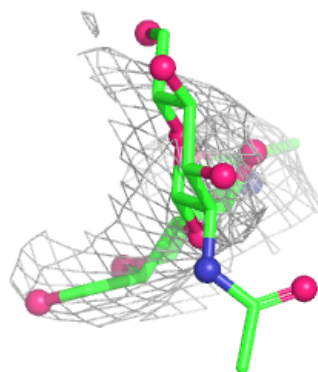
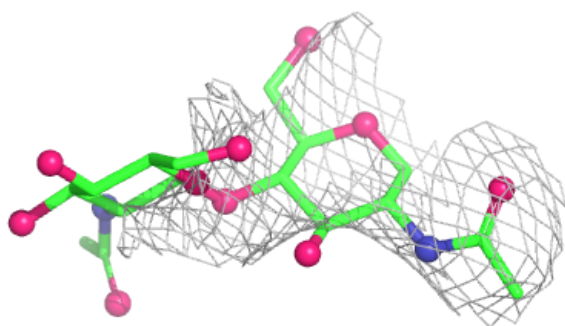
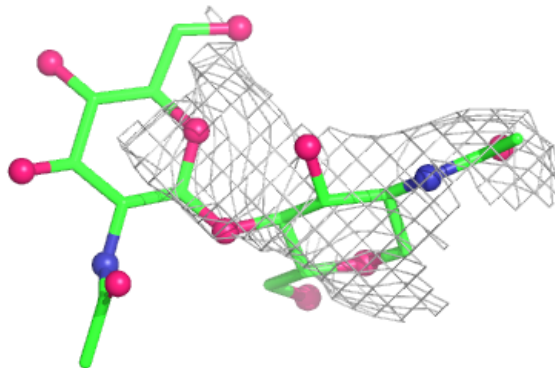
Electron density around Chain J:

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

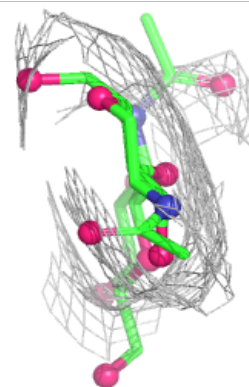
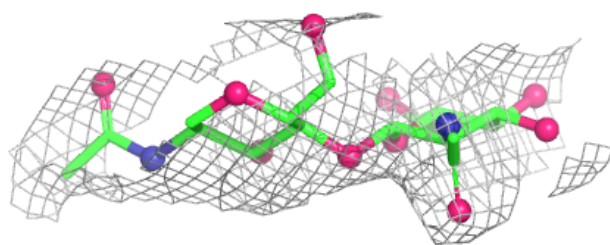
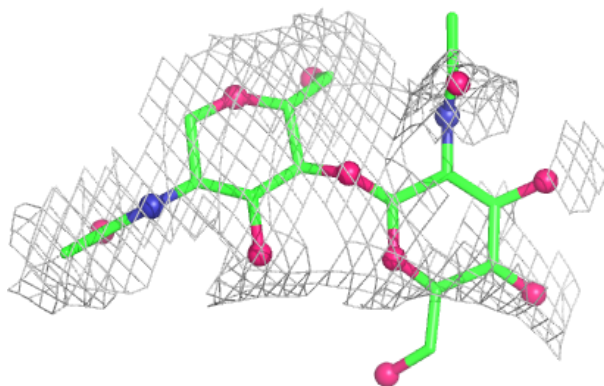


Electron density around Chain K:

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

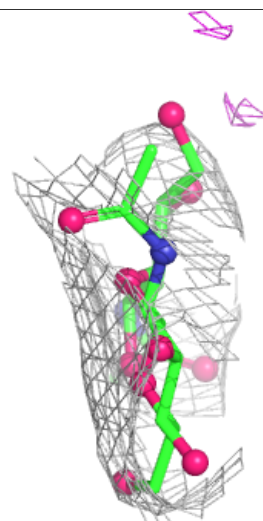
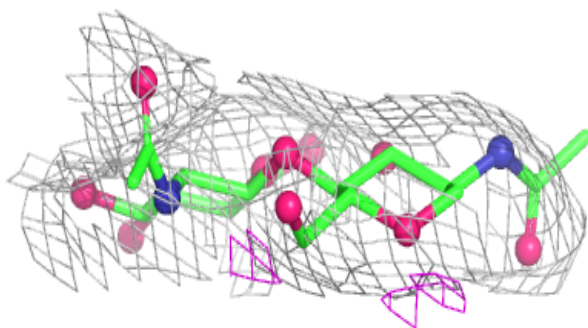
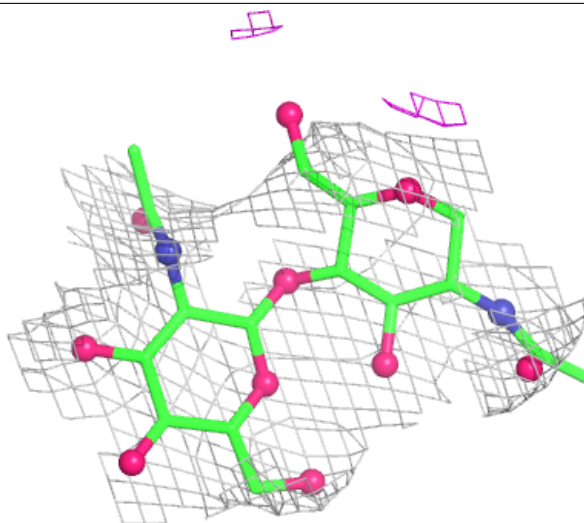
**Electron density around Chain N:**

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



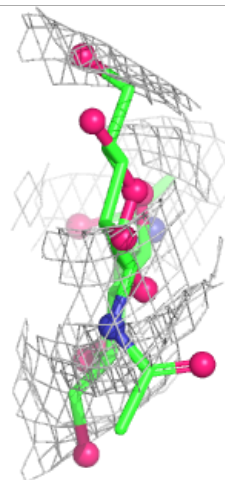
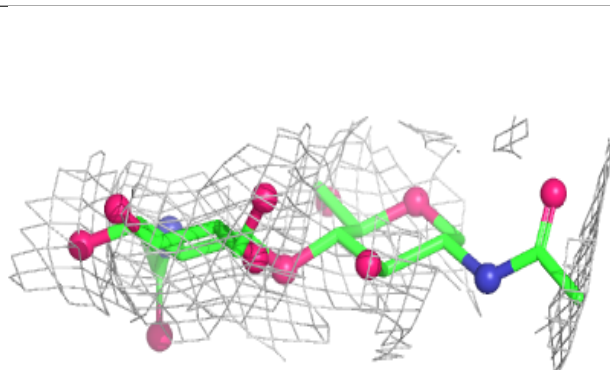
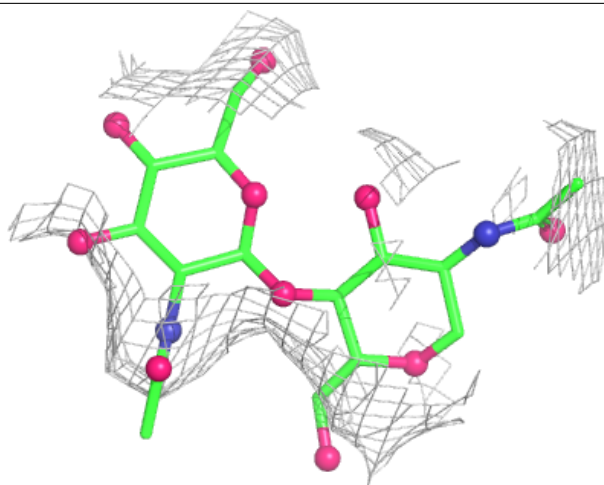
Electron density around Chain O:

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



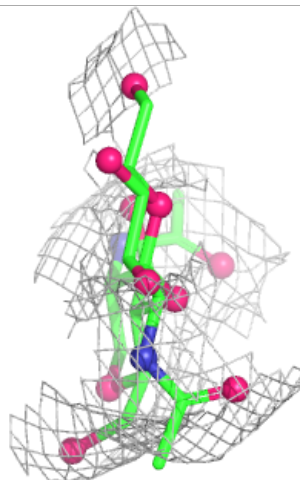
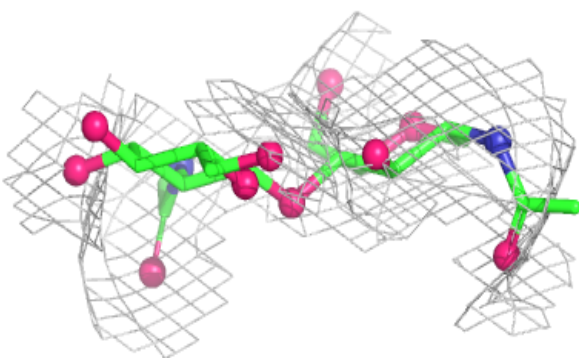
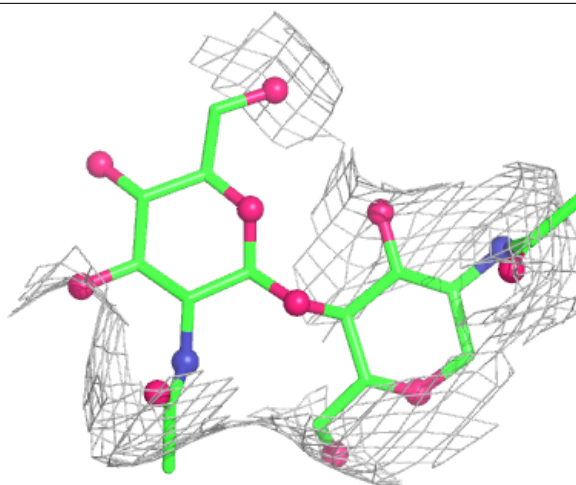
Electron density around Chain Q:

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



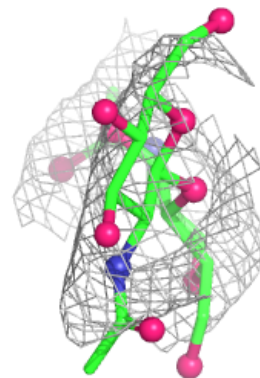
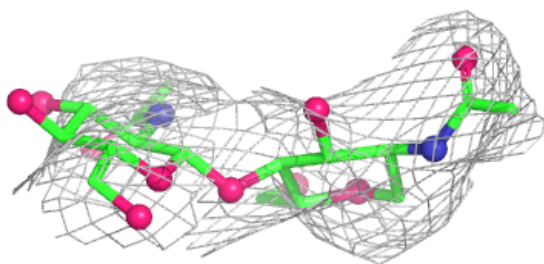
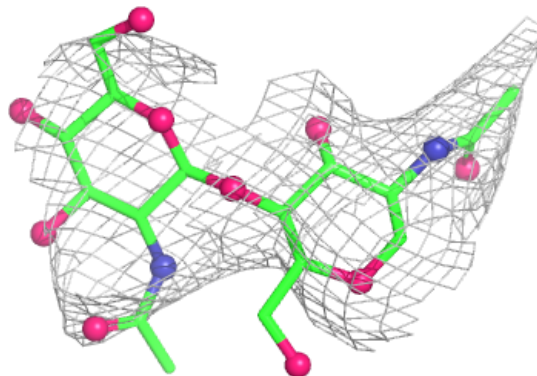
Electron density around Chain R:

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

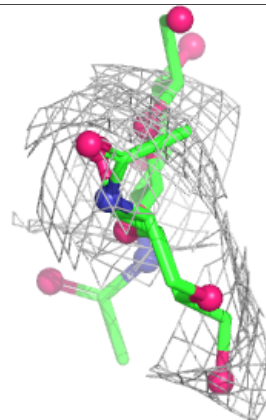
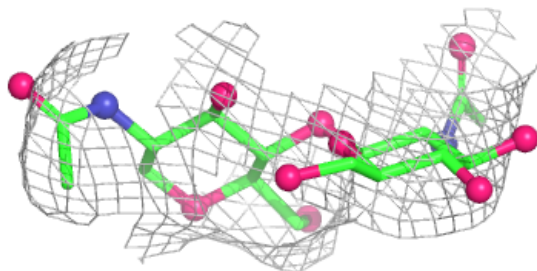
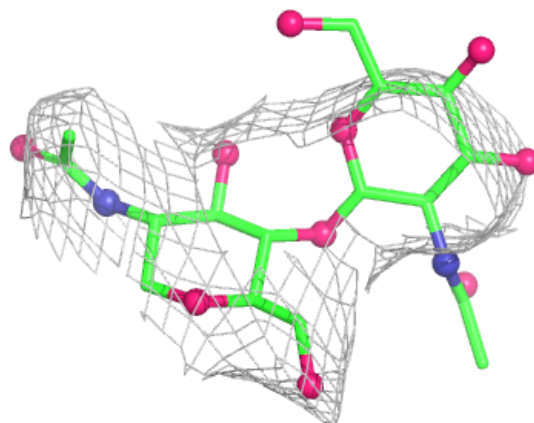


Electron density around Chain S:

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

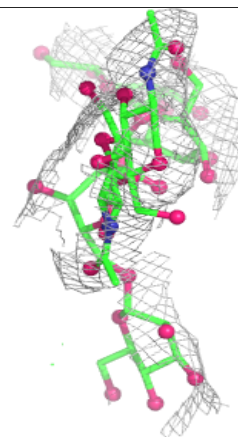
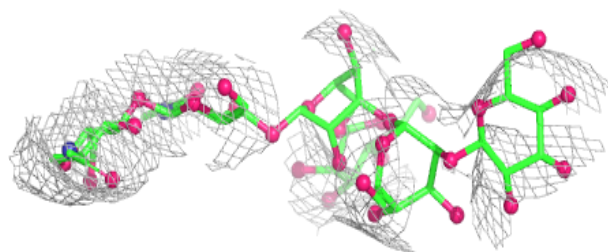
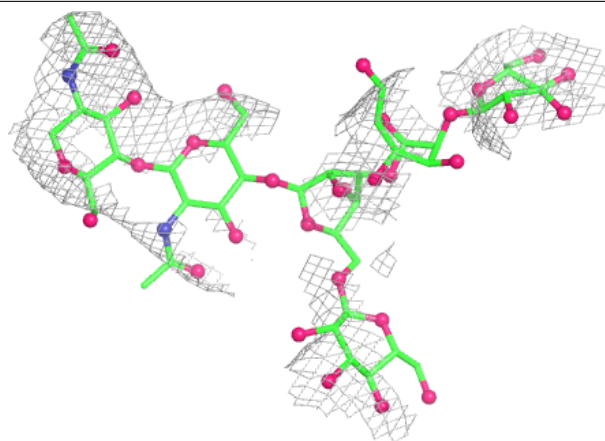
**Electron density around Chain T:**

