



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:05 AM UTC

PDB ID : 7Q15 / pdb_00007q15
Title : Crystal structure of FcRn and beta-2-microglobulin in complex with IgG1-Fc-MST-HN (efgartigimod)
Authors : Pannecoucke, E.; Savvides, S.N.
Deposited on : 2021-10-18
Resolution : 3.30 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

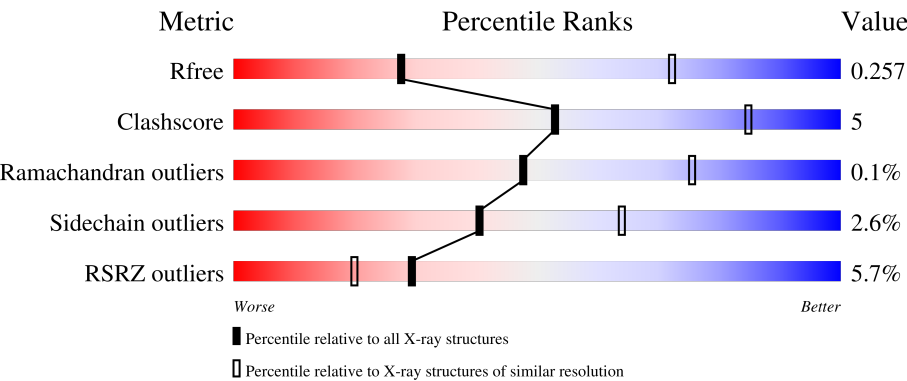
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



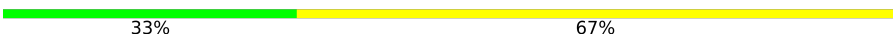
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	338	72%7%21%
1	C	338	9% 71%6%23%
2	B	119	76%8%17%
2	D	119	11% 72%9%18%
3	E	225	2% 81%11%7%

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Mol	Chain	Length	Quality of chain
3	F	225	 6% 74% 16% 9%
4	G	9	 33% 67%
5	H	8	 38% 50% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8522 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	1	0
			1976	1271	331	365	9			
1	C	260	Total	C	N	O	S	0	0	0
			1725	1111	289	319	6			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	GLY	-	expression tag	UNP P55899
A	276	THR	-	expression tag	UNP P55899
A	277	SER	-	expression tag	UNP P55899
A	278	GLY	-	expression tag	UNP P55899
A	279	LEU	-	expression tag	UNP P55899
A	280	VAL	-	expression tag	UNP P55899
A	281	PRO	-	expression tag	UNP P55899
A	282	ARG	-	expression tag	UNP P55899
A	283	GLY	-	expression tag	UNP P55899
A	284	SER	-	expression tag	UNP P55899
A	285	GLY	-	expression tag	UNP P55899
A	286	GLY	-	expression tag	UNP P55899
A	287	SER	-	expression tag	UNP P55899
A	288	GLY	-	expression tag	UNP P55899
A	289	GLY	-	expression tag	UNP P55899
A	290	SER	-	expression tag	UNP P55899
A	291	GLY	-	expression tag	UNP P55899
A	292	LEU	-	expression tag	UNP P55899
A	293	ASN	-	expression tag	UNP P55899
A	294	ASP	-	expression tag	UNP P55899
A	295	ILE	-	expression tag	UNP P55899
A	296	PHE	-	expression tag	UNP P55899
A	297	GLU	-	expression tag	UNP P55899
A	298	ALA	-	expression tag	UNP P55899
A	299	GLN	-	expression tag	UNP P55899

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Chain	Residue	Modelled	Actual	Comment	Reference
A	300	LYS	-	expression tag	UNP P55899
A	301	ILE	-	expression tag	UNP P55899
A	302	GLU	-	expression tag	UNP P55899
A	303	TRP	-	expression tag	UNP P55899
A	304	HIS	-	expression tag	UNP P55899
A	305	GLU	-	expression tag	UNP P55899
A	306	GLY	-	expression tag	UNP P55899
A	307	ARG	-	expression tag	UNP P55899
A	308	THR	-	expression tag	UNP P55899
A	309	LYS	-	expression tag	UNP P55899
A	310	HIS	-	expression tag	UNP P55899
A	311	HIS	-	expression tag	UNP P55899
A	312	HIS	-	expression tag	UNP P55899
A	313	HIS	-	expression tag	UNP P55899
A	314	HIS	-	expression tag	UNP P55899
A	315	HIS	-	expression tag	UNP P55899
C	275	GLY	-	expression tag	UNP P55899
C	276	THR	-	expression tag	UNP P55899
C	277	SER	-	expression tag	UNP P55899
C	278	GLY	-	expression tag	UNP P55899
C	279	LEU	-	expression tag	UNP P55899
C	280	VAL	-	expression tag	UNP P55899
C	281	PRO	-	expression tag	UNP P55899
C	282	ARG	-	expression tag	UNP P55899
C	283	GLY	-	expression tag	UNP P55899
C	284	SER	-	expression tag	UNP P55899
C	285	GLY	-	expression tag	UNP P55899
C	286	GLY	-	expression tag	UNP P55899
C	287	SER	-	expression tag	UNP P55899
C	288	GLY	-	expression tag	UNP P55899
C	289	GLY	-	expression tag	UNP P55899
C	290	SER	-	expression tag	UNP P55899
C	291	GLY	-	expression tag	UNP P55899
C	292	LEU	-	expression tag	UNP P55899
C	293	ASN	-	expression tag	UNP P55899
C	294	ASP	-	expression tag	UNP P55899
C	295	ILE	-	expression tag	UNP P55899
C	296	PHE	-	expression tag	UNP P55899
C	297	GLU	-	expression tag	UNP P55899
C	298	ALA	-	expression tag	UNP P55899
C	299	GLN	-	expression tag	UNP P55899
C	300	LYS	-	expression tag	UNP P55899

