



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:00 AM UTC

PDB ID : 6ZPQ / pdb_00006zpq
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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

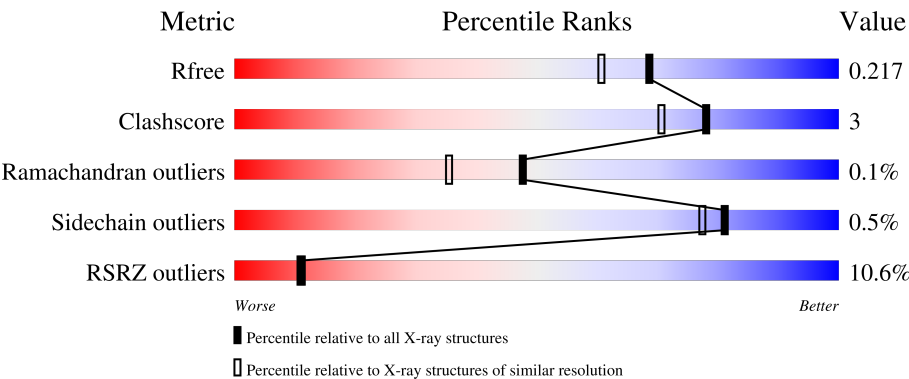
1 Overall quality at a glance i

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.



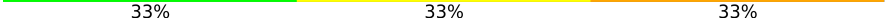
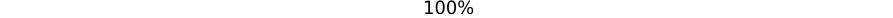
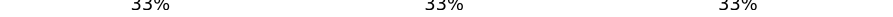
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 $\leq 5\%$. 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	629	7% 91% 6%
1	B	629	17% 89% 7%
1	C	629	10% 91% 5%
1	D	629	8% 90% 7%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	J	2	 50% 50%
3	F	3	 67% 33%
3	G	3	 33% 33% 33%
3	I	3	 100%
3	K	3	 33% 33% 33%

2 Entry composition

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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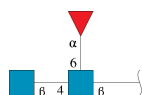
Chain	Residue	Modelled	Actual	Comment	Reference
C	117	GLN	ASN	engineered mutation	UNP P12821
C	131	GLN	ASN	engineered mutation	UNP P12821
C	289	GLN	ASN	engineered mutation	UNP P12821
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
C	629	LEU	-	expression tag	UNP 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 53	C 16	H 25	N 2	O 10	0	0	0
2	H	2	Total 53	C 16	H 25	N 2	O 10	0	0	0
2	J	2	Total 53	C 16	H 25	N 2	O 10	0	0	0

- 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.



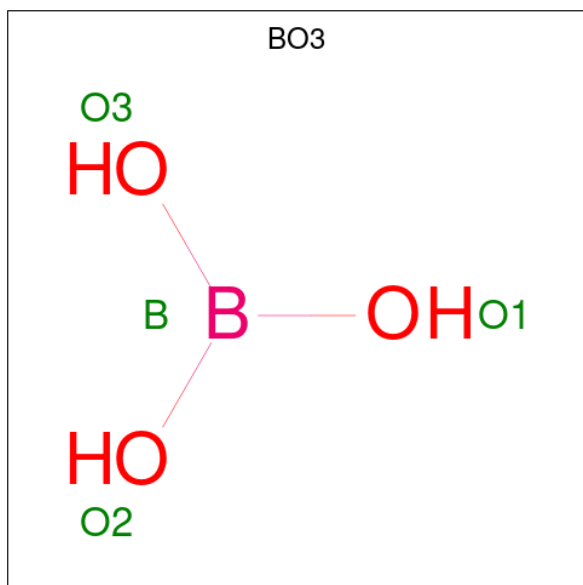
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	3	Total	C	H	N	O	0	0	0
			59	22	21	2	14			

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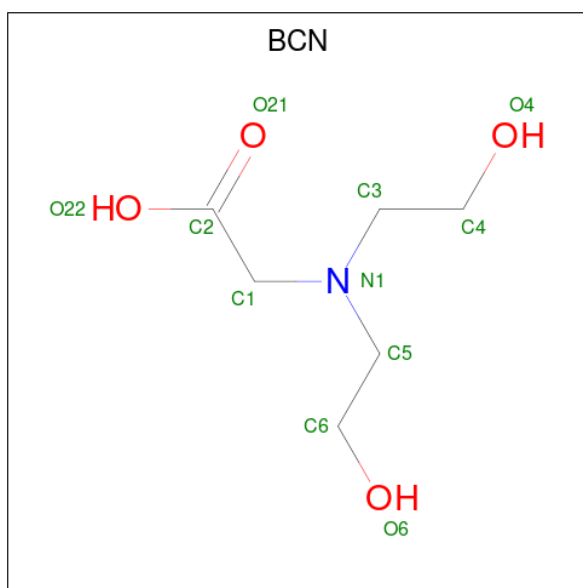
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	H	N	O	0	0	0
			71	22	33	2	14			
3	I	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
3	K	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 4 is BORIC ACID (CCD ID: BO3) (formula: BH_3O_3).



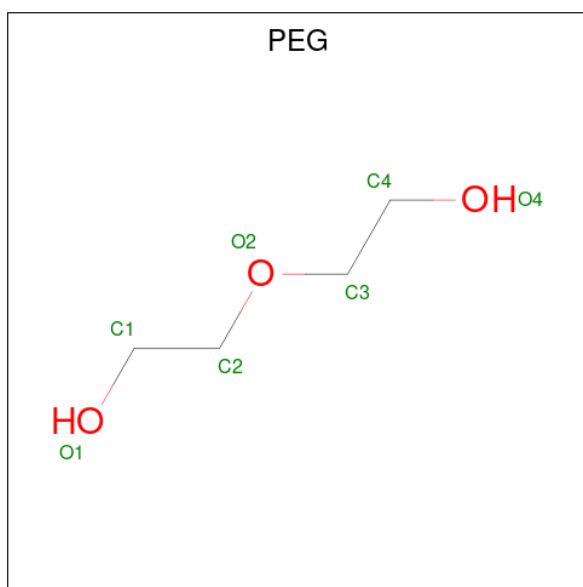
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	B	H	O	0	0
			7	1	3	3		
4	A	1	Total	B	H	O	0	0
			7	1	3	3		
4	A	1	Total	B	H	O	0	0
			7	1	3	3		
4	B	1	Total	B	H	O	0	0
			7	1	3	3		
4	C	1	Total	B	H	O	0	0
			7	1	3	3		
4	D	1	Total	B	H	O	0	0
			7	1	3	3		
4	D	1	Total	B	H	O	0	0
			7	1	3	3		
4	D	1	Total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

- Molecule 5 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).



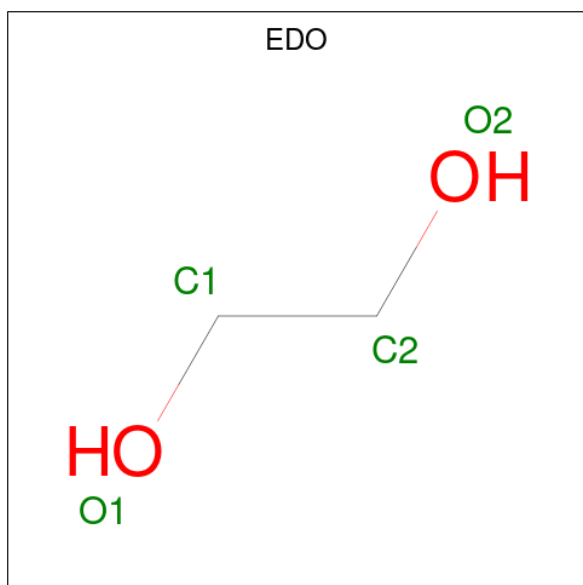
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 23	C 6	H 12	N 1	O 4	0	0
5	A	1	Total 23	C 6	H 12	N 1	O 4	0	0
5	B	1	Total 23	C 6	H 12	N 1	O 4	0	0
5	C	1	Total 23	C 6	H 12	N 1	O 4	0	0
5	D	1	Total 23	C 6	H 12	N 1	O 4	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



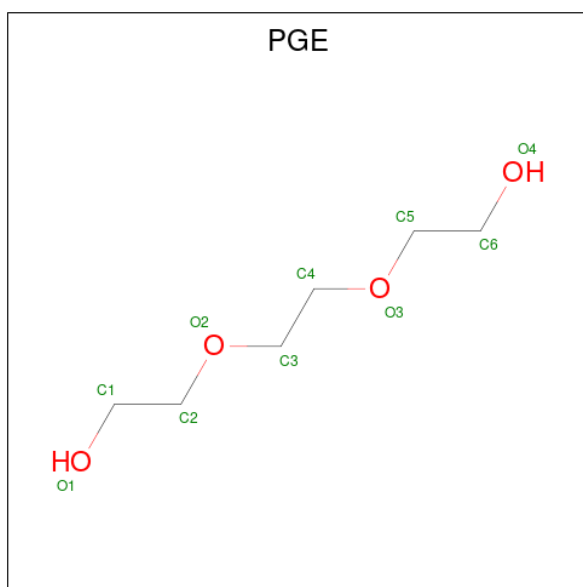
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is CHLORIDE ION (CCD ID: 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

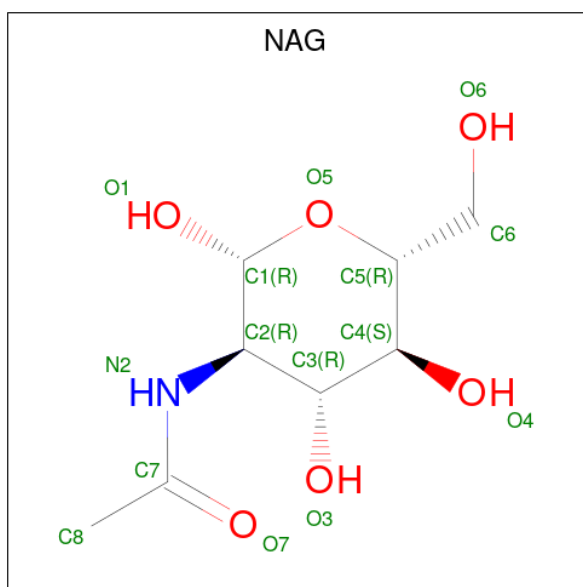
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: CA) (formula: Ca).

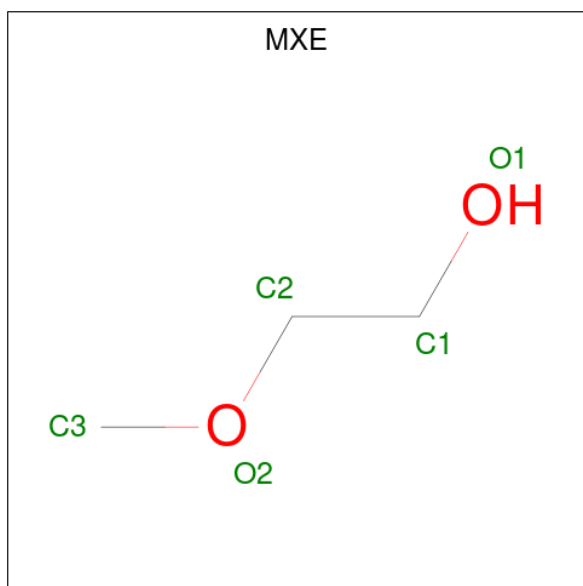
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Ca 1 1	0	0
12	B	1	Total Ca 1 1	0	0
12	C	1	Total Ca 1 1	0	0
12	D	1	Total Ca 1 1	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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 (CCD ID: 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 (CCD ID: NA) (formula: Na).

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

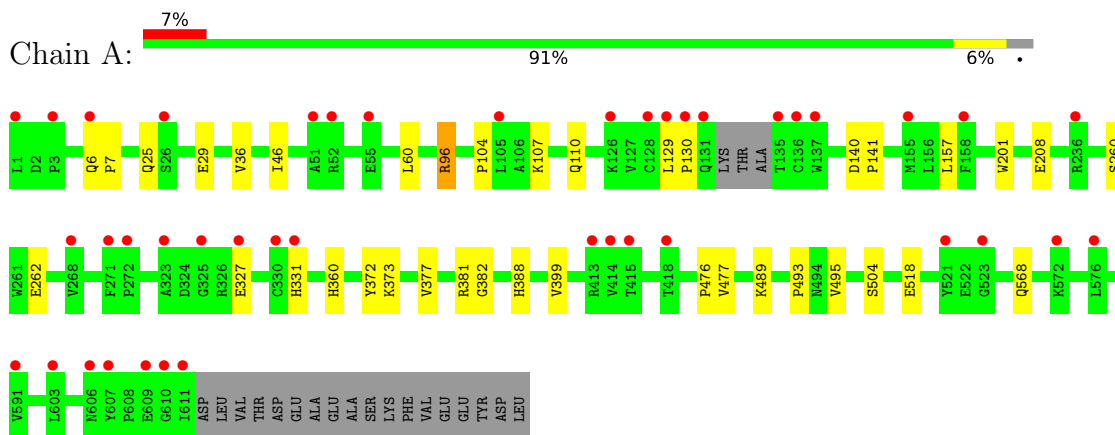
- Molecule 16 is water.

