



Full wwPDB X-ray Structure Validation Report i

Nov 23, 2023 – 02:58 AM JST

PDB ID : 7YIW
Title : The Crystal Structure of Human Tissue Nonspecific Alkaline Phosphatase (ALPL) at Acidic pH
Authors : Yu, Y.T.; Yao, D.Q.; Zhang, Q.; Rao, B.; Xia, Y.; Lu, Y.; Qin, A.; Cao, Y.
Deposited on : 2022-07-18
Resolution : 2.89 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 i symbol.

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

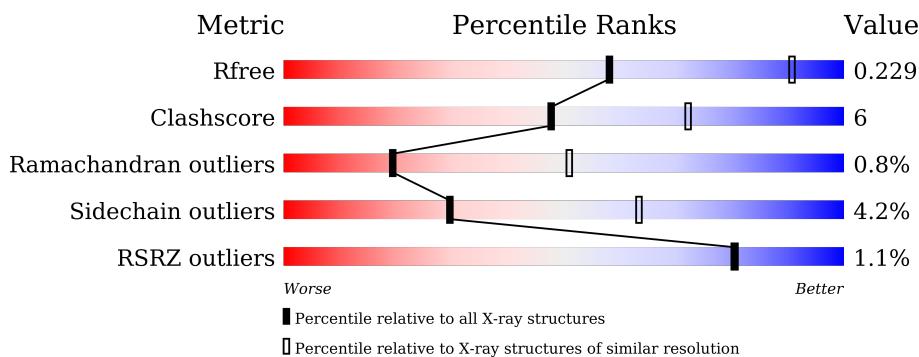
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



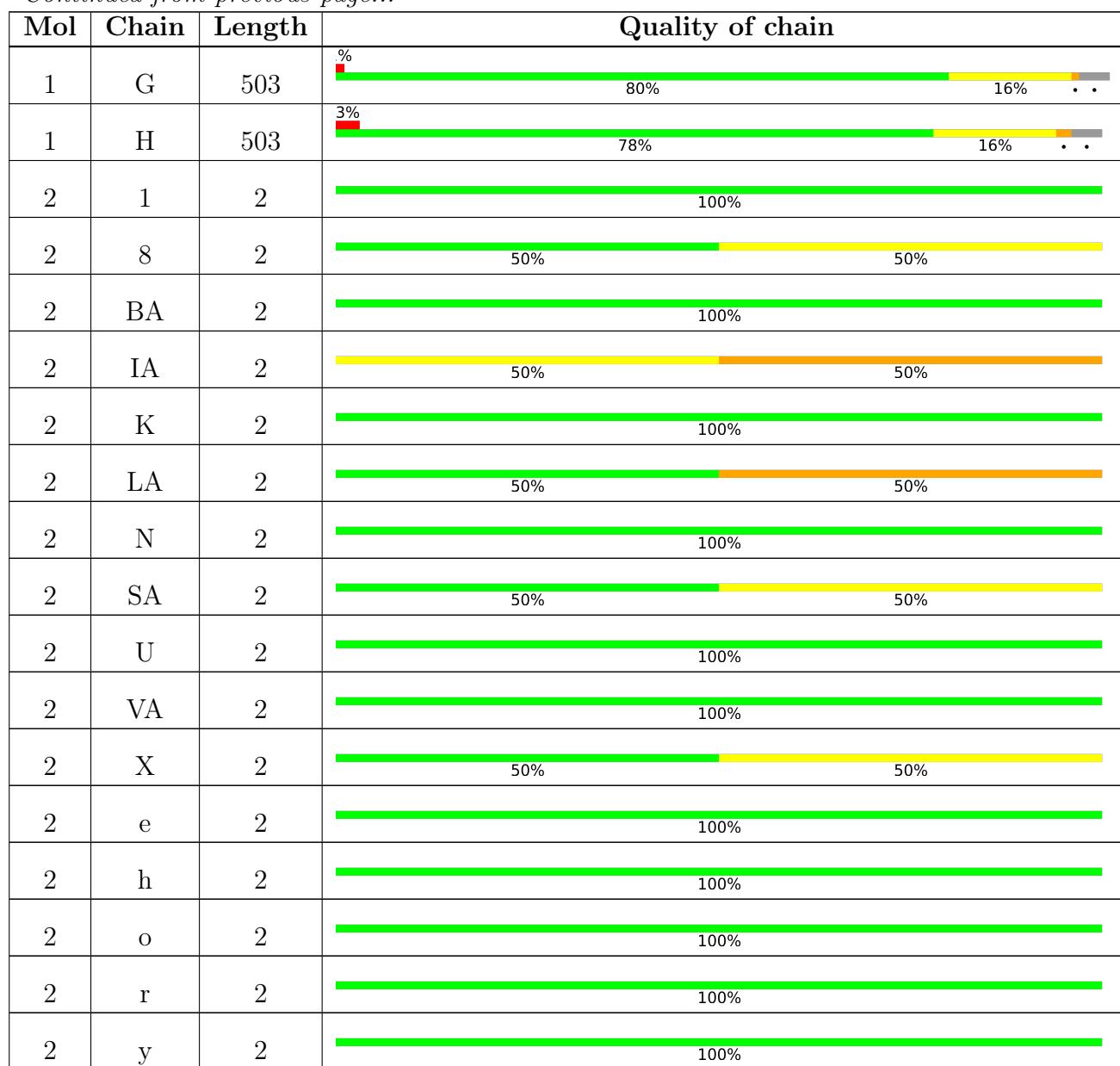
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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.



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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	8	2	-	-	-	X
2	NAG	BA	2	-	-	-	X
2	NAG	IA	2	-	-	-	X
2	NAG	y	2	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 30683 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 Alkaline phosphatase, tissue-nonspecific isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C 3748	N 2345	O 665	S 719	19	0	0
1	D	482	Total	C 3738	N 2339	O 663	S 717	19	0	0
1	C	484	Total	C 3748	N 2345	O 665	S 719	19	0	0
1	B	484	Total	C 3748	N 2345	O 665	S 719	19	0	0
1	G	484	Total	C 3748	N 2345	O 665	S 719	19	0	0
1	H	484	Total	C 3748	N 2345	O 665	S 719	19	0	0
1	F	483	Total	C 3743	N 2342	O 664	S 718	19	0	0
1	E	484	Total	C 3748	N 2345	O 665	S 719	19	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P05186
A	0	LYS	-	expression tag	UNP P05186
A	1	THR	-	expression tag	UNP P05186
A	2	ILE	-	expression tag	UNP P05186
A	3	ILE	-	expression tag	UNP P05186
A	4	ALA	-	expression tag	UNP P05186
A	5	LEU	-	expression tag	UNP P05186
A	6	SER	-	expression tag	UNP P05186
A	7	TYR	-	expression tag	UNP P05186
A	8	ILE	-	expression tag	UNP P05186
A	9	PHE	-	expression tag	UNP P05186
A	10	CYS	-	expression tag	UNP P05186
A	11	LEU	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	VAL	-	expression tag	UNP P05186
A	13	PHE	-	expression tag	UNP P05186
A	14	ALA	-	expression tag	UNP P05186
A	15	GLY	-	expression tag	UNP P05186
A	16	ARG	-	expression tag	UNP P05186
A	17	ALA	-	expression tag	UNP P05186
A	501	ALA	-	expression tag	UNP P05186
D	-1	MET	-	initiating methionine	UNP P05186
D	0	LYS	-	expression tag	UNP P05186
D	1	THR	-	expression tag	UNP P05186
D	2	ILE	-	expression tag	UNP P05186
D	3	ILE	-	expression tag	UNP P05186
D	4	ALA	-	expression tag	UNP P05186
D	5	LEU	-	expression tag	UNP P05186
D	6	SER	-	expression tag	UNP P05186
D	7	TYR	-	expression tag	UNP P05186
D	8	ILE	-	expression tag	UNP P05186
D	9	PHE	-	expression tag	UNP P05186
D	10	CYS	-	expression tag	UNP P05186
D	11	LEU	-	expression tag	UNP P05186
D	12	VAL	-	expression tag	UNP P05186
D	13	PHE	-	expression tag	UNP P05186
D	14	ALA	-	expression tag	UNP P05186
D	15	GLY	-	expression tag	UNP P05186
D	16	ARG	-	expression tag	UNP P05186
D	17	ALA	-	expression tag	UNP P05186
D	501	ALA	-	expression tag	UNP P05186
C	-1	MET	-	initiating methionine	UNP P05186
C	0	LYS	-	expression tag	UNP P05186
C	1	THR	-	expression tag	UNP P05186
C	2	ILE	-	expression tag	UNP P05186
C	3	ILE	-	expression tag	UNP P05186
C	4	ALA	-	expression tag	UNP P05186
C	5	LEU	-	expression tag	UNP P05186
C	6	SER	-	expression tag	UNP P05186
C	7	TYR	-	expression tag	UNP P05186
C	8	ILE	-	expression tag	UNP P05186
C	9	PHE	-	expression tag	UNP P05186
C	10	CYS	-	expression tag	UNP P05186
C	11	LEU	-	expression tag	UNP P05186
C	12	VAL	-	expression tag	UNP P05186
C	13	PHE	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
C	14	ALA	-	expression tag	UNP P05186
C	15	GLY	-	expression tag	UNP P05186
C	16	ARG	-	expression tag	UNP P05186
C	17	ALA	-	expression tag	UNP P05186
C	501	ALA	-	expression tag	UNP P05186
B	-1	MET	-	initiating methionine	UNP P05186
B	0	LYS	-	expression tag	UNP P05186
B	1	THR	-	expression tag	UNP P05186
B	2	ILE	-	expression tag	UNP P05186
B	3	ILE	-	expression tag	UNP P05186
B	4	ALA	-	expression tag	UNP P05186
B	5	LEU	-	expression tag	UNP P05186
B	6	SER	-	expression tag	UNP P05186
B	7	TYR	-	expression tag	UNP P05186
B	8	ILE	-	expression tag	UNP P05186
B	9	PHE	-	expression tag	UNP P05186
B	10	CYS	-	expression tag	UNP P05186
B	11	LEU	-	expression tag	UNP P05186
B	12	VAL	-	expression tag	UNP P05186
B	13	PHE	-	expression tag	UNP P05186
B	14	ALA	-	expression tag	UNP P05186
B	15	GLY	-	expression tag	UNP P05186
B	16	ARG	-	expression tag	UNP P05186
B	17	ALA	-	expression tag	UNP P05186
B	501	ALA	-	expression tag	UNP P05186
G	-1	MET	-	initiating methionine	UNP P05186
G	0	LYS	-	expression tag	UNP P05186
G	1	THR	-	expression tag	UNP P05186
G	2	ILE	-	expression tag	UNP P05186
G	3	ILE	-	expression tag	UNP P05186
G	4	ALA	-	expression tag	UNP P05186
G	5	LEU	-	expression tag	UNP P05186
G	6	SER	-	expression tag	UNP P05186
G	7	TYR	-	expression tag	UNP P05186
G	8	ILE	-	expression tag	UNP P05186
G	9	PHE	-	expression tag	UNP P05186
G	10	CYS	-	expression tag	UNP P05186
G	11	LEU	-	expression tag	UNP P05186
G	12	VAL	-	expression tag	UNP P05186
G	13	PHE	-	expression tag	UNP P05186
G	14	ALA	-	expression tag	UNP P05186
G	15	GLY	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
G	16	ARG	-	expression tag	UNP P05186
G	17	ALA	-	expression tag	UNP P05186
G	501	ALA	-	expression tag	UNP P05186
H	-1	MET	-	initiating methionine	UNP P05186
H	0	LYS	-	expression tag	UNP P05186
H	1	THR	-	expression tag	UNP P05186
H	2	ILE	-	expression tag	UNP P05186
H	3	ILE	-	expression tag	UNP P05186
H	4	ALA	-	expression tag	UNP P05186
H	5	LEU	-	expression tag	UNP P05186
H	6	SER	-	expression tag	UNP P05186
H	7	TYR	-	expression tag	UNP P05186
H	8	ILE	-	expression tag	UNP P05186
H	9	PHE	-	expression tag	UNP P05186
H	10	CYS	-	expression tag	UNP P05186
H	11	LEU	-	expression tag	UNP P05186
H	12	VAL	-	expression tag	UNP P05186
H	13	PHE	-	expression tag	UNP P05186
H	14	ALA	-	expression tag	UNP P05186
H	15	GLY	-	expression tag	UNP P05186
H	16	ARG	-	expression tag	UNP P05186
H	17	ALA	-	expression tag	UNP P05186
H	501	ALA	-	expression tag	UNP P05186
F	-1	MET	-	initiating methionine	UNP P05186
F	0	LYS	-	expression tag	UNP P05186
F	1	THR	-	expression tag	UNP P05186
F	2	ILE	-	expression tag	UNP P05186
F	3	ILE	-	expression tag	UNP P05186
F	4	ALA	-	expression tag	UNP P05186
F	5	LEU	-	expression tag	UNP P05186
F	6	SER	-	expression tag	UNP P05186
F	7	TYR	-	expression tag	UNP P05186
F	8	ILE	-	expression tag	UNP P05186
F	9	PHE	-	expression tag	UNP P05186
F	10	CYS	-	expression tag	UNP P05186
F	11	LEU	-	expression tag	UNP P05186
F	12	VAL	-	expression tag	UNP P05186
F	13	PHE	-	expression tag	UNP P05186
F	14	ALA	-	expression tag	UNP P05186
F	15	GLY	-	expression tag	UNP P05186
F	16	ARG	-	expression tag	UNP P05186
F	17	ALA	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
F	501	ALA	-	expression tag	UNP P05186
E	-1	MET	-	initiating methionine	UNP P05186
E	0	LYS	-	expression tag	UNP P05186
E	1	THR	-	expression tag	UNP P05186
E	2	ILE	-	expression tag	UNP P05186
E	3	ILE	-	expression tag	UNP P05186
E	4	ALA	-	expression tag	UNP P05186
E	5	LEU	-	expression tag	UNP P05186
E	6	SER	-	expression tag	UNP P05186
E	7	TYR	-	expression tag	UNP P05186
E	8	ILE	-	expression tag	UNP P05186
E	9	PHE	-	expression tag	UNP P05186
E	10	CYS	-	expression tag	UNP P05186
E	11	LEU	-	expression tag	UNP P05186
E	12	VAL	-	expression tag	UNP P05186
E	13	PHE	-	expression tag	UNP P05186
E	14	ALA	-	expression tag	UNP P05186
E	15	GLY	-	expression tag	UNP P05186
E	16	ARG	-	expression tag	UNP P05186
E	17	ALA	-	expression tag	UNP P05186
E	501	ALA	-	expression tag	UNP P05186

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



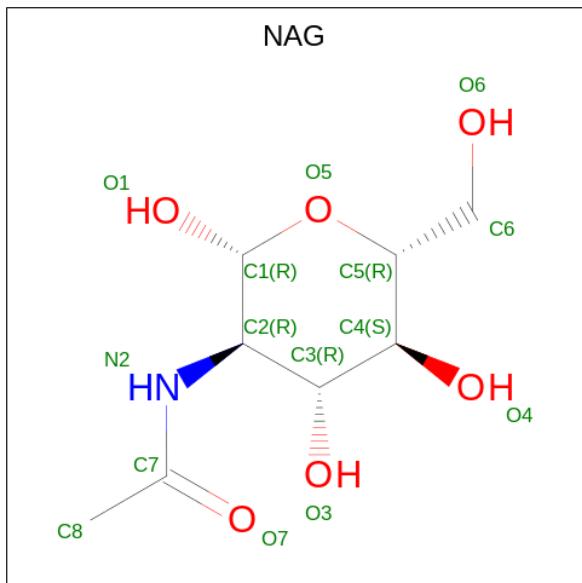
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	h	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	o	2	Total C N O 28 16 2 10	0	0	0
2	r	2	Total C N O 28 16 2 10	0	0	0
2	y	2	Total C N O 28 16 2 10	0	0	0
2	1	2	Total C N O 28 16 2 10	0	0	0
2	8	2	Total C N O 28 16 2 10	0	0	0
2	BA	2	Total C N O 28 16 2 10	0	0	0
2	IA	2	Total C N O 28 16 2 10	0	0	0
2	LA	2	Total C N O 28 16 2 10	0	0	0
2	SA	2	Total C N O 28 16 2 10	0	0	0
2	VA	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0
5	C	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0
5	G	2	Total Zn 2 2	0	0
5	H	2	Total Zn 2 2	0	0
5	F	2	Total Zn 2 2	0	0
5	E	2	Total Zn 2 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0

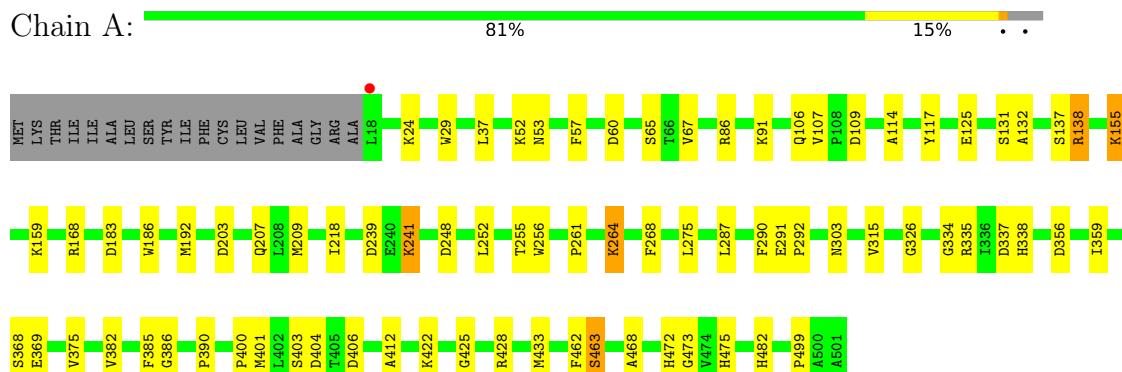
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	2	Total O 2 2	0	0
7	B	4	Total O 4 4	0	0
7	G	2	Total O 2 2	0	0
7	H	1	Total O 1 1	0	0
7	F	1	Total O 1 1	0	0

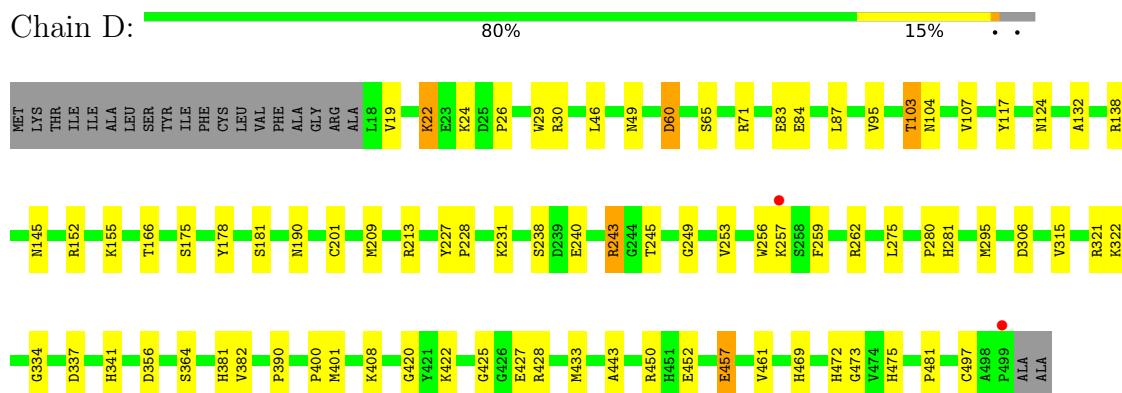
3 Residue-property plots

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.

