



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 3AL4 / pdb_00003al4
Title : Crystal structure of the swine-origin A (H1N1)-2009 influenza A virus hemagglutinin (HA) reveals similar antigenicity to that of the 1918 pandemic virus
Authors : Zhang, W.; Qi, J.X.; Shi, Y.; Li, Q.; Yan, J.H.; Gao, G.F.
Deposited on : 2010-07-22
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

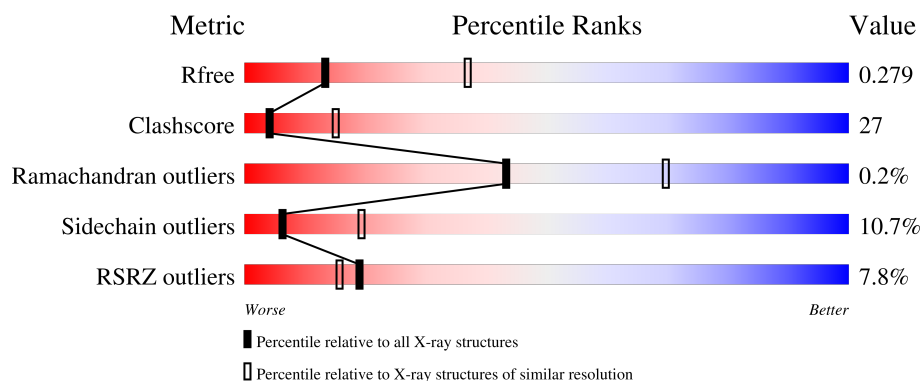
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	333	5% 54% 35% 7% .
1	C	333	3% 53% 38% 6% .
1	E	333	10% 40% 48% 8% .
1	G	333	5% 53% 37% 6% .
1	I	333	9% 53% 36% 6% .

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Mol	Chain	Length	Quality of chain
1	K	333	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
3	M	2	
3	N	2	
3	P	2	
3	Q	2	
3	S	2	
4	O	3	
4	R	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	L	601	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23626 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2505	1584	433	477	11			
1	C	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	E	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	G	321	Total	C	N	O	S	0	0	0
			2505	1584	433	477	11			
1	I	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	K	321	Total	C	N	O	S	0	0	0
			2511	1588	433	479	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP C3W5S1
A	2	ASP	-	expression tag	UNP C3W5S1
A	3	LEU	-	expression tag	UNP C3W5S1
A	4	GLY	-	expression tag	UNP C3W5S1
A	5	SER	-	expression tag	UNP C3W5S1
A	6	ARG	-	expression tag	UNP C3W5S1
C	1	ALA	-	expression tag	UNP C3W5S1
C	2	ASP	-	expression tag	UNP C3W5S1
C	3	LEU	-	expression tag	UNP C3W5S1
C	4	GLY	-	expression tag	UNP C3W5S1
C	5	SER	-	expression tag	UNP C3W5S1
C	6	ARG	-	expression tag	UNP C3W5S1
E	1	ALA	-	expression tag	UNP C3W5S1
E	2	ASP	-	expression tag	UNP C3W5S1
E	3	LEU	-	expression tag	UNP C3W5S1
E	4	GLY	-	expression tag	UNP C3W5S1
E	5	SER	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	ARG	-	expression tag	UNP C3W5S1
G	1	ALA	-	expression tag	UNP C3W5S1
G	2	ASP	-	expression tag	UNP C3W5S1
G	3	LEU	-	expression tag	UNP C3W5S1
G	4	GLY	-	expression tag	UNP C3W5S1
G	5	SER	-	expression tag	UNP C3W5S1
G	6	ARG	-	expression tag	UNP C3W5S1
I	1	ALA	-	expression tag	UNP C3W5S1
I	2	ASP	-	expression tag	UNP C3W5S1
I	3	LEU	-	expression tag	UNP C3W5S1
I	4	GLY	-	expression tag	UNP C3W5S1
I	5	SER	-	expression tag	UNP C3W5S1
I	6	ARG	-	expression tag	UNP C3W5S1
K	1	ALA	-	expression tag	UNP C3W5S1
K	2	ASP	-	expression tag	UNP C3W5S1
K	3	LEU	-	expression tag	UNP C3W5S1
K	4	GLY	-	expression tag	UNP C3W5S1
K	5	SER	-	expression tag	UNP C3W5S1
K	6	ARG	-	expression tag	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	D	162	Total	C	N	O	S	0	0	0
			1300	818	219	257	6			
2	F	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			
2	H	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	J	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	L	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP C3W5S1
B	178	LEU	-	expression tag	UNP C3W5S1
B	179	VAL	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	PRO	-	expression tag	UNP C3W5S1
B	181	ARG	-	expression tag	UNP C3W5S1
D	177	ARG	-	expression tag	UNP C3W5S1
D	178	LEU	-	expression tag	UNP C3W5S1
D	179	VAL	-	expression tag	UNP C3W5S1
D	180	PRO	-	expression tag	UNP C3W5S1
D	181	ARG	-	expression tag	UNP C3W5S1
F	177	ARG	-	expression tag	UNP C3W5S1
F	178	LEU	-	expression tag	UNP C3W5S1
F	179	VAL	-	expression tag	UNP C3W5S1
F	180	PRO	-	expression tag	UNP C3W5S1
F	181	ARG	-	expression tag	UNP C3W5S1
H	177	ARG	-	expression tag	UNP C3W5S1
H	178	LEU	-	expression tag	UNP C3W5S1
H	179	VAL	-	expression tag	UNP C3W5S1
H	180	PRO	-	expression tag	UNP C3W5S1
H	181	ARG	-	expression tag	UNP C3W5S1
J	177	ARG	-	expression tag	UNP C3W5S1
J	178	LEU	-	expression tag	UNP C3W5S1
J	179	VAL	-	expression tag	UNP C3W5S1
J	180	PRO	-	expression tag	UNP C3W5S1
J	181	ARG	-	expression tag	UNP C3W5S1
L	177	ARG	-	expression tag	UNP C3W5S1
L	178	LEU	-	expression tag	UNP C3W5S1
L	179	VAL	-	expression tag	UNP C3W5S1
L	180	PRO	-	expression tag	UNP C3W5S1
L	181	ARG	-	expression tag	UNP C3W5S1

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



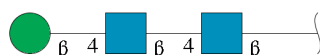
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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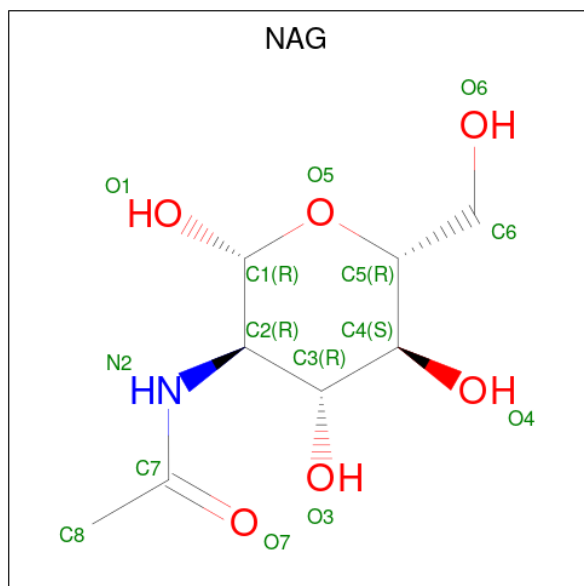
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called 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
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	17	Total	O	0	0
			17	17		
6	C	38	Total	O	0	0
			38	38		
6	D	10	Total	O	0	0
			10	10		
6	E	31	Total	O	0	0
			31	31		

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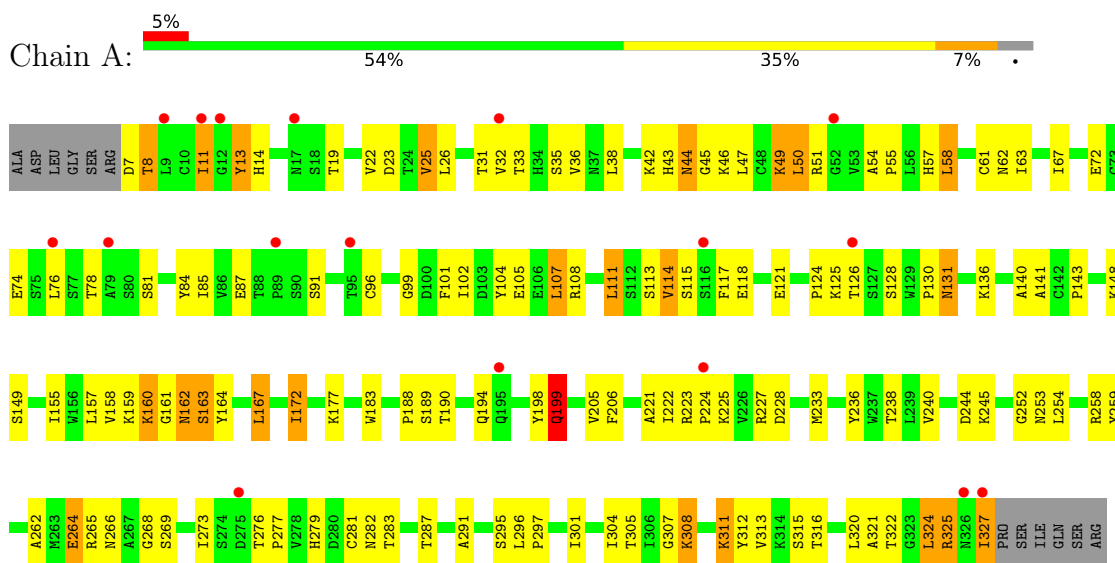
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	13	Total 13	O 13	0	0
6	G	45	Total 45	O 45	0	0
6	H	23	Total 23	O 23	0	0
6	I	37	Total 37	O 37	0	0
6	J	21	Total 21	O 21	0	0
6	K	35	Total 35	O 35	0	0
6	L	11	Total 11	O 11	0	0

