



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:12 AM UTC

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

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:

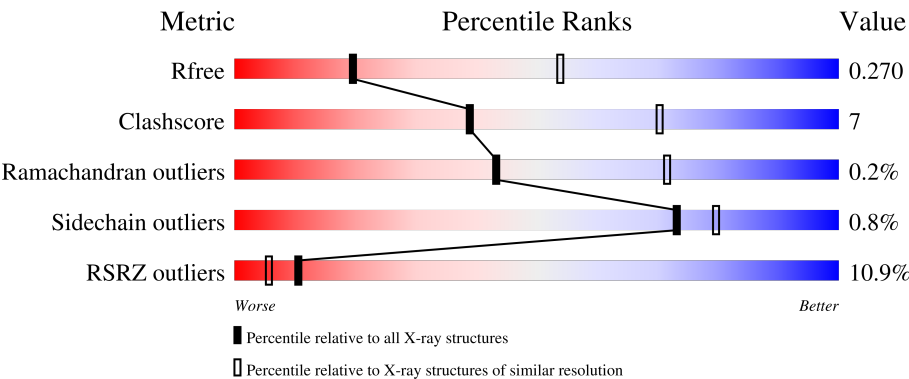
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance 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.



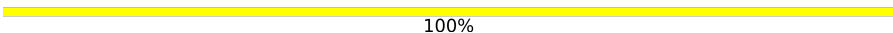
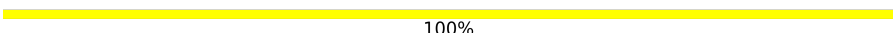
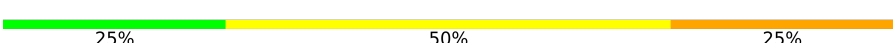
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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 ≥ 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	11% 78% 17% .
1	B	506	12% 78% 18% .
1	C	506	7% 80% 15% 5% .
1	D	506	7% 79% 16% .
1	E	506	8% 81% 14% .

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Mol	Chain	Length	Quality of chain
1	F	506	
2	G	2	
2	H	2	
2	I	2	
3	J	4	
3	K	4	
3	L	4	
3	M	4	
3	N	4	
3	O	4	

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 [i](#)

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.



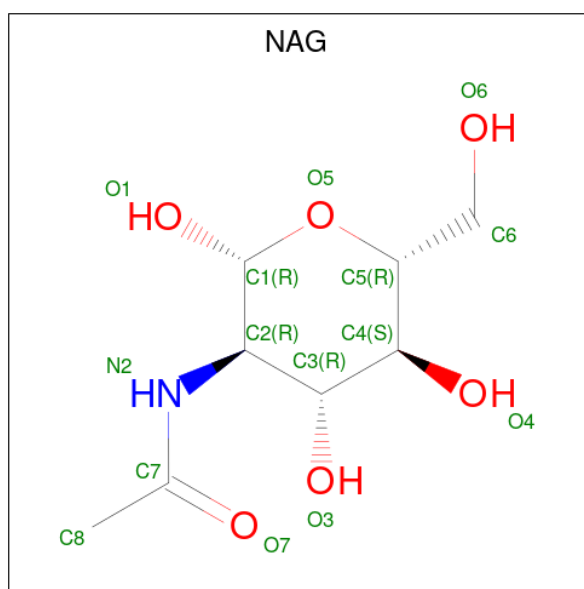
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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: $C_8H_{15}NO_6$).



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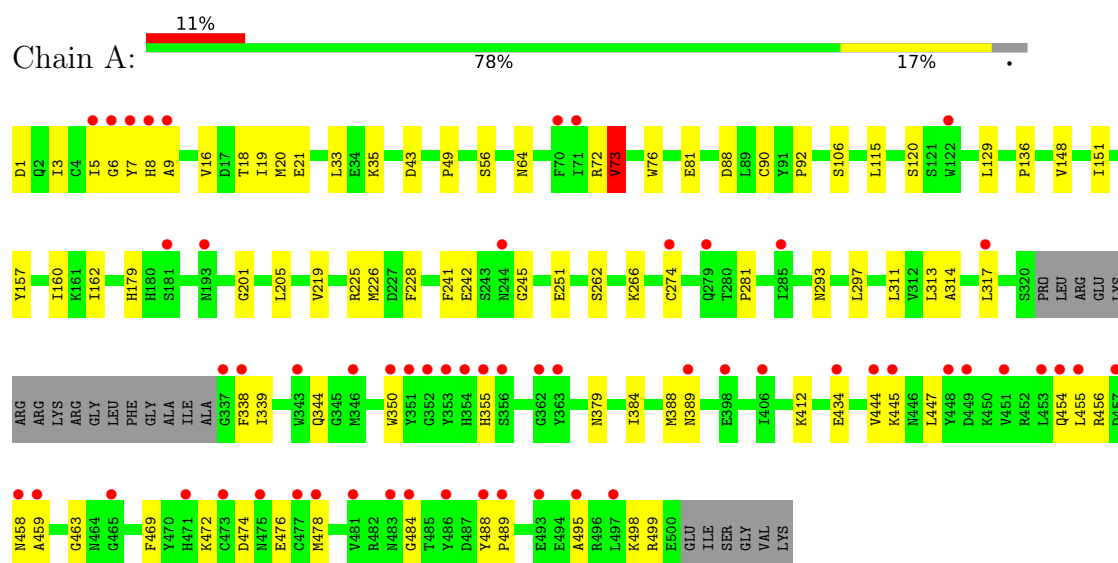
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

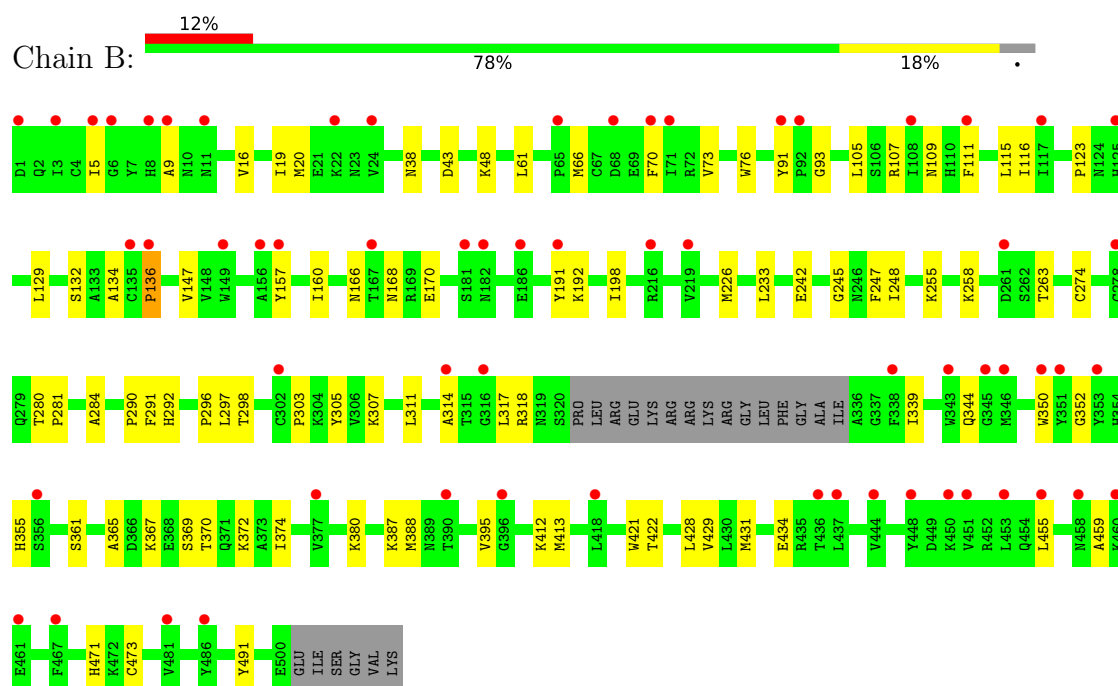
3 Residue-property plots [i](#)

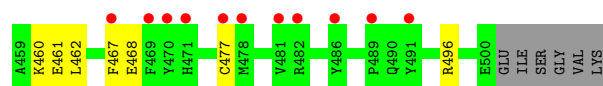
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

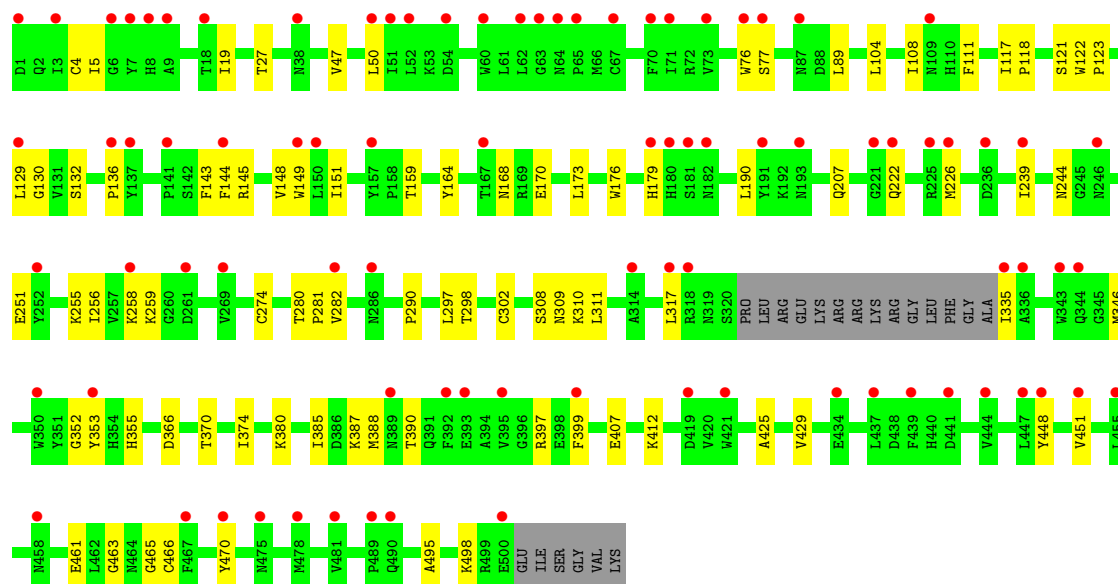
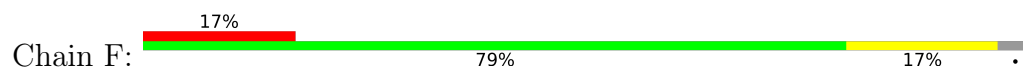


• Molecule 1: Hemagglutinin





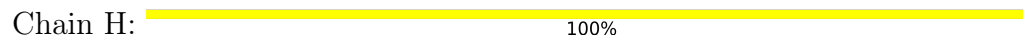
• Molecule 1: Hemagglutinin



• Molecule 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: 

