



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2022 – 06:05 PM EDT

PDB ID : 7SYX
Title : Hendra virus G protein head domain in complex with cross-neutralizing murine antibody hAH1.3
Authors : Xu, K.; Xu, Y.
Deposited on : 2021-11-25
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

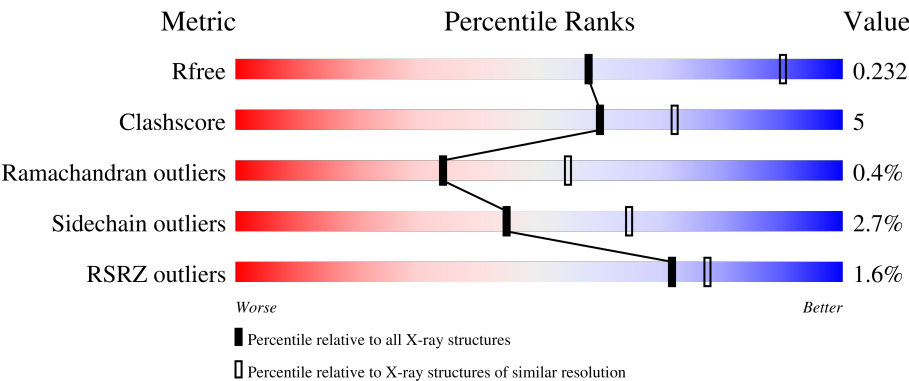
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

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 2.74 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	604	<div><div>%</div><div>58%9%•32%</div></div>
2	H	223	<div><div>%</div><div>86%11%••</div></div>
3	L	221	<div><div>%</div><div>85%13%•</div></div>
4	B	6	<div><div></div><div>67%33%</div></div>
5	C	6	<div><div></div><div>17%67%17%</div></div>

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Mol	Chain	Length	Quality of chain
6	D	2	 100%
7	E	2	 50% 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
10	ZN	A	705	-	-	-	X
11	CL	A	709	-	-	X	-
11	CL	L	301	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 6923 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Attachment glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3227	2062	539	607	19			

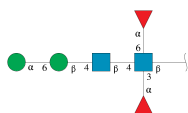
- Molecule 2 is a protein called Antibody hAH1.3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1667	1063	267	328	9			

- Molecule 3 is a protein called Antibody hAH1.3 light chain.

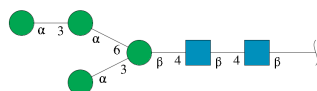
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	218	Total	C	N	O	S	0	0	0
			1690	1061	286	337	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	6	Total	C	N	O	0	0	0
			70	40	2	28			

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



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

- Molecule 6 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
6	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



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

- Molecule 9 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Zn	0	0
			1	1		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	Cl	0	0
			5	5		
11	H	4	Total	Cl	0	0
			4	4		
11	L	1	Total	Cl	0	0
			1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	51	Total	O	0	0
			51	51		
12	H	17	Total	O	0	0
			17	17		
12	L	22	Total	O	0	0
			22	22		



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

Chain B: 67% 33%



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

Chain C: 17% 67% 17%



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

Chain D: 100%



- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.25 Å 137.25 Å 149.97 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.44 – 2.74 44.44 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.44-2.74) 99.9 (44.44-2.74)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.73 Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.211 , 0.233 0.209 , 0.232	Depositor DCC
R_{free} test set	1900 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, FUC, BMA, MAN, CL, SO4

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	0.25	0/3304	0.50	0/4500
2	H	0.26	0/1714	0.48	0/2341
3	L	0.26	0/1729	0.49	0/2346
All	All	0.25	0/6747	0.49	0/9187

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3154	33	0
2	H	1667	0	1612	12	0
3	L	1690	0	1632	17	0
4	B	70	0	61	0	0
5	C	72	0	61	3	0
6	D	28	0	25	0	0
7	E	24	0	22	0	0
8	A	14	0	13	0	0
9	A	15	0	0	2	0
9	H	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	1	0	0	0	0
11	A	5	0	0	2	0
11	H	4	0	0	0	0
11	L	1	0	0	2	0
12	A	51	0	0	1	0
12	H	17	0	0	0	0
12	L	22	0	0	1	0
All	All	6923	0	6580	61	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 5.

