wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 11:30 AM EDT

PDB ID	:	6ZPQ
Title	:	Crystal structure of the open conformation of Angiotensin-1 converting enzyme N-domain.
Authors	:	Cozier, G.E.; Acharya, K.R.
Deposited on	:	2020-07-09
Resolution	:	1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

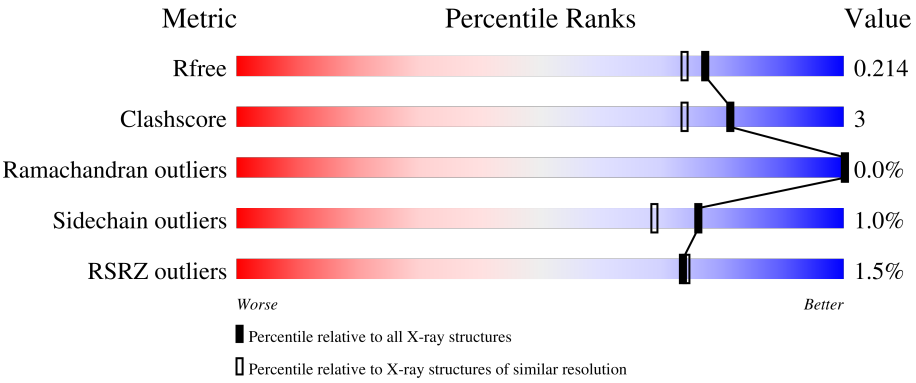
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	629	91% 6% ·
1	B	629	2% 89% 7% ·
1	C	629	% 91% 5% ·
1	D	629	2% 90% 7% ·
2	E	2	100%

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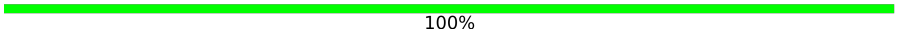
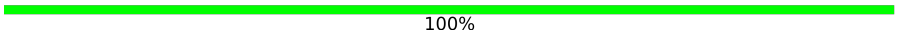
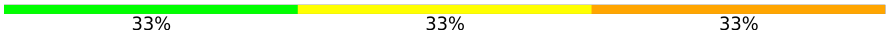
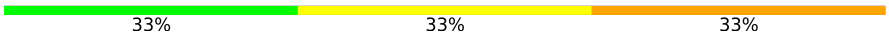
Mol	Chain	Length	Quality of chain
2	H	2	
2	J	2	
3	F	3	
3	G	3	
3	I	3	
3	K	3	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 41964 atoms, of which 19721 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	608	Total	C	H	N	O	S	0	10	0
			9793	3211	4790	859	914	19			
1	B	605	Total	C	H	N	O	S	0	14	0
			9807	3215	4797	861	915	19			
1	C	605	Total	C	H	N	O	S	0	14	0
			9785	3211	4781	857	917	19			
1	D	607	Total	C	H	N	O	S	0	18	0
			9849	3227	4815	866	922	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	-	expression tag	UNP P12821
C	9	GLN	ASN	engineered mutation	UNP P12821
C	25	GLN	ASN	engineered mutation	UNP P12821
C	82	GLN	ASN	engineered mutation	UNP P12821

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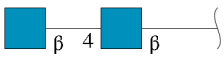
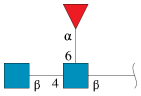
Chain	Residue	Modelled	Actual	Comment	Reference
C	117	GLN	ASN	engineered mutation	UNP P12821
C	131	GLN	ASN	engineered mutation	UNP P12821
C	289	GLN	ASN	engineered mutation	UNP P12821
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
C	629	LEU	-	expression tag	UNP P12821
D	9	GLN	ASN	engineered mutation	UNP P12821
D	25	GLN	ASN	engineered mutation	UNP P12821
D	82	GLN	ASN	engineered mutation	UNP P12821
D	117	GLN	ASN	engineered mutation	UNP P12821
D	131	GLN	ASN	engineered mutation	UNP P12821
D	289	GLN	ASN	engineered mutation	UNP P12821
D	545	ARG	GLN	engineered mutation	UNP P12821
D	576	LEU	PRO	engineered mutation	UNP P12821
D	629	LEU	-	expression tag	UNP P12821

- 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
			53	16	25	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	J	2	Total	C	H	N	O	0	0	0
			53	16	25	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	F	3	Total	C	H	N	O	0	0	0
			59	22	21	2	14			

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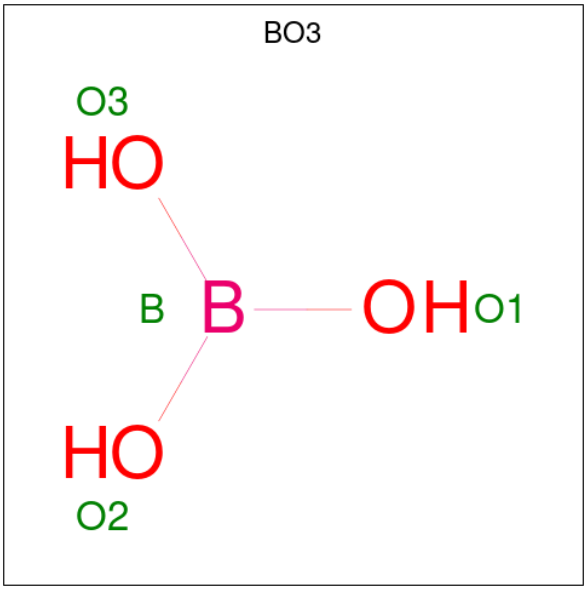
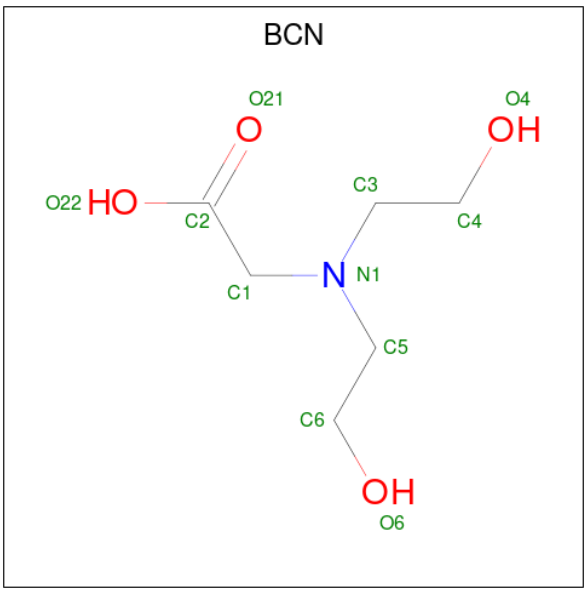
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	H	N	O	0	0	0
			71	22	33	2	14			
3	I	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
3	K	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 4 is BORIC ACID (three-letter code: BO3) (formula: BH_3O_3).



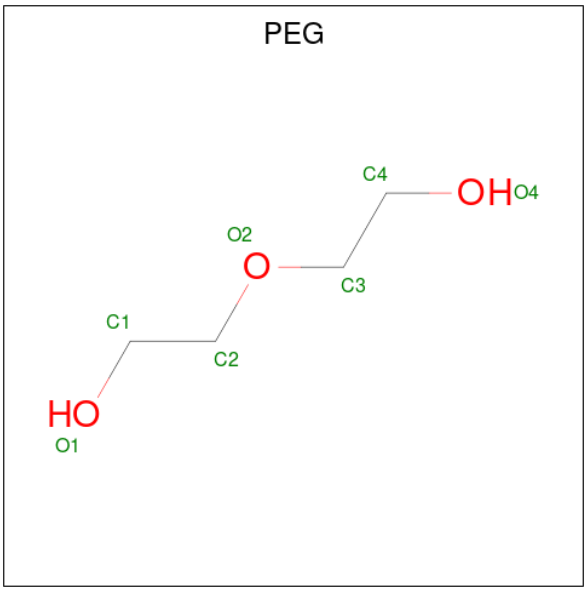
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	B	H	O	0	0
			7	1	3	3		
4	A	1	Total	B	H	O	0	0
			7	1	3	3		
4	A	1	Total	B	H	O	0	0
			7	1	3	3		
4	B	1	Total	B	H	O	0	0
			7	1	3	3		
4	C	1	Total	B	H	O	0	0
			7	1	3	3		
4	D	1	Total	B	H	O	0	0
			7	1	3	3		
4	D	1	Total	B	H	O	0	0
			7	1	3	3		
4	D	1	Total	B	H	O	0	0
			7	1	3	3		

- Molecule 5 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



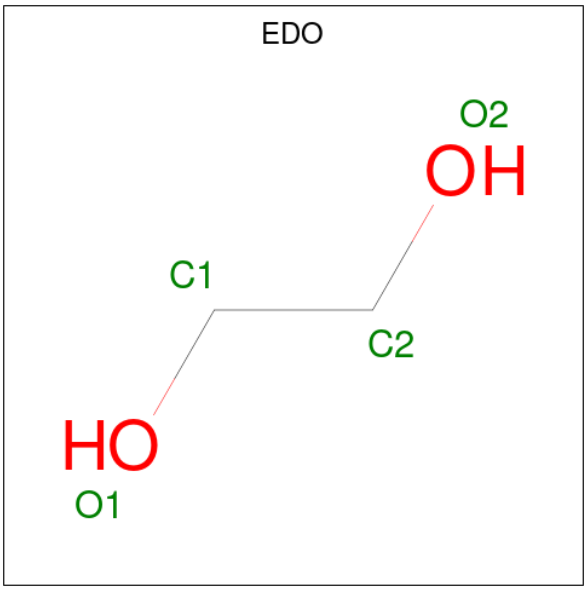
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			23	6	12	1	4		
5	A	1	Total	C	H	N	O	0	0
			23	6	12	1	4		
5	B	1	Total	C	H	N	O	0	0
			23	6	12	1	4		
5	C	1	Total	C	H	N	O	0	0
			23	6	12	1	4		
5	D	1	Total	C	H	N	O	0	0
			23	6	12	1	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



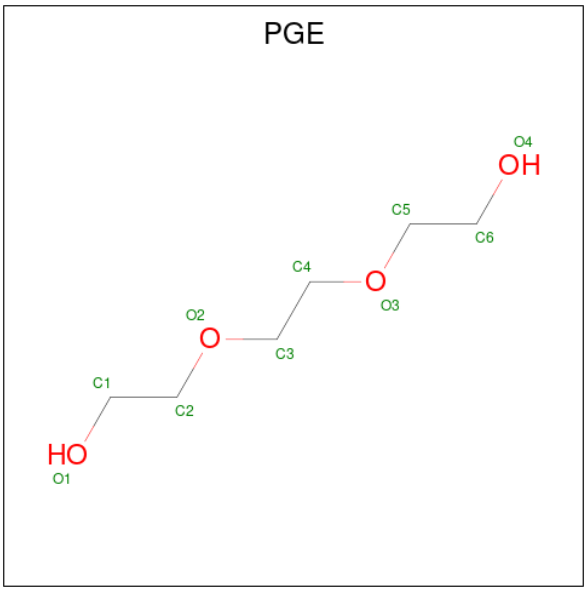
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	1
			20	4	12	4		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	1
			20	4	12	4		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 24 6 14 4	0	0
8	A	1	Total C H O 24 6 14 4	0	0
8	B	1	Total C H O 24 6 14 4	0	0
8	B	1	Total C H O 24 6 14 4	0	0
8	D	1	Total C H O 48 12 28 8	0	1

