



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:31 PM BST

PDB ID : 6PDL
Title : Crystal Structure of Hendra Virus Attachment G Glycoprotein in Complex with Receptor Ephrin-B2
Authors : Xu, K.; Nikolov, D.B.
Deposited on : 2019-06-19
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

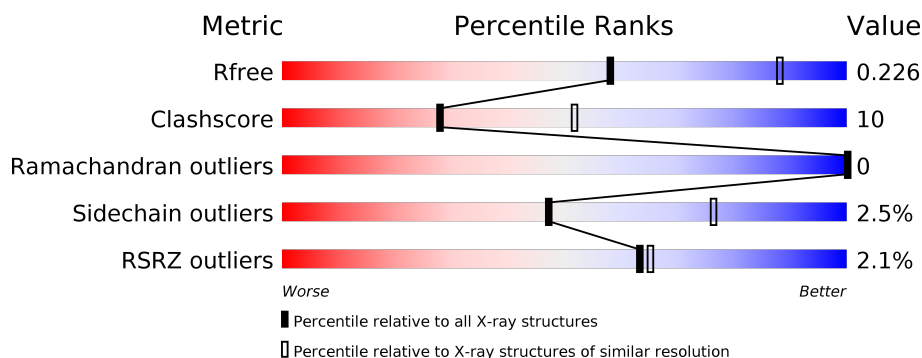
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	441	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	C	441	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	E	441	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	G	441	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• 5%</div> </div> </div>
2	B	141	<div> <div></div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 6%</div> </div> </div>
2	D	141	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	141	
2	H	141	
3	I	2	
3	J	2	
3	L	2	
3	M	2	
3	P	2	
3	S	2	
4	K	7	
4	T	7	
5	N	7	
6	O	3	
6	R	3	
7	Q	5	

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
4	BMA	K	3	X	-	-	-
4	MAN	K	4	X	-	-	-
4	MAN	K	5	-	-	-	X
4	FUC	K	6	X	-	-	-
4	BMA	T	3	X	-	-	-
4	MAN	T	4	X	-	-	-
5	MAN	N	3	X	-	-	-
5	BMA	N	4	X	-	-	-
8	NAG	F	201	-	-	-	X
8	NAG	H	202	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18707 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 Attachment glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3309	2107	555	628	19			
1	C	418	Total	C	N	O	S	0	0	0
			3286	2093	551	623	19			
1	E	421	Total	C	N	O	S	0	0	0
			3309	2107	555	628	19			
1	G	418	Total	C	N	O	S	0	0	0
			3286	2093	551	623	19			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	GLY	-	expression tag	UNP F4YH71
A	606	ARG	-	expression tag	UNP F4YH71
A	607	GLY	-	expression tag	UNP F4YH71
A	608	LEU	-	expression tag	UNP F4YH71
A	609	VAL	-	expression tag	UNP F4YH71
A	610	PRO	-	expression tag	UNP F4YH71
A	611	ARG	-	expression tag	UNP F4YH71
C	605	GLY	-	expression tag	UNP F4YH71
C	606	ARG	-	expression tag	UNP F4YH71
C	607	GLY	-	expression tag	UNP F4YH71
C	608	LEU	-	expression tag	UNP F4YH71
C	609	VAL	-	expression tag	UNP F4YH71
C	610	PRO	-	expression tag	UNP F4YH71
C	611	ARG	-	expression tag	UNP F4YH71
E	605	GLY	-	expression tag	UNP F4YH71
E	606	ARG	-	expression tag	UNP F4YH71
E	607	GLY	-	expression tag	UNP F4YH71
E	608	LEU	-	expression tag	UNP F4YH71
E	609	VAL	-	expression tag	UNP F4YH71
E	610	PRO	-	expression tag	UNP F4YH71
E	611	ARG	-	expression tag	UNP F4YH71

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Chain	Residue	Modelled	Actual	Comment	Reference
G	605	GLY	-	expression tag	UNP F4YH71
G	606	ARG	-	expression tag	UNP F4YH71
G	607	GLY	-	expression tag	UNP F4YH71
G	608	LEU	-	expression tag	UNP F4YH71
G	609	VAL	-	expression tag	UNP F4YH71
G	610	PRO	-	expression tag	UNP F4YH71
G	611	ARG	-	expression tag	UNP F4YH71

- Molecule 2 is a protein called Ephrin-B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1070	687	172	204	7			
2	D	139	Total	C	N	O	S	0	0	0
			1111	711	179	214	7			
2	F	133	Total	C	N	O	S	0	0	0
			1070	687	172	204	7			
2	H	139	Total	C	N	O	S	0	0	0
			1111	711	179	214	7			

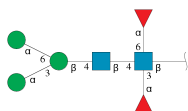
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

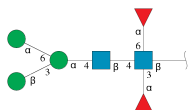
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



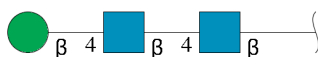
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	7	Total	C	N	O	0	0	0
			81	46	2	33			
4	T	7	Total	C	N	O	0	0	0
			81	46	2	33			

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



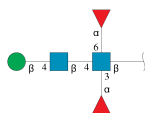
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	7	Total	C	N	O	0	0	0
			81	46	2	33			

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



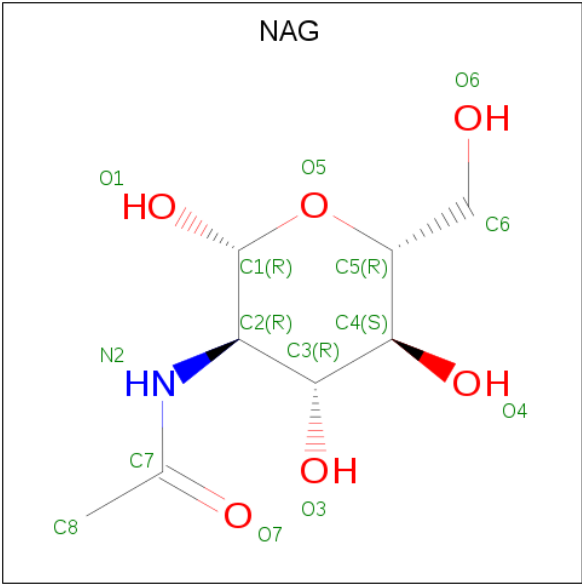
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	Q	5	Total	C	N	O	0	0	0
			59	34	2	23			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

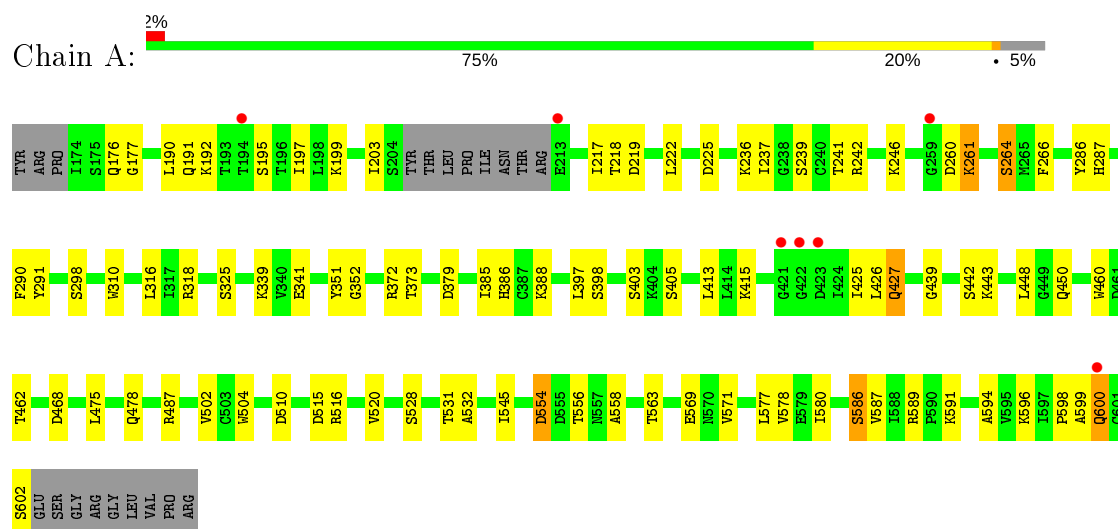
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	75	Total	O	0	0
			75	75		
9	B	21	Total	O	0	0
			21	21		
9	C	104	Total	O	0	0
			104	104		
9	D	11	Total	O	0	0
			11	11		
9	E	127	Total	O	0	0
			127	127		
9	F	22	Total	O	0	0
			22	22		
9	G	47	Total	O	0	0
			47	47		
9	H	18	Total	O	0	0
			18	18		

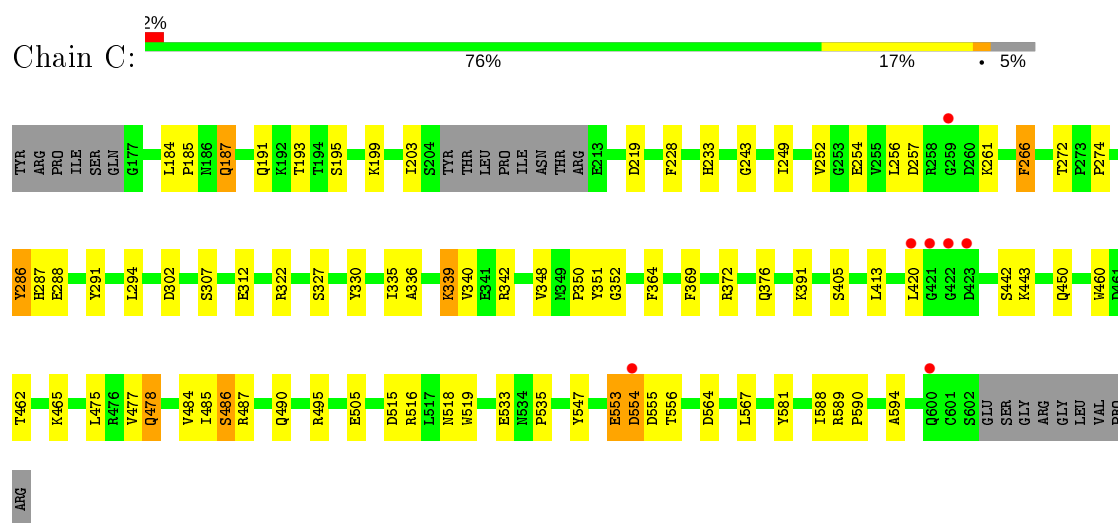
3 Residue-property plots [i](#)

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.

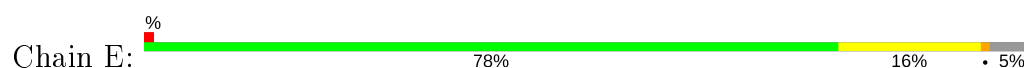
• Molecule 1: Attachment glycoprotein

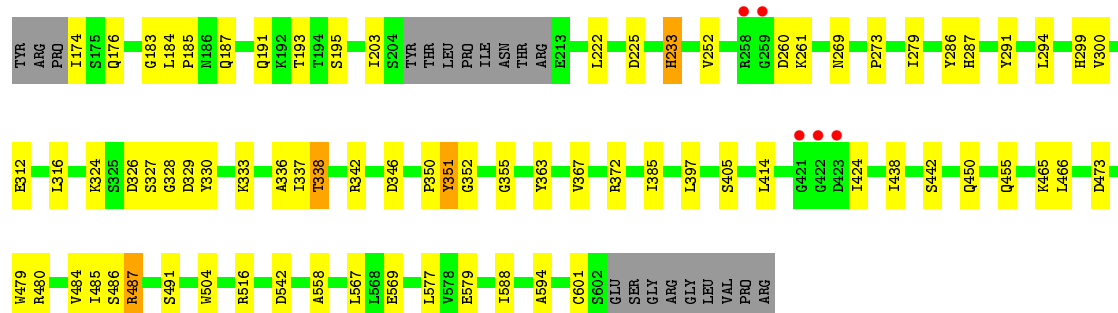


• Molecule 1: Attachment glycoprotein

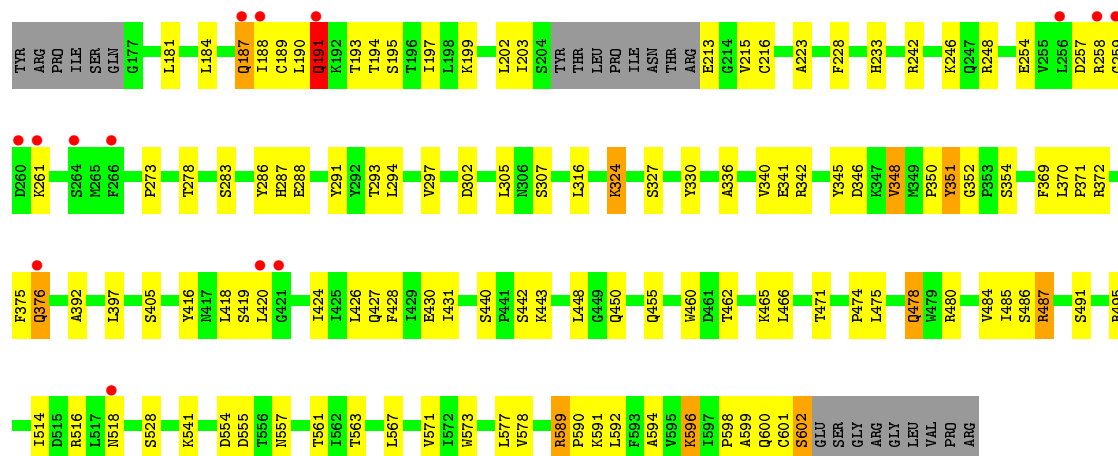


• Molecule 1: Attachment glycoprotein

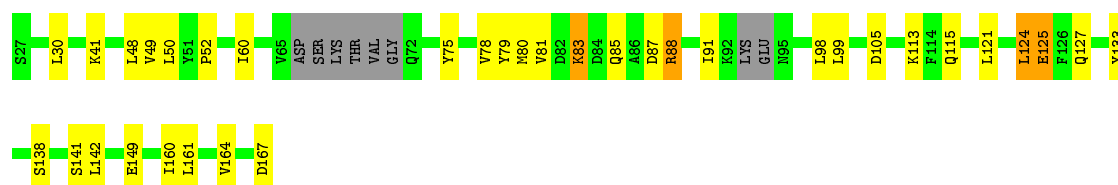




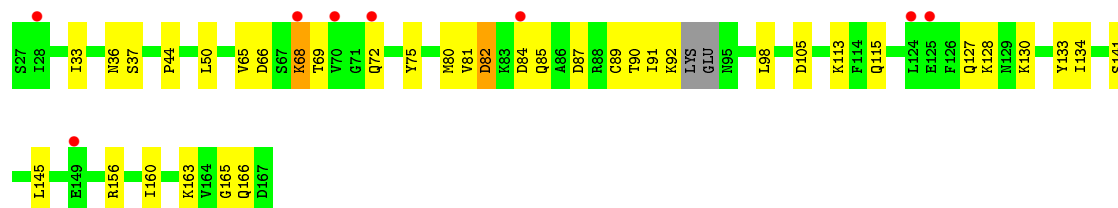
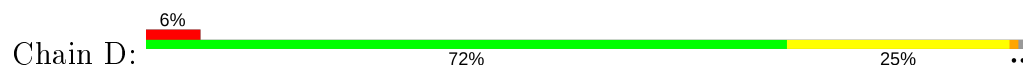
- Molecule 1: Attachment glycoprotein



- Molecule 2: Ephrin-B2

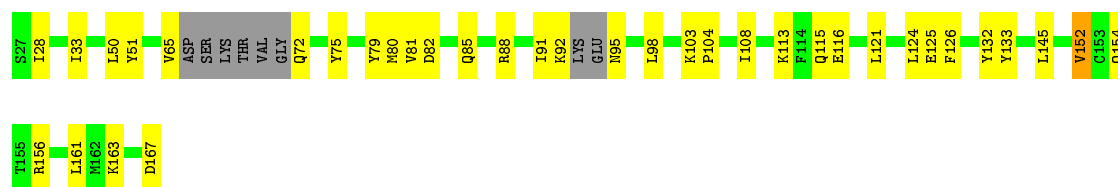


- Molecule 2: Ephrin-B2



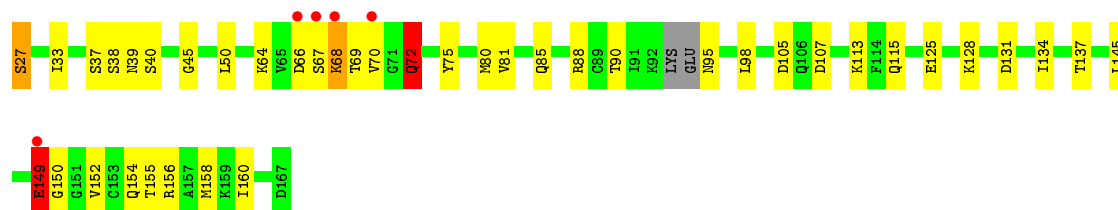
- Molecule 2: Ephrin-B2

Chain F: 



- Molecule 2: Ephrin-B2

Chain H: 



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

Chain I: 



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

Chain J: 



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

Chain L: 



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

Chain M: 



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

Chain P:  100%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain K:  43% 43% 14%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6
FUC7

