



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 12:26 PM BST

PDB ID : 6DXW
Title : Human N-acylethanolamine-hydrolyzing acid amidase (NAAA) precursor (C126A)
Authors : Gorelik, A.; Gebai, A.; Illes, K.; Piomelli, D.; Nagar, B.
Deposited on : 2018-07-01
Resolution : 2.30 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 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

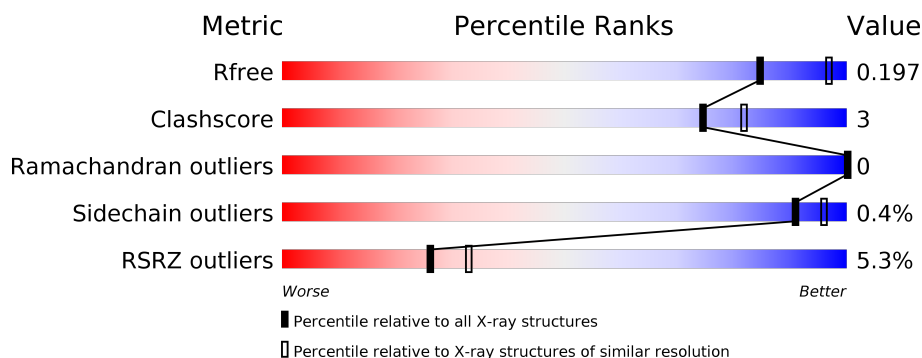
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



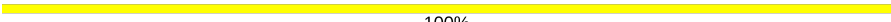
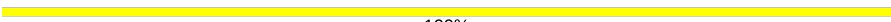
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	341	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	341	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	341	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	D	341	<div> <div>13%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>.</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	G	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	H	3	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22016 atoms, of which 10520 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 N-acylethanolamine-hydrolyzing acid amidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			5190	1679	2584	454	467	6			
1	B	328	Total	C	H	N	O	S	0	0	0
			5190	1679	2584	454	467	6			
1	C	328	Total	C	H	N	O	S	0	0	0
			5189	1679	2583	454	467	6			
1	D	328	Total	C	H	N	O	S	0	0	0
			5191	1679	2585	454	467	6			

There are 48 discrepancies between the modelled and reference sequences:

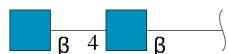
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ASP	-	expression tag	UNP Q02083
A	20	ARG	-	expression tag	UNP Q02083
A	21	HIS	-	expression tag	UNP Q02083
A	22	HIS	-	expression tag	UNP Q02083
A	23	HIS	-	expression tag	UNP Q02083
A	24	HIS	-	expression tag	UNP Q02083
A	25	HIS	-	expression tag	UNP Q02083
A	26	HIS	-	expression tag	UNP Q02083
A	27	LYS	-	expression tag	UNP Q02083
A	28	LEU	-	expression tag	UNP Q02083
A	113	ALA	CYS	conflict	UNP Q02083
A	126	ALA	CYS	engineered mutation	UNP Q02083
B	19	ASP	-	expression tag	UNP Q02083
B	20	ARG	-	expression tag	UNP Q02083
B	21	HIS	-	expression tag	UNP Q02083
B	22	HIS	-	expression tag	UNP Q02083
B	23	HIS	-	expression tag	UNP Q02083
B	24	HIS	-	expression tag	UNP Q02083
B	25	HIS	-	expression tag	UNP Q02083
B	26	HIS	-	expression tag	UNP Q02083
B	27	LYS	-	expression tag	UNP Q02083

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Chain	Residue	Modelled	Actual	Comment	Reference
B	28	LEU	-	expression tag	UNP Q02083
B	113	ALA	CYS	conflict	UNP Q02083
B	126	ALA	CYS	engineered mutation	UNP Q02083
C	19	ASP	-	expression tag	UNP Q02083
C	20	ARG	-	expression tag	UNP Q02083
C	21	HIS	-	expression tag	UNP Q02083
C	22	HIS	-	expression tag	UNP Q02083
C	23	HIS	-	expression tag	UNP Q02083
C	24	HIS	-	expression tag	UNP Q02083
C	25	HIS	-	expression tag	UNP Q02083
C	26	HIS	-	expression tag	UNP Q02083
C	27	LYS	-	expression tag	UNP Q02083
C	28	LEU	-	expression tag	UNP Q02083
C	113	ALA	CYS	conflict	UNP Q02083
C	126	ALA	CYS	engineered mutation	UNP Q02083
D	19	ASP	-	expression tag	UNP Q02083
D	20	ARG	-	expression tag	UNP Q02083
D	21	HIS	-	expression tag	UNP Q02083
D	22	HIS	-	expression tag	UNP Q02083
D	23	HIS	-	expression tag	UNP Q02083
D	24	HIS	-	expression tag	UNP Q02083
D	25	HIS	-	expression tag	UNP Q02083
D	26	HIS	-	expression tag	UNP Q02083
D	27	LYS	-	expression tag	UNP Q02083
D	28	LEU	-	expression tag	UNP Q02083
D	113	ALA	CYS	conflict	UNP Q02083
D	126	ALA	CYS	engineered mutation	UNP Q02083

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

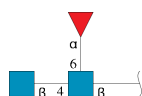
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet

a-D-glucopyranose.



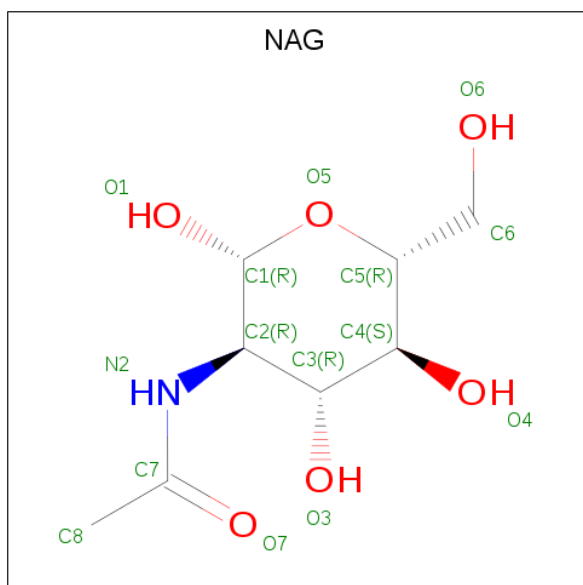
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			