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Chain	Residue	Modelled	Actual	Comment	Reference
C	301	ILE	-	expression tag	UNP P55899
C	302	GLU	-	expression tag	UNP P55899
C	303	TRP	-	expression tag	UNP P55899
C	304	HIS	-	expression tag	UNP P55899
C	305	GLU	-	expression tag	UNP P55899
C	306	GLY	-	expression tag	UNP P55899
C	307	ARG	-	expression tag	UNP P55899
C	308	THR	-	expression tag	UNP P55899
C	309	LYS	-	expression tag	UNP P55899
C	310	HIS	-	expression tag	UNP P55899
C	311	HIS	-	expression tag	UNP P55899
C	312	HIS	-	expression tag	UNP P55899
C	313	HIS	-	expression tag	UNP P55899
C	314	HIS	-	expression tag	UNP P55899
C	315	HIS	-	expression tag	UNP P55899

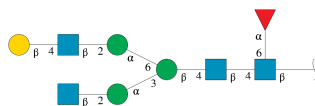
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			759	485	129	142	3			
2	D	98	Total	C	N	O	S	0	0	0
			698	449	119	128	2			

- Molecule 3 is a protein called IgG1-Fc-MST-HN.

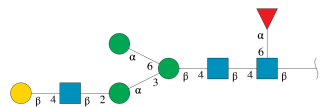
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	209	Total	C	N	O	S	0	0	0
			1595	1020	264	306	5			
3	F	205	Total	C	N	O	S	0	0	0
			1563	1001	257	300	5			

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

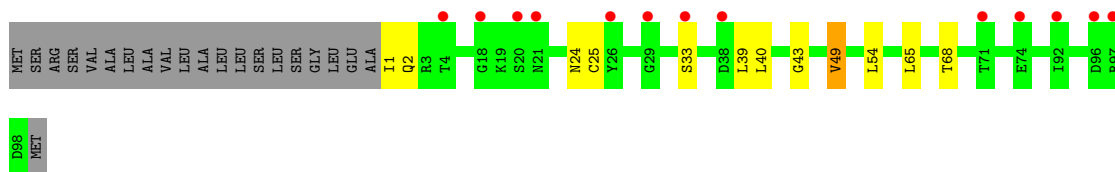


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	9	Total	C	N	O	0	0	0
			110	62	4	44			

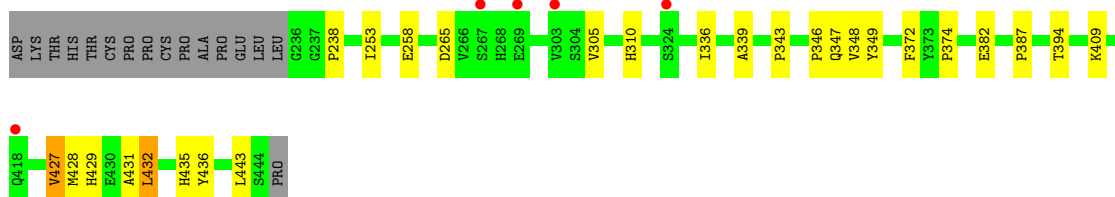
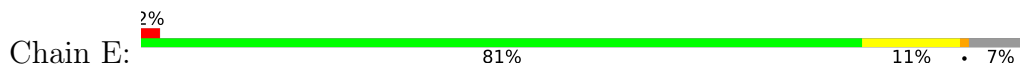
- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



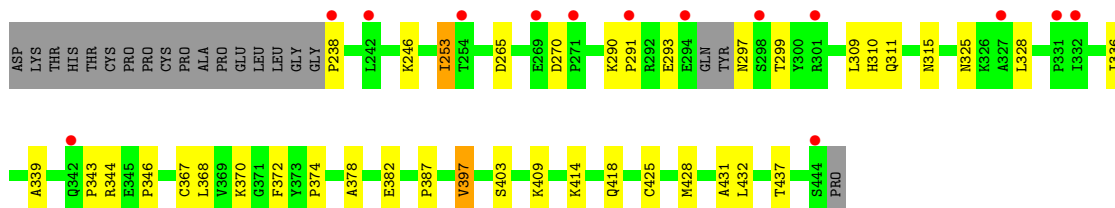
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	8	Total	C	N	O	0	0	0
			96	54	3	39			



