



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:56 AM UTC

PDB ID : 6EN5 / pdb_00006en5
Title : Crystal structure A 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 : 1.75 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

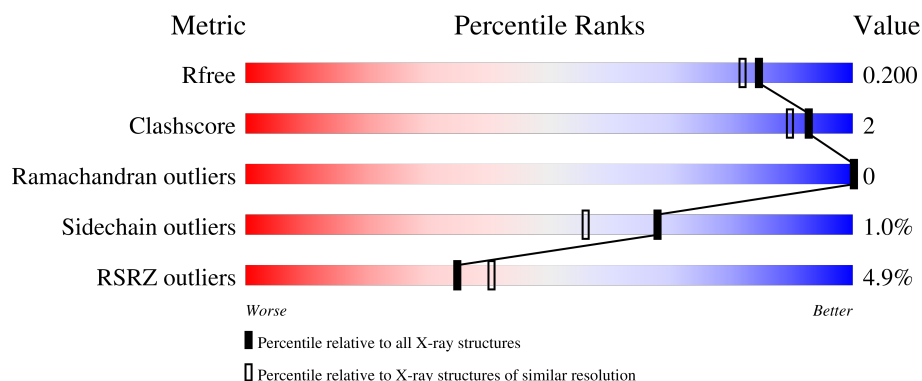
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.



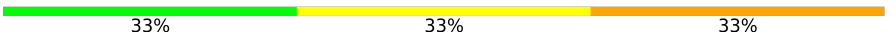
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	3% 92% 5%
1	B	629	10% 93%
1	C	629	4% 93%
1	D	629	2% 94%
2	E	2	100%

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

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 43786 atoms, of which 20257 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	605	Total	C	H	N	O	S	0	11	0
			9849	3228	4811	870	920	20			
1	B	608	Total	C	H	N	O	S	0	9	0
			9851	3231	4810	867	923	20			
1	C	606	Total	C	H	N	O	S	0	9	0
			9789	3213	4779	862	916	19			
1	D	614	Total	C	H	N	O	S	0	14	0
			9957	3264	4865	874	934	20			

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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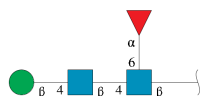
Chain	Residue	Modelled	Actual	Comment	Reference
C	117	GLN	ASN	conflict	UNP P12821
C	131	GLN	ASN	conflict	UNP P12821
C	289	GLN	ASN	conflict	UNP P12821
C	545	ARG	GLN	conflict	UNP P12821
C	576	LEU	PRO	conflict	UNP P12821
C	629	LEU	-	expression tag	UNP P12821
D	9	GLN	ASN	conflict	UNP P12821
D	25	GLN	ASN	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
			55	16	27	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			54	16	26	2	10			
2	K	2	Total	C	H	N	O	0	0	0
			54	16	26	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.



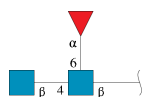
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	4	Total	C	H	N	O	0	0	0
			95	28	46	2	19			

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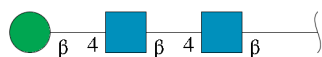
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	4	Total	C	H	N	O	0	0	0
			95	28	46	2	19			

- 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.



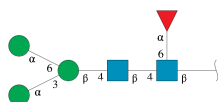
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			
4	J	3	Total	C	H	N	O	0	0	0
			73	22	35	2	14			
4	M	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			
4	P	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 5 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
5	L	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			
5	N	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.

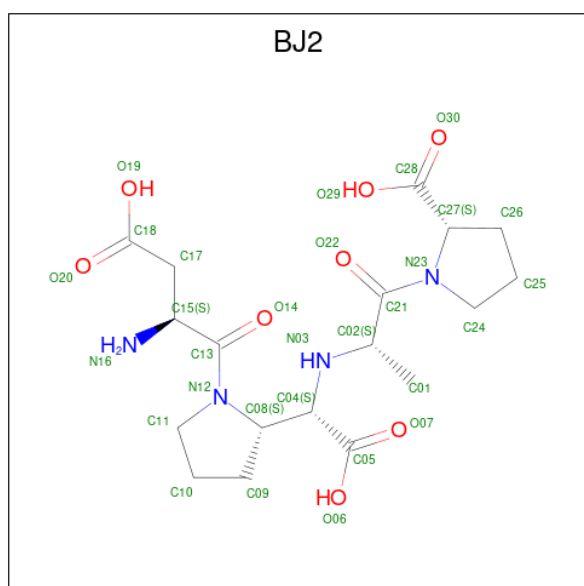


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	6	Total	C	H	N	O	0	0	0
			135	40	64	2	29			

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- 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 (CCD ID: BJ2) (formula: C₁₈H₂₈N₄O₈).



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

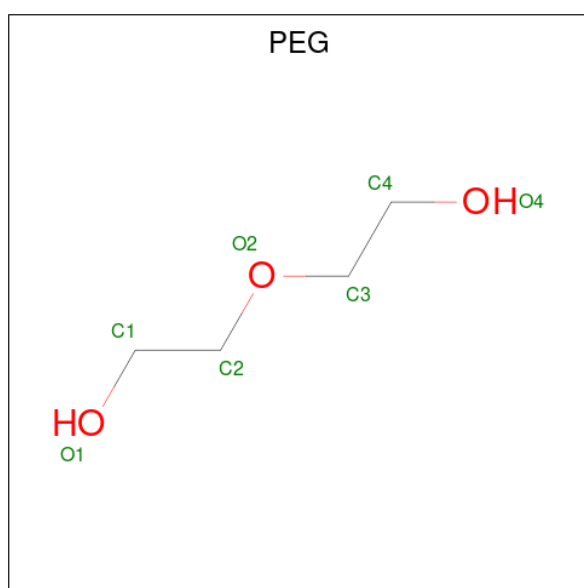
- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



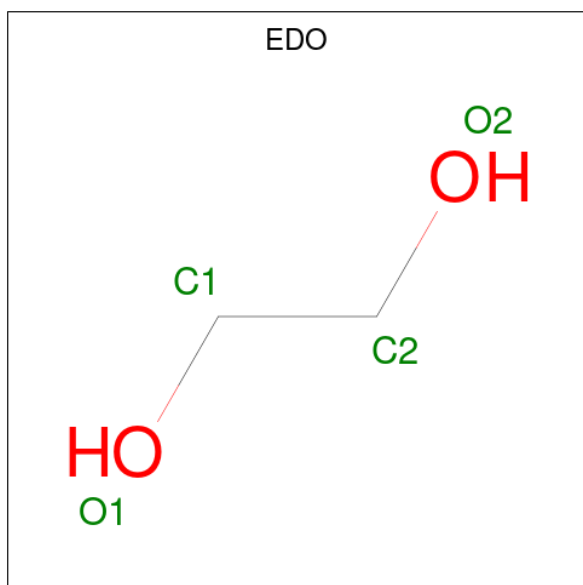
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			17	4	10	3		
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 (CCD ID: EDO) (formula: C₂H₆O₂).



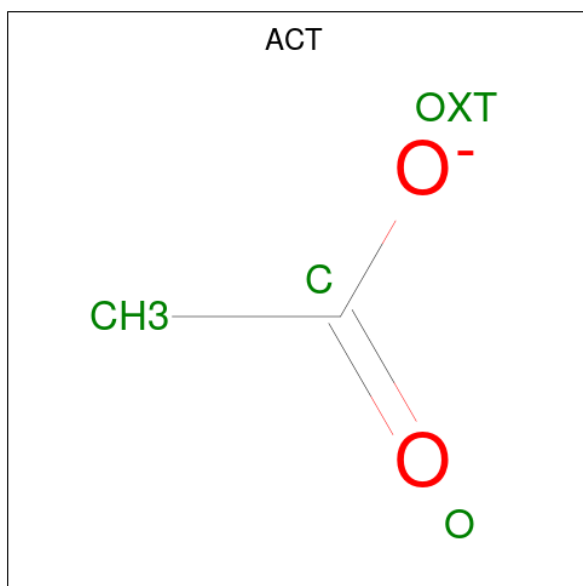
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	B	1	Total	C	H	O	0	0
			10	2	6	2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

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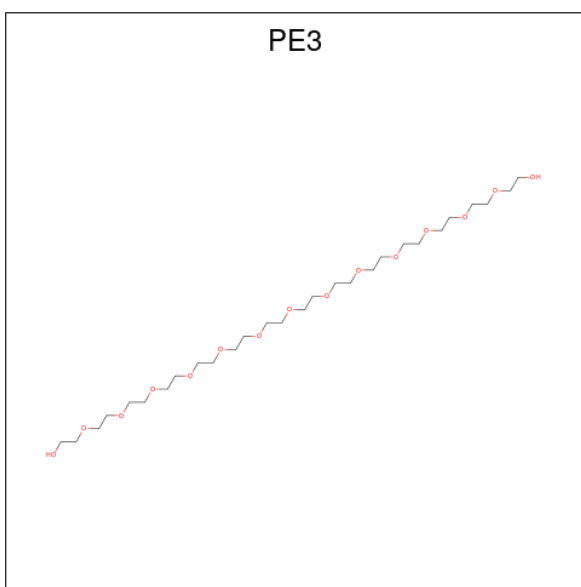
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 13 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



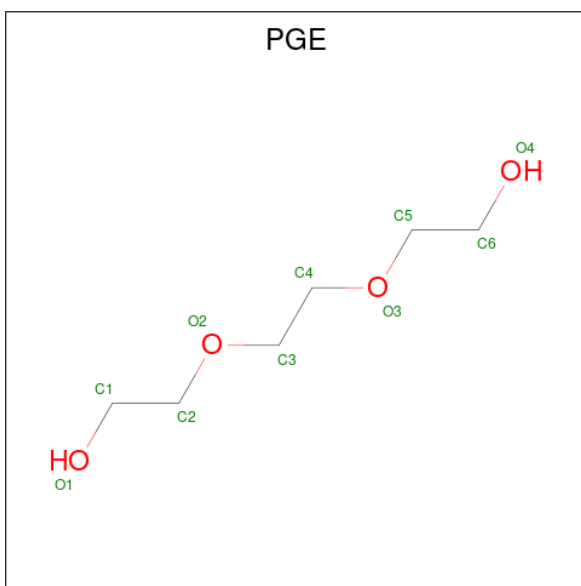
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	H	O	0	0
			7	2	3	2		
13	A	1	Total	C	H	O	0	0
			7	2	3	2		
13	B	1	Total	C	H	O	0	0
			7	2	3	2		
13	C	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 14 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (CCD ID: PE3) (formula: $C_{28}H_{58}O_{15}$).



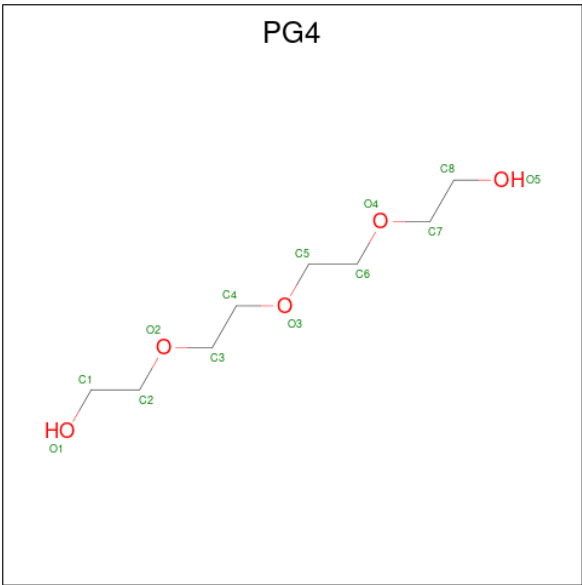
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	H	O	0	0
			101	28	58	15		

- Molecule 15 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



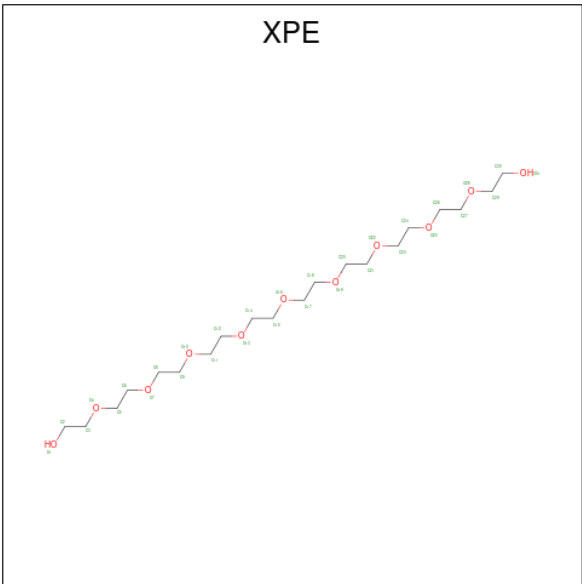
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 16 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	C	H	O	0	0
			31	8	18	5		
16	C	1	Total	C	H	O	0	1
			62	16	36	10		

- Molecule 17 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula: C₂₀H₄₂O₁₁).



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

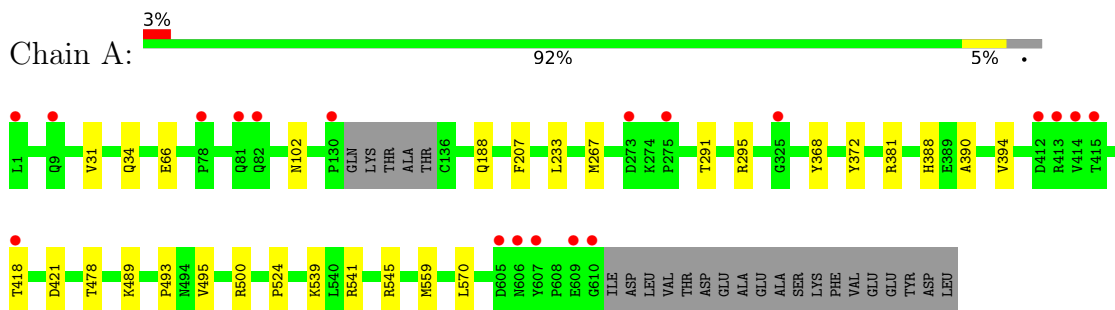
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	584	Total 588	O 588	0	4
18	B	580	Total 581	O 581	0	2
18	C	547	Total 551	O 551	0	4
18	D	682	Total 690	O 690	0	8

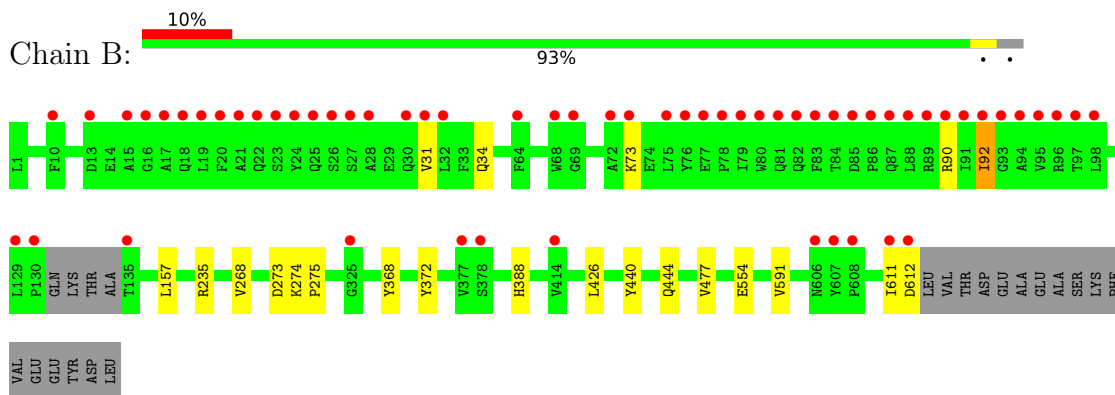
3 Residue-property plots [i](#)

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.

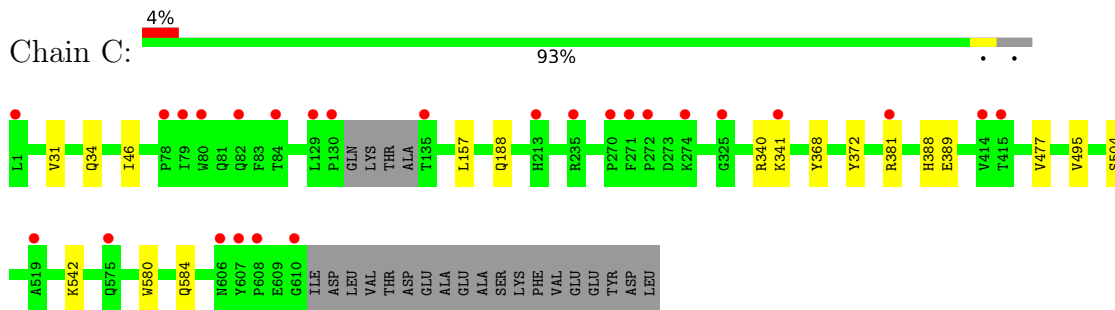
- Molecule 1: Angiotensin-converting enzyme



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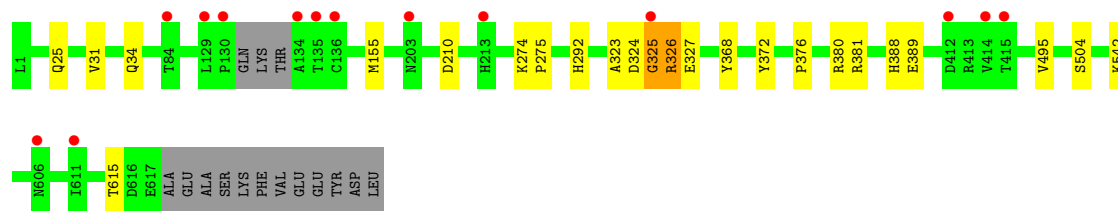


- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme





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

Chain E: 100%



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

Chain H: 50% 50%



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

Chain K: 100%



- 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: 75% 25%



- 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: 100%



- 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: 100%



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

Chain J:  100%



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

Chain M:  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 P:  33% 33% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  67% 33%



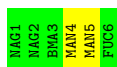
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 O:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.17Å 103.45Å 115.45Å 84.86° 85.49° 81.99°	Depositor
Resolution (Å)	79.48 – 1.75 79.48 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (79.48-1.75) 97.1 (79.48-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.173 , 0.198 0.175 , 0.200	Depositor DCC
R_{free} test set	3195 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	43786	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.30 % 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 4.3807e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, CL, PE3, EDO, PEG, PGE, MAN, ZN, FUC, PG4, MG, ACT, BMA, XPE, BJ2

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	0/5194	0.51	0/7070
1	B	0.40	0/5197	0.52	0/7076
1	C	0.36	0/5181	0.50	0/7055
1	D	0.47	2/5280 (0.0%)	0.55	2/7190 (0.0%)
All	All	0.41	2/20852 (0.0%)	0.52	2/28391 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	327	GLU	C-O	-6.54	1.16	1.24
1	D	326	ARG	CZ-NH2	-5.03	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	GLY	CA-C-N	5.20	128.46	120.82
1	D	325	GLY	C-N-CA	5.20	128.46	120.82