All (61) 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)
3:L:189:HIS:NE2	11:L:301:CL:CL	2.26	1.06
3:L:10:SER:OG	3:L:105:GLU:OE2	2.03	0.76
3:L:181:LEU:HB3	3:L:185:GLU:HG3	1.69	0.71
3:L:150:ILE:HD11	3:L:179:LEU:HD21	1.73	0.70
3:L:185:GLU:OE1	12:L:401:HOH:O	2.10	0.69
2:H:168:ALA:HB2	2:H:177:LEU:HD23	1.82	0.61
1:A:414:LEU:HD22	1:A:426:LEU:HG	1.83	0.60
1:A:376:GLN:N	9:A:704:SO4:O4	2.31	0.60
1:A:201:ARG:NH2	11:A:709:CL:CL	2.71	0.57
1:A:484:VAL:HG23	1:A:485:ILE:HG12	1.87	0.57
1:A:217:ILE:HB	1:A:590:PRO:HD3	1.87	0.56
1:A:568:LEU:O	1:A:571:VAL:HG12	2.06	0.56
3:L:189:HIS:CE1	11:L:301:CL:CL	2.97	0.54
1:A:221:LEU:HB3	1:A:232:SER:HB3	1.90	0.53
1:A:476:ARG:NH2	5:C:5:MAN:O6	2.42	0.53
3:L:37:LEU:HB2	3:L:47:LEU:HD11	1.92	0.51
3:L:184:ASP:O	3:L:188:ARG:HG2	2.11	0.51
1:A:480:ARG:HA	5:C:1:NAG:H82	1.91	0.51
1:A:407:TYR:N	9:A:703:SO4:O3	2.39	0.50
1:A:293:THR:HB	1:A:317:ILE:HG23	1.93	0.49
3:L:27(D):HIS:CD2	3:L:27(E):ILE:H	2.30	0.49
1:A:372:ARG:HH12	1:A:397:LEU:HA	1.78	0.48
1:A:416:TYR:CZ	1:A:424:ILE:HB	2.49	0.48
1:A:204:SER:HB3	1:A:592:LEU:HB2	1.96	0.48
1:A:312:GLU:OE2	1:A:340:VAL:HG11	2.14	0.48
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:106:LEU:O	3:L:166:GLN:NE2	2.39	0.47
1:A:355:GLY:HA3	1:A:363:TYR:O	2.15	0.47
2:H:153:THR:HA	9:H:301:SO4:O4	2.15	0.47
1:A:372:ARG:HG2	1:A:408:ILE:HG23	1.95	0.47
3:L:7:THR:OG1	3:L:22:SER:HB3	2.14	0.47
1:A:181:LEU:HD21	1:A:514:ILE:HA	1.98	0.46
1:A:318:ARG:NH2	1:A:329:ASP:O	2.48	0.46
2:H:4:LEU:HD22	2:H:24:THR:HG22	1.98	0.46
1:A:201:ARG:NE	11:A:709:CL:CL	2.83	0.46
2:H:55:GLY:HA2	2:H:71:LEU:HD21	1.97	0.46
1:A:394:ASN:O	1:A:398:SER:HB2	2.17	0.45
1:A:420:LEU:O	1:A:424:ILE:HG12	2.17	0.45
1:A:345:TYR:CD2	1:A:370:LEU:HB2	2.51	0.44
1:A:252:VAL:HG11	1:A:291:TYR:HB2	1.99	0.44
1:A:294:LEU:HG	1:A:350:PRO:HG3	2.00	0.44
2:H:100(B):LYS:NZ	3:L:91:GLY:O	2.45	0.44
3:L:61:ARG:NH1	3:L:82:ASP:OD1	2.50	0.43
1:A:385:ILE:HG12	1:A:386:HIS:CD2	2.54	0.43
1:A:413:LEU:HG	1:A:475:LEU:HD22	1.99	0.43
3:L:59:PRO:HB2	3:L:61:ARG:HG2	1.99	0.43
1:A:561:THR:HG22	1:A:578:VAL:HG13	2.01	0.43
1:A:286:TYR:OH	1:A:288:GLU:O	2.29	0.42
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.90	0.42
1:A:381:ASN:ND2	12:A:806:HOH:O	2.52	0.42
2:H:119:PRO:HB2	2:H:142:VAL:HG13	2.01	0.42
2:H:69:PHE:CE2	2:H:80:LEU:HD13	2.55	0.42
2:H:43:LYS:HB3	2:H:44:GLY:H	1.70	0.42
5:C:3:BMA:H3	5:C:6:MAN:H2	1.84	0.42
1:A:573:TRP:CZ2	1:A:596:LYS:HB2	2.54	0.42
2:H:46:LYS:HE3	2:H:46:LYS:HB3	1.91	0.42
2:H:114:ALA:HB2	2:H:173:ASP:HB3	2.02	0.41
1:A:233:HIS:CD2	1:A:233:HIS:C	2.94	0.41
1:A:483:SER:HB3	3:L:27(E):ILE:HA	2.03	0.40
3:L:54:ARG:CZ	3:L:60:ASP:HA	2.51	0.40
2:H:94:ARG:O	2:H:100(D):MET:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	407/604 (67%)	389 (96%)	17 (4%)	1 (0%)	47	69
2	H	214/223 (96%)	208 (97%)	5 (2%)	1 (0%)	29	48
3	L	216/221 (98%)	212 (98%)	3 (1%)	1 (0%)	29	48
All	All	837/1048 (80%)	809 (97%)	25 (3%)	3 (0%)	34	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	172	SER
3	L	68	GLY
1	A	288	GLU

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	363/543 (67%)	354 (98%)	9 (2%)	47	67
2	H	189/192 (98%)	183 (97%)	6 (3%)	39	59
3	L	193/198 (98%)	188 (97%)	5 (3%)	46	66
All	All	745/933 (80%)	725 (97%)	20 (3%)	44	65

