



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 07:45 PM EDT

PDB ID : 5UTY
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

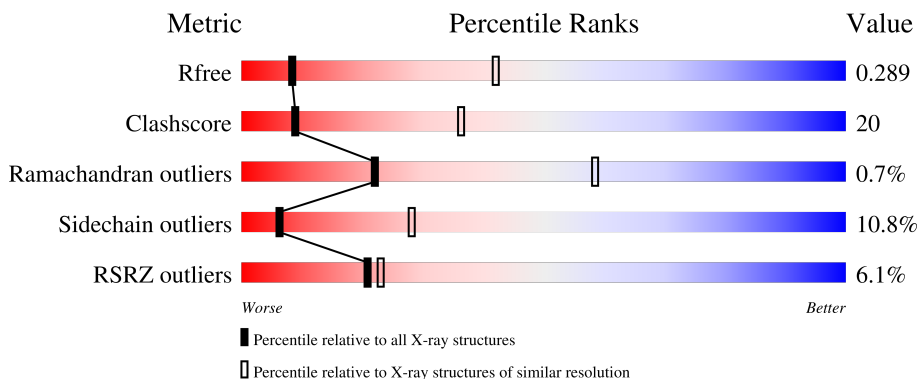
1 Overall quality at a glance

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.







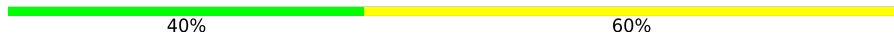




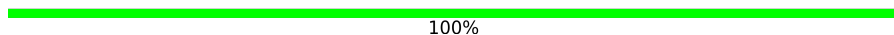
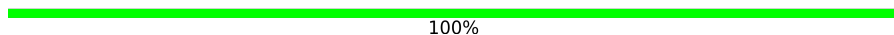


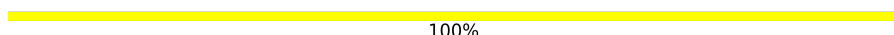

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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
			Total	C	N	O	S			
1	B	122	969	611	168	184	6	0	0	0

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
			Total	C	N	O	S			
2	D	242	1820	1156	303	353	8	0	0	0

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

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

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

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

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

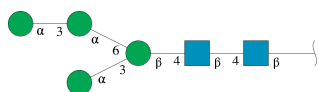
- Molecule 5 is a protein called PGT122 Fab heavy chain.

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

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

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

- 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.



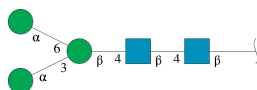
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	A	6	72	40	2	30		0	0	0

- 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
			Total	C	N	O	S			
8	C	4	50	28	2	20		0	0	0

- 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.



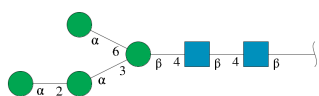
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	F	5	61	34	2	25		0	0	0

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



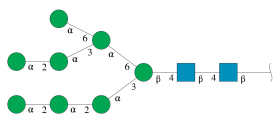
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	2	28	16	2	10	0	0	0
10	J	2	28	16	2	10	0	0	0
10	K	2	28	16	2	10	0	0	0
10	N	2	28	16	2	10	0	0	0
10	O	2	28	16	2	10	0	0	0
10	Q	2	28	16	2	10	0	0	0
10	R	2	28	16	2	10	0	0	0
10	S	2	28	16	2	10	0	0	0
10	T	2	28	16	2	10	0	0	0

- 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.



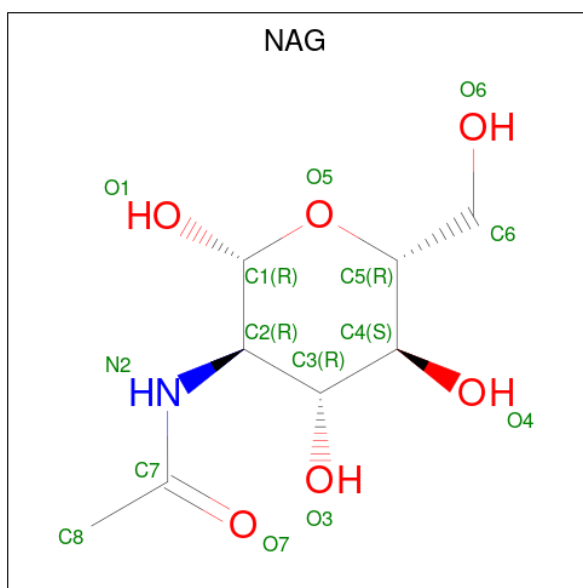
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	M	6	72	40	2	30	0	0	0

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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

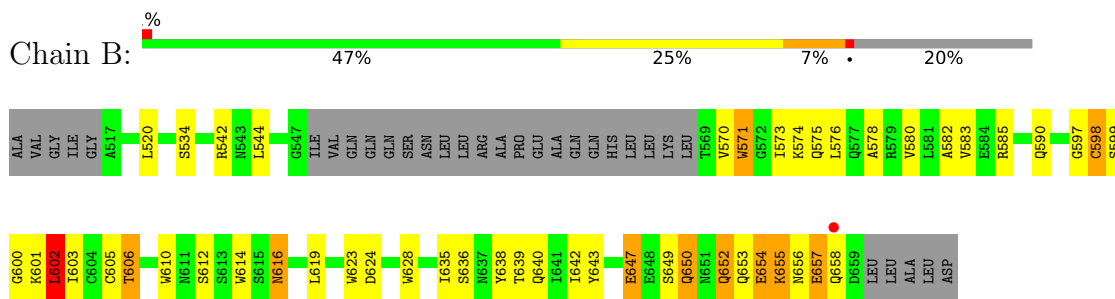


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	H	1	Total	C	N	O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

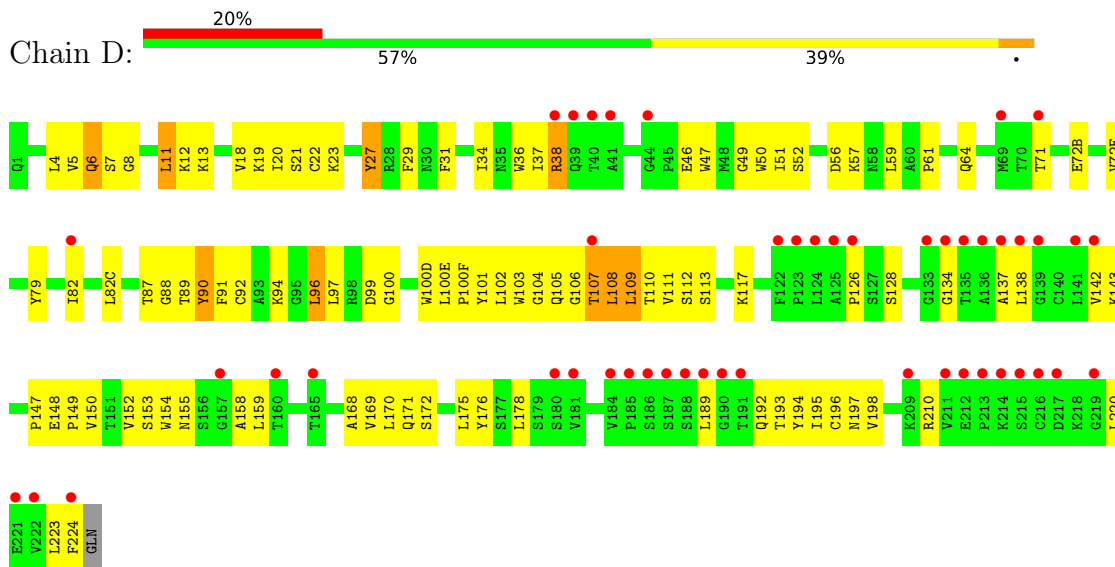
3 Residue-property plots [i](#)

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.

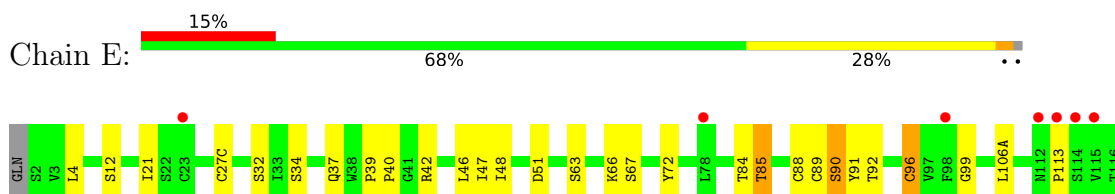
- Molecule 1: HIV-1 BG505 strain Env gp41

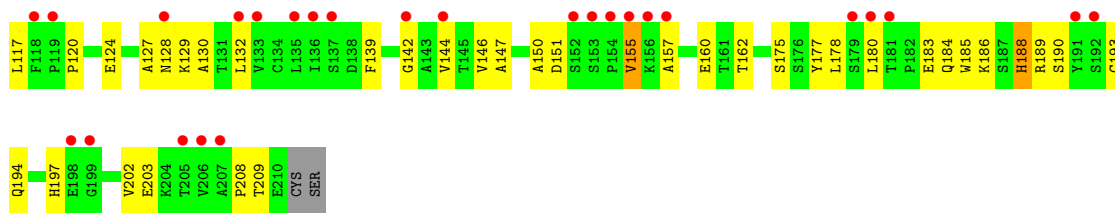


- Molecule 2: 35O22 Fab heavy chain

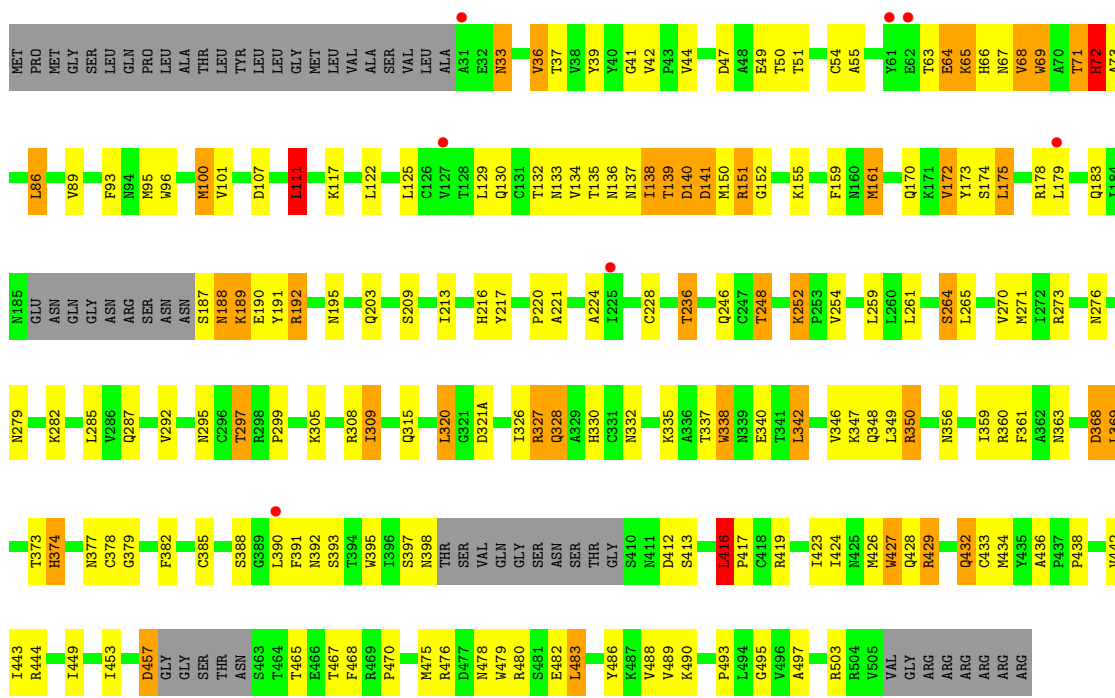


- Molecule 3: 35O22 Fab light chain

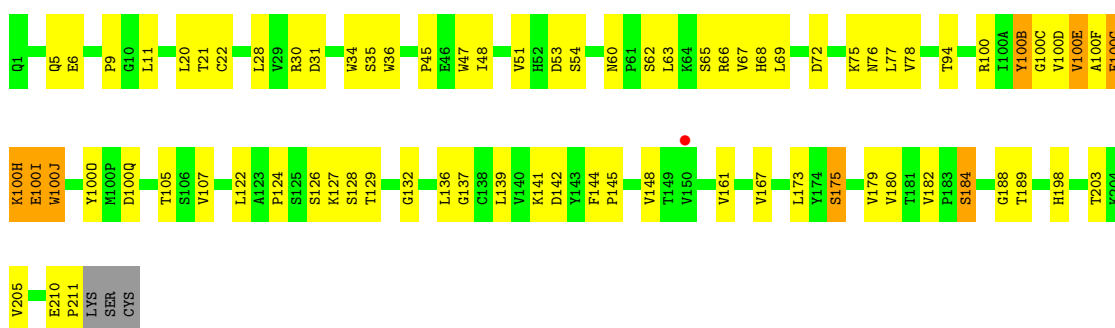




● Molecule 4: HIV-1 BG505 strain Env gp120

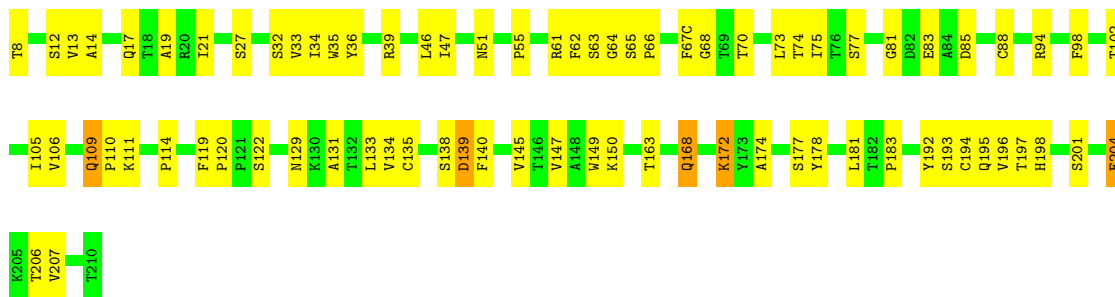


● Molecule 5: PGT122 Fab heavy chain



● Molecule 6: PGT122 Fab light chain





- 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-acetamido-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: 50% 50%



- 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%

MAG1
MAG2

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

Chain N:  50% 50%

MAG1
MAG2

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

Chain O:  100%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

- 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%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 12: 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

Chain P:  20% 80%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.241 , 0.288 0.243 , 0.289	Depositor DCC
R_{free} test set	1269 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.138 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12020	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/987	0.62	1/1338 (0.1%)
2	D	0.29	0/1867	0.55	1/2544 (0.0%)
3	E	0.25	0/1659	0.47	0/2269
4	G	0.35	0/3615	0.62	2/4903 (0.0%)
5	H	0.50	2/1810 (0.1%)	0.53	0/2474
6	L	0.25	0/1619	0.49	0/2217
All	All	0.36	2/11557 (0.0%)	0.56	4/15745 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	100(I)	GLU	CD-OE1	-10.57	1.14	1.25
5	H	100(I)	GLU	CD-OE2	8.65	1.35	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	416	LEU	C-N-CD	-19.82	77.00	120.60
2	D	96	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	600	GLY	N-CA-C	-5.30	99.84	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	111	LEU	CA-CB-CG	5.20	127.26	115.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	969	0	938	42	2
2	D	1820	0	1788	127	0
3	E	1615	0	1542	43	0
4	G	3542	0	3475	140	0
5	H	1762	0	1724	81	0
6	L	1577	0	1518	51	0
7	A	72	0	61	7	0
8	C	50	0	43	2	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	24	0
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	480	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 20.

