



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 10:39 am GMT

PDB ID : 6EN6  
Title : Crystal structure B of the Angiotensin-1 converting enzyme N-domain in complex with a diprolyl inhibitor.  
Authors : Cozier, G.E.; Acharya, K.R.; Fienberg, S.; Chibale, K.; Sturrock, E.D.  
Deposited on : 2017-10-04  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

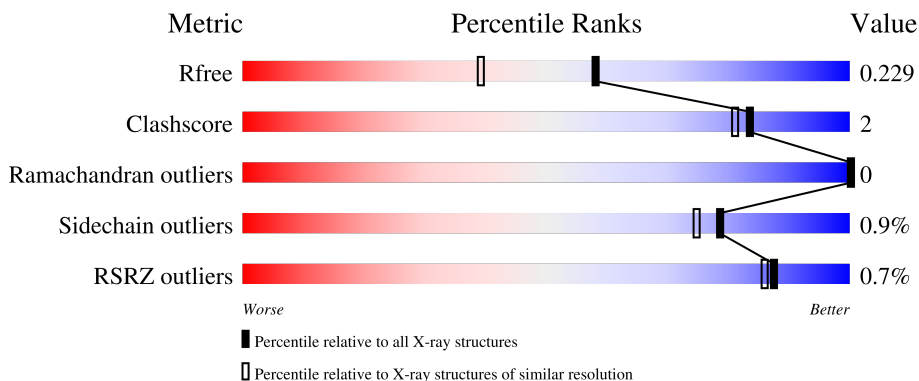
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



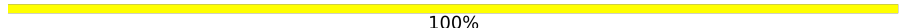


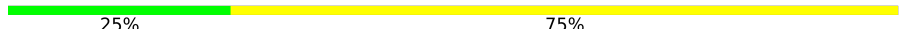





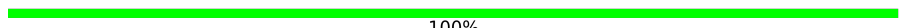
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	629	
1	C	629	
1	D	629	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	M	2	 50% 50%
3	F	4	 50% 25% 25%
3	I	4	 25% 75%
3	N	4	 50% 50%
4	G	3	 67% 33%
4	L	3	 67% 33%
5	J	2	 100%
5	O	2	 50% 50%
6	K	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ACT	D	724	-	-	X	-
13	ACT	D	727	-	-	X	-

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 43754 atoms, of which 20266 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
			Total	C	H	N	O	S			
1	A	605	9801	3214	4791	866	910	20	0	12	0
1	B	605	9862	3230	4823	871	919	19	0	15	0
1	C	606	9838	3227	4804	866	922	19	0	16	0
1	D	614	9975	3269	4876	878	933	19	0	13	0

There are 36 discrepancies between the modelled and reference sequences:

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

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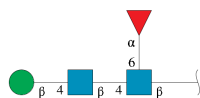
Chain	Residue	Modelled	Actual	Comment	Reference
C	117	GLN	ASN	conflict	UNP P12821
C	131	GLN	ASN	conflict	UNP P12821
C	289	GLN	ASN	conflict	UNP P12821
C	545	ARG	GLN	conflict	UNP P12821
C	576	LEU	PRO	conflict	UNP P12821
C	629	LEU	-	expression tag	UNP P12821
D	9	GLN	ASN	conflict	UNP P12821
D	25	GLN	ASN	conflict	UNP P12821
D	82	GLN	ASN	conflict	UNP P12821
D	117	GLN	ASN	conflict	UNP P12821
D	131	GLN	ASN	conflict	UNP P12821
D	289	GLN	ASN	conflict	UNP P12821
D	545	ARG	GLN	conflict	UNP P12821
D	576	LEU	PRO	conflict	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	M	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



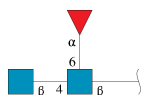
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			
3	N	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



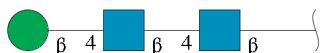
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
4	L	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			
5	O	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

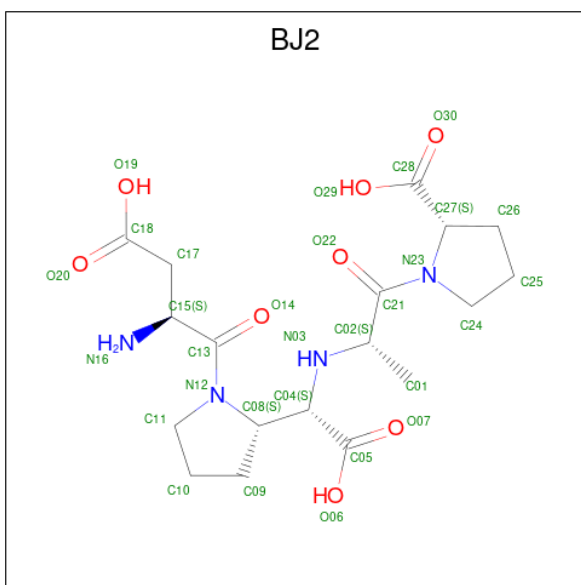


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is (2 {S})-1-[(2 {S})-2-[[1 {S})-1-[(2 {S})-1-[(2 {S})-2-azanyl-4-oxidanyl-4-oxidanylidene-butanoyl]pyrrolidin-2-yl]-2-oxidanyl-2-oxidanylidene-ethyl]amino]propanoyl]pyrrolidine-2-carboxylic acid (three-letter code: BJ2) (formula: C<sub>18</sub>H<sub>28</sub>N<sub>4</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	A	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
8	B	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
8	C	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
8	D	1	Total	C	H	N	O	0	0
			55	18	25	4	8		

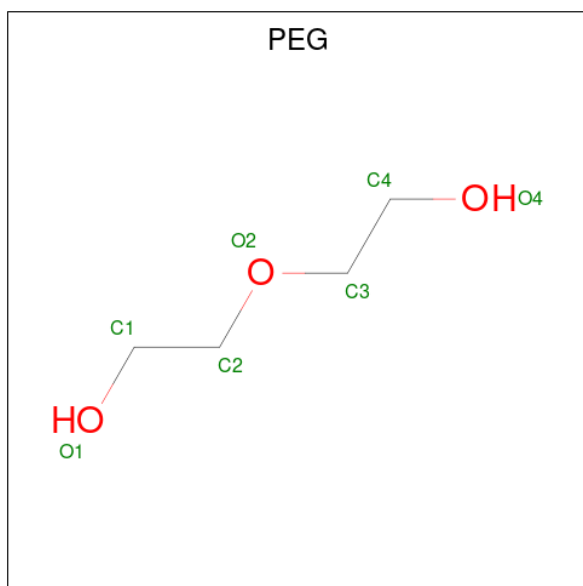
- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

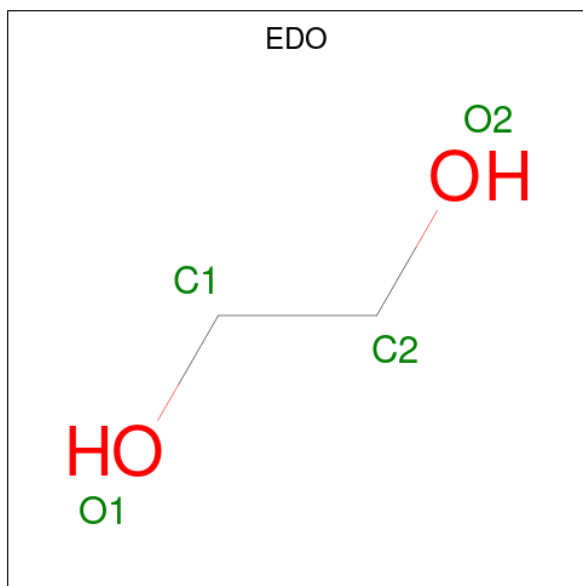
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	C	1	Total	C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

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



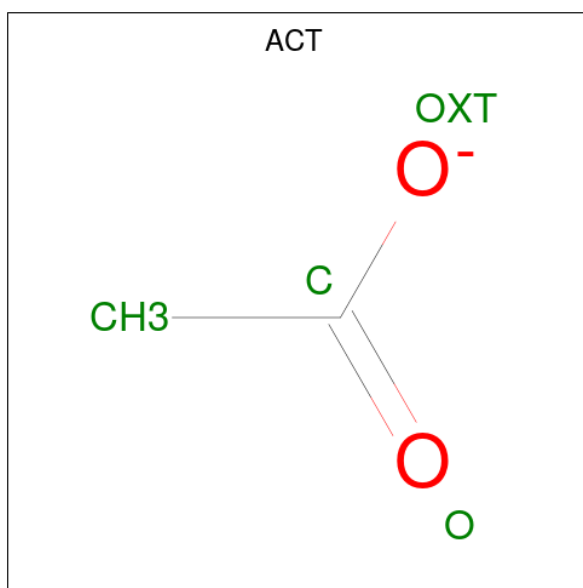
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	A	1	Total	C	H	O	0	0
			10	2	6	2		

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

- Molecule 13 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



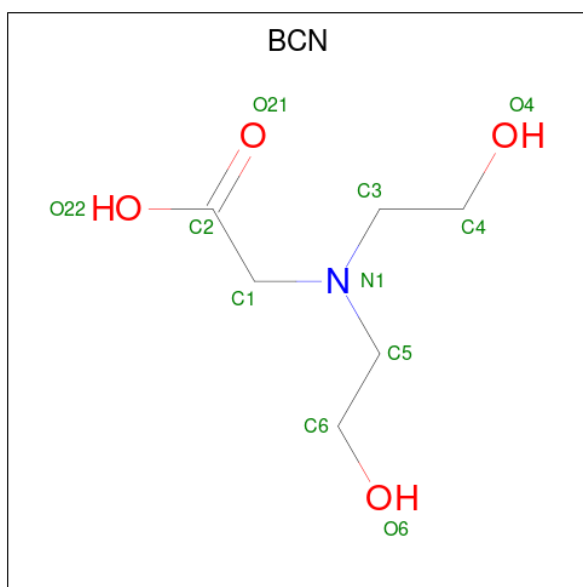
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	H	O	0	0
			7	2	3	2		
13	A	1	Total	C	H	O	0	0
			7	2	3	2		
13	B	1	Total	C	H	O	0	0
			7	2	3	2		
13	B	1	Total	C	H	O	0	0
			7	2	3	2		
13	B	1	Total	C	H	O	0	0
			7	2	3	2		
13	C	1	Total	C	H	O	0	0
			7	2	3	2		
13	C	1	Total	C	H	O	0	0
			7	2	3	2		
13	C	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		

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



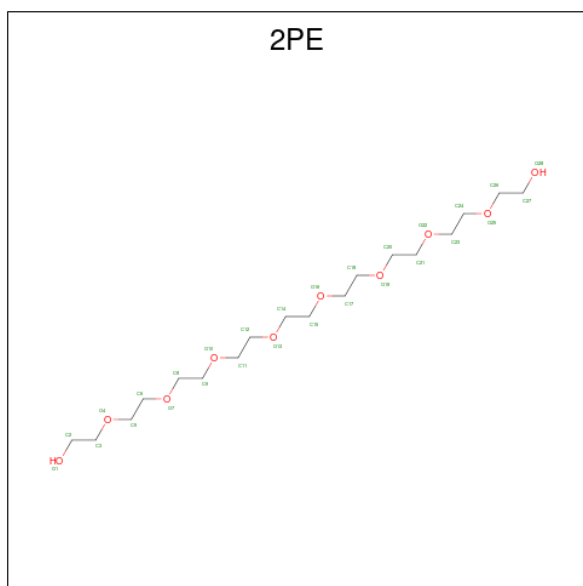
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
14	A	1	24	6	14	4	0	0
14	B	1	24	6	14	4	0	0
14	B	1	48	12	28	8	0	1
14	D	1	24	6	14	4	0	0
14	D	1	24	6	14	4	0	0
14	D	1	24	6	14	4	0	0

- Molecule 15 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



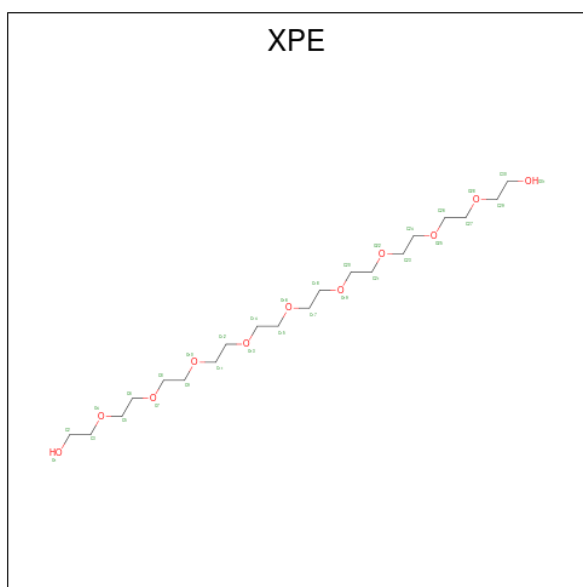
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
15	A	1	23	6	12	1	4	0	0

- Molecule 16 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula:  $C_{18}H_{38}O_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
16	B	1	66	18	38	10	0	0

- Molecule 17 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (three-letter code: XPE) (formula:  $C_{20}H_{42}O_{11}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	H	O	0	0
			73	20	42	11		
17	C	1	Total	C	H	O	0	0
			73	20	42	11		

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

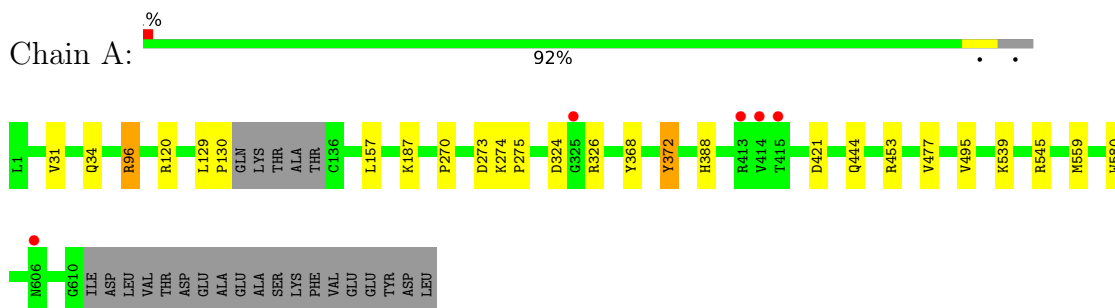
- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	572	Total O 578 578	0	6
19	B	571	Total O 573 573	0	2
19	C	556	Total O 559 559	0	3
19	D	662	Total O 671 671	0	11

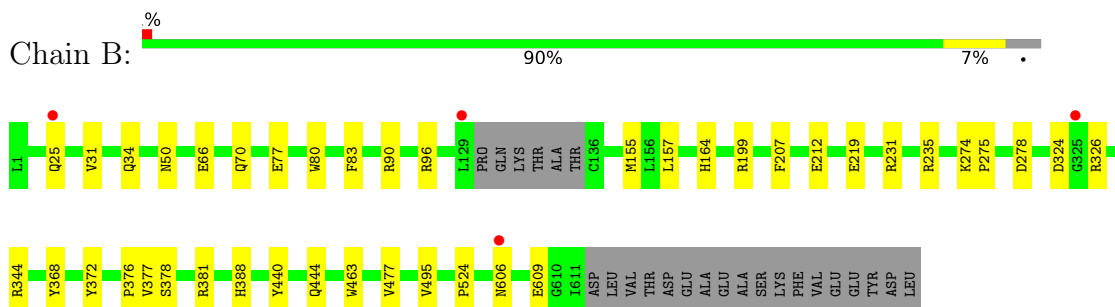
### 3 Residue-property plots

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.

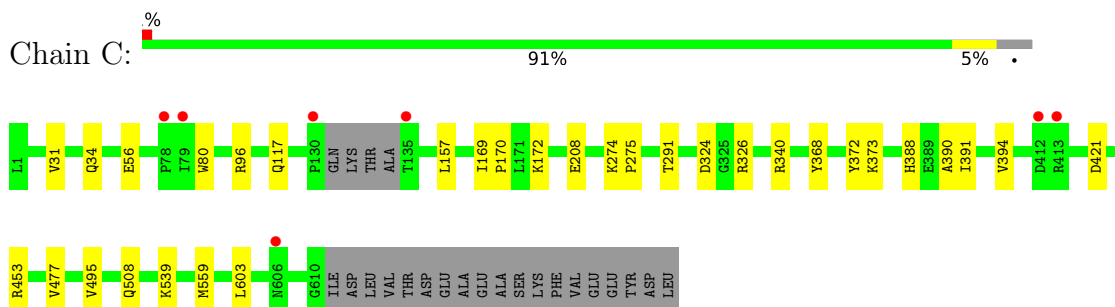
- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme







GLU  
TTR  
ASP  
LEU

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

Chain E: 100%

MAG1  
MAG2

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

Chain H: 100%

MAG1  
MAG2

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

Chain M: 50% 50%

MAG1  
MAG2

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

Chain F: 50% 25% 25%

MAG1  
MAG2  
BMA3  
FUC4

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

Chain I: 25% 75%

MAG1  
MAG2  
BMA3  
FUC4

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

Chain N: 50% 50%



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

Chain G: 67% 33%



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

Chain L: 67% 33%



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 50% 50%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.44Å 103.37Å 115.65Å 84.48° 85.50° 81.61°	Depositor
Resolution (Å)	79.70 – 1.80 101.89 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (79.70-1.80) 97.3 (101.89-1.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 1.80Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.193 , 0.226 0.196 , 0.229	Depositor DCC
$R_{free}$ test set	3041 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	43754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4028e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BJ2, ACT, 2PE, PEG, NAG, CL, EDO, MG, BMA, FUC, XPE, BCN, ZN, PGE

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	0.63	1/5213 (0.0%)	0.65	0/7098
1	B	0.66	1/5225 (0.0%)	0.66	0/7111
1	C	0.60	0/5236	0.63	0/7131
1	D	0.66	0/5278	0.68	0/7187
All	All	0.63	2/20952 (0.0%)	0.65	0/28527

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	GLU	CD-OE1	-7.84	1.17	1.25
1	A	372	TYR	CD1-CE1	5.77	1.48	1.39

