



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:12 PM BST

PDB ID : 6VFU
Title : Crystal structure of human protocadherin 19 EC1-EC4
Authors : Harrison, O.J.; Brasch, J.; Shapiro, L.
Deposited on : 2020-01-06
Resolution : 3.50 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 : 2.13.1
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) : 2.13.1

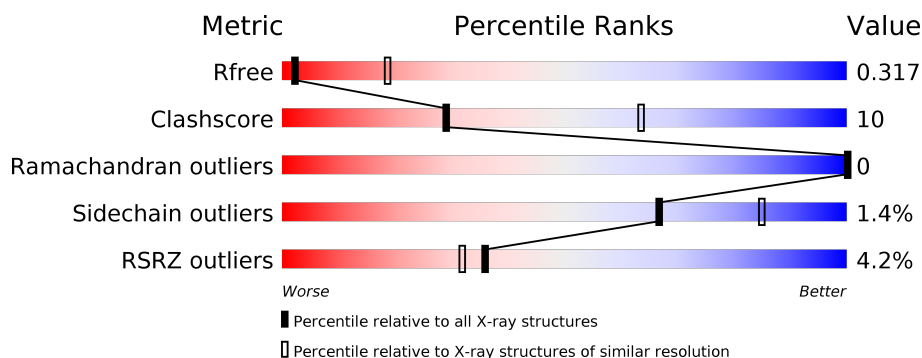
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	430	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>27%</div> </div> </div>
1	B	430	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div></div> </div> </div>
1	C	430	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>17%</div> </div> </div>
2	D	4	<div> <div></div> <div> <div>25%</div> <div>25%</div> <div>50%</div> </div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
4	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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
6	NAG	A	512	-	-	-	X
8	CL	A	515	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19193 atoms, of which 9270 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.

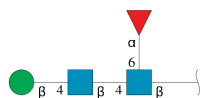
- Molecule 1 is a protein called Protocadherin-19.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	428	Total	C	H	N	O	S	0	0	0
			6365	2049	3073	569	666	8			
1	A	428	Total	C	H	N	O	S	0	0	0
			6402	2049	3110	569	666	8			
1	B	411	Total	C	H	N	O	S	0	1	0
			6173	1969	3017	539	640	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	expression tag	UNP Q8TAB3
C	426	HIS	-	expression tag	UNP Q8TAB3
C	427	HIS	-	expression tag	UNP Q8TAB3
C	428	HIS	-	expression tag	UNP Q8TAB3
C	429	HIS	-	expression tag	UNP Q8TAB3
C	430	HIS	-	expression tag	UNP Q8TAB3
A	425	HIS	-	expression tag	UNP Q8TAB3
A	426	HIS	-	expression tag	UNP Q8TAB3
A	427	HIS	-	expression tag	UNP Q8TAB3
A	428	HIS	-	expression tag	UNP Q8TAB3
A	429	HIS	-	expression tag	UNP Q8TAB3
A	430	HIS	-	expression tag	UNP Q8TAB3
B	425	HIS	-	expression tag	UNP Q8TAB3
B	426	HIS	-	expression tag	UNP Q8TAB3
B	427	HIS	-	expression tag	UNP Q8TAB3
B	428	HIS	-	expression tag	UNP Q8TAB3
B	429	HIS	-	expression tag	UNP Q8TAB3
B	430	HIS	-	expression tag	UNP Q8TAB3

- Molecule 2 is an oligosaccharide called 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
2	D	4	Total	C	H	N	O	0	0	0
			84	28	35	2	19			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	9	Total	Ca	0	0
			9	9		
5	A	9	Total	Ca	0	0
			9	9		
5	C	9	Total	Ca	0	0
			9	9		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O		0	0
			14	8	1	5			
6	A	1	Total	C	N	O		0	0
			14	8	1	5			
6	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ni	0	0
			1	1		
7	C	1	Total	Ni	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Cl	0	0
			2	2		
8	C	2	Total	Cl	0	0
			2	2		

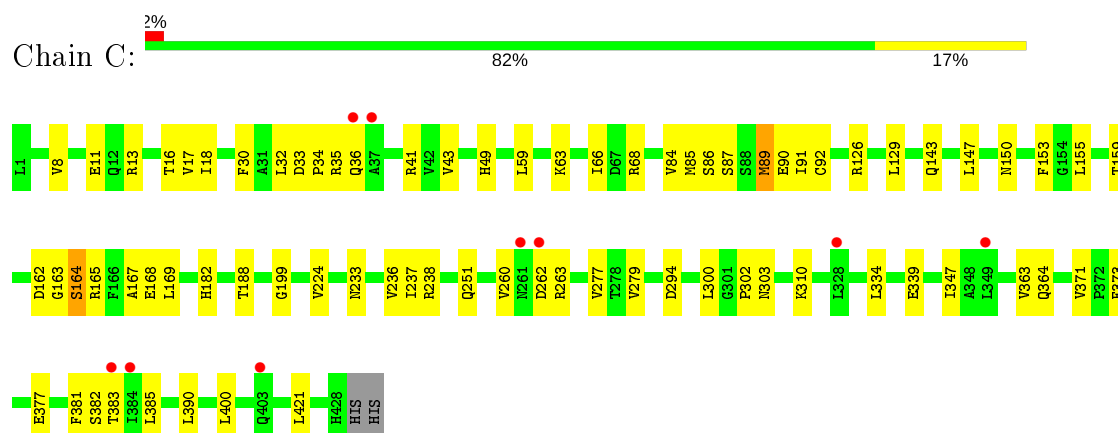
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	4	Total 4	O 4	0	0
9	A	2	Total 2	O 2	0	0
9	B	1	Total 1	O 1	0	0