All (480) 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: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
2:D:109:LEU:HD12	2:D:110:THR:C	1.90	0.89
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
2:D:109:LEU:CD1	2:D:110:THR:C	2.41	0.88
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
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
6:L:131:ALA:HB3	6:L:181:LEU:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:G:138:ILE:HD12	4:G:139:THR:C	2.09	0.73
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
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
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
1:B:652:GLN:HE21	1:B:652:GLN:C	1.96	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:190:GLU:O	4:G:191:TYR:CD1	2.46	0.68
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
4:G:71:THR:O	4:G:72:HIS:C	2.32	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:CYS:HA	4:G:37:THR:HG22	1.77	0.66
3:E:151:ASP:HB2	3:E:188:HIS:HB3	1.78	0.66
2:D:108:LEU:C	2:D:108:LEU:HD23	2.16	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
4:G:427:TRP:O	4:G:428:GLN:C	2.32	0.64
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
4:G:138:ILE:HD12	4:G:138:ILE:C	2.18	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
12:P:8:MAN:HO3	12:P:9:MAN:C1	2.09	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
2:D:36:TRP:C	2:D:37:ILE:HG13	2.20	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
4:G:179:LEU:HD11	4:G:419:ARG:HB3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:109:LEU:HD11	2:D:110:THR:C	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:109:LEU:HD12	2:D:109:LEU:C	2.18	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
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
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
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
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
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
5:H:35:SER:HB3	5:H:47:TRP:HE1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:623:TRP:HH2	4:G:39:TYR:HH	1.56	0.51
3:E:34:SER:O	3:E:88:CYS:HA	2.08	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
5:H:100(B):TYR:CE2	5:H:100(I):GLU:C	2.84	0.51
5:H:100(B):TYR:HE2	5:H:100(I):GLU:C	2.14	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:90:TYR:C	2:D:91:PHE:CD1	2.84	0.51
2:D:117:LYS:HE3	2:D:175:LEU:HD13	1.92	0.50
3:E:162:THR:HG1	3:E:175:SER:H	1.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:100(G):PHE:CD1	5:H:100(H):LYS:C	2.85	0.50
5:H:142:ASP:HA	5:H:173:LEU:HB3	1.93	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
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: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
4:G:189:LYS:C	4:G:190:GLU:HG3	2.33	0.48
4:G:161:MET:O	4:G:170:GLN:HG2	2.13	0.48
6:L:149:TRP:HZ2	6:L:177:SER:HG	1.62	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:19:LYS:C	2:D:20:ILE:HG13	2.34	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
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
6:L:131:ALA:HB3	6:L:181:LEU:C	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:G:429:ARG:C	4:G:429:ARG:HD2	2.36	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:O	5:H:100(J):TRP:CD1	2.70	0.45
6:L:109:GLN:N	6:L:110:PRO:HA	2.31	0.45
1:B:602:LEU:O	1:B:603:ILE:C	2.54	0.45
1:B:655:LYS:HD2	1:B:655:LYS:C	2.36	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
4:G:346:VAL:HG22	4:G:359:ILE:HD13	1.99	0.45
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
2:D:108:LEU:C	2:D:108:LEU:CD2	2.85	0.44
4:G:71:THR:C	4:G:73:ALA:N	2.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:H:100(J):TRP:CD1	5:H:100(J):TRP:C	2.88	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
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
1:B:655:LYS:C	1:B:655:LYS:CD	2.86	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
2:D:189:LEU:HD21	2:D:224:PHE:HE1	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:TRP:CZ3	3:E:208:PRO:HB2	2.54	0.42
4:G:138:ILE:CD1	4:G:139:THR:C	2.86	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
2:D:89:THR:HG22	2:D:90:TYR:N	2.35	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
4:G:361:PHE:CD1	4:G:468:PHE:HB2	2.56	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: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
3:E:144:VAL:HG12	3:E:197:HIS:HB2	2.03	0.41
1:B:649:SER:O	1:B:650:GLN:C	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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 [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	B	118/153 (77%)	109 (92%)	7 (6%)	2 (2%)	9	40
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%)	14	49
5	H	230/235 (98%)	214 (93%)	13 (6%)	3 (1%)	12	45
6	L	206/208 (99%)	190 (92%)	16 (8%)	0	100	100
All	All	1446/1560 (93%)	1353 (94%)	83 (6%)	10 (1%)	22	58

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	104/129 (81%)	83 (80%)	21 (20%)	1	5
2	D	203/206 (98%)	190 (94%)	13 (6%)	17	50
3	E	186/189 (98%)	175 (94%)	11 (6%)	19	52
4	G	403/448 (90%)	333 (83%)	70 (17%)	2	9
5	H	198/205 (97%)	188 (95%)	10 (5%)	24	57
6	L	177/177 (100%)	165 (93%)	12 (7%)	16	48
All	All	1271/1354 (94%)	1134 (89%)	137 (11%)	6	28

All (137) 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
1	B	585	ARG
1	B	602	LEU
1	B	606	THR
1	B	616	ASN
1	B	619	LEU
1	B	638	TYR
1	B	647	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	27	TYR
2	D	38	ARG
2	D	82	ILE
2	D	82(C)	LEU
2	D	90	TYR
2	D	102	LEU
2	D	107	THR

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Mol	Chain	Res	Type
2	D	108	LEU
2	D	109	LEU
2	D	170	LEU
2	D	196	CYS
3	E	27(C)	CYS
3	E	51	ASP
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	155	VAL
3	E	188	HIS
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	72	HIS
4	G	86	LEU
4	G	100	MET
4	G	111	LEU
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

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Mol	Chain	Res	Type
4	G	175	LEU
4	G	188	ASN
4	G	189	LYS
4	G	192	ARG
4	G	213	ILE
4	G	236	THR
4	G	246	GLN
4	G	248	THR
4	G	252	LYS
4	G	264	SER
4	G	265	LEU
4	G	271	MET
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	328	GLN
4	G	338	TRP
4	G	340	GLU
4	G	342	LEU
4	G	350	ARG
4	G	368	ASP
4	G	369	LEU
4	G	374	HIS
4	G	377	ASN
4	G	378	CYS
4	G	390	LEU
4	G	392	ASN
4	G	393	SER
4	G	416	LEU
4	G	429	ARG
4	G	432	GLN
4	G	434	MET
4	G	442	VAL
4	G	457	ASP
4	G	465	THR
4	G	475	MET
4	G	483	LEU

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Mol	Chain	Res	Type
4	G	488	VAL
5	H	21	THR
5	H	62	SER
5	H	65	SER
5	H	100(B)	TYR
5	H	100(J)	TRP
5	H	100(O)	TYR
5	H	105	THR
5	H	175	SER
5	H	182	VAL
5	H	184	SER
6	L	8	THR
6	L	67(C)	PHE
6	L	70	THR
6	L	85	ASP
6	L	109	GLN
6	L	122	SER
6	L	138	SER
6	L	139	ASP
6	L	168	GLN
6	L	172	LYS
6	L	201	SER
6	L	204	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	590	GLN
1	B	652	GLN
2	D	6	GLN
4	G	130	GLN
4	G	188	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

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	0.39	0	17,19,21	0.44	0
7	NAG	A	2	7	14,14,15	0.45	0	17,19,21	1.21	1 (5%)
7	BMA	A	3	7	11,11,12	1.14	1 (9%)	15,15,17	0.91	1 (6%)
7	MAN	A	4	7	11,11,12	1.38	1 (9%)	15,15,17	1.64	3 (20%)
7	MAN	A	5	7	11,11,12	1.17	2 (18%)	15,15,17	1.72	3 (20%)
7	MAN	A	6	7	11,11,12	0.78	1 (9%)	15,15,17	1.22	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.39	0	17,19,21	0.43	0
8	NAG	C	2	8	14,14,15	0.29	0	17,19,21	0.40	0
8	BMA	C	3	8	11,11,12	0.57	0	15,15,17	0.76	0
8	MAN	C	4	8	11,11,12	0.94	1 (9%)	15,15,17	1.31	2 (13%)
9	NAG	F	1	4,9	14,14,15	0.31	0	17,19,21	0.42	0
9	NAG	F	2	9	14,14,15	0.19	0	17,19,21	0.39	0
9	BMA	F	3	9	11,11,12	0.57	0	15,15,17	0.69	0
9	MAN	F	4	9	11,11,12	0.75	1 (9%)	15,15,17	1.19	2 (13%)
9	MAN	F	5	9	11,11,12	0.78	0	15,15,17	0.89	1 (6%)
10	NAG	I	1	10,4	14,14,15	1.73	3 (21%)	17,19,21	1.15	2 (11%)
10	NAG	I	2	10	14,14,15	0.58	0	17,19,21	1.29	2 (11%)
10	NAG	J	1	10,4	14,14,15	0.20	0	17,19,21	0.60	1 (5%)
10	NAG	J	2	10	14,14,15	0.29	0	17,19,21	0.49	0
10	NAG	K	1	10,4	14,14,15	0.21	0	17,19,21	0.68	1 (5%)
10	NAG	K	2	10	14,14,15	0.23	0	17,19,21	0.40	0
11	NAG	M	1	11,4	14,14,15	0.32	0	17,19,21	0.59	0
11	NAG	M	2	11	14,14,15	0.49	0	17,19,21	0.68	0
11	BMA	M	3	11	11,11,12	1.40	3 (27%)	15,15,17	1.37	3 (20%)
11	MAN	M	4	11	11,11,12	1.36	3 (27%)	15,15,17	1.92	3 (20%)
11	MAN	M	5	11	11,11,12	0.78	0	15,15,17	1.15	2 (13%)
11	MAN	M	6	11	11,11,12	1.17	2 (18%)	15,15,17	1.81	5 (33%)
10	NAG	N	1	10,4	14,14,15	0.42	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	N	2	10	14,14,15	0.28	0	17,19,21	0.50	0
10	NAG	O	1	10,4	14,14,15	0.21	0	17,19,21	0.47	0
10	NAG	O	2	10	14,14,15	0.23	0	17,19,21	0.43	0
12	NAG	P	1	4,12	14,14,15	0.97	0	17,19,21	1.72	3 (17%)
12	MAN	P	10	12	11,11,12	0.70	0	15,15,17	1.03	2 (13%)
12	NAG	P	2	12	14,14,15	0.51	0	17,19,21	1.76	5 (29%)
12	BMA	P	3	12	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
12	MAN	P	4	12	11,11,12	0.63	0	15,15,17	1.19	1 (6%)
12	MAN	P	5	12	11,11,12	0.97	0	15,15,17	2.42	4 (26%)
12	MAN	P	6	12	11,11,12	0.79	0	15,15,17	2.00	5 (33%)
12	MAN	P	7	12	11,11,12	0.92	0	15,15,17	2.15	4 (26%)
12	MAN	P	8	12	11,11,12	0.75	0	15,15,17	1.31	2 (13%)
12	MAN	P	9	12	11,11,12	0.45	0	15,15,17	2.05	2 (13%)
10	NAG	Q	1	10,4	14,14,15	0.20	0	17,19,21	0.38	0
10	NAG	Q	2	10	14,14,15	0.22	0	17,19,21	0.44	0
10	NAG	R	1	10,4	14,14,15	0.24	0	17,19,21	0.76	1 (5%)
10	NAG	R	2	10	14,14,15	0.29	0	17,19,21	0.47	0
10	NAG	S	1	10,4	14,14,15	0.99	1 (7%)	17,19,21	0.76	0
10	NAG	S	2	10	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
10	NAG	T	1	10,4	14,14,15	0.23	0	17,19,21	0.54	0
10	NAG	T	2	10	14,14,15	0.23	0	17,19,21	0.39	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	-	3/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	F	2	9	-	0/6/23/26	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	-	3/6/23/26	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	-	4/6/23/26	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	4,12	-	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	-	3/6/23/26	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
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	-	3/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	T	2	10	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	1	NAG	O5-C1	-5.27	1.35	1.43
7	A	4	MAN	C1-C2	3.96	1.61	1.52
10	S	1	NAG	O5-C1	-3.59	1.38	1.43
11	M	3	BMA	C4-C5	2.98	1.59	1.53
11	M	4	MAN	C4-C5	2.95	1.59	1.53
10	I	1	NAG	C1-C2	2.82	1.56	1.52
8	C	4	MAN	C1-C2	2.60	1.58	1.52
11	M	4	MAN	O5-C5	2.37	1.48	1.43
11	M	6	MAN	C1-C2	2.36	1.57	1.52
7	A	3	BMA	O5-C1	-2.29	1.40	1.43
11	M	6	MAN	O5-C5	2.28	1.48	1.43
11	M	3	BMA	O5-C5	2.22	1.47	1.43
7	A	6	MAN	C1-C2	2.20	1.57	1.52
10	I	1	NAG	C3-C2	2.19	1.57	1.52
11	M	3	BMA	C4-C3	2.15	1.57	1.52
9	F	4	MAN	C1-C2	2.12	1.57	1.52
7	A	5	MAN	O5-C5	2.09	1.47	1.43
7	A	5	MAN	C1-C2	2.07	1.56	1.52
11	M	4	MAN	C4-C3	2.06	1.57	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	9	MAN	C1-O5-C5	6.30	120.73	112.19
12	P	5	MAN	O2-C2-C1	-5.47	97.96	109.15
12	P	7	MAN	O5-C1-C2	-5.46	102.34	110.77
12	P	5	MAN	O5-C1-C2	-5.45	102.36	110.77
11	M	4	MAN	C1-O5-C5	5.33	119.41	112.19
7	A	5	MAN	C1-O5-C5	5.03	119.00	112.19
12	P	6	MAN	O2-C2-C3	-4.58	100.97	110.14
11	M	6	MAN	C1-O5-C5	4.42	118.18	112.19
10	I	2	NAG	C2-N2-C7	4.34	129.08	122.90
12	P	7	MAN	C1-C2-C3	-4.20	104.50	109.67
12	P	2	NAG	O5-C1-C2	-4.15	104.74	111.29
7	A	2	NAG	C2-N2-C7	4.12	128.77	122.90
7	A	4	MAN	C1-O5-C5	4.05	117.67	112.19
12	P	3	BMA	O5-C5-C6	3.98	113.44	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	1	NAG	C1-O5-C5	3.69	117.19	112.19
12	P	1	NAG	C3-C4-C5	-3.68	103.67	110.24
12	P	9	MAN	C2-C3-C4	3.55	117.03	110.89
7	A	4	MAN	C1-C2-C3	3.45	113.90	109.67
10	I	1	NAG	C4-C3-C2	3.37	115.95	111.02
12	P	4	MAN	C1-O5-C5	3.27	116.62	112.19
11	M	4	MAN	C3-C4-C5	3.25	116.05	110.24
7	A	6	MAN	C1-O5-C5	3.25	116.60	112.19
8	C	4	MAN	C1-O5-C5	3.18	116.51	112.19
12	P	6	MAN	O3-C3-C4	-3.14	103.08	110.35
11	M	5	MAN	C1-O5-C5	3.07	116.36	112.19
12	P	3	BMA	C1-C2-C3	3.03	113.39	109.67
9	F	4	MAN	C1-O5-C5	2.98	116.23	112.19
12	P	8	MAN	O5-C1-C2	-2.93	106.25	110.77
12	P	6	MAN	O5-C5-C4	-2.85	103.90	110.83
12	P	7	MAN	C1-O5-C5	2.81	116.00	112.19
12	P	8	MAN	O2-C2-C3	-2.81	104.52	110.14
12	P	2	NAG	O4-C4-C3	-2.70	104.10	110.35
12	P	6	MAN	O3-C3-C2	-2.69	104.84	109.99
12	P	2	NAG	O3-C3-C4	-2.69	104.14	110.35
11	M	6	MAN	O5-C1-C2	2.65	114.86	110.77
11	M	3	BMA	O5-C1-C2	-2.60	106.76	110.77
12	P	7	MAN	O4-C4-C3	-2.56	104.42	110.35
11	M	3	BMA	O5-C5-C6	2.43	111.02	107.20
12	P	5	MAN	O3-C3-C4	-2.43	104.74	110.35
12	P	2	NAG	C3-C4-C5	-2.42	105.92	110.24
12	P	6	MAN	O5-C1-C2	-2.38	107.09	110.77
11	M	6	MAN	O2-C2-C3	-2.36	105.41	110.14
12	P	2	NAG	O3-C3-C2	2.35	114.32	109.47
10	R	1	NAG	C1-O5-C5	2.33	115.35	112.19
12	P	3	BMA	O2-C2-C1	-2.29	104.46	109.15
12	P	10	MAN	C1-O5-C5	2.28	115.28	112.19
10	N	1	NAG	C1-O5-C5	2.26	115.26	112.19
7	A	4	MAN	O2-C2-C3	-2.25	105.62	110.14
11	M	3	BMA	C3-C4-C5	2.24	114.24	110.24
11	M	6	MAN	C1-C2-C3	2.24	112.42	109.67
8	C	4	MAN	O2-C2-C3	-2.23	105.67	110.14
12	P	1	NAG	C1-C2-N2	-2.23	106.68	110.49
11	M	4	MAN	O2-C2-C3	-2.22	105.70	110.14
12	P	10	MAN	O2-C2-C3	-2.19	105.76	110.14
10	I	1	NAG	O5-C5-C4	-2.18	105.51	110.83
10	S	2	NAG	C1-O5-C5	2.17	115.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	5	MAN	C6-C5-C4	-2.17	107.92	113.00
7	A	6	MAN	O2-C2-C3	-2.17	105.80	110.14
9	F	5	MAN	O2-C2-C3	-2.13	105.88	110.14
9	F	4	MAN	O2-C2-C3	-2.12	105.89	110.14
7	A	5	MAN	C1-C2-C3	2.11	112.26	109.67
12	P	3	BMA	O5-C5-C4	-2.11	105.70	110.83
11	M	5	MAN	O2-C2-C3	-2.11	105.91	110.14
11	M	6	MAN	C3-C4-C5	-2.02	106.64	110.24
10	J	1	NAG	C1-O5-C5	2.02	114.92	112.19
10	I	2	NAG	C1-C2-N2	2.01	113.93	110.49
7	A	5	MAN	O2-C2-C3	-2.01	106.11	110.14
10	K	1	NAG	C1-O5-C5	2.01	114.91	112.19
7	A	3	BMA	O2-C2-C3	-2.00	106.12	110.14

There are no chirality outliers.