- Molecule 4 is an oligosaccharide called 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	H	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	12	Total	Cl	0	0
			12	12		
6	A	5	Total	Cl	0	0
			5	5		
6	D	4	Total	Cl	0	0
			4	4		
6	C	7	Total	Cl	0	0
			7	7		

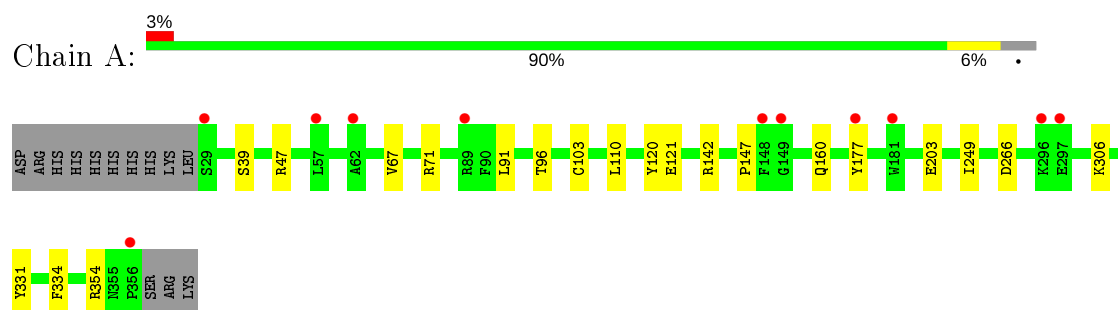
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	248	Total	O	0	0
			248	248		
7	B	244	Total	O	0	0
			244	244		
7	C	273	Total	O	0	0
			273	273		
7	D	91	Total	O	0	0
			91	91		

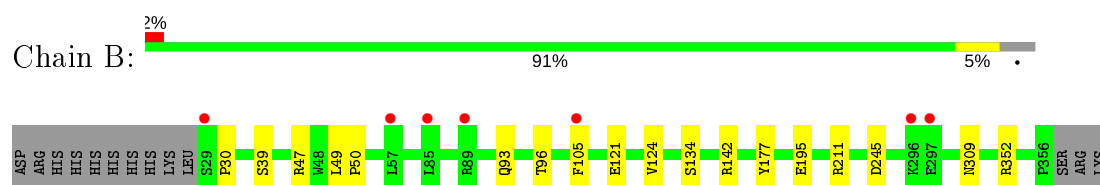
3 Residue-property plots [i](#)

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

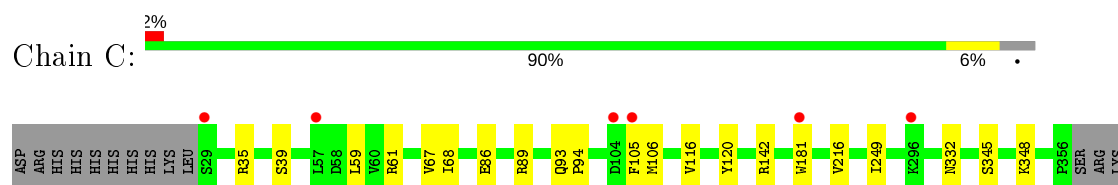
- Molecule 1: N-acylethanolamine-hydrolyzing acid amidase



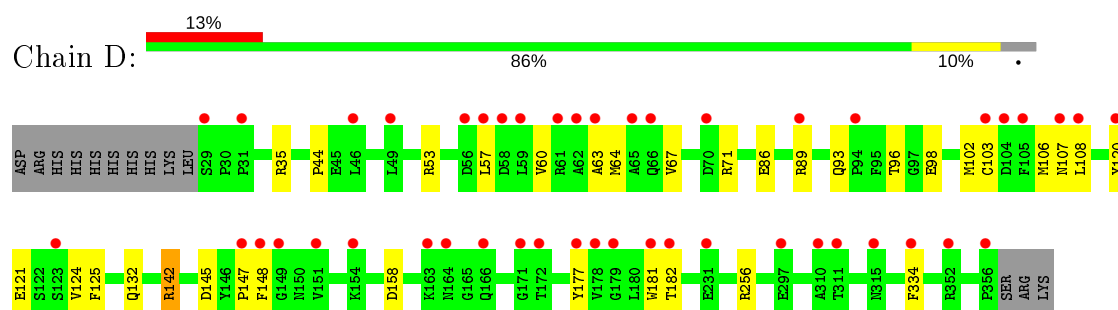
- Molecule 1: N-acylethanolamine-hydrolyzing acid amidase




- Molecule 1: N-acylethanolamine-hydrolyzing acid amidase



- Molecule 1: N-acylethanolamine-hydrolyzing acid amidase




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

Chain E:  50% 50%


MAG1
MAG2

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

Chain G:  50% 50%


MAG1
MAG2

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

Chain F:  100%


MAG1
FUC2

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

Chain H:  100%


MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.91Å 140.01Å 90.12Å 90.00° 115.20° 90.00°	Depositor
Resolution (Å)	38.26 – 2.30 38.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.4 (38.26-2.30) 86.7 (38.26-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.167 , 0.193 0.170 , 0.197	Depositor DCC
R_{free} test set	1796 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22016	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: CL, FUC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/2679	0.52	0/3657
1	B	0.33	0/2679	0.53	0/3657
1	C	0.32	0/2679	0.51	0/3657
1	D	0.33	0/2679	0.56	0/3657
All	All	0.33	0/10716	0.53	0/14628

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	2606	2584	2584	16	0
1	B	2606	2584	2583	10	1
1	C	2606	2583	2583	12	1
1	D	2606	2585	2585	24	0
2	E	28	27	25	0	0
2	G	28	27	25	1	0
3	F	24	24	22	0	0
4	H	38	37	34	2	0
5	A	14	14	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	28	26	2	0
5	C	14	14	13	1	0
5	D	14	13	13	0	0
6	A	5	0	0	0	0
6	B	12	0	0	1	0
6	C	7	0	0	1	0
6	D	4	0	0	0	0
7	A	248	0	0	3	0
7	B	244	0	0	4	0
7	C	273	0	0	4	0
7	D	91	0	0	1	0
All	All	11496	10520	10506	67	1

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 3.