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

Chain T:  43% 57%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6
FUC7

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

Chain N:  29% 71%

MAG1
MAG2
MAN3
BMA4
MAN5
FUC6
FUC7

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  67% 33%


MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 67%

MAG1
MAG2
BMA3

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

Chain Q:  80% 20%

MAG1
MAG2
BMA3
FUC4
FUC5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.76Å 94.64Å 102.52Å 112.86° 97.44° 97.56°	Depositor
Resolution (Å)	37.56 – 2.70 39.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (37.56-2.70) 93.5 (39.78-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.172 , 0.227 0.172 , 0.226	Depositor DCC
R_{free} test set	3225 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18707	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6099e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: FUC, 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	A	0.54	3/3387 (0.1%)	0.75	7/4610 (0.2%)
1	C	0.50	4/3364 (0.1%)	0.76	11/4579 (0.2%)
1	E	0.55	1/3387 (0.0%)	0.64	0/4610
1	G	0.55	6/3364 (0.2%)	0.84	19/4579 (0.4%)
2	B	0.53	0/1091	0.86	3/1471 (0.2%)
2	D	0.59	3/1133 (0.3%)	0.73	1/1529 (0.1%)
2	F	0.41	0/1091	0.72	4/1471 (0.3%)
2	H	0.54	1/1133 (0.1%)	0.85	5/1529 (0.3%)
All	All	0.53	18/17950 (0.1%)	0.76	50/24378 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	G	0	1
2	D	0	1
2	H	0	1
All	All	0	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	LYS	CD-CE	-8.88	1.29	1.51
2	D	68	LYS	CD-CE	-8.38	1.30	1.51
1	G	258	ARG	CG-CD	7.71	1.71	1.51
2	D	68	LYS	CB-CG	-7.62	1.31	1.52
1	G	596	LYS	CD-CE	-6.73	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	68	LYS	CD-CE	-6.47	1.35	1.51
2	D	68	LYS	CE-NZ	6.28	1.64	1.49
1	G	596	LYS	CE-NZ	-6.22	1.33	1.49
1	C	553	GLU	CD-OE2	5.75	1.31	1.25
1	E	225	ASP	C-O	-5.73	1.12	1.23
1	A	225	ASP	C-O	-5.54	1.12	1.23
1	G	478	GLN	CB-CG	-5.51	1.37	1.52
1	C	553	GLU	CB-CG	5.43	1.62	1.52
1	G	187	GLN	CB-CG	5.37	1.67	1.52
1	A	199	LYS	CE-NZ	-5.26	1.35	1.49
1	G	199	LYS	CD-CE	5.24	1.64	1.51
1	C	553	GLU	CG-CD	5.12	1.59	1.51
1	C	286	TYR	CE2-CZ	-5.07	1.31	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	68	LYS	CD-CE-NZ	-12.67	82.57	111.70
1	G	420	LEU	CB-CG-CD1	-11.77	91.00	111.00
1	G	258	ARG	CA-CB-CG	11.30	138.27	113.40
1	A	199	LYS	CD-CE-NZ	-9.91	88.91	111.70
1	G	376	GLN	CA-CB-CG	-9.33	92.87	113.40
1	A	261	LYS	CD-CE-NZ	-8.42	92.34	111.70
1	G	420	LEU	CB-CG-CD2	8.27	125.05	111.00
1	C	553	GLU	CA-CB-CG	8.03	131.06	113.40
1	C	184	LEU	CB-CG-CD1	7.60	123.92	111.00
1	C	187	GLN	CA-CB-CG	-7.55	96.79	113.40
1	A	600	GLN	CA-CB-CG	-7.34	97.24	113.40
1	C	339	LYS	CD-CE-NZ	-7.33	94.83	111.70
1	A	586	SER	CB-CA-C	-7.12	96.58	110.10
1	C	376	GLN	CA-CB-CG	7.08	128.98	113.40
1	G	324	LYS	CA-CB-CG	6.97	128.74	113.40
1	G	187	GLN	CA-CB-CG	6.97	128.73	113.40
1	G	589	ARG	NE-CZ-NH1	-6.94	116.83	120.30
2	H	88	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	G	478	GLN	CA-CB-CG	6.56	127.84	113.40
1	G	348	VAL	CG1-CB-CG2	6.55	121.38	110.90
2	F	82	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	G	258	ARG	CB-CG-CD	-6.38	95.02	111.60
1	G	199	LYS	CA-CB-CG	6.31	127.29	113.40
1	A	427	GLN	N-CA-CB	6.28	121.90	110.60
2	F	152	VAL	CG1-CB-CG2	6.17	120.78	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	72	GLN	CA-CB-CG	-6.07	100.06	113.40
1	C	266	PHE	CB-CG-CD2	-6.05	116.56	120.80
2	B	124	LEU	CA-CB-CG	5.89	128.85	115.30
2	F	82	ASP	CB-CG-OD1	5.82	123.54	118.30
1	G	184	LEU	CA-CB-CG	5.76	128.56	115.30
1	C	199	LYS	CA-CB-CG	5.71	125.97	113.40
1	C	554	ASP	CB-CA-C	-5.68	99.04	110.40
1	G	589	ARG	CG-CD-NE	-5.64	99.95	111.80
1	A	264	SER	N-CA-CB	5.63	118.95	110.50
1	G	478	GLN	CB-CG-CD	-5.61	97.01	111.60
2	H	88	ARG	CA-CB-CG	5.51	125.52	113.40
1	G	199	LYS	N-CA-CB	5.49	120.49	110.60
2	D	68	LYS	CA-CB-CG	-5.49	101.33	113.40
1	G	419	SER	CB-CA-C	5.45	120.45	110.10
1	G	191	GLN	N-CA-CB	-5.44	100.81	110.60
2	H	149	GLU	CG-CD-OE2	-5.39	107.51	118.30
1	G	258	ARG	CG-CD-NE	5.33	122.99	111.80
1	C	477	VAL	C-N-CA	-5.29	108.47	121.70
2	F	82	ASP	CB-CA-C	5.25	120.90	110.40
2	B	88	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	A	403	SER	CB-CA-C	-5.18	100.25	110.10
1	C	266	PHE	CB-CG-CD1	5.14	124.40	120.80
2	B	83	LYS	CA-CB-CG	-5.08	102.23	113.40
1	C	302	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	G	194	THR	OG1-CB-CG2	5.02	121.55	110.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	HIS	Peptide
2	D	82	ASP	Sidechain
1	E	287	HIS	Peptide
1	G	478	GLN	Sidechain
2	H	149	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3309	0	3248	57	1
1	C	3286	0	3224	52	0
1	E	3309	0	3248	48	3
1	G	3286	0	3224	90	1
2	B	1070	0	1057	28	0
2	D	1111	0	1099	25	3
2	F	1070	0	1057	23	1
2	H	1111	0	1098	39	1
3	I	28	0	25	0	0
3	J	28	0	25	2	0
3	L	28	0	25	1	0
3	M	28	0	25	0	0
3	P	28	0	25	1	0
3	S	28	0	25	0	1
4	K	81	0	70	1	1
4	T	81	0	70	0	0
5	N	81	0	70	0	0
6	O	39	0	34	0	0
6	R	39	0	34	0	0
7	Q	59	0	52	0	0
8	A	28	0	26	0	0
8	B	14	0	13	1	0
8	C	28	0	26	0	0
8	D	14	0	13	1	0
8	E	28	0	26	1	0
8	F	14	0	13	0	0
8	G	28	0	26	0	0
8	H	28	0	26	4	0
9	A	75	0	0	9	1
9	B	21	0	0	4	0
9	C	104	0	0	11	0
9	D	11	0	0	2	0
9	E	127	0	0	8	0
9	F	22	0	0	2	0
9	G	47	0	0	7	1
9	H	18	0	0	6	0
All	All	18707	0	17904	359	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (359) 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:H:95:ASN:ND2	9:H:302:HOH:O	1.84	1.08
1:C:553:GLU:HG2	1:C:555:ASP:OD1	1.52	1.08
2:H:27:SER:N	9:H:303:HOH:O	1.86	1.08
1:G:190:LEU:HD22	1:G:518:ASN:OD1	1.59	1.00
2:H:152:VAL:CG2	2:H:158:MET:HE2	1.92	1.00
1:E:174:ILE:N	9:E:801:HOH:O	1.93	0.99
1:G:191:GLN:HE21	1:G:601:CYS:HB2	1.28	0.98
2:H:152:VAL:HG21	2:H:158:MET:CE	1.94	0.97
1:G:191:GLN:HG2	1:G:601:CYS:SG	2.04	0.97
2:D:82:ASP:OD1	2:D:84:ASP:HB2	1.65	0.96
2:H:81:VAL:O	9:H:301:HOH:O	1.82	0.95
1:G:571:VAL:HG11	1:G:596:LYS:HD2	1.50	0.94
1:G:455:GLN:O	9:G:801:HOH:O	1.88	0.92
1:C:335:ILE:O	9:C:801:HOH:O	1.89	0.89
1:G:191:GLN:HE21	1:G:601:CYS:CB	1.86	0.88
2:D:127:GLN:HB2	2:D:130:LYS:HD2	1.55	0.87
1:A:504:TRP:O	9:A:801:HOH:O	1.93	0.87
2:H:107:ASP:O	9:H:304:HOH:O	1.93	0.86
1:G:324:LYS:HG3	1:G:330:TYR:CE2	2.09	0.86
2:B:48:LEU:HD21	2:B:50:LEU:HD13	1.62	0.82
1:E:455:GLN:O	9:E:802:HOH:O	1.98	0.81
1:G:573:TRP:CE2	1:G:596:LYS:HG3	2.15	0.81
1:C:187:GLN:HG3	1:C:187:GLN:O	1.76	0.81
1:C:294:LEU:HG	1:C:350:PRO:HG3	1.60	0.81
2:F:72:GLN:N	9:F:301:HOH:O	2.13	0.80
2:H:152:VAL:HG21	2:H:158:MET:HE1	1.62	0.79
1:G:188:ILE:O	1:G:190:LEU:HD12	1.83	0.78
1:C:553:GLU:CG	1:C:555:ASP:OD1	2.31	0.78
1:C:274:PRO:O	9:C:803:HOH:O	2.02	0.78
1:G:203:ILE:HD11	1:G:594:ALA:HB2	1.66	0.78
1:A:372:ARG:NH1	1:A:405:SER:OG	2.16	0.77
1:C:495:ARG:O	9:C:802:HOH:O	1.99	0.77
2:F:92:LYS:H	2:F:95:ASN:HD21	1.31	0.77
2:H:131:ASP:O	9:H:305:HOH:O	2.03	0.76
1:C:327:SER:O	9:C:805:HOH:O	2.04	0.76
1:G:392:ALA:O	9:G:802:HOH:O	2.04	0.76
2:B:87:ASP:OD2	9:B:301:HOH:O	2.04	0.76
1:C:257:ASP:OD2	9:C:804:HOH:O	2.03	0.75
1:C:203:ILE:HD11	1:C:594:ALA:HB2	1.69	0.75
1:G:193:THR:HG22	1:G:195:SER:H	1.50	0.75
1:G:187:GLN:HE22	1:G:599:ALA:C	1.90	0.75
1:G:187:GLN:NE2	1:G:599:ALA:O	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASP:HB3	1:A:520:VAL:HG12	1.70	0.73
2:F:124:LEU:O	2:F:125:GLU:OE1	2.04	0.73
1:G:518:ASN:O	1:G:541:LYS:NZ	2.21	0.73
2:D:44:PRO:O	9:D:301:HOH:O	2.07	0.72
1:E:328:GLY:O	9:E:803:HOH:O	2.08	0.72
1:G:376:GLN:O	9:G:803:HOH:O	2.08	0.72
2:B:113:LYS:HG2	2:B:115:GLN:HG2	1.72	0.71
1:A:176:GLN:HA	1:A:569:GLU:HG2	1.71	0.71
1:E:504:TRP:CE2	2:F:121:LEU:HD23	2.25	0.71
2:H:152:VAL:CG1	2:H:158:MET:HE2	2.21	0.71
1:E:450:GLN:HB3	9:E:832:HOH:O	1.89	0.71
1:E:261:LYS:NZ	1:E:569:GLU:OE2	2.24	0.71
1:A:372:ARG:HH21	1:A:397:LEU:HA	1.55	0.71
1:C:535:PRO:O	9:C:806:HOH:O	2.09	0.70
1:E:479:TRP:O	9:E:804:HOH:O	2.08	0.70
1:A:241:THR:HG22	1:A:242:ARG:HG3	1.73	0.70
2:H:152:VAL:CG2	2:H:158:MET:CE	2.60	0.70
1:A:439:GLY:O	9:A:802:HOH:O	2.08	0.70
1:C:274:PRO:HB3	2:H:38:SER:HA	1.72	0.70
2:H:152:VAL:HG11	2:H:158:MET:CE	2.22	0.69
2:H:33:ILE:HD11	2:H:50:LEU:HD11	1.74	0.69
2:F:92:LYS:H	2:F:95:ASN:ND2	1.89	0.69
1:E:473:ASP:OD1	9:E:805:HOH:O	2.10	0.69
2:H:113:LYS:HG2	2:H:115:GLN:HG2	1.75	0.69
1:A:510:ASP:O	9:A:803:HOH:O	2.09	0.69
1:C:243:GLY:O	9:C:808:HOH:O	2.11	0.68
2:H:152:VAL:HG11	2:H:158:MET:HE3	1.75	0.68
1:A:388:LYS:NZ	2:B:105:ASP:OD2	2.22	0.68
1:A:379:ASP:O	9:A:804:HOH:O	2.11	0.68
2:D:75:TYR:HB3	2:D:145:LEU:HD13	1.74	0.67
1:E:542:ASP:OD2	9:E:806:HOH:O	2.12	0.67
1:A:504:TRP:CE2	2:B:121:LEU:HD23	2.29	0.67
2:H:152:VAL:HG22	2:H:158:MET:HE2	1.76	0.67
8:H:201:NAG:O4	9:H:306:HOH:O	2.12	0.67
1:G:190:LEU:CD2	1:G:518:ASN:OD1	2.39	0.67
1:G:424:ILE:H	1:G:424:ILE:HD12	1.60	0.67
1:G:191:GLN:NE2	1:G:601:CYS:HB2	2.05	0.67
2:D:82:ASP:OD1	2:D:84:ASP:N	2.28	0.67
2:H:72:GLN:O	2:H:72:GLN:HG3	1.94	0.67
1:G:287:HIS:CD2	1:G:418:LEU:HD13	2.30	0.67
2:H:75:TYR:HB3	2:H:145:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LEU:O	9:B:303:HOH:O	2.14	0.66
1:A:219:ASP:OD2	9:A:805:HOH:O	2.12	0.66
1:C:486:SER:OG	1:C:495:ARG:HG3	1.95	0.65
1:G:430:GLU:OE2	9:G:805:HOH:O	2.15	0.65
1:A:468:ASP:O	1:A:478:GLN:HB3	1.98	0.64
1:G:372:ARG:NH1	1:G:405:SER:OG	2.30	0.64
1:G:340:VAL:HG12	1:G:342:ARG:HG3	1.80	0.64
2:B:80:MET:HB2	2:B:98:LEU:HD11	1.80	0.64
1:A:222:LEU:HB2	1:A:577:LEU:HD12	1.79	0.63
1:G:242:ARG:HH11	1:G:242:ARG:HG2	1.61	0.63
1:A:385:ILE:HD12	1:A:386:HIS:H	1.63	0.63
1:G:577:LEU:HD13	1:G:592:LEU:HG	1.80	0.63
1:G:571:VAL:CG1	1:G:596:LYS:HD2	2.28	0.62
1:C:484:VAL:HG23	1:C:485:ILE:HG12	1.80	0.62
2:H:66:ASP:HB3	2:H:69:THR:HG22	1.81	0.62
1:E:327:SER:HB3	1:E:330:TYR:HB3	1.81	0.62
1:G:197:ILE:HG13	1:G:598:PRO:HG2	1.80	0.62
2:B:30:LEU:HD11	2:B:52:PRO:HB3	1.80	0.62
1:A:203:ILE:HD11	1:A:594:ALA:HB2	1.81	0.62
1:A:339:LYS:HE3	1:A:425:ILE:HG12	1.81	0.62
2:D:80:MET:HB2	2:D:98:LEU:HD11	1.81	0.61
2:D:141:SER:HB3	8:D:201:NAG:H82	1.82	0.61
2:D:69:THR:HG22	2:D:72:GLN:HB2	1.81	0.61
2:H:67:SER:O	2:H:70:VAL:HG23	2.00	0.60
1:C:256:LEU:HD12	1:C:266:PHE:CD2	2.37	0.60
2:H:152:VAL:CG1	2:H:158:MET:CE	2.80	0.60
2:B:49:VAL:HG22	2:B:161:LEU:HB3	1.84	0.60
2:B:81:VAL:O	9:B:304:HOH:O	2.17	0.60
1:G:294:LEU:HG	1:G:350:PRO:HG3	1.84	0.60
1:C:372:ARG:HD2	1:C:405:SER:O	2.01	0.59
2:D:85:GLN:HB3	2:D:90:THR:O	2.02	0.59
2:D:113:LYS:HG2	2:D:115:GLN:HG2	1.83	0.59
1:C:443:LYS:NZ	1:C:564:ASP:OD1	2.36	0.59
2:F:152:VAL:HG22	2:F:156:ARG:HB3	1.84	0.59
1:G:242:ARG:NH1	1:G:242:ARG:HG2	2.18	0.59
1:G:589:ARG:HG2	1:G:590:PRO:N	2.18	0.58
1:E:372:ARG:NH1	1:E:405:SER:OG	2.36	0.58
2:B:141:SER:OG	8:B:201:NAG:H82	2.03	0.58
1:C:193:THR:HG22	1:C:195:SER:H	1.67	0.58
1:E:372:ARG:NH2	1:E:397:LEU:HA	2.19	0.58
1:G:372:ARG:HH21	1:G:397:LEU:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:471:THR:OG1	1:G:474:PRO:O	2.19	0.58
2:D:65:VAL:HG21	2:D:72:GLN:HB3	1.86	0.58
3:J:2:NAG:H83	3:J:2:NAG:H3	1.85	0.58
1:A:372:ARG:NH2	1:A:397:LEU:HA	2.18	0.58
1:G:273:PRO:O	9:G:806:HOH:O	2.17	0.58
1:G:324:LYS:CB	1:G:327:SER:OG	2.52	0.57
1:G:324:LYS:HG3	1:G:330:TYR:CD2	2.39	0.57
2:D:33:ILE:HD11	2:D:50:LEU:HD11	1.85	0.57
1:C:413:LEU:HG	1:C:475:LEU:HD22	1.85	0.57
1:E:185:PRO:HB3	1:E:567:LEU:HD21	1.85	0.57
1:E:294:LEU:HG	1:E:350:PRO:HG3	1.86	0.57
1:A:218:THR:HG21	1:A:236:LYS:HD2	1.85	0.57
1:E:372:ARG:HH21	1:E:397:LEU:HA	1.69	0.57
1:G:484:VAL:HG23	1:G:485:ILE:HG12	1.87	0.57
1:G:431:ILE:HA	1:G:475:LEU:HB3	1.87	0.57
1:C:322:ARG:HD2	1:E:385:ILE:HD11	1.88	0.56
1:C:581:TYR:CG	1:C:588:ILE:HD13	2.40	0.56
1:G:557:ASN:OD1	2:H:113:LYS:HE2	2.06	0.56
1:A:190:LEU:O	1:A:191:GLN:HG2	2.06	0.56
1:A:286:TYR:HB2	1:A:291:TYR:CE2	2.40	0.56
2:F:33:ILE:HD11	2:F:50:LEU:HD11	1.86	0.56
1:A:468:ASP:HB2	1:A:478:GLN:HE21	1.71	0.56
1:E:222:LEU:HB2	1:E:577:LEU:HD12	1.87	0.56
2:H:152:VAL:HG22	2:H:156:ARG:HB2	1.87	0.56
1:G:181:LEU:HD21	1:G:514:ILE:HA	1.87	0.56
2:B:83:LYS:O	2:B:83:LYS:HG2	2.03	0.55
1:C:450:GLN:HB2	1:C:516:ARG:NH2	2.21	0.55
1:G:370:LEU:HD12	1:G:371:PRO:HD2	1.88	0.55
1:G:375:PHE:C	1:G:376:GLN:HG2	2.22	0.55
1:G:448:LEU:HB2	1:G:516:ARG:HH12	1.70	0.55
1:A:571:VAL:HG11	1:A:596:LYS:HE2	1.88	0.55
2:D:36:ASN:ND2	9:D:302:HOH:O	2.27	0.55
1:E:338:THR:HG23	1:E:424:ILE:H	1.72	0.55
2:D:82:ASP:OD1	2:D:84:ASP:CB	2.48	0.55
1:G:416:TYR:CE1	1:G:424:ILE:HG23	2.42	0.55
1:C:462:THR:O	1:C:486:SER:HB2	2.07	0.54
1:A:373:THR:O	9:A:806:HOH:O	2.18	0.54
2:H:85:GLN:HB3	2:H:90:THR:O	2.08	0.54
1:A:478:GLN:NE2	9:A:813:HOH:O	2.40	0.54
1:E:484:VAL:HG23	1:E:485:ILE:HG12	1.90	0.54
1:G:188:ILE:O	1:G:190:LEU:CD1	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:THR:OG1	1:E:195:SER:OG	2.27	0.53
1:A:599:ALA:C	1:A:600:GLN:HG2	2.24	0.53
1:E:329:ASP:HB2	1:E:333:LYS:HG3	1.91	0.53
1:G:600:GLN:C	1:G:602:SER:H	2.10	0.53
1:G:287:HIS:CD2	1:G:418:LEU:CD1	2.91	0.53
2:F:113:LYS:HG2	2:F:115:GLN:HG2	1.91	0.53
1:A:341:GLU:HB2	1:A:427:GLN:HG2	1.91	0.53
2:H:80:MET:HB2	2:H:98:LEU:HD11	1.90	0.52
1:C:420:LEU:CD1	3:L:1:NAG:O5	2.58	0.52
1:E:300:VAL:O	8:E:701:NAG:H83	2.09	0.52
1:A:177:GLY:HA3	9:A:822:HOH:O	2.11	0.51
2:B:88:ARG:NH1	2:B:149:GLU:OE2	2.43	0.51
2:D:81:VAL:HG23	2:D:133:TYR:HB2	1.91	0.51
1:E:450:GLN:HB2	1:E:516:ARG:NH2	2.24	0.51
1:A:197:ILE:HG22	2:F:28:ILE:HG23	1.93	0.51
1:A:532:ALA:HB1	1:A:558:ALA:O	2.11	0.51
1:C:219:ASP:OD1	9:C:809:HOH:O	2.19	0.51
1:G:324:LYS:HB2	1:G:327:SER:OG	2.10	0.51
1:G:555:ASP:N	1:G:555:ASP:OD1	2.42	0.51
1:G:573:TRP:NE1	1:G:596:LYS:HG3	2.25	0.51
2:B:81:VAL:HB	2:B:85:GLN:HB2	1.93	0.51
1:G:352:GLY:HA3	1:G:442:SER:O	2.11	0.51
1:A:528:SER:OG	1:A:531:THR:OG1	2.22	0.50
1:C:249:ILE:HG22	1:C:272:THR:HG22	1.93	0.50
1:E:324:LYS:HB2	1:E:327:SER:OG	2.11	0.50
1:A:578:VAL:HG12	1:A:580:ILE:HB	1.93	0.50
2:B:142:LEU:O	2:B:142:LEU:HD23	2.11	0.50
1:G:248:ARG:O	1:G:273:PRO:HD2	2.12	0.50
1:C:554:ASP:N	1:C:554:ASP:OD1	2.44	0.50
1:G:324:LYS:HB3	1:G:327:SER:OG	2.12	0.50
1:G:336:ALA:HA	9:G:833:HOH:O	2.12	0.49
1:E:286:TYR:HB2	1:E:291:TYR:CE2	2.47	0.49
2:B:138:SER:HB3	9:B:306:HOH:O	2.12	0.49
2:B:78:VAL:HB	2:B:99:LEU:HB2	1.92	0.49
1:E:191:GLN:HG2	1:E:601:CYS:SG	2.52	0.49
1:C:478:GLN:HG3	1:C:478:GLN:O	2.10	0.49
1:E:312:GLU:OE2	1:E:342:ARG:NH1	2.45	0.49
1:C:589:ARG:HG2	1:C:590:PRO:N	2.27	0.49
1:G:345:TYR:CD1	1:G:370:LEU:HB2	2.47	0.49
1:G:345:TYR:CE1	1:G:370:LEU:HB2	2.47	0.49
1:G:286:TYR:HB2	1:G:291:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:SER:O	2:D:156:ARG:NH2	2.38	0.49
2:F:124:LEU:O	2:F:125:GLU:CD	2.51	0.49
2:B:50:LEU:HB3	2:B:52:PRO:HD3	1.95	0.48
2:B:52:PRO:O	2:B:164:VAL:HA	2.13	0.48
2:F:154:GLN:O	9:F:302:HOH:O	2.20	0.48
1:C:352:GLY:HA3	1:C:442:SER:O	2.14	0.48
1:G:351:TYR:CE2	1:G:440:SER:HA	2.48	0.48
1:A:398:SER:OG	1:A:502:VAL:HA	2.14	0.48
2:H:39:ASN:HA	8:H:202:NAG:C8	2.44	0.48
1:A:190:LEU:C	1:A:191:GLN:HG2	2.33	0.48
1:C:252:VAL:HG11	1:C:291:TYR:HB2	1.96	0.48
2:F:133:TYR:CE2	2:F:161:LEU:HD23	2.49	0.47
2:F:80:MET:HB2	2:F:98:LEU:HD11	1.96	0.47
1:G:340:VAL:HG22	1:G:426:LEU:HB2	1.96	0.47
1:E:336:ALA:O	1:E:424:ILE:HG13	2.14	0.47
2:H:152:VAL:HA	2:H:155:THR:HG22	1.97	0.47
2:F:65:VAL:HG12	2:F:104:PRO:O	2.14	0.47
1:A:239:SER:HG	1:A:242:ARG:H	1.62	0.47
1:G:302:ASP:HB3	1:G:305:LEU:HD12	1.97	0.47
2:H:152:VAL:HG13	2:H:158:MET:HB2	1.96	0.47
1:G:341:GLU:HB2	1:G:427:GLN:HG3	1.96	0.47
1:G:516:ARG:NH1	1:G:516:ARG:HB2	2.30	0.47
2:H:39:ASN:HA	8:H:202:NAG:H82	1.96	0.47
2:H:72:GLN:O	2:H:72:GLN:CG	2.61	0.47
1:C:312:GLU:OE1	1:C:340:VAL:HG21	2.15	0.47
2:D:128:LYS:HG3	2:D:165:GLY:HA3	1.96	0.47
2:F:103:LYS:HB2	2:F:108:ILE:HD11	1.97	0.47
1:G:465:LYS:HA	9:G:820:HOH:O	2.13	0.47
1:C:460:TRP:O	1:C:462:THR:HG23	2.14	0.47
2:D:91:ILE:O	2:D:92:LYS:HD3	2.15	0.47
1:A:528:SER:HB3	1:A:531:THR:O	2.15	0.46
1:G:193:THR:HG22	1:G:195:SER:N	2.26	0.46
1:E:337:ILE:HA	1:E:424:ILE:HB	1.97	0.46
2:F:115:GLN:O	2:F:125:GLU:OE2	2.32	0.46
1:A:413:LEU:HD11	1:A:475:LEU:HD13	1.97	0.46
2:H:134:ILE:HB	2:H:160:ILE:HB	1.98	0.46
1:G:466:LEU:O	1:G:480:ARG:HG2	2.15	0.46
1:A:443:LYS:NZ	1:A:563:THR:O	2.48	0.46
1:G:187:GLN:HE22	1:G:599:ALA:CA	2.28	0.46
1:C:287:HIS:NE2	1:C:288:GLU:HG3	2.30	0.46
2:F:75:TYR:HB3	2:F:145:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:460:TRP:O	1:G:462:THR:HG23	2.16	0.46
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.79	0.46
1:A:260:ASP:O	1:A:261:LYS:HB2	2.16	0.46
1:A:586:SER:HB2	1:A:587:VAL:HG23	1.96	0.46
1:C:286:TYR:HB2	1:C:291:TYR:CE2	2.50	0.46
1:E:286:TYR:HB2	1:E:291:TYR:CZ	2.51	0.46
1:E:203:ILE:HD11	1:E:594:ALA:HB2	1.97	0.45
1:E:260:ASP:OD2	1:E:260:ASP:N	2.41	0.45
1:G:348:VAL:HG11	1:G:428:PHE:HB2	1.97	0.45
1:G:486:SER:OG	1:G:487:ARG:N	2.48	0.45
2:H:137:THR:HG21	2:H:149:GLU:N	2.31	0.45
2:B:133:TYR:CE2	2:B:161:LEU:HD23	2.51	0.45
1:A:237:ILE:HD11	1:A:246:LYS:HG3	1.98	0.45
1:A:192:LYS:NZ	1:A:545:ILE:O	2.46	0.45
2:H:37:SER:O	2:H:156:ARG:NH2	2.49	0.45
9:A:807:HOH:O	4:K:4:MAN:O3	2.20	0.45
1:E:486:SER:OG	1:E:487:ARG:N	2.48	0.45
1:G:443:LYS:NZ	1:G:563:THR:O	2.44	0.45
1:G:573:TRP:CD2	1:G:596:LYS:HG3	2.51	0.45
1:G:257:ASP:OD1	1:G:261:LYS:N	2.46	0.45
2:D:85:GLN:O	2:D:89:CYS:N	2.49	0.45
2:H:64:LYS:HG3	2:H:105:ASP:O	2.16	0.45
1:A:450:GLN:HB2	1:A:516:ARG:NH2	2.32	0.45
1:G:307:SER:HG	1:G:369:PHE:HE1	1.63	0.45
1:C:581:TYR:CD2	1:C:588:ILE:HD13	2.52	0.45
1:C:254:GLU:HG3	1:C:256:LEU:HD11	1.99	0.44
1:C:307:SER:HG	1:C:369:PHE:HE1	1.61	0.44
1:E:355:GLY:HA3	1:E:363:TYR:O	2.17	0.44
1:A:460:TRP:O	1:A:462:THR:HG23	2.17	0.44
1:C:342:ARG:HG2	1:C:348:VAL:HG13	2.00	0.44
2:F:79:TYR:CE1	2:F:91:ILE:HD13	2.52	0.44
1:A:298:SER:HB2	1:A:310:TRP:CD1	2.53	0.44
2:B:48:LEU:HD22	2:B:160:ILE:HG23	2.00	0.44
2:B:41:LYS:HB3	2:B:48:LEU:HD12	1.99	0.44
2:F:81:VAL:HB	2:F:85:GLN:HB2	2.00	0.44
1:G:213:GLU:HB3	1:G:215:VAL:HG13	1.99	0.44
1:G:340:VAL:HG11	1:G:348:VAL:CG2	2.47	0.44
1:E:351:TYR:HD2	1:E:367:VAL:HB	1.81	0.44
1:A:580:ILE:HG21	1:A:591:LYS:HD2	1.98	0.44
1:E:176:GLN:HA	1:E:569:GLU:HG2	2.00	0.44
2:D:87:ASP:N	2:D:87:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:SER:OG	1:A:266:PHE:CE2	2.71	0.43
1:G:561:THR:HG22	1:G:578:VAL:HG22	2.00	0.43
3:J:1:NAG:H61	3:J:2:NAG:C7	2.48	0.43
2:H:152:VAL:CB	2:H:158:MET:HE2	2.46	0.43
2:D:66:ASP:HB2	2:D:69:THR:HB	2.00	0.43
1:E:438:ILE:HD13	1:E:504:TRP:CD1	2.53	0.43
2:D:134:ILE:HB	2:D:160:ILE:HB	2.00	0.43
1:E:352:GLY:HA3	1:E:442:SER:O	2.18	0.43
1:C:533:GLU:HB2	1:C:556:THR:O	2.18	0.43
1:E:233:HIS:C	1:E:233:HIS:CD2	2.91	0.43
1:G:571:VAL:HG12	1:G:573:TRP:CD1	2.54	0.43
2:B:125:GLU:OE2	2:B:127:GLN:NE2	2.29	0.43
1:C:261:LYS:HD3	1:C:261:LYS:N	2.34	0.43
1:G:424:ILE:CD1	1:G:424:ILE:H	2.30	0.43
2:B:83:LYS:HE2	2:B:87:ASP:OD1	2.18	0.43
2:F:51:TYR:CE2	2:F:163:LYS:HD3	2.54	0.43
1:C:490:GLN:HB2	1:C:505:GLU:CD	2.38	0.43
1:E:465:LYS:HB3	1:E:465:LYS:HE2	1.70	0.43
2:B:60:ILE:HG22	2:B:99:LEU:HD11	2.00	0.43
1:C:287:HIS:CE1	1:C:288:GLU:HG3	2.53	0.43
1:C:364:PHE:O	1:C:413:LEU:HA	2.19	0.43
2:F:126:PHE:HA	2:F:132:TYR:CZ	2.54	0.43
1:G:278:THR:O	1:G:297:VAL:HA	2.18	0.43
1:G:567:LEU:HA	1:G:571:VAL:O	2.19	0.43
1:A:286:TYR:HB2	1:A:291:TYR:CZ	2.54	0.42
2:B:79:TYR:CE1	2:B:91:ILE:HD13	2.54	0.42
1:C:465:LYS:HB3	1:C:465:LYS:HE2	1.72	0.42
2:F:92:LYS:HE3	2:F:92:LYS:HB3	1.81	0.42
2:B:88:ARG:O	2:B:88:ARG:HG3	2.19	0.42
1:C:185:PRO:HB3	1:C:567:LEU:HD21	2.01	0.42
2:D:65:VAL:HG22	2:D:66:ASP:H	1.83	0.42
1:C:228:PHE:HA	1:C:254:GLU:HA	2.01	0.42
1:C:327:SER:HB2	1:C:330:TYR:HB3	2.01	0.42
1:G:283:SER:O	1:G:293:THR:HA	2.19	0.42
1:G:202:LEU:HD11	1:G:591:LYS:HD3	2.01	0.42
1:G:465:LYS:HE2	1:G:465:LYS:HB3	1.75	0.42
1:E:252:VAL:HG22	1:E:269:ASN:HB3	2.01	0.42
1:G:257:ASP:CG	1:G:259:GLY:H	2.23	0.42
1:A:352:GLY:HA3	1:A:442:SER:O	2.20	0.42
1:C:515:ASP:OD2	1:C:518:ASN:HB2	2.20	0.42
9:C:867:HOH:O	2:H:45:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:CD2	1:A:318:ARG:HD2	2.55	0.42
2:B:75:TYR:CZ	2:B:142:LEU:HD12	2.54	0.42
1:G:228:PHE:HA	1:G:254:GLU:HA	2.02	0.42
2:H:39:ASN:CG	8:H:202:NAG:H82	2.40	0.42
2:D:163:LYS:HB3	2:D:166:GLN:CD	2.40	0.41
1:A:217:ILE:HD12	1:A:589:ARG:HG3	2.02	0.41
1:E:466:LEU:O	1:E:480:ARG:HG2	2.18	0.41
1:A:197:ILE:HG13	1:A:598:PRO:HG2	2.01	0.41
1:E:299:HIS:ND1	9:E:811:HOH:O	2.37	0.41
1:G:327:SER:HB3	1:G:330:TYR:HB3	2.03	0.41
1:G:351:TYR:HE2	1:G:440:SER:HA	1.84	0.41
1:A:478:GLN:CG	1:A:478:GLN:O	2.69	0.41
1:C:372:ARG:NH1	9:C:824:HOH:O	2.53	0.41
1:A:554:ASP:C	1:A:556:THR:H	2.23	0.41
1:C:336:ALA:HA	9:C:844:HOH:O	2.20	0.41
1:E:273:PRO:HG2	1:E:279:ILE:HD13	2.03	0.41
1:G:450:GLN:HB2	1:G:516:ARG:NH2	2.36	0.41
2:H:69:THR:HG23	2:H:69:THR:O	2.21	0.41
1:E:351:TYR:CD2	1:E:367:VAL:HB	2.56	0.41
1:G:223:ALA:HB2	1:G:354:SER:HB3	2.03	0.41
1:G:287:HIS:HD2	1:G:418:LEU:HD13	1.81	0.41
2:H:150:GLY:HA2	2:H:154:GLN:HB2	2.03	0.41
1:E:414:LEU:HD23	1:E:414:LEU:HA	1.93	0.40
2:D:33:ILE:CD1	2:D:50:LEU:HD11	2.48	0.40
1:A:415:LYS:O	1:A:426:LEU:HA	2.21	0.40
1:E:558:ALA:HA	1:E:579:GLU:O	2.21	0.40
3:P:1:NAG:H62	3:P:2:NAG:H82	2.04	0.40
1:A:218:THR:OG1	1:A:219:ASP:N	2.54	0.40
1:E:588:ILE:CD1	2:F:116:GLU:HG3	2.52	0.40
1:G:486:SER:OG	1:G:495:ARG:HG3	2.21	0.40