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	5038	4811	4799	17	0
1	B	5041	4810	4802	13	0
1	C	5010	4779	4758	9	0
1	D	5092	4865	4820	12	0
2	E	28	27	25	0	0
2	H	28	26	25	0	0
2	K	28	26	25	0	0
3	F	49	46	43	1	0
3	I	49	46	43	0	0
4	G	38	36	34	3	0
4	J	38	35	34	0	0
4	M	38	36	34	0	0
4	P	38	34	34	2	0
5	L	39	36	34	0	0
5	N	39	36	34	0	0
6	O	71	64	61	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	0	0
8	C	30	25	0	1	0
8	D	30	25	0	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	21	30	30	2	0
11	B	35	50	50	0	0
11	C	14	20	20	3	0
11	D	14	20	20	0	0
12	A	28	42	42	3	0
12	B	20	30	30	0	0
12	C	32	48	48	0	0
12	D	12	18	18	0	0
13	A	8	6	6	0	0
13	B	4	3	3	0	0
13	C	4	3	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	8	6	6	1	0
14	A	43	58	58	4	0
15	B	10	14	14	0	0
16	B	13	18	18	2	0
16	C	26	36	36	0	0
17	D	31	42	42	0	0
18	A	588	0	0	3	0
18	B	581	0	0	3	0
18	C	551	0	0	2	0
18	D	690	0	0	4	0
All	All	23529	20257	20049	62	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 (62) 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)
13:D:723:ACT:H1	18:D:1087:HOH:O	1.89	0.71
1:D:542:LYS:NZ	18:D:804:HOH:O	2.25	0.69
1:C:340[A]:ARG:O	1:C:341:LYS:HE2	1.99	0.62
1:C:340[B]:ARG:O	1:C:341:LYS:HE2	1.99	0.62
1:A:381[B]:ARG:NH1	18:A:803:HOH:O	2.34	0.61
4:G:2:NAG:H83	4:G:2:NAG:H3	1.81	0.61
1:C:542:LYS:NZ	18:C:804:HOH:O	2.27	0.61
1:D:324:ASP:OD1	1:D:326:ARG:HB2	2.01	0.60
1:B:554:GLU:OE2	18:B:801:HOH:O	2.17	0.58
1:A:31:VAL:O	1:A:34:GLN:HG3	2.05	0.56
1:A:295:ARG:HG3	14:A:726:PE3:H381	1.86	0.55
8:C:702:BJ2:N16	11:C:713:PEG:O1	2.39	0.55
1:D:155[A]:MET:SD	1:D:615:THR:HG22	2.47	0.54
14:A:726:PE3:H392	14:A:726:PE3:O31	2.08	0.54
1:B:73:LYS:HE3	18:B:1097:HOH:O	2.09	0.53
1:C:31:VAL:O	1:C:34:GLN:HG3	2.10	0.51
1:B:31:VAL:O	1:B:34:GLN:HG3	2.10	0.51
1:A:418:THR:HG22	3:F:4:FUC:O4	2.12	0.50
4:G:1:NAG:H61	4:G:3:FUC:O2	2.11	0.50
4:P:1:NAG:H61	4:P:3:FUC:O2	2.12	0.49
1:A:539:LYS:HE3	1:A:559:MET:O	2.11	0.49
1:B:440:TYR:O	1:B:444[B]:GLN:HG2	2.13	0.48
1:D:25:GLN:OE1	1:D:376:PRO:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:716:PEG:H31	18:A:827:HOH:O	2.15	0.46
1:D:31:VAL:O	1:D:34:GLN:HG3	2.15	0.46
1:D:274:LYS:HB3	1:D:275:PRO:CD	2.45	0.46
12:A:723:EDO:H22	18:A:1009:HOH:O	2.16	0.45
1:B:92:ILE:CD1	1:B:92:ILE:N	2.80	0.45
1:C:580:TRP:O	1:C:584:GLN:HG2	2.17	0.45
1:B:611:ILE:O	1:B:612:ASP:HB2	2.15	0.45
1:B:235:ARG:HH11	16:B:726:PG4:C6	2.30	0.44
1:A:541:ARG:HG2	1:A:545:ARG:HD2	1.99	0.44
1:A:570:LEU:C	1:A:570:LEU:HD23	2.43	0.44
1:B:274:LYS:HB3	1:B:275:PRO:CD	2.48	0.44
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.98	0.43
11:C:713:PEG:H31	18:C:1234:HOH:O	2.16	0.43
1:C:495:VAL:O	1:C:495:VAL:HG12	2.18	0.43
1:C:46:ILE:HG22	11:C:714:PEG:H31	1.99	0.43
1:B:73:LYS:HG3	18:B:1097:HOH:O	2.18	0.43
1:D:210:ASP:OD2	18:D:801:HOH:O	2.22	0.43
1:A:524:PRO:HB3	12:A:719:EDO:H12	2.00	0.43
1:D:380:ARG:O	1:D:381[A]:ARG:HD2	2.19	0.42
4:P:3:FUC:O4	4:P:3:FUC:C1	2.66	0.42
1:B:235:ARG:HH11	16:B:726:PG4:H62	1.83	0.42
1:B:92:ILE:N	1:B:92:ILE:HD12	2.34	0.42
1:A:233:LEU:HD23	1:A:267[B]:MET:HE1	2.00	0.42
1:A:390:ALA:O	1:A:394:VAL:HG23	2.20	0.41
1:A:500:ARG:HH12	12:A:723:EDO:C1	2.32	0.41
1:D:495:VAL:O	1:D:495:VAL:HG12	2.20	0.41
1:A:495:VAL:O	1:A:495:VAL:HG12	2.21	0.41
1:A:291:THR:HG21	14:A:726:PE3:H391	2.01	0.41
1:A:478:THR:HB	4:G:3:FUC:H63	2.02	0.41
1:A:489:LYS:O	1:A:493:PRO:HD2	2.21	0.41
1:B:157:LEU:HD11	1:B:477:VAL:HG13	2.02	0.41
1:D:389:GLU:HB2	1:D:504:SER:HB2	2.03	0.41
1:D:292:HIS:HD2	18:D:1316:HOH:O	2.04	0.41
1:D:323:ALA:C	1:D:325:GLY:H	2.29	0.41
14:A:726:PE3:H271	14:A:726:PE3:H382	2.02	0.40
1:C:389:GLU:HB2	1:C:504:SER:HB2	2.02	0.40
1:A:102:ASN:HB3	1:A:188:GLN:HG3	2.02	0.40
1:B:268:VAL:HG23	1:B:426:LEU:HD11	2.02	0.40
1:A:207:PHE:HB3	11:A:716:PEG:H12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	612/629 (97%)	603 (98%)	9 (2%)	0	100	100
1	B	613/629 (98%)	605 (99%)	8 (1%)	0	100	100
1	C	611/629 (97%)	603 (99%)	8 (1%)	0	100	100
1	D	624/629 (99%)	615 (99%)	9 (1%)	0	100	100
All	All	2460/2516 (98%)	2426 (99%)	34 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	531/541 (98%)	526 (99%)	5 (1%)	70	60
1	B	532/541 (98%)	525 (99%)	7 (1%)	61	46
1	C	530/541 (98%)	525 (99%)	5 (1%)	70	60
1	D	542/541 (100%)	539 (99%)	3 (1%)	78	71
All	All	2135/2164 (99%)	2115 (99%)	20 (1%)	68	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	368	TYR

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Mol	Chain	Res	Type
1	A	372	TYR
1	A	388	HIS
1	A	421	ASP
1	B	90	ARG
1	B	92	ILE
1	B	273	ASP
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	591	VAL
1	C	188	GLN
1	C	368	TYR
1	C	372	TYR
1	C	381	ARG
1	C	388	HIS
1	D	368	TYR
1	D	372	TYR
1	D	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	371	GLN
1	B	371	GLN
1	C	224	ASN
1	C	585	ASN
1	D	224	ASN
1	D	585	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 ⓘ

38 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	0.41	0	17,19,21	0.60	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	F	1	1,3	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	F	2	3	14,14,15	0.29	0	17,19,21	0.41	0
3	BMA	F	3	3	11,11,12	0.53	0	15,15,17	0.73	0
3	FUC	F	4	3	10,10,11	0.77	0	14,14,16	0.76	0
4	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	0.93	1 (5%)
4	NAG	G	2	4	14,14,15	0.40	0	17,19,21	1.09	2 (11%)
4	FUC	G	3	4	10,10,11	0.95	0	14,14,16	1.44	2 (14%)
2	NAG	H	1	1,2	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
2	NAG	H	2	2	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	I	1	1,3	14,14,15	0.58	0	17,19,21	0.69	0
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.37	0
3	BMA	I	3	3	11,11,12	0.71	0	15,15,17	0.68	0
3	FUC	I	4	3	10,10,11	0.64	0	14,14,16	0.73	0
4	NAG	J	1	1,4	14,14,15	0.49	0	17,19,21	0.59	0
4	NAG	J	2	4	14,14,15	0.35	0	17,19,21	0.41	0
4	FUC	J	3	4	10,10,11	0.90	0	14,14,16	0.88	0
2	NAG	K	1	1,2	14,14,15	0.32	0	17,19,21	0.57	0
2	NAG	K	2	2	14,14,15	0.31	0	17,19,21	0.51	0
5	NAG	L	1	1,5	14,14,15	0.16	0	17,19,21	0.51	0
5	NAG	L	2	5	14,14,15	0.39	0	17,19,21	0.59	0
5	BMA	L	3	5	11,11,12	0.70	0	15,15,17	0.89	1 (6%)
4	NAG	M	1	1,4	14,14,15	0.25	0	17,19,21	0.72	0
4	NAG	M	2	4	14,14,15	0.34	0	17,19,21	0.41	0
4	FUC	M	3	4	10,10,11	1.08	1 (10%)	14,14,16	1.22	1 (7%)
5	NAG	N	1	1,5	14,14,15	0.36	0	17,19,21	0.71	0
5	NAG	N	2	5	14,14,15	0.31	0	17,19,21	0.49	0
5	BMA	N	3	5	11,11,12	0.63	0	15,15,17	0.67	0
6	NAG	O	1	1,6	14,14,15	0.66	0	17,19,21	0.82	0
6	NAG	O	2	6	14,14,15	0.47	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	O	3	6	11,11,12	0.77	0	15,15,17	0.85	0
6	MAN	O	4	6	11,11,12	1.03	1 (9%)	15,15,17	1.17	2 (13%)
6	MAN	O	5	6	11,11,12	0.88	1 (9%)	15,15,17	0.90	1 (6%)
6	FUC	O	6	6	10,10,11	0.90	0	14,14,16	0.63	0
4	NAG	P	1	1,4	14,14,15	0.37	0	17,19,21	0.78	0
4	NAG	P	2	4	14,14,15	0.52	0	17,19,21	0.42	0
4	FUC	P	3	4	10,10,11	1.43	1 (10%)	14,14,16	0.95	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	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	-	2/2/19/22	0/1/1/1
3	FUC	I	4	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	M	3	4	-	-	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	BMA	N	3	5	-	1/2/19/22	0/1/1/1
6	NAG	O	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	1/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
6	FUC	O	6	6	-	-	0/1/1/1
4	NAG	P	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	FUC	P	3	4	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	3	FUC	C1-C2	4.02	1.61	1.52
6	O	4	MAN	C1-C2	2.63	1.58	1.52
6	O	5	MAN	O5-C1	-2.08	1.40	1.43
4	M	3	FUC	O5-C1	-2.01	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C2-N2-C7	3.51	127.60	122.90
4	G	3	FUC	O5-C5-C4	3.23	115.36	109.55
6	O	4	MAN	C1-O5-C5	2.79	115.93	112.19
5	L	3	BMA	C1-O5-C5	2.43	115.44	112.19
4	P	3	FUC	O2-C2-C1	2.39	114.70	109.22
4	G	3	FUC	O2-C2-C1	2.38	114.66	109.22
4	G	1	NAG	C1-O5-C5	2.34	115.33	112.19
6	O	4	MAN	O2-C2-C3	-2.33	105.33	110.15
4	M	3	FUC	O2-C2-C1	2.17	114.20	109.22
2	H	1	NAG	C1-O5-C5	2.08	114.97	112.19
6	O	5	MAN	O2-C2-C3	-2.07	105.86	110.15
4	G	2	NAG	C1-C2-N2	2.03	113.64	110.43

There are no chirality outliers.

All (47) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
4	M	1	NAG	C3-C2-N2-C7

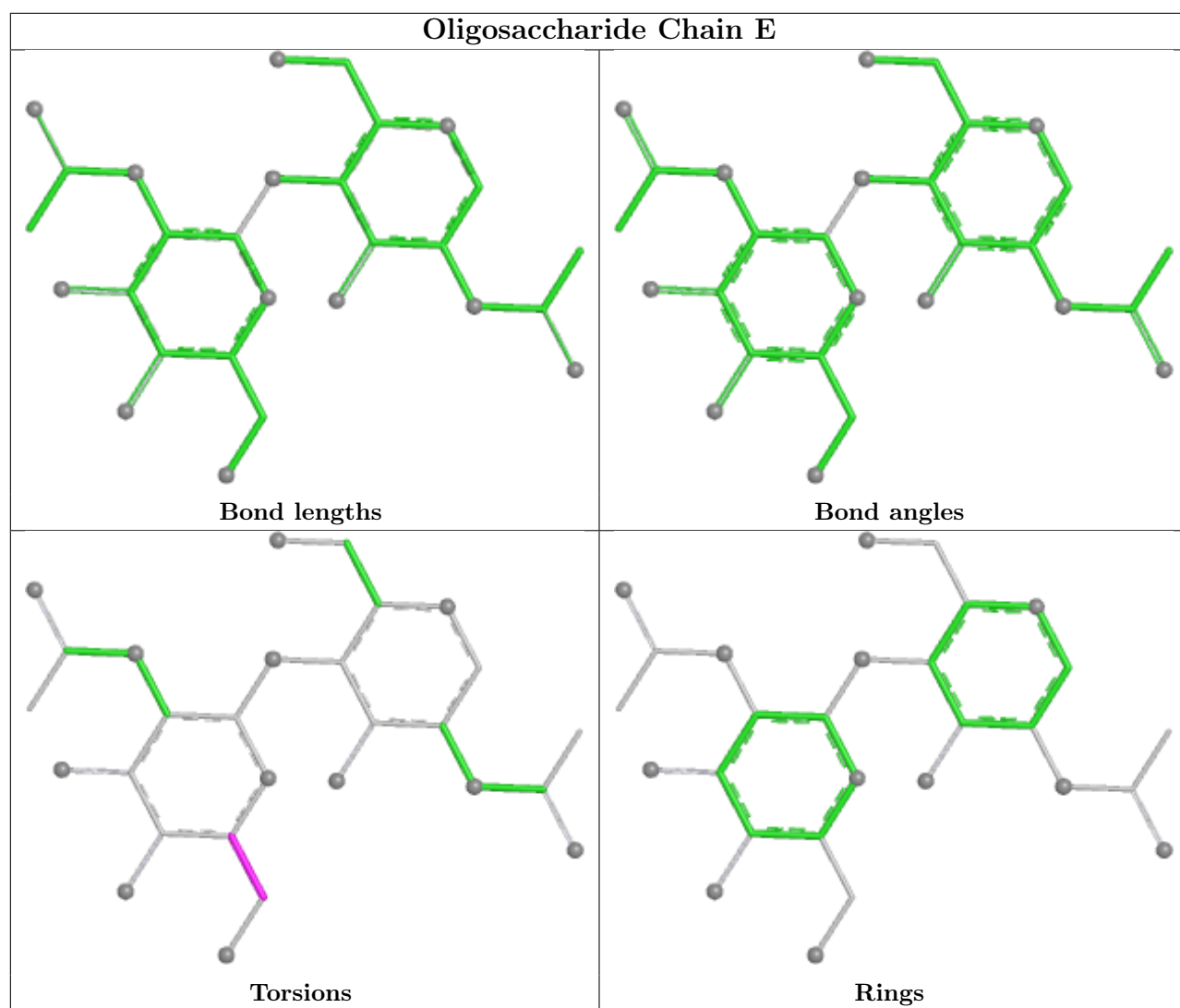
All (1) ring outliers are listed below:

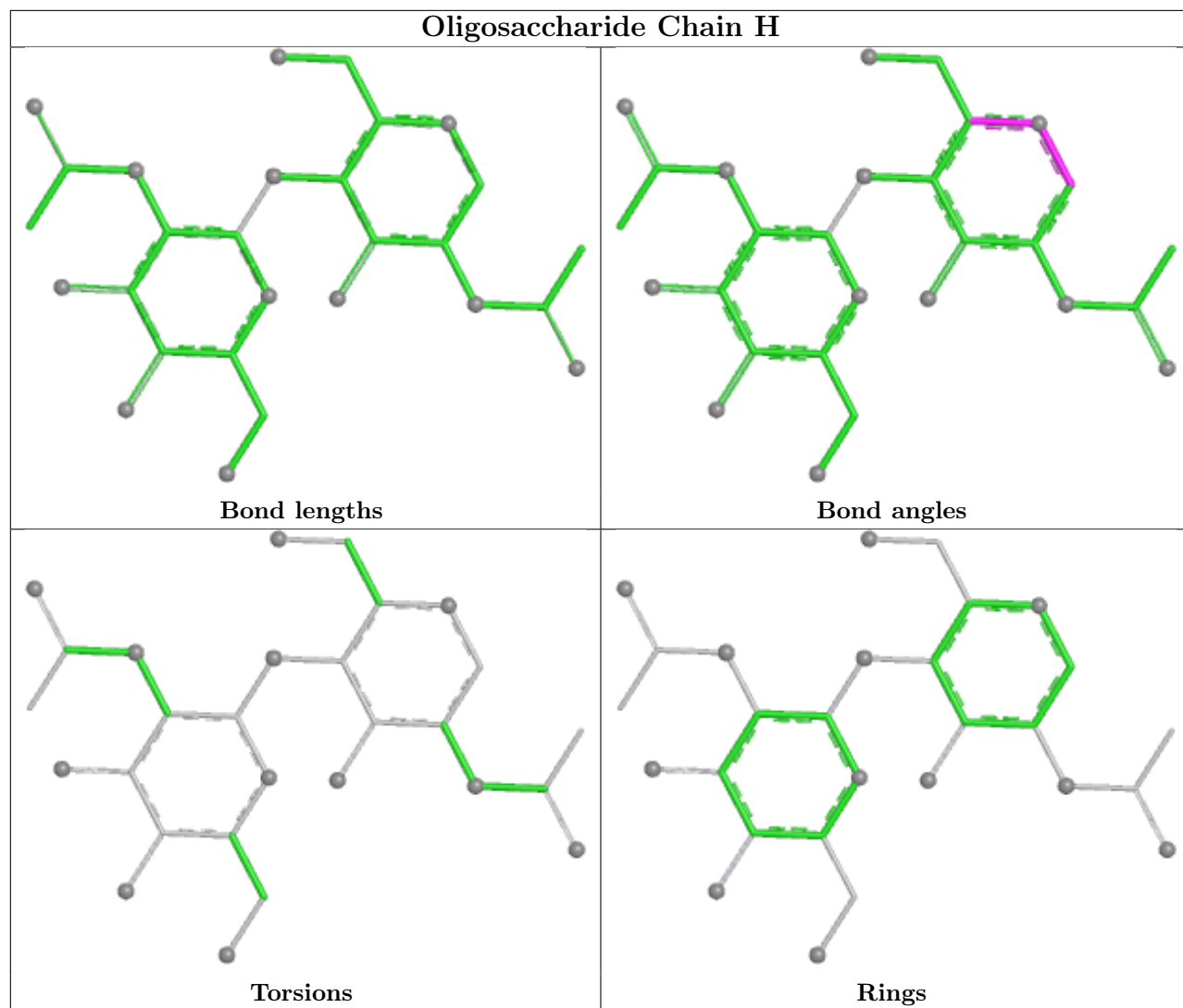
Mol	Chain	Res	Type	Atoms
6	O	4	MAN	C1-C2-C3-C4-C5-O5