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Zn 1 1	0	0
9	B	1	Total Zn 1 1	0	0
9	C	1	Total Zn 1 1	0	0
9	D	1	Total Zn 1 1	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0
10	B	1	Total Cl 1 1	0	0
10	C	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

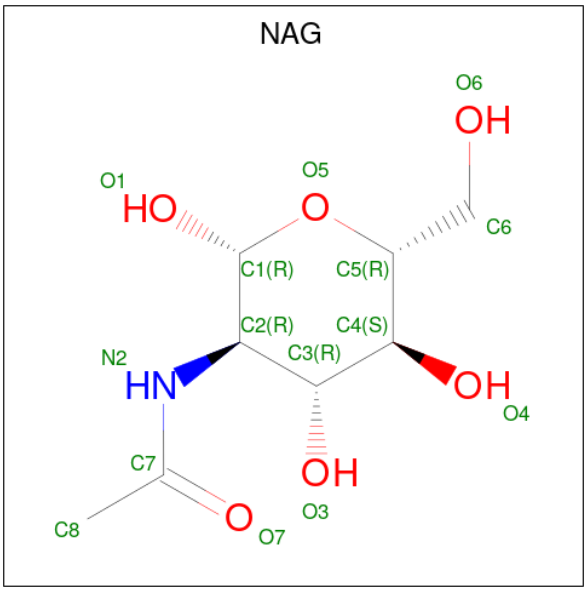
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Mg 1 1	0	0
11	B	1	Total Mg 1 1	0	0
11	C	1	Total Mg 1 1	0	0

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

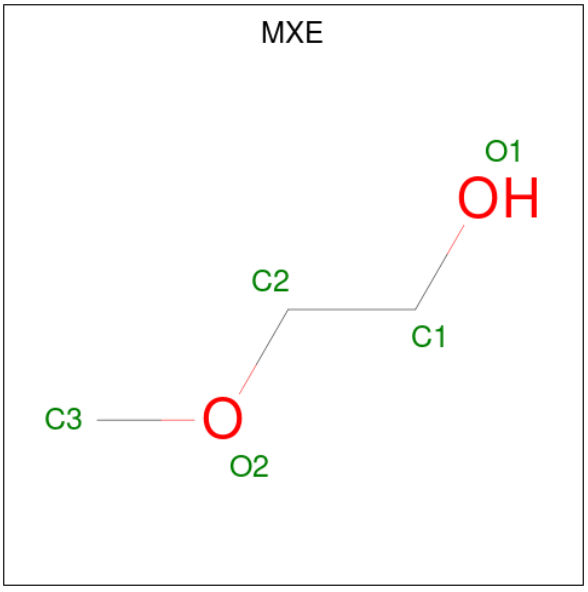
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Ca 1 1	0	0
12	B	1	Total Ca 1 1	0	0
12	C	1	Total Ca 1 1	0	0
12	D	1	Total Ca 1 1	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 14 is 2-METHOXYETHANOL (three-letter code: MXE) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	H	O	0	0
			13	3	8	2		
14	C	1	Total	C	H	O	0	1
			26	6	16	4		

- Molecule 15 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total Na 1 1	0	0

- Molecule 16 is water.

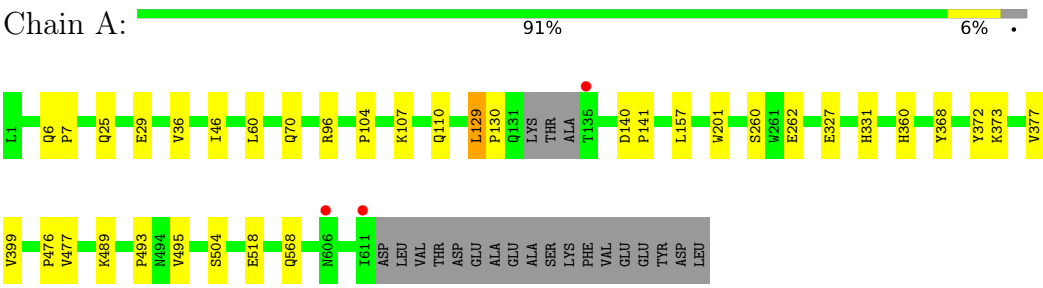
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	435	Total O 436 436	0	1
16	B	403	Total O 403 403	0	0
16	C	389	Total O 389 389	0	0
16	D	443	Total O 444 444	0	1

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.

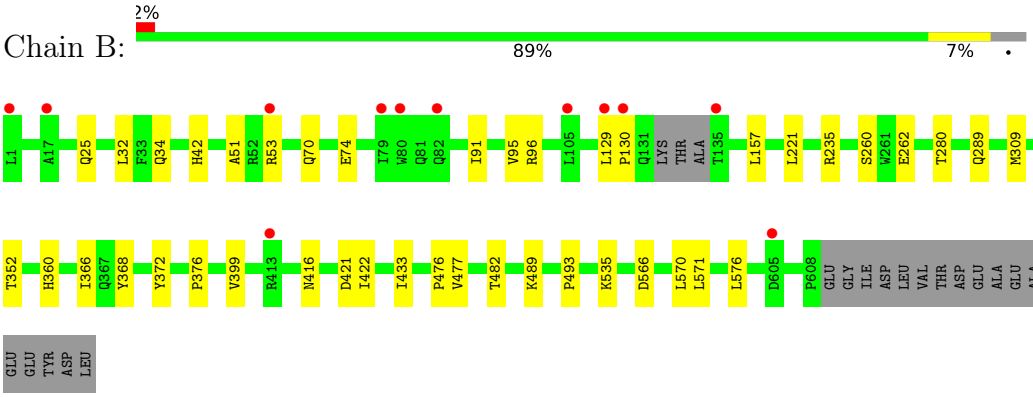
• Molecule 1: Angiotensin-converting enzyme

Chain A:



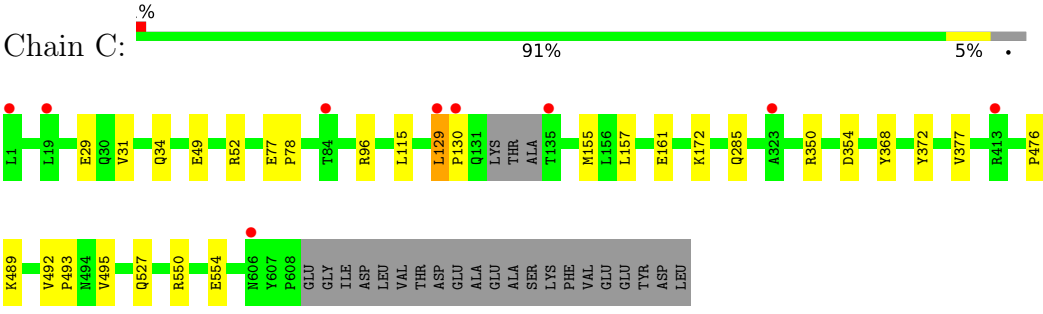
• Molecule 1: Angiotensin-converting enzyme

Chain B:



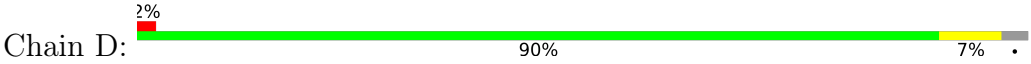
• Molecule 1: Angiotensin-converting enzyme

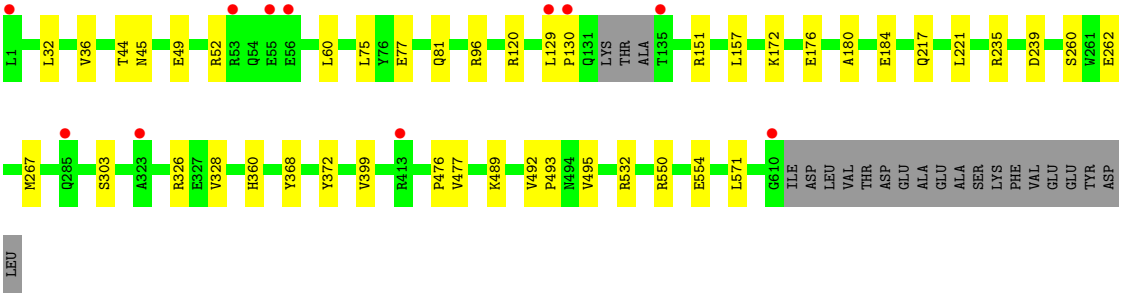
Chain C:



• Molecule 1: Angiotensin-converting enzyme

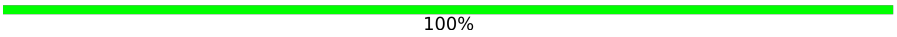
Chain D:





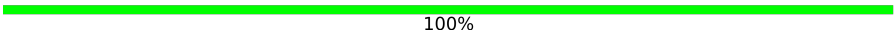
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain H:

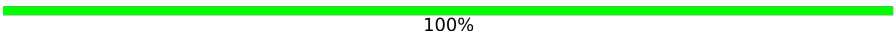


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

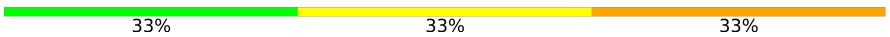
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• 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:

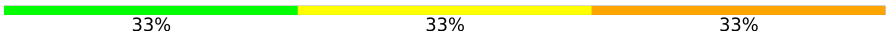


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.68Å 99.93Å 128.70Å 97.76° 90.21° 111.06°	Depositor
Resolution (Å)	80.50 – 1.85 92.26 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (80.50-1.85) 97.6 (92.26-1.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.184 , 0.214 0.185 , 0.214	Depositor DCC
R_{free} test set	2025 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	41964	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, CA, BCN, MXE, ZN, MG, PEG, EDO, BO3, PGE, NAG, CL, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/5211	0.50	0/7097
1	B	0.49	0/5213	0.52	0/7101
1	C	0.45	0/5214	0.49	0/7101
1	D	0.51	0/5259	0.52	0/7162
All	All	0.47	0/20897	0.51	0/28461

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	5003	4790	4743	27	0
1	B	5010	4797	4749	27	0
1	C	5004	4781	4732	17	1
1	D	5034	4815	4742	28	1
2	E	28	25	25	0	0
2	H	28	25	25	0	0
2	J	28	25	25	2	0
3	F	38	21	34	0	0
3	G	38	33	34	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	38	34	34	0	0
3	K	38	34	34	1	0
4	A	12	9	9	0	0
4	B	4	3	3	0	0
4	C	4	3	3	0	0
4	D	12	9	9	1	0
5	A	22	24	20	2	0
5	B	11	12	10	0	0
5	C	11	12	10	0	0
5	D	11	12	11	0	0
6	A	7	10	10	0	0
6	B	21	30	30	2	0
7	A	20	30	30	1	0
7	B	8	12	12	0	0
7	C	16	24	24	0	0
7	D	20	30	29	0	0
8	A	20	28	28	6	0
8	B	20	28	28	0	0
8	D	20	28	28	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	B	14	13	13	0	0
14	B	5	8	8	0	0
14	C	10	16	16	0	0
15	B	1	0	0	0	0
16	A	436	0	0	6	0
16	B	403	0	0	5	0
16	C	389	0	0	6	0
16	D	444	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22243	19721	19508	104	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.