All (67) 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:D:121:GLU:OE2	1:D:177:TYR:OH	2.00	0.79
5:C:403:NAG:O7	7:C:501:HOH:O	2.01	0.79
1:A:203:GLU:OE1	7:A:501:HOH:O	2.01	0.78
1:D:103:CYS:O	1:D:107:ASN:N	2.18	0.76
1:A:121:GLU:OE2	1:A:177:TYR:OH	2.03	0.76
1:D:142:ARG:NH2	1:D:181:TRP:O	2.20	0.73
1:A:121:GLU:O	7:A:502:HOH:O	2.07	0.73
1:D:142:ARG:NE	1:D:182:THR:OG1	2.21	0.70
1:B:245:ASP:O	7:B:501:HOH:O	2.09	0.69
1:B:93:GLN:OE1	1:B:96:THR:OG1	2.10	0.69
1:A:103:CYS:SG	1:A:110:LEU:HA	2.37	0.65
6:B:415:CL:CL	7:B:657:HOH:O	2.51	0.65
1:A:306:LYS:HG3	5:A:403:NAG:H81	1.78	0.65
1:C:67:VAL:HG11	1:C:120:TYR:OH	2.03	0.59
1:C:59:LEU:HD23	1:C:59:LEU:C	2.23	0.58
1:D:93:GLN:OE1	1:D:96:THR:OG1	2.21	0.54
1:D:147:PRO:HA	1:D:334:PHE:CD1	2.43	0.53
1:D:67:VAL:O	1:D:71:ARG:N	2.37	0.53
1:B:211:ARG:NH1	7:B:504:HOH:O	2.30	0.53
1:D:35:ARG:HA	1:D:158:ASP:O	2.09	0.52
1:B:124:VAL:O	1:B:195:GLU:HG2	2.10	0.52
1:D:57:LEU:HD13	1:D:106:MET:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HB3	1:A:71:ARG:CZ	2.42	0.50
1:B:309:ASN:ND2	5:B:402:NAG:O7	2.46	0.48
1:C:345:SER:HB3	1:C:348:LYS:HD2	1.95	0.48
1:A:120:TYR:HB2	1:A:177:TYR:CE1	2.49	0.47
1:D:120:TYR:O	1:D:124:VAL:HG21	2.14	0.47
6:C:413:CL:CL	7:C:761:HOH:O	2.58	0.46
1:D:132:GLN:OE1	1:D:256:ARG:N	2.46	0.46
1:B:39:SER:O	1:B:47:ARG:HG2	2.16	0.46
1:C:61:ARG:NE	1:C:106:MET:O	2.48	0.46
1:A:67:VAL:HG21	1:A:120:TYR:OH	2.16	0.45
1:C:35:ARG:HD2	7:C:709:HOH:O	2.16	0.45
1:D:64:MET:O	1:D:67:VAL:HG22	2.16	0.45
1:D:142:ARG:HH21	1:D:181:TRP:C	2.17	0.45
1:A:266:ASP:HB3	4:H:1:NAG:H5	1.97	0.45
1:D:125:PHE:HB2	1:D:145:ASP:HB2	1.98	0.45
1:A:39:SER:O	1:A:47:ARG:HG2	2.16	0.45
1:D:71:ARG:HB3	1:D:71:ARG:CZ	2.46	0.45
1:D:60:VAL:O	1:D:63:ALA:N	2.48	0.45
1:D:57:LEU:HD13	1:D:106:MET:CG	2.47	0.44
1:D:86:GLU:OE2	1:D:89:ARG:NH1	2.50	0.44
1:C:68:ILE:HD11	1:C:116:VAL:HG23	2.00	0.44
1:C:332:ASN:HA	4:H:1:NAG:O7	2.18	0.44
1:D:71:ARG:HD3	1:D:148:PHE:HD2	1.83	0.43
1:D:98:GLU:O	1:D:102:MET:HG2	2.18	0.43
1:D:142:ARG:NH2	1:D:181:TRP:HB3	2.33	0.43
1:B:30:PRO:HB2	1:B:352:ARG:HB3	2.01	0.43
1:C:93:GLN:OE1	1:C:94:PRO:HA	2.19	0.43
1:D:53:ARG:NH1	7:D:509:HOH:O	2.43	0.43
1:B:49:LEU:HD21	1:B:105:PHE:CE1	2.55	0.42
1:A:249:ILE:HD12	1:A:249:ILE:N	2.35	0.42
1:A:331:TYR:HE1	1:A:354:ARG:HB3	1.83	0.42
1:A:147:PRO:HA	1:A:334:PHE:CD1	2.54	0.42
1:D:106:MET:HE3	1:D:108:LEU:HD12	2.00	0.42
5:B:401:NAG:H82	7:B:700:HOH:O	2.20	0.42
1:B:49:LEU:HB2	1:B:50:PRO:HD3	2.02	0.41
1:C:249:ILE:N	1:C:249:ILE:HD12	2.34	0.41
1:D:44:PRO:HB3	1:D:98:GLU:HG3	2.03	0.41
1:C:181:TRP:CH2	1:C:216:VAL:HG21	2.55	0.41
1:C:86:GLU:OE2	1:C:89:ARG:NH1	2.52	0.41
1:A:91:LEU:HB2	1:A:96:THR:HG21	2.03	0.40
1:A:160:GLN:HG3	7:A:587:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:573:HOH:O	2:G:2:NAG:H4	2.21	0.40
1:A:306:LYS:CG	5:A:403:NAG:H81	2.49	0.40
1:B:121:GLU:OE2	1:B:177:TYR:OH	2.34	0.40
1:C:105:PHE:N	1:C:105:PHE:CD1	2.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:O	1:C:39:SER:HG[2_555]	1.59	0.01

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	326/341 (96%)	319 (98%)	7 (2%)	0	100	100
1	B	326/341 (96%)	318 (98%)	8 (2%)	0	100	100
1	C	326/341 (96%)	318 (98%)	8 (2%)	0	100	100
1	D	326/341 (96%)	317 (97%)	9 (3%)	0	100	100
All	All	1304/1364 (96%)	1272 (98%)	32 (2%)	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	278/291 (96%)	277 (100%)	1 (0%)	91	96
1	B	278/291 (96%)	277 (100%)	1 (0%)	91	96
1	C	278/291 (96%)	277 (100%)	1 (0%)	91	96
1	D	278/291 (96%)	277 (100%)	1 (0%)	91	96
All	All	1112/1164 (96%)	1108 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	B	142	ARG
1	C	142	ARG
1	D	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	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 ⓘ