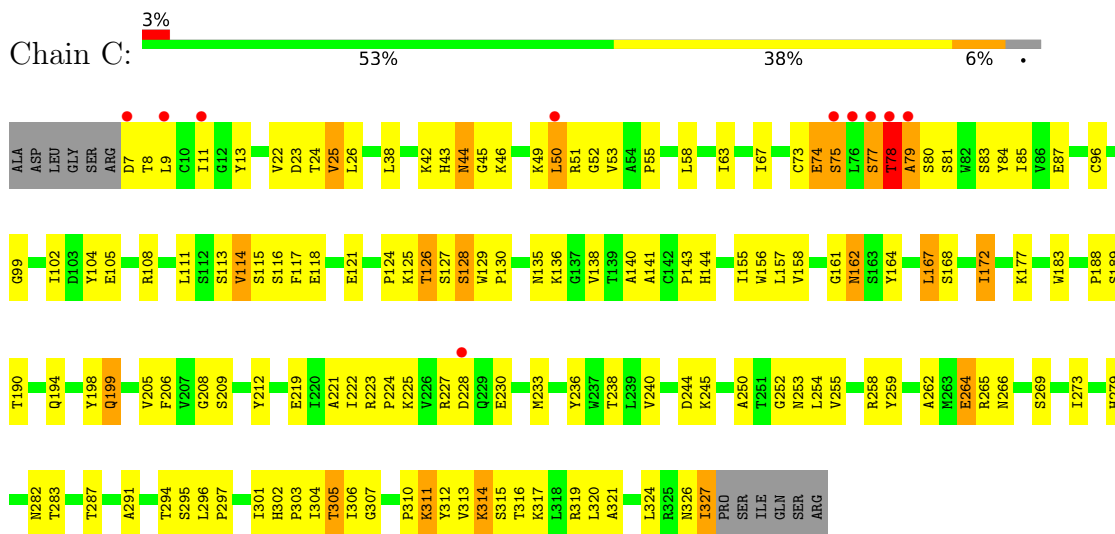
3 Residue-property plots [i](#)

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

• Molecule 1: Hemagglutinin

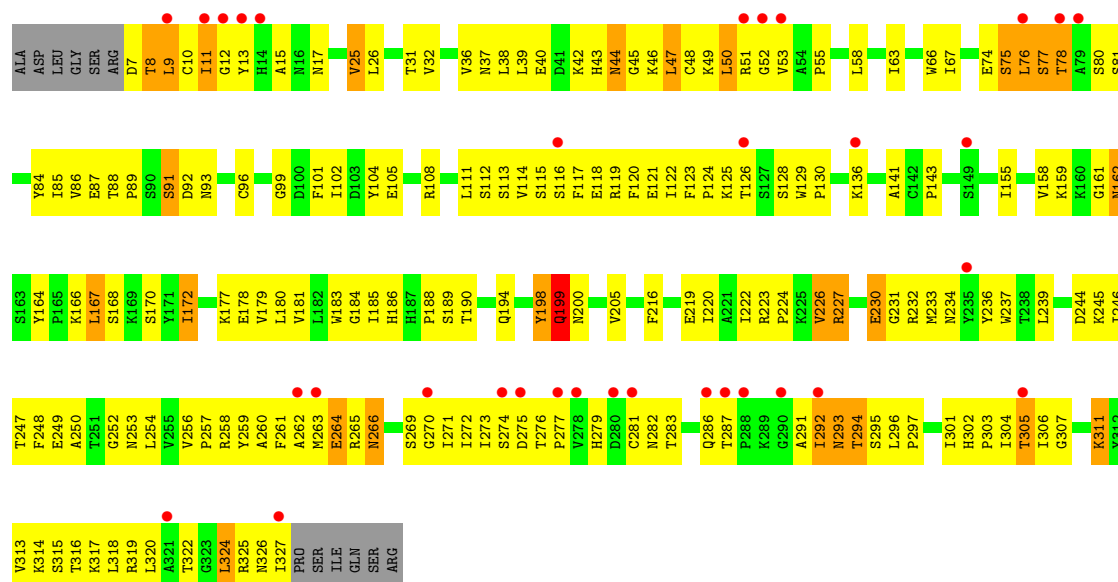


• Molecule 1: Hemagglutinin

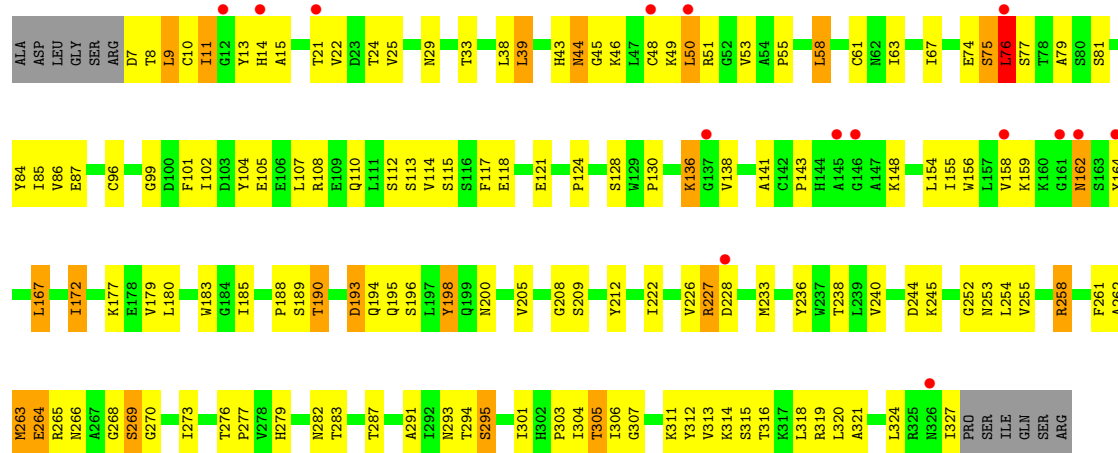


• Molecule 1: Hemagglutinin

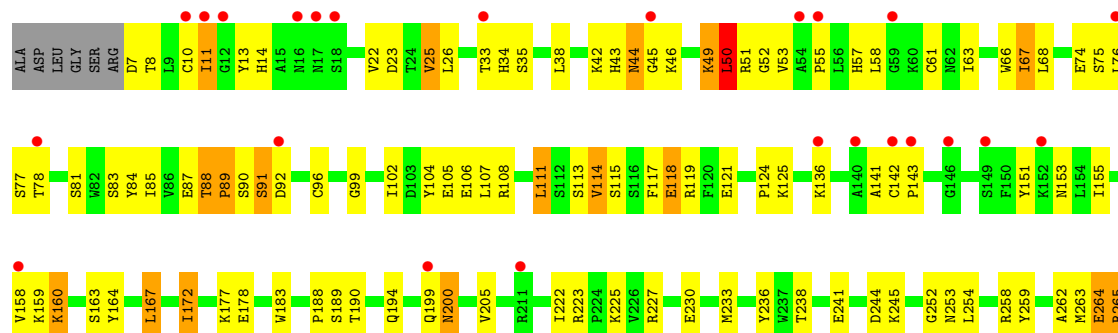




• Molecule 1: Hemagglutinin

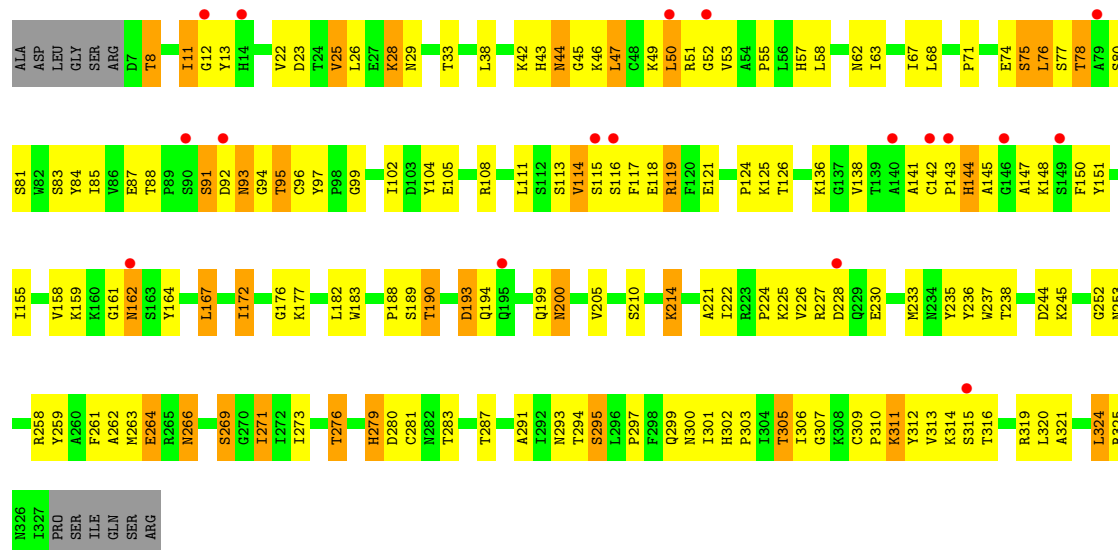


• Molecule 1: Hemagglutinin

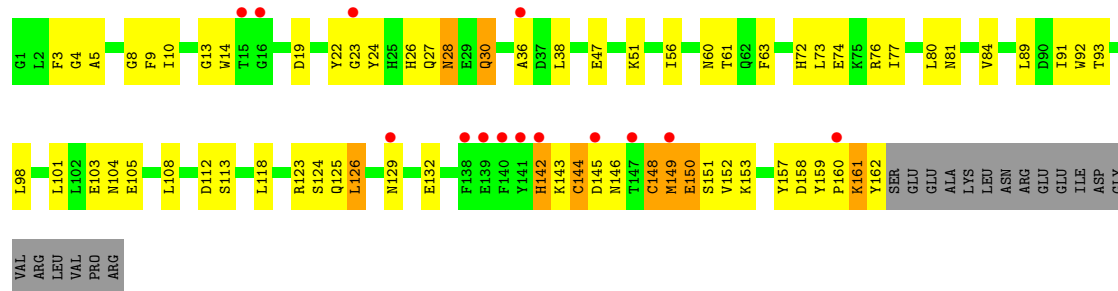




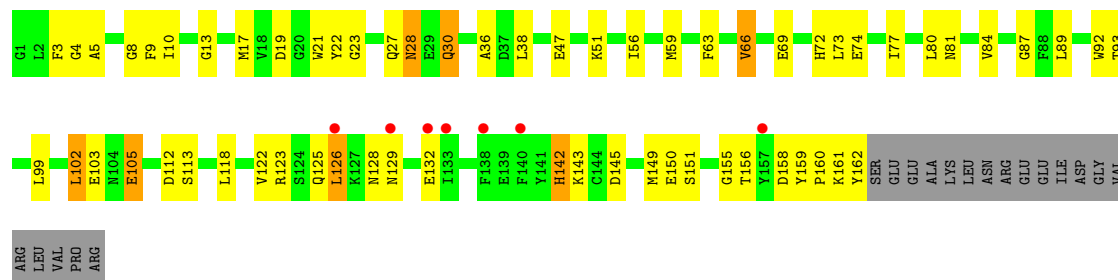
• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin

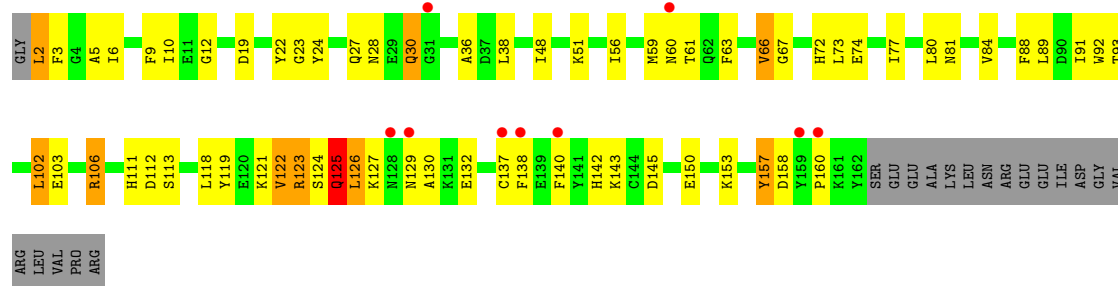


• Molecule 2: Hemagglutinin

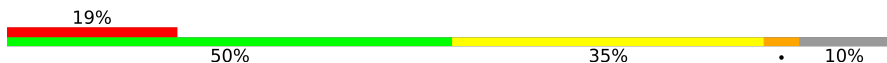


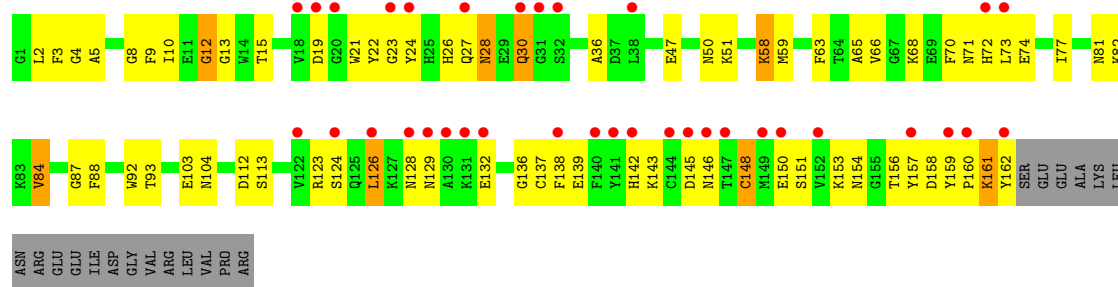
- Molecule 2: Hemagglutinin

Chain F: 



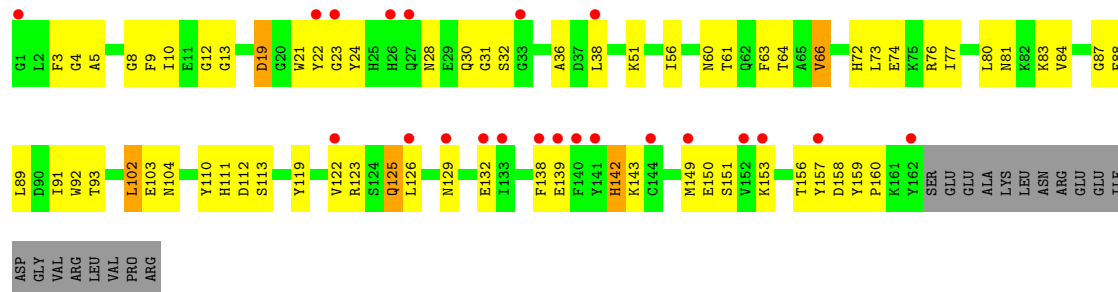
- Molecule 2: Hemagglutinin

Chain H: 



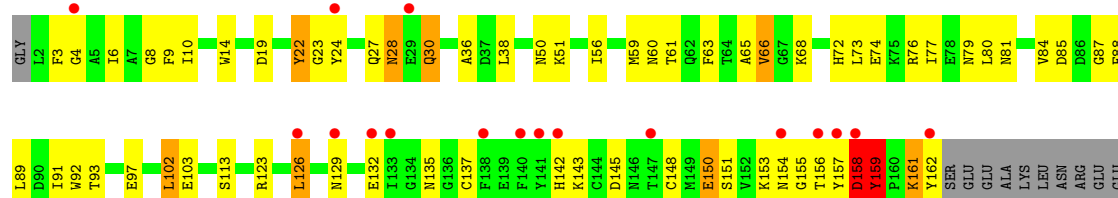
- Molecule 2: Hemagglutinin

Chain J: 



- Molecule 2: Hemagglutinin

Chain L: 



ILE
ASP
GLY
VAL
ARG
LEU
VAL
PRO
ARG

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

Chain M:  100%

NAG1
NAG2

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

Chain N:  100%

NAG1
NAG2

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

Chain P:  100%

NAG1
NAG2

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

Chain Q:  50% 50%

NAG1
NAG2

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

Chain S:  100%

NAG1
NAG2

- Molecule 4: 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%

NAG1
NAG2
BMA3

- Molecule 4: 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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.02Å 115.19Å 114.98Å 62.31° 77.94° 81.05°	Depositor
Resolution (Å)	24.19 – 2.87 24.19 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.6 (24.19-2.87) 96.9 (24.19-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.85Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.246 , 0.270 0.256 , 0.279	Depositor DCC
R_{free} test set	3296 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23626	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 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	A	0.30	0/2568	0.85	6/3488 (0.2%)
1	C	0.29	0/2572	0.84	8/3493 (0.2%)
1	E	0.30	0/2572	0.98	11/3493 (0.3%)
1	G	0.31	0/2568	0.84	5/3488 (0.1%)
1	I	0.30	0/2572	0.84	8/3493 (0.2%)
1	K	0.37	0/2574	0.90	8/3497 (0.2%)
2	B	0.30	0/1333	0.73	1/1797 (0.1%)
2	D	0.27	0/1328	0.69	0/1791
2	F	0.28	0/1330	0.76	1/1794 (0.1%)
2	H	0.30	0/1333	0.73	3/1797 (0.2%)
2	J	0.30	0/1333	0.66	0/1797
2	L	0.29	0/1330	0.78	3/1794 (0.2%)
All	All	0.30	0/23413	0.83	54/31722 (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	C	0	2
1	E	0	1
2	F	0	1
2	L	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	226	VAL	O-C-N	-22.55	99.75	122.30
1	K	92	ASP	N-CA-C	13.61	130.77	111.30
1	E	76	LEU	N-CA-CB	-12.27	89.75	110.49
1	A	199	GLN	N-CA-CB	-12.23	89.81	110.49
1	E	78	THR	N-CA-C	-12.14	96.19	114.16

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	73	CYS	Peptide
1	C	77	SER	Peptide
1	E	226	VAL	Mainchain
2	F	125	GLN	Peptide
2	L	159	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2442	160	0
1	C	2509	0	2447	136	3
1	E	2509	0	2450	216	0
1	G	2505	0	2443	143	0
1	I	2509	0	2450	145	0
1	K	2511	0	2454	166	3
2	B	1305	0	1228	76	0
2	D	1300	0	1216	55	0
2	F	1302	0	1224	73	0
2	H	1305	0	1228	97	0
2	J	1305	0	1228	79	0
2	L	1302	0	1225	77	0
3	M	28	0	25	9	0
3	N	28	0	25	4	0
3	P	28	0	25	2	0
3	Q	28	0	25	3	0
3	S	28	0	25	5	0
4	O	39	0	34	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	39	0	34	3	0
5	A	28	0	26	1	0
5	C	28	0	26	3	0
5	E	42	0	39	2	0
5	F	14	0	13	0	0
5	G	42	0	39	3	0
5	K	56	0	52	9	0
5	L	14	0	13	10	0
6	A	36	0	0	19	0
6	B	17	0	0	10	0
6	C	38	0	0	15	0
6	D	10	0	0	2	0
6	E	31	0	0	10	0
6	F	13	0	0	4	0
6	G	45	0	0	25	0
6	H	23	0	0	14	0
6	I	37	0	0	21	0
6	J	21	0	0	6	0
6	K	35	0	0	16	0
6	L	11	0	0	2	0
All	All	23626	0	22436	1252	3

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 27.