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

Mol	Chain	Res	Type
1	A	201	ARG
1	A	241	THR
1	A	340	VAL
1	A	351	TYR
1	A	357	LYS
1	A	398	SER
1	A	487	ARG
1	A	519	TRP
1	A	534	ASN
2	H	4	LEU
2	H	100(A)	LEU
2	H	140	CYS
2	H	173	ASP
2	H	194	THR
2	H	195	CYS
3	L	33	LEU
3	L	42	GLN
3	L	61	ARG
3	L	77	ARG
3	L	163	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	543	ASN
3	L	30	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 ⓘ

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1	1,4	14,14,15	0.24	0	17,19,21	0.84	1 (5%)
4	NAG	B	2	4	14,14,15	0.33	0	17,19,21	0.37	0
4	BMA	B	3	4	11,11,12	0.58	0	15,15,17	0.83	0
4	MAN	B	4	4	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
4	FUC	B	5	4	10,10,11	0.69	0	14,14,16	0.89	0
4	FUC	B	6	4	10,10,11	0.74	0	14,14,16	0.65	0
5	NAG	C	1	1,5	14,14,15	0.27	0	17,19,21	0.38	0
5	NAG	C	2	5	14,14,15	0.25	0	17,19,21	0.35	0
5	BMA	C	3	5	11,11,12	0.61	0	15,15,17	0.74	0
5	MAN	C	4	5	11,11,12	0.70	0	15,15,17	1.17	2 (13%)
5	MAN	C	5	5	11,11,12	0.80	0	15,15,17	1.01	0
5	MAN	C	6	5	11,11,12	0.78	0	15,15,17	0.97	2 (13%)
6	NAG	D	1	6,1	14,14,15	0.57	0	17,19,21	0.54	0
6	NAG	D	2	6	14,14,15	0.30	0	17,19,21	0.37	0
7	NAG	E	1	1,7	14,14,15	0.17	0	17,19,21	0.81	1 (5%)
7	FUC	E	2	7	10,10,11	0.72	0	14,14,16	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	FUC	B	5	4	-	-	0/1/1/1
4	FUC	B	6	4	-	-	0/1/1/1
5	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1
5	MAN	C	5	5	-	0/2/19/22	0/1/1/1
5	MAN	C	6	5	-	0/2/19/22	0/1/1/1
6	NAG	D	1	6,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
7	NAG	E	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	E	2	7	-	-	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4	MAN	C1-O5-C5	2.64	115.77	112.19
4	B	4	MAN	C1-O5-C5	2.59	115.70	112.19
4	B	1	NAG	C1-O5-C5	2.58	115.69	112.19
7	E	1	NAG	C1-O5-C5	2.39	115.43	112.19
5	C	6	MAN	O2-C2-C3	-2.23	105.67	110.14
4	B	4	MAN	O2-C2-C3	-2.20	105.73	110.14
5	C	6	MAN	C1-O5-C5	2.15	115.11	112.19
5	C	4	MAN	O2-C2-C3	-2.10	105.94	110.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