9 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	E	1	1,2	14,14,15	0.43	0	17,19,21	0.62	0
2	NAG	E	2	2	14,14,15	0.78	1 (7%)	17,19,21	1.01	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.74	1 (7%)	17,19,21	0.66	0
3	FUC	F	2	3	10,10,11	1.01	1 (10%)	14,14,16	0.96	0
2	NAG	G	1	1,2	14,14,15	0.86	1 (7%)	17,19,21	0.68	0
2	NAG	G	2	2	14,14,15	0.38	0	17,19,21	0.73	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.66	0	17,19,21	0.53	0
4	NAG	H	2	4	14,14,15	0.79	1 (7%)	17,19,21	0.94	1 (5%)
4	FUC	H	3	4	10,10,11	1.36	2 (20%)	14,14,16	1.59	2 (14%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	-2.94	1.39	1.43
4	H	3	FUC	O5-C1	-2.76	1.39	1.43
4	H	3	FUC	C4-C5	2.42	1.58	1.52
3	F	1	NAG	O5-C1	-2.41	1.39	1.43
2	E	2	NAG	C1-C2	-2.41	1.48	1.52
4	H	2	NAG	O5-C1	-2.40	1.39	1.43
3	F	2	FUC	O5-C1	-2.17	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	H	3	FUC	O5-C5-C4	3.99	116.68	109.52
4	H	2	NAG	C1-O5-C5	2.53	115.61	112.19
2	E	2	NAG	C4-C3-C2	-2.39	107.52	111.02
2	E	2	NAG	C1-O5-C5	2.19	115.17	112.19
2	G	2	NAG	C1-O5-C5	-2.13	109.31	112.19
4	H	3	FUC	C2-C3-C4	-2.08	107.29	110.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

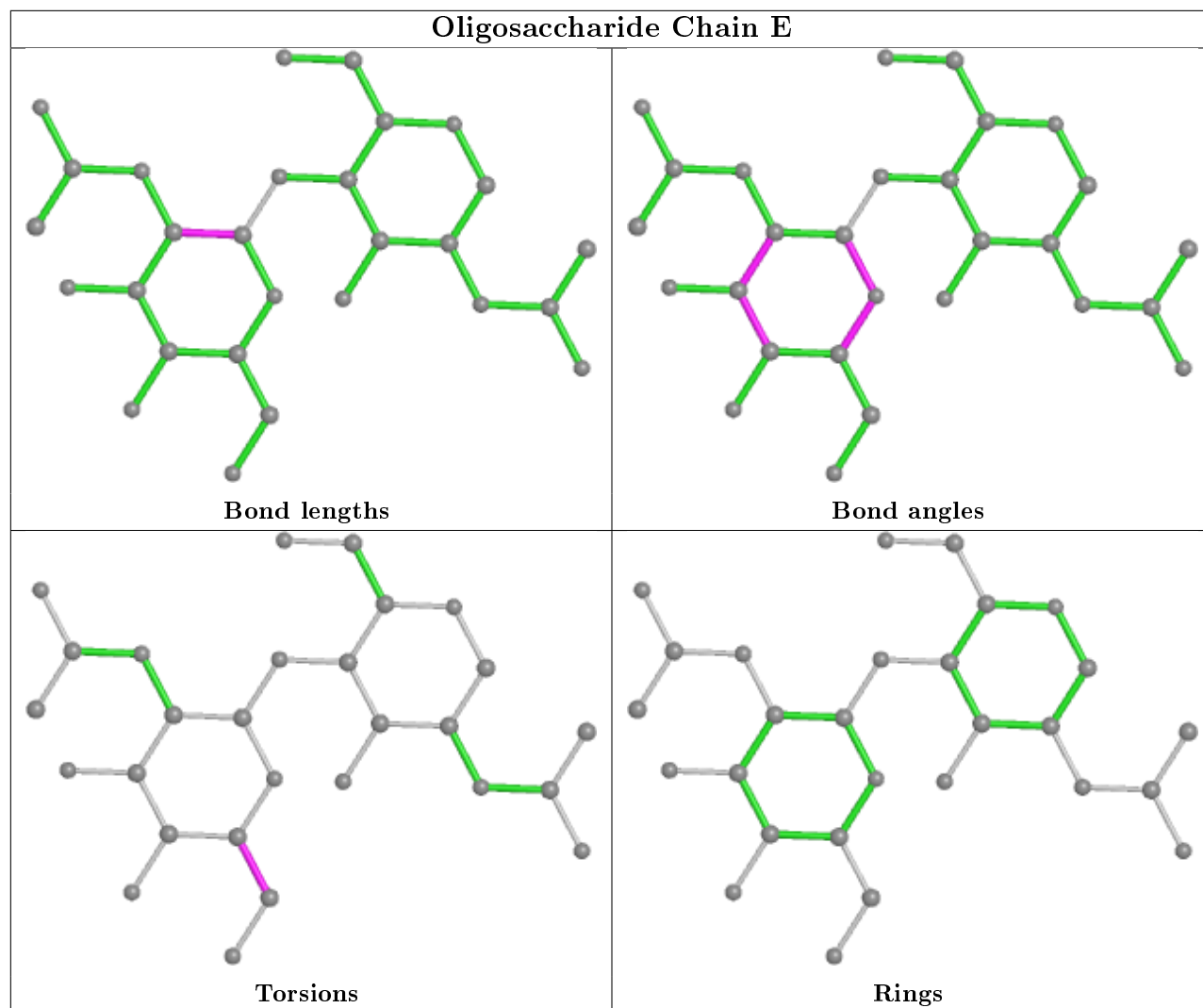
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

