



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:30 PM UTC

PDB ID : 6FB3 / pdb_00006fb3
Title : Teneurin 2 Partial Extracellular Domain
Authors : Jackson, V.A.; Carrasquero, M.; Lowe, E.D.; Seiradake, E.
Deposited on : 2017-12-18
Resolution : 2.38 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

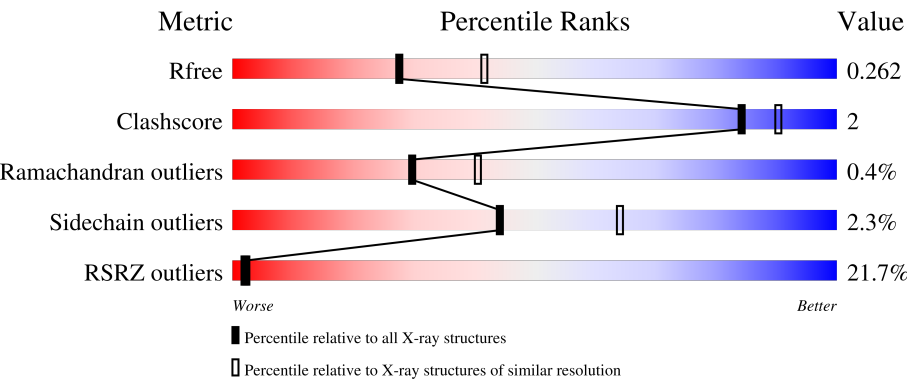
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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.



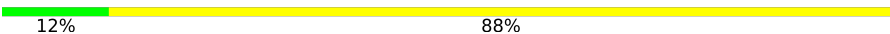
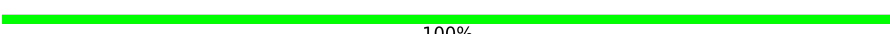
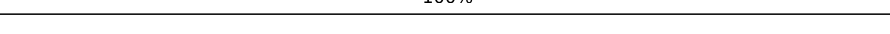
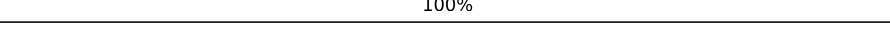
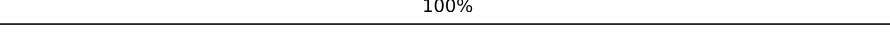
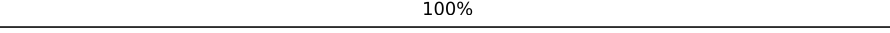
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	1859	26% 89% 9% ..
1	B	1859	23% 89% 9% ..
1	C	1859	14% 89% 9% ..
1	D	1859	23% 89% 9% ..
2	E	8	12% 88%

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Mol	Chain	Length	Quality of chain
2	K	8	 25% 75%
2	Q	8	 12% 88%
2	W	8	 25% 75%
3	F	2	 100%
3	G	2	 100%
3	H	2	 50% 50%
3	I	2	 100%
3	J	2	 100%
3	L	2	 100%
3	M	2	 100%
3	N	2	 50% 50%
3	O	2	 50% 50%
3	P	2	 100%
3	R	2	 50% 50%
3	S	2	 100%
3	T	2	 50% 50%
3	U	2	 50% 50%
3	V	2	 100%
3	X	2	 100%
3	Y	2	 100%
3	Z	2	 50% 50%
3	a	2	 50% 50%
3	b	2	 50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 59451 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 Teneurin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			
1	B	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			
1	C	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			
1	D	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			

There are 44 discrepancies between the modelled and reference sequences:

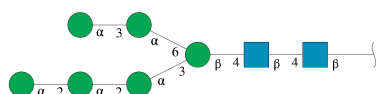
Chain	Residue	Modelled	Actual	Comment	Reference
A	953	THR	-	expression tag	UNP Q9DER5
A	954	GLY	-	expression tag	UNP Q9DER5
A	2803	GLY	-	expression tag	UNP Q9DER5
A	2804	THR	-	expression tag	UNP Q9DER5
A	2805	LYS	-	expression tag	UNP Q9DER5
A	2806	HIS	-	expression tag	UNP Q9DER5
A	2807	HIS	-	expression tag	UNP Q9DER5
A	2808	HIS	-	expression tag	UNP Q9DER5
A	2809	HIS	-	expression tag	UNP Q9DER5
A	2810	HIS	-	expression tag	UNP Q9DER5
A	2811	HIS	-	expression tag	UNP Q9DER5
B	953	THR	-	expression tag	UNP Q9DER5
B	954	GLY	-	expression tag	UNP Q9DER5
B	2803	GLY	-	expression tag	UNP Q9DER5
B	2804	THR	-	expression tag	UNP Q9DER5
B	2805	LYS	-	expression tag	UNP Q9DER5
B	2806	HIS	-	expression tag	UNP Q9DER5
B	2807	HIS	-	expression tag	UNP Q9DER5
B	2808	HIS	-	expression tag	UNP Q9DER5
B	2809	HIS	-	expression tag	UNP Q9DER5
B	2810	HIS	-	expression tag	UNP Q9DER5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2811	HIS	-	expression tag	UNP Q9DER5
C	953	THR	-	expression tag	UNP Q9DER5
C	954	GLY	-	expression tag	UNP Q9DER5
C	2803	GLY	-	expression tag	UNP Q9DER5
C	2804	THR	-	expression tag	UNP Q9DER5
C	2805	LYS	-	expression tag	UNP Q9DER5
C	2806	HIS	-	expression tag	UNP Q9DER5
C	2807	HIS	-	expression tag	UNP Q9DER5
C	2808	HIS	-	expression tag	UNP Q9DER5
C	2809	HIS	-	expression tag	UNP Q9DER5
C	2810	HIS	-	expression tag	UNP Q9DER5
C	2811	HIS	-	expression tag	UNP Q9DER5
D	953	THR	-	expression tag	UNP Q9DER5
D	954	GLY	-	expression tag	UNP Q9DER5
D	2803	GLY	-	expression tag	UNP Q9DER5
D	2804	THR	-	expression tag	UNP Q9DER5
D	2805	LYS	-	expression tag	UNP Q9DER5
D	2806	HIS	-	expression tag	UNP Q9DER5
D	2807	HIS	-	expression tag	UNP Q9DER5
D	2808	HIS	-	expression tag	UNP Q9DER5
D	2809	HIS	-	expression tag	UNP Q9DER5
D	2810	HIS	-	expression tag	UNP Q9DER5
D	2811	HIS	-	expression tag	UNP Q9DER5

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]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
2	E	8	Total	C	N	O	0	0	0
			94	52	2	40			
2	K	8	Total	C	N	O	0	0	0
			94	52	2	40			
2	Q	8	Total	C	N	O	0	0	0
			94	52	2	40			
2	W	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



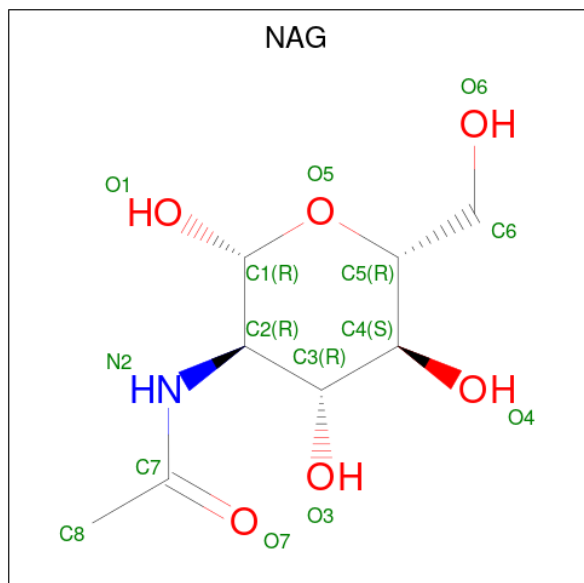
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