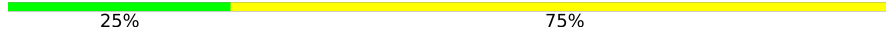


- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain K: 

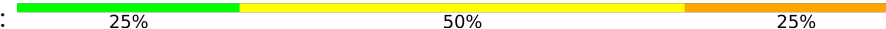


- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	1979 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, SIA, 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	0.32	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%)	43	71
1	B	481/506 (95%)	456 (95%)	24 (5%)	1 (0%)	43	71
1	C	479/506 (95%)	466 (97%)	13 (3%)	0	100	100
1	D	480/506 (95%)	458 (95%)	21 (4%)	1 (0%)	43	71
1	E	481/506 (95%)	468 (97%)	12 (2%)	1 (0%)	43	71
1	F	482/506 (95%)	456 (95%)	25 (5%)	1 (0%)	43	71
All	All	2883/3036 (95%)	2759 (96%)	119 (4%)	5 (0%)	43	71

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%)	81	83
1	B	428/445 (96%)	425 (99%)	3 (1%)	76	80
1	C	428/445 (96%)	424 (99%)	4 (1%)	70	78
1	D	428/445 (96%)	426 (100%)	2 (0%)	81	83
1	E	427/445 (96%)	421 (99%)	6 (1%)	59	74
1	F	429/445 (96%)	426 (99%)	3 (1%)	76	80
All	All	2567/2670 (96%)	2547 (99%)	20 (1%)	73	80

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	2,1	14,14,15	0.74	0	17,19,21	1.09	1 (5%)
2	NAG	G	2	2	14,14,15	0.59	0	17,19,21	1.22	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.91	1 (7%)	17,19,21	1.93	4 (23%)
2	NAG	H	2	2	14,14,15	0.86	1 (7%)	17,19,21	1.68	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	1	2,1	14,14,15	0.79	0	17,19,21	1.03	1 (5%)
2	NAG	I	2	2	14,14,15	2.12	4 (28%)	17,19,21	0.98	0
3	GAL	J	1	3	12,12,12	0.23	0	17,17,17	0.66	0
3	NAG	J	2	3	14,14,15	0.41	0	17,19,21	1.65	3 (17%)
3	GAL	J	3	3	11,11,12	0.68	0	15,15,17	1.16	1 (6%)
3	SIA	J	4	3	20,20,21	1.63	2 (10%)	21,28,31	1.87	5 (23%)
3	GAL	K	1	3	12,12,12	0.21	0	17,17,17	0.53	0
3	NAG	K	2	3	14,14,15	0.40	0	17,19,21	0.84	0
3	GAL	K	3	3	11,11,12	0.67	0	15,15,17	1.16	1 (6%)
3	SIA	K	4	3	20,20,21	1.63	2 (10%)	21,28,31	1.87	5 (23%)
3	GAL	L	1	3	12,12,12	0.17	0	17,17,17	0.45	0
3	NAG	L	2	3	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
3	GAL	L	3	3	11,11,12	0.69	0	15,15,17	1.16	1 (6%)
3	SIA	L	4	3	20,20,21	1.65	3 (15%)	21,28,31	1.88	5 (23%)
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	0.37	0	17,19,21	1.15	1 (5%)
3	GAL	M	3	3	11,11,12	0.66	0	15,15,17	1.17	1 (6%)
3	SIA	M	4	3	20,20,21	1.63	2 (10%)	21,28,31	1.87	5 (23%)
3	GAL	N	1	3	12,12,12	0.23	0	17,17,17	0.52	0
3	NAG	N	2	3	14,14,15	0.40	0	17,19,21	0.51	0
3	GAL	N	3	3	11,11,12	0.67	0	15,15,17	1.16	1 (6%)
3	SIA	N	4	3	20,20,21	1.64	2 (10%)	21,28,31	1.87	5 (23%)
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	0.90	1 (5%)
3	GAL	O	3	3	11,11,12	0.67	0	15,15,17	1.16	1 (6%)
3	SIA	O	4	3	20,20,21	1.63	2 (10%)	21,28,31	1.87	5 (23%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
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	-	2/6/23/26	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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	4	SIA	C2-C1	5.82	1.59	1.52
3	L	4	SIA	C2-C1	5.81	1.59	1.52
3	M	4	SIA	C2-C1	5.80	1.59	1.52
3	J	4	SIA	C2-C1	5.78	1.59	1.52
3	K	4	SIA	C2-C1	5.78	1.59	1.52
3	O	4	SIA	C2-C1	5.73	1.59	1.52
2	I	2	NAG	O5-C1	4.57	1.51	1.43
2	I	2	NAG	C7-N2	3.94	1.47	1.34
2	H	2	NAG	C1-C2	2.96	1.56	1.52
2	I	2	NAG	C2-N2	2.95	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	O5-C5	2.61	1.48	1.43
3	J	4	SIA	O6-C2	2.21	1.47	1.43
3	L	4	SIA	O6-C2	2.19	1.47	1.43
3	N	4	SIA	O6-C2	2.17	1.47	1.43
3	K	4	SIA	O6-C2	2.16	1.47	1.43
2	H	1	NAG	O4-C4	2.15	1.48	1.43
3	M	4	SIA	O6-C2	2.15	1.47	1.43
3	O	4	SIA	O6-C2	2.13	1.47	1.43
3	L	4	SIA	C7-C6	2.00	1.55	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	NAG	O5-C1-C2	-5.44	102.87	111.29
2	H	2	NAG	C2-N2-C7	5.40	130.14	122.90
3	L	4	SIA	O1A-C1-C2	-5.22	111.57	122.85
3	N	4	SIA	O1A-C1-C2	-5.22	111.58	122.85
3	M	4	SIA	O1A-C1-C2	-5.20	111.62	122.85
3	J	4	SIA	O1A-C1-C2	-5.19	111.62	122.85
3	K	4	SIA	O1A-C1-C2	-5.18	111.65	122.85
3	O	4	SIA	O1A-C1-C2	-5.16	111.69	122.85
2	H	1	NAG	O4-C4-C5	4.18	119.61	109.32
2	H	1	NAG	O5-C1-C2	4.16	117.73	111.29
3	L	4	SIA	O6-C2-C3	-3.91	105.30	110.56
3	J	4	SIA	O6-C2-C3	-3.89	105.33	110.56
3	K	4	SIA	O6-C2-C3	-3.87	105.35	110.56
3	M	4	SIA	O6-C2-C3	-3.86	105.36	110.56
3	O	4	SIA	O6-C2-C3	-3.86	105.37	110.56
3	N	4	SIA	O6-C2-C3	-3.85	105.38	110.56
2	H	1	NAG	C4-C3-C2	-3.28	106.22	111.02
2	G	2	NAG	O5-C1-C2	3.02	115.97	111.29
3	M	2	NAG	C1-C2-N2	2.89	114.99	110.43
3	J	2	NAG	C1-C2-N2	2.88	114.98	110.43
3	K	3	GAL	O3-C3-C2	-2.84	104.26	110.05
3	J	3	GAL	O3-C3-C2	-2.83	104.28	110.05
3	N	3	GAL	O3-C3-C2	-2.82	104.29	110.05
3	L	3	GAL	O3-C3-C2	-2.82	104.30	110.05
3	M	3	GAL	O3-C3-C2	-2.81	104.31	110.05
3	O	3	GAL	O3-C3-C2	-2.80	104.35	110.05
2	I	1	NAG	O5-C5-C4	-2.74	104.16	110.83
2	H	1	NAG	O5-C5-C4	-2.71	104.23	110.83
2	G	2	NAG	C1-O5-C5	2.61	115.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	4	SIA	O1B-C1-O1A	2.43	129.59	124.08
3	L	4	SIA	O1B-C1-O1A	2.42	129.57	124.08
3	J	4	SIA	O1B-C1-O1A	2.42	129.56	124.08
3	M	4	SIA	O1B-C1-O1A	2.41	129.55	124.08
3	K	4	SIA	O1B-C1-O1A	2.40	129.53	124.08
3	O	4	SIA	O1B-C1-O1A	2.38	129.49	124.08
3	L	4	SIA	O1B-C1-C2	2.36	118.84	112.71
3	M	4	SIA	O1B-C1-C2	2.35	118.82	112.71
3	N	4	SIA	O1B-C1-C2	2.35	118.82	112.71
3	K	4	SIA	O1B-C1-C2	2.35	118.81	112.71
3	J	4	SIA	O1B-C1-C2	2.34	118.80	112.71
3	O	4	SIA	O1B-C1-C2	2.34	118.80	112.71
3	M	4	SIA	C6-C5-N5	-2.28	107.28	110.91
3	N	4	SIA	C6-C5-N5	-2.27	107.28	110.91
3	K	4	SIA	C6-C5-N5	-2.27	107.29	110.91
3	J	4	SIA	C6-C5-N5	-2.26	107.30	110.91
3	O	4	SIA	C6-C5-N5	-2.26	107.30	110.91
3	L	4	SIA	C6-C5-N5	-2.26	107.31	110.91
2	H	2	NAG	C1-C2-N2	2.19	113.89	110.43
2	H	2	NAG	O7-C7-N2	2.15	125.78	121.98
3	J	2	NAG	C2-N2-C7	-2.14	120.04	122.90
3	O	2	NAG	O5-C1-C2	-2.11	108.03	111.29
2	G	1	NAG	O5-C5-C6	-2.07	103.62	107.66
3	L	2	NAG	C1-C2-N2	2.06	113.69	110.43

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	I	2	NAG	C1-C2-N2-C7
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	J	4	SIA	C6-C7-C8-O8
3	K	4	SIA	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
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
2	G	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
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
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	C1-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
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
2	H	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C3-C2-N2-C7

There are no ring outliers.