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

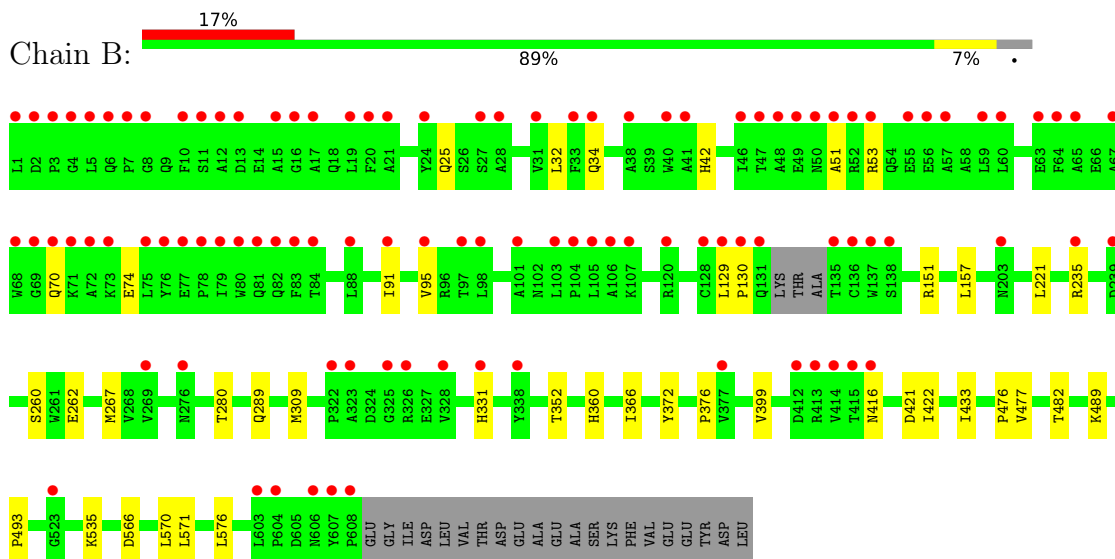
3 Residue-property plots [i](#)

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.

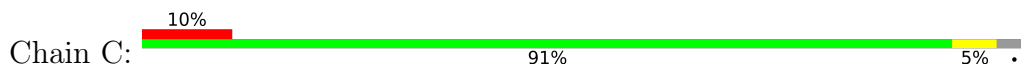
- Molecule 1: Angiotensin-converting enzyme

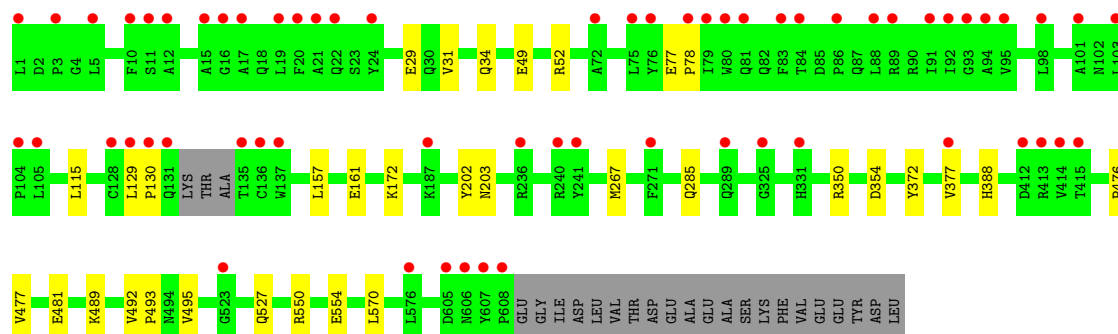


- Molecule 1: Angiotensin-converting enzyme

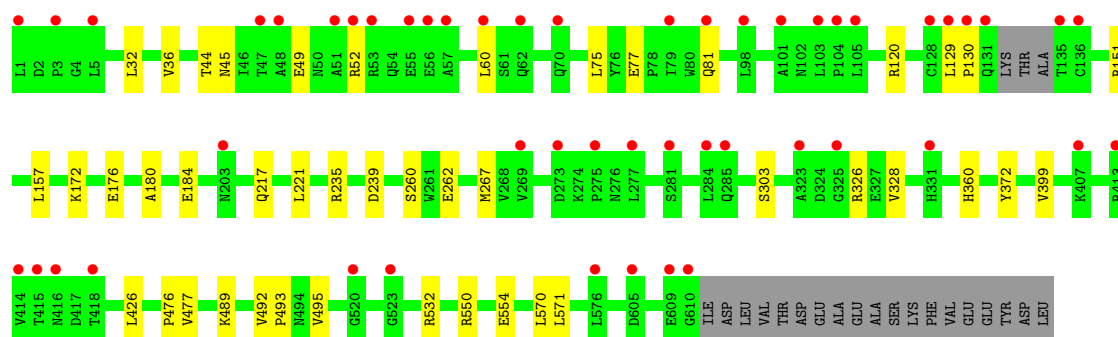


- Molecule 1: Angiotensin-converting enzyme





- Molecule 1: Angiotensin-converting enzyme



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



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



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



- 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%



- 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% 33% 33%



- 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:  100%



- 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:  33% 33% 33%



4 Data and refinement statistics

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 80.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (80.50-1.85) 97.6 (80.50-1.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 0.187 , 0.217	Depositor DCC
R_{free} test set	2027 reflections (0.69%)	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)	0.41 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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, PGE, NAG, ZN, PEG, MG, BCN, FUC, BO3, MXE, EDO, NA, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/5211	0.44	0/7097
1	B	0.47	0/5213	0.47	0/7101
1	C	0.40	0/5214	0.43	0/7101
1	D	0.47	0/5259	0.45	0/7162
All	All	0.44	0/20897	0.45	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 [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	5003	4790	4743	29	0
1	B	5010	4797	4749	30	0
1	C	5004	4781	4732	20	1
1	D	5034	4815	4742	30	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	1	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	7	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	114	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 (114) 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
3:G:1:NAG:H83	3:G:1:NAG:H3	1.69	0.74
1:C:554:GLU:OE1	16:C:801:HOH:O	2.06	0.72
1:B:566:ASP:OD2	16:B:801:HOH:O	2.08	0.70
1:C:550:ARG:NH1	16:C:804:HOH:O	2.23	0.70
7:A:711:EDO:O1	16:A:801:HOH:O	2.12	0.68
1:B:331:HIS:ND1	16:B:804:HOH:O	2.26	0.67
1:D:151:ARG:HD2	1:D:267:MET:HE2	1.77	0.67
1:C:527:GLN:NE2	16:C:808:HOH:O	2.28	0.67
1:A:201:TRP:O	8:A:716:PGE:H12	1.96	0.66
1:B:260:SER:OG	1:B:262:GLU:OE1	2.08	0.66
1:C:354[B]:ASP:OD1	16:C:802:HOH:O	2.15	0.64
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.80	0.63
1:D:75:LEU:O	16:D:802:HOH:O	2.14	0.63
1:C:49:GLU:OE1	1:C:52:ARG:NH1	2.31	0.63
1:D:157:LEU:HD11	1:D:477:VAL:HG13	1.82	0.61
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.82	0.61
1:A:518:GLU:OE2	16:A:802:HOH:O	2.16	0.61
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.81	0.61
1:A:110[A]:GLN:NE2	16:A:812:HOH:O	2.36	0.58
1:A:504[B]:SER:OG	16:A:803:HOH:O	2.17	0.57
1:A:46:ILE:HD12	1:A:327:GLU:HG2	1.86	0.57
1:B:25:GLN:OE1	1:B:376:PRO:HA	2.07	0.55
1:A:381:ARG:HB2	8:A:716:PGE:H5	1.89	0.55
1:C:157:LEU:HD13	1:C:476:PRO:HB2	1.89	0.54
1:D:360:HIS:CD2	1:D:399:VAL:HG21	2.43	0.54
1:B:34:GLN:OE1	1:B:53:ARG:NH1	2.39	0.54
1:B:482:THR:HG23	3:G:1:NAG:H82	1.89	0.54
1:A:25:GLN:NE2	16:A:807:HOH:O	2.31	0.53
2:J:1:NAG:H62	2:J:2:NAG:C1	2.40	0.52
1:D:81[B]:GLN:CD	1:D:81[B]:GLN:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD21	6:B:707:PEG:H32	1.91	0.52
1:D:129:LEU:HB3	1:D:130:PRO:HD2	1.92	0.52
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.93	0.51
1:C:31:VAL:O	1:C:34:GLN:HG3	2.11	0.51
1:D:44:THR:C	1:D:328:VAL:HG12	2.36	0.50
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.94	0.50
1:D:217[B]:GLN:OE1	16:D:803:HOH:O	2.20	0.50
1:B:151:ARG:HD2	1:B:267:MET:HE2	1.93	0.49
1:B:566:ASP:OD1	16:B:802:HOH:O	2.20	0.49
1:C:77:GLU:HB3	1:C:78:PRO:HD3	1.95	0.48
1:D:495:VAL:O	1:D:495:VAL:HG12	2.13	0.47
1:B:482:THR:CG2	3:G:1:NAG:H82	2.43	0.47
1:A:201:TRP:O	8:A:716:PGE:C1	2.61	0.47
1:A:104:PRO:HG2	1:A:107:LYS:HD2	1.97	0.46
1:A:129:LEU:HB3	1:A:130:PRO:HD2	1.97	0.46
1:B:42:HIS:CD2	1:B:51:ALA:HB2	2.51	0.46
3:K:1:NAG:H62	3:K:3:FUC:O2	2.14	0.46
1:B:32:LEU:HD11	6:B:707:PEG:H31	1.97	0.46
1:B:280:THR:HG23	1:B:352:THR:HA	1.97	0.46
1:D:492:VAL:HB	1:D:493:PRO:CD	2.45	0.46
1:C:489:LYS:O	1:C:493:PRO:HD2	2.16	0.45
1:D:49:GLU:OE2	1:D:52:ARG:NH2	2.50	0.45
1:B:489:LYS:O	1:B:493:PRO:HD2	2.17	0.45
1:C:570:LEU:C	1:C:570:LEU:HD23	2.42	0.45
1:D:550:ARG:HD2	16:D:801:HOH:O	2.16	0.45
1:A:489:LYS:O	1:A:493:PRO:HD2	2.17	0.44
1:A:331:HIS:NE2	5:A:709:BCN:C1	2.80	0.44
1:B:129:LEU:HB3	1:B:130:PRO:HD2	2.00	0.44
3:G:1:NAG:H3	3:G:1:NAG:C8	2.42	0.44
1:D:221:LEU:CD1	1:D:571:LEU:HD22	2.47	0.44
1:A:331:HIS:NE2	5:A:709:BCN:H12	2.32	0.44
1:D:77:GLU:O	1:D:81[B]:GLN:OE1	2.36	0.44
1:D:157:LEU:HD13	1:D:476:PRO:HB2	2.00	0.44
1:B:576[B]:LEU:HD12	16:B:988:HOH:O	2.18	0.43
1:C:492:VAL:HB	1:C:493:PRO:CD	2.47	0.43
1:B:570:LEU:C	1:B:570:LEU:HD23	2.43	0.43
1:B:235[B]:ARG:NH2	16:B:830:HOH:O	2.51	0.43
1:C:129:LEU:HB3	1:C:130:PRO:HD2	2.00	0.43
1:D:60:LEU:O	1:D:60:LEU:HD23	2.18	0.43
1:A:495:VAL:HG12	1:A:495:VAL:O	2.18	0.43
1:C:172:LYS:NZ	1:C:481:GLU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:NH1	16:C:824:HOH:O	2.48	0.43
1:A:6:GLN:HB2	1:A:7:PRO:HD2	2.00	0.42
1:A:373:LYS:HE3	1:B:535:LYS:HG2	2.01	0.42
1:D:489:LYS:O	1:D:493:PRO:HD2	2.19	0.42
1:D:239:ASP:OD2	16:D:804:HOH:O	2.21	0.42
1:B:70:GLN:O	1:B:74:GLU:HG3	2.20	0.42
1:A:29:GLU:HG2	1:A:377:VAL:HG11	2.01	0.42
1:A:96:ARG:C	1:A:96:ARG:HD3	2.43	0.42
1:C:29:GLU:CG	1:C:377:VAL:HG11	2.50	0.42
1:B:91:ILE:O	1:B:95:VAL:HG23	2.20	0.42
1:B:53:ARG:O	1:B:53:ARG:HD2	2.20	0.42
1:B:422:ILE:HD11	1:B:576[B]:LEU:HG	2.01	0.42
1:C:267:MET:HE1	16:C:962:HOH:O	2.20	0.42
1:D:221:LEU:HD11	1:D:571:LEU:HD22	2.01	0.42
1:B:221:LEU:CD1	1:B:571:LEU:HD22	2.50	0.41
1:D:120:ARG:NH1	16:D:835:HOH:O	2.52	0.41
1:A:568:GLN:OE1	16:A:804:HOH:O	2.22	0.41
1:D:180:ALA:O	1:D:184[B]:GLU:HG3	2.20	0.41
1:B:151:ARG:CD	1:B:267:MET:HE2	2.50	0.41
1:D:32:LEU:O	1:D:36:VAL:HG23	2.20	0.41
1:A:382:GLY:O	8:A:716:PGE:H4	2.21	0.41
1:C:161:GLU:OE2	16:C:803:HOH:O	2.22	0.41
1:A:208:GLU:OE2	4:A:706:BO3:O1	2.34	0.41
1:A:36:VAL:HG22	8:A:712:PGE:H22	2.02	0.41
1:A:382:GLY:O	8:A:716:PGE:C4	2.68	0.41
1:B:360:HIS:CD2	1:B:399:VAL:HG21	2.55	0.41
1:C:202:TYR:O	1:C:203:ASN:C	2.64	0.41
1:D:570:LEU:C	1:D:570:LEU:HD23	2.46	0.41
1:B:309:MET:SD	1:B:366:ILE:HG21	2.60	0.41
1:D:426:LEU:C	1:D:426:LEU:HD13	2.46	0.41
1:A:360:HIS:CD2	1:A:399:VAL:HG21	2.56	0.40
1:D:303:SER:HB2	1:D:532:ARG:HG2	2.01	0.40
1:D:326:ARG:NE	2:J:1:NAG:H82	2.36	0.40
1:A:60:LEU:HD23	1:A:60:LEU:O	2.22	0.40
1:B:433[B]:ILE:HD11	1:B:570:LEU:HD21	2.03	0.40
1:C:115:LEU:CD2	1:C:495:VAL:HG21	2.51	0.40
1:D:550:ARG:NH2	16:D:821:HOH:O	2.46	0.40
1:A:140:ASP:HA	1:A:141:PRO:HA	1.96	0.40
1:D:172:LYS:O	1:D:176[A]:GLU:HG3	2.22	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: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	1/629 (0%)	1 (100%)	0	0	100	100
1	C	30/629 (5%)	30 (100%)	0	0	100	100
1	D	621/629 (99%)	607 (98%)	13 (2%)	1 (0%)	43	31
All	All	1266/2516 (50%)	1240 (98%)	25 (2%)	1 (0%)	48	35

