



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 06:20 PM BST

PDB ID : 2OXE
Title : Structure of the Human Pancreatic Lipase-related Protein 2
Authors : Walker, J.R.; Davis, T.; Seitova, A.; Finerty Jr., P.J.; Butler-Cole, C.; Kozieradzki, I.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2007-02-20
Resolution : 2.80 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

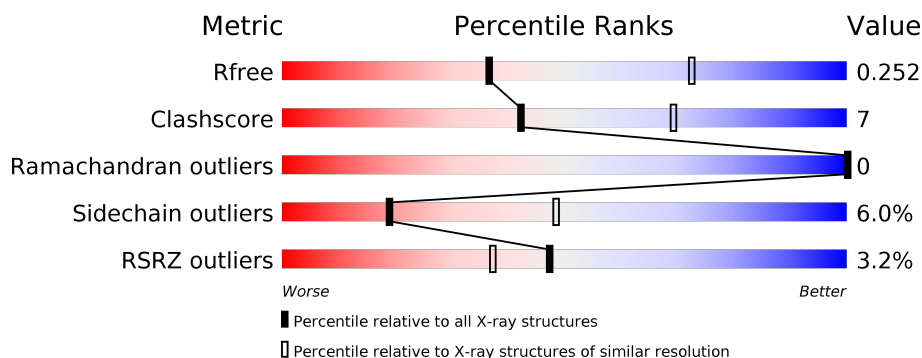
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	466	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>• 7%</div> </div> </div>
1	B	466	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 8%</div> </div> </div>
2	C	5	<div> <div></div> <div>100%</div> </div>
2	D	5	<div> <div></div> <div>60%</div> <div>40%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1	X	-	-	-
2	MAN	D	5	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6886 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 Pancreatic lipase-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	2	0
			3353	2118	561	653	21			
1	B	431	Total	C	N	O	S	0	2	0
			3328	2098	560	649	21			

There are 28 discrepancies between the modelled and reference sequences:

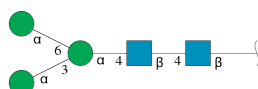
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	cloning artifact	UNP P54317
A	17	ALA	-	cloning artifact	UNP P54317
A	470	GLU	-	cloning artifact	UNP P54317
A	471	PHE	-	cloning artifact	UNP P54317
A	472	VAL	-	cloning artifact	UNP P54317
A	473	GLU	-	cloning artifact	UNP P54317
A	474	HIS	-	cloning artifact	UNP P54317
A	475	HIS	-	cloning artifact	UNP P54317
A	476	HIS	-	cloning artifact	UNP P54317
A	477	HIS	-	cloning artifact	UNP P54317
A	478	HIS	-	cloning artifact	UNP P54317
A	479	HIS	-	cloning artifact	UNP P54317
A	480	HIS	-	cloning artifact	UNP P54317
A	481	HIS	-	cloning artifact	UNP P54317
B	16	ALA	-	cloning artifact	UNP P54317
B	17	ALA	-	cloning artifact	UNP P54317
B	470	GLU	-	cloning artifact	UNP P54317
B	471	PHE	-	cloning artifact	UNP P54317
B	472	VAL	-	cloning artifact	UNP P54317
B	473	GLU	-	cloning artifact	UNP P54317
B	474	HIS	-	cloning artifact	UNP P54317
B	475	HIS	-	cloning artifact	UNP P54317
B	476	HIS	-	cloning artifact	UNP P54317
B	477	HIS	-	cloning artifact	UNP P54317
B	478	HIS	-	cloning artifact	UNP P54317

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Chain	Residue	Modelled	Actual	Comment	Reference
B	479	HIS	-	cloning artifact	UNP P54317
B	480	HIS	-	cloning artifact	UNP P54317
B	481	HIS	-	cloning artifact	UNP P54317

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total	O	0	0
			44	44		
5	B	32	Total	O	0	0
			32	32		

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.