11 monomers are involved in 20 short contacts:

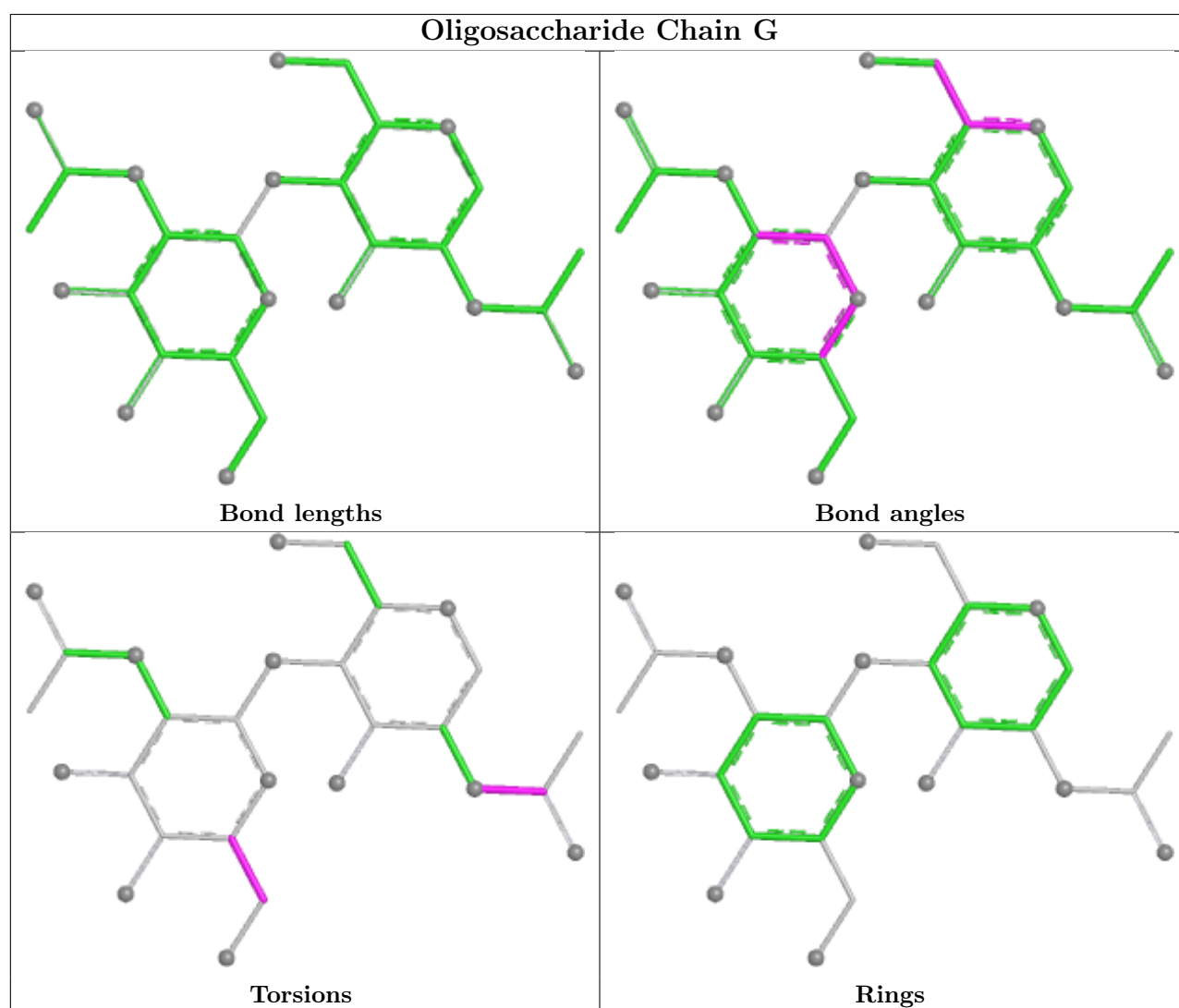
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
3	M	4	SIA	2	0
3	K	4	SIA	3	0

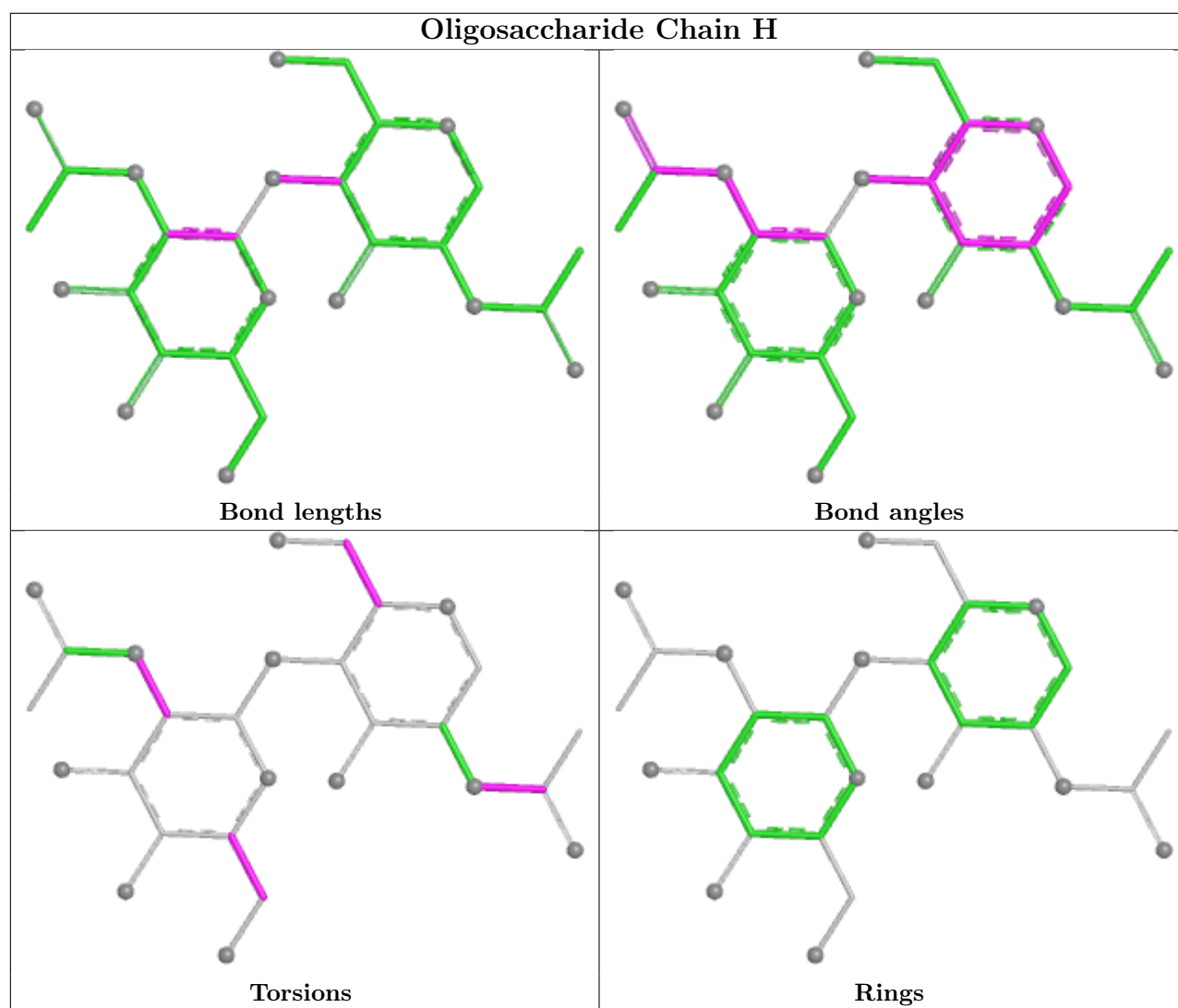
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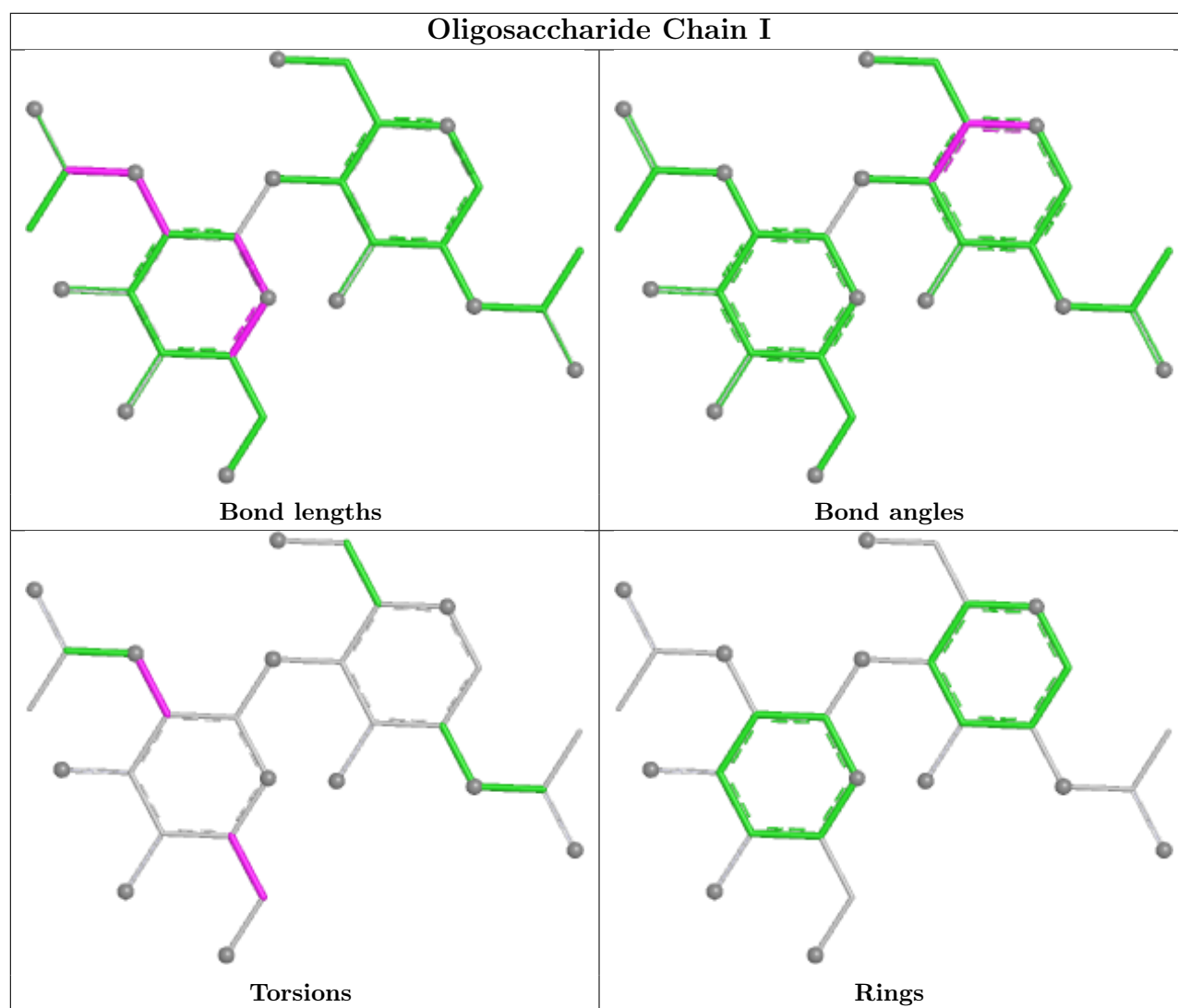
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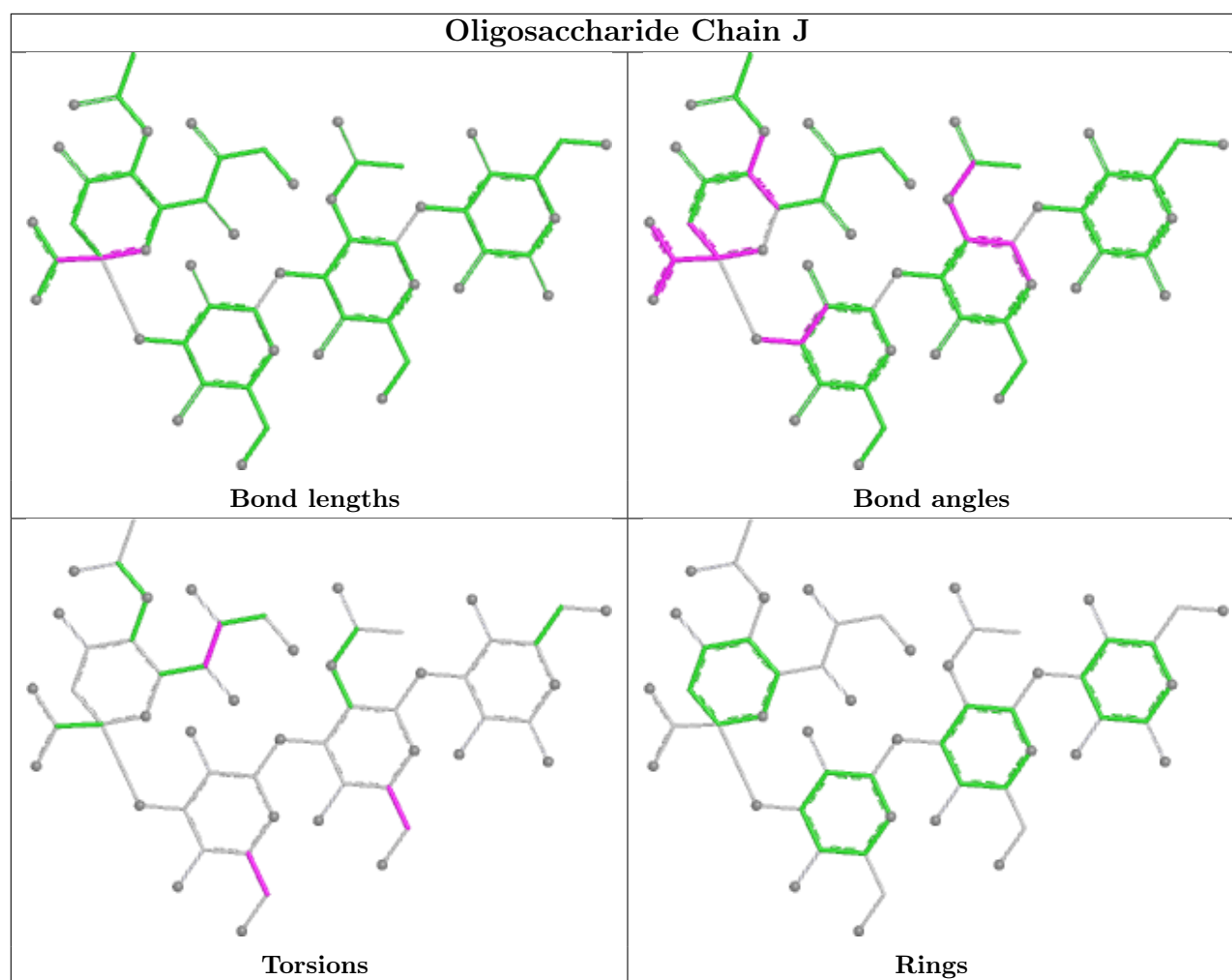
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
3	N	4	SIA	9	0
3	K	3	GAL	1	0
3	J	3	GAL	1	0
3	O	3	GAL	1	0
3	O	4	SIA	3	0
3	N	3	GAL	1	0
3	J	4	SIA	2	0