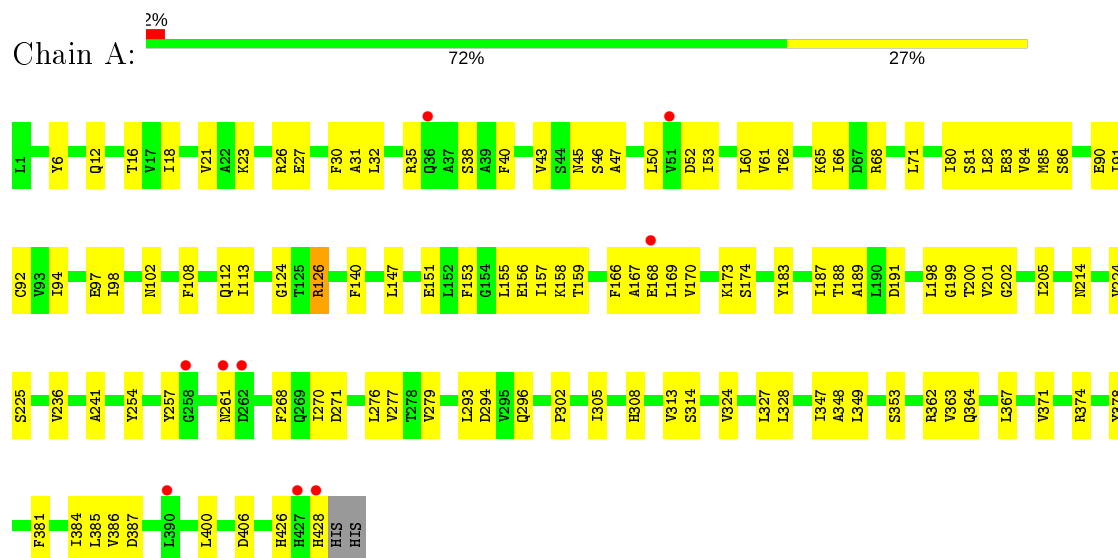
3 Residue-property plots

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

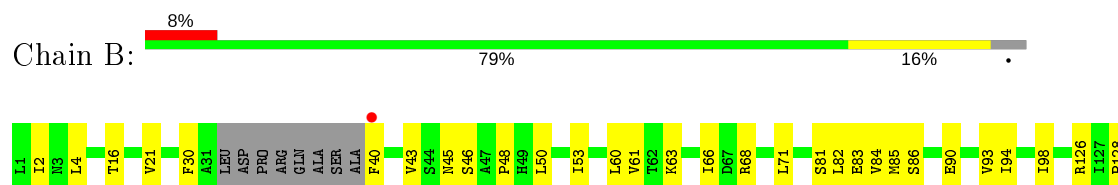
• Molecule 1: Protocadherin-19

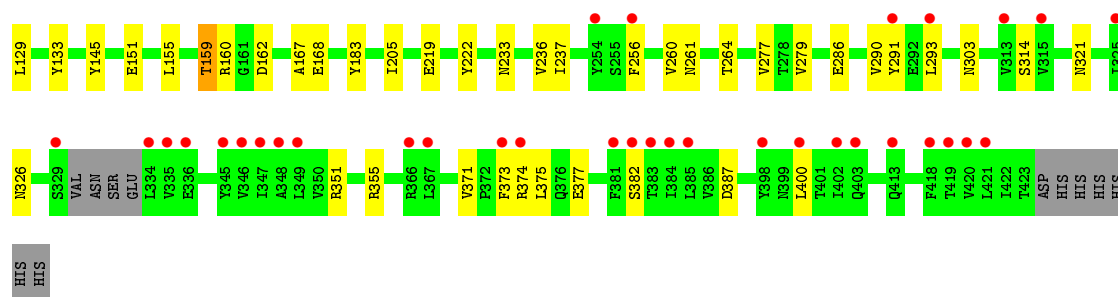


• Molecule 1: Protocadherin-19



• Molecule 1: Protocadherin-19





- Molecule 2: 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

Chain D: 25% 25% 50%



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

Chain E: 100%



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

Chain F: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.97Å 108.97Å 309.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.50 37.53 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-3.50) 88.3 (37.53-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.265 , 0.291 0.276 , 0.317	Depositor DCC
R_{free} test set	1387 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	123.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19193	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: NI, BMA, NAG, CL, CA, FUC

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	0.33	0/3354	0.55	0/4569
1	B	0.31	0/3214	0.53	0/4374
1	C	0.28	0/3354	0.52	0/4569
All	All	0.30	0/9922	0.53	0/13512

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

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	3292	3110	3216	90	1
1	B	3156	3017	3096	46	1
1	C	3292	3073	3216	53	0
2	D	49	35	43	2	0
3	E	24	22	22	0	0
4	F	28	0	25	4	0
5	A	9	0	0	0	0
5	B	9	0	0	0	0
5	C	9	0	0	0	0
6	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	13	13	2	0
6	C	14	0	13	2	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	2	0	0	0	0
8	C	2	0	0	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
9	C	4	0	0	0	0
All	All	9923	9270	9657	187	2

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 10.