All (7) 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)
9:A:859:HOH:O	9:G:844:HOH:O[1_556]	1.87	0.33
2:D:68:LYS:NZ	1:E:183:GLY:O[1_665]	1.94	0.26
1:G:288:GLU:OE1	4:K:4:MAN:O4[1_444]	1.97	0.23
2:D:68:LYS:CD	1:E:183:GLY:N[1_665]	2.01	0.19
2:F:88:ARG:NH1	3:S:2:NAG:O6[1_656]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:O	2:H:68:LYS:NZ[1_556]	2.09	0.11
2:D:68:LYS:CE	1:E:183:GLY:N[1_665]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/441 (95%)	405 (97%)	12 (3%)	0	100	100
1	C	414/441 (94%)	404 (98%)	10 (2%)	0	100	100
1	E	417/441 (95%)	407 (98%)	10 (2%)	0	100	100
1	G	414/441 (94%)	402 (97%)	12 (3%)	0	100	100
2	B	127/141 (90%)	125 (98%)	2 (2%)	0	100	100
2	D	135/141 (96%)	133 (98%)	2 (2%)	0	100	100
2	F	127/141 (90%)	125 (98%)	2 (2%)	0	100	100
2	H	135/141 (96%)	132 (98%)	3 (2%)	0	100	100
All	All	2186/2328 (94%)	2133 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/394 (95%)	369 (98%)	7 (2%)	57	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	373/394 (95%)	363 (97%)	10 (3%)	44	74
1	E	376/394 (95%)	366 (97%)	10 (3%)	44	74
1	G	373/394 (95%)	360 (96%)	13 (4%)	36	65
2	B	121/128 (94%)	119 (98%)	2 (2%)	60	84
2	D	126/128 (98%)	125 (99%)	1 (1%)	81	93
2	F	121/128 (94%)	120 (99%)	1 (1%)	81	93
2	H	126/128 (98%)	121 (96%)	5 (4%)	31	60
All	All	1992/2088 (95%)	1943 (98%)	49 (2%)	47	76