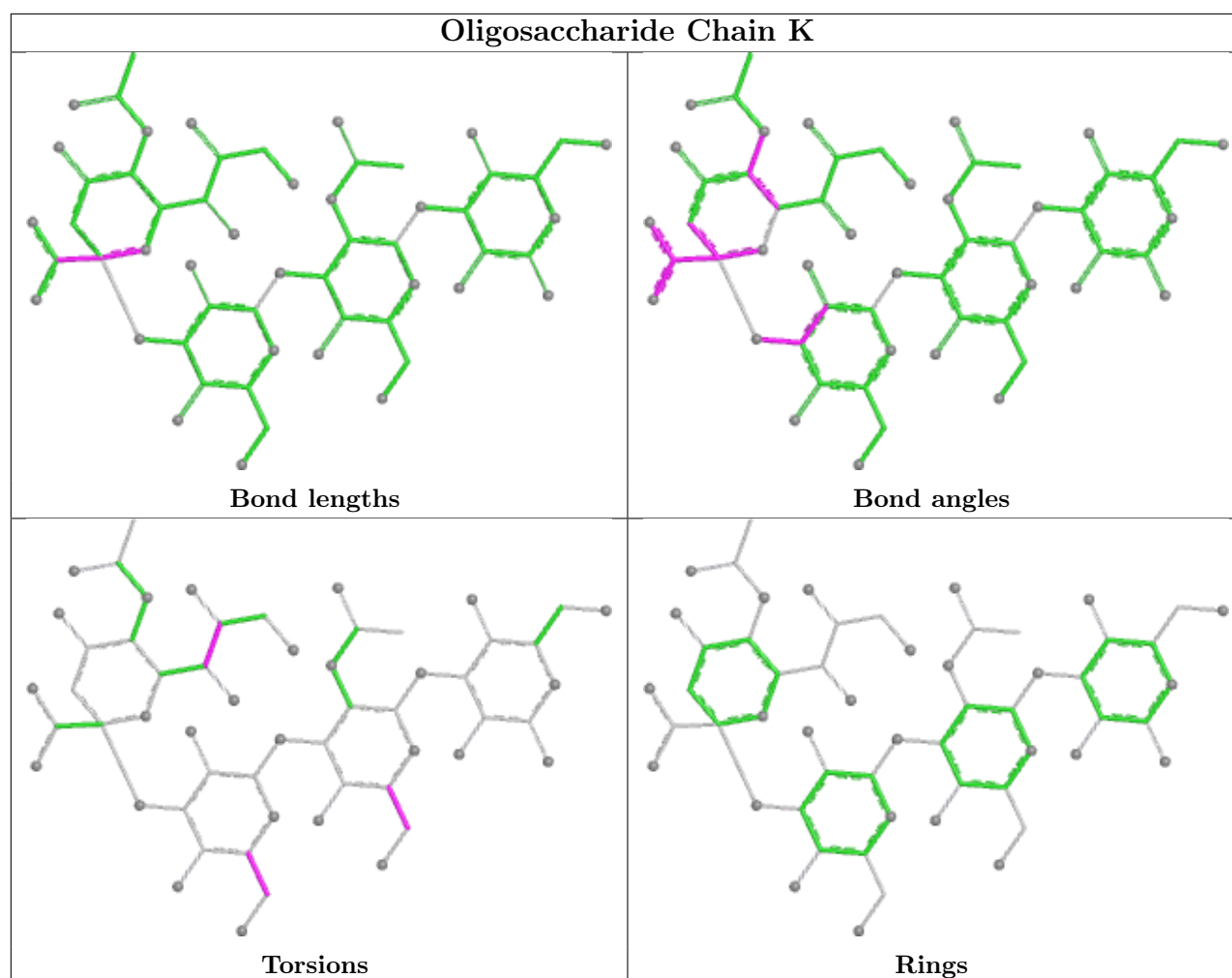
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