All (187) 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)
4:F:1:NAG:H3	4:F:1:NAG:H83	1.50	0.93
1:A:31:ALA:HB3	1:A:86:SER:OG	1.70	0.91
1:A:31:ALA:HB3	1:A:86:SER:HG	1.48	0.76
1:B:126:ARG:HD3	1:B:168:GLU:OE2	1.92	0.69
6:B:510:NAG:O3	6:B:510:NAG:O7	2.10	0.67
4:F:1:NAG:H3	4:F:1:NAG:C8	2.25	0.67
1:B:53:ILE:HG12	1:B:60:LEU:HD23	1.76	0.65
1:B:46:SER:N	1:B:81:SER:O	2.27	0.64
1:C:182:HIS:NE2	1:B:151:GLU:OE2	2.33	0.62
1:C:238:ARG:HH12	6:C:514:NAG:H81	1.65	0.61
1:A:66:ILE:HG21	1:A:98:ILE:HD13	1.83	0.60
1:B:236:VAL:HB	1:B:277:VAL:O	2.01	0.60
1:C:8:VAL:HG11	1:C:18:ILE:HG12	1.83	0.60
1:C:339:GLU:HG3	1:C:390:LEU:O	2.03	0.59
1:A:112:GLN:HA	1:A:202:GLY:O	2.03	0.58
1:B:21:VAL:HG13	1:B:60:LEU:HG	1.85	0.58
1:C:294:ASP:OD2	1:C:310:LYS:NZ	2.34	0.58
1:A:45:ASN:HB3	1:A:82:LEU:HG	1.86	0.58
1:A:84:VAL:HG22	1:A:92:CYS:O	2.05	0.56
1:A:45:ASN:CB	1:A:82:LEU:HG	2.36	0.56
1:A:53:ILE:HD12	1:A:82:LEU:HD23	1.86	0.56
1:A:126:ARG:NE	1:A:168:GLU:OE2	2.39	0.56
1:A:188:THR:HA	1:A:199:GLY:O	2.06	0.55
1:A:102:ASN:HB2	1:A:140:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HB3	1:A:32:LEU:HD22	1.89	0.55
6:B:510:NAG:C7	6:B:510:NAG:HO3	2.15	0.55
1:B:128:PRO:HA	1:B:168:GLU:HB3	1.89	0.54
1:C:371:VAL:HG21	1:C:400:LEU:CD2	2.38	0.54
1:B:374:ARG:NE	1:B:387:ASP:OD2	2.39	0.54
1:C:11:GLU:N	1:C:66:ILE:O	2.36	0.54
1:C:30:PHE:HD2	1:C:32:LEU:HB2	1.73	0.54
1:C:233:ASN:N	1:C:279:VAL:O	2.41	0.54
1:A:241:ALA:N	1:A:254:TYR:OH	2.32	0.53
1:B:290:VAL:HG12	1:B:314:SER:HA	1.90	0.53
1:C:236:VAL:HB	1:C:277:VAL:O	2.07	0.53
1:A:23:LYS:O	1:A:26:ARG:HG2	2.09	0.53
1:A:189:ALA:O	1:A:198:LEU:HA	2.09	0.52
1:C:238:ARG:NH1	6:C:514:NAG:H81	2.24	0.52
1:C:262:ASP:OD1	1:C:263:ARG:N	2.43	0.52
1:B:86:SER:N	1:B:90:GLU:O	2.42	0.52
1:A:53:ILE:HD12	1:A:82:LEU:CD2	2.40	0.52
1:C:302:PRO:HG3	1:A:302:PRO:HG2	1.91	0.52
1:A:371:VAL:HG21	1:A:400:LEU:CD2	2.40	0.51
1:C:143:GLN:O	1:C:165:ARG:NH1	2.44	0.51
1:B:50:LEU:O	1:B:63:LYS:N	2.41	0.51
1:B:30:PHE:CE1	1:B:86:SER:HB2	2.45	0.51
1:C:86:SER:HB3	1:C:90:GLU:HB3	1.92	0.51
4:F:1:NAG:H82	4:F:1:NAG:C1	2.41	0.51
1:C:188:THR:HA	1:C:199:GLY:O	2.12	0.50
1:B:387:ASP:OD1	1:B:387:ASP:O	2.29	0.50
1:C:43:VAL:HG13	1:A:328:LEU:HD12	1.94	0.50
1:B:256:PHE:CE1	1:B:293:LEU:HB3	2.47	0.50
1:A:268:PHE:CD1	1:A:293:LEU:HD21	2.46	0.50
4:F:1:NAG:C3	4:F:1:NAG:H83	2.34	0.49
1:A:378:TYR:HB2	1:A:381:PHE:O	2.12	0.49
1:C:150:ASN:HD21	1:C:153:PHE:HB2	1.77	0.49
1:C:251:GLN:HB3	1:C:300:LEU:HD12	1.95	0.49
1:C:153:PHE:HB3	1:C:169:LEU:HD11	1.94	0.49
1:A:126:ARG:HD2	1:A:170:VAL:HG22	1.95	0.49
1:C:381:PHE:CE2	1:A:91:ILE:HD13	2.48	0.49
1:A:147:LEU:HD23	1:A:155:LEU:HG	1.95	0.49
1:A:157:ILE:N	1:A:157:ILE:HD12	2.27	0.49
1:A:374:ARG:HG2	1:A:387:ASP:HB2	1.93	0.49
1:A:47:ALA:CB	1:A:50:LEU:HD12	2.43	0.49
1:B:50:LEU:CD2	1:B:71:LEU:HD11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PHE:CZ	1:B:84:VAL:HG21	2.48	0.49
1:C:49:HIS:HA	1:C:63:LYS:HD3	1.94	0.49
1:A:21:VAL:HG21	1:A:53:ILE:HG12	1.95	0.48
1:B:129:LEU:HB2	1:B:167:ALA:O	2.13	0.48
1:B:43:VAL:HG11	1:B:85:MET:HB2	1.95	0.48
1:A:153:PHE:HB3	1:A:169:LEU:HD11	1.95	0.48
1:C:260:VAL:O	1:C:260:VAL:HG12	2.13	0.48
1:A:214:ASN:CG	1:A:305:ILE:HB	2.34	0.48
1:A:84:VAL:O	1:A:91:ILE:HG13	2.14	0.48
1:C:126:ARG:NH1	1:C:168:GLU:OE2	2.46	0.48
1:C:129:LEU:HB2	1:C:167:ALA:O	2.14	0.48
1:C:377:GLU:HA	1:C:382:SER:HA	1.96	0.48
1:B:145:TYR:HB2	1:B:155:LEU:HD21	1.95	0.48
1:C:86:SER:N	1:C:90:GLU:O	2.44	0.47
1:A:367:LEU:HD12	1:A:367:LEU:O	2.15	0.47
1:C:163:GLY:O	1:C:164:SER:C	2.52	0.47
1:B:83:GLU:HG2	1:B:93:VAL:HG22	1.97	0.47
1:A:225:SER:HA	1:A:314:SER:O	2.14	0.47
1:A:183:TYR:HB2	1:A:205:ILE:HB	1.96	0.47
1:A:16:THR:O	1:A:61:VAL:HA	2.14	0.47
1:A:270:ILE:HG13	1:A:277:VAL:HG22	1.97	0.46
1:A:43:VAL:N	1:A:83:GLU:O	2.43	0.46
1:C:33:ASP:HB3	1:C:35:ARG:HG3	1.97	0.46
2:D:2:NAG:O7	2:D:2:NAG:H3	2.16	0.46
1:B:377:GLU:HA	1:B:382:SER:HA	1.98	0.46
1:B:43:VAL:CG1	1:B:85:MET:HB2	2.46	0.46
1:A:158:LYS:HB2	1:A:166:PHE:CE2	2.51	0.46
1:A:159:THR:O	1:A:159:THR:HG23	2.16	0.46
1:B:183:TYR:HB2	1:B:205:ILE:HB	1.97	0.45
1:C:347:ILE:CD1	1:C:373:PHE:CD1	2.99	0.45
1:A:108:PHE:HB2	1:A:201:VAL:CG1	2.46	0.45
1:A:80:ILE:HG22	1:A:82:LEU:CD1	2.47	0.45
1:B:264:THR:HG22	1:B:291:TYR:HD1	1.82	0.45
1:B:373:PHE:CD2	1:B:400:LEU:HD21	2.52	0.45
1:C:310:LYS:HE3	1:A:166:PHE:CE1	2.51	0.45
1:A:26:ARG:CB	1:A:32:LEU:HD22	2.46	0.45
1:B:40:PHE:HZ	1:B:84:VAL:HG21	1.80	0.45
1:C:35:ARG:HD2	1:C:87:SER:OG	2.17	0.45
1:A:151:GLU:N	1:A:151:GLU:OE1	2.50	0.45
1:C:89:MET:CE	1:A:348:ALA:HA	2.47	0.45
1:A:50:LEU:CD1	1:A:71:LEU:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:O	1:C:16:THR:OG1	2.31	0.45
1:A:108:PHE:CB	1:A:201:VAL:HG11	2.47	0.45
1:A:236:VAL:CG2	1:A:279:VAL:HG23	2.47	0.45
1:C:147:LEU:HD23	1:C:155:LEU:HB2	1.99	0.45
2:D:4:FUC:C1	2:D:4:FUC:O4	2.64	0.45
1:A:347:ILE:HD11	1:A:386:VAL:HG12	1.98	0.45
1:B:260:VAL:HG22	1:B:261:ASN:H	1.81	0.45
1:B:45:ASN:HD21	1:B:48:PRO:HA	1.81	0.44
1:A:30:PHE:CE2	1:A:86:SER:HB2	2.52	0.44
1:A:18:ILE:HD11	1:A:62:THR:HG22	1.99	0.44
1:A:271:ASP:HB3	1:A:276:LEU:H	1.83	0.44
1:A:46:SER:HB3	1:A:80:ILE:HG23	1.99	0.44
1:C:89:MET:SD	1:C:89:MET:N	2.90	0.44
1:B:375:LEU:O	1:B:375:LEU:HD23	2.18	0.44
1:B:45:ASN:HA	1:B:82:LEU:HA	1.99	0.44
1:A:108:PHE:HB2	1:A:201:VAL:HG13	2.00	0.44
1:C:36:GLN:HG3	1:C:36:GLN:O	2.18	0.44
1:A:126:ARG:NH2	1:A:158:LYS:HE2	2.33	0.44
1:C:33:ASP:OD1	1:C:34:PRO:HD2	2.17	0.43
1:C:41:ARG:NH2	1:A:328:LEU:HB3	2.33	0.43
1:A:384:ILE:C	1:A:385:LEU:HD12	2.39	0.43
1:A:6:TYR:O	1:A:97:GLU:HG2	2.17	0.43
1:A:257:TYR:O	1:A:294:ASP:HB2	2.17	0.43
1:C:334:LEU:HD21	1:C:421:LEU:HD23	2.00	0.43
1:C:43:VAL:CG2	1:C:85:MET:HB2	2.48	0.43
1:A:86:SER:N	1:A:90:GLU:O	2.46	0.43
1:B:233:ASN:N	1:B:279:VAL:O	2.51	0.43
1:C:363:VAL:HG12	1:C:364:GLN:N	2.33	0.43
1:A:324:VAL:CG1	1:A:353:SER:OG	2.67	0.43
1:A:50:LEU:HD22	1:A:66:ILE:HG12	2.01	0.43
1:C:224:VAL:HG21	1:C:237:ILE:HB	2.01	0.42
1:A:126:ARG:CD	1:A:168:GLU:OE2	2.67	0.42
1:C:182:HIS:CD2	1:B:151:GLU:OE2	2.72	0.42
1:A:113:ILE:N	1:A:202:GLY:O	2.48	0.42
1:A:108:PHE:HB3	1:A:201:VAL:HG11	2.00	0.42
1:A:124:GLY:O	1:A:126:ARG:HG2	2.19	0.42
1:A:188:THR:HG22	1:A:200:THR:HG23	2.02	0.42
1:A:224:VAL:HG12	1:A:225:SER:N	2.35	0.42
1:C:91:ILE:HD11	1:A:381:PHE:CE2	2.55	0.42
1:B:236:VAL:HG12	1:B:237:ILE:HG22	1.99	0.42
1:B:126:ARG:CD	1:B:168:GLU:OE2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:PHE:CD2	1:C:400:LEU:HD21	2.55	0.42
1:A:81:SER:HA	1:A:94:ILE:O	2.20	0.42
1:A:362:ARG:O	1:A:406:ASP:HA	2.20	0.41
1:C:85:MET:SD	1:A:349:LEU:HD12	2.61	0.41
1:B:159:THR:O	1:B:159:THR:OG1	2.35	0.41
1:C:383:THR:HG23	1:C:385:LEU:HD13	2.02	0.41
1:A:173:LYS:HG2	1:A:174:SER:N	2.35	0.41
1:B:321:ASN:OD1	1:B:355:ARG:HD3	2.20	0.41
1:B:53:ILE:HD12	1:B:84:VAL:HG11	2.02	0.41
1:B:2:ILE:HD11	1:B:90:GLU:OE2	2.20	0.41
1:C:30:PHE:CD2	1:C:32:LEU:HB2	2.52	0.41
1:C:17:VAL:HG13	1:C:59:LEU:HD21	2.02	0.41
1:A:26:ARG:HG3	1:A:27:GLU:N	2.35	0.41
1:B:219:GLU:H	1:B:222:TYR:HH	1.68	0.41
1:B:371:VAL:HG21	1:B:400:LEU:CD2	2.50	0.41
1:C:43:VAL:HG22	1:C:85:MET:HB2	2.02	0.41
1:A:296:GLN:HB3	1:A:308:HIS:HD2	1.86	0.41
1:C:84:VAL:HG22	1:C:92:CYS:O	2.21	0.41
1:A:12:GLN:O	1:A:65:LYS:HG2	2.21	0.41
1:B:326:ASN:HD22	1:B:351:ARG:NH2	2.19	0.41
1:A:294:ASP:N	1:A:294:ASP:OD1	2.52	0.41
1:B:286:GLU:HG2	1:B:355:ARG:HE	1.85	0.41
1:B:66:ILE:HG21	1:B:98:ILE:HD13	2.03	0.41
1:A:293:LEU:HD11	1:A:313:VAL:HG21	2.03	0.41
1:A:18:ILE:HB	1:A:60:LEU:HG	2.02	0.41
1:B:4:LEU:O	1:B:94:ILE:HA	2.21	0.41
1:A:108:PHE:CB	1:A:201:VAL:CG1	2.99	0.41
1:A:102:ASN:ND2	1:A:191:ASP:OD2	2.47	0.41
1:A:187:ILE:CG2	1:A:201:VAL:HG23	2.51	0.41
1:A:35:ARG:NE	1:A:38:SER:OG	2.54	0.41
1:A:112:GLN:CA	1:A:202:GLY:O	2.68	0.40
1:A:40:PHE:HA	1:A:85:MET:O	2.22	0.40
1:A:268:PHE:CE1	1:A:293:LEU:HD21	2.56	0.40
1:A:327:LEU:O	1:A:327:LEU:HD12	2.22	0.40
1:B:16:THR:O	1:B:61:VAL:HA	2.22	0.40
1:A:363:VAL:HG12	1:A:364:GLN:N	2.36	0.40
1:B:30:PHE:CZ	1:B:40:PHE:HD1	2.39	0.40
1:C:373:PHE:HD2	1:C:400:LEU:HD21	1.87	0.40
1:A:156:GLU:O	1:A:167:ALA:HA	2.22	0.40
1:A:296:GLN:HB3	1:A:308:HIS:CD2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:OD1	1:A:261:ASN:ND2[3_455]	2.08	0.12
1:B:63:LYS:O	1:B:133:TYR:HH[6_554]	1.60	0.00