- Chain A:
-
- 4% 79% 12% 7%
- ALA
K18
K32
R40
L57
T60
N61
E62
N63
I70
E74
I78
E79
K88
R89
I93
L97
W104
P105
K110
V123
R126
R130
Q135
I140
Q152
Y160
D164
V165
H166
V167
I168
G169
L172
T176
- R183
T192
G193
P199
C200
F201
Q202
S226
P227
I228
V229
P230
S231
K239
C256
LVS
ASN
VAL
LEU
SER
THR
THR
ASP
ILE
D268
V271
E272
G275
V278
L283
R284
Y288
L294
V295
P296
D297
L300
C304
F316
F336
T337
T343

- Chain B:
-
- 2.96
76%
15%
8%
- ALA
ALA
E19
V34
T37
L38
Q39
R40
L44
L45
P46
N47
S48
P49
E50
T54
T60
I70
P75
D76
T77
I78
D86
F91
T92
T93
A100
V104
P105
K111
I121
G122
V123
R126
A131
T134
Q135
A136
V137
N139
Q138
I140
R141
- V142
E146
Q157
I168
G169
S171
T192
G193
P199
C200
V218
I228
V229
H242
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D244
F245
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A843
S844
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V847
A848
S849
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A853
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A858
S859
T860
L861

- Chain C:  100%

MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain D:



MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	216.92Å 216.92Å 123.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.80 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.88-2.80) 99.3 (29.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.261 0.217 , 0.252	Depositor DCC
R_{free} test set	1811 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.3	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	0.93	EDS
Total number of atoms	6886	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.21% 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: CA, CL, NAG, MAN

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	0.40	0/3438	0.54	0/4667
1	B	0.40	0/3411	0.53	0/4628
All	All	0.40	0/6849	0.53	0/9295

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	3353	0	3108	45	0
1	B	3328	0	3095	43	0
2	C	61	0	52	0	0
2	D	61	0	52	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	44	0	0	0	0
5	B	32	0	0	0	0
All	All	6886	0	6307	90	0