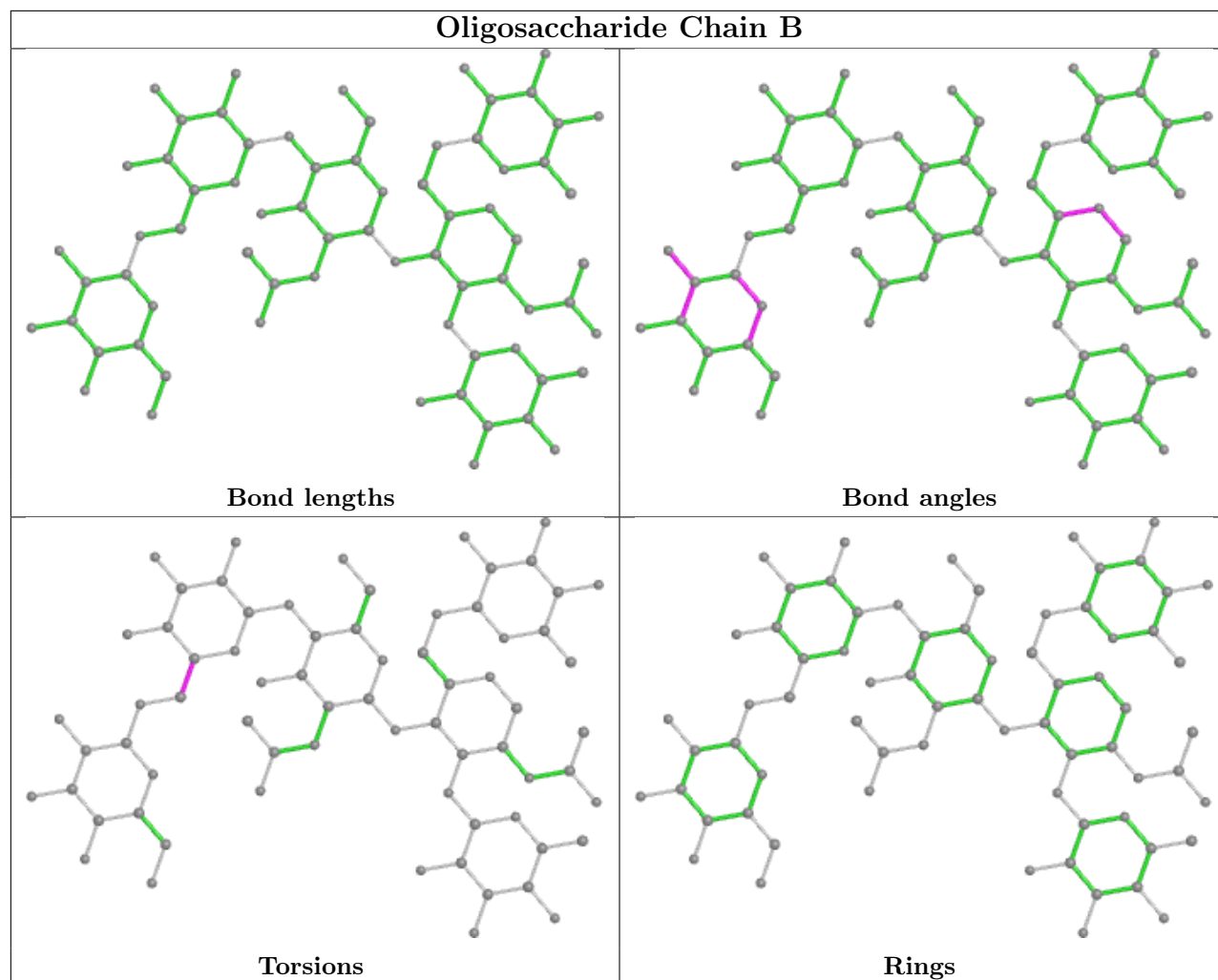
Mol	Chain	Res	Type	Atoms
4	B	3	BMA	O5-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
7	E	1	NAG	C4-C5-C6-O6
7	E	1	NAG	O5-C5-C6-O6

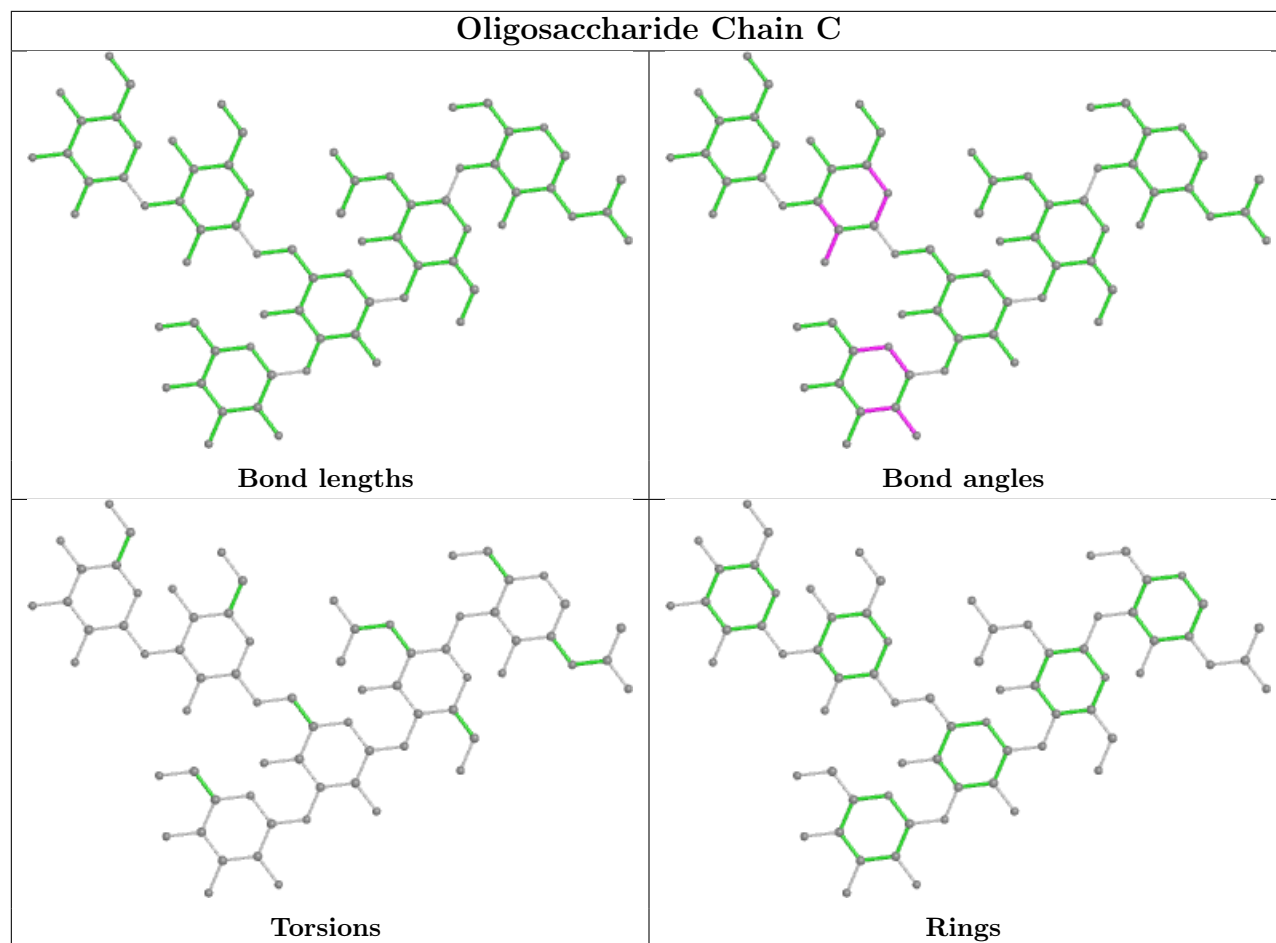
There are no ring outliers.