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	5010	4791	4736	16	0
1	B	5039	4823	4791	30	0
1	C	5034	4804	4748	20	0
1	D	5099	4876	4838	17	0
2	E	28	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	28	25	25	0	0
2	M	28	25	25	0	0
3	F	49	43	43	1	0
3	I	49	43	43	1	0
3	N	49	43	43	0	0
4	G	38	34	34	0	0
4	L	38	34	34	0	0
5	J	24	22	22	2	0
5	O	24	22	22	1	0
6	K	39	34	34	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	30	25	0	0	0
8	B	30	25	0	1	0
8	C	30	25	0	1	0
8	D	30	25	0	1	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	14	20	20	0	0
11	B	28	40	40	2	0
11	C	14	20	20	3	0
11	D	14	20	20	1	0
12	A	8	12	12	0	0
12	B	32	48	48	4	0
12	C	16	24	24	0	0
12	D	36	54	54	0	0
13	A	8	6	6	0	0
13	B	12	9	9	1	0
13	C	12	9	9	2	0
13	D	20	15	15	3	0
14	A	10	14	14	0	0
14	B	30	42	42	4	0
14	D	30	42	42	3	0
15	A	11	12	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	28	38	38	4	0
17	B	31	42	42	0	0
17	C	31	42	42	2	0
18	C	14	13	13	0	0
19	A	578	0	0	6	0
19	B	573	0	0	7	0
19	C	559	0	0	7	0
19	D	671	0	0	5	0
All	All	23488	20266	19985	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ARG:NH1	19:A:803:HOH:O	2.25	0.69
1:D:378:SER:O	1:D:381[B]:ARG:NH2	2.26	0.69
13:D:724:ACT:H3	13:D:727:ACT:H3	1.76	0.68
1:A:444[B]:GLN:NE2	19:A:802:HOH:O	2.23	0.67
13:D:724:ACT:H3	13:D:727:ACT:CH3	2.26	0.64
13:D:728:ACT:H2	19:D:923:HOH:O	1.97	0.61
1:B:274:LYS:HB3	1:B:275:PRO:CD	2.34	0.58
1:B:235:ARG:NH1	16:B:730:2PE:O16	2.36	0.57
1:A:120:ARG:NH2	19:A:810:HOH:O	2.37	0.57
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.87	0.56
5:J:1:NAG:H61	5:J:2:FUC:O2	2.07	0.55
8:B:710:BJ2:N16	11:B:714:PEG:O1	2.41	0.54
1:A:453:ARG:NH1	1:B:212:GLU:OE2	2.41	0.53
1:D:25:GLN:OE1	1:D:376:PRO:HA	2.09	0.53
1:B:66:GLU:O	1:B:70:GLN:HG3	2.10	0.52
16:B:730:2PE:H172	19:B:919:HOH:O	2.10	0.51
1:D:245:ARG:HG2	1:D:591:VAL:HG21	1.92	0.51
1:B:77:GLU:OE2	1:B:96:ARG:NH2	2.39	0.51
1:B:199:ARG:HE	14:B:728:PGE:H4	1.76	0.51
1:B:235:ARG:HH22	16:B:730:2PE:H81	1.76	0.51
1:B:278:ASP:OD2	19:B:801:HOH:O	2.20	0.51
1:B:324:ASP:OD1	1:B:326:ARG:HB2	2.11	0.51
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.42	0.50
1:B:25:GLN:CD	1:B:376:PRO:HB3	2.33	0.49
13:B:726:ACT:H3	19:B:1344:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ARG:O	1:D:381[A]:ARG:HD2	2.13	0.49
1:B:25:GLN:HG3	19:B:1206:HOH:O	2.13	0.48
1:C:56[B]:GLU:HG2	19:C:1094:HOH:O	2.13	0.48
1:C:539:LYS:HE3	1:C:559:MET:O	2.12	0.48
1:B:90:ARG:NH2	19:B:822:HOH:O	2.45	0.48
1:D:541[A]:ARG:NH1	19:D:808:HOH:O	2.31	0.48
1:C:96:ARG:NH1	19:C:825:HOH:O	2.45	0.48
1:B:155:MET:HE3	1:B:155:MET:HA	1.96	0.48
5:J:2:FUC:O4	5:J:2:FUC:C1	2.61	0.48
1:D:22:GLN:OE1	19:D:802:HOH:O	2.21	0.47
1:A:270:PRO:HB3	1:A:580:TRP:CH2	2.50	0.47
1:C:390:ALA:O	1:C:394[A]:VAL:HG23	2.15	0.47
1:B:274:LYS:HB3	1:B:275:PRO:HD2	1.96	0.47
1:A:324:ASP:OD1	1:A:326:ARG:HB2	2.15	0.47
1:B:440:TYR:O	1:B:444[B]:GLN:HG2	2.14	0.47
1:C:603:LEU:HG	13:C:719:ACT:H2	1.96	0.47
8:C:709:BJ2:N16	11:C:712:PEG:O4	2.47	0.47
1:A:495:VAL:HG12	1:A:495:VAL:O	2.16	0.46
1:B:495:VAL:HG12	1:B:495:VAL:O	2.16	0.46
1:D:542:LYS:HB3	1:D:542:LYS:HE3	1.82	0.46
1:B:606:ASN:O	1:B:609:GLU:O	2.34	0.45
1:D:478:THR:HB	5:O:2:FUC:H2	1.99	0.45
1:D:274:LYS:HB3	1:D:275:PRO:CD	2.46	0.45
1:A:187:LYS:CE	19:A:1159:HOH:O	2.64	0.45
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.98	0.45
1:D:321:LYS:O	14:D:731:PGE:H32	2.17	0.45
8:D:710:BJ2:N16	11:D:713:PEG:O1	2.50	0.45
1:C:31:VAL:O	1:C:34:GLN:HG3	2.16	0.45
11:C:713:PEG:H41	17:C:721:XPE:H141	1.99	0.45
1:C:391:ILE:O	1:C:394[B]:VAL:HG22	2.17	0.45
1:B:157:LEU:HD11	1:B:477:VAL:HG13	2.00	0.44
1:B:381[B]:ARG:NH2	19:B:830:HOH:O	2.50	0.44
15:A:721:BCN:H51	19:A:1019:HOH:O	2.17	0.43
1:C:291:THR:HG23	19:C:1017:HOH:O	2.17	0.43
1:B:207:PHE:N	14:B:728:PGE:H12	2.33	0.43
1:A:539:LYS:HE3	1:A:559:MET:O	2.18	0.43
1:B:344:ARG:HH12	11:B:715:PEG:C4	2.32	0.43
1:D:18:GLN:O	1:D:22:GLN:HG3	2.18	0.43
1:C:539:LYS:HA	19:C:1265:HOH:O	2.18	0.43
1:C:495:VAL:O	1:C:495:VAL:HG12	2.18	0.43
1:A:129:LEU:HB3	1:A:130:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:713:PEG:C4	17:C:721:XPE:H141	2.48	0.42
1:D:495:VAL:O	1:D:495:VAL:HG12	2.18	0.42
1:B:463:TRP:NE1	12:B:718:EDO:H21	2.35	0.42
1:A:187:LYS:HE3	19:A:1159:HOH:O	2.18	0.42
1:C:208:GLU:OE2	19:C:801:HOH:O	2.22	0.42
1:D:66:GLU:OE2	19:D:801:HOH:O	2.20	0.42
3:F:1:NAG:H62	3:F:4:FUC:O2	2.19	0.42
1:B:463:TRP:HE1	12:B:718:EDO:H21	1.85	0.42
1:A:31:VAL:O	1:A:34:GLN:HG3	2.19	0.42
16:B:730:2PE:H151	19:B:919:HOH:O	2.20	0.42
1:C:274:LYS:HB3	1:C:275:PRO:CD	2.50	0.42
1:B:80:TRP:HA	1:B:83:PHE:CE2	2.55	0.41
1:A:96:ARG:C	1:A:96:ARG:HD3	2.41	0.41
1:B:207:PHE:HB3	14:B:728:PGE:H12	2.01	0.41
1:D:321:LYS:O	14:D:731:PGE:C3	2.69	0.41
14:D:731:PGE:H22	19:D:1355:HOH:O	2.21	0.41
1:C:340[A]:ARG:HG2	1:C:373:LYS:O	2.20	0.41
1:B:50:ASN:OD1	12:B:722:EDO:C1	2.68	0.41
1:B:231:ARG:HH22	14:B:729[B]:PGE:C4	2.34	0.41
1:C:117:GLN:NE2	13:C:720:ACT:H1	2.35	0.41
1:D:274:LYS:HB3	1:D:275:PRO:HD2	2.02	0.41
1:C:394[B]:VAL:HG12	1:C:508:GLN:HB2	2.03	0.41
1:D:31:VAL:O	1:D:34:GLN:HG3	2.20	0.41
1:B:164:HIS:CD2	12:B:718:EDO:H22	2.56	0.41
19:C:943:HOH:O	1:D:292:HIS:CD2	2.73	0.41
1:B:31:VAL:O	1:B:34:GLN:HG3	2.21	0.40
1:C:324:ASP:OD1	1:C:326:ARG:HB2	2.21	0.40
1:A:157:LEU:HD11	1:A:477:VAL:HG13	2.01	0.40
15:A:721:BCN:O6	15:A:721:BCN:H12	2.20	0.40
1:C:169:ILE:HB	1:C:170:PRO:HD3	2.03	0.40
1:B:524:PRO:HG3	3:I:2:NAG:O7	2.21	0.40
1:C:80:TRP:CZ2	1:C:96:ARG:HD3	2.57	0.40
1:C:172:LYS:CE	19:C:822:HOH:O	2.70	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	613/629 (98%)	602 (98%)	11 (2%)	0	100	100
1	B	616/629 (98%)	606 (98%)	10 (2%)	0	100	100
1	C	618/629 (98%)	606 (98%)	12 (2%)	0	100	100
1	D	623/629 (99%)	614 (99%)	9 (1%)	0	100	100
All	All	2470/2516 (98%)	2428 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	532/541 (98%)	526 (99%)	6 (1%)	73	68
1	B	535/541 (99%)	530 (99%)	5 (1%)	78	75
1	C	536/541 (99%)	531 (99%)	5 (1%)	78	75
1	D	541/541 (100%)	538 (99%)	3 (1%)	86	84
All	All	2144/2164 (99%)	2125 (99%)	19 (1%)	78	75

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	273	ASP

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Mol	Chain	Res	Type
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	421	ASP
1	B	368	TYR
1	B	372	TYR
1	B	377	VAL
1	B	378	SER
1	B	388	HIS
1	C	368	TYR
1	C	372	TYR
1	C	388	HIS
1	C	421	ASP
1	C	453	ARG
1	D	368	TYR
1	D	372	TYR
1	D	388	HIS

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](#)

31 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	0.55	0	17,19,21	0.61	0
2	NAG	E	2	2	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	F	1	1,3	14,14,15	0.36	0	17,19,21	0.48	0
3	NAG	F	2	3	14,14,15	0.48	0	17,19,21	0.40	0
3	BMA	F	3	3	11,11,12	0.54	0	15,15,17	0.74	0
3	FUC	F	4	3	10,10,11	1.07	0	14,14,16	0.92	2 (14%)
4	NAG	G	1	1,4	14,14,15	0.39	0	17,19,21	0.66	0
4	NAG	G	2	4	14,14,15	0.21	0	17,19,21	0.62	0
4	FUC	G	3	4	10,10,11	1.47	2 (20%)	14,14,16	1.85	3 (21%)
2	NAG	H	1	1,2	14,14,15	0.23	0	17,19,21	0.70	1 (5%)
2	NAG	H	2	2	14,14,15	0.43	0	17,19,21	0.68	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.78	1 (7%)	17,19,21	0.78	0
3	NAG	I	2	3	14,14,15	0.24	0	17,19,21	0.35	0
3	BMA	I	3	3	11,11,12	0.73	0	15,15,17	0.80	0
3	FUC	I	4	3	10,10,11	1.40	2 (20%)	14,14,16	1.23	1 (7%)
5	NAG	J	1	1,5	14,14,15	1.09	1 (7%)	17,19,21	0.87	0
5	FUC	J	2	5	10,10,11	1.69	2 (20%)	14,14,16	1.19	1 (7%)
6	NAG	K	1	1,6	14,14,15	0.29	0	17,19,21	0.38	0
6	NAG	K	2	6	14,14,15	0.44	0	17,19,21	0.49	0
6	BMA	K	3	6	11,11,12	0.74	0	15,15,17	0.72	0
4	NAG	L	1	1,4	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	L	2	4	14,14,15	0.30	0	17,19,21	0.64	0
4	FUC	L	3	4	10,10,11	1.24	2 (20%)	14,14,16	1.15	1 (7%)
2	NAG	M	1	1,2	14,14,15	0.36	0	17,19,21	0.60	1 (5%)
2	NAG	M	2	2	14,14,15	0.28	0	17,19,21	0.55	0
3	NAG	N	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	0.56	0
3	NAG	N	2	3	14,14,15	0.42	0	17,19,21	0.54	0
3	BMA	N	3	3	11,11,12	0.80	0	15,15,17	1.81	3 (20%)
3	FUC	N	4	3	10,10,11	0.69	0	14,14,16	0.96	0
5	NAG	O	1	1,5	14,14,15	0.94	1 (7%)	17,19,21	0.74	0
5	FUC	O	2	5	10,10,11	1.41	2 (20%)	14,14,16	1.43	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. '2' 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

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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	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	FUC	G	3	4	-	-	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	FUC	I	4	3	-	-	0/1/1/1
5	NAG	J	1	1,5	-	3/6/23/26	0/1/1/1
5	FUC	J	2	5	-	-	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	FUC	N	4	3	-	-	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	O	2	5	-	-	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	FUC	C1-C2	4.55	1.62	1.52
5	J	1	NAG	O5-C1	3.84	1.49	1.43
5	O	1	NAG	O5-C1	3.33	1.49	1.43
4	G	3	FUC	O5-C1	-3.32	1.38	1.43
5	O	2	FUC	O5-C1	-2.52	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4	FUC	O5-C1	-2.31	1.40	1.43
5	O	2	FUC	C4-C3	2.27	1.58	1.52
3	N	1	NAG	O5-C1	-2.21	1.40	1.43
4	G	3	FUC	C2-C3	2.21	1.55	1.52
4	L	3	FUC	O5-C5	2.14	1.48	1.43
5	J	2	FUC	C2-C3	2.07	1.55	1.52
4	L	3	FUC	O5-C1	-2.04	1.40	1.43
3	I	4	FUC	O2-C2	-2.04	1.39	1.43
3	I	1	NAG	O5-C1	-2.02	1.40	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	FUC	C1-C2-C3	5.35	116.24	109.67
3	N	3	BMA	O5-C5-C6	3.81	113.17	107.20
3	N	3	BMA	C1-C2-C3	3.56	114.05	109.67
3	I	4	FUC	O5-C1-C2	-3.34	105.61	110.77
5	O	2	FUC	O5-C5-C4	3.27	115.39	109.52
5	J	2	FUC	O2-C2-C1	3.11	115.52	109.15
5	O	2	FUC	O2-C2-C1	2.95	115.19	109.15
4	G	3	FUC	C2-C3-C4	2.84	115.80	110.89
4	L	3	FUC	O2-C2-C1	2.66	114.60	109.15
3	N	3	BMA	O5-C1-C2	2.57	114.74	110.77
2	H	2	NAG	C1-O5-C5	2.41	115.45	112.19
4	G	3	FUC	O3-C3-C4	-2.15	105.37	110.35
2	H	1	NAG	C1-O5-C5	2.15	115.11	112.19
3	F	4	FUC	O5-C1-C2	-2.07	107.57	110.77
3	F	4	FUC	O2-C2-C1	2.02	113.28	109.15
2	M	1	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6

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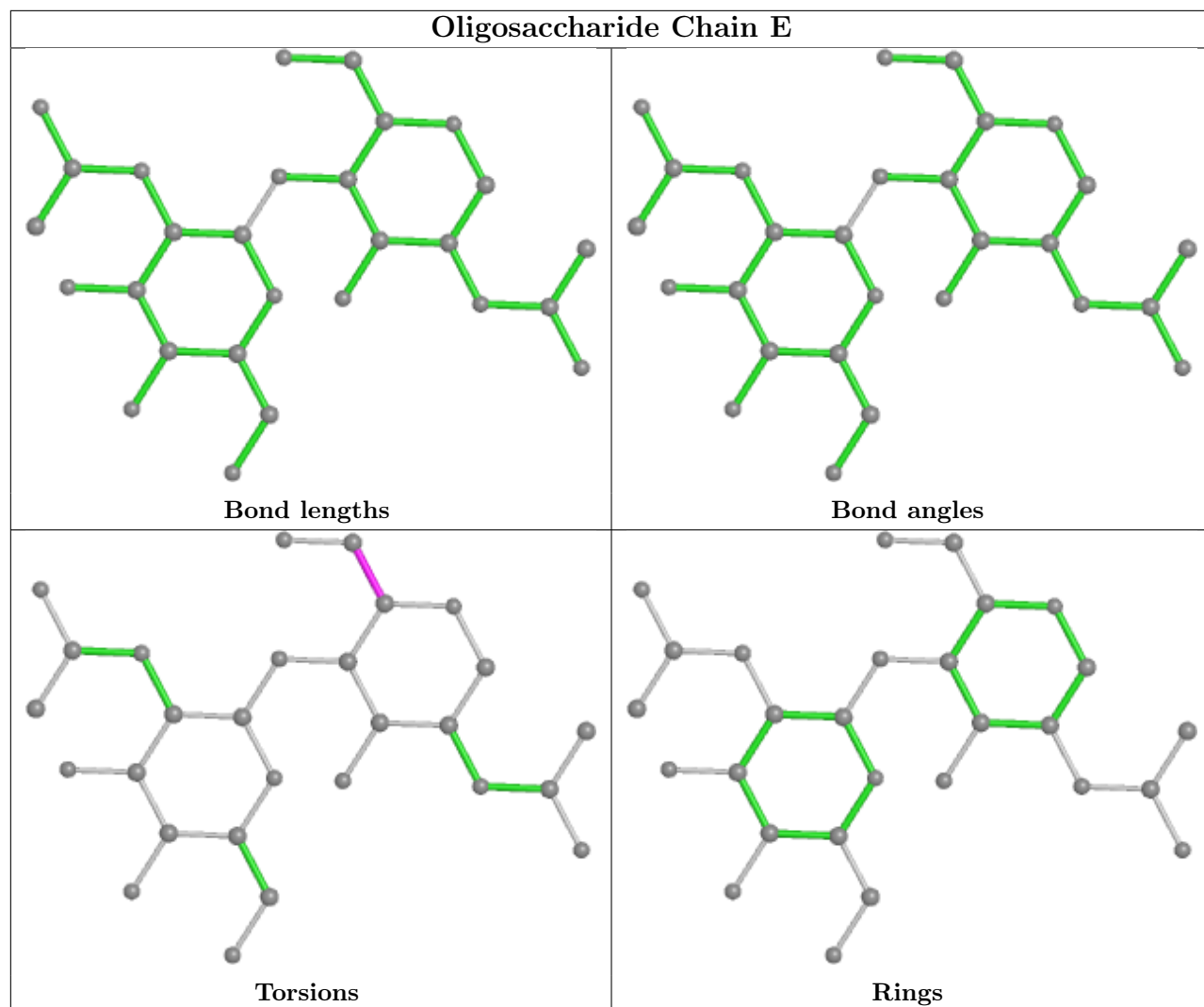
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C4-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
4	G	1	NAG	C3-C2-N2-C7
4	L	1	NAG	C3-C2-N2-C7
5	J	1	NAG	C3-C2-N2-C7
3	N	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6
5	O	1	NAG	C3-C2-N2-C7
5	O	1	NAG	C1-C2-N2-C7

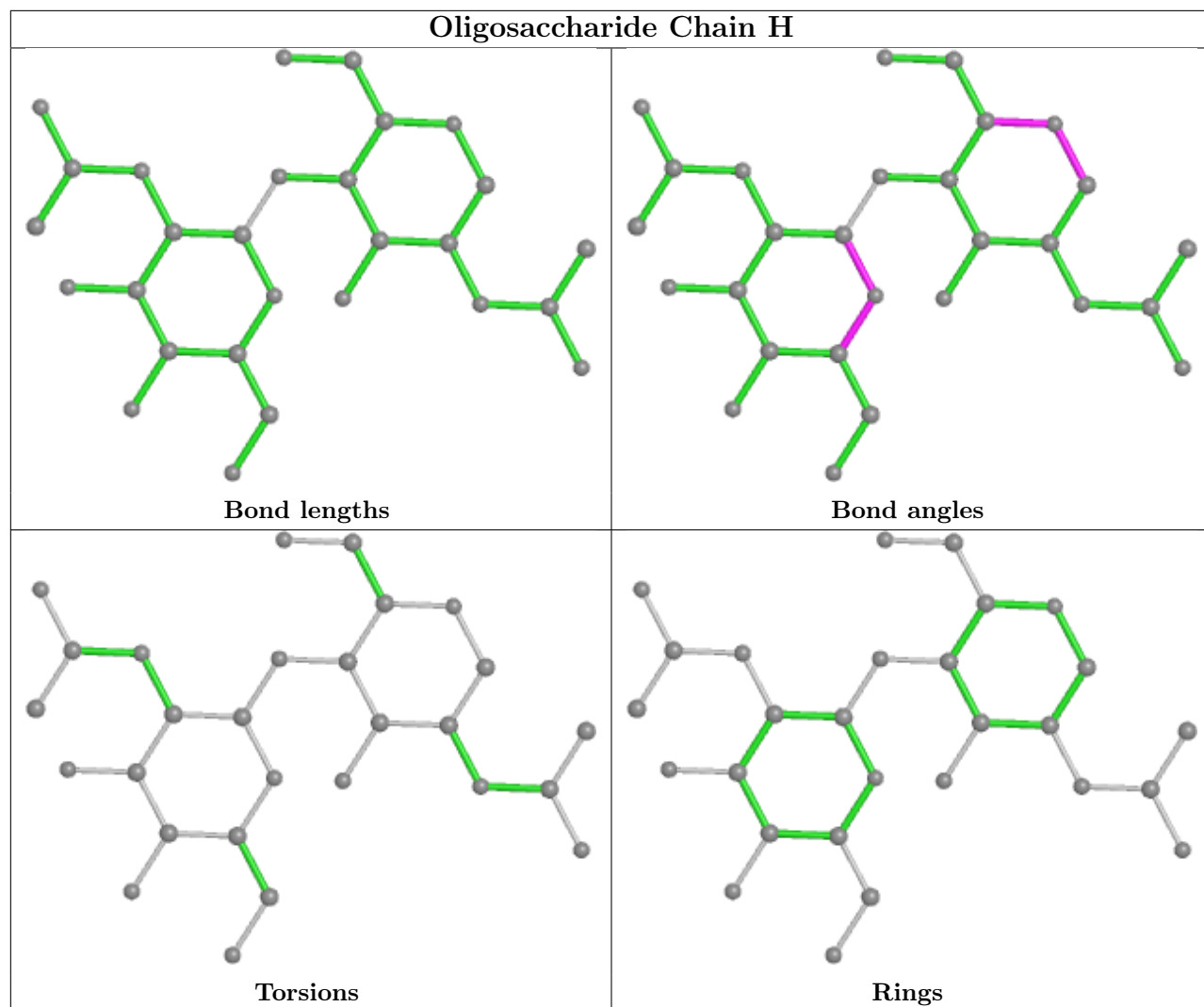
There are no ring outliers.