The worst 5 of 104 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:554:GLU:OE1	16:D:801:HOH:O	1.94	0.85
1:A:260:SER:OG	1:A:262:GLU:OE1	2.01	0.77
1:D:260:SER:OG	1:D:262:GLU:OE1	2.03	0.76
1:D:151:ARG:HD2	1:D:267:MET:HE2	1.67	0.76
3:G:1:NAG:H83	3:G:1:NAG:H3	1.69	0.74

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:C:285:GLN:OE1	1:D:235[B]:ARG:HH21[1_556]	1.56	0.04

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	614/629 (98%)	602 (98%)	12 (2%)	0	100 100
1	B	615/629 (98%)	602 (98%)	13 (2%)	0	100 100
1	C	615/629 (98%)	602 (98%)	13 (2%)	0	100 100
1	D	621/629 (99%)	607 (98%)	13 (2%)	1 (0%)	47 33
All	All	2465/2516 (98%)	2413 (98%)	51 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	45	ASN

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	533/541 (98%)	528 (99%)	5 (1%)	78	72
1	B	534/541 (99%)	527 (99%)	7 (1%)	69	58
1	C	533/541 (98%)	528 (99%)	5 (1%)	78	72
1	D	538/541 (99%)	535 (99%)	3 (1%)	86	83
All	All	2138/2164 (99%)	2118 (99%)	20 (1%)	76	72

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	155	MET
1	D	96	ARG
1	D	372	TYR
1	D	368	TYR
1	B	289	GLN

Sometimes 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)

18 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	0.22	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	F	1	1,3	14,14,15	0.41	0	17,19,21	0.46	0
3	NAG	F	2	3	14,14,15	0.71	0	17,19,21	0.51	0
3	FUC	F	3	3	10,10,11	0.77	0	14,14,16	0.79	0
3	NAG	G	1	1,3	14,14,15	0.63	0	17,19,21	1.14	1 (5%)
3	NAG	G	2	3	14,14,15	0.93	1 (7%)	17,19,21	0.87	0
3	FUC	G	3	3	10,10,11	0.85	0	14,14,16	0.84	0
2	NAG	H	1	1,2	14,14,15	0.17	0	17,19,21	0.60	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.46	0
3	NAG	I	1	1,3	14,14,15	0.50	0	17,19,21	0.51	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.60	0
3	FUC	I	3	3	10,10,11	0.69	0	14,14,16	0.79	0
2	NAG	J	1	1,2	14,14,15	0.75	1 (7%)	17,19,21	0.82	1 (5%)
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.43	0
3	NAG	K	1	1,3	14,14,15	0.31	0	17,19,21	0.77	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	FUC	K	3	3	10,10,11	1.02	0	14,14,16	1.21	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	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	FUC	K	3	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	C1-C2	3.15	1.57	1.52
2	J	1	NAG	O5-C1	-2.62	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C2-N2-C7	3.23	127.50	122.90
3	K	3	FUC	C1-C2-C3	2.46	112.69	109.67
2	J	1	NAG	C1-O5-C5	2.39	115.43	112.19
3	K	3	FUC	C1-O5-C5	2.26	117.90	112.78

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6

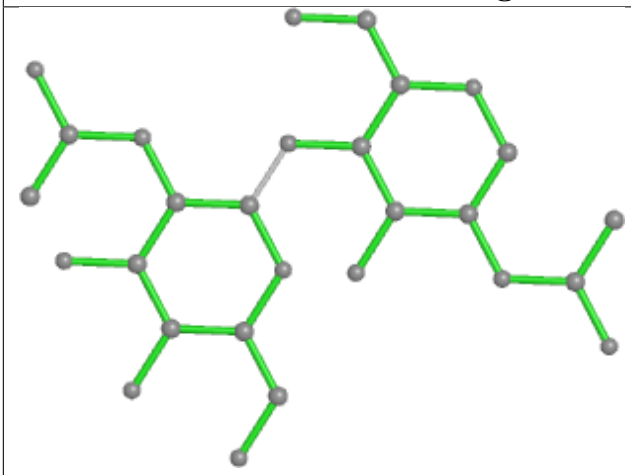
There are no ring outliers.

5 monomers are involved in 7 short contacts:

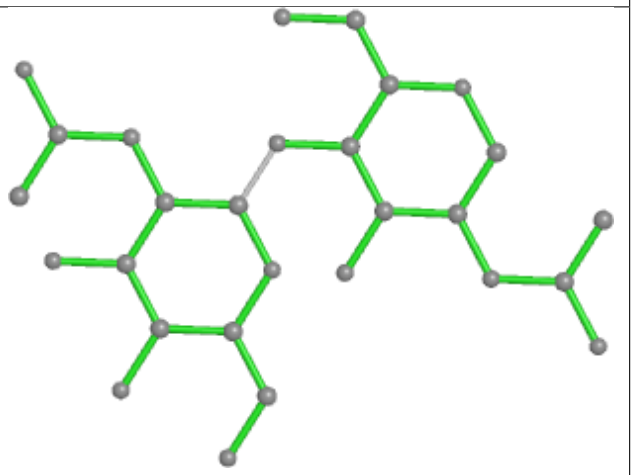
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	4	0
3	K	1	NAG	1	0
2	J	2	NAG	1	0
2	J	1	NAG	2	0
3	K	3	FUC	1	0

