



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2025 – 12:29 AM JST

PDB ID : 8X26 / pdb\_00008x26  
Title : Crystal structure of H5 hemagglutinin from human-infecting H5N8 influenza virus in complex with LSTa  
Authors : Jin, X.Y.; Song, H.; Han, P.; Qi, J.X.  
Deposited on : 2023-11-09  
Resolution : 3.12 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

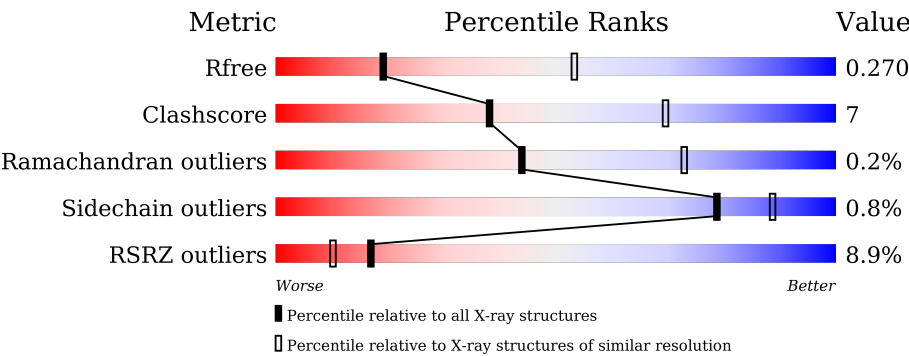
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.12 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.




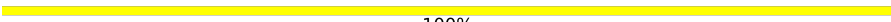







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1668 (3.14-3.10)
Clashscore	180529	1788 (3.14-3.10)
Ramachandran outliers	177936	1696 (3.14-3.10)
Sidechain outliers	177891	1696 (3.14-3.10)
RSRZ outliers	164620	1668 (3.14-3.10)

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  $\geq 3$ , 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	506	<div><div>9%</div><div><div></div><div>78%</div><div>17%</div><div>.</div></div></div>
1	B	506	<div><div>10%</div><div><div></div><div>78%</div><div>18%</div><div>.</div></div></div>
1	C	506	<div><div>5%</div><div><div></div><div>80%</div><div>15%</div><div>5%</div></div></div>
1	D	506	<div><div>6%</div><div><div></div><div>79%</div><div>16%</div><div>.</div></div></div>
1	E	506	<div><div>7%</div><div><div></div><div>81%</div><div>14%</div><div>.</div></div></div>
1	F	506	<div><div>13%</div><div><div></div><div>79%</div><div>17%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
3	J	4	 25% 25% 50%
3	K	4	 50% 50%
3	L	4	 50% 50%
3	M	4	 25% 50% 25%
3	N	4	 50% 50%
3	O	4	 25% 25% 50%

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
3	SIA	N	4	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23778 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	484	Total	C	N	O	S	0	0	0
			3877	2437	675	743	22			
1	B	485	Total	C	N	O	S	0	0	0
			3883	2441	676	744	22			
1	C	483	Total	C	N	O	S	0	0	0
			3873	2435	674	742	22			
1	D	484	Total	C	N	O	S	0	0	0
			3877	2437	675	743	22			
1	E	485	Total	C	N	O	S	0	0	0
			3882	2440	676	744	22			
1	F	486	Total	C	N	O	S	0	0	0
			3890	2446	677	745	22			

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



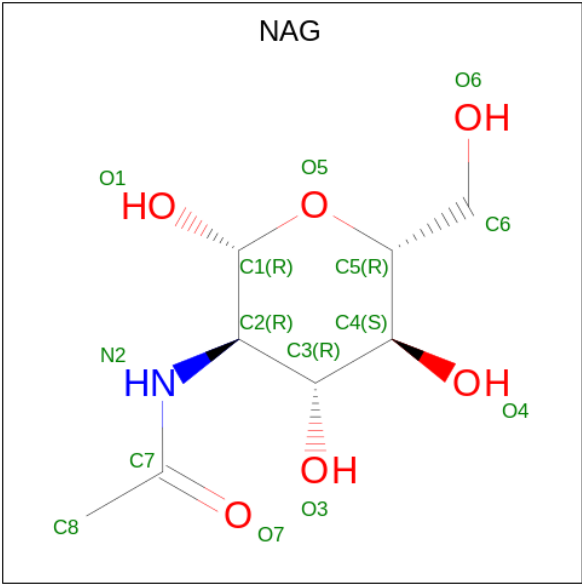
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	4	Total	C	N	O	0	0	0
			57	31	2	24			
3	K	4	Total	C	N	O	0	0	0
			57	31	2	24			
3	L	4	Total	C	N	O	0	0	0
			57	31	2	24			
3	M	4	Total	C	N	O	0	0	0
			57	31	2	24			
3	N	4	Total	C	N	O	0	0	0
			57	31	2	24			
3	O	4	Total	C	N	O	0	0	0
			57	31	2	24			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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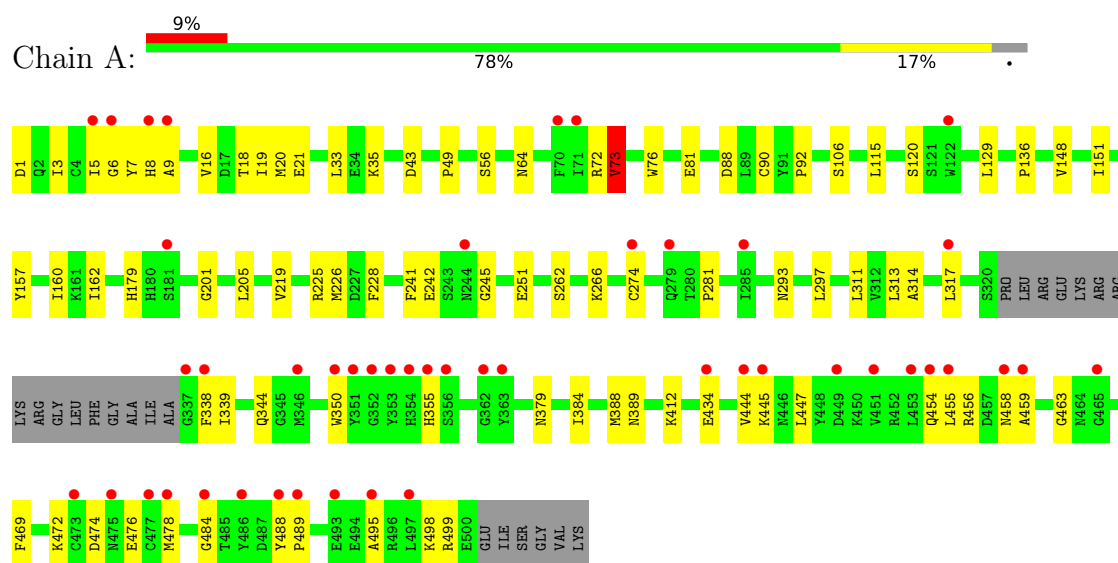
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

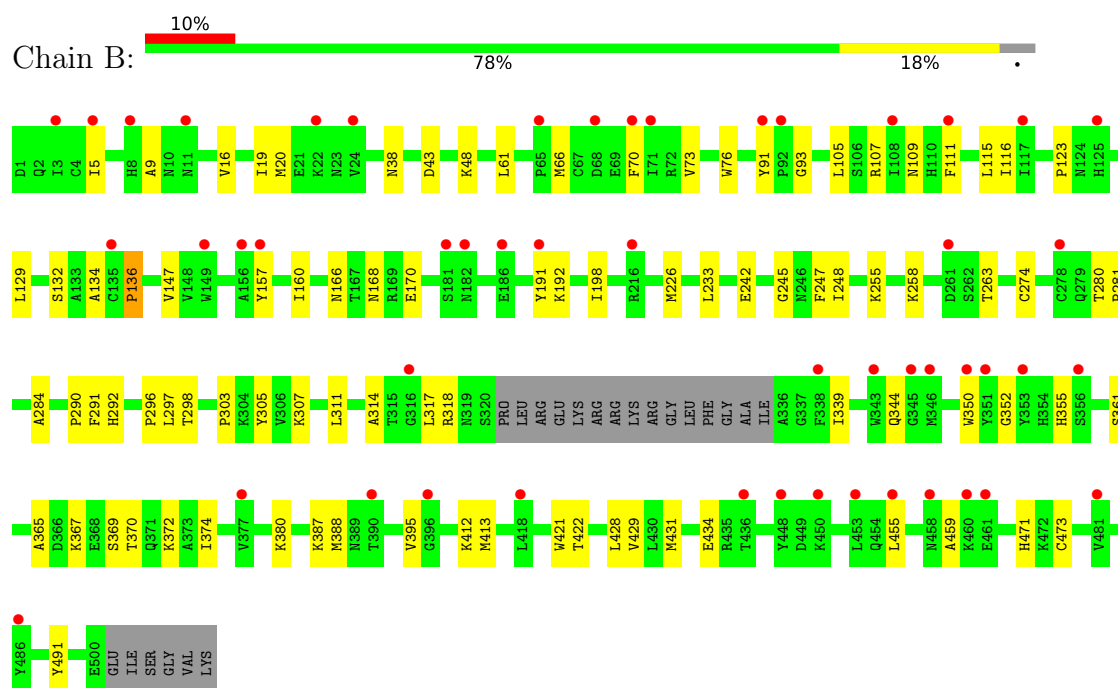
### 3 Residue-property plots

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

#### • Molecule 1: Hemagglutinin

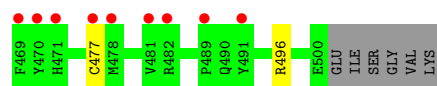


#### • Molecule 1: Hemagglutinin

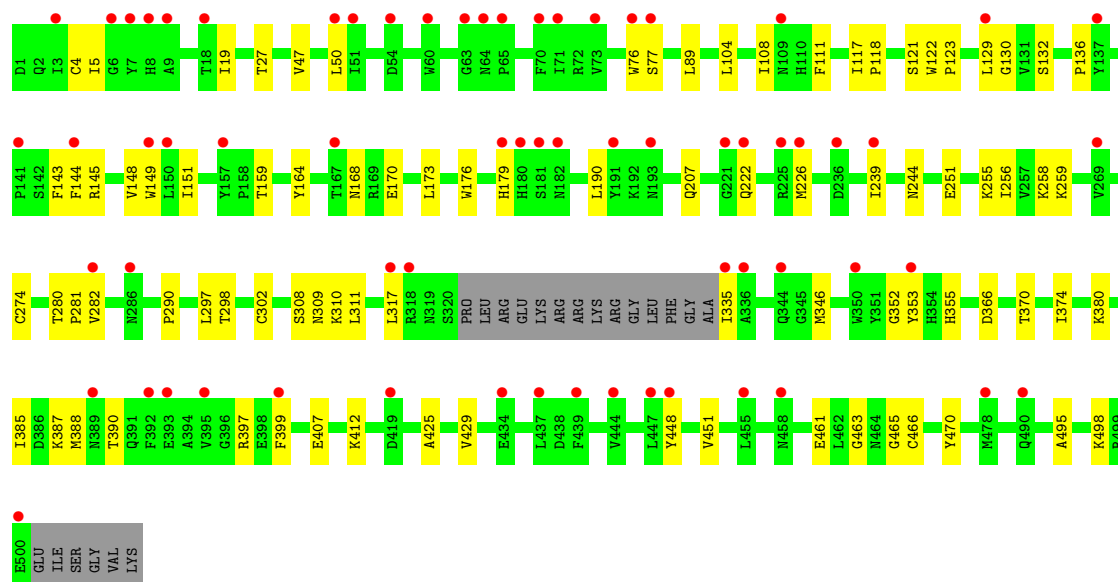
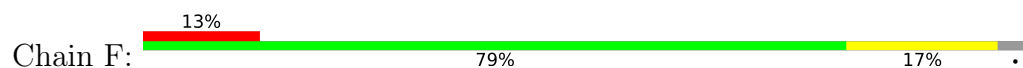








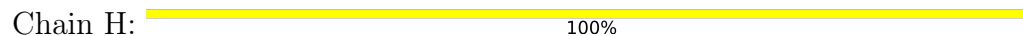
• Molecule 1: Hemagglutinin



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




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



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



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain J: 



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain K: 



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain L: 



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain M: 

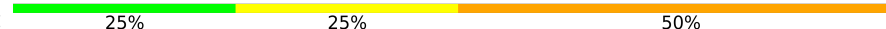


- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain N: 



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain O: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.98Å 263.81Å 131.62Å 90.00° 101.64° 90.00°	Depositor
Resolution (Å)	48.28 – 3.12 48.28 – 3.12	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.28-3.12) 90.8 (48.28-3.12)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.265 , 0.271 0.264 , 0.270	Depositor DCC
$R_{free}$ test set	82630 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	23778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: NAG, SIA, GAL

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	0.32	0/3966	0.62	4/5370 (0.1%)
1	B	0.38	0/3972	0.64	3/5379 (0.1%)
1	C	0.34	1/3962 (0.0%)	0.61	3/5365 (0.1%)
1	D	0.22	0/3966	0.49	0/5370
1	E	0.40	1/3971 (0.0%)	0.70	3/5377 (0.1%)
1	F	0.28	0/3979	0.54	2/5388 (0.0%)
All	All	0.33	2/23816 (0.0%)	0.61	15/32249 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	SER	CA-CB	-6.73	1.45	1.54
1	E	262	SER	CA-CB	-5.11	1.46	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	CA-C-N	-7.26	117.02	123.33
1	A	72	ARG	C-N-CA	-7.26	117.02	123.33
1	C	88	ASP	CB-CA-C	-7.14	108.32	116.54
1	F	222	GLN	N-CA-C	6.34	117.80	108.86
1	B	116	ILE	N-CA-C	-5.96	107.00	112.96
1	B	123	PRO	CB-CA-C	-5.53	104.26	112.55
1	E	63	GLY	N-CA-C	-5.51	105.82	112.48
1	E	63	GLY	CA-C-O	-5.30	117.63	122.24
1	A	73	VAL	CB-CA-C	5.25	115.22	110.13
1	C	120	SER	N-CA-C	-5.21	105.77	111.82
1	A	120	SER	N-CA-C	-5.19	105.75	111.71
1	E	280	THR	CB-CA-C	5.13	116.53	108.63
1	B	91	TYR	N-CA-C	-5.12	103.20	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	475	ASN	N-CA-C	-5.04	105.78	111.28
1	F	145	ARG	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

