



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:09 PM BST

PDB ID : 5HQN
Title : Catalytic domain of murine Acid Sphingomyelinase (ASMase, ASM, SMPD1)
Authors : Gorelik, A.; Illes, K.; Heinz, L.X.; Superti-Furga, G.; Nagar, B.
Deposited on : 2016-01-21
Resolution : 2.60 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

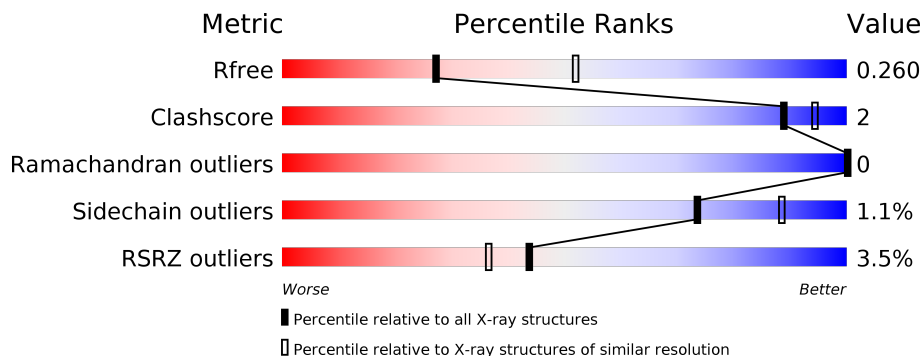
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	473	 3% 89% 5% 7%
1	B	473	 4% 90% 7%
2	C	2	 100%
2	E	2	 100%
2	H	2	 100%
3	D	3	 67% 33%

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Mol	Chain	Length	Quality of chain
3	F	3	 67% 33%
3	G	3	 33% 67%

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
3	FUC	D	3	-	-	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 14288 atoms, of which 6938 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 Spingomyelin phosphodiesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	442	6889	2274	3364	606	630	15	0	0	0
1	B	442	6894	2274	3369	606	630	15	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

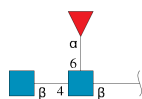
Chain	Residue	Modelled	Actual	Comment	Reference
A	155	ASP	-	expression tag	UNP Q04519
A	156	ARG	-	expression tag	UNP Q04519
A	157	HIS	-	expression tag	UNP Q04519
A	158	HIS	-	expression tag	UNP Q04519
A	159	HIS	-	expression tag	UNP Q04519
A	160	HIS	-	expression tag	UNP Q04519
A	161	HIS	-	expression tag	UNP Q04519
A	162	HIS	-	expression tag	UNP Q04519
A	163	LYS	-	expression tag	UNP Q04519
A	164	LEU	-	expression tag	UNP Q04519
B	155	ASP	-	expression tag	UNP Q04519
B	156	ARG	-	expression tag	UNP Q04519
B	157	HIS	-	expression tag	UNP Q04519
B	158	HIS	-	expression tag	UNP Q04519
B	159	HIS	-	expression tag	UNP Q04519
B	160	HIS	-	expression tag	UNP Q04519
B	161	HIS	-	expression tag	UNP Q04519
B	162	HIS	-	expression tag	UNP Q04519
B	163	LYS	-	expression tag	UNP Q04519
B	164	LEU	-	expression tag	UNP Q04519

- 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	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 3 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.

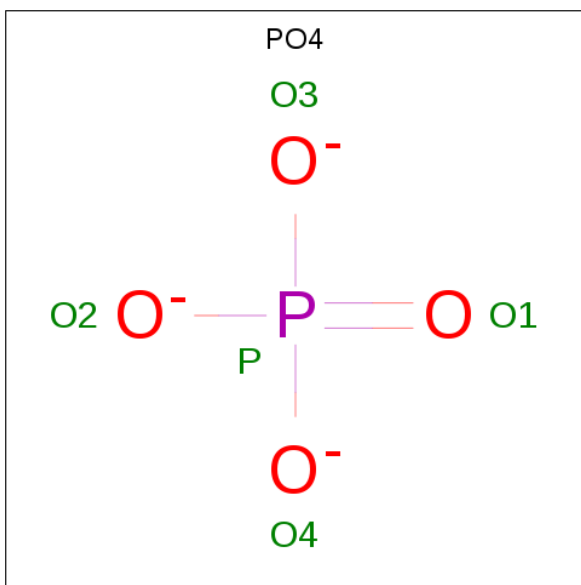


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	D	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
3	F	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			
3	G	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

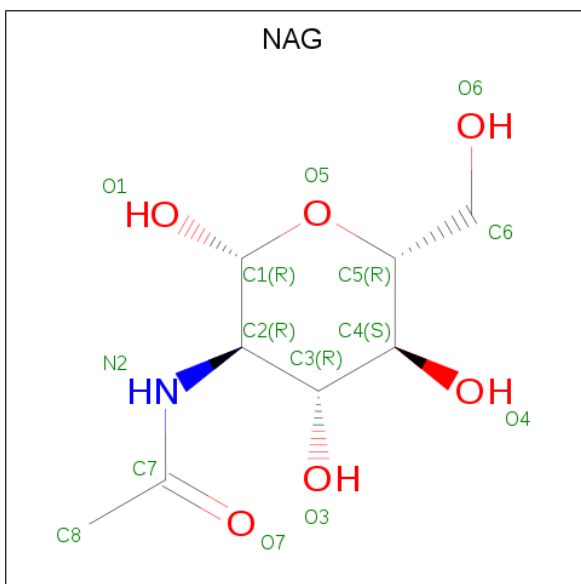
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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


- Molecule 7 is water.

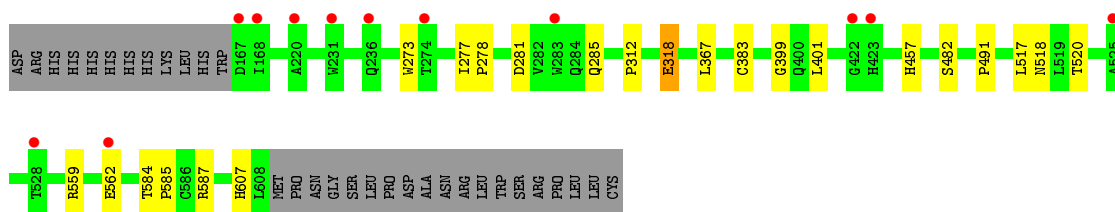
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total 39	O 39	0	0
7	B	35	Total 35	O 35	0	0

3 Residue-property plots [i](#)

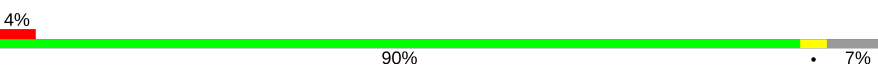
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