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

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HD11	1:A:172:LEU:HB3	1.27	1.15
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.34	0.91
1:A:183:ARG:CG	1:A:183:ARG:HH21	1.85	0.89
1:A:183:ARG:HH21	1:A:183:ARG:HG2	1.39	0.87
1:A:60:THR:HB	1:A:63:ASN:OD1	1.84	0.77
1:B:361:VAL:HG11	1:B:377:ILE:HD13	1.67	0.77
1:B:218:VAL:H	1:B:242:HIS:HD2	1.32	0.76
1:A:40:ARG:NH2	1:A:200:CYS:O	2.22	0.72
1:B:284:ARG:HG2	1:B:288:TYR:CZ	2.26	0.70
1:A:358:ARG:CG	1:A:358:ARG:HH11	2.05	0.70
1:A:140:ILE:CD1	1:A:172:LEU:HB3	2.16	0.69
1:A:60:THR:HG22	1:A:62:GLU:H	1.58	0.67
1:A:140:ILE:HG12	1:A:176:THR:OG1	1.97	0.65
1:A:410:PHE:CE2	1:A:412:VAL:HG12	2.37	0.60
1:A:140:ILE:HD12	1:A:172:LEU:HD22	1.85	0.58
1:A:239:LYS:HE2	1:A:343:THR:OG1	2.04	0.58
1:B:37:THR:HG23	1:B:40:ARG:HG2	1.85	0.58
1:B:218:VAL:H	1:B:242:HIS:CD2	2.18	0.56
1:A:284:ARG:HG2	1:A:288:TYR:CZ	2.41	0.55
1:B:228:ILE:HG22	1:B:229:VAL:HG23	1.87	0.55
1:B:218:VAL:N	1:B:242:HIS:HD2	2.03	0.55
1:A:183:ARG:NH2	1:A:183:ARG:HG2	2.12	0.55
1:B:46:PRO:HD3	1:B:138:GLN:HG3	1.88	0.55
1:B:34:TRP:CZ3	1:B:141:ARG:HD3	2.42	0.54
1:A:183:ARG:CG	1:A:183:ARG:NH2	2.56	0.54
1:B:377:ILE:HD11	1:B:439:ILE:HD13	1.90	0.54
1:B:37:THR:HG23	1:B:40:ARG:CG	2.37	0.53
1:A:97:LEU:HD23	1:A:130[A]:ARG:HG3	1.92	0.52
1:B:142:VAL:O	1:B:146:GLU:HG3	2.09	0.52
1:A:183:ARG:HH21	1:A:183:ARG:HG3	1.74	0.52
1:A:304:CYS:HB3	1:A:345:PHE:HD1	1.73	0.52
1:B:375:ILE:HD12	1:B:420:PHE:CE1	2.45	0.51
1:B:361:VAL:CG1	1:B:377:ILE:HD13	2.39	0.51
1:B:353:ASN:HB2	1:B:355:THR:HG23	1.92	0.51
1:B:423:ASN:HA	1:B:460:GLU:HG3	1.92	0.51
1:B:111:LYS:HE3	1:B:290:SER:HB3	1.92	0.51
1:B:34:TRP:CE3	1:B:141:ARG:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ASN:N	1:B:423:ASN:HD22	2.10	0.50
1:B:104:TRP:CG	1:B:105:PRO:HD3	2.48	0.49
1:A:90:ARG:HG2	1:A:166:HIS:HB3	1.95	0.49
1:B:70:ILE:HB	1:B:78:ILE:HD13	1.94	0.49
1:A:377:ILE:HD12	1:A:391:ILE:HD13	1.95	0.49
1:A:126:ARG:O	1:A:130[A]:ARG:HD2	2.13	0.48
1:A:70:ILE:HB	1:A:78:ILE:HD13	1.94	0.48
1:B:171:SER:HB3	1:B:282:HIS:CE1	2.48	0.48
1:B:44:LEU:HD23	1:B:134:THR:HG22	1.95	0.48
1:B:398:PRO:O	1:B:399:ASP:HB2	2.14	0.48
1:A:140:ILE:CD1	1:A:172:LEU:HD22	2.44	0.47
1:A:60:THR:HG22	1:A:61:ASN:N	2.30	0.47
1:A:93:ILE:HG12	1:A:123:VAL:HB	1.97	0.47
1:B:86:ASP:N	1:B:86:ASP:OD1	2.45	0.47
1:B:137:VAL:O	1:B:140:ILE:HG12	2.15	0.47
1:A:375:ILE:HD12	1:A:420:PHE:CE1	2.50	0.47
1:B:47:TRP:CH2	1:B:131:ALA:HB2	2.50	0.46
1:B:276:GLY:O	1:B:279:SER:HB3	2.16	0.45
2:D:1:NAG:H61	2:D:2:NAG:HN2	1.81	0.45
1:A:336:LYS:HG3	1:A:337:THR:HG23	1.99	0.45
1:A:377:ILE:HD12	1:A:391:ILE:CD1	2.46	0.45
1:B:93:ILE:HG12	1:B:123:VAL:HB	1.98	0.45
1:A:377:ILE:HB	1:A:391:ILE:HD12	1.97	0.45
1:B:311:GLN:HE21	1:B:311:GLN:HA	1.82	0.45
1:B:48:SER:OG	1:B:50:GLU:HG2	2.17	0.45
1:A:160:TYR:CE2	1:A:164:ASP:HB2	2.52	0.45
1:A:275:GLY:O	1:A:278:VAL:HG12	2.18	0.44
1:B:100:ALA:HA	1:B:105:PRO:HG2	2.00	0.44
1:B:363:VAL:O	1:B:401:SER:HA	2.16	0.44
1:B:75:PRO:HB3	1:B:157:GLN:HG2	1.98	0.44
1:B:168:ILE:HG23	1:B:192:THR:HB	1.99	0.44
2:D:1:NAG:H61	2:D:2:NAG:N2	2.32	0.44
1:A:60:THR:CG2	1:A:61:ASN:N	2.81	0.43
1:B:289:TYR:O	1:B:292:SER:HB3	2.18	0.43
1:A:375:ILE:HG23	1:A:420:PHE:CE1	2.54	0.43
1:A:278:VAL:HA	1:A:283:LEU:HD21	2.01	0.43
1:A:32:LYS:HG2	1:A:32:LYS:H	1.59	0.42
1:B:199:PRO:O	1:B:200:CYS:HB2	2.19	0.42
1:B:91:PHE:HA	1:B:121:ILE:O	2.20	0.42
1:A:358:ARG:NH1	1:A:358:ARG:CG	2.72	0.42
1:A:104:TRP:CG	1:A:105:PRO:HD3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:LYS:HG2	1:B:457:THR:O	2.21	0.41
1:A:375:ILE:HD12	1:A:420:PHE:HE1	1.86	0.41
1:A:304:CYS:HB3	1:A:345:PHE:CD1	2.55	0.41
1:A:294:LEU:O	1:A:296:PRO:HD3	2.20	0.41
1:A:316:PHE:CE2	1:A:444:GLY:HA2	2.54	0.41
1:B:245:PHE:CG	1:B:326:MET:HG3	2.55	0.41
1:A:202:GLN:HG2	1:A:228:ILE:HD13	2.03	0.41
1:A:199:PRO:O	1:A:200:CYS:HB2	2.21	0.41
1:B:37:THR:CG2	1:B:40:ARG:HG3	2.51	0.40
1:A:297:ASP:HB2	1:A:300:LEU:HD21	2.03	0.40
1:B:375:ILE:HG12	1:B:396:LEU:HD22	2.03	0.40
1:B:37:THR:CG2	1:B:40:ARG:CG	2.99	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	431/466 (92%)	403 (94%)	28 (6%)	0	100	100
1	B	427/466 (92%)	410 (96%)	17 (4%)	0	100	100
All	All	858/932 (92%)	813 (95%)	45 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	359/400 (90%)	337 (94%)	22 (6%)	18	48
1	B	358/400 (90%)	337 (94%)	21 (6%)	19	49
All	All	717/800 (90%)	674 (94%)	43 (6%)	19	48