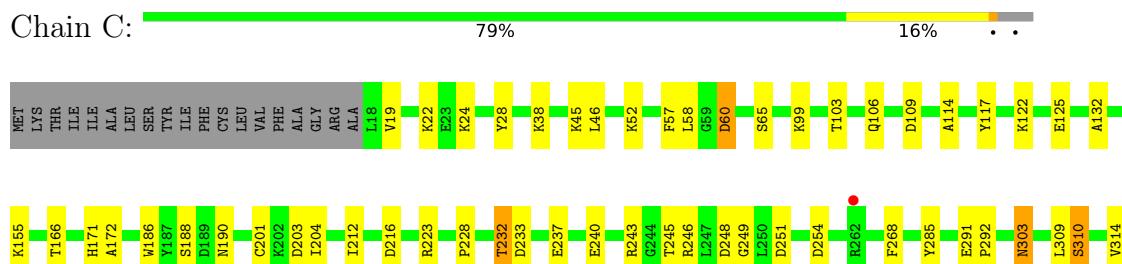
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

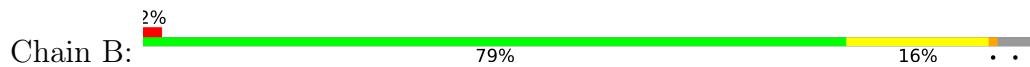


- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

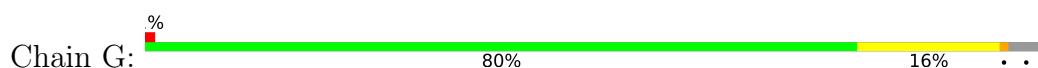




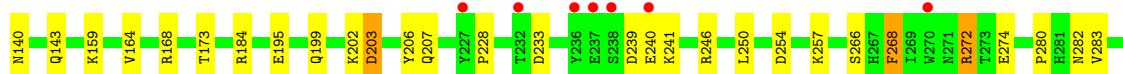
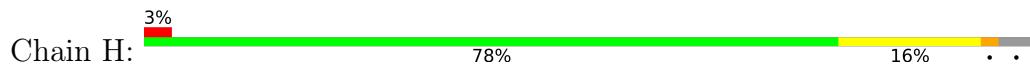
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

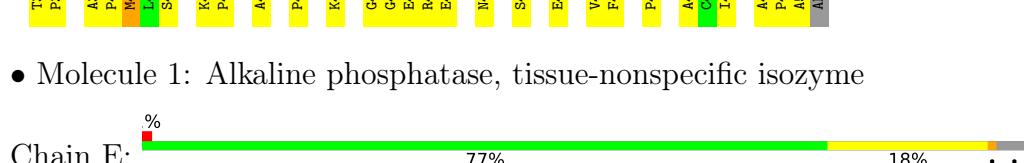
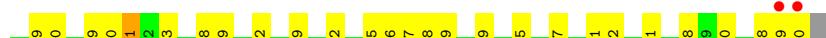
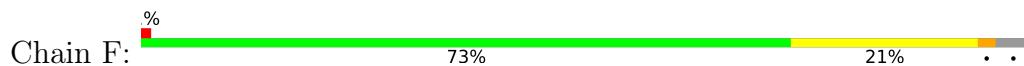


- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme





- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



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



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





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

Chain U:  100%

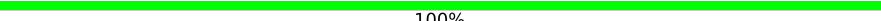


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50%  50%

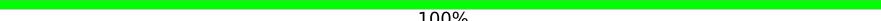


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%



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

Chain h:  100%

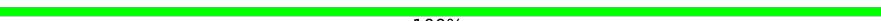


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%

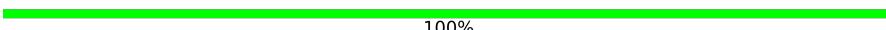


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%



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

Chain y:  100%



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

Chain 1:  100%

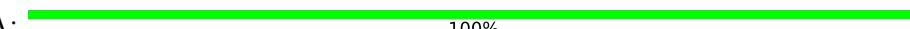


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:  50% 50%



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

Chain BA:  100%



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

Chain IA:  50% 50%



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

Chain LA:  50% 50%



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

Chain SA:  50% 50%

MAG1
MAG2

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

Chain VA:  100%

MAG1
MAG2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	159.36 Å 166.53 Å 181.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 2.89 48.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.96-2.89) 99.8 (48.96-2.89)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.43 (at 2.91 Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ????)	Depositor
R , R_{free}	0.201 , 0.230 0.198 , 0.229	Depositor DCC
R_{free} test set	2003 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30683	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, NAG, ZN

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	0.24	0/3834	0.49	0/5201
1	B	0.24	0/3834	0.49	0/5201
1	C	0.24	0/3834	0.48	0/5201
1	D	0.25	0/3824	0.50	0/5187
1	E	0.25	0/3834	0.50	0/5201
1	F	0.25	0/3829	0.51	0/5194
1	G	0.24	0/3834	0.49	0/5201
1	H	0.25	0/3834	0.50	1/5201 (0.0%)
All	All	0.25	0/30657	0.50	1/41587 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	168	ARG	NE-CZ-NH1	5.11	122.85	120.30

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	3748	0	3628	38	0
1	B	3748	0	3629	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3748	0	3629	47	0
1	D	3738	0	3619	41	0
1	E	3748	0	3628	54	0
1	F	3743	0	3624	67	0
1	G	3748	0	3629	48	0
1	H	3748	0	3629	50	0
2	1	28	0	25	0	0
2	8	28	0	25	1	0
2	BA	28	0	25	0	0
2	IA	28	0	25	2	0
2	K	28	0	25	0	0
2	LA	28	0	25	1	0
2	N	28	0	25	0	0
2	SA	28	0	25	1	0
2	U	28	0	25	0	0
2	VA	28	0	25	0	0
2	X	28	0	25	1	0
2	e	28	0	25	0	0
2	h	28	0	25	0	0
2	o	28	0	25	0	0
2	r	28	0	25	0	0
2	y	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	1	0
3	C	28	0	26	1	0
3	D	28	0	26	0	0
3	E	28	0	26	2	0
3	F	28	0	26	1	0
3	G	28	0	26	1	0
3	H	28	0	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	B	4	0	0	0	0
7	D	2	0	0	0	0
7	F	1	0	0	0	0
7	G	2	0	0	0	0
7	H	1	0	0	0	0
All	All	30683	0	29623	368	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 6.

All (368) 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:F:239:ASP:OD1	1:F:241:LYS:HD2	1.68	0.94
1:F:246:ARG:HH11	1:F:252:LEU:HD11	1.38	0.88
1:E:109:ASP:OD2	1:E:184:ARG:NH1	2.10	0.83
1:C:390:PRO:HD3	1:C:400:PRO:HG3	1.60	0.82
1:F:268:PHE:HD1	1:F:287:LEU:HD12	1.48	0.78
1:F:132:ALA:HB3	1:E:24:LYS:HA	1.67	0.77
1:G:107:VAL:HG21	1:H:386:GLY:HA2	1.69	0.75
1:A:472:HIS:H	1:A:475:HIS:HE1	1.36	0.74
1:F:386:GLY:HA2	1:E:107:VAL:HG21	1.70	0.74
1:G:240:GLU:HG2	1:G:243:ARG:HE	1.53	0.73
1:D:275:LEU:HD11	1:D:315:VAL:HG21	1.69	0.73
1:B:390:PRO:HD3	1:B:400:PRO:HG3	1.70	0.73
1:G:132:ALA:HB3	1:H:24:LYS:HA	1.69	0.73
1:E:390:PRO:HD3	1:E:400:PRO:HG3	1.71	0.73
1:C:463:SER:HB3	1:C:468:ALA:HB1	1.69	0.73
1:G:390:PRO:HD3	1:G:400:PRO:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:GLU:OE1	1:H:240:GLU:N	2.24	0.70
1:D:24:LYS:HA	1:C:132:ALA:HB3	1.72	0.70
1:G:60:ASP:HB3	1:G:337:ASP:HB2	1.73	0.70
1:A:386:GLY:HA2	1:B:107:VAL:HG21	1.74	0.69
1:E:281:HIS:HA	1:E:322:LYS:HE2	1.74	0.69
1:F:57:PHE:HB2	1:F:375:VAL:HG22	1.74	0.68
1:G:24:LYS:HA	1:H:132:ALA:HB3	1.74	0.68
1:C:473:GLY:H	1:C:475:HIS:CE1	2.11	0.68
1:B:473:GLY:H	1:B:475:HIS:CE1	2.12	0.67
1:D:473:GLY:H	1:D:475:HIS:CE1	2.13	0.66
1:A:107:VAL:HG21	1:B:386:GLY:HA2	1.78	0.66
1:E:248:ASP:HB3	1:E:250:LEU:HG	1.78	0.65
1:C:346:LYS:HD3	1:C:439:ASN:HA	1.77	0.65
1:B:346:LYS:HD3	1:B:439:ASN:HA	1.78	0.65
1:G:448:PRO:O	1:H:403:SER:OG	2.15	0.65
1:E:283:VAL:O	1:E:322:LYS:NZ	2.31	0.64
1:D:390:PRO:HD3	1:D:400:PRO:HG3	1.80	0.63
1:C:408:LYS:NZ	1:C:428:ARG:O	2.31	0.63
1:G:283:VAL:O	1:G:322:LYS:NZ	2.31	0.62
1:G:246:ARG:NH2	1:G:248:ASP:OD2	2.32	0.62
1:F:390:PRO:HD3	1:F:400:PRO:HG3	1.80	0.62
1:F:102:ASN:HB2	1:F:105:ALA:HB3	1.81	0.62
1:H:110:SER:HB2	1:H:184:ARG:HH12	1.65	0.61
1:F:403:SER:OG	1:E:448:PRO:O	2.18	0.61
1:A:24:LYS:HA	1:B:132:ALA:HB3	1.82	0.61
1:D:472:HIS:H	1:D:475:HIS:HE1	1.47	0.61
1:F:310:SER:OG	1:F:354:GLU:OE2	2.19	0.61
1:D:60:ASP:HB2	1:D:334:GLY:HA2	1.82	0.61
1:F:346:LYS:HD3	1:F:439:ASN:HA	1.83	0.61
1:H:390:PRO:HD3	1:H:400:PRO:HG3	1.83	0.60
1:D:83:GLU:OE2	1:C:106:GLN:HB2	2.02	0.60
1:F:226:MET:HA	1:F:252:LEU:HD12	1.84	0.60
1:H:310:SER:OG	1:H:354:GLU:OE2	2.19	0.59
1:F:278:LEU:HD13	1:F:283:VAL:HG21	1.83	0.59
1:A:482:HIS:HD2	1:B:34:GLN:HE21	1.50	0.59
1:H:274:GLU:OE2	2:8:1:NAG:H62	2.03	0.59
1:C:228:PRO:HB3	1:C:249:GLY:HA2	1.85	0.59
1:G:248:ASP:HB3	1:G:250:LEU:H	1.67	0.59
1:A:473:GLY:H	1:A:475:HIS:CE1	2.21	0.59
1:H:375:VAL:HB	1:H:462:PHE:HB2	1.84	0.59
1:A:261:PRO:HB2	1:A:264:LYS:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:386:GLY:HA2	1:H:107:VAL:HG21	1.85	0.59
1:F:248:ASP:HB3	1:F:250:LEU:HD13	1.83	0.59
1:H:380:SER:OG	1:H:381:HIS:N	2.36	0.58
1:F:274:GLU:OE2	2:IA:1:NAG:H62	2.03	0.58
1:A:132:ALA:HB3	1:B:24:LYS:HA	1.86	0.58
1:F:55:ILE:HB	1:F:373:THR:HG23	1.85	0.58
1:F:268:PHE:CD1	1:F:287:LEU:HD12	2.34	0.58
1:F:408:LYS:HG2	2:LA:1:NAG:H82	1.87	0.57
1:A:106:GLN:HB2	1:B:83:GLU:OE2	2.05	0.57
1:H:140:ASN:N	1:H:140:ASN:OD1	2.37	0.57
1:F:255:THR:HG22	1:F:259:PHE:CE1	2.39	0.57
1:G:332:GLU:OE2	1:G:334:GLY:HA2	2.04	0.56
1:E:274:GLU:OE2	2:SA:1:NAG:H62	2.05	0.56
1:A:406:ASP:OD2	1:A:428:ARG:HD3	2.05	0.56
1:F:126:GLY:HA2	1:F:184:ARG:HG2	1.88	0.56
1:C:240:GLU:HA	1:C:243:ARG:HG3	1.87	0.56
1:C:251:ASP:OD2	1:C:254:ASP:HB2	2.05	0.56
1:C:467:MET:HB3	1:C:470:LEU:HD22	1.87	0.56
1:E:409:PRO:O	1:E:428:ARG:NH2	2.38	0.56
1:E:346:LYS:HD3	1:E:439:ASN:HA	1.88	0.56
1:D:22:LYS:NZ	1:B:80:ASN:OD1	2.36	0.55
1:F:97:LEU:HG	1:E:95:VAL:HG11	1.89	0.55
1:F:46:LEU:HD13	1:E:44:GLN:HG2	1.89	0.55
1:A:57:PHE:HB2	1:A:375:VAL:HG22	1.88	0.55
1:H:104:ASN:HB2	1:H:124:ASN:HA	1.89	0.55
1:F:214:ASP:OD1	1:F:214:ASP:N	2.38	0.55
1:F:223:ARG:NH1	1:F:233:ASP:OD2	2.33	0.55
1:B:291:GLU:HG3	1:B:295:MET:HA	1.87	0.55
1:G:310:SER:OG	1:G:354:GLU:OE2	2.25	0.54
1:A:218:ILE:HB	1:A:287:LEU:HD12	1.90	0.54
1:H:122:LYS:NZ	1:H:476:GLU:OE1	2.36	0.54
1:A:356:ASP:HA	1:A:359:ILE:HD12	1.90	0.54
1:C:57:PHE:HB2	1:C:375:VAL:HG22	1.89	0.54
1:H:409:PRO:O	1:H:428:ARG:NH2	2.41	0.54
1:C:223:ARG:NH1	1:C:233:ASP:OD2	2.42	0.53
1:A:209:MET:SD	1:A:256:TRP:HB2	2.48	0.53
1:A:60:ASP:HB2	1:A:334:GLY:HA2	1.90	0.53
1:B:140:ASN:OD1	1:B:140:ASN:N	2.37	0.53
1:A:65:SER:HA	1:B:457:GLU:HB3	1.90	0.53
1:E:84:GLU:OE1	1:E:391:ARG:NH2	2.33	0.53
1:F:24:LYS:HA	1:E:132:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:SER:HA	1:H:457:GLU:HB3	1.91	0.52
1:G:349:LEU:O	1:G:353:VAL:HG23	2.09	0.52
1:E:117:TYR:HE2	1:E:378:ASP:HB3	1.74	0.52
1:E:202:LYS:HD3	1:E:206:TYR:CE1	2.45	0.52
1:G:118:LEU:HD12	1:G:176:ALA:HB3	1.91	0.52
1:D:104:ASN:HB2	1:D:124:ASN:HA	1.92	0.52
1:B:481:PRO:HA	1:B:484:MET:HE2	1.92	0.52
1:F:254:ASP:O	1:F:258:SER:OG	2.27	0.52
1:F:275:LEU:HD11	1:F:315:VAL:HG21	1.91	0.52
1:F:378:ASP:OD1	1:F:378:ASP:N	2.41	0.52
1:D:427:GLU:HA	1:D:427:GLU:OE1	2.11	0.51
1:C:314:VAL:HG13	1:C:365:LEU:HD11	1.93	0.51
1:H:60:ASP:HB2	1:H:334:GLY:HA2	1.92	0.51
1:F:54:VAL:HG12	1:F:328:PHE:HD2	1.76	0.51
1:F:209:MET:HG3	1:F:252:LEU:HB3	1.92	0.51
1:D:337:ASP:OD1	1:D:381:HIS:NE2	2.40	0.51
1:B:173:THR:HG21	1:B:332:GLU:HG3	1.92	0.51
1:G:228:PRO:HA	1:G:246:ARG:HB2	1.92	0.51
1:H:53:ASN:HB2	1:H:371:THR:HG23	1.92	0.51
1:F:60:ASP:OD2	1:F:332:GLU:OE2	2.27	0.51
1:A:114:ALA:HA	1:A:117:TYR:CZ	2.46	0.51
1:H:202:LYS:HD3	1:H:206:TYR:CE1	2.46	0.51
1:E:317:ILE:O	1:E:321:ARG:HG3	2.11	0.51
1:D:49:ASN:OD1	1:B:281:HIS:NE2	2.43	0.51
1:B:60:ASP:HB2	1:B:334:GLY:HA2	1.92	0.51
1:H:342:GLU:HB3	1:H:344:LYS:HE3	1.93	0.51
1:G:57:PHE:HB2	1:G:375:VAL:HG22	1.93	0.51
1:D:46:LEU:HB3	1:D:469:HIS:CE1	2.46	0.51
1:D:87:LEU:HB3	1:D:356:ASP:OD2	2.11	0.50
1:C:473:GLY:H	1:C:475:HIS:HE1	1.58	0.50
1:F:255:THR:HG22	1:F:259:PHE:HE1	1.76	0.50
1:D:281:HIS:NE2	1:B:49:ASN:OD1	2.34	0.50
1:C:166:THR:HG23	1:C:309:LEU:HD13	1.92	0.50
1:B:346:LYS:HG3	1:B:396:PHE:CZ	2.46	0.50
1:B:195:GLU:O	1:B:199:GLN:HG3	2.12	0.50
1:H:173:THR:HG21	1:H:332:GLU:HG3	1.93	0.50
1:C:228:PRO:HA	1:C:246:ARG:HB2	1.93	0.50
1:D:213:ARG:HD3	1:D:259:PHE:CD2	2.47	0.50
1:B:261:PRO:HB2	1:B:263:TYR:CE1	2.47	0.50
1:F:111:ALA:HB1	1:F:128:VAL:HG12	1.93	0.50
1:E:57:PHE:HB2	1:E:375:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:LYS:NZ	1:F:214:ASP:O	2.38	0.49
1:G:166:THR:HG23	1:G:309:LEU:HD13	1.95	0.49
1:E:472:HIS:H	1:E:475:HIS:HE1	1.60	0.49
1:D:132:ALA:HB3	1:C:24:LYS:HA	1.93	0.49
1:B:46:LEU:HB3	1:B:469:HIS:CE1	2.47	0.49
1:G:38:LYS:O	1:G:42:GLU:HG3	2.12	0.49
1:C:171:HIS:CG	1:C:172:ALA:N	2.81	0.49
1:F:114:ALA:HA	1:F:117:TYR:CZ	2.48	0.49
3:B:602:NAG:HG83	3:B:602:NAG:H3	1.93	0.49
1:F:457:GLU:HB2	1:E:65:SER:HA	1.93	0.49
1:H:463:SER:HB3	1:H:468:ALA:HB1	1.95	0.48
1:E:417:ASN:HB2	1:E:449:LEU:HD12	1.94	0.48
1:F:239:ASP:OD1	1:F:240:GLU:N	2.46	0.48
1:H:164:VAL:HG23	1:H:329:LEU:HD11	1.95	0.48
1:F:117:TYR:HA	1:F:481:PRO:HD3	1.94	0.48
1:C:472:HIS:H	1:C:475:HIS:HE1	1.60	0.48
1:G:173:THR:HG21	1:G:332:GLU:HG3	1.95	0.48
1:E:430:ASN:OD1	1:E:432:SER:OG	2.31	0.48
1:D:473:GLY:H	1:D:475:HIS:HE1	1.60	0.48
1:B:406:ASP:OD2	1:B:428:ARG:NH1	2.47	0.48
1:B:472:HIS:H	1:B:475:HIS:HE1	1.62	0.48
1:F:63:GLY:O	1:F:67:VAL:HG13	2.14	0.48
1:C:46:LEU:HD13	1:C:469:HIS:CD2	2.49	0.48
1:E:63:GLY:O	1:E:67:VAL:HG13	2.13	0.48
1:H:240:GLU:H	1:H:240:GLU:CD	2.15	0.47
1:F:488:ALA:HB3	1:F:490:ILE:HG12	1.96	0.47
1:C:401:MET:SD	1:C:401:MET:N	2.87	0.47
1:B:114:ALA:O	1:B:118:LEU:HB2	2.14	0.47
1:D:240:GLU:OE1	1:D:243:ARG:NH1	2.48	0.47
1:G:223:ARG:HA	1:G:289:LEU:HD23	1.96	0.47
1:F:117:TYR:CE2	1:F:378:ASP:HB3	2.49	0.47
1:B:473:GLY:H	1:B:475:HIS:HE1	1.59	0.47
1:D:253:VAL:HG12	1:D:257:LYS:HE3	1.96	0.47
1:G:388:TYR:HA	1:H:107:VAL:HB	1.96	0.47
1:B:219:MET:HG2	1:B:290:PHE:HE2	1.80	0.47
1:F:498:ALA:O	1:F:500:ALA:N	2.48	0.47
1:H:73:LEU:HD22	1:H:349:LEU:HB3	1.97	0.47
1:A:155:LYS:NZ	1:A:159:LYS:O	2.44	0.46
1:D:95:VAL:HA	1:D:461:VAL:O	2.15	0.46
1:D:227:TYR:HB3	1:D:231:LYS:HD3	1.97	0.46
1:B:302:ASN:OD1	1:B:304:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TRP:CG	1:A:192:MET:HG2	2.50	0.46
1:A:463:SER:HB3	1:A:468:ALA:HB1	1.98	0.46
1:D:253:VAL:O	1:D:257:LYS:HG3	2.15	0.46
1:B:337:ASP:OD1	1:B:381:HIS:NE2	2.46	0.46
1:G:114:ALA:HA	1:G:117:TYR:CZ	2.50	0.46
1:F:60:ASP:HB3	1:F:337:ASP:HB2	1.97	0.46
1:F:117:TYR:HE2	1:F:378:ASP:HB3	1.80	0.46
1:E:467:MET:HA	1:E:469:HIS:CE1	2.50	0.46
1:F:227:TYR:HE1	1:F:253:VAL:HG21	1.81	0.46
1:D:420:GLY:HA3	1:D:443:ALA:O	2.16	0.46
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.98	0.46
1:G:117:TYR:CE2	1:G:378:ASP:HB3	2.51	0.46
1:H:272:ARG:NH1	1:H:311:GLU:OE2	2.49	0.46
1:G:92:PHE:CZ	1:G:464:LYS:HE2	2.51	0.46
1:E:269:ILE:HD13	1:E:286:LEU:HD11	1.97	0.46
1:D:228:PRO:HB3	1:D:249:GLY:HA2	1.99	0.45
1:E:240:GLU:HG2	1:E:243:ARG:HE	1.81	0.45
1:D:71:ARG:HG3	1:D:87:LEU:HG	1.97	0.45
1:H:239:ASP:OD1	1:H:241:LYS:N	2.49	0.45
1:E:188:SER:HB3	1:E:225:TYR:HD1	1.82	0.45
1:A:192:MET:HE2	1:A:203:ASP:HB3	1.97	0.45
1:D:103:THR:HG21	1:D:132:ALA:HB1	1.99	0.45
1:E:420:GLY:HA3	1:E:443:ALA:O	2.16	0.45
1:D:26:PRO:O	1:D:30:ARG:HG3	2.17	0.45
1:B:117:TYR:HE2	1:B:378:ASP:HB3	1.82	0.45
1:F:239:ASP:OD1	1:F:241:LYS:N	2.49	0.45
1:B:140:ASN:HA	1:B:143:GLN:HE22	1.82	0.45
1:F:271:ASN:OD1	1:F:274:GLU:HG3	2.17	0.45
1:E:301:ARG:O	3:E:602:NAG:H82	2.16	0.45
1:C:38:LYS:HA	1:C:38:LYS:HD3	1.82	0.45
1:F:409:PRO:O	1:F:428:ARG:NH2	2.50	0.45
1:E:312:MET:HB2	1:E:312:MET:HE2	1.72	0.45
1:H:423:VAL:HA	1:H:428:ARG:HA	1.98	0.45
1:F:408:LYS:NZ	1:F:427:GLU:HG3	2.31	0.45
1:G:117:TYR:HE2	1:G:378:ASP:HB3	1.80	0.45
1:A:131:SER:HB3	1:B:26:PRO:HG3	1.99	0.45
1:F:401:MET:SD	1:F:401:MET:N	2.89	0.45
1:C:216:ASP:HA	1:C:285:TYR:HD1	1.80	0.45
1:F:188:SER:HA	1:F:203:ASP:OD2	2.16	0.45
3:E:602:NAG:O7	3:E:602:NAG:O3	2.32	0.45
1:D:107:VAL:HG21	1:C:386:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASP:O	1:B:35:GLU:HG3	2.18	0.44
1:B:272:ARG:HG2	1:B:276:LEU:HD23	1.98	0.44
1:G:273:THR:O	1:G:277:THR:OG1	2.30	0.44
1:G:317:ILE:O	1:G:321:ARG:HG2	2.17	0.44
1:H:117:TYR:HE2	1:H:378:ASP:HB3	1.82	0.44
1:H:291:GLU:HG3	1:H:295:MET:HA	2.00	0.44
1:F:230:ASN:HA	1:F:243:ARG:HD2	1.98	0.44
1:A:86:ARG:NH1	1:A:91:LYS:HG2	2.33	0.44
1:A:239:ASP:OD1	1:A:241:LYS:N	2.50	0.44
1:D:166:THR:O	1:D:295:MET:HB2	2.17	0.44
1:C:186:TRP:O	1:C:204:ILE:HG13	2.18	0.44
1:B:344:LYS:HD3	1:B:440:ASN:HA	2.00	0.44
1:G:323:ASN:OD1	1:G:325:LYS:HG3	2.18	0.44
1:G:344:LYS:HE2	1:G:440:ASN:HB3	1.99	0.44
1:F:203:ASP:OD1	1:F:203:ASP:N	2.45	0.44
1:D:457:GLU:HB3	1:C:65:SER:HA	2.00	0.44
1:C:52:LYS:O	1:C:326:GLY:HA3	2.18	0.44
1:C:114:ALA:HA	1:C:117:TYR:CZ	2.53	0.44
1:D:381:HIS:ND1	1:D:452:GLU:OE1	2.50	0.44
1:C:381:HIS:HB3	1:C:452:GLU:OE2	2.17	0.44
1:E:117:TYR:CE2	1:E:378:ASP:HB3	2.53	0.44
1:D:84:GLU:H	1:D:84:GLU:CD	2.20	0.44
1:H:424:VAL:N	1:H:427:GLU:O	2.51	0.44
1:G:291:GLU:HG3	1:G:292:PRO:HD2	1.99	0.44
1:C:60:ASP:O	1:C:336:ILE:HB	2.18	0.44
1:E:240:GLU:OE1	1:E:241:LYS:HD2	2.17	0.44
1:A:275:LEU:HD12	1:A:290:PHE:CZ	2.52	0.44
1:B:42:GLU:O	1:B:45:LYS:HG2	2.18	0.44
1:E:173:THR:HG21	1:E:332:GLU:HG3	1.99	0.44
1:A:291:GLU:HG3	1:A:292:PRO:HD2	2.00	0.43
1:D:280:PRO:O	1:D:322:LYS:HE3	2.17	0.43
1:G:303:ASN:ND2	3:G:602:NAG:O7	2.51	0.43
1:F:95:VAL:HA	1:F:461:VAL:O	2.18	0.43
1:F:308:SER:O	1:F:312:MET:HG3	2.18	0.43
1:A:239:ASP:OD1	1:A:241:LYS:HE3	2.18	0.43
1:A:252:LEU:HA	1:A:255:THR:HB	1.99	0.43
1:A:390:PRO:HD3	1:A:400:PRO:HG3	2.00	0.43
1:C:448:PRO:O	1:C:449:LEU:HD23	2.18	0.43
1:H:22:LYS:HD2	1:H:28:TYR:CE1	2.52	0.43
1:H:203:ASP:O	1:H:207:GLN:HG3	2.17	0.43
1:A:401:MET:SD	1:A:401:MET:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:SER:HA	1:D:178:TYR:CZ	2.53	0.43
1:B:38:LYS:O	1:B:42:GLU:HG3	2.18	0.43
1:H:117:TYR:HA	1:H:481:PRO:HD3	1.99	0.43
1:E:68:THR:O	1:E:72:ILE:HG13	2.17	0.43
1:E:117:TYR:HA	1:E:481:PRO:HD3	2.00	0.43
1:C:310:SER:OG	1:C:354:GLU:OE2	2.36	0.43
1:H:381:HIS:HB3	1:H:452:GLU:OE2	2.18	0.43
1:E:355:MET:O	1:E:359:ILE:HG13	2.19	0.43
1:A:203:ASP:O	1:A:207:GLN:HG3	2.18	0.43
1:E:314:VAL:O	1:E:318:GLN:HG3	2.18	0.43
1:B:214:ASP:OD1	1:B:214:ASP:N	2.52	0.43
1:H:228:PRO:HA	1:H:246:ARG:HB2	2.01	0.43
3:F:601:NAG:O7	3:F:601:NAG:O3	2.36	0.43
1:B:264:LYS:HD2	1:B:264:LYS:HA	1.69	0.43
1:F:52:LYS:O	1:F:326:GLY:HA3	2.19	0.43
1:E:385:PHE:HA	1:E:412:ALA:O	2.19	0.43
1:C:45:LYS:HD2	1:C:45:LYS:HA	1.75	0.43
1:C:99:LYS:O	1:C:477:GLN:HB2	2.19	0.43
1:C:232:THR:HG22	1:C:237:GLU:HA	2.01	0.43
1:G:74:LYS:HD2	1:G:87:LEU:HD23	2.01	0.43
1:G:420:GLY:HA3	1:G:443:ALA:O	2.18	0.43
1:E:114:ALA:HA	1:E:117:TYR:CZ	2.54	0.43
1:F:375:VAL:HB	1:F:462:PHE:HB2	2.01	0.42
1:E:168:ARG:HG3	1:E:294:ASP:OD1	2.19	0.42
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.54	0.42
1:G:378:ASP:N	1:G:378:ASP:OD1	2.50	0.42
1:H:195:GLU:O	1:H:199:GLN:HB2	2.19	0.42
1:E:84:GLU:CD	1:E:84:GLU:H	2.22	0.42
1:G:381:HIS:ND1	1:G:452:GLU:OE1	2.52	0.42
1:H:228:PRO:HD3	1:H:250:LEU:O	2.19	0.42
1:F:268:PHE:HA	1:F:287:LEU:O	2.19	0.42
1:G:160:SER:HB3	1:G:320:LEU:HD22	2.01	0.42
1:G:274:GLU:O	1:G:278:LEU:HD13	2.20	0.42
1:E:186:TRP:HB3	1:E:192:MET:HG2	2.00	0.42
1:B:45:LYS:HG2	1:B:45:LYS:H	1.67	0.42
1:B:336:ILE:HD11	1:B:352:ALA:HA	2.00	0.42
1:F:26:PRO:O	1:F:30:ARG:HG3	2.19	0.42
1:B:228:PRO:HB3	1:B:249:GLY:HA2	2.02	0.42
1:G:92:PHE:CE1	1:G:464:LYS:HE2	2.54	0.42
1:H:52:LYS:O	1:H:159:LYS:HE3	2.20	0.42
1:A:52:LYS:O	1:A:326:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:THR:HG22	1:F:399:ALA:HA	2.02	0.42
1:A:385:PHE:HA	1:A:412:ALA:O	2.20	0.42
1:C:155:LYS:HG2	1:C:212:ILE:HD11	2.01	0.42
1:C:303:ASN:HD22	3:C:602:NAG:C7	2.30	0.42
1:H:114:ALA:HA	1:H:117:TYR:CZ	2.54	0.42
1:H:257:LYS:HE3	1:H:257:LYS:HB2	1.71	0.42
1:C:404:ASP:OD1	1:C:404:ASP:N	2.51	0.42
1:B:59:GLY:HA3	1:B:355:MET:HE1	2.02	0.42
1:B:372:LEU:HD21	1:B:484:MET:HG2	2.01	0.42
1:G:111:ALA:HB2	1:G:172:ALA:HB1	2.02	0.42
1:F:104:ASN:HB3	1:E:19:VAL:HG22	2.02	0.41
1:E:140:ASN:OD1	1:E:140:ASN:N	2.53	0.41
1:E:280:PRO:O	1:E:282:ASN:N	2.49	0.41
1:C:303:ASN:OD1	1:C:303:ASN:N	2.50	0.41
1:G:417:ASN:HB2	1:G:449:LEU:HD12	2.02	0.41
1:E:488:ALA:HB3	1:E:490:ILE:HG12	2.03	0.41
1:H:57:PHE:HB2	1:H:375:VAL:HG22	2.01	0.41
1:D:117:TYR:HA	1:D:481:PRO:HD3	2.01	0.41
1:F:103:THR:HG21	1:F:132:ALA:HB2	2.02	0.41
1:F:422:LYS:HD3	1:F:429:GLU:OE2	2.21	0.41
1:B:117:TYR:CE2	1:B:378:ASP:HB3	2.56	0.41
1:E:155:LYS:NZ	1:E:216:ASP:OD1	2.52	0.41
1:C:188:SER:HA	1:C:203:ASP:OD2	2.21	0.41
1:H:268:PHE:HA	1:H:287:LEU:O	2.21	0.41
2:IA:1:NAG:H61	2:IA:2:NAG:H82	2.02	0.41
1:D:190:ASN:HB2	1:D:245:THR:O	2.20	0.41
1:B:409:PRO:O	1:B:428:ARG:NH2	2.54	0.41
1:G:72:ILE:O	1:G:76:GLN:HG3	2.20	0.41
1:F:155:LYS:HD3	1:F:214:ASP:CG	2.41	0.41
1:A:29:TRP:CE2	1:B:122:LYS:HB2	2.56	0.41
1:G:126:GLY:HA2	1:G:184:ARG:HG2	2.03	0.41
1:H:280:PRO:O	1:H:322:LYS:HE2	2.20	0.41
1:A:60:ASP:HB3	1:A:337:ASP:HB2	2.03	0.41
1:D:341:HIS:ND1	1:D:452:GLU:O	2.54	0.41
1:C:190:ASN:HB2	1:C:245:THR:O	2.20	0.41
1:C:382:VAL:HG23	1:C:416:GLY:H	1.86	0.41
1:G:406:ASP:OD2	1:G:428:ARG:NH1	2.53	0.41
1:H:126:GLY:HA2	1:H:184:ARG:HG2	2.03	0.41
1:F:246:ARG:NH1	1:F:252:LEU:HD11	2.20	0.41
1:E:74:LYS:HD2	1:E:353:VAL:HG13	2.02	0.41
1:E:235:GLU:HG3	1:E:270:TRP:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:TRP:CE2	1:C:122:LYS:HB2	2.55	0.41
1:D:408:LYS:HG3	2:X:1:NAG:H82	2.03	0.41
1:B:104:ASN:HB2	1:B:124:ASN:HA	2.02	0.41
1:G:168:ARG:HB3	1:G:170:ASN:OD1	2.20	0.41
1:H:114:ALA:O	1:H:118:LEU:HB2	2.21	0.41
1:B:103:THR:HG21	1:B:132:ALA:HB1	2.02	0.40
1:G:409:PRO:O	1:G:428:ARG:NH2	2.54	0.40
1:A:138:ARG:HD3	1:A:138:ARG:HA	1.75	0.40
1:A:335:ARG:HD2	1:A:338:HIS:ND1	2.35	0.40
1:D:209:MET:SD	1:D:256:TRP:HB2	2.61	0.40
1:H:49:ASN:OD1	1:H:49:ASN:N	2.54	0.40
1:F:149:SER:OG	1:F:177:ALA:O	2.32	0.40
1:F:385:PHE:HA	1:F:412:ALA:O	2.21	0.40
1:E:113:THR:OG1	1:E:378:ASP:HB2	2.20	0.40
1:G:114:ALA:HA	1:G:117:TYR:CE2	2.56	0.40
1:C:22:LYS:HD2	1:C:28:TYR:CE1	2.57	0.40
1:C:335:ARG:HB2	1:C:351:GLU:OE1	2.22	0.40
1:B:189:ASP:OD2	1:B:248:ASP:N	2.54	0.40
1:B:378:ASP:OD1	1:B:378:ASP:N	2.49	0.40
1:E:126:GLY:HA3	1:E:136:ARG:HD2	2.03	0.40
1:E:171:HIS:CG	1:E:172:ALA:H	2.40	0.40
1:A:375:VAL:HB	1:A:462:PHE:HB2	2.02	0.40
1:H:467:MET:HA	1:H:469:HIS:CE1	2.56	0.40
1:E:167:THR:HG23	1:E:334:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	482/503 (96%)	464 (96%)	13 (3%)	5 (1%)	15 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	482/503 (96%)	459 (95%)	19 (4%)	4 (1%)	19 51
1	C	482/503 (96%)	460 (95%)	19 (4%)	3 (1%)	25 58
1	D	480/503 (95%)	460 (96%)	16 (3%)	4 (1%)	19 51
1	E	482/503 (96%)	454 (94%)	25 (5%)	3 (1%)	25 58
1	F	481/503 (96%)	451 (94%)	24 (5%)	6 (1%)	13 40
1	G	482/503 (96%)	464 (96%)	16 (3%)	2 (0%)	34 66
1	H	482/503 (96%)	461 (96%)	19 (4%)	2 (0%)	34 66
All	All	3853/4024 (96%)	3673 (95%)	151 (4%)	29 (1%)	19 51