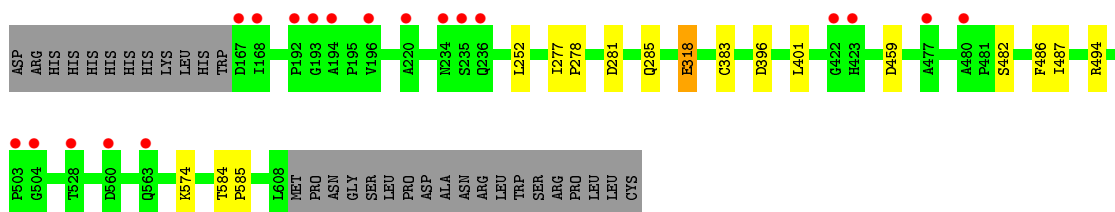
- Molecule 1: SpHINGOMYELIN phosphodiesterase

Chain A: 



- Molecule 1: SpHINGOMYELIN phosphodiesterase

Chain B: 



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

Chain C: 

MAG1
MAG2

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

Chain E: 

MAG1
MAG2

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

Chain H:  100%

■ NAG1
■ NAG2

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

Chain D:  67% 33%

■ NAG1
■ NAG2
■ FUC3

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

Chain F:  67% 33%

■ NAG1
■ NAG2
■ FUC3

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

Chain G:  33% 67%

■ NAG1
■ NAG2
■ FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.84Å 127.30Å 102.52Å 90.00° 121.67° 90.00°	Depositor
Resolution (Å)	38.86 – 2.60 38.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.86-2.60) 88.0 (38.86-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.60 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.213 , 0.258 0.214 , 0.260	Depositor DCC
R_{free} test set	2000 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14288	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.24% 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: FUC, PO4, ZN, 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	0.30	0/3655	0.45	0/5008
1	B	0.29	0/3655	0.43	0/5008
All	All	0.29	0/7310	0.44	0/10016

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	3525	3364	3370	13	0
1	B	3525	3369	3369	8	0
2	C	28	27	25	1	0
2	E	28	27	25	0	0
2	H	28	27	25	0	0
3	D	38	37	34	0	0
3	F	38	36	34	2	0
3	G	38	37	34	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
6	B	14	14	13	0	0
7	A	39	0	0	1	0
7	B	35	0	0	0	0
All	All	7350	6938	6929	27	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 2.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:NAG:O3	3:F:2:NAG:O7	2.00	0.79
3:G:2:NAG:O7	3:G:2:NAG:O3	2.07	0.73
2:C:1:NAG:O3	2:C:2:NAG:O5	2.13	0.63
1:B:396:ASP:O	3:G:3:FUC:O4	2.19	0.61
1:A:562:GLU:OE2	1:A:587:ARG:NH1	2.37	0.57
1:A:318:GLU:OE1	1:A:318:GLU:N	2.38	0.56
3:F:2:NAG:C3	3:F:2:NAG:O7	2.54	0.55
1:A:518:ASN:OD1	1:A:520:THR:OG1	2.24	0.54
1:B:318:GLU:N	1:B:318:GLU:OE1	2.42	0.51
3:G:2:NAG:C7	3:G:2:NAG:HO3	2.16	0.50
1:A:281:ASP:OD2	1:A:285:GLN:NE2	2.46	0.49
1:A:273:TRP:O	1:A:312:PRO:HA	2.14	0.47
1:B:482:SER:O	1:B:574:LYS:NZ	2.35	0.47
3:G:1:NAG:H62	3:G:3:FUC:O2	2.15	0.46
1:B:281:ASP:OD1	1:B:285:GLN:NE2	2.48	0.45
1:A:277:ILE:HB	1:A:278:PRO:HD3	1.98	0.44
1:B:584:THR:N	1:B:585:PRO:CD	2.80	0.44
1:B:277:ILE:HB	1:B:278:PRO:HD3	2.00	0.43
1:A:584:THR:N	1:A:585:PRO:HD2	2.33	0.43
1:A:457:HIS:HA	1:A:482:SER:HB3	2.02	0.42
1:B:459:ASP:OD2	1:B:494:ARG:NH2	2.53	0.41
1:A:584:THR:N	1:A:585:PRO:CD	2.84	0.41
1:A:559:ARG:NH1	1:A:607:HIS:O	2.52	0.41
1:A:491:PRO:HG2	1:A:517:LEU:HB3	2.03	0.41
1:A:584:THR:HG23	1:A:585:PRO:HD3	2.02	0.41
1:A:399:GLY:O	7:A:802:HOH:O	2.21	0.41
1:B:486:PHE:HA	1:B:487:ILE:HA	1.87	0.40

There are no symmetry-related clashes.

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	440/473 (93%)	413 (94%)	27 (6%)	0	100	100
1	B	440/473 (93%)	419 (95%)	21 (5%)	0	100	100
All	All	880/946 (93%)	832 (94%)	48 (6%)	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	376/405 (93%)	372 (99%)	4 (1%)	73	88
1	B	376/405 (93%)	372 (99%)	4 (1%)	73	88
All	All	752/810 (93%)	744 (99%)	8 (1%)	73	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	GLU
1	A	367	LEU
1	A	383	CYS
1	A	401	LEU
1	B	252	LEU
1	B	318	GLU
1	B	383	CYS
1	B	401	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

15 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	0.22	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	D	1	1,3	14,14,15	0.30	0	17,19,21	0.43	0
3	NAG	D	2	3	14,14,15	0.42	0	17,19,21	0.54	0
3	FUC	D	3	3	10,10,11	1.27	1 (10%)	14,14,16	1.09	2 (14%)
2	NAG	E	1	1,2	14,14,15	0.17	0	17,19,21	0.44	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.63	0
3	FUC	F	3	3	10,10,11	0.64	0	14,14,16	0.97	0
3	NAG	G	1	1,3	14,14,15	0.57	1 (7%)	17,19,21	0.75	0
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	0.44	0
3	FUC	G	3	3	10,10,11	1.40	2 (20%)	14,14,16	1.82	5 (35%)
2	NAG	H	1	1,2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	H	2	2	14,14,15	0.37	0	17,19,21	0.41	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1
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	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	FUC	C1-C2	3.33	1.59	1.52
3	G	3	FUC	C1-C2	3.29	1.59	1.52
3	G	3	FUC	O5-C5	2.53	1.49	1.43
3	G	1	NAG	O5-C1	-2.00	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	FUC	C1-O5-C5	4.28	122.49	112.78
3	G	3	FUC	O5-C5-C4	2.91	114.73	109.52
3	G	3	FUC	O2-C2-C1	2.89	115.06	109.15
3	D	3	FUC	C1-C2-C3	2.85	113.17	109.67
3	D	3	FUC	O2-C2-C1	2.17	113.60	109.15
3	G	3	FUC	C1-C2-C3	2.03	112.16	109.67
3	G	3	FUC	O5-C1-C2	2.01	113.87	110.77

There are no chirality outliers.