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

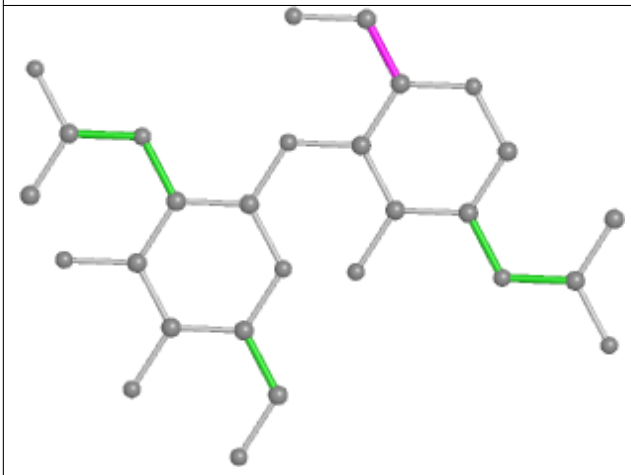
Oligosaccharide Chain E



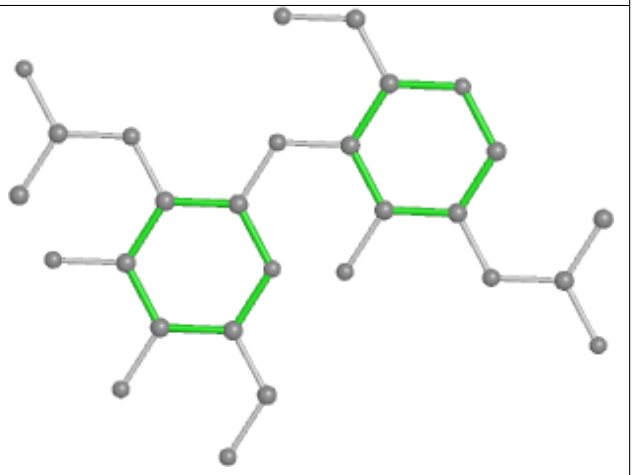
Bond lengths



Bond angles

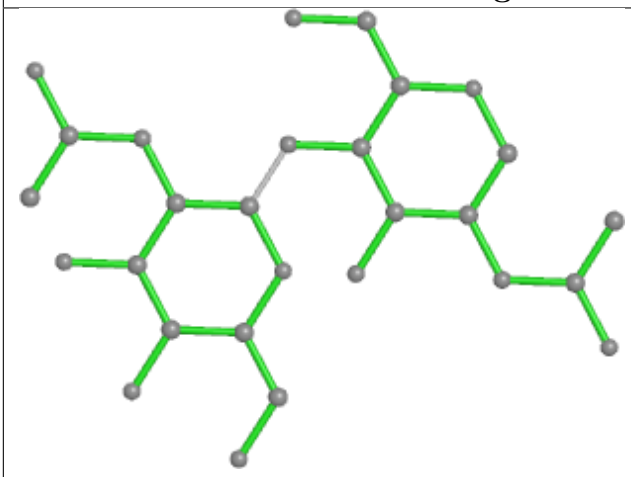


Torsions

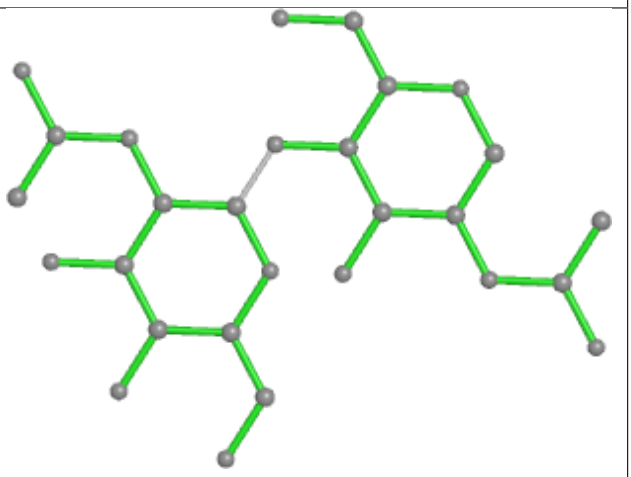


Rings

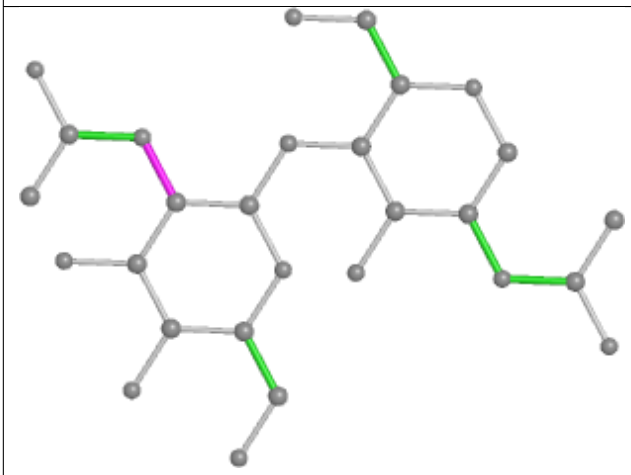
Oligosaccharide Chain H



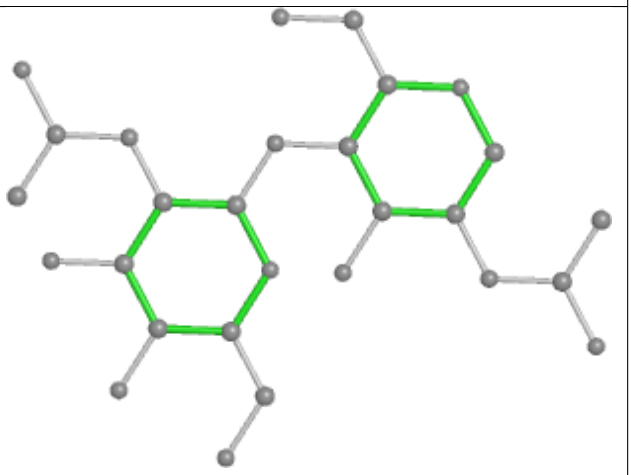
Bond lengths



Bond angles

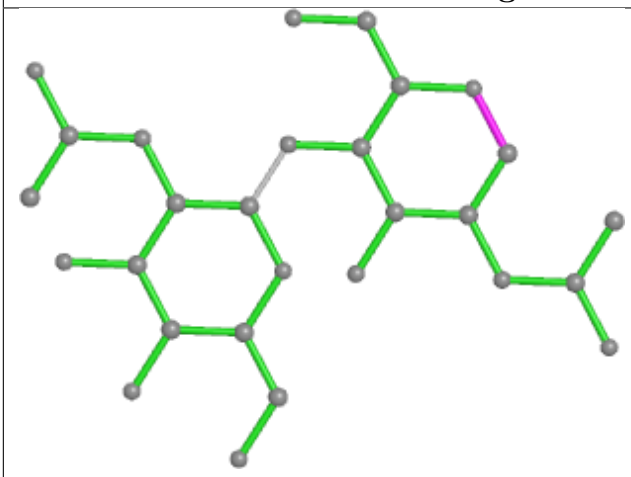


Torsions

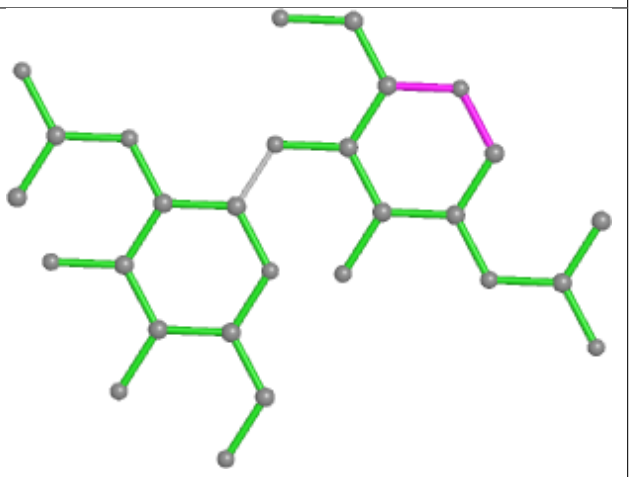


Rings

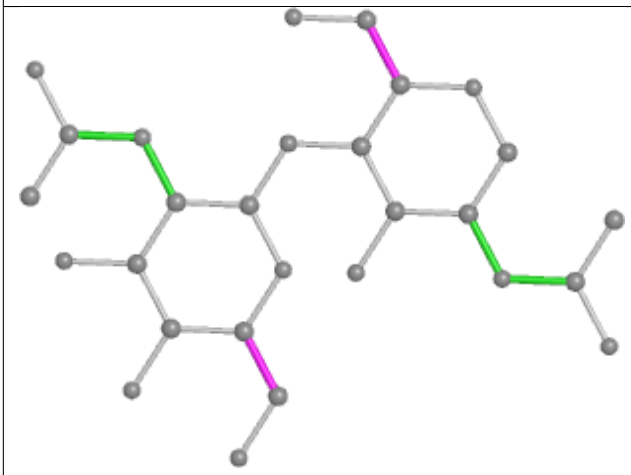
Oligosaccharide Chain J



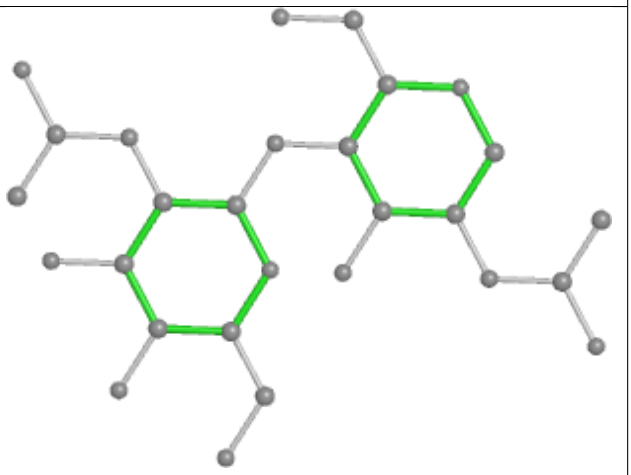
Bond lengths



Bond angles

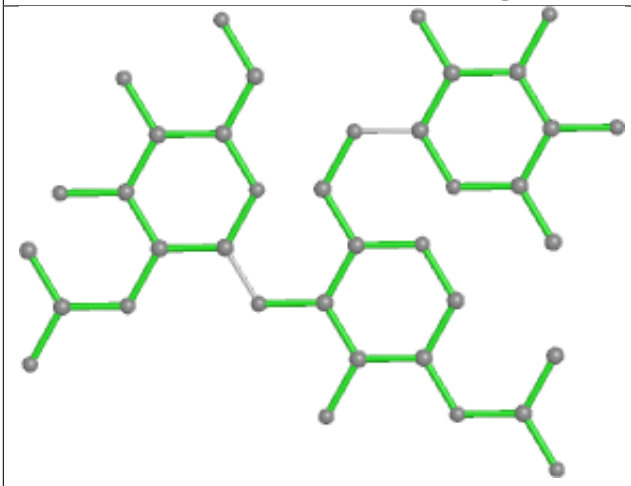


Torsions

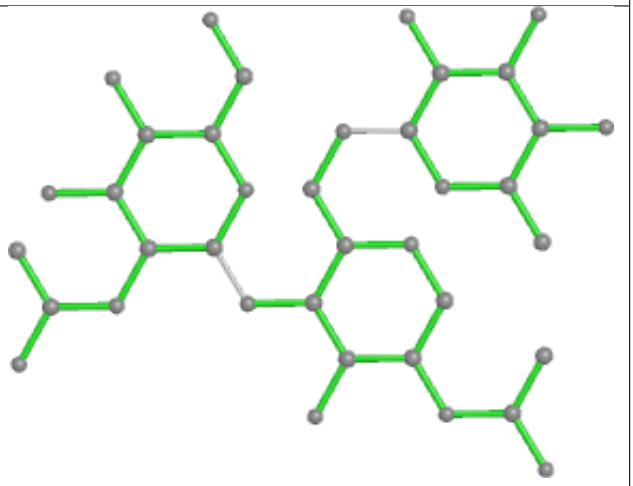


Rings

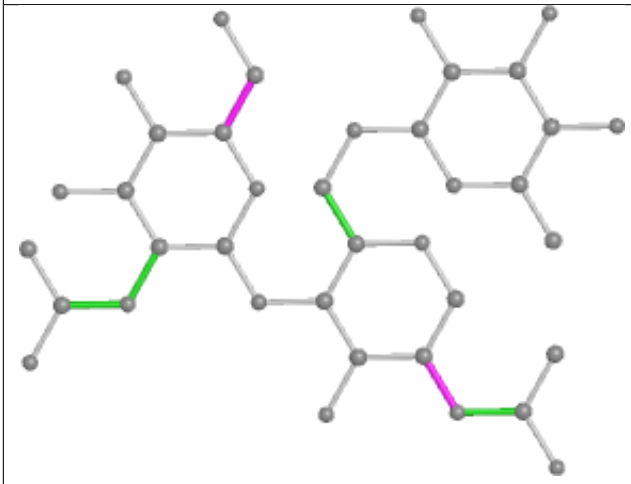
Oligosaccharide Chain F



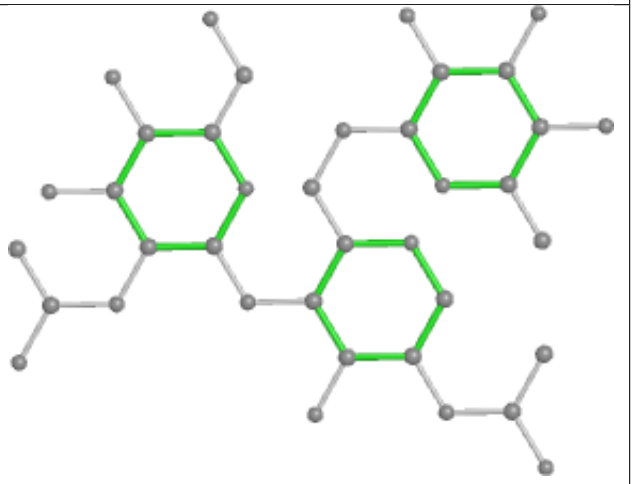
Bond lengths



Bond angles

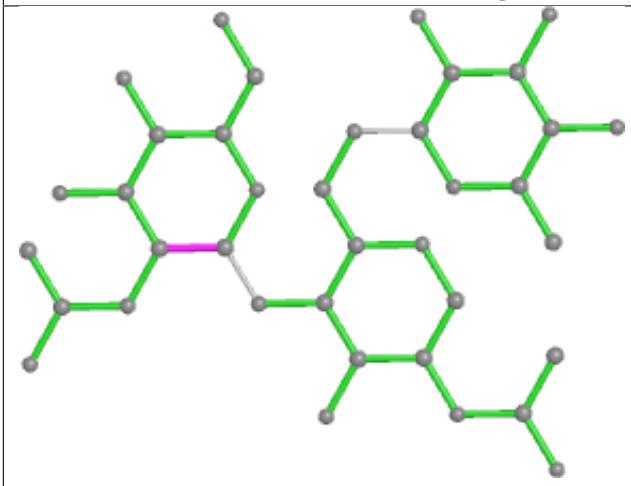


Torsions

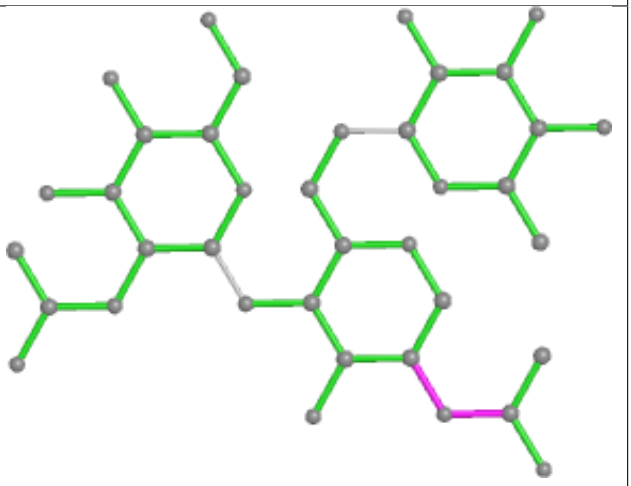


Rings

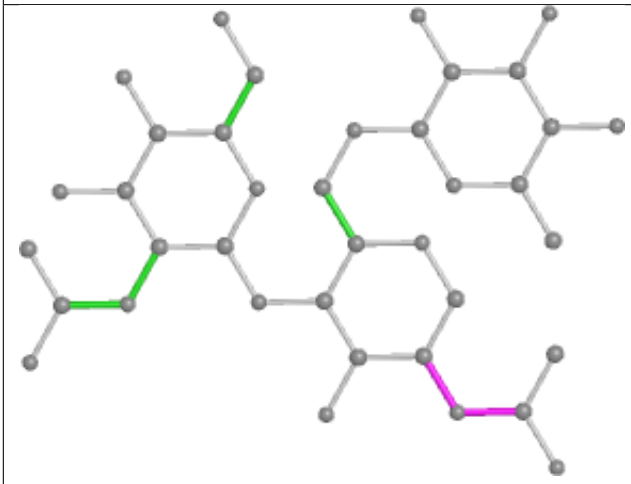
Oligosaccharide Chain G



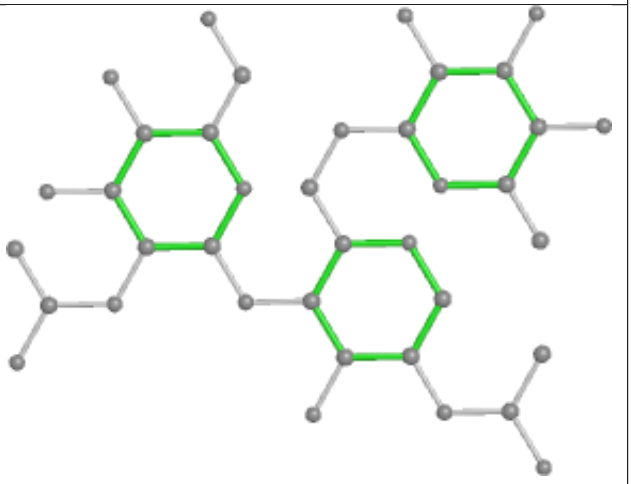
Bond lengths



Bond angles

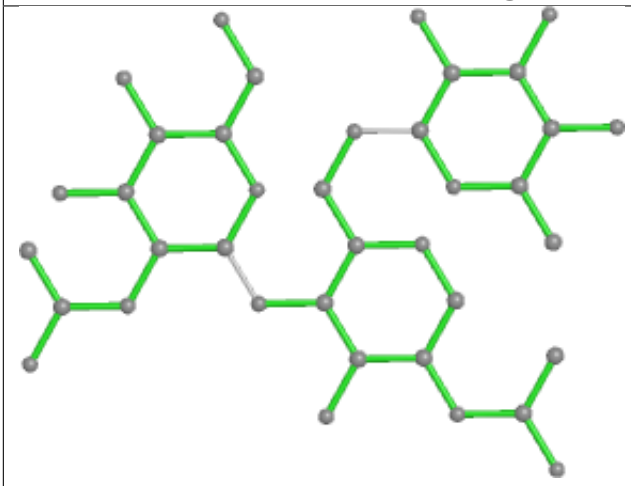


Torsions

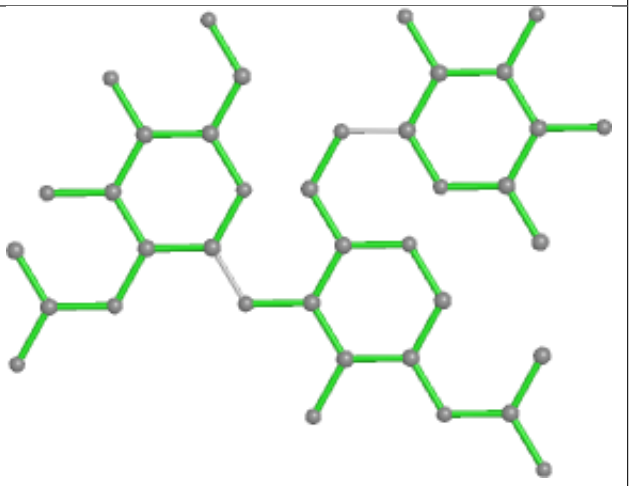


Rings

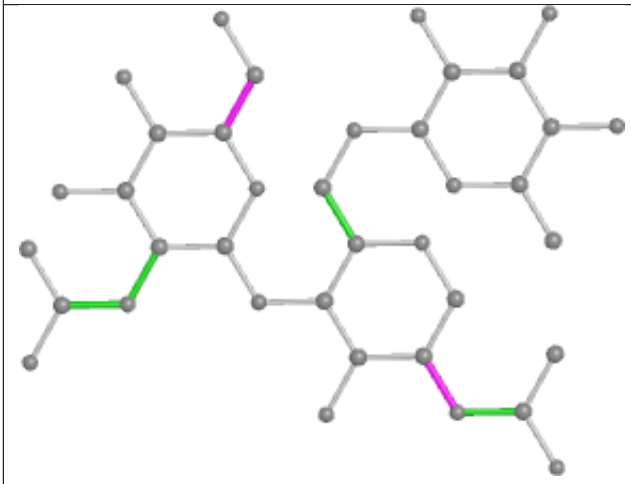
Oligosaccharide Chain I



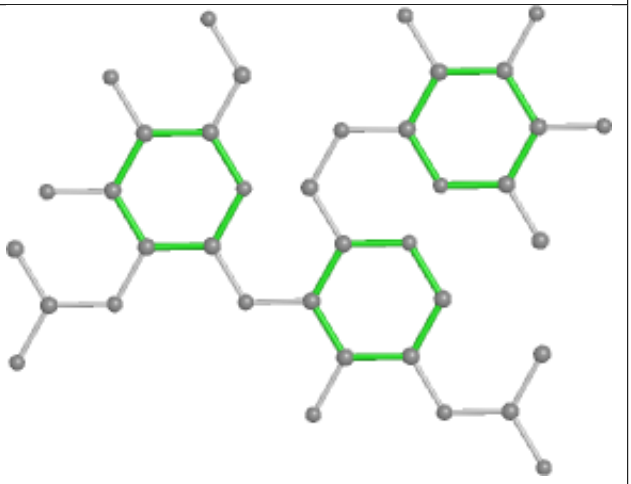
Bond lengths



Bond angles

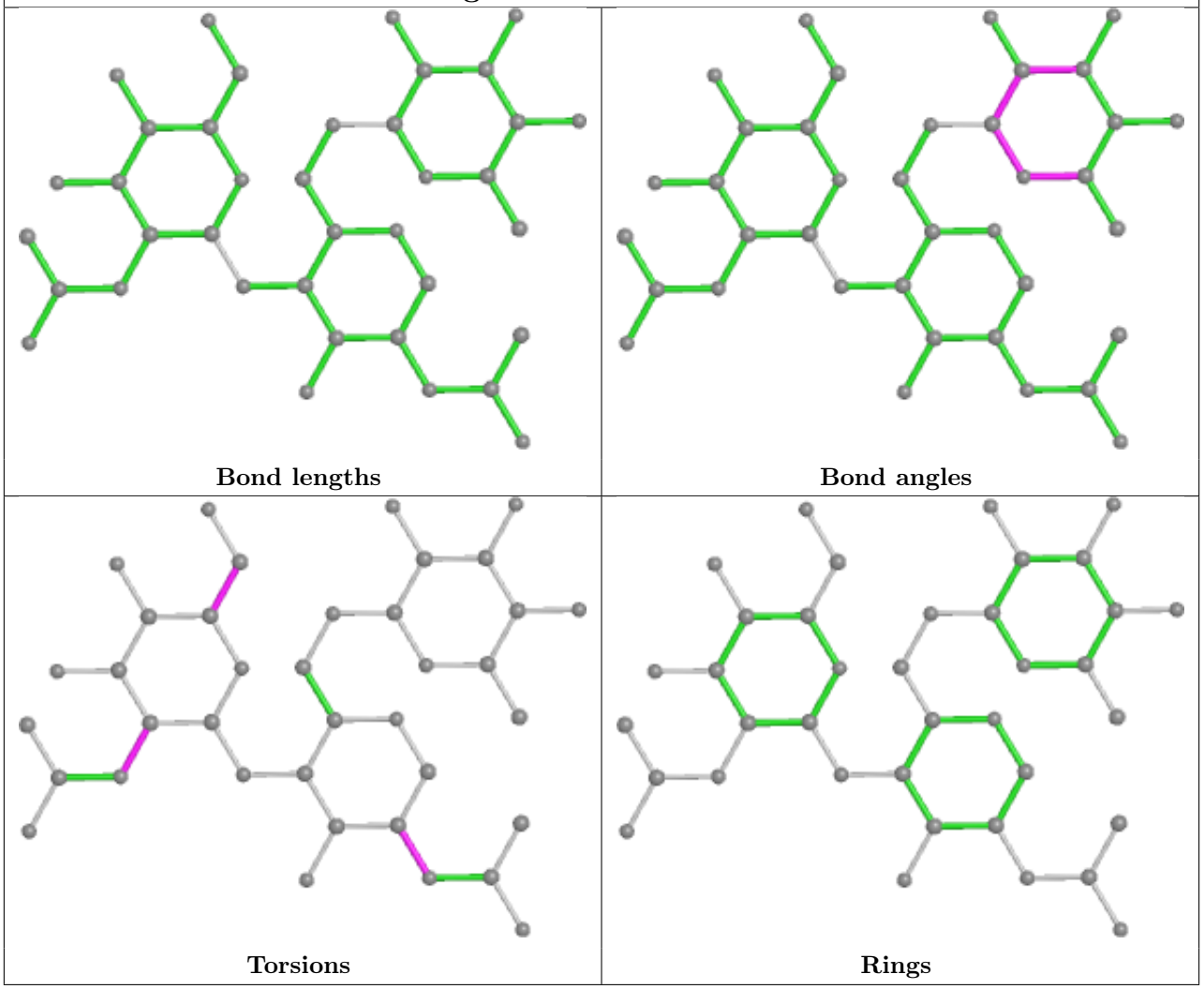


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 59 ligands modelled in this entry, 16 are monoatomic - leaving 43 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	BCN	B	706	12	10,10,10	1.02	1 (10%)	11,11,11	1.27	1 (9%)
7	EDO	D	710	-	3,3,3	0.51	0	2,2,2	0.27	0
5	BCN	D	707	12	10,10,10	0.75	0	11,11,11	1.07	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BO3	D	714	-	3,3,3	0.34	0	3,3,3	0.34	0
7	EDO	C	709[A]	-	3,3,3	0.53	0	2,2,2	0.46	0
7	EDO	C	711	-	3,3,3	0.51	0	2,2,2	0.39	0
7	EDO	D	709	-	3,3,3	0.40	0	2,2,2	0.31	0
5	BCN	A	709	12	10,10,10	1.00	0	11,11,11	0.99	0
6	PEG	B	707	-	6,6,6	0.47	0	5,5,5	0.24	0
7	EDO	A	711	-	3,3,3	0.44	0	2,2,2	0.37	0
4	BO3	D	713	-	3,3,3	0.54	0	3,3,3	0.24	0
14	MXE	C	707[B]	-	4,4,4	0.44	0	3,3,3	0.37	0
4	BO3	A	706	-	3,3,3	0.18	0	3,3,3	0.06	0
4	BO3	B	705	-	3,3,3	0.28	0	3,3,3	0.15	0