• Molecule 3: IgG1-Fc-MST-HN



• Molecule 3: IgG1-Fc-MST-HN



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.43Å 53.11Å 195.75Å 90.00° 92.18° 90.00°	Depositor
Resolution (Å)	48.90 – 3.30 48.90 – 3.30	Depositor EDS
% Data completeness (in resolution range)	66.7 (48.90-3.30) 66.7 (48.90-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.206 , 0.231 0.230 , 0.257	Depositor DCC
R_{free} test set	1003 reflections (5.50%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	8522	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: NAG, MAN, FUC, BMA, 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	0.55	0/2037	0.87	0/2792
1	C	0.55	1/1779 (0.1%)	0.88	1/2454 (0.0%)
2	B	0.47	0/782	0.84	0/1072
2	D	0.50	0/720	0.85	0/995
3	E	0.57	0/1642	0.92	2/2256 (0.1%)
3	F	0.55	0/1608	0.91	1/2206 (0.0%)
All	All	0.54	1/8568 (0.0%)	0.88	4/11775 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204	TYR	C-N	5.28	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	TYR	CA-C-O	-7.18	110.32	120.16
3	F	297	ASN	OD1-CG-ND2	-5.12	117.48	122.60
3	E	429	HIS	CA-C-N	5.07	127.32	120.38
3	E	429	HIS	C-N-CA	5.07	127.32	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	SER	Mainchain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1976	0	1755	13	0
1	C	1725	0	1354	15	0
2	B	759	0	657	6	0
2	D	698	0	560	10	0
3	E	1595	0	1478	18	0
3	F	1563	0	1436	25	0
4	G	110	0	94	0	0
5	H	96	0	82	1	0
All	All	8522	0	7416	79	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 (79) 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:F:238:PRO:HA	3:F:265:ASP:HB2	1.55	0.86
3:E:346:PRO:HB3	3:E:372:PHE:HB3	1.64	0.80
3:F:346:PRO:HB3	3:F:372:PHE:HB3	1.67	0.75
3:E:238:PRO:HA	3:E:265:ASP:HB2	1.73	0.71
3:E:348:VAL:HG21	3:E:427:VAL:HG11	1.73	0.70
2:B:17:ASN:HD21	2:B:97:ARG:HH22	1.37	0.70
3:E:347:GLN:NE2	3:E:349:TYR:OH	2.27	0.68
2:B:17:ASN:ND2	2:B:97:ARG:HH22	1.92	0.66
1:A:117:PHE:HB3	3:E:253:ILE:HD12	1.76	0.66
1:C:81:ALA:HB2	1:C:140:ARG:HG3	1.76	0.66
3:F:238:PRO:HA	3:F:265:ASP:CB	2.27	0.65
3:E:346:PRO:HG2	3:E:432:LEU:HD23	1.79	0.63
1:A:67:ASP:O	1:A:70:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:343:PRO:HB2	3:E:431:ALA:HB2	1.84	0.60
3:F:343:PRO:HB2	3:F:431:ALA:HB2	1.84	0.59
3:F:270:ASP:OD2	3:F:325:ASN:ND2	2.37	0.58
1:A:117:PHE:HB3	3:E:253:ILE:CD1	2.34	0.57
1:C:118:MET:HE2	1:C:134:ALA:HA	1.85	0.57
2:B:17:ASN:HD21	2:B:97:ARG:NH2	2.04	0.56
1:C:79:PHE:CE2	1:C:88:TYR:HB2	2.41	0.55
3:E:394:THR:HG22	3:F:397:VAL:HG21	1.89	0.54
1:A:117:PHE:CB	3:E:253:ILE:HD12	2.39	0.53
1:C:10:HIS:CE1	1:C:29:TRP:CD1	2.98	0.52
3:F:368:LEU:HD21	3:F:370:LYS:HB2	1.91	0.52
1:C:188:PRO:O	1:C:193:PHE:O	2.27	0.52
1:A:188:PRO:O	1:A:193:PHE:O	2.27	0.52
1:C:117:PHE:HB3	3:F:253:ILE:HD12	1.92	0.51
3:F:378:ALA:HB3	3:F:428:MET:CG	2.40	0.51
3:E:253:ILE:HA	3:E:310:HIS:CE1	2.45	0.51
3:E:339:ALA:HB3	3:E:374:PRO:HB3	1.93	0.51
1:A:64:GLU:O	1:A:68:LEU:HD12	2.11	0.51
1:C:10:HIS:ND1	1:C:29:TRP:CD1	2.80	0.50
3:E:348:VAL:HG21	3:E:427:VAL:CG1	2.39	0.50
3:F:339:ALA:HB3	3:F:374:PRO:HB3	1.94	0.50
3:F:290:LYS:HG3	3:F:291:PRO:HD2	1.92	0.49
3:F:253:ILE:HA	3:F:310:HIS:CE1	2.46	0.49
1:C:10:HIS:HD2	1:C:93:LEU:HD13	1.77	0.49
3:E:258:GLU:HB3	3:E:305:VAL:HG13	1.94	0.49
1:A:132:PRO:HD3	3:E:435:HIS:HB2	1.94	0.49
3:F:414:LYS:NZ	3:F:418:GLN:HE21	2.10	0.49
3:F:367:CYS:HG	3:F:425:CYS:HG	1.59	0.49
2:B:20:SER:HA	2:B:71:THR:HG22	1.94	0.48
1:C:22:PRO:HB3	1:C:41:LEU:HG	1.95	0.48
3:F:432:LEU:HD13	3:F:437:THR:HG22	1.96	0.48
3:E:238:PRO:HA	3:E:265:ASP:CB	2.43	0.47
3:F:344:ARG:HH21	3:F:403:SER:HA	1.79	0.46
1:A:186:ALA:HB2	1:A:196:LEU:HD23	1.97	0.46
1:C:7:LEU:CD1	1:C:30:LEU:HD23	2.46	0.46
2:D:1:ILE:HG22	2:D:2:GLN:N	2.31	0.45
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.98	0.45
2:D:25:CYS:HB2	2:D:39:LEU:HD21	1.99	0.45
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.99	0.45
2:D:39:LEU:HD12	2:D:49:VAL:HG12	1.99	0.45
1:A:77:GLU:HG3	1:A:140:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:LEU:HD23	2:D:43:GLY:HA2	1.99	0.44
3:E:382:GLU:HA	3:E:387:PRO:HA	1.99	0.44
1:C:79:PHE:HE2	1:C:88:TYR:HB2	1.83	0.44
1:C:10:HIS:CD2	1:C:93:LEU:HD13	2.52	0.44
3:F:382:GLU:HA	3:F:387:PRO:HA	1.99	0.44
1:A:112:LEU:HB2	1:A:117:PHE:CE1	2.53	0.44
1:C:10:HIS:CD2	1:C:93:LEU:CD1	3.01	0.43
3:F:325:ASN:HB3	3:F:328:LEU:HD13	2.01	0.43
2:D:1:ILE:HD12	3:F:309:LEU:HD23	2.00	0.43
3:F:290:LYS:NZ	3:F:291:PRO:HD2	2.32	0.43
2:D:33:SER:HB2	2:D:54:LEU:HD21	2.00	0.43
1:A:8:LEU:HD23	1:A:95:GLY:HA3	2.01	0.43
1:A:242:VAL:HG22	1:A:243:LYS:N	2.33	0.43
1:C:79:PHE:CD2	1:C:88:TYR:HB2	2.54	0.43
2:D:1:ILE:CG2	2:D:2:GLN:N	2.82	0.43
2:D:49:VAL:HG12	2:D:68:THR:HB	2.01	0.43
3:F:368:LEU:CD2	3:F:370:LYS:HB2	2.49	0.43
3:E:428:MET:HE3	3:E:436:TYR:HE1	1.84	0.43
2:B:33:SER:HB2	2:B:54:LEU:HD21	2.00	0.42
3:F:299:THR:CB	5:H:1:NAG:HN2	2.32	0.42
2:D:1:ILE:HD11	3:F:309:LEU:HA	2.01	0.42
1:A:120:PHE:HE2	1:A:152:LEU:HD12	1.83	0.42
1:C:11:LEU:HD13	1:C:94:LEU:HD12	2.02	0.42
3:F:311:GLN:O	3:F:315:ASN:OD1	2.39	0.41
3:F:414:LYS:HZ3	3:F:418:GLN:HG3	1.86	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	265/338 (78%)	253 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	254/338 (75%)	243 (96%)	10 (4%)	1 (0%)	30	60
2	B	97/119 (82%)	97 (100%)	0	0	100	100
2	D	96/119 (81%)	96 (100%)	0	0	100	100
3	E	207/225 (92%)	199 (96%)	8 (4%)	0	100	100
3	F	201/225 (89%)	196 (98%)	5 (2%)	0	100	100
All	All	1120/1364 (82%)	1084 (97%)	35 (3%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	204	TYR