The worst 5 of 1252 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:ASN:HD21	5:E:601:NAG:C1	1.30	1.42
1:E:7:ASP:HA	2:F:27:GLN:O	1.37	1.21
1:E:66:TRP:HE1	1:E:77:SER:HB2	1.08	1.14
1:K:280:ASP:OD1	3:M:2:NAG:O7	1.65	1.14
1:C:282:ASN:OD1	5:C:607:NAG:O7	1.67	1.13

All (3) 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:C:74:GLU:OE1	1:K:144:HIS:NE2[1_455]	1.89	0.31
1:C:74:GLU:OE1	1:K:144:HIS:CD2[1_455]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLU:OE2	1:K:144:HIS:ND1[1_455]	2.13	0.07

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	319/333 (96%)	286 (90%)	32 (10%)	1 (0%)	36	62
1	C	319/333 (96%)	296 (93%)	22 (7%)	1 (0%)	36	62
1	E	319/333 (96%)	291 (91%)	24 (8%)	4 (1%)	9	29
1	G	319/333 (96%)	299 (94%)	19 (6%)	1 (0%)	36	62
1	I	319/333 (96%)	294 (92%)	25 (8%)	0	100	100
1	K	319/333 (96%)	288 (90%)	31 (10%)	0	100	100
2	B	160/181 (88%)	143 (89%)	17 (11%)	0	100	100
2	D	160/181 (88%)	146 (91%)	14 (9%)	0	100	100
2	F	159/181 (88%)	147 (92%)	12 (8%)	0	100	100
2	H	160/181 (88%)	145 (91%)	15 (9%)	0	100	100
2	J	160/181 (88%)	148 (92%)	12 (8%)	0	100	100
2	L	159/181 (88%)	145 (91%)	14 (9%)	0	100	100
All	All	2872/3084 (93%)	2628 (92%)	237 (8%)	7 (0%)	43	70

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	92	ASP
1	E	199	GLN
1	A	199	GLN
1	E	75	SER
1	G	268	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/292 (96%)	246 (88%)	35 (12%)	4	13
1	C	282/292 (97%)	255 (90%)	27 (10%)	8	23
1	E	282/292 (97%)	247 (88%)	35 (12%)	4	13
1	G	281/292 (96%)	250 (89%)	31 (11%)	6	18
1	I	282/292 (97%)	252 (89%)	30 (11%)	6	19
1	K	282/292 (97%)	244 (86%)	38 (14%)	4	11
2	B	139/156 (89%)	127 (91%)	12 (9%)	10	28
2	D	138/156 (88%)	127 (92%)	11 (8%)	11	31
2	F	139/156 (89%)	122 (88%)	17 (12%)	5	14
2	H	139/156 (89%)	131 (94%)	8 (6%)	18	46
2	J	139/156 (89%)	126 (91%)	13 (9%)	8	24
2	L	139/156 (89%)	126 (91%)	13 (9%)	8	24
All	All	2523/2688 (94%)	2253 (89%)	270 (11%)	6	19

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	91	SER
1	K	142	CYS
2	L	38	LEU
1	E	91	SER
1	E	74	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	199	GLN
1	I	144	HIS
2	L	125	GLN
1	G	266	ASN

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Mol	Chain	Res	Type
2	H	125	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 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	M	1	1,3	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
3	NAG	M	2	3	14,14,15	0.55	0	17,19,21	1.60	3 (17%)
3	NAG	N	1	1,3	14,14,15	0.56	0	17,19,21	0.60	0
3	NAG	N	2	3	14,14,15	0.45	0	17,19,21	0.96	0
4	NAG	O	1	4,1	14,14,15	0.60	0	17,19,21	1.15	1 (5%)
4	NAG	O	2	4	14,14,15	0.53	0	17,19,21	1.04	0
4	BMA	O	3	4	11,11,12	0.25	0	15,15,17	0.52	0
3	NAG	P	1	1,3	14,14,15	0.54	0	17,19,21	0.83	0
3	NAG	P	2	3	14,14,15	0.44	0	17,19,21	2.03	4 (23%)
3	NAG	Q	1	1,3	14,14,15	0.55	0	17,19,21	0.62	0
3	NAG	Q	2	3	14,14,15	0.57	0	17,19,21	0.78	0
4	NAG	R	1	4,1	14,14,15	0.52	0	17,19,21	1.76	3 (17%)
4	NAG	R	2	4	14,14,15	0.41	0	17,19,21	1.90	4 (23%)
4	BMA	R	3	4	11,11,12	0.26	0	15,15,17	0.54	0
3	NAG	S	1	1,3	14,14,15	0.54	0	17,19,21	1.77	3 (17%)
3	NAG	S	2	3	14,14,15	0.60	0	17,19,21	1.10	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
3	NAG	M	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	BMA	R	3	4	-	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	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	2	NAG	C1-O5-C5	6.23	120.54	112.19
4	R	1	NAG	C2-N2-C7	-5.23	115.90	122.90
4	R	2	NAG	C1-O5-C5	5.15	119.08	112.19
3	S	1	NAG	O4-C4-C3	4.85	121.81	110.38
3	M	2	NAG	C2-N2-C7	-4.55	116.80	122.90

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6

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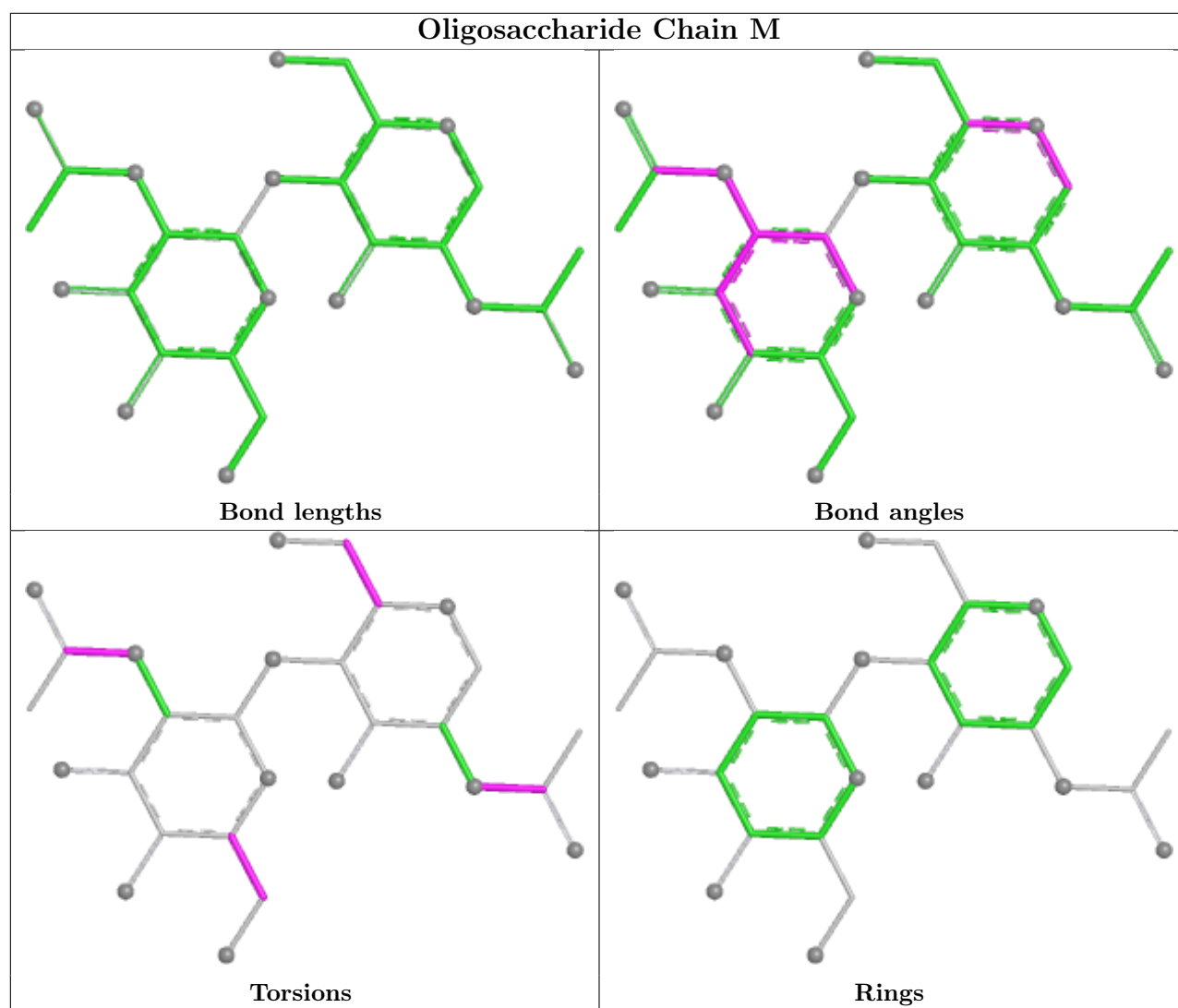
Mol	Chain	Res	Type	Atoms
4	O	1	NAG	O5-C5-C6-O6

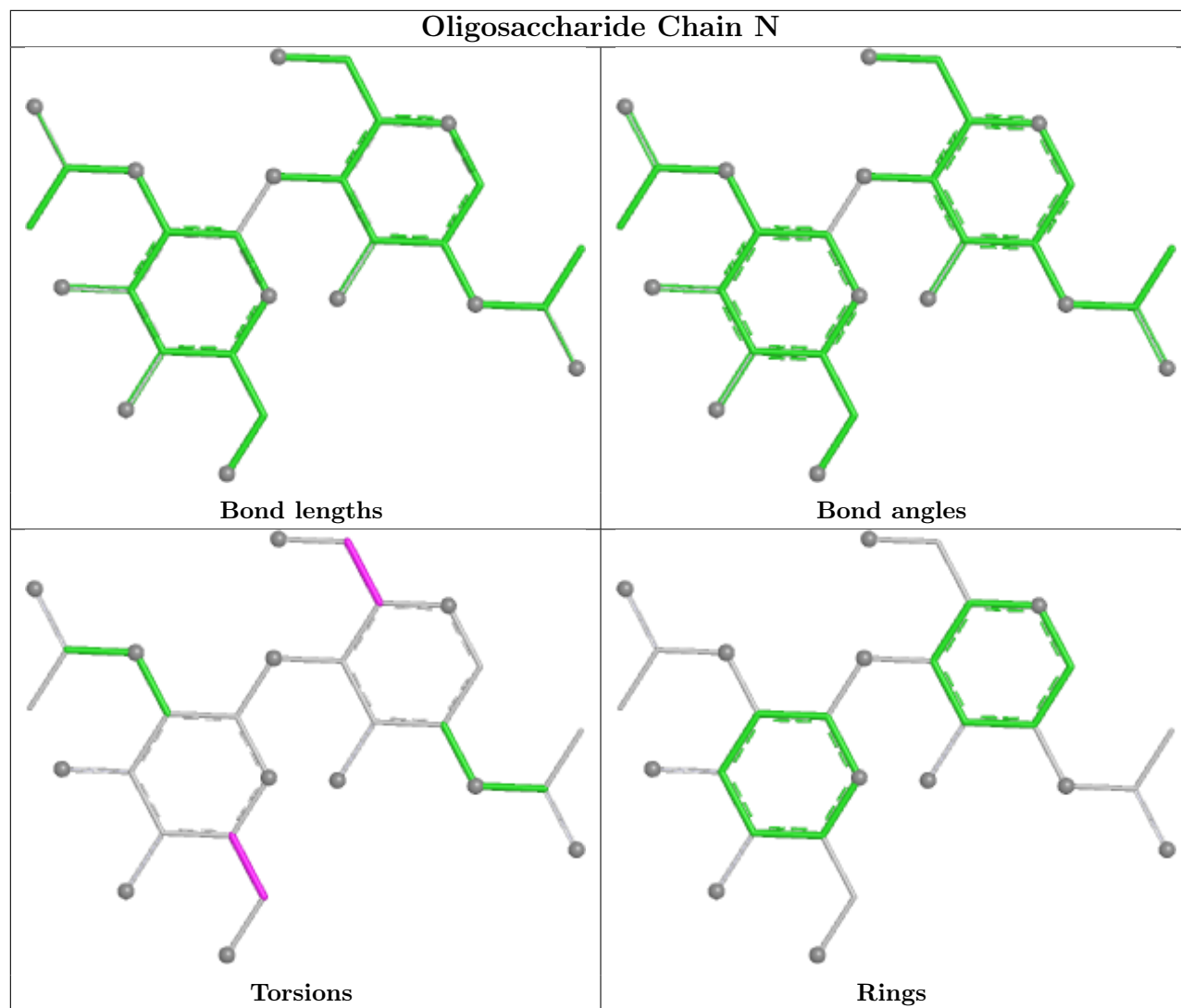
There are no ring outliers.