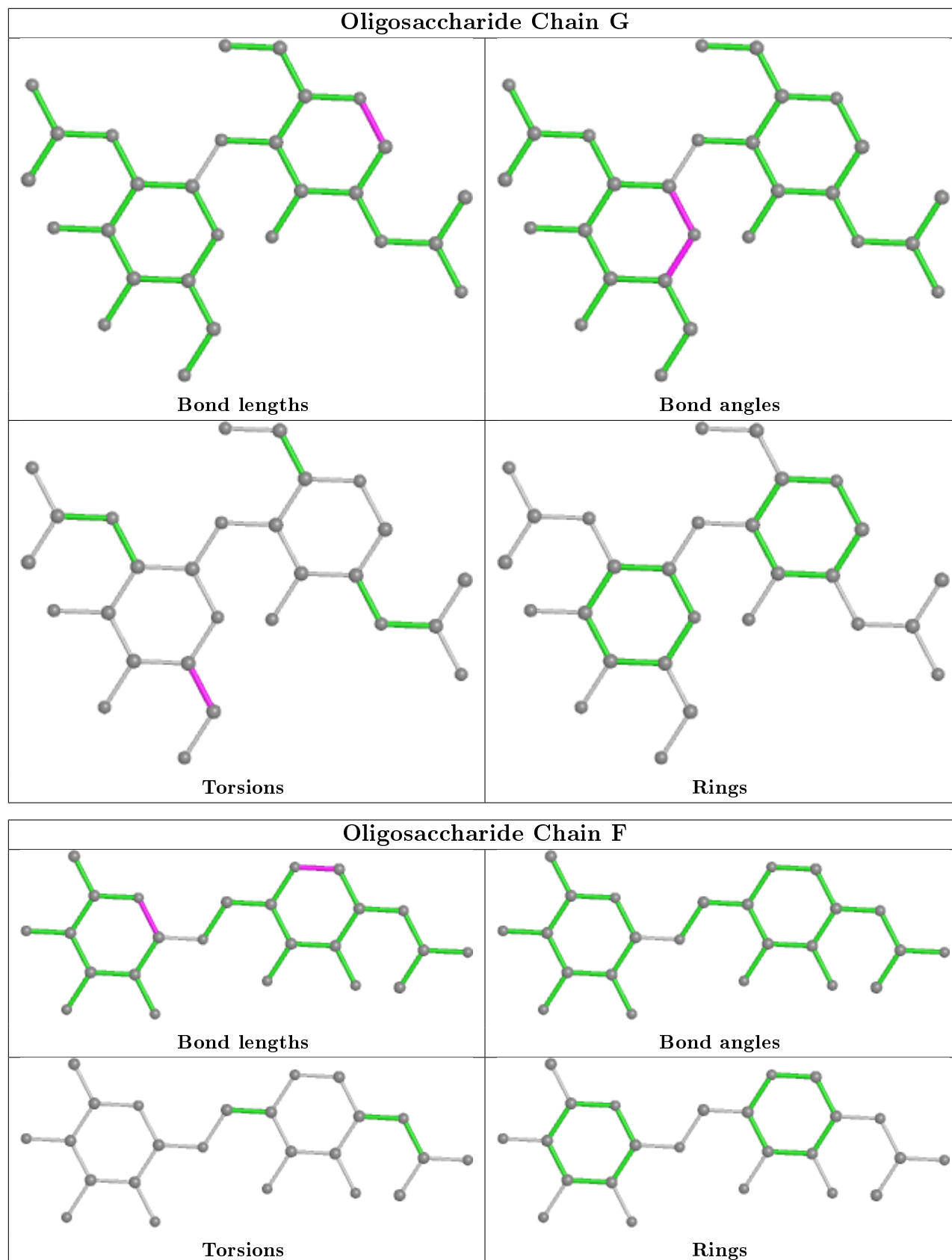
There are no ring outliers.

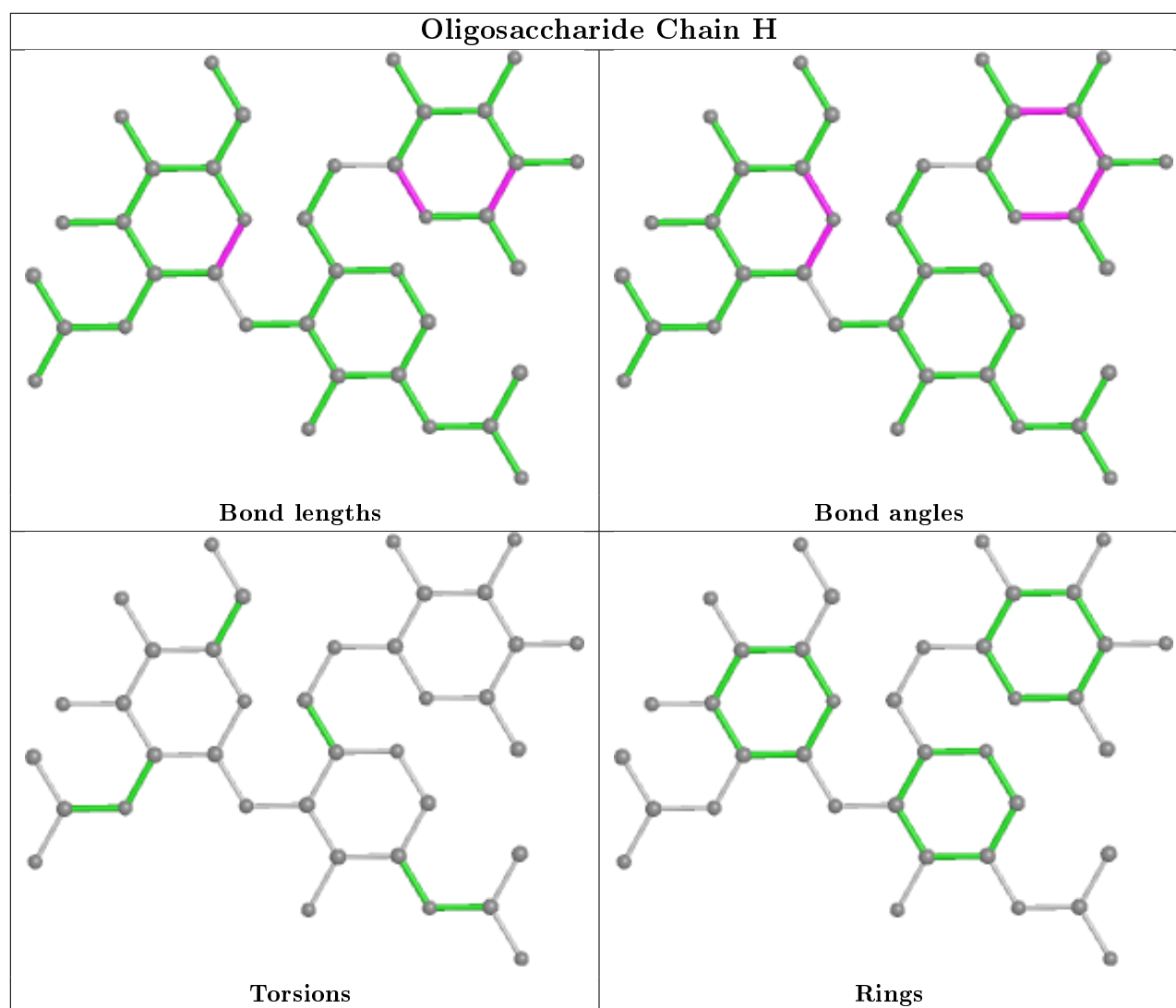
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
4	H	1	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 ⓘ