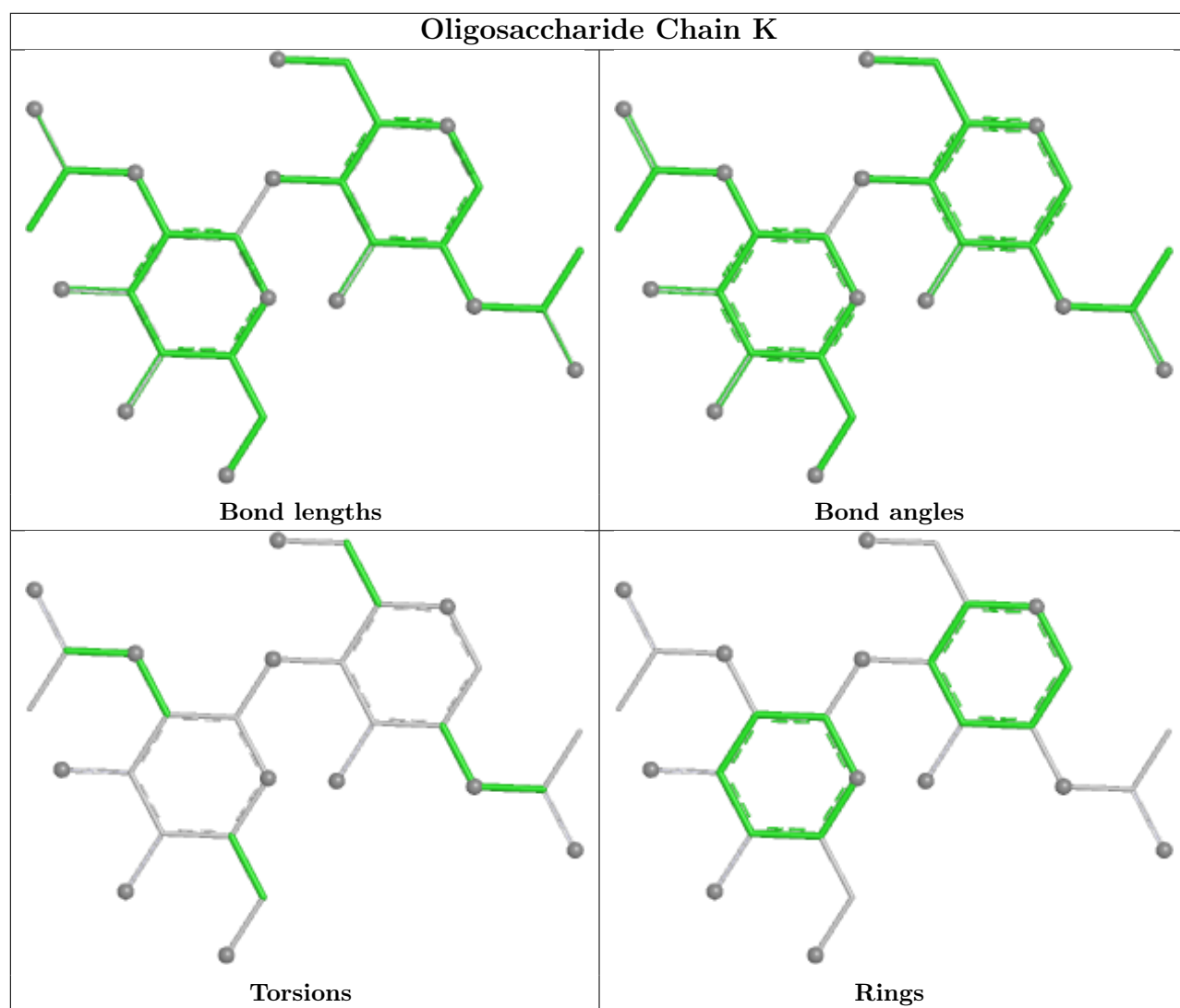
6 monomers are involved in 6 short contacts:

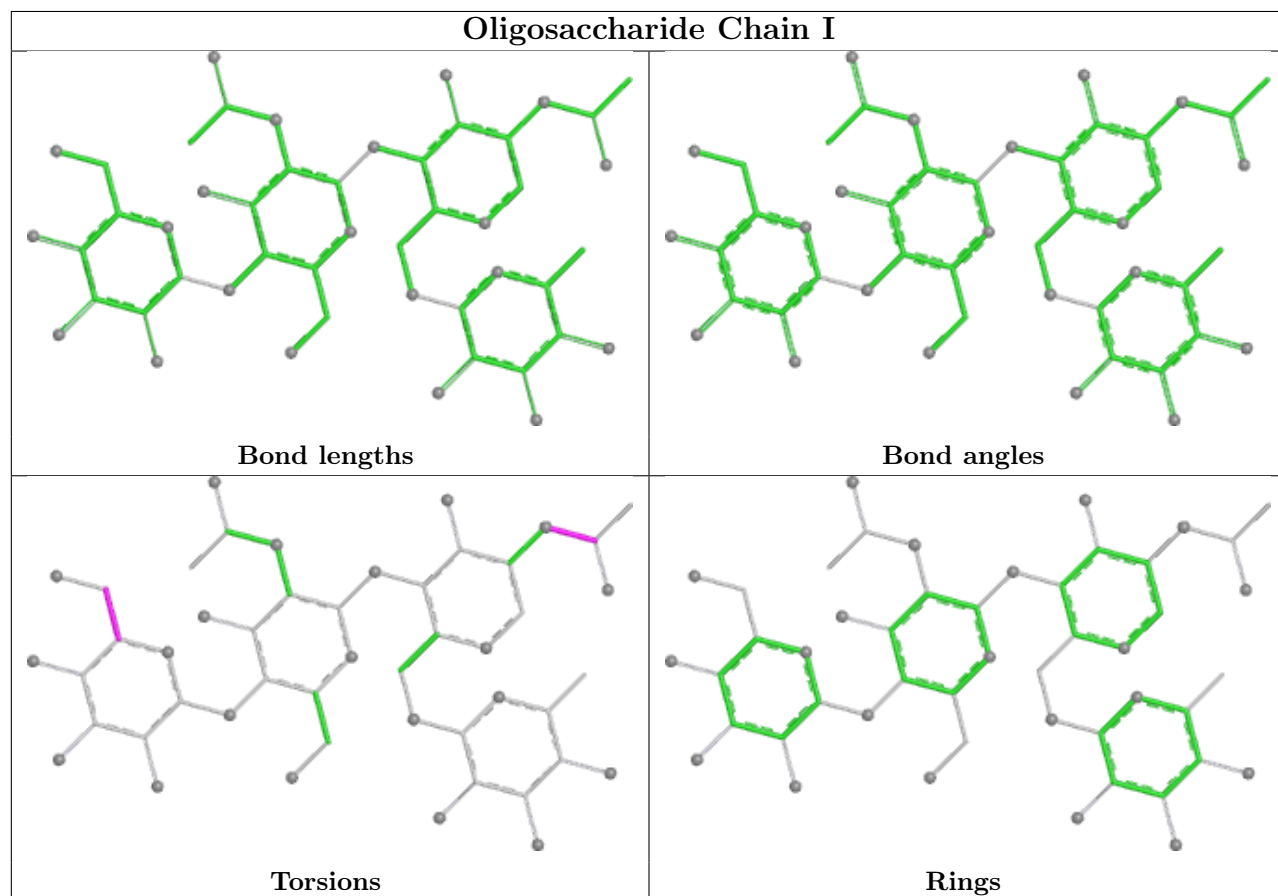
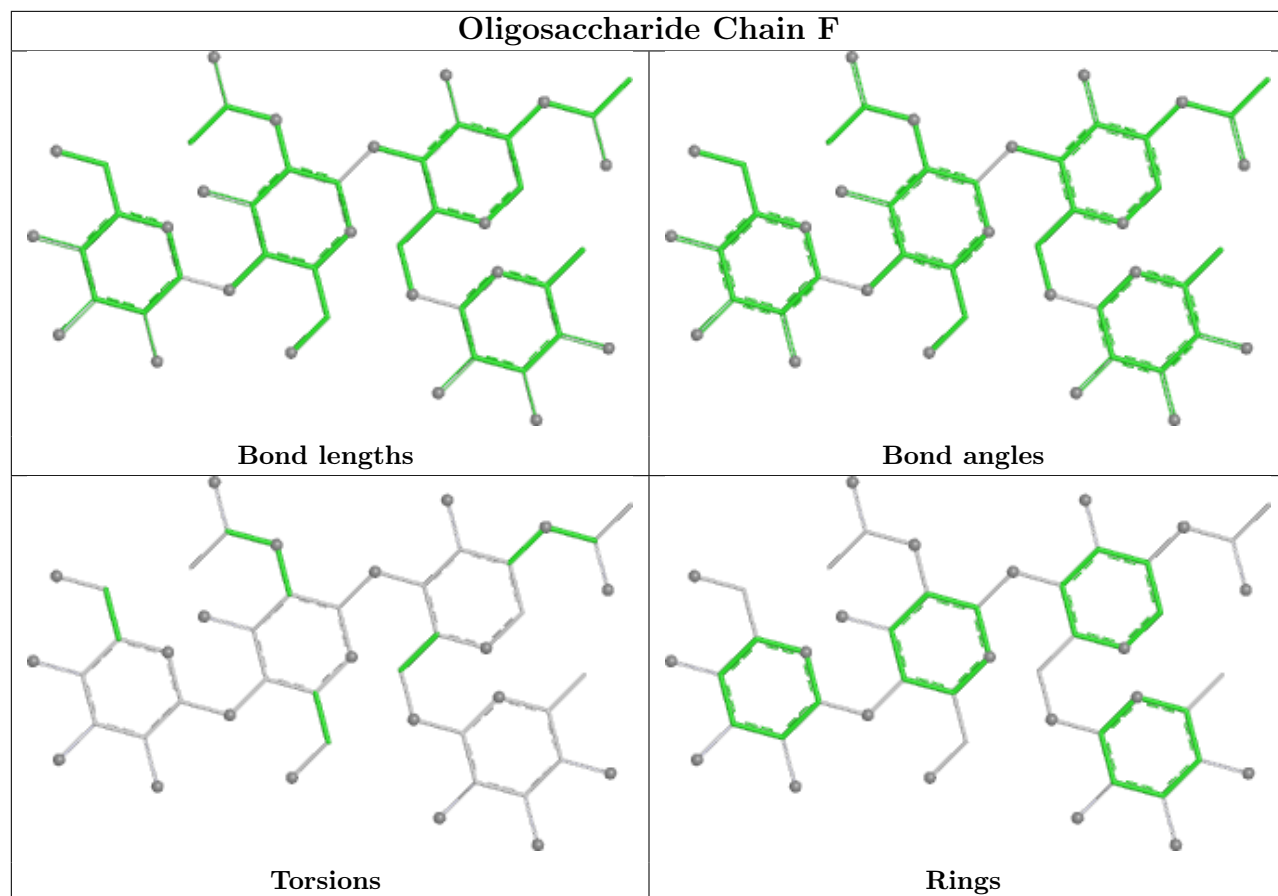
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3	FUC	2	0
4	G	2	NAG	1	0
4	G	1	NAG	1	0
4	P	1	NAG	1	0
3	F	4	FUC	1	0
4	P	3	FUC	2	0

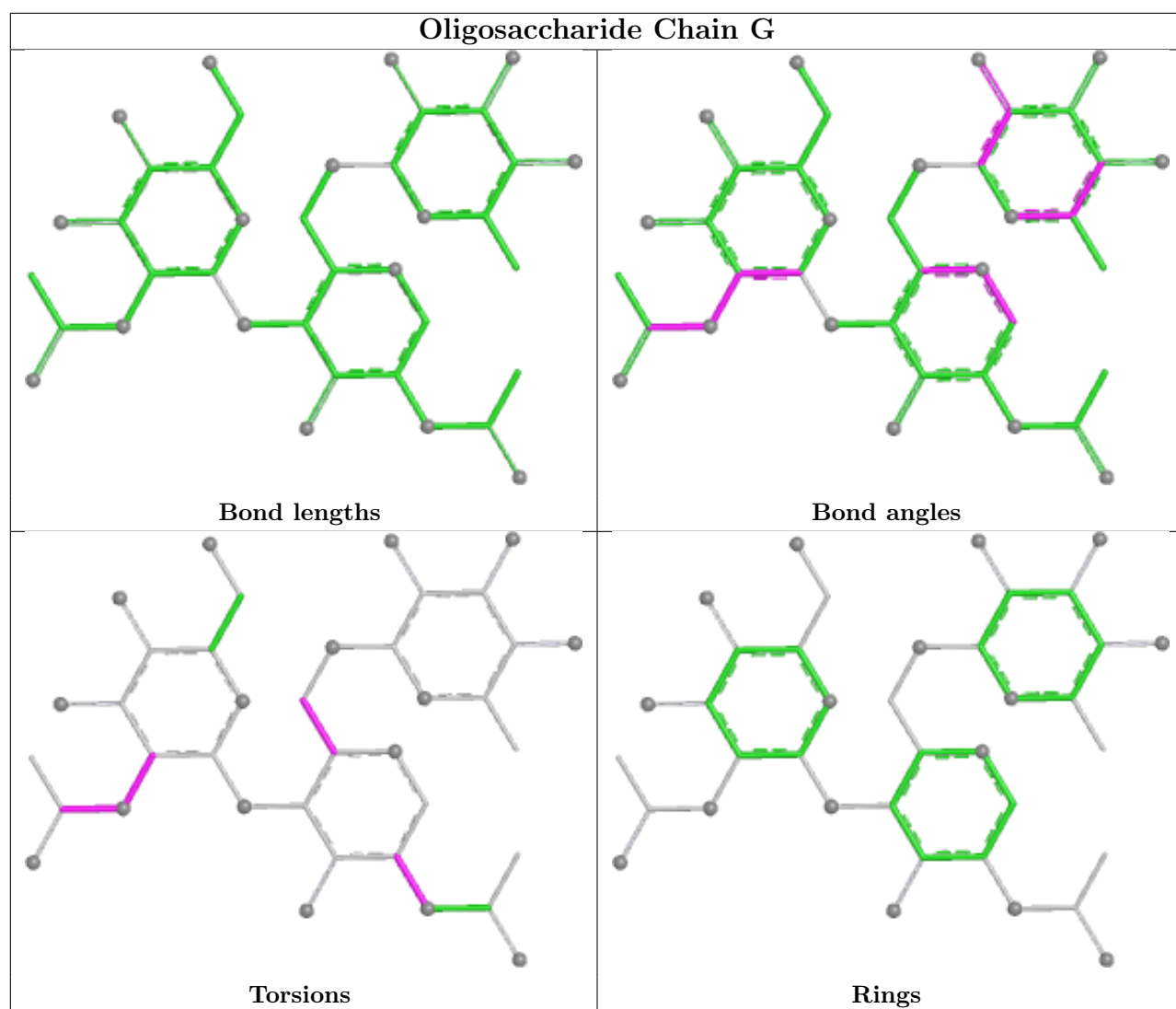
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