5	BCN	C	706	12	10,10,10	0.95	0	11,11,11	0.85	0
8	PGE	A	716	-	9,9,9	0.48	0	8,8,8	0.79	0
8	PGE	D	708[A]	-	9,9,9	0.28	0	8,8,8	0.32	0
7	EDO	C	710	-	3,3,3	0.49	0	2,2,2	0.33	0
7	EDO	D	712[B]	-	3,3,3	0.53	0	2,2,2	0.48	0
7	EDO	B	710	-	3,3,3	0.49	0	2,2,2	0.33	0
13	NAG	B	701	1	14,14,15	0.35	0	17,19,21	0.55	0
6	PEG	A	710	-	6,6,6	0.49	0	5,5,5	0.42	0
6	PEG	B	714	-	6,6,6	0.49	0	5,5,5	0.32	0
7	EDO	A	717	-	3,3,3	0.37	0	2,2,2	0.50	0
8	PGE	B	709	-	9,9,9	0.33	0	8,8,8	0.32	0
7	EDO	C	709[B]	-	3,3,3	0.45	0	2,2,2	0.23	0
5	BCN	A	707	12	10,10,10	1.02	0	11,11,11	0.95	0
4	BO3	D	706	-	3,3,3	0.36	0	3,3,3	0.32	0
7	EDO	A	715	-	3,3,3	0.48	0	2,2,2	0.62	0
7	EDO	A	718	-	3,3,3	0.51	0	2,2,2	0.61	0
7	EDO	B	711	-	3,3,3	0.48	0	2,2,2	0.35	0
4	BO3	C	708	-	3,3,3	0.31	0	3,3,3	0.16	0
8	PGE	A	712	-	9,9,9	0.33	0	8,8,8	0.30	0
7	EDO	D	711	12	3,3,3	0.47	0	2,2,2	0.46	0
7	EDO	A	714	-	3,3,3	0.46	0	2,2,2	0.35	0
8	PGE	D	708[B]	-	9,9,9	0.29	0	8,8,8	0.35	0
6	PEG	B	713	-	6,6,6	0.47	0	5,5,5	0.40	0
14	MXE	C	707[A]	-	4,4,4	0.36	0	3,3,3	0.33	0
4	BO3	A	713	-	3,3,3	0.31	0	3,3,3	0.27	0
14	MXE	B	712	-	4,4,4	0.39	0	3,3,3	0.31	0
8	PGE	B	708	-	9,9,9	0.30	0	8,8,8	0.32	0
4	BO3	A	708	-	3,3,3	0.50	0	3,3,3	0.16	0
7	EDO	D	712[A]	-	3,3,3	0.58	0	2,2,2	0.36	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	BCN	B	706	12	-	2/10/10/10	-
7	EDO	D	710	-	-	1/1/1/1	-
5	BCN	D	707	12	-	2/10/10/10	-
7	EDO	C	709[A]	-	-	0/1/1/1	-
7	EDO	C	711	-	-	1/1/1/1	-
7	EDO	D	709	-	-	0/1/1/1	-
5	BCN	A	709	12	-	3/10/10/10	-
6	PEG	B	707	-	-	3/4/4/4	-
7	EDO	A	711	-	-	0/1/1/1	-
14	MXE	C	707[B]	-	-	1/2/2/2	-
5	BCN	C	706	12	-	2/10/10/10	-
8	PGE	A	716	-	-	4/7/7/7	-
8	PGE	D	708[A]	-	-	2/7/7/7	-
7	EDO	C	710	-	-	0/1/1/1	-
7	EDO	D	712[B]	-	-	0/1/1/1	-
7	EDO	B	710	-	-	0/1/1/1	-
7	EDO	A	717	-	-	1/1/1/1	-
6	PEG	A	710	-	-	2/4/4/4	-
6	PEG	B	714	-	-	1/4/4/4	-
8	PGE	B	709	-	-	3/7/7/7	-
7	EDO	C	709[B]	-	-	0/1/1/1	-
5	BCN	A	707	12	-	0/10/10/10	-
7	EDO	A	715	-	-	1/1/1/1	-
7	EDO	A	718	-	-	0/1/1/1	-
7	EDO	B	711	-	-	0/1/1/1	-
8	PGE	A	712	-	-	3/7/7/7	-
7	EDO	D	711	12	-	1/1/1/1	-
7	EDO	A	714	-	-	1/1/1/1	-
8	PGE	D	708[B]	-	-	1/7/7/7	-
6	PEG	B	713	-	-	1/4/4/4	-
14	MXE	C	707[A]	-	-	1/2/2/2	-
14	MXE	B	712	-	-	0/2/2/2	-
8	PGE	B	708	-	-	0/7/7/7	-
13	NAG	B	701	1	-	2/6/23/26	0/1/1/1