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	A	316	LEU
1	A	325	SER
1	A	351	TYR
1	A	487	ARG
1	A	554	ASP
1	A	602	SER
2	B	125	GLU
2	B	167	ASP
1	C	191	GLN
1	C	233	HIS
1	C	339	LYS
1	C	351	TYR
1	C	391	LYS
1	C	478	GLN
1	C	486	SER
1	C	487	ARG
1	C	519	TRP
1	C	547	TYR
2	D	105	ASP
1	E	184	LEU
1	E	187	GLN
1	E	233	HIS
1	E	316	LEU
1	E	326	ASP
1	E	338	THR
1	E	346	ASP
1	E	351	TYR

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Mol	Chain	Res	Type
1	E	487	ARG
1	E	491	SER
2	F	167	ASP
1	G	189	CYS
1	G	191	GLN
1	G	216	CYS
1	G	233	HIS
1	G	246	LYS
1	G	316	LEU
1	G	346	ASP
1	G	351	TYR
1	G	487	ARG
1	G	491	SER
1	G	528	SER
1	G	554	ASP
1	G	602	SER
2	H	27	SER
2	H	40	SER
2	H	72	GLN
2	H	125	GLU
2	H	128	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	478	GLN
1	C	518	ASN
1	C	559	GLN
2	F	85	GLN
2	F	95	ASN
2	F	106	GLN
2	F	148	GLN
1	G	187	GLN
1	G	191	GLN
1	G	287	HIS

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 ⓘ

44 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$
3	NAG	I	1	1,3	14,14,15	0.21	0	17,19,21	0.57	0
3	NAG	I	2	3	14,14,15	1.16	1 (7%)	17,19,21	2.54	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.24	0	17,19,21	0.62	1 (5%)
3	NAG	J	2	3	14,14,15	0.37	0	17,19,21	1.26	1 (5%)
4	NAG	K	1	1,4	14,14,15	0.38	0	17,19,21	0.44	0
4	NAG	K	2	4	14,14,15	0.34	0	17,19,21	0.39	0
4	BMA	K	3	4	11,11,12	0.87	0	15,15,17	1.17	1 (6%)
4	MAN	K	4	4	11,11,12	0.97	0	15,15,17	1.32	2 (13%)
4	MAN	K	5	4	11,11,12	0.85	0	15,15,17	1.21	2 (13%)
4	FUC	K	6	4	10,10,11	1.03	2 (20%)	14,14,16	1.27	2 (14%)
4	FUC	K	7	4	10,10,11	0.91	0	14,14,16	0.94	0
3	NAG	L	1	1,3	14,14,15	0.25	0	17,19,21	0.62	1 (5%)
3	NAG	L	2	3	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.39	0	17,19,21	0.35	0
3	NAG	M	2	3	14,14,15	0.36	0	17,19,21	0.62	0
5	NAG	N	1	1,5	14,14,15	0.36	0	17,19,21	0.42	0
5	NAG	N	2	5	14,14,15	0.42	0	17,19,21	0.45	0
5	MAN	N	3	5	11,11,12	0.94	1 (9%)	15,15,17	0.95	1 (6%)
5	BMA	N	4	5	11,11,12	0.67	0	15,15,17	1.01	1 (6%)
5	MAN	N	5	5	11,11,12	0.70	0	15,15,17	1.25	1 (6%)
5	FUC	N	6	5	10,10,11	0.92	1 (10%)	14,14,16	0.80	0
5	FUC	N	7	5	10,10,11	0.83	0	14,14,16	1.03	1 (7%)
6	NAG	O	1	1,6	14,14,15	0.24	0	17,19,21	0.69	0
6	NAG	O	2	6	14,14,15	0.18	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	O	3	6	11,11,12	0.53	0	15,15,17	1.05	0
3	NAG	P	1	1,3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	P	2	3	14,14,15	0.20	0	17,19,21	0.51	0
7	NAG	Q	1	1,7	14,14,15	0.24	0	17,19,21	0.48	0
7	NAG	Q	2	7	14,14,15	0.37	0	17,19,21	0.40	0
7	BMA	Q	3	7	11,11,12	0.71	0	15,15,17	1.01	0
7	FUC	Q	4	7	10,10,11	0.81	0	14,14,16	0.92	0
7	FUC	Q	5	7	10,10,11	0.82	1 (10%)	14,14,16	0.90	0
6	NAG	R	1	1,6	14,14,15	0.18	0	17,19,21	0.71	1 (5%)
6	NAG	R	2	6	14,14,15	0.46	0	17,19,21	0.75	1 (5%)
6	BMA	R	3	6	11,11,12	0.98	0	15,15,17	0.92	0
3	NAG	S	1	1,3	14,14,15	0.42	0	17,19,21	0.46	0
3	NAG	S	2	3	14,14,15	0.38	0	17,19,21	0.45	0
4	NAG	T	1	1,4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	T	2	4	14,14,15	0.18	0	17,19,21	0.52	0
4	BMA	T	3	4	11,11,12	0.93	0	15,15,17	1.41	3 (20%)
4	MAN	T	4	4	11,11,12	0.91	0	15,15,17	1.19	2 (13%)
4	MAN	T	5	4	11,11,12	0.73	0	15,15,17	1.49	2 (13%)
4	FUC	T	6	4	10,10,11	0.92	1 (10%)	14,14,16	0.85	0
4	FUC	T	7	4	10,10,11	0.65	0	14,14,16	0.78	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
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	5/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	K	4	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	K	5	4	-	2/2/19/22	0/1/1/1
4	FUC	K	6	4	1/1/4/5	-	0/1/1/1
4	FUC	K	7	4	-	-	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	2	NAG	O5-C1	4.13	1.50	1.43
5	N	3	MAN	O5-C1	-2.74	1.39	1.43
5	N	6	FUC	O5-C1	-2.44	1.39	1.43
7	Q	5	FUC	O5-C1	-2.19	1.40	1.43
4	T	6	FUC	O5-C1	-2.11	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	6	FUC	O5-C1	-2.06	1.40	1.43
4	K	6	FUC	C2-C3	2.02	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C1-O5-C5	10.29	126.14	112.19
3	J	2	NAG	C2-N2-C7	4.31	129.04	122.90
6	O	2	NAG	C1-O5-C5	3.60	117.07	112.19
4	T	5	MAN	C1-O5-C5	3.40	116.80	112.19
3	L	2	NAG	C1-O5-C5	3.35	116.73	112.19
4	T	4	MAN	O2-C2-C3	-3.29	103.54	110.14
5	N	5	MAN	C1-O5-C5	3.24	116.58	112.19
4	K	6	FUC	C1-C2-C3	3.14	113.52	109.67
4	T	5	MAN	O5-C1-C2	2.89	115.24	110.77
4	K	5	MAN	C1-O5-C5	2.82	116.01	112.19
6	R	2	NAG	C1-O5-C5	2.78	115.95	112.19
4	K	4	MAN	O5-C1-C2	2.50	114.64	110.77
4	K	4	MAN	C1-O5-C5	2.49	115.56	112.19
6	R	1	NAG	C1-O5-C5	2.48	115.56	112.19
4	T	4	MAN	C1-O5-C5	2.42	115.48	112.19
4	K	3	BMA	O5-C1-C2	2.42	114.51	110.77
4	K	6	FUC	O5-C1-C2	2.41	114.48	110.77
4	T	3	BMA	O2-C2-C3	-2.36	105.40	110.14
4	T	3	BMA	C2-C3-C4	-2.26	106.99	110.89
4	K	5	MAN	O5-C1-C2	2.17	114.13	110.77
3	L	1	NAG	C1-O5-C5	2.17	115.14	112.19
5	N	3	MAN	O2-C2-C3	-2.17	105.79	110.14
4	T	3	BMA	C1-O5-C5	2.13	115.08	112.19
5	N	4	BMA	O5-C5-C4	-2.08	105.78	110.83
3	J	1	NAG	C1-O5-C5	2.04	114.95	112.19
5	N	7	FUC	C1-O5-C5	2.02	117.36	112.78

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	K	6	FUC	C1
4	T	4	MAN	C1
4	T	3	BMA	C1
4	K	4	MAN	C1
5	N	3	MAN	C1
5	N	4	BMA	C1

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Mol	Chain	Res	Type	Atom
4	K	3	BMA	C1

All (37) torsion outliers are listed below:

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

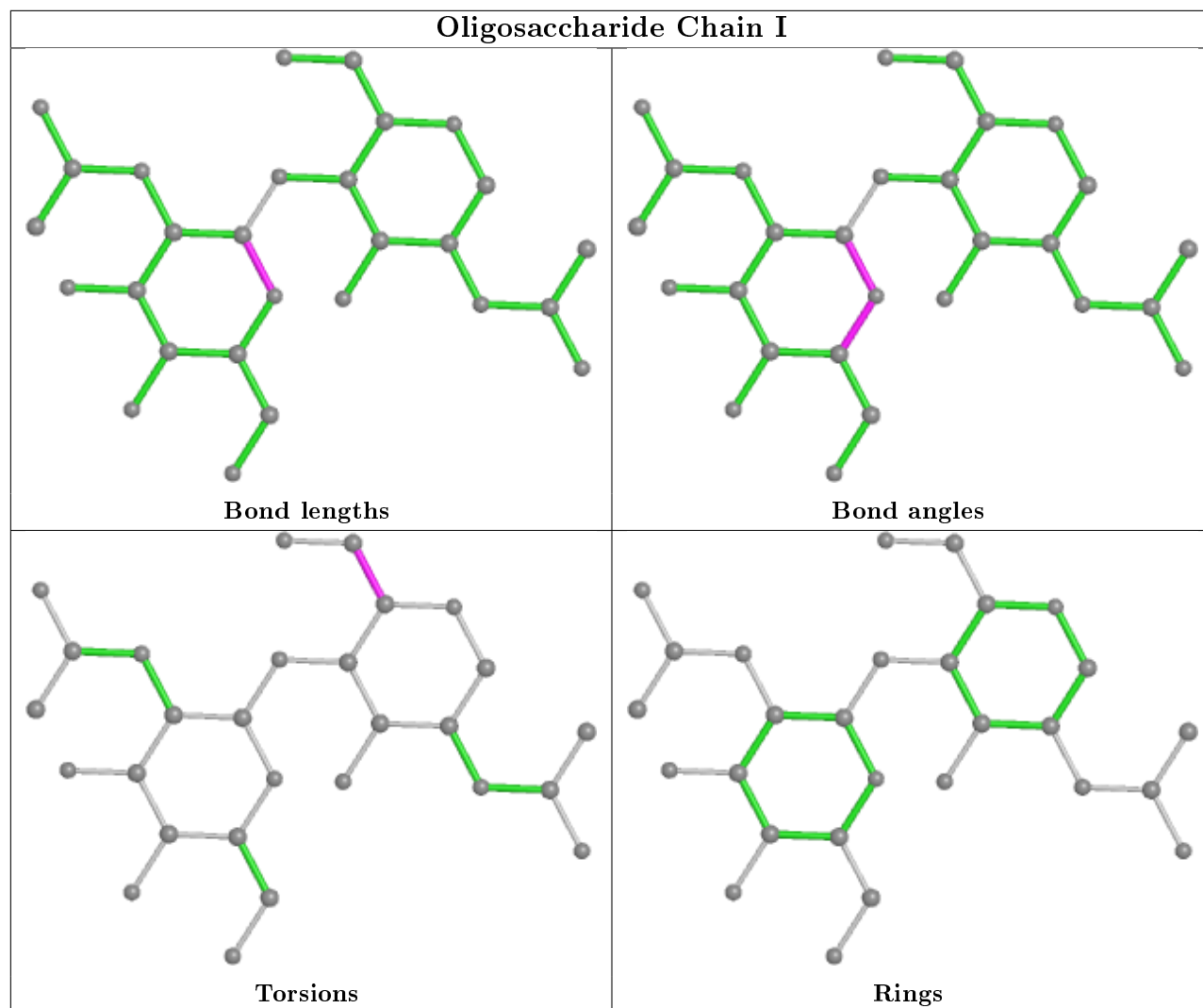
All (1) ring outliers are listed below:

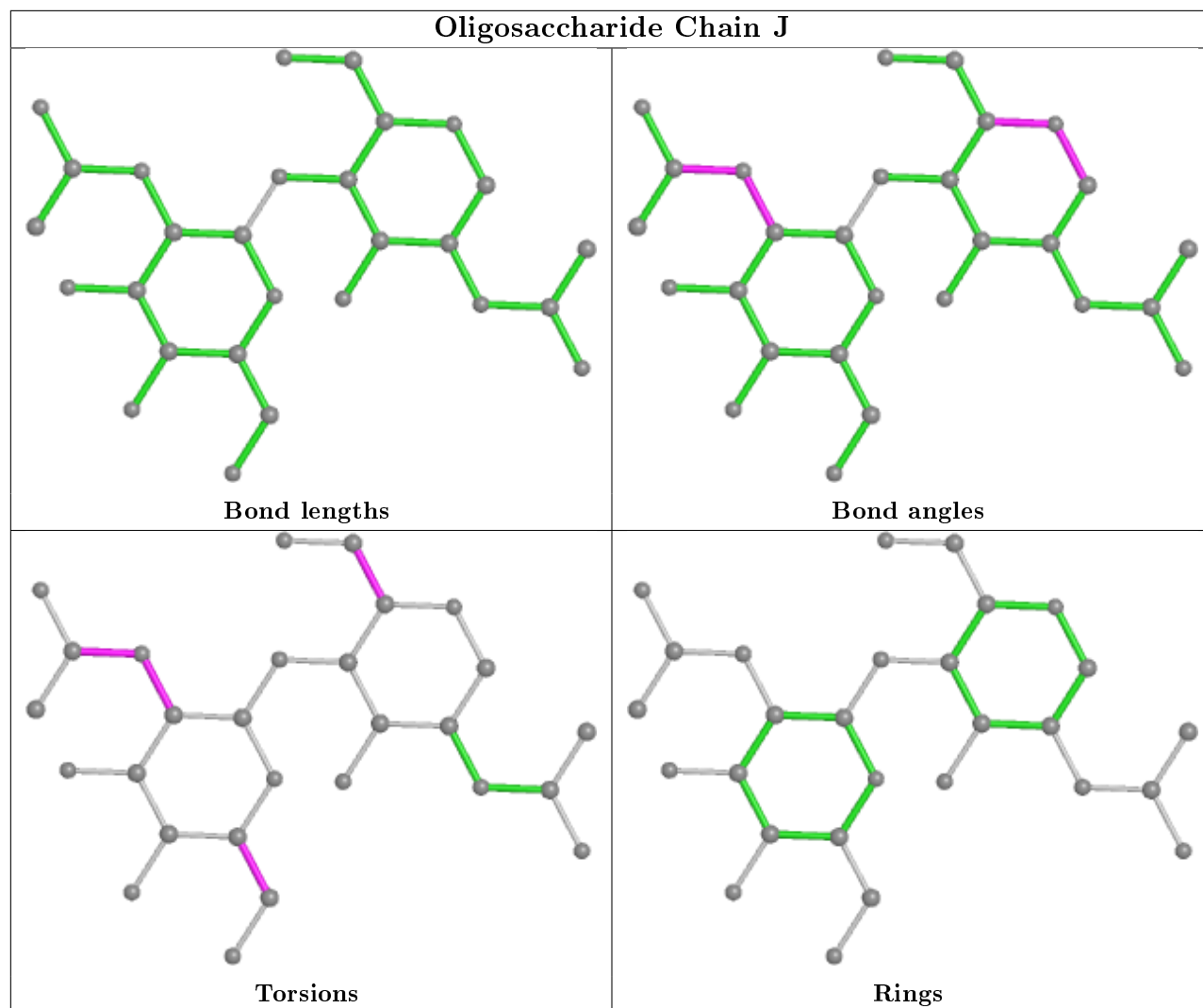
Mol	Chain	Res	Type	Atoms
4	T	3	BMA	C1-C2-C3-C4-C5-O5