## 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	3877	0	3734	61	0
1	B	3883	0	3739	57	0
1	C	3873	0	3726	52	0
1	D	3877	0	3731	55	0
1	E	3882	0	3735	49	0
1	F	3890	0	3746	54	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	J	57	0	49	2	0
3	K	57	0	49	3	0
3	L	57	0	49	0	0
3	M	57	0	49	2	0
3	N	57	0	49	9	0
3	O	57	0	49	3	0
4	B	14	0	13	0	0
4	C	28	0	26	0	0
4	D	14	0	13	0	0
4	F	14	0	13	0	0
All	All	23778	0	22845	315	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (315) 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:178:ILE:HD12	1:E:246:ASN:O	1.80	0.82
1:C:7:TYR:HB2	1:C:317:LEU:HD13	1.63	0.81
1:D:476:GLU:O	1:D:479:GLU:HG3	1.80	0.81
1:B:132:SER:OG	3:O:4:SIA:O1B	1.99	0.80
1:B:129:LEU:O	3:O:4:SIA:H113	1.81	0.79
1:D:102:LYS:HB3	1:D:264:ILE:HD11	1.65	0.78
1:F:132:SER:OG	3:N:4:SIA:O1B	2.01	0.78
1:D:106:SER:HB3	1:D:262:SER:O	1.85	0.77
1:F:290:PRO:HD3	1:F:385:ILE:HG23	1.66	0.76
1:D:102:LYS:HB3	1:D:264:ILE:CD1	2.17	0.75
1:B:38:ASN:HD21	1:B:284:ALA:HB3	1.53	0.74
1:F:151:ILE:HD11	3:N:4:SIA:H111	1.70	0.72
1:E:64:ASN:HB3	1:E:67:CYS:HB2	1.72	0.72
1:B:134:ALA:O	1:B:136:PRO:HD3	1.90	0.71
1:D:487:ASP:HB3	1:D:490:GLN:HB2	1.72	0.71
1:E:2:GLN:HE21	1:E:462:LEU:HD11	1.54	0.71
1:A:456:ARG:HH12	1:D:460:LYS:HA	1.56	0.70
1:A:106:SER:HB2	1:A:262:SER:O	1.92	0.70
1:A:412:LYS:HE2	1:C:393:GLU:HB3	1.74	0.69
1:F:47:VAL:HB	1:F:77:SER:HB3	1.75	0.69
1:A:455:LEU:HD13	1:A:459:ALA:HB3	1.74	0.69
1:C:6:GLY:HA2	1:C:339:ILE:HD13	1.75	0.69
1:D:37:HIS:HB3	1:D:294:ILE:HD13	1.75	0.69
1:F:151:ILE:CD1	3:N:4:SIA:H111	2.23	0.68
1:B:61:LEU:HD11	1:B:105:LEU:HD11	1.75	0.67
1:E:129:LEU:O	3:M:4:SIA:H113	1.95	0.67
1:E:18:THR:HG23	1:E:434:GLU:HB2	1.76	0.67
1:A:355:HIS:HB3	1:A:478:MET:HE2	1.76	0.66
1:D:280:THR:HG23	1:D:295:HIS:HB3	1.77	0.66
1:E:110:HIS:HB3	1:E:257:VAL:HG22	1.77	0.66
1:F:280:THR:HG22	1:F:298:THR:HG22	1.79	0.65
1:A:456:ARG:NH1	1:D:460:LYS:HA	2.12	0.65
1:F:50:LEU:HB2	1:F:76:TRP:CD1	2.32	0.64
1:F:132:SER:CB	3:N:4:SIA:O1B	2.45	0.64
1:D:350:TRP:HB2	1:D:370:THR:HG23	1.79	0.63
1:B:352:GLY:HA3	1:B:365:ALA:HA	1.79	0.63
1:C:280:THR:HG22	1:C:298:THR:HG22	1.81	0.63
1:A:92:PRO:HB2	1:A:225:ARG:HE	1.64	0.63
1:B:263:THR:HB	1:B:395:VAL:HG23	1.79	0.63
1:B:9:ALA:HB3	1:B:344:GLN:HA	1.82	0.62
1:B:109:ASN:HB2	1:B:258:LYS:HG3	1.81	0.62
1:F:118:PRO:HG2	1:F:121:SER:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ILE:HG23	1:B:20:MET:HG3	1.81	0.61
1:B:134:ALA:C	1:B:136:PRO:HD3	2.25	0.61
1:B:16:VAL:HG21	1:B:314:ALA:HB2	1.81	0.61
1:A:162:ILE:HG22	1:A:241:PHE:HB2	1.83	0.61
1:B:280:THR:HG22	1:B:298:THR:HG22	1.82	0.60
1:E:63:GLY:O	1:E:144:PHE:HD1	1.84	0.60
1:D:152:LYS:HD3	1:D:155:ASP:HA	1.83	0.60
1:A:379:ASN:HB3	1:D:22:LYS:HE2	1.82	0.60
1:C:459:ALA:HB1	1:C:467:PHE:HB3	1.83	0.60
1:B:471:HIS:CD2	1:B:491:TYR:HB3	2.38	0.59
1:A:160:ILE:O	1:A:242:GLU:HA	2.03	0.58
1:A:6:GLY:HA2	1:A:339:ILE:HG12	1.86	0.58
1:C:359:GLN:NE2	1:C:474:ASP:HA	2.19	0.58
1:E:172:LEU:HD23	1:E:255:LYS:HA	1.86	0.58
1:F:346:MET:HE1	1:F:352:GLY:HA3	1.85	0.58
1:E:280:THR:HG21	1:E:294:ILE:HG22	1.85	0.57
1:A:129:LEU:HB2	1:A:151:ILE:HD11	1.85	0.57
1:A:458:ASN:HB3	1:A:469:PHE:HE1	1.68	0.57
1:A:19:ILE:HG13	1:A:20:MET:HG3	1.87	0.57
1:D:19:ILE:HG23	1:D:20:MET:HG3	1.86	0.56
1:D:134:ALA:C	1:D:136:PRO:HD3	2.30	0.56
1:D:75:GLU:HG3	1:D:109:ASN:HA	1.86	0.56
1:D:104:LEU:HD21	1:D:232:ILE:HD11	1.87	0.56
1:E:455:LEU:HD23	1:E:458:ASN:HB3	1.86	0.56
1:E:380:LYS:HE3	1:E:432:GLU:HB3	1.88	0.56
1:E:104:LEU:HD12	1:E:258:LYS:HD2	1.89	0.55
1:F:4:CYS:HA	1:F:466:CYS:HA	1.89	0.55
1:A:6:GLY:HA2	1:A:339:ILE:CG1	2.36	0.55
1:E:20:MET:HG2	1:F:380:LYS:HB2	1.87	0.55
1:C:359:GLN:HE22	1:C:474:ASP:HA	1.71	0.55
1:C:226:MET:HE2	1:C:248:ILE:HD11	1.89	0.55
1:A:389:ASN:HB2	1:D:307:LYS:NZ	2.22	0.54
1:D:280:THR:HB	1:D:283:GLY:O	2.08	0.54
1:C:300:GLY:HA2	1:C:392:PHE:HD1	1.73	0.54
1:E:423:TYR:O	1:E:427:LEU:HD23	2.08	0.54
1:A:474:ASP:HB3	1:A:476:GLU:HG2	1.90	0.53
1:C:114:ILE:HD11	1:C:172:LEU:HD21	1.91	0.53
1:E:160:ILE:O	1:E:242:GLU:HA	2.08	0.53
1:A:474:ASP:O	1:A:478:MET:HG2	2.07	0.53
1:D:102:LYS:HD2	1:D:264:ILE:HD12	1.89	0.53
1:C:93:GLY:HA3	1:C:226:MET:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:TRP:HZ3	1:B:111:PHE:HD1	1.55	0.53
1:C:129:LEU:O	3:J:4:SIA:H113	2.09	0.53
1:E:315:THR:HA	1:E:377:VAL:HG11	1.91	0.53
1:F:179:HIS:HA	1:F:226:MET:HG2	1.90	0.53
1:B:428:LEU:HA	1:B:431:MET:HE2	1.90	0.53
1:C:1:ASP:HB2	1:C:469:PHE:HB2	1.92	0.52
1:C:181:SER:HB2	1:C:213:ILE:HG12	1.91	0.52
1:D:216:ARG:HH21	1:D:224:GLY:HA2	1.73	0.52
1:F:173:LEU:HD22	1:F:256:ILE:HD11	1.91	0.52
1:F:190:LEU:HD21	3:N:4:SIA:O10	2.08	0.52
1:F:470:TYR:HB3	1:F:495:ALA:HB1	1.92	0.52
1:B:73:VAL:HB	1:B:111:PHE:HE1	1.75	0.52
1:C:370:THR:O	1:C:374:ILE:HG23	2.10	0.52
1:A:338:PHE:CE2	1:A:445:LYS:HD2	2.45	0.52
1:A:339:ILE:HD11	1:A:444:VAL:HG11	1.92	0.52
1:D:102:LYS:HD2	1:D:264:ILE:CD1	2.40	0.52
1:A:281:PRO:HD3	1:A:297:LEU:O	2.10	0.52
1:F:148:VAL:HG23	1:F:251:GLU:HB2	1.92	0.51
1:B:380:LYS:HE2	1:F:19:ILE:HD12	1.91	0.51
1:E:132:SER:OG	3:M:4:SIA:O1B	2.27	0.51
1:E:432:GLU:HA	1:E:435:ARG:HG2	1.92	0.51
1:C:459:ALA:HA	1:C:468:GLU:O	2.10	0.51
1:C:300:GLY:HA2	1:C:392:PHE:CD1	2.46	0.51
1:F:104:LEU:HA	1:F:258:LYS:HZ1	1.76	0.51
1:B:455:LEU:HD11	1:B:459:ALA:HB3	1.92	0.51
1:C:160:ILE:O	1:C:242:GLU:HA	2.11	0.51
1:C:263:THR:HG21	1:C:396:GLY:HA3	1.93	0.51
1:C:16:VAL:HG21	1:C:314:ALA:HB2	1.93	0.51
1:B:367:LYS:C	1:B:369:SER:H	2.19	0.50
1:D:280:THR:HG22	1:D:282:VAL:H	1.76	0.50
1:E:178:ILE:HD11	1:E:211:PRO:HG3	1.92	0.50
1:D:355:HIS:HB2	1:D:478:MET:HE3	1.93	0.50
1:A:201:GLY:HA2	1:A:205:LEU:O	2.12	0.50
1:B:372:LYS:HZ1	1:F:335:ILE:N	2.10	0.50
1:C:474:ASP:N	1:C:477:CYS:HB3	2.27	0.50
1:D:148:VAL:HG23	1:D:251:GLU:HB2	1.94	0.50
1:D:7:TYR:HB2	1:D:317:LEU:HD13	1.93	0.50
1:B:38:ASN:ND2	1:B:284:ALA:HB3	2.26	0.50
1:B:434:GLU:HG2	1:E:435:ARG:NH2	2.26	0.50
1:F:308:SER:HB2	1:F:311:LEU:HD11	1.94	0.50
1:D:393:GLU:HG3	1:D:394:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLU:HB3	1:D:151:ILE:HG13	1.94	0.49
1:E:5:ILE:CD1	1:E:448:TYR:HB2	2.42	0.49
1:E:216:ARG:HH21	1:E:224:GLY:HA2	1.78	0.49
1:F:76:TRP:CZ3	1:F:108:ILE:HB	2.46	0.49
1:E:18:THR:CG2	1:E:434:GLU:HB2	2.41	0.49
1:A:3:ILE:HD12	1:A:478:MET:HE1	1.95	0.49
1:C:352:GLY:HA2	1:C:365:ALA:HA	1.95	0.49
1:E:111:PHE:HA	1:E:255:LYS:O	2.12	0.49
1:A:19:ILE:HD12	1:C:380:LYS:HE2	1.95	0.48
1:E:134:ALA:O	1:E:136:PRO:HD3	2.13	0.48
1:F:159:THR:HG22	1:F:244:ASN:HB3	1.95	0.48
1:A:495:ALA:HB1	1:A:498:LYS:HB2	1.96	0.48
1:C:19:ILE:HG23	1:C:20:MET:HG3	1.93	0.48
1:D:202:THR:HG22	1:D:239:ILE:HA	1.95	0.48
1:A:18:THR:OG1	1:A:434:GLU:HB2	2.13	0.48
1:E:5:ILE:HD11	1:E:448:TYR:HB2	1.96	0.48
1:A:148:VAL:HG23	1:A:251:GLU:HB2	1.95	0.47
1:D:423:TYR:CZ	1:D:427:LEU:HD11	2.49	0.47
1:F:399:PHE:HB2	1:F:407:GLU:HG3	1.96	0.47
1:E:280:THR:HG21	1:E:294:ILE:CG2	2.43	0.47
1:F:353:TYR:CE2	1:F:366:ASP:HB2	2.49	0.47
1:A:355:HIS:HB3	1:A:478:MET:CE	2.44	0.47
1:B:307:LYS:HZ2	1:E:389:ASN:HB3	1.78	0.47
1:C:193:ASN:HD22	1:C:244:ASN:HB2	1.79	0.47
1:A:9:ALA:HB3	1:A:344:GLN:HA	1.95	0.47
1:E:109:ASN:HB2	1:E:257:VAL:HG23	1.96	0.47
1:A:115:LEU:HD22	1:A:251:GLU:O	2.14	0.47
1:A:226:MET:HE3	1:A:228:PHE:CZ	2.50	0.47
1:A:463:GLY:HA3	1:C:453:LEU:HD13	1.96	0.47
1:F:425:ALA:O	1:F:429:VAL:HG23	2.14	0.47
1:F:164:TYR:H	1:F:239:ILE:HG22	1.80	0.47
1:A:7:TYR:CD1	1:A:317:LEU:HD13	2.50	0.47
1:B:355:HIS:O	1:B:361:SER:HA	2.15	0.47
1:D:160:ILE:O	1:D:242:GLU:HA	2.14	0.47
1:D:388:MET:HB3	1:D:388:MET:HE2	1.74	0.47
1:B:350:TRP:HB2	1:B:370:THR:HG23	1.97	0.46
1:A:488:TYR:CG	1:A:489:PRO:HD3	2.50	0.46
1:B:43:ASP:OD1	1:B:48:LYS:HA	2.15	0.46
1:C:16:VAL:HG12	1:C:312:VAL:HG22	1.96	0.46
1:C:440:HIS:O	1:C:444:VAL:HG23	2.16	0.46
1:E:117:ILE:HD12	1:E:250:PRO:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:HD3	1:A:499:ARG:HA	1.63	0.46
1:F:130:GLY:HA2	3:N:4:SIA:C11	2.45	0.46
1:B:307:LYS:HB2	1:B:422:THR:HG21	1.98	0.46
1:B:395:VAL:HG12	1:F:412:LYS:HD2	1.96	0.46
1:B:281:PRO:HD3	1:B:297:LEU:O	2.16	0.46
1:A:92:PRO:HB3	1:A:219:VAL:HB	1.97	0.46
1:E:373:ALA:O	1:E:377:VAL:HG23	2.16	0.46
1:B:70:PHE:HB3	1:B:73:VAL:HG21	1.97	0.46
1:D:102:LYS:HB3	1:D:264:ILE:HD12	1.95	0.45
1:A:157:TYR:CZ	1:A:245:GLY:HA2	2.52	0.45
1:A:455:LEU:O	1:A:455:LEU:HD12	2.16	0.45
1:C:281:PRO:HD3	1:C:297:LEU:O	2.16	0.45
1:C:413:MET:HE2	1:C:413:MET:HB3	1.76	0.45
1:A:129:LEU:O	3:K:4:SIA:H113	2.16	0.45
1:A:8:HIS:HB2	1:A:350:TRP:HA	1.98	0.45
1:C:346:MET:SD	1:C:352:GLY:HA3	2.56	0.45
1:D:2:GLN:HB2	1:D:356:SER:HB2	1.98	0.45
1:E:460:LYS:HB3	1:E:468:GLU:HB3	1.99	0.45
1:E:496:ARG:HD2	1:E:496:ARG:HA	1.71	0.45
1:A:16:VAL:HG21	1:A:314:ALA:HB2	1.98	0.45
1:B:198:ILE:HD11	1:B:247:PHE:HA	1.98	0.45
1:A:388:MET:HE3	1:A:388:MET:HA	1.99	0.45
1:E:280:THR:HG22	1:E:282:VAL:H	1.82	0.45
1:A:18:THR:HG23	1:A:21:GLU:H	1.81	0.45
1:A:454:GLN:CD	1:A:484:GLY:HA2	2.42	0.45
1:F:129:LEU:O	3:N:4:SIA:H113	2.16	0.45
2:G:1:NAG:H4	2:G:2:NAG:H2	1.40	0.45
1:D:487:ASP:HB3	1:D:490:GLN:CB	2.46	0.45
1:E:352:GLY:HA3	1:E:365:ALA:HA	1.98	0.45
1:F:5:ILE:HD11	1:F:451:VAL:HG21	1.99	0.45
1:B:168:ASN:O	1:B:170:GLU:HG2	2.16	0.45
1:D:380:LYS:HE3	1:D:432:GLU:HB3	1.98	0.45
1:B:455:LEU:HD21	1:B:459:ALA:HB3	1.99	0.44
1:C:61:LEU:HD11	1:C:105:LEU:HD11	1.98	0.44
1:D:299:ILE:HG22	1:D:395:VAL:HA	1.98	0.44
1:E:16:VAL:HG21	1:E:314:ALA:HB2	1.99	0.44
1:F:412:LYS:HB3	1:F:412:LYS:HE2	1.70	0.44
1:A:5:ILE:HD11	1:A:447:LEU:HB2	1.99	0.44
1:A:339:ILE:CD1	1:A:444:VAL:HG11	2.47	0.44
1:D:393:GLU:HG3	1:D:394:ALA:H	1.81	0.44
1:E:66:MET:HB3	1:E:66:MET:HE2	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:ASP:H	1:D:477:CYS:HB3	1.82	0.44
1:F:495:ALA:HA	1:F:498:LYS:HB3	1.99	0.44
1:B:111:PHE:HA	1:B:255:LYS:O	2.18	0.44
1:B:370:THR:O	1:B:374:ILE:HG22	2.18	0.44
1:C:61:LEU:HD11	1:C:105:LEU:CD1	2.47	0.44
1:C:372:LYS:HE3	1:C:372:LYS:HB2	1.79	0.44
1:B:73:VAL:HB	1:B:111:PHE:CE1	2.52	0.43
1:F:298:THR:HB	1:F:302:CYS:SG	2.57	0.43
1:B:296:PRO:HG3	1:B:305:TYR:CE2	2.53	0.43
1:B:412:LYS:HB3	1:E:413:MET:HE1	1.99	0.43
1:C:339:ILE:H	1:C:339:ILE:HG13	1.42	0.43
1:A:313:LEU:HD11	1:A:384:ILE:HD13	2.01	0.43
1:C:345:GLY:O	1:C:347:VAL:HG13	2.17	0.43
1:F:89:LEU:HA	1:F:144:PHE:HZ	1.83	0.43
1:A:1:ASP:OD2	1:A:472:LYS:HA	2.18	0.43
1:B:166:ASN:HB2	1:B:233:LEU:HD23	2.01	0.43
1:B:388:MET:HE1	1:B:421:TRP:CZ3	2.53	0.43
1:D:201:GLY:HA2	1:D:205:LEU:O	2.18	0.43
1:F:281:PRO:HD3	1:F:297:LEU:O	2.19	0.43
1:F:388:MET:HG3	1:F:390:THR:HG23	2.01	0.43
1:A:33:LEU:HB2	1:A:311:LEU:HB2	1.99	0.43
1:B:93:GLY:HA3	1:B:226:MET:O	2.18	0.43
1:D:48:LYS:HE2	1:D:271:TYR:CE2	2.54	0.43
1:D:346:MET:HG3	1:D:346:MET:O	2.18	0.43
1:C:456:ARG:HD2	1:C:456:ARG:HA	1.78	0.43
1:C:488:TYR:N	1:C:489:PRO:HD2	2.34	0.43
1:D:345:GLY:HA3	1:D:363:TYR:CE2	2.54	0.43
1:F:143:PHE:CE2	1:F:149:TRP:HB2	2.54	0.43
1:A:81:GLU:O	1:A:266:LYS:HA	2.18	0.43
3:N:3:GAL:H3	3:N:4:SIA:H32	1.91	0.43
1:B:157:TYR:CZ	1:B:245:GLY:HA2	2.54	0.43
1:C:104:LEU:HD21	1:C:232:ILE:HD11	2.00	0.42
1:A:18:THR:HG22	1:A:21:GLU:HB2	2.00	0.42
1:C:460:LYS:O	1:C:467:PHE:HA	2.18	0.42
1:E:38:ASN:ND2	1:E:284:ALA:HB3	2.34	0.42
1:F:130:GLY:HA2	3:N:4:SIA:H113	2.01	0.42
1:A:73:VAL:HG12	1:A:76:TRP:HE3	1.83	0.42
1:B:107:ARG:HE	1:B:107:ARG:HB3	1.56	0.42
1:D:1:ASP:HB2	1:D:469:PHE:HB2	2.02	0.42
1:E:3:ILE:HD12	1:E:3:ILE:HA	1.92	0.42
1:B:5:ILE:O	1:B:339:ILE:HD12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LYS:HA	1:B:387:LYS:HD3	1.69	0.42
1:C:151:ILE:HG22	1:C:152:LYS:N	2.34	0.42
1:C:162:ILE:HG22	1:C:241:PHE:HB2	2.01	0.42
1:D:71:ILE:HG12	1:D:73:VAL:HG23	2.02	0.42
1:D:92:PRO:HG2	1:D:219:VAL:O	2.19	0.42
1:A:56:SER:OG	1:A:88:ASP:HA	2.20	0.42
1:A:92:PRO:HB2	1:A:225:ARG:NE	2.33	0.42
1:A:412:LYS:HE3	1:C:395:VAL:HG22	2.01	0.42
1:B:66:MET:HE3	1:B:66:MET:HB3	1.91	0.42
1:B:317:LEU:HD12	1:B:318:ARG:O	2.20	0.42
1:C:395:VAL:HG12	1:C:395:VAL:O	2.18	0.42
1:A:64:ASN:HD21	1:A:90:CYS:HB3	1.84	0.42
1:A:43:ASP:OD1	1:A:49:PRO:HD2	2.19	0.42
1:B:147:VAL:HG22	1:B:248:ILE:HG22	2.01	0.42
1:D:39:GLY:H	1:D:283:GLY:HA3	1.83	0.42
3:J:3:GAL:H3	3:J:4:SIA:H32	1.91	0.42
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.92	0.42
1:F:176:TRP:HZ2	1:F:207:GLN:HE22	1.67	0.42
1:B:413:MET:HE2	1:B:413:MET:HB3	1.67	0.42
1:F:121:SER:C	1:F:123:PRO:HD3	2.45	0.42
3:O:3:GAL:H3	3:O:4:SIA:H32	1.91	0.42
1:B:160:ILE:O	1:B:242:GLU:HA	2.20	0.41
1:D:88:ASP:CG	1:D:89:LEU:H	2.28	0.41
1:E:198:ILE:HD13	1:E:247:PHE:HD1	1.85	0.41
1:E:450:LYS:HE2	1:E:450:LYS:HB3	1.90	0.41
1:A:7:TYR:HD2	1:A:339:ILE:HD13	1.85	0.41
1:C:34:GLU:OE2	1:C:287:SER:HB2	2.19	0.41
1:F:168:ASN:C	1:F:170:GLU:H	2.28	0.41
1:A:35:LYS:HG2	1:A:293:ASN:OD1	2.20	0.41
1:E:53:LYS:HE3	1:E:53:LYS:HB2	1.83	0.41
1:F:259:LYS:HE2	1:F:259:LYS:HB3	1.89	0.41
1:F:387:LYS:HD3	1:F:387:LYS:HA	1.86	0.41
1:C:63:GLY:O	1:C:144:PHE:HA	2.20	0.41
1:C:134:ALA:O	1:C:136:PRO:HD3	2.21	0.41
1:D:498:LYS:O	1:D:498:LYS:HG3	2.21	0.41
1:B:290:PRO:HG2	1:B:291:PHE:CD2	2.55	0.41
1:B:311:LEU:HD22	1:B:429:VAL:HG21	2.02	0.41
1:E:148:VAL:HG23	1:E:251:GLU:HB2	2.03	0.41
1:D:313:LEU:HD23	1:D:313:LEU:HA	1.95	0.41
1:C:339:ILE:HD11	1:C:444:VAL:HG11	2.01	0.41
1:D:178:ILE:HD11	1:D:211:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:SER:O	1:D:387:LYS:HB2	2.21	0.41
1:D:427:LEU:HD23	1:D:427:LEU:HA	1.97	0.41
1:A:179:HIS:NE2	3:K:4:SIA:H91	2.36	0.41
1:C:371:GLN:HA	1:C:374:ILE:HG12	2.02	0.41
1:E:226:MET:HE2	1:E:226:MET:HB2	1.94	0.41
1:E:412:LYS:HD3	1:F:397:ARG:HH12	1.85	0.41
1:E:461:GLU:HG2	1:E:467:PHE:HE1	1.86	0.41
1:F:111:PHE:CE1	1:F:256:ILE:HG12	2.56	0.41
1:F:117:ILE:HG21	1:F:122:TRP:CZ2	2.56	0.41
1:F:310:LYS:HB2	1:F:310:LYS:HE2	1.81	0.41
1:F:448:TYR:HE2	1:F:465:GLY:HA2	1.86	0.41
1:A:389:ASN:HB2	1:D:307:LYS:HZ3	1.86	0.41
1:F:309:ASN:O	1:F:310:LYS:HG3	2.21	0.41
3:K:3:GAL:H3	3:K:4:SIA:H32	1.91	0.41
1:F:111:PHE:HA	1:F:255:LYS:O	2.21	0.40
1:F:370:THR:O	1:F:374:ILE:HG13	2.21	0.40
1:F:27:THR:HG23	1:F:317:LEU:O	2.21	0.40
1:B:192:LYS:HA	1:B:192:LYS:HD2	1.64	0.40
1:C:42:CYS:HB3	1:C:274:CYS:C	2.46	0.40
1:E:42:CYS:HB3	1:E:274:CYS:C	2.45	0.40
1:E:110:HIS:HB3	1:E:257:VAL:CG2	2.46	0.40
1:D:108:ILE:HD13	1:D:256:ILE:HG23	2.03	0.40
1:B:157:TYR:CE2	1:B:191:TYR:HD1	2.40	0.40
1:B:292:HIS:HB3	1:B:303:PRO:HB2	2.04	0.40
1:C:20:MET:HE2	1:D:376:GLY:C	2.46	0.40
1:C:359:GLN:H	1:C:359:GLN:HG3	1.53	0.40
1:F:461:GLU:HG2	1:F:463:GLY:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/506 (95%)	455 (95%)	24 (5%)	1 (0%)	44	73
1	B	481/506 (95%)	456 (95%)	24 (5%)	1 (0%)	44	73
1	C	479/506 (95%)	466 (97%)	13 (3%)	0	100	100
1	D	480/506 (95%)	458 (95%)	21 (4%)	1 (0%)	44	73
1	E	481/506 (95%)	468 (97%)	12 (2%)	1 (0%)	44	73
1	F	482/506 (95%)	456 (95%)	25 (5%)	1 (0%)	44	73
All	All	2883/3036 (95%)	2759 (96%)	119 (4%)	5 (0%)	44	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	136	PRO
1	B	136	PRO
1	E	194	PRO
1	D	136	PRO
1	A	136	PRO