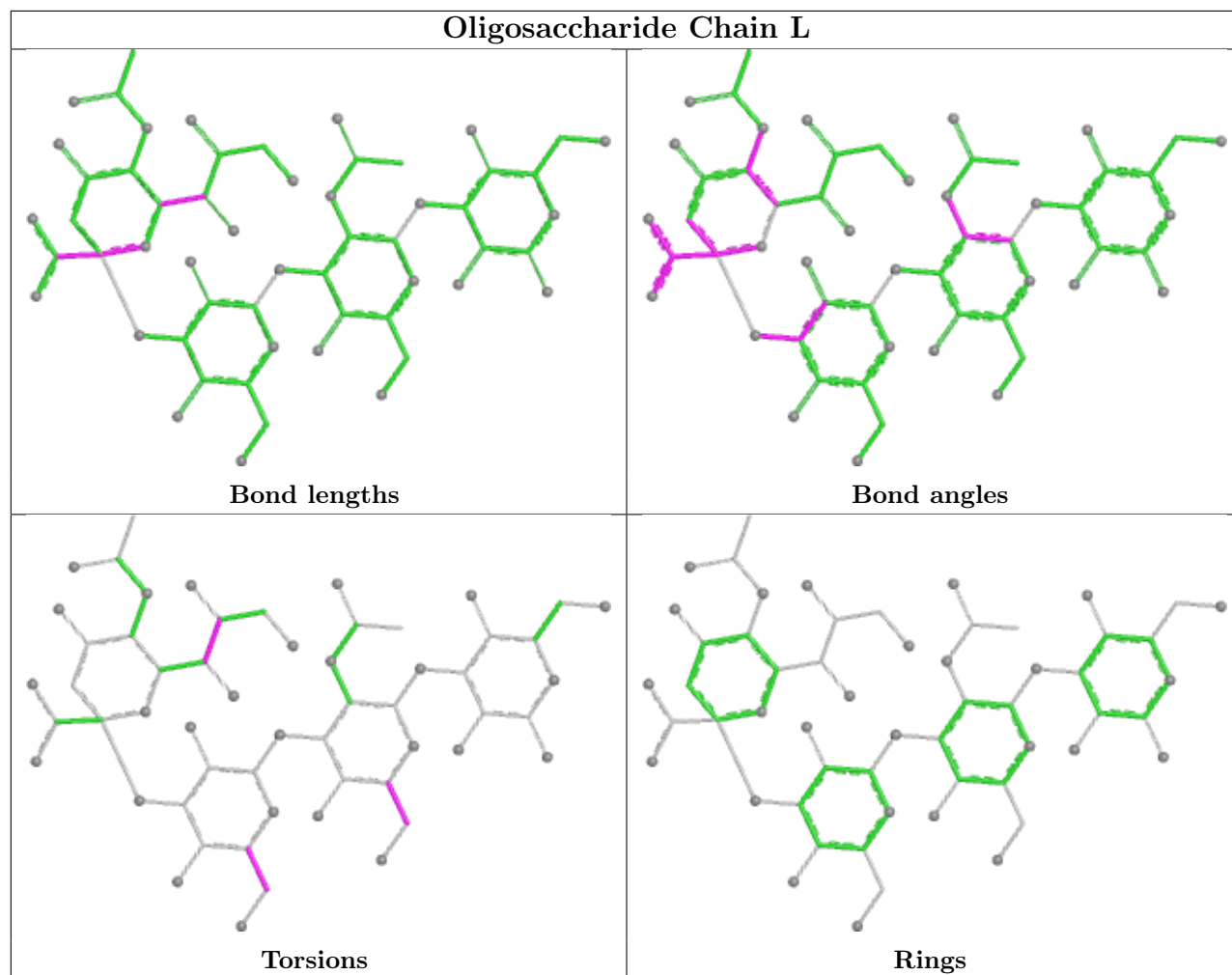


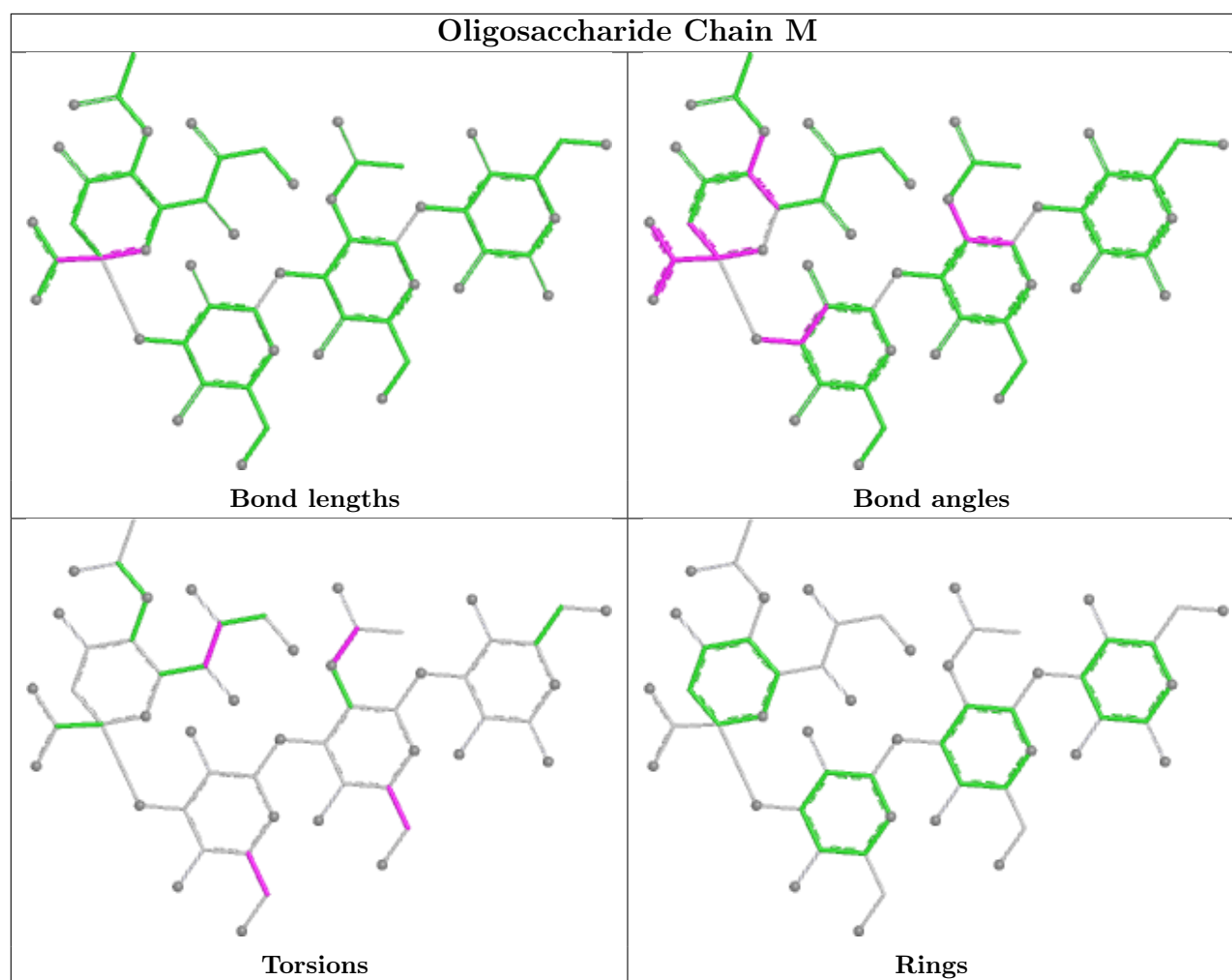


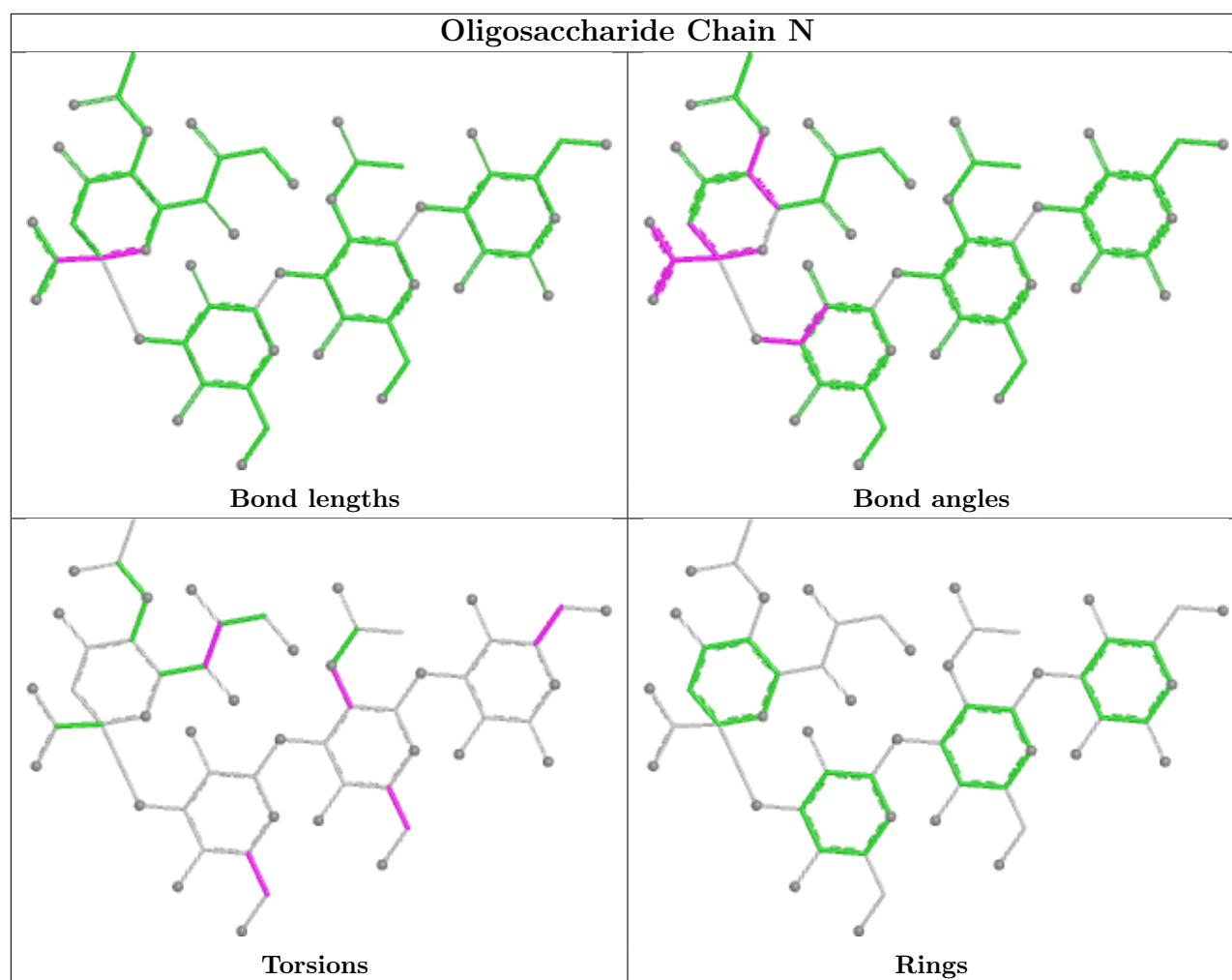


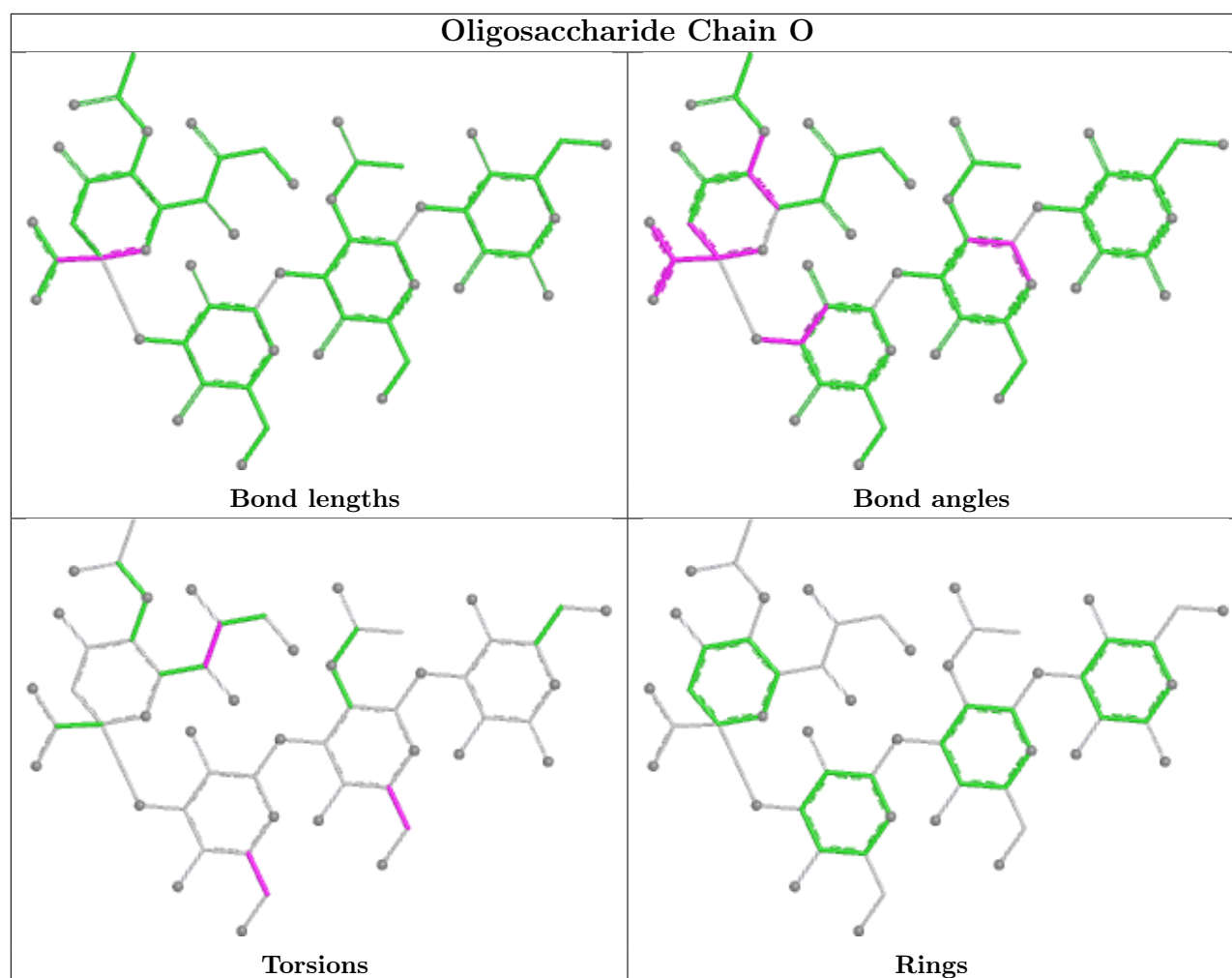












5.6 Ligand geometry [i](#)

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	701	1	14,14,15	0.71	0	17,19,21	1.11	2 (11%)
4	NAG	B	701	1	14,14,15	0.39	0	17,19,21	1.62	3 (17%)
4	NAG	D	601	1	14,14,15	2.02	4 (28%)	17,19,21	1.22	2 (11%)
4	NAG	C	702	1	14,14,15	2.00	4 (28%)	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	601	1	14,14,15	0.40	0	17,19,21	1.23	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	701	1	-	2/6/23/26	0/1/1/1
4	NAG	B	701	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	702	1	-	2/6/23/26	0/1/1/1
4	NAG	F	601	1	-	4/6/23/26	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	4.36	1.51	1.43
4	C	702	NAG	O5-C1	4.27	1.50	1.43
4	D	601	NAG	C7-N2	3.89	1.46	1.34
4	C	702	NAG	C7-N2	3.83	1.46	1.34
4	D	601	NAG	C2-N2	2.52	1.50	1.46
4	C	702	NAG	C2-N2	2.49	1.50	1.46
4	D	601	NAG	O5-C5	2.32	1.48	1.43
4	C	702	NAG	O5-C5	2.28	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	NAG	O5-C1-C2	-3.98	105.13	111.29
4	B	701	NAG	C2-N2-C7	-3.42	118.31	122.90
4	B	701	NAG	C1-O5-C5	2.78	115.92	112.19
4	C	702	NAG	C2-N2-C7	-2.73	119.24	122.90
4	C	702	NAG	C8-C7-N2	2.48	120.23	116.12
4	D	601	NAG	C8-C7-N2	2.47	120.21	116.12
4	C	701	NAG	C2-N2-C7	-2.47	119.60	122.90
4	F	601	NAG	O3-C3-C4	-2.35	104.84	110.38
4	C	701	NAG	C1-O5-C5	-2.05	109.44	112.19
4	F	601	NAG	C1-C2-N2	-2.03	107.23	110.43
4	D	601	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (10) 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	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, 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	484/506 (95%)	0.87	58 (11%)	9 5	47, 77, 206, 236	0
1	B	485/506 (95%)	1.05	62 (12%)	7 4	64, 107, 214, 256	0
1	C	483/506 (95%)	0.58	33 (6%)	23 12	31, 64, 184, 205	0
1	D	484/506 (95%)	0.69	34 (7%)	22 12	38, 77, 174, 220	0
1	E	485/506 (95%)	0.88	43 (8%)	15 8	45, 86, 220, 240	0
1	F	486/506 (96%)	1.26	87 (17%)	3 2	75, 127, 231, 259	0
All	All	2907/3036 (95%)	0.89	317 (10%)	10 6	31, 93, 212, 259	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	PHE	5.6
1	A	356	SER	5.5
1	A	6	GLY	5.4
1	F	478	MET	5.0
1	C	316	GLY	4.7
1	A	71	ILE	4.4
1	B	351	TYR	4.3
1	A	354	HIS	4.2
1	F	76	TRP	4.2
1	C	317	LEU	4.1
1	A	455	LEU	4.1
1	A	5	ILE	4.1
1	E	182	ASN	4.1
1	F	448	TYR	4.0
1	C	182	ASN	4.0
1	B	65	PRO	4.0
1	F	222	GLN	3.9
1	F	399	PHE	3.9
1	F	71	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	181	SER	3.8
1	A	486	TYR	3.8
1	A	244	ASN	3.8
1	E	350	TRP	3.8
1	A	451	VAL	3.7
1	F	434	GLU	3.7
1	F	167	THR	3.7
1	D	497	LEU	3.7
1	B	24	VAL	3.7
1	A	338	PHE	3.7
1	C	486	TYR	3.6
1	F	393	GLU	3.6
1	A	352	GLY	3.6
1	A	355	HIS	3.6
1	D	9	ALA	3.6
1	C	356	SER	3.6
1	C	477	CYS	3.5
1	F	444	VAL	3.5
1	D	262	SER	3.5
1	F	54	ASP	3.5
1	B	481	VAL	3.5
1	E	398	GLU	3.5
1	E	317	LEU	3.4
1	F	419	ASP	3.4
1	B	157	TYR	3.4
1	B	108	ILE	3.4
1	B	353	TYR	3.4
1	B	3	ILE	3.4
1	D	455	LEU	3.3
1	F	389	ASN	3.3
1	A	495	ALA	3.3
1	C	478	MET	3.3
1	A	449	ASP	3.3
1	C	338	PHE	3.2
1	F	350	TRP	3.2
1	E	353	TYR	3.2
1	B	343	TRP	3.1
1	D	353	TYR	3.1
1	B	68	ASP	3.1
1	A	350	TRP	3.1
1	F	225	ARG	3.1
1	B	5	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	180	HIS	3.1
1	A	351	TYR	3.1
1	D	469	PHE	3.1
1	F	51	ILE	3.1
1	E	191	TYR	3.1
1	F	137	TYR	3.1
1	F	455	LEU	3.0
1	B	191	TYR	3.0
1	C	480	SER	3.0
1	E	489	PRO	3.0
1	D	451	VAL	3.0
1	E	351	TYR	3.0
1	E	491	TYR	3.0
1	E	68	ASP	3.0
1	F	181	SER	2.9
1	A	279	GLN	2.9
1	A	488	TYR	2.9
1	A	465	GLY	2.9
1	A	458	ASN	2.9
1	F	269	VAL	2.9
1	F	109	ASN	2.9
1	B	486	TYR	2.9
1	E	356	SER	2.9
1	B	186	GLU	2.9
1	B	461	GLU	2.9
1	F	182	ASN	2.9
1	A	122	TRP	2.9
1	A	444	VAL	2.9
1	F	70	PHE	2.9
1	A	346	MET	2.9
1	B	396	GLY	2.8
1	D	259	LYS	2.8
1	D	338	PHE	2.8
1	B	125	HIS	2.8
1	E	434	GLU	2.8