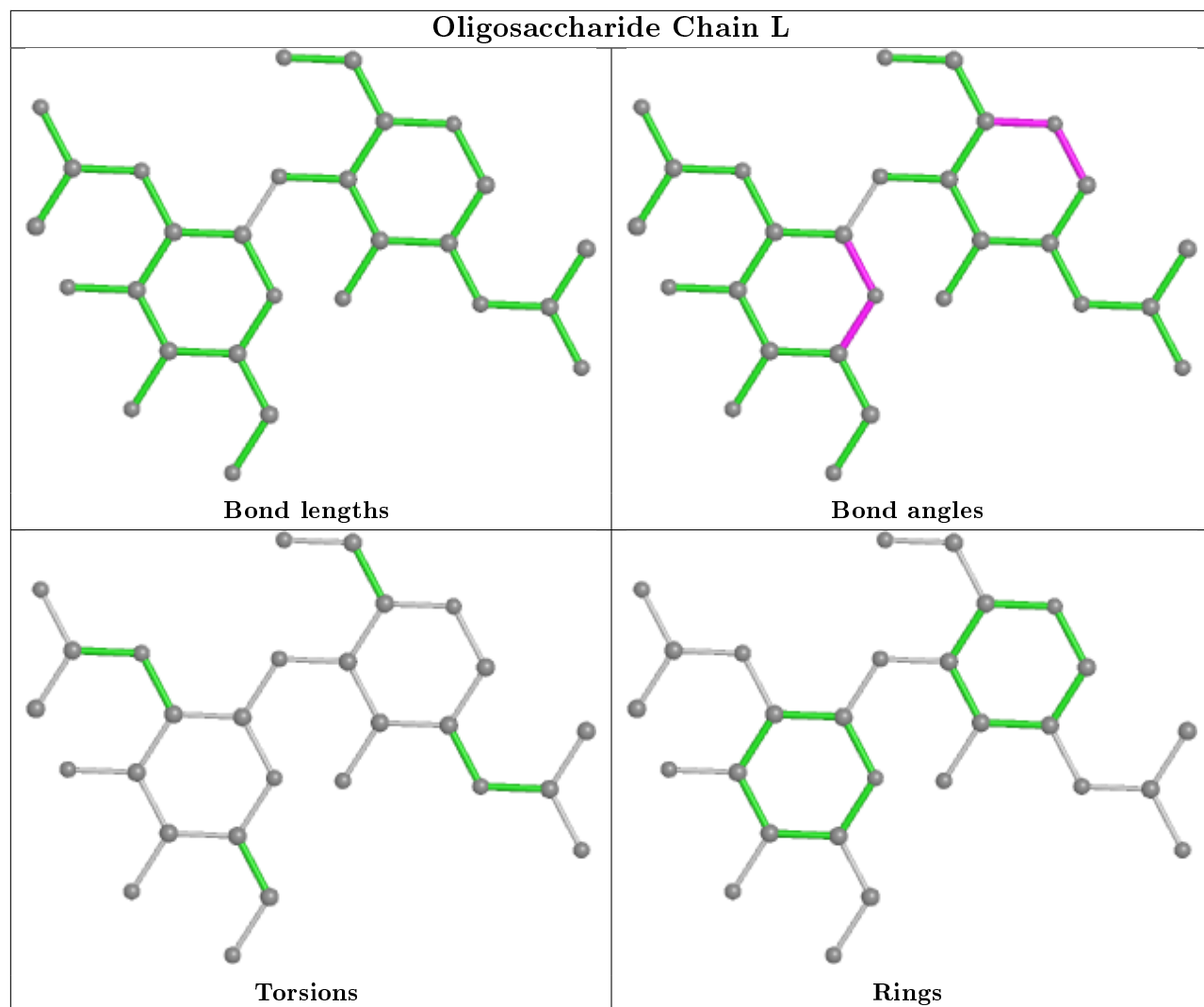
7 monomers are involved in 7 short contacts:

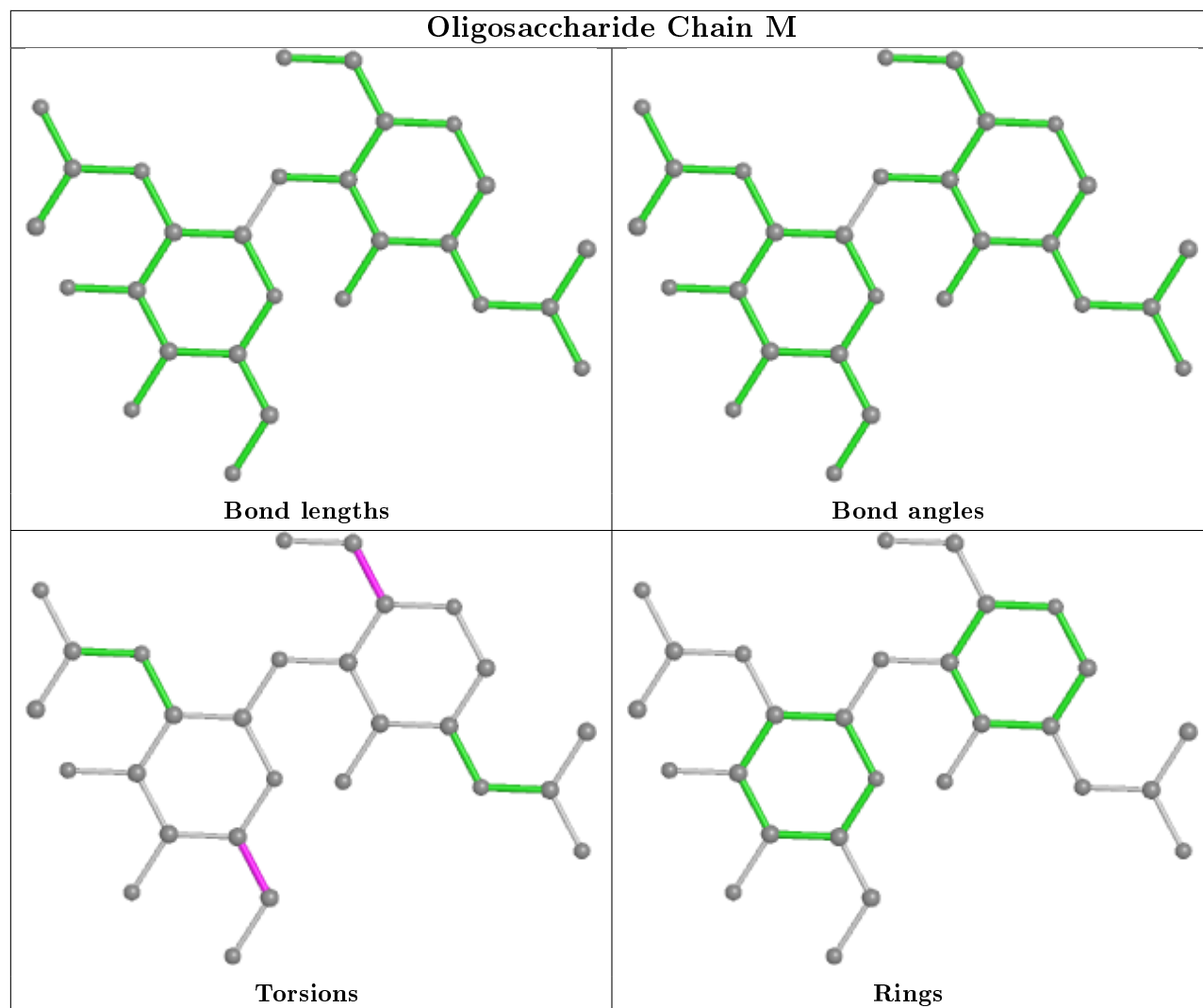
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	1	0
3	P	2	NAG	1	0
4	K	4	MAN	1	1
3	J	2	NAG	2	0
3	L	1	NAG	1	0
3	P	1	NAG	1	0
3	S	2	NAG	0	1

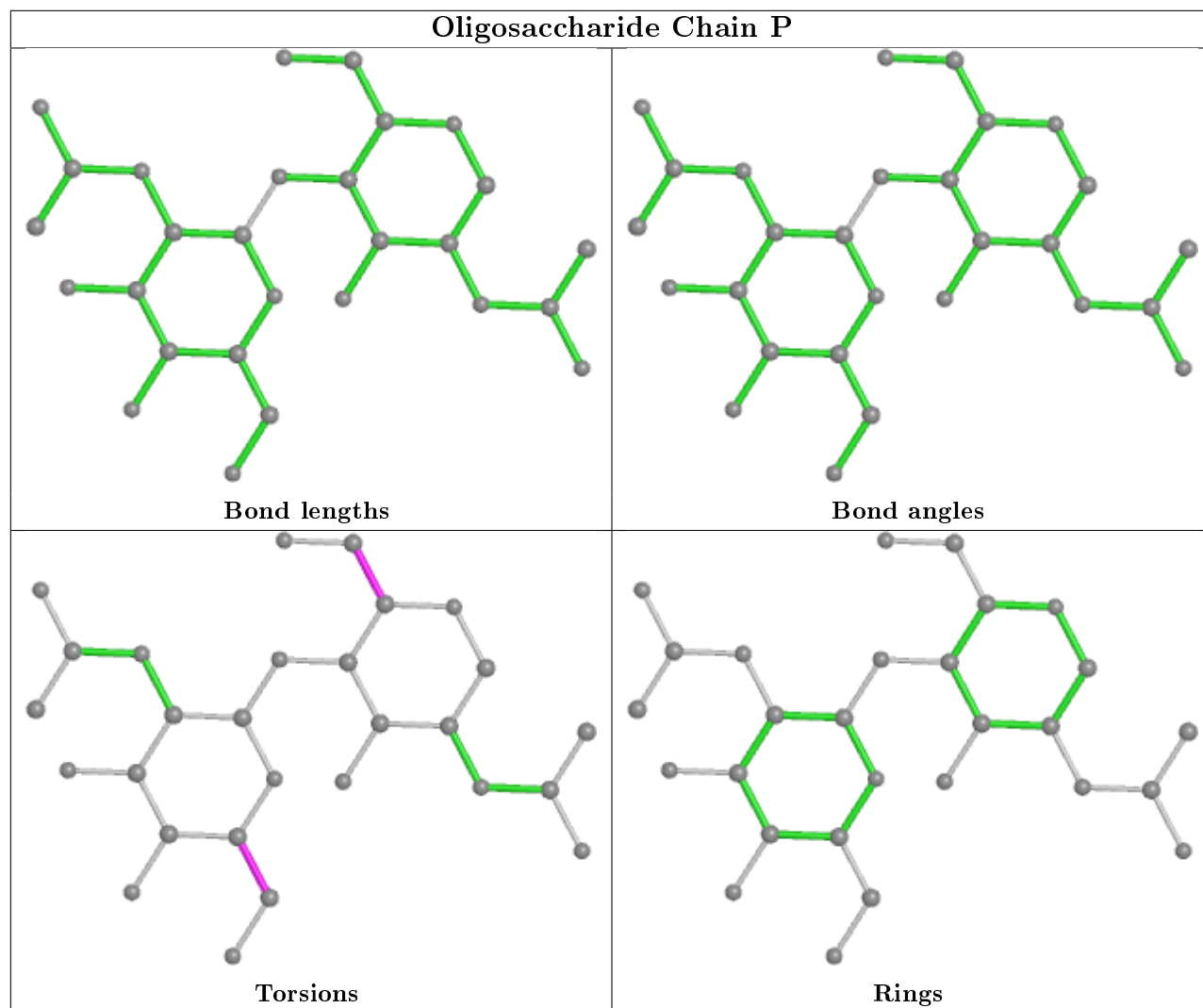
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