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	426/430 (99%)	407 (96%)	19 (4%)	0	100	100
1	B	406/430 (94%)	392 (97%)	14 (3%)	0	100	100
1	C	426/430 (99%)	407 (96%)	19 (4%)	0	100	100
All	All	1258/1290 (98%)	1206 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	375/377 (100%)	371 (99%)	4 (1%)	73	88
1	B	360/377 (96%)	355 (99%)	5 (1%)	67	85
1	C	375/377 (100%)	369 (98%)	6 (2%)	62	83
All	All	1110/1131 (98%)	1095 (99%)	15 (1%)	67	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	68	ARG
1	C	89	MET
1	C	159	THR
1	C	162	ASP
1	C	164	SER
1	C	303	ASN
1	A	68	ARG
1	A	126	ARG
1	A	426	HIS
1	A	428	HIS
1	B	68	ARG
1	B	159	THR
1	B	160	ARG
1	B	162	ASP
1	B	303	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	426	HIS
1	B	182	HIS
1	B	413	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 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	D	1	1,2	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
2	NAG	D	2	2	14,14,15	0.55	0	17,19,21	0.69	1 (5%)
2	BMA	D	3	2	11,11,12	0.56	0	15,15,17	0.70	0
2	FUC	D	4	2	10,10,11	1.45	2 (20%)	14,14,16	1.47	2 (14%)
3	NAG	E	1	1,3	14,14,15	0.33	0	17,19,21	0.48	0
3	FUC	E	2	3	10,10,11	0.74	0	14,14,16	0.76	0
4	NAG	F	1	1,4	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
4	NAG	F	2	4	14,14,15	0.38	0	17,19,21	0.38	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	FUC	C4-C3	2.42	1.58	1.52
2	D	4	FUC	O5-C1	-2.20	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	FUC	O5-C5-C6	-3.71	99.34	107.33
2	D	1	NAG	C1-O5-C5	2.60	115.72	112.19
4	F	1	NAG	C1-O5-C5	2.36	115.39	112.19
2	D	4	FUC	O2-C2-C1	2.26	113.78	109.15
2	D	2	NAG	C1-O5-C5	2.14	115.08	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