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	40	ARG
1	A	57	LEU
1	A	74	GLU
1	A	79	GLU
1	A	88	LYS
1	A	110	LYS
1	A	126	ARG
1	A	135	GLN
1	A	140	ILE
1	A	152	GLN
1	A	183	ARG
1	A	226	SER
1	A	228	ILE
1	A	231	SER
1	A	268	ASP
1	A	272	GLU
1	A	304	CYS
1	A	358	ARG
1	A	364	THR
1	A	385	ASN
1	A	423	ASN
1	B	37	THR
1	B	38	LEU
1	B	40	ARG
1	B	54	THR
1	B	60	THR
1	B	76	ASP
1	B	126	ARG
1	B	135	GLN
1	B	138	GLN
1	B	243	LEU
1	B	278	VAL
1	B	284	ARG

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Mol	Chain	Res	Type
1	B	290	SER
1	B	304	CYS
1	B	311	GLN
1	B	346	LEU
1	B	353	ASN
1	B	358	ARG
1	B	409	ASP
1	B	412	VAL
1	B	423	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	423	ASN
1	B	152	GLN
1	B	242	HIS
1	B	311	GLN
1	B	385	ASN
1	B	423	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 ⓘ

10 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	C	1	1,2	14,14,15	0.54	0	17,19,21	2.15	5 (29%)
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	1.63	4 (23%)
2	MAN	C	3	2	11,11,12	0.91	1 (9%)	15,15,17	2.05	3 (20%)
2	MAN	C	4	2	11,11,12	0.55	0	15,15,17	2.10	3 (20%)
2	MAN	C	5	2	11,11,12	0.60	0	15,15,17	1.32	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.73	0	17,19,21	1.37	2 (11%)
2	NAG	D	2	2	14,14,15	0.47	0	17,19,21	1.21	1 (5%)
2	MAN	D	3	2	11,11,12	0.50	0	15,15,17	2.28	5 (33%)
2	MAN	D	4	2	11,11,12	0.70	0	15,15,17	1.06	1 (6%)
2	MAN	D	5	2	11,11,12	0.62	0	15,15,17	0.90	1 (6%)

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	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	1,2	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	MAN	D	3	2	-	0/2/19/22	1/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	MAN	C2-C3	2.22	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	6.79	121.39	112.19
2	C	4	MAN	C1-O5-C5	6.77	121.36	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	MAN	C1-C2-C3	6.14	117.21	109.67
2	D	3	MAN	C1-O5-C5	5.57	119.74	112.19
2	D	3	MAN	O3-C3-C4	4.21	120.08	110.35
2	C	2	NAG	C1-O5-C5	3.79	117.33	112.19
2	D	1	NAG	O5-C1-C2	-3.67	105.49	111.29
2	C	3	MAN	C2-C3-C4	3.59	117.11	110.89
2	D	3	MAN	O5-C5-C6	3.18	112.18	107.20
2	C	5	MAN	C1-O5-C5	3.15	116.46	112.19
2	C	2	NAG	O4-C4-C3	3.11	117.54	110.35
2	C	2	NAG	C4-C3-C2	-3.07	106.52	111.02
2	D	3	MAN	C3-C4-C5	-2.95	104.97	110.24
2	C	1	NAG	C4-C3-C2	-2.87	106.81	111.02
2	C	5	MAN	C3-C4-C5	2.78	115.19	110.24
2	C	1	NAG	C2-N2-C7	2.69	126.73	122.90
2	C	4	MAN	C3-C4-C5	2.64	114.94	110.24
2	C	3	MAN	O5-C5-C6	2.59	111.27	107.20
2	D	1	NAG	C2-N2-C7	2.45	126.39	122.90
2	C	4	MAN	O5-C5-C4	2.33	116.48	110.83
2	D	2	NAG	C1-O5-C5	2.25	115.24	112.19
2	D	5	MAN	C1-O5-C5	2.25	115.23	112.19
2	C	2	NAG	O4-C4-C5	2.22	114.80	109.30
2	C	1	NAG	C1-C2-N2	2.21	114.26	110.49
2	D	3	MAN	O5-C1-C2	2.21	114.17	110.77
2	D	4	MAN	O5-C1-C2	-2.17	107.42	110.77
2	C	1	NAG	O5-C5-C6	2.13	110.54	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C3-C2-N2-C7
2	D	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	5	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