### 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	427/445 (96%)	425 (100%)	2 (0%)	86	92
1	B	428/445 (96%)	425 (99%)	3 (1%)	81	90
1	C	428/445 (96%)	424 (99%)	4 (1%)	75	87
1	D	428/445 (96%)	426 (100%)	2 (0%)	86	92
1	E	427/445 (96%)	421 (99%)	6 (1%)	62	79
1	F	429/445 (96%)	426 (99%)	3 (1%)	81	90
All	All	2567/2670 (96%)	2547 (99%)	20 (1%)	79	89

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	A	274	CYS
1	B	115	LEU
1	B	274	CYS
1	B	473	CYS
1	C	261	ASP
1	C	274	CYS
1	C	339	ILE
1	C	477	CYS
1	D	274	CYS
1	D	282	VAL
1	E	264	ILE
1	E	274	CYS
1	E	280	THR
1	E	317	LEU
1	E	319	ASN
1	E	477	CYS
1	F	274	CYS
1	F	282	VAL
1	F	355	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	168	ASN
1	A	193	ASN
1	A	222	GLN
1	B	28	HIS
1	B	64	ASN
1	B	124	ASN
1	B	166	ASN
1	B	168	ASN
1	B	279	GLN
1	C	146	ASN
1	C	222	GLN
1	C	408	ASN
1	D	2	GLN
1	D	38	ASN
1	D	45	ASN
1	D	103	HIS
1	D	109	ASN

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Mol	Chain	Res	Type
1	D	110	HIS
1	E	2	GLN
1	E	103	HIS
1	E	146	ASN
1	E	182	ASN
1	E	354	HIS
1	E	359	GLN
1	E	379	ASN
1	F	15	GLN
1	F	168	ASN
1	F	189	ASN
1	F	207	GLN
1	F	292	HIS
1	F	475	ASN

### 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 ⓘ

30 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	$\# Z  > 2$
2	NAG	G	1	1,2	14,14,15	0.73	0	17,19,21	1.11	1 (5%)
2	NAG	G	2	2	14,14,15	0.57	0	17,19,21	1.20	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.92	1 (7%)	17,19,21	1.91	4 (23%)
2	NAG	H	2	2	14,14,15	0.80	1 (7%)	17,19,21	1.60	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	I	1	1,2	14,14,15	0.80	0	17,19,21	1.04	1 (5%)
2	NAG	I	2	2	14,14,15	2.10	4 (28%)	17,19,21	1.00	0
3	GAL	J	1	3	12,12,12	0.23	0	17,17,17	0.67	0
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	1.60	3 (17%)
3	GAL	J	3	3	11,11,12	0.70	0	15,15,17	1.27	2 (13%)
3	SIA	J	4	3	20,20,21	2.04	2 (10%)	24,28,31	1.92	7 (29%)
3	GAL	K	1	3	12,12,12	0.22	0	17,17,17	0.53	0
3	NAG	K	2	3	14,14,15	0.40	0	17,19,21	0.81	0
3	GAL	K	3	3	11,11,12	0.69	0	15,15,17	1.28	2 (13%)
3	SIA	K	4	3	20,20,21	2.04	2 (10%)	24,28,31	1.92	7 (29%)
3	GAL	L	1	3	12,12,12	0.17	0	17,17,17	0.46	0
3	NAG	L	2	3	14,14,15	0.40	0	17,19,21	0.77	0
3	GAL	L	3	3	11,11,12	0.71	0	15,15,17	1.27	2 (13%)
3	SIA	L	4	3	20,20,21	2.05	2 (10%)	24,28,31	1.93	7 (29%)
3	GAL	M	1	3	12,12,12	0.19	0	17,17,17	0.60	0
3	NAG	M	2	3	14,14,15	0.38	0	17,19,21	1.09	1 (5%)
3	GAL	M	3	3	11,11,12	0.68	0	15,15,17	1.29	2 (13%)
3	SIA	M	4	3	20,20,21	2.04	2 (10%)	24,28,31	1.92	7 (29%)
3	GAL	N	1	3	12,12,12	0.24	0	17,17,17	0.52	0
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	0.49	0
3	GAL	N	3	3	11,11,12	0.69	0	15,15,17	1.27	2 (13%)
3	SIA	N	4	3	20,20,21	2.05	2 (10%)	24,28,31	1.92	7 (29%)
3	GAL	O	1	3	12,12,12	0.13	0	17,17,17	0.48	0
3	NAG	O	2	3	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
3	GAL	O	3	3	11,11,12	0.69	0	15,15,17	1.28	2 (13%)
3	SIA	O	4	3	20,20,21	2.02	2 (10%)	24,28,31	1.91	7 (29%)