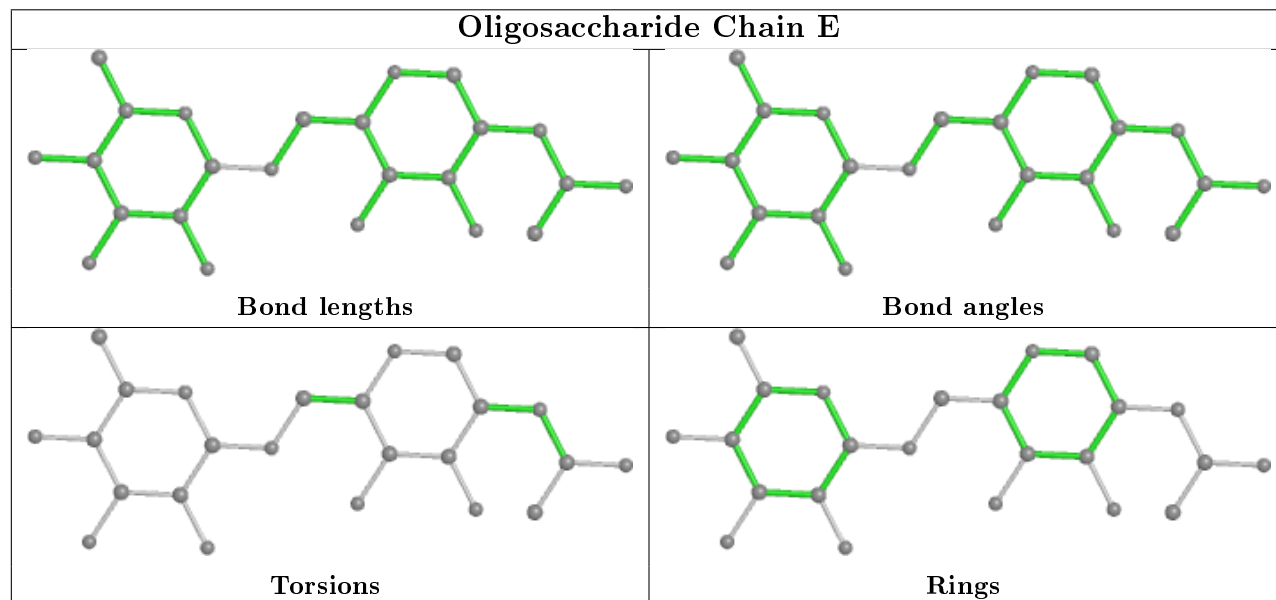
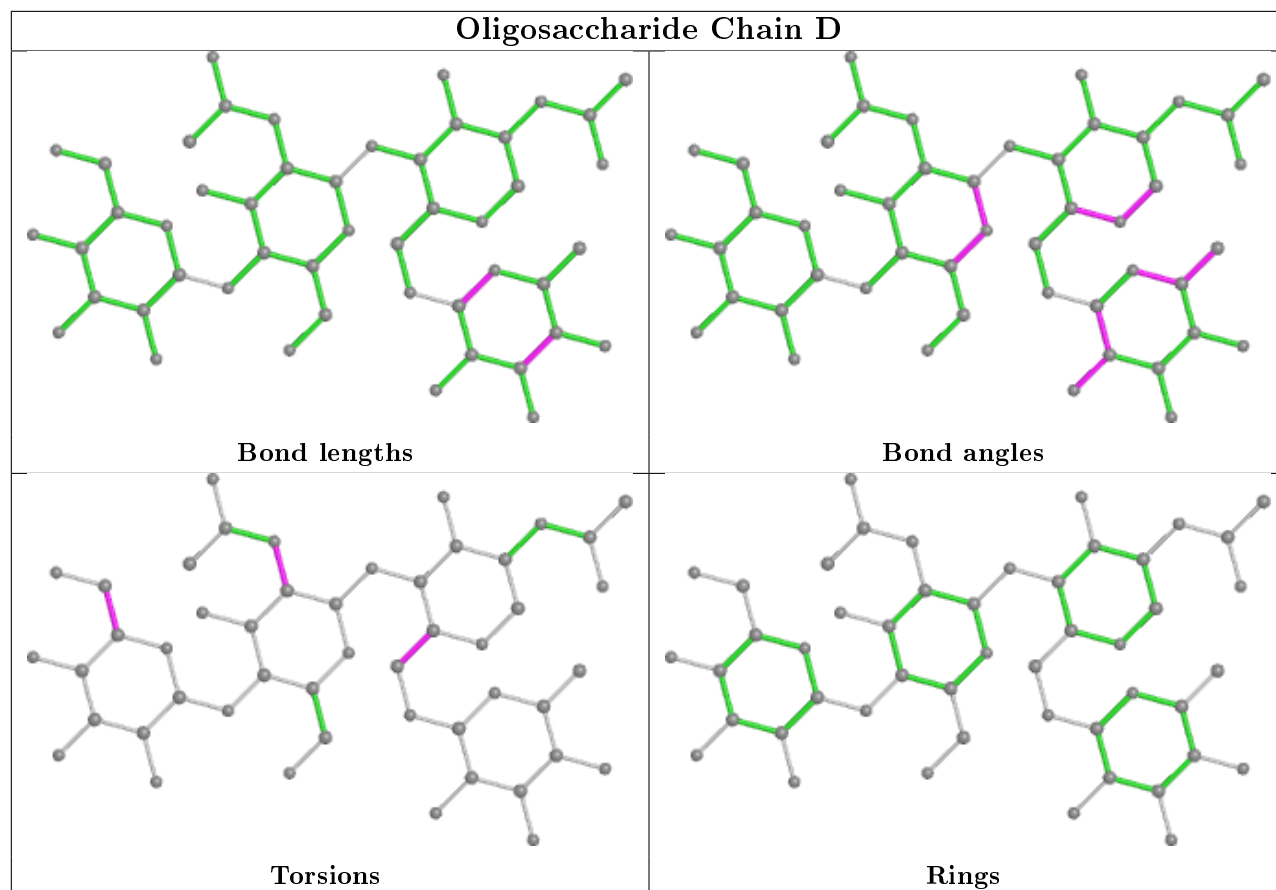
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
2	D	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7