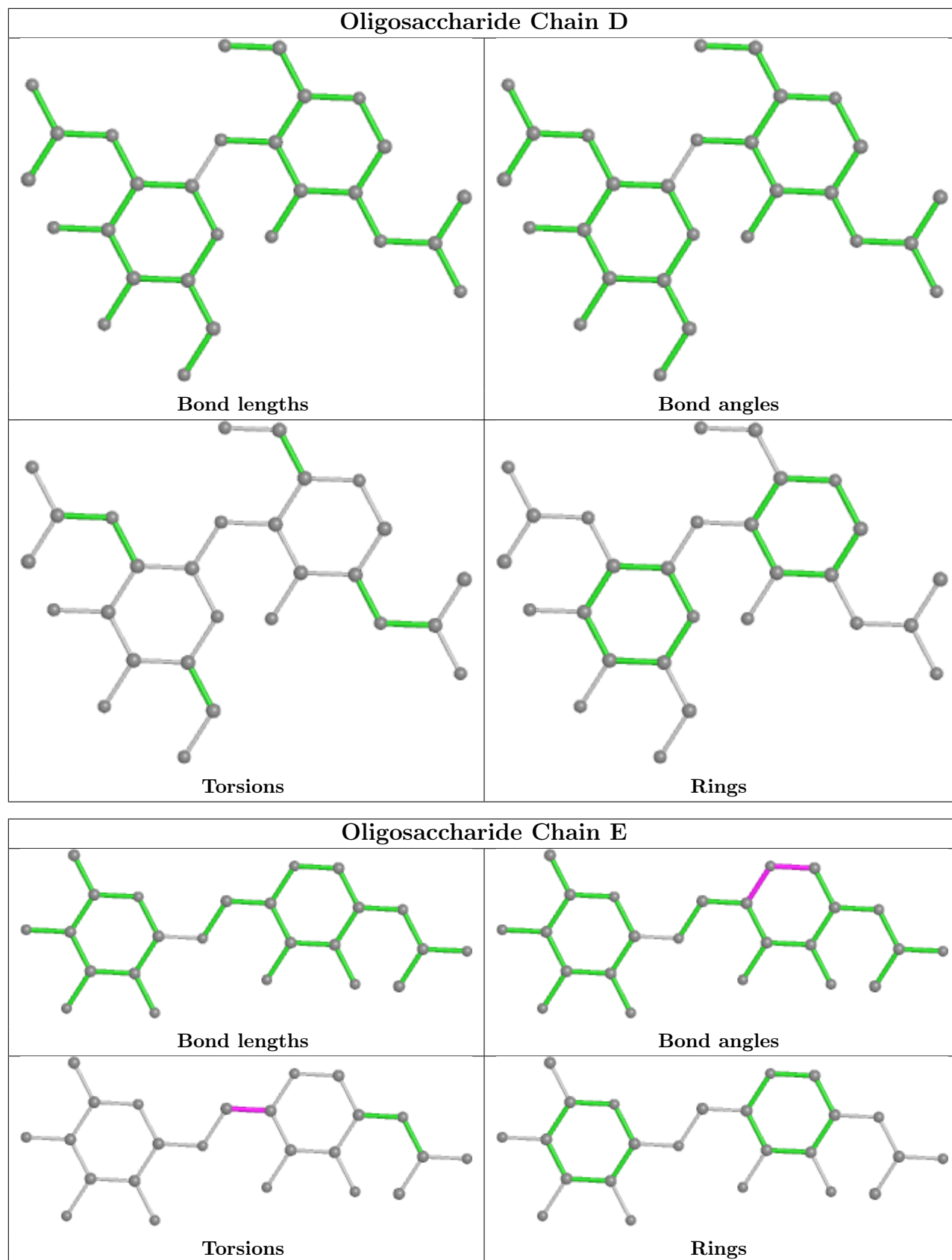
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5	MAN	1	0
5	C	3	BMA	1	0
5	C	1	NAG	1	0
5	C	6	MAN	1	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

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 for Mogul analysis.