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
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1
3	GAL	J	1	3	-	0/2/22/22	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	GAL	J	3	3	-	1/2/19/22	0/1/1/1
3	SIA	J	4	3	-	3/18/34/38	0/1/1/1
3	GAL	K	1	3	-	0/2/22/22	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	GAL	K	3	3	-	1/2/19/22	0/1/1/1
3	SIA	K	4	3	-	3/18/34/38	0/1/1/1
3	GAL	L	1	3	-	0/2/22/22	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	GAL	L	3	3	-	1/2/19/22	0/1/1/1
3	SIA	L	4	3	-	3/18/34/38	0/1/1/1
3	GAL	M	1	3	-	0/2/22/22	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	GAL	M	3	3	-	1/2/19/22	0/1/1/1
3	SIA	M	4	3	-	3/18/34/38	0/1/1/1
3	GAL	N	1	3	-	1/2/22/22	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	GAL	N	3	3	-	1/2/19/22	0/1/1/1
3	SIA	N	4	3	-	3/18/34/38	0/1/1/1
3	GAL	O	1	3	-	0/2/22/22	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	GAL	O	3	3	-	1/2/19/22	0/1/1/1
3	SIA	O	4	3	-	3/18/34/38	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	4	SIA	C2-C1	7.79	1.59	1.52
3	L	4	SIA	C2-C1	7.77	1.59	1.52
3	M	4	SIA	C2-C1	7.76	1.59	1.52
3	J	4	SIA	C2-C1	7.74	1.59	1.52
3	K	4	SIA	C2-C1	7.73	1.59	1.52
3	O	4	SIA	C2-C1	7.66	1.59	1.52
2	I	2	NAG	O5-C1	4.80	1.51	1.43
2	I	2	NAG	C7-N2	3.70	1.47	1.34
3	J	4	SIA	O6-C2	3.06	1.47	1.43
3	L	4	SIA	O6-C2	3.03	1.47	1.43
3	N	4	SIA	O6-C2	3.00	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	4	SIA	O6-C2	2.98	1.47	1.43
3	M	4	SIA	O6-C2	2.97	1.47	1.43
3	O	4	SIA	O6-C2	2.94	1.47	1.43
2	I	2	NAG	C2-N2	2.83	1.51	1.46
2	H	2	NAG	C1-C2	2.71	1.56	1.52
2	I	2	NAG	O5-C5	2.51	1.48	1.43
2	H	1	NAG	O4-C4	2.26	1.48	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	NAG	O5-C1-C2	-5.33	102.87	111.29
2	H	2	NAG	C2-N2-C7	5.08	130.14	122.90
3	L	4	SIA	O1A-C1-C2	-4.66	111.57	122.57
3	N	4	SIA	O1A-C1-C2	-4.65	111.58	122.57
3	M	4	SIA	O1A-C1-C2	-4.64	111.62	122.57
3	J	4	SIA	O1A-C1-C2	-4.63	111.62	122.57
3	K	4	SIA	O1A-C1-C2	-4.62	111.65	122.57
3	O	4	SIA	O1A-C1-C2	-4.60	111.69	122.57
3	K	4	SIA	C6-O6-C2	4.34	120.62	111.34
3	M	4	SIA	C6-O6-C2	4.33	120.61	111.34
3	L	4	SIA	C6-O6-C2	4.33	120.60	111.34
3	N	4	SIA	C6-O6-C2	4.33	120.60	111.34
3	O	4	SIA	C6-O6-C2	4.32	120.58	111.34
3	J	4	SIA	C6-O6-C2	4.32	120.58	111.34
2	H	1	NAG	O4-C4-C5	4.16	119.61	109.30
2	H	1	NAG	O5-C1-C2	4.08	117.73	111.29
3	L	4	SIA	O6-C2-C3	-3.75	105.30	110.46
3	J	4	SIA	O6-C2-C3	-3.73	105.33	110.46
3	K	4	SIA	O6-C2-C3	-3.71	105.35	110.46
3	M	4	SIA	O6-C2-C3	-3.71	105.36	110.46
3	O	4	SIA	O6-C2-C3	-3.70	105.37	110.46
3	N	4	SIA	O6-C2-C3	-3.69	105.38	110.46
2	H	1	NAG	C4-C3-C2	-3.28	106.22	111.02
3	K	3	GAL	O3-C3-C2	-3.00	104.26	109.99
3	J	3	GAL	O3-C3-C2	-2.98	104.28	109.99
3	N	3	GAL	O3-C3-C2	-2.98	104.29	109.99
3	L	3	GAL	O3-C3-C2	-2.97	104.30	109.99
3	M	3	GAL	O3-C3-C2	-2.97	104.31	109.99
2	G	2	NAG	O5-C1-C2	2.96	115.97	111.29
3	O	3	GAL	O3-C3-C2	-2.95	104.35	109.99
2	I	1	NAG	O5-C5-C4	-2.74	104.16	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	O5-C5-C4	-2.71	104.23	110.83
3	M	2	NAG	C1-C2-N2	2.64	114.99	110.49
3	J	2	NAG	C1-C2-N2	2.63	114.98	110.49
2	G	2	NAG	C1-O5-C5	2.58	115.69	112.19
3	N	4	SIA	O1B-C1-O1A	2.42	129.59	124.09
3	L	4	SIA	O1B-C1-O1A	2.42	129.57	124.09
3	J	4	SIA	O1B-C1-O1A	2.41	129.56	124.09
3	M	4	SIA	O1B-C1-O1A	2.40	129.55	124.09
3	K	4	SIA	O1B-C1-O1A	2.40	129.53	124.09
3	O	4	SIA	O1B-C1-O1A	2.38	129.49	124.09
2	G	1	NAG	O5-C5-C6	-2.28	103.62	107.20
3	M	4	SIA	C3-C4-C5	-2.26	108.73	111.46
3	K	4	SIA	C3-C4-C5	-2.23	108.76	111.46
3	L	4	SIA	C3-C4-C5	-2.23	108.77	111.46
3	J	4	SIA	C3-C4-C5	-2.22	108.78	111.46
3	N	4	SIA	C3-C4-C5	-2.19	108.81	111.46
3	M	4	SIA	C6-C5-N5	-2.19	107.28	110.91
3	N	4	SIA	C6-C5-N5	-2.19	107.28	110.91
3	K	4	SIA	C6-C5-N5	-2.18	107.29	110.91
3	O	4	SIA	C3-C4-C5	-2.18	108.82	111.46
3	J	4	SIA	C6-C5-N5	-2.18	107.30	110.91
3	O	4	SIA	C6-C5-N5	-2.18	107.30	110.91
3	L	4	SIA	C6-C5-N5	-2.17	107.31	110.91
2	H	2	NAG	O7-C7-N2	2.08	125.78	121.95
3	O	2	NAG	O5-C1-C2	-2.06	108.03	111.29
3	M	3	GAL	O5-C5-C6	2.06	110.43	107.20
3	L	3	GAL	O5-C5-C6	2.04	110.41	107.20
3	L	4	SIA	O1B-C1-C2	2.04	118.84	113.03
3	O	3	GAL	O5-C5-C6	2.03	110.39	107.20
3	M	4	SIA	O1B-C1-C2	2.03	118.82	113.03
3	N	4	SIA	O1B-C1-C2	2.03	118.82	113.03
3	K	4	SIA	O1B-C1-C2	2.02	118.81	113.03
3	J	3	GAL	O5-C5-C6	2.02	110.38	107.20
3	J	4	SIA	O1B-C1-C2	2.02	118.80	113.03
3	O	4	SIA	O1B-C1-C2	2.02	118.80	113.03
3	K	3	GAL	O5-C5-C6	2.02	110.37	107.20
3	J	2	NAG	C2-N2-C7	-2.01	120.04	122.90
3	N	3	GAL	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	I	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	N	1	GAL	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C8-C7-N2-C2
3	N	2	NAG	C1-C2-N2-C7
2	H	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	J	4	SIA	C6-C7-C8-O8
3	K	4	SIA	C6-C7-C8-O8
3	L	4	SIA	C6-C7-C8-O8
3	M	4	SIA	C6-C7-C8-O8
3	N	4	SIA	C6-C7-C8-O8
3	O	4	SIA	C6-C7-C8-O8
3	L	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O7-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C1-C2-N2-C7
3	M	3	GAL	C4-C5-C6-O6
3	K	3	GAL	C4-C5-C6-O6
3	L	3	GAL	C4-C5-C6-O6
3	O	3	GAL	C4-C5-C6-O6
3	N	3	GAL	C4-C5-C6-O6
3	J	3	GAL	C4-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C3-C2-N2-C7
3	J	4	SIA	C6-C7-C8-C9
3	K	4	SIA	C6-C7-C8-C9
3	L	4	SIA	C6-C7-C8-C9
3	M	4	SIA	C6-C7-C8-C9
3	N	4	SIA	C6-C7-C8-C9
3	O	4	SIA	C6-C7-C8-C9
3	J	4	SIA	O7-C7-C8-O8
3	K	4	SIA	O7-C7-C8-O8

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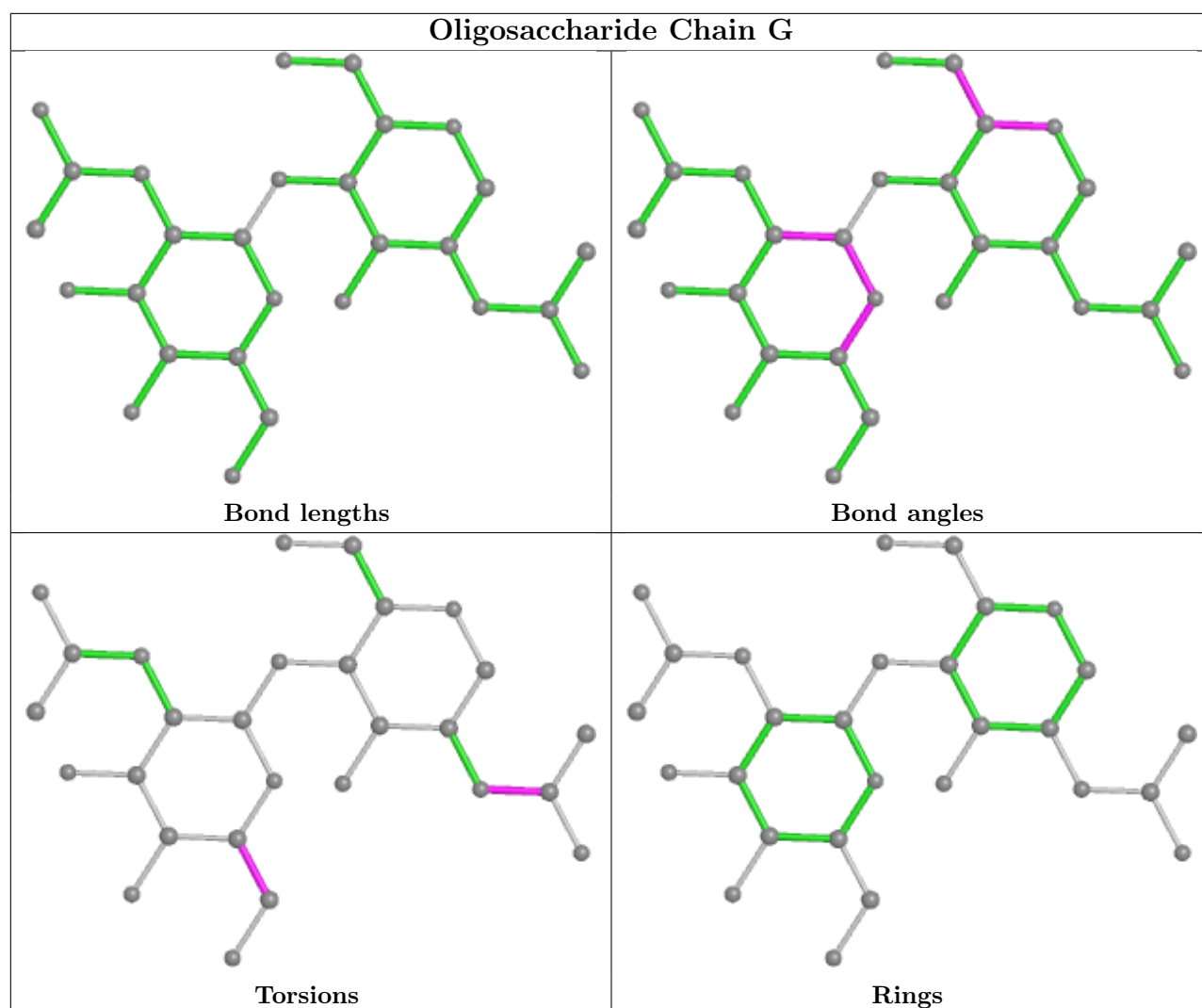
Mol	Chain	Res	Type	Atoms
3	L	4	SIA	O7-C7-C8-O8
3	M	4	SIA	O7-C7-C8-O8
3	N	4	SIA	O7-C7-C8-O8
3	O	4	SIA	O7-C7-C8-O8