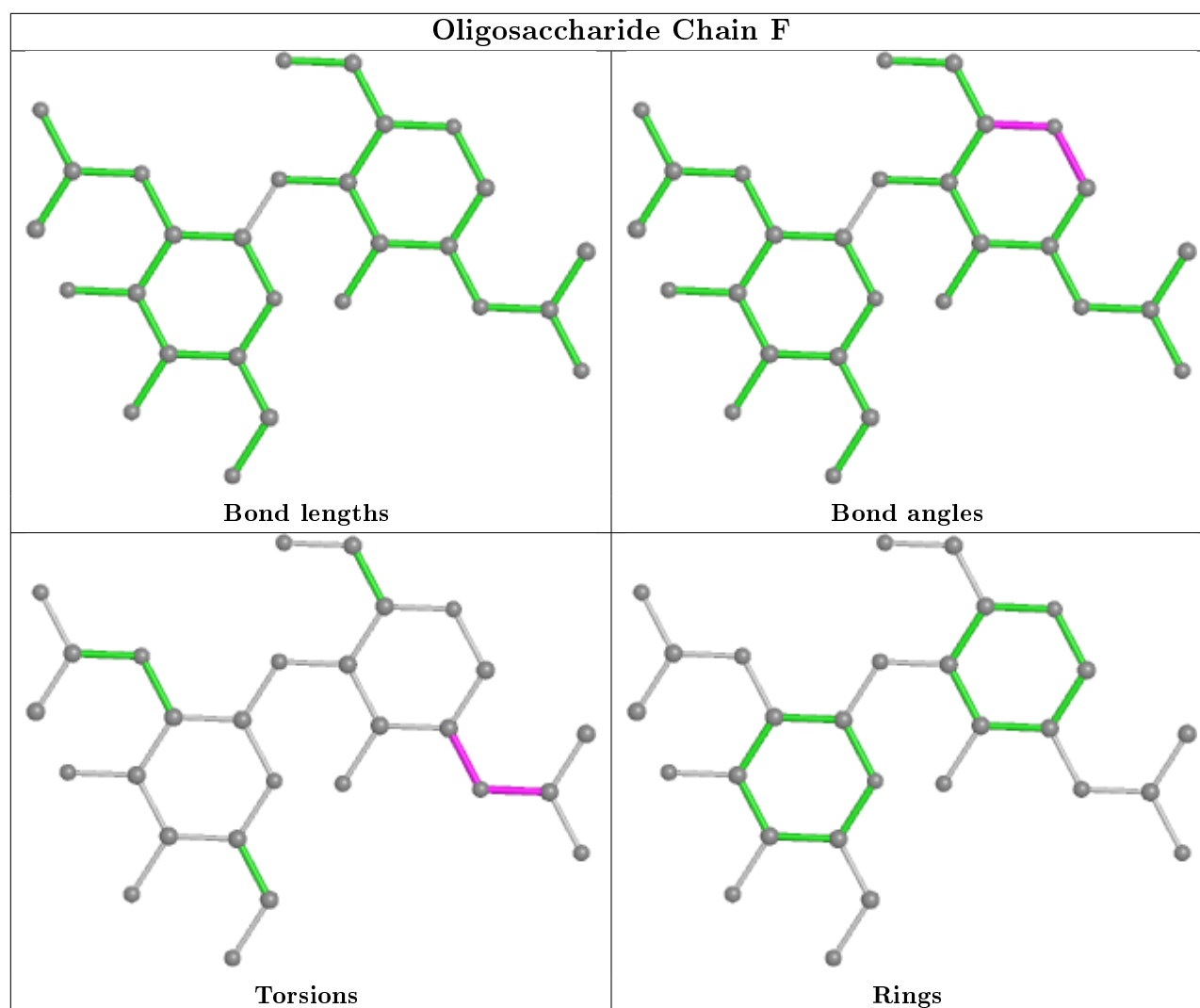
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	4	0
2	D	2	NAG	1	0
2	D	4	FUC	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](#)

Of 36 ligands modelled in this entry, 33 are monoatomic - leaving 3 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	$\# Z > 2$
6	NAG	C	514	1	14,14,15	0.37	0	17,19,21	0.53	0
6	NAG	B	510	1	14,14,15	0.43	0	17,19,21	0.39	0
6	NAG	A	512	1	14,14,15	0.39	0	17,19,21	0.44	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
6	NAG	C	514	1	-	0/6/23/26	0/1/1/1
6	NAG	B	510	1	-	2/6/23/26	0/1/1/1
6	NAG	A	512	1	-	0/6/23/26	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
6	B	510	NAG	C1-C2-N2-C7
6	B	510	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	514	NAG	2	0
6	B	510	NAG	2	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	428/430 (99%)	-0.05	9 (2%) 63 58	134, 162, 217, 285	0
1	B	411/430 (95%)	0.26	35 (8%) 10 11	115, 192, 275, 357	0
1	C	428/430 (99%)	-0.12	9 (2%) 63 58	111, 163, 224, 293	0
All	All	1267/1290 (98%)	0.03	53 (4%) 36 32	111, 167, 252, 357	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	VAL	13.0
1	B	348	ALA	9.6
1	B	419	THR	6.7
1	B	334	LEU	6.7
1	B	383	THR	6.6
1	A	36	GLN	6.4
1	B	367	LEU	6.4
1	B	418	PHE	6.2
1	B	398	TYR	5.9
1	B	335	VAL	5.6
1	A	427	HIS	5.0
1	B	325	ILE	4.7
1	B	315	VAL	4.7
1	B	421	LEU	4.5
1	B	384	ILE	4.5
1	B	347	ILE	4.3
1	B	345	TYR	4.2
1	A	262	ASP	4.2
1	A	428	HIS	4.0
1	C	37	ALA	3.9
1	C	36	GLN	3.8
1	B	382	SER	3.6
1	A	390	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	373	PHE	3.4
1	B	366	ARG	3.4
1	B	313	VAL	3.2
1	C	383	THR	3.2
1	A	258	GLY	3.2
1	B	413	GLN	3.2
1	B	349	LEU	3.2
1	B	40	PHE	3.0
1	C	384	ILE	2.9
1	B	346	VAL	2.9
1	C	349	LEU	2.9
1	C	262	ASP	2.8
1	B	385	LEU	2.7
1	C	261	ASN	2.7
1	B	336	GLU	2.6
1	B	403	GLN	2.6
1	B	256	PHE	2.5
1	B	374	ARG	2.4
1	B	254	TYR	2.4
1	B	402	ILE	2.4
1	A	51	VAL	2.3
1	B	293	LEU	2.3
1	B	400	LEU	2.3
1	C	403	GLN	2.2
1	B	329	SER	2.2
1	A	261	ASN	2.1
1	B	291	TYR	2.0
1	C	328	LEU	2.0
1	A	168	GLU	2.0
1	B	381	PHE	2.0