All (67) 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
7	A	3	BMA	C4-C5-C6-O6
11	M	2	NAG	O5-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6
10	Q	2	NAG	O5-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
12	P	7	MAN	O5-C5-C6-O6
12	P	2	NAG	O5-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
12	P	6	MAN	O5-C5-C6-O6
10	Q	2	NAG	C4-C5-C6-O6
11	M	3	BMA	O5-C5-C6-O6
11	M	2	NAG	C4-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
11	M	1	NAG	O5-C5-C6-O6
12	P	5	MAN	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
11	M	2	NAG	C1-C2-N2-C7
10	O	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	P	2	NAG	C4-C5-C6-O6
10	O	1	NAG	C4-C5-C6-O6
11	M	1	NAG	C4-C5-C6-O6
10	S	2	NAG	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
10	R	1	NAG	C4-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
12	P	7	MAN	C4-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
12	P	5	MAN	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
10	N	1	NAG	O5-C5-C6-O6
7	A	4	MAN	C4-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
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
7	A	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	I	2	NAG	C3-C2-N2-C7

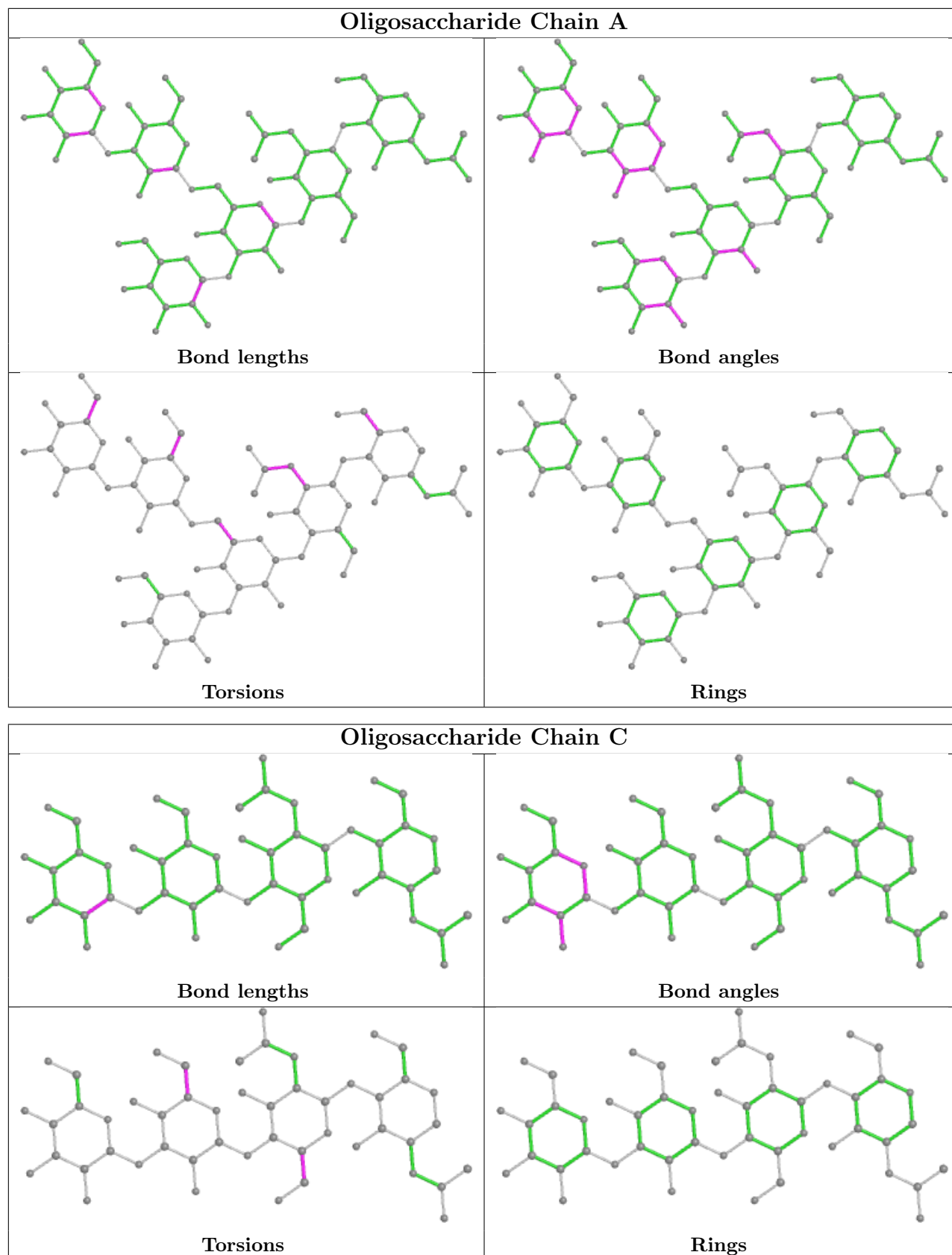
All (1) ring outliers are listed below:

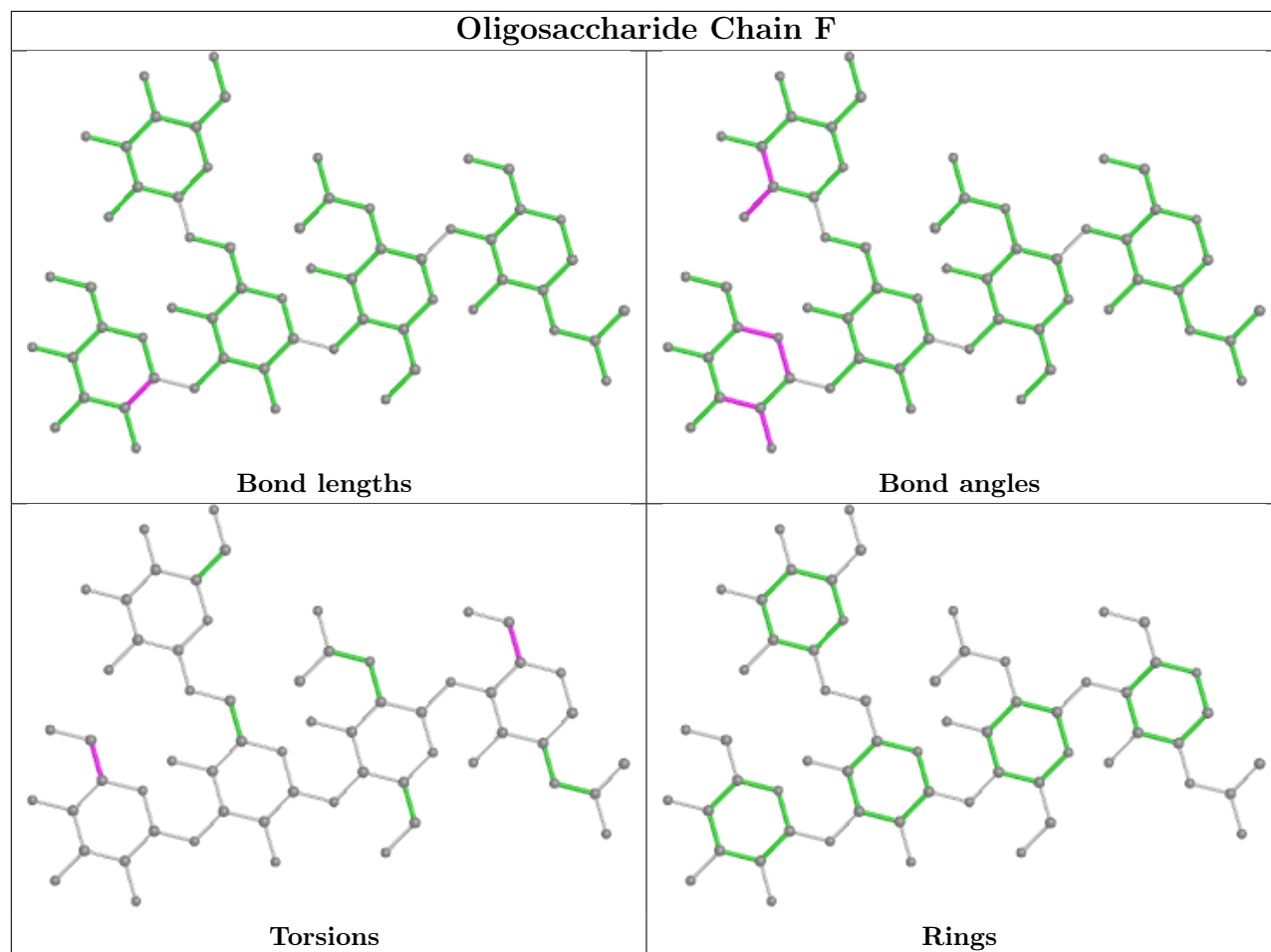
Mol	Chain	Res	Type	Atoms
11	M	5	MAN	C1-C2-C3-C4-C5-O5

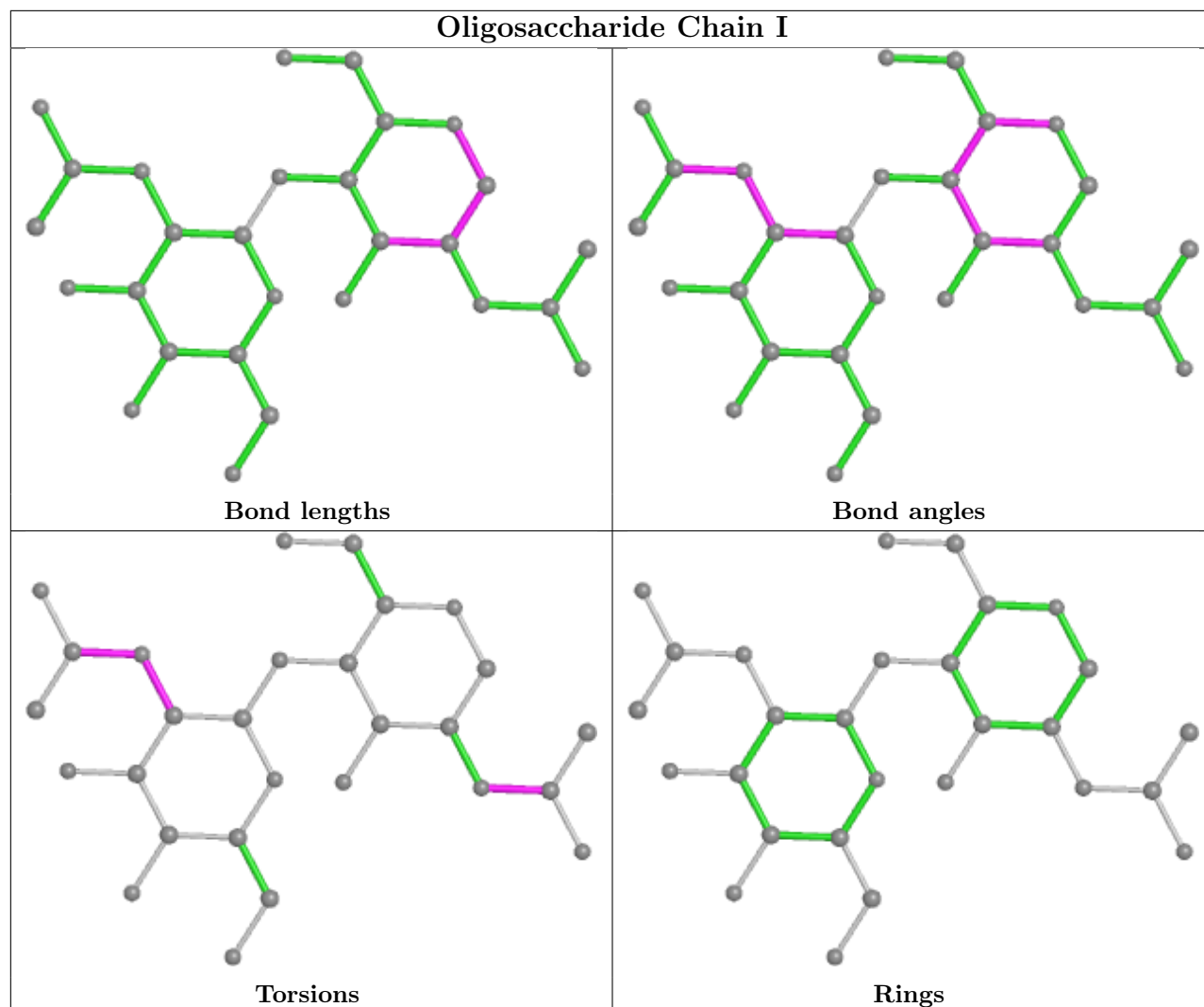
24 monomers are involved in 44 short contacts:

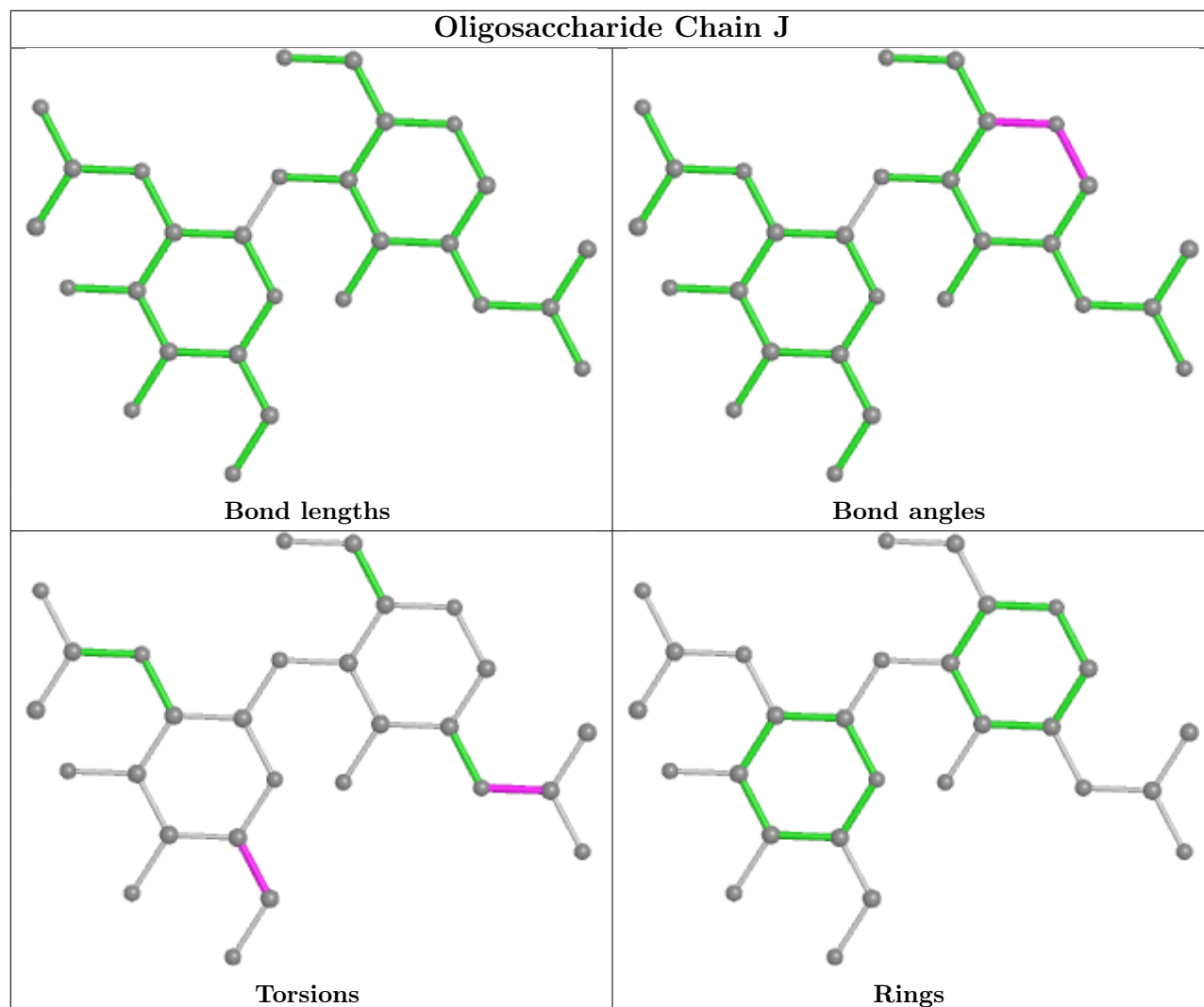
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	2	NAG	1	0
11	M	1	NAG	1	0
11	M	2	NAG	3	0
12	P	5	MAN	6	0
12	P	2	NAG	7	0
12	P	3	BMA	1	0
12	P	7	MAN	1	0
8	C	1	NAG	2	0
10	I	1	NAG	1	0
12	P	9	MAN	2	0
7	A	3	BMA	1	0
9	F	1	NAG	1	0
7	A	1	NAG	3	0
10	K	1	NAG	1	0
10	I	2	NAG	1	0
10	K	2	NAG	1	0
12	P	8	MAN	3	0
10	S	2	NAG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

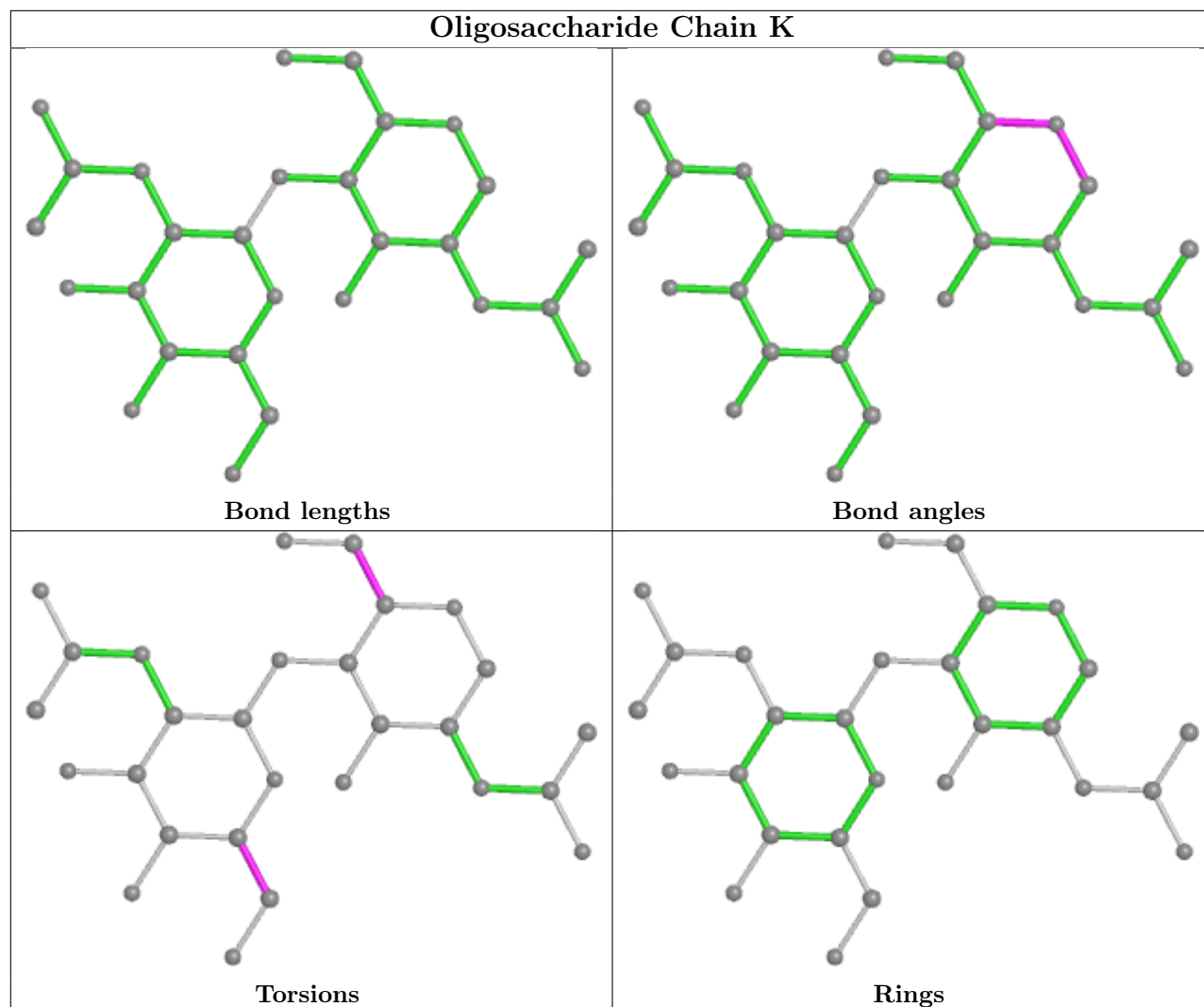
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