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	184/275 (67%)	180 (98%)	4 (2%)	45	66
1	C	124/275 (45%)	121 (98%)	3 (2%)	43	65
2	B	76/109 (70%)	75 (99%)	1 (1%)	61	74
2	D	61/109 (56%)	60 (98%)	1 (2%)	55	72
3	E	173/209 (83%)	168 (97%)	5 (3%)	37	62
3	F	167/209 (80%)	161 (96%)	6 (4%)	31	58
All	All	785/1186 (66%)	765 (98%)	20 (2%)	40	64

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

Mol	Chain	Res	Type
1	A	48	CYS
1	A	56	GLN
1	A	152	LEU
1	A	208	LEU
2	B	6	LYS

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Mol	Chain	Res	Type
1	C	30	LEU
1	C	143	GLN
1	C	208	LEU
2	D	49	VAL
3	E	336	ILE
3	E	409	LYS
3	E	427	VAL
3	E	432	LEU
3	E	443	LEU
3	F	246	LYS
3	F	253	ILE
3	F	293	GLU
3	F	336	ILE
3	F	397	VAL
3	F	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	139	GLN
1	A	215	ASN
2	B	17	ASN
2	B	24	ASN
1	C	139	GLN
1	C	215	ASN
2	D	24	ASN
3	E	311	GLN
3	E	315	ASN
3	E	325	ASN
3	E	347	GLN
3	F	311	GLN
3	F	315	ASN
3	F	325	ASN
3	F	418	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