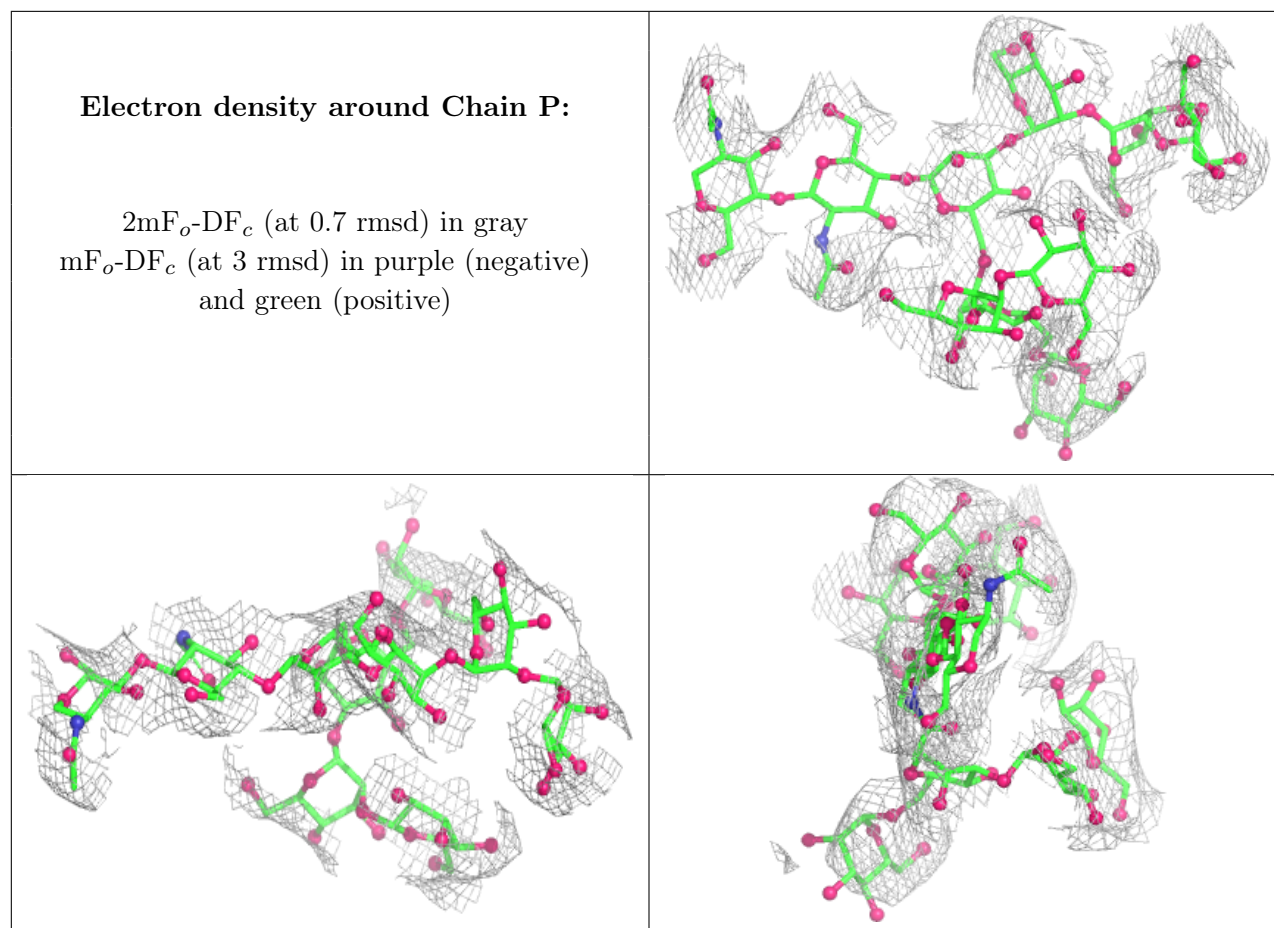
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	NAG	B	702	14/15	0.96	0.04	156,178,188,194	0
13	NAG	G	607	14/15	0.97	0.05	94,114,126,137	0
13	NAG	H	301	14/15	0.97	0.04	189,207,211,211	0
13	NAG	G	629	14/15	0.98	0.07	141,150,156,167	0
13	NAG	G	644	14/15	0.98	0.03	106,139,147,149	0
13	NAG	G	653	14/15	0.98	0.07	161,201,208,213	0
13	NAG	B	701	14/15	0.98	0.04	176,194,207,212	0
13	NAG	B	703	14/15	0.99	0.03	157,164,173,174	0

6.5 Other polymers [i](#)

There are no such residues in this entry.