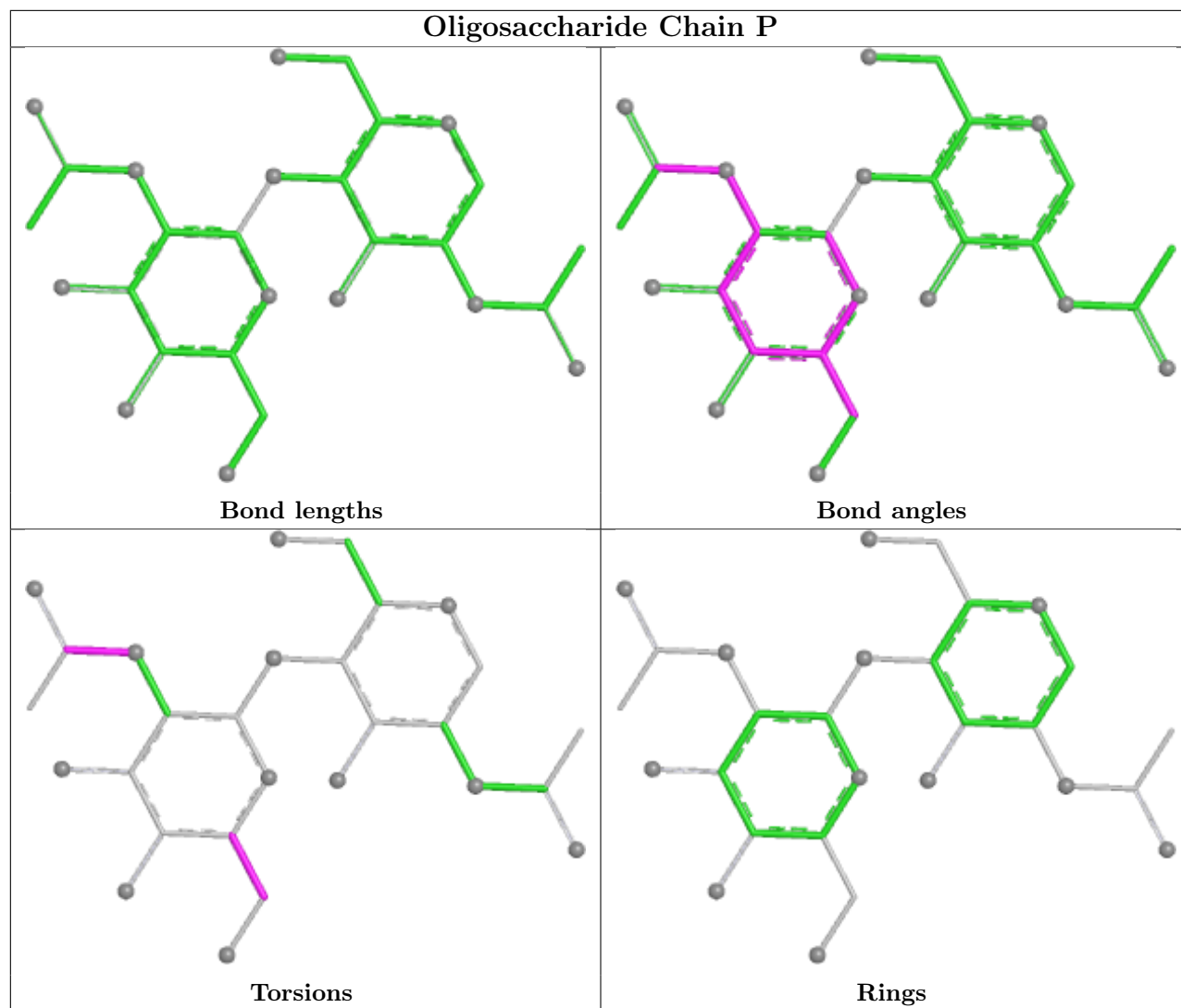
12 monomers are involved in 30 short contacts:

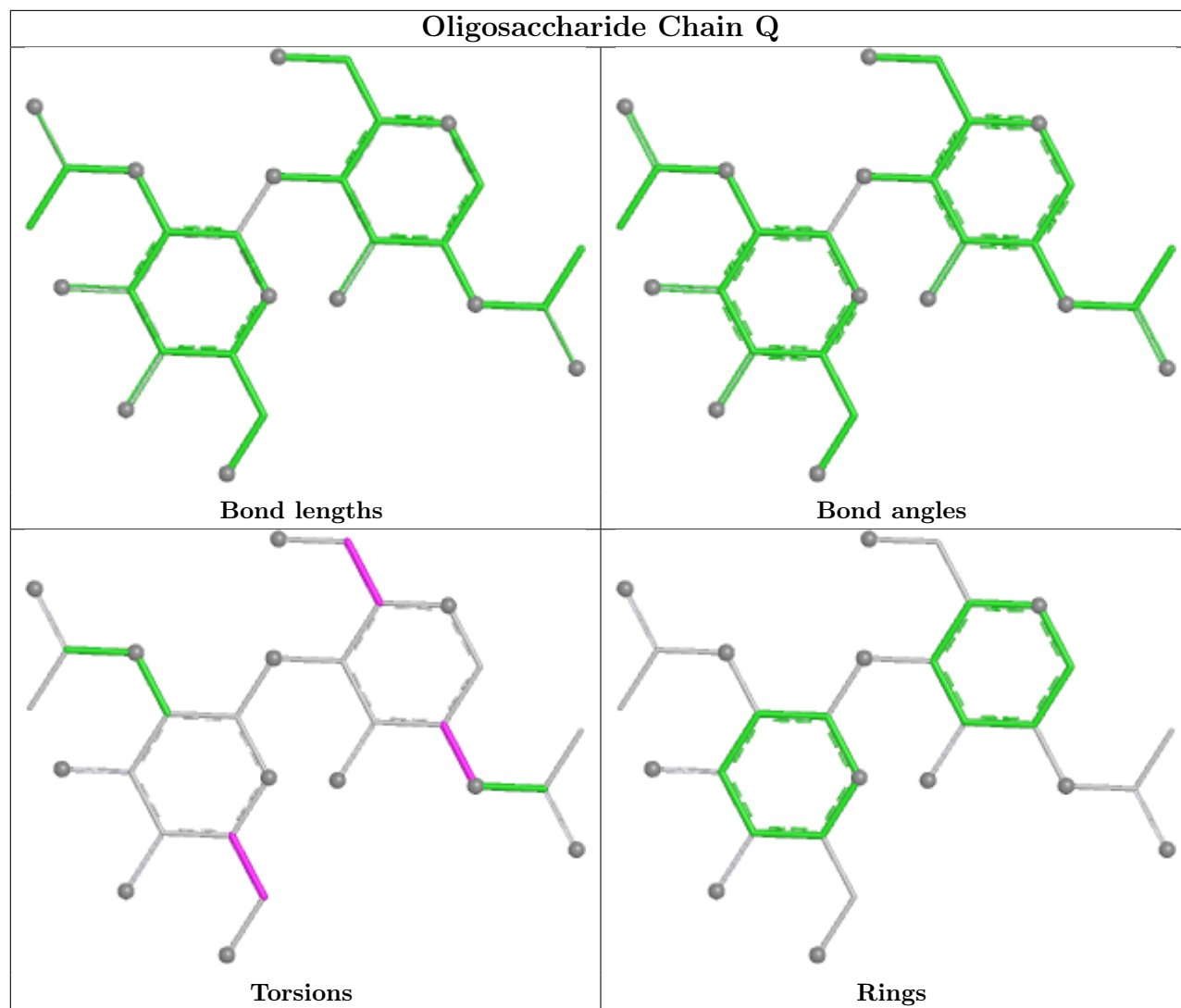
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	NAG	3	0
3	N	2	NAG	1	0
3	Q	1	NAG	3	0
4	O	1	NAG	4	0
4	R	3	BMA	2	0
3	M	1	NAG	6	0
3	N	1	NAG	4	0
3	P	1	NAG	2	0
4	R	2	NAG	2	0
3	S	1	NAG	3	0
4	R	1	NAG	1	0
3	S	2	NAG	3	0