All (19) torsion outliers are listed below:

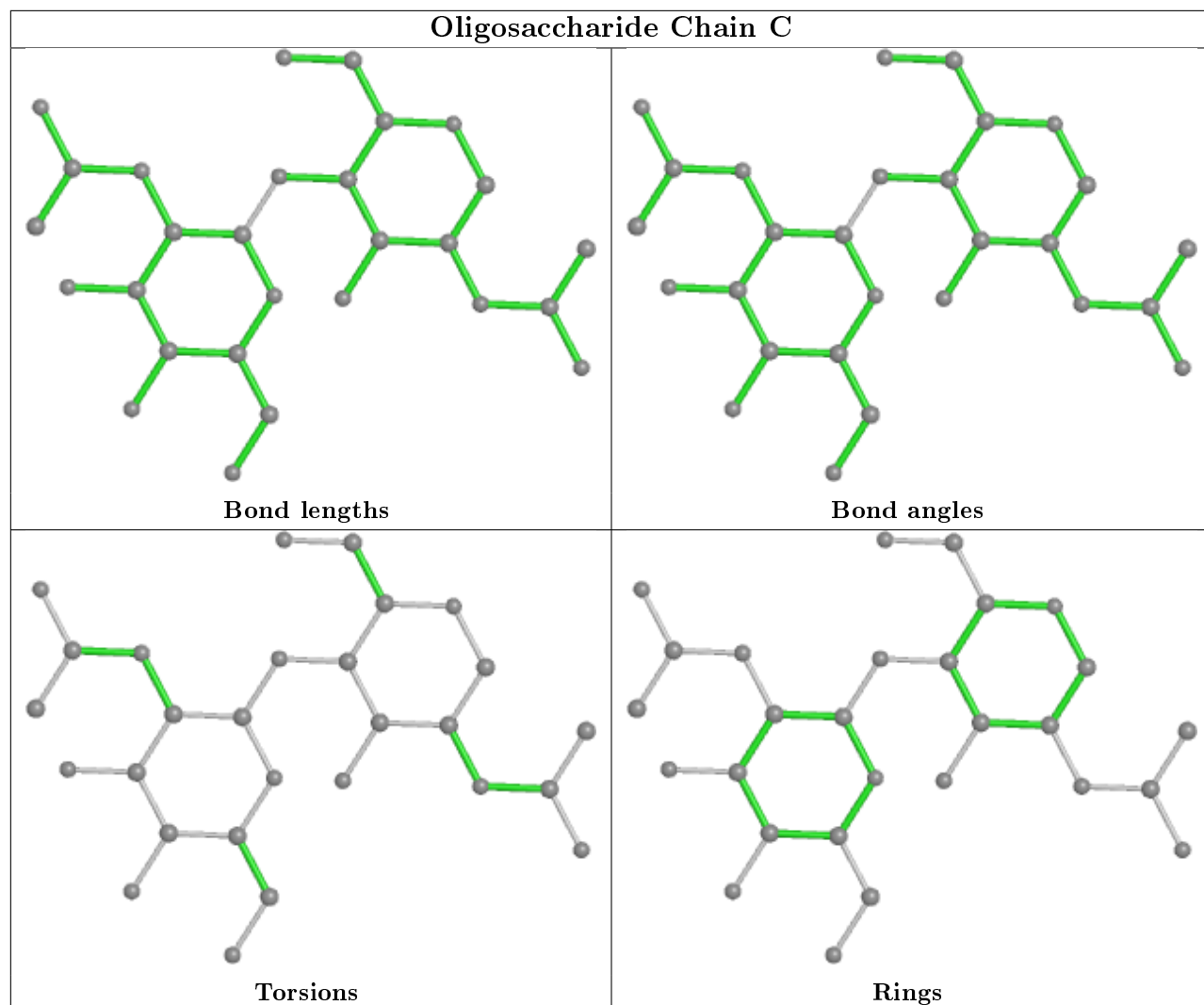
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C3-C2-N2-C7
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
3	G	2	NAG	C4-C5-C6-O6

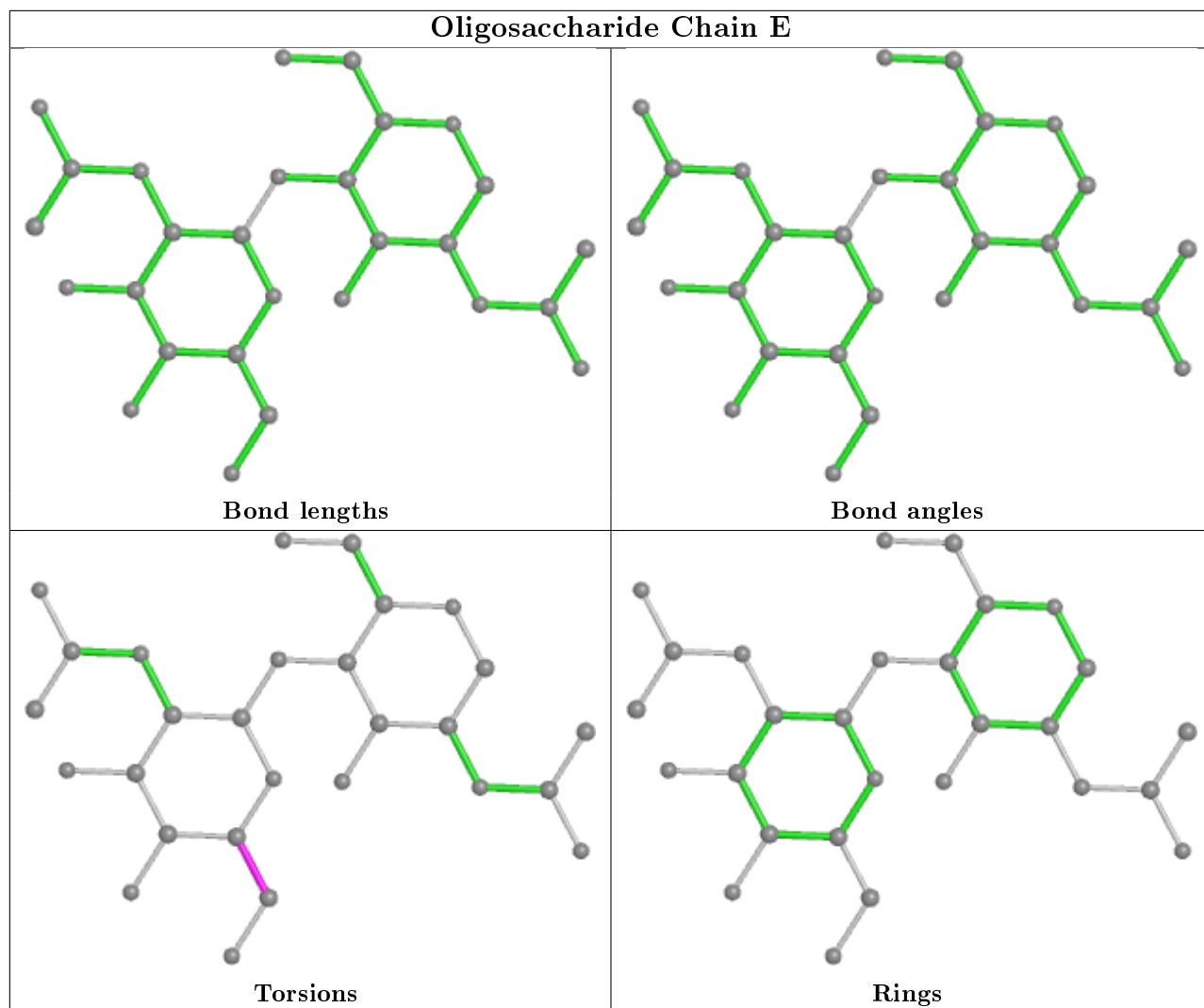
There are no ring outliers.