6 monomers are involved in 5 short contacts:

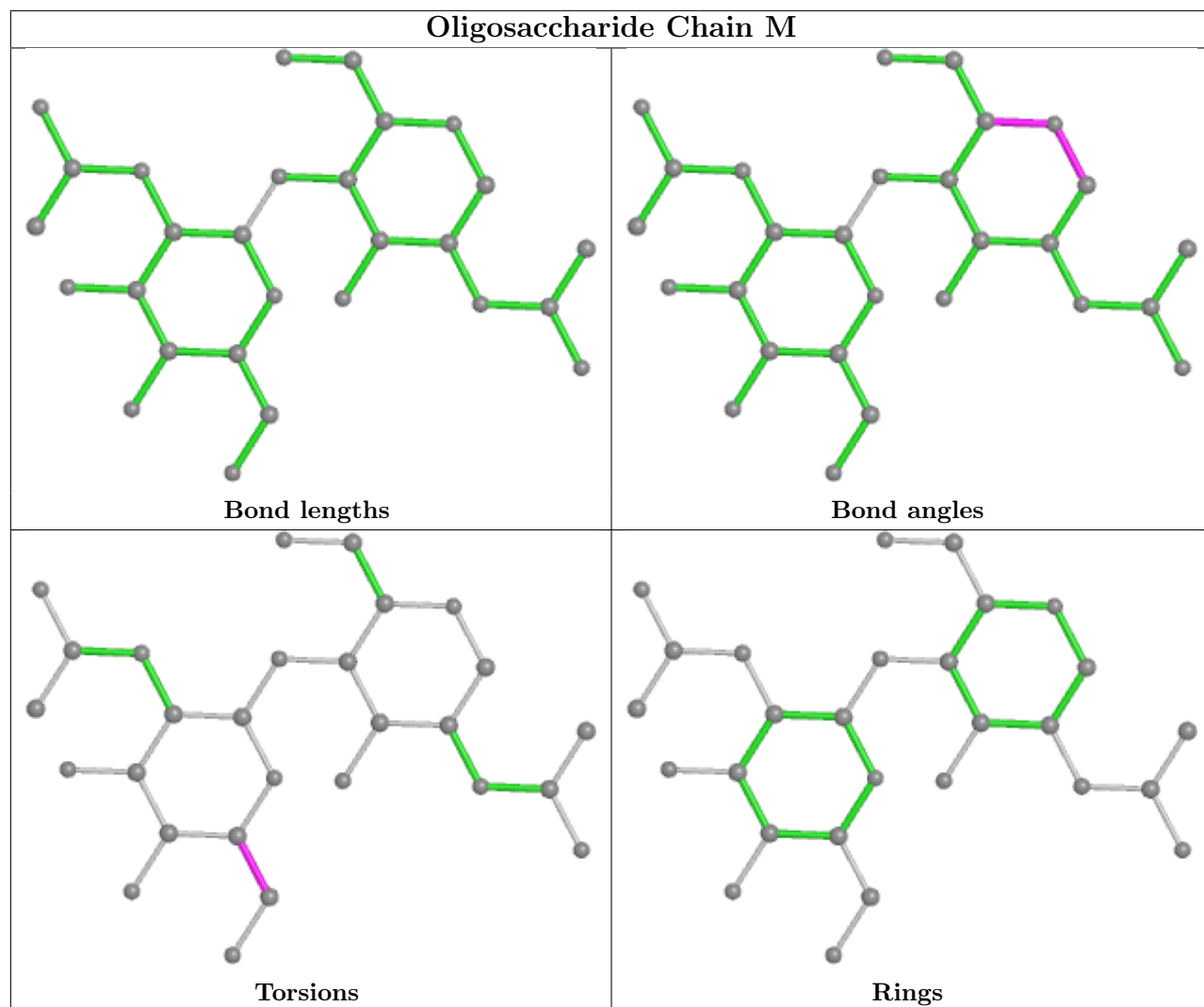
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	1	0
5	J	2	FUC	2	0
3	F	1	NAG	1	0
5	O	2	FUC	1	0
3	F	4	FUC	1	0
3	I	2	NAG	1	0

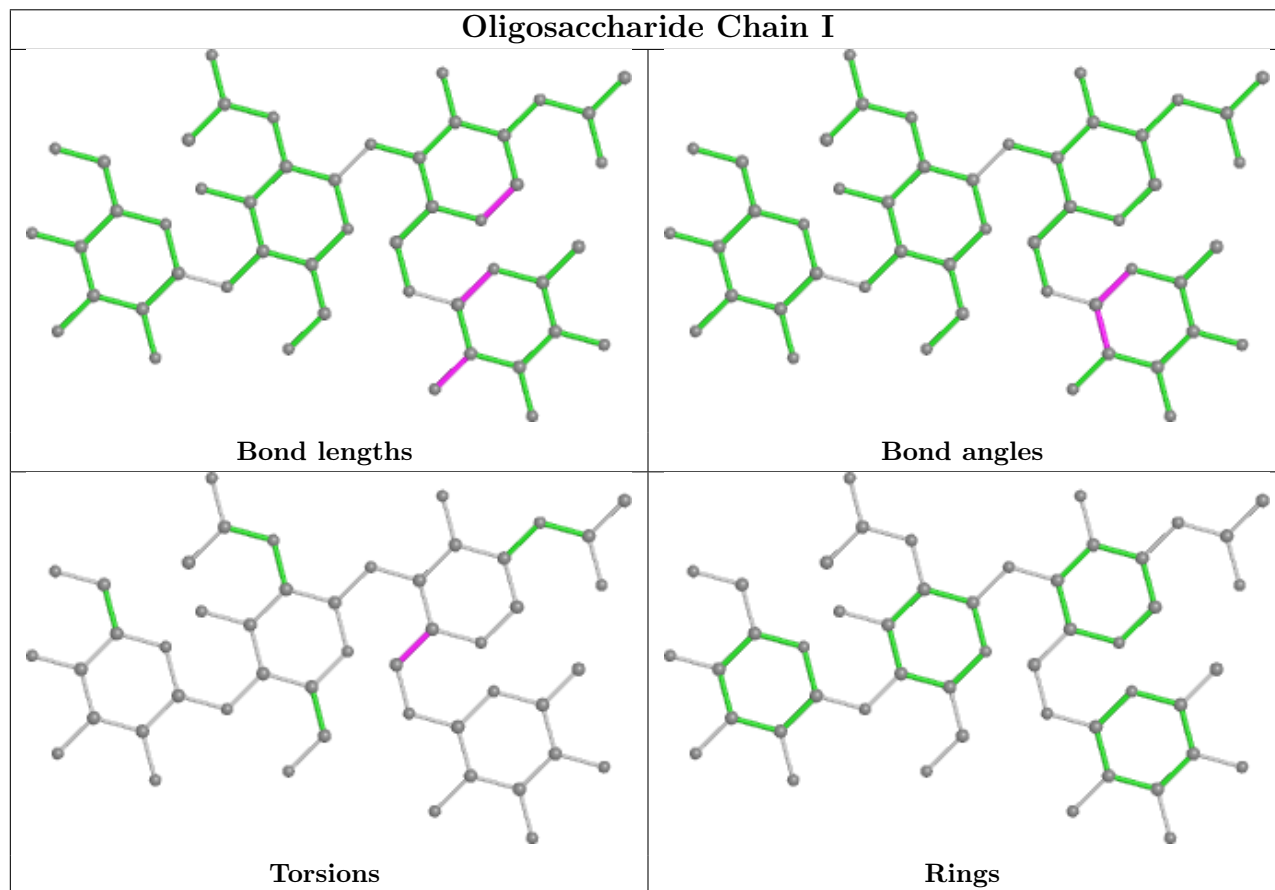
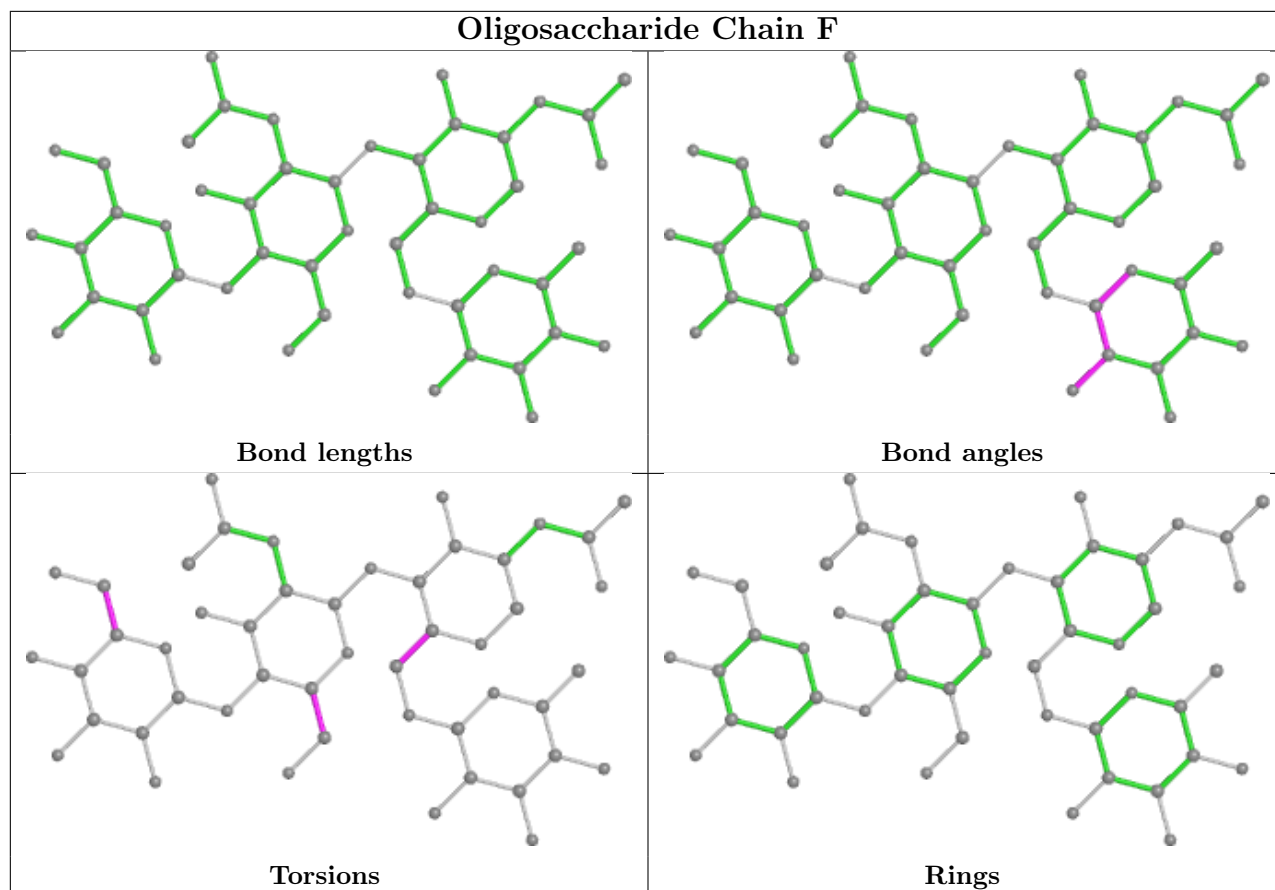
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