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	497	CYS
1	A	268	PHE
1	E	282	ASN
1	C	268	PHE
1	H	268	PHE
1	A	241	LYS
1	C	19	VAL
1	B	268	PHE
1	F	268	PHE
1	A	425	GLY
1	D	19	VAL
1	B	430	ASN
1	F	499	PRO
1	E	19	VAL
1	G	19	VAL
1	F	19	VAL
1	D	425	GLY
1	B	382	VAL
1	F	426	GLY
1	A	382	VAL
1	D	382	VAL
1	C	382	VAL
1	B	19	VAL
1	G	382	VAL
1	F	382	VAL
1	F	425	GLY
1	H	382	VAL
1	E	382	VAL

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Mol	Chain	Res	Type
1	A	499	PRO

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	398/413 (96%)	377 (95%)	21 (5%)	22 54
1	B	398/413 (96%)	383 (96%)	15 (4%)	33 67
1	C	398/413 (96%)	385 (97%)	13 (3%)	38 72
1	D	398/413 (96%)	376 (94%)	22 (6%)	21 53
1	E	398/413 (96%)	388 (98%)	10 (2%)	47 78
1	F	398/413 (96%)	374 (94%)	24 (6%)	19 49
1	G	398/413 (96%)	387 (97%)	11 (3%)	43 76
1	H	398/413 (96%)	380 (96%)	18 (4%)	27 61
All	All	3184/3304 (96%)	3050 (96%)	134 (4%)	30 63

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	53	ASN
1	A	67	VAL
1	A	109	ASP
1	A	125	GLU
1	A	137	SER
1	A	138	ARG
1	A	155	LYS
1	A	168	ARG
1	A	183	ASP
1	A	248	ASP
1	A	264	LYS
1	A	303	ASN
1	A	315	VAL

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Mol	Chain	Res	Type
1	A	368	SER
1	A	369	GLU
1	A	403	SER
1	A	404	ASP
1	A	422	LYS
1	A	433	MET
1	A	463	SER
1	D	22	LYS
1	D	60	ASP
1	D	65	SER
1	D	103	THR
1	D	138	ARG
1	D	145	ASN
1	D	152	ARG
1	D	155	LYS
1	D	181	SER
1	D	201	CYS
1	D	238	SER
1	D	243	ARG
1	D	262	ARG
1	D	306	ASP
1	D	321	ARG
1	D	364	SER
1	D	401	MET
1	D	422	LYS
1	D	428	ARG
1	D	433	MET
1	D	450	ARG
1	D	457	GLU
1	C	58	LEU
1	C	60	ASP
1	C	103	THR
1	C	109	ASP
1	C	125	GLU
1	C	201	CYS
1	C	232	THR
1	C	248	ASP
1	C	303	ASN
1	C	310	SER
1	C	368	SER
1	C	401	MET
1	C	432	SER

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Mol	Chain	Res	Type
1	B	53	ASN
1	B	67	VAL
1	B	103	THR
1	B	140	ASN
1	B	152	ARG
1	B	155	LYS
1	B	168	ARG
1	B	190	ASN
1	B	283	VAL
1	B	304	VAL
1	B	332	GLU
1	B	357	ARG
1	B	384	THR
1	B	428	ARG
1	B	457	GLU
1	G	60	ASP
1	G	168	ARG
1	G	195	GLU
1	G	231	LYS
1	G	243	ARG
1	G	310	SER
1	G	368	SER
1	G	401	MET
1	G	422	LYS
1	G	428	ARG
1	G	432	SER
1	H	18	LEU
1	H	45	LYS
1	H	49	ASN
1	H	109	ASP
1	H	143	GLN
1	H	203	ASP
1	H	233	ASP
1	H	254	ASP
1	H	266	SER
1	H	272	ARG
1	H	282	ASN
1	H	283	VAL
1	H	303	ASN
1	H	306	ASP
1	H	310	SER
1	H	349	LEU

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Mol	Chain	Res	Type
1	H	428	ARG
1	H	457	GLU
1	F	38	LYS
1	F	53	ASN
1	F	60	ASP
1	F	103	THR
1	F	109	ASP
1	F	128	VAL
1	F	130	VAL
1	F	137	SER
1	F	151	LEU
1	F	152	ARG
1	F	198	SER
1	F	229	LYS
1	F	241	LYS
1	F	247	LEU
1	F	254	ASP
1	F	260	LYS
1	F	262	ARG
1	F	310	SER
1	F	325	LYS
1	F	349	LEU
1	F	364	SER
1	F	401	MET
1	F	419	PRO
1	F	445	SER
1	E	45	LYS
1	E	58	LEU
1	E	198	SER
1	E	202	LYS
1	E	224	LYS
1	E	269	ILE
1	E	364	SER
1	E	401	MET
1	E	428	ARG
1	E	445	SER

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

Mol	Chain	Res	Type
1	A	230	ASN
1	A	475	HIS

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Mol	Chain	Res	Type
1	A	482	HIS
1	A	496	HIS
1	D	78	HIS
1	D	475	HIS
1	C	102	ASN
1	C	361	GLN
1	C	475	HIS
1	B	44	GLN
1	B	143	GLN
1	B	199	GLN
1	B	475	HIS
1	F	282	ASN
1	F	469	HIS
1	E	44	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

32 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	1	1	1,2	14,14,15	0.38	0	17,19,21	0.76	0
2	NAG	1	2	2	14,14,15	0.41	0	17,19,21	0.49	0
2	NAG	8	1	1,2	14,14,15	0.22	0	17,19,21	0.39	0
2	NAG	8	2	2	14,14,15	0.29	0	17,19,21	0.42	0
2	NAG	BA	1	1,2	14,14,15	0.30	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	BA	2	2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	IA	1	1,2	14,14,15	0.23	0	17,19,21	0.60	1 (5%)
2	NAG	IA	2	2	14,14,15	0.36	0	17,19,21	0.46	0
2	NAG	K	1	1,2	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	K	2	2	14,14,15	0.26	0	17,19,21	0.42	0
2	NAG	LA	1	1,2	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
2	NAG	LA	2	2	14,14,15	0.38	0	17,19,21	0.74	0
2	NAG	N	1	1,2	14,14,15	0.34	0	17,19,21	0.70	0
2	NAG	N	2	2	14,14,15	0.47	0	17,19,21	0.49	0
2	NAG	SA	1	1,2	14,14,15	0.52	0	17,19,21	0.76	0
2	NAG	SA	2	2	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	U	1	1,2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	U	2	2	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	VA	1	1,2	14,14,15	0.27	0	17,19,21	0.58	0
2	NAG	VA	2	2	14,14,15	0.32	0	17,19,21	0.46	0
2	NAG	X	1	1,2	14,14,15	0.24	0	17,19,21	0.56	0
2	NAG	X	2	2	14,14,15	0.20	0	17,19,21	0.69	0
2	NAG	e	1	1,2	14,14,15	0.20	0	17,19,21	0.50	0
2	NAG	e	2	2	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	h	1	1,2	14,14,15	0.24	0	17,19,21	0.57	0
2	NAG	h	2	2	14,14,15	0.29	0	17,19,21	0.33	0
2	NAG	o	1	1,2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	o	2	2	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	r	1	1,2	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	r	2	2	14,14,15	0.36	0	17,19,21	0.52	0
2	NAG	y	1	1,2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	y	2	2	14,14,15	0.34	0	17,19,21	0.42	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
2	NAG	1	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	1	2	2	-	3/6/23/26	0/1/1/1
2	NAG	8	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	8	2	2	-	0/6/23/26	0/1/1/1
2	NAG	BA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	IA	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	IA	2	2	-	2/6/23/26	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
2	NAG	LA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	LA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	SA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	VA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	VA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	3/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	NAG	o	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	NAG	r	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	r	2	2	-	3/6/23/26	0/1/1/1
2	NAG	y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	y	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	LA	1	NAG	C1-O5-C5	2.28	115.28	112.19
2	IA	1	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	IA	2	NAG	O5-C5-C6-O6
2	SA	2	NAG	O5-C5-C6-O6
2	LA	2	NAG	O5-C5-C6-O6
2	BA	1	NAG	C4-C5-C6-O6
2	IA	2	NAG	C4-C5-C6-O6
2	h	2	NAG	O5-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	SA	2	NAG	C4-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6
2	o	2	NAG	C4-C5-C6-O6
2	LA	2	NAG	C4-C5-C6-O6
2	VA	2	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	r	1	NAG	O5-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	LA	2	NAG	C1-C2-N2-C7
2	r	2	NAG	C4-C5-C6-O6
2	1	2	NAG	O5-C5-C6-O6
2	VA	2	NAG	C4-C5-C6-O6
2	r	2	NAG	C3-C2-N2-C7
2	VA	1	NAG	C4-C5-C6-O6
2	r	1	NAG	C4-C5-C6-O6
2	r	2	NAG	O5-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C3-C2-N2-C7
2	1	2	NAG	C3-C2-N2-C7
2	BA	2	NAG	C3-C2-N2-C7
2	VA	1	NAG	O5-C5-C6-O6
2	1	2	NAG	C1-C2-N2-C7
2	BA	2	NAG	C1-C2-N2-C7
2	X	2	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