Of 33 ligands modelled in this entry, 28 are monoatomic - leaving 5 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	$\# Z > 2$
5	NAG	B	402	1	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
5	NAG	C	403	1	14,14,15	0.26	0	17,19,21	0.61	0
5	NAG	D	401	1	14,14,15	0.87	1 (7%)	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	403	1	14,14,15	0.65	1 (7%)	17,19,21	0.77	1 (5%)
5	NAG	B	401	1	14,14,15	0.24	0	17,19,21	0.74	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
5	NAG	B	402	1	-	3/6/23/26	0/1/1/1
5	NAG	C	403	1	-	0/6/23/26	0/1/1/1
5	NAG	D	401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	401	1	-	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)
5	D	401	NAG	O5-C1	3.04	1.48	1.43
5	A	403	NAG	O5-C1	-2.10	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	NAG	C1-O5-C5	3.18	116.50	112.19
5	D	401	NAG	C1-O5-C5	2.89	116.11	112.19
5	A	403	NAG	C1-O5-C5	2.32	115.34	112.19
5	D	401	NAG	C1-C2-N2	2.11	114.09	110.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	401	NAG	O5-C5-C6-O6
5	D	401	NAG	C4-C5-C6-O6
5	A	403	NAG	O5-C5-C6-O6
5	B	402	NAG	O5-C5-C6-O6
5	A	403	NAG	C4-C5-C6-O6
5	B	402	NAG	C4-C5-C6-O6
5	B	402	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	NAG	1	0
5	C	403	NAG	1	0
5	A	403	NAG	2	0
5	B	401	NAG	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	328/341 (96%)	-0.12	11 (3%) 45 52	16, 32, 64, 82	0
1	B	328/341 (96%)	-0.19	7 (2%) 63 70	17, 32, 59, 87	0
1	C	328/341 (96%)	-0.14	6 (1%) 68 74	19, 30, 57, 80	0
1	D	328/341 (96%)	0.68	46 (14%) 2 4	31, 61, 100, 124	0
All	All	1312/1364 (96%)	0.06	70 (5%) 26 33	16, 35, 83, 124	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	PHE	9.8
1	D	59	LEU	7.9
1	D	148	PHE	7.0
1	D	107	ASN	6.6
1	D	29	SER	6.6
1	D	356	PRO	5.3
1	C	29	SER	5.2
1	D	108	LEU	4.8
1	A	29	SER	4.5
1	D	62	ALA	4.4
1	B	29	SER	4.2
1	C	105	PHE	4.1
1	D	58	ASP	4.1
1	D	63	ALA	3.9
1	D	166	GLN	3.8
1	A	356	PRO	3.8
1	D	61	ARG	3.6
1	D	297	GLU	3.6
1	D	123	SER	3.6
1	D	56	ASP	3.6
1	A	148	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	179	GLY	3.5
1	D	177	TYR	3.5
1	B	89	ARG	3.3
1	D	181	TRP	3.3
1	B	105	PHE	3.1
1	C	296	LYS	3.1
1	D	149	GLY	3.0
1	D	66	GLN	2.9
1	D	311	THR	2.9
1	D	151	VAL	2.8
1	D	310	ALA	2.8
1	D	65	ALA	2.8
1	D	147	PRO	2.8
1	A	149	GLY	2.8
1	D	104	ASP	2.8
1	D	172	THR	2.7
1	D	103	CYS	2.7
1	D	46	LEU	2.7
1	D	163	LYS	2.7
1	D	31	PRO	2.6
1	D	154	LYS	2.6
1	D	164	ASN	2.6
1	D	94	PRO	2.6
1	A	177	TYR	2.5
1	D	120	TYR	2.5
1	D	89	ARG	2.5
1	B	297	GLU	2.5
1	D	57	LEU	2.5
1	D	49	LEU	2.5
1	A	297	GLU	2.4
1	A	57	LEU	2.4
1	B	57	LEU	2.4
1	A	296	LYS	2.4
1	A	62	ALA	2.3
1	D	171	GLY	2.3
1	B	296	LYS	2.3
1	D	352	ARG	2.3
1	D	182	THR	2.2
1	D	178	VAL	2.2
1	D	334	PHE	2.2
1	C	57	LEU	2.2
1	C	104	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	89	ARG	2.2
1	D	315	ASN	2.1
1	C	181	TRP	2.1
1	D	231	GLU	2.1
1	D	70	ASP	2.0
1	B	85	LEU	2.0
1	A	181	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