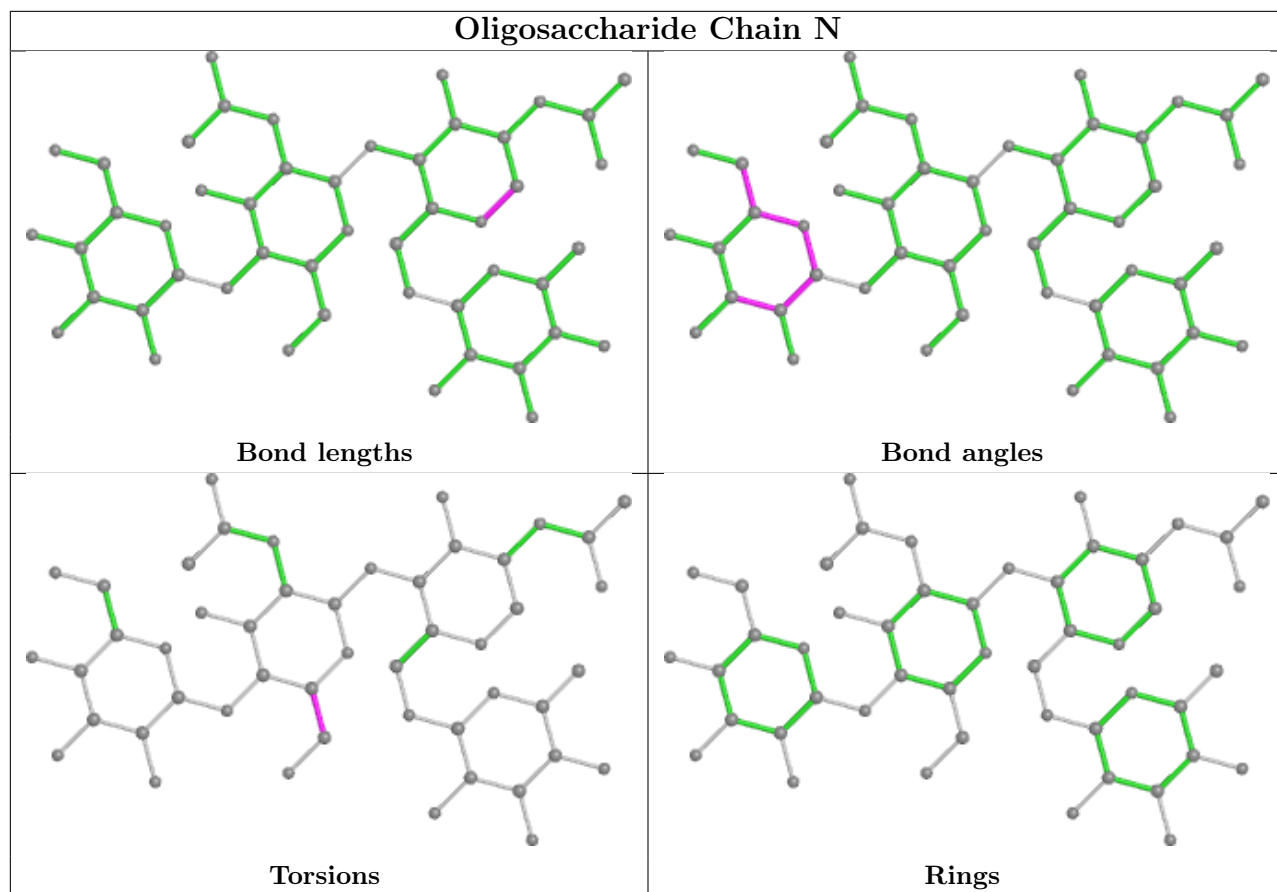


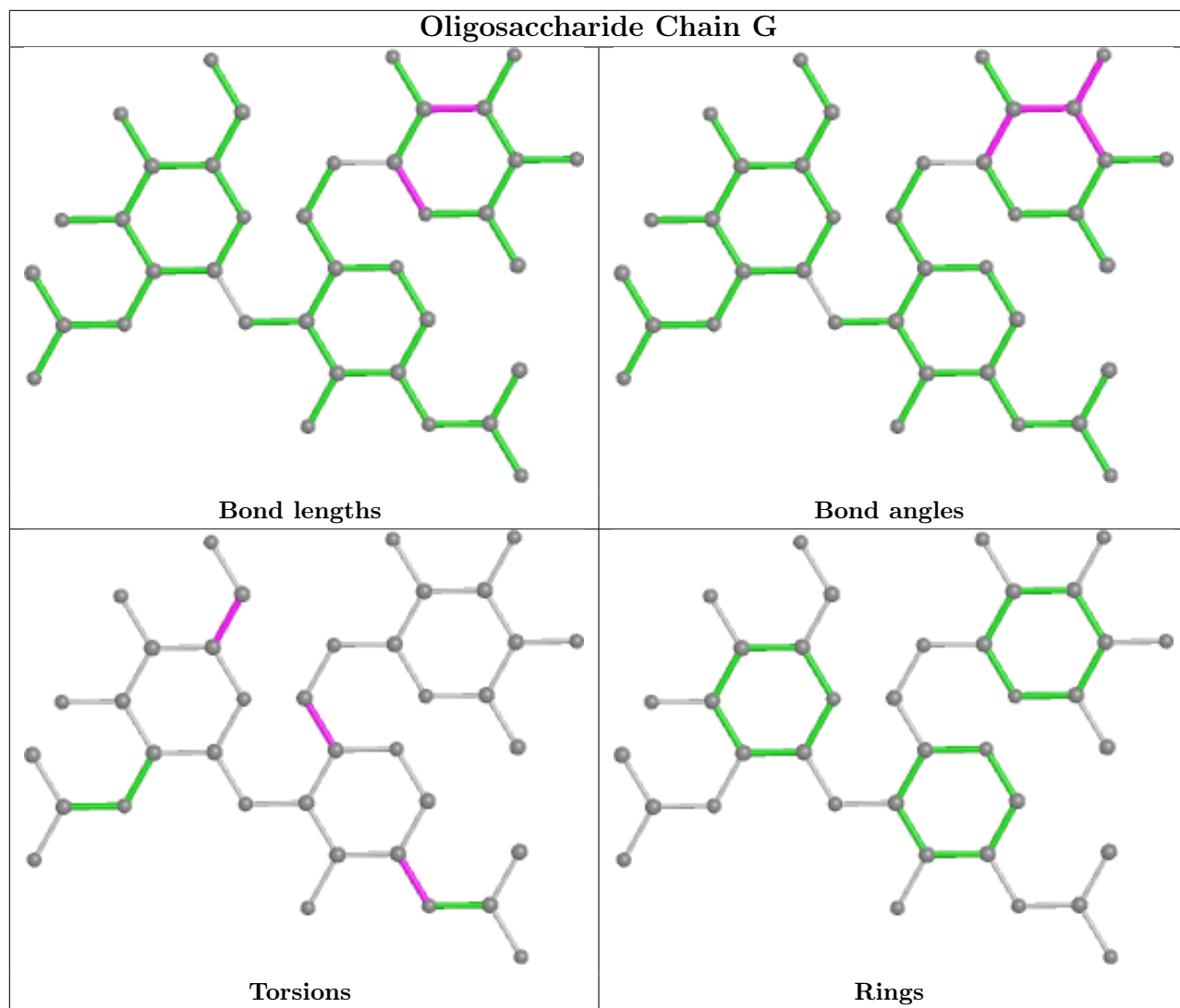


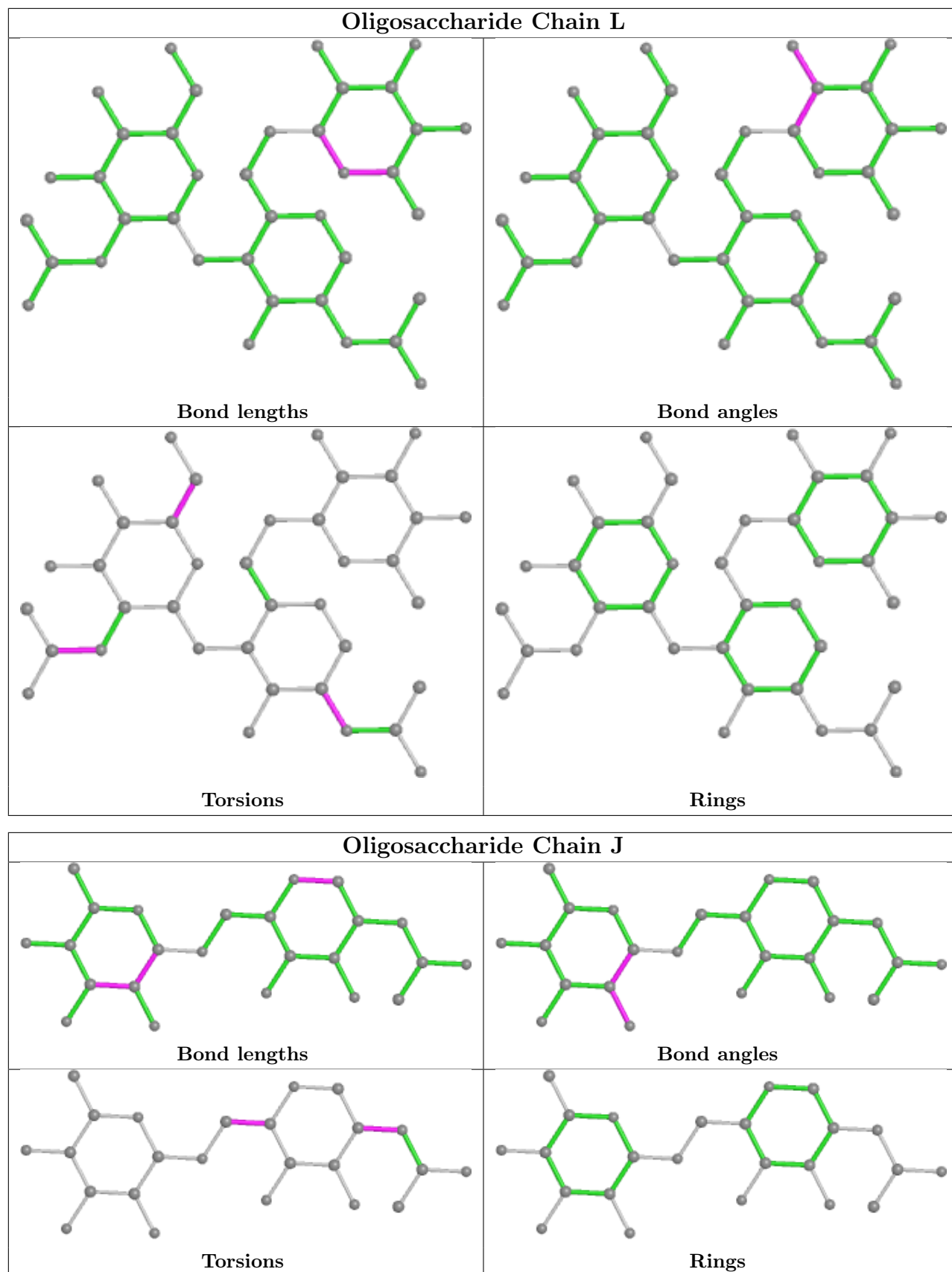


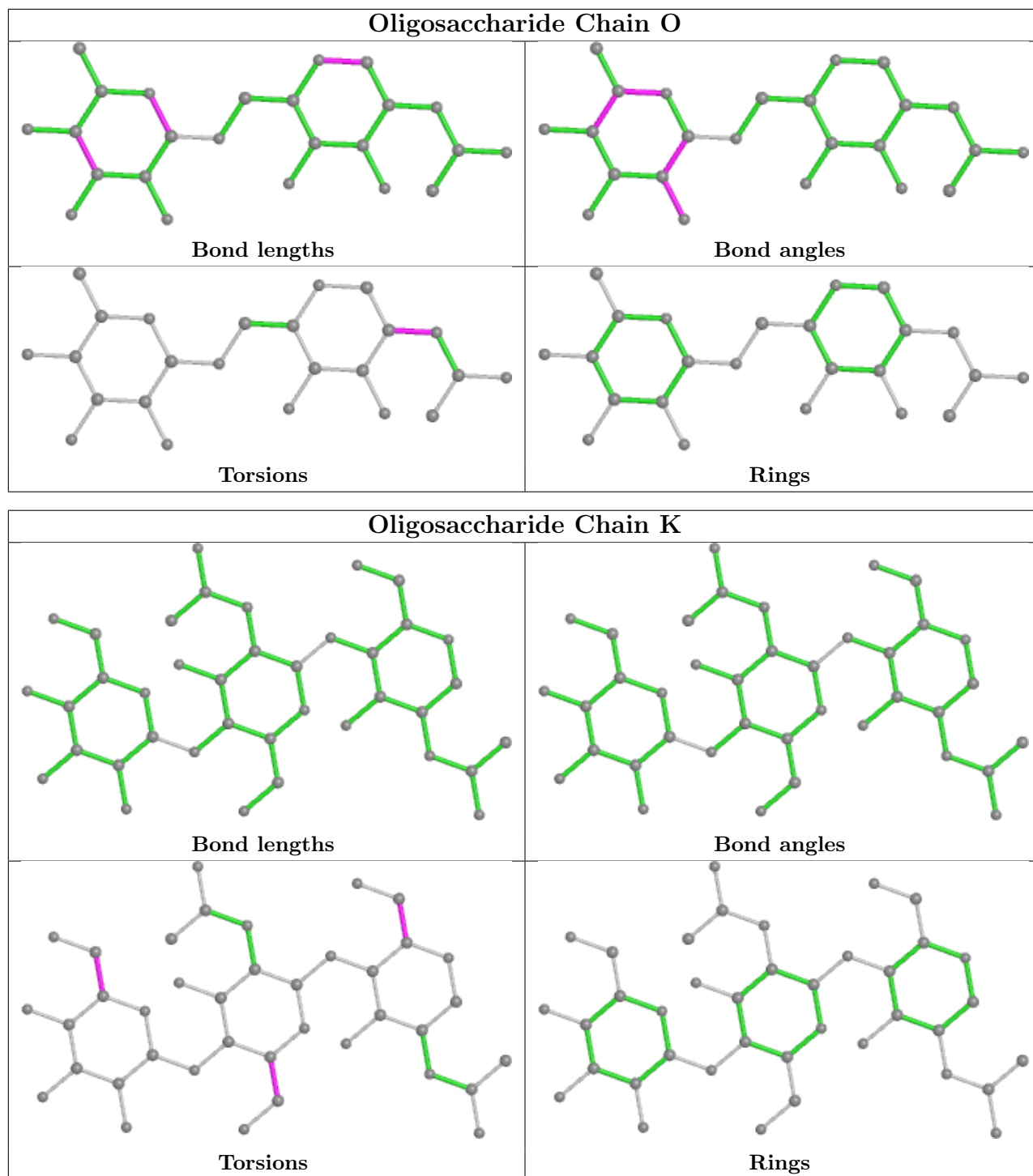












## 5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 12 are monoatomic - leaving 62 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
13	ACT	D	724	-	3,3,3	1.17	0	3,3,3	1.54	1 (33%)
12	EDO	D	718	-	3,3,3	0.49	0	2,2,2	0.30	0
14	PGE	D	730	-	9,9,9	0.64	0	8,8,8	0.94	0
13	ACT	D	726	-	3,3,3	1.24	0	3,3,3	1.64	2 (66%)
14	PGE	B	729[B]	-	9,9,9	0.32	0	8,8,8	0.47	0
12	EDO	B	724	-	3,3,3	0.46	0	2,2,2	0.41	0
8	BJ2	A	711	7	30,31,31	3.69	12 (40%)	36,44,44	1.41	6 (16%)
14	PGE	B	729[A]	-	9,9,9	0.35	0	8,8,8	0.26	0
11	PEG	C	712	-	6,6,6	0.45	0	5,5,5	0.34	0
13	ACT	D	728	-	3,3,3	0.91	0	3,3,3	1.48	0
12	EDO	D	719	-	3,3,3	0.49	0	2,2,2	0.31	0
16	2PE	B	730	-	27,27,27	0.56	0	26,26,26	0.53	0
13	ACT	D	727	-	3,3,3	1.55	0	3,3,3	1.51	1 (33%)
12	EDO	B	722	-	3,3,3	0.39	0	2,2,2	0.41	0
13	ACT	C	719	-	3,3,3	1.38	0	3,3,3	1.44	0
11	PEG	A	714	-	6,6,6	0.45	0	5,5,5	0.53	0
12	EDO	A	716	-	3,3,3	0.64	0	2,2,2	0.15	0
12	EDO	C	714	-	3,3,3	0.51	0	2,2,2	0.31	0
12	EDO	D	716	-	3,3,3	0.47	0	2,2,2	0.27	0
17	XPE	B	731	-	30,30,30	0.65	0	29,29,29	0.76	0
13	ACT	B	725	-	3,3,3	1.00	0	3,3,3	1.62	1 (33%)
12	EDO	C	716	-	3,3,3	0.50	0	2,2,2	0.29	0
12	EDO	B	723	-	3,3,3	0.54	0	2,2,2	0.06	0
12	EDO	B	718	-	3,3,3	0.14	0	2,2,2	0.83	0
12	EDO	D	723[A]	-	3,3,3	0.55	0	2,2,2	0.25	0
11	PEG	B	715	-	6,6,6	0.48	0	5,5,5	0.27	0
12	EDO	B	721	-	3,3,3	0.58	0	2,2,2	0.11	0
12	EDO	B	719	-	3,3,3	0.43	0	2,2,2	0.38	0
11	PEG	C	713	-	6,6,6	0.44	0	5,5,5	0.62	0
11	PEG	D	713	-	6,6,6	0.49	0	5,5,5	0.38	0
12	EDO	B	720	-	3,3,3	0.48	0	2,2,2	0.33	0
13	ACT	B	726	-	3,3,3	1.12	0	3,3,3	1.92	2 (66%)
14	PGE	A	720	-	9,9,9	0.48	0	8,8,8	0.89	0
14	PGE	D	731	-	9,9,9	0.28	0	8,8,8	0.54	0
12	EDO	A	717	-	3,3,3	0.44	0	2,2,2	0.19	0
12	EDO	D	721	-	3,3,3	0.86	0	2,2,2	0.22	0
12	EDO	C	717	-	3,3,3	0.51	0	2,2,2	0.25	0
13	ACT	B	727	-	3,3,3	1.34	0	3,3,3	1.65	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	PEG	A	715	-	6,6,6	0.47	0	5,5,5	0.48	0
8	BJ2	B	710	7	30,31,31	3.39	11 (36%)	36,44,44	1.33	3 (8%)
8	BJ2	D	710	7	30,31,31	3.50	13 (43%)	36,44,44	1.36	4 (11%)
12	EDO	C	715	-	3,3,3	0.51	0	2,2,2	0.29	0
15	BCN	A	721	-	10,10,10	0.98	0	11,11,11	1.09	0
12	EDO	D	720	-	3,3,3	0.40	0	2,2,2	0.47	0
14	PGE	B	728	-	9,9,9	0.56	0	8,8,8	0.63	0
12	EDO	D	715	-	3,3,3	0.56	0	2,2,2	0.15	0
11	PEG	B	714	-	6,6,6	0.47	0	5,5,5	0.29	0
12	EDO	D	717	-	3,3,3	0.53	0	2,2,2	0.43	0
11	PEG	B	713	-	6,6,6	0.49	0	5,5,5	0.41	0
12	EDO	D	722	-	3,3,3	0.56	0	2,2,2	0.41	0
13	ACT	C	720	-	3,3,3	1.41	0	3,3,3	1.52	1 (33%)
14	PGE	D	729	-	9,9,9	0.38	0	8,8,8	0.44	0
11	PEG	B	716	-	6,6,6	0.48	0	5,5,5	0.38	0
11	PEG	D	714	-	6,6,6	0.47	0	5,5,5	0.37	0
13	ACT	A	719	-	3,3,3	1.10	0	3,3,3	1.48	0
12	EDO	B	717	-	3,3,3	0.38	0	2,2,2	0.31	0
13	ACT	A	718	-	3,3,3	1.03	0	3,3,3	1.61	1 (33%)
13	ACT	C	718	-	3,3,3	1.39	0	3,3,3	1.52	0
8	BJ2	C	709	7	30,31,31	3.77	15 (50%)	36,44,44	1.66	9 (25%)
17	XPE	C	721	-	30,30,30	0.56	0	29,29,29	0.59	0
13	ACT	D	725	-	3,3,3	1.46	1 (33%)	3,3,3	1.61	1 (33%)
18	NAG	C	701	1	14,14,15	0.29	0	17,19,21	0.65	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	EDO	D	718	-	-	0/1/1/1	-
14	PGE	D	730	-	-	5/7/7/7	-
14	PGE	B	729[B]	-	-	1/7/7/7	-
12	EDO	B	724	-	-	1/1/1/1	-
8	BJ2	A	711	7	-	5/36/56/56	0/2/2/2
14	PGE	B	729[A]	-	-	3/7/7/7	-
11	PEG	C	712	-	-	1/4/4/4	-
12	EDO	D	719	-	-	1/1/1/1	-
16	2PE	B	730	-	-	9/25/25/25	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	EDO	B	722	-	-	0/1/1/1	-
17	XPE	B	731	-	-	14/28/28/28	-
11	PEG	A	714	-	-	3/4/4/4	-
12	EDO	A	716	-	-	0/1/1/1	-
12	EDO	C	714	-	-	0/1/1/1	-
12	EDO	D	716	-	-	0/1/1/1	-
12	EDO	C	716	-	-	1/1/1/1	-
12	EDO	B	723	-	-	1/1/1/1	-
12	EDO	B	718	-	-	0/1/1/1	-
12	EDO	D	723[A]	-	-	1/1/1/1	-
11	PEG	B	715	-	-	2/4/4/4	-
12	EDO	B	721	-	-	1/1/1/1	-
12	EDO	B	719	-	-	1/1/1/1	-
11	PEG	C	713	-	-	2/4/4/4	-
11	PEG	D	713	-	-	4/4/4/4	-
12	EDO	B	720	-	-	0/1/1/1	-
14	PGE	A	720	-	-	3/7/7/7	-
14	PGE	D	731	-	-	5/7/7/7	-
12	EDO	A	717	-	-	0/1/1/1	-
12	EDO	D	721	-	-	0/1/1/1	-
12	EDO	C	717	-	-	1/1/1/1	-
11	PEG	A	715	-	-	3/4/4/4	-
8	BJ2	B	710	7	-	2/36/56/56	0/2/2/2
8	BJ2	D	710	7	-	5/36/56/56	0/2/2/2
12	EDO	C	715	-	-	0/1/1/1	-
15	BCN	A	721	-	-	6/10/10/10	-
12	EDO	D	720	-	-	0/1/1/1	-
14	PGE	B	728	-	-	4/7/7/7	-
12	EDO	D	715	-	-	1/1/1/1	-
11	PEG	B	714	-	-	2/4/4/4	-
12	EDO	D	717	-	-	1/1/1/1	-
11	PEG	B	713	-	-	2/4/4/4	-
12	EDO	D	722	-	-	0/1/1/1	-
14	PGE	D	729	-	-	4/7/7/7	-
11	PEG	B	716	-	-	3/4/4/4	-
11	PEG	D	714	-	-	2/4/4/4	-
12	EDO	B	717	-	-	0/1/1/1	-
8	BJ2	C	709	7	-	4/36/56/56	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	XPE	C	721	-	-	16/28/28/28	-
18	NAG	C	701	1	-	0/6/23/26	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	709	BJ2	C08-N12	9.46	1.59	1.47
8	A	711	BJ2	C08-N12	9.12	1.58	1.47
8	D	710	BJ2	C08-N12	8.86	1.58	1.47
8	A	711	BJ2	C09-C08	-7.90	1.39	1.53
8	D	710	BJ2	C09-C08	-7.82	1.40	1.53
8	B	710	BJ2	C09-C08	-7.62	1.40	1.53
8	C	709	BJ2	C09-C08	-7.61	1.40	1.53
8	B	710	BJ2	C08-N12	7.13	1.56	1.47
8	A	711	BJ2	C27-N23	6.68	1.60	1.47
8	D	710	BJ2	C26-C27	-6.32	1.38	1.53
8	A	711	BJ2	C24-N23	-6.26	1.35	1.47
8	B	710	BJ2	C26-C27	-6.15	1.39	1.53
8	A	711	BJ2	C26-C27	-6.05	1.39	1.53
8	C	709	BJ2	C11-N12	-6.03	1.36	1.47
8	B	710	BJ2	C27-N23	5.94	1.59	1.47
8	C	709	BJ2	C26-C27	-5.91	1.39	1.53
8	D	710	BJ2	C24-N23	-5.87	1.36	1.47
8	C	709	BJ2	C21-N23	5.84	1.48	1.34
8	C	709	BJ2	C27-N23	5.82	1.58	1.47
8	A	711	BJ2	C11-N12	-5.72	1.36	1.47
8	B	710	BJ2	C11-N12	-5.63	1.36	1.47
8	C	709	BJ2	C04-C08	5.54	1.60	1.54
8	C	709	BJ2	C24-N23	-5.44	1.37	1.47
8	A	711	BJ2	C21-N23	5.42	1.47	1.34
8	B	710	BJ2	C21-N23	5.33	1.46	1.34
8	D	710	BJ2	C11-N12	-5.32	1.37	1.47
8	D	710	BJ2	C27-N23	5.30	1.57	1.47
8	B	710	BJ2	C24-N23	-5.18	1.37	1.47
8	B	710	BJ2	C13-N12	4.92	1.45	1.34
8	D	710	BJ2	C13-N12	4.78	1.45	1.34
8	D	710	BJ2	C21-N23	4.73	1.45	1.34
8	A	711	BJ2	C04-C08	4.65	1.59	1.54
8	C	709	BJ2	C13-N12	4.47	1.44	1.34
8	A	711	BJ2	C13-N12	4.14	1.44	1.34
8	B	710	BJ2	C04-C08	3.73	1.58	1.54
8	C	709	BJ2	C04-C05	3.70	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	710	BJ2	C04-C08	3.05	1.57	1.54
8	A	711	BJ2	C04-C05	3.03	1.57	1.52
8	D	710	BJ2	C04-C05	2.72	1.56	1.52
8	A	711	BJ2	C04-N03	2.48	1.49	1.46
8	C	709	BJ2	C10-C11	2.45	1.60	1.51
8	B	710	BJ2	C10-C11	2.43	1.60	1.51
8	C	709	BJ2	O07-C05	2.35	1.29	1.22
8	B	710	BJ2	O22-C21	-2.31	1.18	1.22
8	D	710	BJ2	C10-C11	2.21	1.59	1.51
8	C	709	BJ2	C17-C18	2.16	1.56	1.51
13	D	725	ACT	CH3-C	2.11	1.58	1.49
8	C	709	BJ2	C04-N03	2.09	1.48	1.46
8	A	711	BJ2	O20-C18	2.09	1.29	1.22
8	D	710	BJ2	C04-N03	2.06	1.48	1.46
8	D	710	BJ2	C17-C18	2.05	1.56	1.51
8	C	709	BJ2	O30-C28	2.02	1.28	1.22