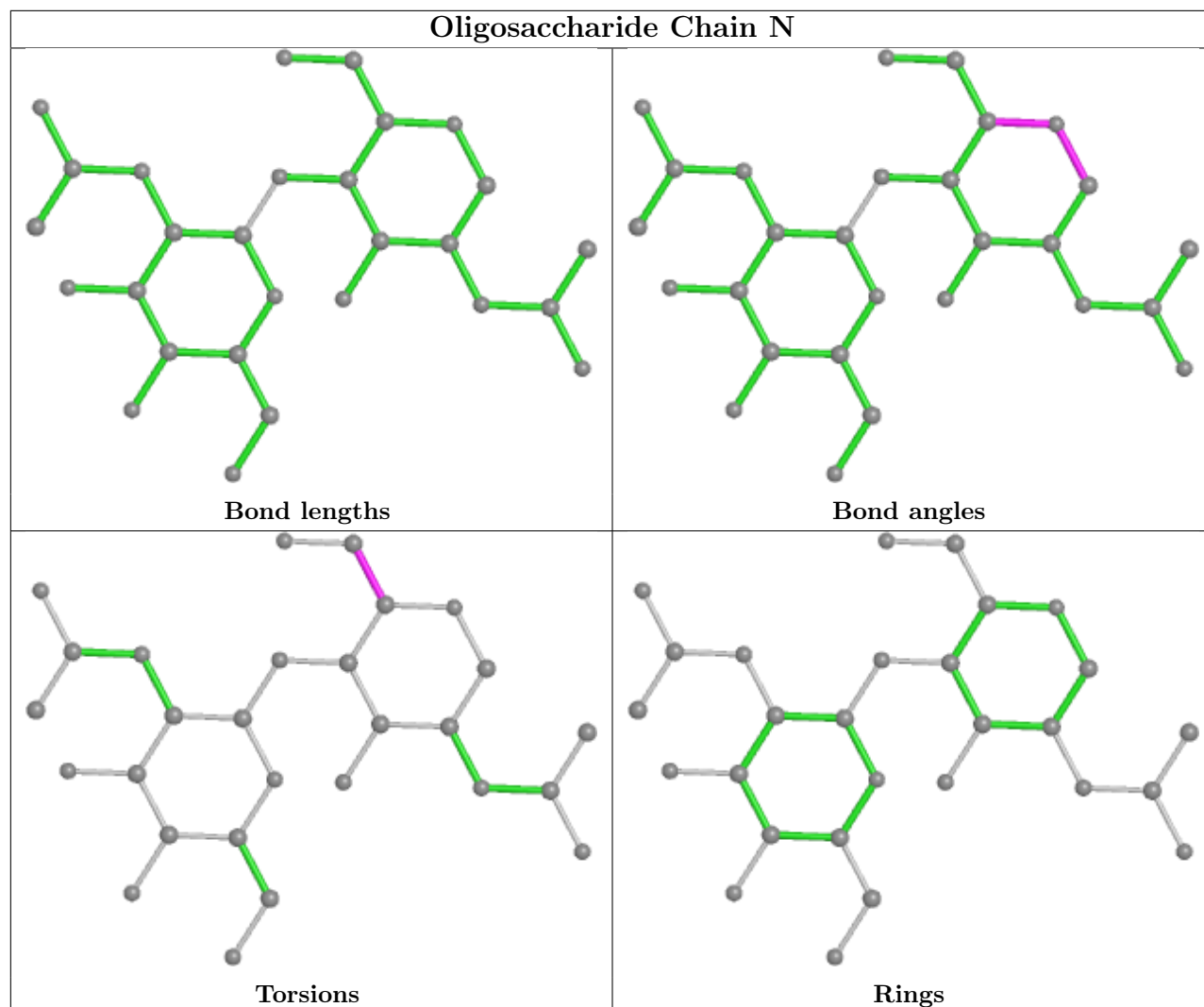


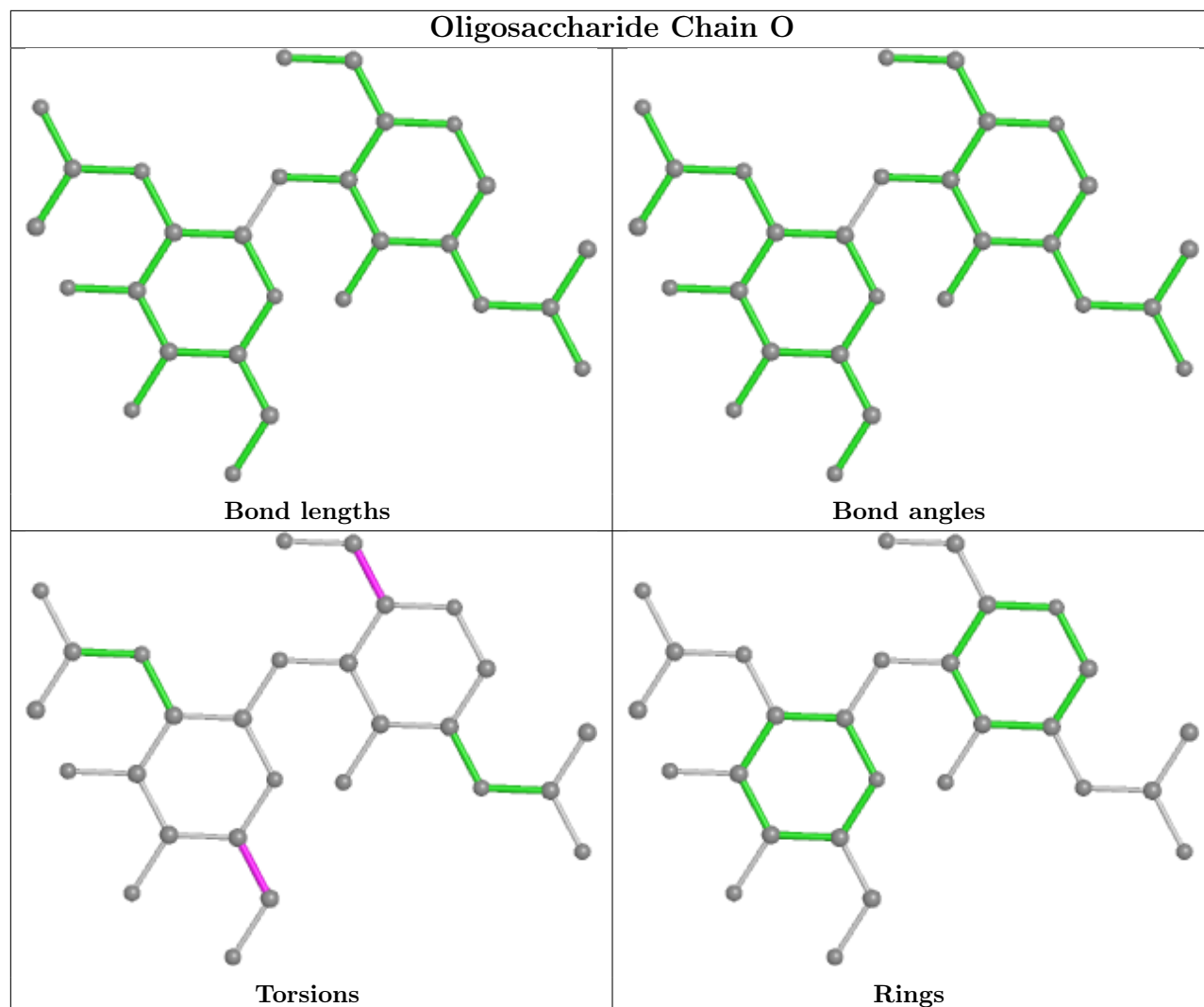


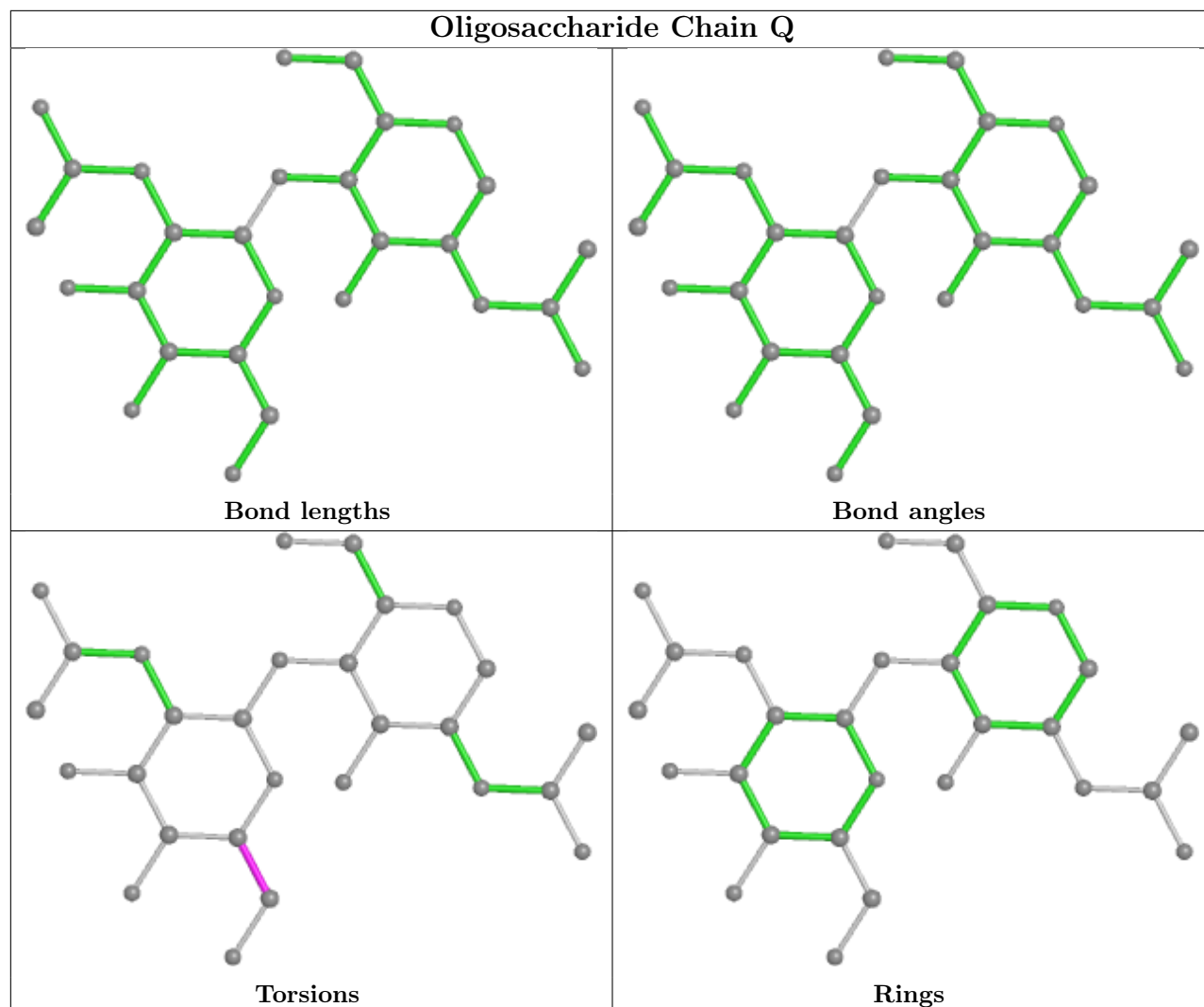


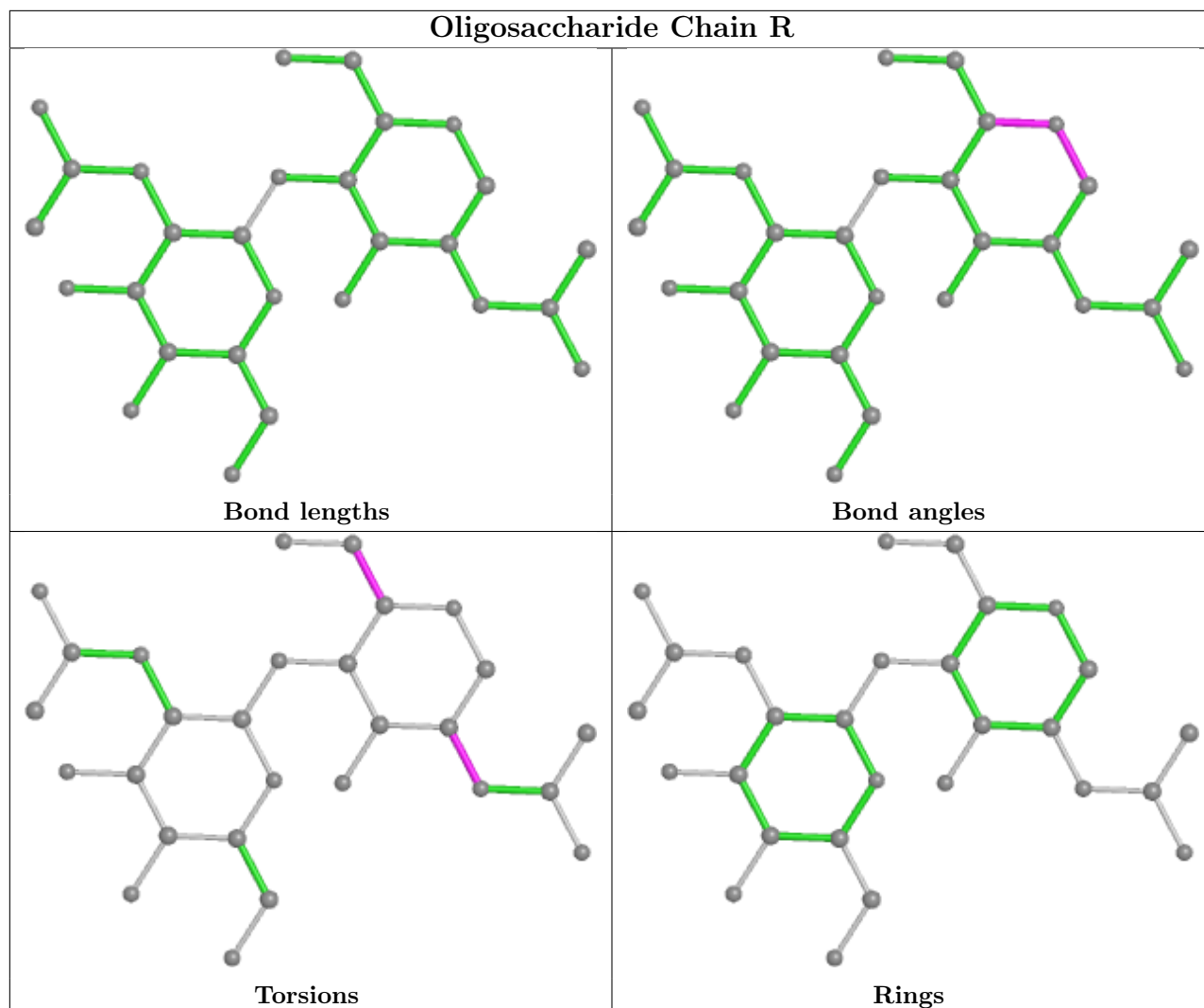


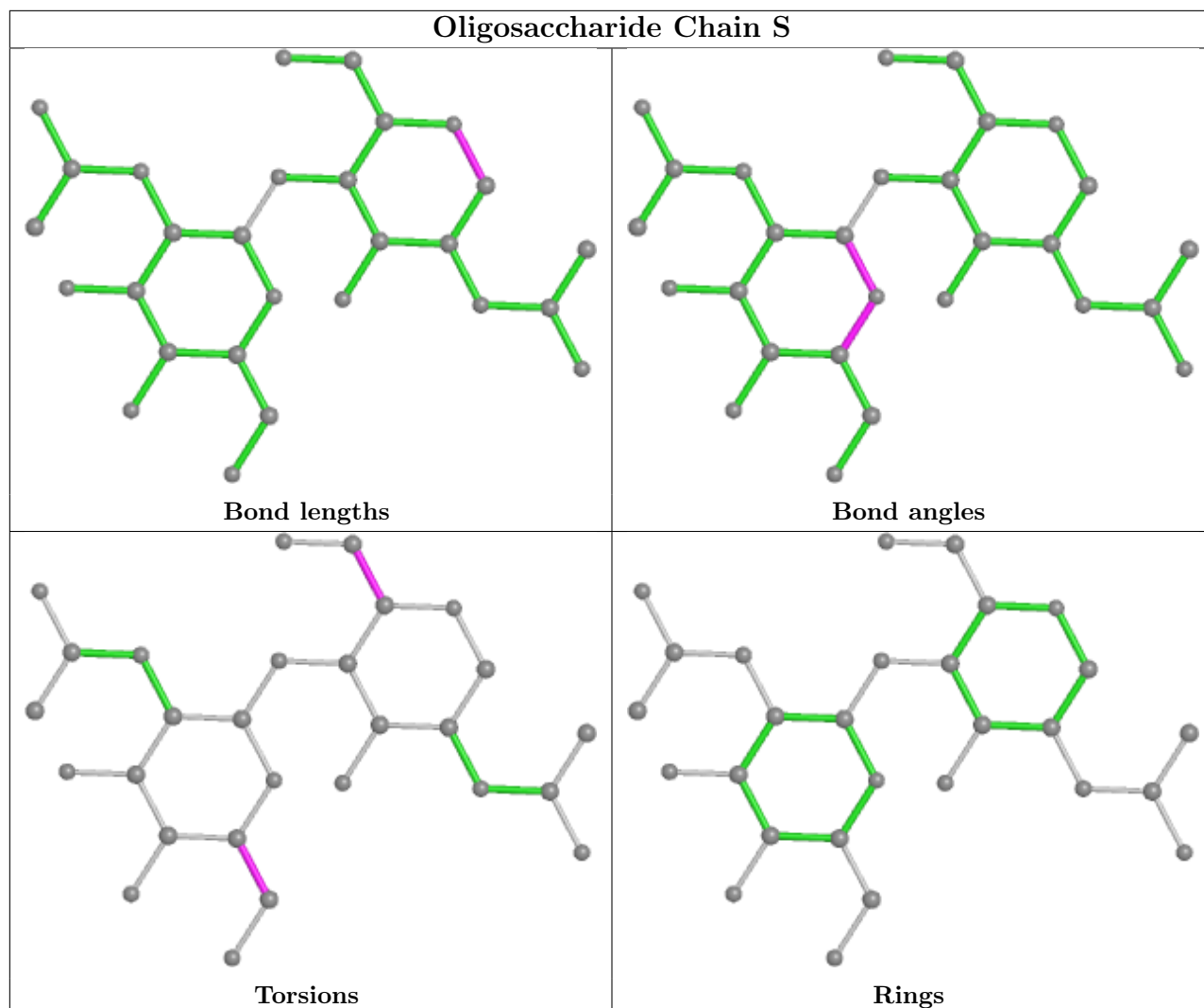


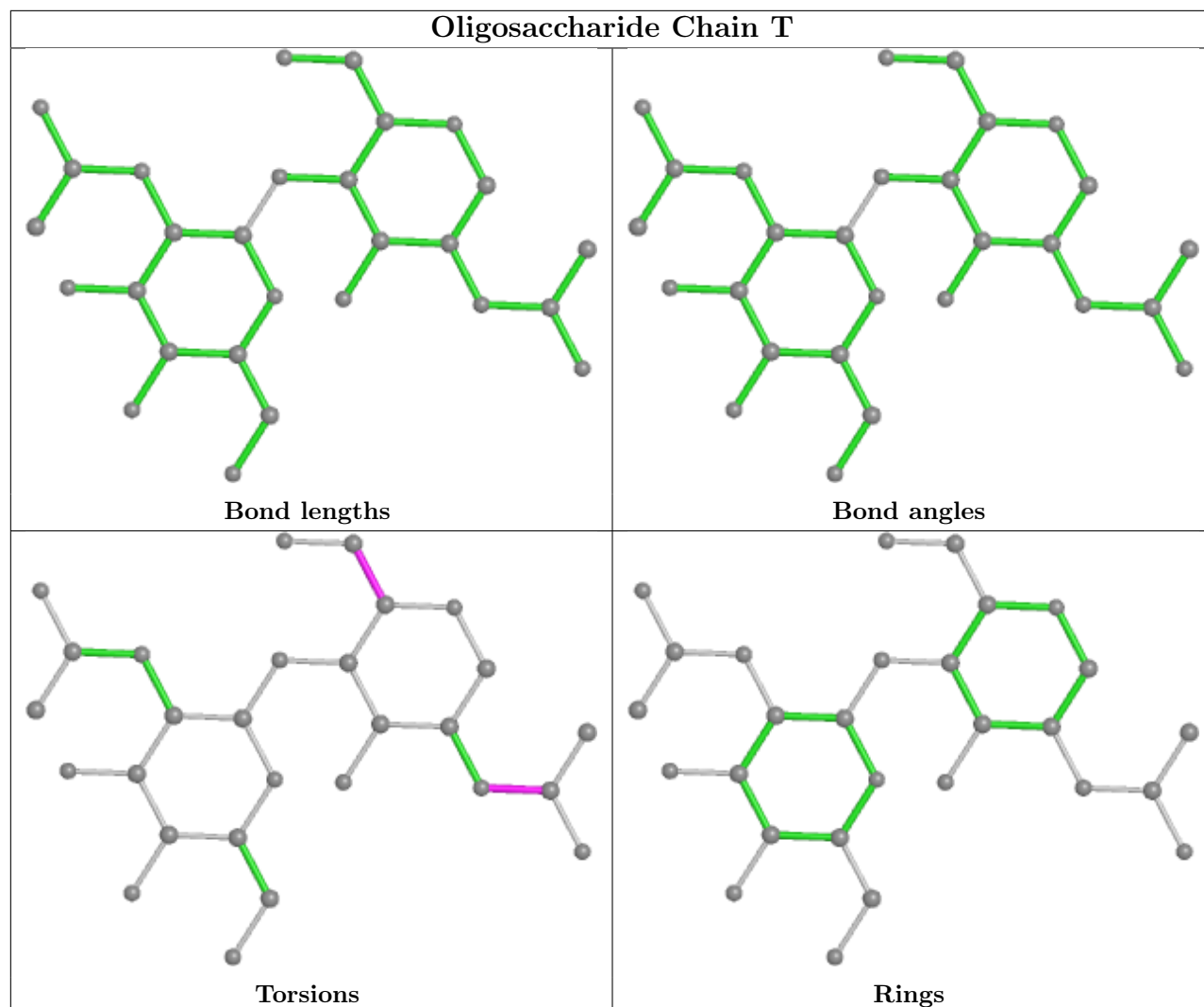


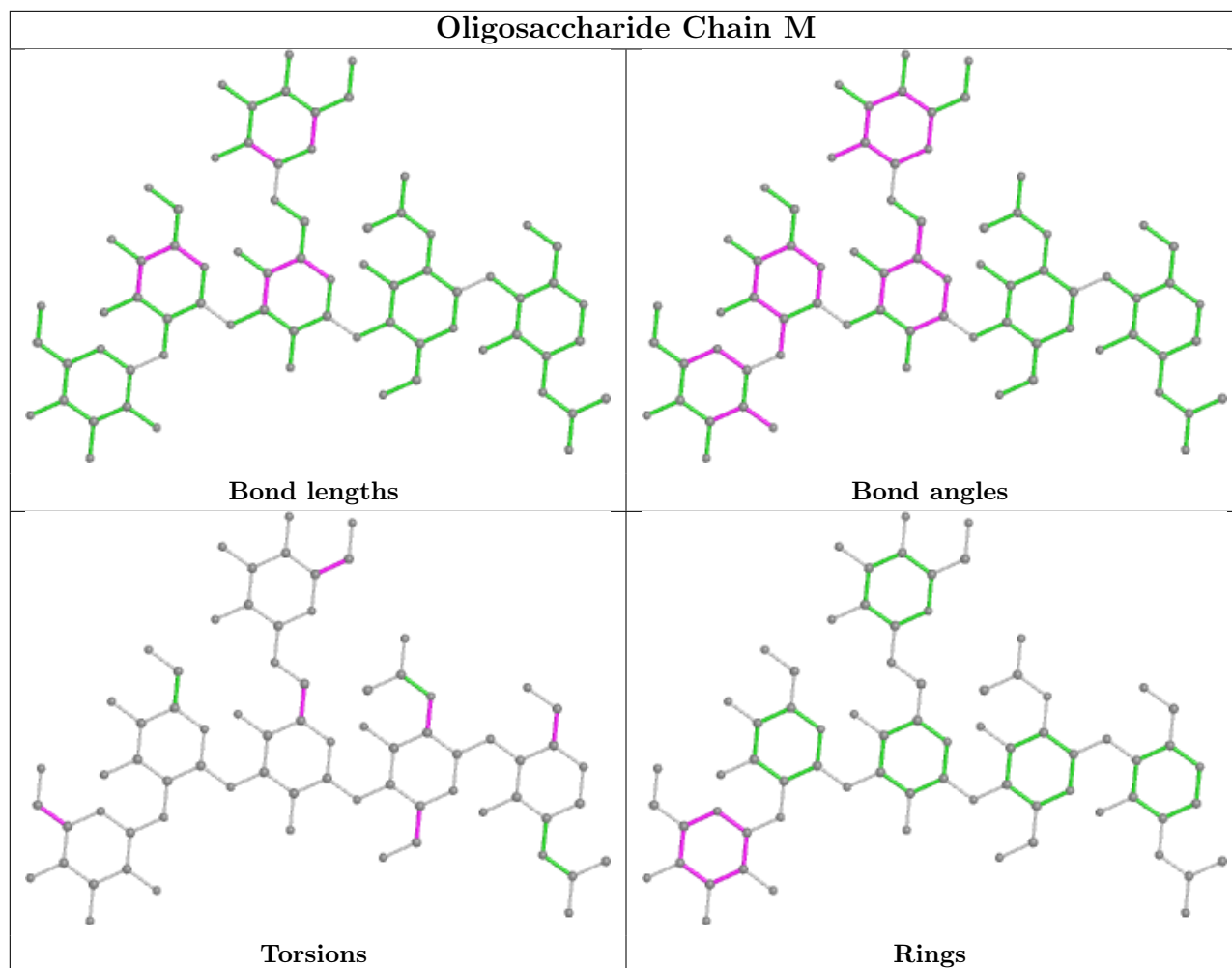


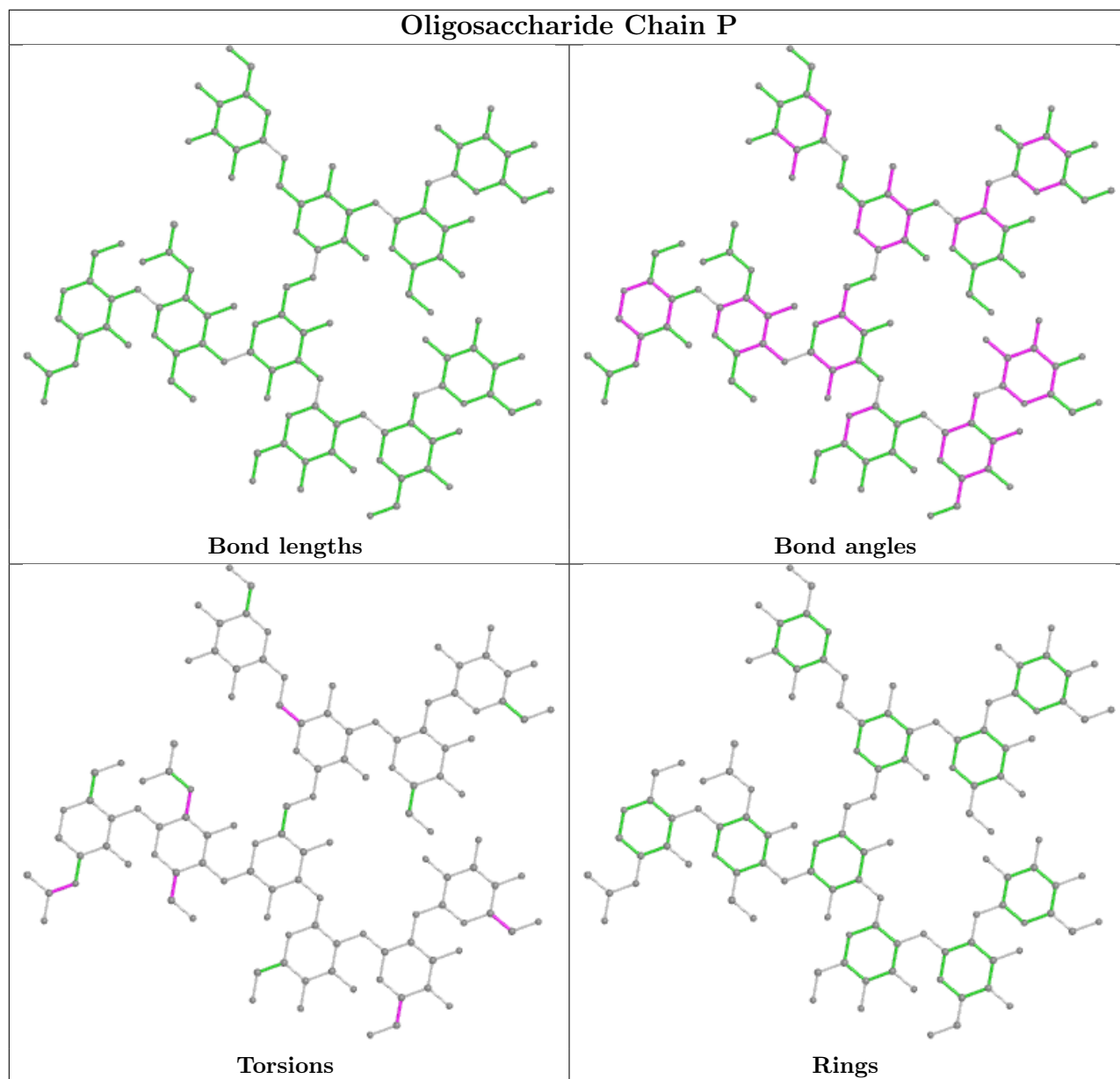












5.6 Ligand geometry [i](#)

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	B	702	1	14,14,15	0.24	0	17,19,21	0.50	0
13	NAG	G	607	4	14,14,15	0.53	0	17,19,21	0.54	0
13	NAG	B	701	1	14,14,15	0.47	0	17,19,21	0.44	0
13	NAG	G	629	4	14,14,15	0.42	0	17,19,21	1.31	1 (5%)
13	NAG	G	653	4	14,14,15	0.24	0	17,19,21	0.42	0
13	NAG	B	703	1	14,14,15	0.26	0	17,19,21	0.47	0
13	NAG	G	644	4	14,14,15	0.36	0	17,19,21	0.55	0
13	NAG	H	301	5	14,14,15	0.17	0	17,19,21	0.63	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	B	702	1	-	3/6/23/26	0/1/1/1
13	NAG	G	607	4	-	3/6/23/26	0/1/1/1
13	NAG	B	701	1	-	3/6/23/26	0/1/1/1
13	NAG	G	629	4	-	5/6/23/26	0/1/1/1
13	NAG	G	653	4	-	2/6/23/26	0/1/1/1
13	NAG	B	703	1	-	2/6/23/26	0/1/1/1
13	NAG	G	644	4	-	4/6/23/26	0/1/1/1
13	NAG	H	301	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	629	NAG	C2-N2-C7	4.27	128.99	122.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	629	NAG	O5-C5-C6-O6
13	G	629	NAG	C4-C5-C6-O6
13	B	701	NAG	O5-C5-C6-O6
13	G	607	NAG	C8-C7-N2-C2
13	G	607	NAG	O7-C7-N2-C2

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

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	B	122/153 (79%)	0.13	1 (0%) 86 84	21, 77, 141, 229	0
2	D	242/243 (99%)	1.03	48 (19%) 1 1	82, 179, 336, 392	0
3	E	213/216 (98%)	0.62	33 (15%) 2 3	89, 186, 303, 337	0
4	G	449/505 (88%)	0.10	7 (1%) 72 71	28, 80, 170, 246	0
5	H	232/235 (98%)	-0.08	1 (0%) 92 91	48, 104, 179, 228	0
6	L	208/208 (100%)	-0.10	0 100 100	35, 78, 142, 198	0
All	All	1466/1560 (93%)	0.28	90 (6%) 21 23	21, 105, 266, 392	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	CYS	19.6
2	D	215	SER	17.7
2	D	214	LYS	16.5
3	E	115	VAL	12.0
2	D	213	PRO	11.9
2	D	212	GLU	11.8
2	D	188	SER	10.4
2	D	187	SER	9.8
3	E	114	SER	8.6
2	D	185	PRO	8.6
3	E	113	PRO	8.1
2	D	211	VAL	8.0
2	D	217	ASP	7.8
2	D	190	GLY	7.1
2	D	138	LEU	6.5
3	E	156	LYS	6.5
2	D	189	LEU	6.5
2	D	124	LEU	6.4
2	D	180	SER	6.4

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Mol	Chain	Res	Type	RSRZ
2	D	126	PRO	6.3
3	E	119	PRO	6.0
3	E	157	ALA	5.8
2	D	184	VAL	5.8
2	D	165	THR	5.7
3	E	154	PRO	5.7
4	G	31	ALA	4.9
2	D	224	PHE	4.7
3	E	128	ASN	4.6
2	D	160	THR	4.6
3	E	191	TYR	4.4
2	D	125	ALA	4.3
2	D	44	GLY	4.1
2	D	222	VAL	4.1
3	E	152	SER	4.0
3	E	153	SER	3.8
2	D	136	ALA	3.8
3	E	135	LEU	3.8
3	E	155	VAL	3.8
2	D	69	MET	3.8
3	E	118	PHE	3.7
3	E	207	ALA	3.7
3	E	205	THR	3.7
2	D	191	THR	3.7
2	D	135	THR	3.6
2	D	133	GLY	3.5
4	G	179	LEU	3.5
4	G	62	GLU	3.5
4	G	61	TYR	3.4