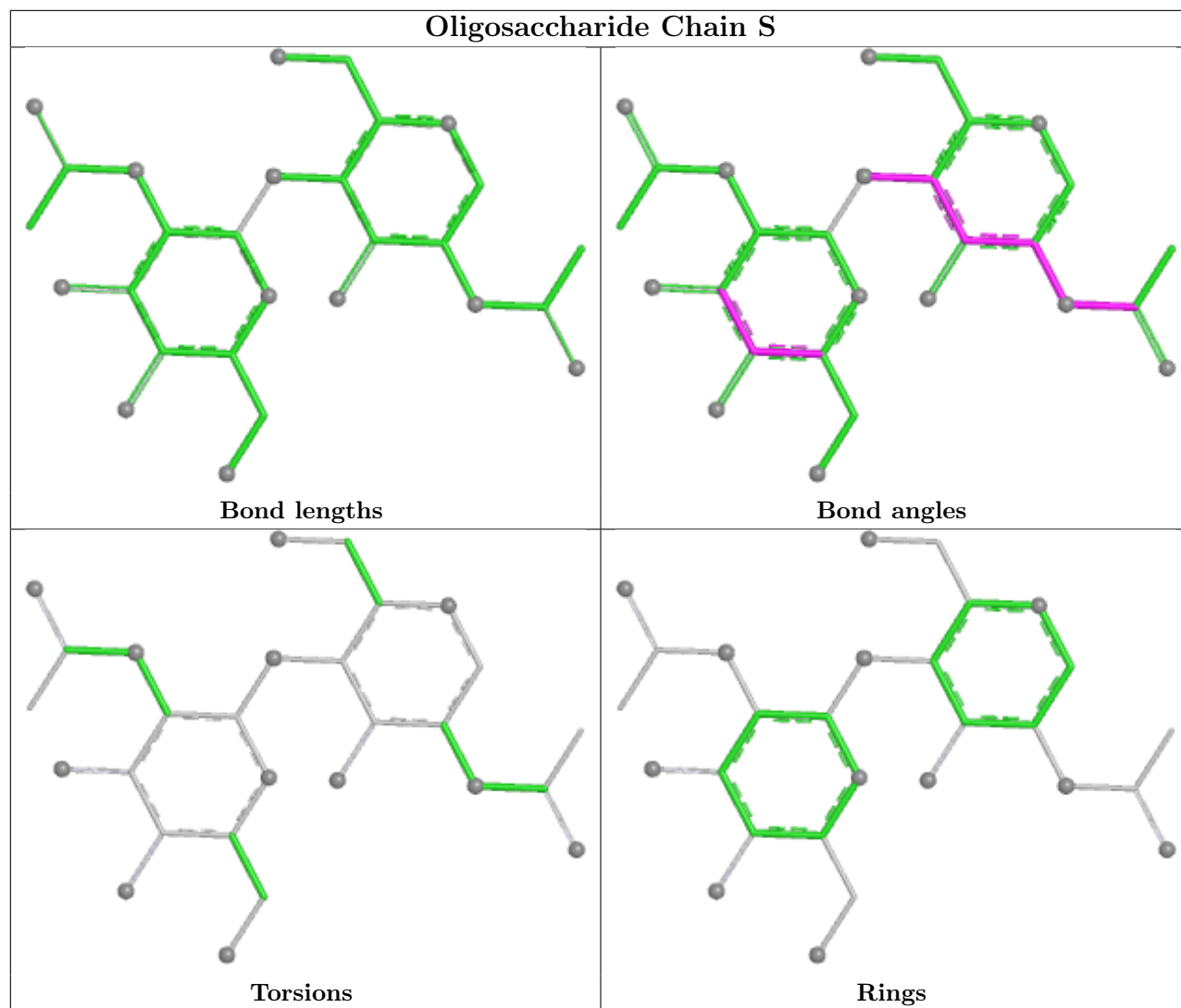
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

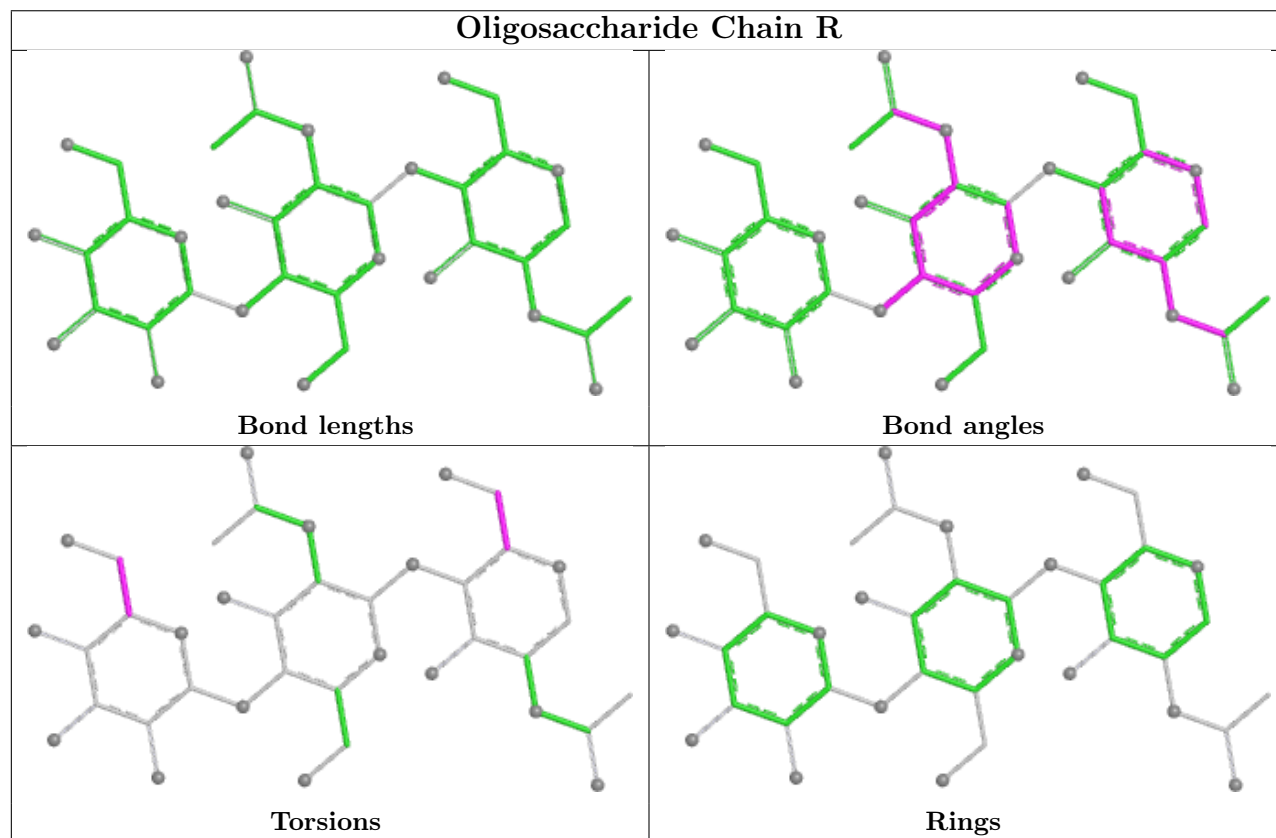
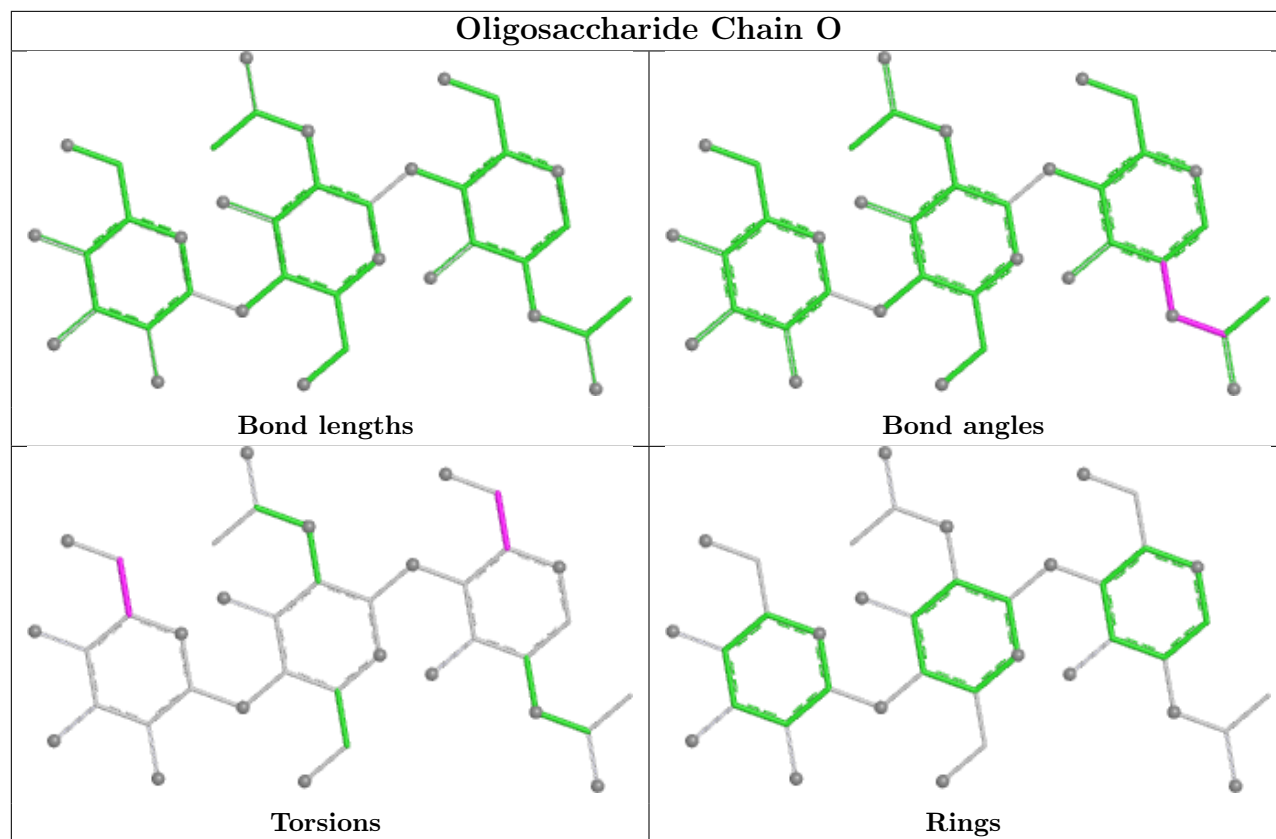












