



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:55 AM UTC

PDB ID : 6YDX / pdb_00006ydx
Title : Insulin-regulated aminopeptidase complexed with a macrocyclic peptidic inhibitor
Authors : Mpakali, A.; Saridakis, E.; Giastas, P.; Stratikos, E.
Deposited on : 2020-03-21
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

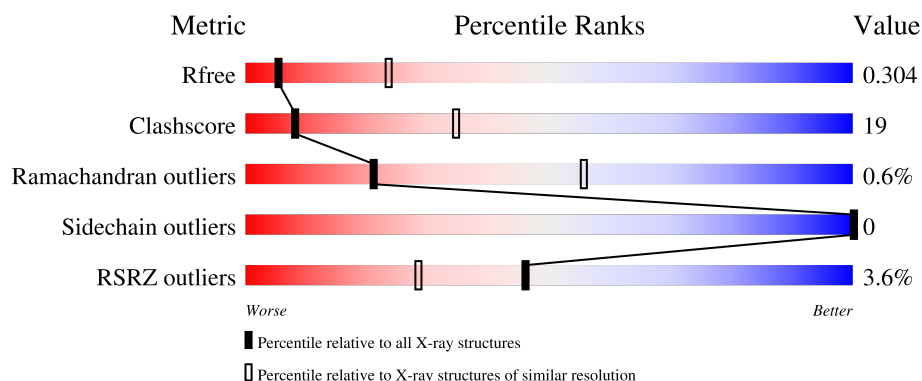
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	912	4% 56% 38% 6%
1	B	912	3% 59% 34% 6%
2	C	2	100%
2	E	2	100%
2	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	I	2	 100%
3	D	3	 67% 33%
3	H	3	 33% 67%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14298 atoms, of which 0 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 Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	856	Total	C	N	O	S	0	4	0
			6868	4448	1118	1276	26			
1	B	853	Total	C	N	O	S	0	0	0
			6827	4422	1113	1266	26			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9UIQ6
A	125	GLY	-	expression tag	UNP Q9UIQ6
A	126	ILE	-	expression tag	UNP Q9UIQ6
A	127	LEU	-	expression tag	UNP Q9UIQ6
A	128	PRO	-	expression tag	UNP Q9UIQ6
A	129	SER	-	expression tag	UNP Q9UIQ6
A	130	PRO	-	expression tag	UNP Q9UIQ6
A	131	GLY	-	expression tag	UNP Q9UIQ6
A	132	ASN	-	expression tag	UNP Q9UIQ6
A	133	PRO	-	expression tag	UNP Q9UIQ6
A	134	ALA	-	expression tag	UNP Q9UIQ6
A	135	LEU	-	expression tag	UNP Q9UIQ6
A	136	LEU	-	expression tag	UNP Q9UIQ6
A	137	SER	-	expression tag	UNP Q9UIQ6
A	138	LEU	-	expression tag	UNP Q9UIQ6
A	139	VAL	-	expression tag	UNP Q9UIQ6
A	140	SER	-	expression tag	UNP Q9UIQ6
A	141	LEU	-	expression tag	UNP Q9UIQ6
A	142	LEU	-	expression tag	UNP Q9UIQ6
A	143	SER	-	expression tag	UNP Q9UIQ6
A	144	VAL	-	expression tag	UNP Q9UIQ6
A	145	LEU	-	expression tag	UNP Q9UIQ6
A	146	LEU	-	expression tag	UNP Q9UIQ6
A	147	MET	-	expression tag	UNP Q9UIQ6
A	148	GLY	-	expression tag	UNP Q9UIQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	149	CYS	-	expression tag	UNP Q9UIQ6
A	150	VAL	-	expression tag	UNP Q9UIQ6
A	151	ALA	-	expression tag	UNP Q9UIQ6
A	152	GLU	-	expression tag	UNP Q9UIQ6
A	153	THR	-	expression tag	UNP Q9UIQ6
A	154	GLY	-	expression tag	UNP Q9UIQ6
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	124	MET	-	initiating methionine	UNP Q9UIQ6
B	125	GLY	-	expression tag	UNP Q9UIQ6
B	126	ILE	-	expression tag	UNP Q9UIQ6
B	127	LEU	-	expression tag	UNP Q9UIQ6
B	128	PRO	-	expression tag	UNP Q9UIQ6
B	129	SER	-	expression tag	UNP Q9UIQ6
B	130	PRO	-	expression tag	UNP Q9UIQ6
B	131	GLY	-	expression tag	UNP Q9UIQ6
B	132	ASN	-	expression tag	UNP Q9UIQ6
B	133	PRO	-	expression tag	UNP Q9UIQ6
B	134	ALA	-	expression tag	UNP Q9UIQ6
B	135	LEU	-	expression tag	UNP Q9UIQ6
B	136	LEU	-	expression tag	UNP Q9UIQ6
B	137	SER	-	expression tag	UNP Q9UIQ6
B	138	LEU	-	expression tag	UNP Q9UIQ6
B	139	VAL	-	expression tag	UNP Q9UIQ6
B	140	SER	-	expression tag	UNP Q9UIQ6
B	141	LEU	-	expression tag	UNP Q9UIQ6
B	142	LEU	-	expression tag	UNP Q9UIQ6
B	143	SER	-	expression tag	UNP Q9UIQ6
B	144	VAL	-	expression tag	UNP Q9UIQ6
B	145	LEU	-	expression tag	UNP Q9UIQ6
B	146	LEU	-	expression tag	UNP Q9UIQ6
B	147	MET	-	expression tag	UNP Q9UIQ6
B	148	GLY	-	expression tag	UNP Q9UIQ6
B	149	CYS	-	expression tag	UNP Q9UIQ6

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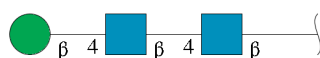
Chain	Residue	Modelled	Actual	Comment	Reference
B	150	VAL	-	expression tag	UNP Q9UIQ6
B	151	ALA	-	expression tag	UNP Q9UIQ6
B	152	GLU	-	expression tag	UNP Q9UIQ6
B	153	THR	-	expression tag	UNP Q9UIQ6
B	154	GLY	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

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



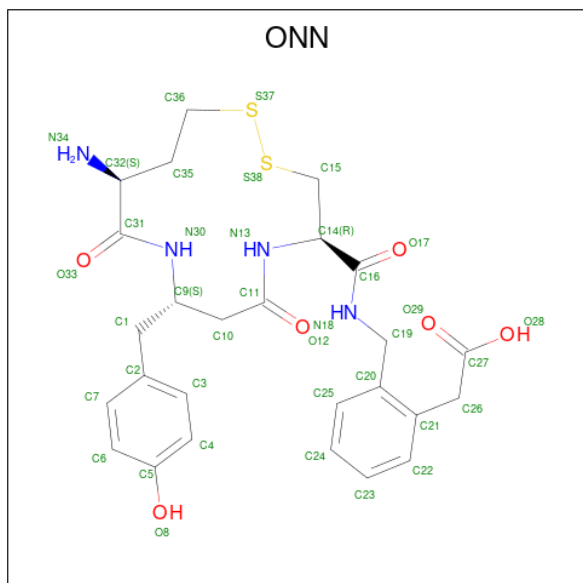
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-[2-[[[(4 {R},8 {S},11 {S})-11-azanyl-8-[(4-hydroxyphenyl)methyl]-6,10-bis(oxidanylidene)-1,2-dithia-5,9-diazacyclotridec-4-yl]carbonylamino]methyl]phenyl]ethanoic acid (CCD ID: ONN) (formula: C₂₆H₃₂N₄O₆S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			76	52	8	12	4		
4	B	1	Total	C	N	O	S	0	1
			76	52	8	12	4		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

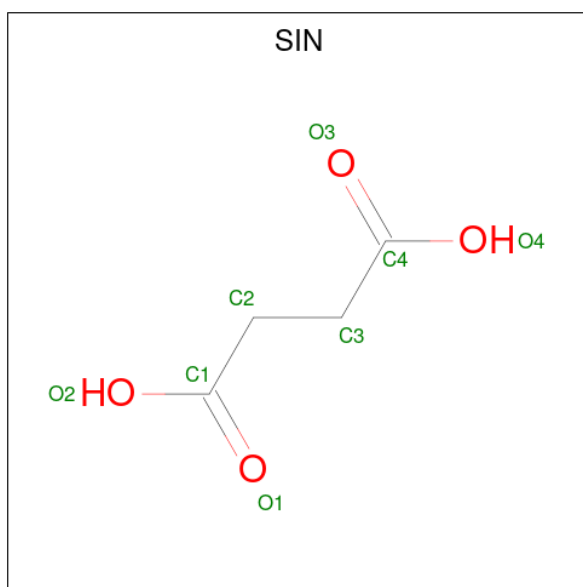
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



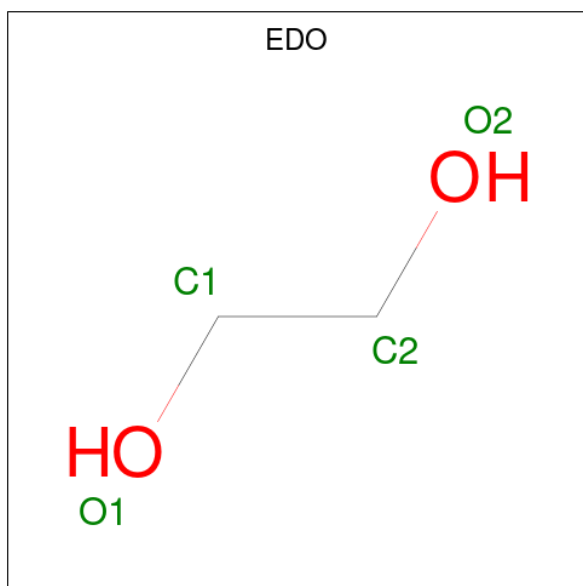
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1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

- Molecule 7 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



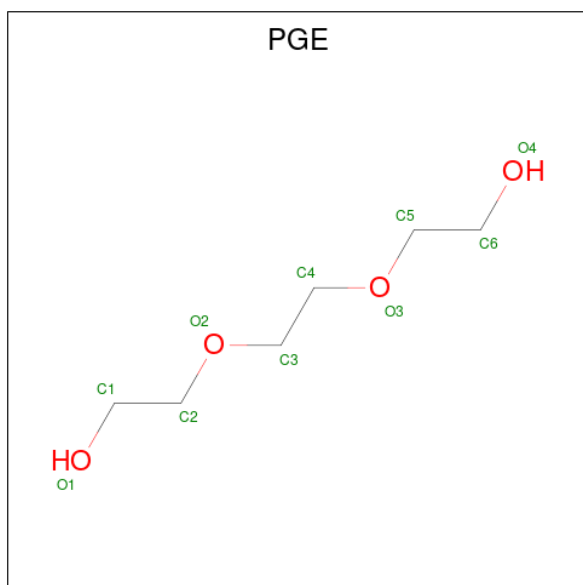
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

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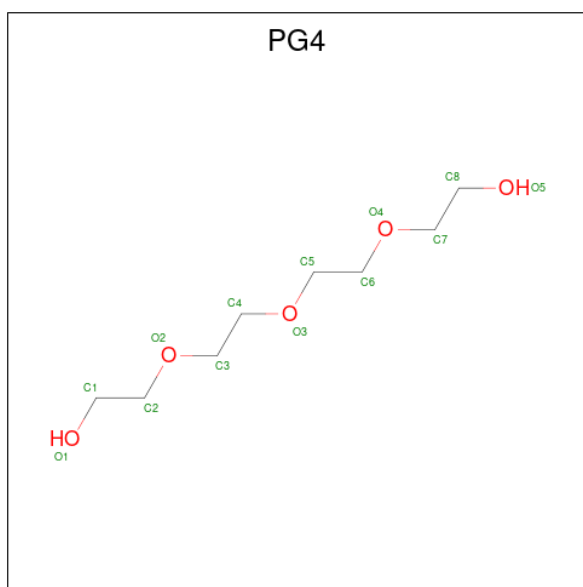
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