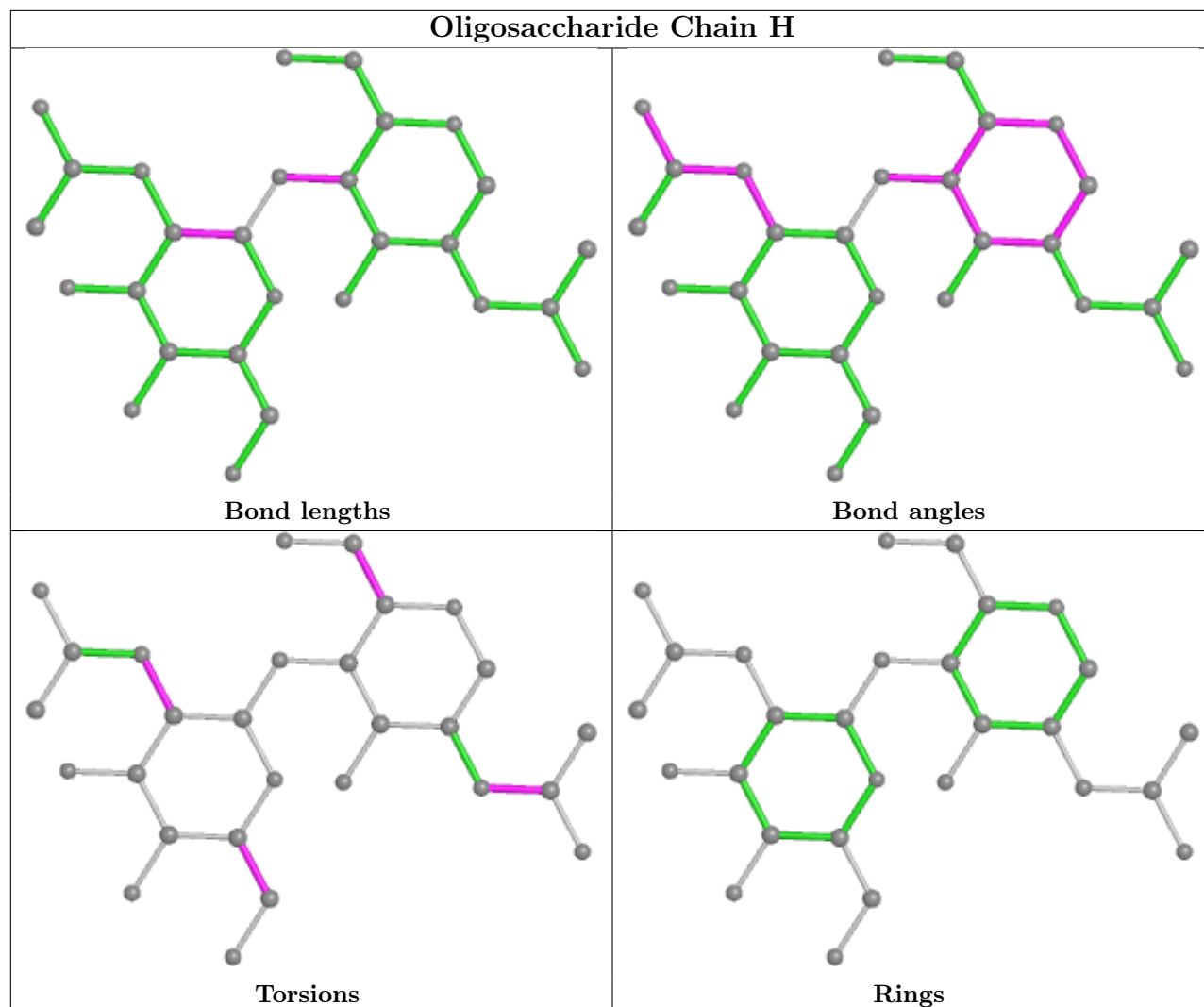
There are no ring outliers.

11 monomers are involved in 20 short contacts:

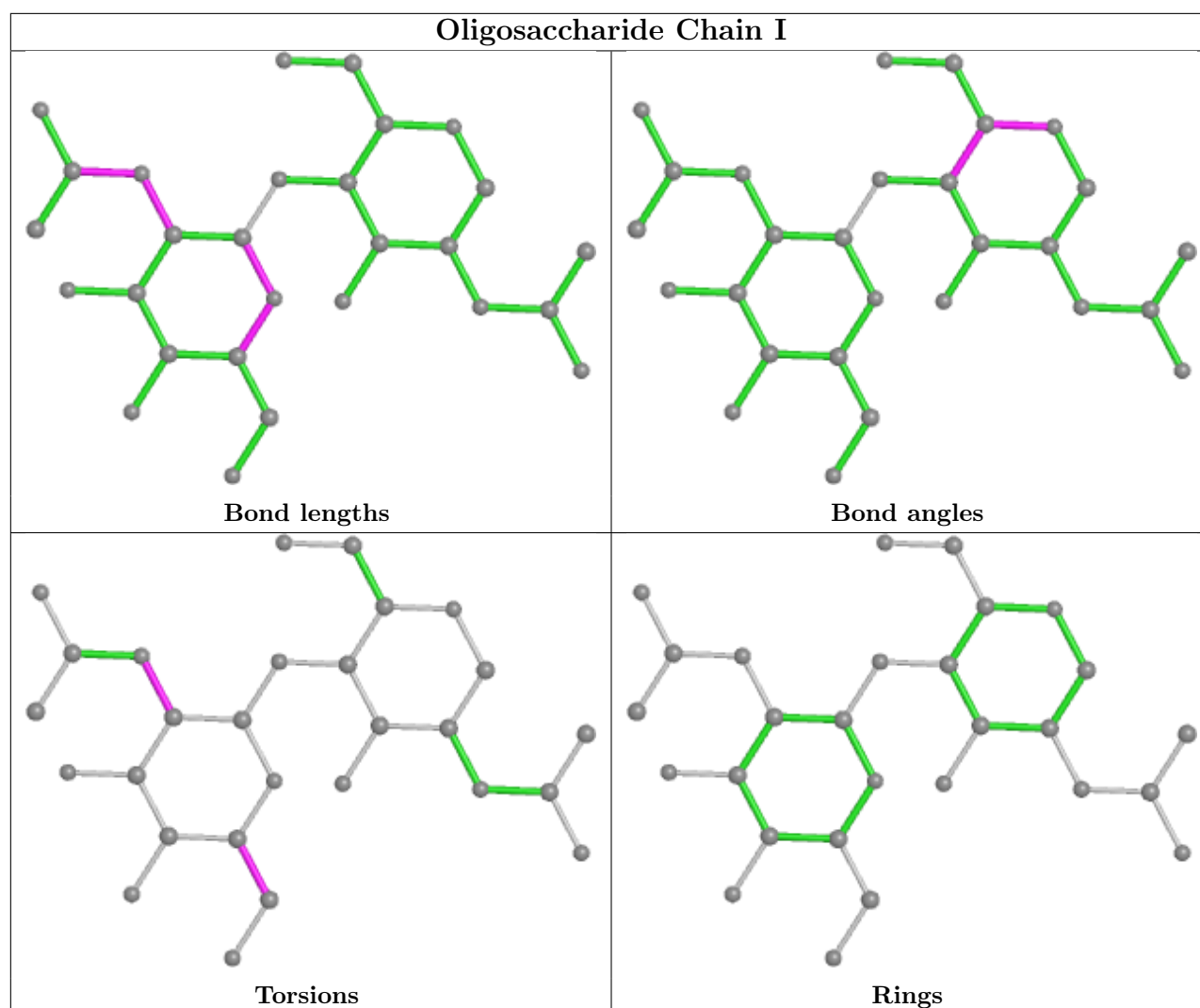
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	G	2	NAG	1	0
3	K	3	GAL	1	0
3	N	3	GAL	1	0
3	O	3	GAL	1	0
3	K	4	SIA	3	0
3	N	4	SIA	9	0
3	O	4	SIA	3	0
3	J	3	GAL	1	0
3	M	4	SIA	2	0
3	J	4	SIA	2	0

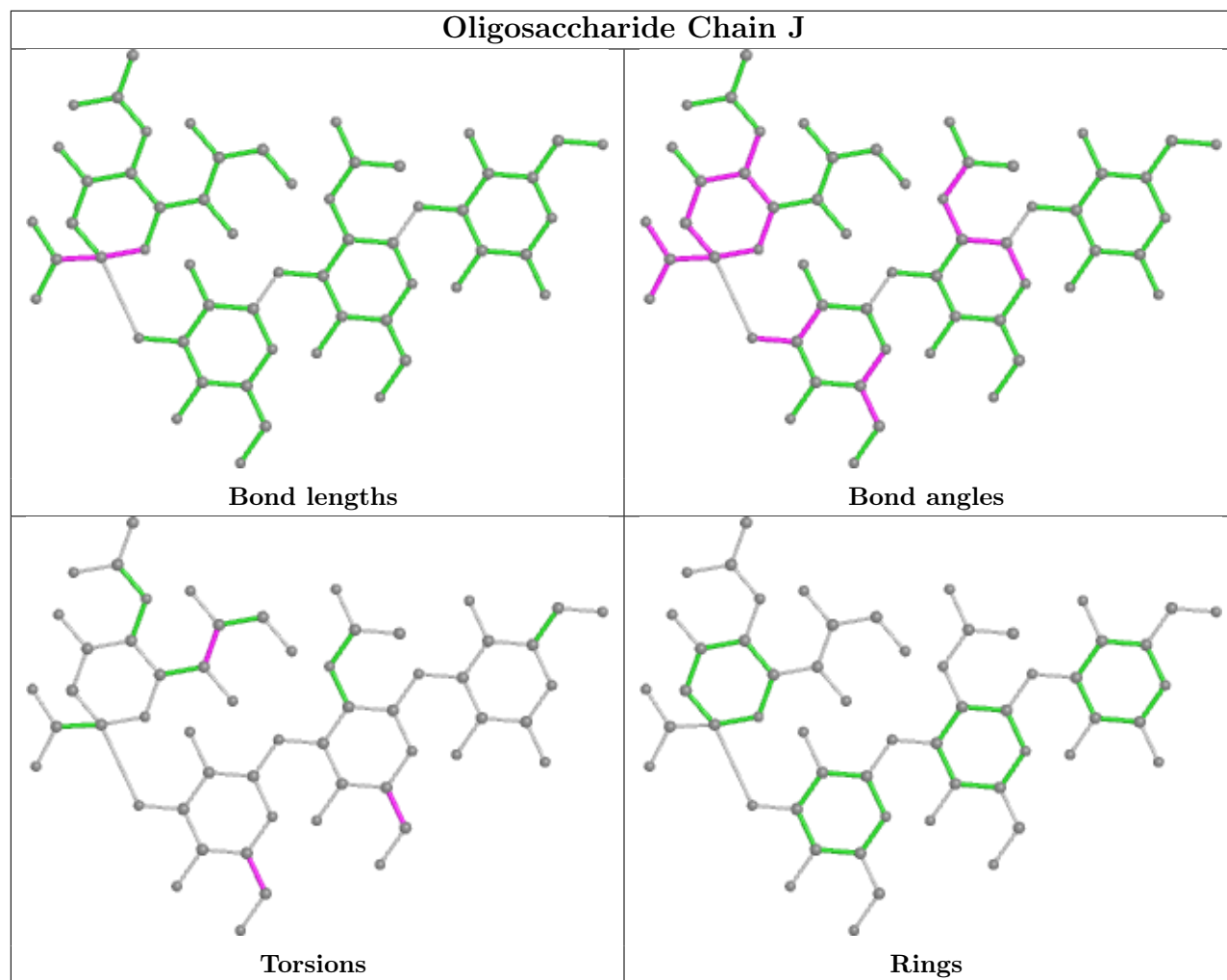
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