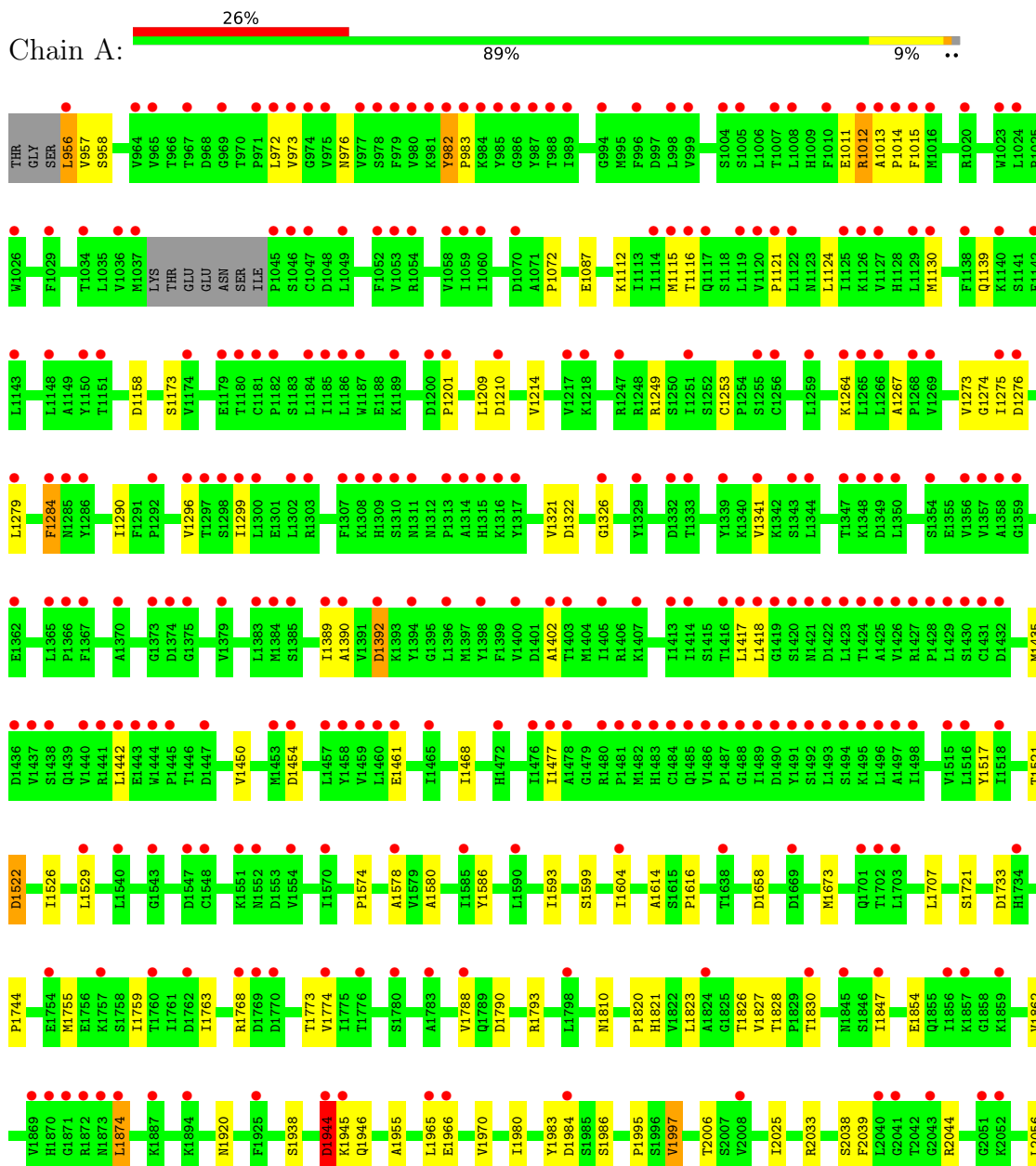
- Molecule 5 is water.