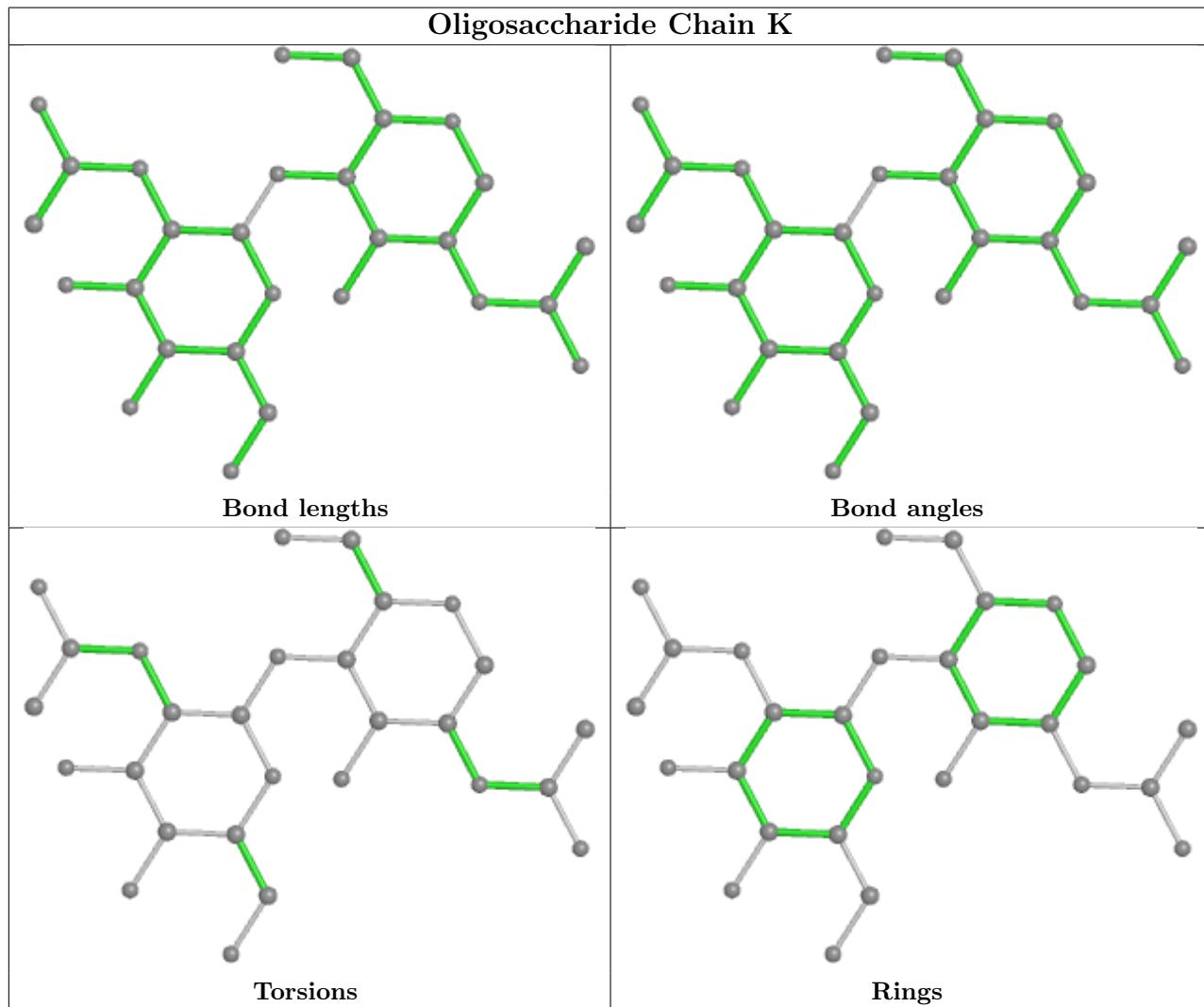
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	IA	1	NAG	2	0
2	8	1	NAG	1	0
2	LA	1	NAG	1	0
2	IA	2	NAG	1	0

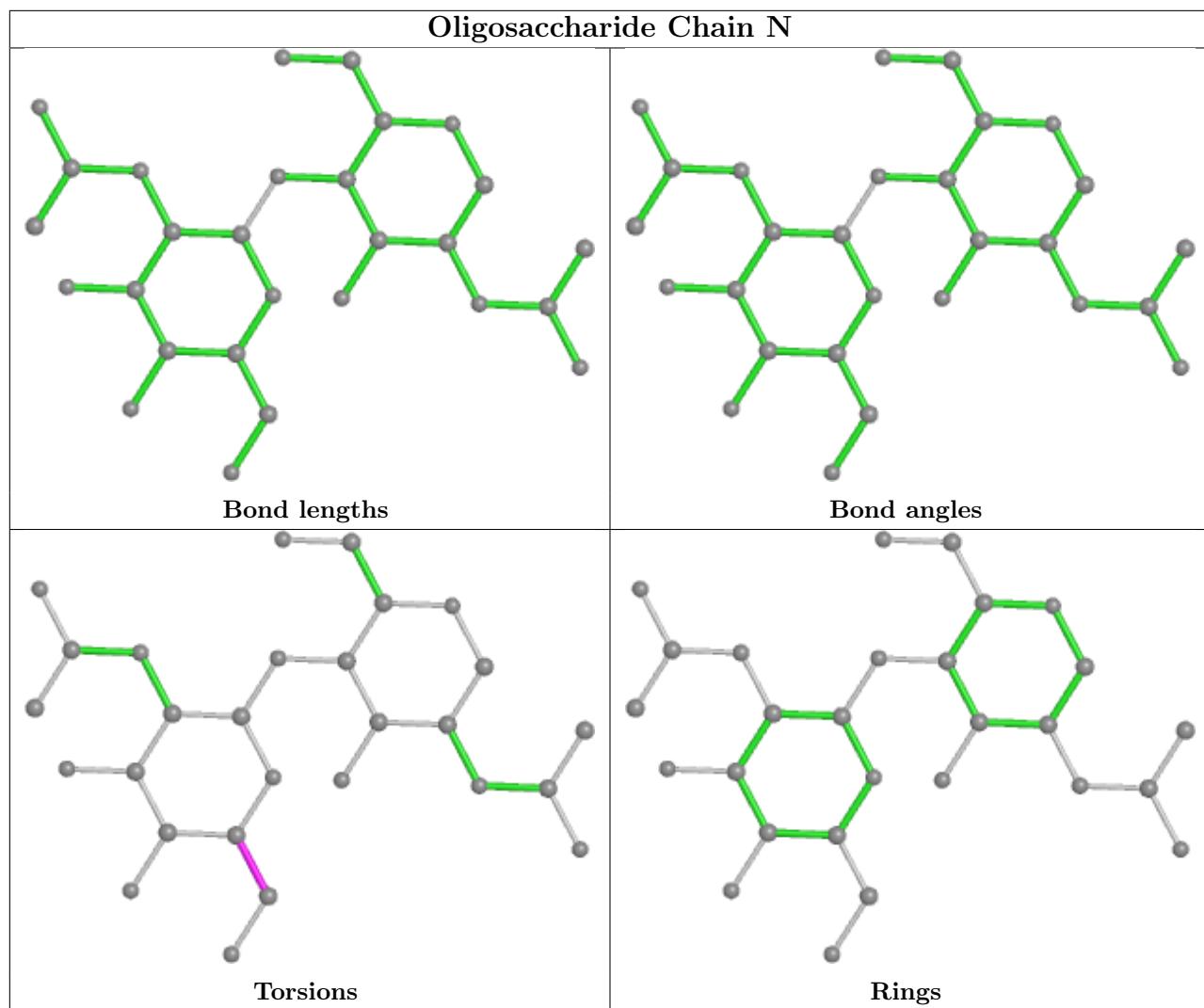
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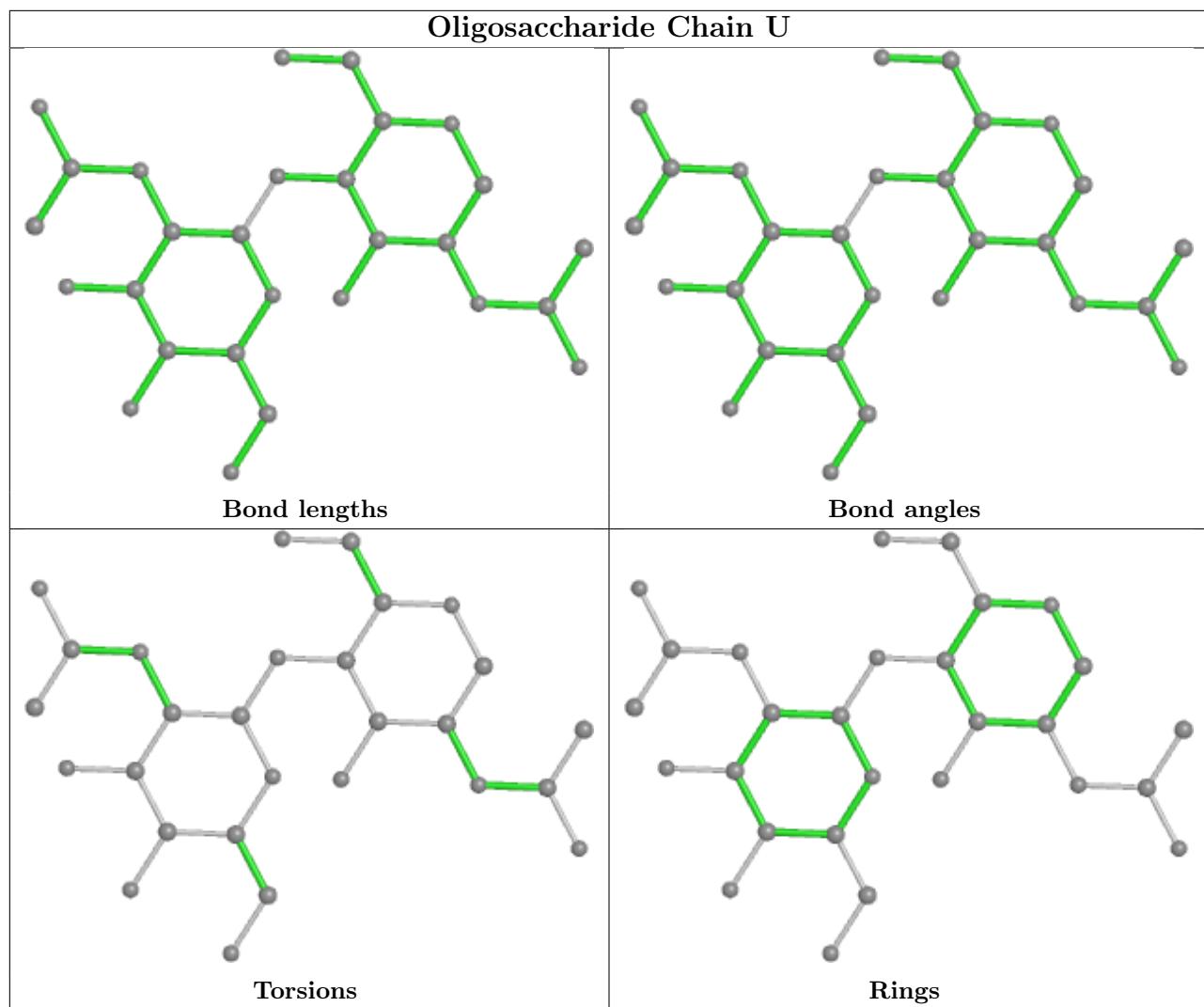
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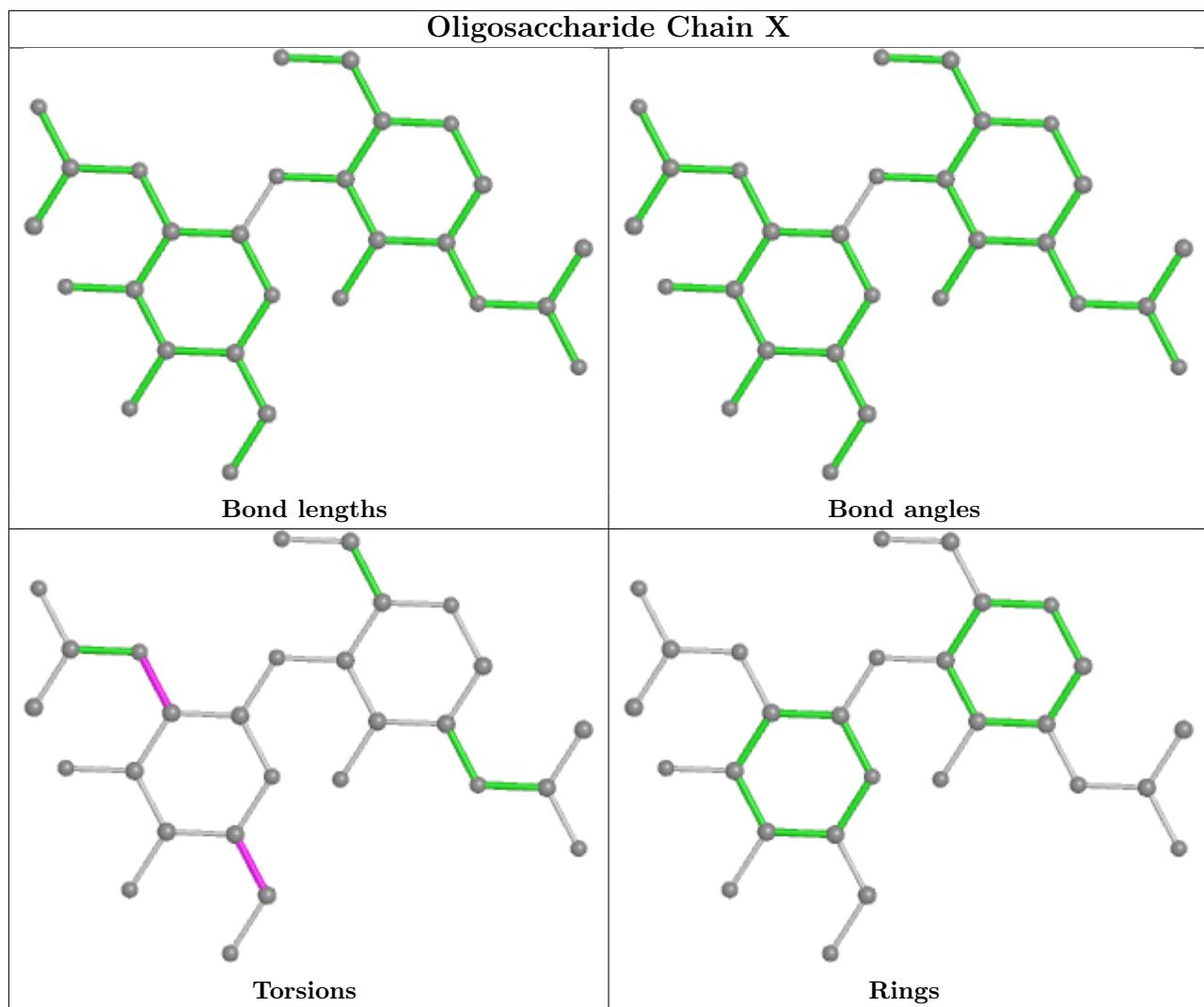
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	SA	1	NAG	1	0
2	X	1	NAG	1	0

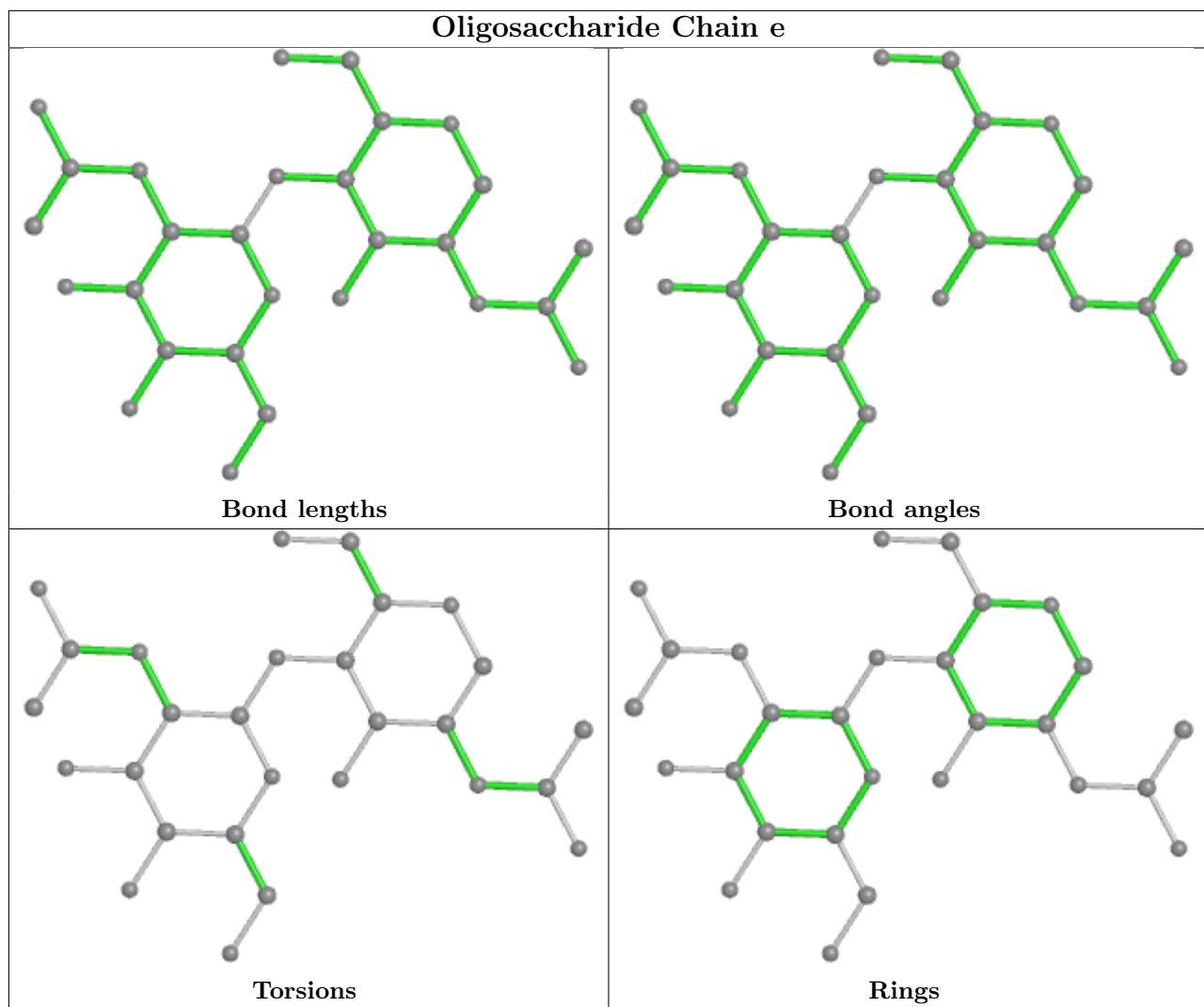
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