7	EDO	D	712[A]	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	706	BCN	O21-C2	2.16	1.29	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	706	BCN	O22-C2-C1	2.28	122.44	113.45
5	D	707	BCN	C1-N1-C3	-2.09	106.85	111.94

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	708[A]	PGE	O1-C1-C2-O2
5	D	707	BCN	N1-C5-C6-O6
8	A	712	PGE	O1-C1-C2-O2
13	B	701	NAG	O5-C5-C6-O6
5	C	706	BCN	N1-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	714	BO3	1	0
5	A	709	BCN	2	0
6	B	707	PEG	2	0
7	A	711	EDO	1	0
8	A	716	PGE	5	0
8	A	712	PGE	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, 95^{th} 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	608/629 (96%)	-0.11	3 (0%)	91	91	23, 36, 62, 93	0
1	B	605/629 (96%)	0.03	13 (2%)	63	63	20, 34, 76, 98	0
1	C	605/629 (96%)	-0.06	9 (1%)	73	74	22, 37, 66, 105	0
1	D	607/629 (96%)	-0.05	11 (1%)	68	68	19, 34, 64, 102	0
All	All	2425/2516 (96%)	-0.05	36 (1%)	73	74	19, 35, 68, 105	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	LEU	5.0
1	B	1	LEU	4.6
1	D	130	PRO	4.6
1	B	130	PRO	3.7
1	B	105	LEU	3.6

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, 95^{th} 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	NAG	F	2	14/15	0.63	0.21	59,77,82,87	0
3	NAG	K	2	14/15	0.68	0.19	62,81,101,106	0

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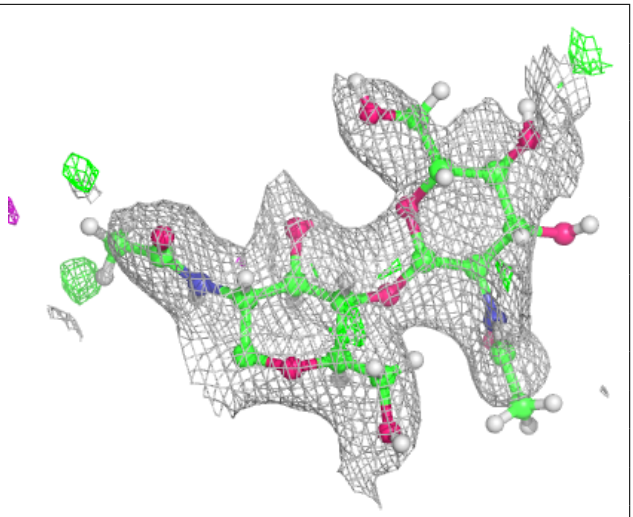
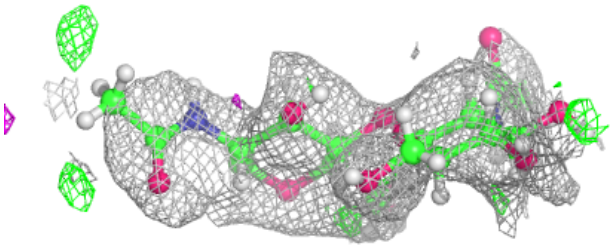
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	J	2	14/15	0.71	0.22	82,97,113,116	0
3	NAG	G	2	14/15	0.74	0.29	62,86,113,117	0
2	NAG	E	2	14/15	0.75	0.22	75,90,108,115	0
3	FUC	K	3	10/11	0.76	0.30	59,74,89,89	0
3	NAG	I	2	14/15	0.79	0.18	51,76,95,102	0
2	NAG	J	1	14/15	0.80	0.19	67,90,106,110	0
3	NAG	K	1	14/15	0.80	0.14	42,58,68,80	0
2	NAG	E	1	14/15	0.83	0.13	55,70,83,88	0
3	NAG	G	1	14/15	0.85	0.13	31,45,60,64	0
2	NAG	H	2	14/15	0.85	0.17	79,93,109,121	0
2	NAG	H	1	14/15	0.85	0.13	52,64,80,87	0
3	NAG	I	1	14/15	0.88	0.12	38,47,57,66	0
3	FUC	G	3	10/11	0.89	0.18	45,58,83,90	0
3	FUC	I	3	10/11	0.90	0.13	46,57,73,76	0
3	FUC	F	3	10/11	0.91	0.14	48,59,74,77	0
3	NAG	F	1	14/15	0.91	0.11	40,54,64,68	0

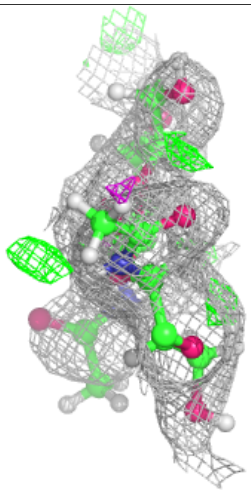
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

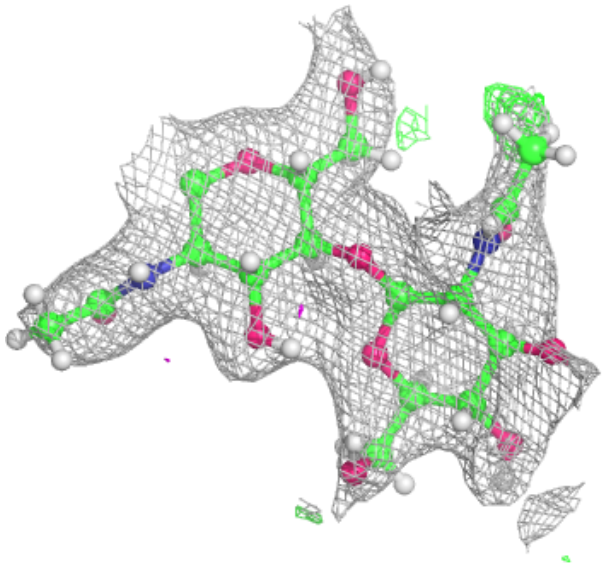


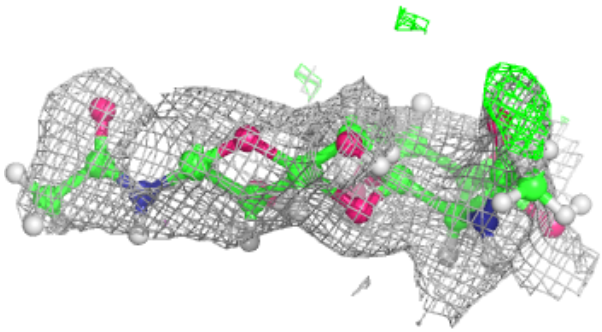


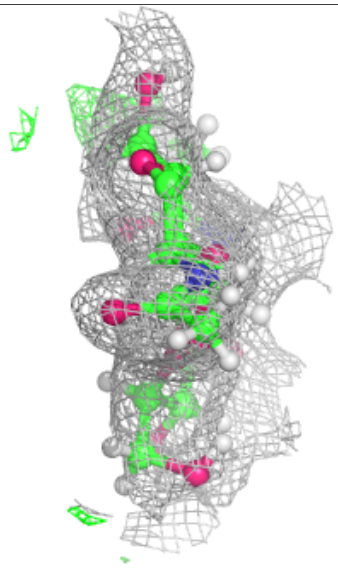


Electron density around Chain H:

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

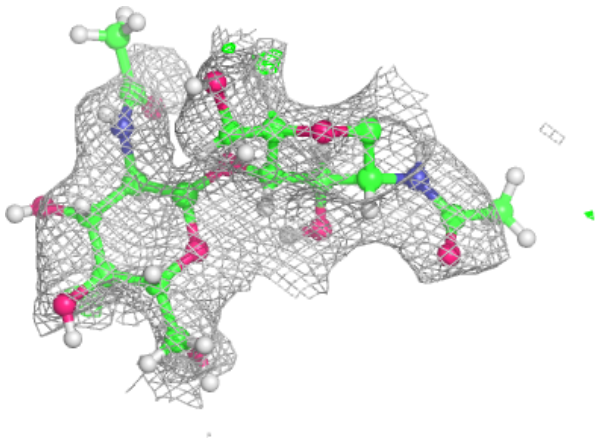


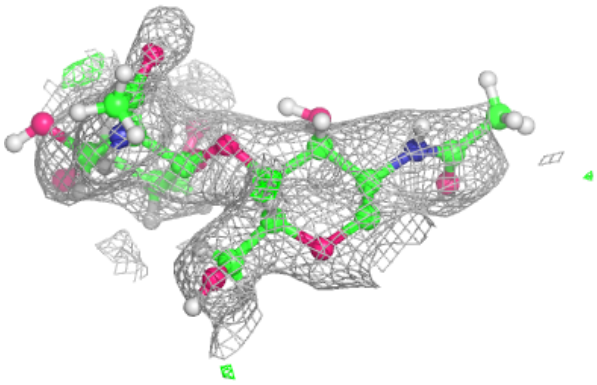


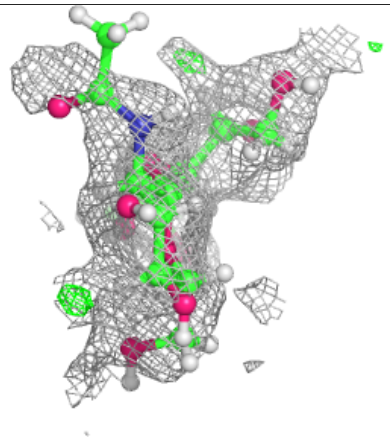


Electron density around Chain J:

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

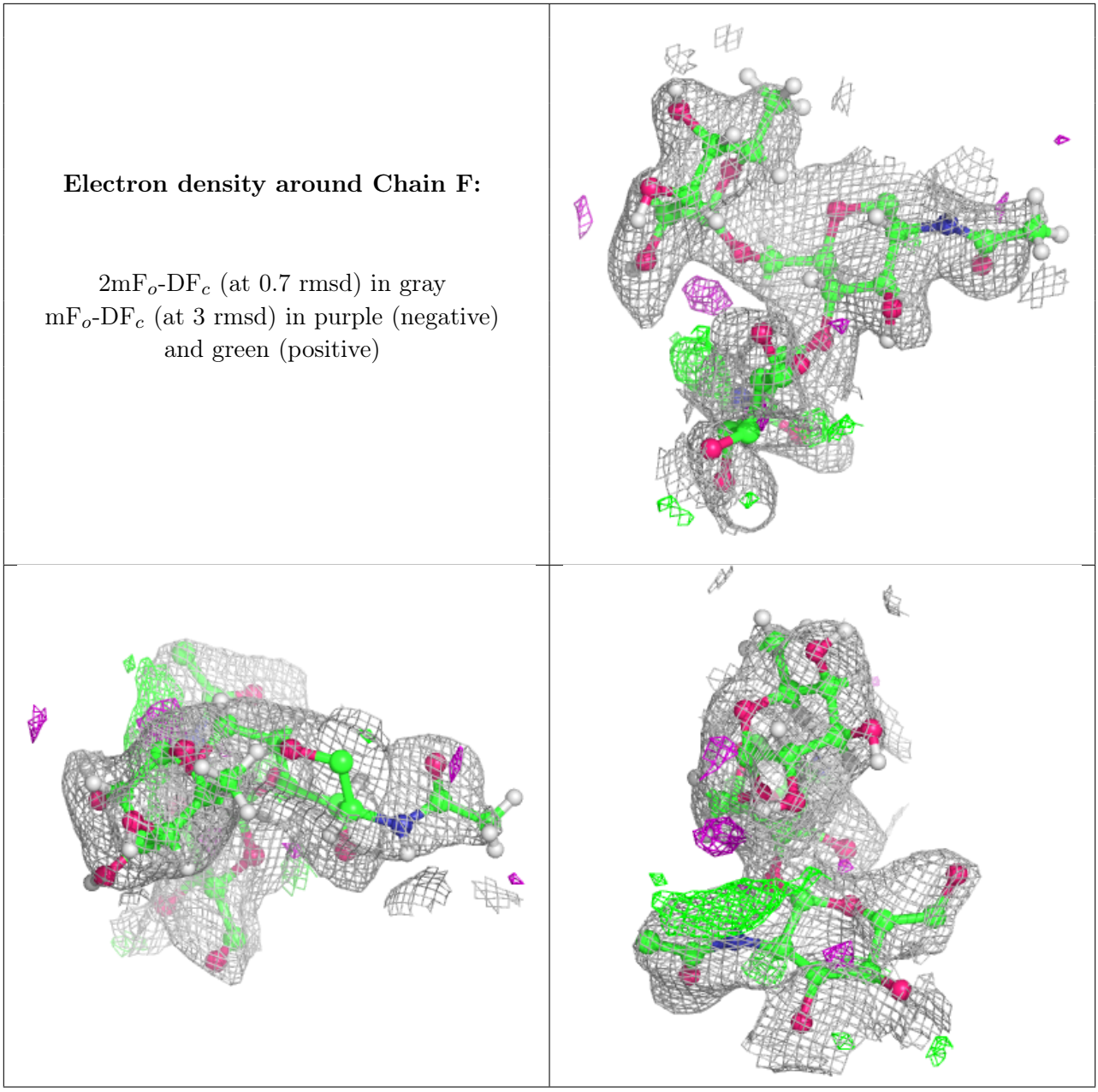






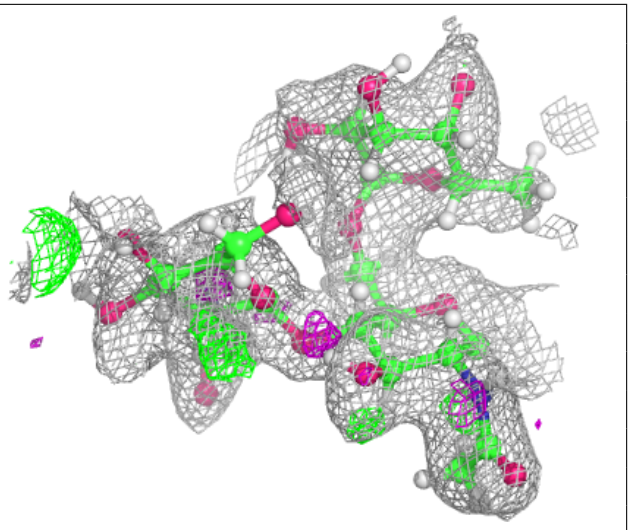
Electron density around Chain F:

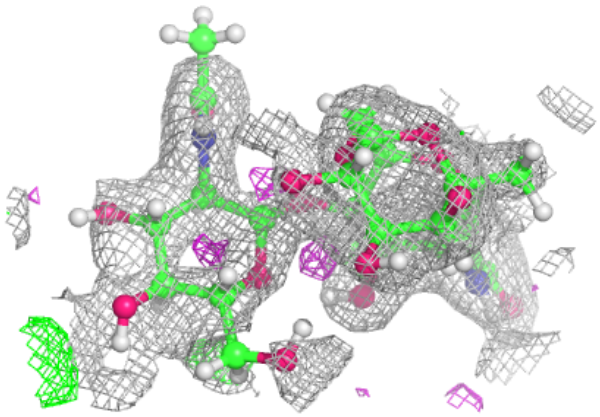
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

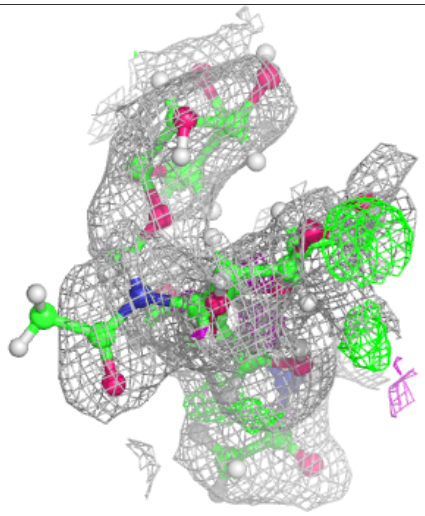


Electron density around Chain G:

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

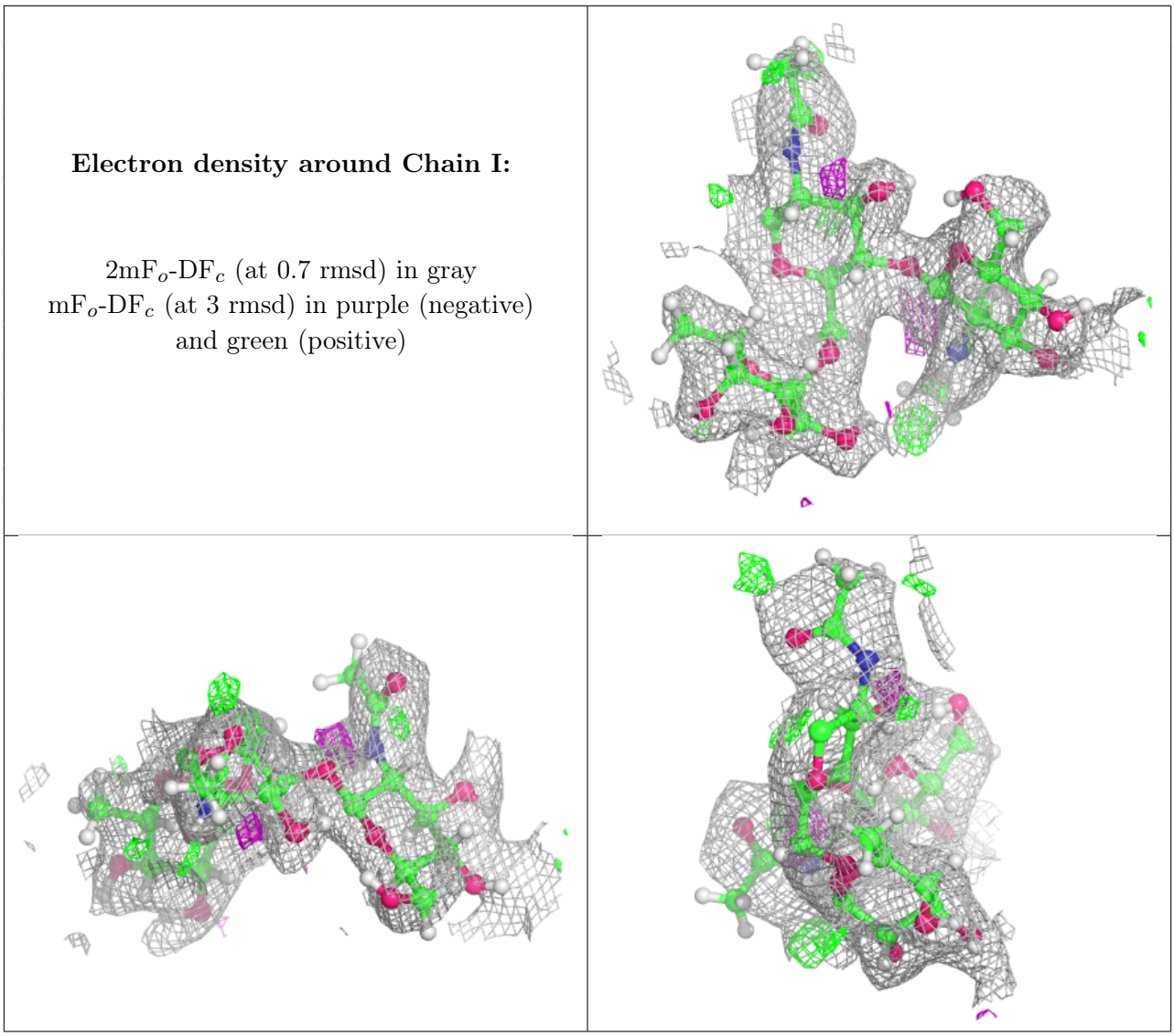






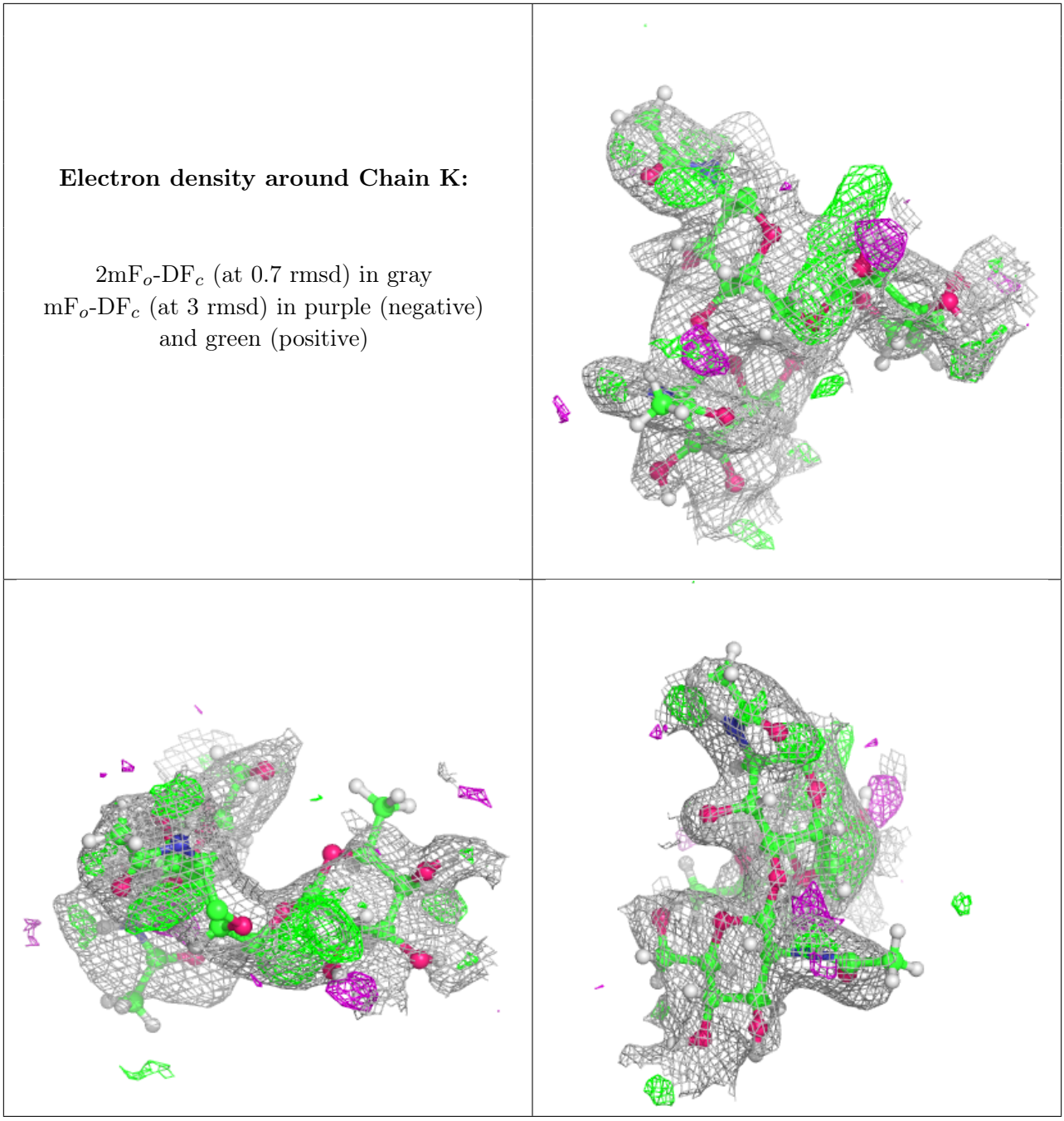
Electron density around Chain I:

$2mF_o$-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 K:

$2mF_o$-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, 95^{th} 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
11	MG	A	721	1/1	0.35	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	C	710	4/4	0.58	0.21	59,71,77,85	0
7	EDO	A	718	4/4	0.61	0.22	59,70,80,81	0
6	PEG	B	707	7/7	0.62	0.18	56,70,85,85	0
4	BO3	D	714	4/4	0.63	0.16	42,50,67,81	0
14	MXE	C	707[A]	5/5	0.67	0.21	43,53,62,65	13
14	MXE	C	707[B]	5/5	0.67	0.21	34,47,61,62	13
11	MG	B	717	1/1	0.69	0.16	63,63,63,63	0
7	EDO	C	711	4/4	0.70	0.33	60,72,75,78	0
8	PGE	D	708[A]	10/10	0.72	0.18	45,59,71,71	24
8	PGE	D	708[B]	10/10	0.72	0.18	45,59,71,71	24
7	EDO	C	709[A]	4/4	0.73	0.16	40,48,55,57	10
7	EDO	C	709[B]	4/4	0.73	0.16	37,45,55,57	10
4	BO3	A	706	4/4	0.77	0.26	45,51,59,62	0
7	EDO	D	712[A]	4/4	0.78	0.19	38,48,57,58	10
7	EDO	D	712[B]	4/4	0.78	0.19	38,49,54,59	10
6	PEG	B	714	7/7	0.78	0.19	50,61,74,74	0
7	EDO	D	710	4/4	0.78	0.13	50,62,70,84	0
15	NA	B	719	1/1	0.79	0.11	63,63,63,63	0
8	PGE	A	712	10/10	0.80	0.15	44,63,72,75	0
13	NAG	B	701	14/15	0.81	0.17	61,83,105,106	0
7	EDO	D	711	4/4	0.81	0.14	45,54,62,74	0
6	PEG	B	713	7/7	0.82	0.15	37,49,59,67	17
7	EDO	B	710	4/4	0.84	0.19	44,53,64,69	0
6	PEG	A	710	7/7	0.85	0.17	55,66,75,82	0
5	BCN	A	709	11/11	0.86	0.25	48,63,70,73	0
8	PGE	B	708	10/10	0.86	0.15	51,68,76,76	0
7	EDO	B	711	4/4	0.87	0.14	48,59,70,74	0
8	PGE	B	709	10/10	0.87	0.13	46,55,66,76	0
4	BO3	B	705	4/4	0.88	0.16	33,36,40,43	0
7	EDO	A	711	4/4	0.88	0.11	50,60,66,70	0
4	BO3	D	713	4/4	0.90	0.16	34,41,57,69	0
8	PGE	A	716	10/10	0.90	0.26	21,53,60,63	24
4	BO3	D	706	4/4	0.91	0.14	31,37,44,44	0
7	EDO	A	717	4/4	0.91	0.13	48,58,70,72	0
4	BO3	A	713	4/4	0.91	0.18	47,51,59,61	0
7	EDO	D	709	4/4	0.91	0.09	57,69,75,75	0
4	BO3	C	708	4/4	0.92	0.15	40,44,53,60	0
11	MG	C	714	1/1	0.92	0.11	44,44,44,44	1
7	EDO	A	714	4/4	0.92	0.11	48,58,63,64	0
7	EDO	A	715	4/4	0.93	0.09	51,61,68,75	0
14	MXE	B	712	5/5	0.94	0.12	46,55,65,65	0
5	BCN	B	706	11/11	0.95	0.10	24,39,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BCN	D	707	11/11	0.95	0.11	24,38,46,50	0
5	BCN	C	706	11/11	0.96	0.11	26,35,45,54	0
4	BO3	A	708	4/4	0.96	0.13	35,38,44,50	0
5	BCN	A	707	11/11	0.96	0.13	29,42,51,53	0
12	CA	D	717	1/1	0.98	0.09	26,26,26,26	0
12	CA	A	722	1/1	0.98	0.07	31,31,31,31	0
10	CL	A	720	1/1	0.99	0.17	26,26,26,26	0
12	CA	B	718	1/1	0.99	0.08	28,28,28,28	0
10	CL	B	716	1/1	1.00	0.15	23,23,23,23	0
12	CA	C	715	1/1	1.00	0.07	30,30,30,30	0
10	CL	C	713	1/1	1.00	0.14	26,26,26,26	0
10	CL	D	716	1/1	1.00	0.19	23,23,23,23	0
9	ZN	B	715	1/1	1.00	0.14	27,27,27,27	0
9	ZN	C	712	1/1	1.00	0.16	27,27,27,27	0
9	ZN	D	715	1/1	1.00	0.14	27,27,27,27	0
9	ZN	A	719	1/1	1.00	0.16	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.