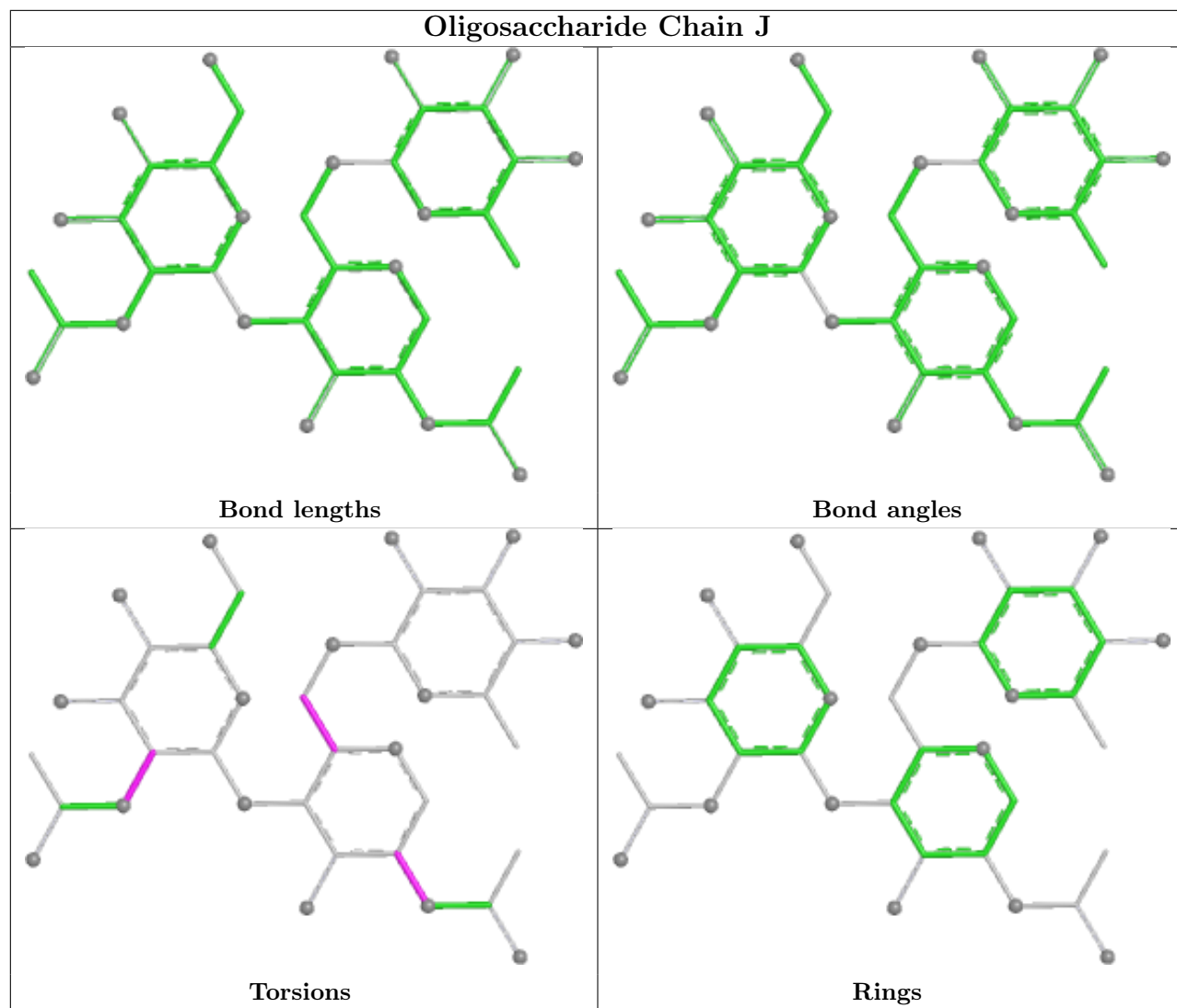


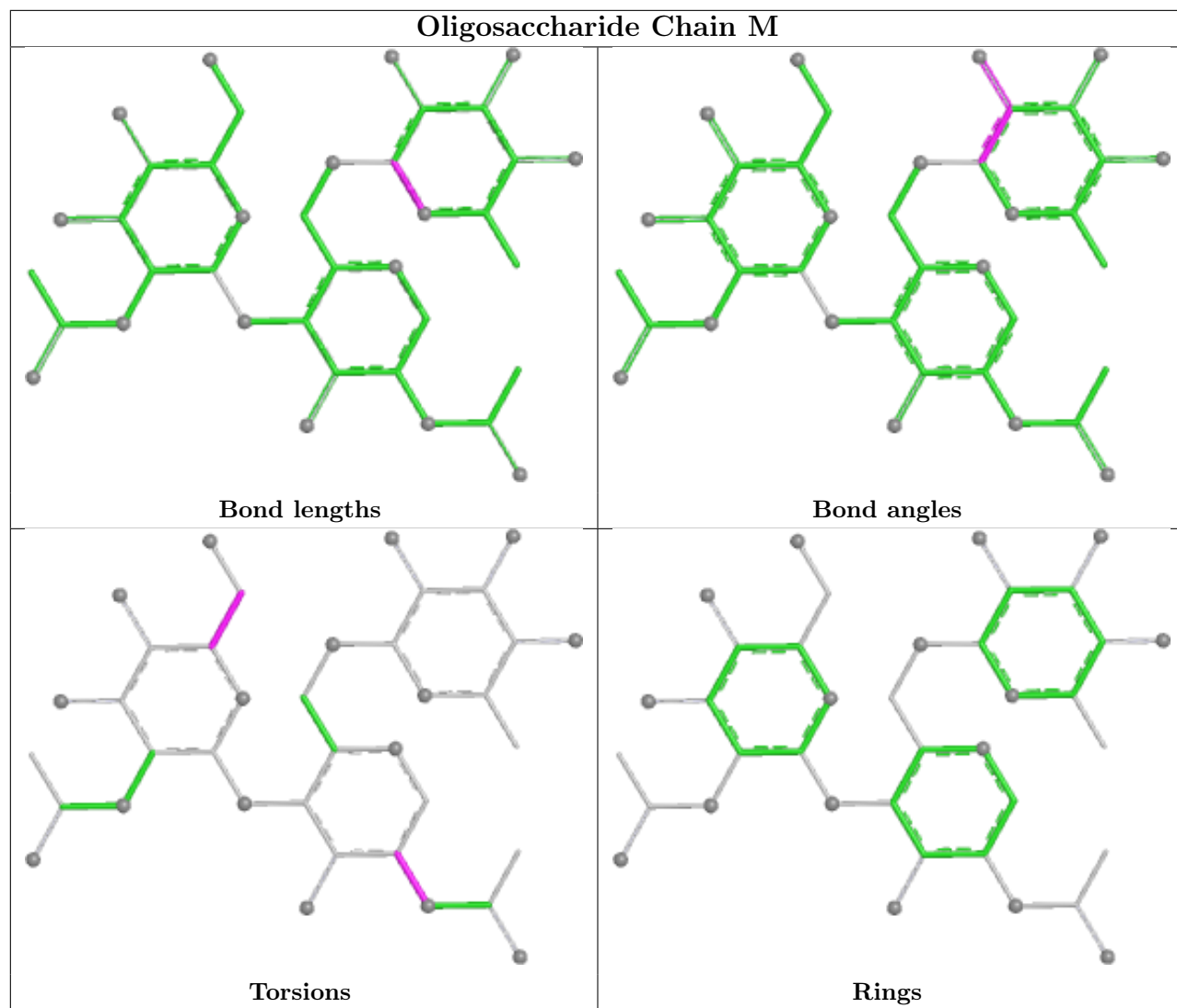


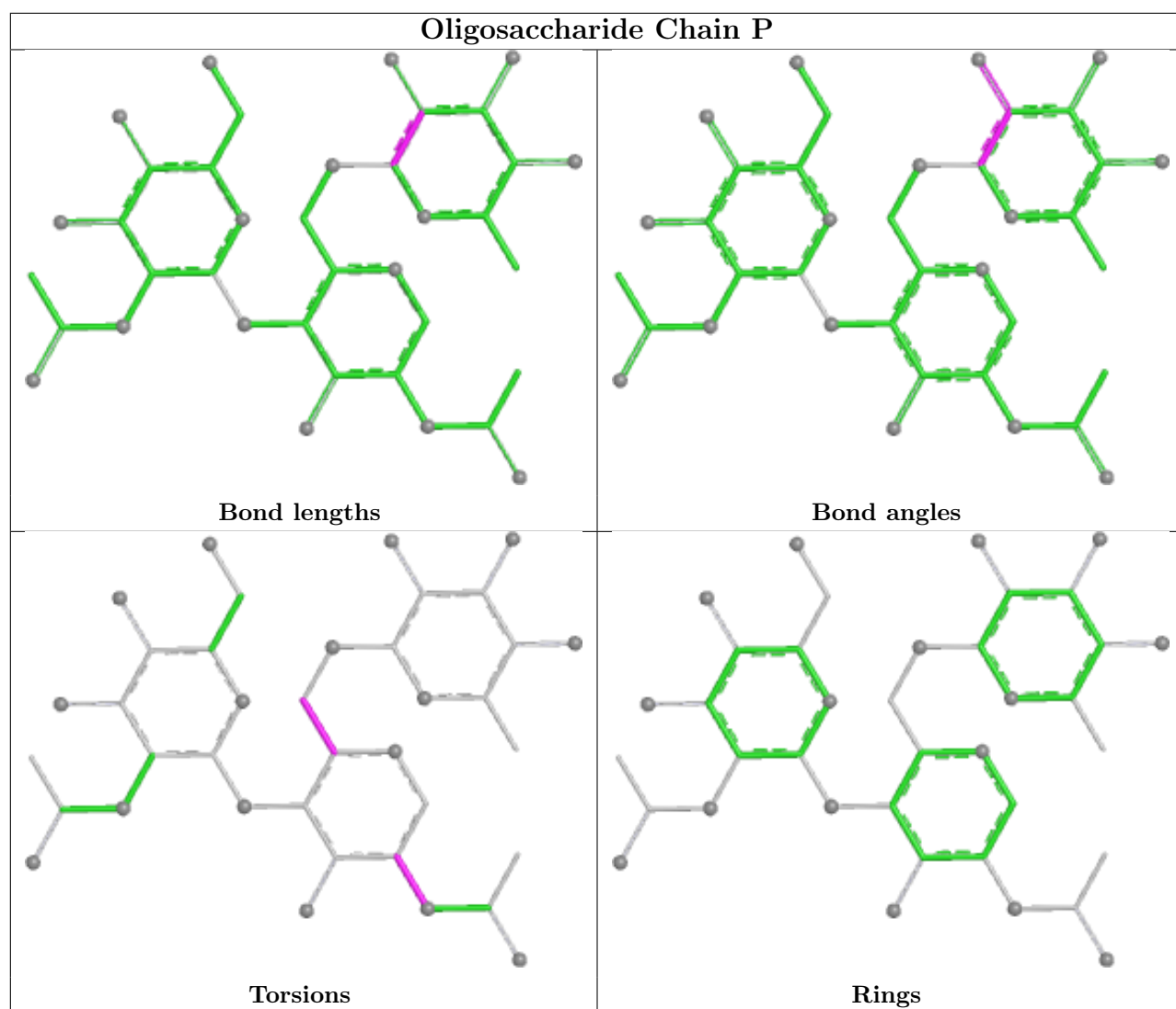


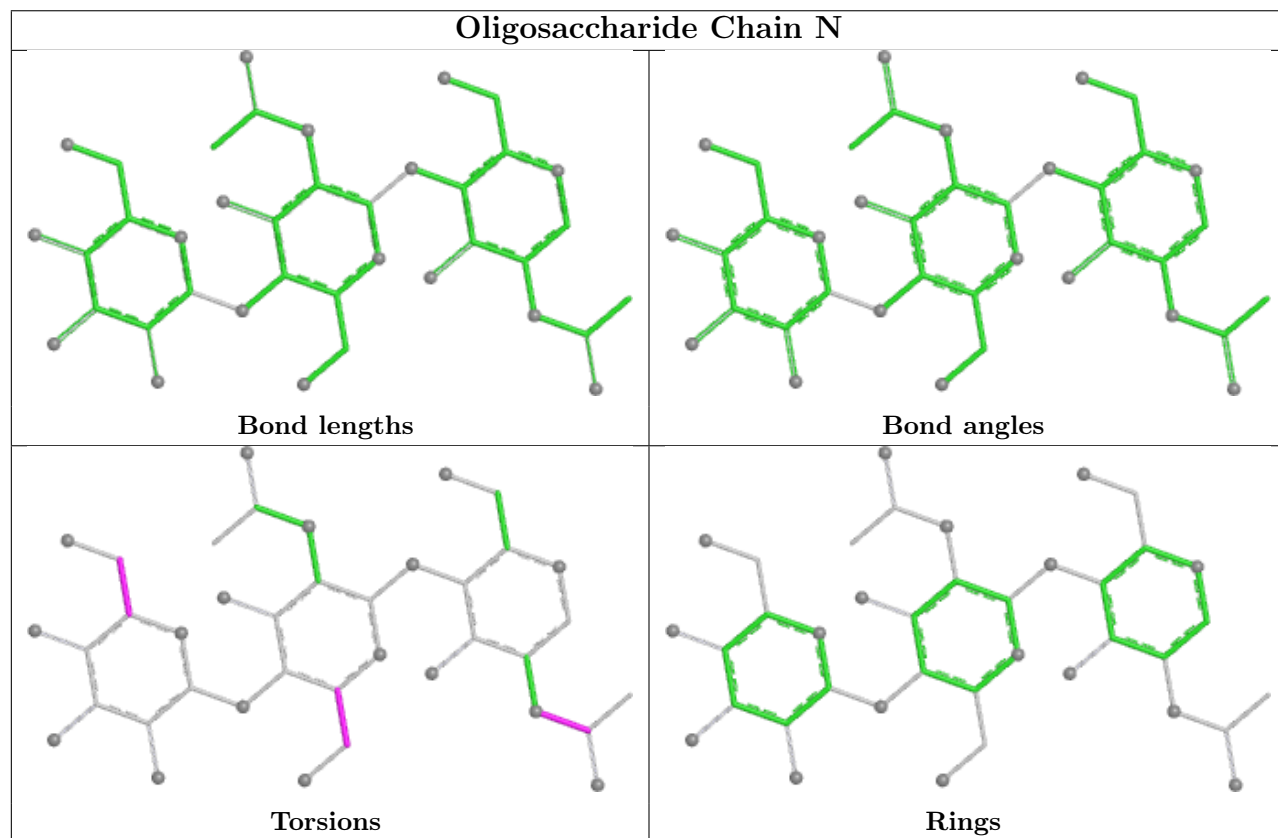
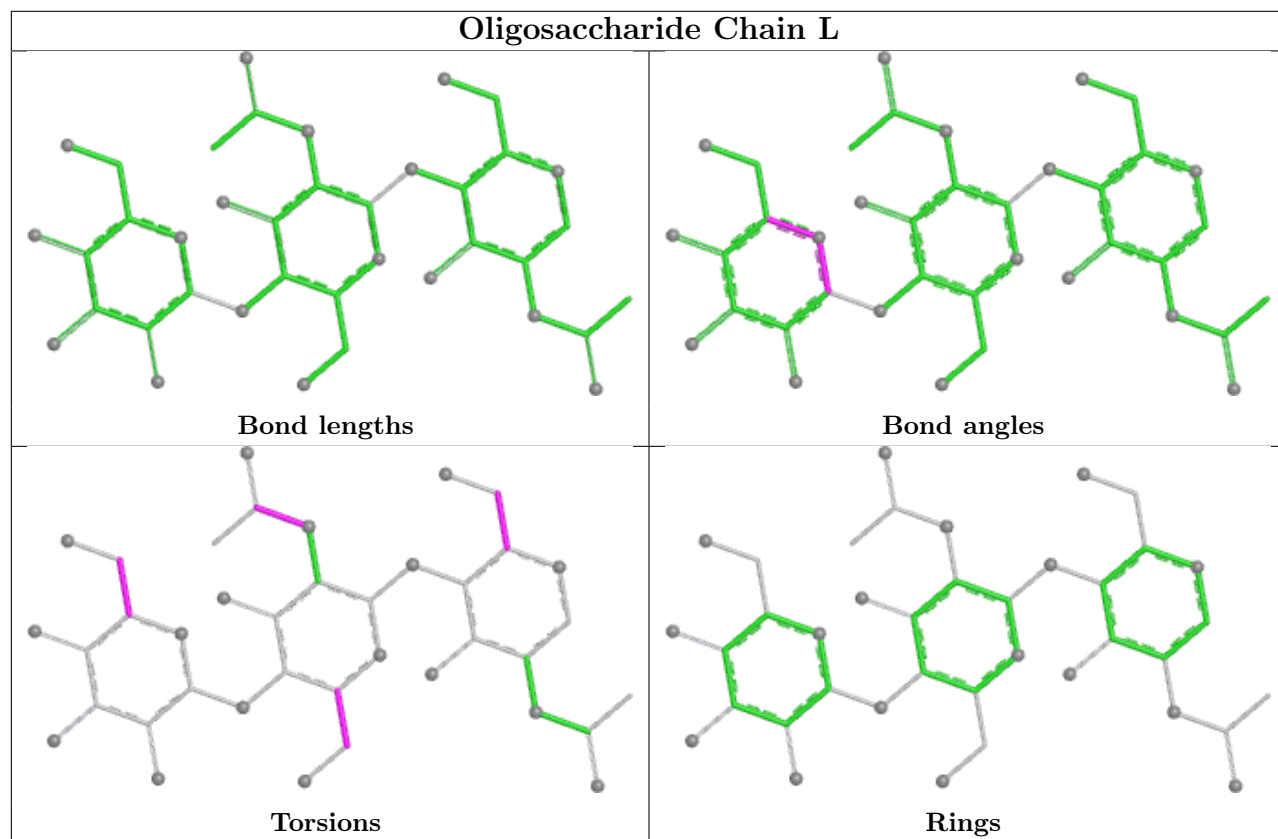