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

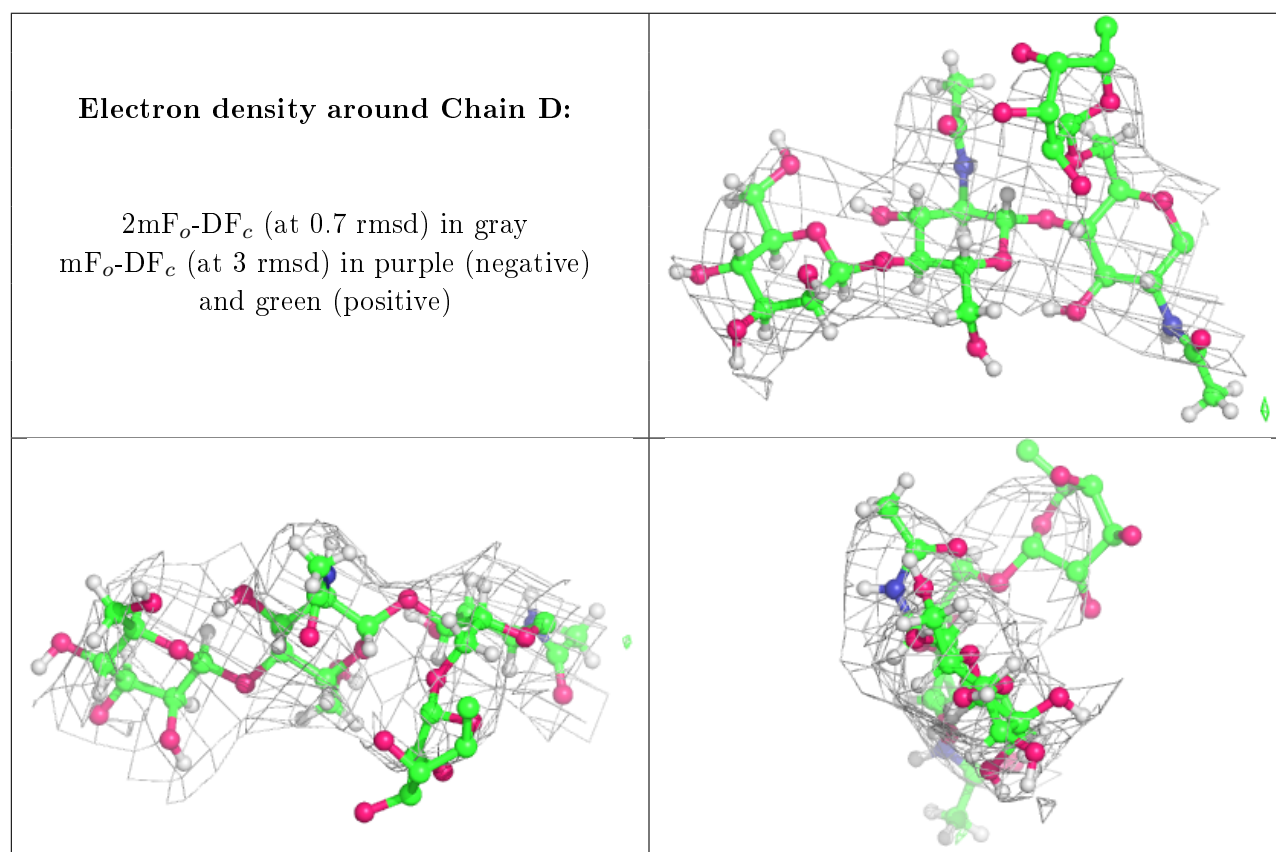
There are no non-standard protein/DNA/RNA residues in this entry.

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.

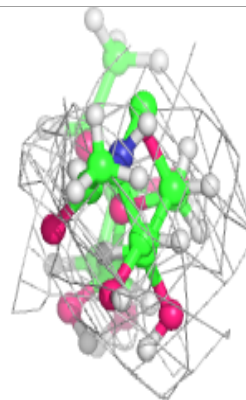
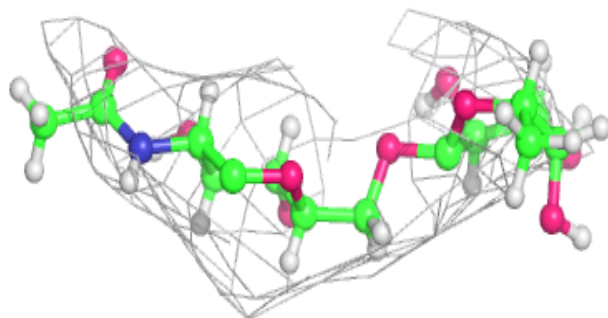
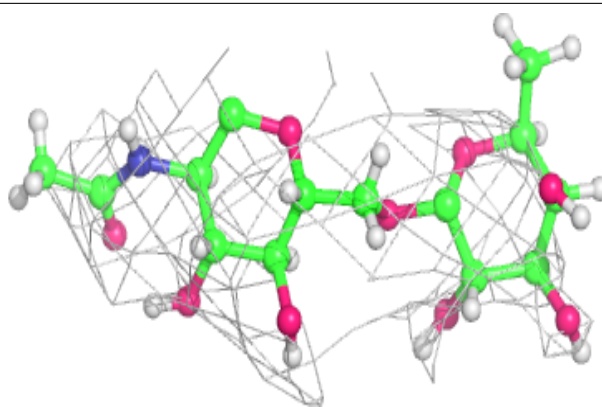
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FUC	E	2	10/11	0.80	0.32	187,237,291,327	0
2	NAG	D	2	14/15	0.82	0.32	146,220,281,294	0
2	NAG	D	1	14/15	0.84	0.24	197,230,261,263	0
4	NAG	F	1	14/15	0.85	0.13	146,204,234,236	0
3	NAG	E	1	14/15	0.85	0.14	153,197,257,265	0
2	FUC	D	4	10/11	0.85	0.41	188,204,226,234	0
4	NAG	F	2	14/15	0.86	0.17	146,194,231,242	0
2	BMA	D	3	11/12	0.88	0.37	168,221,263,284	0