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	709	BJ2	O06-C05-C04	4.31	129.44	114.21
8	A	711	BJ2	C08-C04-N03	-3.81	102.14	109.99
8	B	710	BJ2	C28-C27-N23	-3.72	104.71	112.26
8	C	709	BJ2	C28-C27-N23	-3.57	105.03	112.26
8	C	709	BJ2	O06-C05-O07	-3.53	116.07	124.09
8	A	711	BJ2	C28-C27-N23	-3.13	105.91	112.26
8	D	710	BJ2	C08-C04-N03	-3.00	103.80	109.99
8	B	710	BJ2	C08-C04-N03	-2.99	103.82	109.99
8	D	710	BJ2	O22-C21-C02	2.87	126.12	120.19
8	A	711	BJ2	O06-C05-O07	-2.78	117.77	124.09
8	C	709	BJ2	C08-C04-N03	-2.74	104.33	109.99
8	C	709	BJ2	C26-C27-N23	2.57	106.85	103.03
8	A	711	BJ2	C26-C27-N23	2.51	106.75	103.03
8	A	711	BJ2	O06-C05-C04	2.44	122.81	114.21
13	B	726	ACT	O-C-CH3	-2.42	112.91	122.33
8	D	710	BJ2	C11-N12-C08	-2.26	108.18	111.74
13	B	726	ACT	OXT-C-O	2.23	130.29	122.05
8	C	709	BJ2	O22-C21-C02	2.23	124.80	120.19
8	A	711	BJ2	O29-C28-O30	-2.22	119.05	124.09
8	B	710	BJ2	C26-C27-N23	2.22	106.32	103.03
8	C	709	BJ2	O29-C28-C27	2.19	120.96	113.38
13	D	724	ACT	OXT-C-O	2.18	130.09	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	727	ACT	OXT-C-O	2.14	129.93	122.05
8	C	709	BJ2	O07-C05-C04	-2.10	114.47	121.70
13	C	720	ACT	OXT-C-O	2.07	129.67	122.05
13	B	727	ACT	O-C-CH3	-2.06	114.32	122.33
8	D	710	BJ2	C17-C15-C13	-2.05	104.36	109.27
8	C	709	BJ2	C26-C27-C28	2.05	114.72	111.36
13	B	725	ACT	OXT-C-O	2.02	129.51	122.05
13	A	718	ACT	OXT-C-O	2.02	129.49	122.05
13	D	725	ACT	O-C-CH3	-2.01	114.50	122.33
13	D	726	ACT	O-C-CH3	-2.01	114.52	122.33
13	D	726	ACT	OXT-C-O	2.00	129.43	122.05

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	711	BJ2	N03-C04-C08-C09
8	C	709	BJ2	C05-C04-C08-C09
8	C	709	BJ2	C05-C04-C08-N12
8	D	710	BJ2	N03-C04-C08-C09
15	A	721	BCN	N1-C1-C2-O21
14	D	730	PGE	C1-C2-O2-C3
14	A	720	PGE	C1-C2-O2-C3
15	A	721	BCN	N1-C1-C2-O22
14	D	731	PGE	O2-C3-C4-O3
16	B	730	2PE	O4-C5-C6-O7
16	B	730	2PE	O10-C11-C12-O13
17	C	721	XPE	O22-C23-C24-O25
14	A	720	PGE	O2-C3-C4-O3
14	D	730	PGE	O2-C3-C4-O3
16	B	730	2PE	O13-C14-C15-O16
14	B	729[A]	PGE	O2-C3-C4-O3
14	B	729[B]	PGE	O2-C3-C4-O3
17	B	731	XPE	O22-C23-C24-O25
17	B	731	XPE	O19-C20-C21-O22
16	B	730	2PE	O7-C8-C9-O10
17	B	731	XPE	O7-C8-C9-O10
11	D	713	PEG	C1-C2-O2-C3
17	C	721	XPE	O10-C11-C12-O13
17	C	721	XPE	O19-C20-C21-O22
11	A	714	PEG	O2-C3-C4-O4
11	B	714	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
11	C	712	PEG	O2-C3-C4-O4
14	D	731	PGE	O1-C1-C2-O2
16	B	730	2PE	O25-C26-C27-O28
17	B	731	XPE	O28-C29-C30-O31
17	C	721	XPE	O7-C8-C9-O10
15	A	721	BCN	N1-C3-C4-O4
17	B	731	XPE	O16-C17-C18-O19
11	A	714	PEG	O1-C1-C2-O2
11	A	715	PEG	O2-C3-C4-O4
11	B	715	PEG	O1-C1-C2-O2
14	B	728	PGE	O3-C5-C6-O4
14	D	729	PGE	O3-C5-C6-O4
14	D	731	PGE	O3-C5-C6-O4
11	C	713	PEG	C4-C3-O2-C2
14	A	720	PGE	C6-C5-O3-C4
11	B	713	PEG	O1-C1-C2-O2
11	D	714	PEG	O2-C3-C4-O4
11	B	715	PEG	O2-C3-C4-O4
12	B	721	EDO	O1-C1-C2-O2
12	B	723	EDO	O1-C1-C2-O2
12	C	716	EDO	O1-C1-C2-O2
12	C	717	EDO	O1-C1-C2-O2
12	D	717	EDO	O1-C1-C2-O2
12	D	723[A]	EDO	O1-C1-C2-O2
14	D	729	PGE	O2-C3-C4-O3
11	B	716	PEG	O1-C1-C2-O2
17	C	721	XPE	O28-C29-C30-O31
17	B	731	XPE	O1-C2-C3-O4
12	B	719	EDO	O1-C1-C2-O2
12	D	715	EDO	O1-C1-C2-O2
15	A	721	BCN	C6-C5-N1-C1
11	C	713	PEG	O1-C1-C2-O2
14	B	728	PGE	C1-C2-O2-C3
17	B	731	XPE	C21-C20-O19-C18
8	B	710	BJ2	N03-C04-C08-C09
8	C	709	BJ2	N03-C04-C08-C09
14	D	731	PGE	C3-C4-O3-C5
14	B	729[A]	PGE	C6-C5-O3-C4
11	B	713	PEG	C4-C3-O2-C2
17	B	731	XPE	C9-C8-O7-C6
17	C	721	XPE	C30-C29-O28-C27
17	C	721	XPE	C24-C23-O22-C21

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Mol	Chain	Res	Type	Atoms
8	A	711	BJ2	C05-C04-C08-C09
8	D	710	BJ2	C15-C17-C18-O19
8	D	710	BJ2	C15-C17-C18-O20
14	B	728	PGE	C3-C4-O3-C5
14	D	730	PGE	C6-C5-O3-C4
11	D	714	PEG	C1-C2-O2-C3
8	A	711	BJ2	C05-C04-C08-N12
8	D	710	BJ2	C05-C04-C08-N12
14	D	730	PGE	C3-C4-O3-C5
17	B	731	XPE	C12-C11-O10-C9
14	B	729[A]	PGE	C1-C2-O2-C3
15	A	721	BCN	N1-C5-C6-O6
11	D	713	PEG	O2-C3-C4-O4
17	C	721	XPE	O1-C2-C3-O4
8	D	710	BJ2	N03-C04-C08-N12
17	C	721	XPE	C9-C8-O7-C6
11	B	716	PEG	C1-C2-O2-C3
16	B	730	2PE	C5-C6-O7-C8
17	B	731	XPE	C6-C5-O4-C3
11	A	715	PEG	O1-C1-C2-O2
17	C	721	XPE	O4-C5-C6-O7
16	B	730	2PE	C12-C11-O10-C9
17	B	731	XPE	C5-C6-O7-C8
11	A	715	PEG	C1-C2-O2-C3
17	C	721	XPE	C6-C5-O4-C3
11	D	713	PEG	O1-C1-C2-O2
16	B	730	2PE	C23-C24-O25-C26
17	C	721	XPE	C26-C27-O28-C29
8	A	711	BJ2	C15-C17-C18-O20
17	C	721	XPE	C12-C11-O10-C9
11	D	713	PEG	C4-C3-O2-C2
17	B	731	XPE	C24-C23-O22-C21
16	B	730	2PE	C8-C9-O10-C11
17	C	721	XPE	C20-C21-O22-C23
14	D	730	PGE	O1-C1-C2-O2
17	C	721	XPE	O13-C14-C15-O16
17	B	731	XPE	C26-C27-O28-C29
17	C	721	XPE	O16-C17-C18-O19
12	D	719	EDO	O1-C1-C2-O2
14	D	729	PGE	O1-C1-C2-O2
17	B	731	XPE	O10-C11-C12-O13
14	D	729	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
14	B	728	PGE	O2-C3-C4-O3
12	B	724	EDO	O1-C1-C2-O2
8	A	711	BJ2	C15-C17-C18-O19
8	C	709	BJ2	C15-C17-C18-O20
11	A	714	PEG	C4-C3-O2-C2
11	B	714	PEG	C4-C3-O2-C2
15	A	721	BCN	C2-C1-N1-C5
8	B	710	BJ2	C15-C17-C18-O20
11	B	716	PEG	O2-C3-C4-O4
14	D	731	PGE	C4-C3-O2-C2

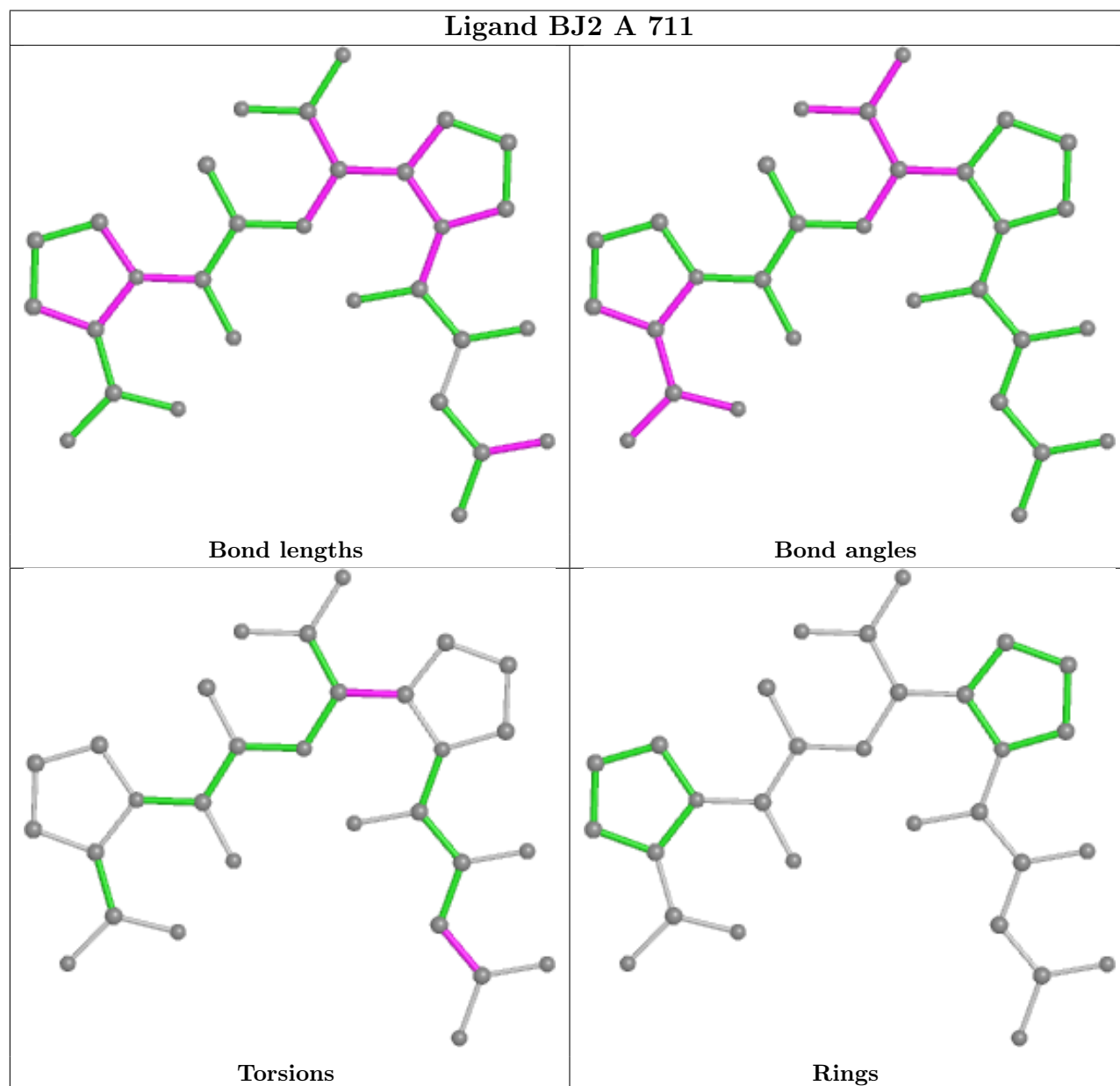
There are no ring outliers.

22 monomers are involved in 29 short contacts:

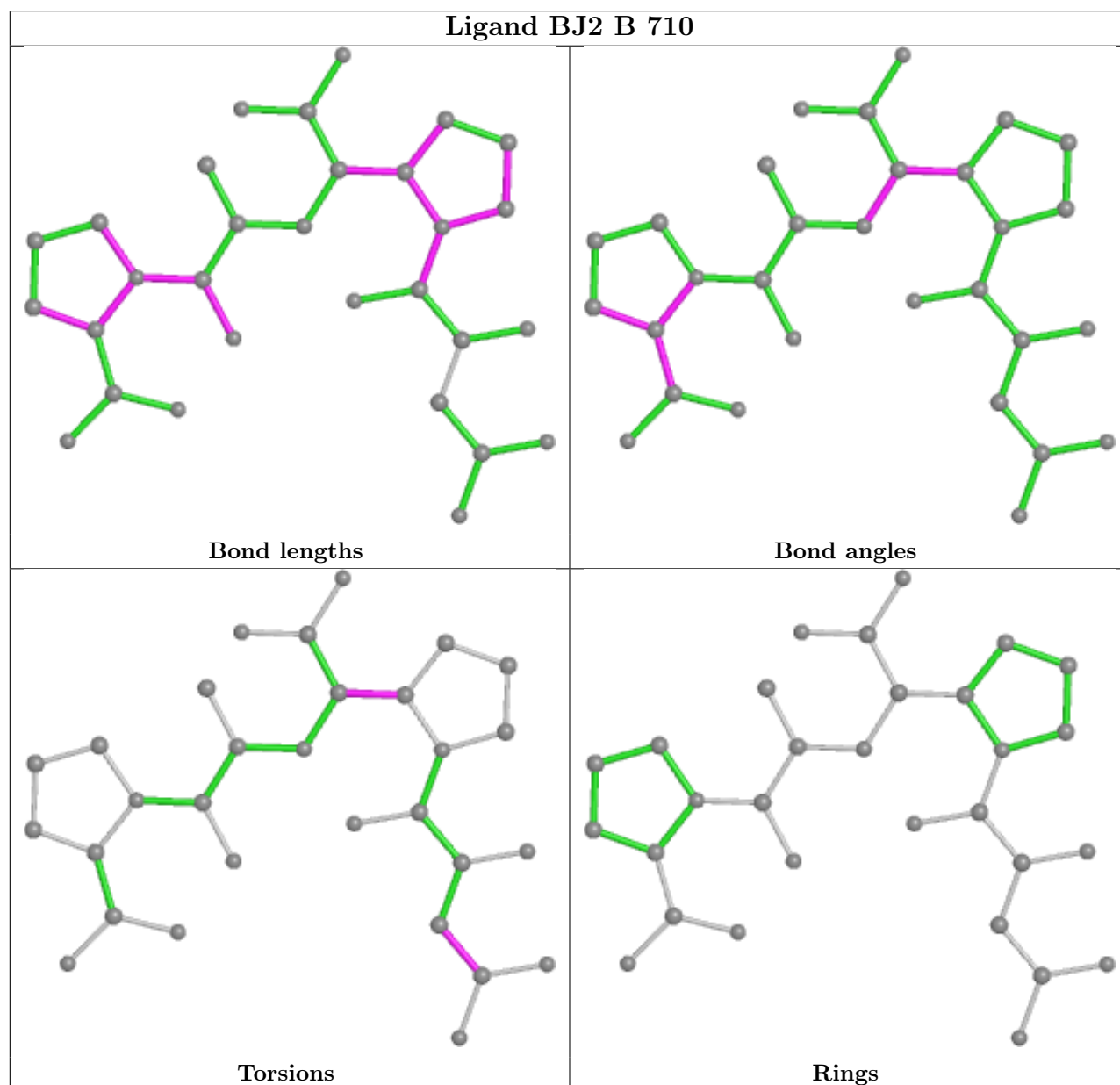
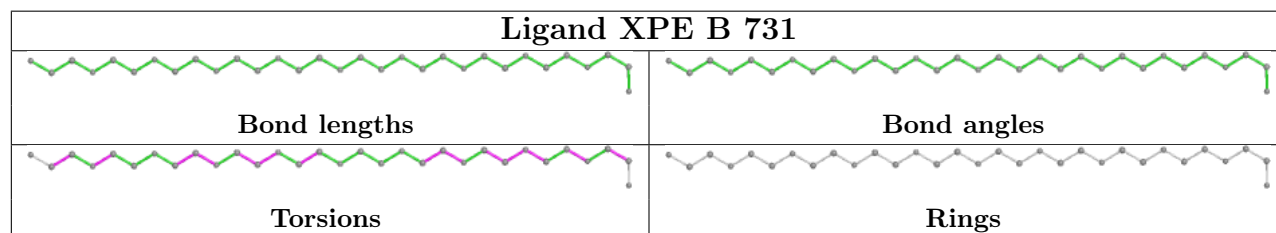
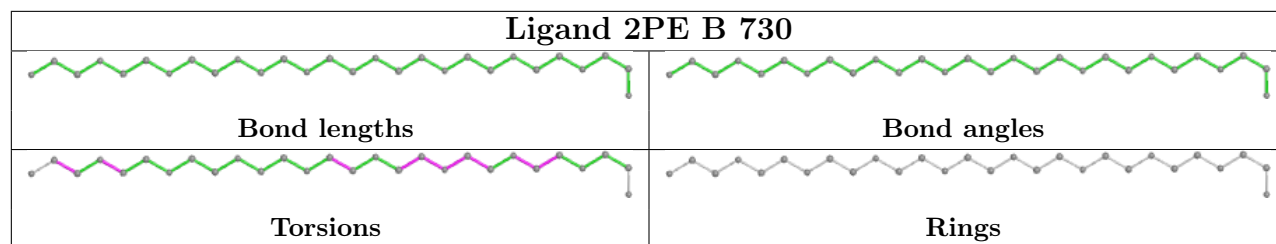
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	724	ACT	2	0
14	B	729[B]	PGE	1	0
11	C	712	PEG	1	0
13	D	728	ACT	1	0
16	B	730	2PE	4	0
13	D	727	ACT	2	0
12	B	722	EDO	1	0
13	C	719	ACT	1	0
12	B	718	EDO	3	0
11	B	715	PEG	1	0
11	C	713	PEG	2	0
11	D	713	PEG	1	0
13	B	726	ACT	1	0
14	D	731	PGE	3	0
8	B	710	BJ2	1	0
8	D	710	BJ2	1	0
15	A	721	BCN	2	0
14	B	728	PGE	3	0
11	B	714	PEG	1	0
13	C	720	ACT	1	0
8	C	709	BJ2	1	0
17	C	721	XPE	2	0