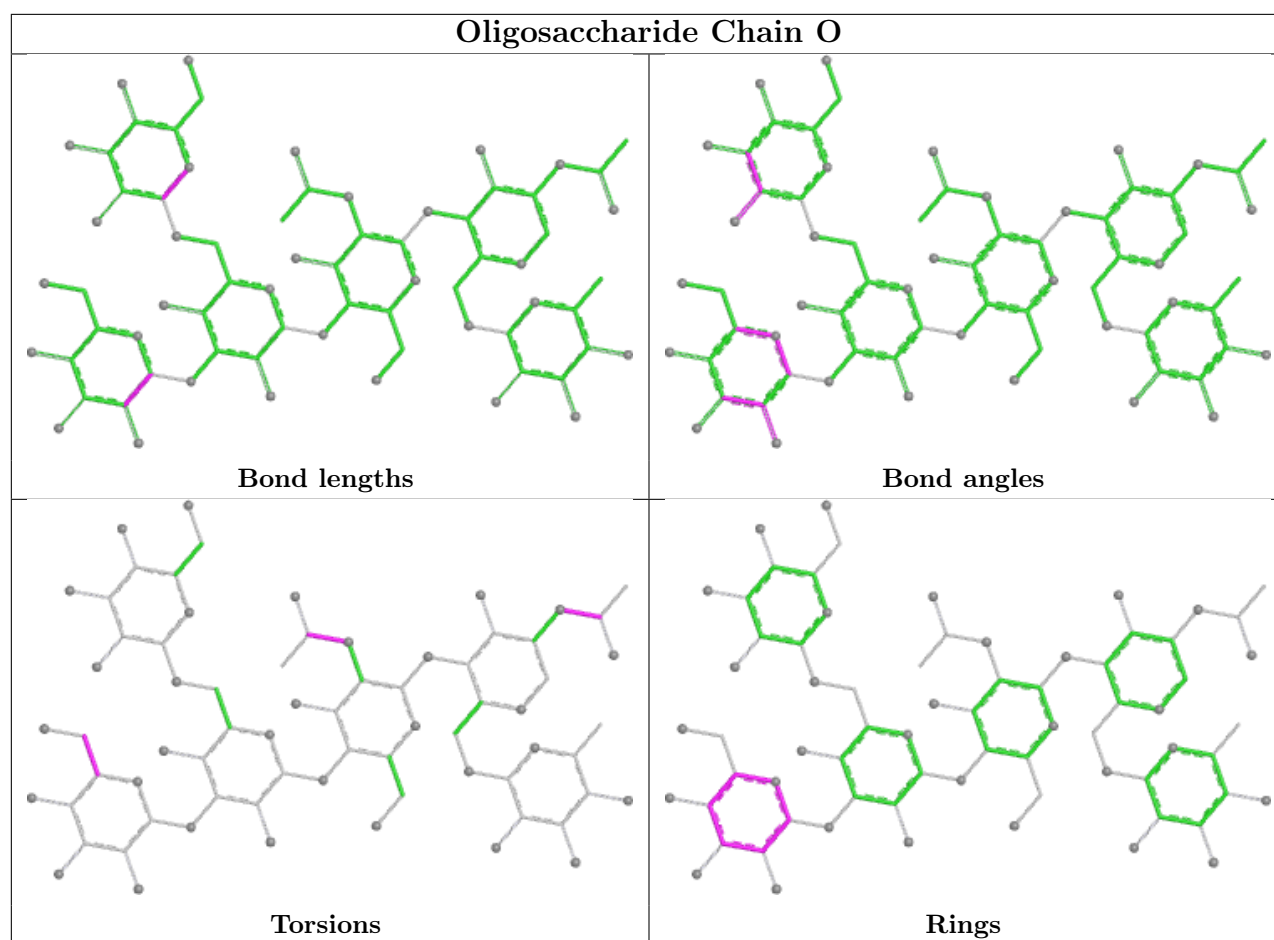












5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 12 are monoatomic - leaving 51 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
8	BJ2	A	702	7	31,31,31	3.63	12 (38%)	37,44,44	1.50	5 (13%)
13	ACT	D	723	-	3,3,3	1.29	0	3,3,3	1.40	0
11	PEG	B	714	-	6,6,6	0.48	0	5,5,5	0.35	0
15	PGE	B	725	-	9,9,9	0.32	0	8,8,8	0.31	0
8	BJ2	B	702	7	31,31,31	3.58	10 (32%)	37,44,44	1.39	5 (13%)
12	EDO	A	721	-	3,3,3	0.46	0	2,2,2	0.46	0
12	EDO	C	721	-	3,3,3	0.47	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PEG	B	716	-	6,6,6	0.50	0	5,5,5	0.32	0
13	ACT	D	722	-	3,3,3	0.92	0	3,3,3	1.77	2 (66%)
12	EDO	B	720	-	3,3,3	0.51	0	2,2,2	0.30	0
11	PEG	B	715	-	6,6,6	0.50	0	5,5,5	0.31	0
12	EDO	D	719	-	3,3,3	0.49	0	2,2,2	0.25	0
11	PEG	B	718	-	6,6,6	0.47	0	5,5,5	0.40	0
8	BJ2	D	702	7	31,31,31	3.55	14 (45%)	37,44,44	1.45	7 (18%)
12	EDO	B	719	-	3,3,3	0.48	0	2,2,2	0.27	0
16	PG4	C	724[B]	-	12,12,12	0.53	0	11,11,11	0.32	0
13	ACT	C	723	-	3,3,3	1.34	0	3,3,3	1.48	0
12	EDO	B	721	-	3,3,3	0.43	0	2,2,2	0.34	0
12	EDO	A	722	-	3,3,3	0.44	0	2,2,2	0.32	0
12	EDO	B	722	-	3,3,3	0.42	0	2,2,2	0.37	0
12	EDO	D	720	-	3,3,3	0.47	0	2,2,2	0.34	0
12	EDO	A	718	-	3,3,3	0.45	0	2,2,2	0.38	0
11	PEG	C	714	-	6,6,6	0.48	0	5,5,5	0.32	0
13	ACT	B	724	-	3,3,3	1.50	1 (33%)	3,3,3	1.43	0
12	EDO	A	723	-	3,3,3	0.40	0	2,2,2	0.24	0
11	PEG	D	718	-	6,6,6	0.44	0	5,5,5	0.29	0
12	EDO	C	719	-	3,3,3	0.46	0	2,2,2	0.31	0
16	PG4	B	726	-	12,12,12	0.60	0	11,11,11	0.55	0
12	EDO	C	715	-	3,3,3	0.45	0	2,2,2	0.30	0
17	XPE	D	724	-	30,30,30	0.55	0	29,29,29	0.51	0
12	EDO	A	720	-	3,3,3	0.45	0	2,2,2	0.12	0
12	EDO	C	720	-	3,3,3	0.41	0	2,2,2	0.45	0
14	PE3	A	726	-	42,42,42	0.56	0	41,41,41	0.47	0
16	PG4	C	724[A]	-	12,12,12	0.53	0	11,11,11	0.38	0
13	ACT	A	725	-	3,3,3	1.44	1 (33%)	3,3,3	1.42	0
8	BJ2	C	702	7	31,31,31	3.77	12 (38%)	37,44,44	1.42	7 (18%)
11	PEG	A	714	-	6,6,6	0.50	0	5,5,5	0.28	0
12	EDO	C	717	-	3,3,3	0.47	0	2,2,2	0.29	0
11	PEG	D	717	-	6,6,6	0.47	0	5,5,5	0.25	0
12	EDO	D	721	-	3,3,3	0.38	0	2,2,2	0.41	0
12	EDO	A	717	-	3,3,3	0.54	0	2,2,2	0.25	0
11	PEG	B	717	-	6,6,6	0.49	0	5,5,5	0.49	0
12	EDO	C	716	-	3,3,3	0.48	0	2,2,2	0.20	0
12	EDO	B	723	-	3,3,3	0.44	0	2,2,2	0.35	0
11	PEG	C	713	-	6,6,6	0.49	0	5,5,5	0.54	0
13	ACT	A	724	-	3,3,3	1.63	1 (33%)	3,3,3	1.38	0
12	EDO	C	722	-	3,3,3	0.48	0	2,2,2	0.05	0
12	EDO	C	718	-	3,3,3	0.50	0	2,2,2	0.29	0
11	PEG	A	716	-	6,6,6	0.41	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	EDO	A	719	-	3,3,3	0.52	0	2,2,2	0.24	0
11	PEG	A	715	-	6,6,6	0.47	0	5,5,5	0.35	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
8	BJ2	A	702	7	-	7/36/56/56	0/2/2/2
11	PEG	B	714	-	-	1/4/4/4	-
15	PGE	B	725	-	-	4/7/7/7	-
8	BJ2	B	702	7	-	7/36/56/56	0/2/2/2
12	EDO	A	721	-	-	0/1/1/1	-
12	EDO	C	721	-	-	0/1/1/1	-
11	PEG	B	716	-	-	0/4/4/4	-
12	EDO	B	720	-	-	1/1/1/1	-
11	PEG	B	715	-	-	2/4/4/4	-
12	EDO	D	719	-	-	1/1/1/1	-
11	PEG	B	718	-	-	1/4/4/4	-
8	BJ2	D	702	7	-	7/36/56/56	0/2/2/2
12	EDO	B	719	-	-	1/1/1/1	-
16	PG4	C	724[B]	-	-	6/10/10/10	-
12	EDO	B	721	-	-	0/1/1/1	-
12	EDO	A	722	-	-	0/1/1/1	-
12	EDO	B	722	-	-	1/1/1/1	-
12	EDO	D	720	-	-	1/1/1/1	-
12	EDO	A	718	-	-	0/1/1/1	-
11	PEG	C	714	-	-	1/4/4/4	-
12	EDO	A	723	-	-	0/1/1/1	-
11	PEG	D	718	-	-	3/4/4/4	-
12	EDO	C	719	-	-	0/1/1/1	-
16	PG4	B	726	-	-	4/10/10/10	-
12	EDO	C	715	-	-	1/1/1/1	-
17	XPE	D	724	-	-	14/28/28/28	-
12	EDO	A	720	-	-	1/1/1/1	-
12	EDO	C	720	-	-	0/1/1/1	-
14	PE3	A	726	-	-	22/40/40/40	-
16	PG4	C	724[A]	-	-	2/10/10/10	-
8	BJ2	C	702	7	-	7/36/56/56	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PEG	A	714	-	-	1/4/4/4	-
12	EDO	C	717	-	-	0/1/1/1	-
11	PEG	D	717	-	-	2/4/4/4	-
12	EDO	D	721	-	-	0/1/1/1	-
12	EDO	A	717	-	-	0/1/1/1	-
11	PEG	B	717	-	-	3/4/4/4	-
12	EDO	C	716	-	-	1/1/1/1	-
12	EDO	B	723	-	-	1/1/1/1	-
11	PEG	C	713	-	-	2/4/4/4	-
12	EDO	C	722	-	-	0/1/1/1	-
12	EDO	C	718	-	-	1/1/1/1	-
11	PEG	A	716	-	-	0/4/4/4	-
12	EDO	A	719	-	-	1/1/1/1	-
11	PEG	A	715	-	-	0/4/4/4	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	702	BJ2	C08-N12	9.96	1.58	1.46
8	A	702	BJ2	C08-N12	9.37	1.58	1.46
8	D	702	BJ2	C08-N12	9.21	1.58	1.46
8	B	702	BJ2	C08-N12	8.93	1.57	1.46
8	B	702	BJ2	C09-C08	-7.87	1.40	1.53
8	D	702	BJ2	C09-C08	-7.67	1.40	1.53
8	C	702	BJ2	C09-C08	-7.66	1.40	1.53
8	A	702	BJ2	C09-C08	-7.61	1.40	1.53
8	C	702	BJ2	C27-N23	7.04	1.60	1.47
8	D	702	BJ2	C27-N23	6.57	1.59	1.47
8	B	702	BJ2	C27-N23	6.49	1.59	1.47
8	A	702	BJ2	C26-C27	-6.44	1.38	1.53
8	C	702	BJ2	C26-C27	-6.30	1.38	1.53
8	B	702	BJ2	C26-C27	-6.23	1.38	1.53
8	D	702	BJ2	C24-N23	-6.21	1.35	1.47
8	A	702	BJ2	C27-N23	6.19	1.59	1.47
8	A	702	BJ2	C24-N23	-6.15	1.35	1.47
8	C	702	BJ2	C24-N23	-6.14	1.35	1.47
8	D	702	BJ2	C26-C27	-5.99	1.39	1.53
8	B	702	BJ2	C24-N23	-5.92	1.36	1.47
8	B	702	BJ2	C21-N23	5.77	1.47	1.34
8	C	702	BJ2	C21-N23	5.74	1.47	1.34
8	A	702	BJ2	C11-N12	-5.61	1.36	1.47
8	C	702	BJ2	C11-N12	-5.55	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	702	BJ2	C21-N23	5.43	1.46	1.34
8	B	702	BJ2	C11-N12	-5.28	1.37	1.47
8	A	702	BJ2	C21-N23	5.25	1.46	1.34
8	A	702	BJ2	C04-C08	4.78	1.60	1.54
8	C	702	BJ2	C04-C08	4.64	1.60	1.54
8	C	702	BJ2	C13-N12	4.50	1.44	1.34
8	D	702	BJ2	C11-N12	-4.48	1.39	1.47
8	B	702	BJ2	C04-C08	4.40	1.59	1.54
8	B	702	BJ2	C13-N12	4.27	1.44	1.34
8	A	702	BJ2	C13-N12	4.11	1.43	1.34
8	D	702	BJ2	C13-N12	3.97	1.43	1.34
8	D	702	BJ2	C04-C08	3.67	1.58	1.54
8	D	702	BJ2	C04-C05	3.15	1.57	1.52
8	C	702	BJ2	C04-C05	3.08	1.57	1.52
8	A	702	BJ2	C04-C05	2.89	1.57	1.52
8	C	702	BJ2	C04-N03	2.82	1.49	1.46
8	D	702	BJ2	C04-N03	2.58	1.49	1.46
8	B	702	BJ2	C04-C05	2.55	1.56	1.52
8	A	702	BJ2	O07-C05	2.52	1.29	1.22
13	A	724	ACT	CH3-C	2.47	1.58	1.49
8	A	702	BJ2	C04-N03	2.23	1.49	1.46
13	B	724	ACT	CH3-C	2.17	1.57	1.49
8	D	702	BJ2	C25-C24	2.16	1.59	1.51
8	D	702	BJ2	O30-C28	2.16	1.28	1.22
8	D	702	BJ2	O07-C05	2.11	1.28	1.22
13	A	725	ACT	CH3-C	2.11	1.57	1.49
8	C	702	BJ2	O07-C05	2.11	1.28	1.22

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	702	BJ2	C28-C27-N23	-4.18	104.17	112.54
8	D	702	BJ2	C28-C27-N23	-4.00	104.51	112.54
8	A	702	BJ2	C08-C04-N03	-4.00	101.90	110.02
8	C	702	BJ2	C08-C04-N03	-3.55	102.81	110.02
8	A	702	BJ2	C28-C27-N23	-3.37	105.77	112.54
8	C	702	BJ2	C28-C27-N23	-3.26	106.00	112.54
8	B	702	BJ2	C08-C04-N03	-2.93	104.06	110.02
8	D	702	BJ2	C08-C04-N03	-2.74	104.45	110.02
8	D	702	BJ2	O22-C21-C02	2.72	125.75	120.15
8	C	702	BJ2	O29-C28-O30	-2.67	118.01	124.08
8	B	702	BJ2	C26-C27-N23	2.63	106.88	103.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	702	BJ2	O29-C28-C27	2.59	121.78	113.34
8	C	702	BJ2	O29-C28-C27	2.34	120.99	113.34
8	D	702	BJ2	O29-C28-C27	2.34	120.97	113.34
8	A	702	BJ2	O29-C28-O30	-2.33	118.80	124.08
13	D	722	ACT	OXT-C-O	2.31	130.59	122.03
8	B	702	BJ2	O29-C28-C27	2.29	120.83	113.34
8	D	702	BJ2	C26-C27-N23	2.22	106.27	103.02
8	C	702	BJ2	C26-C27-N23	2.20	106.25	103.02
8	C	702	BJ2	O06-C05-C04	2.16	121.64	114.15
8	D	702	BJ2	C11-N12-C08	-2.08	108.41	111.69
8	C	702	BJ2	O06-C05-O07	-2.04	119.44	124.08
8	B	702	BJ2	O06-C05-O07	-2.03	119.47	124.08
8	D	702	BJ2	O29-C28-O30	-2.03	119.47	124.08
13	D	722	ACT	O-C-CH3	-2.02	114.26	122.53
8	A	702	BJ2	C26-C27-N23	2.01	105.97	103.02

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	702	BJ2	N03-C04-C08-C09
8	B	702	BJ2	N03-C04-C08-C09
8	C	702	BJ2	N03-C04-C08-C09
14	A	726	PE3	C42-C41-O40-C39
16	B	726	PG4	O3-C5-C6-O4
14	A	726	PE3	O37-C38-C39-O40
14	A	726	PE3	O13-C14-C15-O16
11	C	714	PEG	O2-C3-C4-O4
11	D	717	PEG	O2-C3-C4-O4
15	B	725	PGE	O1-C1-C2-O2
16	B	726	PG4	O4-C7-C8-O5
16	C	724[B]	PG4	O4-C7-C8-O5
16	C	724[B]	PG4	O2-C3-C4-O3
17	D	724	XPE	O13-C14-C15-O16
15	B	725	PGE	O2-C3-C4-O3
17	D	724	XPE	O19-C20-C21-O22
16	C	724[B]	PG4	C6-C5-O3-C4
11	B	714	PEG	O2-C3-C4-O4
11	C	713	PEG	O1-C1-C2-O2
14	A	726	PE3	O1-C2-C3-O4
16	C	724[B]	PG4	O1-C1-C2-O2
14	A	726	PE3	O22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
14	A	726	PE3	O4-C5-C6-O7
14	A	726	PE3	O34-C35-C36-O37
11	D	718	PEG	O2-C3-C4-O4
14	A	726	PE3	O40-C41-C42-O43
12	A	719	EDO	O1-C1-C2-O2
12	A	720	EDO	O1-C1-C2-O2
12	B	723	EDO	O1-C1-C2-O2
16	B	726	PG4	C8-C7-O4-C6
11	B	715	PEG	O1-C1-C2-O2
12	B	722	EDO	O1-C1-C2-O2
12	C	718	EDO	O1-C1-C2-O2
11	D	717	PEG	O1-C1-C2-O2
8	A	702	BJ2	N03-C04-C05-O06
8	B	702	BJ2	N03-C04-C05-O06
8	D	702	BJ2	N03-C04-C05-O06
14	A	726	PE3	O7-C8-C9-O10
14	A	726	PE3	C23-C24-O25-C26
14	A	726	PE3	C14-C15-O16-C17
14	A	726	PE3	C39-C38-O37-C36
14	A	726	PE3	C11-C12-O13-C14
11	B	717	PEG	C1-C2-O2-C3
17	D	724	XPE	C12-C11-O10-C9
11	B	717	PEG	C4-C3-O2-C2
17	D	724	XPE	C17-C18-O19-C20
17	D	724	XPE	C11-C12-O13-C14
17	D	724	XPE	C23-C24-O25-C26
16	C	724[B]	PG4	C4-C3-O2-C2
14	A	726	PE3	C35-C36-O37-C38
11	D	718	PEG	O1-C1-C2-O2
17	D	724	XPE	O28-C29-C30-O31
14	A	726	PE3	C26-C27-O28-C29
11	B	718	PEG	C1-C2-O2-C3
8	A	702	BJ2	C05-C04-C08-C09
8	B	702	BJ2	C05-C04-C08-C09
8	C	702	BJ2	C05-C04-C08-C09
8	D	702	BJ2	C05-C04-C08-C09
17	D	724	XPE	C2-C3-O4-C5
16	C	724[A]	PG4	O3-C5-C6-O4
11	B	715	PEG	C1-C2-O2-C3
14	A	726	PE3	C36-C35-O34-C33
16	C	724[A]	PG4	O2-C3-C4-O3
14	A	726	PE3	O16-C17-C18-O19

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Mol	Chain	Res	Type	Atoms
16	B	726	PG4	C6-C5-O3-C4
15	B	725	PGE	C3-C4-O3-C5
8	D	702	BJ2	N03-C04-C08-C09
12	D	720	EDO	O1-C1-C2-O2
8	B	702	BJ2	C05-C04-C08-N12
8	C	702	BJ2	C05-C04-C08-N12
8	D	702	BJ2	C05-C04-C08-N12
11	D	718	PEG	C1-C2-O2-C3
17	D	724	XPE	O25-C26-C27-O28
11	C	713	PEG	C1-C2-O2-C3
14	A	726	PE3	O10-C11-C12-O13
17	D	724	XPE	C18-C17-O16-C15
12	D	719	EDO	O1-C1-C2-O2
17	D	724	XPE	C26-C27-O28-C29
15	B	725	PGE	C6-C5-O3-C4
16	C	724[B]	PG4	O3-C5-C6-O4
8	C	702	BJ2	C15-C17-C18-O19
11	B	717	PEG	O1-C1-C2-O2
14	A	726	PE3	C27-C26-O25-C24
17	D	724	XPE	C21-C20-O19-C18
12	B	719	EDO	O1-C1-C2-O2
12	B	720	EDO	O1-C1-C2-O2
17	D	724	XPE	C14-C15-O16-C17
8	A	702	BJ2	C15-C17-C18-O20
8	B	702	BJ2	N03-C04-C05-O07
14	A	726	PE3	C20-C21-O22-C23
12	C	715	EDO	O1-C1-C2-O2
14	A	726	PE3	C12-C11-O10-C9
8	A	702	BJ2	C15-C17-C18-O19
8	B	702	BJ2	C15-C17-C18-O19
8	B	702	BJ2	C15-C17-C18-O20
8	C	702	BJ2	C15-C17-C18-O20
8	D	702	BJ2	C15-C17-C18-O19
8	D	702	BJ2	C15-C17-C18-O20
11	A	714	PEG	C1-C2-O2-C3
14	A	726	PE3	O25-C26-C27-O28
12	C	716	EDO	O1-C1-C2-O2
8	A	702	BJ2	N03-C04-C05-O07
8	C	702	BJ2	N03-C04-C05-O06
8	C	702	BJ2	N03-C04-C05-O07
8	D	702	BJ2	N03-C04-C05-O07
8	A	702	BJ2	C05-C04-N03-C02

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Mol	Chain	Res	Type	Atoms
17	D	724	XPE	C15-C14-O13-C12

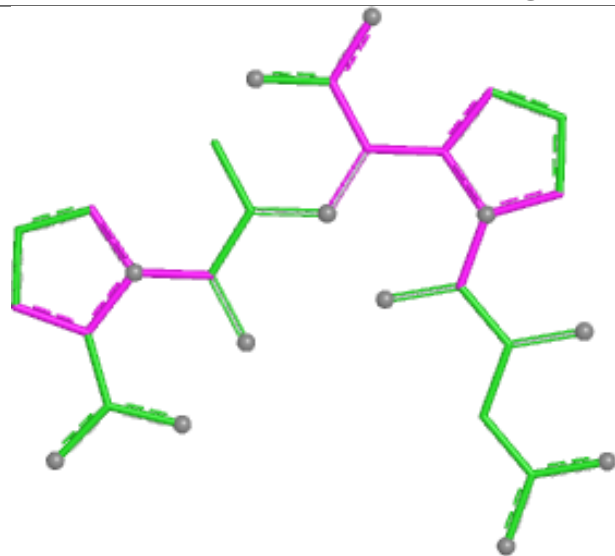
There are no ring outliers.

9 monomers are involved in 15 short contacts:

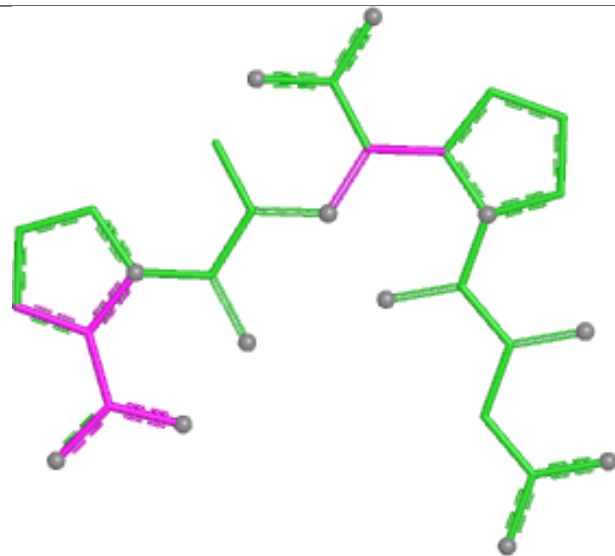
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	723	ACT	1	0
11	C	714	PEG	1	0
12	A	723	EDO	2	0
16	B	726	PG4	2	0
14	A	726	PE3	4	0
8	C	702	BJ2	1	0
11	C	713	PEG	2	0
11	A	716	PEG	2	0
12	A	719	EDO	1	0