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%)	530 (99%)	3 (1%)	78	73
1	B	534/541 (99%)	530 (99%)	4 (1%)	76	70
1	C	533/541 (98%)	531 (100%)	2 (0%)	84	82
1	D	538/541 (99%)	537 (100%)	1 (0%)	87	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2138/2164 (99%)	2128 (100%)	10 (0%)	81	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	372	TYR
1	A	388	HIS
1	B	289	GLN
1	B	372	TYR
1	B	416	ASN
1	B	421	ASP
1	C	372	TYR
1	C	388	HIS
1	D	372	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	444	GLN
1	A	568	GLN
1	A	598	GLN
1	B	234	HIS
1	B	331	HIS
1	B	568	GLN
1	B	579	GLN
1	B	588	ASN
1	C	82	GLN
1	C	331	HIS
1	C	444	GLN
1	D	289	GLN
1	D	579	GLN
1	D	588	ASN
1	D	606	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	2,1	14,14,15	0.22	0	17,19,21	0.59	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	F	1	1,3	14,14,15	0.41	0	17,19,21	0.48	0
3	NAG	F	2	3	14,14,15	0.73	1 (7%)	17,19,21	0.52	0
3	FUC	F	3	3	10,10,11	0.74	0	14,14,16	0.74	0
3	NAG	G	1	1,3	14,14,15	0.64	0	17,19,21	1.20	3 (17%)
3	NAG	G	2	3	14,14,15	1.00	1 (7%)	17,19,21	0.88	0
3	FUC	G	3	3	10,10,11	0.82	0	14,14,16	0.78	0
2	NAG	H	1	2,1	14,14,15	0.16	0	17,19,21	0.61	0
2	NAG	H	2	2	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	I	1	1,3	14,14,15	0.50	0	17,19,21	0.53	0
3	NAG	I	2	3	14,14,15	0.21	0	17,19,21	0.62	0
3	FUC	I	3	3	10,10,11	0.69	0	14,14,16	0.73	0
2	NAG	J	1	2,1	14,14,15	0.72	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	J	2	2	14,14,15	0.34	0	17,19,21	0.44	0
3	NAG	K	1	1,3	14,14,15	0.31	0	17,19,21	0.79	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.44	0
3	FUC	K	3	3	10,10,11	1.03	1 (10%)	14,14,16	1.11	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	2,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	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	2,1	-	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	-	3/6/23/26	0/1/1/1
3	FUC	K	3	3	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	C1-C2	3.45	1.57	1.52
2	J	1	NAG	O5-C1	-2.48	1.39	1.43
3	K	3	FUC	O5-C5	2.13	1.47	1.43
3	F	2	NAG	C1-C2	2.01	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C2-N2-C7	3.43	127.50	122.90
2	J	1	NAG	C1-O5-C5	2.42	115.43	112.19
3	G	1	NAG	C1-C2-N2	2.12	113.77	110.43
3	K	3	FUC	C1-C2-C3	2.09	112.69	109.64
3	K	3	FUC	C1-O5-C5	2.09	117.90	112.97
3	G	1	NAG	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

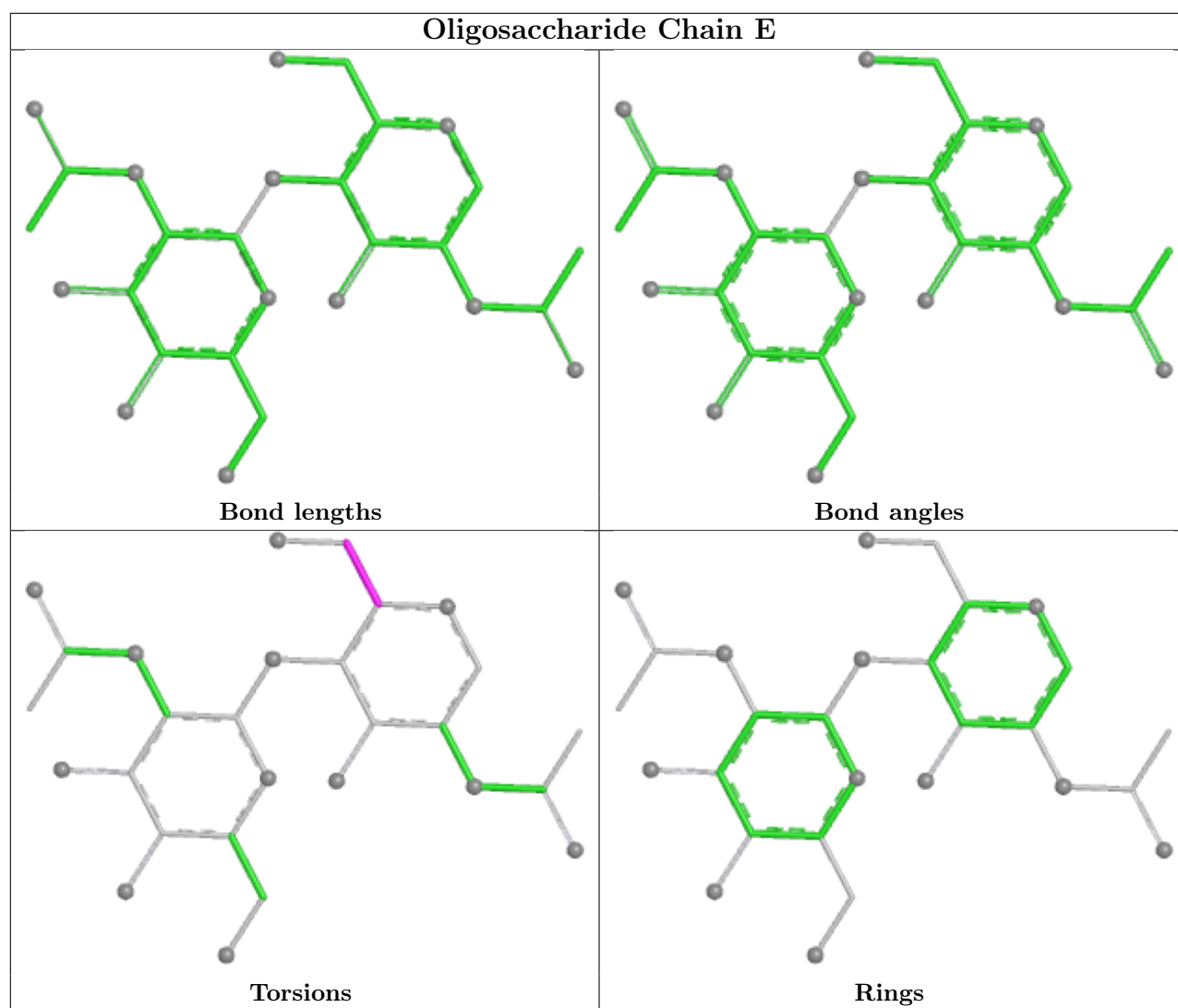
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
3	K	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	K	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6

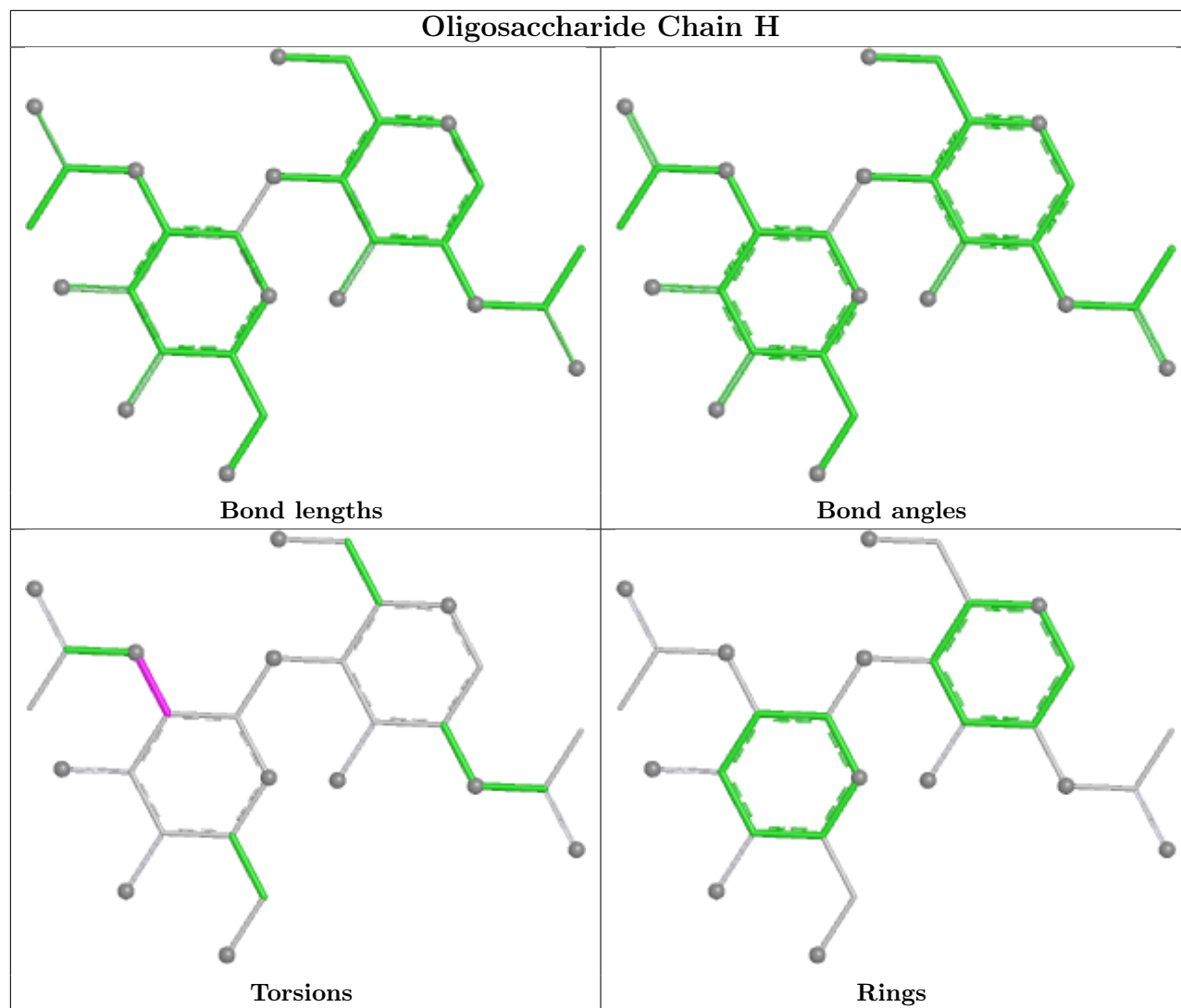
There are no ring outliers.