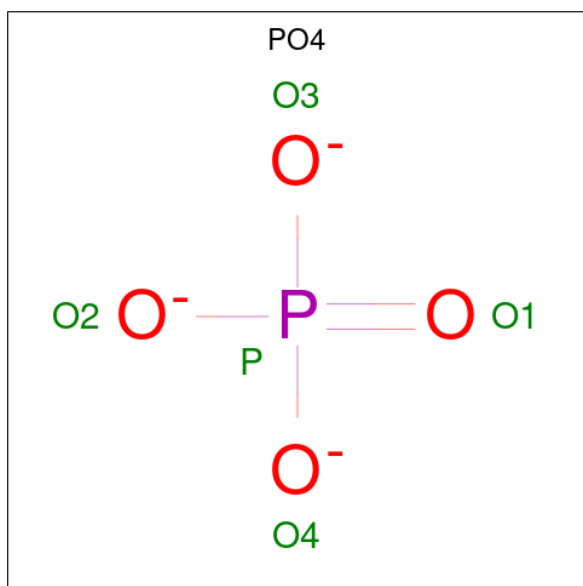
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



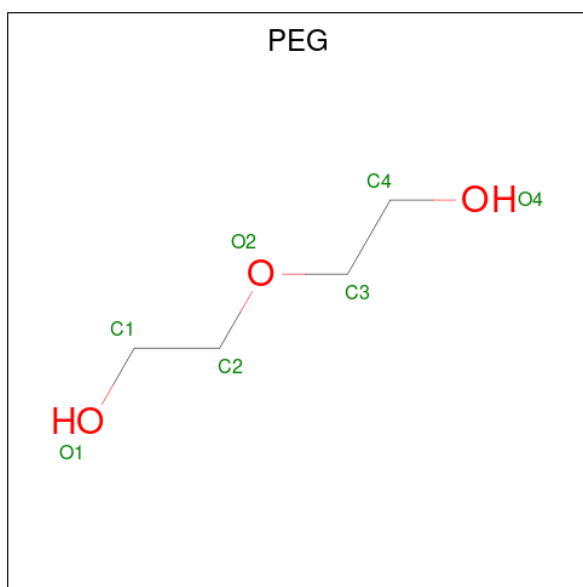
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			7	4	3		

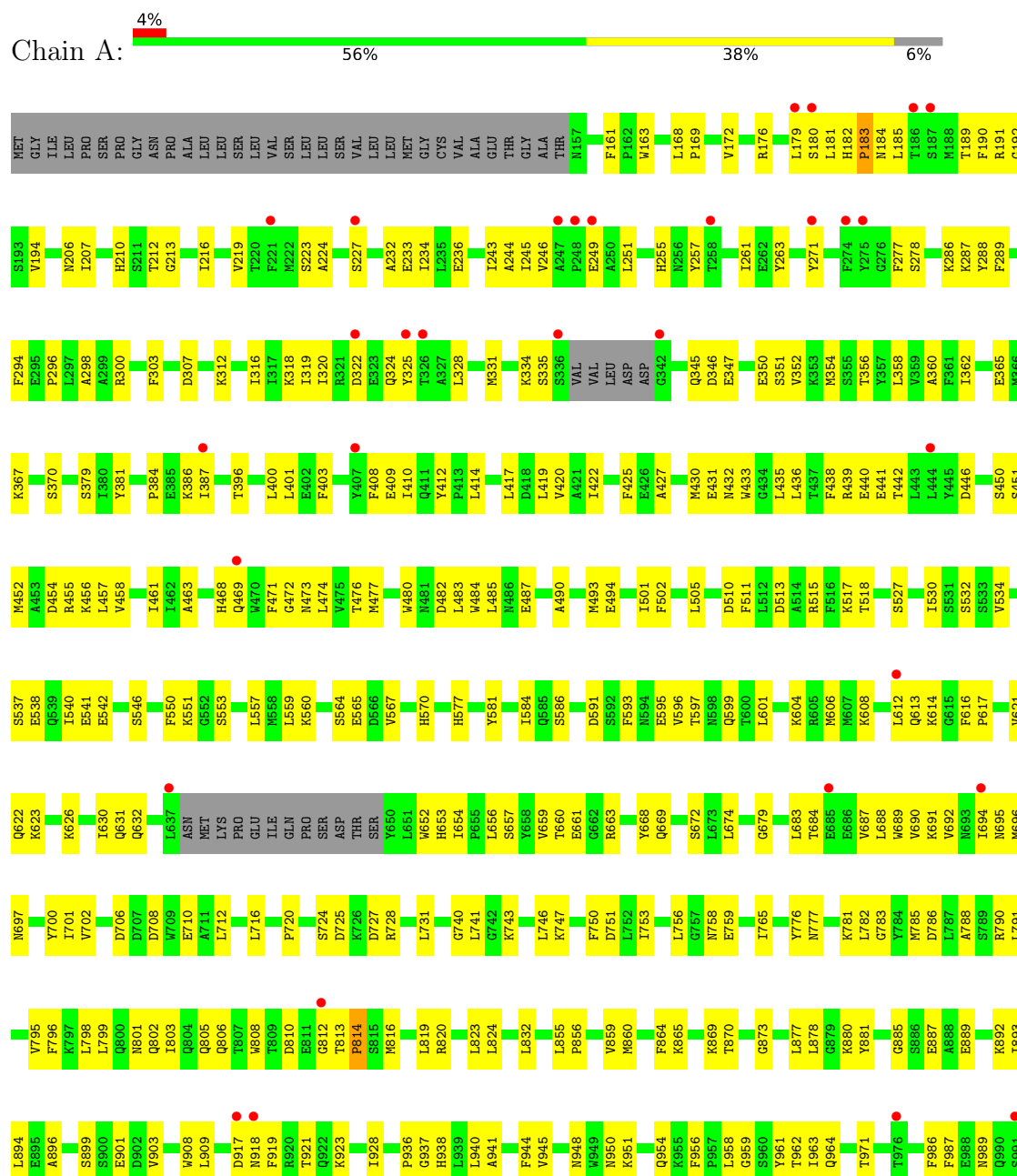
- Molecule 13 is water.

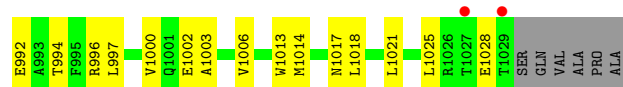
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	11	Total	O	0	0
			11	11		
13	B	17	Total	O	0	0
			17	17		

3 Residue-property plots

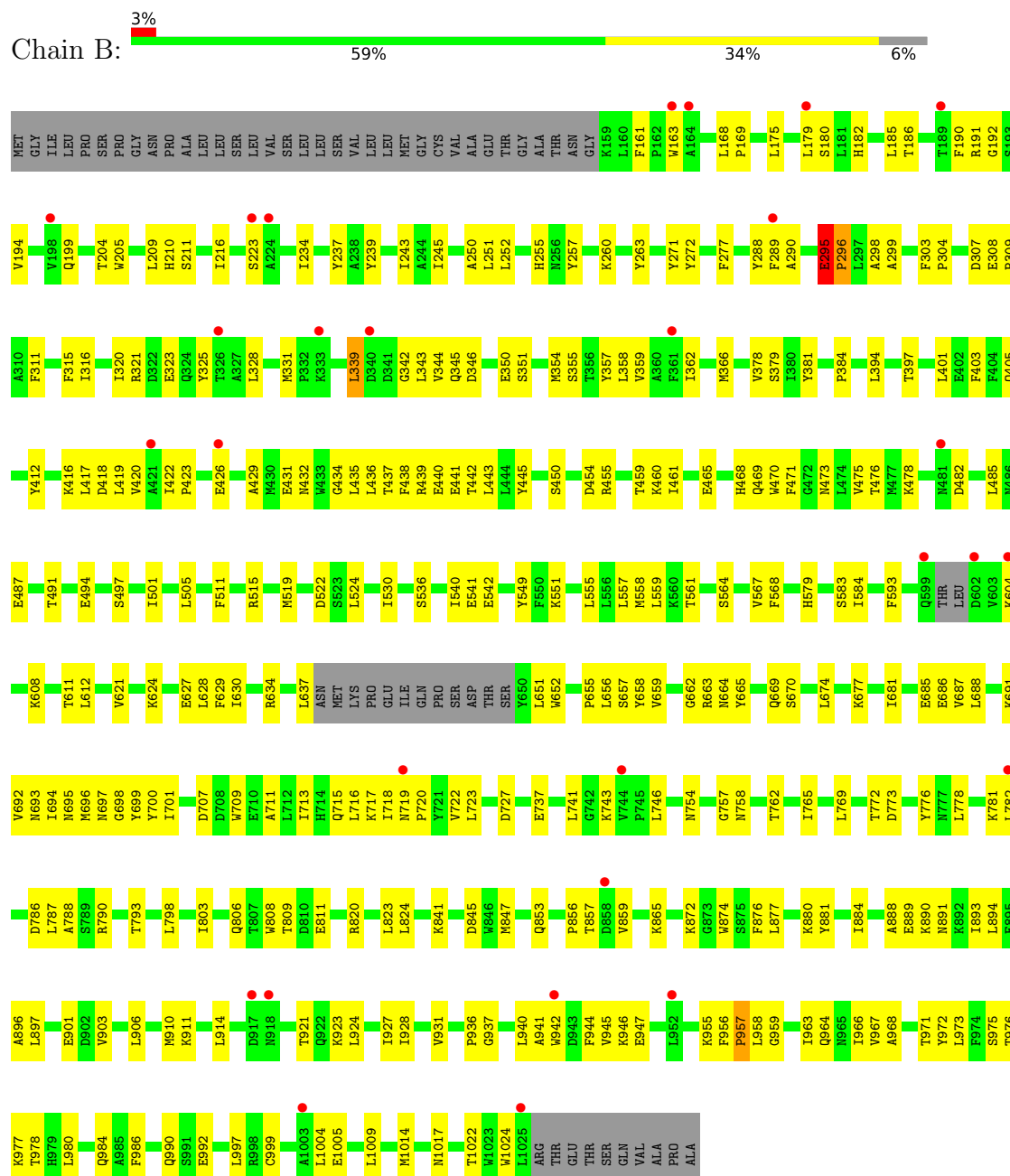
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: Leucyl-cystinyl aminopeptidase



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



HA61
HA62

- 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 F:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%

MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.42Å 118.63Å 141.39Å 90.00° 102.77° 90.00°	Depositor
Resolution (Å)	45.96 – 3.20 45.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	81.7 (45.96-3.20) 81.8 (45.96-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.277 , 0.314 0.271 , 0.304	Depositor DCC
R_{free} test set	1597 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	14298	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 25.17 % 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 3.3379e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PEG, EDO, BMA, PO4, ZN, PG4, ONN, SIN, 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	0.36	0/7047	0.75	4/9566 (0.0%)
1	B	0.35	1/6994 (0.0%)	0.75	2/9498 (0.0%)
All	All	0.36	1/14041 (0.0%)	0.75	6/19064 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	PHE	C-N	-5.12	1.29	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	GLY	N-CA-C	6.46	118.09	111.95
1	B	295	GLU	C-N-CD	-6.43	98.65	125.00
1	A	422	ILE	N-CA-C	6.26	114.02	108.63
1	B	957	PRO	N-CA-C	5.62	121.23	113.98
1	A	695	ASN	CA-C-N	-5.18	111.65	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	295	GLU	Peptide

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	6868	0	6703	274	0
1	B	6827	0	6664	254	0
2	C	28	0	25	1	0
2	E	28	0	25	3	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
3	D	39	0	34	3	0
3	H	39	0	34	3	0
4	A	76	0	0	3	0
4	B	76	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	70	0	64	6	0
6	B	70	0	65	0	0
7	A	8	0	4	0	0
8	A	8	0	12	1	0
8	B	12	0	18	0	0
9	A	10	0	14	0	0
10	A	13	0	18	0	0
11	A	5	0	0	0	0
12	B	7	0	10	1	0
13	A	11	0	0	0	0
13	B	17	0	0	1	0
All	All	14298	0	13765	545	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 19.