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

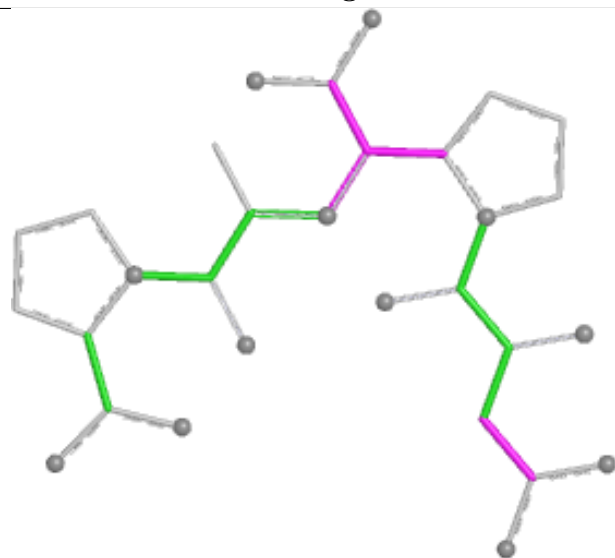
Ligand BJ2 A 702



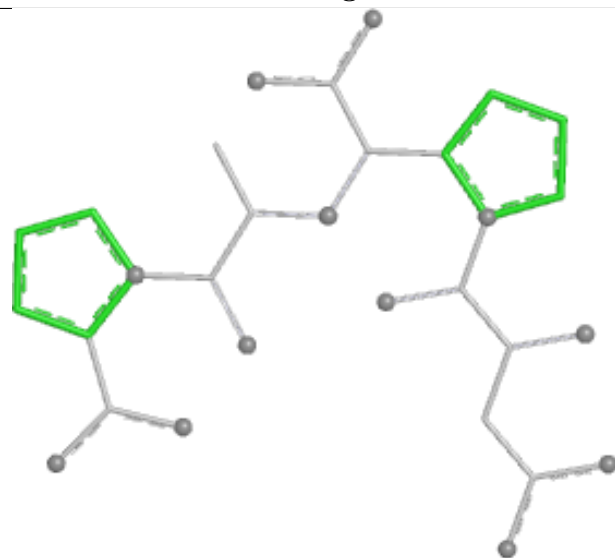
Bond lengths



Bond angles

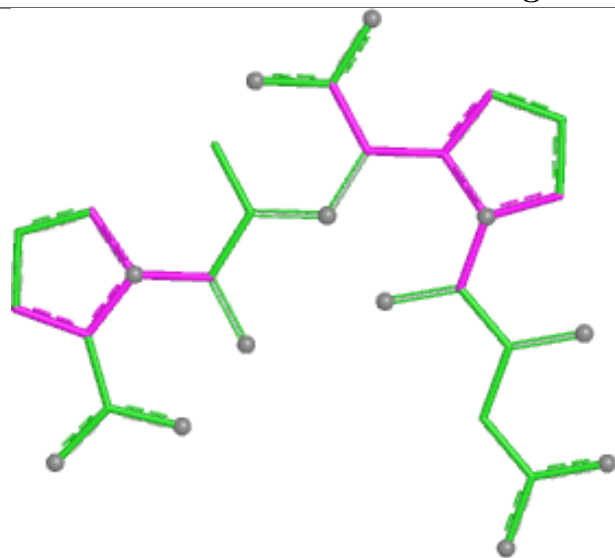


Torsions

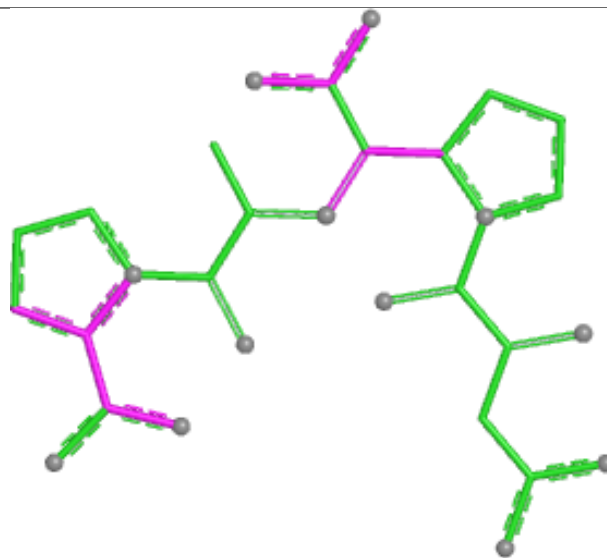


Rings

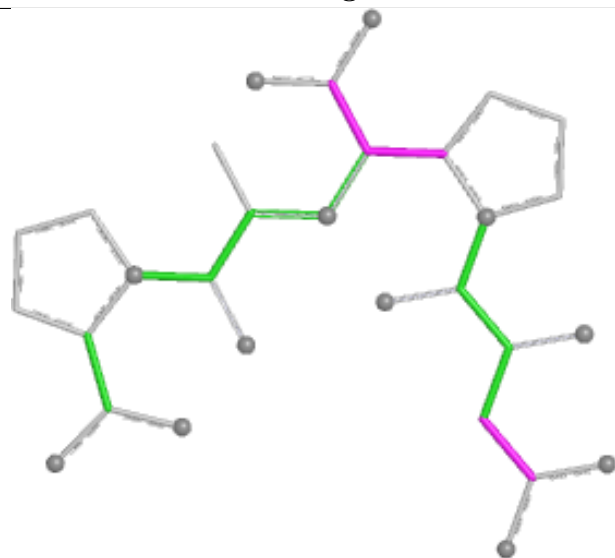
Ligand BJ2 B 702



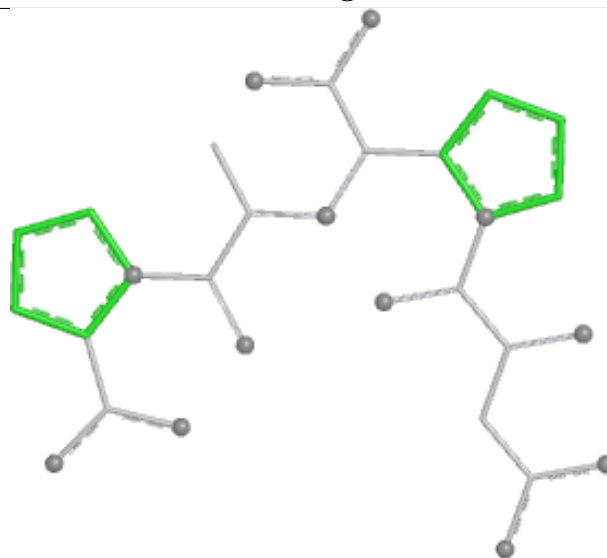
Bond lengths



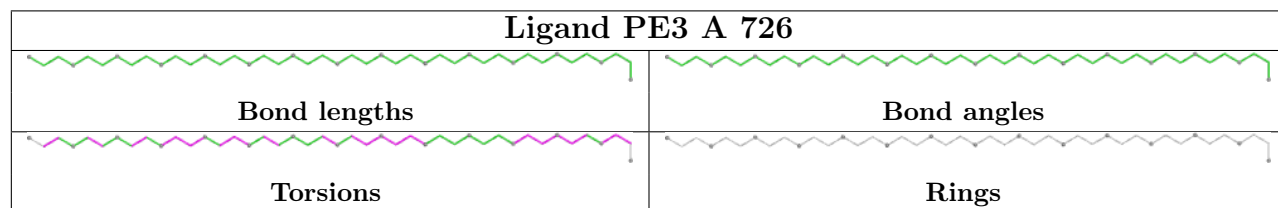
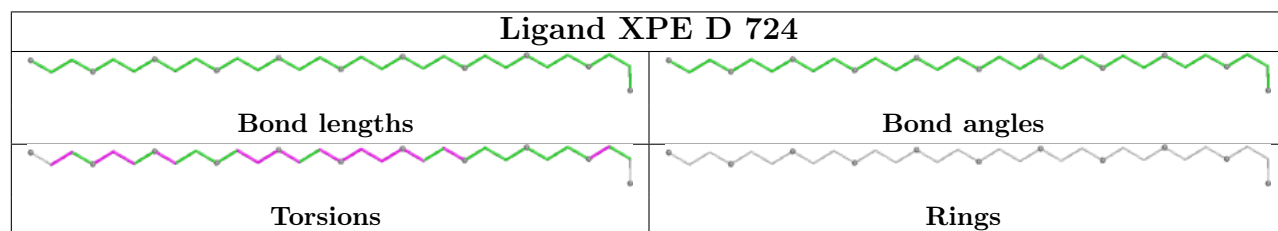
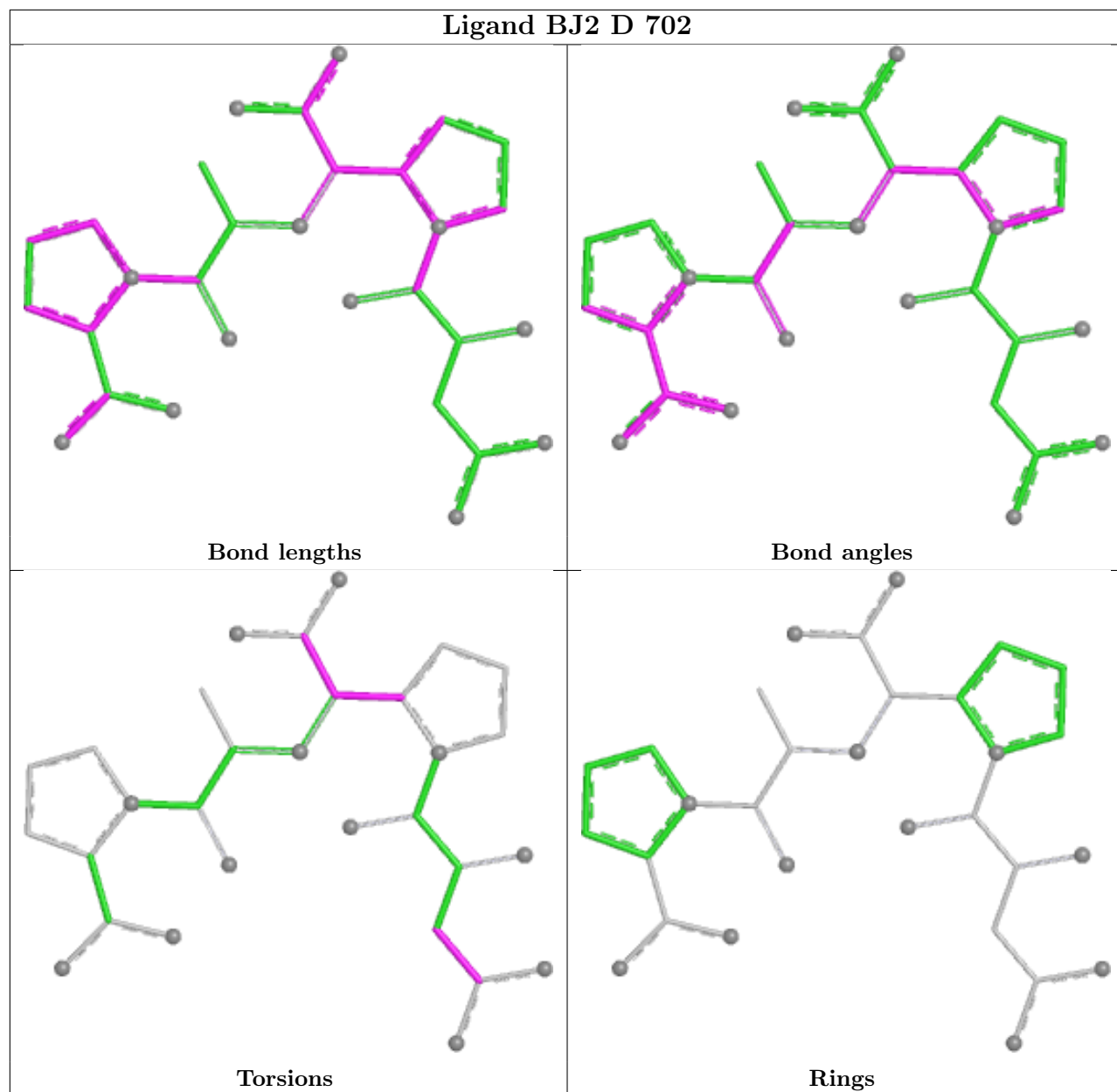
Bond angles

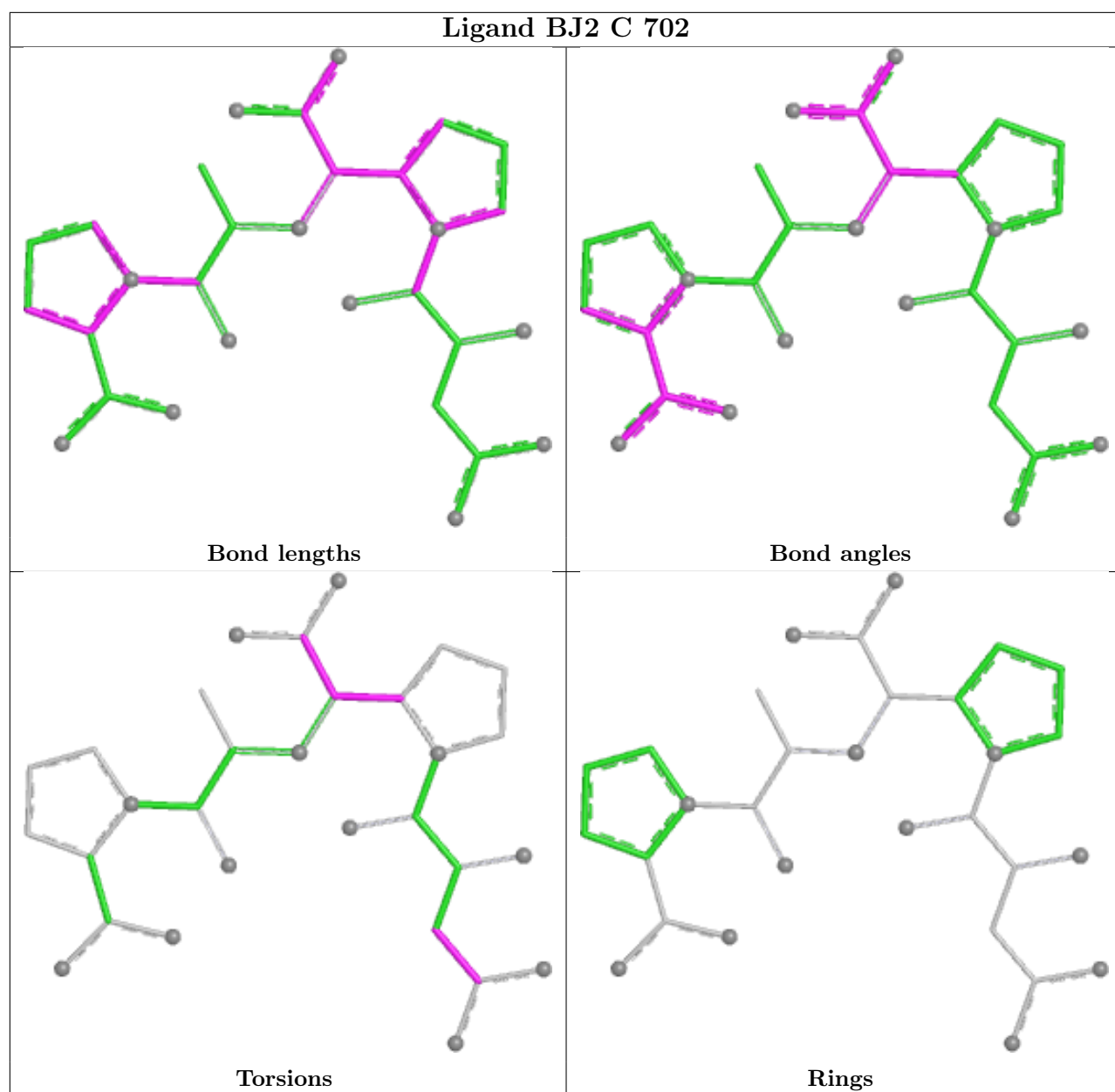


Torsions



Rings





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	605/629 (96%)	0.04	19 (3%)	51	58	12, 28, 51, 113	11 (1%)
1	B	608/629 (96%)	0.27	60 (9%)	13	15	12, 28, 49, 84	59 (9%)
1	C	606/629 (96%)	0.30	26 (4%)	40	46	13, 33, 59, 92	7 (1%)
1	D	614/629 (97%)	-0.11	14 (2%)	61	67	10, 26, 46, 77	10 (1%)
All	All	2433/2516 (96%)	0.12	119 (4%)	35	40	10, 29, 52, 113	87 (3%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	6.7
1	B	91	ILE	6.7
1	B	24	TYR	6.7
1	B	80	TRP	6.1
1	B	83	PHE	6.0
1	B	15	ALA	5.9
1	B	95	VAL	5.7
1	B	21	ALA	5.6
1	B	88	LEU	5.6
1	B	76	TYR	5.6
1	C	130	PRO	5.1
1	B	79	ILE	5.0
1	D	135	THR	4.9
1	B	20	PHE	4.9
1	B	135	THR	4.7
1	A	130	PRO	4.6
1	A	610	GLY	4.6
1	B	92	ILE	4.5
1	B	73	LYS	4.5
1	D	414	VAL	4.4
1	B	72	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	94	ALA	4.3
1	C	135	THR	4.2
1	A	606	ASN	4.2
1	B	19	LEU	4.2
1	B	90	ARG	4.2
1	C	79	ILE	4.2
1	B	16	GLY	4.1
1	B	84	THR	4.0
1	A	325	GLY	4.0
1	B	130	PRO	3.9
1	B	25	GLN	3.9
1	A	415	THR	3.8
1	A	9	GLN	3.8
1	C	1	LEU	3.8
1	B	78	PRO	3.8
1	D	130	PRO	3.8
1	B	93	GLY	3.7
1	C	325	GLY	3.7
1	B	28	ALA	3.7
1	B	85	ASP	3.7
1	C	610	GLY	3.7
1	B	86	PRO	3.6
1	B	325	GLY	3.5
1	B	87	GLN	3.5
1	B	89	ARG	3.5
1	B	97	THR	3.5
1	B	82	GLN	3.5
1	C	414	VAL	3.5
1	B	75	LEU	3.4
1	D	134	ALA	3.4
1	A	412	ASP	3.4
1	B	377	VAL	3.4
1	B	10	PHE	3.3
1	C	606	ASN	3.3
1	B	18	GLN	3.3
1	B	81	GLN	3.3
1	A	607	TYR	3.2
1	C	129	LEU	3.2
1	C	608	PRO	3.2
1	B	26	SER	3.2
1	B	27	SER	3.2
1	B	69	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	31	VAL	3.2
1	B	606	ASN	3.1
1	B	96	ARG	3.1
1	C	213[A]	HIS	3.1
1	B	22	GLN	3.0
1	B	129	LEU	3.0
1	C	78	PRO	2.9
1	A	413	ARG	2.9
1	C	270	PRO	2.9
1	B	608	PRO	2.8
1	B	98	LEU	2.8
1	C	82	GLN	2.7
1	C	271	PHE	2.7
1	C	84	THR	2.7
1	C	415	THR	2.7
1	D	415	THR	2.7
1	B	23	SER	2.7
1	A	273	ASP	2.7
1	C	519	ALA	2.6
1	A	275	PRO	2.6
1	B	612	ASP	2.5
1	D	611	ILE	2.5
1	A	418	THR	2.5
1	B	68	TRP	2.5
1	A	82	GLN	2.5
1	B	17	ALA	2.5
1	C	607	TYR	2.5
1	A	609	GLU	2.4
1	B	414	VAL	2.4
1	B	30	GLN	2.3
1	D	606	ASN	2.3
1	D	84	THR	2.3
1	D	136	CYS	2.3
1	C	80	TRP	2.2
1	B	77	GLU	2.2
1	B	13	ASP	2.2
1	B	607	TYR	2.2
1	D	129	LEU	2.2
1	D	325	GLY	2.2
1	C	575	GLN	2.2
1	A	78	PRO	2.2
1	A	605	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	64	PHE	2.2
1	C	274	LYS	2.2
1	C	272	PRO	2.1
1	C	381	ARG	2.1
1	A	1	LEU	2.1
1	A	81	GLN	2.1
1	B	611	ILE	2.1
1	D	213[A]	HIS	2.1
1	D	203	ASN	2.1
1	D	412	ASP	2.1
1	B	32	LEU	2.1
1	C	235	ARG	2.1
1	C	341	LYS	2.1
1	B	378	SER	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	N	3	11/12	0.40	0.17	84,102,122,126	0
6	MAN	O	4	11/12	0.48	0.19	75,92,108,116	0
6	MAN	O	5	11/12	0.48	0.17	71,86,101,106	21
5	BMA	L	3	11/12	0.51	0.15	76,95,114,115	0
2	NAG	E	2	14/15	0.56	0.18	66,86,105,126	28
3	BMA	F	3	11/12	0.57	0.20	57,70,85,88	22
4	NAG	J	2	14/15	0.63	0.20	52,70,88,93	27
4	NAG	P	2	14/15	0.63	0.23	59,79,102,109	27
2	NAG	K	2	14/15	0.63	0.20	56,71,86,94	27
4	NAG	M	2	14/15	0.64	0.18	52,79,101,112	27
4	NAG	G	2	14/15	0.64	0.19	53,80,99,111	28
2	NAG	H	2	14/15	0.64	0.19	57,68,87,95	27
3	BMA	I	3	11/12	0.68	0.12	64,74,89,90	0
4	FUC	P	3	10/11	0.69	0.23	52,65,78,82	19

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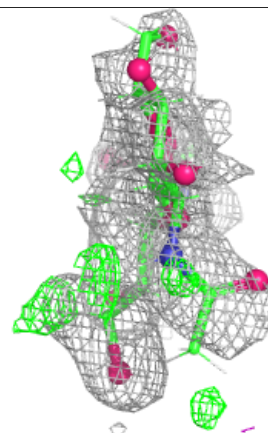
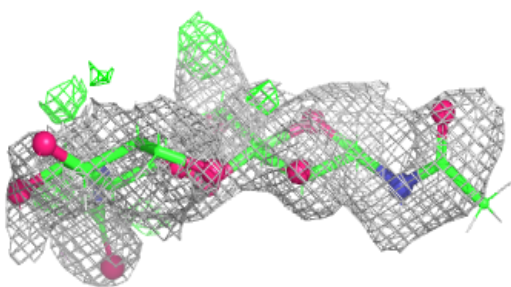
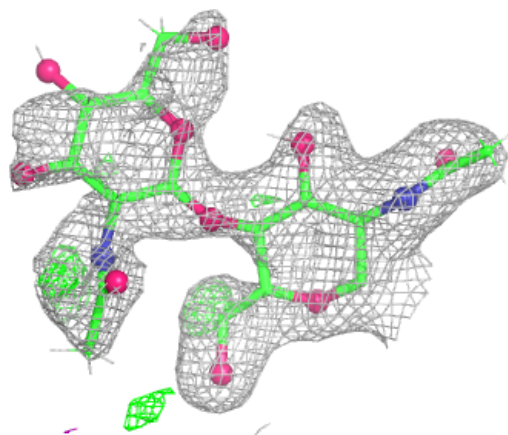
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FUC	M	3	10/11	0.71	0.19	51,62,71,79	21
6	BMA	O	3	11/12	0.74	0.15	63,70,84,84	0
4	FUC	J	3	10/11	0.74	0.20	53,65,78,81	20
5	NAG	L	2	14/15	0.74	0.18	67,82,93,95	27
5	NAG	N	2	14/15	0.77	0.18	44,64,87,96	27
4	FUC	G	3	10/11	0.79	0.20	48,66,76,80	20
2	NAG	E	1	14/15	0.80	0.15	44,61,76,80	0
3	FUC	F	4	10/11	0.80	0.18	42,51,63,72	20
6	FUC	O	6	10/11	0.80	0.13	42,53,64,67	0
3	FUC	I	4	10/11	0.81	0.13	45,55,65,67	0
6	NAG	O	2	14/15	0.83	0.17	39,49,70,71	0
5	NAG	L	1	14/15	0.84	0.13	56,70,88,88	0
4	NAG	M	1	14/15	0.85	0.13	37,50,65,69	0
3	NAG	F	2	14/15	0.86	0.14	44,55,64,64	27
2	NAG	K	1	14/15	0.86	0.13	36,53,63,67	0
4	NAG	P	1	14/15	0.86	0.14	37,50,65,74	0
2	NAG	H	1	14/15	0.87	0.12	33,50,60,68	0
3	NAG	I	2	14/15	0.87	0.13	41,55,68,68	0
4	NAG	J	1	14/15	0.88	0.11	35,46,60,66	0
3	NAG	F	1	14/15	0.89	0.12	40,48,60,60	26
4	NAG	G	1	14/15	0.90	0.11	30,43,57,61	0
5	NAG	N	1	14/15	0.91	0.11	30,45,54,59	0
6	NAG	O	1	14/15	0.93	0.09	29,40,46,52	0
3	NAG	I	1	14/15	0.93	0.09	32,41,49,50	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.