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
9	SO4	A	703	-	4,4,4	0.15	0	6,6,6	0.06	0
8	NAG	A	701	1	14,14,15	0.17	0	17,19,21	0.45	0
9	SO4	H	302	-	4,4,4	0.13	0	6,6,6	0.05	0
9	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.13	0
9	SO4	H	303	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	A	704	-	4,4,4	0.17	0	6,6,6	0.05	0
9	SO4	A	702	-	4,4,4	0.15	0	6,6,6	0.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	701	NAG	C4-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	703	SO4	1	0
9	H	301	SO4	1	0
9	A	704	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	413/604 (68%)	-0.02	9 (2%) 62 69	54, 69, 98, 137	0
2	H	218/223 (97%)	-0.19	3 (1%) 75 80	57, 70, 97, 148	0
3	L	218/221 (98%)	-0.04	2 (0%) 84 88	58, 74, 100, 128	0
All	All	849/1048 (81%)	-0.07	14 (1%) 72 78	54, 70, 98, 148	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	GLY	5.0
1	A	587	VAL	3.7
2	H	215	CYS	3.0
3	L	213	GLU	2.9
1	A	581	TYR	2.7
1	A	244	ILE	2.6
3	L	77	ARG	2.6
1	A	603	GLU	2.4
2	H	59	TYR	2.4
1	A	237	ILE	2.4
1	A	177	GLY	2.3
1	A	425	ILE	2.1
2	H	51	ILE	2.1
1	A	355	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

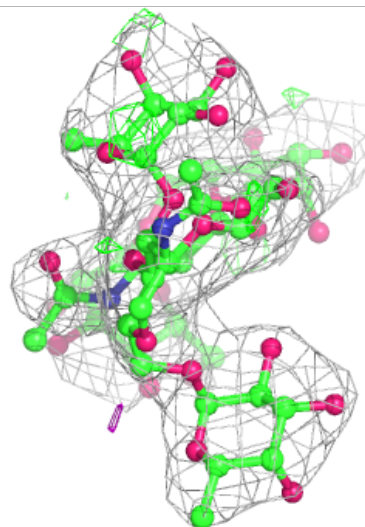
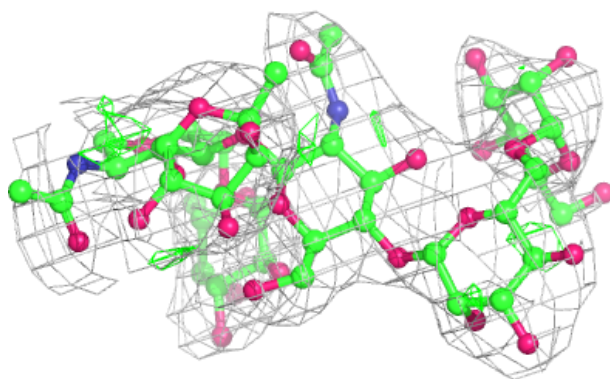
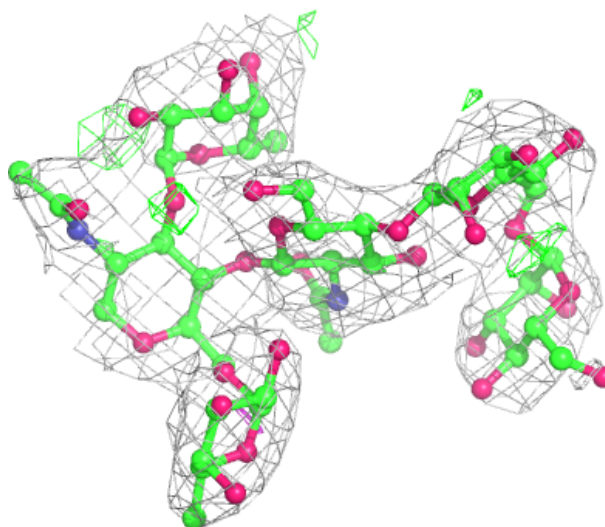
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	C	3	11/12	0.65	0.22	125,127,133,137	0
5	MAN	C	6	11/12	0.77	0.31	128,137,139,139	0
6	NAG	D	2	14/15	0.78	0.26	113,123,130,133	0
7	NAG	E	1	14/15	0.80	0.27	100,119,125,127	0
5	MAN	C	4	11/12	0.81	0.25	115,120,121,121	0
7	FUC	E	2	10/11	0.83	0.32	119,128,129,130	0
4	BMA	B	3	11/12	0.84	0.16	110,114,116,121	0
5	MAN	C	5	11/12	0.84	0.52	95,108,112,116	0
5	NAG	C	2	14/15	0.85	0.23	90,101,110,122	0
4	MAN	B	4	11/12	0.85	0.31	101,109,114,115	0
6	NAG	D	1	14/15	0.88	0.17	69,92,104,113	0
4	NAG	B	1	14/15	0.90	0.17	71,78,85,86	0
4	NAG	B	2	14/15	0.91	0.12	86,90,97,105	0
4	FUC	B	6	10/11	0.95	0.17	68,79,83,86	0
5	NAG	C	1	14/15	0.96	0.15	67,76,85,90	0
4	FUC	B	5	10/11	0.96	0.12	81,83,84,85	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.