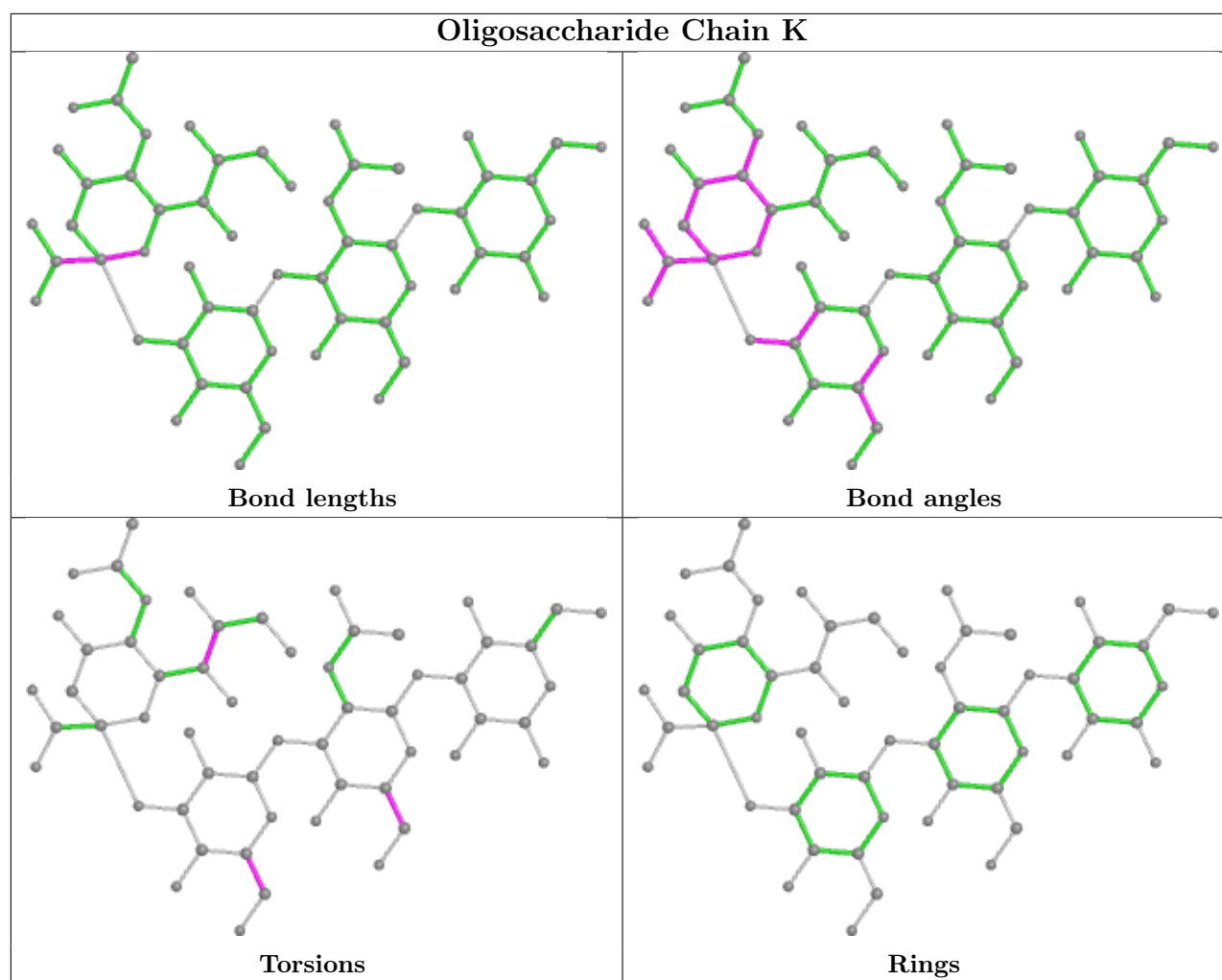


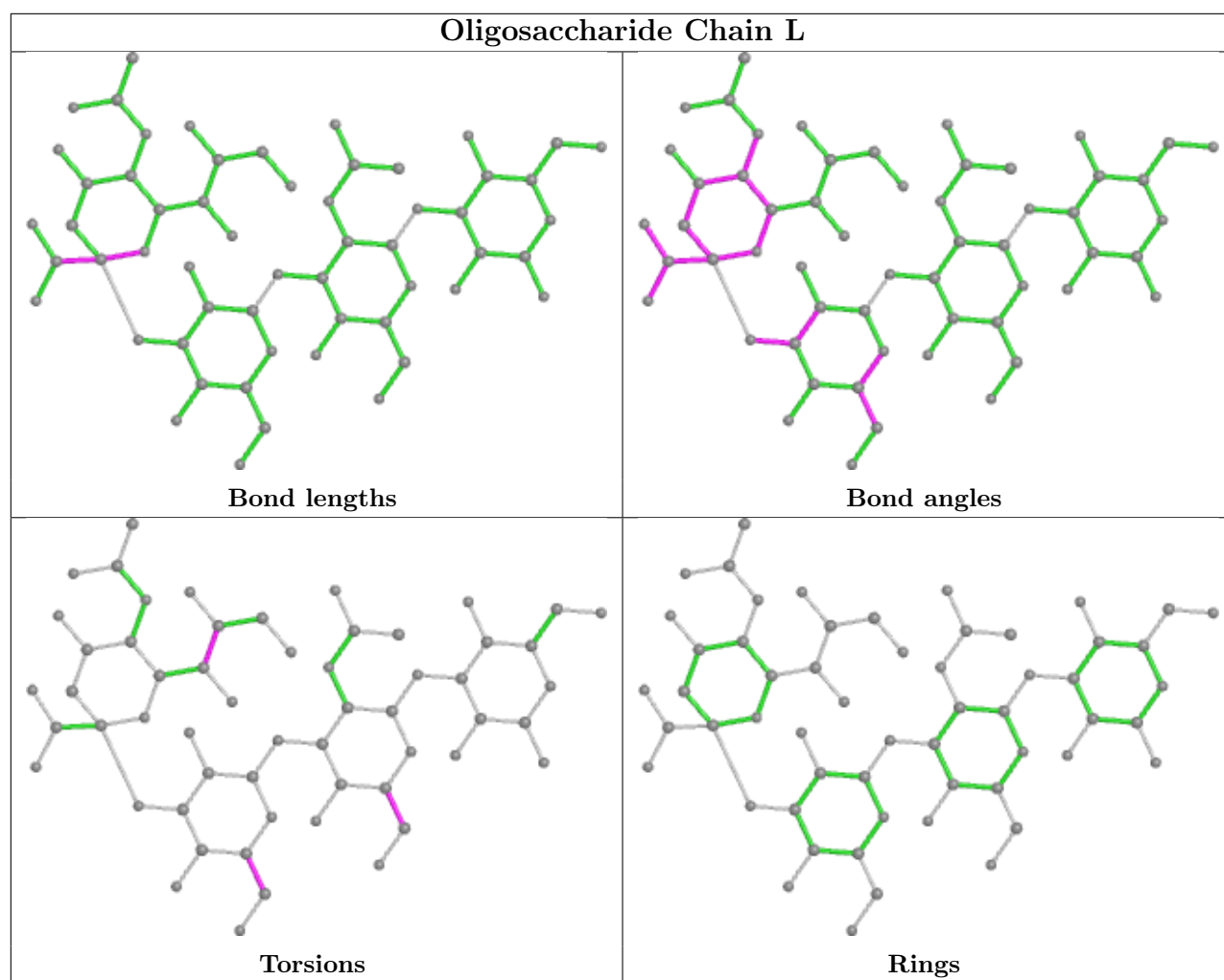


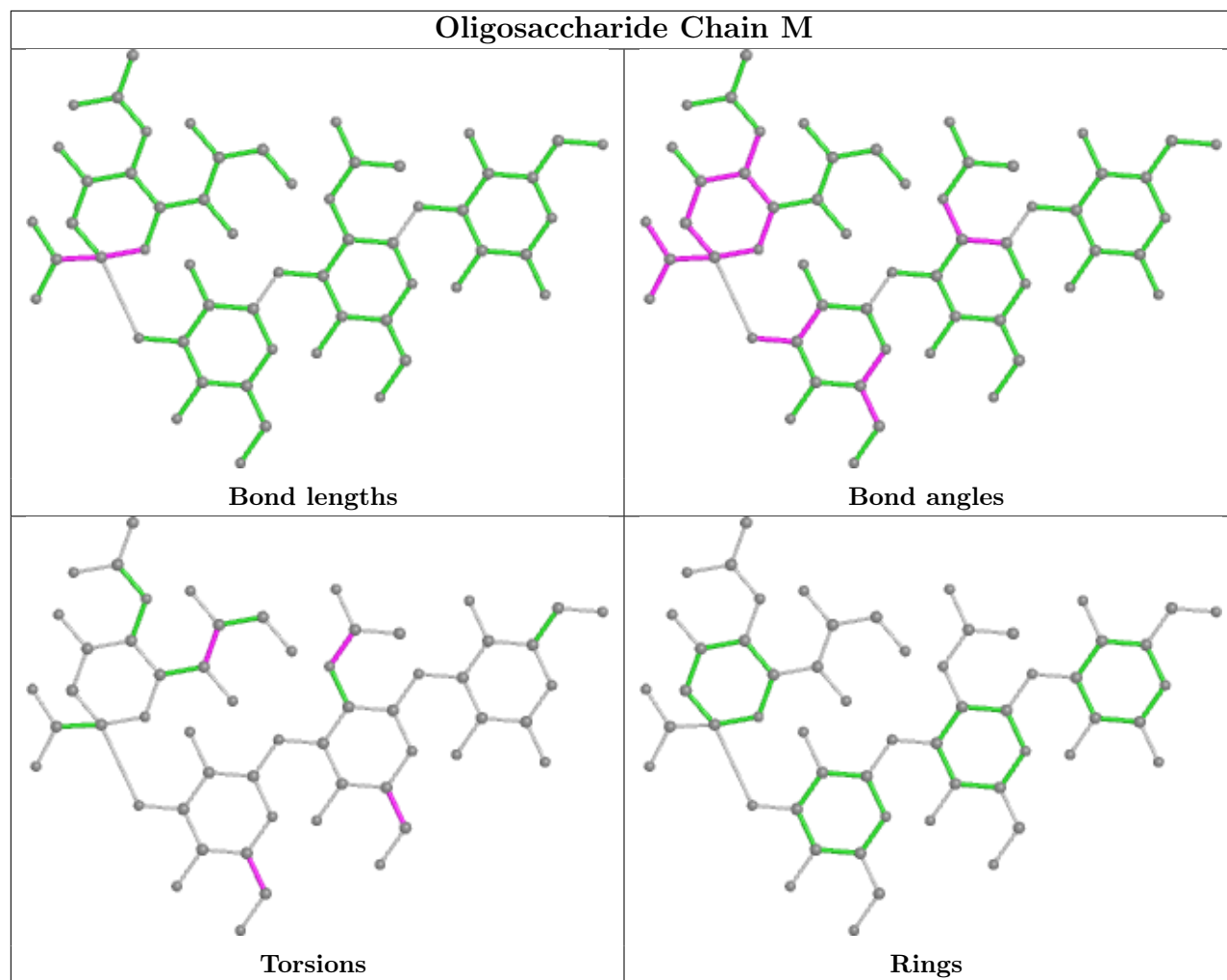


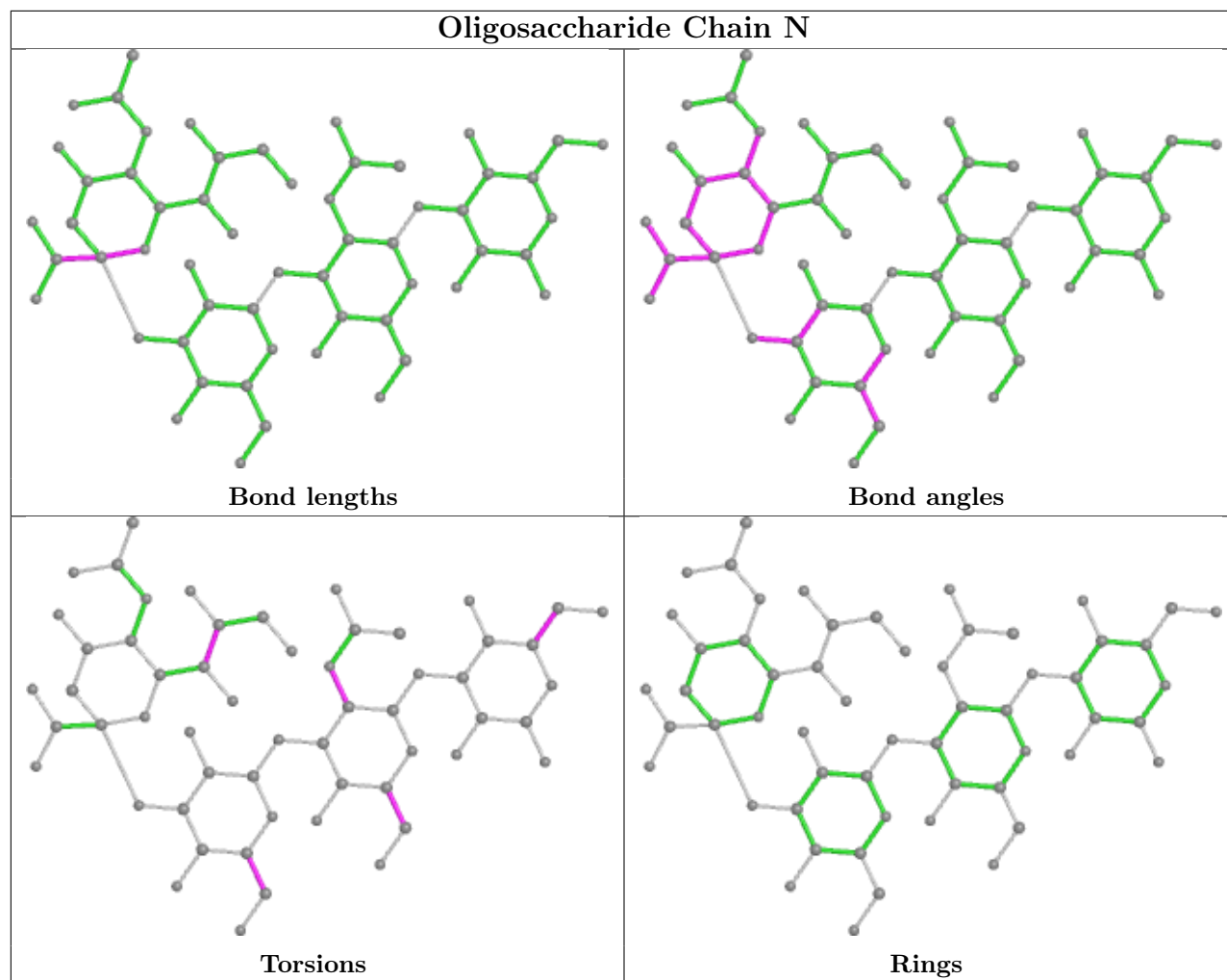


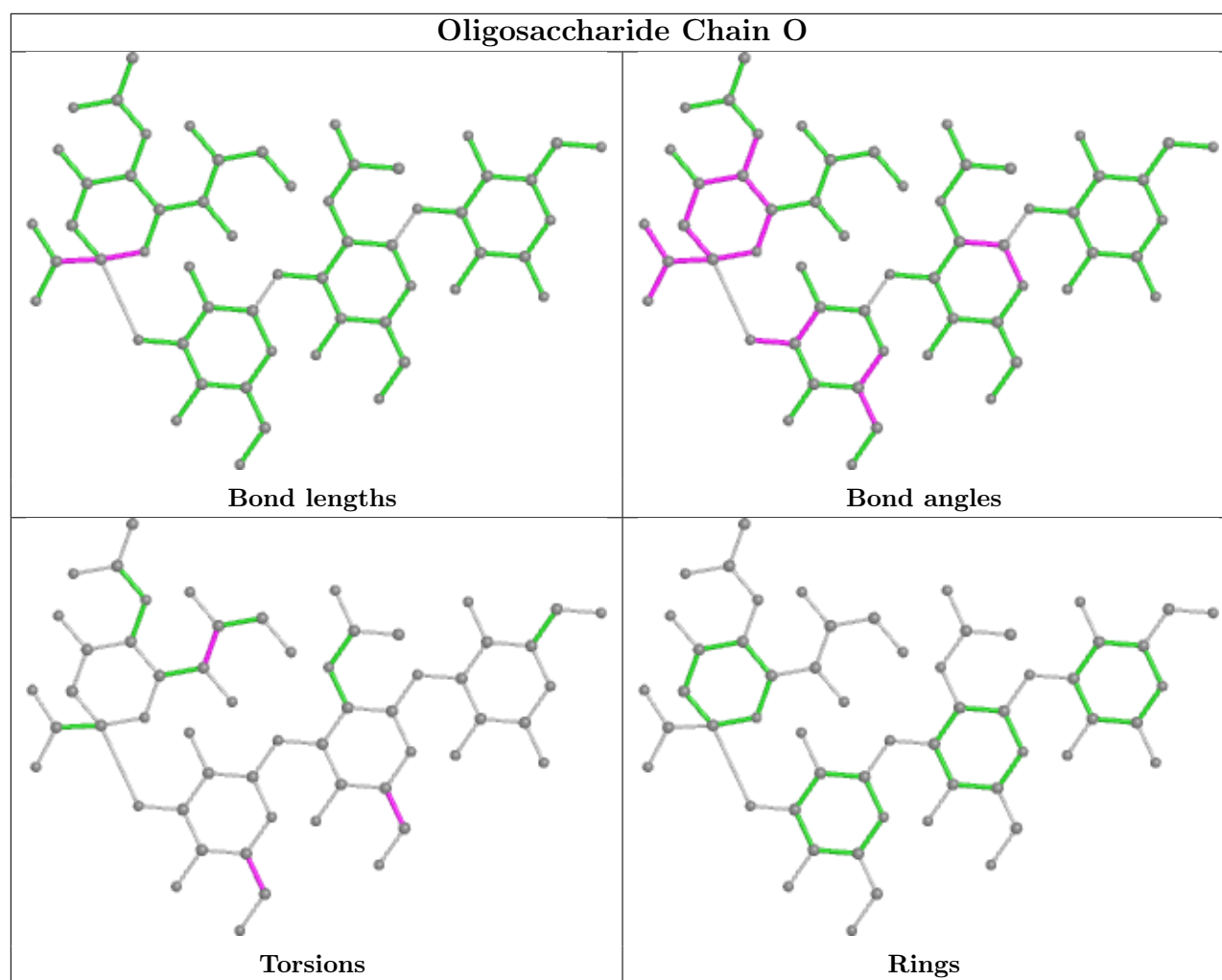












## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
4	NAG	C	702	1	14,14,15	1.99	4 (28%)	17,19,21	1.17	2 (11%)
4	NAG	B	701	1	14,14,15	0.39	0	17,19,21	1.58	3 (17%)
4	NAG	F	601	1	14,14,15	0.40	0	17,19,21	1.21	1 (5%)
4	NAG	D	601	1	14,14,15	2.00	4 (28%)	17,19,21	1.23	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	701	1	14,14,15	0.71	0	17,19,21	1.09	2 (11%)

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
4	NAG	C	702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	701	1	-	2/6/23/26	0/1/1/1
4	NAG	F	601	1	-	5/6/23/26	0/1/1/1
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	701	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	NAG	O5-C1	4.57	1.51	1.43
4	C	702	NAG	O5-C1	4.48	1.50	1.43
4	D	601	NAG	C7-N2	3.65	1.46	1.34
4	C	702	NAG	C7-N2	3.59	1.46	1.34
4	D	601	NAG	C2-N2	2.42	1.50	1.46
4	C	702	NAG	C2-N2	2.39	1.50	1.46
4	D	601	NAG	O5-C5	2.22	1.48	1.43
4	C	702	NAG	O5-C5	2.18	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	NAG	O5-C1-C2	-3.90	105.13	111.29
4	B	701	NAG	C2-N2-C7	-3.22	118.31	122.90
4	B	701	NAG	C1-O5-C5	2.75	115.92	112.19
4	C	702	NAG	C2-N2-C7	-2.57	119.24	122.90
4	C	702	NAG	C8-C7-N2	2.44	120.23	116.10
4	D	601	NAG	C8-C7-N2	2.43	120.21	116.10
4	F	601	NAG	O3-C3-C4	-2.38	104.84	110.35
4	C	701	NAG	C2-N2-C7	-2.32	119.60	122.90
4	C	701	NAG	C1-O5-C5	-2.03	109.44	112.19

There are no chirality outliers.