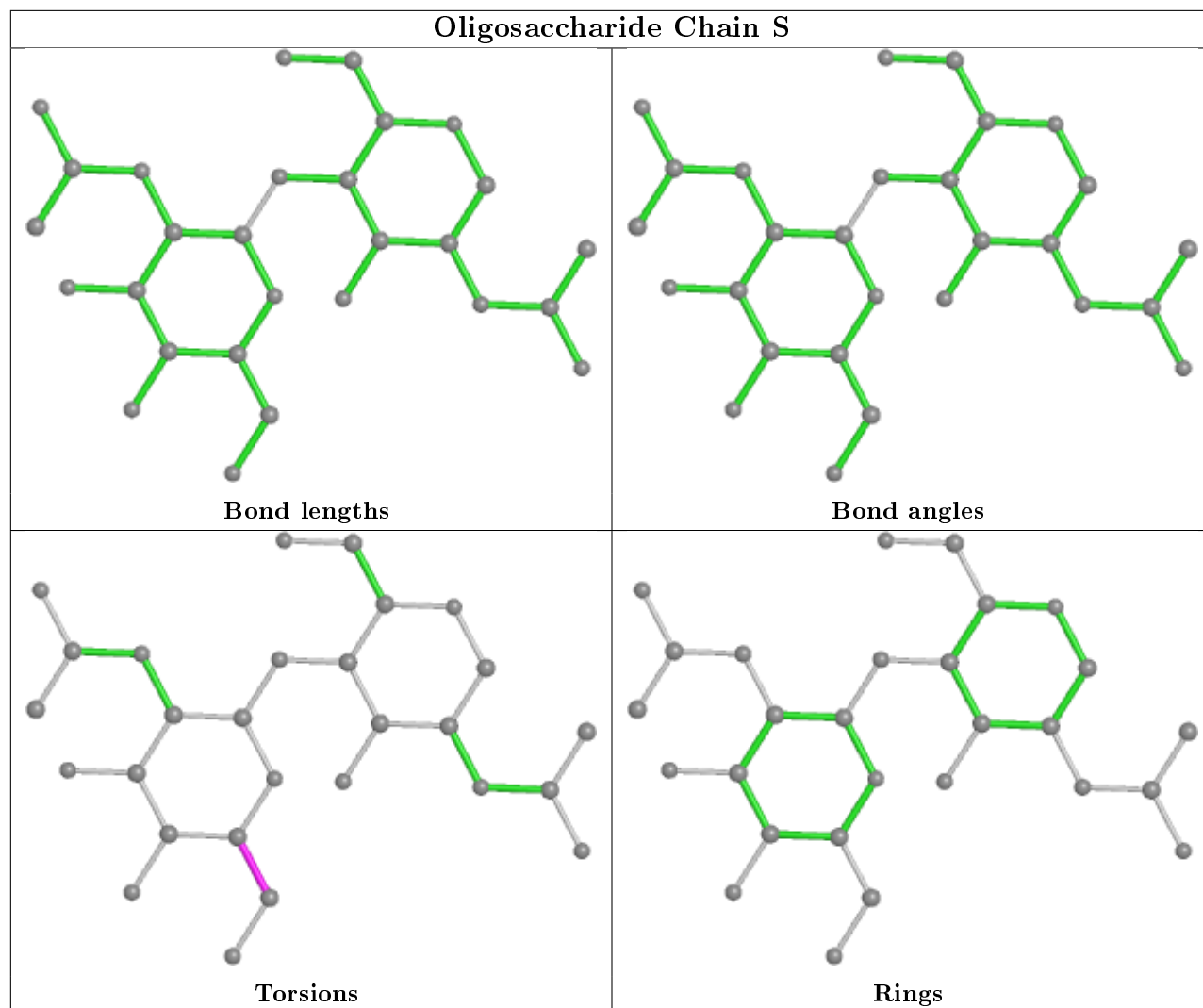


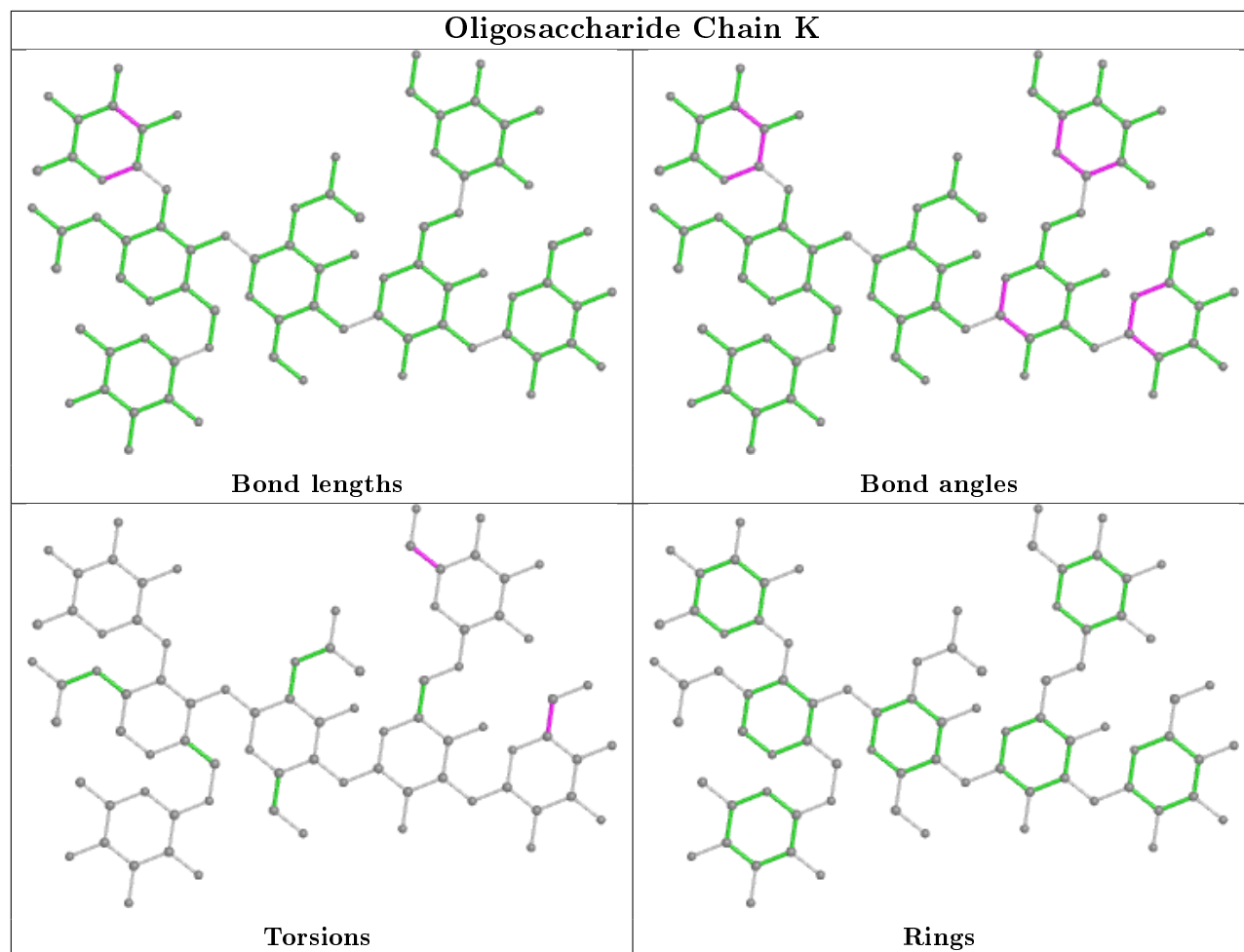


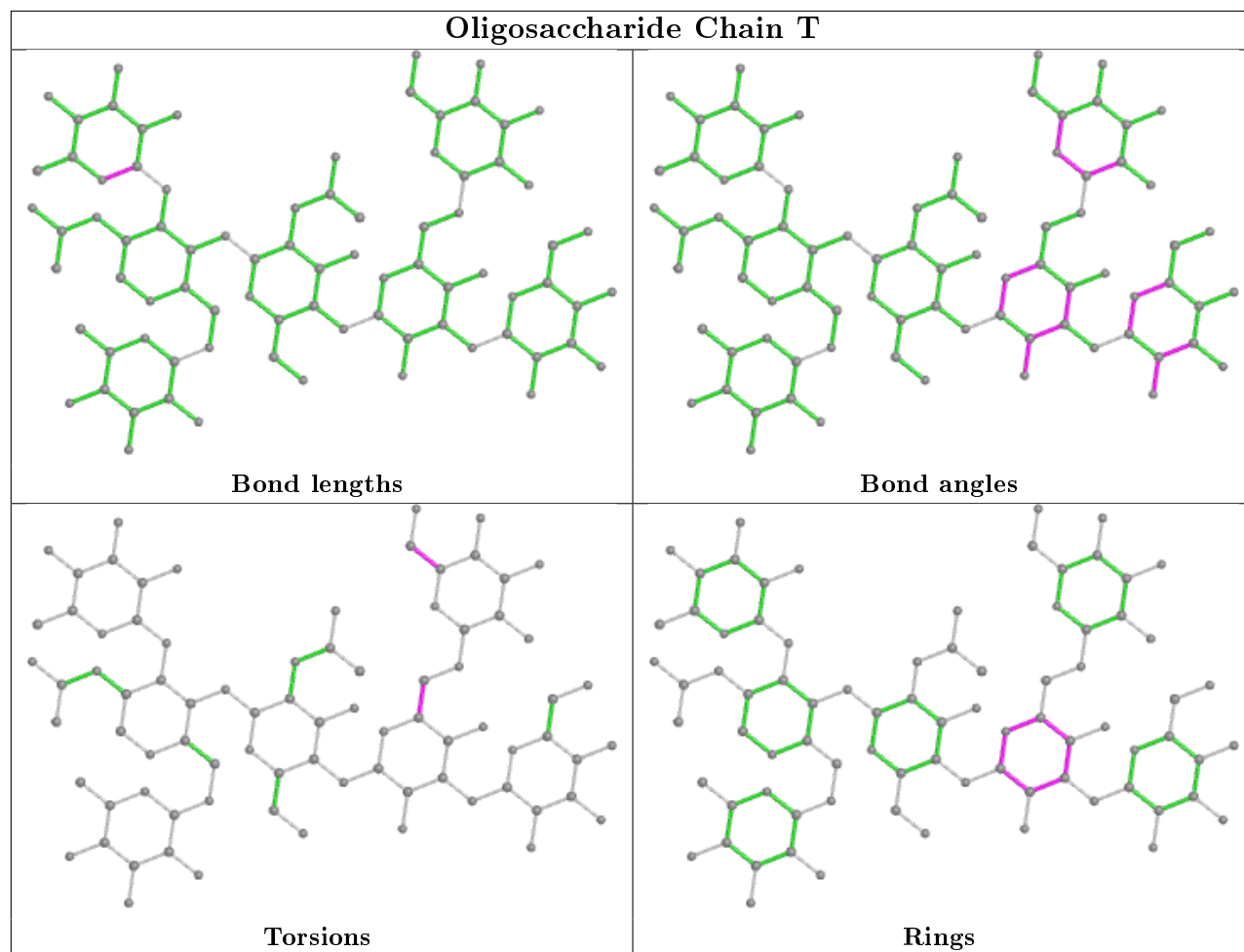


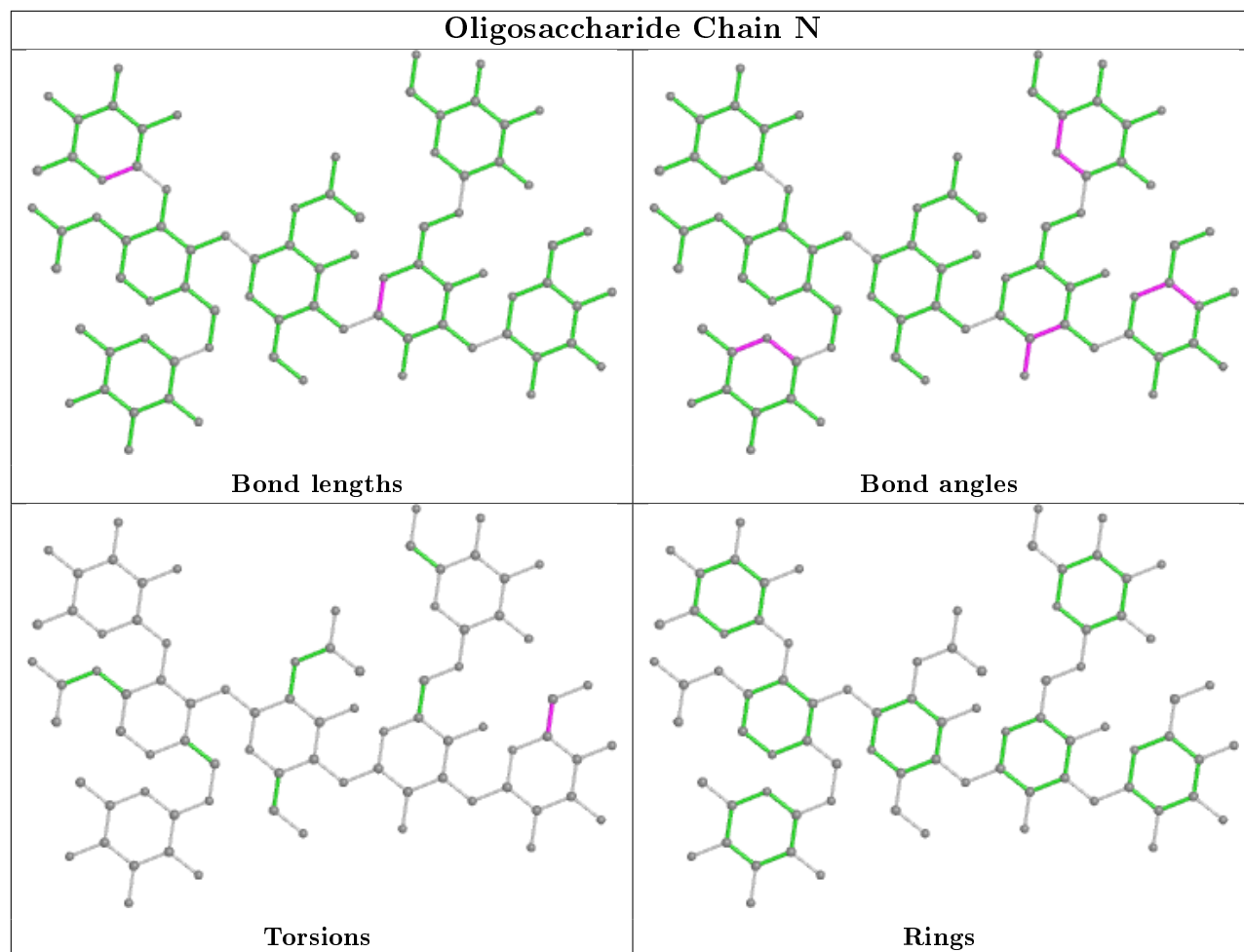


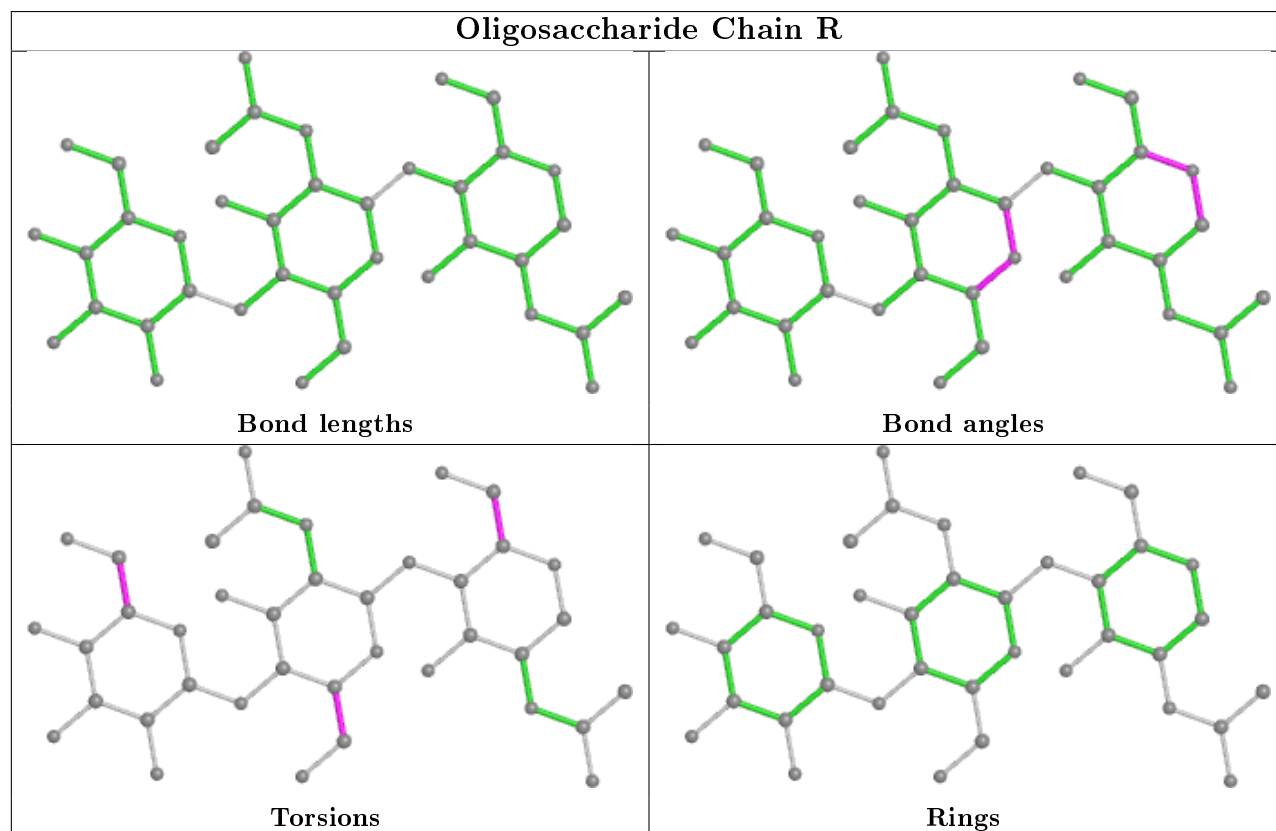
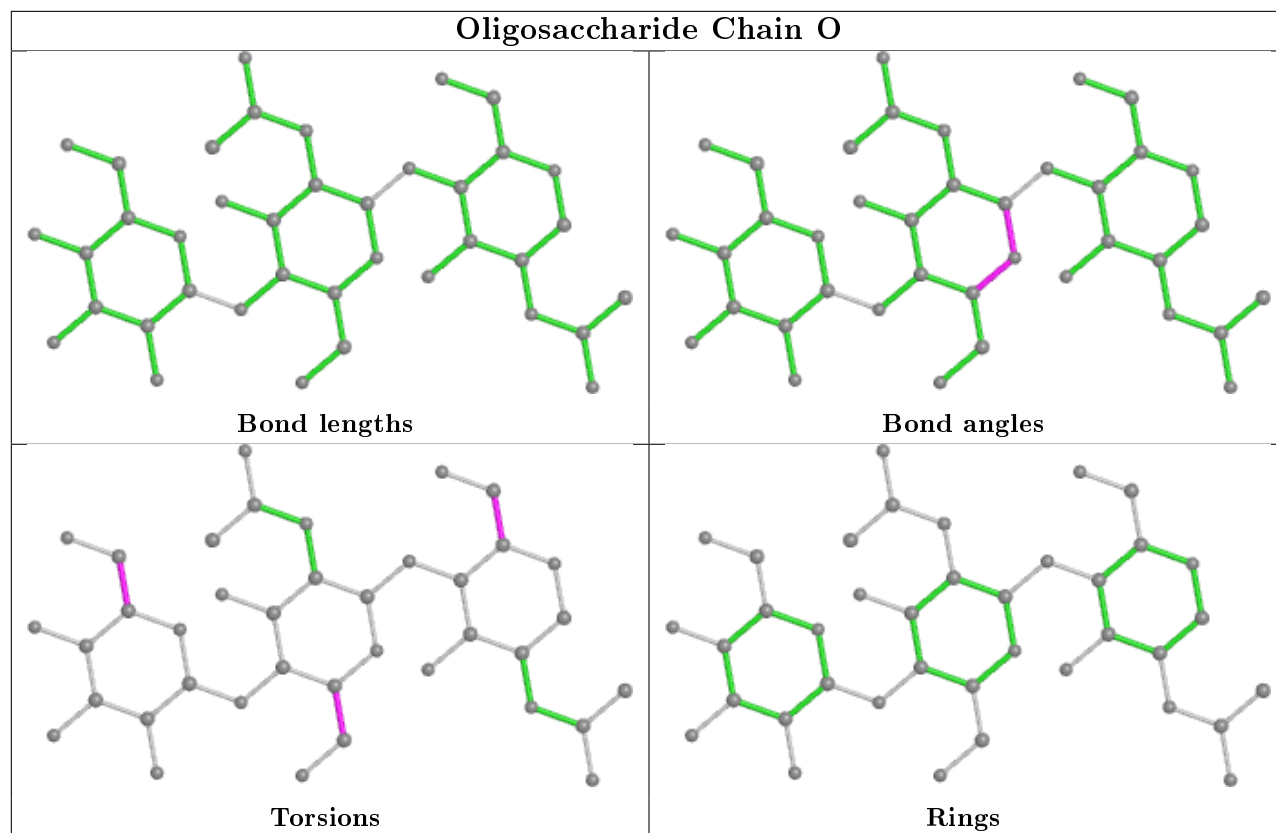