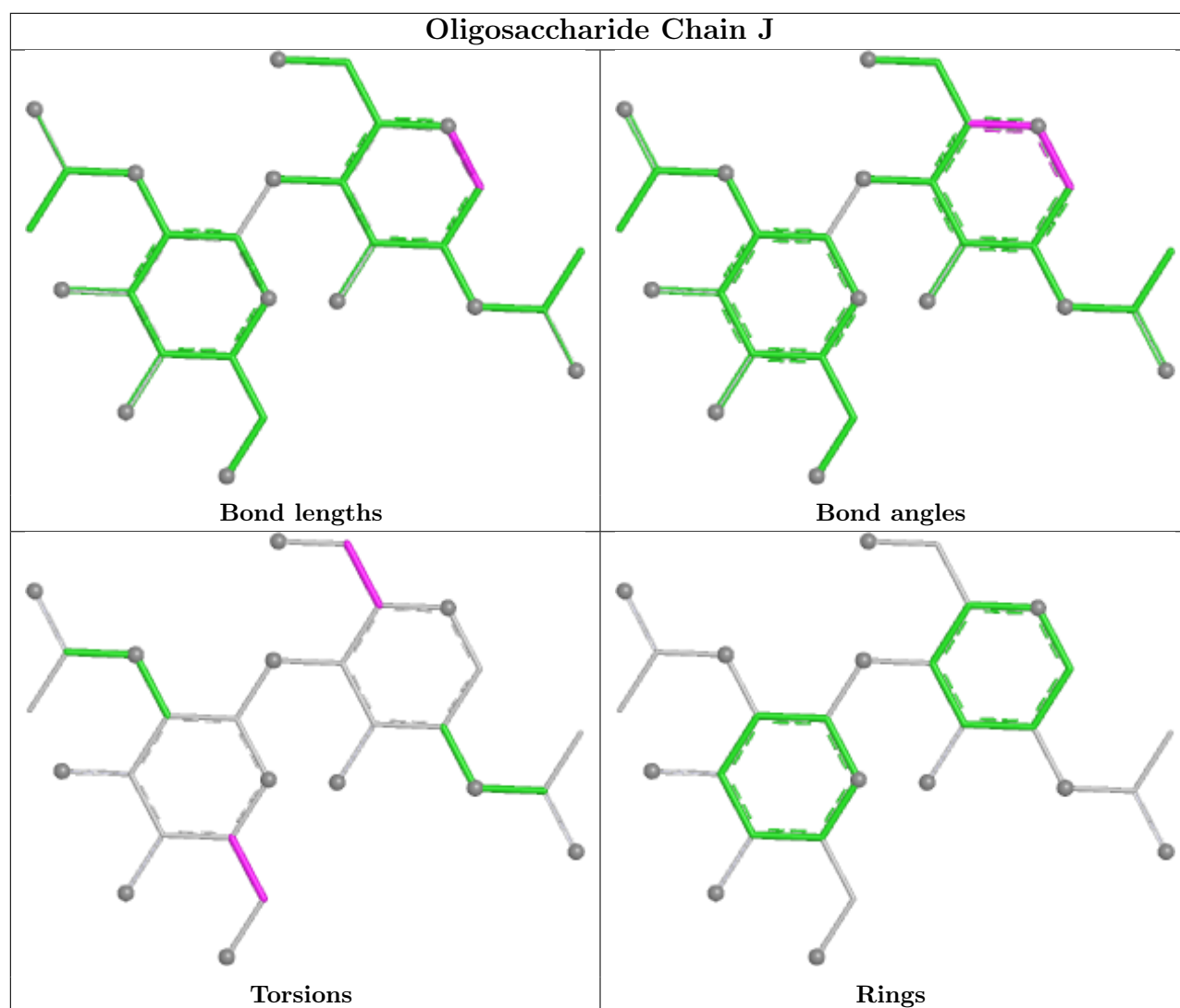
5 monomers are involved in 7 short contacts:

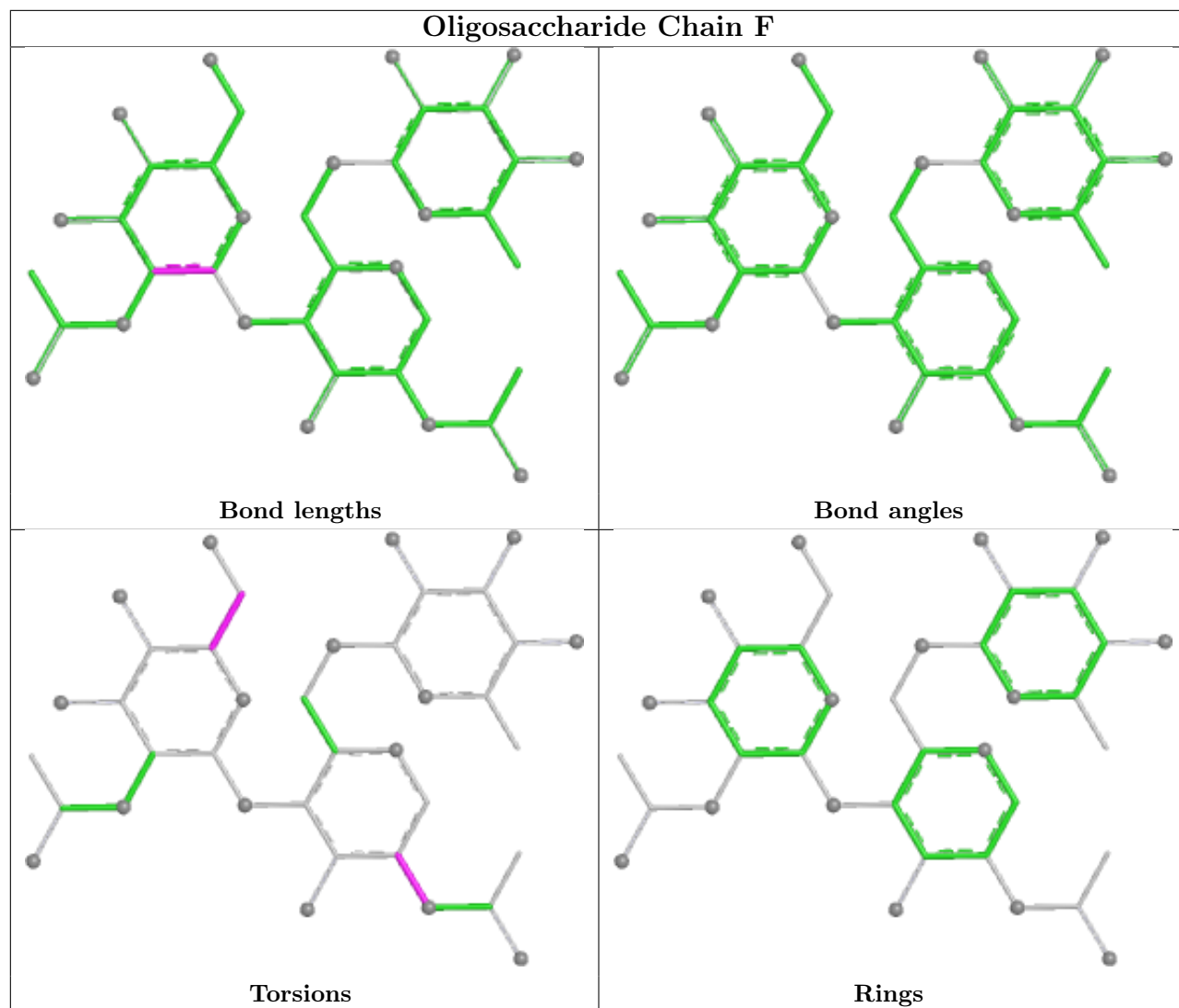
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	4	0
3	K	1	NAG	1	0
2	J	1	NAG	2	0
2	J	2	NAG	1	0
3	K	3	FUC	1	0

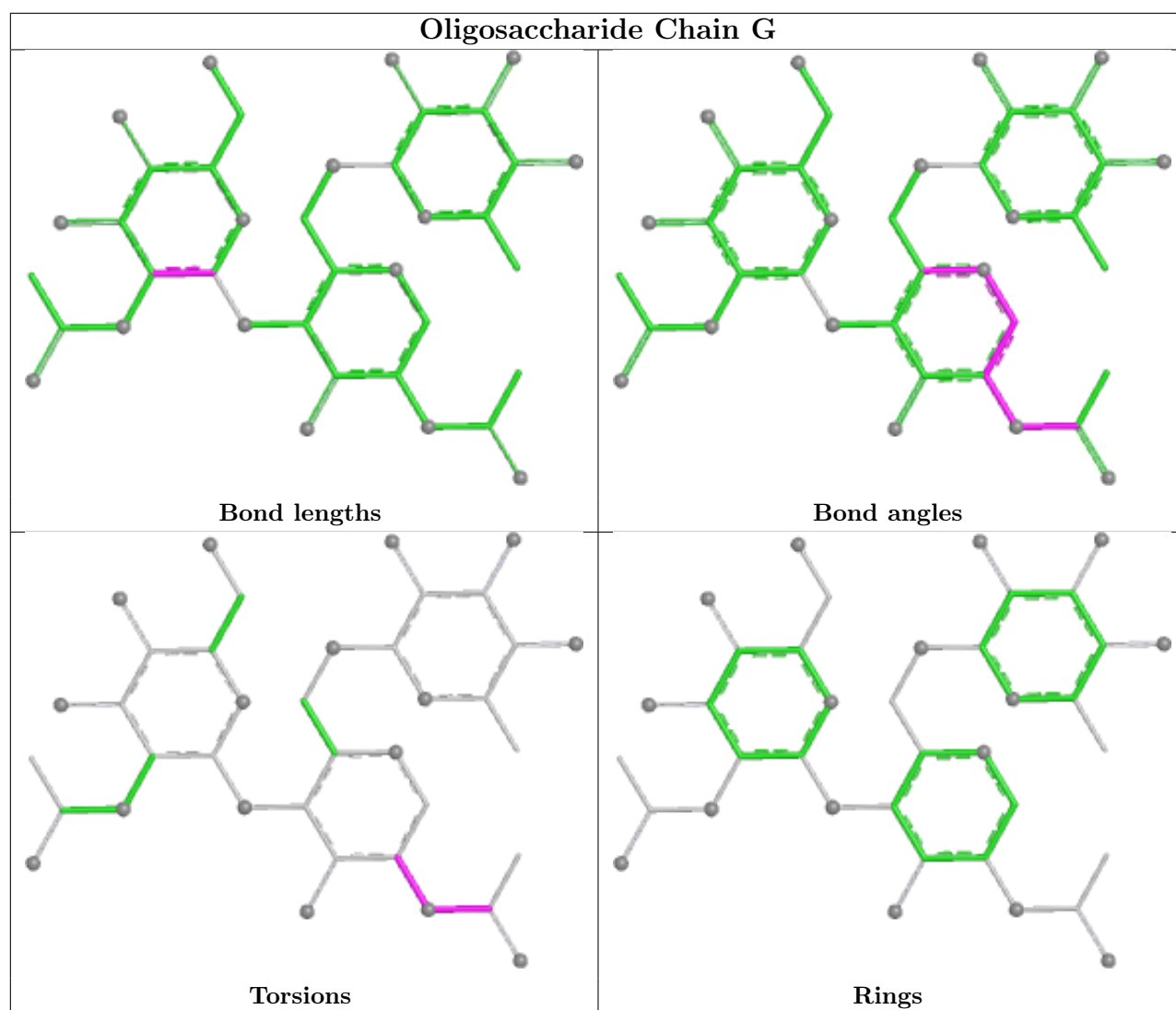
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