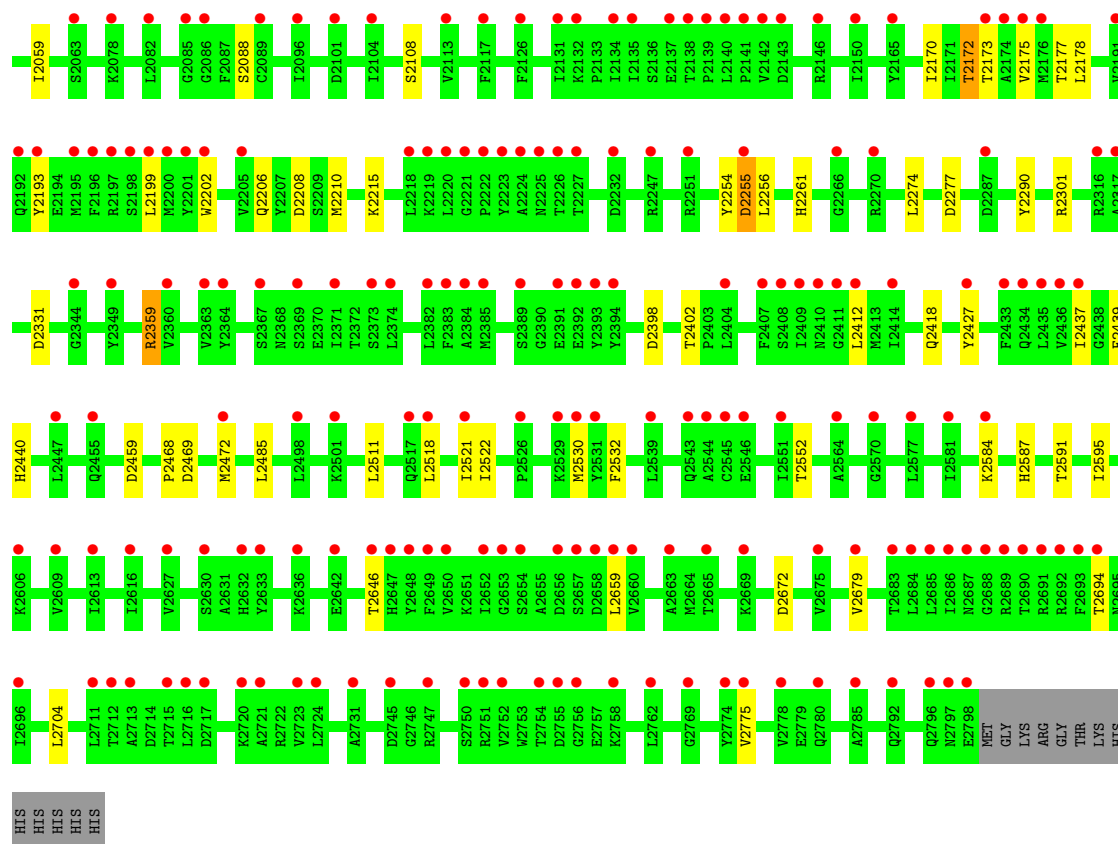
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	29	Total	O	0	0
			29	29		
5	C	105	Total	O	0	0
			105	105		
5	D	32	Total	O	0	0
			32	32		

3 Residue-property plots

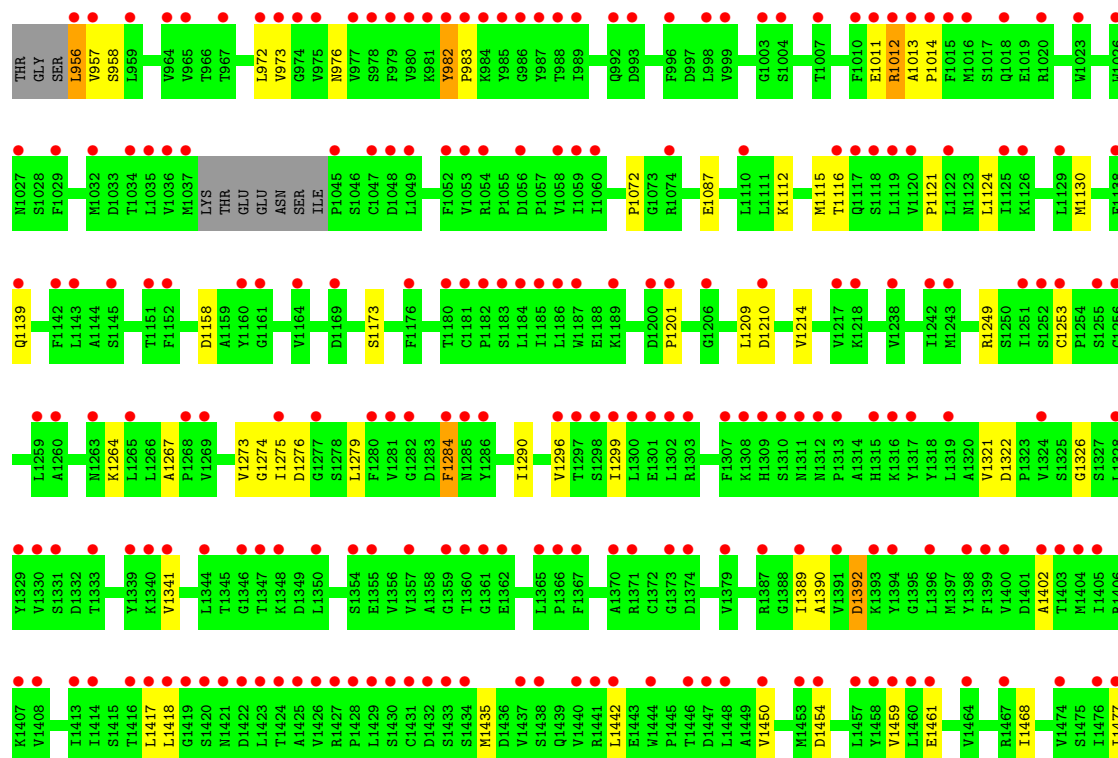
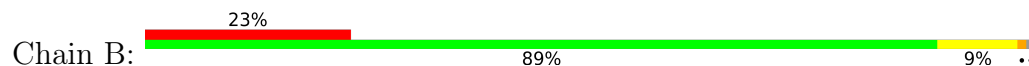
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