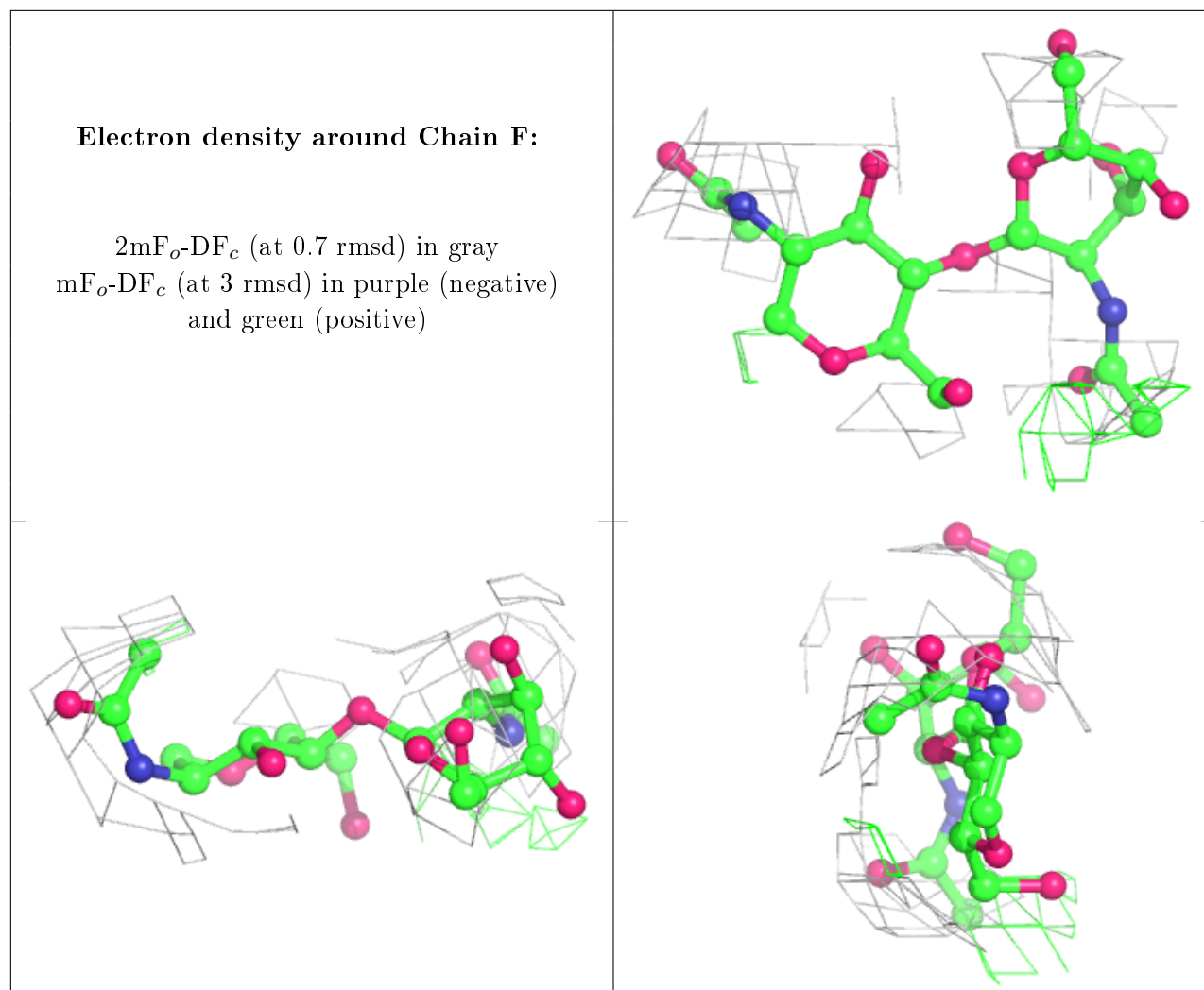
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

$2mF_o - DF_c$ (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
8	CL	A	515	1/1	0.59	0.62	146,146,146,146	0
6	NAG	A	512	14/15	0.60	0.42	146,203,223,234	0
8	CL	C	517	1/1	0.66	0.10	146,146,146,146	0
8	CL	A	514	1/1	0.77	0.13	152,152,152,152	0
6	NAG	B	510	14/15	0.80	0.27	146,238,289,294	0
6	NAG	C	514	14/15	0.80	0.26	170,223,241,249	0
7	NI	A	513	1/1	0.83	0.24	194,194,194,194	0
5	CA	B	508	1/1	0.84	0.17	242,242,242,242	0
8	CL	C	516	1/1	0.84	0.28	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	B	504	1/1	0.85	0.15	146,146,146,146	0
5	CA	C	506	1/1	0.85	0.23	181,181,181,181	0
7	NI	C	515	1/1	0.85	0.27	165,165,165,165	0
5	CA	B	501	1/1	0.89	0.26	146,146,146,146	0
5	CA	B	509	1/1	0.90	0.10	259,259,259,259	0
5	CA	B	502	1/1	0.91	0.22	146,146,146,146	0
5	CA	B	506	1/1	0.91	0.17	146,146,146,146	0
5	CA	B	507	1/1	0.91	0.16	219,219,219,219	0
5	CA	A	507	1/1	0.93	0.14	146,146,146,146	0
5	CA	A	505	1/1	0.93	0.17	146,146,146,146	0
5	CA	C	504	1/1	0.94	0.22	146,146,146,146	0
5	CA	C	507	1/1	0.94	0.10	161,161,161,161	0
5	CA	A	501	1/1	0.95	0.20	146,146,146,146	0
5	CA	C	509	1/1	0.96	0.10	146,146,146,146	0
5	CA	A	508	1/1	0.96	0.28	146,146,146,146	0
5	CA	A	504	1/1	0.96	0.19	146,146,146,146	0
5	CA	A	509	1/1	0.96	0.17	162,162,162,162	0
5	CA	B	503	1/1	0.97	0.23	146,146,146,146	0
5	CA	A	503	1/1	0.97	0.20	146,146,146,146	0
5	CA	A	502	1/1	0.97	0.21	160,160,160,160	0
5	CA	B	505	1/1	0.97	0.13	146,146,146,146	0
5	CA	C	505	1/1	0.97	0.18	146,146,146,146	0
5	CA	C	508	1/1	0.98	0.09	146,146,146,146	0
5	CA	C	502	1/1	0.98	0.20	146,146,146,146	0
5	CA	C	501	1/1	0.98	0.29	146,146,146,146	0
5	CA	A	506	1/1	0.98	0.19	146,146,146,146	0
5	CA	C	503	1/1	0.99	0.21	146,146,146,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.