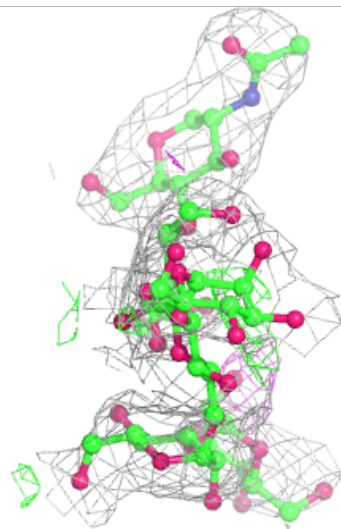
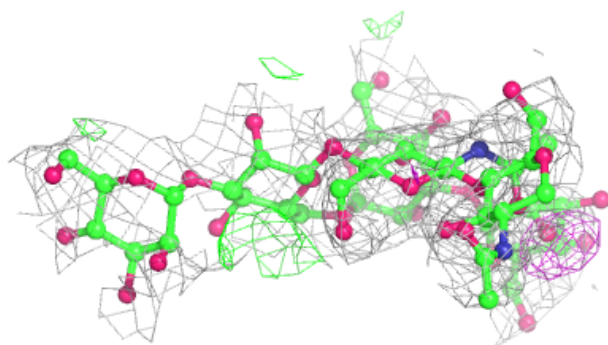
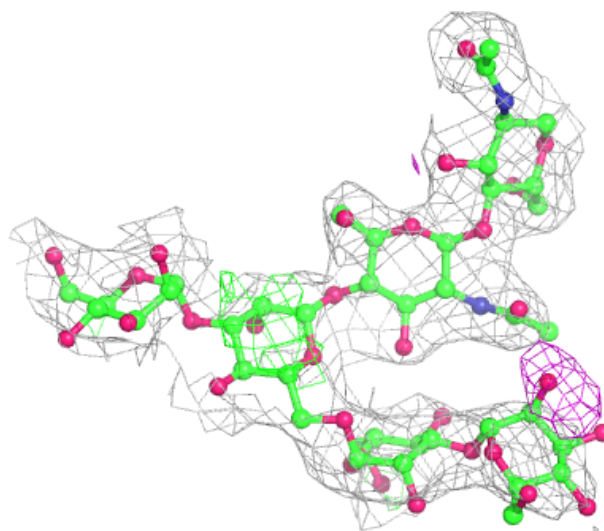
Electron density around Chain B:

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



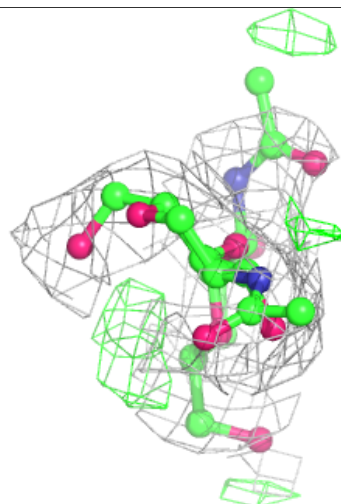
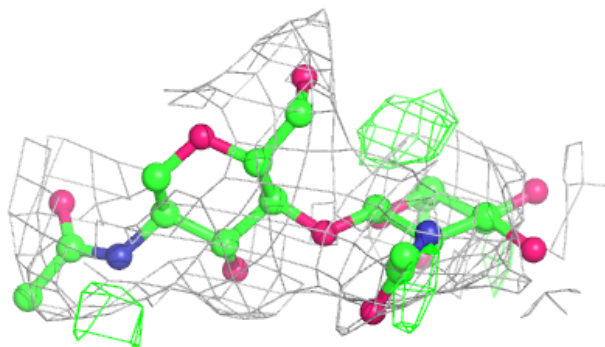
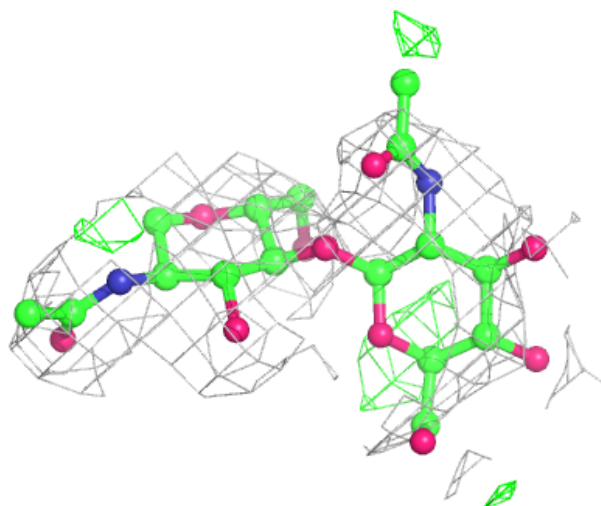
Electron density around Chain C:

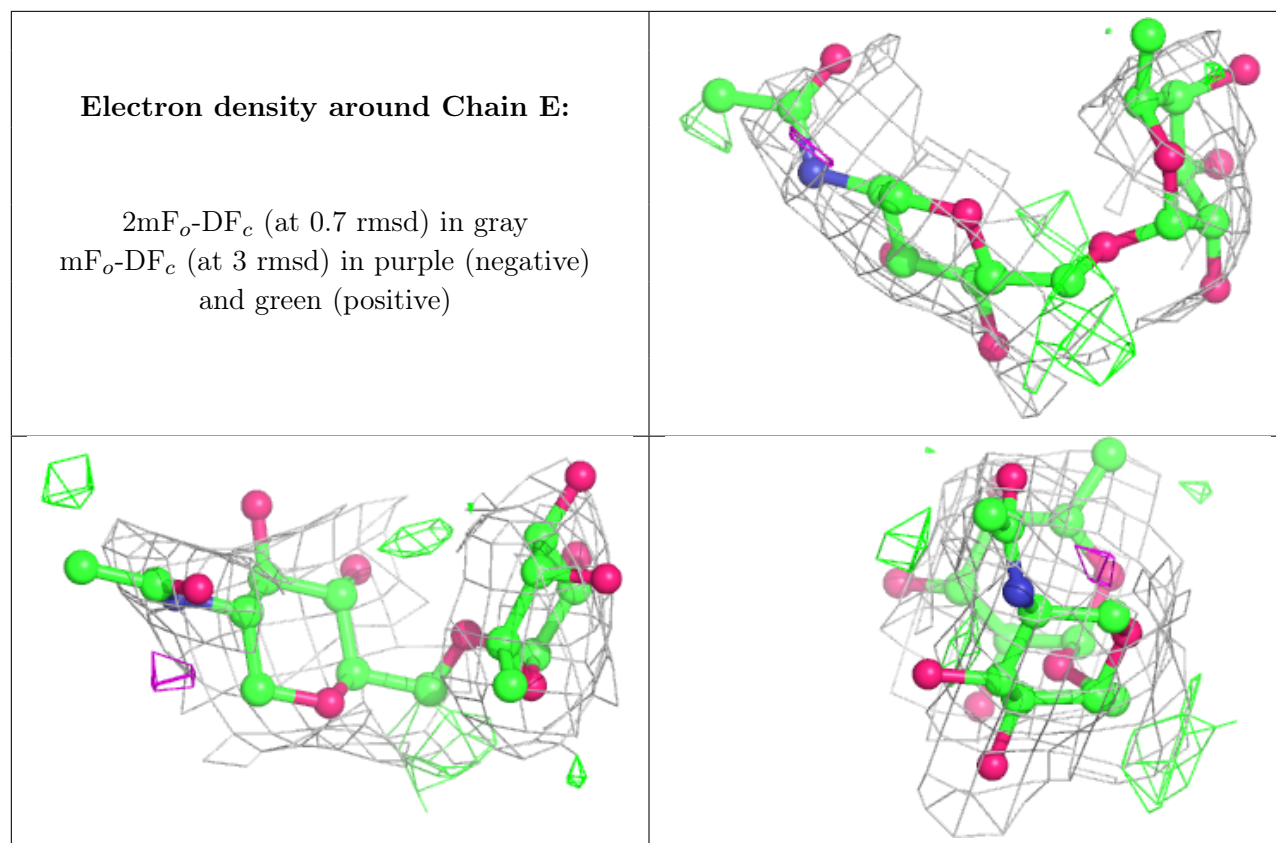
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (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
10	ZN	A	705	1/1	0.51	0.62	246,246,246,246	0
8	NAG	A	701	14/15	0.81	0.32	107,117,132,137	0
11	CL	A	708	1/1	0.83	0.14	89,89,89,89	0
11	CL	H	304	1/1	0.86	0.10	88,88,88,88	0
9	SO4	H	303	5/5	0.92	0.35	96,96,111,117	0
11	CL	H	307	1/1	0.93	0.56	74,74,74,74	0
9	SO4	A	703	5/5	0.95	0.17	78,78,83,86	0
11	CL	H	305	1/1	0.96	0.12	72,72,72,72	0
11	CL	A	707	1/1	0.96	0.09	71,71,71,71	0
9	SO4	H	302	5/5	0.97	0.31	74,75,81,86	0
9	SO4	H	301	5/5	0.97	0.16	73,75,85,88	0
11	CL	L	301	1/1	0.97	0.51	32,32,32,32	0
11	CL	A	710	1/1	0.98	0.22	62,62,62,62	0
11	CL	A	706	1/1	0.98	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SO4	A	702	5/5	0.98	0.19	79,79,90,90	0
9	SO4	A	704	5/5	0.98	0.11	81,82,91,95	0
11	CL	A	709	1/1	0.98	0.05	67,67,67,67	0
11	CL	H	306	1/1	0.99	0.25	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.