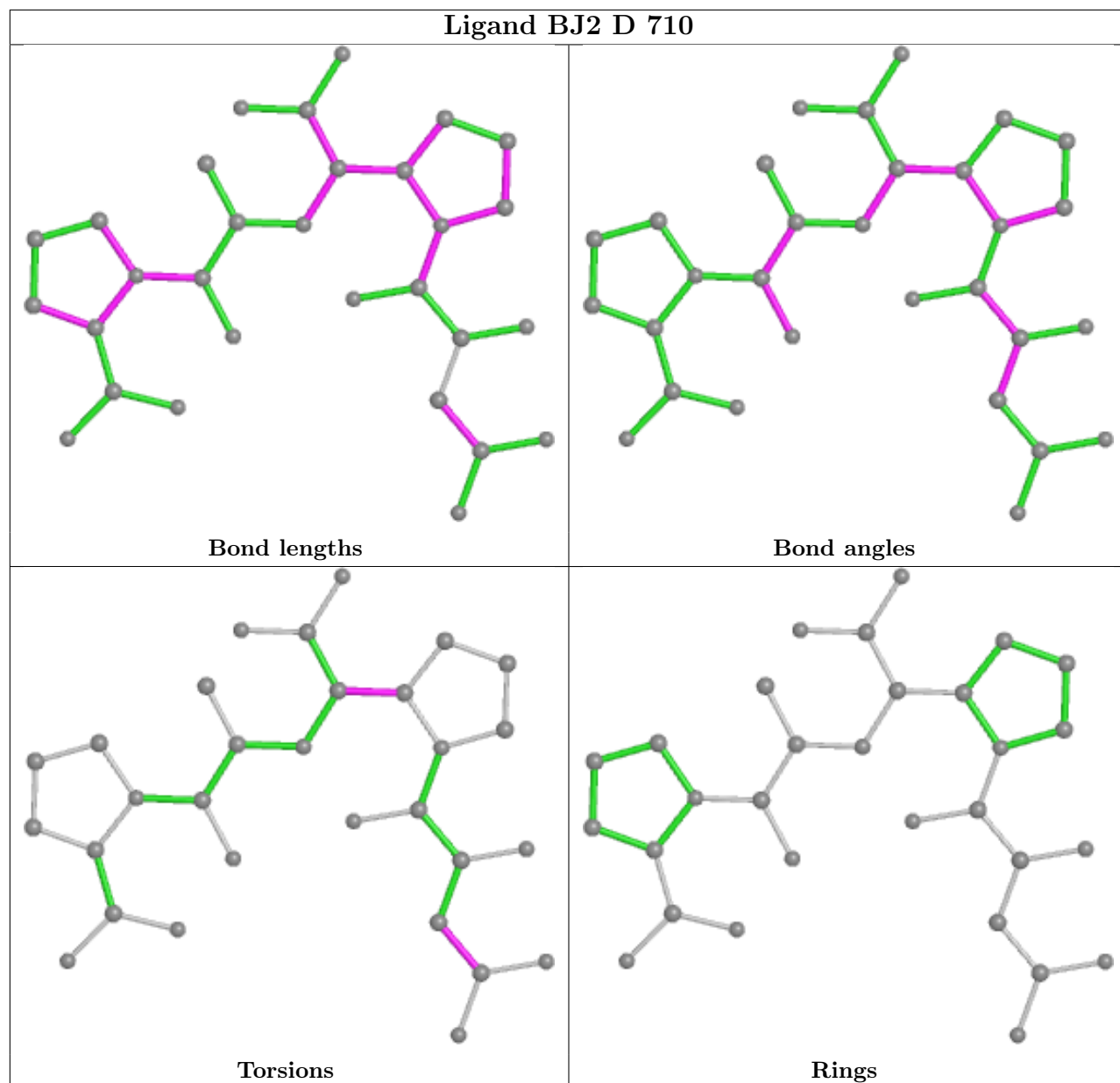
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

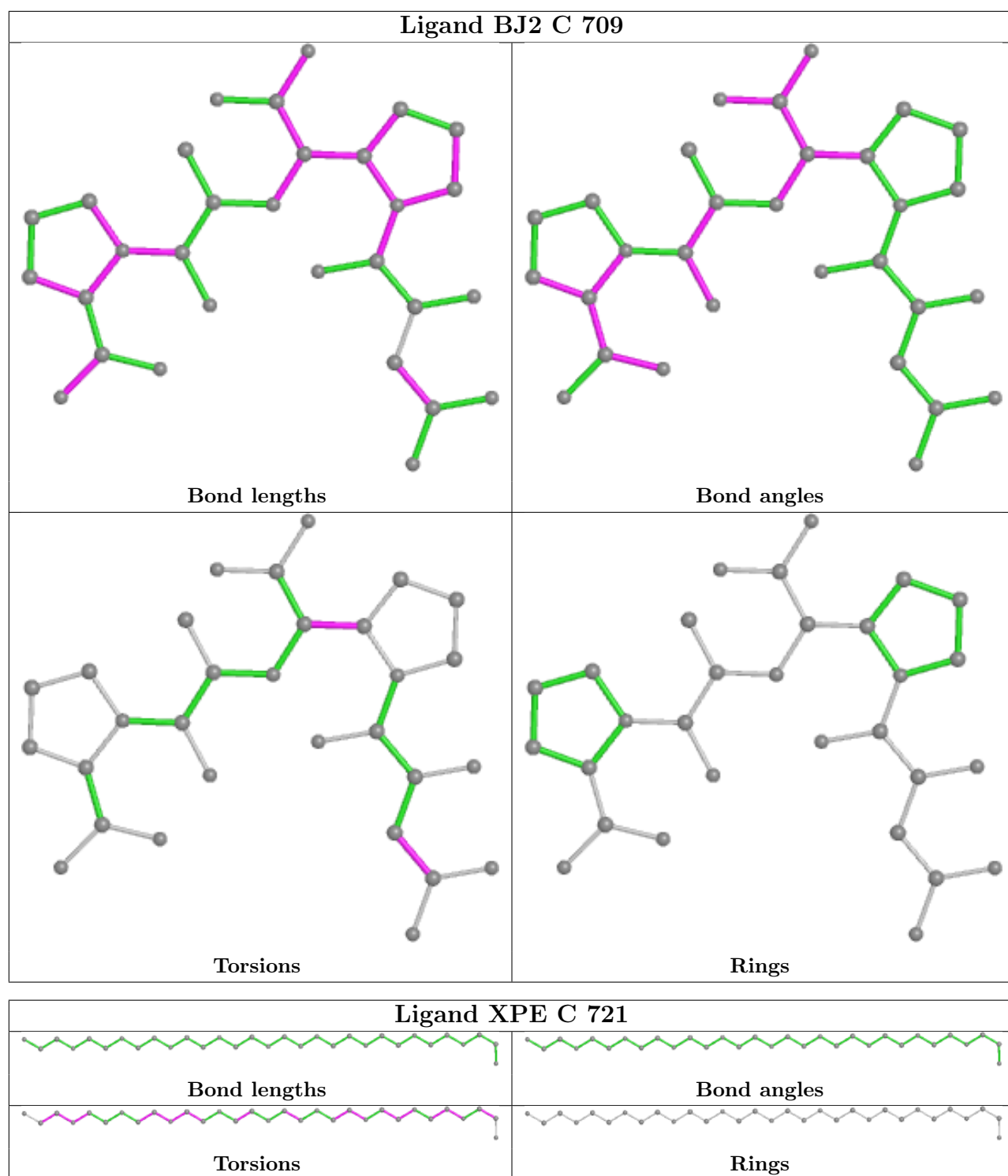
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	605/629 (96%)	-0.26	5 (0%) 86 84	15, 25, 43, 77	0
1	B	605/629 (96%)	-0.23	4 (0%) 87 86	15, 25, 41, 64	0
1	C	606/629 (96%)	-0.11	7 (1%) 79 76	17, 28, 45, 78	0
1	D	614/629 (97%)	-0.30	1 (0%) 95 93	15, 23, 37, 61	0
All	All	2430/2516 (96%)	-0.23	17 (0%) 87 86	15, 25, 42, 78	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	4.8
1	B	25	GLN	4.5
1	D	618	ALA	4.4
1	B	606	ASN	3.6
1	A	413	ARG	3.5
1	C	135	THR	3.4
1	C	78	PRO	3.3
1	A	606	ASN	3.1
1	B	325	GLY	2.9
1	C	130	PRO	2.8
1	C	606	ASN	2.8
1	C	79	ILE	2.5
1	C	413	ARG	2.4
1	A	325	GLY	2.3
1	C	412	ASP	2.1
1	A	415	THR	2.1
1	B	129	LEU	2.1

### 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](#)

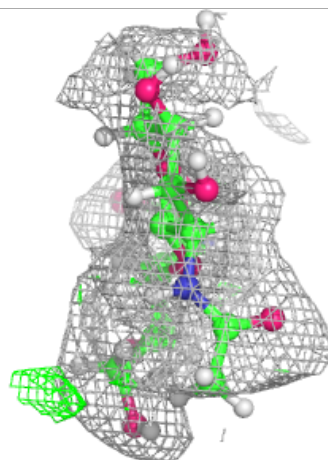
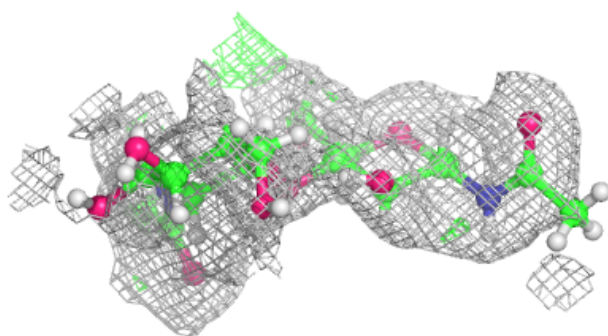
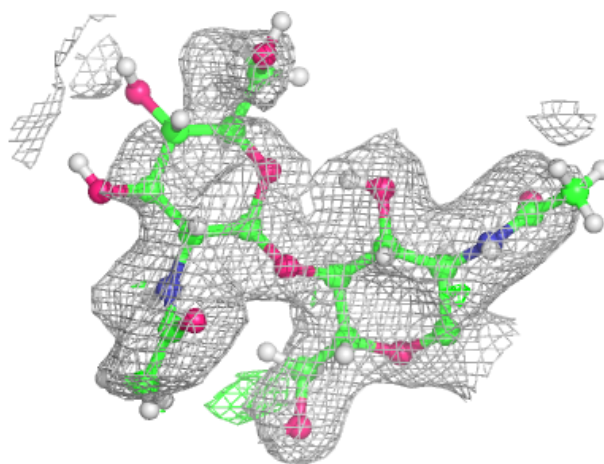
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	G	2	14/15	0.51	0.24	54,69,89,94	27
2	NAG	E	2	14/15	0.67	0.21	63,82,100,110	0
5	FUC	J	2	10/11	0.68	0.24	43,56,64,69	20
6	BMA	K	3	11/12	0.68	0.15	63,67,80,81	21
3	BMA	N	3	11/12	0.72	0.17	49,52,61,67	21
2	NAG	M	2	14/15	0.73	0.24	48,60,68,73	27
2	NAG	E	1	14/15	0.74	0.15	46,60,72,77	0
3	FUC	N	4	10/11	0.76	0.12	37,45,55,57	20
6	NAG	K	1	14/15	0.77	0.23	50,65,82,82	26
4	NAG	L	2	14/15	0.77	0.16	57,72,90,92	27
3	FUC	I	4	10/11	0.80	0.14	46,55,66,70	20
3	BMA	I	3	11/12	0.80	0.14	58,70,85,86	0
3	FUC	F	4	10/11	0.81	0.24	48,54,65,65	20
3	BMA	F	3	11/12	0.82	0.13	55,59,70,72	21
4	FUC	G	3	10/11	0.82	0.17	42,53,63,66	20
2	NAG	H	2	14/15	0.82	0.16	40,52,65,66	27
4	NAG	G	1	14/15	0.84	0.10	34,43,55,59	0
6	NAG	K	2	14/15	0.84	0.14	55,65,79,79	26
5	NAG	O	1	14/15	0.84	0.11	32,39,50,55	0
5	FUC	O	2	10/11	0.86	0.17	34,40,55,55	20
3	NAG	N	2	14/15	0.86	0.16	39,49,59,59	0
3	NAG	F	2	14/15	0.87	0.17	44,53,65,65	26
5	NAG	J	1	14/15	0.87	0.11	33,41,53,64	0
3	NAG	I	2	14/15	0.89	0.13	44,53,66,70	0
2	NAG	M	1	14/15	0.90	0.11	36,46,56,56	0
4	FUC	L	3	10/11	0.90	0.10	45,56,74,74	0
3	NAG	N	1	14/15	0.90	0.09	33,41,47,49	0
2	NAG	H	1	14/15	0.91	0.11	33,44,53,59	26
3	NAG	F	1	14/15	0.91	0.12	43,47,57,58	25
3	NAG	I	1	14/15	0.93	0.11	36,44,53,53	0
4	NAG	L	1	14/15	0.94	0.09	33,44,55,58	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.

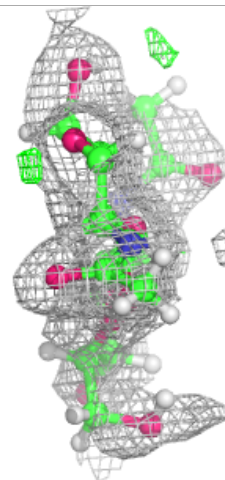
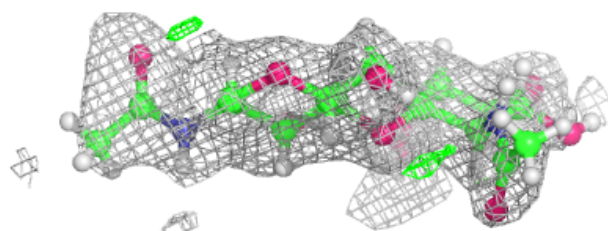
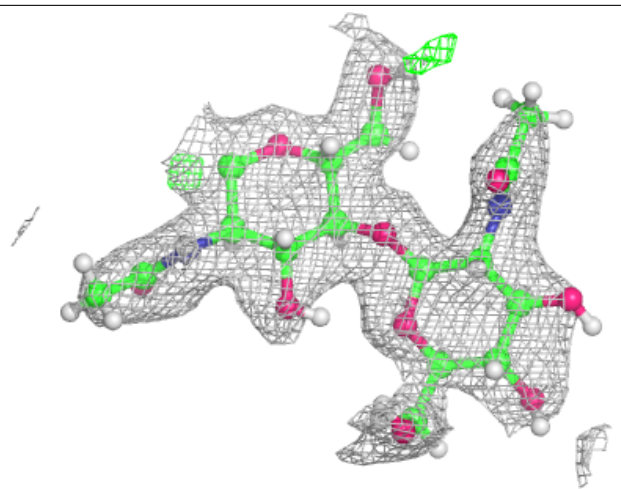
**Electron density around Chain E:**

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



**Electron density around Chain H:**

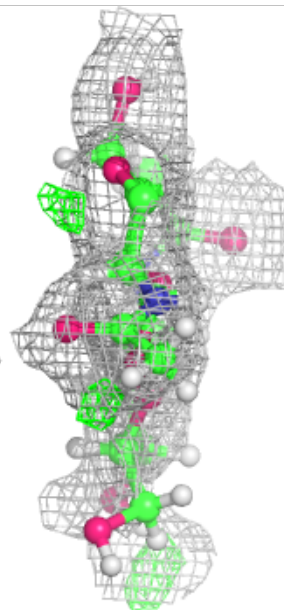
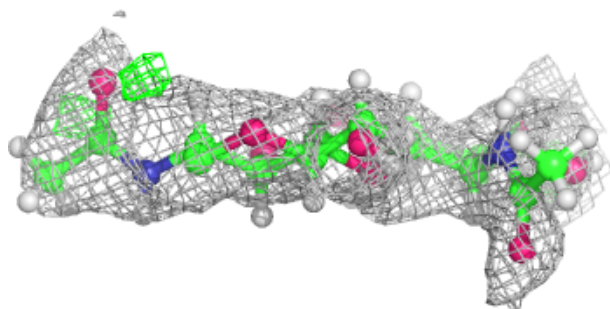
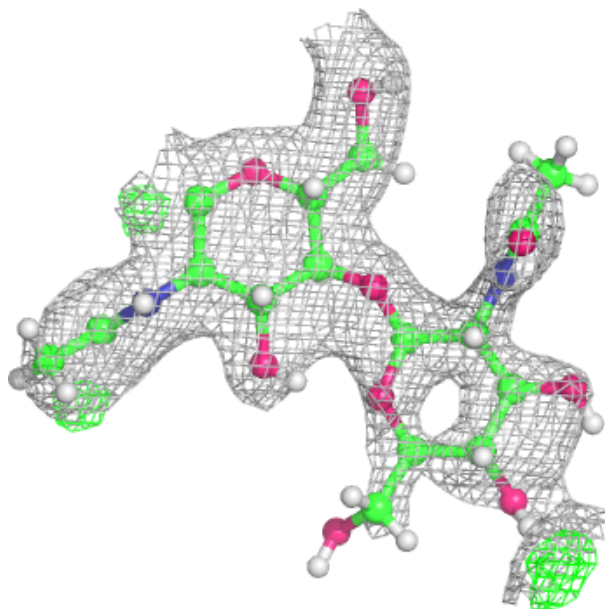
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