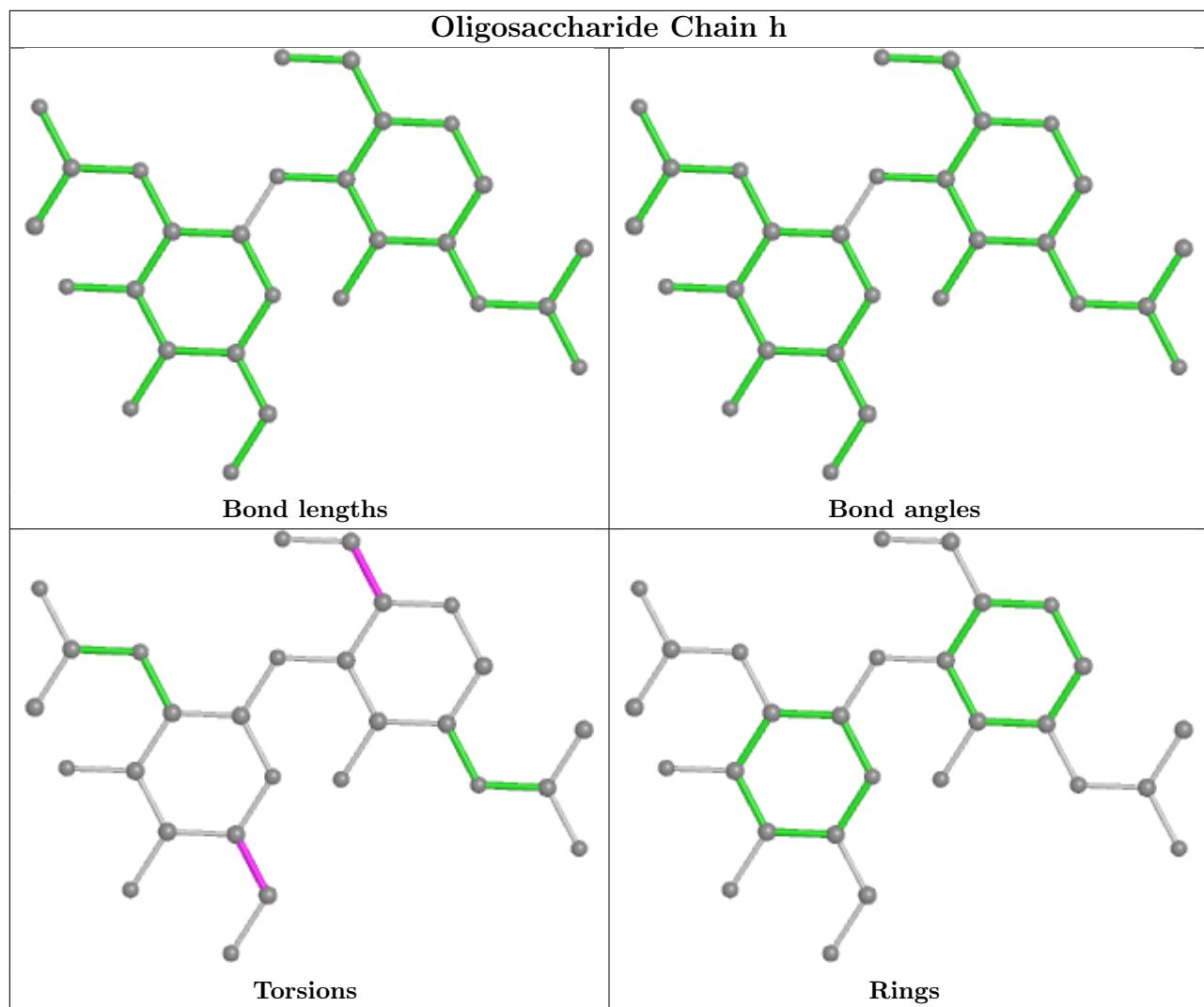


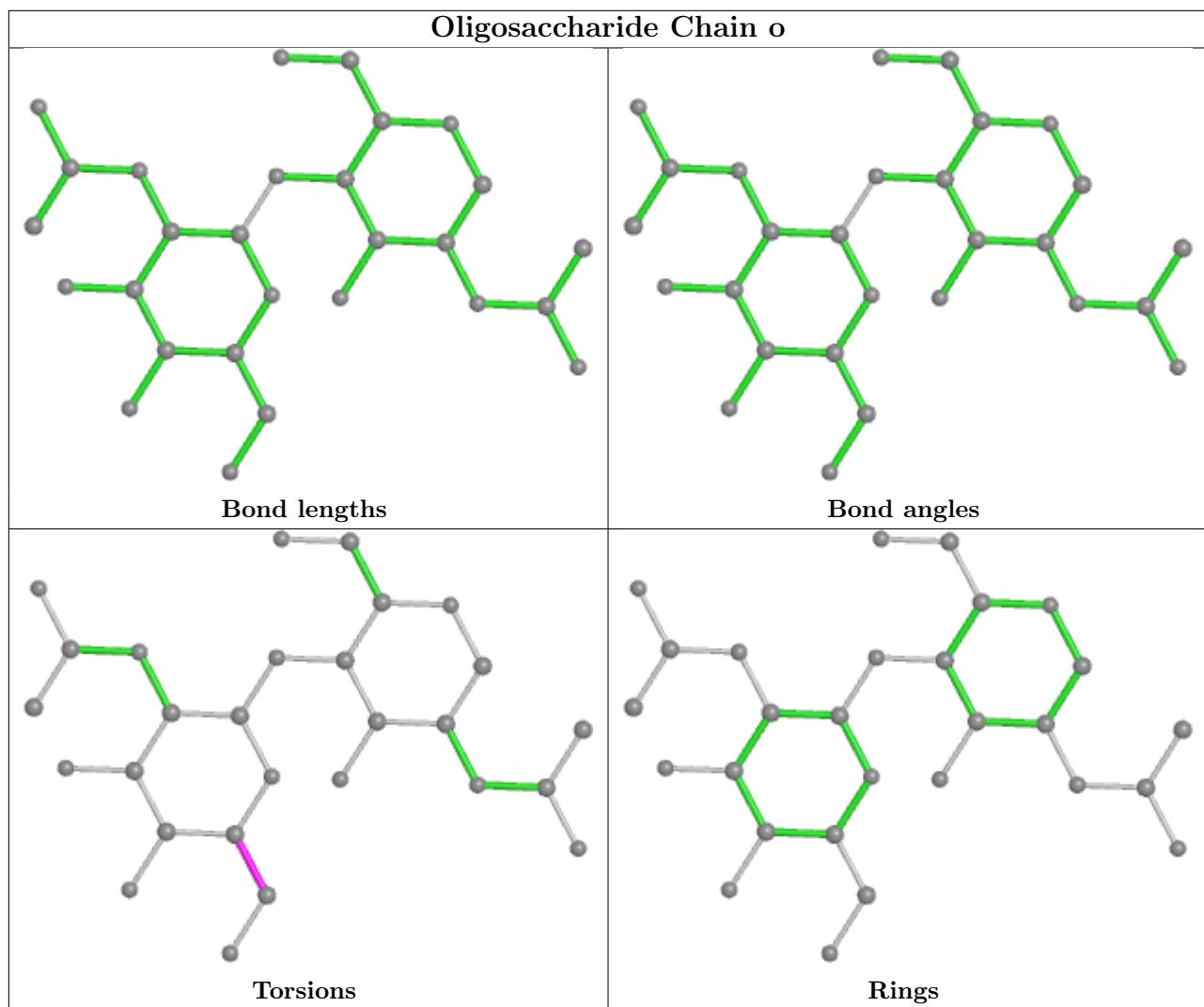


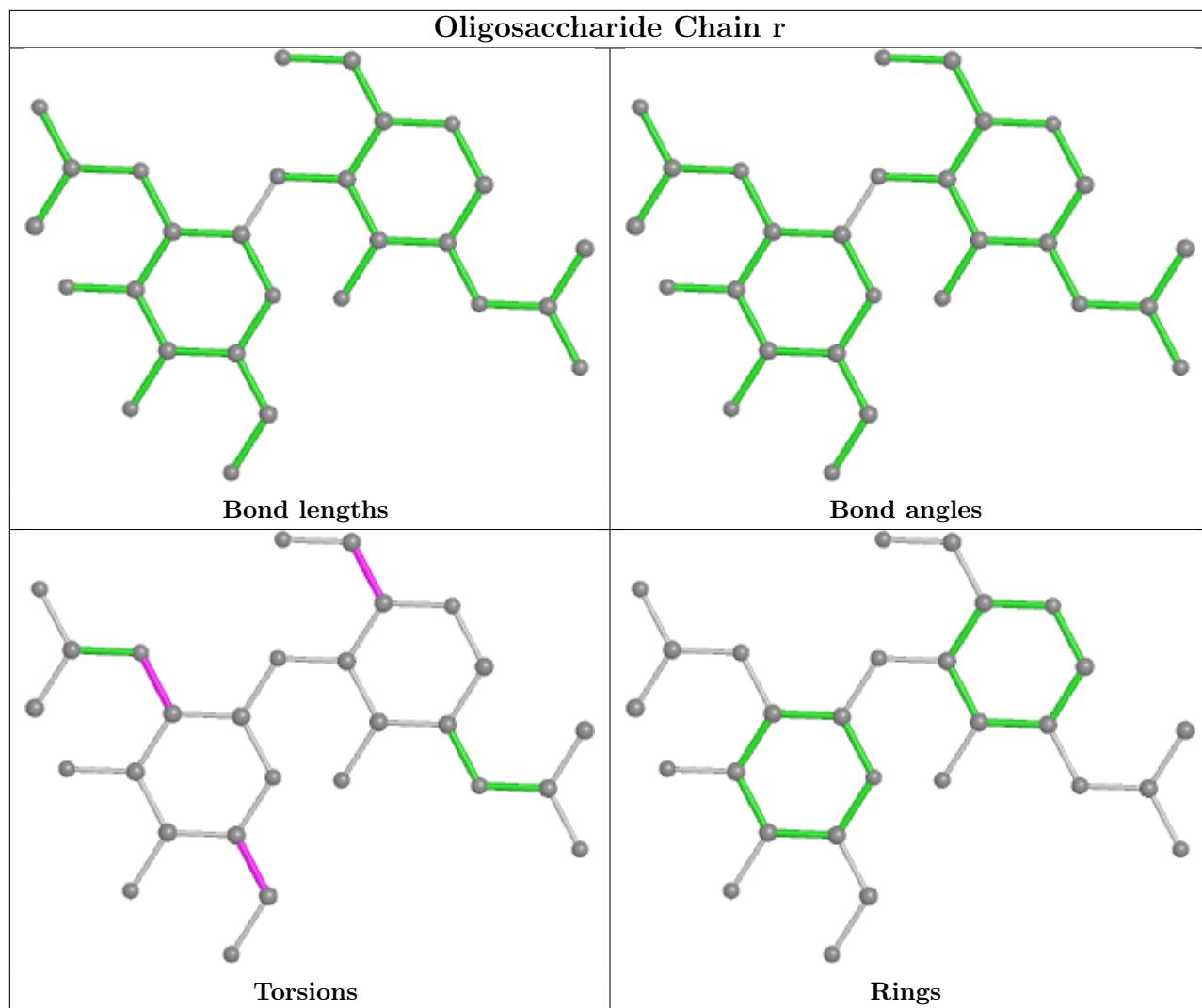


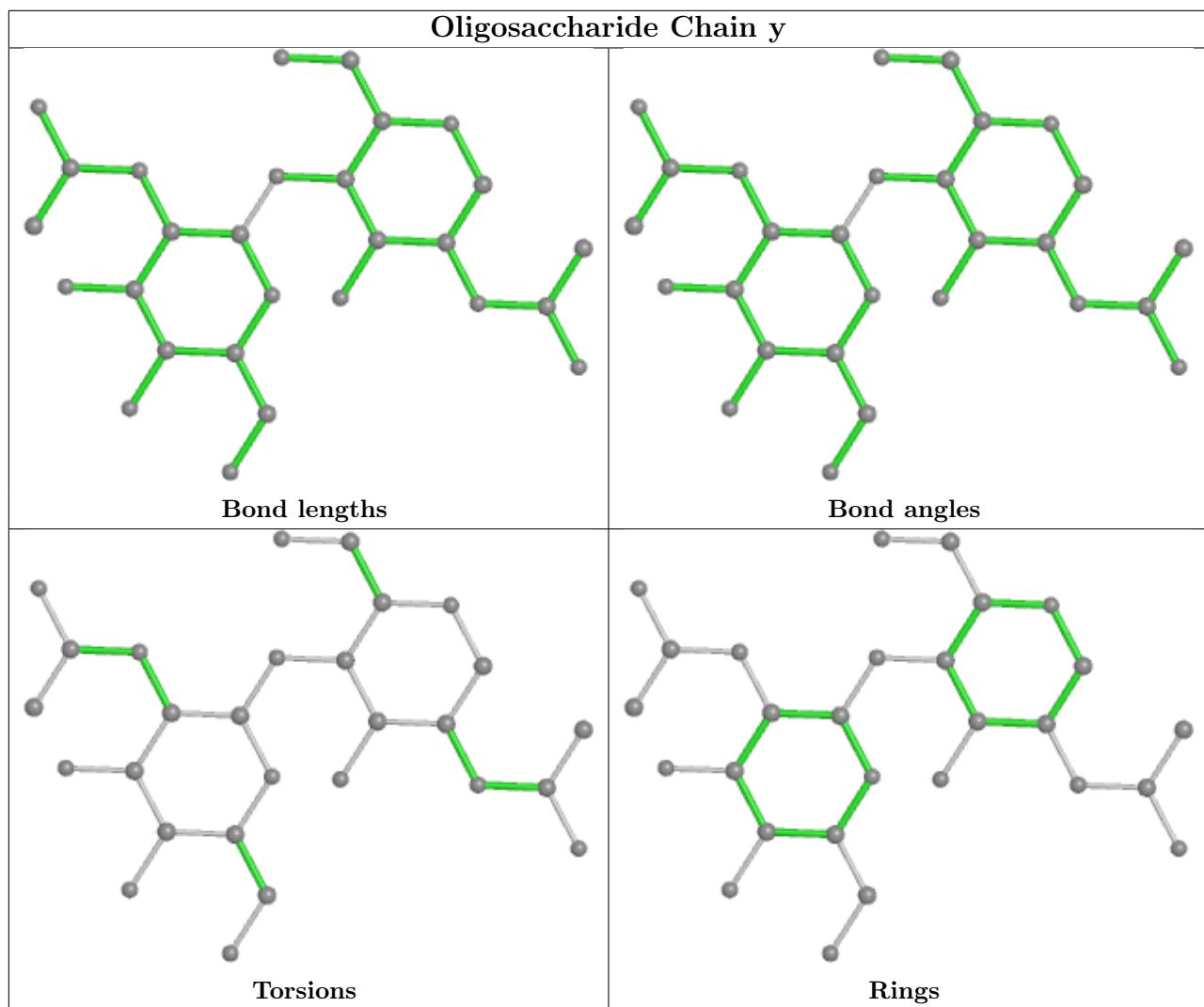


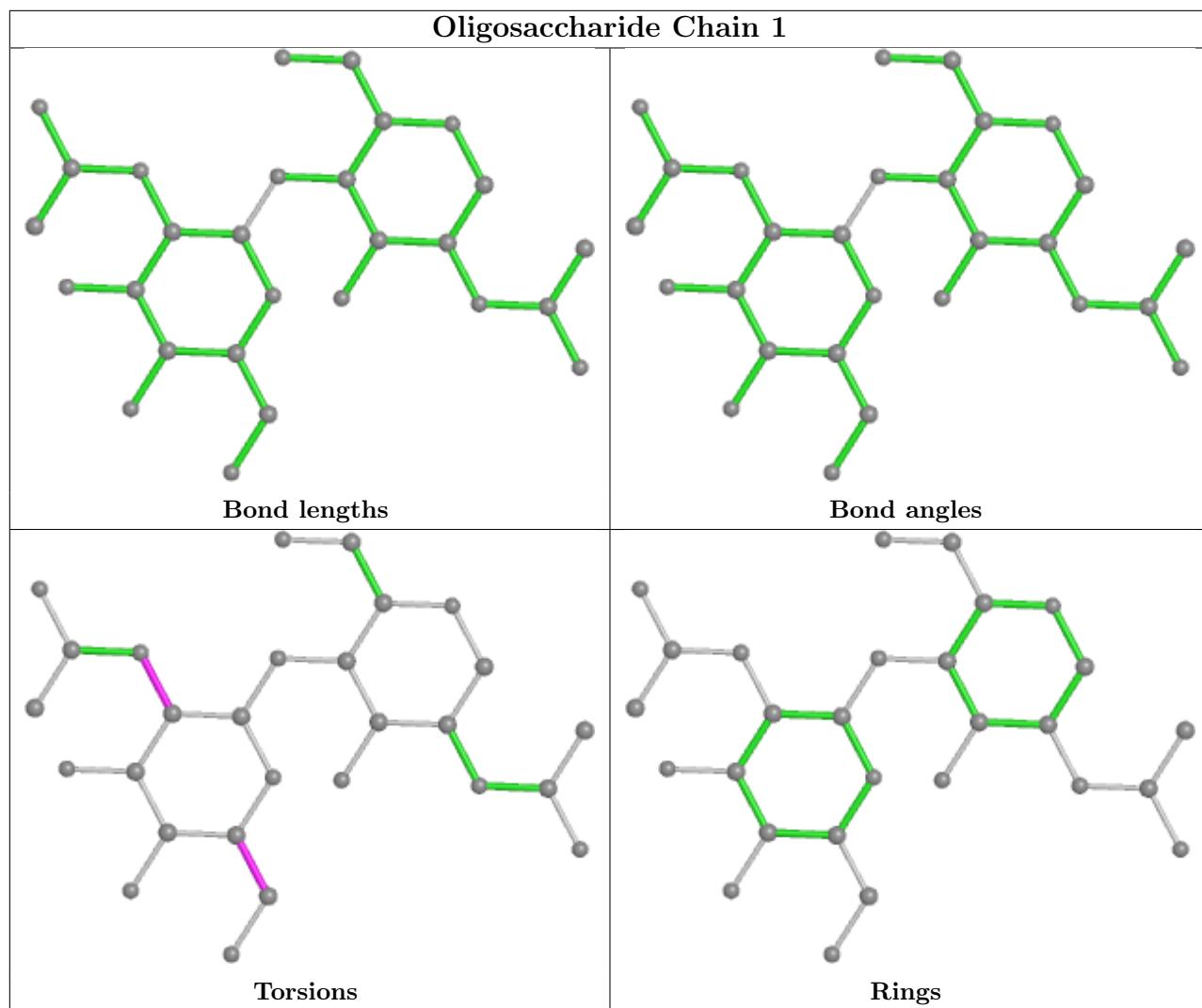


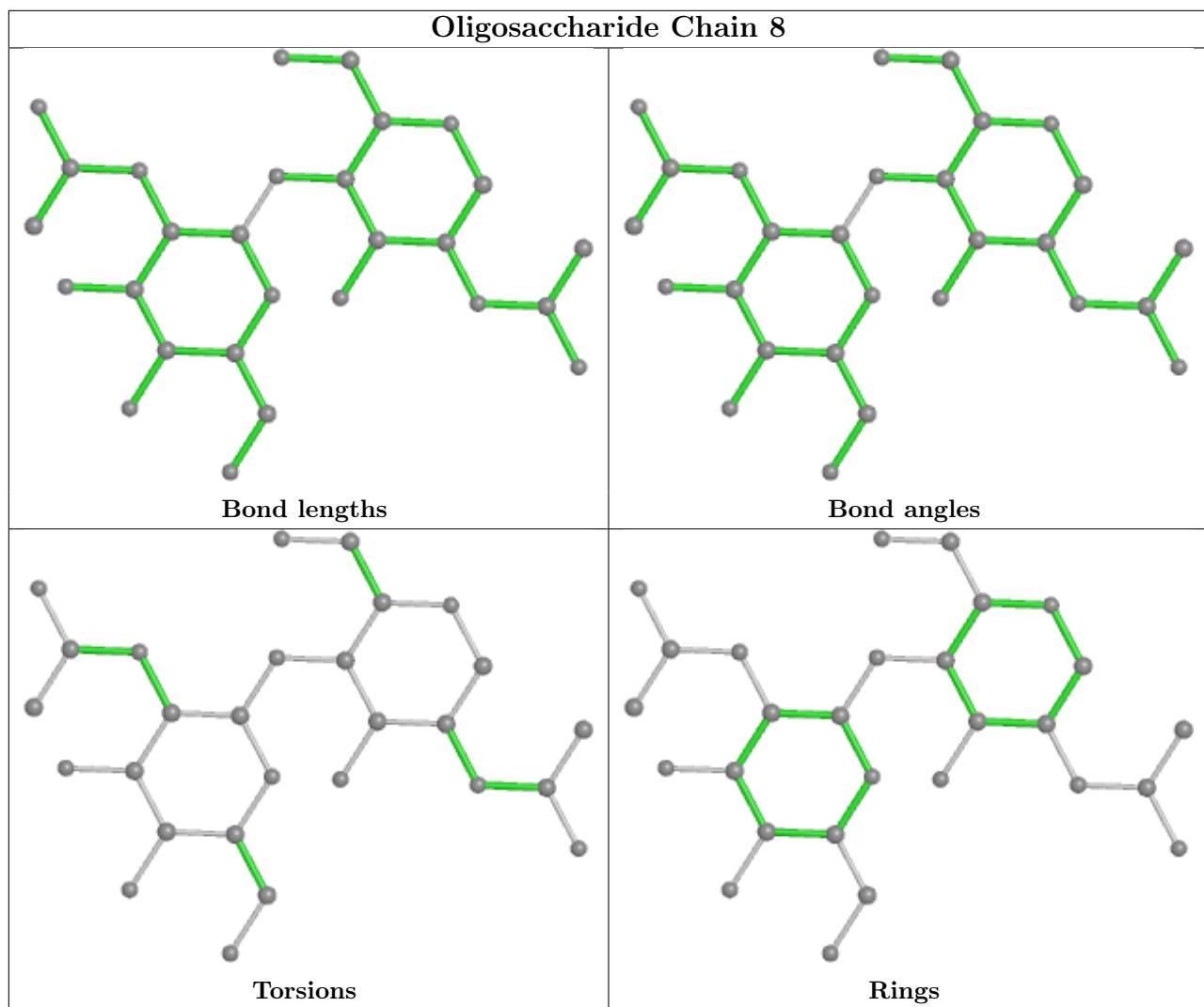


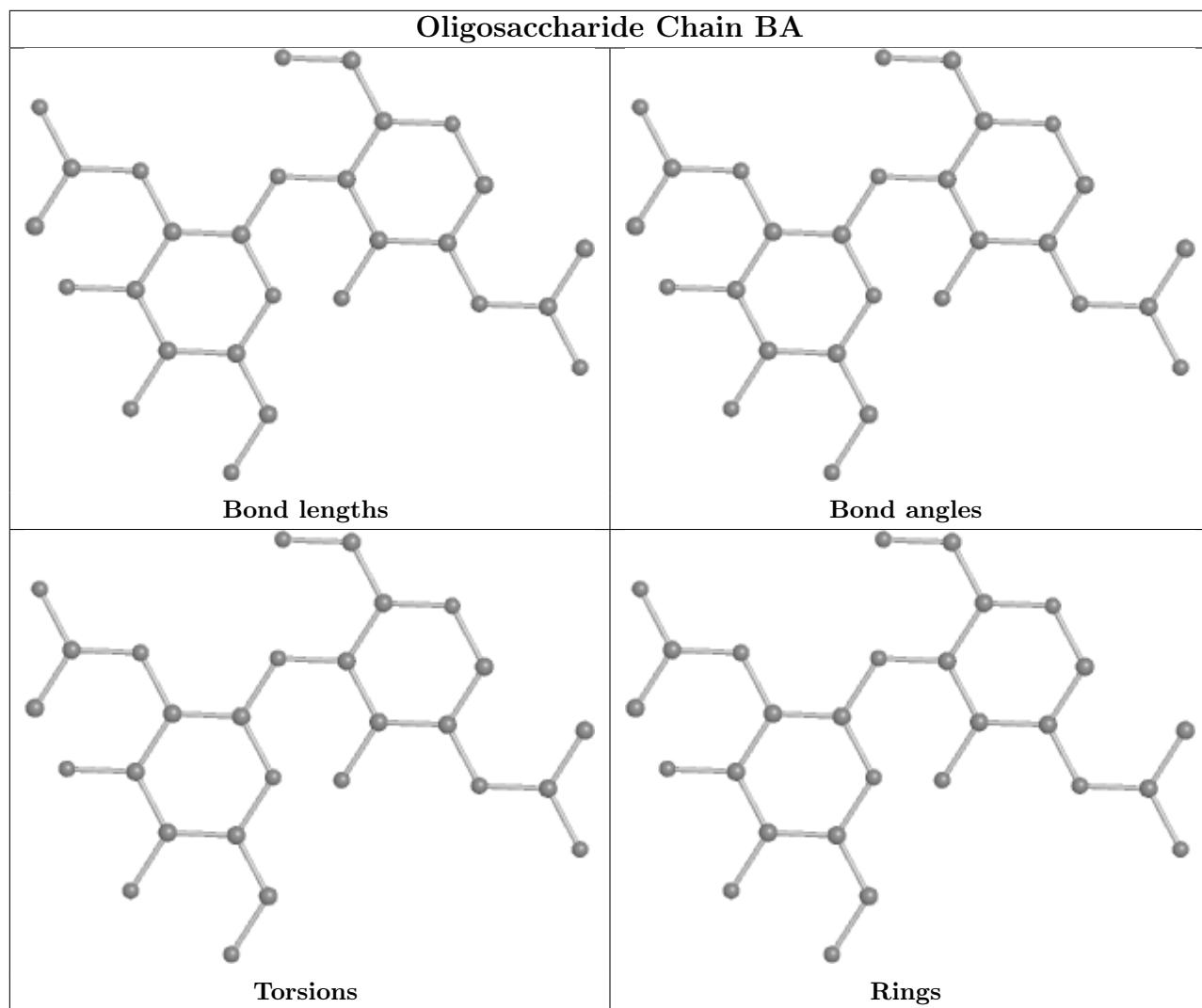


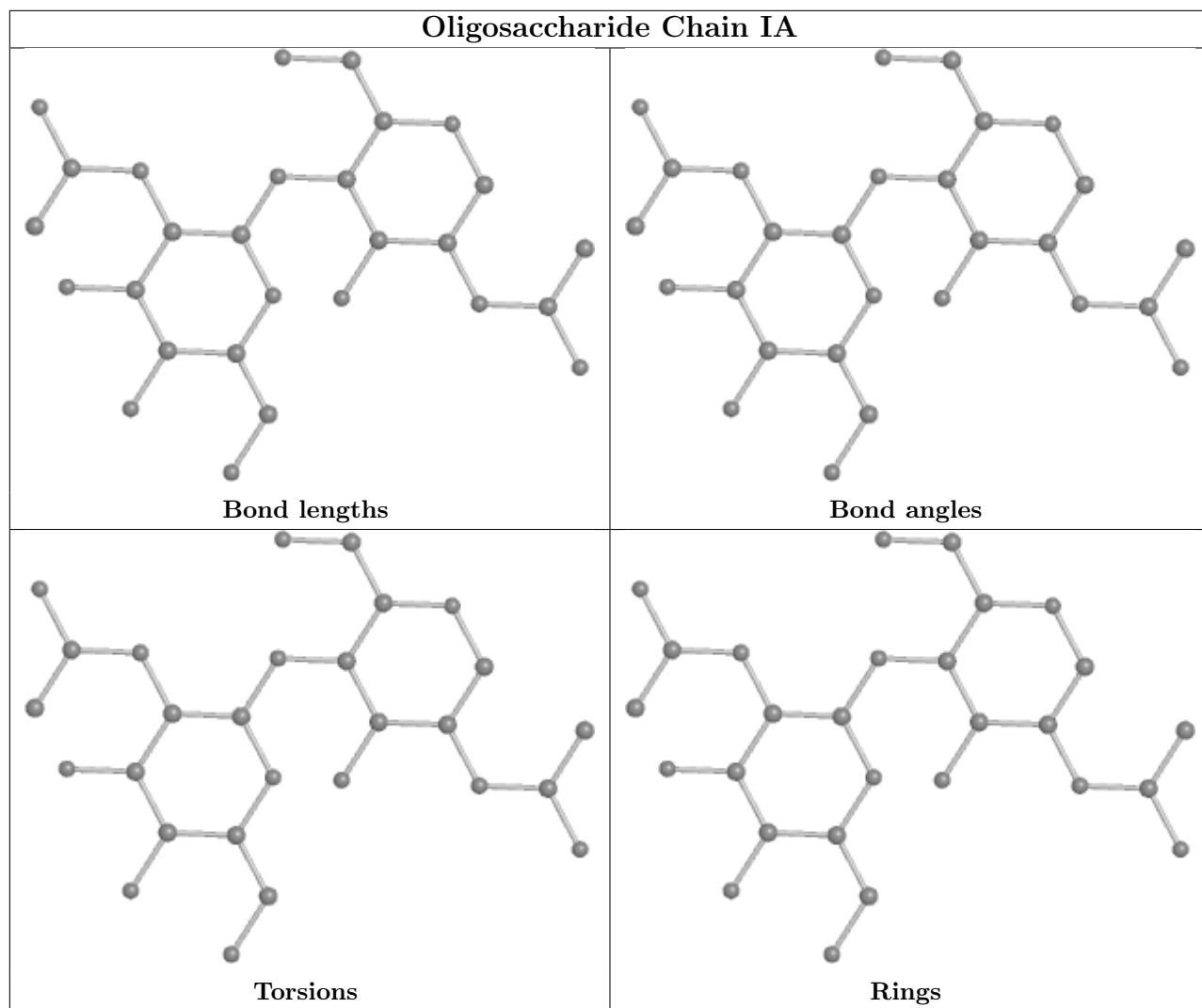


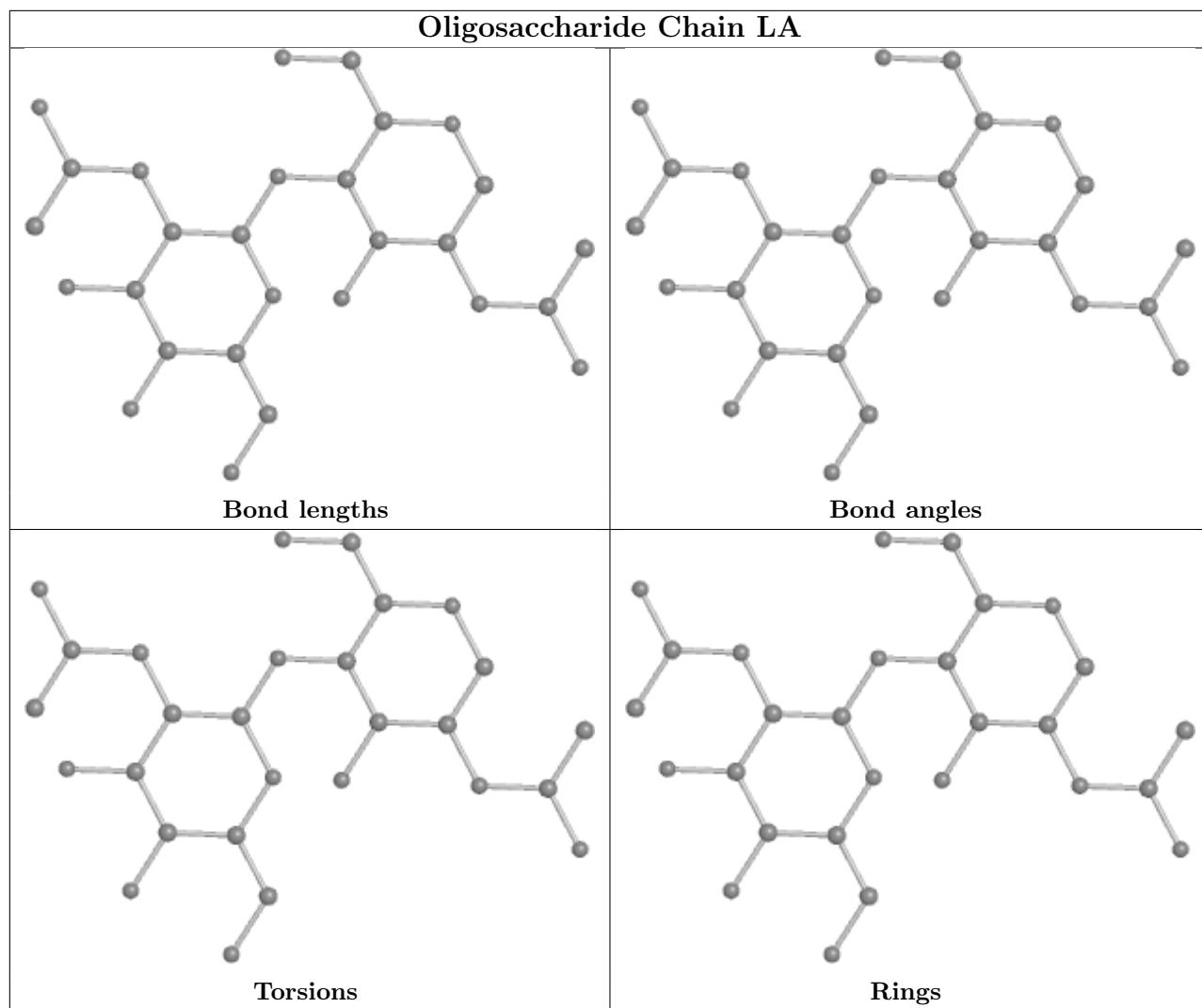


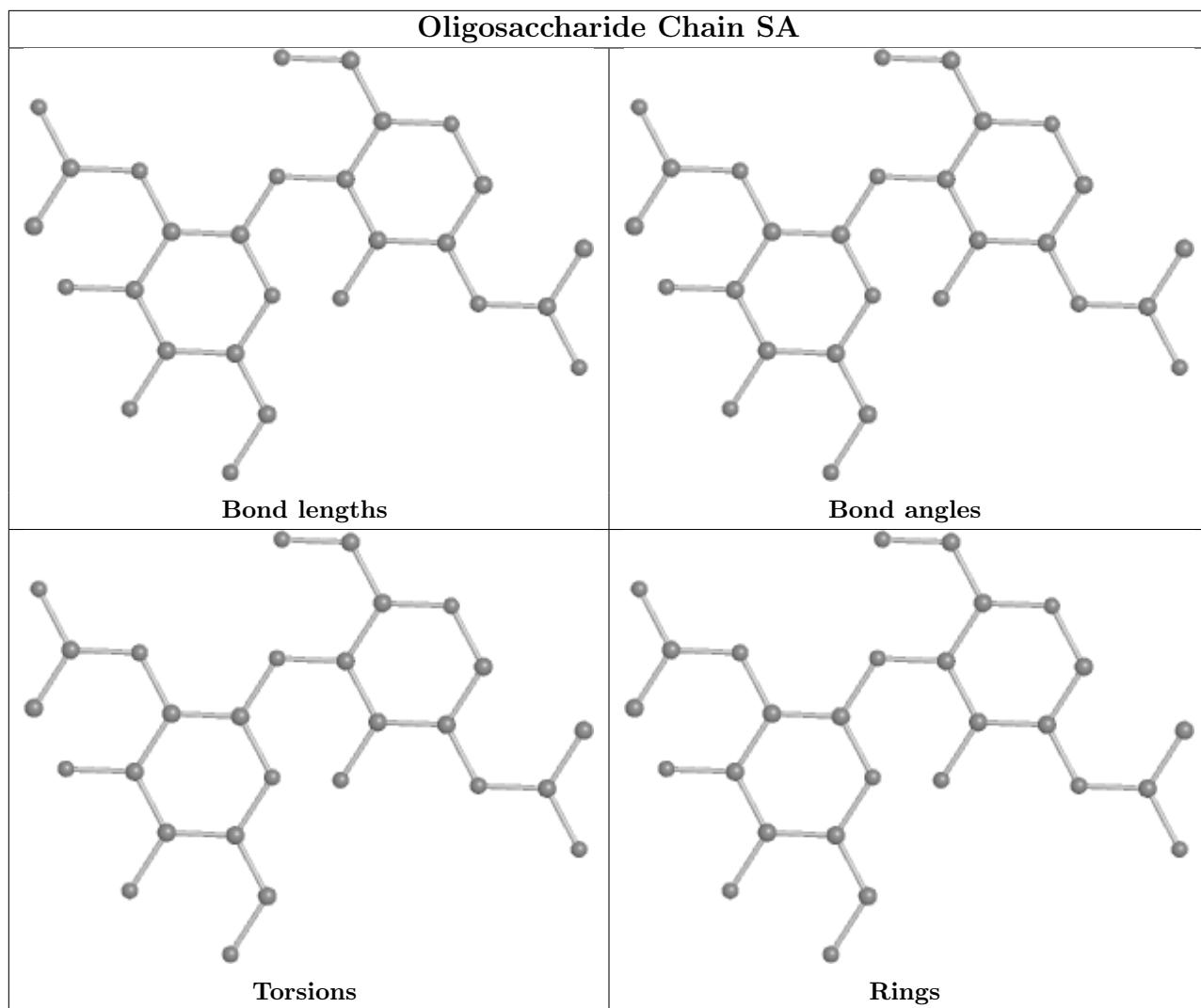


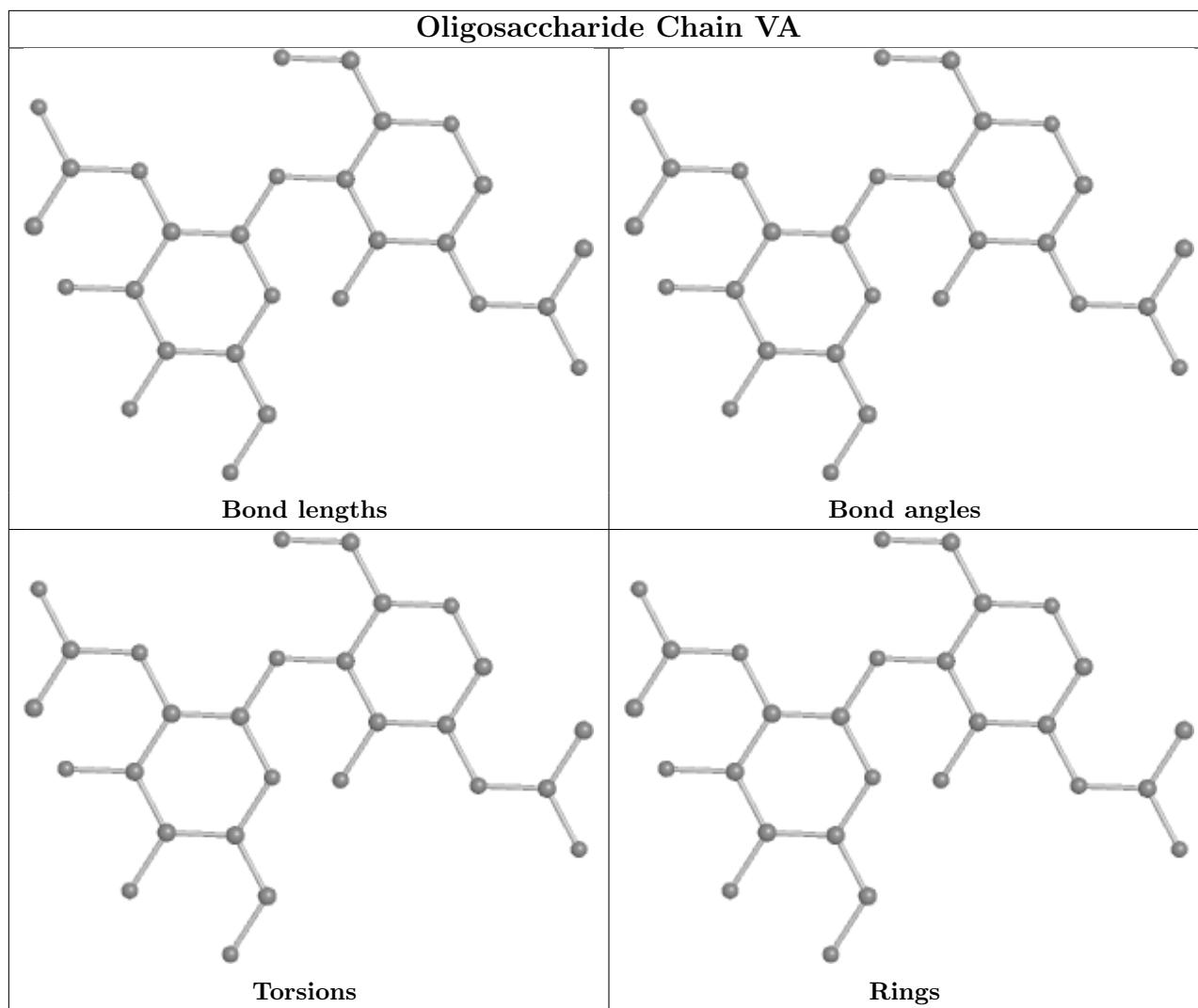












5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 32 are monoatomic - leaving 16 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
3	NAG	D	601	1	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	C	601	1	14,14,15	0.35	0	17,19,21	0.54	0
3	NAG	A	602	1	14,14,15	0.32	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	602	1	14,14,15	0.50	0	17,19,21	0.79	1 (5%)
3	NAG	E	602	1	14,14,15	0.63	1 (7%)	17,19,21	0.42	0
3	NAG	D	602	1	14,14,15	0.52	0	17,19,21	0.60	0
3	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.42	0
3	NAG	B	601	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	602	1	14,14,15	0.30	0	17,19,21	0.39	0
3	NAG	B	602	1	14,14,15	0.34	0	17,19,21	1.35	2 (11%)
3	NAG	G	601	1	14,14,15	0.58	0	17,19,21	0.66	1 (5%)
3	NAG	H	602	1	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
3	NAG	E	601	1	14,14,15	0.62	0	17,19,21	0.72	1 (5%)
3	NAG	H	601	1	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	F	602	1	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	F	601	1	14,14,15	0.43	0	17,19,21	0.37	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
3	NAG	D	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	1/6/23/26	0/1/1/1
3	NAG	A	602	1	-	1/6/23/26	0/1/1/1
3	NAG	G	602	1	-	3/6/23/26	0/1/1/1
3	NAG	E	602	1	-	2/6/23/26	0/1/1/1
3	NAG	D	602	1	-	1/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	601	1	-	1/6/23/26	0/1/1/1
3	NAG	C	602	1	-	3/6/23/26	0/1/1/1
3	NAG	B	602	1	-	3/6/23/26	0/1/1/1
3	NAG	G	601	1	-	4/6/23/26	0/1/1/1
3	NAG	H	602	1	-	2/6/23/26	0/1/1/1
3	NAG	E	601	1	-	2/6/23/26	0/1/1/1
3	NAG	H	601	1	-	2/6/23/26	0/1/1/1
3	NAG	F	602	1	-	2/6/23/26	0/1/1/1
3	NAG	F	601	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	NAG	C1-C2	2.13	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAG	C2-N2-C7	4.51	129.32	122.90
3	G	602	NAG	C1-O5-C5	2.63	115.75	112.19
3	E	601	NAG	C1-O5-C5	2.51	115.59	112.19
3	B	602	NAG	C1-C2-N2	2.28	114.38	110.49
3	G	601	NAG	C1-O5-C5	2.23	115.22	112.19
3	H	602	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	C4-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
3	F	601	NAG	O5-C5-C6-O6
3	F	602	NAG	C4-C5-C6-O6
3	F	602	NAG	O5-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	G	601	NAG	O5-C5-C6-O6
3	E	602	NAG	C1-C2-N2-C7
3	H	601	NAG	O5-C5-C6-O6
3	C	602	NAG	C8-C7-N2-C2
3	C	602	NAG	O7-C7-N2-C2
3	B	602	NAG	C8-C7-N2-C2
3	B	602	NAG	O7-C7-N2-C2
3	H	602	NAG	O5-C5-C6-O6
3	H	601	NAG	C4-C5-C6-O6
3	G	602	NAG	O5-C5-C6-O6
3	F	601	NAG	C4-C5-C6-O6
3	F	601	NAG	C1-C2-N2-C7
3	C	601	NAG	O5-C5-C6-O6
3	G	601	NAG	C1-C2-N2-C7
3	G	602	NAG	C4-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	D	602	NAG	O5-C5-C6-O6
3	C	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	G	602	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	602	NAG	C3-C2-N2-C7