The worst 5 of 545 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:B:168:LEU:HD13	1:B:210:HIS:CE1	1.81	1.15
1:B:695:ASN:N	1:B:727:ASP:OD1	1.83	1.11
1:A:482:ASP:HB3	1:A:485:LEU:HD12	1.37	1.07
1:A:207:ILE:HG22	1:A:245:ILE:HB	1.47	0.97
1:B:717:LYS:HE2	1:B:754:ASN:HB2	1.47	0.96

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	854/912 (94%)	811 (95%)	36 (4%)	7 (1%)	16	50
1	B	847/912 (93%)	813 (96%)	30 (4%)	4 (0%)	24	59
All	All	1701/1824 (93%)	1624 (96%)	66 (4%)	11 (1%)	21	56

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	PRO
1	B	664	ASN
1	A	697	ASN
1	A	425	PHE
1	A	918	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	742/813 (91%)	742 (100%)	0	100	100
1	B	738/813 (91%)	738 (100%)	0	100	100
All	All	1480/1626 (91%)	1480 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	577	HIS
1	B	719	ASN
1	B	918	ASN
1	B	734	ASN
1	B	891	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 ⓘ

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.35	0	17,19,21	0.62	0
2	NAG	C	2	2	14,14,15	2.08	2 (14%)	17,19,21	1.84	3 (17%)
3	NAG	D	1	3,1	14,14,15	1.07	2 (14%)	17,19,21	1.73	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	2	3	14,14,15	0.16	0	17,19,21	0.61	0
3	BMA	D	3	3	11,11,12	1.17	1 (9%)	15,15,17	0.99	1 (6%)
2	NAG	E	1	2,1	14,14,15	1.81	2 (14%)	17,19,21	1.28	1 (5%)
2	NAG	E	2	2	14,14,15	0.86	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.38	0	17,19,21	0.96	1 (5%)
2	NAG	F	2	2	14,14,15	0.88	1 (7%)	17,19,21	0.81	0
2	NAG	G	1	2,1	14,14,15	0.96	2 (14%)	17,19,21	1.16	1 (5%)
2	NAG	G	2	2	14,14,15	0.90	1 (7%)	17,19,21	0.42	0
3	NAG	H	1	3,1	14,14,15	1.19	1 (7%)	17,19,21	1.92	4 (23%)
3	NAG	H	2	3	14,14,15	0.66	1 (7%)	17,19,21	1.20	1 (5%)
3	BMA	H	3	3	11,11,12	0.88	1 (9%)	15,15,17	1.43	2 (13%)
2	NAG	I	1	2,1	14,14,15	1.25	1 (7%)	17,19,21	2.24	5 (29%)
2	NAG	I	2	2	14,14,15	1.13	1 (7%)	17,19,21	2.79	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	7.25	1.55	1.43
2	E	1	NAG	O5-C1	5.54	1.53	1.43
3	H	1	NAG	O5-C1	-4.09	1.36	1.43
2	I	2	NAG	O5-C1	3.82	1.50	1.43
2	E	1	NAG	C1-C2	3.79	1.57	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C2-N2-C7	10.10	136.43	122.90
2	I	1	NAG	C2-N2-C7	6.03	130.99	122.90
3	H	1	NAG	O4-C4-C5	-5.45	95.89	109.32
3	D	1	NAG	C2-N2-C7	5.00	129.60	122.90
2	C	2	NAG	C2-N2-C7	4.62	129.09	122.90

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

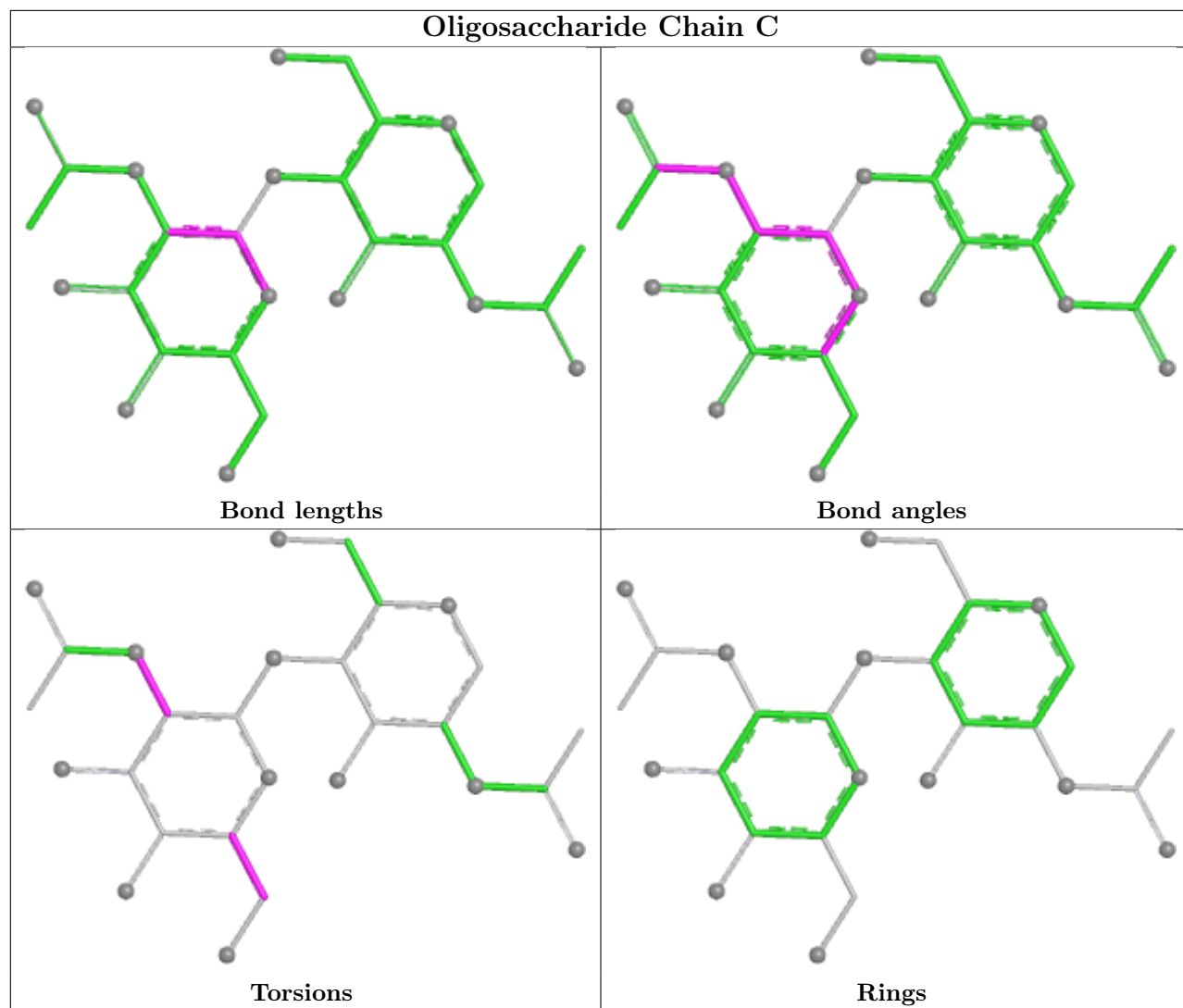
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6

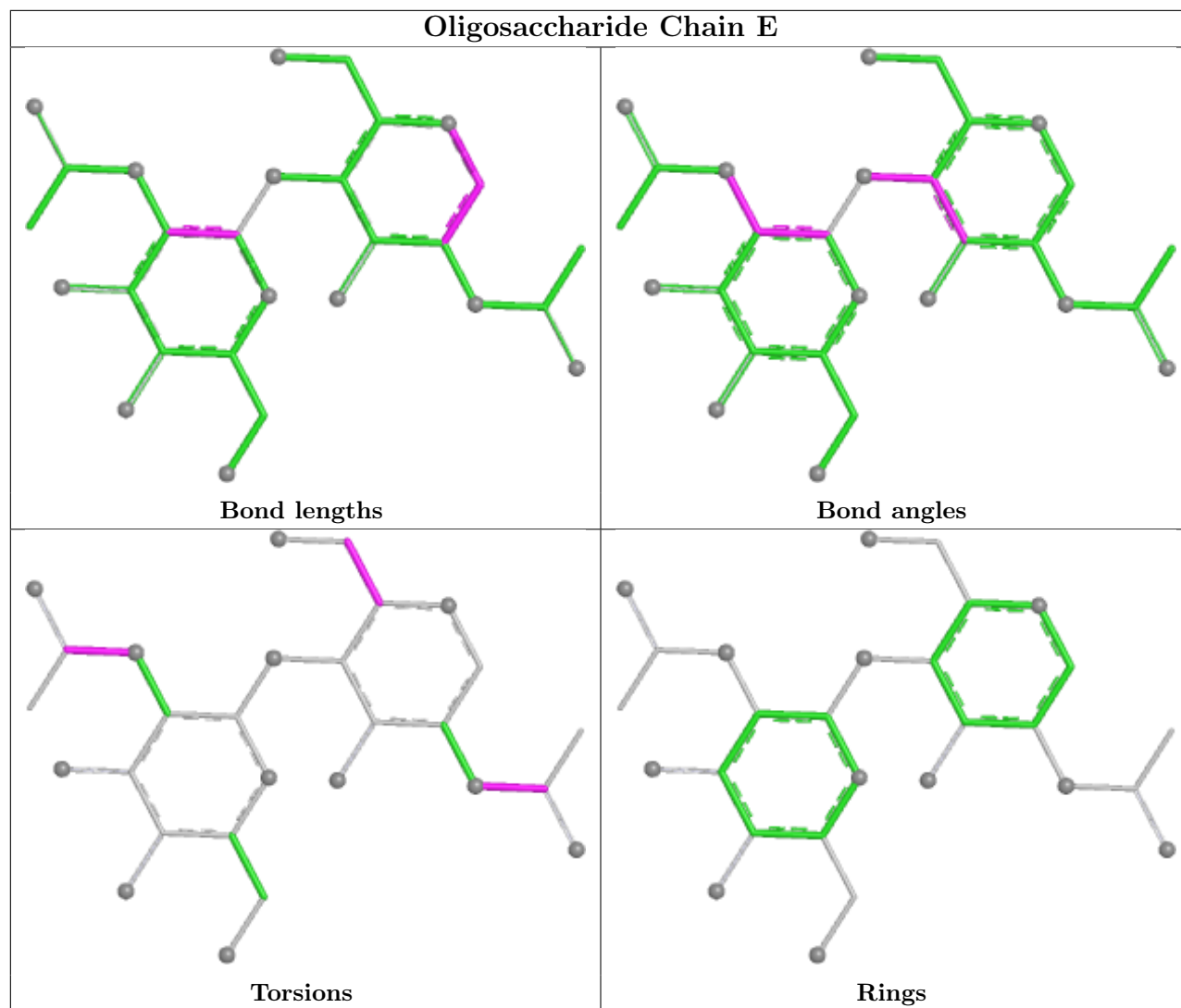
There are no ring outliers.

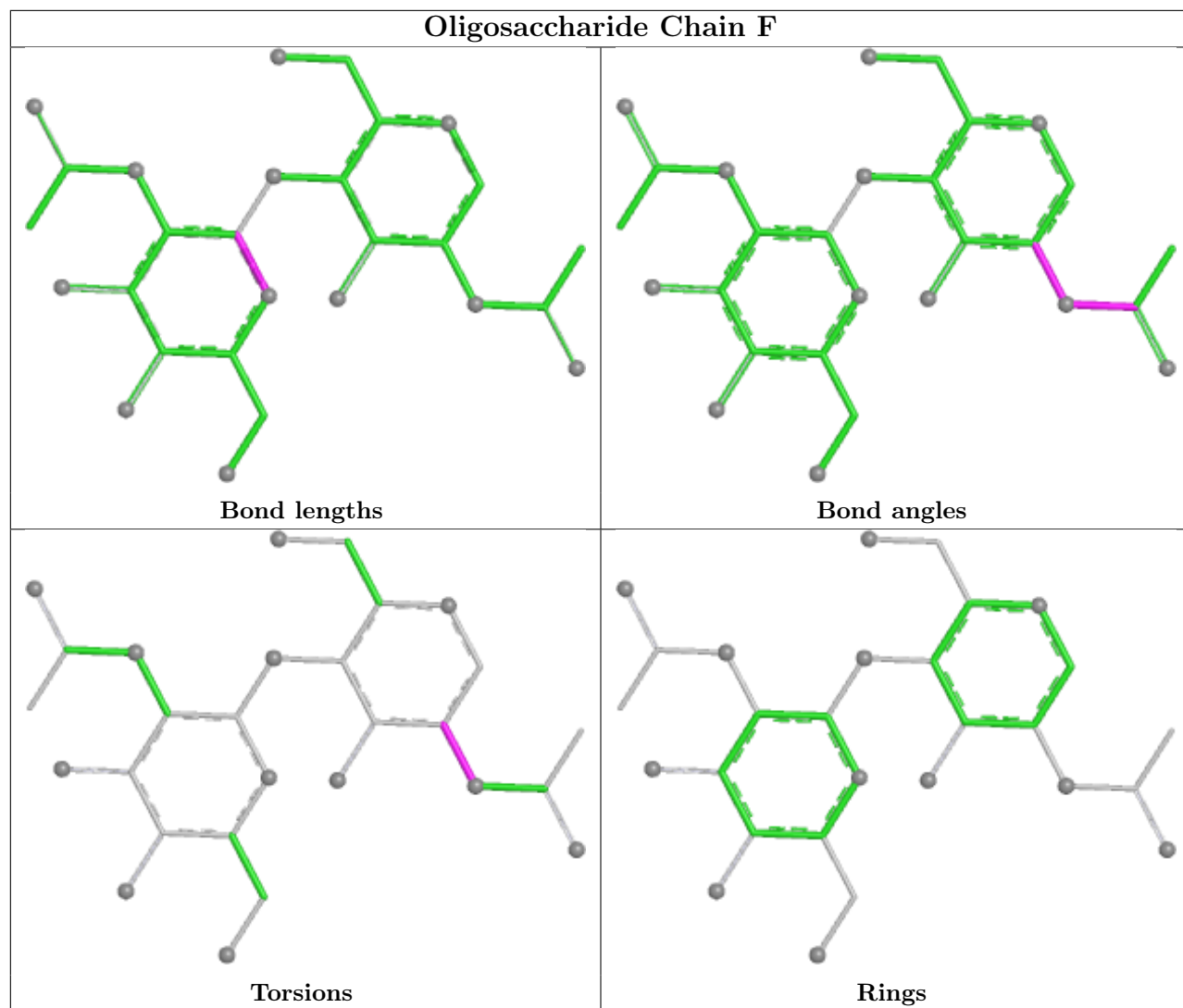
8 monomers are involved in 11 short contacts:

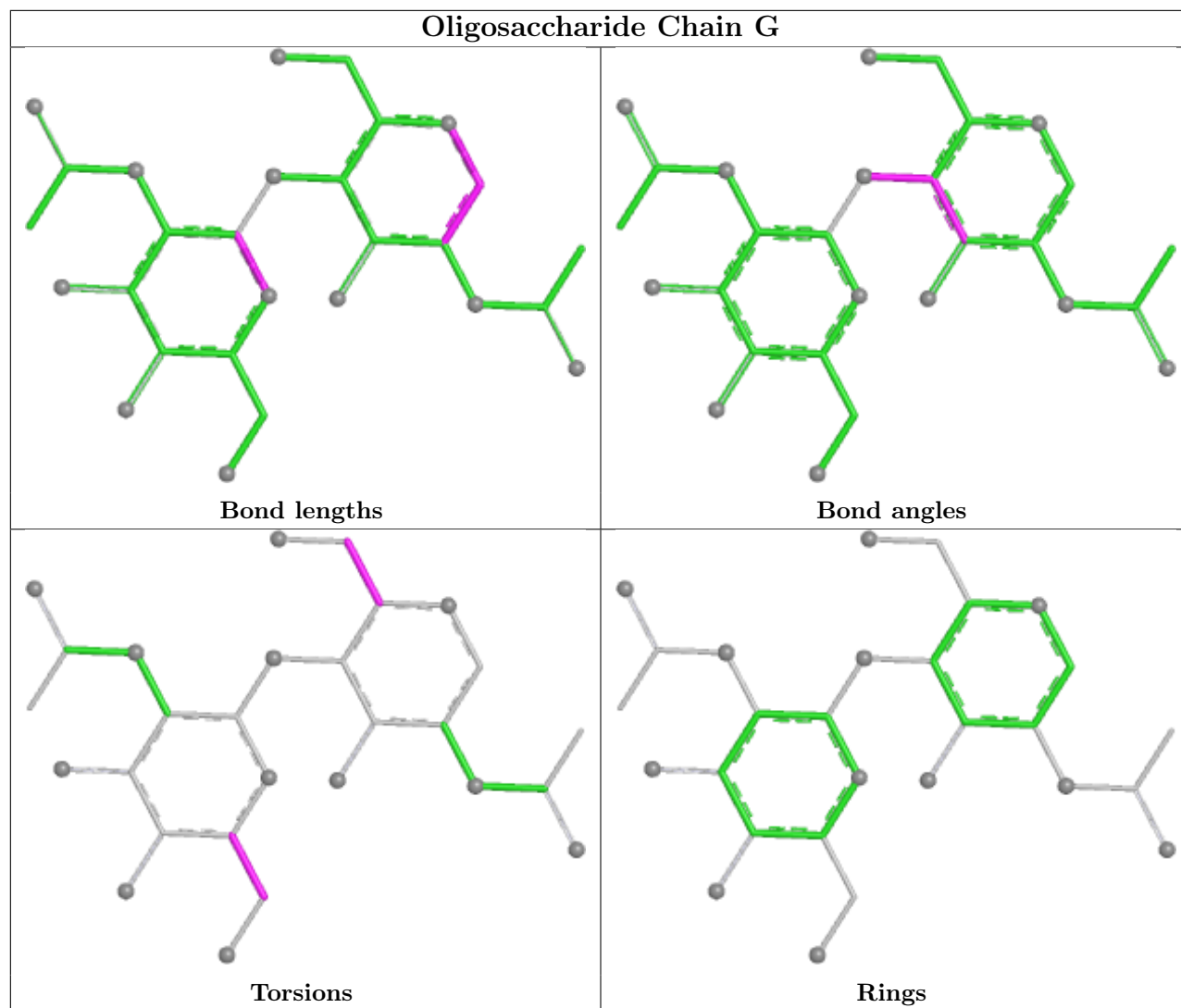
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3	BMA	1	0
2	C	1	NAG	1	0
2	F	1	NAG	1	0
3	D	2	NAG	2	0
2	E	2	NAG	2	0
3	H	2	NAG	2	0
2	E	1	NAG	1	0
3	D	1	NAG	2	0

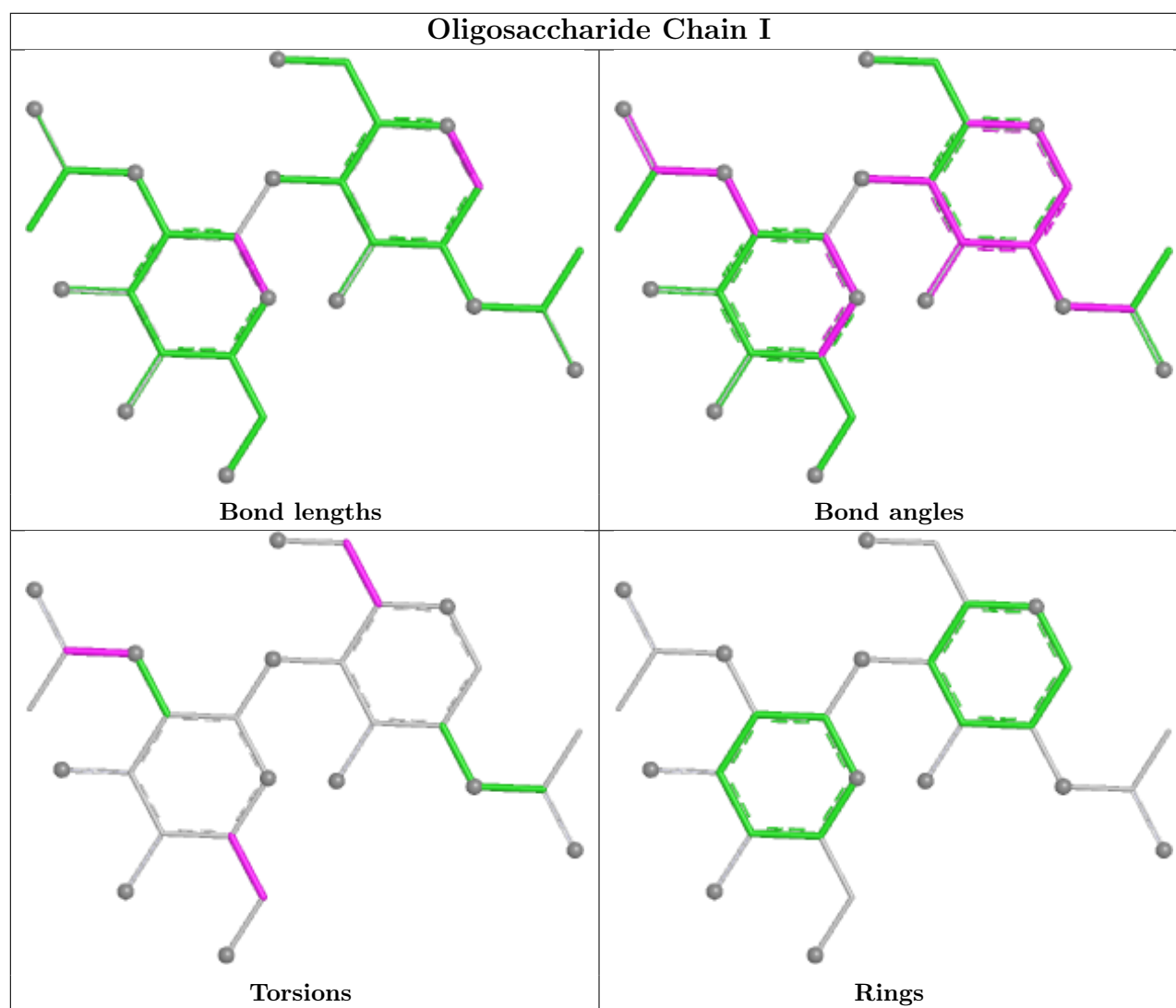
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