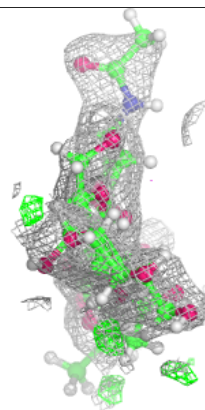
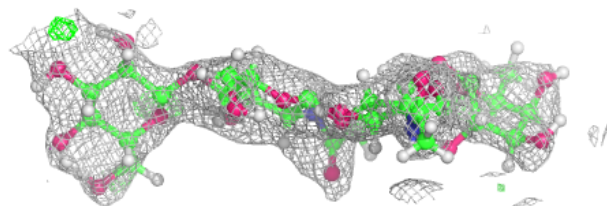
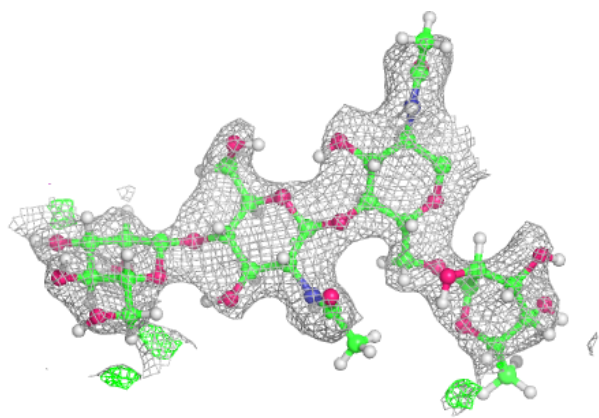
**Electron density around Chain M:**

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



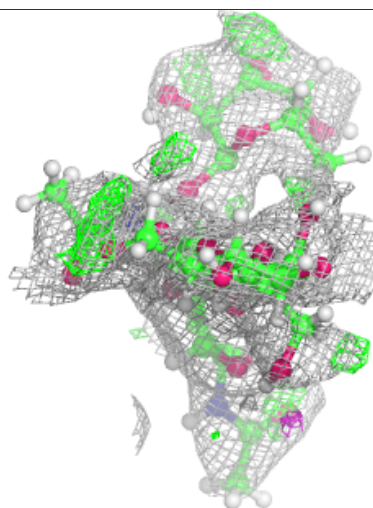
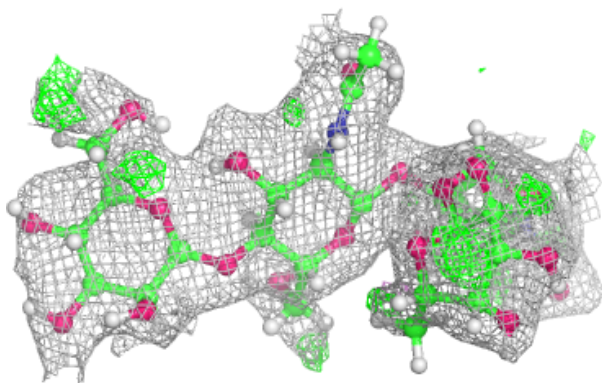
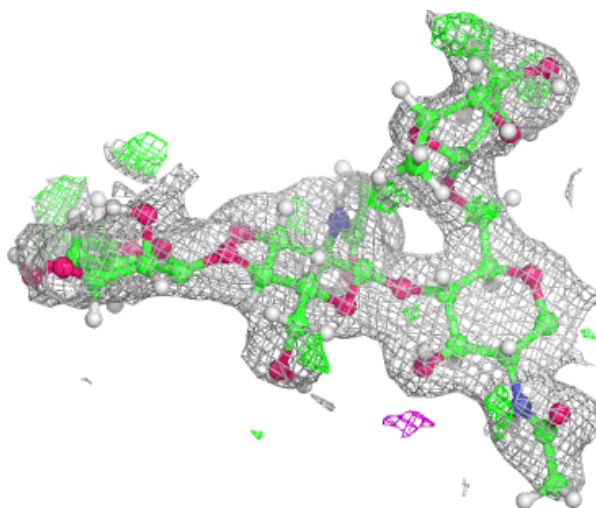
**Electron density around Chain F:**

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



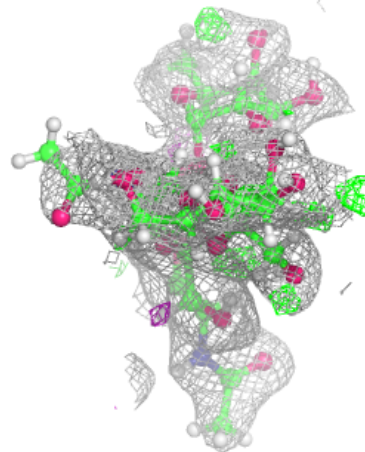
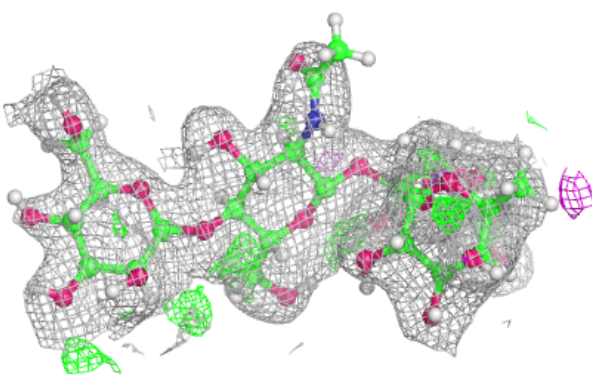
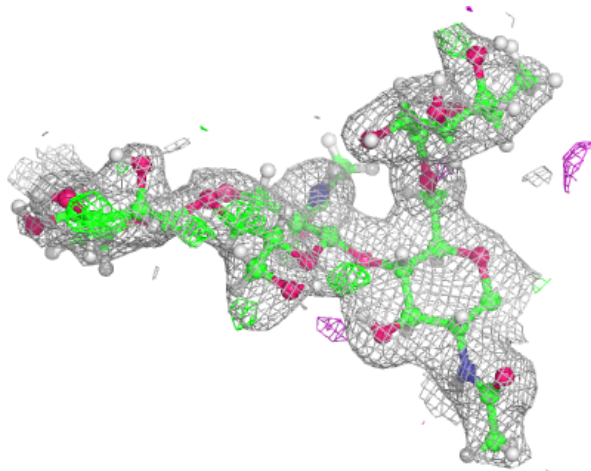
**Electron density around Chain I:**

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



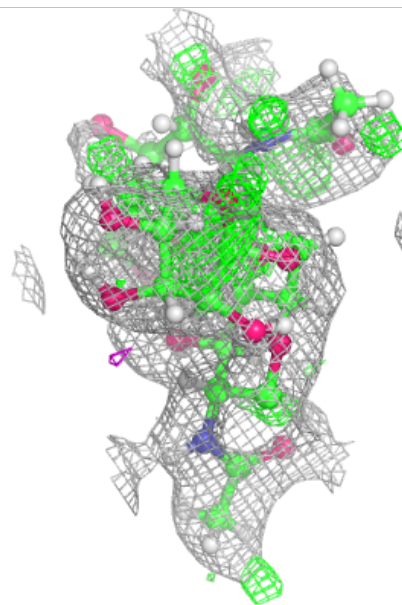
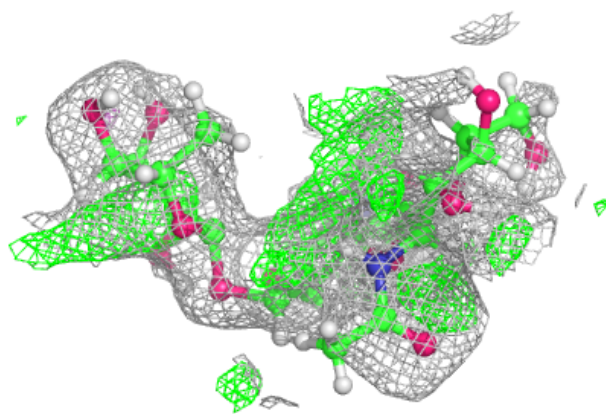
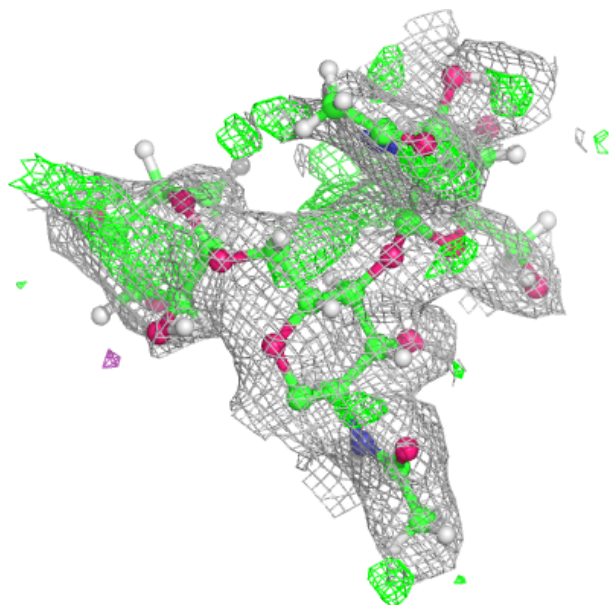
**Electron density around Chain N:**

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



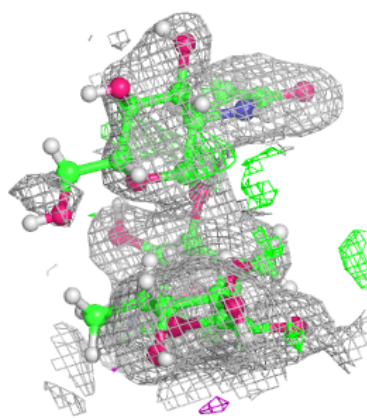
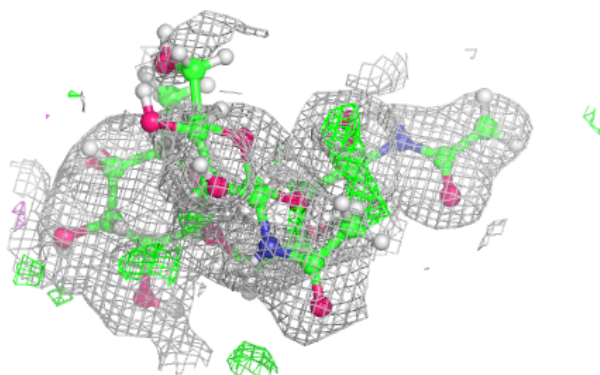
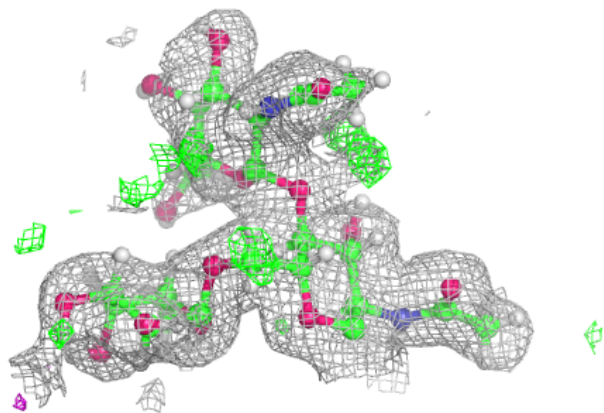
**Electron density around Chain G:**

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



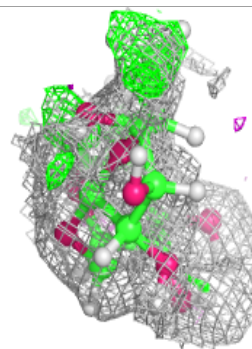
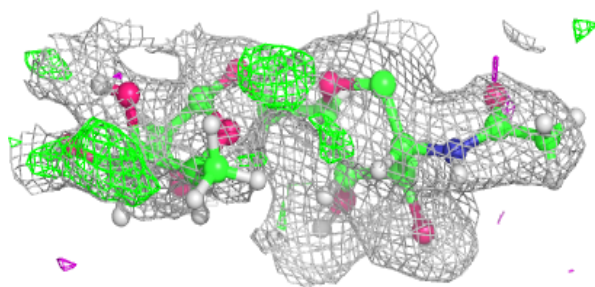
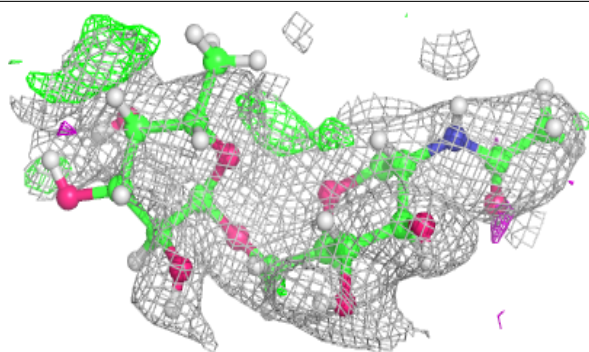
**Electron density around Chain L:**

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

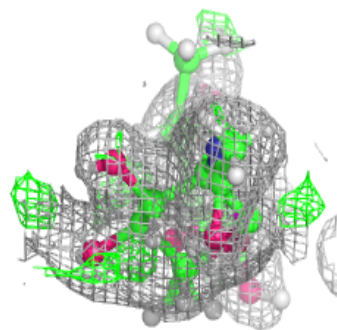
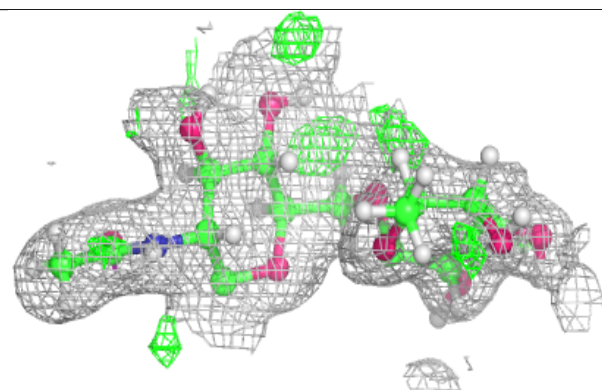
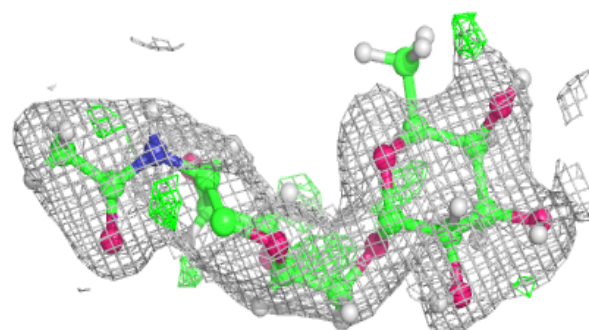