2	D	186	SER	3.4
2	D	209	LYS	3.3
2	D	142	VAL	3.3
2	D	82	ILE	3.2
2	D	139	GLY	3.2
2	D	137	ALA	3.1
3	E	98	PHE	3.1
3	E	198	GLU	3.1
3	E	133	VAL	3.1
3	E	142	GLY	3.1
3	E	206	VAL	3.0
2	D	41	ALA	2.9
2	D	39	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	192	SER	2.8
3	E	199	GLY	2.8
3	E	132	LEU	2.8
2	D	219	GLY	2.7
3	E	136	ILE	2.7
3	E	181	THR	2.7
3	E	112	ASN	2.7
2	D	221	GLU	2.7
2	D	122	PHE	2.6
3	E	137	SER	2.6
3	E	179	SER	2.5
2	D	123	PRO	2.4
3	E	78	LEU	2.4
2	D	40	THR	2.4
2	D	181	VAL	2.4
2	D	71	THR	2.4
3	E	180	LEU	2.4
2	D	134	GLY	2.3
2	D	157	GLY	2.3
3	E	144	VAL	2.2
4	G	127	VAL	2.2
2	D	141	LEU	2.2
4	G	225	ILE	2.2
3	E	23	CYS	2.2
1	B	658	GLN	2.1
2	D	38	ARG	2.1
5	H	150	VAL	2.1
4	G	390	LEU	2.0
2	D	107	THR	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.

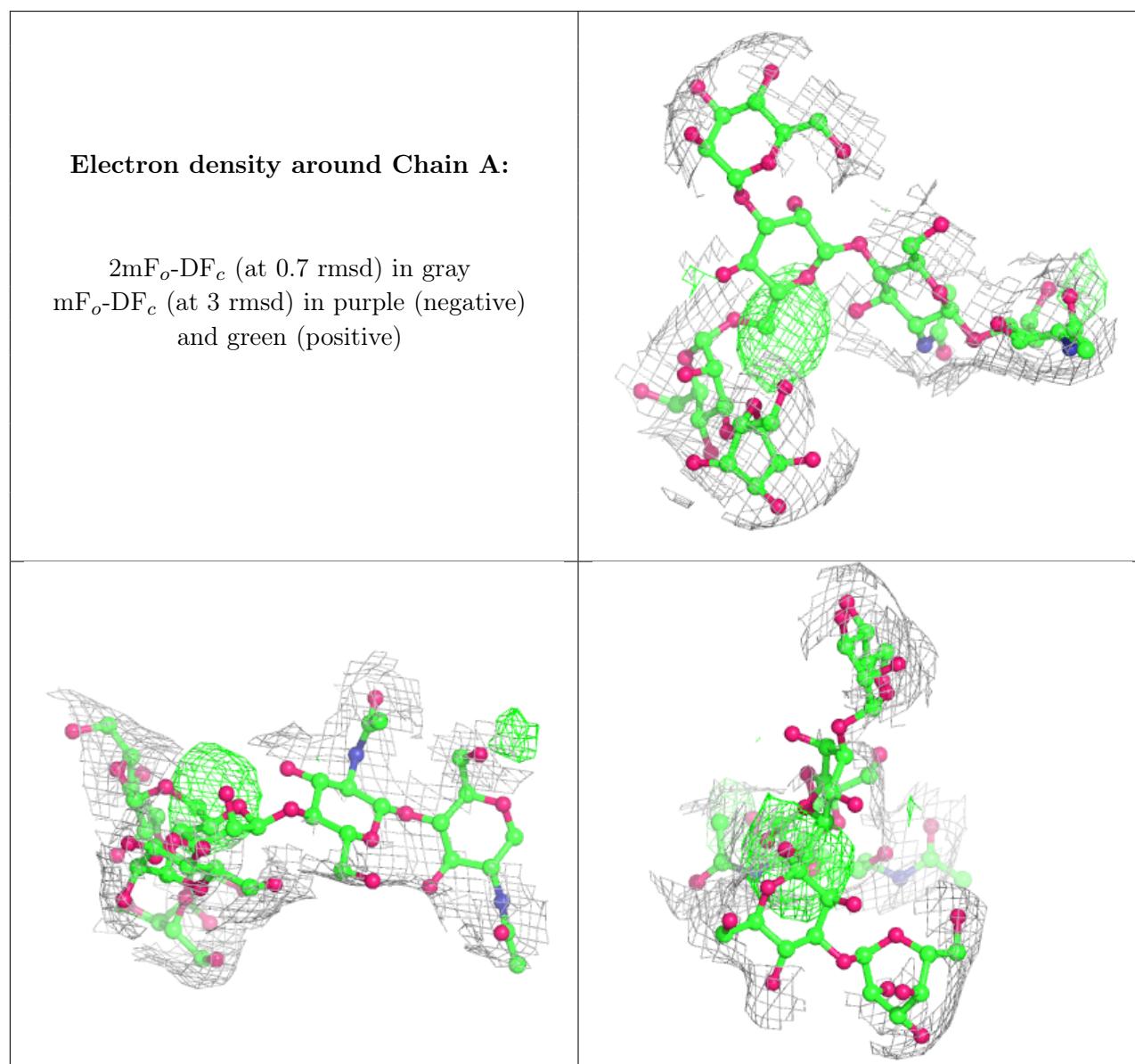
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NAG	J	2	14/15	0.69	0.38	178,208,220,224	0
10	NAG	J	1	14/15	0.79	0.17	133,159,187,193	0
10	NAG	K	2	14/15	0.82	0.57	175,193,201,202	0
10	NAG	O	2	14/15	0.82	0.23	137,151,165,171	0
12	MAN	P	7	11/12	0.82	0.17	141,147,162,166	0
12	MAN	P	10	11/12	0.82	0.17	154,157,159,160	0
9	MAN	F	5	11/12	0.83	0.14	125,144,153,154	0
10	NAG	I	2	14/15	0.84	0.21	113,138,175,178	0
9	BMA	F	3	11/12	0.85	0.12	121,143,150,157	0
10	NAG	Q	2	14/15	0.85	0.23	154,160,187,192	0
10	NAG	R	2	14/15	0.86	0.14	116,130,146,153	0
10	NAG	S	2	14/15	0.86	0.39	150,172,182,188	0
7	MAN	A	4	11/12	0.86	0.17	138,154,176,182	0
8	BMA	C	3	11/12	0.86	0.10	176,187,198,207	0
10	NAG	K	1	14/15	0.87	0.17	94,149,177,180	0
11	MAN	M	6	11/12	0.88	0.13	103,117,139,141	0
10	NAG	T	1	14/15	0.88	0.17	74,132,158,161	0
11	MAN	M	5	11/12	0.88	0.15	151,168,188,200	0
7	BMA	A	3	11/12	0.89	0.19	78,113,127,141	0
8	NAG	C	2	14/15	0.89	0.11	116,144,163,180	0
12	MAN	P	9	11/12	0.89	0.15	154,182,188,190	0
10	NAG	N	2	14/15	0.89	0.20	108,129,138,138	0
11	MAN	M	4	11/12	0.90	0.13	115,135,152,174	0
9	NAG	F	1	14/15	0.90	0.20	59,103,114,116	0
9	NAG	F	2	14/15	0.90	0.17	118,131,139,146	0
8	NAG	C	1	14/15	0.90	0.26	108,140,173,177	0
9	MAN	F	4	11/12	0.90	0.20	108,121,130,130	0
10	NAG	T	2	14/15	0.90	0.31	161,172,192,195	0
8	MAN	C	4	11/12	0.91	0.32	140,169,187,189	0
7	NAG	A	2	14/15	0.91	0.14	121,124,132,138	0
7	NAG	A	1	14/15	0.91	0.20	76,102,129,143	0
10	NAG	S	1	14/15	0.92	0.28	123,161,167,173	0
10	NAG	Q	1	14/15	0.92	0.14	106,122,146,148	0
11	BMA	M	3	11/12	0.92	0.11	125,141,151,160	0
7	MAN	A	5	11/12	0.93	0.15	137,141,157,167	0
10	NAG	N	1	14/15	0.93	0.15	83,102,127,127	0
12	MAN	P	8	11/12	0.94	0.14	149,153,163,174	0
12	NAG	P	2	14/15	0.94	0.16	107,122,133,141	0
12	NAG	P	1	14/15	0.94	0.15	51,96,122,126	0
11	NAG	M	1	14/15	0.95	0.22	42,73,91,100	0
11	NAG	M	2	14/15	0.95	0.18	91,112,147,147	0
12	BMA	P	3	11/12	0.95	0.16	102,130,146,147	0
12	MAN	P	4	11/12	0.95	0.17	60,76,97,104	0