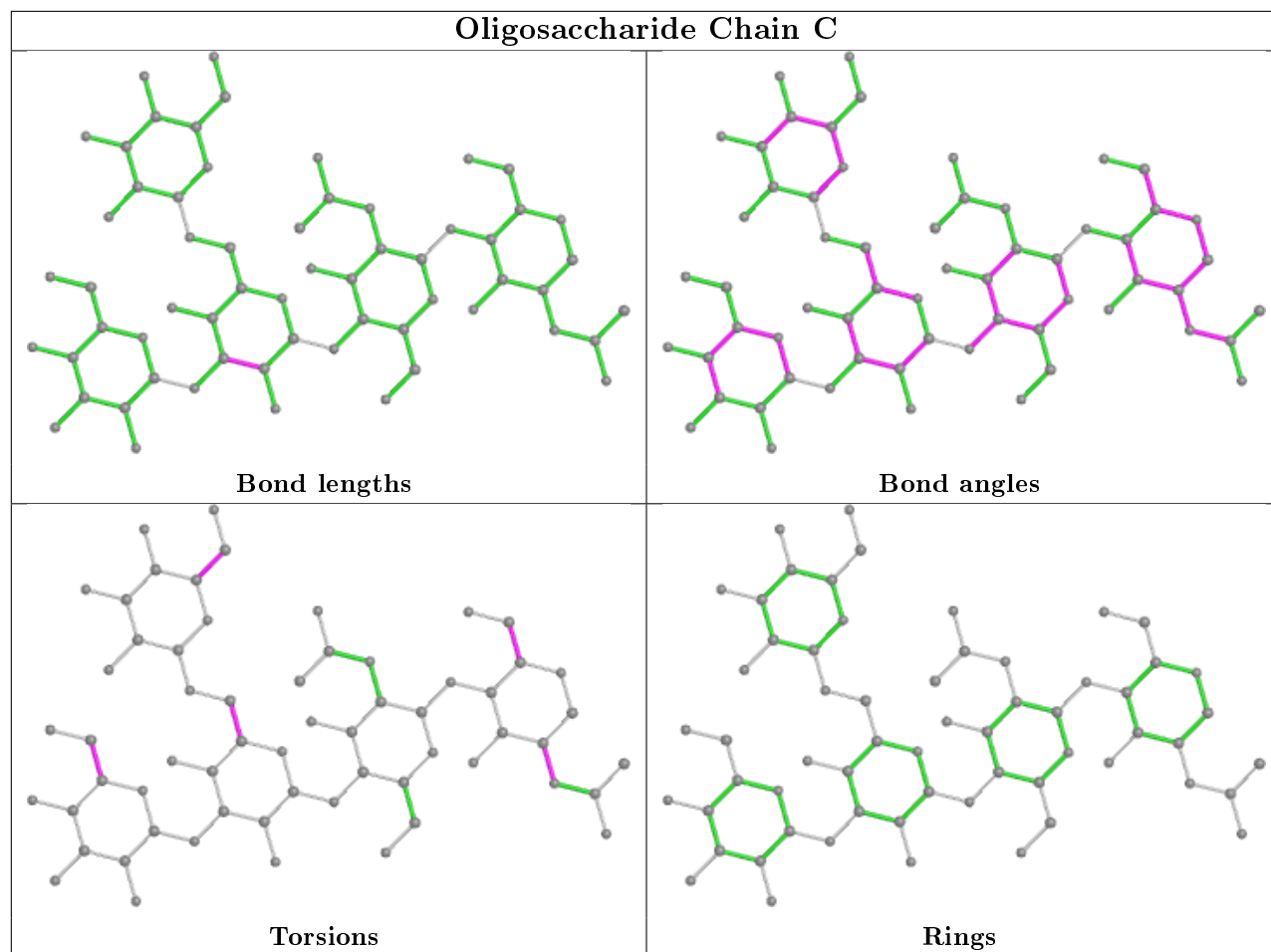
All (1) ring outliers are listed below:

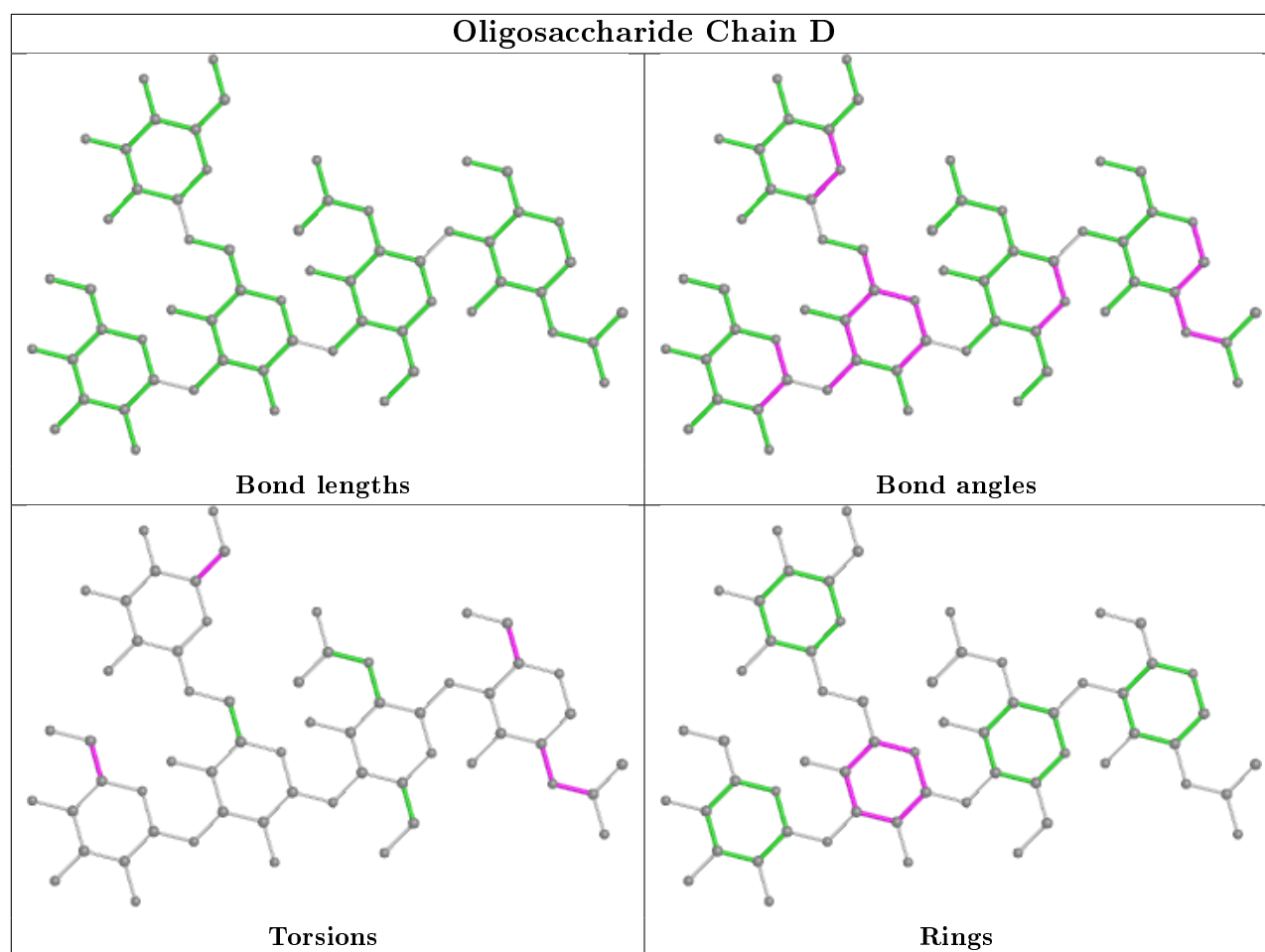
Mol	Chain	Res	Type	Atoms
2	D	3	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
2	D	2	NAG	2	0