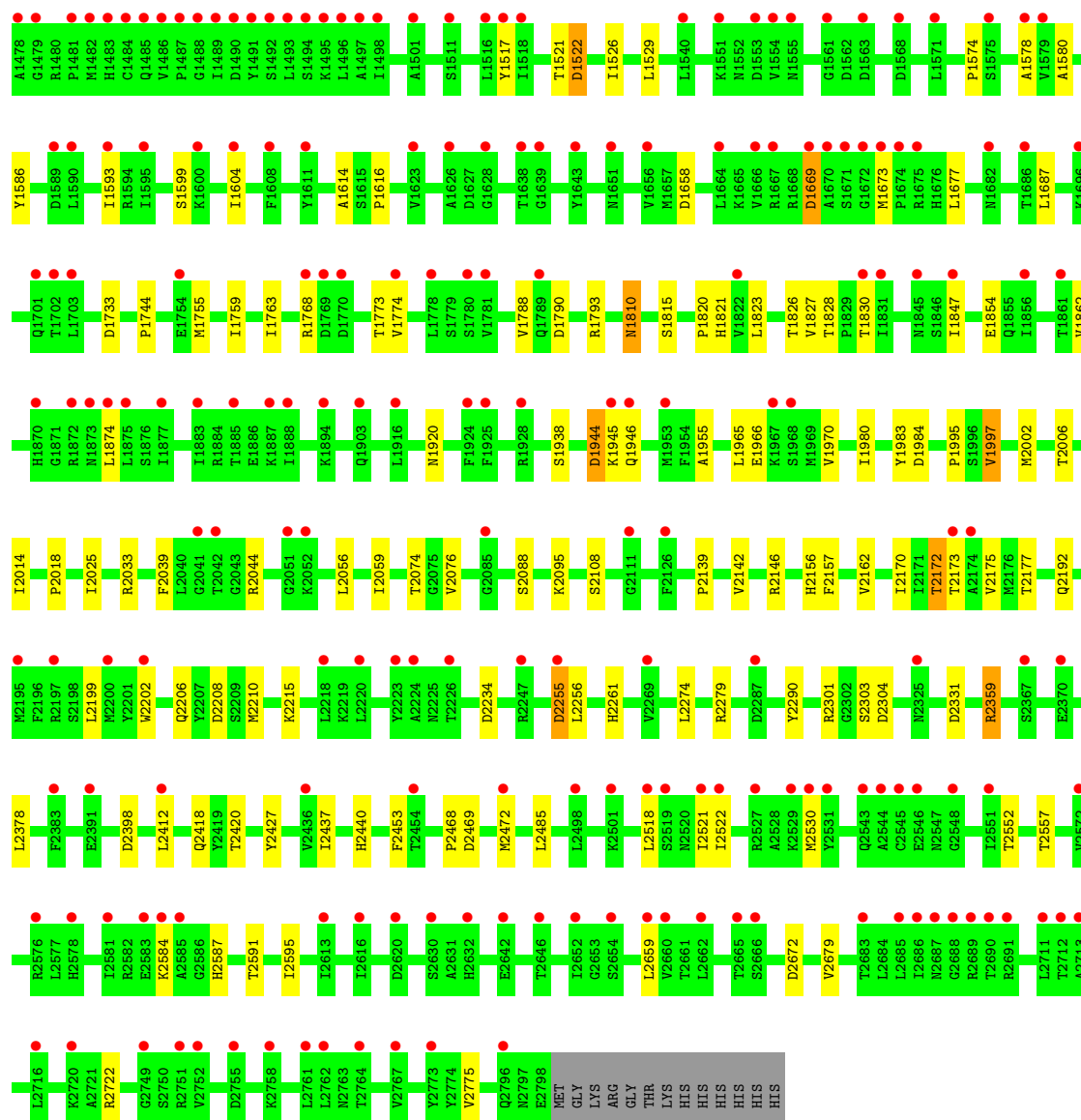
• Molecule 1: Teneurin-2



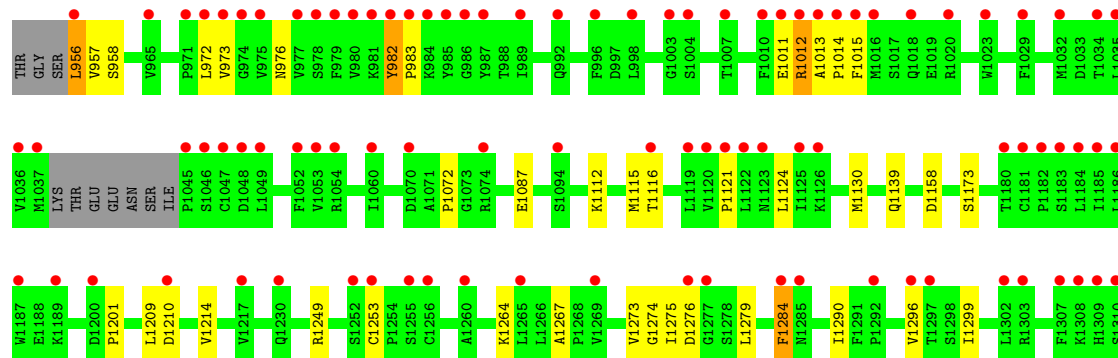