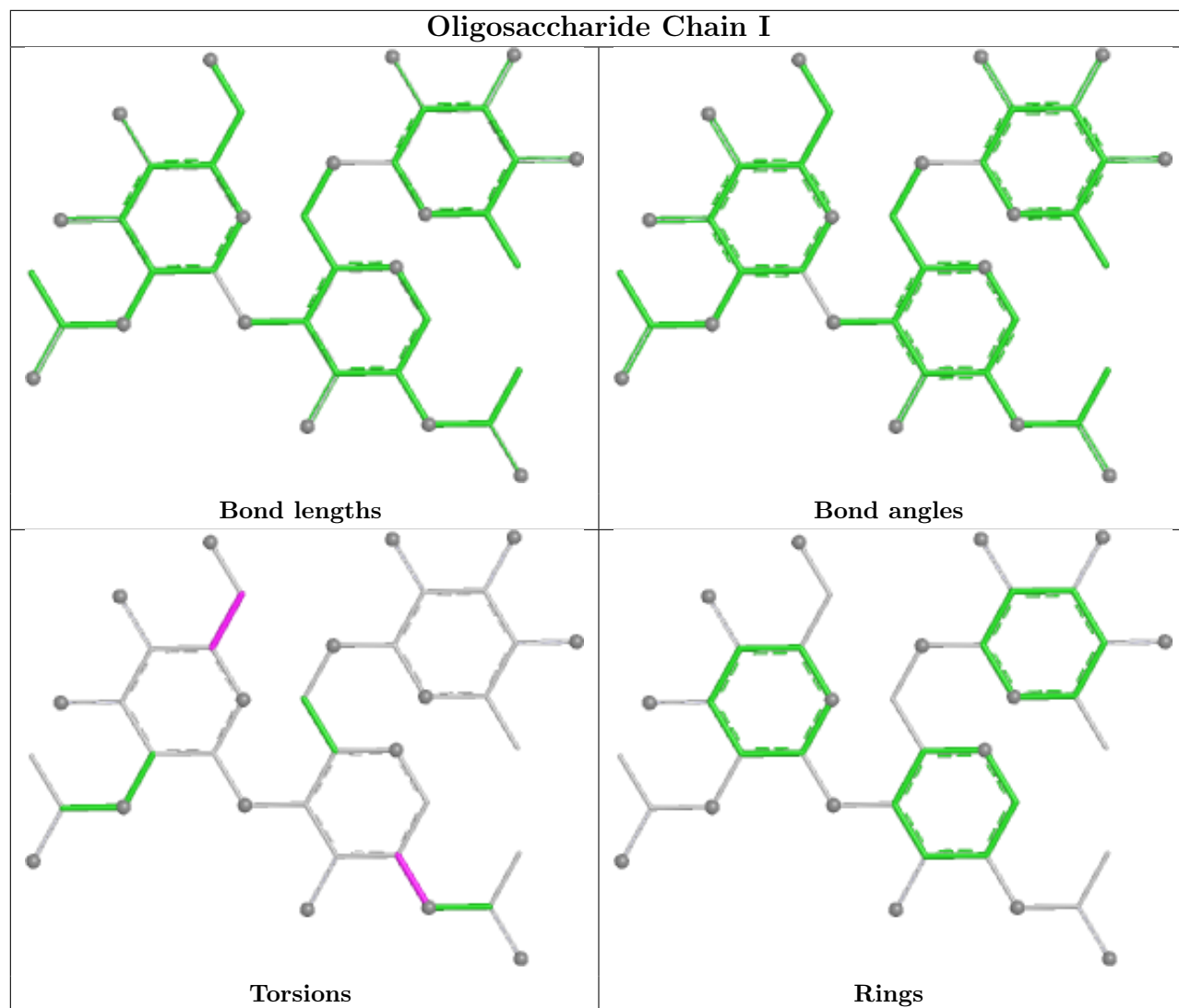


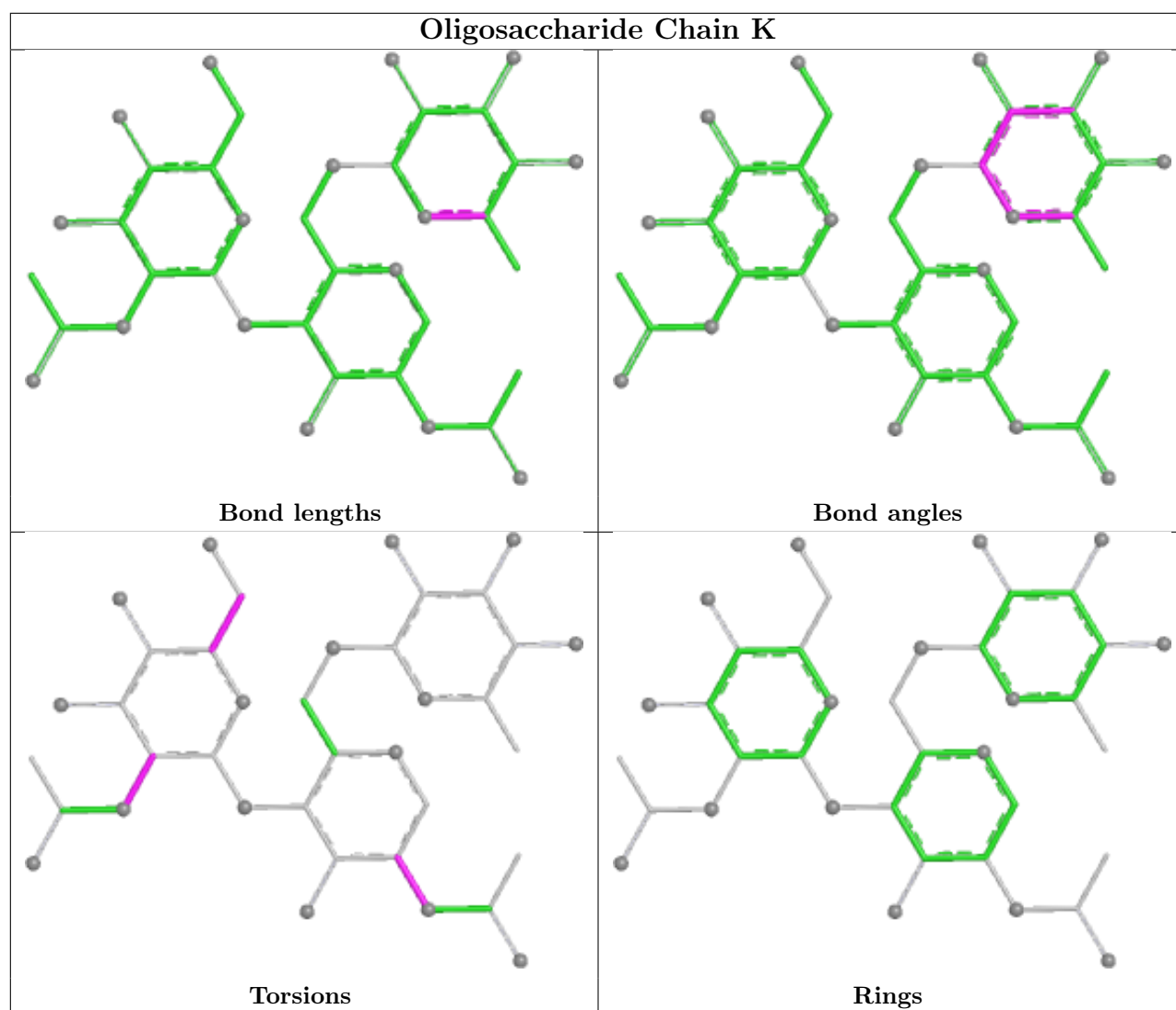












5.6 Ligand geometry [i](#)

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	A	707	12	10,10,10	1.05	0	11,11,11	0.96	0
7	EDO	D	709	-	3,3,3	0.37	0	2,2,2	0.36	0
6	PEG	B	707	-	6,6,6	0.49	0	5,5,5	0.24	0

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	1.05	1 (10%)	11,11,11	1.26	1 (9%)
4	BO3	B	705	-	3,3,3	0.32	0	3,3,3	0.17	0
14	MXE	C	707[A]	-	4,4,4	0.37	0	3,3,3	0.32	0
7	EDO	A	711	-	3,3,3	0.41	0	2,2,2	0.41	0
8	PGE	B	709	-	9,9,9	0.34	0	8,8,8	0.32	0
8	PGE	D	708[A]	-	9,9,9	0.29	0	8,8,8	0.32	0
14	MXE	B	712	-	4,4,4	0.40	0	3,3,3	0.31	0
7	EDO	A	718	-	3,3,3	0.48	0	2,2,2	0.64	0
7	EDO	A	714	-	3,3,3	0.43	0	2,2,2	0.39	0
6	PEG	B	714	-	6,6,6	0.50	0	5,5,5	0.32	0
4	BO3	A	708	-	3,3,3	0.57	0	3,3,3	0.16	0
7	EDO	D	712[A]	-	3,3,3	0.55	0	2,2,2	0.39	0
4	BO3	D	714	-	3,3,3	0.38	0	3,3,3	0.35	0
5	BCN	C	706	12	10,10,10	0.97	0	11,11,11	0.86	0
4	BO3	A	706	-	3,3,3	0.22	0	3,3,3	0.07	0
8	PGE	B	708	-	9,9,9	0.30	0	8,8,8	0.31	0
7	EDO	C	709[B]	-	3,3,3	0.42	0	2,2,2	0.28	0
13	NAG	B	701	1	14,14,15	0.37	0	17,19,21	0.56	0
8	PGE	A	716	-	9,9,9	0.49	0	8,8,8	0.78	0
8	PGE	A	712	-	9,9,9	0.33	0	8,8,8	0.30	0
7	EDO	A	717	-	3,3,3	0.33	0	2,2,2	0.53	0
7	EDO	B	711	-	3,3,3	0.45	0	2,2,2	0.40	0
7	EDO	A	715	-	3,3,3	0.45	0	2,2,2	0.65	0
7	EDO	B	710	-	3,3,3	0.46	0	2,2,2	0.37	0
4	BO3	A	713	-	3,3,3	0.36	0	3,3,3	0.29	0
7	EDO	C	709[A]	-	3,3,3	0.49	0	2,2,2	0.49	0
14	MXE	C	707[B]	-	4,4,4	0.46	0	3,3,3	0.37	0
4	BO3	D	713	-	3,3,3	0.62	0	3,3,3	0.25	0
6	PEG	A	710	-	6,6,6	0.50	0	5,5,5	0.41	0
4	BO3	C	708	-	3,3,3	0.36	0	3,3,3	0.16	0
7	EDO	D	712[B]	-	3,3,3	0.50	0	2,2,2	0.51	0
6	PEG	B	713	-	6,6,6	0.48	0	5,5,5	0.39	0
8	PGE	D	708[B]	-	9,9,9	0.30	0	8,8,8	0.34	0
4	BO3	D	706	-	3,3,3	0.42	0	3,3,3	0.32	0
7	EDO	C	710	-	3,3,3	0.46	0	2,2,2	0.37	0
7	EDO	D	710	-	3,3,3	0.47	0	2,2,2	0.32	0
7	EDO	D	711	12	3,3,3	0.46	0	2,2,2	0.48	0
5	BCN	D	707	12	10,10,10	0.77	0	11,11,11	1.07	1 (9%)
7	EDO	C	711	-	3,3,3	0.48	0	2,2,2	0.43	0
5	BCN	A	709	12	10,10,10	1.03	0	11,11,11	1.02	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	A	707	12	-	0/10/10/10	-
7	EDO	D	709	-	-	0/1/1/1	-
6	PEG	B	707	-	-	3/4/4/4	-
5	BCN	B	706	12	-	2/10/10/10	-
14	MXE	C	707[A]	-	-	1/2/2/2	-
7	EDO	A	711	-	-	0/1/1/1	-
8	PGE	B	709	-	-	4/7/7/7	-
8	PGE	D	708[A]	-	-	2/7/7/7	-
14	MXE	B	712	-	-	0/2/2/2	-
7	EDO	A	718	-	-	0/1/1/1	-
7	EDO	A	714	-	-	1/1/1/1	-
6	PEG	B	714	-	-	2/4/4/4	-
7	EDO	D	712[A]	-	-	0/1/1/1	-
5	BCN	C	706	12	-	2/10/10/10	-
8	PGE	B	708	-	-	0/7/7/7	-
7	EDO	C	709[B]	-	-	0/1/1/1	-
13	NAG	B	701	1	-	2/6/23/26	0/1/1/1
8	PGE	A	716	-	-	4/7/7/7	-
8	PGE	A	712	-	-	3/7/7/7	-
7	EDO	A	717	-	-	1/1/1/1	-
7	EDO	B	711	-	-	0/1/1/1	-
7	EDO	A	715	-	-	1/1/1/1	-
7	EDO	B	710	-	-	0/1/1/1	-
7	EDO	C	709[A]	-	-	0/1/1/1	-
14	MXE	C	707[B]	-	-	1/2/2/2	-
6	PEG	A	710	-	-	2/4/4/4	-
7	EDO	D	712[B]	-	-	0/1/1/1	-
6	PEG	B	713	-	-	1/4/4/4	-
8	PGE	D	708[B]	-	-	1/7/7/7	-
7	EDO	C	710	-	-	0/1/1/1	-
7	EDO	D	710	-	-	1/1/1/1	-
7	EDO	D	711	12	-	1/1/1/1	-
5	BCN	D	707	12	-	2/10/10/10	-
7	EDO	C	711	-	-	1/1/1/1	-
5	BCN	A	709	12	-	3/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	706	BCN	O21-C2	2.20	1.29	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	706	BCN	O22-C2-C1	2.30	122.44	113.38
5	D	707	BCN	C1-N1-C3	-2.10	106.85	111.91