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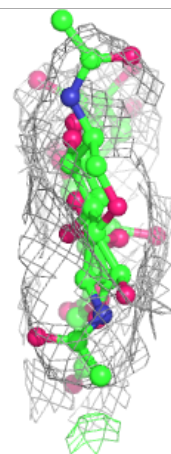
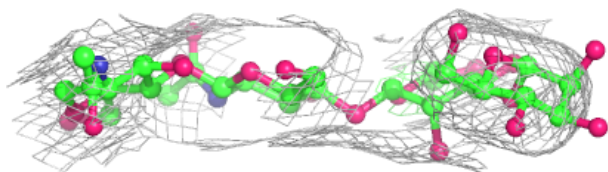
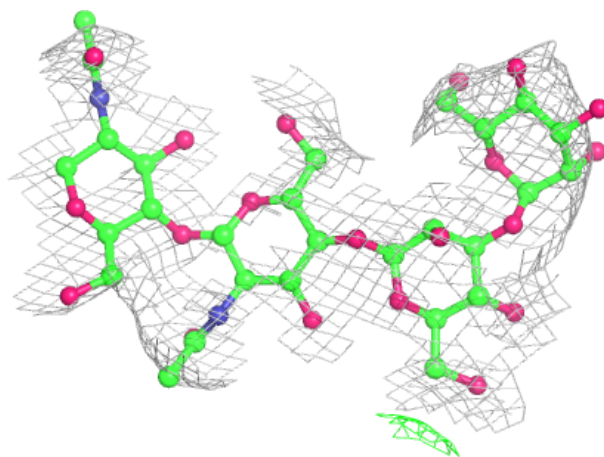
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	MAN	P	5	11/12	0.95	0.15	72,87,111,116	0
7	MAN	A	6	11/12	0.95	0.14	90,101,137,152	0
10	NAG	O	1	14/15	0.95	0.25	68,106,128,130	0
10	NAG	R	1	14/15	0.95	0.16	94,123,148,151	0
10	NAG	I	1	14/15	0.95	0.13	93,109,128,135	0
12	MAN	P	6	11/12	0.96	0.12	98,116,138,147	0

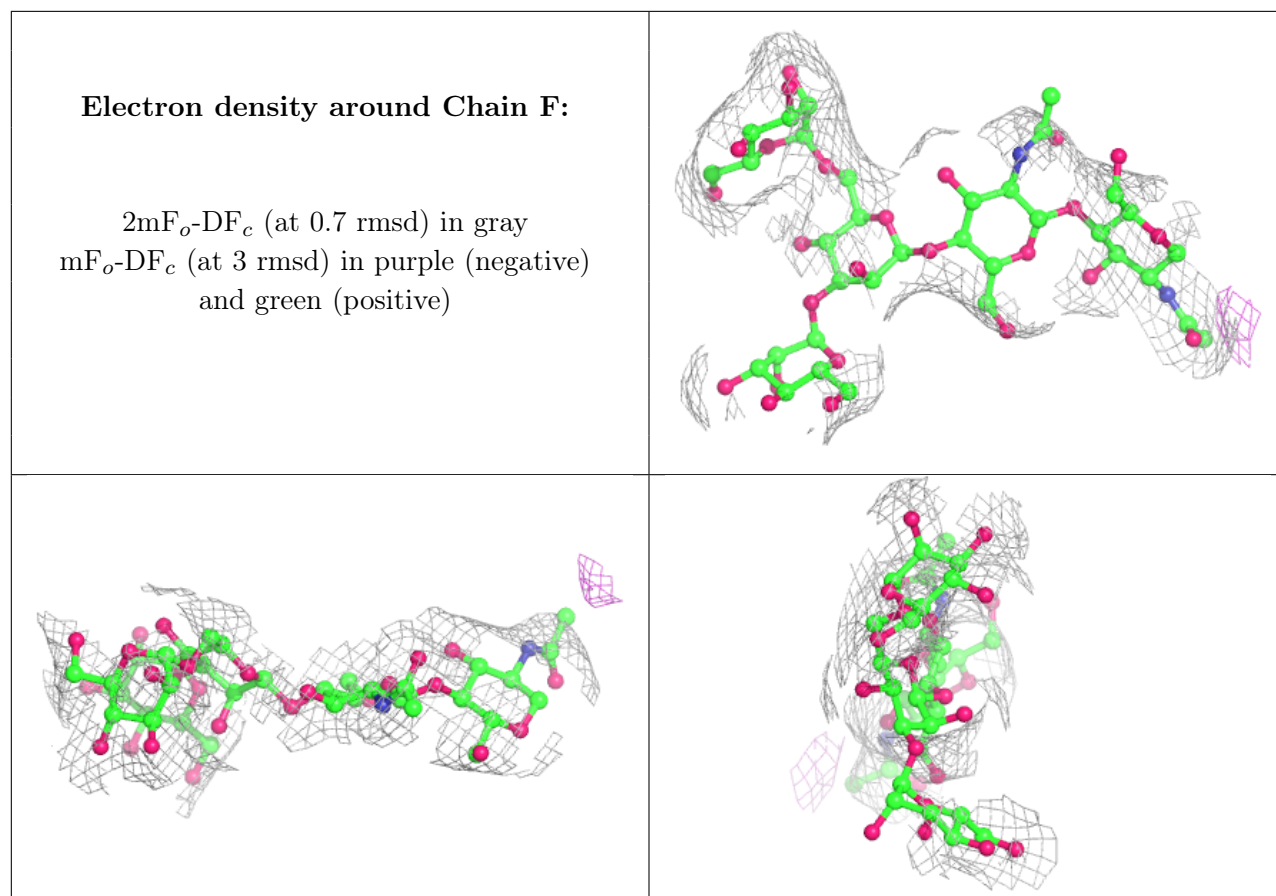
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain C:

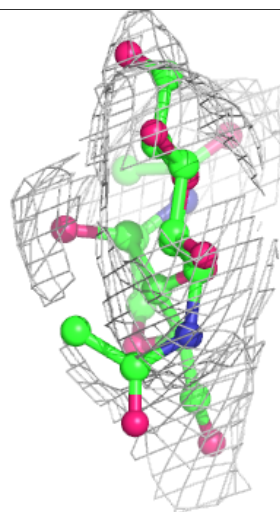
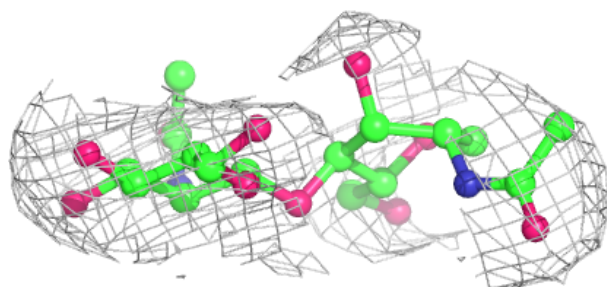
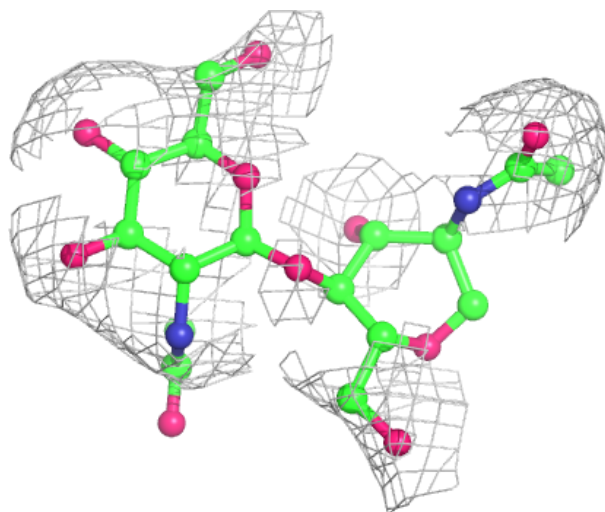
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





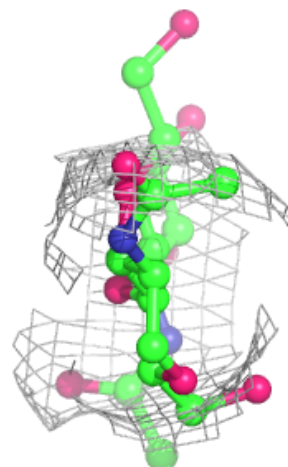
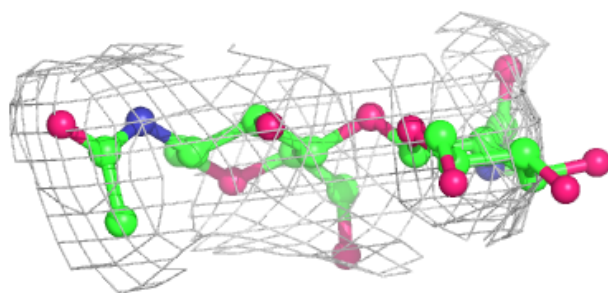
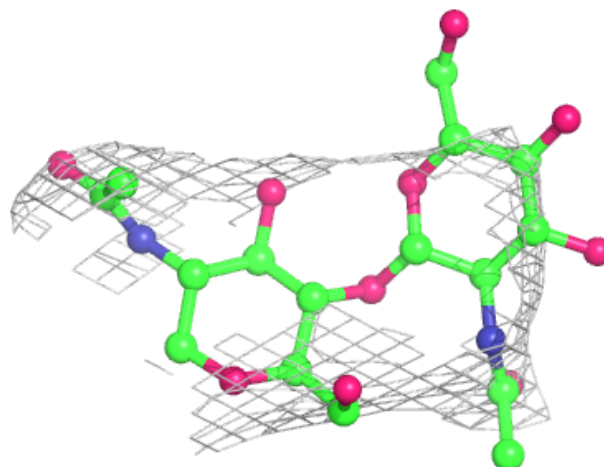
Electron density around Chain I:

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



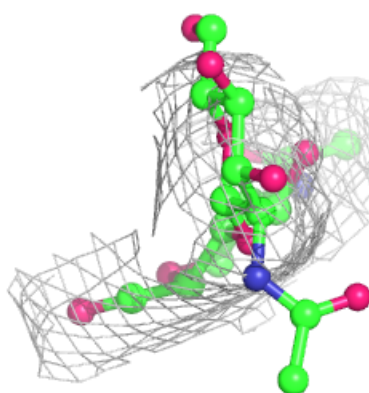
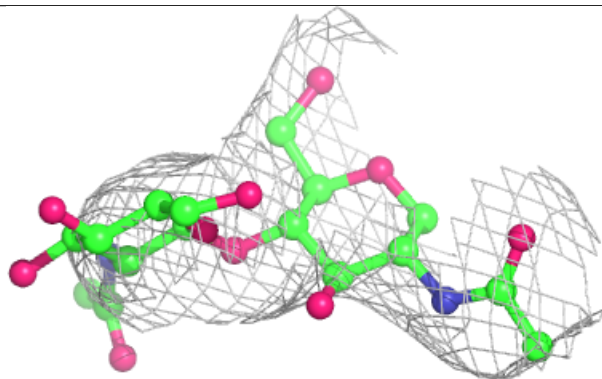
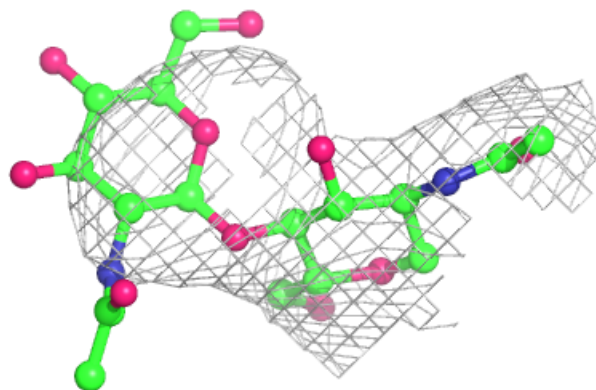
Electron density around Chain J:

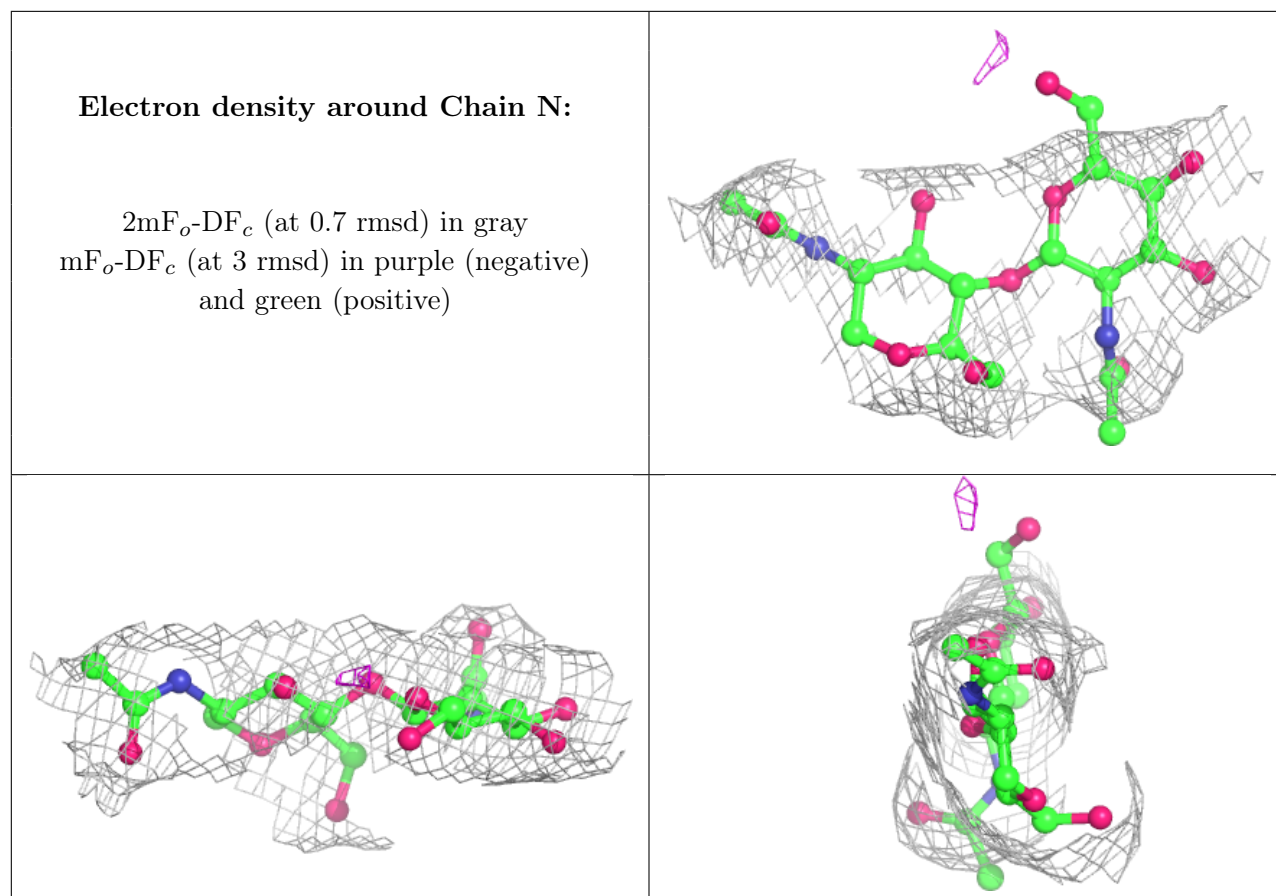
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