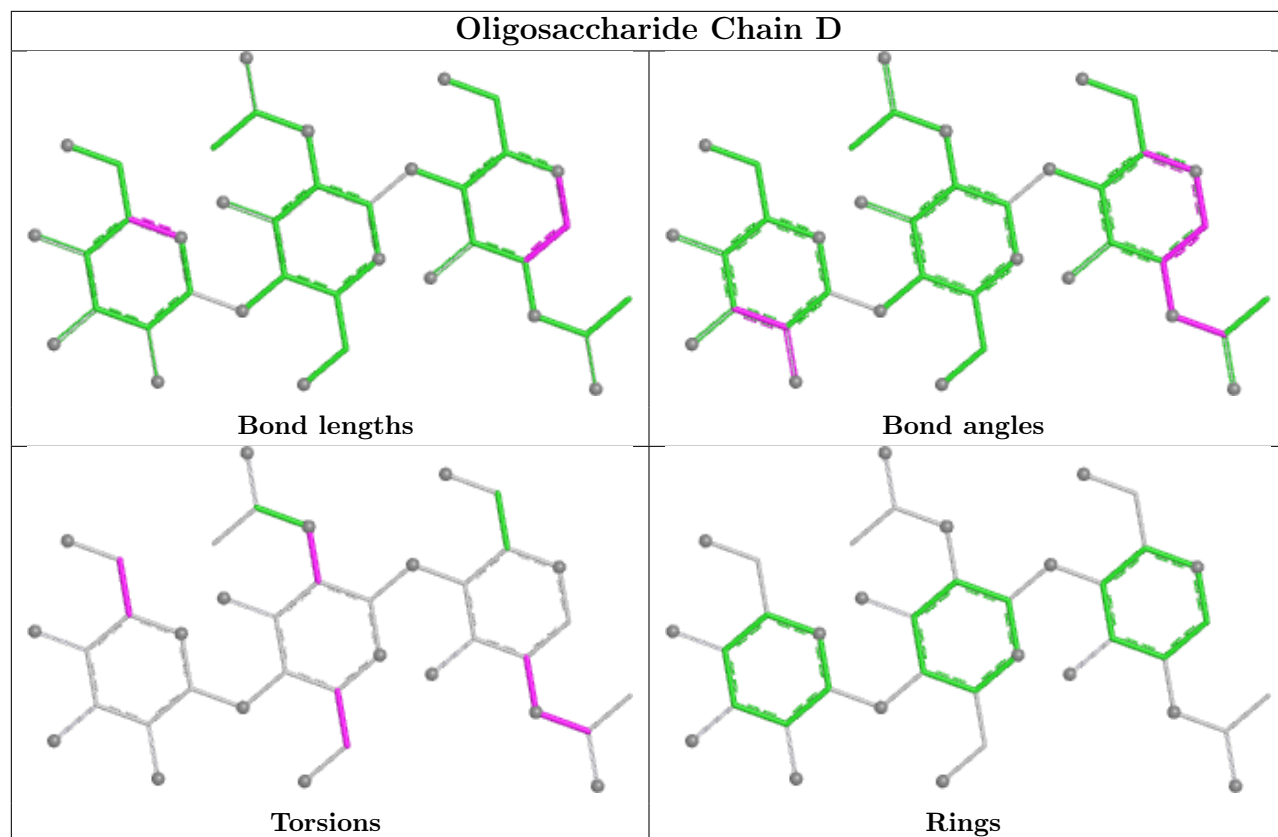




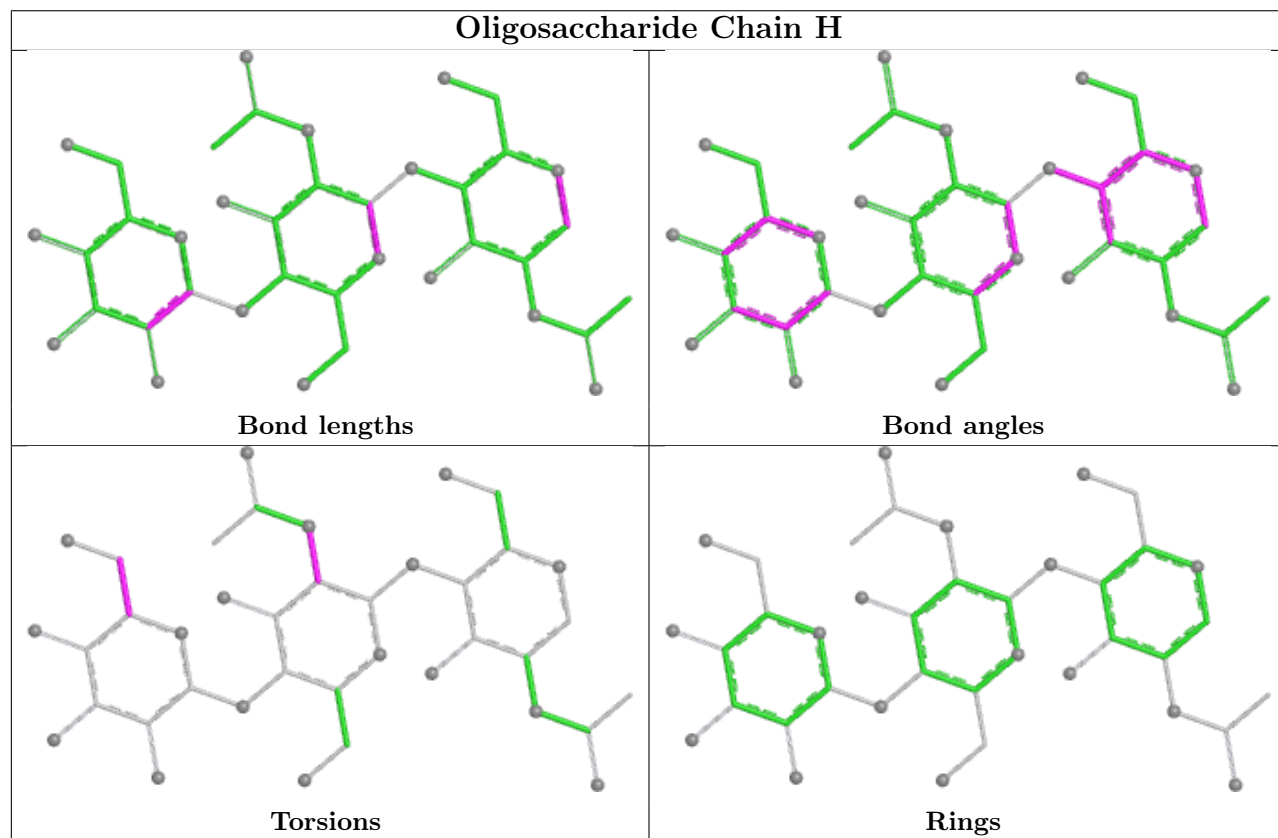




Oligosaccharide Chain D



Oligosaccharide Chain H



5.6 Ligand geometry

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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
6	NAG	B	1106	1	14,14,15	0.47	0	17,19,21	0.69	0
12	PEG	B	1111	-	6,6,6	0.50	0	5,5,5	0.38	0
6	NAG	A	1107	1	14,14,15	1.89	2 (14%)	17,19,21	2.67	4 (23%)
6	NAG	B	1105	1	14,14,15	0.45	0	17,19,21	0.67	0
4	ONN	A	1101[B]	5	40,40,40	2.99	12 (30%)	52,53,53	1.97	11 (21%)
7	SIN	A	1108	-	7,7,7	1.09	0	8,8,8	1.73	3 (37%)
11	PO4	A	1113	-	4,4,4	0.91	0	6,6,6	0.65	0
8	EDO	A	1109	-	3,3,3	0.36	0	2,2,2	0.71	0
8	EDO	A	1110	-	3,3,3	0.50	0	2,2,2	0.31	0
9	PGE	A	1111	-	9,9,9	0.56	0	8,8,8	0.59	0
4	ONN	A	1101[A]	5	40,40,40	3.01	12 (30%)	52,53,53	1.79	13 (25%)
6	NAG	B	1107	1	14,14,15	0.28	0	17,19,21	1.36	2 (11%)
6	NAG	A	1106	1	14,14,15	1.63	2 (14%)	17,19,21	1.10	2 (11%)
10	PG4	A	1112	-	12,12,12	0.55	0	11,11,11	0.26	0
4	ONN	B	1101[B]	5	40,40,40	3.02	13 (32%)	52,53,53	1.85	9 (17%)
6	NAG	A	1105	1	14,14,15	1.92	2 (14%)	17,19,21	1.31	2 (11%)
8	EDO	B	1108	-	3,3,3	0.48	0	2,2,2	0.33	0
6	NAG	B	1103	1	14,14,15	0.84	1 (7%)	17,19,21	1.31	2 (11%)
6	NAG	A	1104	1	14,14,15	0.75	0	17,19,21	1.25	2 (11%)
6	NAG	B	1104	1	14,14,15	1.50	1 (7%)	17,19,21	1.67	3 (17%)
8	EDO	B	1109	-	3,3,3	0.43	0	2,2,2	0.40	0
4	ONN	B	1101[A]	5	40,40,40	2.97	11 (27%)	52,53,53	1.71	10 (19%)
6	NAG	A	1103	1	14,14,15	0.89	1 (7%)	17,19,21	0.68	0
8	EDO	B	1110	-	3,3,3	0.48	0	2,2,2	0.27	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
6	NAG	B	1106	1	-	4/6/23/26	0/1/1/1
12	PEG	B	1111	-	-	2/4/4/4	-
6	NAG	A	1107	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1105	1	-	2/6/23/26	0/1/1/1
4	ONN	A	1101[B]	5	-	15/41/41/41	0/2/3/3
7	SIN	A	1108	-	-	1/5/5/5	-
8	EDO	A	1109	-	-	0/1/1/1	-
8	EDO	A	1110	-	-	0/1/1/1	-
9	PGE	A	1111	-	-	6/7/7/7	-
4	ONN	A	1101[A]	5	-	21/41/41/41	0/2/3/3
6	NAG	B	1107	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1106	1	-	4/6/23/26	0/1/1/1
10	PG4	A	1112	-	-	8/10/10/10	-
4	ONN	B	1101[B]	5	-	19/41/41/41	0/2/3/3
6	NAG	A	1105	1	-	3/6/23/26	0/1/1/1
8	EDO	B	1108	-	-	0/1/1/1	-
6	NAG	B	1103	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1104	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1104	1	-	1/6/23/26	0/1/1/1
8	EDO	B	1109	-	-	0/1/1/1	-
4	ONN	B	1101[A]	5	-	14/41/41/41	0/2/3/3
6	NAG	A	1103	1	-	0/6/23/26	0/1/1/1
8	EDO	B	1110	-	-	1/1/1/1	-

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101[B]	ONN	C7-C6	8.94	1.53	1.38
4	A	1101[B]	ONN	C7-C6	8.83	1.53	1.38
4	A	1101[A]	ONN	C7-C6	8.82	1.53	1.38
4	B	1101[A]	ONN	C7-C6	8.62	1.52	1.38
4	B	1101[A]	ONN	C4-C5	7.63	1.53	1.39

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1101[B]	ONN	C10-C9-N30	-7.56	101.14	110.14
6	A	1107	NAG	C1-C2-N2	-7.37	98.82	110.43
4	A	1101[B]	ONN	C9-C10-C11	-6.54	103.14	112.41
4	B	1101[A]	ONN	C10-C9-N30	-6.44	102.47	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101[B]	ONN	C10-C9-N30	-5.79	103.25	110.14

There are no chirality outliers.

5 of 107 torsion outliers are listed below:

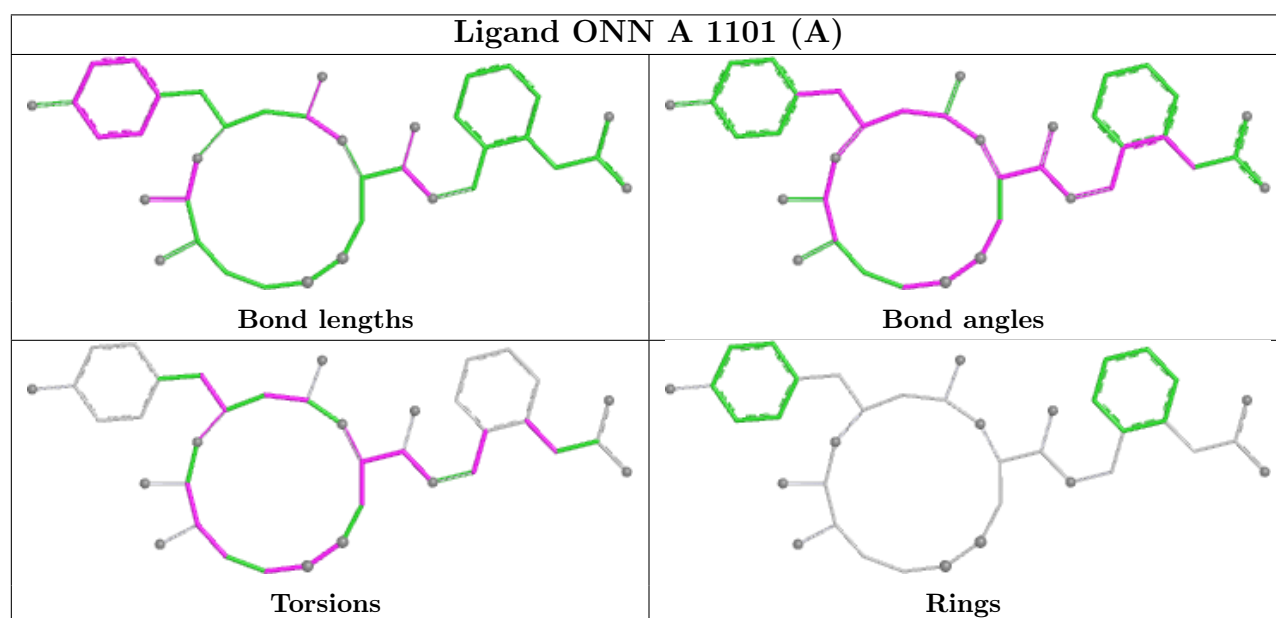
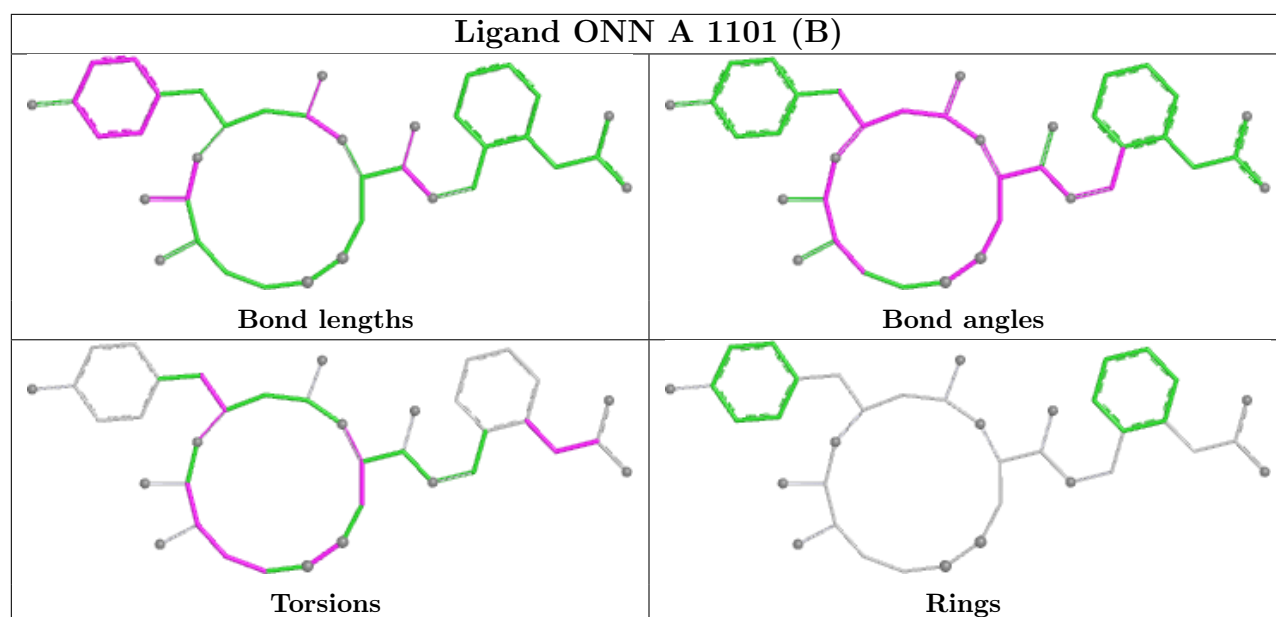
Mol	Chain	Res	Type	Atoms
4	A	1101[A]	ONN	C16-C14-C15-S38
4	A	1101[A]	ONN	N13-C14-C15-S38
4	A	1101[A]	ONN	C16-C14-N13-C11
4	A	1101[A]	ONN	N30-C31-C32-C35
4	A	1101[A]	ONN	O33-C31-C32-C35