5.6 Ligand geometry

16 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
5	NAG	G	601	1	14,14,15	0.53	0	17,19,21	0.73	0
5	NAG	K	603	1	14,14,15	0.56	0	17,19,21	0.61	0
5	NAG	L	601	2	14,14,15	0.56	0	17,19,21	0.61	0
5	NAG	F	601	2	14,14,15	0.54	0	17,19,21	0.62	0
5	NAG	G	603	1	14,14,15	0.55	0	17,19,21	0.61	0
5	NAG	A	606	1	14,14,15	0.55	0	17,19,21	0.87	0
5	NAG	E	604	1	14,14,15	0.53	0	17,19,21	0.69	0
5	NAG	E	605	1	14,14,15	0.55	0	17,19,21	1.27	4 (23%)
5	NAG	K	604	1	14,14,15	0.55	0	17,19,21	0.62	0
5	NAG	A	601	1	14,14,15	0.55	0	17,19,21	0.61	0
5	NAG	G	602	1	14,14,15	0.55	0	17,19,21	0.61	0
5	NAG	E	601	1	14,14,15	0.55	0	17,19,21	0.61	0
5	NAG	C	601	1	14,14,15	0.56	0	17,19,21	0.61	0
5	NAG	K	601	1	14,14,15	0.46	0	17,19,21	2.48	4 (23%)
5	NAG	C	607	1	14,14,15	0.54	0	17,19,21	0.62	0
5	NAG	K	602	1	14,14,15	0.55	0	17,19,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	601	1	-	2/6/23/26	0/1/1/1
5	NAG	K	603	1	-	2/6/23/26	0/1/1/1
5	NAG	L	601	2	-	2/6/23/26	0/1/1/1
5	NAG	F	601	2	-	2/6/23/26	0/1/1/1
5	NAG	G	603	1	-	3/6/23/26	0/1/1/1
5	NAG	A	606	1	-	2/6/23/26	0/1/1/1
5	NAG	E	604	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	605	1	-	2/6/23/26	0/1/1/1
5	NAG	K	604	1	-	1/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	G	602	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	NAG	K	601	1	-	4/6/23/26	0/1/1/1
5	NAG	C	607	1	-	2/6/23/26	0/1/1/1
5	NAG	K	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	601	NAG	C1-O5-C5	8.83	124.03	112.19
5	K	601	NAG	O5-C1-C2	3.17	116.20	111.29
5	E	605	NAG	O5-C1-C2	-2.74	107.05	111.29
5	E	605	NAG	C6-C5-C4	-2.32	107.32	113.02
5	K	601	NAG	O5-C5-C4	2.19	116.16	110.83

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	606	NAG	C8-C7-N2-C2
5	A	606	NAG	O7-C7-N2-C2
5	K	604	NAG	C1-C2-N2-C7
5	K	602	NAG	C4-C5-C6-O6
5	G	601	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	603	NAG	3	0
5	L	601	NAG	10	0
5	G	603	NAG	1	0
5	K	604	NAG	2	0
5	A	601	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	602	NAG	2	0
5	E	601	NAG	2	0
5	C	607	NAG	3	0
5	K	602	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/333 (96%)	0.58	17 (5%) 32 25	39, 70, 122, 226	0
1	C	321/333 (96%)	0.36	10 (3%) 51 42	36, 67, 116, 196	0
1	E	321/333 (96%)	0.86	33 (10%) 12 10	41, 74, 130, 215	0
1	G	321/333 (96%)	0.68	15 (4%) 36 29	46, 76, 128, 232	0
1	I	321/333 (96%)	0.78	30 (9%) 14 12	37, 70, 120, 228	0
1	K	321/333 (96%)	0.55	18 (5%) 30 23	38, 70, 121, 195	0
2	B	162/181 (89%)	0.67	14 (8%) 16 13	32, 77, 167, 209	0
2	D	162/181 (89%)	0.37	7 (4%) 40 32	34, 72, 186, 246	0
2	F	161/181 (88%)	0.40	9 (5%) 30 23	34, 74, 178, 241	0
2	H	162/181 (89%)	1.07	35 (21%) 2 2	33, 80, 174, 289	0
2	J	162/181 (89%)	0.76	22 (13%) 7 5	32, 69, 165, 200	0
2	L	161/181 (88%)	0.72	17 (10%) 11 10	36, 73, 169, 199	0
All	All	2896/3084 (93%)	0.64	227 (7%) 19 16	32, 72, 157, 289	0

The worst 5 of 227 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	12	GLY	6.9
2	H	149	MET	4.9
2	H	130	ALA	4.9
2	H	140	PHE	4.9
1	E	12	GLY	4.8

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 ⓘ

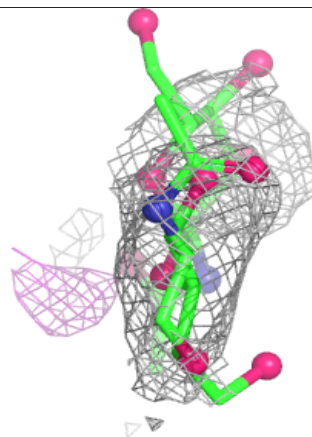
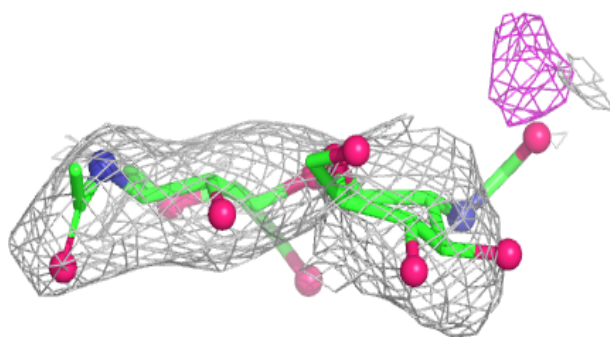
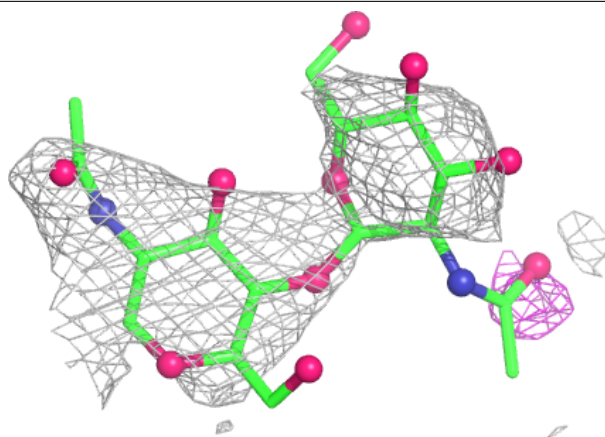
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	R	3	11/12	0.16	0.17	108,135,142,143	0
3	NAG	N	2	14/15	0.37	0.14	124,134,147,148	0
3	NAG	M	2	14/15	0.39	0.15	120,148,155,174	0
4	BMA	O	3	11/12	0.45	0.14	89,112,124,151	0
3	NAG	Q	2	14/15	0.49	0.16	119,139,166,193	0
3	NAG	N	1	14/15	0.63	0.10	68,108,117,126	0
4	NAG	R	1	14/15	0.65	0.13	72,82,95,97	0
3	NAG	P	2	14/15	0.68	0.12	91,106,136,144	0
3	NAG	S	2	14/15	0.69	0.13	128,134,141,147	0
3	NAG	Q	1	14/15	0.70	0.15	108,129,134,135	0
4	NAG	O	2	14/15	0.71	0.13	55,84,111,120	0
3	NAG	M	1	14/15	0.71	0.14	82,113,129,130	0
4	NAG	R	2	14/15	0.78	0.11	92,117,138,145	0
3	NAG	S	1	14/15	0.78	0.13	94,114,139,150	0
4	NAG	O	1	14/15	0.83	0.10	61,76,95,102	0
3	NAG	P	1	14/15	0.83	0.11	70,86,98,99	0

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

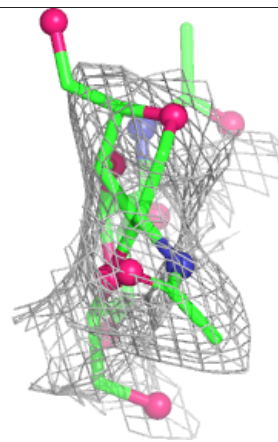
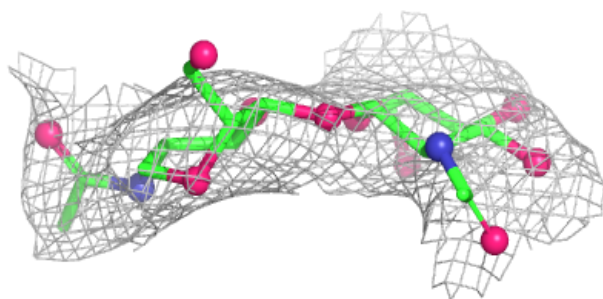
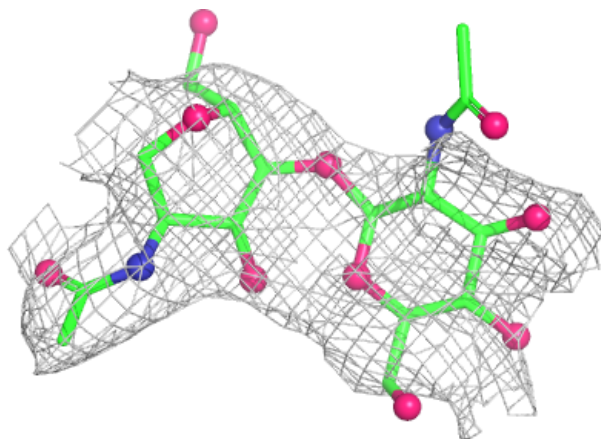
Electron density around Chain M:

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



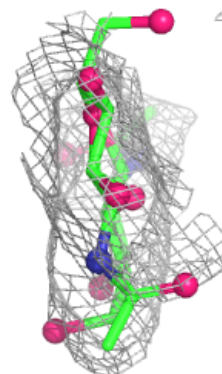
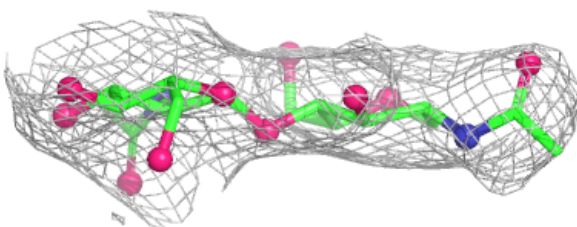
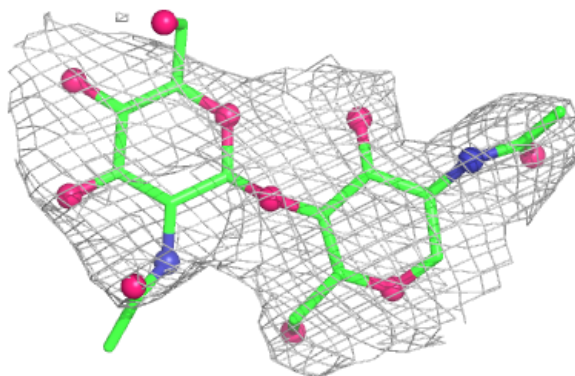
Electron density around Chain N:

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

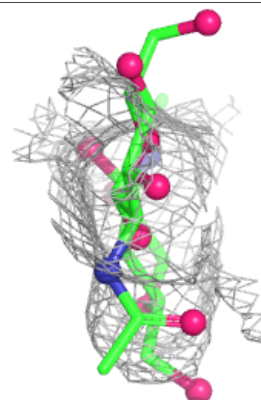
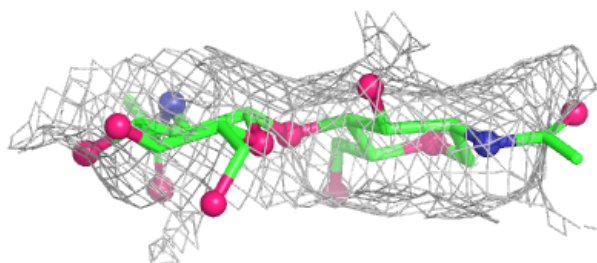
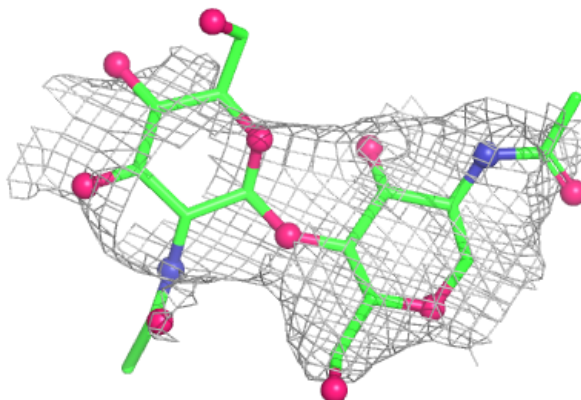


Electron density around Chain P:

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

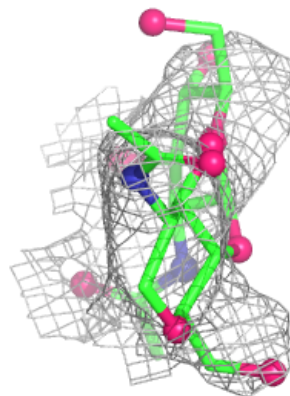
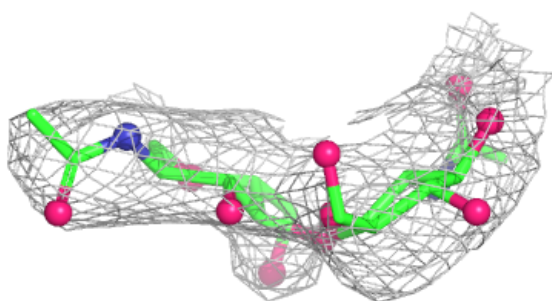
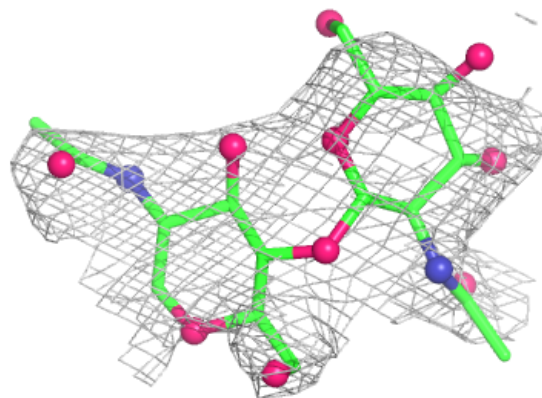
**Electron density around Chain Q:**

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

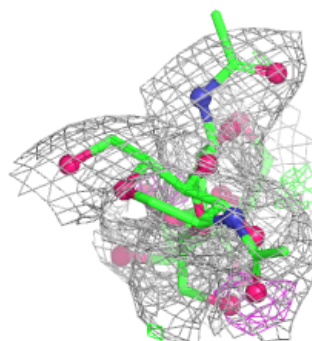
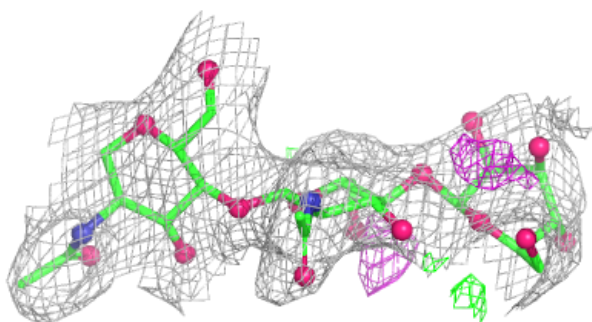
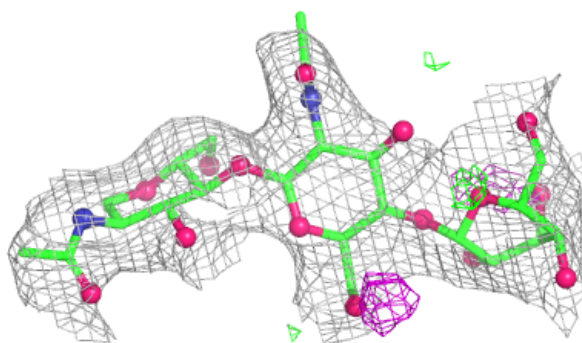


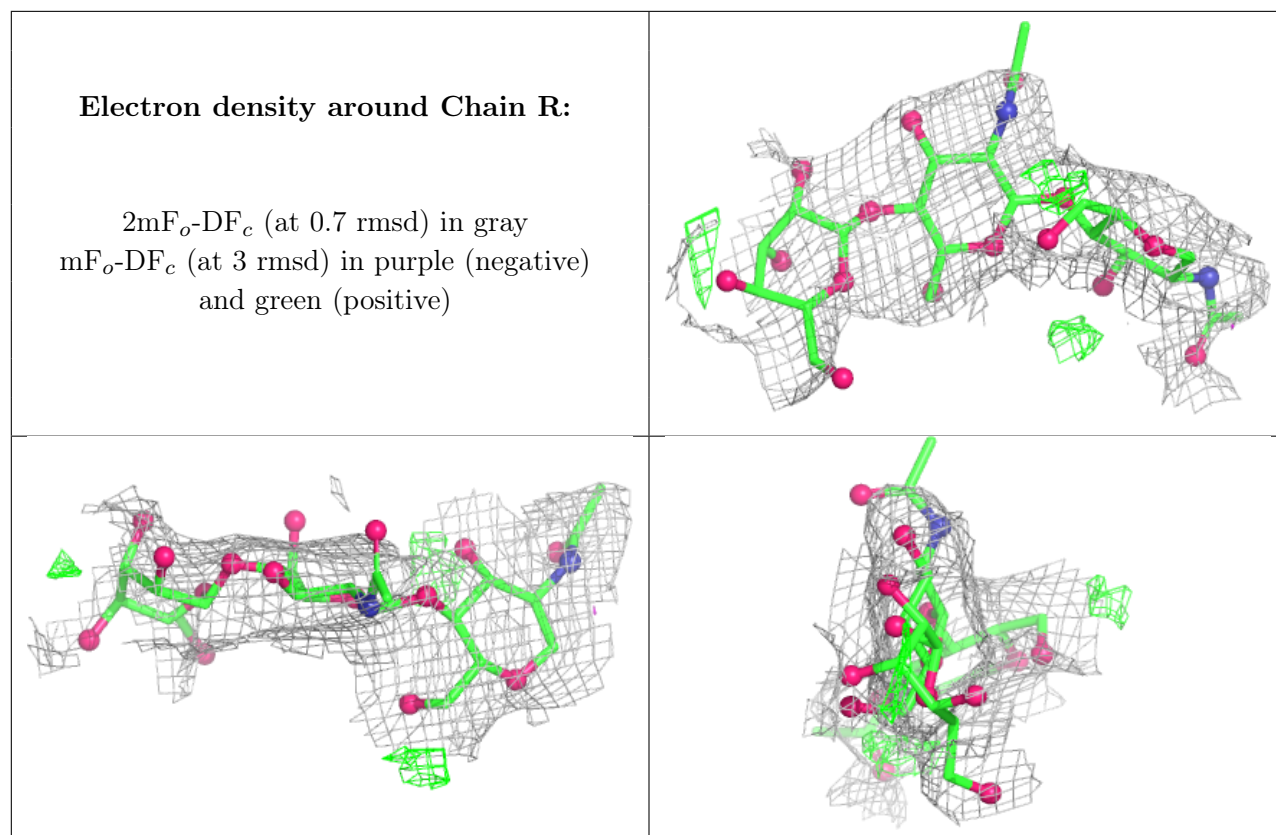
Electron density around Chain S:

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

**Electron density around Chain O:**

$2mF_o-DF_c$ (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
5	NAG	A	606	14/15	0.17	0.16	103,126,141,143	0
5	NAG	E	601	14/15	0.36	0.13	117,156,185,194	0
5	NAG	E	605	14/15	0.43	0.16	134,171,193,199	0
5	NAG	K	601	14/15	0.44	0.15	88,113,140,142	0
5	NAG	K	603	14/15	0.44	0.15	84,126,147,153	0
5	NAG	A	601	14/15	0.45	0.15	53,78,94,104	0
5	NAG	L	601	14/15	0.45	0.18	132,161,178,187	0
5	NAG	F	601	14/15	0.49	0.12	154,173,188,194	0
5	NAG	C	601	14/15	0.49	0.13	157,180,192,198	0
5	NAG	G	601	14/15	0.50	0.16	141,158,176,181	0
5	NAG	K	604	14/15	0.56	0.12	108,133,146,153	0
5	NAG	K	602	14/15	0.56	0.13	68,115,138,139	0
5	NAG	E	604	14/15	0.57	0.29	26,28,30,30	0
5	NAG	G	602	14/15	0.58	0.14	171,186,198,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	607	14/15	0.60	0.15	95,116,142,146	0
5	NAG	G	603	14/15	0.67	0.14	139,163,185,199	0

6.5 Other polymers [i](#)

There are no such residues in this entry.