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





5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	435/466 (93%)	0.10	20 (4%) 32 22	40, 64, 109, 158	0
1	B	431/466 (92%)	0.03	8 (1%) 66 59	40, 67, 100, 134	0
All	All	866/932 (92%)	0.07	28 (3%) 47 37	40, 65, 104, 158	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLY	5.7
1	B	305	ALA	4.0
1	A	228	ILE	3.9
1	A	229	VAL	3.9
1	A	383	ASN	3.8
1	A	372	ASN	3.7
1	B	169	GLY	3.6
1	A	192	THR	3.3
1	A	271	TRP	3.1
1	A	227	PRO	3.1
1	A	231	SER	3.0
1	A	167	VAL	3.0
1	A	399	ASP	2.7
1	A	374	TYR	2.6
1	B	304	CYS	2.6
1	A	382	SER	2.5
1	A	193	GLY	2.5
1	A	169	GLY	2.5
1	A	400	ALA	2.4
1	B	373	GLY	2.4
1	B	399	ASP	2.3
1	A	226	SER	2.3
1	A	375	ILE	2.3
1	A	432	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	192	THR	2.2
1	B	19	GLU	2.2
1	B	193	GLY	2.1
1	A	373	GLY	2.1

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 ⓘ

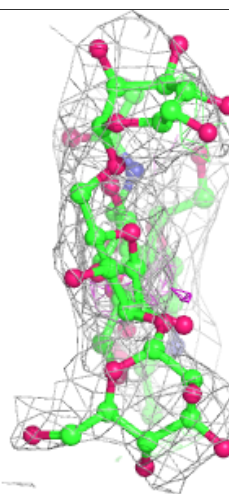
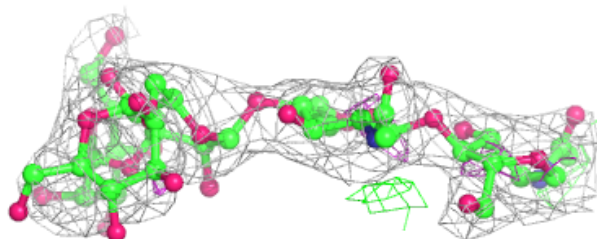
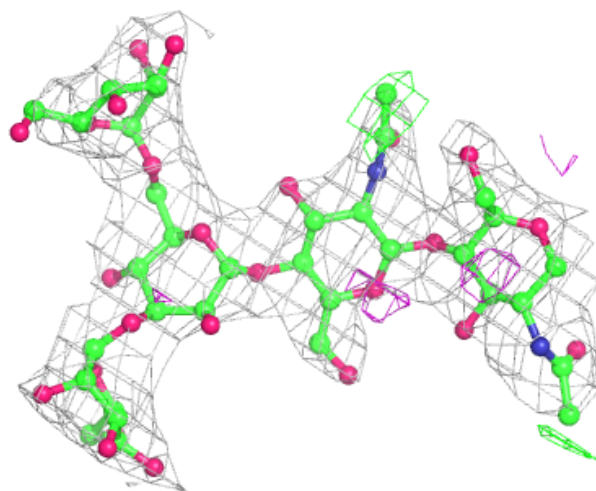
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