1	B	458	ASN	2.8
1	F	144	PHE	2.8
1	F	317	LEU	2.8
1	D	448	TYR	2.8
1	F	179	HIS	2.8
1	B	350	TRP	2.8
1	A	70	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	447	LEU	2.8
1	F	7	TYR	2.8
1	E	467	PHE	2.8
1	B	346	MET	2.8
1	F	458	ASN	2.8
1	F	353	TYR	2.8
1	B	8	HIS	2.8
1	C	285	ILE	2.8
1	E	71	ILE	2.8
1	B	149	TRP	2.7
1	D	342	GLY	2.7
1	B	182	ASN	2.7
1	D	478	MET	2.7
1	F	236	ASP	2.7
1	A	475	ASN	2.7
1	E	477	CYS	2.7
1	C	389	ASN	2.7
1	F	129	LEU	2.7
1	A	353	TYR	2.7
1	A	497	LEU	2.7
1	E	481	VAL	2.7
1	F	282	VAL	2.7
1	C	1	ASP	2.7
1	D	344	GLN	2.6
1	F	439	PHE	2.6
1	E	214	ALA	2.6
1	E	451	VAL	2.6
1	F	141	PRO	2.6
1	D	87	ASN	2.6
1	A	434	GLU	2.6
1	D	69	GLU	2.6
1	E	453	LEU	2.6
1	E	454	GLN	2.6
1	B	316	GLY	2.6
1	B	418	LEU	2.6
1	F	335	ILE	2.6
1	E	478	MET	2.6
1	B	181	SER	2.6
1	F	65	PRO	2.6
1	E	6	GLY	2.6
1	E	224	GLY	2.6
1	B	11	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	3	ILE	2.5
1	E	470	TYR	2.5
1	B	22	LYS	2.5
1	F	73	VAL	2.5
1	B	156	ALA	2.5
1	F	149	TRP	2.5
1	D	488	TYR	2.5
1	F	437	LEU	2.5
1	B	216	ARG	2.5
1	B	450	LYS	2.5
1	B	460	LYS	2.5
1	E	469	PHE	2.5
1	D	354	HIS	2.5
1	F	50	LEU	2.5
1	A	8	HIS	2.5
1	B	455	LEU	2.5
1	E	450	LYS	2.5
1	F	344	GLN	2.5
1	B	261	ASP	2.5
1	F	64	ASN	2.5
1	C	350	TRP	2.5
1	A	181	SER	2.4
1	E	302	CYS	2.4
1	A	478	MET	2.4
1	B	70	PHE	2.4
1	C	13	THR	2.4
1	D	390	THR	2.4
1	B	345	GLY	2.4
1	F	3	ILE	2.4
1	D	181	SER	2.4
1	D	320	SER	2.4
1	F	392	PHE	2.4
1	B	453	LEU	2.4
1	A	363	TYR	2.4
1	F	9	ALA	2.4
1	A	454	GLN	2.4
1	F	490	GLN	2.4
1	E	316	GLY	2.4
1	E	471	HIS	2.4
1	F	191	TYR	2.4
1	B	71	ILE	2.4
1	B	377	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	2.4
1	B	448	TYR	2.4
1	D	470	TYR	2.4
1	D	70	PHE	2.4
1	E	455	LEU	2.4
1	D	500	GLU	2.4
1	C	287	SER	2.4
1	B	92	PRO	2.4
1	F	8	HIS	2.3
1	A	453	LEU	2.3
1	B	390	THR	2.3
1	D	4	CYS	2.3
1	F	336	ALA	2.3
1	F	226	MET	2.3
1	D	457	ASP	2.3
1	A	489	PRO	2.3
1	B	356	SER	2.3
1	C	339	ILE	2.3
1	D	285	ILE	2.3
1	F	60	TRP	2.3
1	F	221	GLY	2.3
1	B	278	CYS	2.3
1	D	278	CYS	2.3
1	E	278	CYS	2.3
1	A	317	LEU	2.3
1	C	469	PHE	2.3
1	C	398	GLU	2.3
1	E	192	LYS	2.3
1	C	455	LEU	2.3
1	B	91	TYR	2.3
1	A	274	CYS	2.3
1	B	338	PHE	2.3
1	F	395	VAL	2.3
1	A	362	GLY	2.3
1	A	459	ALA	2.3
1	A	484	GLY	2.3
1	F	6	GLY	2.3
1	D	480	SER	2.3
1	F	77	SER	2.3
1	C	351	TYR	2.3
1	F	157	TYR	2.3
1	F	193	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	500	GLU	2.2
1	A	337	GLY	2.2
1	F	18	THR	2.2
1	C	470	TYR	2.2
1	F	318	ARG	2.2
1	A	473	CYS	2.2
1	C	393	GLU	2.2
1	F	447	LEU	2.2
1	C	481	VAL	2.2
1	D	444	VAL	2.2
1	D	299	ILE	2.2
1	C	236	ASP	2.2
1	C	462	LEU	2.2
1	B	436	THR	2.2
1	C	471	HIS	2.2
1	E	87	ASN	2.2
1	F	286	ASN	2.2
1	A	477	CYS	2.2
1	B	135	CYS	2.2
1	C	300	GLY	2.2
1	F	63	GLY	2.2
1	A	448	TYR	2.2
1	B	117	ILE	2.2
1	F	150	LEU	2.2
1	A	457	ASP	2.2
1	F	467	PHE	2.2
1	A	471	HIS	2.2
1	D	8	HIS	2.2
1	A	285	ILE	2.1
1	F	239	ILE	2.1
1	B	437	LEU	2.1
1	D	472	LYS	2.1
1	A	493	GLU	2.1
1	B	302	CYS	2.1
1	E	43	ASP	2.1
1	F	261	ASP	2.1
1	A	481	VAL	2.1
1	F	343	TRP	2.1
1	F	481	VAL	2.1
1	E	157	TYR	2.1
1	F	470	TYR	2.1
1	A	445	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	344	GLN	2.1
1	B	9	ALA	2.1
1	E	482	ARG	2.1
1	F	38	ASN	2.1
1	A	343	TRP	2.1
1	B	219	VAL	2.1
1	D	350	TRP	2.1
1	F	67	CYS	2.1
1	F	258	LYS	2.1
1	A	398	GLU	2.1
1	F	136	PRO	2.1
1	A	483	ASN	2.1
1	C	347	VAL	2.1
1	A	406	ILE	2.1
1	C	406	ILE	2.1
1	C	418	LEU	2.1
1	F	62	LEU	2.1
1	F	441	ASP	2.1
1	F	314	ALA	2.1
1	B	467	PHE	2.1
1	E	65	PRO	2.1
1	B	1	ASP	2.1
1	C	487	ASP	2.1
1	A	7	TYR	2.1
1	E	486	TYR	2.1
1	B	136	PRO	2.1
1	B	444	VAL	2.0
1	F	87	ASN	2.0
1	C	353	TYR	2.0
1	F	1	ASP	2.0
1	F	252	TYR	2.0
1	B	6	GLY	2.0
1	C	344	GLN	2.0
1	E	392	PHE	2.0
1	B	451	VAL	2.0
1	A	193	ASN	2.0
1	A	389	ASN	2.0
1	E	246	ASN	2.0
1	F	246	ASN	2.0
1	F	475	ASN	2.0
1	F	421	TRP	2.0
1	B	167	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	314	ALA	2.0
1	F	489	PRO	2.0
1	F	451	VAL	2.0
1	F	52	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