17 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	G	1	3,4	14,14,15	0.28	0	17,19,21	1.25	1 (5%)
4	NAG	G	2	4	14,14,15	0.32	0	17,19,21	0.55	0
4	BMA	G	3	4	11,11,12	0.27	0	15,15,17	0.66	1 (6%)
4	MAN	G	4	4	11,11,12	0.26	0	15,15,17	0.87	1 (6%)
4	NAG	G	5	4	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
4	GAL	G	6	4	11,11,12	0.28	0	15,15,17	0.47	0
4	MAN	G	7	4	11,11,12	0.26	0	15,15,17	0.73	1 (6%)
4	NAG	G	8	4	14,14,15	0.33	0	17,19,21	0.57	0
4	FUC	G	9	4	10,10,11	0.80	0	14,14,16	1.47	3 (21%)
5	NAG	H	1	5,3	14,14,15	0.37	0	17,19,21	1.42	1 (5%)
5	NAG	H	2	5	14,14,15	0.34	0	17,19,21	0.58	0
5	BMA	H	3	5	11,11,12	0.36	0	15,15,17	0.76	1 (6%)
5	MAN	H	4	5	11,11,12	0.33	0	15,15,17	0.84	1 (6%)
5	NAG	H	5	5	14,14,15	0.34	0	17,19,21	1.10	1 (5%)
5	GAL	H	6	5	11,11,12	0.31	0	15,15,17	0.45	0
5	MAN	H	7	5	11,11,12	0.31	0	15,15,17	0.73	1 (6%)
5	FUC	H	8	5	10,10,11	0.35	0	14,14,16	0.45	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	G	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	NAG	G	5	4	-	1/6/23/26	0/1/1/1
4	GAL	G	6	4	-	0/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1
4	NAG	G	8	4	-	0/6/23/26	0/1/1/1
4	FUC	G	9	4	-	-	0/1/1/1
5	NAG	H	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	-	0/6/23/26	0/1/1/1
5	GAL	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	1/2/19/22	0/1/1/1
5	FUC	H	8	5	-	-	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-O5-C5	5.19	119.14	112.19
4	G	1	NAG	C1-O5-C5	4.63	118.39	112.19
5	H	5	NAG	O5-C1-C2	-3.83	105.36	111.29
4	G	9	FUC	C1-O5-C5	3.63	121.54	112.97
4	G	4	MAN	C1-O5-C5	3.22	116.50	112.19
5	H	4	MAN	C1-O5-C5	2.95	116.14	112.19
4	G	7	MAN	C1-O5-C5	2.57	115.63	112.19
5	H	3	BMA	C1-O5-C5	2.56	115.61	112.19
5	H	7	MAN	C1-O5-C5	2.50	115.54	112.19
4	G	5	NAG	O5-C1-C2	-2.39	107.59	111.29
4	G	3	BMA	C1-O5-C5	2.24	115.19	112.19
4	G	9	FUC	C1-C2-C3	2.11	112.71	109.64
4	G	9	FUC	O2-C2-C1	2.06	113.94	109.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1	NAG	O5-C5-C6-O6

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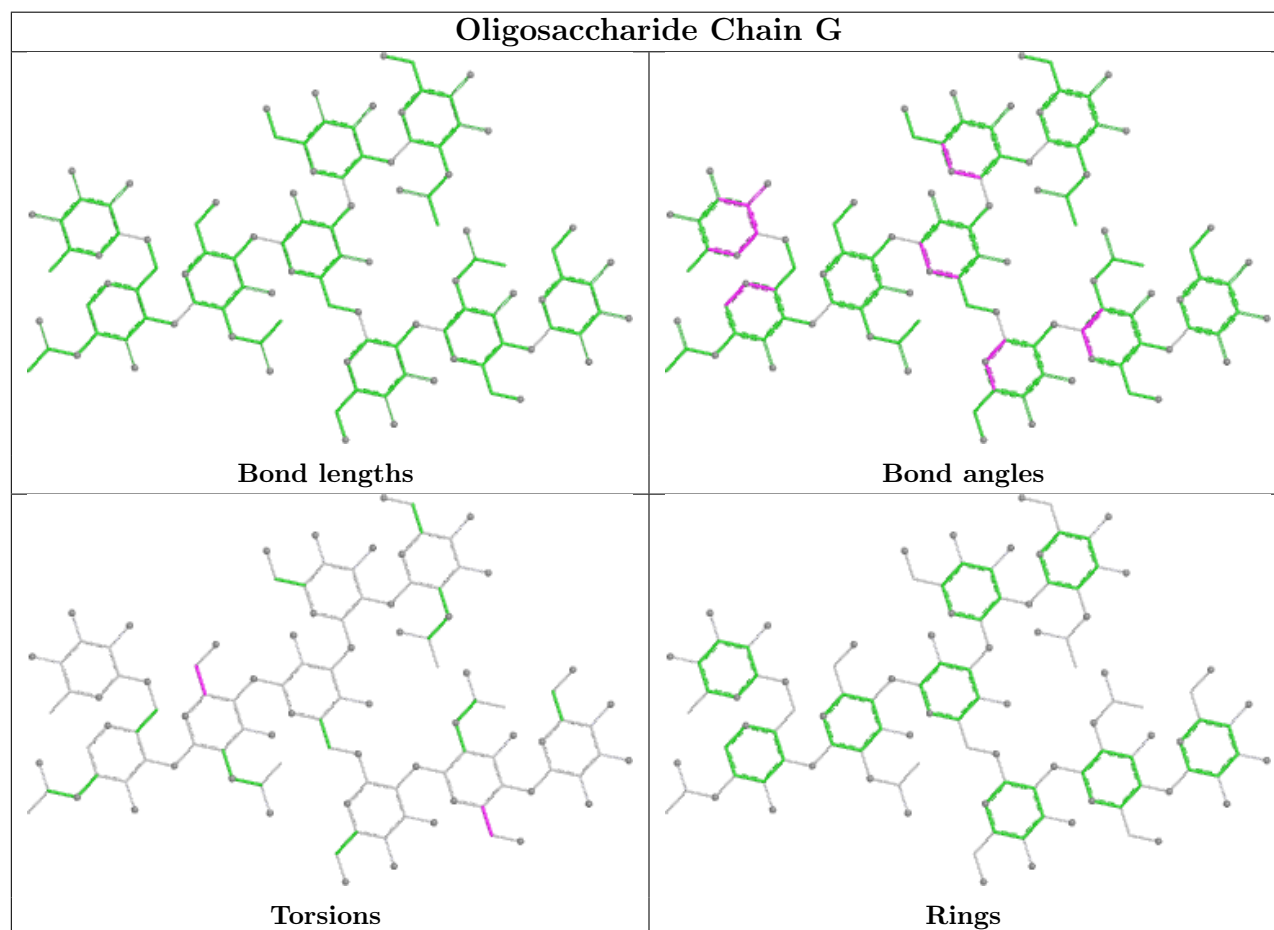
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	H	7	MAN	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	H	3	BMA	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	G	5	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