All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	NAG	C8-C7-N2-C2
4	F	601	NAG	O7-C7-N2-C2
4	C	701	NAG	C8-C7-N2-C2
4	C	701	NAG	O7-C7-N2-C2
4	C	702	NAG	O5-C5-C6-O6
4	C	702	NAG	C4-C5-C6-O6
4	B	701	NAG	C8-C7-N2-C2
4	B	701	NAG	O7-C7-N2-C2
4	F	601	NAG	C1-C2-N2-C7
4	F	601	NAG	O5-C5-C6-O6
4	F	601	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	484/506 (95%)	0.72	47 (9%)	15 9	47, 77, 206, 236	0
1	B	485/506 (95%)	0.90	50 (10%)	13 8	64, 107, 214, 256	0
1	C	483/506 (95%)	0.43	27 (5%)	31 19	31, 64, 184, 205	0
1	D	484/506 (95%)	0.54	32 (6%)	26 15	38, 77, 174, 220	0
1	E	485/506 (95%)	0.73	36 (7%)	22 13	45, 86, 220, 240	0
1	F	486/506 (96%)	1.11	66 (13%)	8 5	75, 127, 231, 259	0
All	All	2907/3036 (95%)	0.74	258 (8%)	17 10	31, 93, 212, 259	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	PHE	5.4
1	A	356	SER	5.3
1	A	6	GLY	5.2
1	F	478	MET	4.8
1	C	316	GLY	4.5
1	A	71	ILE	4.2
1	B	351	TYR	4.1
1	A	354	HIS	4.0
1	C	317	LEU	4.0
1	A	5	ILE	4.0
1	A	455	LEU	4.0
1	F	76	TRP	3.9
1	E	182	ASN	3.9
1	C	182	ASN	3.9
1	F	448	TYR	3.9
1	F	222	GLN	3.8
1	B	65	PRO	3.8
1	F	71	ILE	3.7
1	F	399	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	244	ASN	3.7
1	E	181	SER	3.6
1	F	434	GLU	3.6
1	A	486	TYR	3.6
1	A	451	VAL	3.6
1	F	167	THR	3.6
1	D	497	LEU	3.5
1	E	350	TRP	3.5
1	B	24	VAL	3.5
1	F	393	GLU	3.5
1	C	486	TYR	3.5
1	A	338	PHE	3.5
1	D	9	ALA	3.4
1	A	352	GLY	3.4
1	A	355	HIS	3.4
1	F	444	VAL	3.4
1	C	356	SER	3.4
1	E	398	GLU	3.4
1	C	477	CYS	3.3
1	B	481	VAL	3.3
1	F	54	ASP	3.3
1	D	262	SER	3.3
1	E	317	LEU	3.3
1	B	108	ILE	3.2
1	F	419	ASP	3.2
1	B	3	ILE	3.2
1	B	157	TYR	3.2
1	B	353	TYR	3.2
1	D	455	LEU	3.2
1	F	389	ASN	3.2
1	A	495	ALA	3.2
1	C	478	MET	3.1
1	A	449	ASP	3.1
1	C	338	PHE	3.1
1	F	225	ARG	3.0
1	F	350	TRP	3.0
1	E	353	TYR	3.0
1	B	5	ILE	3.0
1	D	353	TYR	3.0
1	B	68	ASP	3.0
1	F	180	HIS	2.9
1	A	351	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	343	TRP	2.9
1	F	51	ILE	2.9
1	F	455	LEU	2.9
1	A	350	TRP	2.9
1	D	469	PHE	2.9
1	E	191	TYR	2.9
1	F	137	TYR	2.9
1	D	451	VAL	2.9
1	B	191	TYR	2.9
1	C	480	SER	2.8
1	E	489	PRO	2.8
1	E	351	TYR	2.8
1	A	279	GLN	2.8
1	E	68	ASP	2.8
1	E	491	TYR	2.8
1	F	181	SER	2.8
1	A	458	ASN	2.8
1	F	269	VAL	2.8
1	A	465	GLY	2.8
1	A	488	TYR	2.7
1	F	109	ASN	2.7
1	B	186	GLU	2.7
1	B	461	GLU	2.7
1	D	259	LYS	2.7
1	A	444	VAL	2.7
1	F	182	ASN	2.7
1	B	486	TYR	2.7
1	E	356	SER	2.7
1	E	434	GLU	2.7
1	A	346	MET	2.7
1	B	458	ASN	2.7
1	B	396	GLY	2.7
1	F	70	PHE	2.7
1	B	125	HIS	2.7
1	F	317	LEU	2.7
1	D	338	PHE	2.6
1	E	447	LEU	2.6
1	F	179	HIS	2.6
1	A	122	TRP	2.6
1	D	448	TYR	2.6
1	F	144	PHE	2.6
1	F	458	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	7	TYR	2.6
1	C	285	ILE	2.6
1	E	71	ILE	2.6
1	A	70	PHE	2.6
1	B	182	ASN	2.6
1	B	8	HIS	2.6
1	B	346	MET	2.6
1	F	353	TYR	2.6
1	E	467	PHE	2.6
1	D	342	GLY	2.6
1	A	475	ASN	2.6
1	B	350	TRP	2.6
1	D	478	MET	2.6
1	F	236	ASP	2.6
1	C	389	ASN	2.6
1	E	477	CYS	2.5
1	B	149	TRP	2.5
1	F	129	LEU	2.5
1	E	481	VAL	2.5
1	F	282	VAL	2.5
1	A	497	LEU	2.5
1	D	344	GLN	2.5
1	E	214	ALA	2.5
1	E	451	VAL	2.5
1	C	1	ASP	2.5
1	A	353	TYR	2.5
1	A	434	GLU	2.5
1	D	69	GLU	2.5
1	F	439	PHE	2.5
1	D	87	ASN	2.5
1	F	141	PRO	2.5
1	E	453	LEU	2.4
1	E	454	GLN	2.4
1	F	335	ILE	2.4
1	B	418	LEU	2.4
1	B	22	LYS	2.4
1	B	316	GLY	2.4
1	B	11	ASN	2.4
1	B	216	ARG	2.4
1	D	3	ILE	2.4
1	B	450	LYS	2.4
1	B	460	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	6	GLY	2.4
1	E	224	GLY	2.4
1	B	156	ALA	2.4
1	E	478	MET	2.4
1	F	73	VAL	2.4
1	B	181	SER	2.4
1	F	65	PRO	2.4
1	E	470	TYR	2.4
1	F	437	LEU	2.4
1	E	450	LYS	2.4
1	D	488	TYR	2.3
1	F	50	LEU	2.3
1	D	354	HIS	2.3
1	B	455	LEU	2.3
1	F	344	GLN	2.3
1	E	469	PHE	2.3
1	F	64	ASN	2.3
1	A	8	HIS	2.3
1	F	149	TRP	2.3
1	B	261	ASP	2.3
1	F	3	ILE	2.3
1	C	13	THR	2.3
1	D	390	THR	2.3
1	A	478	MET	2.3
1	A	181	SER	2.3
1	B	345	GLY	2.3
1	F	9	ALA	2.3
1	B	453	LEU	2.3
1	E	302	CYS	2.3
1	A	454	GLN	2.3
1	B	70	PHE	2.3
1	F	490	GLN	2.3
1	D	181	SER	2.3
1	D	320	SER	2.3
1	B	71	ILE	2.2
1	C	350	TRP	2.2
1	F	392	PHE	2.2
1	A	363	TYR	2.2
1	B	377	VAL	2.2
1	A	9	ALA	2.2
1	E	316	GLY	2.2
1	D	500	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	471	HIS	2.2
1	F	191	TYR	2.2
1	E	455	LEU	2.2
1	B	448	TYR	2.2
1	D	470	TYR	2.2
1	A	453	LEU	2.2
1	F	336	ALA	2.2
1	F	8	HIS	2.2
1	C	287	SER	2.2
1	D	70	PHE	2.2
1	B	92	PRO	2.2
1	E	192	LYS	2.2
1	B	390	THR	2.2
1	C	339	ILE	2.2
1	D	285	ILE	2.2
1	C	398	GLU	2.2
1	F	226	MET	2.2
1	A	317	LEU	2.2
1	D	457	ASP	2.2
1	F	221	GLY	2.1
1	D	4	CYS	2.1
1	A	489	PRO	2.1
1	B	356	SER	2.1
1	C	455	LEU	2.1
1	F	395	VAL	2.1
1	A	459	ALA	2.1
1	B	278	CYS	2.1
1	D	278	CYS	2.1
1	E	278	CYS	2.1
1	F	318	ARG	2.1
1	C	469	PHE	2.1
1	F	500	GLU	2.1
1	B	91	TYR	2.1
1	F	193	ASN	2.1
1	A	362	GLY	2.1
1	A	484	GLY	2.1
1	F	6	GLY	2.1
1	B	338	PHE	2.1
1	A	274	CYS	2.1
1	C	393	GLU	2.1
1	F	60	TRP	2.1
1	D	480	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	18	THR	2.1
1	F	77	SER	2.1
1	A	337	GLY	2.1
1	C	351	TYR	2.1
1	F	157	TYR	2.1
1	F	447	LEU	2.1
1	C	481	VAL	2.1
1	D	444	VAL	2.1
1	D	299	ILE	2.1
1	C	470	TYR	2.1
1	C	462	LEU	2.1
1	A	473	CYS	2.1
1	B	436	THR	2.0
1	E	87	ASN	2.0
1	F	286	ASN	2.0
1	C	236	ASP	2.0
1	C	471	HIS	2.0
1	D	472	LYS	2.0
1	B	117	ILE	2.0
1	C	300	GLY	2.0
1	F	63	GLY	2.0
1	F	150	LEU	2.0
1	A	445	LYS	2.0
1	E	482	ARG	2.0
1	A	285	ILE	2.0
1	A	493	GLU	2.0
1	F	239	ILE	2.0
1	A	477	CYS	2.0
1	B	135	CYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

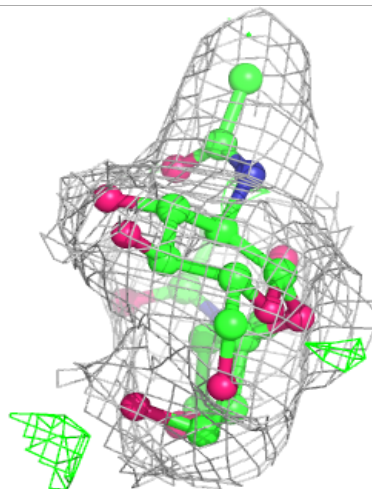
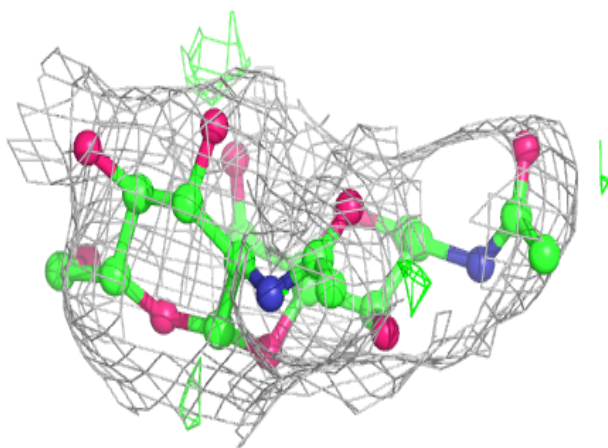
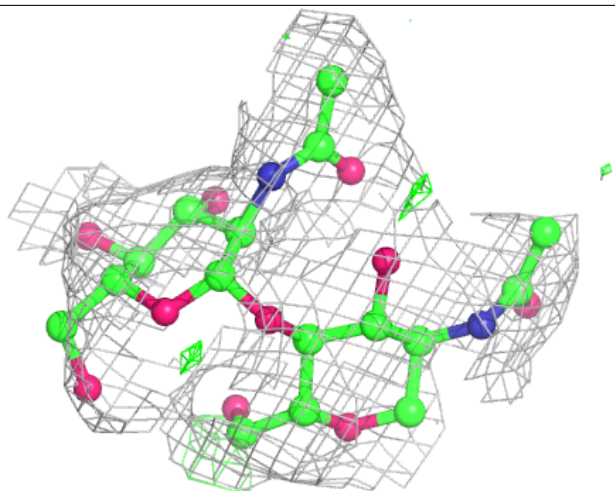


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	N	1	12/12	0.28	0.15	119,128,135,137	0
3	GAL	O	1	12/12	0.32	0.13	119,128,135,137	0
3	NAG	O	2	14/15	0.42	0.16	106,114,122,126	0
3	GAL	L	1	12/12	0.50	0.10	119,128,135,137	0
3	NAG	N	2	14/15	0.51	0.14	106,114,122,126	0
3	GAL	M	1	12/12	0.54	0.12	119,128,135,137	0
3	GAL	K	1	12/12	0.57	0.11	119,128,135,137	0
2	NAG	G	2	14/15	0.58	0.15	64,122,139,144	0
2	NAG	H	2	14/15	0.61	0.15	82,107,124,124	0
2	NAG	I	2	14/15	0.63	0.15	99,140,169,174	0
3	GAL	J	1	12/12	0.66	0.12	119,128,135,137	0
3	NAG	L	2	14/15	0.68	0.12	106,114,122,126	0
3	GAL	O	3	11/12	0.68	0.15	68,76,87,90	0
3	GAL	N	3	11/12	0.69	0.12	68,76,87,90	0
3	NAG	K	2	14/15	0.69	0.13	106,114,122,126	0
3	NAG	J	2	14/15	0.76	0.13	106,114,122,126	0
3	NAG	M	2	14/15	0.78	0.12	106,114,122,126	0
3	SIA	N	4	20/21	0.79	0.12	49,64,82,83	0
2	NAG	I	1	14/15	0.81	0.12	80,105,140,142	0
3	SIA	O	4	20/21	0.83	0.14	49,64,82,83	0
2	NAG	G	1	14/15	0.84	0.14	83,99,123,137	0
3	GAL	J	3	11/12	0.86	0.12	68,76,87,90	0
2	NAG	H	1	14/15	0.87	0.15	51,85,109,110	0
3	GAL	M	3	11/12	0.87	0.10	68,76,87,90	0
3	GAL	L	3	11/12	0.88	0.09	68,76,87,90	0
3	SIA	M	4	20/21	0.92	0.09	49,64,82,83	0
3	GAL	K	3	11/12	0.93	0.09	68,76,87,90	0
3	SIA	J	4	20/21	0.93	0.11	49,64,82,83	0
3	SIA	L	4	20/21	0.93	0.12	49,64,82,83	0
3	SIA	K	4	20/21	0.95	0.09	49,64,82,83	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.