There are no chirality outliers.

All (41) 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
5	C	706	BCN	N1-C5-C6-O6
13	B	701	NAG	O5-C5-C6-O6
8	A	712	PGE	O1-C1-C2-O2
14	C	707[B]	MXE	O1-C1-C2-O2
13	B	701	NAG	C4-C5-C6-O6
8	D	708[B]	PGE	O1-C1-C2-O2
6	B	707	PEG	O2-C3-C4-O4
14	C	707[A]	MXE	O1-C1-C2-O2
8	B	709	PGE	O1-C1-C2-O2
7	D	710	EDO	O1-C1-C2-O2
7	D	711	EDO	O1-C1-C2-O2
8	A	712	PGE	O3-C5-C6-O4
8	A	716	PGE	C1-C2-O2-C3
5	B	706	BCN	N1-C3-C4-O4
6	B	707	PEG	O1-C1-C2-O2
6	B	714	PEG	O2-C3-C4-O4
8	A	716	PGE	O3-C5-C6-O4
8	D	708[A]	PGE	O3-C5-C6-O4
6	A	710	PEG	C1-C2-O2-C3
6	B	707	PEG	C4-C3-O2-C2
8	B	709	PGE	O3-C5-C6-O4
6	A	710	PEG	C4-C3-O2-C2
8	A	712	PGE	O2-C3-C4-O3
5	A	709	BCN	C2-C1-N1-C5
7	A	717	EDO	O1-C1-C2-O2
8	A	716	PGE	C4-C3-O2-C2
7	A	714	EDO	O1-C1-C2-O2
5	C	706	BCN	C6-C5-N1-C1

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Mol	Chain	Res	Type	Atoms
5	A	709	BCN	C4-C3-N1-C5
6	B	713	PEG	C1-C2-O2-C3
8	B	709	PGE	C4-C3-O2-C2
7	A	715	EDO	O1-C1-C2-O2
7	C	711	EDO	O1-C1-C2-O2
5	B	706	BCN	C4-C3-N1-C1
5	A	709	BCN	C4-C3-N1-C1
5	D	707	BCN	C6-C5-N1-C1
8	A	716	PGE	O2-C3-C4-O3
8	B	709	PGE	C3-C4-O3-C5
6	B	714	PEG	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	707	PEG	2	0
7	A	711	EDO	1	0
4	D	714	BO3	1	0
4	A	706	BO3	1	0
8	A	716	PGE	5	0
8	A	712	PGE	1	0
5	A	709	BCN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	608/629 (96%)	0.46	42 (6%) 23 25	14, 39, 67, 102	5 (0%)
1	B	605/629 (96%)	0.69	104 (17%) 4 3	12, 37, 82, 109	8 (1%)
1	C	605/629 (96%)	0.69	62 (10%) 12 12	13, 40, 72, 113	7 (1%)
1	D	607/629 (96%)	0.48	50 (8%) 17 18	13, 38, 71, 111	9 (1%)
All	All	2425/2516 (96%)	0.58	258 (10%) 11 11	12, 39, 74, 113	29 (1%)

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	THR	7.1
1	D	135	THR	6.6
1	D	130	PRO	6.6
1	B	105	LEU	6.3
1	C	135	THR	5.7
1	B	130	PRO	5.4
1	C	129	LEU	5.2
1	D	129	LEU	5.2
1	C	130	PRO	5.1
1	C	79	ILE	5.0
1	B	1	LEU	5.0
1	C	80	TRP	4.7
1	B	75	LEU	4.7
1	B	129	LEU	4.7
1	A	611	ILE	4.6
1	A	131	GLN	4.6
1	C	83	PHE	4.5
1	B	79	ILE	4.4
1	B	51	ALA	4.4
1	C	608	PRO	4.3
1	B	10	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	4.2
1	B	8	GLY	4.2
1	D	325	GLY	4.1
1	C	607	TYR	4.1
1	B	135	THR	4.1
1	C	1	LEU	4.1
1	D	1	LEU	4.1
1	D	131	GLN	4.0
1	B	48	ALA	4.0
1	C	131	GLN	4.0
1	C	78	PRO	4.0
1	B	78	PRO	3.9
1	A	610	GLY	3.9
1	B	325	GLY	3.9
1	B	608	PRO	3.9
1	A	325	GLY	3.8
1	D	610	GLY	3.8
1	C	88	LEU	3.8
1	D	413	ARG	3.8
1	B	57	ALA	3.8
1	A	130	PRO	3.7
1	B	98	LEU	3.7
1	B	131	GLN	3.7
1	C	19	LEU	3.6
1	B	13	ASP	3.6
1	B	331	HIS	3.6
1	B	73	LYS	3.6
1	B	60	LEU	3.5
1	C	412	ASP	3.5
1	B	15	ALA	3.4
1	C	15	ALA	3.4
1	C	17	ALA	3.4
1	B	24	TYR	3.4
1	B	63	GLU	3.4
1	B	4	GLY	3.4
1	B	12	ALA	3.3
1	B	323	ALA	3.3
1	B	19	LEU	3.3
1	B	68	TRP	3.3
1	B	53	ARG	3.3
1	B	607	TYR	3.3
1	C	105	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	606	ASN	3.3
1	C	325	GLY	3.3
1	D	128	CYS	3.3
1	D	331	HIS	3.2
1	C	21	ALA	3.2
1	D	323	ALA	3.2
1	B	2	ASP	3.2
1	B	3	PRO	3.2
1	D	416	ASN	3.2
1	C	12	ALA	3.2
1	D	418	THR	3.2
1	C	75	LEU	3.2
1	C	93	GLY	3.2
1	D	105	LEU	3.2
1	B	80	TRP	3.1
1	B	47	THR	3.1
1	D	285	GLN	3.1
1	B	20	PHE	3.1
1	C	606	ASN	3.1
1	C	10	PHE	3.1
1	C	20	PHE	3.1
1	B	101	ALA	3.1
1	B	76	TYR	3.0
1	B	137	TRP	3.0
1	D	203[A]	ASN	3.0
1	C	5	LEU	3.0
1	D	414	VAL	3.0
1	B	40	TRP	3.0
1	B	104	PRO	3.0
1	B	70	GLN	3.0
1	C	101	ALA	3.0
1	B	203[A]	ASN	3.0
1	B	5	LEU	3.0
1	B	64	PHE	3.0
1	B	71	LYS	3.0
1	B	88	LEU	2.9
1	B	16	GLY	2.9
1	B	7	PRO	2.9
1	A	137	TRP	2.9
1	D	56	GLU	2.9
1	B	95	VAL	2.9
1	C	72	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	92	ILE	2.9
1	C	137	TRP	2.8
1	C	84	THR	2.8
1	C	331	HIS	2.8
1	B	322	PRO	2.8
1	C	76	TYR	2.8
1	C	136	CYS	2.8
1	B	50	ASN	2.8
1	D	415	THR	2.8
1	D	104	PRO	2.8
1	B	21	ALA	2.8
1	A	128	CYS	2.8
1	A	136	CYS	2.8
1	B	136	CYS	2.8
1	A	572[A]	LYS	2.8
1	B	97	THR	2.8
1	D	55	GLU	2.8
1	B	11	SER	2.7
1	B	77	GLU	2.7
1	D	523	GLY	2.7
1	C	289	GLN	2.7
1	B	523	GLY	2.7
1	C	91	ILE	2.7
1	A	52	ARG	2.7
1	C	95	VAL	2.7
1	B	412	ASP	2.7
1	B	46	ILE	2.7
1	B	106	ALA	2.6
1	D	57	ALA	2.6
1	A	3	PRO	2.6
1	D	5	LEU	2.6
1	A	414	VAL	2.6
1	D	605	ASP	2.6
1	A	1	LEU	2.6
1	D	273	ASP	2.6
1	B	414	VAL	2.6
1	D	275	PRO	2.6
1	B	103	LEU	2.6
1	B	413	ARG	2.6
1	D	60	LEU	2.6
1	B	6	GLN	2.6
1	C	605	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	27	SER	2.6
1	A	327	GLU	2.5
1	B	59	LEU	2.5
1	B	416	ASN	2.5
1	B	235[A]	ARG	2.5
1	B	82	GLN	2.5
1	D	284	LEU	2.5
1	B	269	VAL	2.5
1	C	3	PRO	2.5
1	A	330	CYS	2.5
1	A	26	SER	2.5
1	A	55	GLU	2.5
1	A	415	THR	2.5
1	B	83	PHE	2.4
1	D	281	SER	2.4
1	A	323	ALA	2.4
1	B	72	ALA	2.4
1	C	187	LYS	2.4
1	C	415	THR	2.4
1	D	47	THR	2.4
1	D	101	ALA	2.4
1	D	269	VAL	2.4
1	C	240	ARG	2.4
1	C	523	GLY	2.4
1	B	107	LYS	2.4
1	A	418	THR	2.4
1	B	17	ALA	2.4
1	C	104	PRO	2.4
1	C	377	VAL	2.4
1	D	70	GLN	2.4
1	C	128	CYS	2.4
1	C	241	TYR	2.4
1	B	49	GLU	2.4
1	B	606	ASN	2.4
1	B	31	VAL	2.4
1	C	236	ARG	2.3
1	D	103	LEU	2.3
1	A	607	TYR	2.3
1	A	271	PHE	2.3
1	C	22	GLN	2.3
1	C	94	ALA	2.3
1	C	11	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	414	VAL	2.3
1	D	53	ARG	2.3
1	A	609	GLU	2.3
1	C	98	LEU	2.3
1	B	415	THR	2.3
1	B	34	GLN	2.3
1	B	276	ASN	2.3
1	B	33	PHE	2.3
1	A	272	PRO	2.3
1	B	41	ALA	2.3
1	B	67	ALA	2.3
1	D	3	PRO	2.3
1	D	48	ALA	2.3
1	B	55	GLU	2.3
1	A	576	LEU	2.3
1	C	576	LEU	2.3
1	B	38	ALA	2.2
1	C	86	PRO	2.2
1	C	271	PHE	2.2
1	D	81[A]	GLN	2.2
1	A	413	ARG	2.2
1	D	136	CYS	2.2
1	A	603	LEU	2.2
1	C	16	GLY	2.2
1	D	520	GLY	2.2
1	B	65	ALA	2.2
1	A	268	VAL	2.2
1	B	128	CYS	2.2
1	A	51	ALA	2.2
1	D	407	LYS	2.2
1	B	52	ARG	2.2
1	C	89	ARG	2.2
1	D	609	GLU	2.2
1	A	6	GLN	2.2
1	C	81	GLN	2.2
1	D	79	ILE	2.1
1	B	81	GLN	2.1
1	A	591	VAL	2.1
1	A	126	LYS	2.1
1	B	120	ARG	2.1
1	C	413	ARG	2.1
1	D	277	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	576	LEU	2.1
1	D	51	ALA	2.1
1	A	158	PHE	2.1
1	B	239	ASP	2.1
1	A	236	ARG	2.1
1	A	523	GLY	2.1
1	B	377	VAL	2.1
1	D	98	LEU	2.1
1	B	28	ALA	2.1
1	D	62	GLN	2.1
1	B	338	TYR	2.1
1	B	56	GLU	2.1
1	B	69	GLY	2.1
1	B	328	VAL	2.1
1	C	103	LEU	2.1
1	B	138	SER	2.0
1	A	331	HIS	2.0
1	A	105	LEU	2.0
1	B	603	LEU	2.0
1	B	326	ARG	2.0
1	A	155	MET	2.0
1	B	91	ILE	2.0
1	B	84	THR	2.0
1	A	521	TYR	2.0
1	C	24	TYR	2.0
1	B	604	PRO	2.0
1	D	52	ARG	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($\text{\AA}^2$)	Q<0.9
2	NAG	J	2	14/15	0.53	0.19	82,97,113,116	0