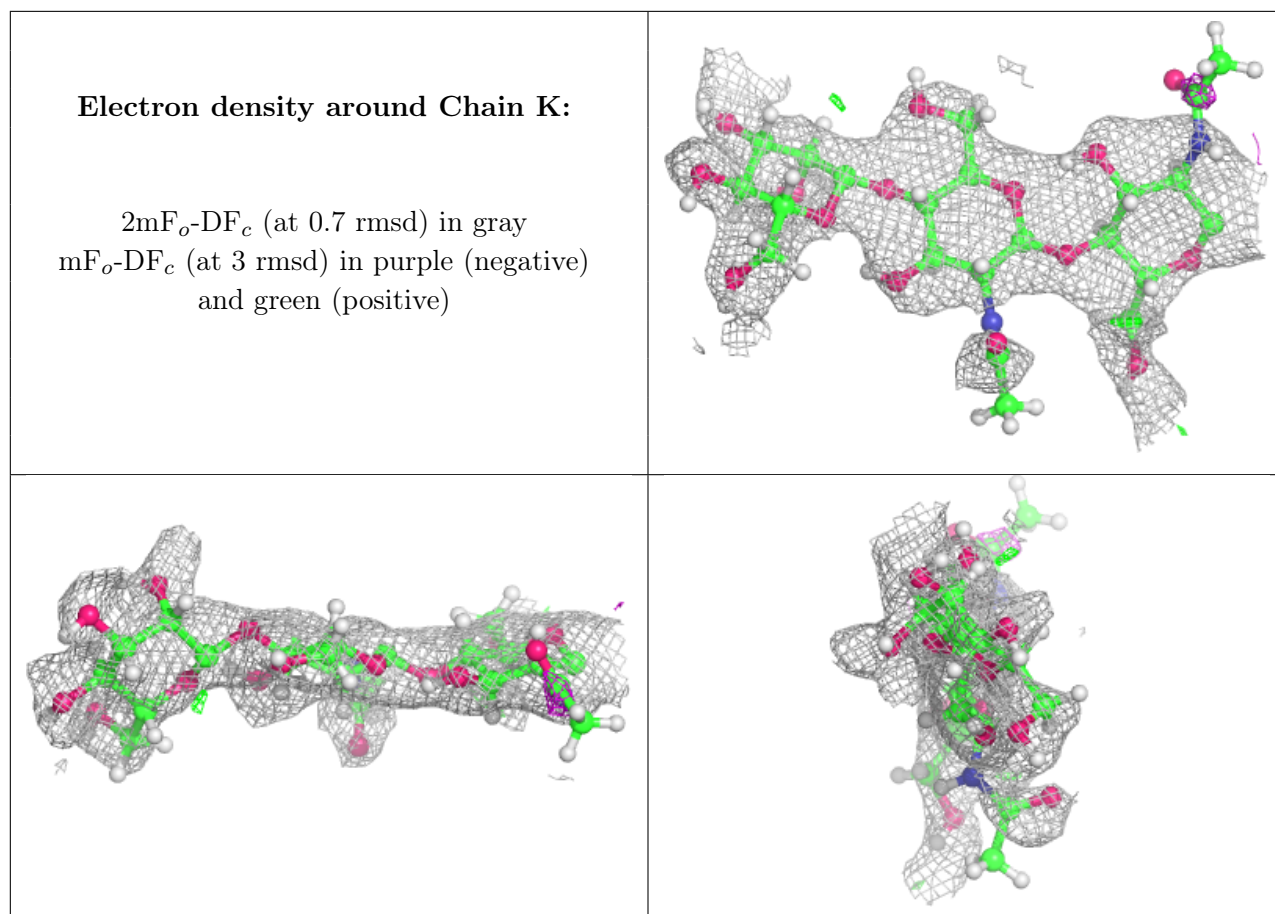
**Electron density around Chain J:**

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

**Electron density around Chain O:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
13	ACT	B	726	4/4	0.60	0.19	29,31,35,35	7
14	PGE	B	729[A]	10/10	0.68	0.21	31,40,47,47	24
14	PGE	B	729[B]	10/10	0.68	0.21	29,37,42,45	24
12	EDO	D	721	4/4	0.69	0.16	30,38,46,46	0
11	PEG	B	715	7/7	0.69	0.20	33,40,47,47	17
14	PGE	A	720	10/10	0.71	0.25	34,51,61,64	0
14	PGE	B	728	10/10	0.73	0.35	37,47,55,60	0
12	EDO	B	721	4/4	0.74	0.23	31,38,42,43	10
14	PGE	D	730	10/10	0.74	0.24	28,40,46,50	0
11	PEG	C	713	7/7	0.75	0.25	29,36,42,45	17
16	2PE	B	730	28/28	0.76	0.22	36,61,79,85	0
13	ACT	D	727	4/4	0.77	0.20	26,32,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	ACT	C	718	4/4	0.78	0.15	30,37,38,40	0
12	EDO	C	715	4/4	0.78	0.13	35,42,44,46	10
12	EDO	D	718	4/4	0.80	0.17	53,64,70,76	0
12	EDO	D	719	4/4	0.80	0.12	33,40,47,50	10
12	EDO	C	716	4/4	0.80	0.21	37,44,50,51	10
17	XPE	B	731	31/31	0.80	0.15	30,43,56,69	0
15	BCN	A	721	11/11	0.81	0.24	35,43,52,53	0
11	PEG	D	714	7/7	0.81	0.11	39,51,61,61	17
12	EDO	D	723[A]	4/4	0.81	0.17	36,44,47,51	10
14	PGE	D	731	10/10	0.82	0.50	34,49,60,67	0
12	EDO	A	716	4/4	0.82	0.20	25,30,33,38	10
18	NAG	C	701	14/15	0.82	0.12	38,46,56,56	27
11	PEG	A	714	7/7	0.83	0.12	27,35,42,45	17
12	EDO	C	714	4/4	0.83	0.14	27,33,39,43	10
12	EDO	A	717	4/4	0.83	0.20	25,35,40,42	10
12	EDO	D	722	4/4	0.83	0.20	36,43,50,50	0
12	EDO	B	720	4/4	0.83	0.29	57,68,69,74	0
12	EDO	D	716	4/4	0.83	0.13	38,47,53,57	10
11	PEG	D	713	7/7	0.84	0.13	26,41,48,57	17
13	ACT	C	720	4/4	0.85	0.26	39,43,47,47	0
13	ACT	B	727	4/4	0.85	0.20	41,43,49,49	0
12	EDO	C	717	4/4	0.85	0.15	34,41,44,47	10
13	ACT	C	719	4/4	0.85	0.18	36,43,47,48	0
12	EDO	B	724	4/4	0.86	0.13	49,58,61,65	0
11	PEG	C	712	7/7	0.86	0.15	29,35,39,46	17
11	PEG	B	716	7/7	0.86	0.15	43,54,69,73	0
14	PGE	D	729	10/10	0.87	0.15	31,40,49,52	0
11	PEG	A	715	7/7	0.88	0.14	33,43,51,56	17
12	EDO	D	715	4/4	0.88	0.13	31,40,42,50	10
11	PEG	B	713	7/7	0.88	0.12	36,44,51,58	17
12	EDO	B	722	4/4	0.88	0.27	37,44,45,52	10
17	XPE	C	721	31/31	0.88	0.12	29,42,52,54	0
12	EDO	B	723	4/4	0.88	0.14	28,38,41,49	10
12	EDO	D	717	4/4	0.89	0.12	31,39,47,48	10
12	EDO	B	719	4/4	0.90	0.12	27,32,37,39	10
12	EDO	B	717	4/4	0.90	0.17	22,26,32,32	10
13	ACT	A	718	4/4	0.91	0.17	25,30,31,34	0
13	ACT	B	725	4/4	0.91	0.11	23,28,34,35	0
12	EDO	D	720	4/4	0.92	0.12	23,32,39,40	10
11	PEG	B	714	7/7	0.92	0.11	27,35,47,57	17
13	ACT	D	725	4/4	0.93	0.16	24,29,32,34	0
8	BJ2	C	709	30/30	0.94	0.10	17,23,28,28	0

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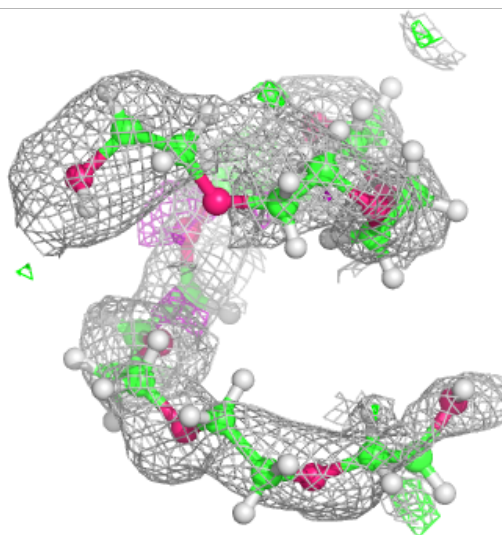
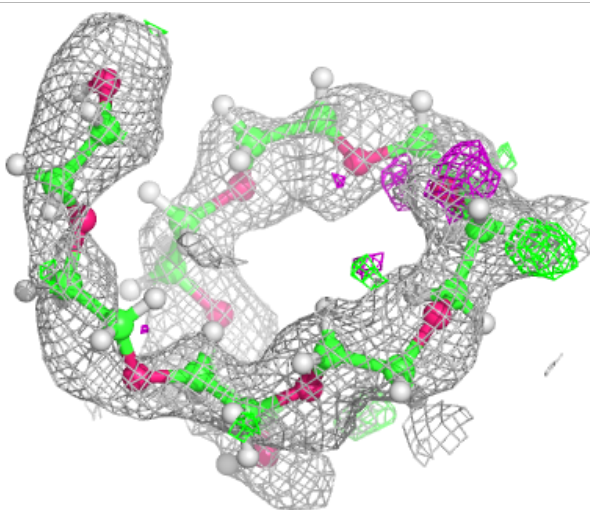
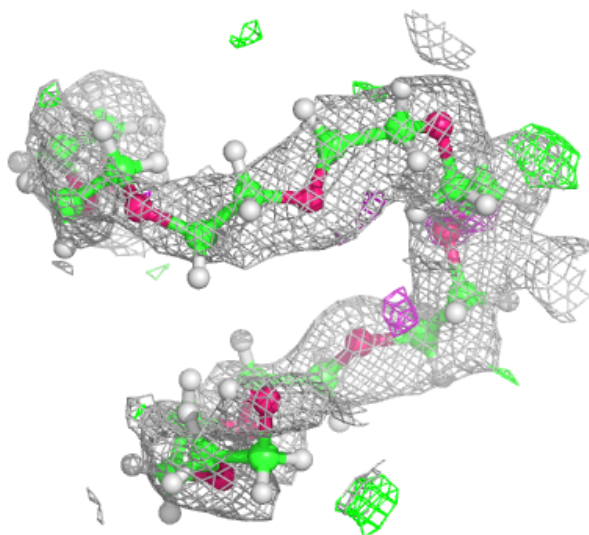
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	ACT	A	719	4/4	0.94	0.08	39,41,47,47	0
13	ACT	D	728	4/4	0.94	0.15	29,36,39,40	0
13	ACT	D	724	4/4	0.95	0.09	22,26,27,28	0
12	EDO	B	718	4/4	0.95	0.20	15,18,21,21	10
8	BJ2	D	710	30/30	0.96	0.09	15,20,24,25	0
13	ACT	D	726	4/4	0.97	0.20	37,39,45,45	0
8	BJ2	B	710	30/30	0.97	0.09	14,20,24,24	0
8	BJ2	A	711	30/30	0.97	0.09	15,20,24,26	0
10	MG	A	713	1/1	0.98	0.11	23,23,23,23	0
10	MG	B	712	1/1	0.99	0.07	24,24,24,24	0
10	MG	D	712	1/1	0.99	0.14	13,13,13,13	0
9	CL	D	711	1/1	1.00	0.12	18,18,18,18	0
7	ZN	A	710	1/1	1.00	0.13	16,16,16,16	0
7	ZN	B	709	1/1	1.00	0.13	17,17,17,17	0
10	MG	C	711	1/1	1.00	0.08	25,25,25,25	0
7	ZN	C	708	1/1	1.00	0.11	18,18,18,18	0
7	ZN	D	709	1/1	1.00	0.12	17,17,17,17	0
9	CL	A	712	1/1	1.00	0.10	17,17,17,17	0
9	CL	B	711	1/1	1.00	0.12	19,19,19,19	0
9	CL	C	710	1/1	1.00	0.08	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

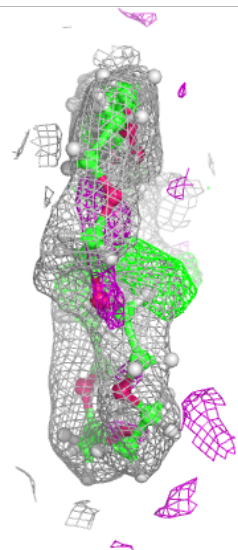
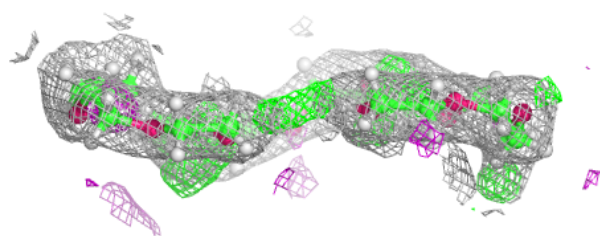
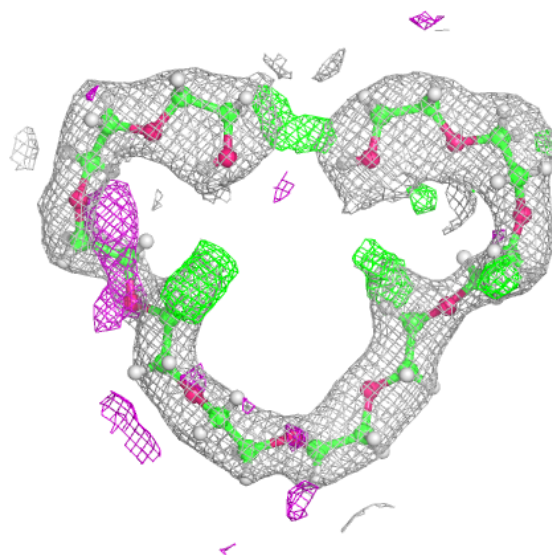
**Electron density around 2PE B 730:**

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



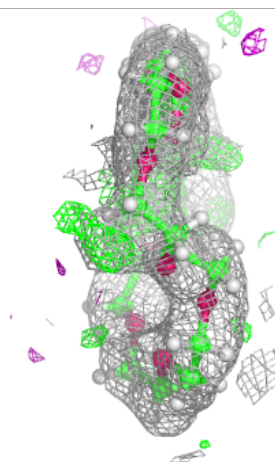
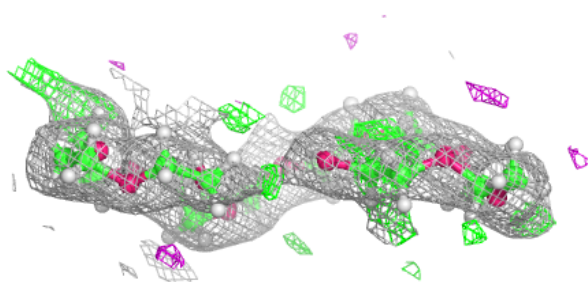
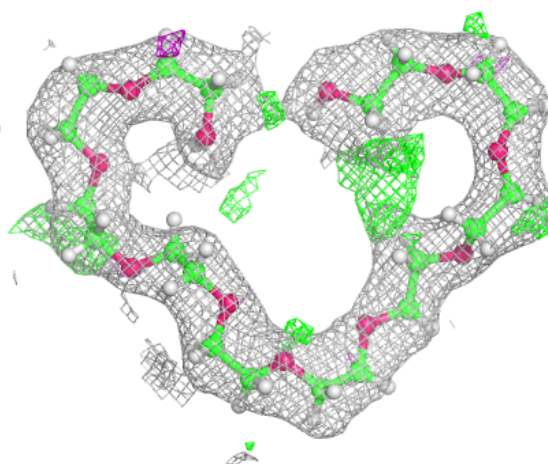
**Electron density around XPE B 731:**

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



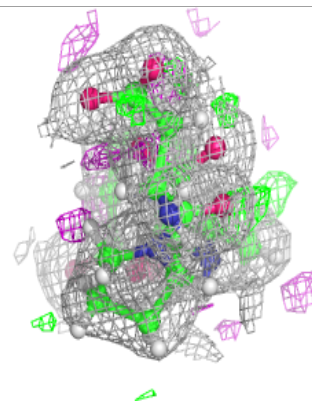
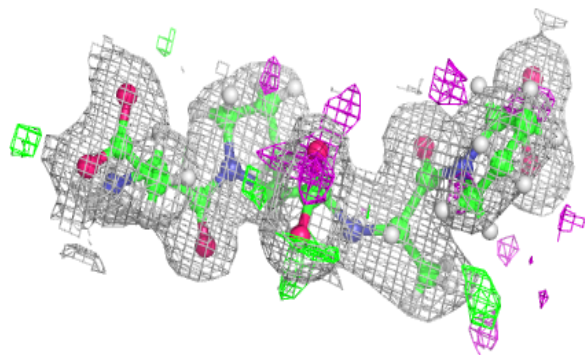
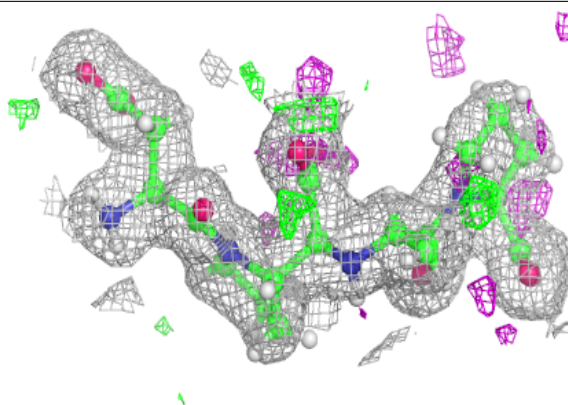
**Electron density around XPE C 721:**

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

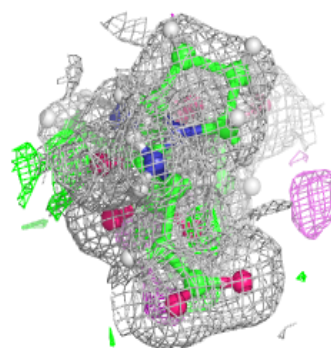
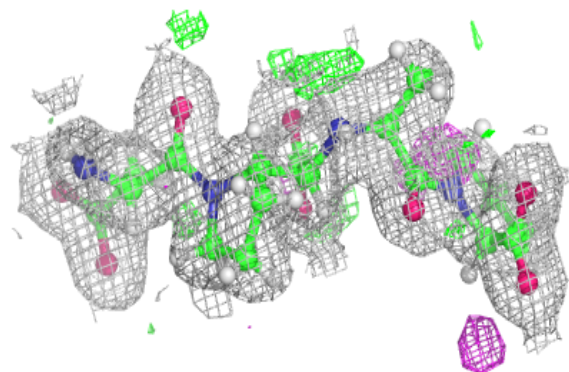
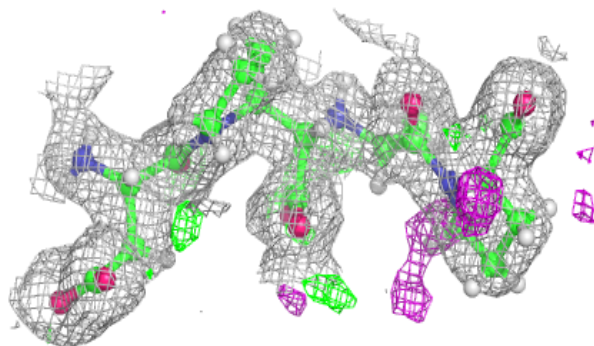


**Electron density around BJ2 C 709:**

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

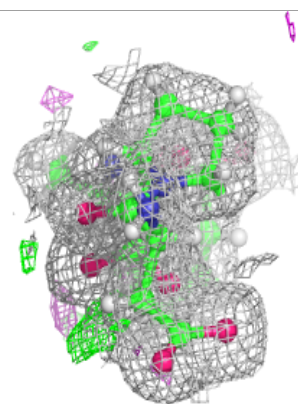
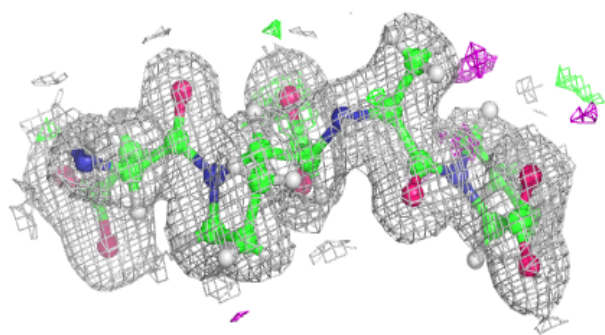
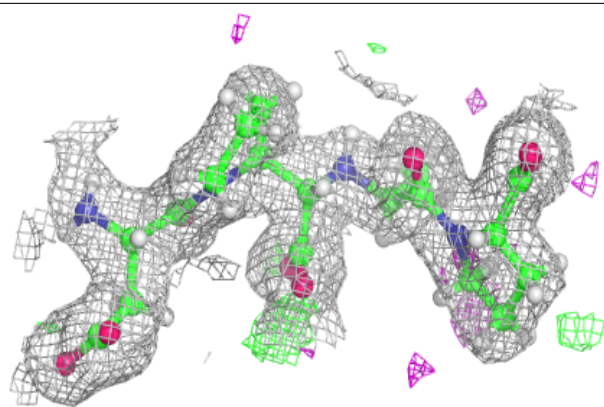
**Electron density around BJ2 D 710:**

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

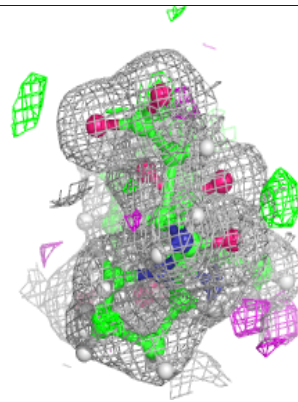
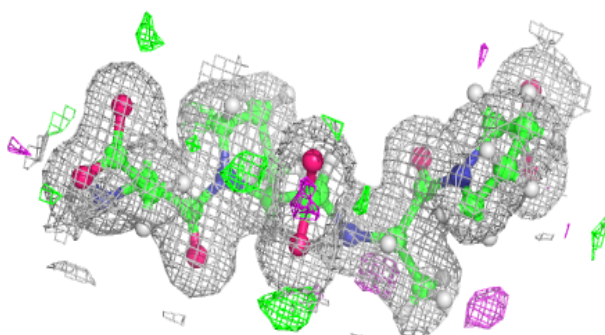
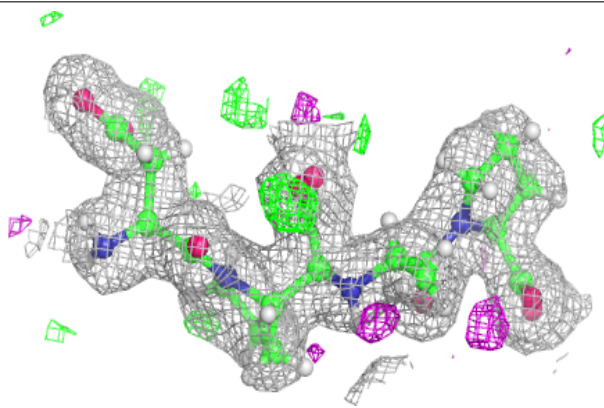


**Electron density around BJ2 B 710:**

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

**Electron density around BJ2 A 711:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.