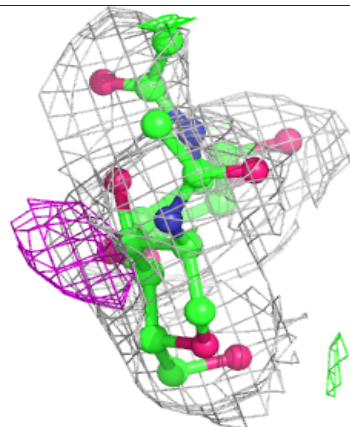
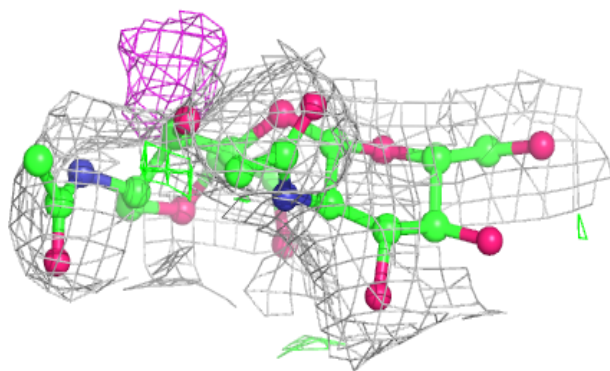
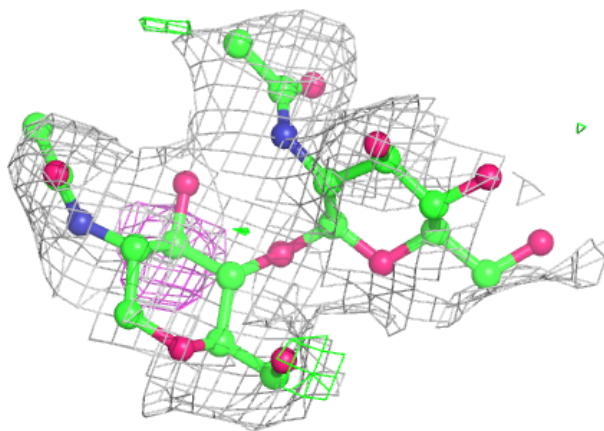
**Electron density around Chain G:**

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

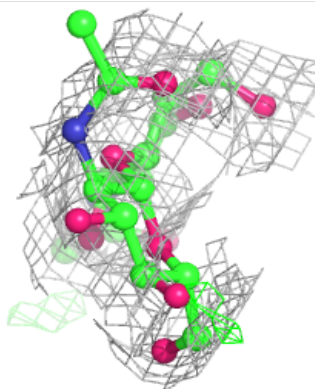
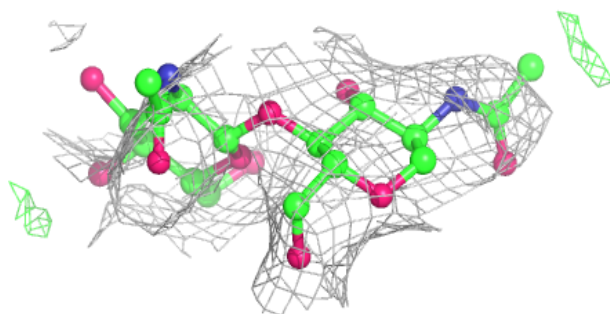
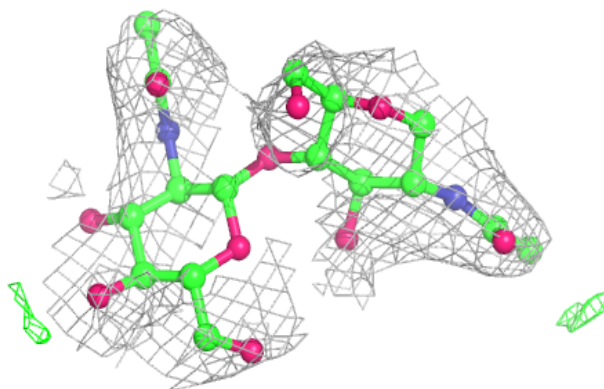


**Electron density around Chain H:**

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

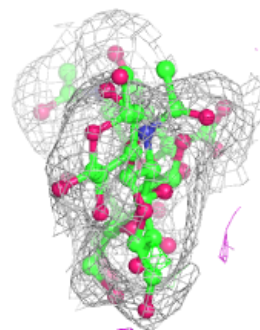
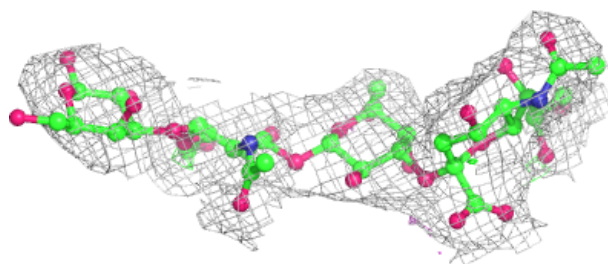
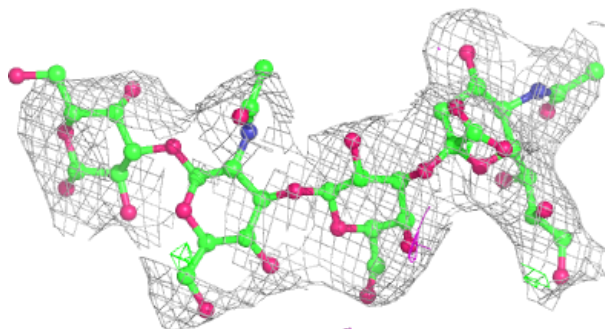
**Electron density around Chain I:**

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

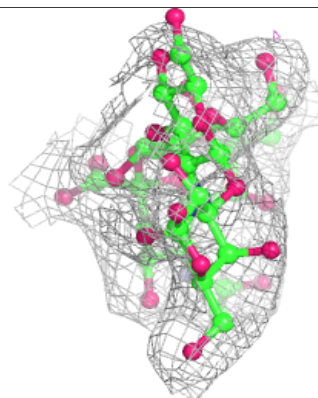
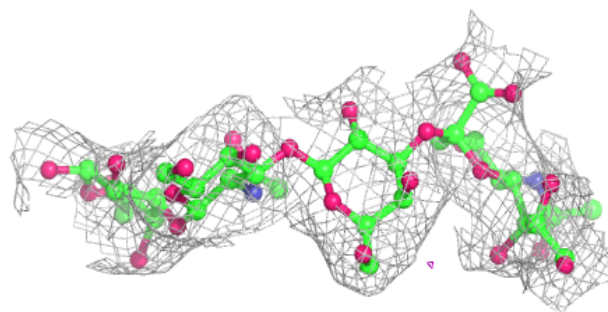
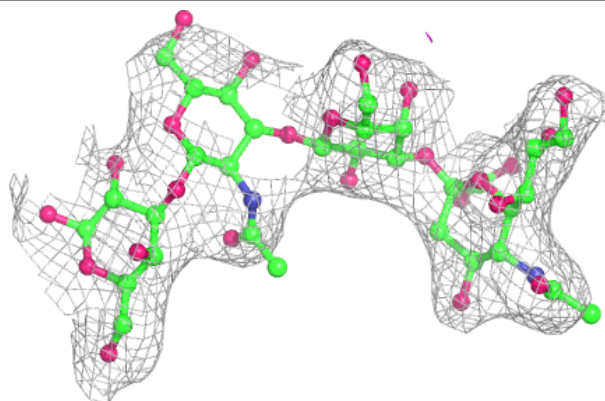


**Electron density around Chain J:**

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

**Electron density around Chain K:**

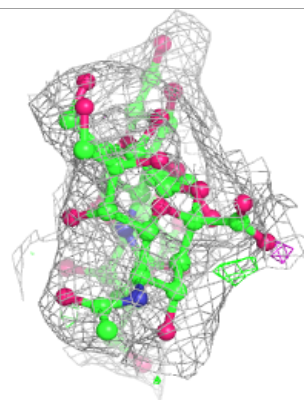
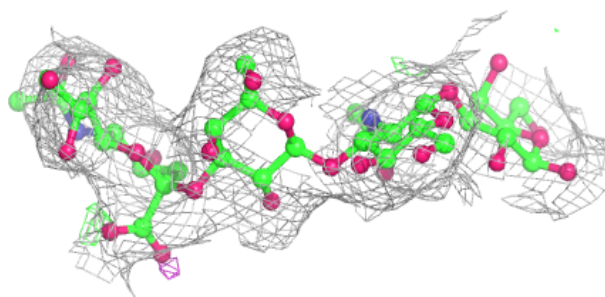
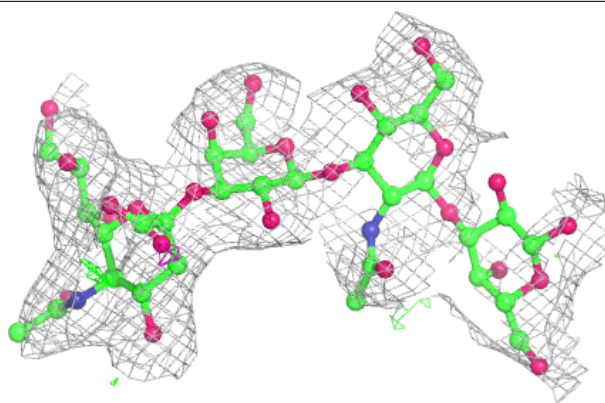
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



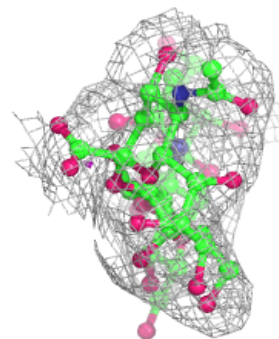
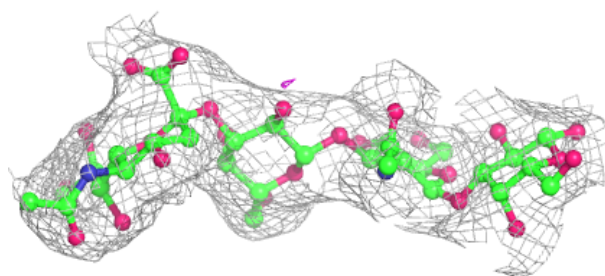
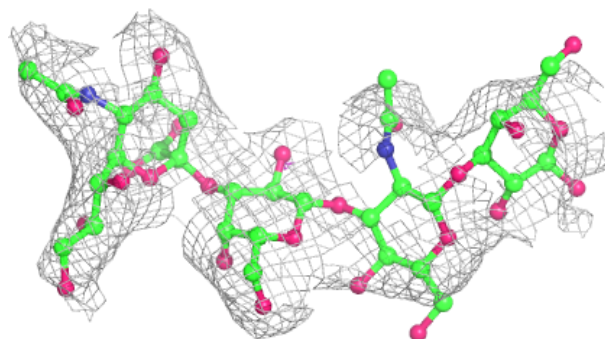


**Electron density around Chain L:**

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

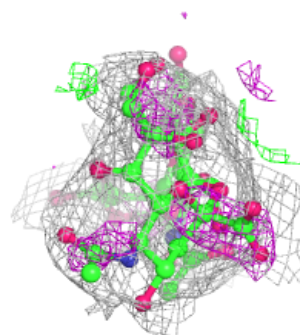
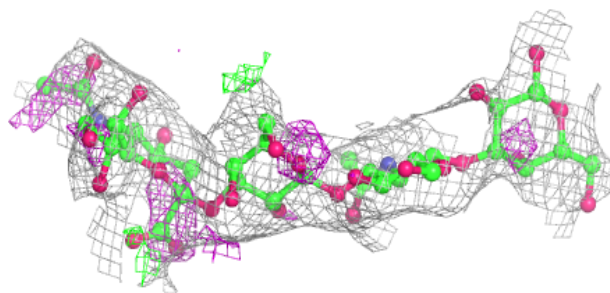
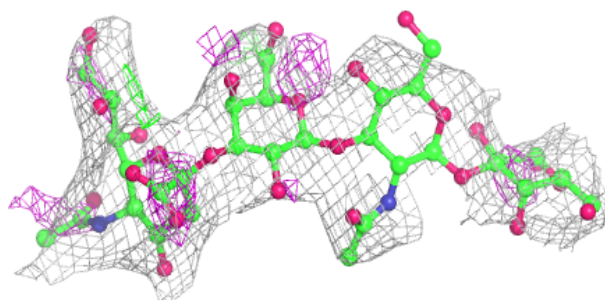
**Electron density around Chain M:**

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

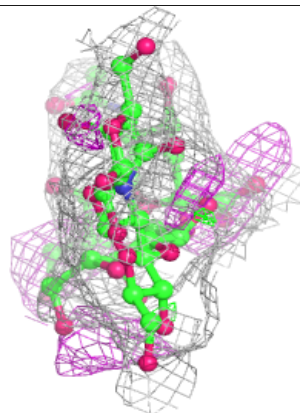
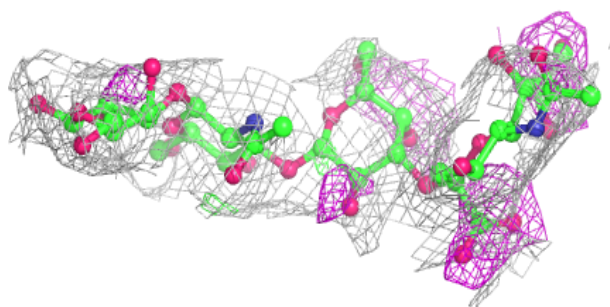
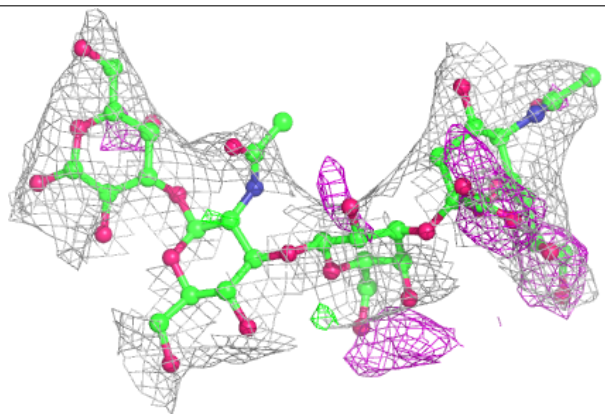


**Electron density around Chain N:**

$2mF_o-DF_c$  (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)



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	D	601	14/15	0.26	0.15	126,154,178,179	0
4	NAG	C	702	14/15	0.66	0.14	125,142,158,166	0
4	NAG	B	701	14/15	0.76	0.17	107,142,155,156	0
4	NAG	F	601	14/15	0.81	0.15	98,115,132,140	0
4	NAG	C	701	14/15	0.88	0.11	76,91,103,110	0

## 6.5 Other polymers

There are no such residues in this entry.