3	E	602	NAG	C3-C2-N2-C7
3	H	602	NAG	C4-C5-C6-O6
3	G	601	NAG	C3-C2-N2-C7
3	F	601	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	602	NAG	1	0
3	E	602	NAG	2	0
3	C	602	NAG	1	0
3	B	602	NAG	1	0
3	F	601	NAG	1	0

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

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	484/503 (96%)	-0.44	1 (0%)	95	95	22, 32, 50, 70	0
1	B	484/503 (96%)	-0.32	8 (1%)	70	69	21, 35, 57, 95	0
1	C	484/503 (96%)	-0.33	1 (0%)	95	95	22, 35, 59, 72	0
1	D	482/503 (95%)	-0.38	2 (0%)	92	93	20, 31, 49, 74	0
1	E	484/503 (96%)	-0.21	3 (0%)	89	89	25, 43, 63, 82	0
1	F	483/503 (96%)	-0.16	6 (1%)	79	79	27, 48, 74, 109	0
1	G	484/503 (96%)	-0.26	6 (1%)	79	79	26, 40, 57, 79	0
1	H	484/503 (96%)	-0.17	14 (2%)	51	47	26, 42, 65, 96	0
All	All	3869/4024 (96%)	-0.28	41 (1%)	80	80	20, 38, 63, 109	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	ALA	6.4
1	H	499	PRO	4.4
1	F	499	PRO	4.4
1	B	500	ALA	4.1
1	F	500	ALA	4.0
1	H	424	VAL	3.8
1	H	501	ALA	3.7
1	G	424	VAL	3.5
1	G	425	GLY	3.5
1	H	500	ALA	3.4
1	E	281	HIS	3.0
1	B	263	TYR	2.9
1	F	293	GLY	2.9
1	H	236	TYR	2.9
1	B	230	ASN	2.8
1	D	499	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	238	SER	2.6
1	B	18	LEU	2.6
1	B	499	PRO	2.5
1	A	18	LEU	2.5
1	B	424	VAL	2.5
1	G	501	ALA	2.5
1	B	267	HIS	2.4
1	H	237	GLU	2.4
1	E	195	GLU	2.4
1	H	232	THR	2.4
1	H	270	TRP	2.3
1	G	427	GLU	2.3
1	F	242	ALA	2.3
1	H	426	GLY	2.2
1	D	257	LYS	2.2
1	E	270	TRP	2.2
1	C	262	ARG	2.2
1	H	240	GLU	2.2
1	H	423	VAL	2.1
1	F	236	TYR	2.1
1	H	18	LEU	2.0
1	G	405	THR	2.0
1	G	423	VAL	2.0
1	H	227	TYR	2.0
1	F	143	GLN	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
2	NAG	y	2	14/15	0.68	0.47	72,94,102,103	0
2	NAG	BA	2	14/15	0.69	0.40	88,95,100,101	0
2	NAG	N	2	14/15	0.73	0.26	74,78,88,88	0

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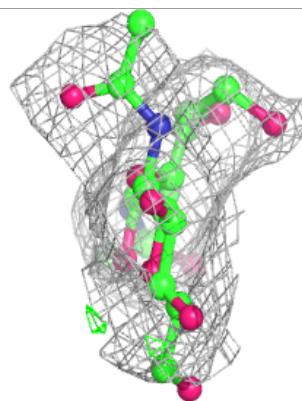
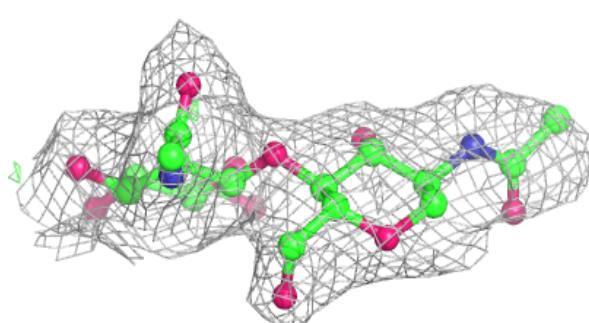
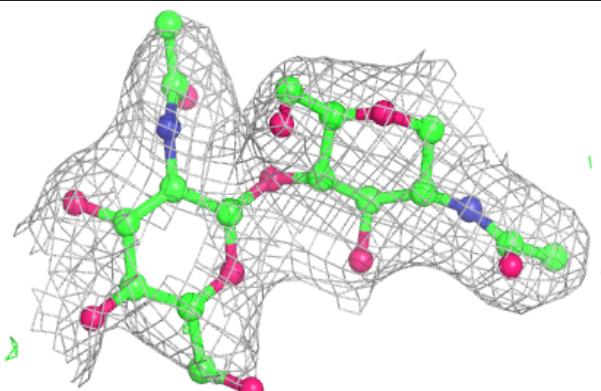
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	SA	2	14/15	0.73	0.27	56,76,83,84	0
2	NAG	o	2	14/15	0.78	0.35	60,72,83,84	0
2	NAG	IA	2	14/15	0.78	0.41	78,91,98,99	0
2	NAG	8	2	14/15	0.78	0.50	77,89,96,100	0
2	NAG	r	2	14/15	0.79	0.24	74,81,88,88	0
2	NAG	h	2	14/15	0.79	0.38	74,83,90,91	0
2	NAG	e	2	14/15	0.80	0.38	71,81,90,90	0
2	NAG	K	2	14/15	0.81	0.30	55,70,80,80	0
2	NAG	IA	1	14/15	0.83	0.30	63,71,78,86	0
2	NAG	VA	2	14/15	0.83	0.37	77,86,90,90	0
2	NAG	U	2	14/15	0.84	0.38	48,69,78,80	0
2	NAG	N	1	14/15	0.84	0.19	42,57,72,77	0
2	NAG	X	2	14/15	0.85	0.25	73,80,84,86	0
2	NAG	1	2	14/15	0.85	0.29	67,86,89,90	0
2	NAG	y	1	14/15	0.86	0.20	53,68,74,85	0
2	NAG	SA	1	14/15	0.86	0.27	54,64,71,72	0
2	NAG	LA	2	14/15	0.87	0.27	73,79,83,85	0
2	NAG	h	1	14/15	0.87	0.18	60,68,72,78	0
2	NAG	1	1	14/15	0.89	0.19	51,66,75,77	0
2	NAG	VA	1	14/15	0.90	0.19	53,69,76,80	0
2	NAG	X	1	14/15	0.90	0.19	50,60,68,75	0
2	NAG	r	1	14/15	0.91	0.16	43,57,68,72	0
2	NAG	BA	1	14/15	0.91	0.17	37,58,76,77	0
2	NAG	LA	1	14/15	0.93	0.14	52,59,71,72	0
2	NAG	8	1	14/15	0.93	0.39	48,62,77,86	0
2	NAG	K	1	14/15	0.94	0.22	40,50,60,67	0
2	NAG	e	1	14/15	0.94	0.22	49,54,64,73	0
2	NAG	U	1	14/15	0.94	0.26	31,50,59,66	0
2	NAG	o	1	14/15	0.95	0.26	48,52,62,68	0