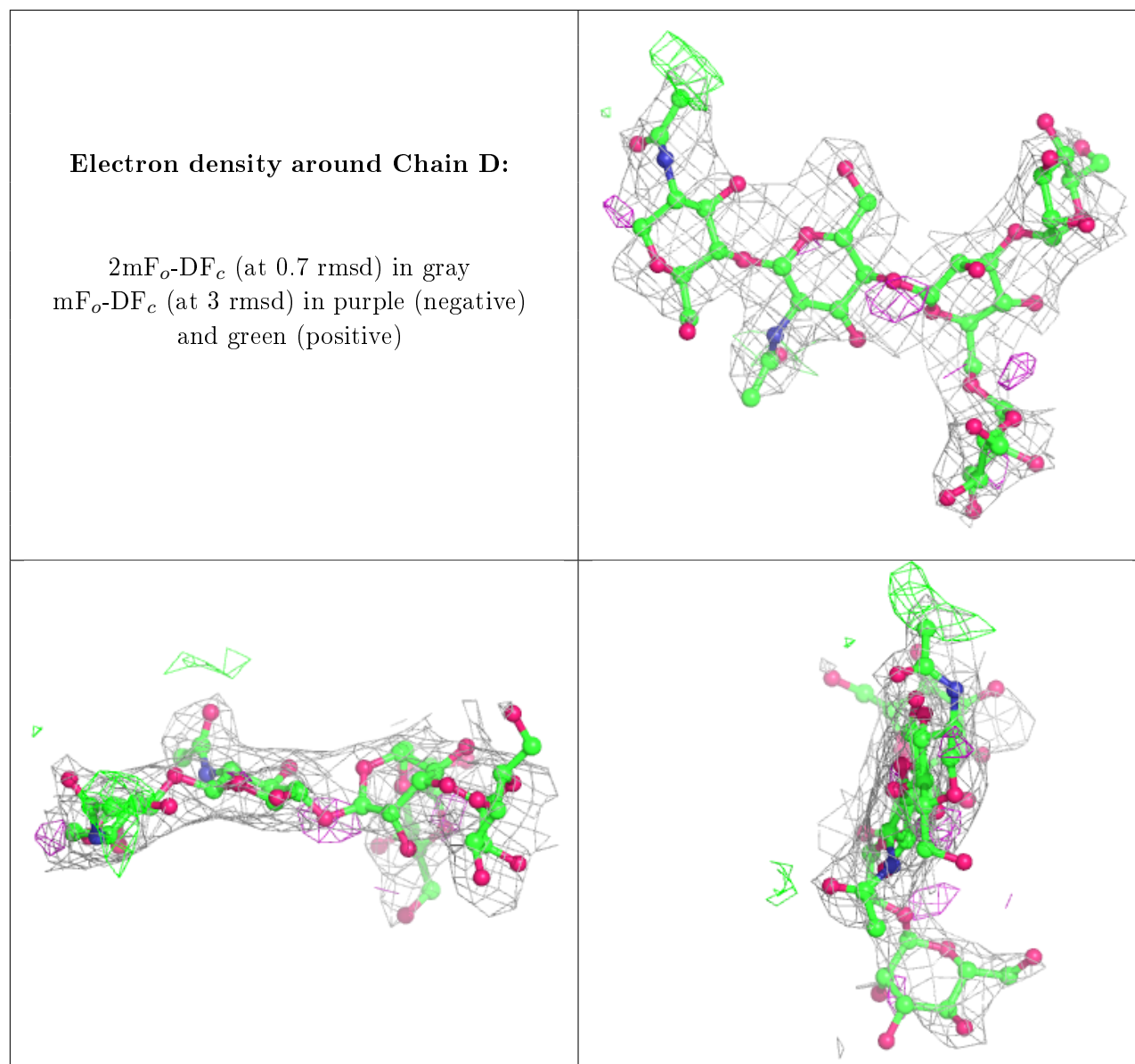
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	D	5	11/12	0.69	0.58	115,116,116,116	0
2	NAG	D	2	14/15	0.76	0.37	93,96,100,104	0
2	MAN	C	3	11/12	0.78	0.23	100,103,105,106	0
2	MAN	C	4	11/12	0.80	0.37	106,107,108,108	0
2	MAN	D	4	11/12	0.81	0.45	113,113,114,114	0
2	MAN	D	3	11/12	0.82	0.32	107,110,111,113	0
2	MAN	C	5	11/12	0.83	0.39	108,109,109,110	0
2	NAG	D	1	14/15	0.83	0.35	72,79,82,88	0
2	NAG	C	2	14/15	0.87	0.33	86,89,92,96	0
2	NAG	C	1	14/15	0.91	0.31	66,72,76,81	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 C:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	A	1	1/1	0.91	0.17	59,59,59,59	0
3	CA	A	600	1/1	0.95	0.18	40,40,40,40	0
4	CL	B	5	1/1	0.95	0.08	65,65,65,65	0
3	CA	B	600	1/1	0.95	0.17	67,67,67,67	0
4	CL	B	2	1/1	0.95	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	A	3	1/1	0.97	0.16	57,57,57,57	0
4	CL	B	4	1/1	0.98	0.14	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.