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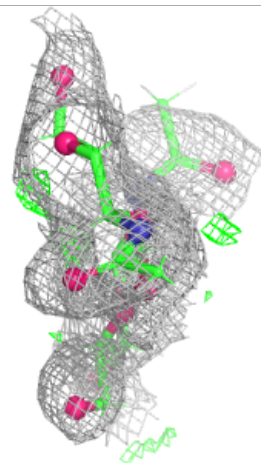
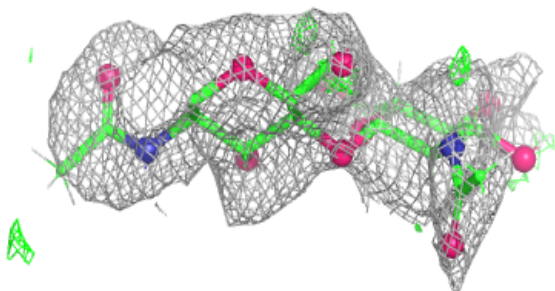
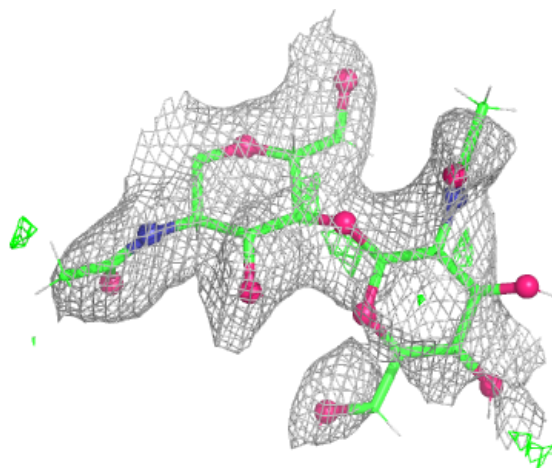
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	H	2	14/15	0.60	0.17	79,93,109,121	0
3	NAG	F	2	14/15	0.63	0.22	59,77,82,87	0
3	NAG	G	2	14/15	0.64	0.19	62,86,113,117	0
2	NAG	E	2	14/15	0.67	0.18	75,90,108,115	0
3	NAG	I	2	14/15	0.70	0.18	51,76,95,102	0
3	FUC	K	3	10/11	0.71	0.25	59,74,89,89	0
3	NAG	K	2	14/15	0.74	0.18	62,81,101,106	0
2	NAG	J	1	14/15	0.78	0.15	67,90,106,110	0
3	NAG	K	1	14/15	0.81	0.17	42,58,68,80	0
2	NAG	H	1	14/15	0.83	0.13	52,64,80,87	0
3	FUC	G	3	10/11	0.85	0.14	45,58,83,90	0
2	NAG	E	1	14/15	0.86	0.14	55,70,83,88	0
3	FUC	F	3	10/11	0.87	0.12	48,59,74,77	0
3	FUC	I	3	10/11	0.89	0.11	46,57,73,76	0
3	NAG	G	1	14/15	0.89	0.12	31,45,60,64	0
3	NAG	I	1	14/15	0.90	0.11	38,47,57,66	0
3	NAG	F	1	14/15	0.91	0.12	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.

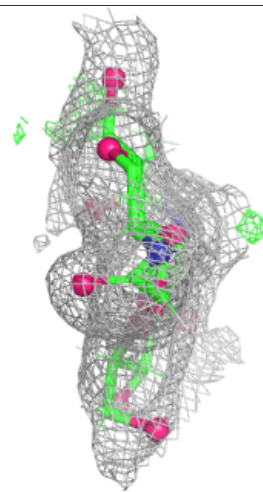
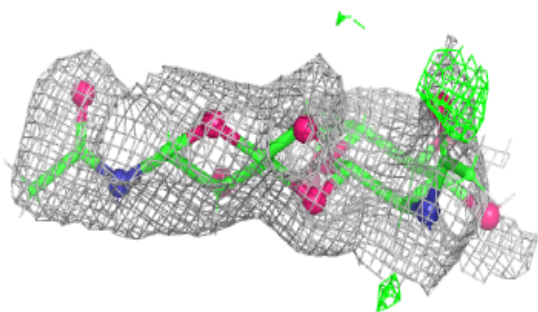
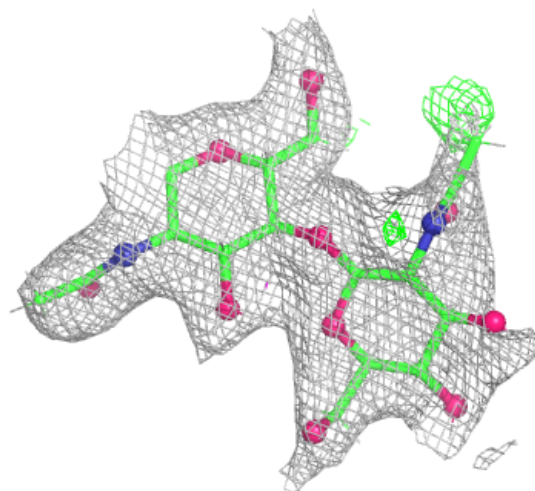
Electron density around Chain E:

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



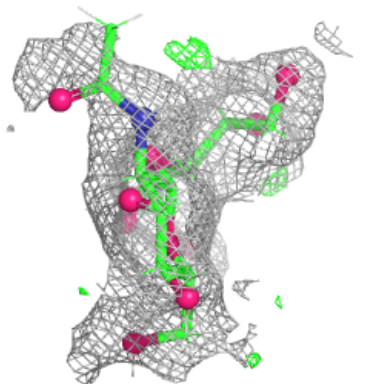
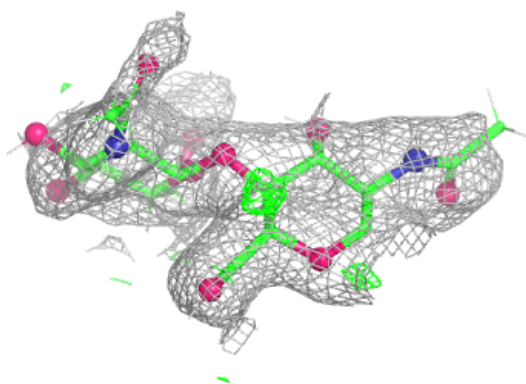
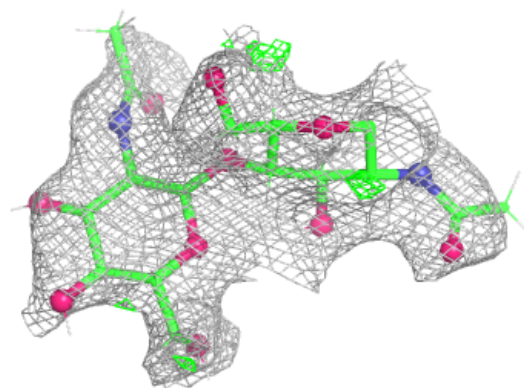
Electron density around Chain H:

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



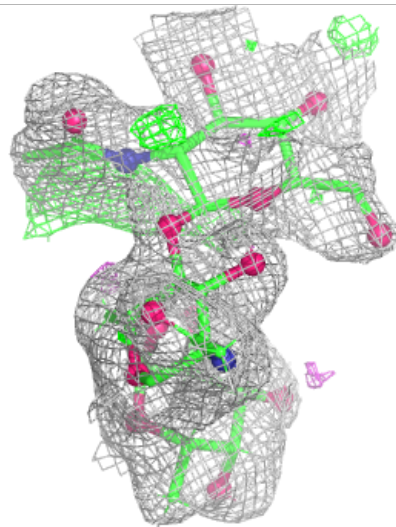
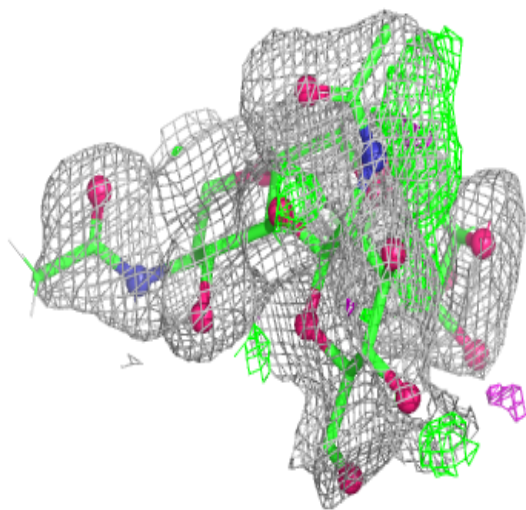
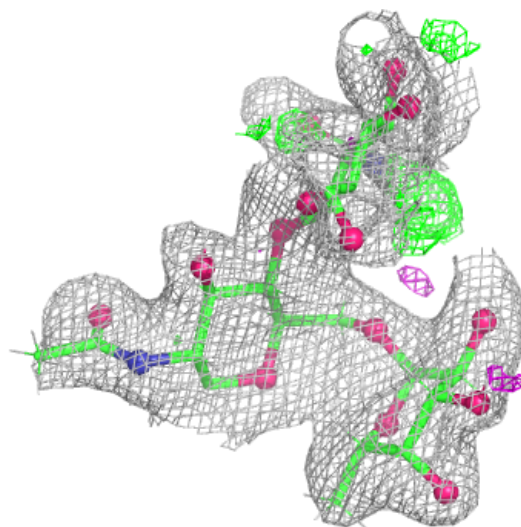
Electron density around Chain J:

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



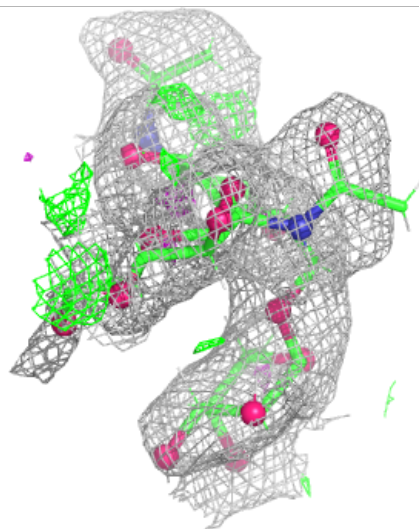
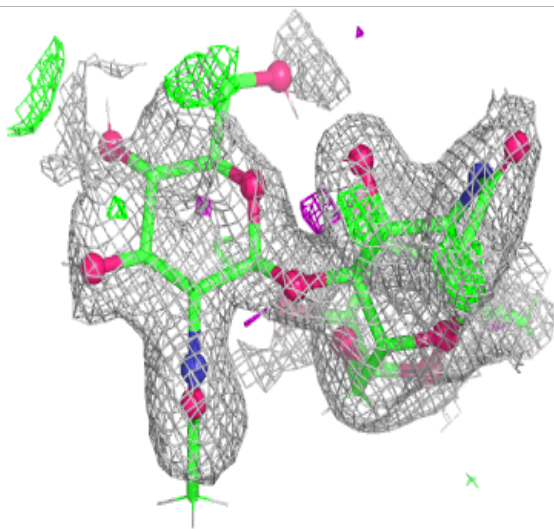
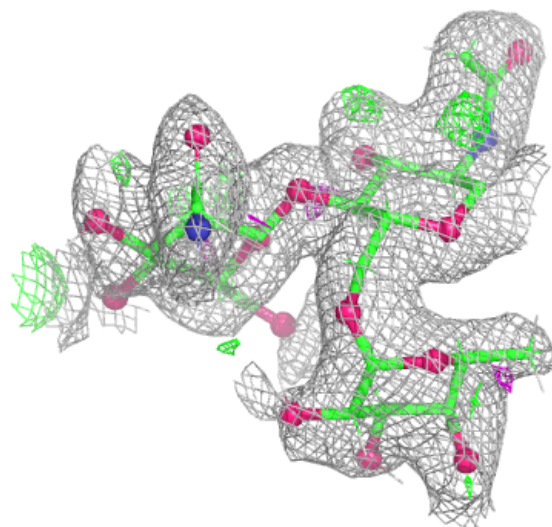
Electron density around Chain F:

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



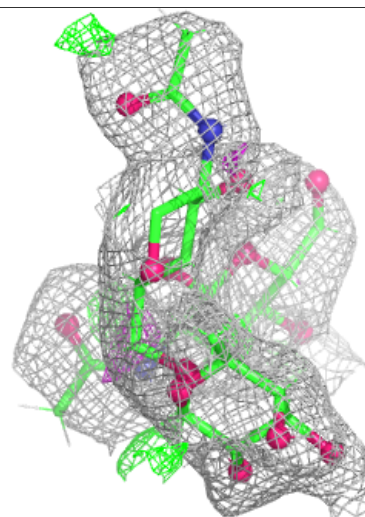
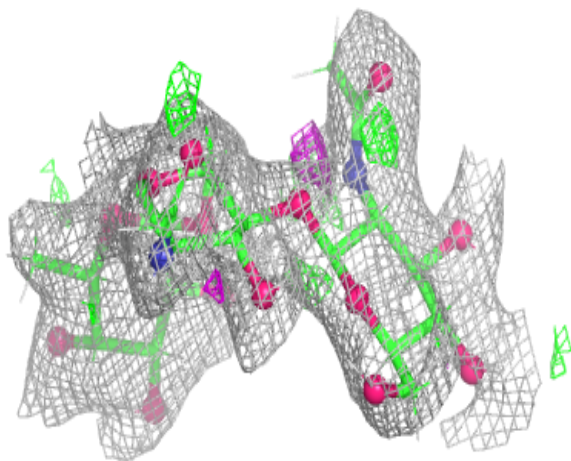
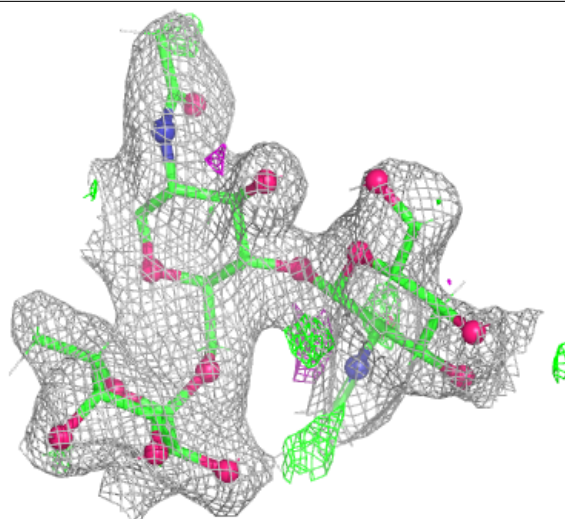
Electron density around Chain G:

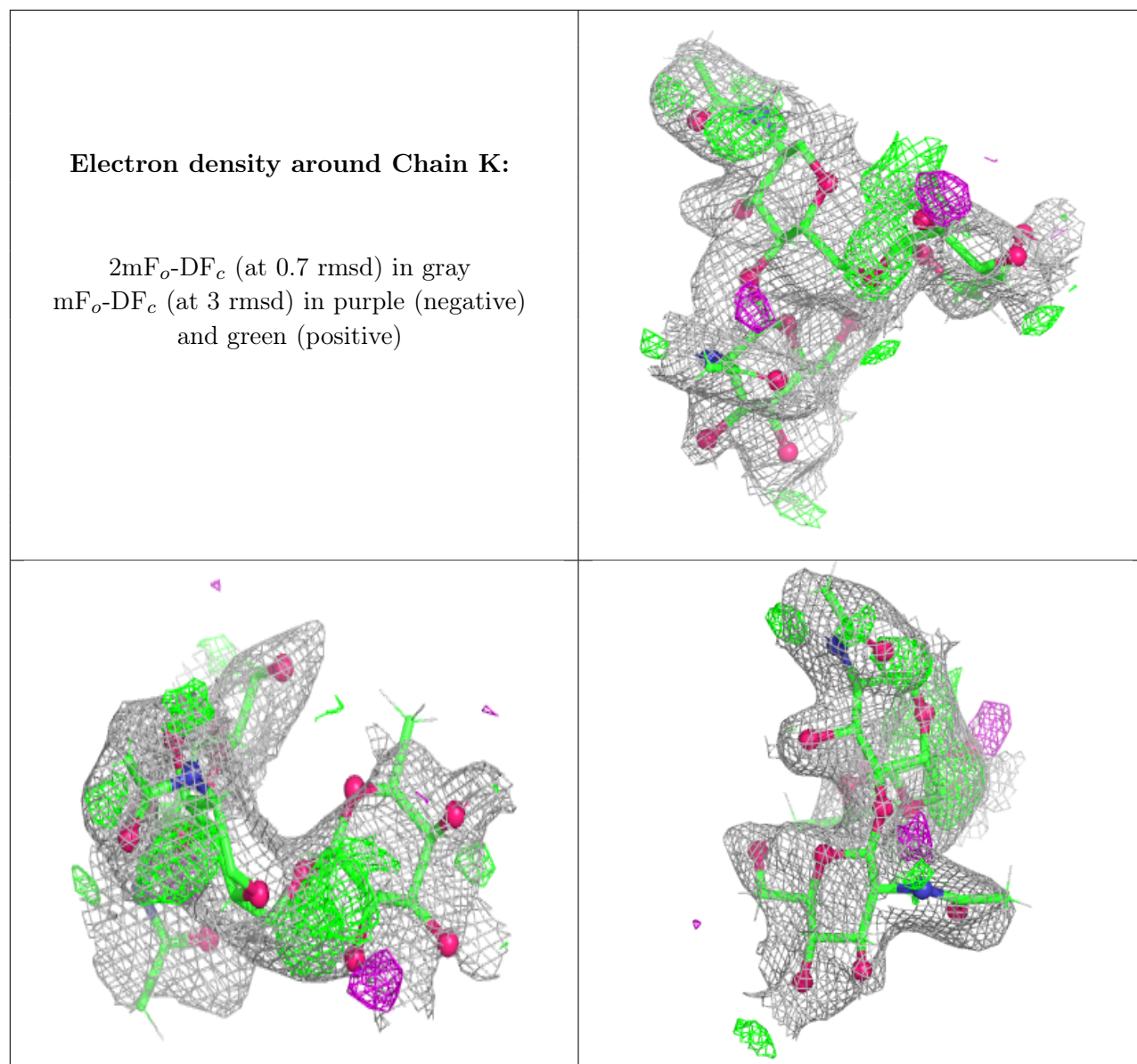
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
11	MG	A	721	1/1	0.64	0.27	72,72,72,72	0
13	NAG	B	701	14/15	0.69	0.17	61,83,105,106	0
6	PEG	B	707	7/7	0.73	0.20	56,70,85,85	0
7	EDO	A	718	4/4	0.73	0.18	59,70,80,81	0
7	EDO	D	711	4/4	0.74	0.18	45,54,62,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	MXE	C	707[A]	5/5	0.74	0.27	43,53,62,65	13
14	MXE	C	707[B]	5/5	0.74	0.27	34,47,61,62	13
7	EDO	D	709	4/4	0.75	0.20	57,69,75,75	0
7	EDO	A	717	4/4	0.75	0.21	48,58,70,72	0
7	EDO	C	709[A]	4/4	0.76	0.23	40,48,55,57	10
7	EDO	C	709[B]	4/4	0.76	0.23	37,45,55,57	10
15	NA	B	719	1/1	0.77	0.15	63,63,63,63	0
7	EDO	C	710	4/4	0.78	0.18	59,71,77,85	0
7	EDO	C	711	4/4	0.79	0.18	60,72,75,78	0
5	BCN	A	709	11/11	0.81	0.15	48,63,70,73	0
11	MG	B	717	1/1	0.81	0.12	63,63,63,63	0
8	PGE	A	712	10/10	0.81	0.17	44,63,72,75	0
7	EDO	B	710	4/4	0.82	0.17	44,53,64,69	0
8	PGE	D	708[A]	10/10	0.83	0.16	45,59,71,71	24
8	PGE	D	708[B]	10/10	0.83	0.16	45,59,71,71	24
7	EDO	D	712[B]	4/4	0.83	0.18	38,49,54,59	10
7	EDO	D	712[A]	4/4	0.83	0.18	38,48,57,58	10
6	PEG	A	710	7/7	0.84	0.16	55,66,75,82	0
4	BO3	A	713	4/4	0.85	0.14	47,51,59,61	0
8	PGE	B	709	10/10	0.85	0.14	46,55,66,76	0
14	MXE	B	712	5/5	0.85	0.15	46,55,65,65	0
6	PEG	B	713	7/7	0.85	0.20	37,49,59,67	17
7	EDO	A	711	4/4	0.85	0.17	50,60,66,70	0
7	EDO	B	711	4/4	0.85	0.13	48,59,70,74	0
4	BO3	D	714	4/4	0.86	0.11	42,50,67,81	0
6	PEG	B	714	7/7	0.86	0.14	50,61,74,74	0
8	PGE	A	716	10/10	0.87	0.21	21,53,60,63	24
8	PGE	B	708	10/10	0.87	0.15	51,68,76,76	0
11	MG	C	714	1/1	0.88	0.09	44,44,44,44	1
4	BO3	D	713	4/4	0.88	0.17	34,41,57,69	0
4	BO3	A	706	4/4	0.88	0.13	45,51,59,62	0
7	EDO	D	710	4/4	0.89	0.12	50,62,70,84	0
4	BO3	C	708	4/4	0.90	0.17	40,44,53,60	0
7	EDO	A	714	4/4	0.91	0.13	48,58,63,64	0
7	EDO	A	715	4/4	0.92	0.12	51,61,68,75	0
4	BO3	B	705	4/4	0.93	0.15	33,36,40,43	0
5	BCN	D	707	11/11	0.93	0.10	24,38,46,50	0
5	BCN	A	707	11/11	0.93	0.09	29,42,51,53	0
5	BCN	C	706	11/11	0.94	0.09	26,35,45,54	0
4	BO3	A	708	4/4	0.94	0.09	35,38,44,50	0
4	BO3	D	706	4/4	0.94	0.11	31,37,44,44	0
5	BCN	B	706	11/11	0.96	0.07	24,39,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	CA	D	717	1/1	0.98	0.07	26,26,26,26	0
10	CL	A	720	1/1	0.99	0.03	26,26,26,26	0
10	CL	B	716	1/1	0.99	0.03	23,23,23,23	0
10	CL	C	713	1/1	0.99	0.04	26,26,26,26	0
12	CA	A	722	1/1	0.99	0.06	31,31,31,31	0
12	CA	B	718	1/1	0.99	0.06	28,28,28,28	0
12	CA	C	715	1/1	0.99	0.07	30,30,30,30	0
9	ZN	B	715	1/1	1.00	0.01	27,27,27,27	0
9	ZN	C	712	1/1	1.00	0.01	27,27,27,27	0
10	CL	D	716	1/1	1.00	0.03	23,23,23,23	0
9	ZN	D	715	1/1	1.00	0.02	27,27,27,27	0
9	ZN	A	719	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.