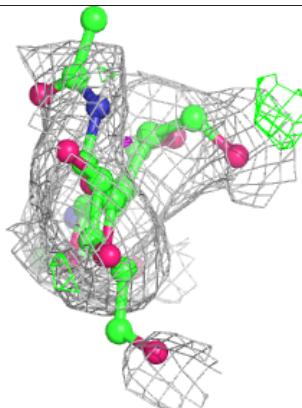
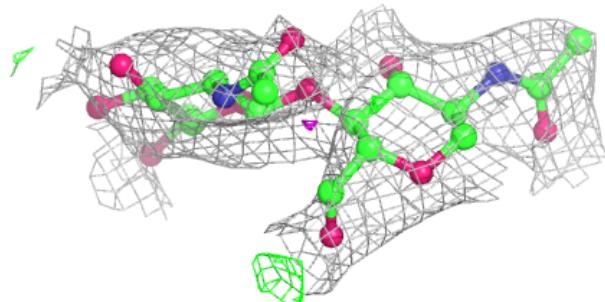
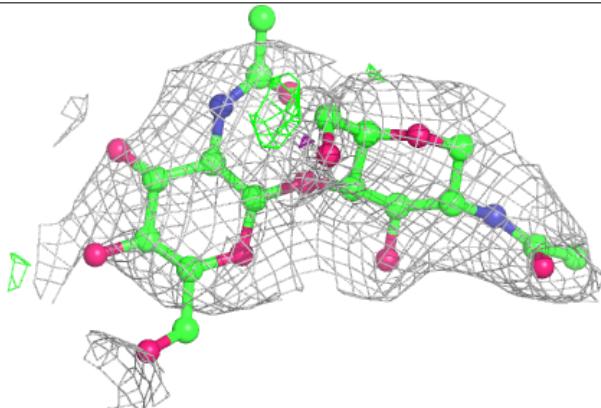
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

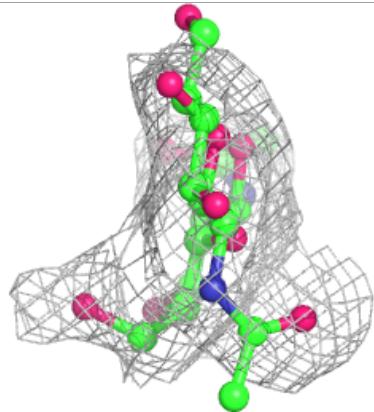
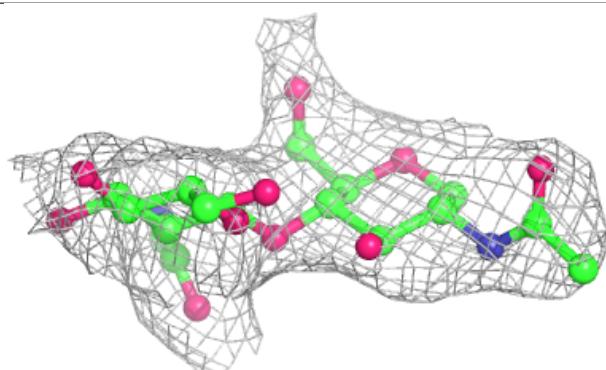
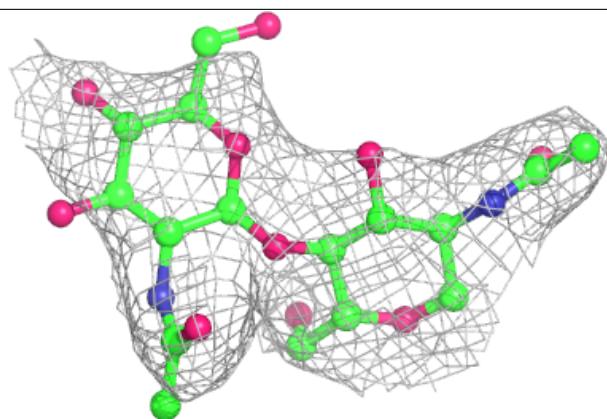
**Electron density around Chain N:**

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

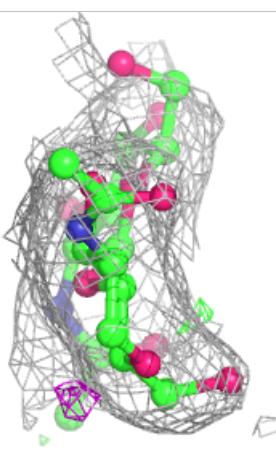
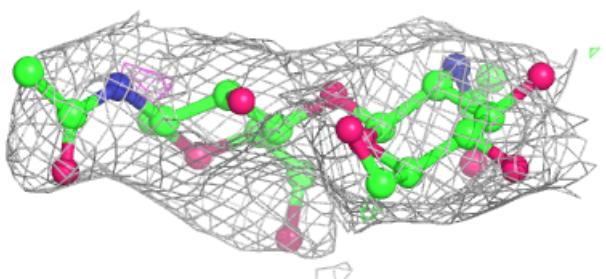
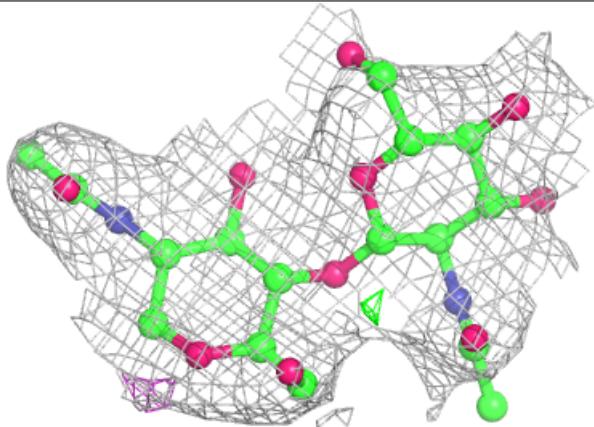


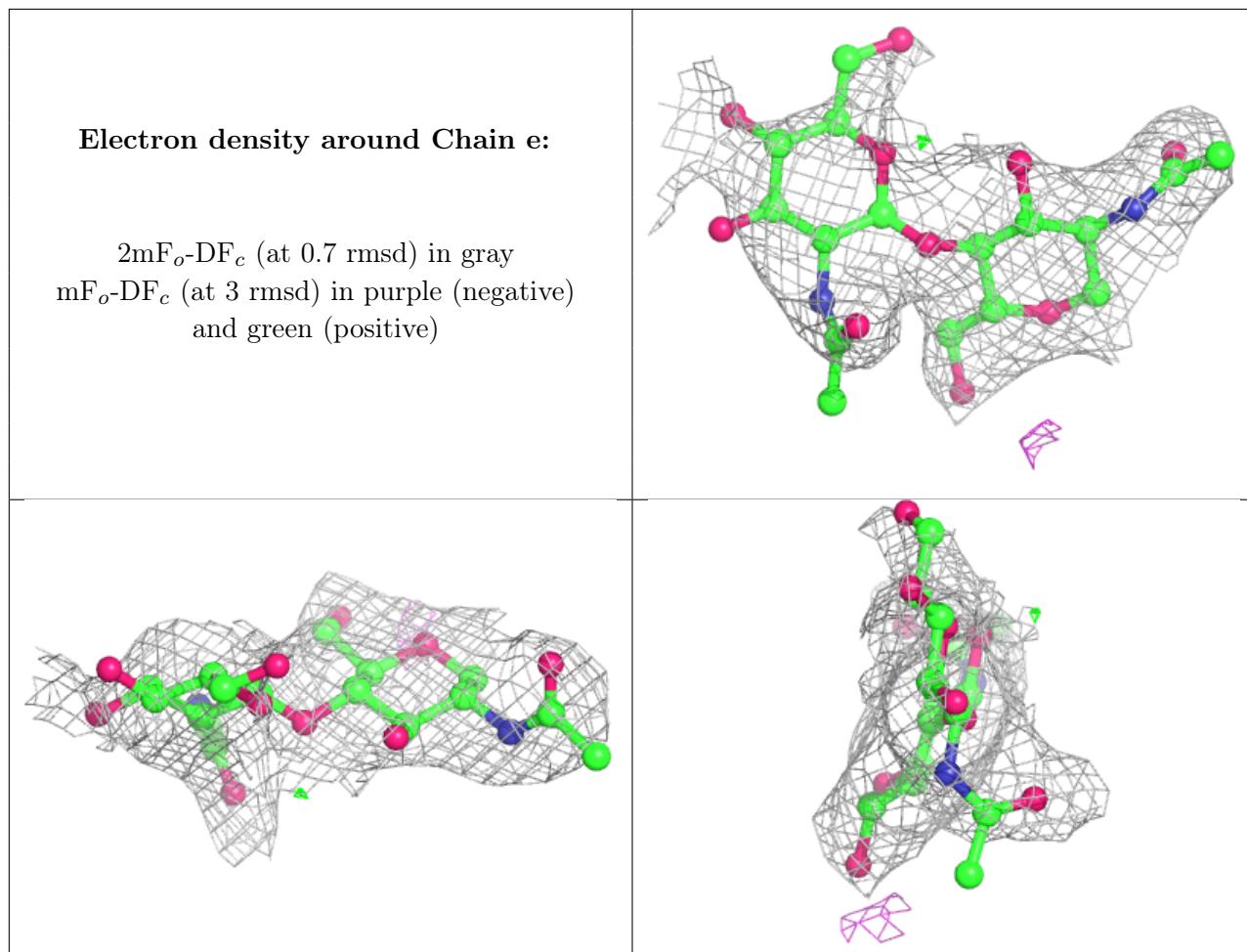
Electron density around Chain U:

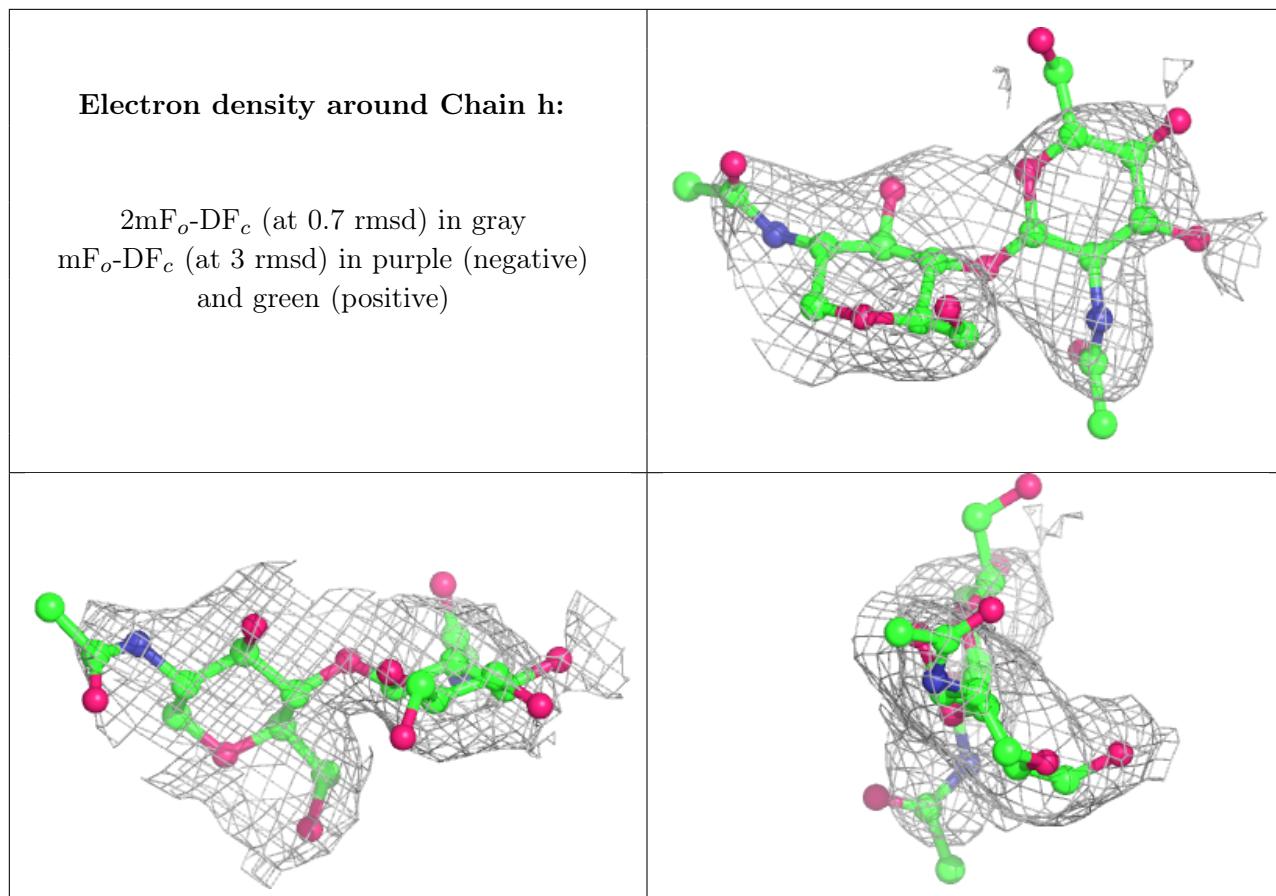
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

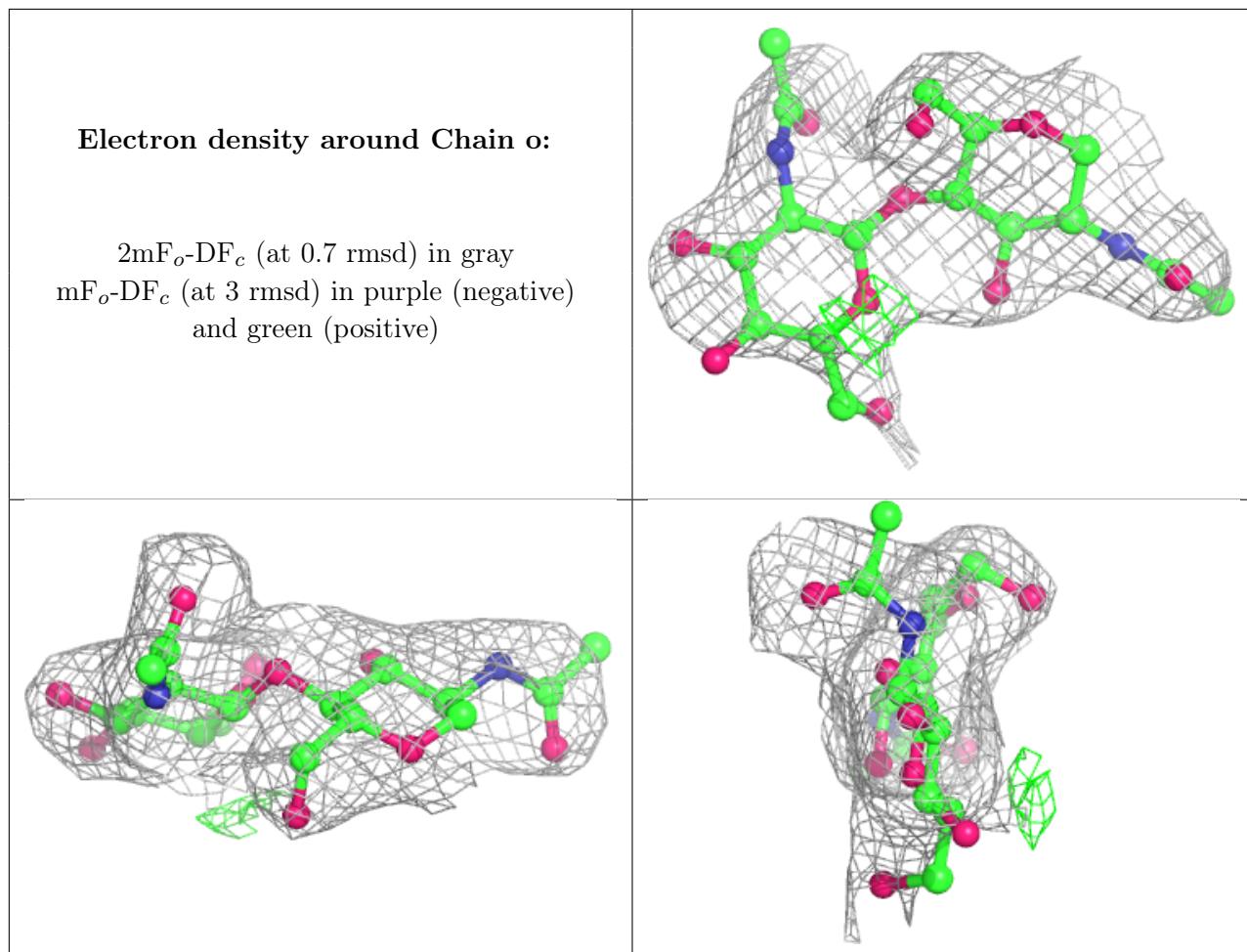
**Electron density around Chain X:**

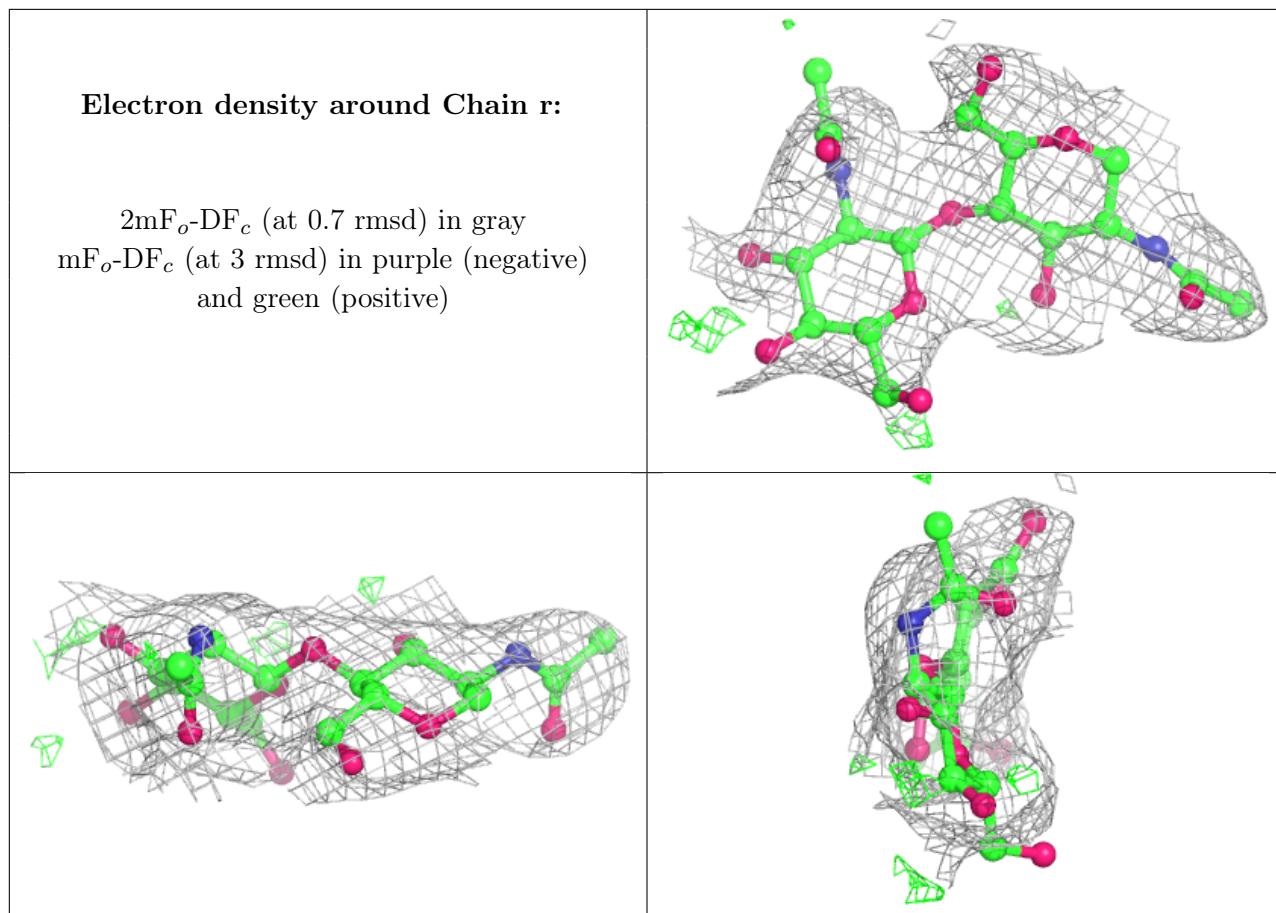
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