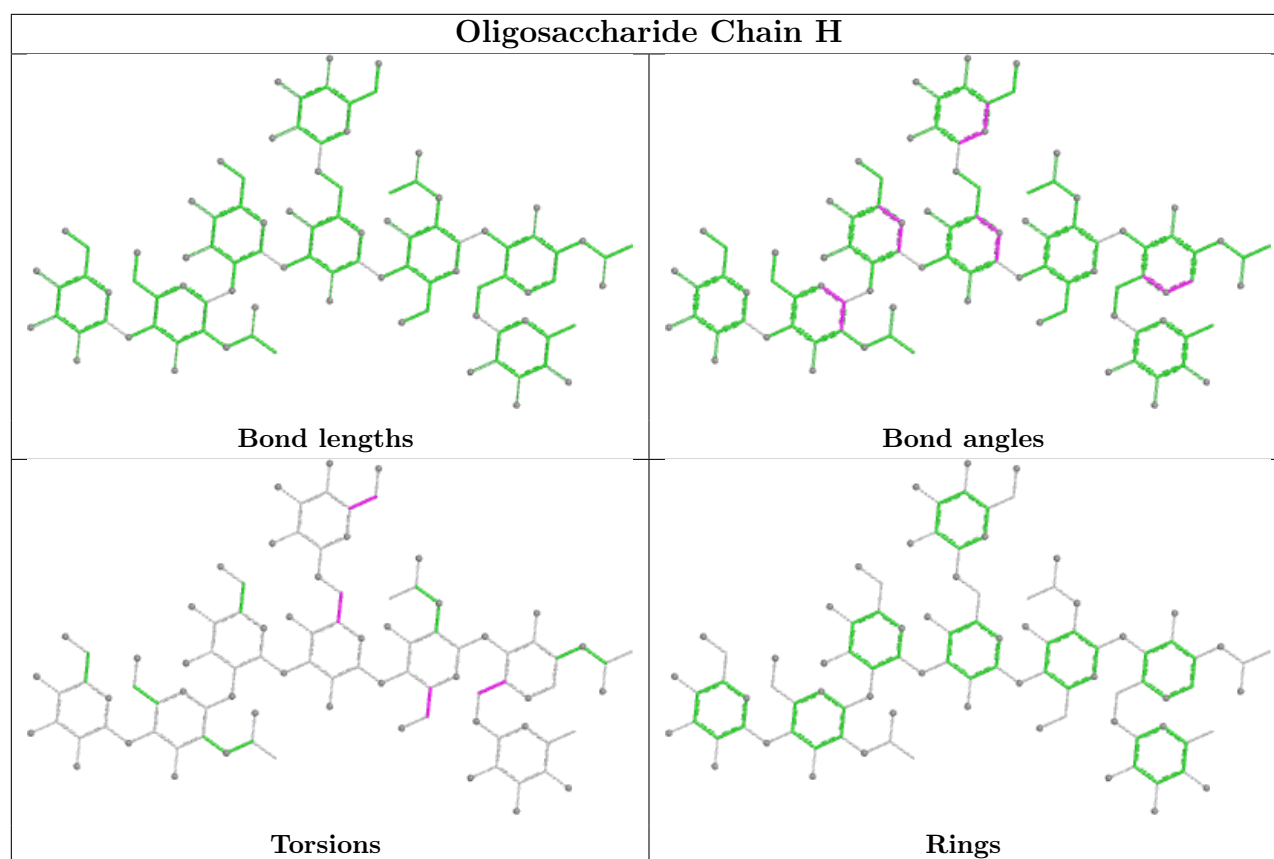
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	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 [i](#)

There are no ligands in this entry.