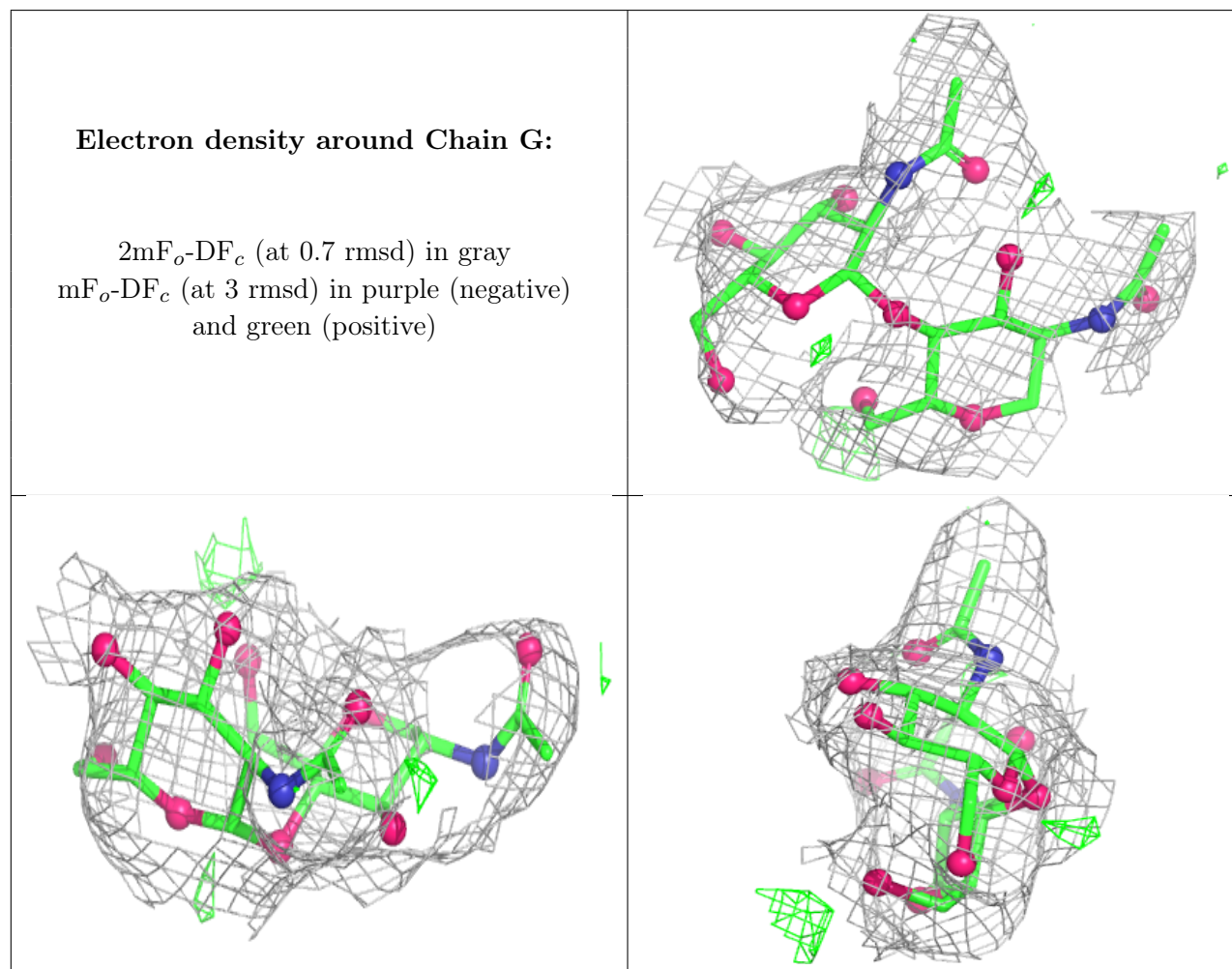
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GAL	N	1	12/12	0.28	0.15	119,128,135,137	0
3	GAL	O	1	12/12	0.32	0.13	119,128,135,137	0
3	NAG	O	2	14/15	0.42	0.16	106,114,122,126	0
3	GAL	L	1	12/12	0.50	0.10	119,128,135,137	0
3	NAG	N	2	14/15	0.51	0.14	106,114,122,126	0
3	GAL	M	1	12/12	0.54	0.12	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

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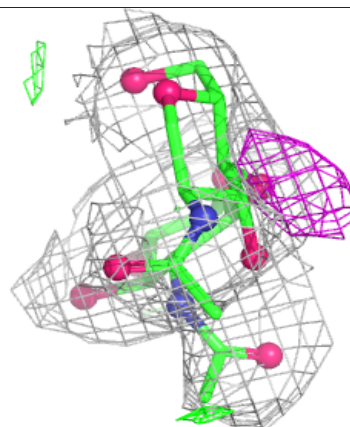
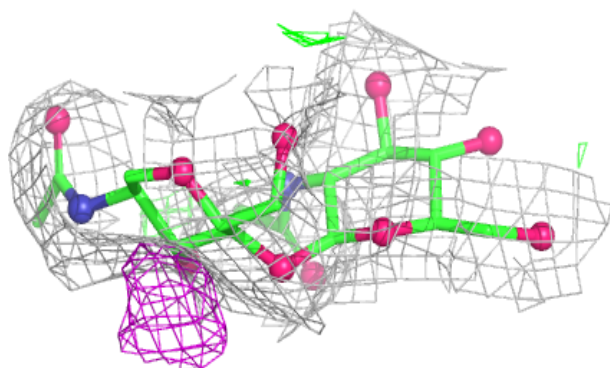
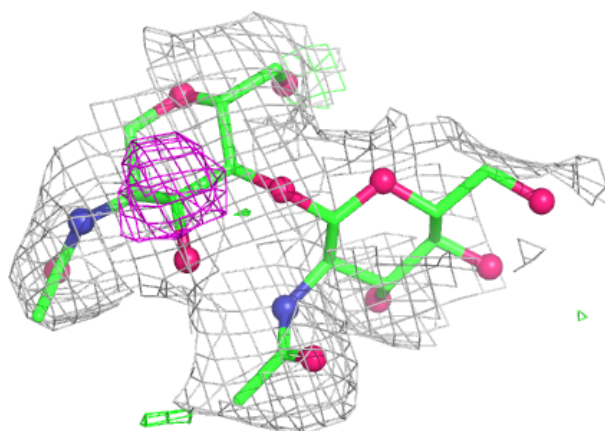
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GAL	L	3	11/12	0.88	0.09	68,76,87,90	0
3	SIA	M	4	20/21	0.92	0.09	49,64,82,83	0
3	GAL	K	3	11/12	0.93	0.09	68,76,87,90	0
3	SIA	J	4	20/21	0.93	0.11	49,64,82,83	0
3	SIA	L	4	20/21	0.93	0.12	49,64,82,83	0
3	SIA	K	4	20/21	0.95	0.09	49,64,82,83	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.