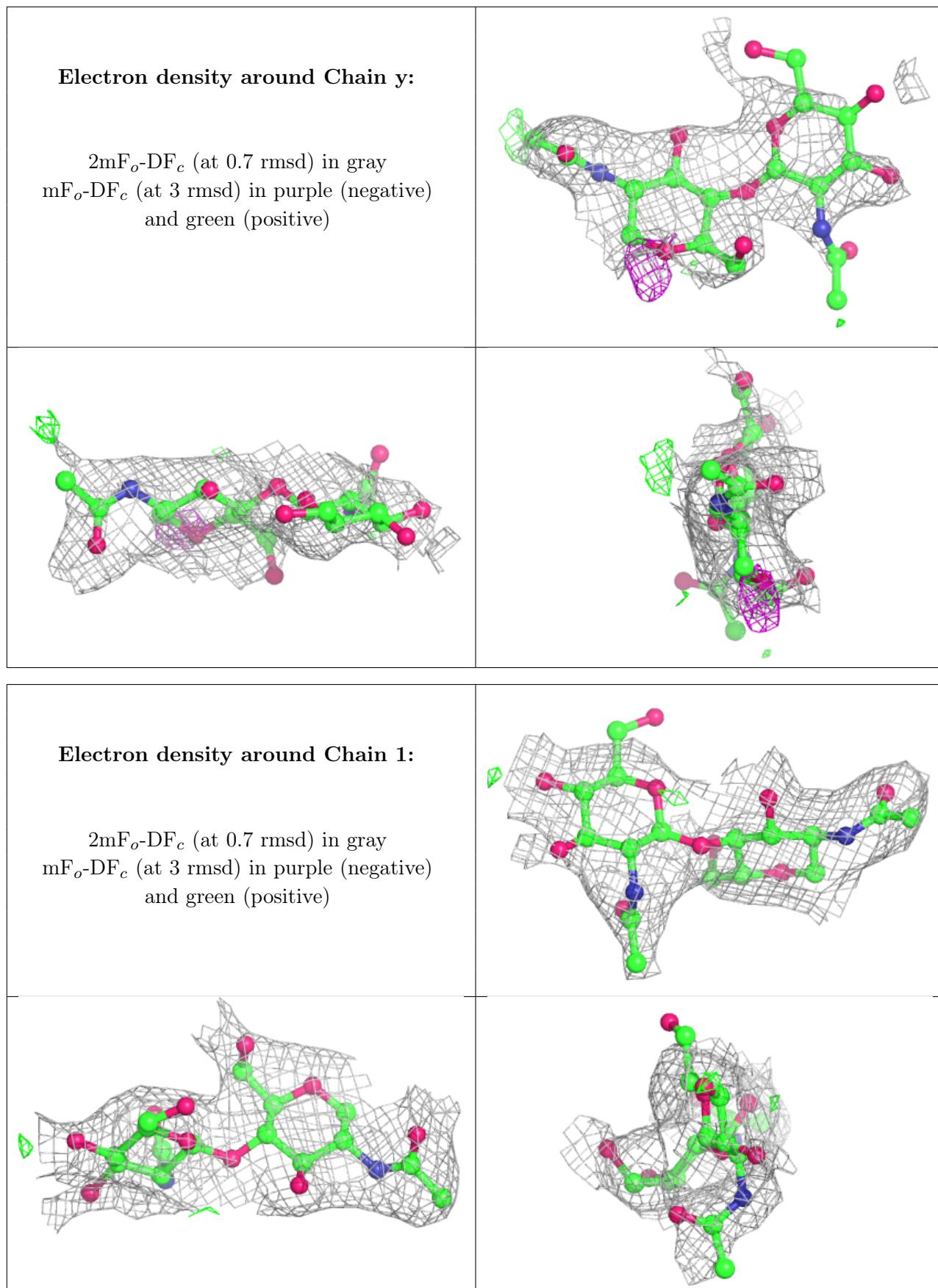






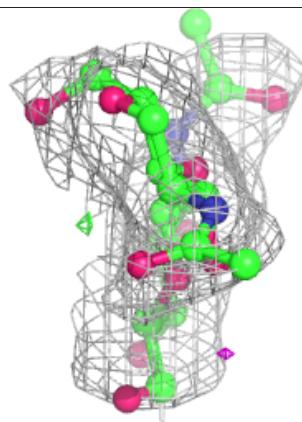
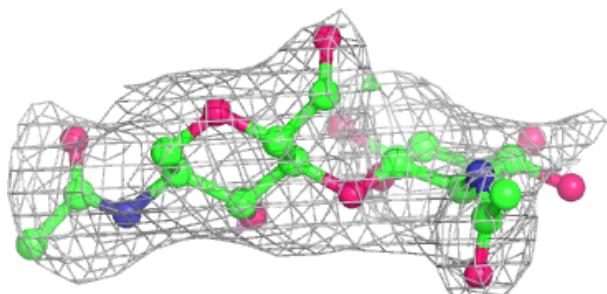
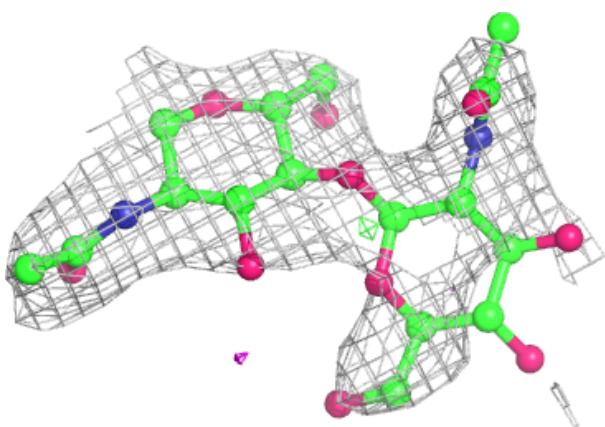




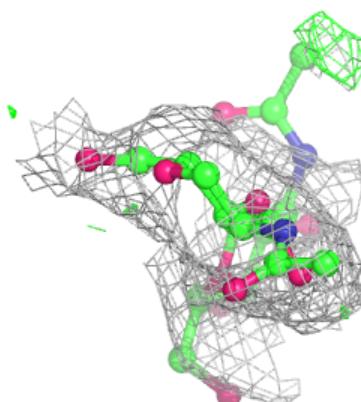
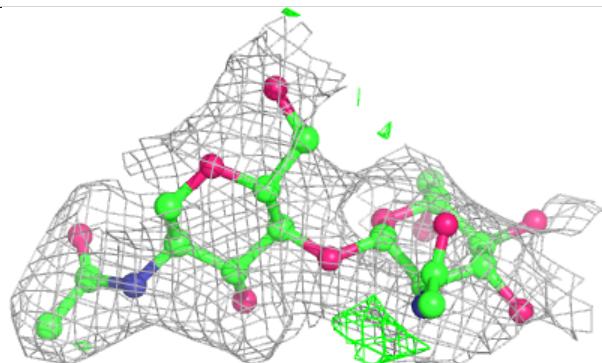
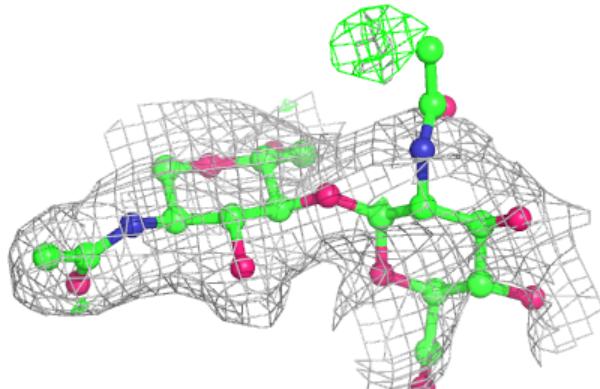


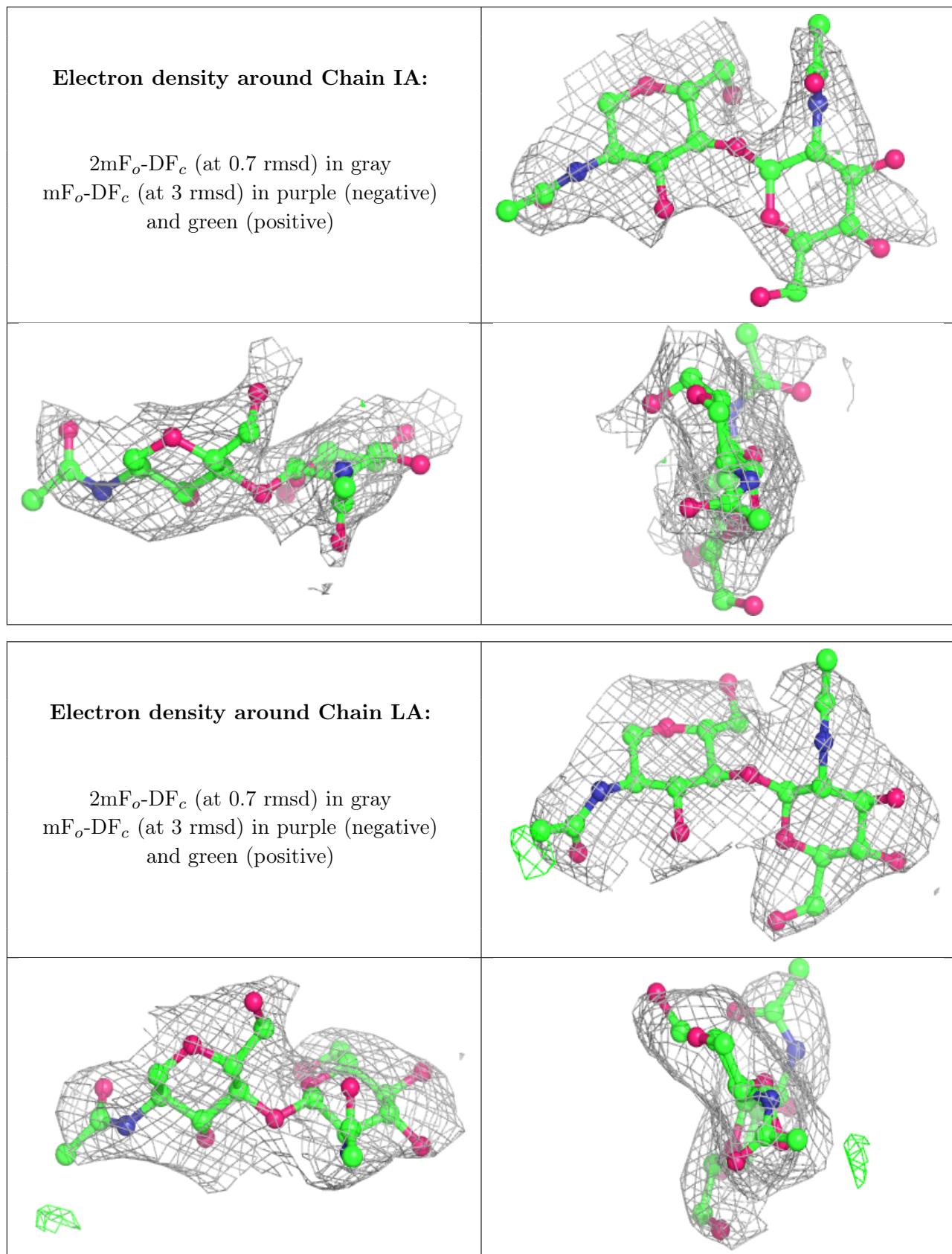
Electron density around Chain 8:

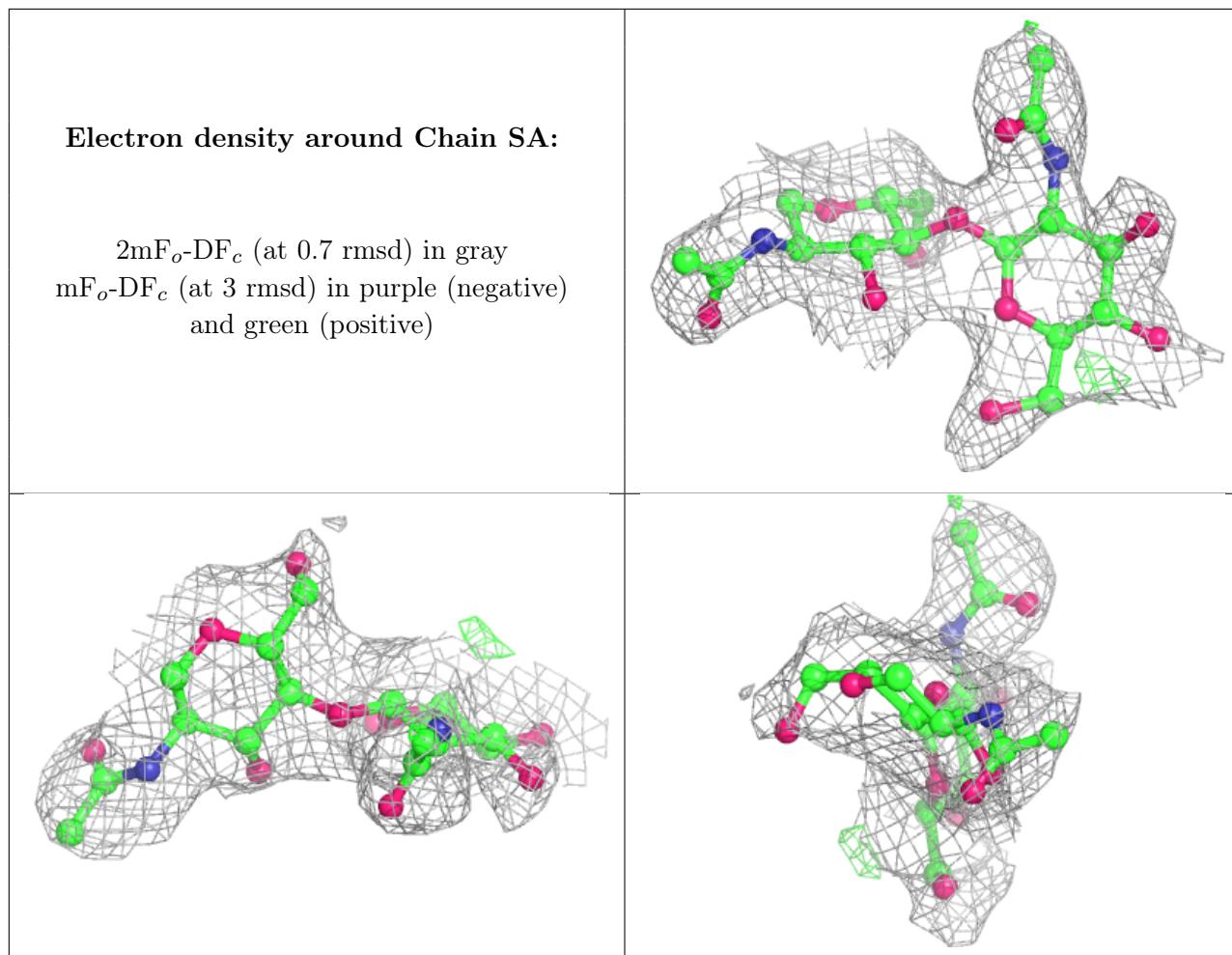
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

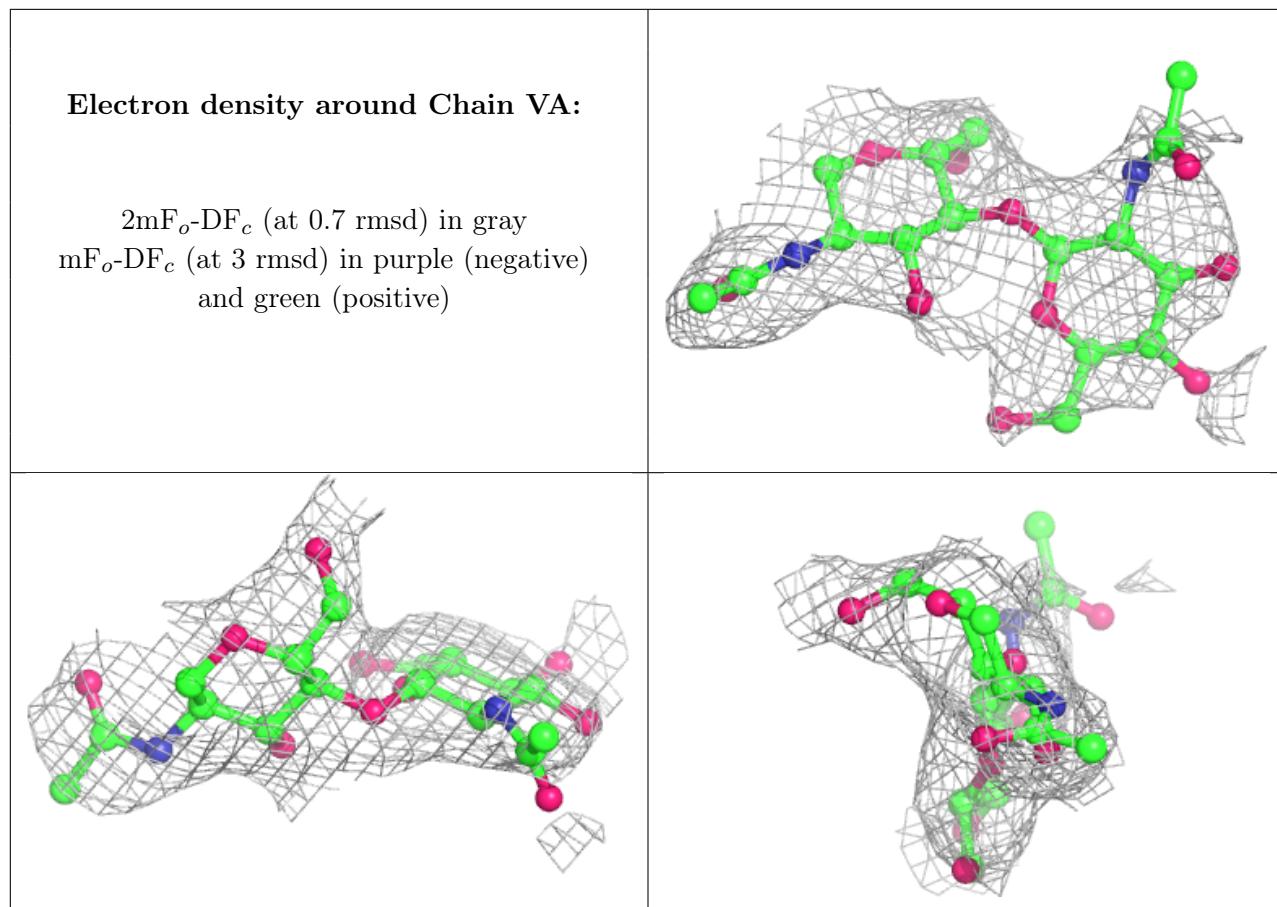
**Electron density around Chain BA:**

$2mF_o-DF_c$ (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
3	NAG	H	601	14/15	0.51	0.33	63,88,92,95	0
3	NAG	E	602	14/15	0.51	0.31	85,96,103,105	0
3	NAG	B	601	14/15	0.64	0.36	71,80,87,92	0
3	NAG	F	602	14/15	0.65	0.26	65,73,84,85	0
3	NAG	A	602	14/15	0.65	0.28	53,65,75,79	0
3	NAG	D	602	14/15	0.66	0.28	48,65,73,74	0
3	NAG	F	601	14/15	0.66	0.26	85,95,106,106	0
3	NAG	C	601	14/15	0.69	0.32	78,83,90,91	0
3	NAG	H	602	14/15	0.70	0.24	58,74,82,83	0
3	NAG	G	601	14/15	0.73	0.26	79,88,95,98	0
3	NAG	G	602	14/15	0.74	0.30	60,67,77,79	0
3	NAG	D	601	14/15	0.74	0.32	56,69,76,79	0
3	NAG	A	601	14/15	0.77	0.28	54,71,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	601	14/15	0.82	0.19	67,73,83,85	0
4	MG	H	603	1/1	0.83	0.34	59,59,59,59	0
3	NAG	B	602	14/15	0.84	0.19	54,62,67,68	0
4	MG	G	603	1/1	0.84	0.12	51,51,51,51	0
3	NAG	C	602	14/15	0.84	0.21	59,70,80,81	0
5	ZN	C	606	1/1	0.84	0.08	71,71,71,71	0
6	CA	H	605	1/1	0.85	0.10	50,50,50,50	0
5	ZN	B	606	1/1	0.87	0.10	80,80,80,80	0
5	ZN	C	604	1/1	0.88	0.13	35,35,35,35	0
4	MG	B	603	1/1	0.90	0.19	51,51,51,51	0
6	CA	G	605	1/1	0.92	0.17	40,40,40,40	0
4	MG	F	603	1/1	0.93	0.13	60,60,60,60	0
4	MG	C	603	1/1	0.93	0.10	43,43,43,43	0
6	CA	F	605	1/1	0.93	0.07	61,61,61,61	0
6	CA	A	605	1/1	0.94	0.08	42,42,42,42	0
5	ZN	A	606	1/1	0.95	0.05	68,68,68,68	0
4	MG	D	603	1/1	0.95	0.09	44,44,44,44	0
6	CA	E	605	1/1	0.95	0.05	53,53,53,53	0
5	ZN	F	606	1/1	0.96	0.07	75,75,75,75	0
5	ZN	D	606	1/1	0.96	0.07	67,67,67,67	0
6	CA	D	605	1/1	0.96	0.05	37,37,37,37	0
6	CA	C	605	1/1	0.96	0.10	43,43,43,43	0
5	ZN	B	604	1/1	0.96	0.37	69,69,69,69	0
4	MG	E	603	1/1	0.96	0.12	50,50,50,50	0
5	ZN	H	604	1/1	0.96	0.12	43,43,43,43	0
5	ZN	H	606	1/1	0.96	0.07	73,73,73,73	0
5	ZN	F	604	1/1	0.97	0.10	41,41,41,41	0
6	CA	B	605	1/1	0.97	0.07	42,42,42,42	0
5	ZN	E	604	1/1	0.97	0.17	43,43,43,43	0
5	ZN	D	604	1/1	0.98	0.12	28,28,28,28	0
5	ZN	E	606	1/1	0.98	0.04	62,62,62,62	0
5	ZN	A	604	1/1	0.98	0.10	29,29,29,29	0
4	MG	A	603	1/1	0.98	0.16	41,41,41,41	0
5	ZN	G	606	1/1	0.98	0.07	68,68,68,68	0
5	ZN	G	604	1/1	0.99	0.14	34,34,34,34	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.