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	268/338 (79%)	0.21	1 (0%) 88 79	12, 37, 68, 87	1 (0%)
1	C	260/338 (76%)	1.05	32 (12%) 8 7	38, 87, 124, 145	0
2	B	99/119 (83%)	0.20	0 100 100	15, 49, 81, 90	0
2	D	98/119 (82%)	0.93	13 (13%) 7 6	48, 75, 115, 126	0
3	E	209/225 (92%)	0.47	5 (2%) 59 40	22, 50, 111, 141	0
3	F	205/225 (91%)	0.74	14 (6%) 23 16	17, 64, 131, 145	0
All	All	1139/1364 (83%)	0.60	65 (5%) 29 20	12, 58, 117, 145	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	59	TRP	4.3
3	F	298	SER	4.2
1	C	237	SER	3.9
1	C	231	ASP	3.8
1	C	48	CYS	3.7
1	C	174	LEU	3.7
1	C	32	PRO	3.6
1	C	232	GLY	3.5
1	C	173	ASN	3.4
1	C	166	HIS	3.4
1	C	58	SER	3.1
2	D	38	ASP	3.1
3	F	269	GLU	3.1
1	C	124	GLN	3.0
1	C	104	SER	3.0
1	C	230	SER	3.0
3	E	267	SER	3.0
1	C	50	ALA	3.0
1	C	33	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	213	LEU	2.9
1	C	61	TRP	2.8
2	D	26	TYR	2.8
1	C	62	GLU	2.8
1	C	121	ASP	2.8
3	E	269	GLU	2.8
3	F	327	ALA	2.7
3	F	331	PRO	2.7
1	C	226	PHE	2.7
2	D	71	THR	2.7
1	C	204	TYR	2.7
1	C	54	GLU	2.6
2	D	29	GLY	2.6
3	E	324	SER	2.6
2	D	21	ASN	2.6
3	F	294	GLU	2.6
1	C	191	PRO	2.5
3	F	444	SER	2.5
3	F	271	PRO	2.4
1	C	255	GLN	2.4
3	E	418	GLN	2.4
2	D	96	ASP	2.4
3	F	242	LEU	2.4
1	C	97	GLU	2.4
2	D	97	ARG	2.3
1	A	20	GLY	2.3
1	C	103	THR	2.3
2	D	92	ILE	2.2
3	F	238	PRO	2.2
3	F	301	ARG	2.2
2	D	33	SER	2.2
1	C	252	CYS	2.2
1	C	63	LYS	2.2
2	D	18	GLY	2.2
2	D	4	THR	2.1
3	E	303	VAL	2.1
1	C	93	LEU	2.1
2	D	20	SER	2.1
1	C	233	SER	2.1
3	F	254	THR	2.1
2	D	74	GLU	2.1
3	F	291	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	176	TRP	2.0
3	F	342	GLN	2.0
1	C	190	SER	2.0
3	F	332	ILE	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](#)

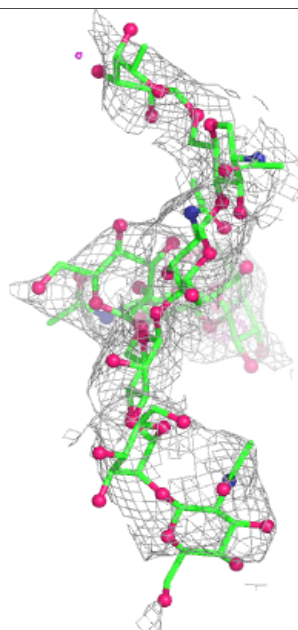
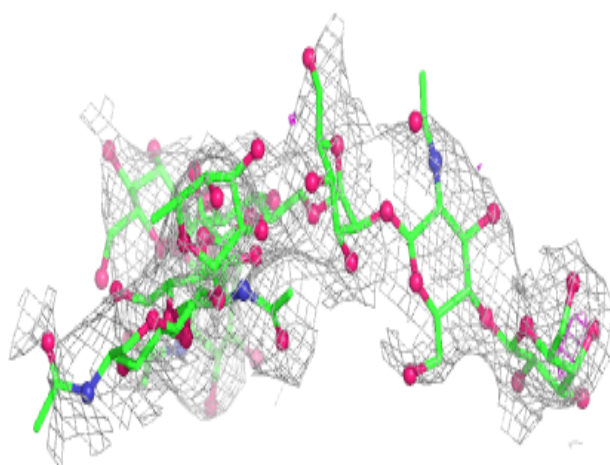
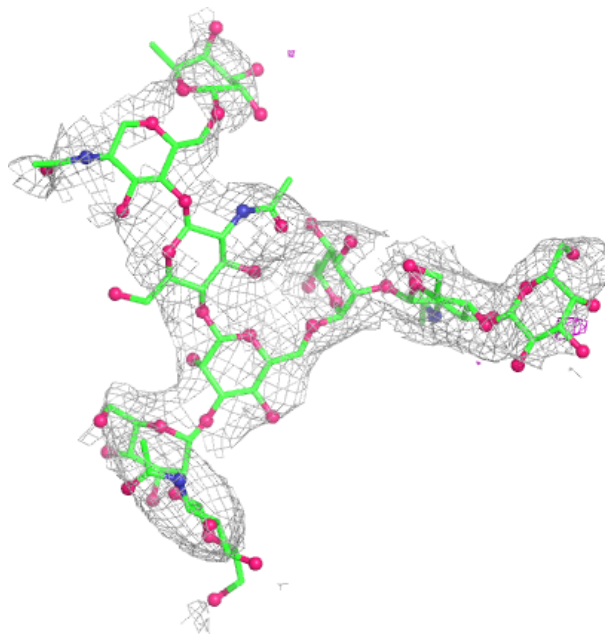
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