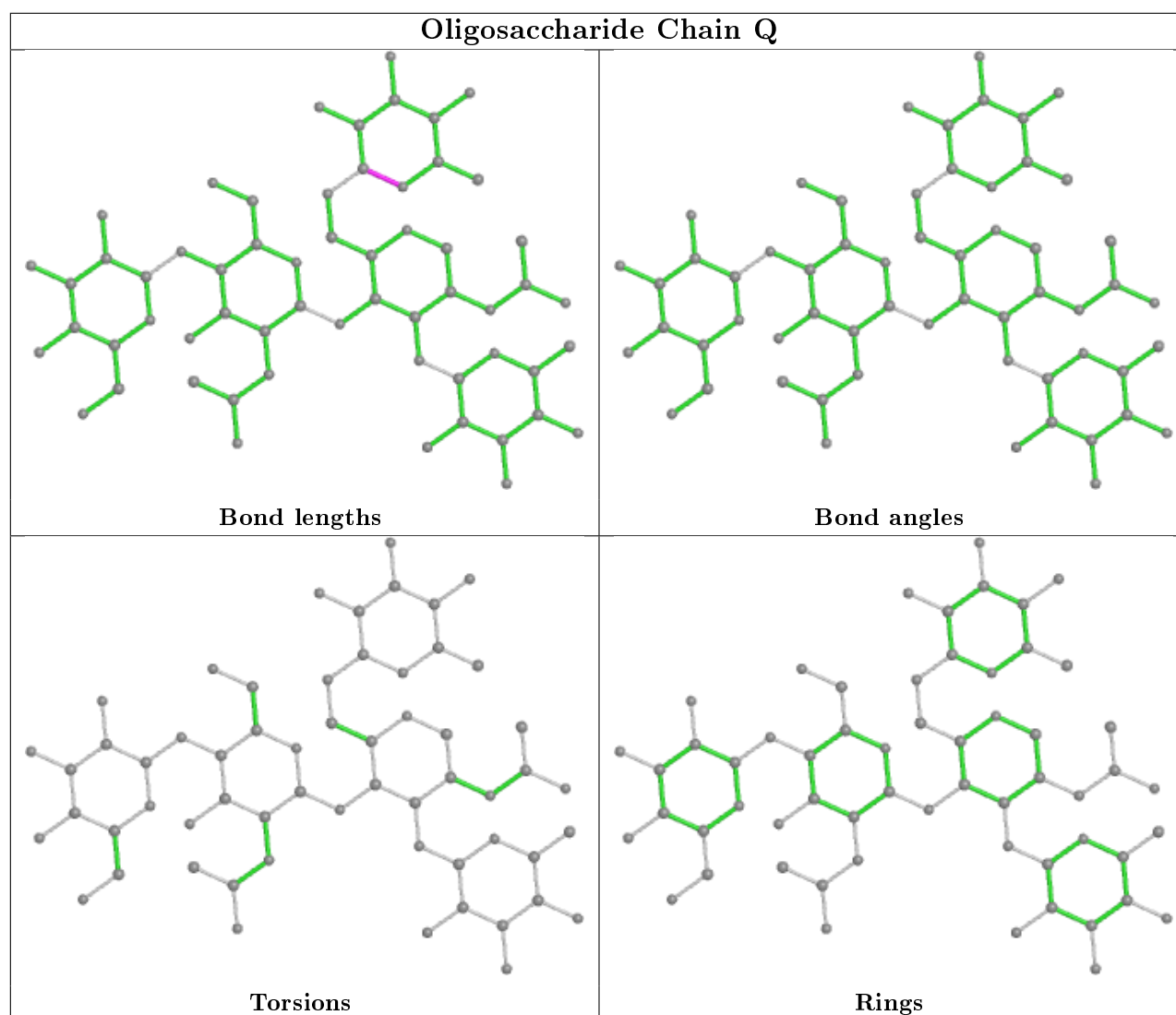












5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	NAG	F	201	2	14,14,15	0.58	0	17,19,21	1.03	1 (5%)
8	NAG	D	201	2	14,14,15	0.61	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	702	1	14,14,15	0.47	0	17,19,21	0.73	1 (5%)
8	NAG	E	702	1	14,14,15	0.56	0	17,19,21	0.85	1 (5%)
8	NAG	A	702	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	0
8	NAG	G	701	1	14,14,15	0.75	1 (7%)	17,19,21	0.56	0
8	NAG	E	701	1	14,14,15	0.45	0	17,19,21	0.78	0
8	NAG	H	202	2	14,14,15	1.27	2 (14%)	17,19,21	0.73	0
8	NAG	C	701	1	14,14,15	0.68	1 (7%)	17,19,21	0.66	1 (5%)
8	NAG	G	702	1	14,14,15	0.72	1 (7%)	17,19,21	0.61	0
8	NAG	A	701	1	14,14,15	0.57	0	17,19,21	0.67	1 (5%)
8	NAG	H	201	2	14,14,15	0.66	0	17,19,21	0.89	1 (5%)
8	NAG	B	201	2	14,14,15	0.74	1 (7%)	17,19,21	0.85	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	201	2	-	1/6/23/26	0/1/1/1
8	NAG	D	201	2	-	0/6/23/26	0/1/1/1
8	NAG	C	702	1	-	2/6/23/26	0/1/1/1
8	NAG	E	702	1	-	2/6/23/26	0/1/1/1
8	NAG	A	702	1	-	2/6/23/26	0/1/1/1
8	NAG	G	701	1	-	0/6/23/26	0/1/1/1
8	NAG	E	701	1	-	2/6/23/26	0/1/1/1
8	NAG	H	202	2	-	2/6/23/26	0/1/1/1
8	NAG	C	701	1	-	0/6/23/26	0/1/1/1
8	NAG	G	702	1	-	0/6/23/26	0/1/1/1
8	NAG	A	701	1	-	0/6/23/26	0/1/1/1
8	NAG	H	201	2	-	1/6/23/26	0/1/1/1
8	NAG	B	201	2	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	202	NAG	C1-C2	3.66	1.57	1.52
8	H	202	NAG	O5-C1	2.70	1.48	1.43
8	G	701	NAG	O5-C1	2.59	1.47	1.43
8	B	201	NAG	O5-C1	2.48	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	702	NAG	O5-C1	2.21	1.47	1.43
8	C	701	NAG	O5-C1	2.12	1.47	1.43
8	G	702	NAG	O5-C1	2.11	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	201	NAG	C1-O5-C5	3.34	116.72	112.19
8	F	201	NAG	C1-O5-C5	2.88	116.09	112.19
8	B	201	NAG	C1-O5-C5	2.85	116.06	112.19
8	D	201	NAG	C1-O5-C5	2.79	115.97	112.19
8	E	702	NAG	C1-O5-C5	2.61	115.73	112.19
8	C	702	NAG	C1-O5-C5	2.54	115.63	112.19
8	A	701	NAG	C1-O5-C5	2.15	115.10	112.19
8	C	701	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	702	NAG	O5-C5-C6-O6
8	H	202	NAG	O5-C5-C6-O6
8	A	702	NAG	C4-C5-C6-O6
8	E	701	NAG	C8-C7-N2-C2
8	E	701	NAG	O7-C7-N2-C2
8	H	201	NAG	O5-C5-C6-O6
8	H	202	NAG	C4-C5-C6-O6
8	F	201	NAG	O5-C5-C6-O6
8	C	702	NAG	C4-C5-C6-O6
8	E	702	NAG	C4-C5-C6-O6
8	B	201	NAG	O5-C5-C6-O6
8	C	702	NAG	O5-C5-C6-O6
8	E	702	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	201	NAG	1	0
8	E	701	NAG	1	0
8	H	202	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	201	NAG	1	0
8	B	201	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	A	421/441 (95%)	-0.26	7 (1%) 70 72	12, 29, 57, 84	0
1	C	418/441 (94%)	-0.28	7 (1%) 70 72	14, 27, 58, 82	0
1	E	421/441 (95%)	-0.28	5 (1%) 79 80	12, 23, 46, 74	0
1	G	418/441 (94%)	0.01	14 (3%) 46 46	17, 36, 68, 97	0
2	B	133/141 (94%)	-0.16	0 100 100	20, 40, 70, 76	0
2	D	139/141 (98%)	0.10	8 (5%) 23 22	22, 46, 82, 93	0
2	F	133/141 (94%)	-0.25	0 100 100	18, 35, 60, 71	0
2	H	139/141 (98%)	-0.12	5 (3%) 42 42	17, 36, 64, 80	0
All	All	2222/2328 (95%)	-0.18	46 (2%) 63 65	12, 31, 64, 97	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	GLY	5.1
1	G	259	GLY	4.8
2	D	72	GLN	4.2
2	D	68	LYS	4.1
1	E	259	GLY	3.9
2	H	68	LYS	3.7
1	C	421	GLY	3.7
1	G	258	ARG	3.7
1	G	187	GLN	3.5
1	G	260	ASP	3.3
1	G	421	GLY	3.3
1	C	554	ASP	3.2
1	A	600	GLN	3.2
2	D	125	GLU	3.1
1	C	259	GLY	3.0
1	G	420	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	84	ASP	2.9
2	D	28	ILE	2.9
1	G	266	PHE	2.8
1	E	423	ASP	2.8
2	H	70	VAL	2.8
2	D	124	LEU	2.7
2	D	70	VAL	2.7
2	H	67	SER	2.7
2	H	66	ASP	2.7
1	C	600	GLN	2.6
1	A	259	GLY	2.6
1	A	213	GLU	2.5
1	E	421	GLY	2.5
1	G	188	ILE	2.5
1	C	423	ASP	2.5
1	E	258	ARG	2.5
1	G	261	LYS	2.4
1	G	518	ASN	2.4
1	A	423	ASP	2.4
1	G	191	GLN	2.4
1	E	422	GLY	2.3
1	G	256	LEU	2.3
1	G	376	GLN	2.3
1	A	422	GLY	2.2
2	D	149	GLU	2.2
1	A	194	THR	2.1
1	G	264	SER	2.1
1	C	422	GLY	2.0
1	C	420	LEU	2.0
2	H	149	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

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.

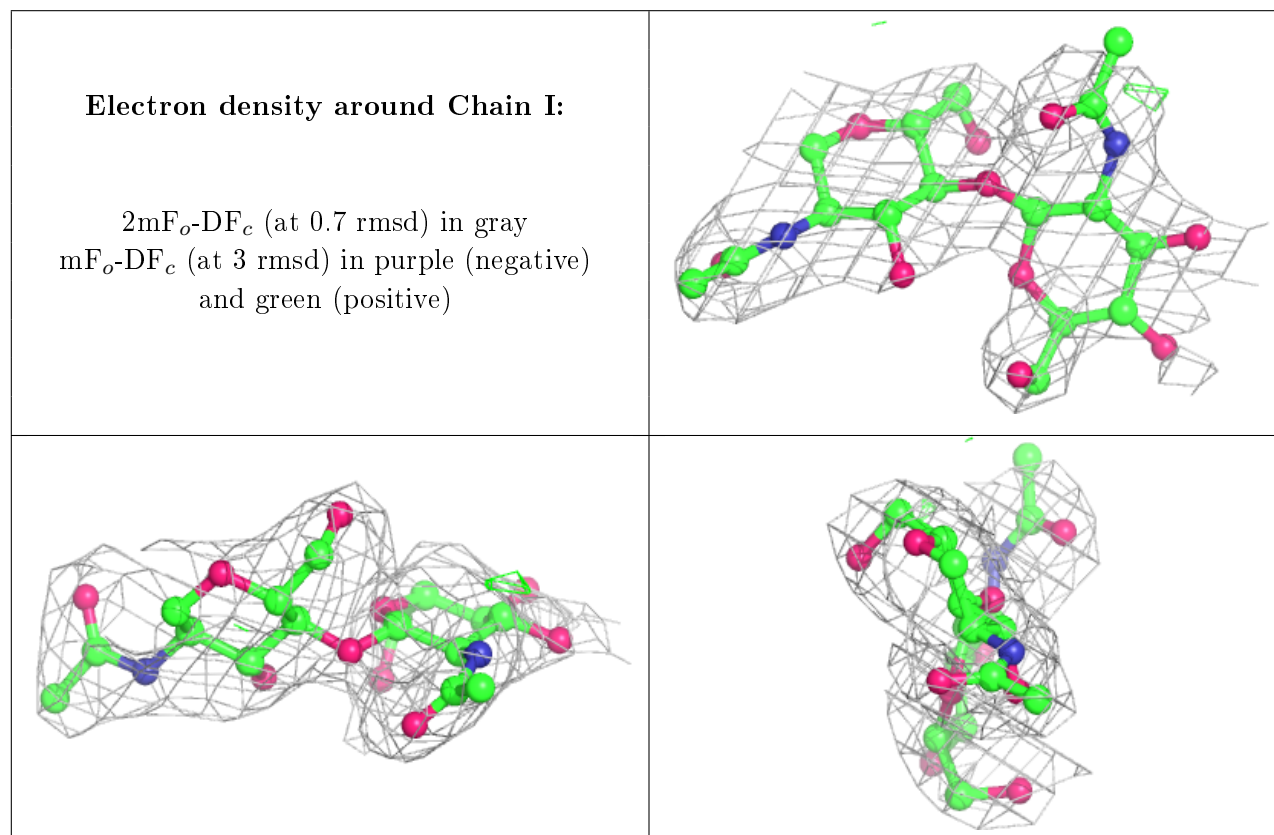
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	K	5	11/12	0.75	0.50	92,103,113,116	0
6	BMA	O	3	11/12	0.81	0.33	75,83,92,94	0
7	BMA	Q	3	11/12	0.81	0.35	74,84,90,91	0
6	NAG	R	1	14/15	0.81	0.37	56,77,90,103	0
6	BMA	R	3	11/12	0.82	0.34	65,80,91,93	0
3	NAG	P	2	14/15	0.83	0.32	50,63,73,81	0
6	NAG	R	2	14/15	0.83	0.47	74,87,93,102	0
4	MAN	K	4	11/12	0.83	0.32	74,93,102,105	0
3	NAG	I	2	14/15	0.84	0.37	53,71,85,87	0
3	NAG	S	2	14/15	0.84	0.40	65,76,80,81	0
4	BMA	K	3	11/12	0.84	0.23	85,95,101,103	0
3	NAG	L	2	14/15	0.84	0.48	55,79,90,93	0
3	NAG	M	2	14/15	0.85	0.31	60,77,89,98	0
3	NAG	J	1	14/15	0.88	0.21	30,62,85,91	0
3	NAG	J	2	14/15	0.88	0.34	52,82,87,88	0
6	NAG	O	2	14/15	0.89	0.33	40,65,83,90	0
4	BMA	T	3	11/12	0.90	0.19	29,42,58,68	0
3	NAG	L	1	14/15	0.90	0.27	28,55,69,83	0
4	NAG	K	2	14/15	0.91	0.18	38,57,82,86	0
3	NAG	I	1	14/15	0.91	0.21	28,46,53,67	0
7	NAG	Q	2	14/15	0.91	0.24	42,53,74,83	0
4	MAN	T	4	11/12	0.92	0.12	25,32,40,48	0
4	FUC	K	6	10/11	0.93	0.17	43,51,61,72	0
3	NAG	S	1	14/15	0.93	0.18	24,38,60,75	0
3	NAG	P	1	14/15	0.93	0.18	21,39,56,68	0
4	FUC	K	7	10/11	0.94	0.11	33,36,45,46	0
7	FUC	Q	4	10/11	0.94	0.22	34,47,51,55	0
5	BMA	N	4	11/12	0.95	0.12	27,31,43,44	0
4	MAN	T	5	11/12	0.95	0.19	36,44,51,57	0
3	NAG	M	1	14/15	0.95	0.14	24,38,60,70	0
5	NAG	N	1	14/15	0.96	0.10	15,20,28,31	0
4	NAG	K	1	14/15	0.96	0.11	30,39,51,56	0
6	NAG	O	1	14/15	0.96	0.23	30,40,58,61	0
4	NAG	T	2	14/15	0.96	0.13	20,29,37,41	0
7	FUC	Q	5	10/11	0.97	0.13	20,28,46,48	0
5	MAN	N	5	11/12	0.97	0.13	18,25,32,35	0
4	FUC	T	6	10/11	0.97	0.17	26,36,41,57	0
7	NAG	Q	1	14/15	0.97	0.08	18,34,43,50	0
5	FUC	N	7	10/11	0.97	0.07	15,27,32,32	0
5	MAN	N	3	11/12	0.97	0.10	27,33,41,44	0
5	NAG	N	2	14/15	0.97	0.12	16,29,38,42	0
4	NAG	T	1	14/15	0.98	0.09	18,23,29,33	0
5	FUC	N	6	10/11	0.98	0.14	21,28,33,42	0

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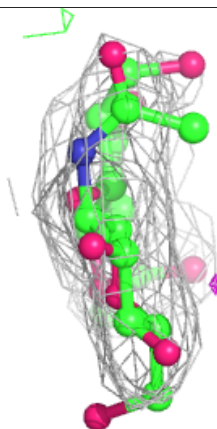
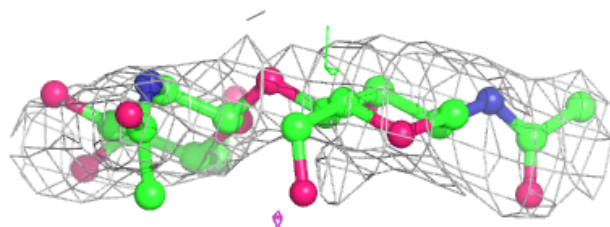
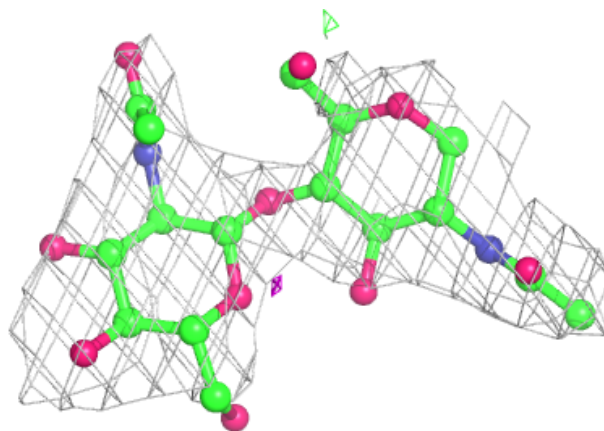
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FUC	T	7	10/11	0.98	0.11	23,28,40,53	0

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.



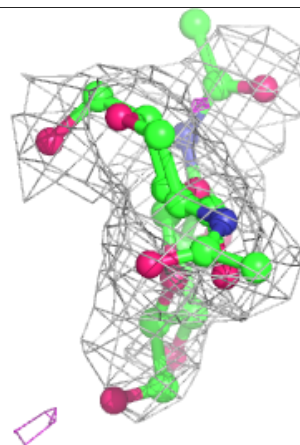
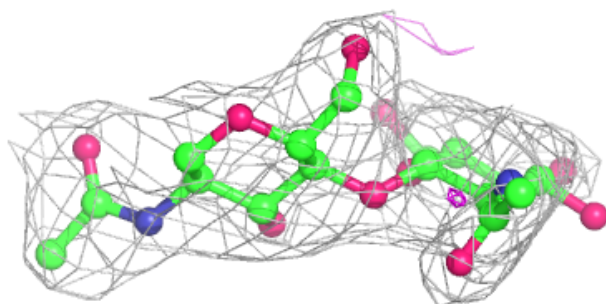
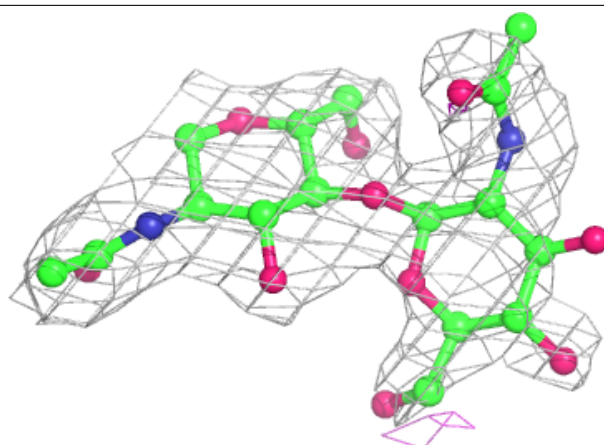
Electron density around Chain J:

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



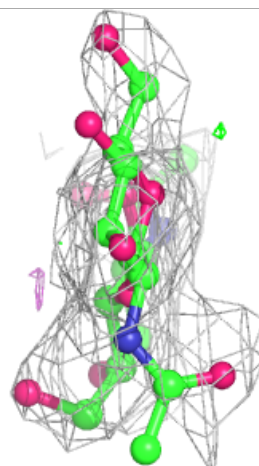
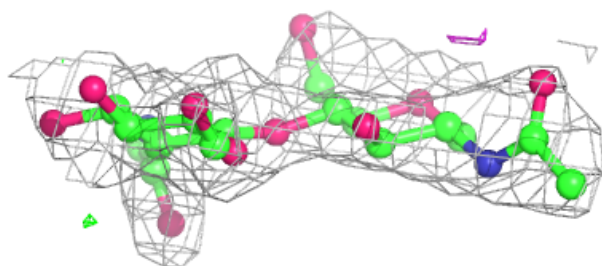
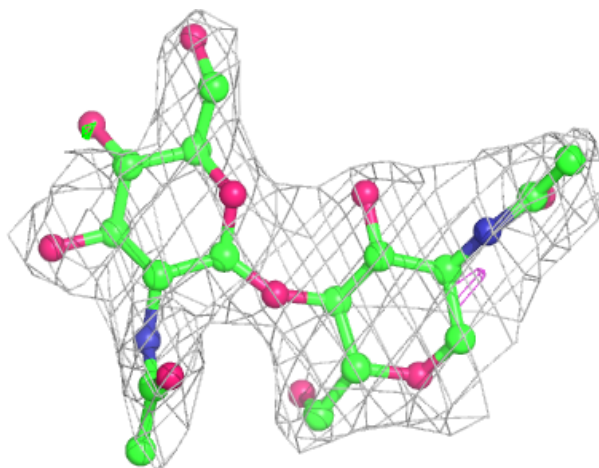
Electron density around Chain L:

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



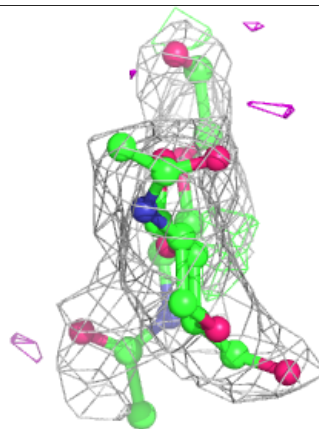
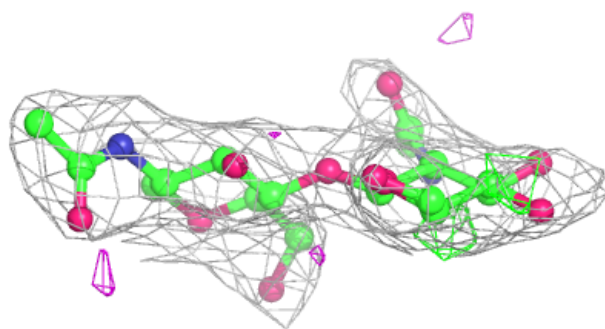
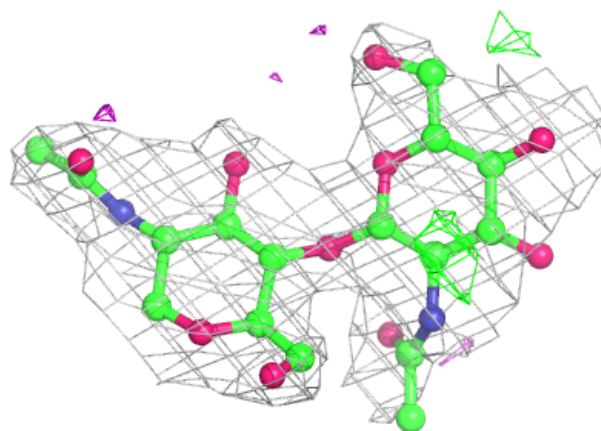
Electron density around Chain M:

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



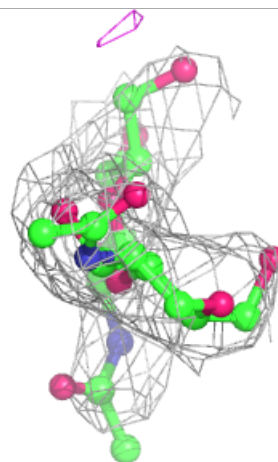
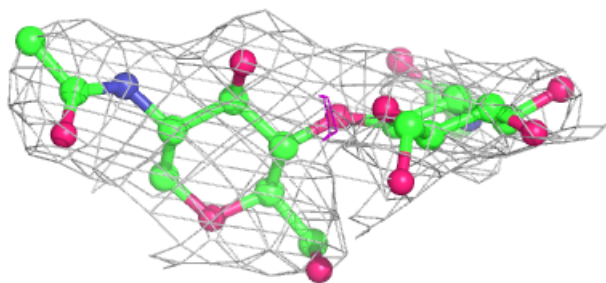
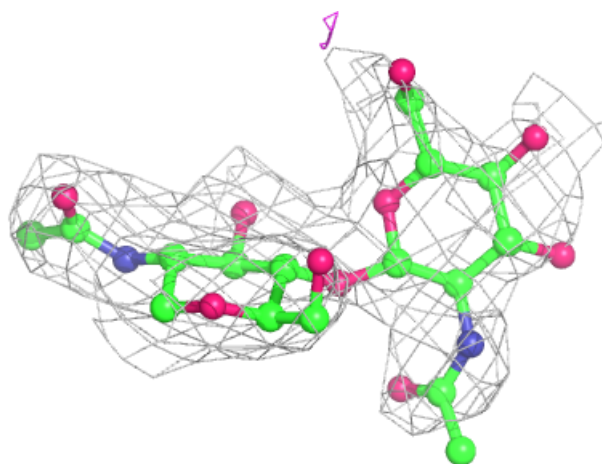
Electron density around Chain P:

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



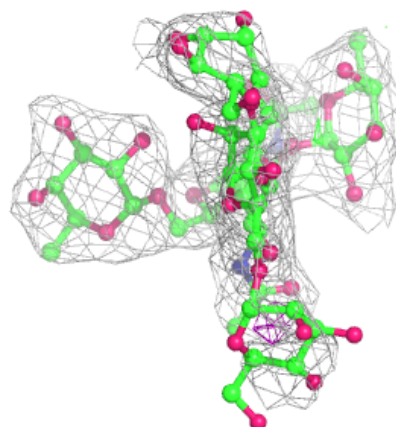
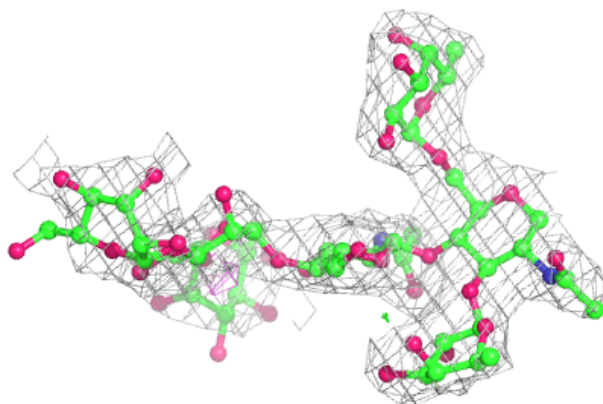
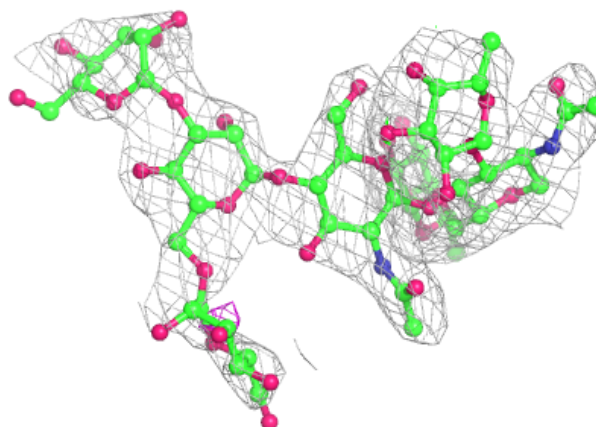
Electron density around Chain S:

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



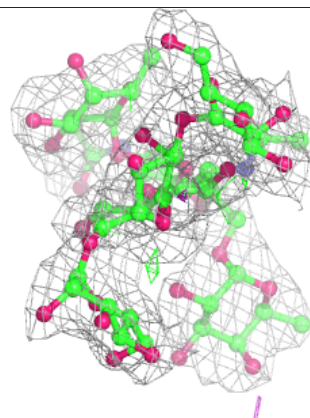
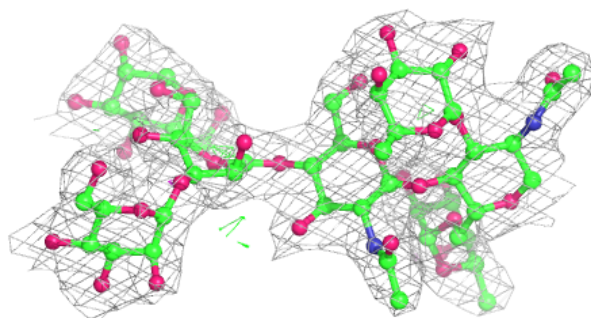
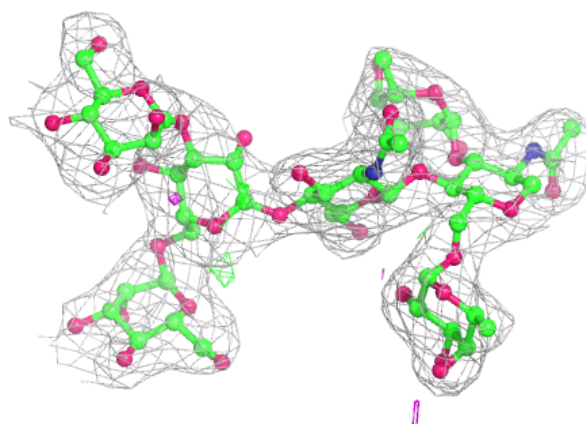
Electron density around Chain K:

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

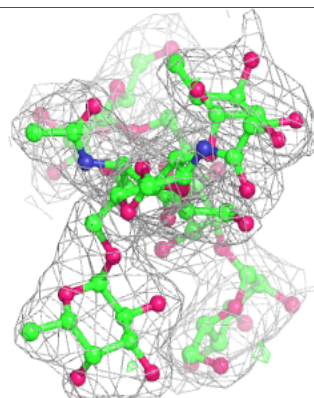
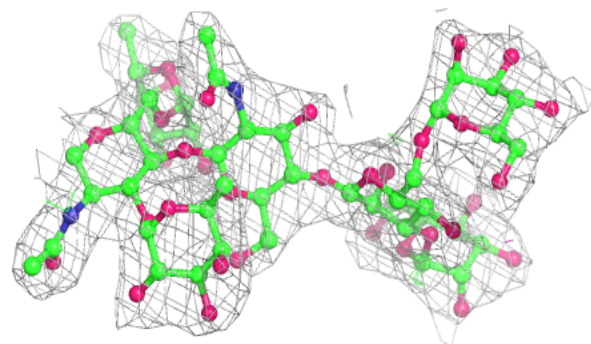
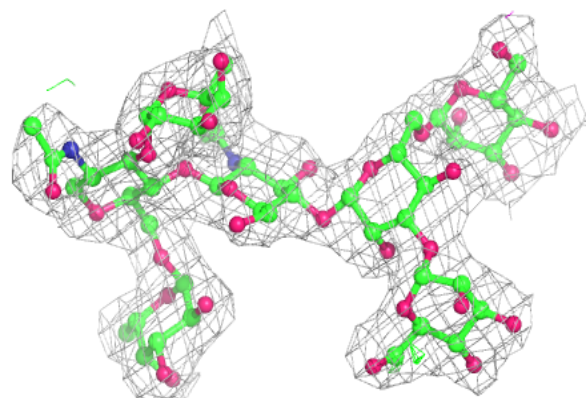


Electron density around Chain T:

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

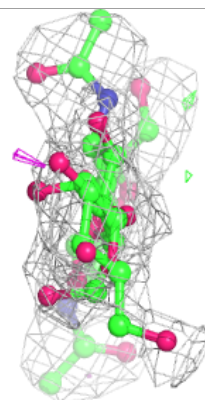
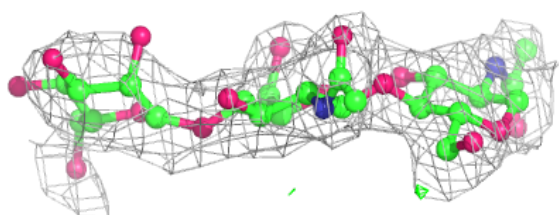
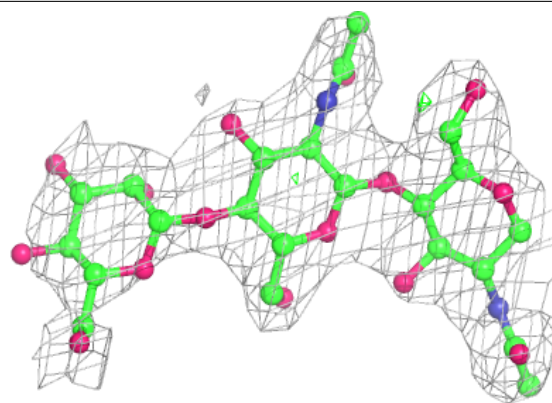
**Electron density around Chain N:**

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

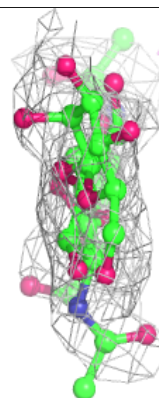
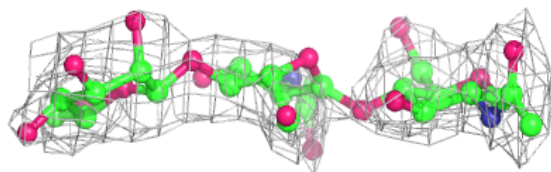
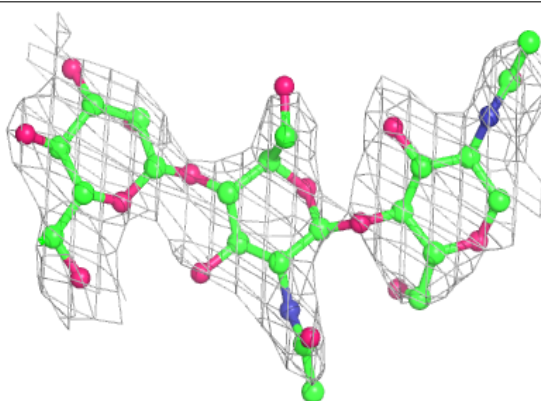


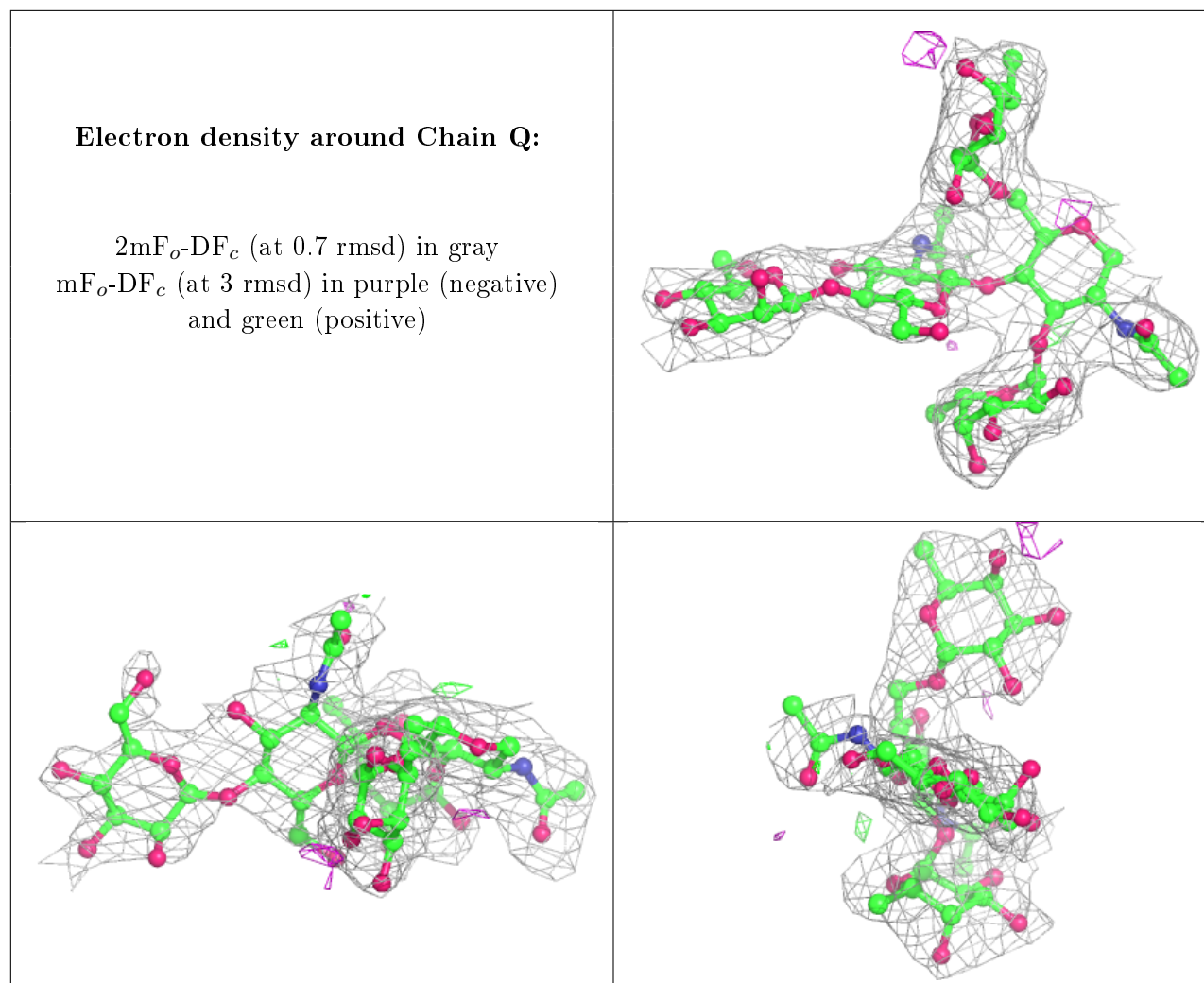
Electron density around Chain O:

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

**Electron density around Chain R:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	G	702	14/15	0.65	0.39	42,81,91,94	0
8	NAG	E	702	14/15	0.67	0.34	47,67,81,83	0
8	NAG	F	201	14/15	0.69	0.43	60,88,103,105	0
8	NAG	G	701	14/15	0.72	0.40	70,78,100,102	0
8	NAG	A	702	14/15	0.76	0.38	58,81,91,95	0
8	NAG	H	202	14/15	0.78	0.43	41,75,88,92	0
8	NAG	C	702	14/15	0.78	0.34	46,73,89,89	0
8	NAG	E	701	14/15	0.81	0.32	44,70,79,86	0
8	NAG	B	201	14/15	0.81	0.31	52,69,93,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	H	201	14/15	0.82	0.43	56,70,87,95	0
8	NAG	D	201	14/15	0.83	0.27	55,61,68,80	0
8	NAG	C	701	14/15	0.87	0.25	55,62,81,102	0
8	NAG	A	701	14/15	0.90	0.30	47,71,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.