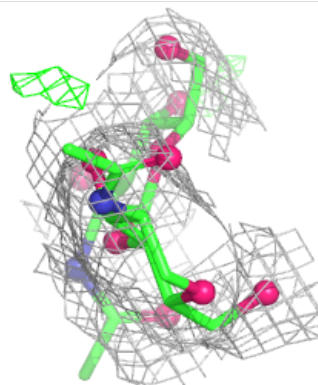
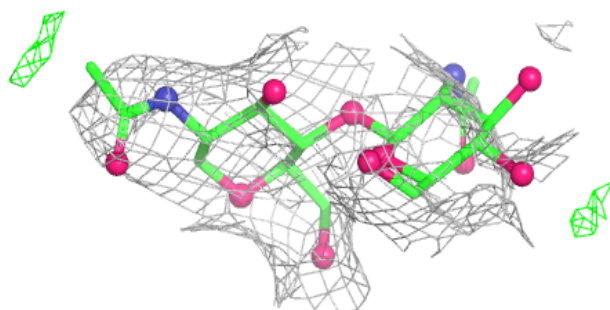
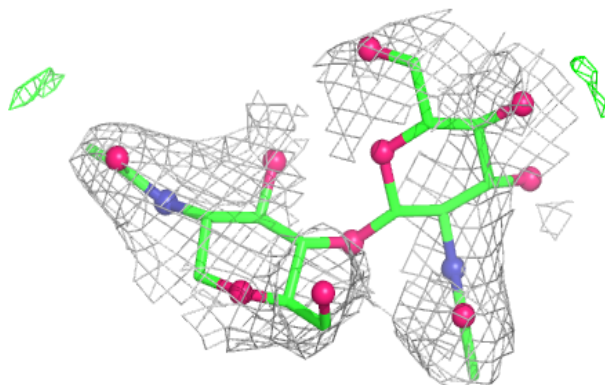


Electron density around Chain H:

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

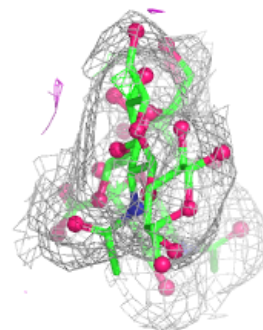
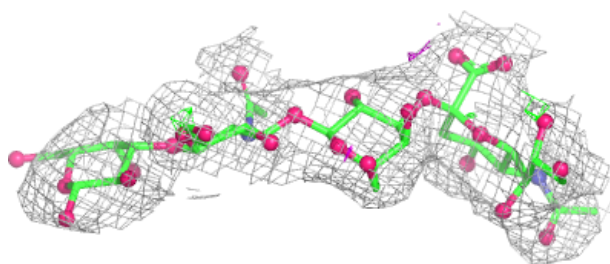
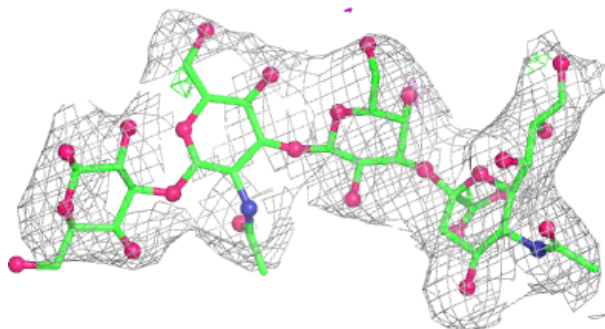
**Electron density around Chain I:**

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

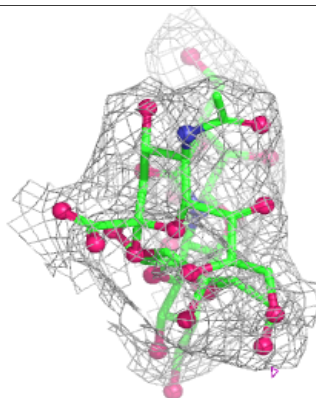
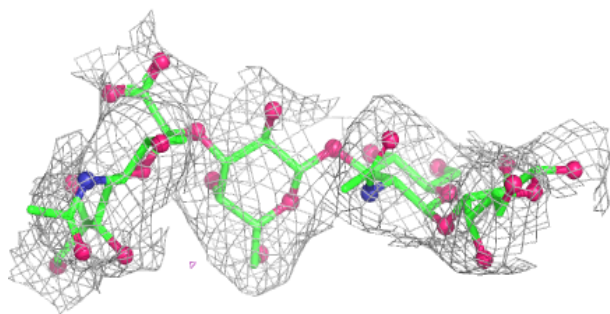
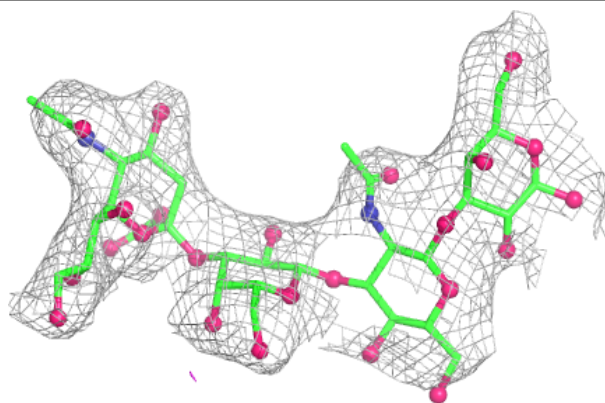


Electron density around Chain J:

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

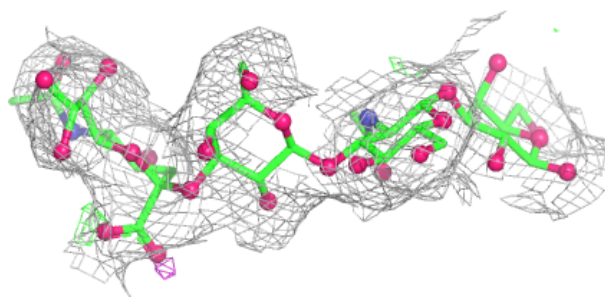
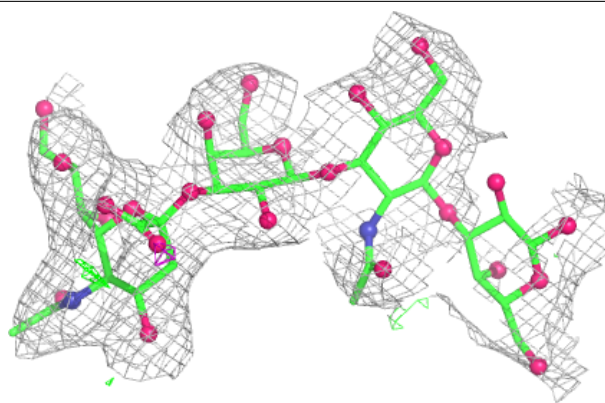
**Electron density around Chain K:**

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

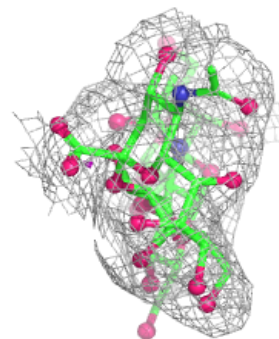
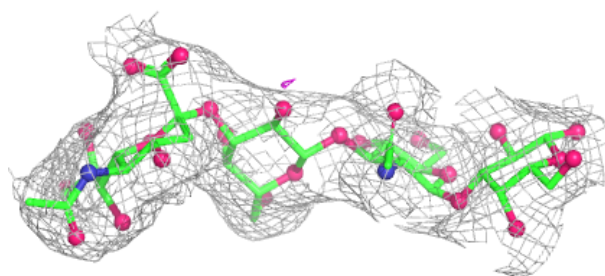
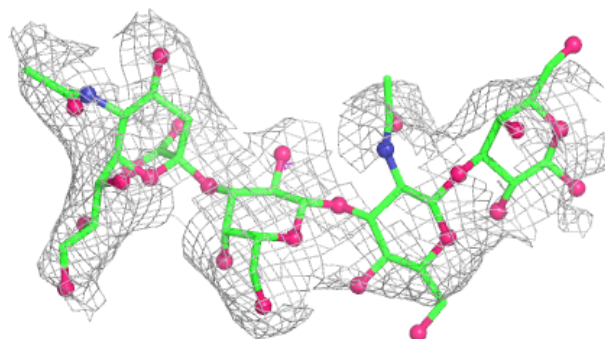


Electron density around Chain L:

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

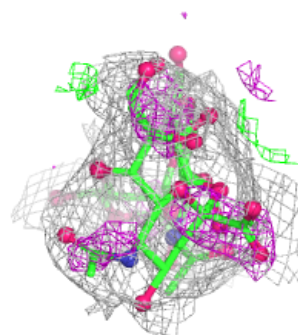
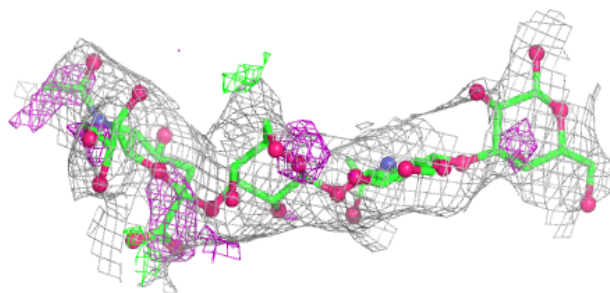
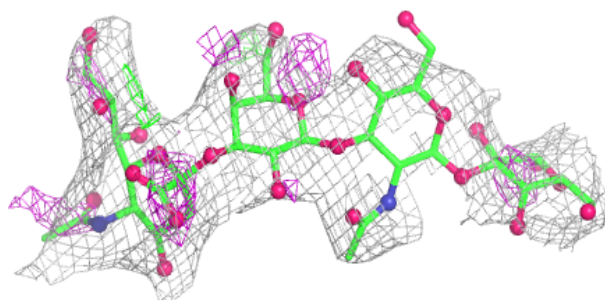
**Electron density around Chain M:**

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

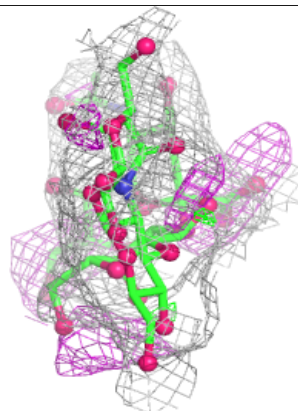
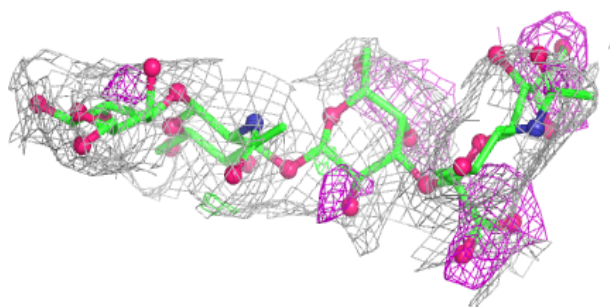
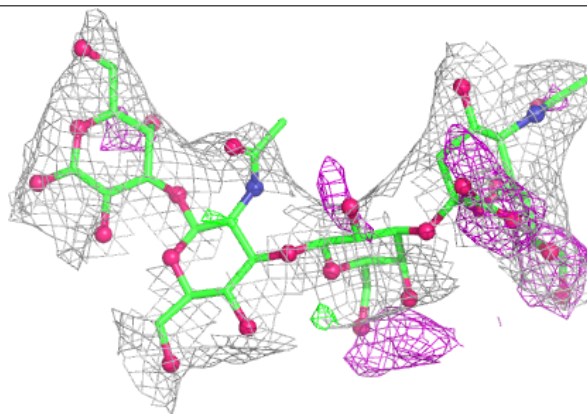


Electron density around Chain N:

$2mF_o-DF_c$ (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, 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	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.