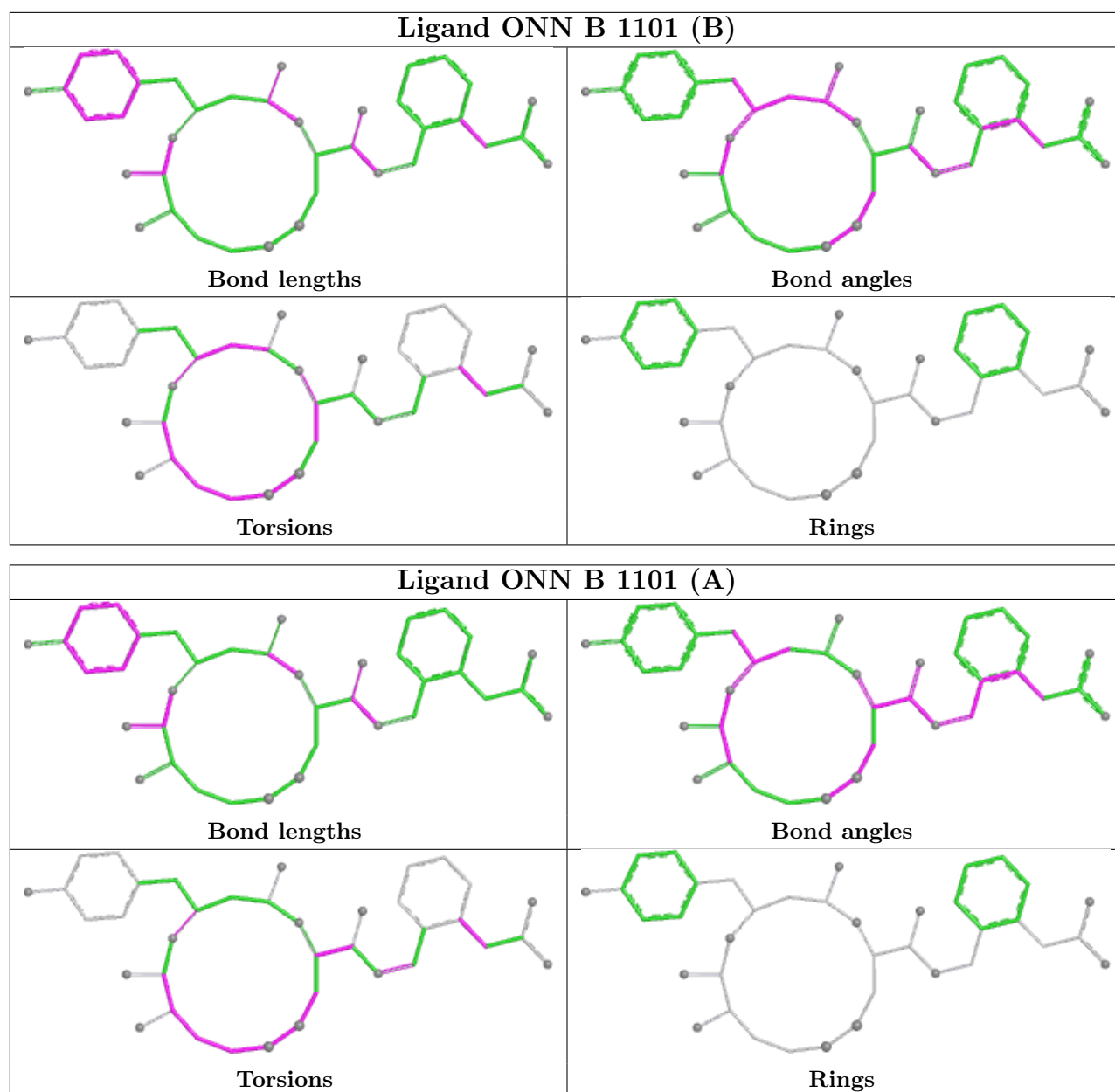
There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1111	PEG	1	0
6	A	1107	NAG	1	0
4	A	1101[B]	ONN	3	0
8	A	1109	EDO	1	0
6	A	1106	NAG	1	0
4	B	1101[B]	ONN	2	0
6	A	1105	NAG	2	0
6	A	1104	NAG	2	0
4	B	1101[A]	ONN	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.





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 [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, 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	856/912 (93%)	0.48	33 (3%) 43 27	16, 38, 64, 103	4 (0%)
1	B	853/912 (93%)	0.47	28 (3%) 49 30	18, 34, 53, 90	0
All	All	1709/1824 (93%)	0.47	61 (3%) 46 28	16, 35, 59, 103	4 (0%)

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	ALA	5.2
1	B	918	ASN	4.9
1	B	223	SER	4.6
1	A	694	ILE	4.2
1	A	248	PRO	4.1

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, 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.

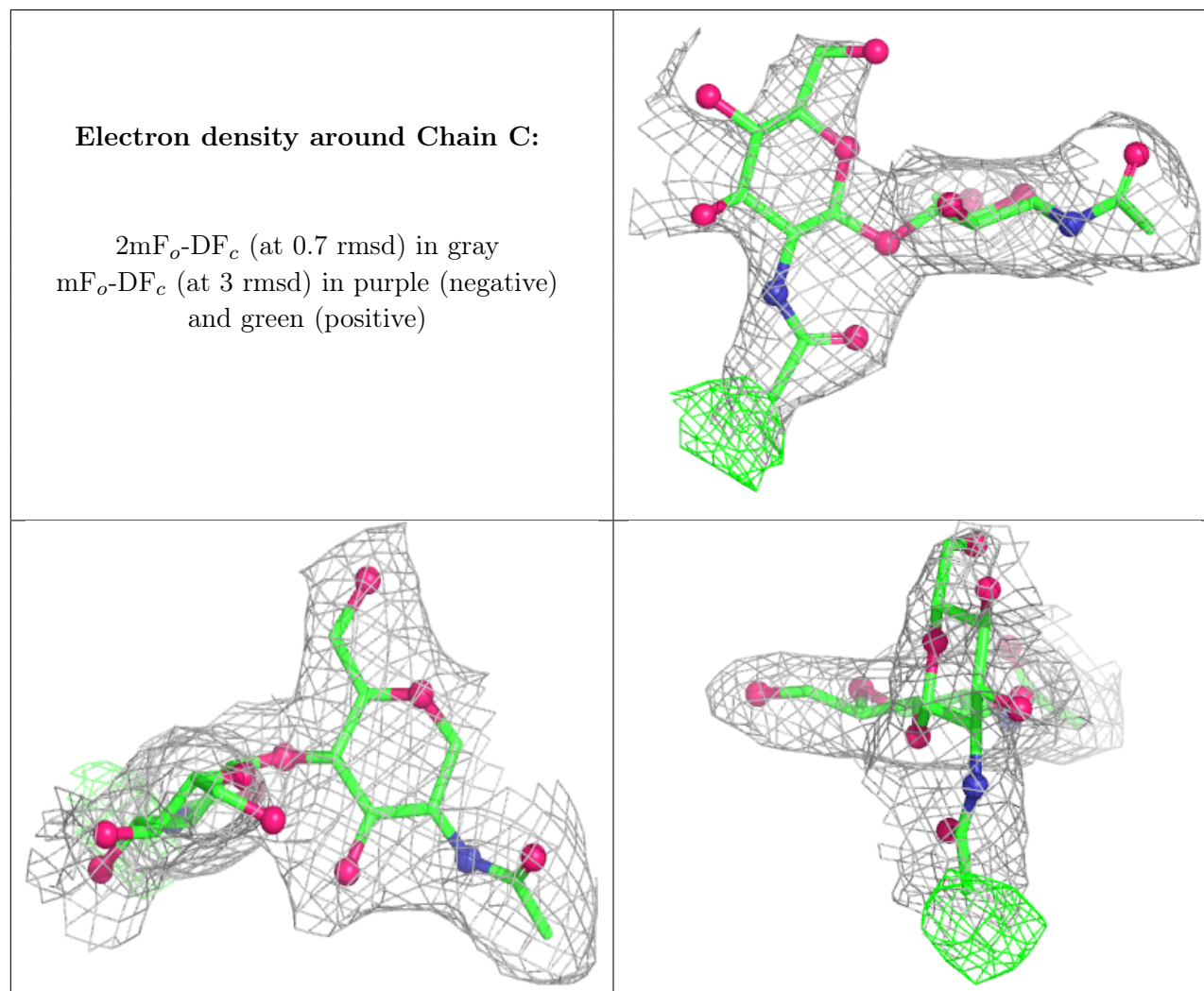
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.35	0.20	58,60,61,61	0
2	NAG	G	2	14/15	0.47	0.16	63,70,79,80	0
2	NAG	F	2	14/15	0.59	0.13	66,66,67,67	0
3	BMA	D	3	11/12	0.63	0.12	74,75,75,75	0
3	BMA	H	3	11/12	0.63	0.13	53,54,54,54	0

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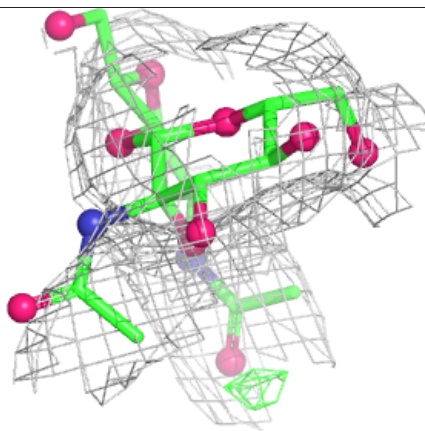
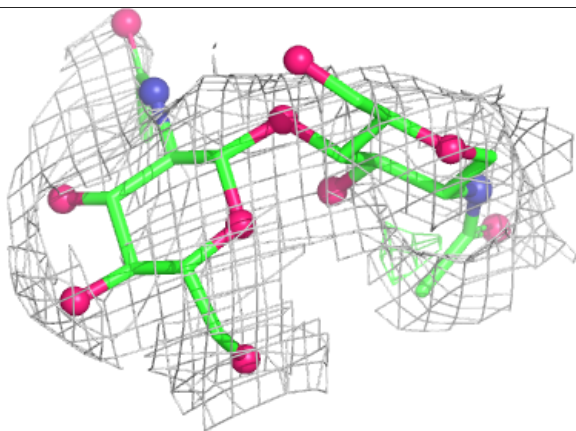
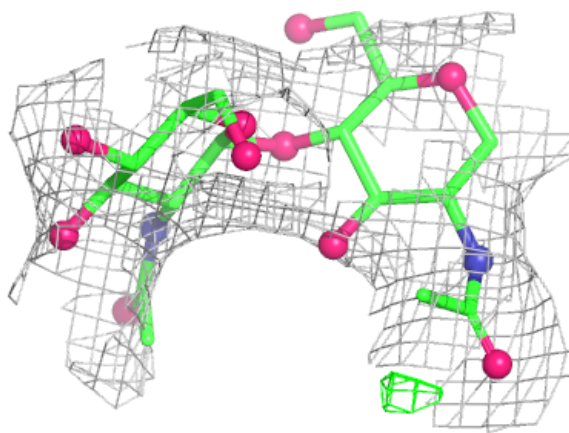
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	2	14/15	0.64	0.16	70,71,73,73	0
2	NAG	C	1	14/15	0.66	0.12	46,54,59,62	0
2	NAG	E	1	14/15	0.70	0.13	69,73,80,81	0
3	NAG	H	2	14/15	0.71	0.15	50,50,51,51	0
2	NAG	I	1	14/15	0.72	0.19	54,54,55,55	0
2	NAG	G	1	14/15	0.72	0.13	54,61,72,73	0
3	NAG	D	1	14/15	0.73	0.13	71,78,82,83	0
2	NAG	I	2	14/15	0.74	0.12	54,55,55,55	0
3	NAG	D	2	14/15	0.80	0.12	67,72,74,75	0
2	NAG	F	1	14/15	0.82	0.11	56,56,57,57	0
3	NAG	H	1	14/15	0.84	0.11	41,42,43,43	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.