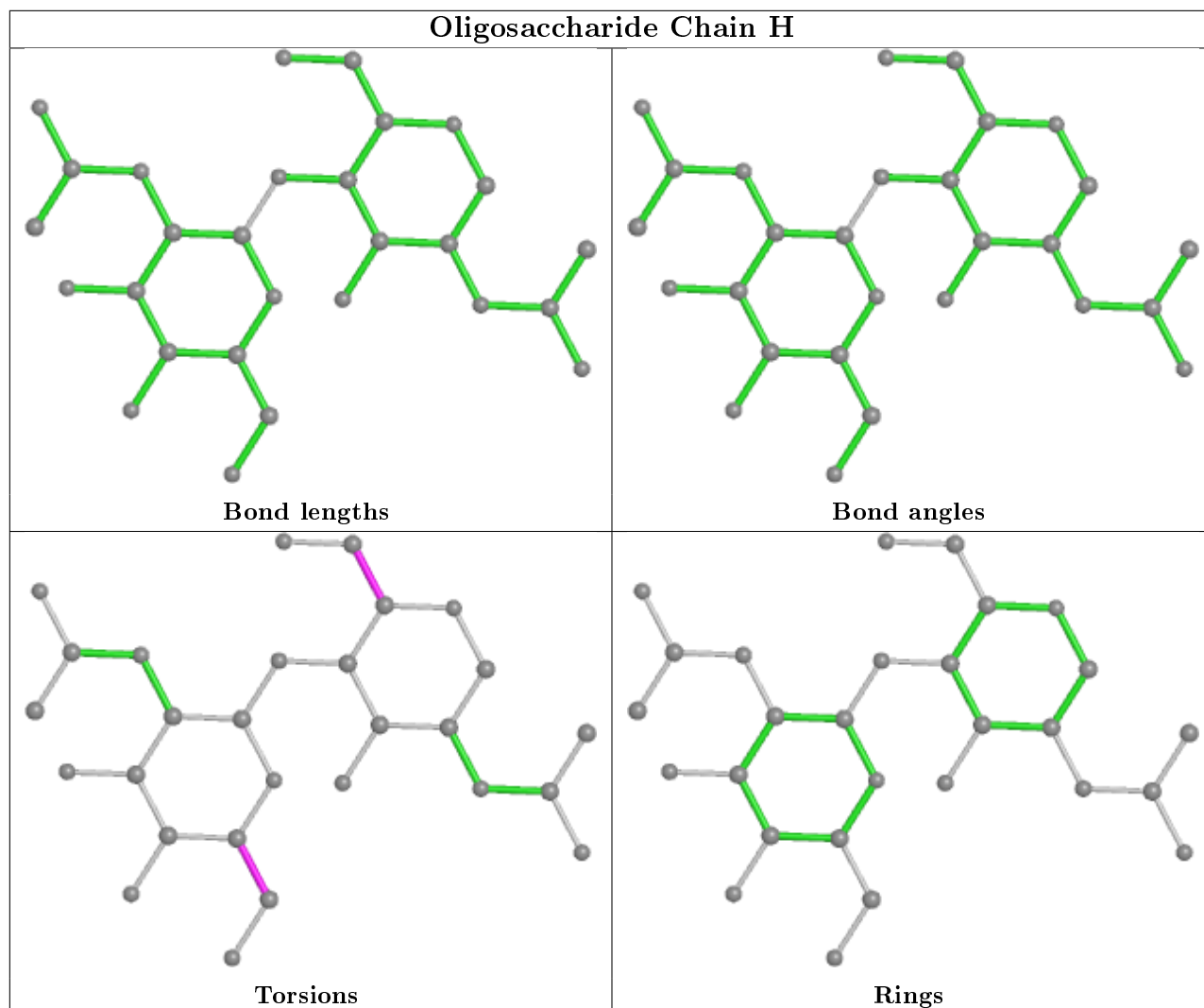
6 monomers are involved in 7 short contacts:

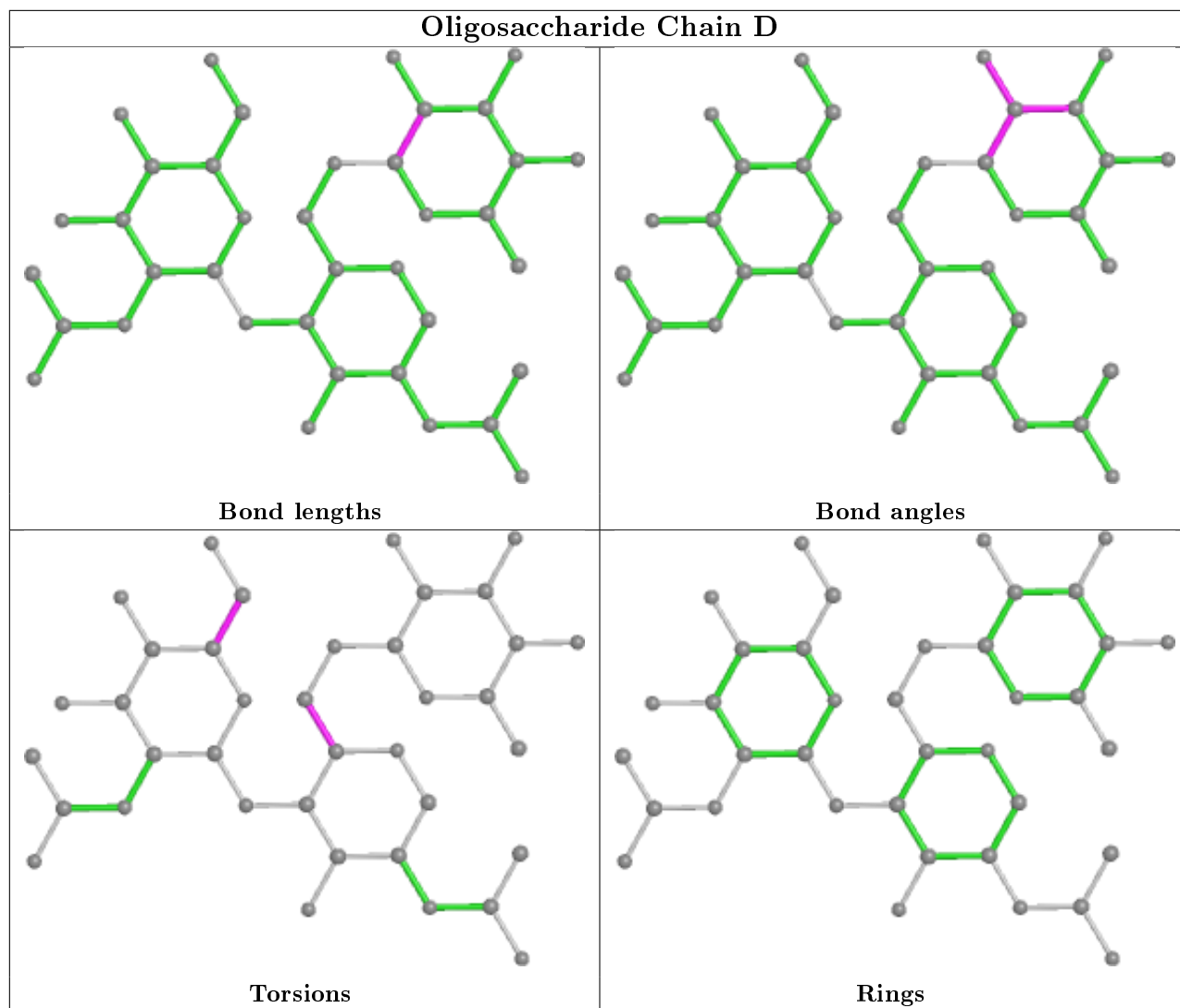
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
3	G	2	NAG	2	0
3	G	3	FUC	2	0
3	F	2	NAG	2	0
3	G	1	NAG	1	0
2	C	1	NAG	1	0

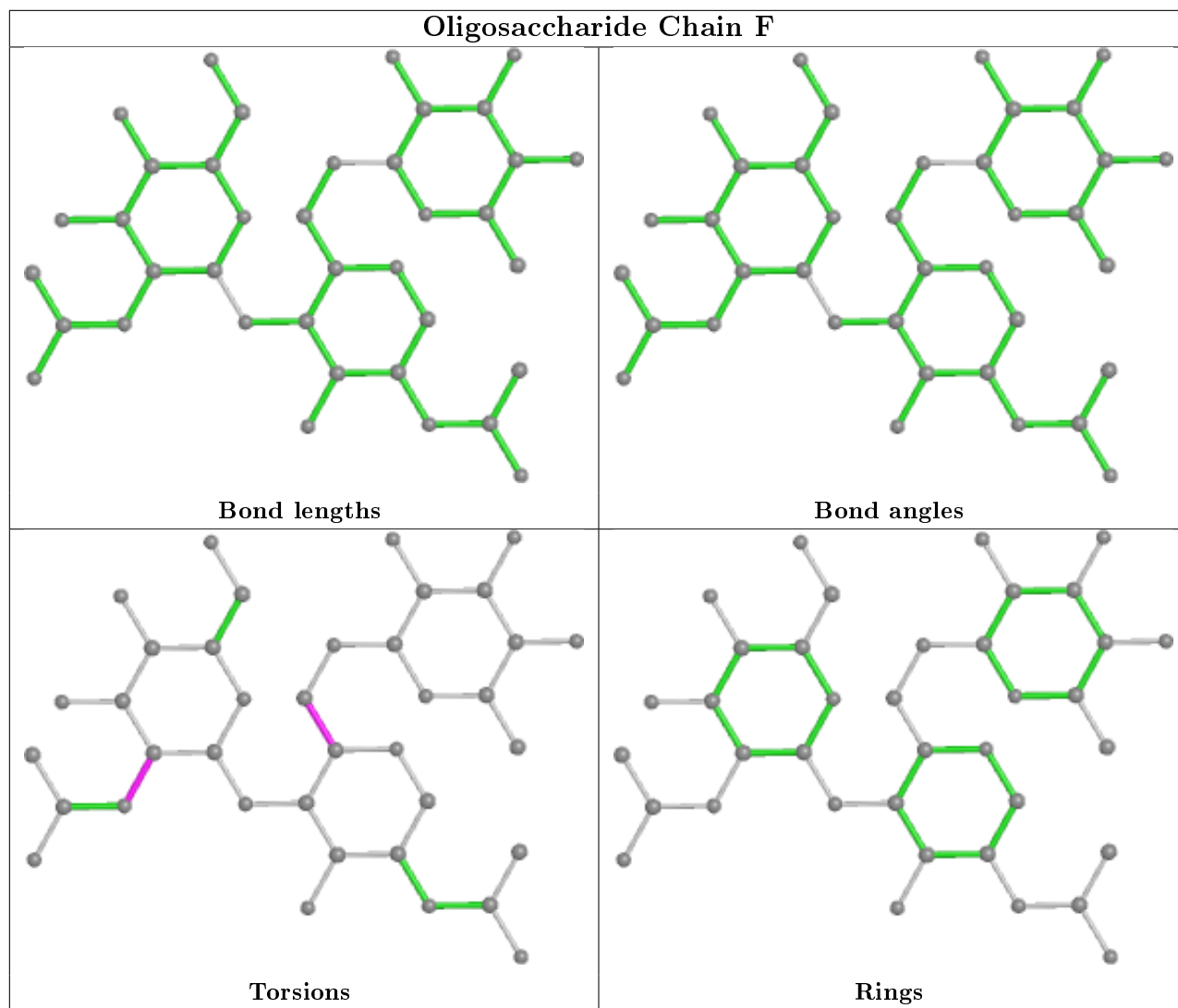
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