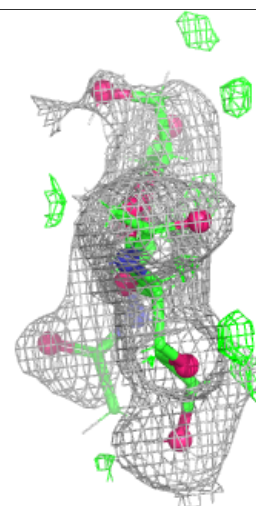
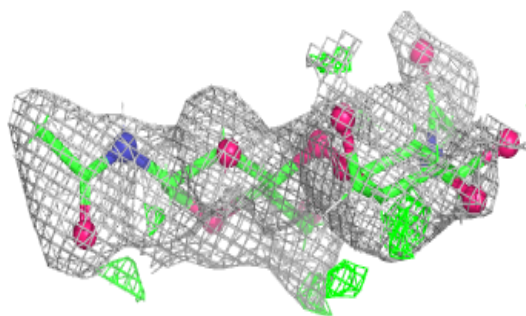
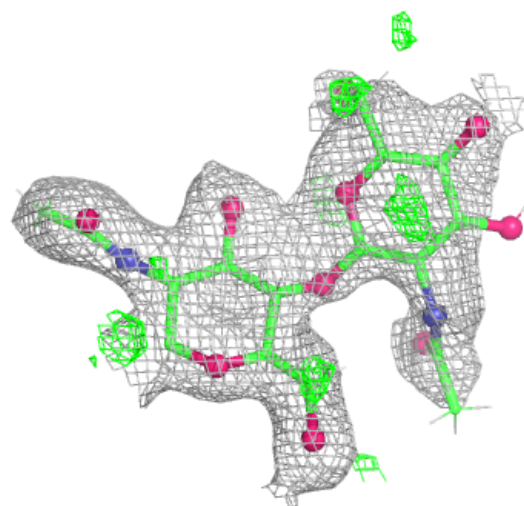
Electron density around Chain E:

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



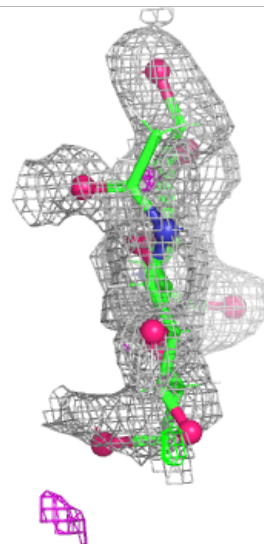
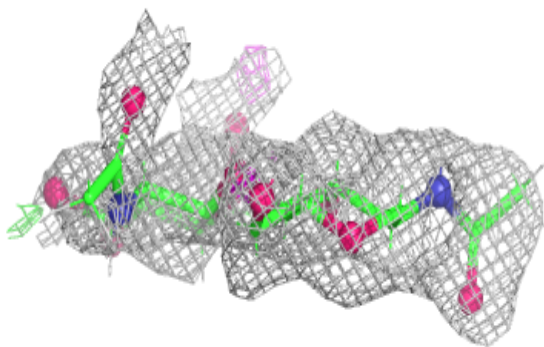
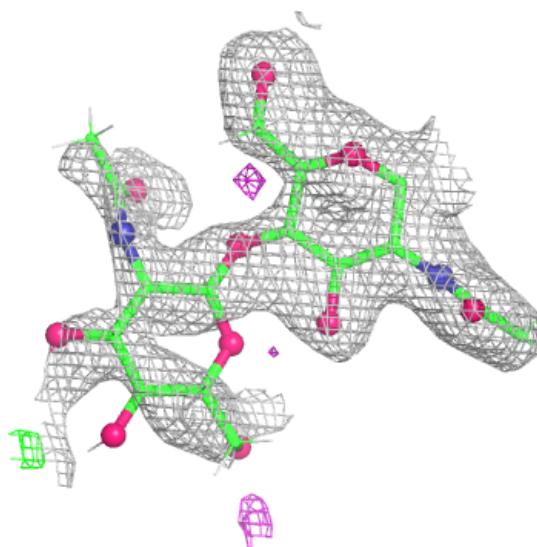
Electron density around Chain H:

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



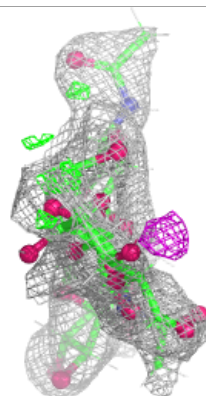
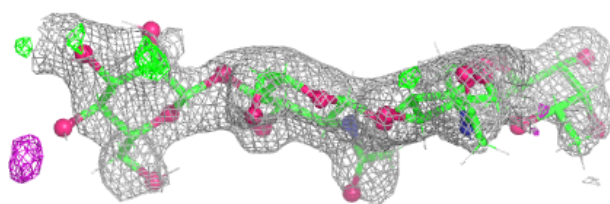
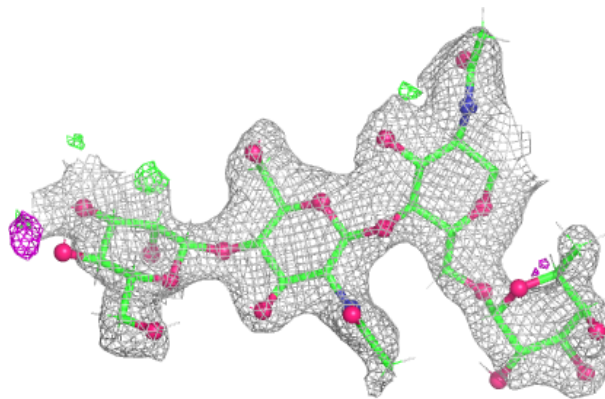
Electron density around Chain K:

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



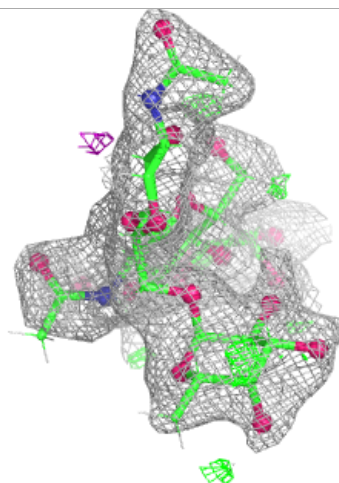
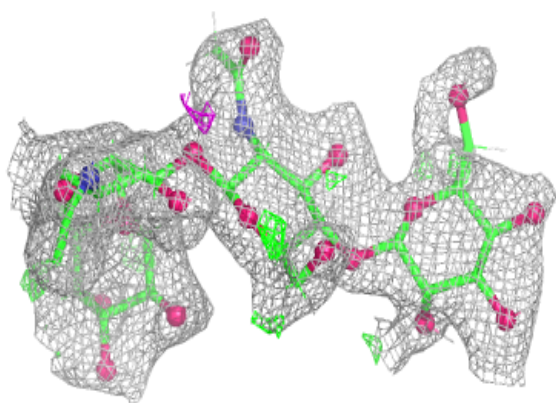
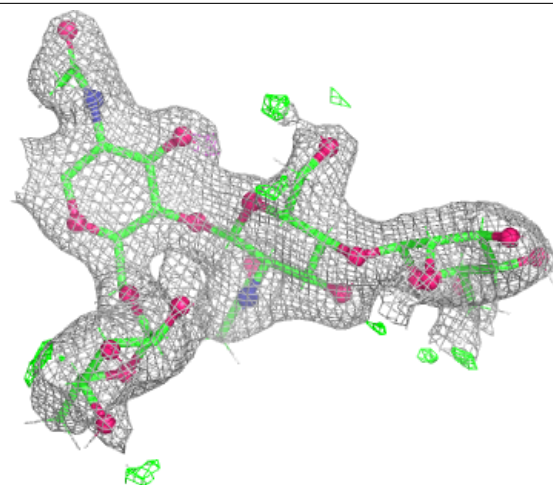
Electron density around Chain F:

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



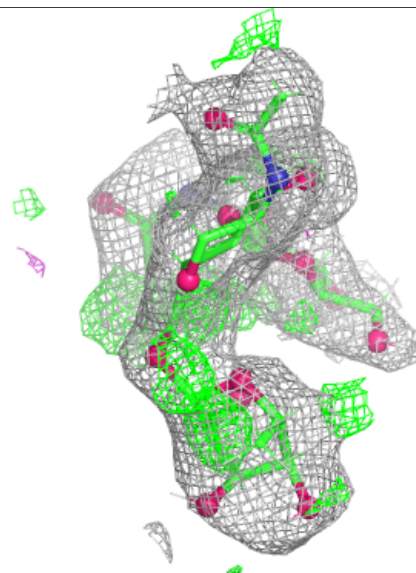
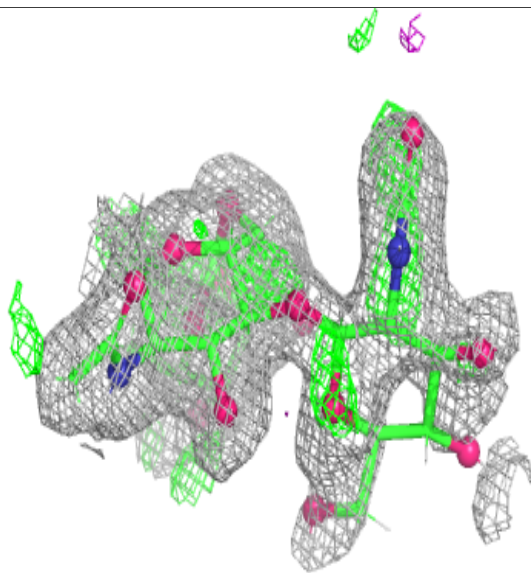
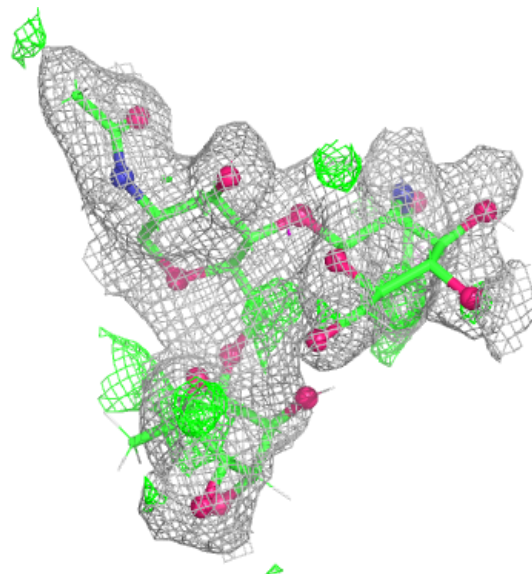
Electron density around Chain I:

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



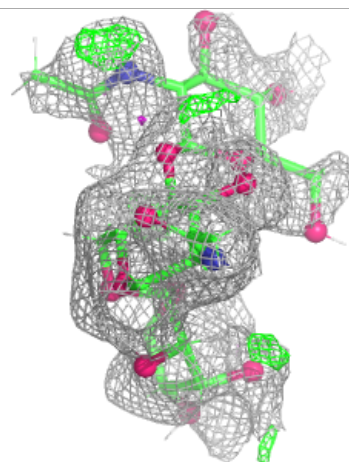
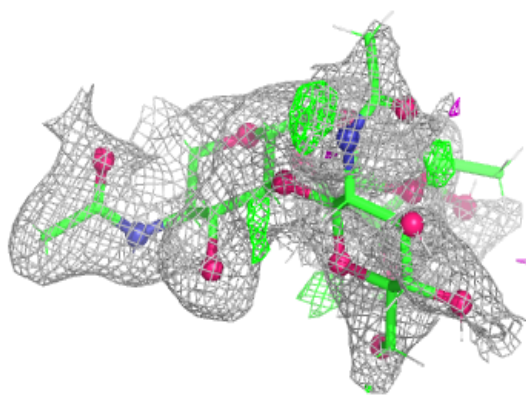
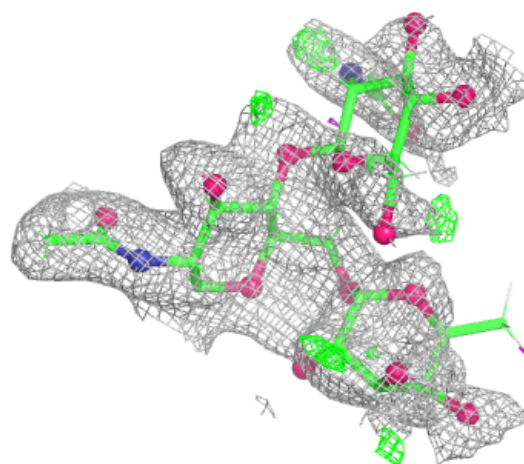
Electron density around Chain G:

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



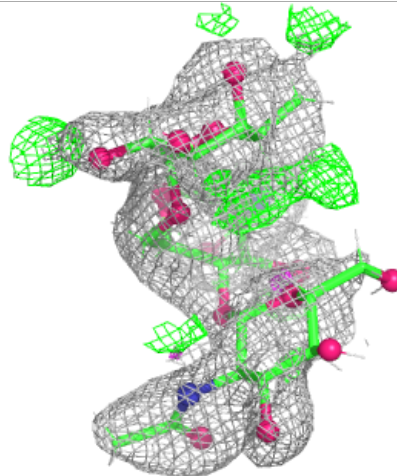
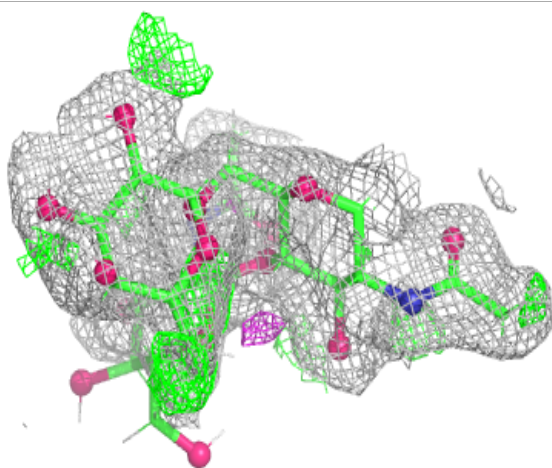
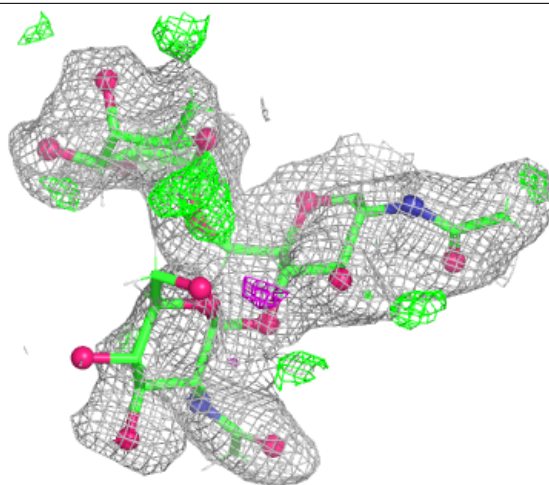
Electron density around Chain J:

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



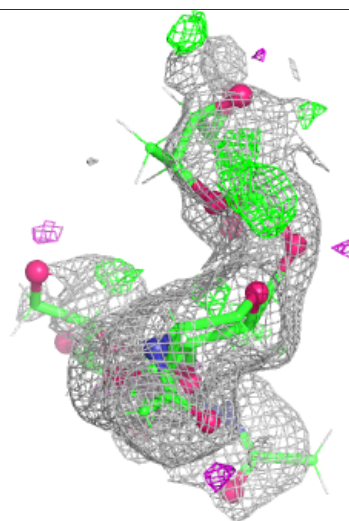
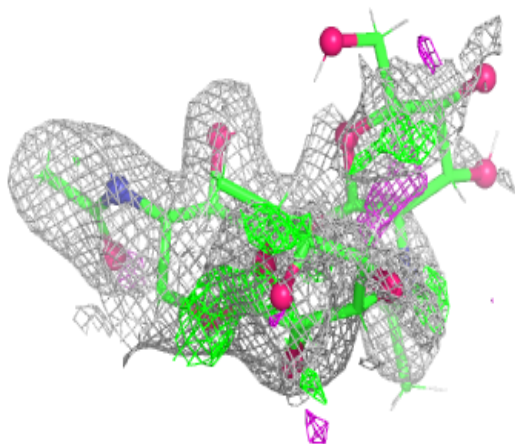
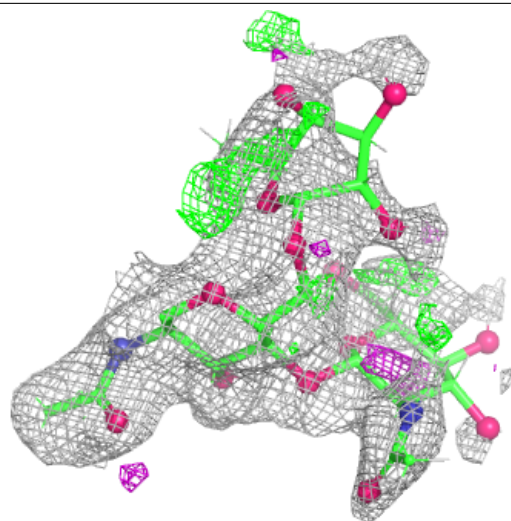
Electron density around Chain M:

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



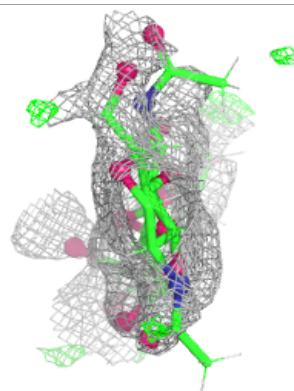
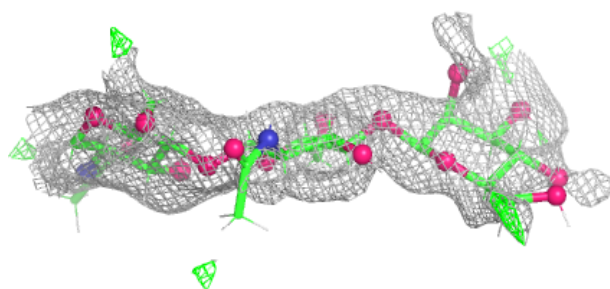
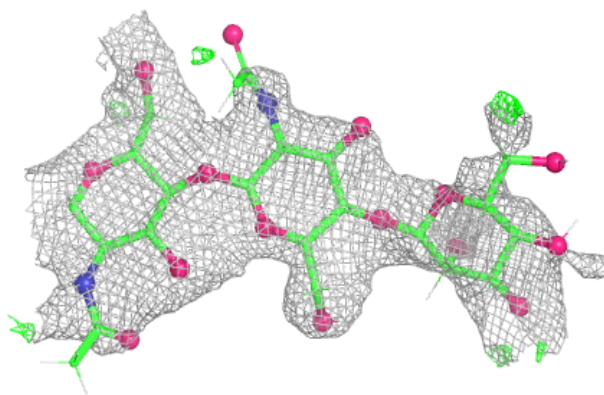
Electron density around Chain P:

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

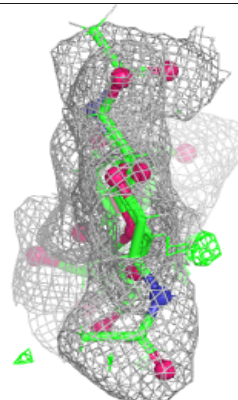
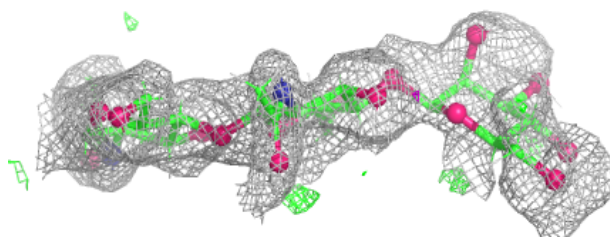
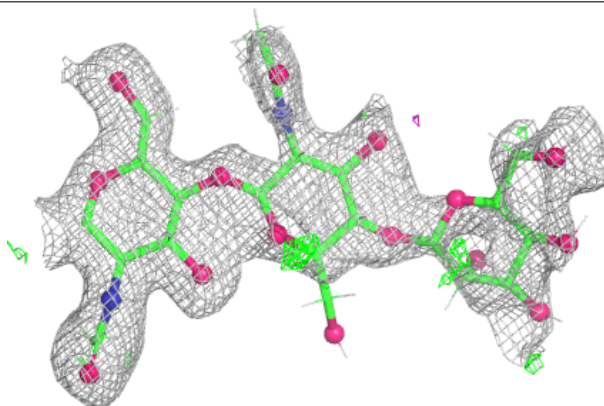


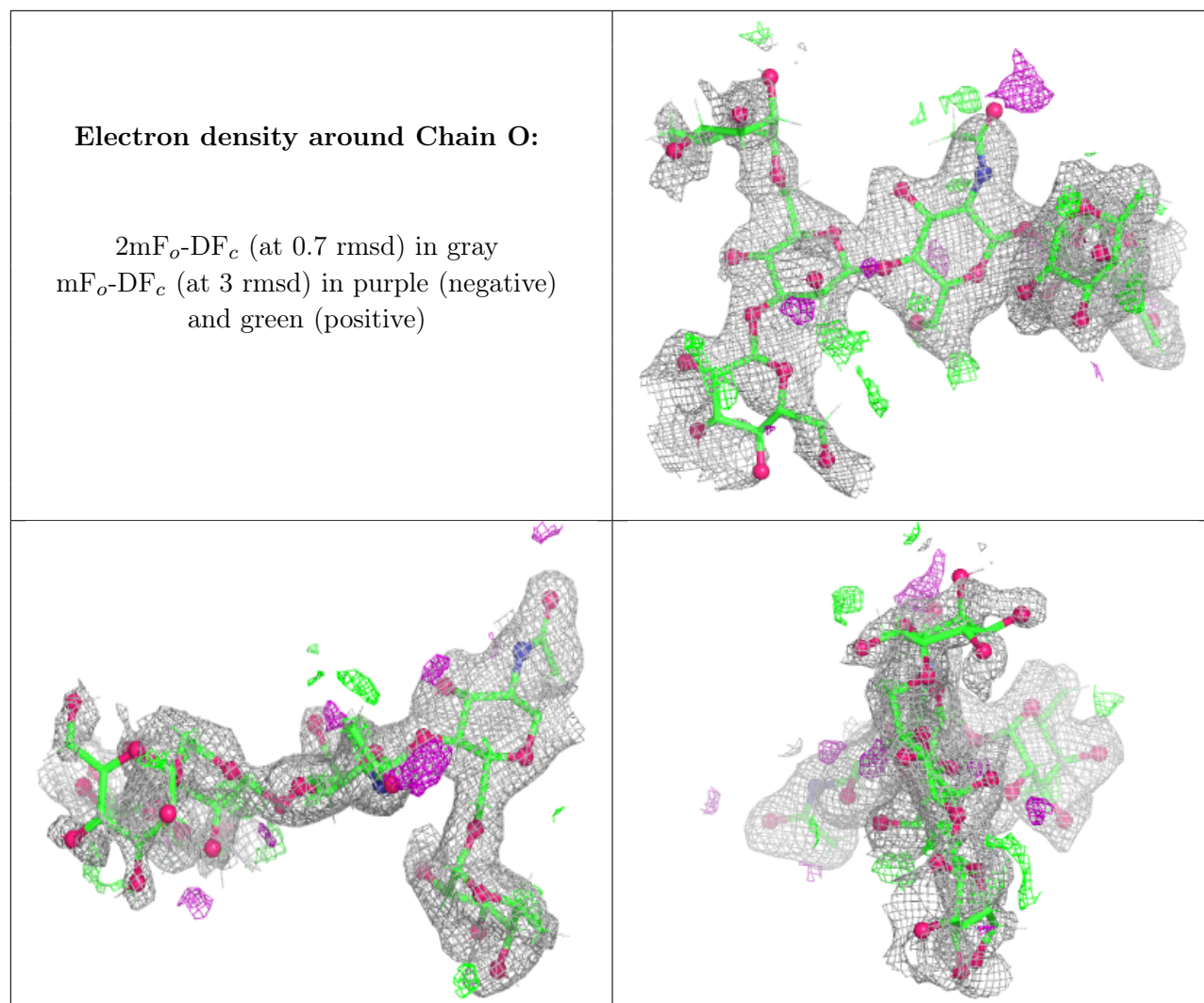
Electron density around Chain L:

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

**Electron density around Chain N:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
12	EDO	B	723	4/4	0.71	0.17	48,61,63,75	0
12	EDO	C	718	4/4	0.72	0.20	46,56,58,58	10
12	EDO	A	721	4/4	0.75	0.18	40,49,55,59	10
12	EDO	C	720	4/4	0.75	0.18	38,48,58,63	10
12	EDO	C	719	4/4	0.77	0.17	46,57,69,69	10
12	EDO	C	716	4/4	0.78	0.19	56,67,80,80	0
11	PEG	A	716	7/7	0.78	0.20	30,36,42,48	17
13	ACT	C	723	4/4	0.78	0.18	34,41,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	EDO	A	718	4/4	0.79	0.16	49,59,60,63	0
12	EDO	A	723	4/4	0.80	0.17	31,37,49,58	10
12	EDO	D	720	4/4	0.80	0.17	49,63,65,78	0
12	EDO	C	717	4/4	0.80	0.16	64,76,83,92	0
11	PEG	B	716	7/7	0.81	0.19	39,47,63,63	17
12	EDO	C	721	4/4	0.82	0.16	49,59,65,67	0
14	PE3	A	726	43/43	0.82	0.16	28,42,56,63	101
12	EDO	C	722	4/4	0.83	0.17	36,44,60,60	10
11	PEG	A	715	7/7	0.83	0.18	26,41,49,52	17
12	EDO	D	721	4/4	0.83	0.16	38,46,52,53	10
11	PEG	B	715	7/7	0.83	0.20	33,43,52,55	17
12	EDO	A	720	4/4	0.83	0.16	33,43,51,59	10
16	PG4	C	724[A]	13/13	0.83	0.16	30,37,42,53	31
16	PG4	C	724[B]	13/13	0.83	0.16	27,34,41,42	31
12	EDO	A	717	4/4	0.84	0.18	17,30,36,38	10
11	PEG	C	713	7/7	0.84	0.14	39,47,54,55	17
11	PEG	C	714	7/7	0.84	0.16	31,42,51,51	17
13	ACT	A	725	4/4	0.84	0.14	46,49,59,59	0
17	XPE	D	724	31/31	0.84	0.14	31,47,60,71	0
11	PEG	B	717	7/7	0.85	0.14	46,55,62,62	17
12	EDO	B	720	4/4	0.85	0.16	31,38,43,48	10
12	EDO	A	719	4/4	0.85	0.19	36,44,46,48	10
12	EDO	D	719	4/4	0.86	0.13	29,38,43,49	10
12	EDO	C	715	4/4	0.86	0.14	42,50,55,59	0
15	PGE	B	725	10/10	0.86	0.15	30,43,49,51	24
11	PEG	B	714	7/7	0.87	0.12	45,55,66,76	0
12	EDO	B	721	4/4	0.87	0.12	48,58,70,71	0
11	PEG	B	718	7/7	0.87	0.12	41,50,68,68	0
16	PG4	B	726	13/13	0.88	0.12	26,42,54,55	0
11	PEG	D	717	7/7	0.88	0.13	32,42,51,51	17
13	ACT	A	724	4/4	0.88	0.17	30,36,44,46	0
11	PEG	A	714	7/7	0.88	0.12	35,46,55,55	17
12	EDO	A	722	4/4	0.89	0.11	43,52,57,61	0
11	PEG	D	718	7/7	0.89	0.10	44,53,63,73	0
12	EDO	B	722	4/4	0.89	0.11	29,38,46,48	10
12	EDO	B	719	4/4	0.89	0.11	40,48,55,60	0
13	ACT	D	722	4/4	0.91	0.13	24,29,37,46	0
13	ACT	D	723	4/4	0.93	0.14	27,33,35,39	0
13	ACT	B	724	4/4	0.94	0.09	32,41,42,47	0
10	MG	C	704	1/1	0.96	0.08	31,31,31,31	0
8	BJ2	B	702	30/30	0.97	0.06	16,23,28,31	0
8	BJ2	C	702	30/30	0.97	0.06	17,24,31,31	0

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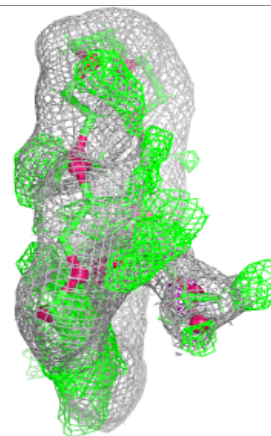
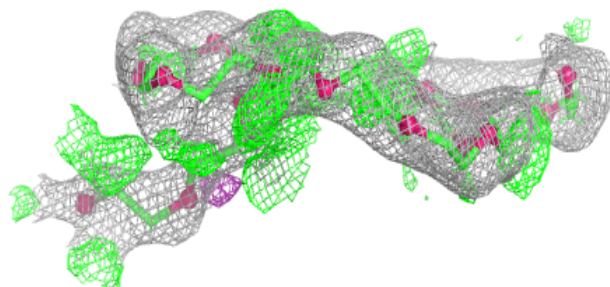
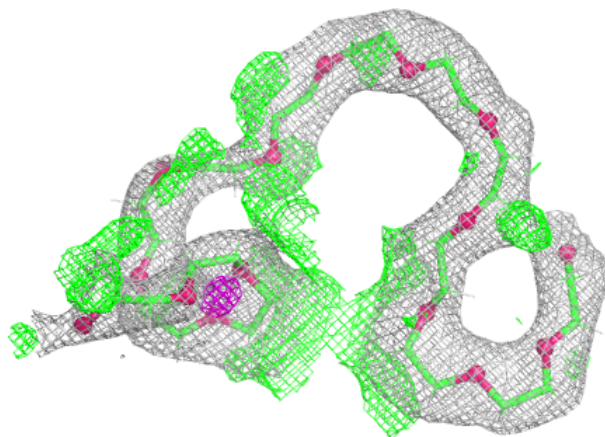
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	BJ2	D	702	30/30	0.97	0.05	13,20,24,28	0
10	MG	A	704	1/1	0.97	0.05	23,23,23,23	0
8	BJ2	A	702	30/30	0.98	0.05	14,21,28,29	0
10	MG	D	704	1/1	0.99	0.07	17,17,17,17	0
10	MG	B	704	1/1	0.99	0.05	29,29,29,29	0
9	CL	D	703	1/1	0.99	0.02	18,18,18,18	0
7	ZN	D	701	1/1	1.00	0.01	16,16,16,16	0
9	CL	A	703	1/1	1.00	0.03	19,19,19,19	0
9	CL	B	703	1/1	1.00	0.02	20,20,20,20	0
9	CL	C	703	1/1	1.00	0.02	22,22,22,22	0
7	ZN	A	701	1/1	1.00	0.02	17,17,17,17	0
7	ZN	B	701	1/1	1.00	0.01	18,18,18,18	0
7	ZN	C	701	1/1	1.00	0.01	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.

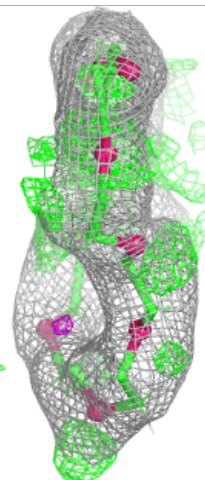
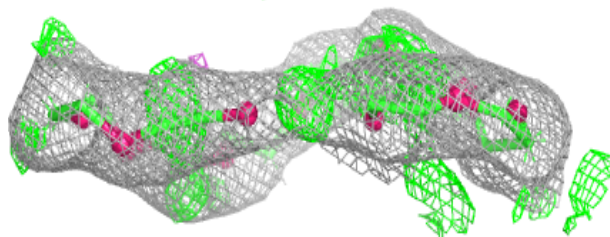
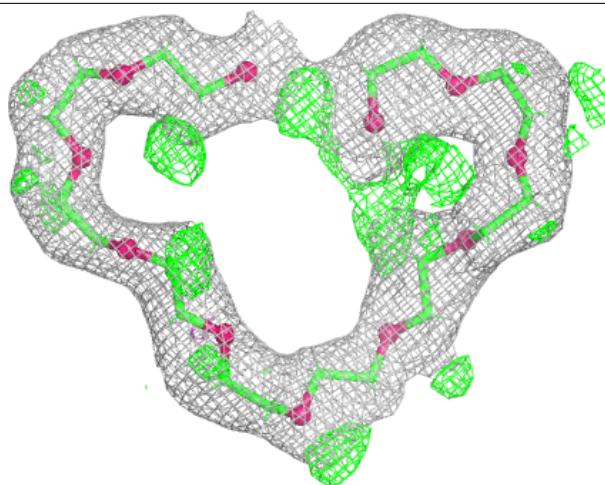
Electron density around PE3 A 726:

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



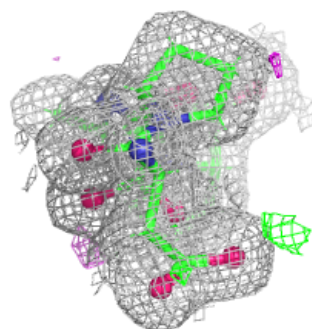
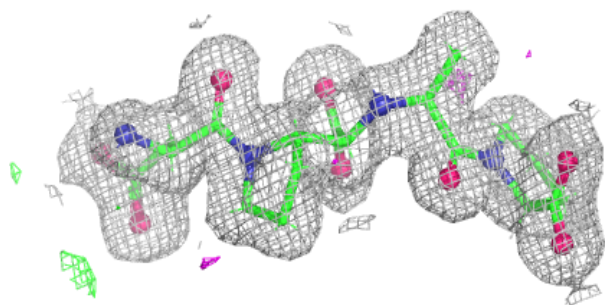
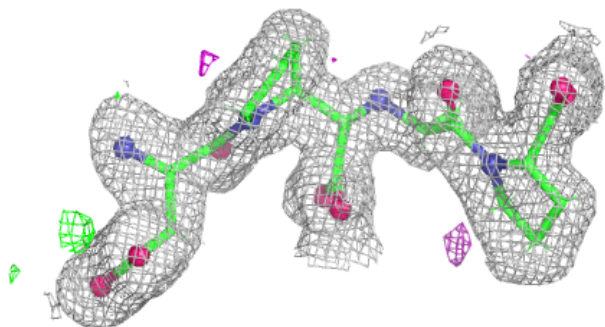
Electron density around XPE D 724:

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

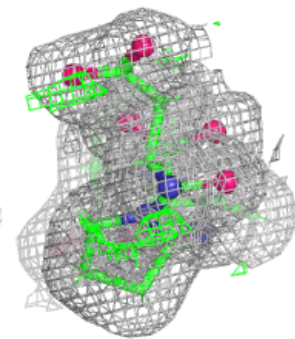
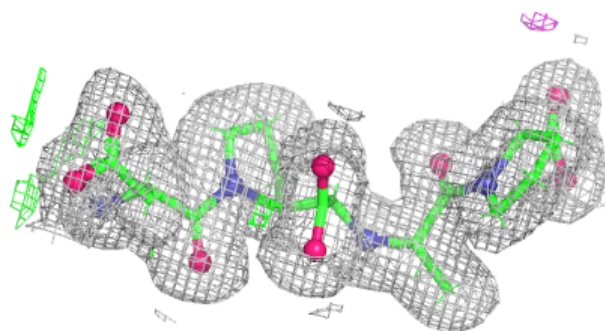
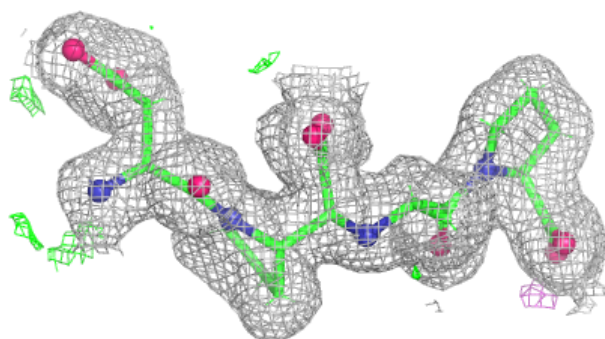


Electron density around BJ2 B 702:

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

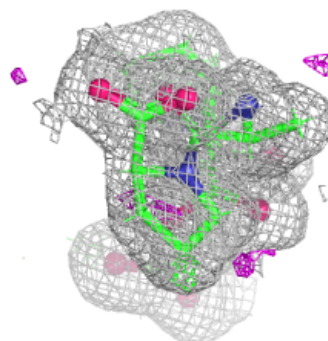
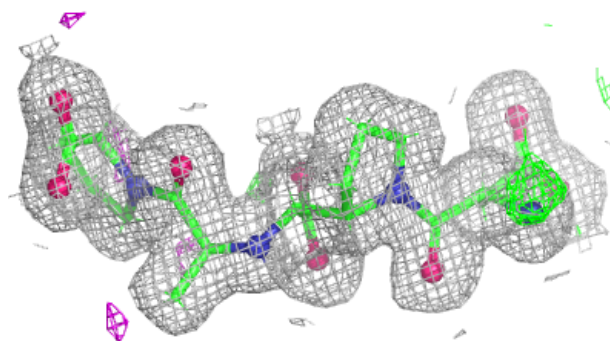
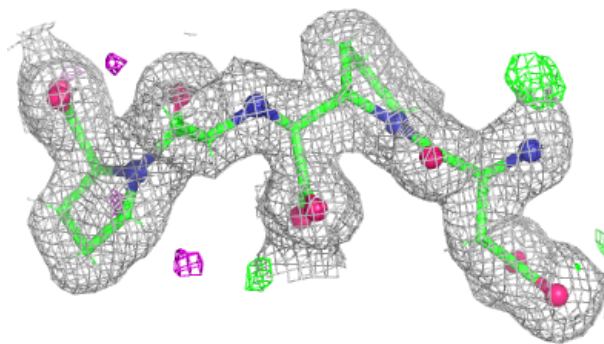
**Electron density around BJ2 C 702:**

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

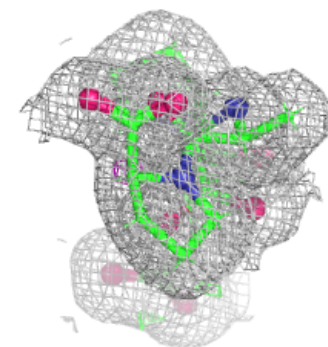
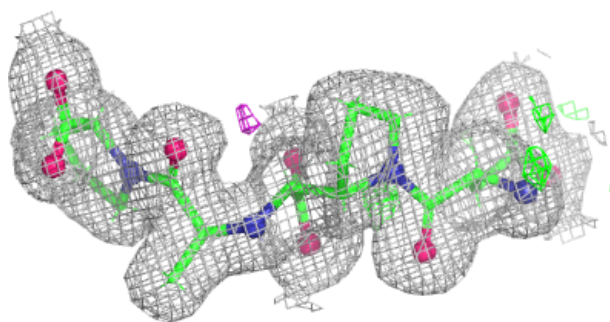
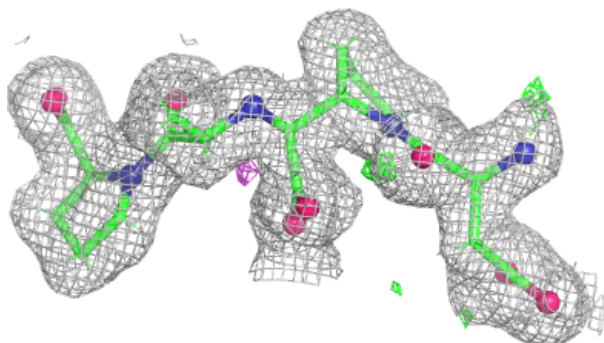


Electron density around BJ2 D 702:

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

**Electron density around BJ2 A 702:**

$2mF_o-DF_c$ (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.