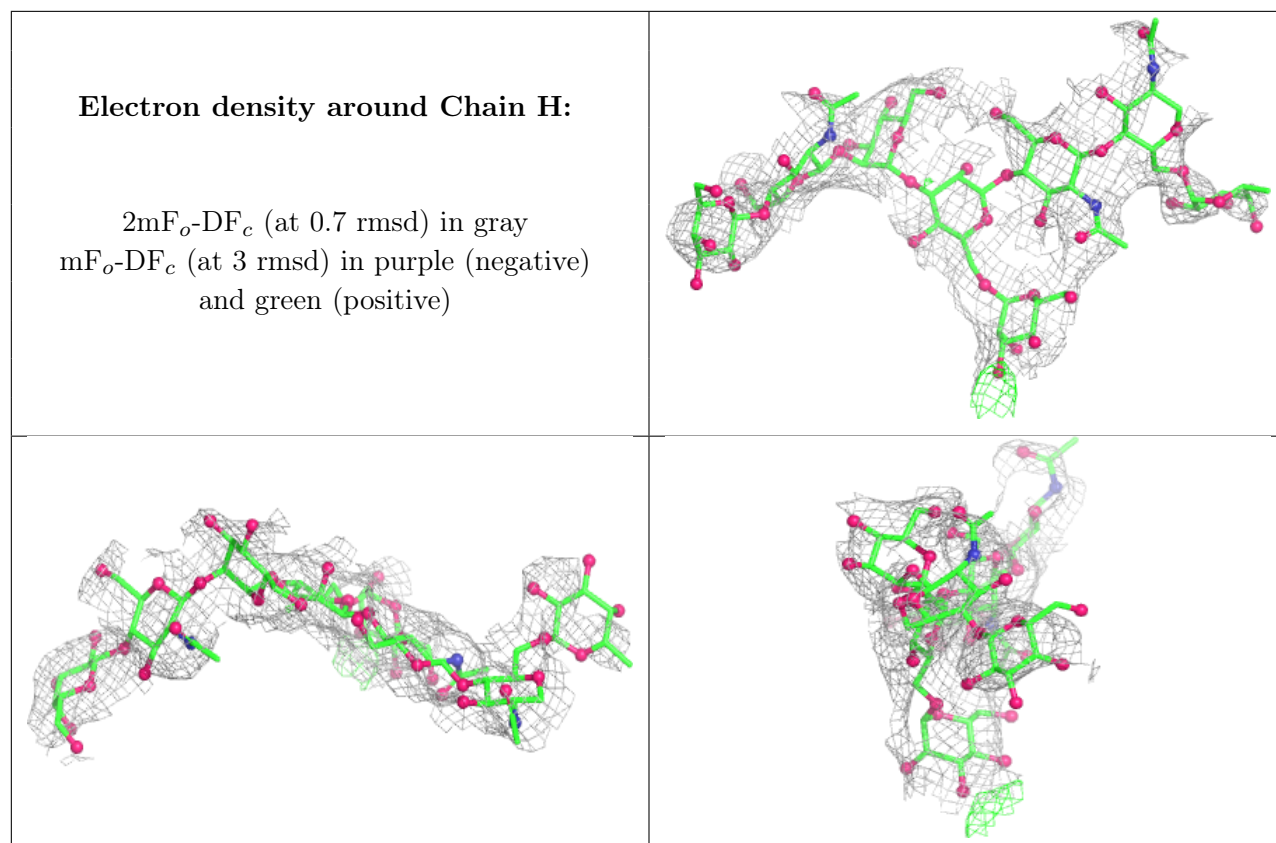
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FUC	G	9	10/11	0.47	0.28	131,137,142,146	0
5	FUC	H	8	10/11	0.48	0.31	134,139,141,143	0
5	NAG	H	5	14/15	0.61	0.20	127,129,136,137	0
5	MAN	H	7	11/12	0.63	0.21	110,113,117,117	0
4	BMA	G	3	11/12	0.63	0.18	116,118,123,124	0
4	NAG	G	8	14/15	0.67	0.19	117,120,127,128	0
5	GAL	H	6	11/12	0.70	0.25	125,128,132,134	0
4	MAN	G	7	11/12	0.71	0.17	123,126,132,132	0
4	NAG	G	1	14/15	0.74	0.14	129,134,144,145	0
5	NAG	H	2	14/15	0.75	0.18	123,127,132,132	0
4	MAN	G	4	11/12	0.77	0.17	114,118,120,122	0
5	MAN	H	4	11/12	0.80	0.10	127,130,136,136	0
5	BMA	H	3	11/12	0.81	0.16	115,120,125,126	0
5	NAG	H	1	14/15	0.83	0.14	132,139,149,151	0
4	NAG	G	5	14/15	0.86	0.20	109,111,113,115	0
4	NAG	G	2	14/15	0.87	0.14	120,124,128,132	0
4	GAL	G	6	11/12	0.88	0.24	106,108,111,111	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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.