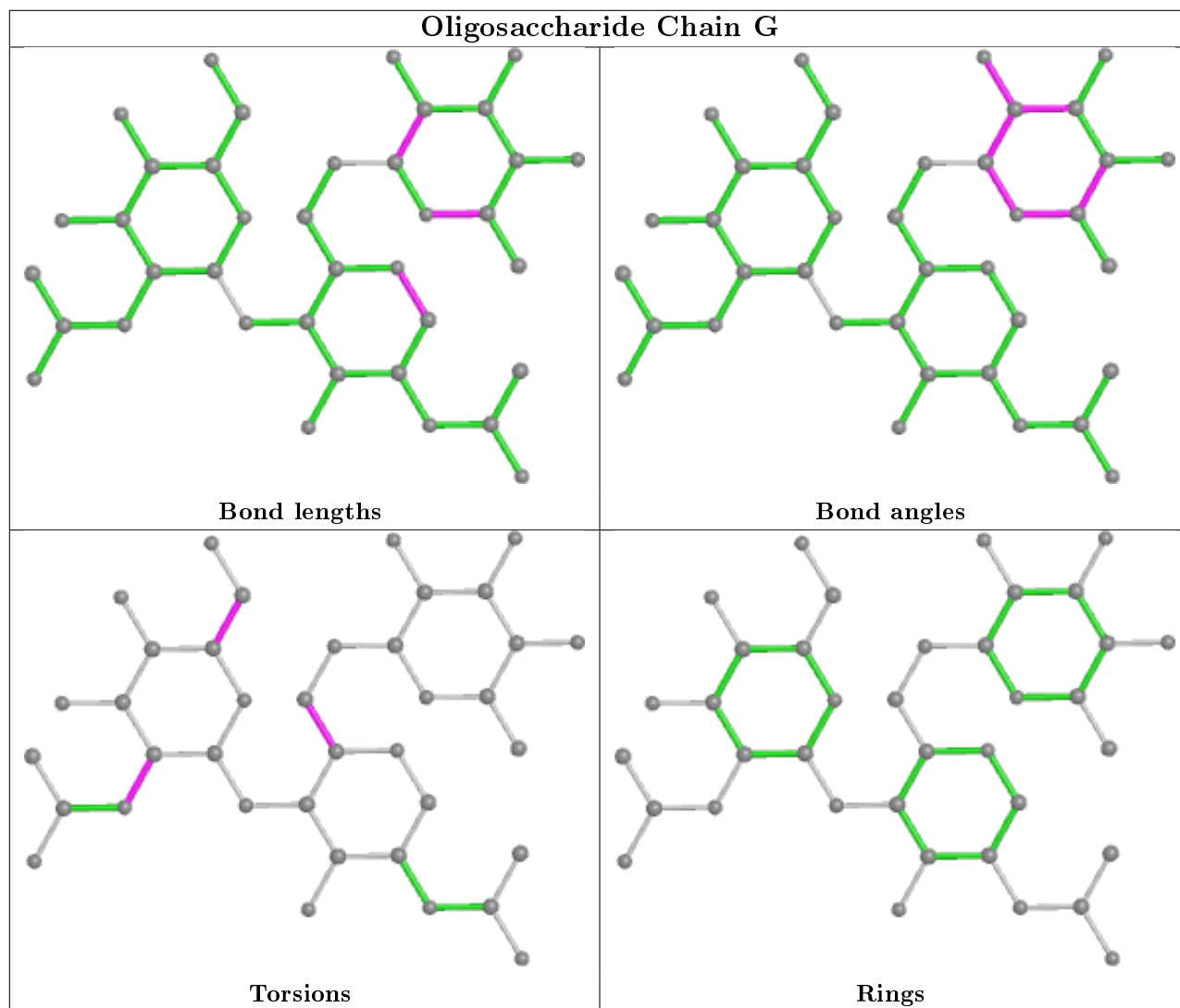












5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 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$
5	PO4	A	710	4	4,4,4	0.84	0	6,6,6	0.78	0
5	PO4	B	712	4	4,4,4	0.88	0	6,6,6	0.75	0
6	NAG	B	703	1	14,14,15	0.68	1 (7%)	17,19,21	0.84	1 (5%)

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	B	703	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	703	NAG	O5-C1	2.06	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	703	NAG	C1-O5-C5	3.21	116.55	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	703	NAG	C1-C2-N2-C7
6	B	703	NAG	C3-C2-N2-C7

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 [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	442/473 (93%)	-0.03	12 (2%) 54 48	31, 46, 68, 114	0
1	B	442/473 (93%)	0.09	19 (4%) 35 28	34, 52, 76, 106	0
All	All	884/946 (93%)	0.03	31 (3%) 44 36	31, 49, 73, 114	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	THR	4.6
1	A	168	ILE	4.2
1	A	167	ASP	3.8
1	B	236	GLN	3.8
1	B	193	GLY	3.5
1	B	167	ASP	3.5
1	A	283	TRP	3.3
1	A	423	HIS	3.1
1	B	192	PRO	3.0
1	B	560	ASP	2.9
1	B	196	VAL	2.8
1	B	504	GLY	2.6
1	B	194	ALA	2.6
1	A	562	GLU	2.5
1	A	236	GLN	2.5
1	B	503	PRO	2.4
1	B	168	ILE	2.4
1	B	422	GLY	2.3
1	B	220	ALA	2.3
1	B	234	ASN	2.3
1	B	235	SER	2.3
1	A	274	THR	2.3
1	A	422	GLY	2.2
1	B	423	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	563	GLN	2.2
1	A	231	TRP	2.2
1	B	480	ALA	2.2
1	A	220	ALA	2.1
1	B	477	ALA	2.1
1	A	525	ALA	2.0
1	B	528	THR	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](#)

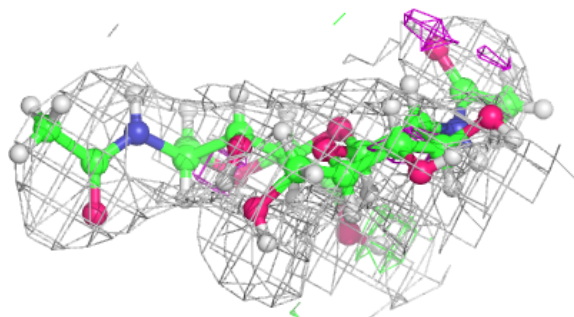
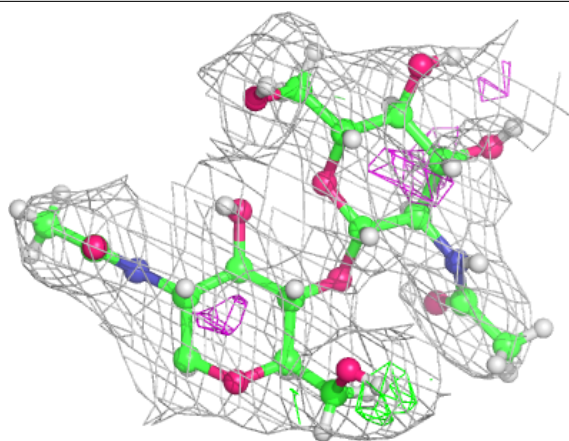
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	D	3	10/11	0.68	0.53	76,94,108,123	0
3	NAG	F	2	14/15	0.69	0.39	75,121,147,154	0
2	NAG	C	2	14/15	0.72	0.33	64,103,125,133	0
2	NAG	C	1	14/15	0.74	0.28	76,96,117,123	0
3	FUC	F	3	10/11	0.79	0.36	120,167,201,208	0
3	NAG	D	2	14/15	0.79	0.35	80,100,121,124	0
2	NAG	E	2	14/15	0.80	0.25	56,82,98,101	0
2	NAG	H	2	14/15	0.81	0.34	76,116,140,142	0
3	NAG	F	1	14/15	0.83	0.24	80,100,121,123	0
3	FUC	G	3	10/11	0.84	0.32	65,81,90,98	0
3	NAG	G	2	14/15	0.85	0.29	81,98,118,123	0
2	NAG	H	1	14/15	0.89	0.20	63,83,105,114	0
3	NAG	G	1	14/15	0.90	0.14	54,67,88,97	0
2	NAG	E	1	14/15	0.90	0.17	44,70,85,87	0
3	NAG	D	1	14/15	0.93	0.20	48,67,87,89	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.