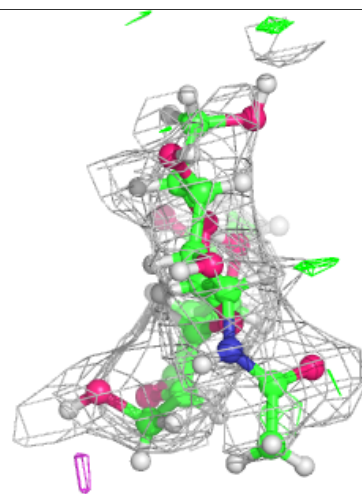
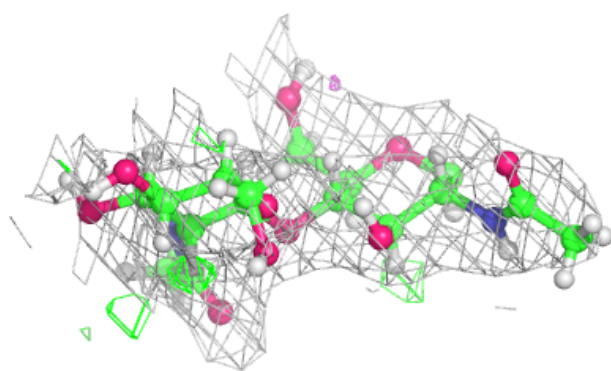
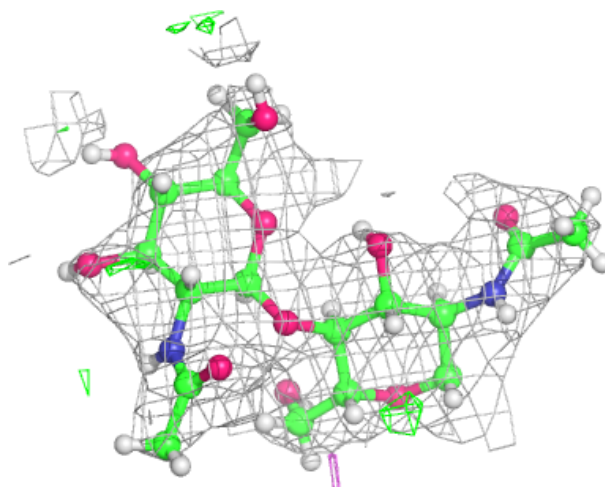
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	2	14/15	0.77	0.35	83,100,119,123	0
4	NAG	H	2	14/15	0.77	0.30	66,121,152,156	0
4	FUC	H	3	10/11	0.80	0.30	94,115,138,138	0
2	NAG	E	2	14/15	0.83	0.31	75,107,131,139	0
3	FUC	F	2	10/11	0.89	0.30	72,88,100,117	0
4	NAG	H	1	14/15	0.93	0.19	50,63,79,96	0
2	NAG	E	1	14/15	0.93	0.15	40,58,70,71	0
2	NAG	G	1	14/15	0.94	0.11	30,59,83,83	0
3	NAG	F	1	14/15	0.94	0.11	38,54,74,85	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.

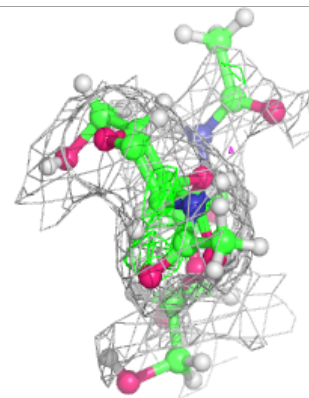
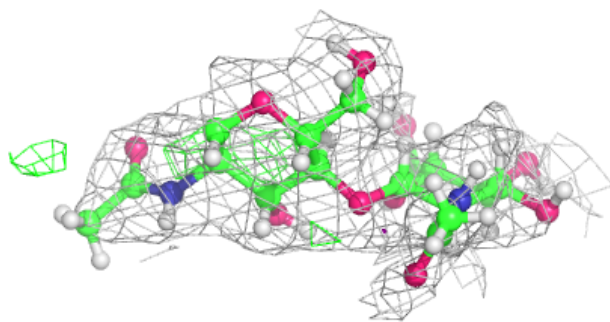
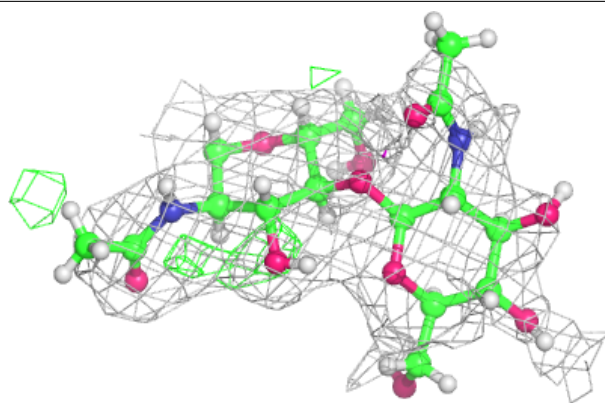
Electron density around Chain E:

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



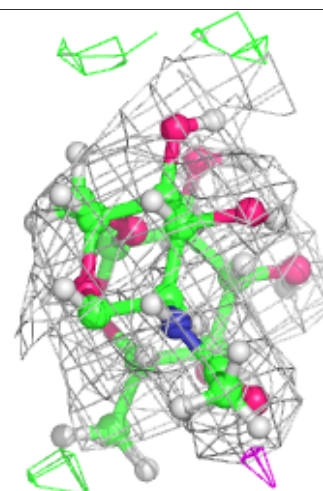
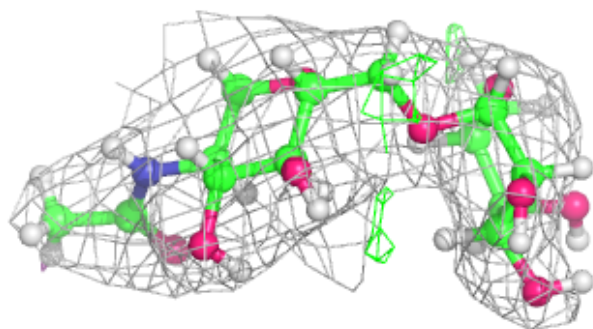
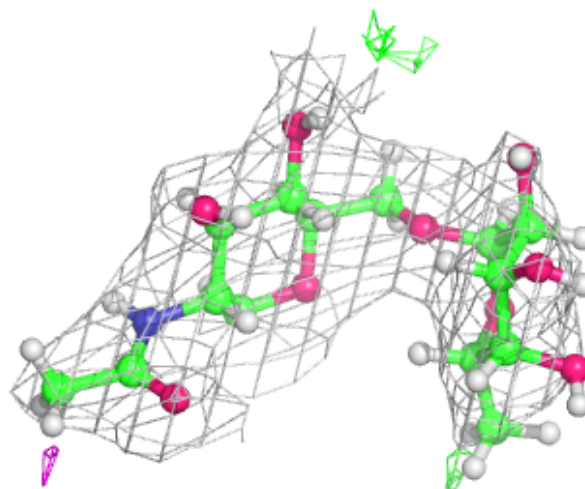
Electron density around Chain G:

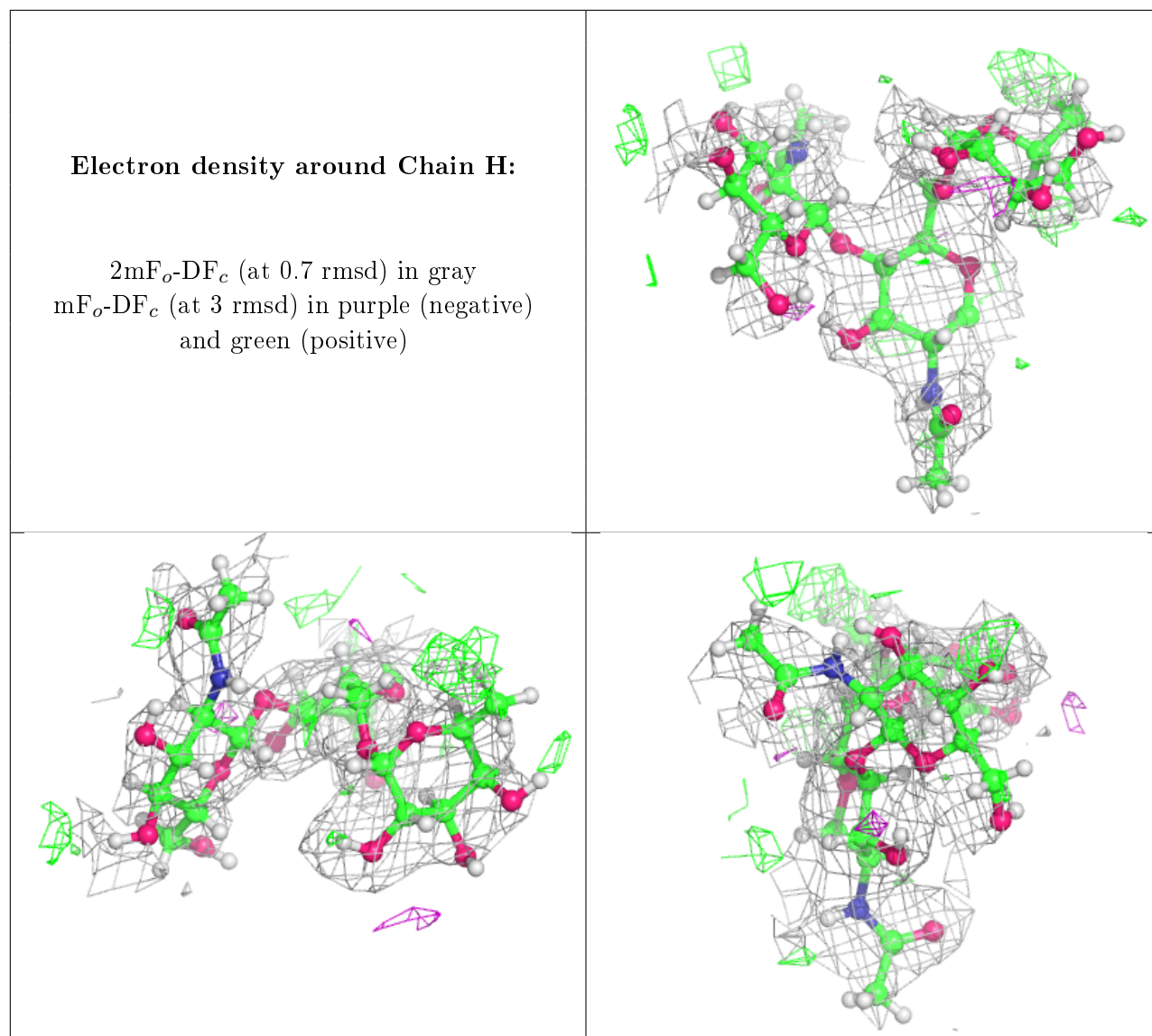
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

$2mF_o-DF_c$ (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
5	NAG	D	401	14/15	0.70	0.23	69,92,131,136	0
6	CL	D	405	1/1	0.80	0.22	82,82,82,82	0
6	CL	B	410	1/1	0.84	0.14	67,67,67,67	0
5	NAG	B	402	14/15	0.85	0.17	54,67,85,96	0
5	NAG	A	403	14/15	0.86	0.13	68,83,106,114	0
6	CL	C	412	1/1	0.86	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	B	401	14/15	0.90	0.17	52,85,105,118	0
5	NAG	C	403	14/15	0.91	0.17	48,60,70,77	0
6	CL	B	411	1/1	0.92	0.07	66,66,66,66	0
6	CL	C	409	1/1	0.93	0.14	51,51,51,51	0
6	CL	B	414	1/1	0.94	0.16	74,74,74,74	0
6	CL	B	409	1/1	0.94	0.09	55,55,55,55	0
6	CL	B	415	1/1	0.95	0.13	63,63,63,63	0
6	CL	B	416	1/1	0.95	0.09	57,57,57,57	0
6	CL	B	412	1/1	0.95	0.06	56,56,56,56	0
6	CL	B	408	1/1	0.95	0.13	58,58,58,58	0
6	CL	A	408	1/1	0.96	0.09	57,57,57,57	0
6	CL	B	413	1/1	0.96	0.06	60,60,60,60	0
6	CL	D	403	1/1	0.97	0.08	55,55,55,55	0
6	CL	C	411	1/1	0.97	0.13	60,60,60,60	0
6	CL	A	407	1/1	0.97	0.06	46,46,46,46	0
6	CL	D	404	1/1	0.98	0.06	63,63,63,63	0
6	CL	B	407	1/1	0.98	0.05	47,47,47,47	0
6	CL	A	406	1/1	0.98	0.06	40,40,40,40	0
6	CL	C	413	1/1	0.98	0.11	61,61,61,61	0
6	CL	C	410	1/1	0.98	0.10	42,42,42,42	0
6	CL	A	405	1/1	0.99	0.13	35,35,35,35	0
6	CL	A	404	1/1	0.99	0.09	26,26,26,26	0
6	CL	B	406	1/1	0.99	0.09	40,40,40,40	0
6	CL	D	402	1/1	0.99	0.11	36,36,36,36	0
6	CL	C	408	1/1	0.99	0.07	44,44,44,44	0
6	CL	C	407	1/1	0.99	0.07	28,28,28,28	0
6	CL	B	405	1/1	1.00	0.07	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.