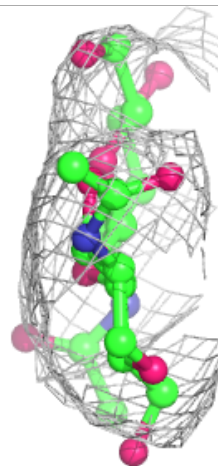
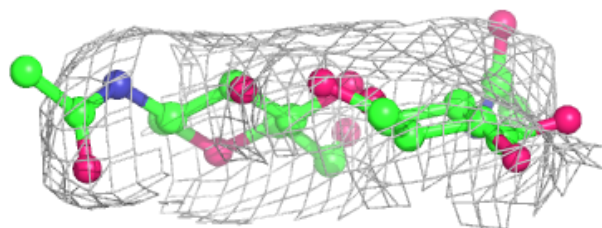
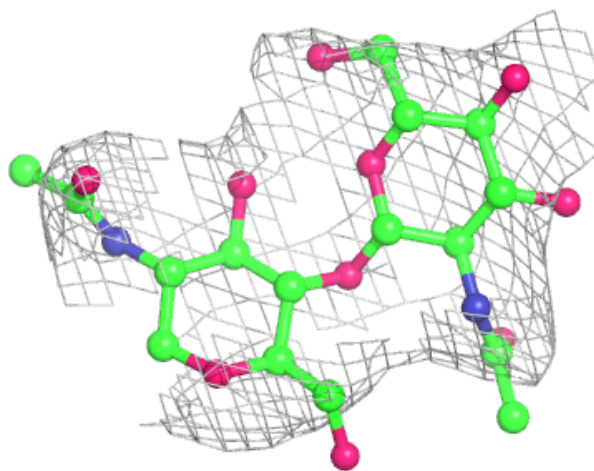
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





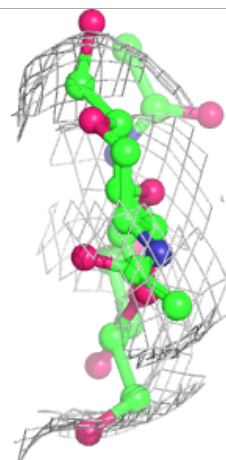
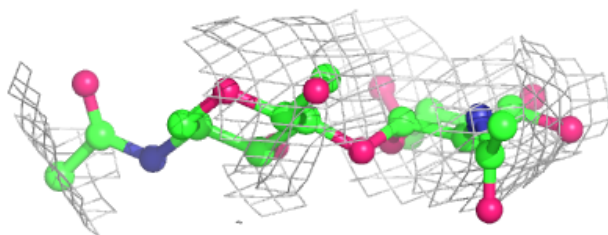
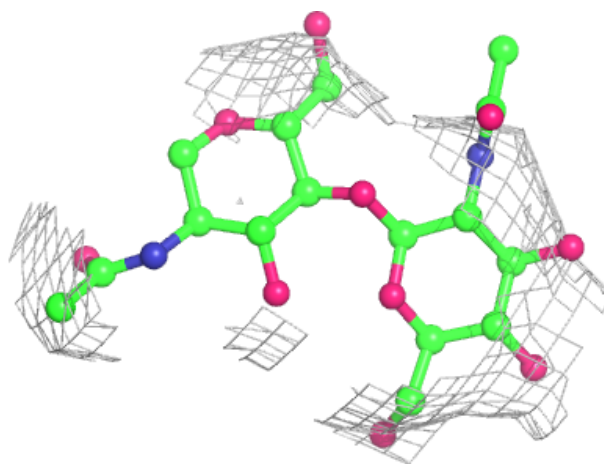
Electron density around Chain O:

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



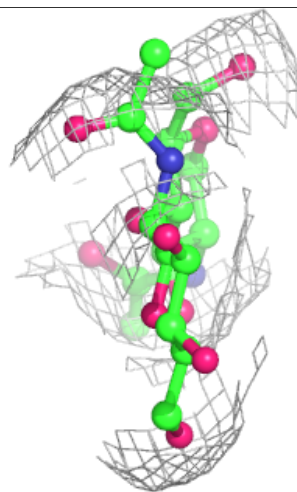
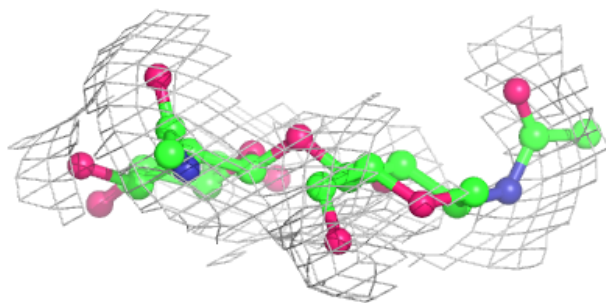
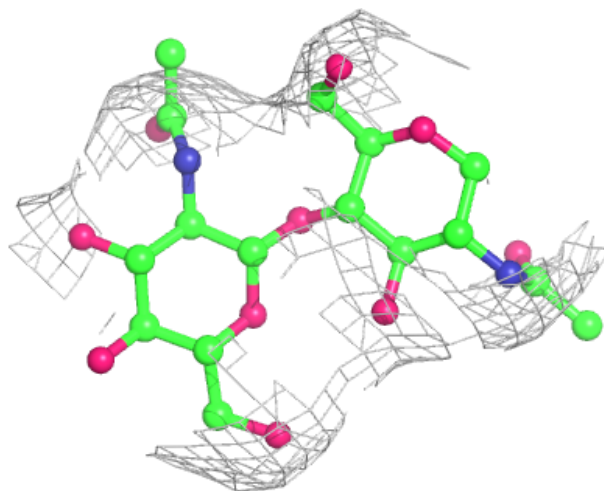
Electron density around Chain Q:

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



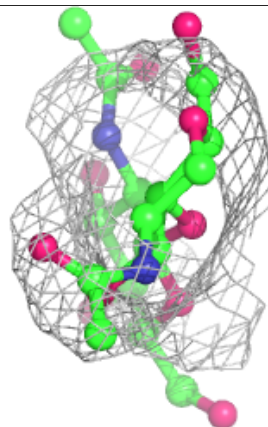
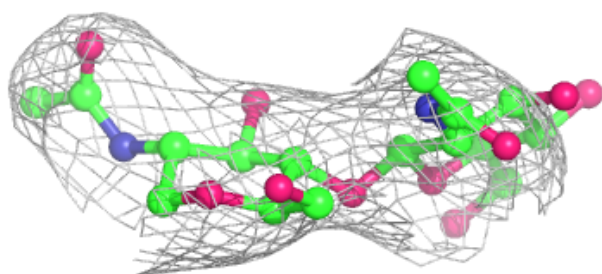
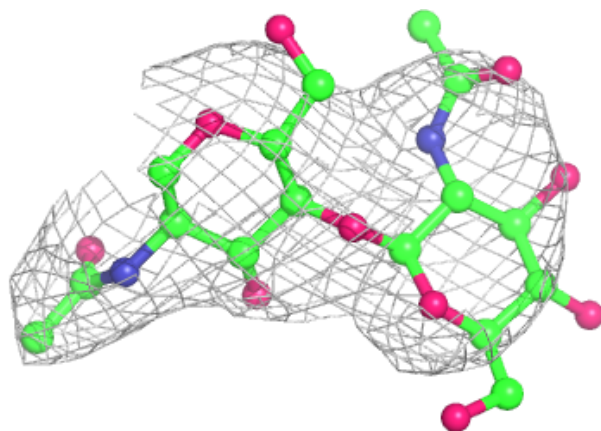
Electron density around Chain R:

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

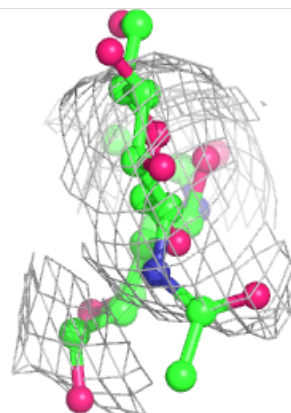
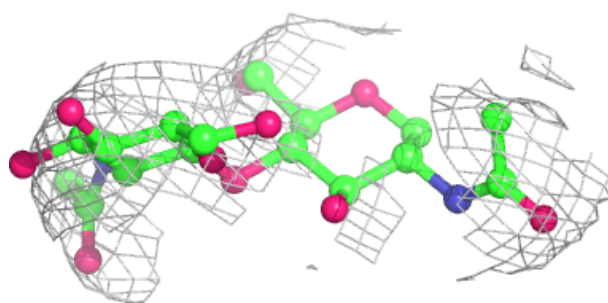
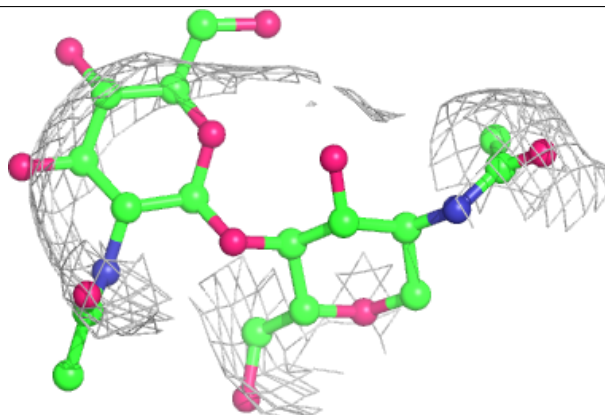


Electron density around Chain S:

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

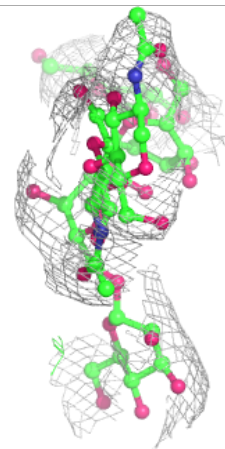
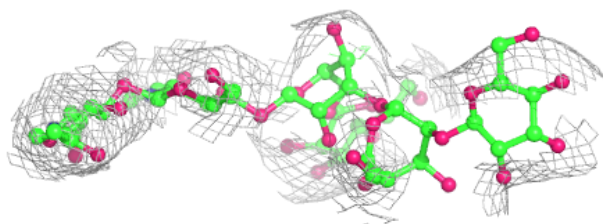
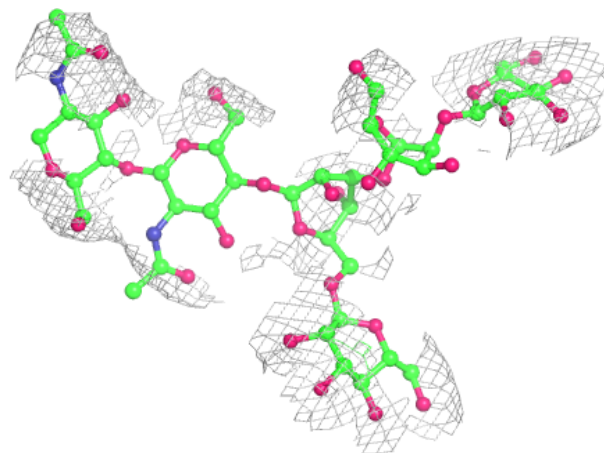
**Electron density around Chain T:**

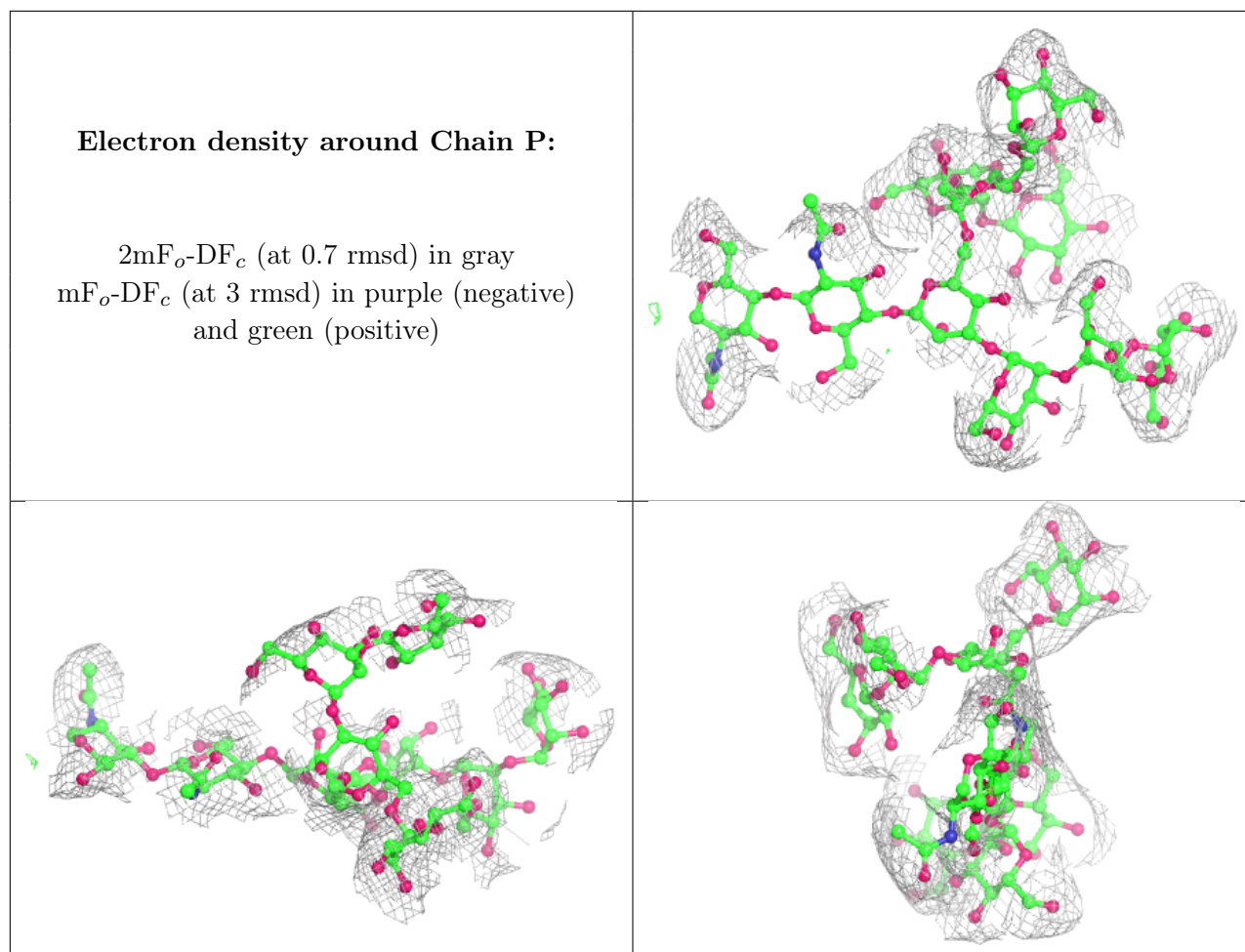
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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	H	301	14/15	0.63	0.33	189,207,211,211	0
13	NAG	B	703	14/15	0.71	0.39	157,164,173,174	0
13	NAG	B	701	14/15	0.76	0.26	176,194,207,212	0
13	NAG	G	644	14/15	0.78	0.16	106,139,147,149	0
13	NAG	G	629	14/15	0.82	0.32	141,150,156,167	0
13	NAG	G	653	14/15	0.83	0.26	161,201,208,213	0
13	NAG	G	607	14/15	0.85	0.19	94,114,126,137	0
13	NAG	B	702	14/15	0.86	0.25	156,178,188,194	0

6.5 Other polymers [i](#)

There are no such residues in this entry.