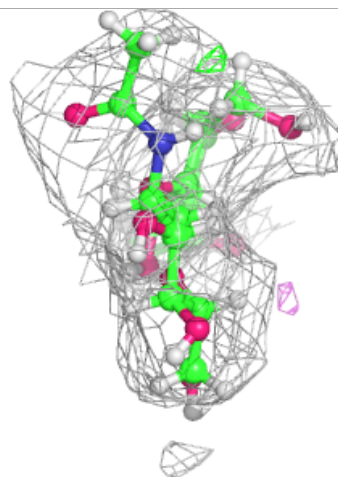
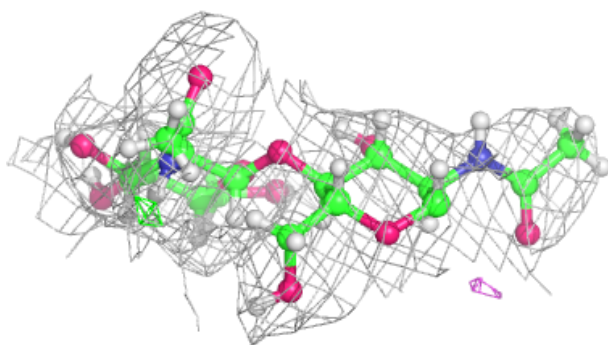
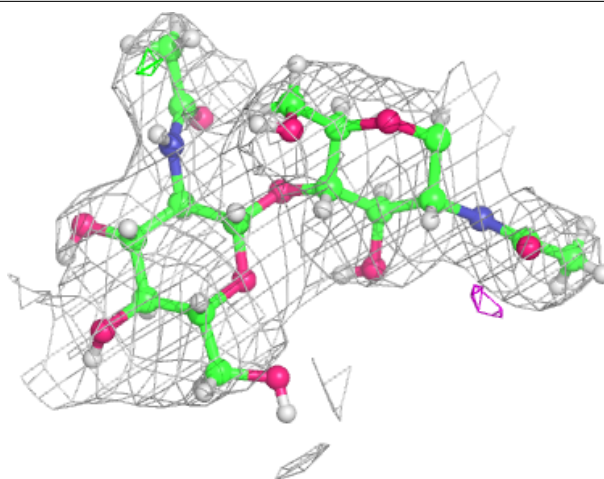
Electron density around Chain C:

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



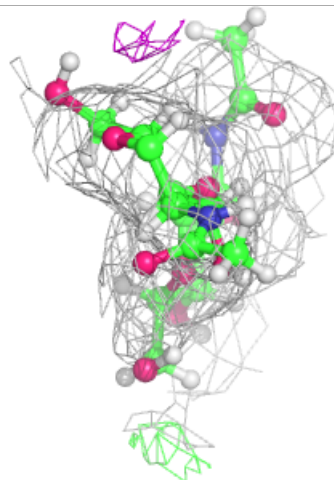
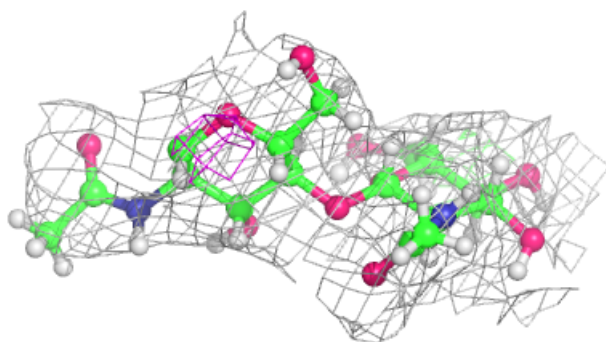
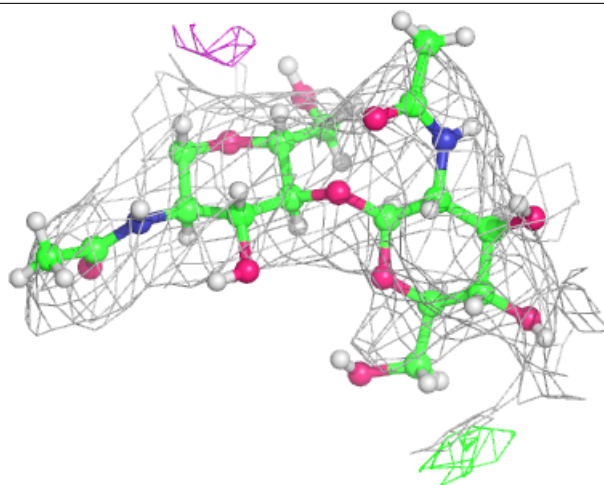
Electron density around Chain E:

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



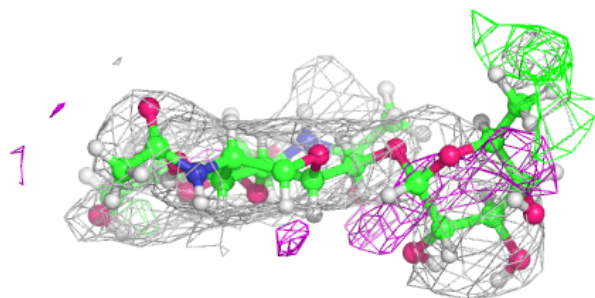
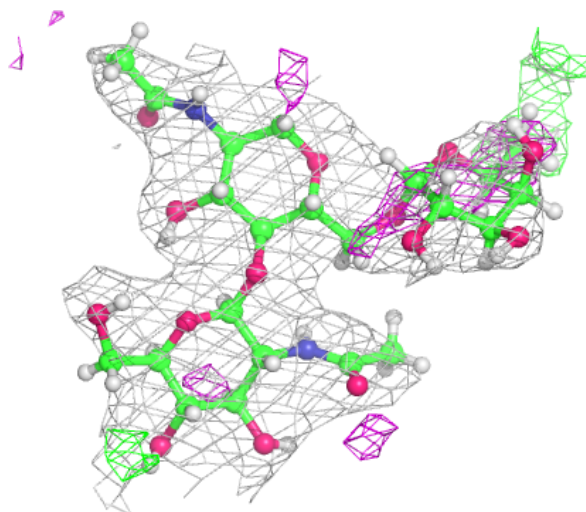
Electron density around Chain H:

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



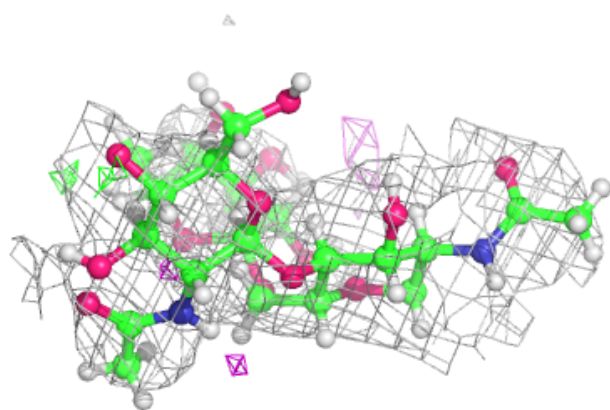
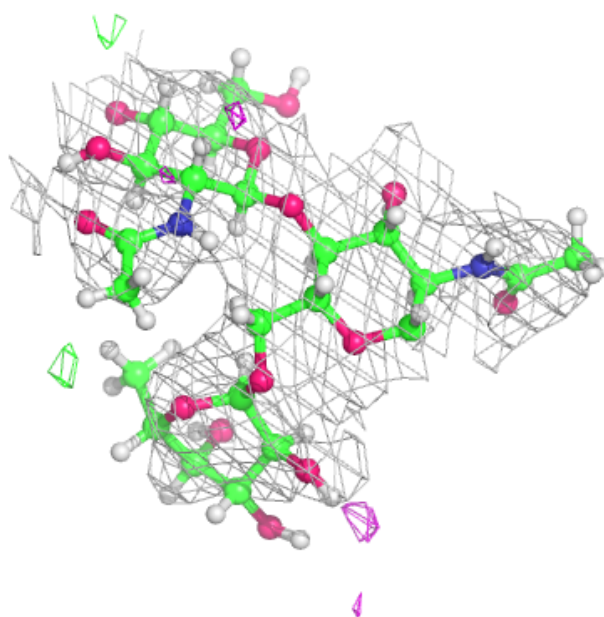
Electron density around Chain D:

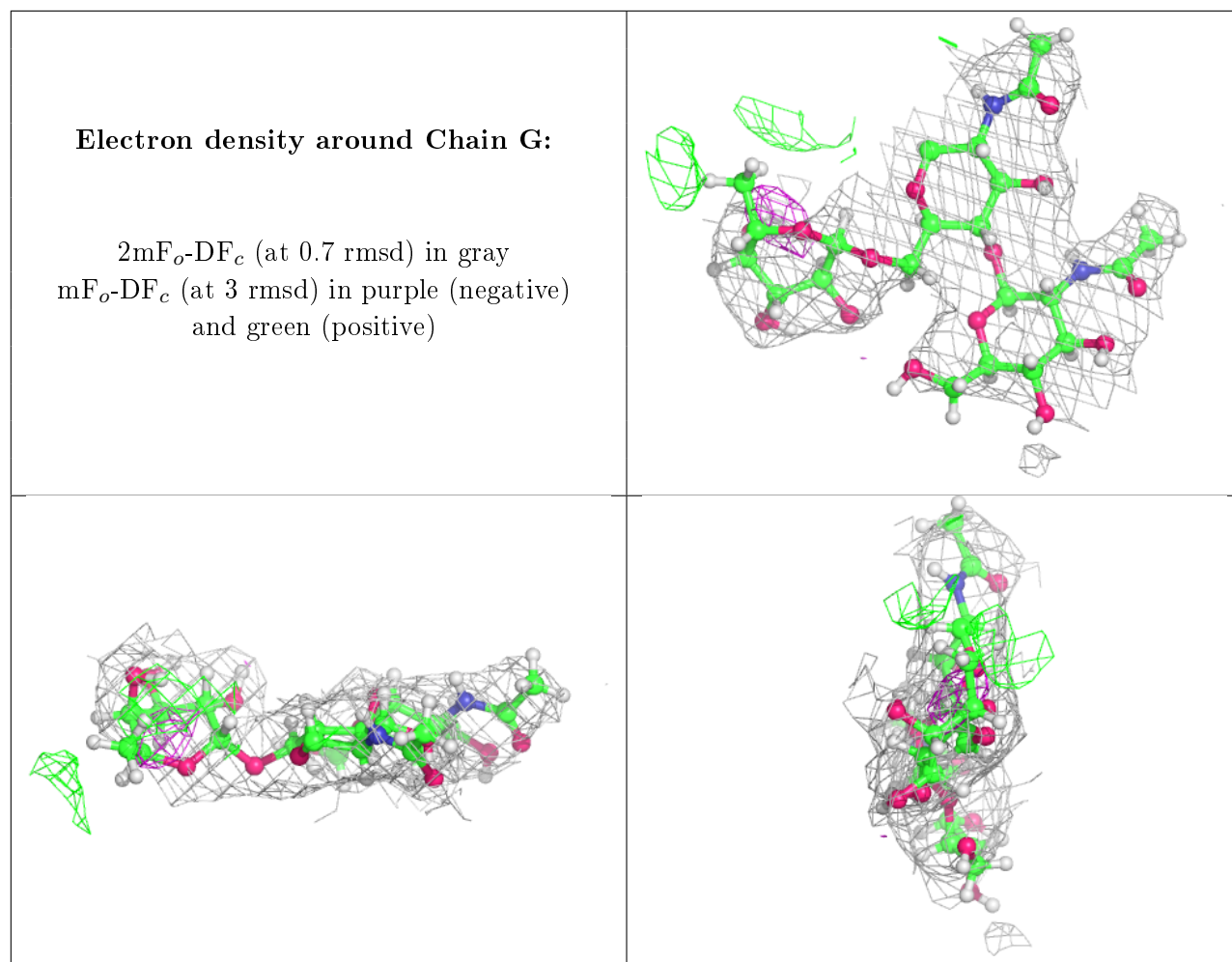
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [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
6	NAG	B	703	14/15	0.55	0.26	100,131,157,165	0
5	PO4	B	712	5/5	0.97	0.27	31,40,43,47	0
5	PO4	A	710	5/5	0.97	0.18	31,37,45,46	0
4	ZN	B	702	1/1	0.99	0.20	27,27,27,27	0
4	ZN	B	701	1/1	0.99	0.17	28,28,28,28	0
4	ZN	A	702	1/1	1.00	0.17	23,23,23,23	0
4	ZN	A	701	1/1	1.00	0.14	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.