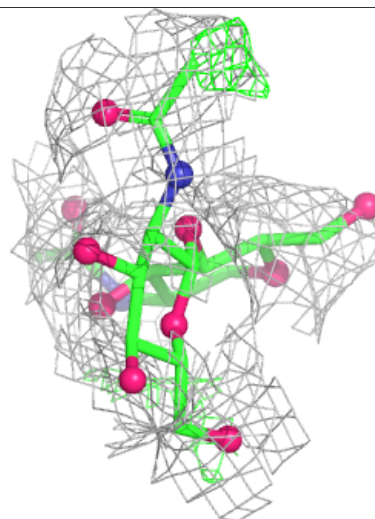
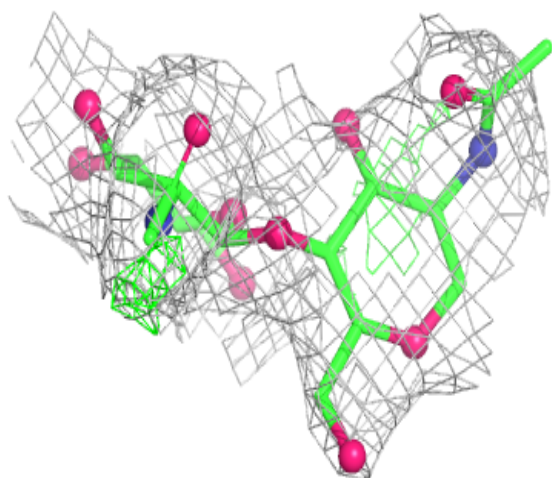
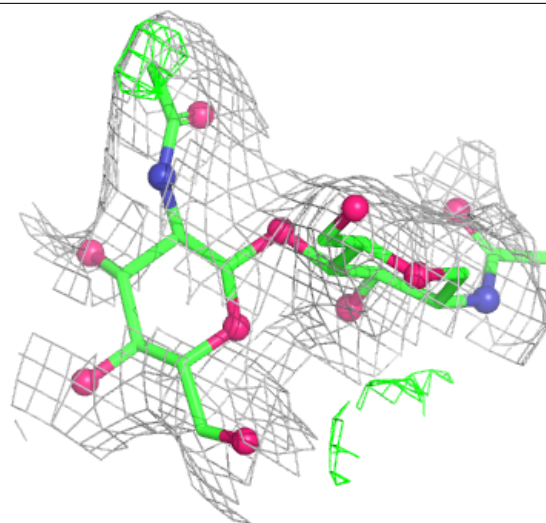
Electron density around Chain E:

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



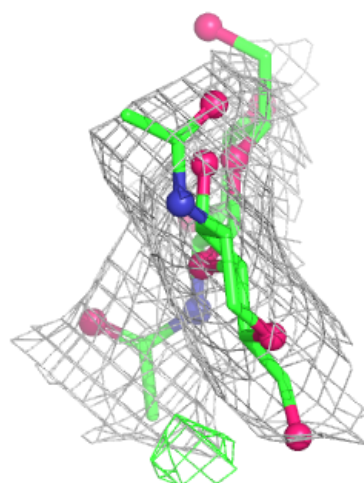
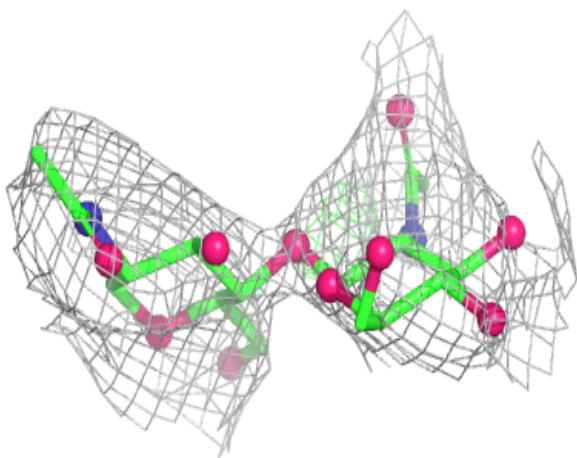
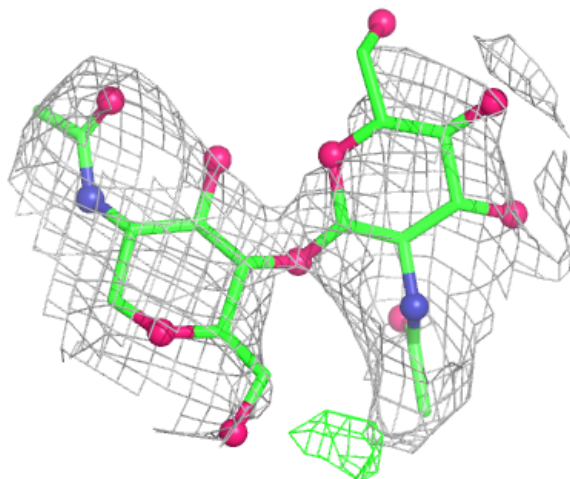
Electron density around Chain F:

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



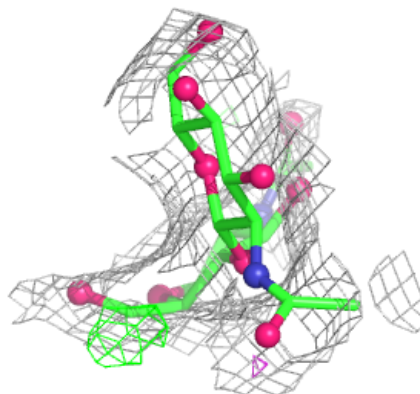
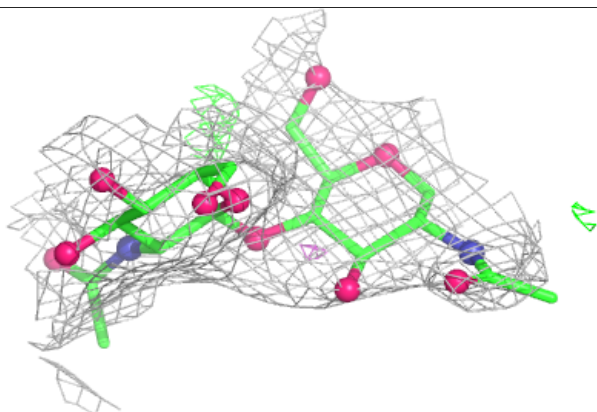
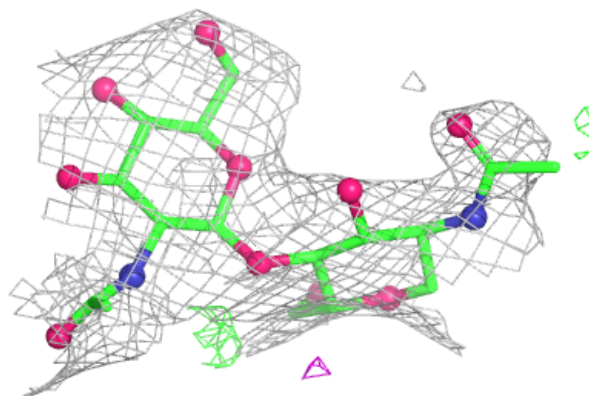
Electron density around Chain G:

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

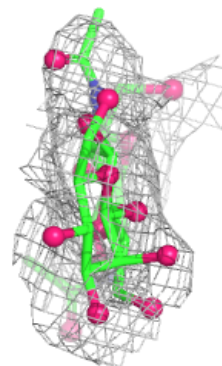
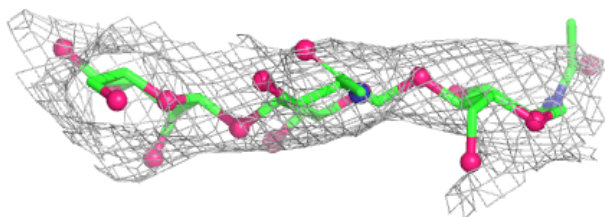
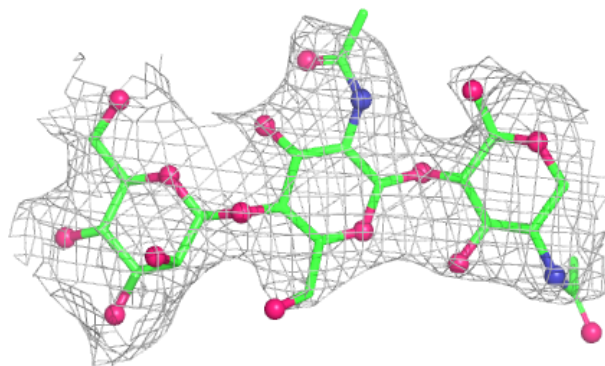


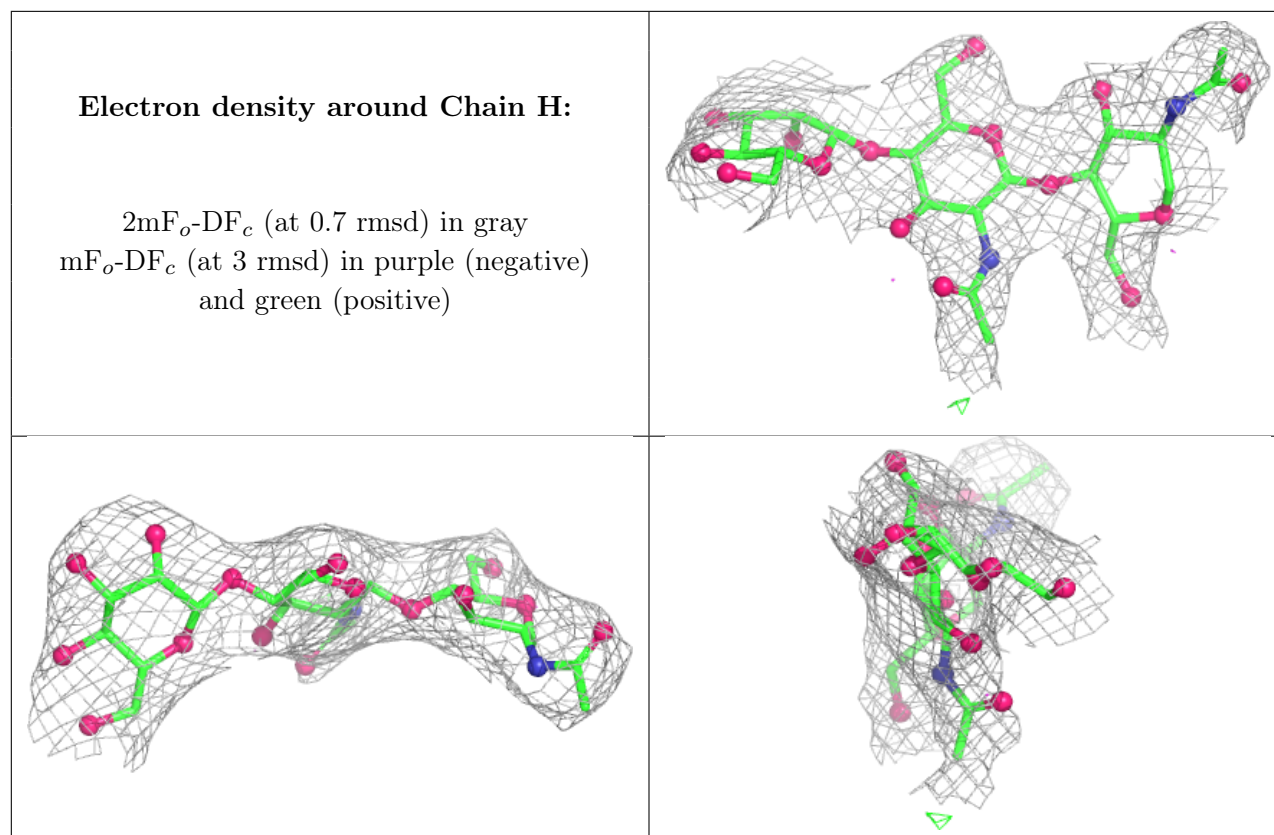
Electron density around Chain I:

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

**Electron density around Chain D:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	B	1105	14/15	0.56	0.16	58,59,59,59	0
9	PGE	A	1111	10/10	0.57	0.14	41,51,55,60	0
6	NAG	A	1107	14/15	0.61	0.13	75,76,77,77	0
6	NAG	A	1106	14/15	0.62	0.13	57,57,57,57	0
12	PEG	B	1111	7/7	0.62	0.23	56,56,56,56	0
6	NAG	A	1103	14/15	0.66	0.12	77,81,84,85	0
6	NAG	B	1106	14/15	0.66	0.12	60,60,61,61	0
6	NAG	B	1107	14/15	0.68	0.12	49,50,50,50	0
6	NAG	A	1104	14/15	0.70	0.11	55,66,69,69	0
8	EDO	B	1109	4/4	0.72	0.14	37,39,40,41	0
6	NAG	A	1105	14/15	0.73	0.12	50,54,58,64	0
8	EDO	B	1108	4/4	0.75	0.14	36,39,39,41	0
10	PG4	A	1112	13/13	0.78	0.13	41,49,55,56	0
7	SIN	A	1108	8/8	0.79	0.12	38,42,45,48	0

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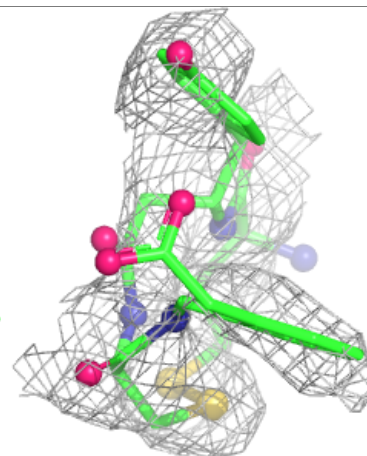
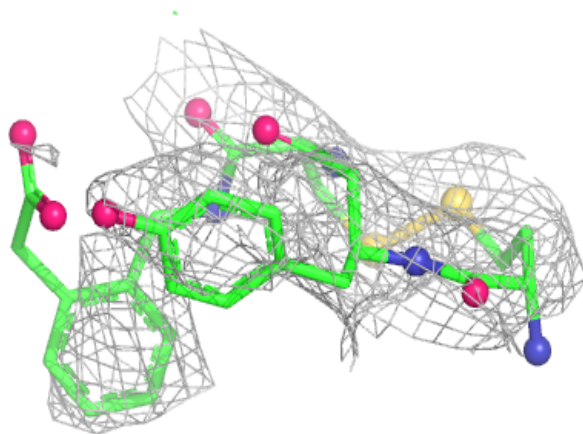
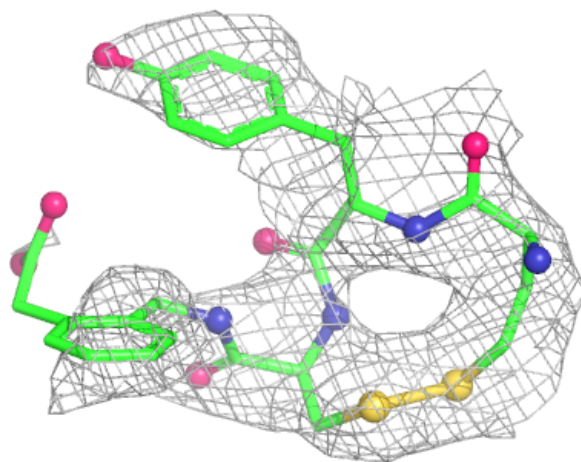
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	EDO	B	1110	4/4	0.81	0.19	24,28,31,33	0
6	NAG	B	1104	14/15	0.83	0.10	55,60,63,64	0
8	EDO	A	1110	4/4	0.84	0.15	26,26,26,26	0
4	ONN	B	1101[B]	38/38	0.85	0.20	40,48,53,59	38
4	ONN	B	1101[A]	38/38	0.85	0.20	33,38,40,46	38
6	NAG	B	1103	14/15	0.85	0.12	52,57,65,66	0
4	ONN	A	1101[A]	38/38	0.86	0.25	33,39,43,48	38
8	EDO	A	1109	4/4	0.86	0.13	35,38,38,40	0
4	ONN	A	1101[B]	38/38	0.86	0.25	33,38,42,48	38
11	PO4	A	1113	5/5	0.90	0.15	59,59,59,59	0
5	ZN	A	1102	1/1	0.99	0.02	49,49,49,49	0
5	ZN	B	1102	1/1	1.00	0.03	35,35,35,35	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.

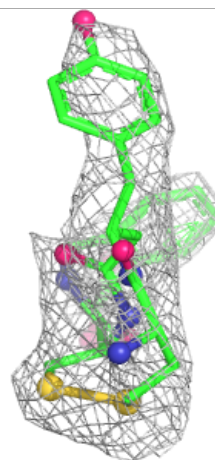
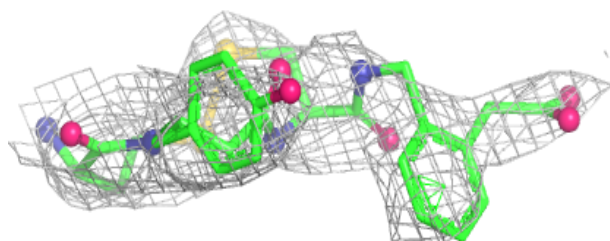
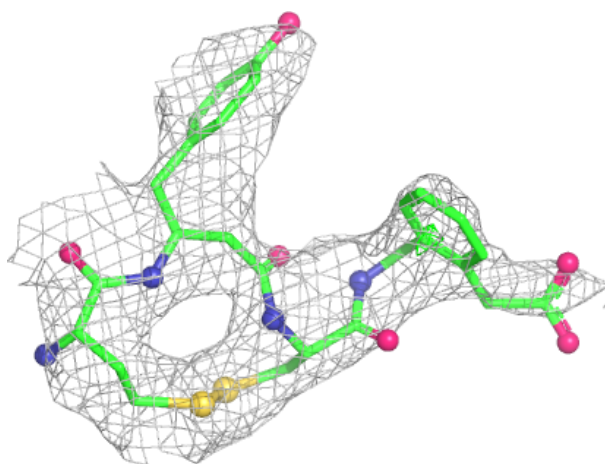
Electron density around ONN B 1101 (B):

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



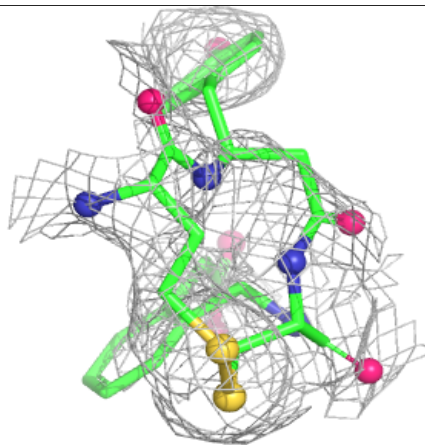
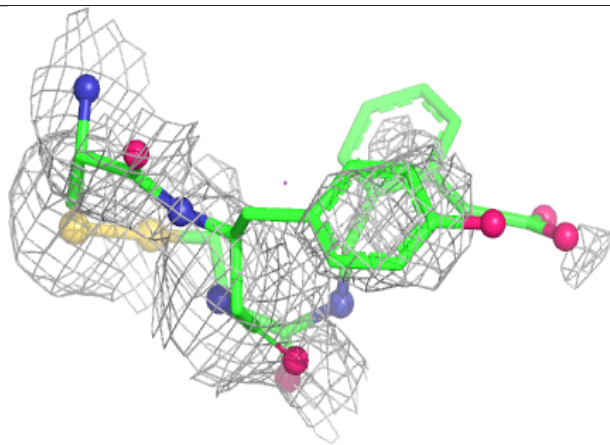
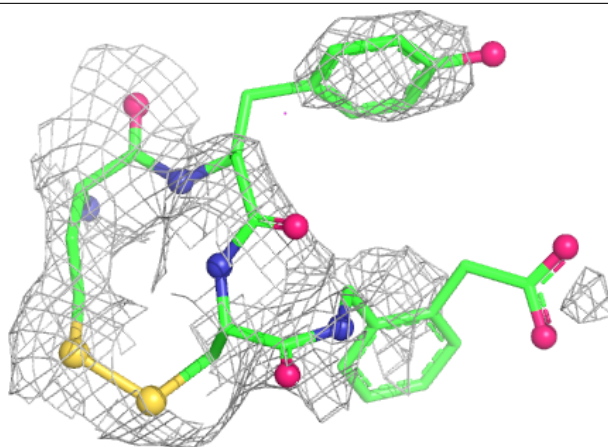
Electron density around ONN B 1101 (A):

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



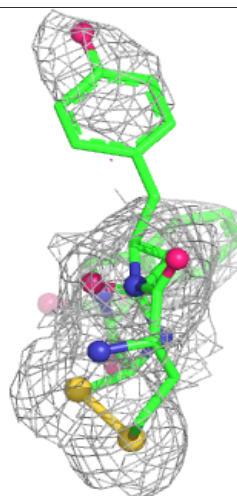
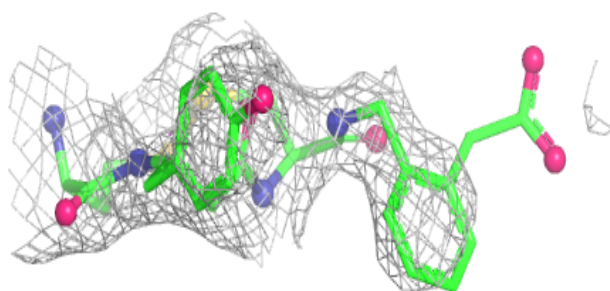
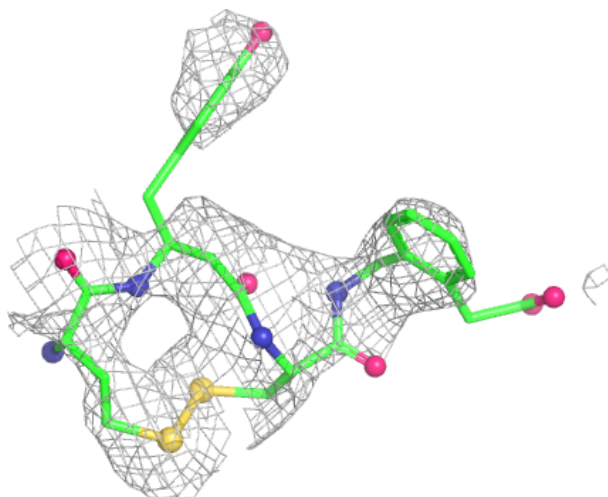
Electron density around ONN A 1101 (A):

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



Electron density around ONN A 1101 (B):

$2mF_o-DF_c$ (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.