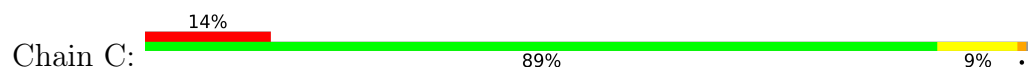


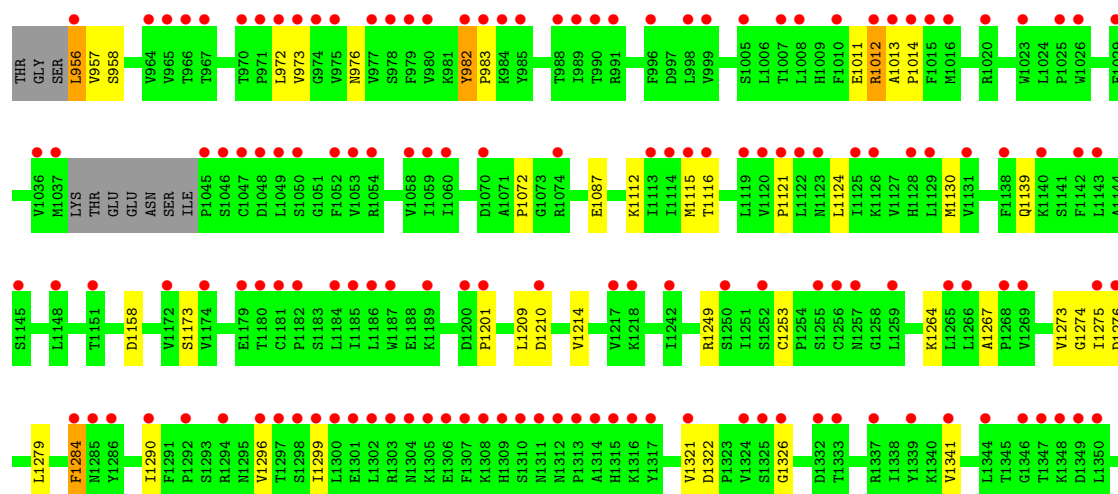
● Molecule 1: Teneurin-2

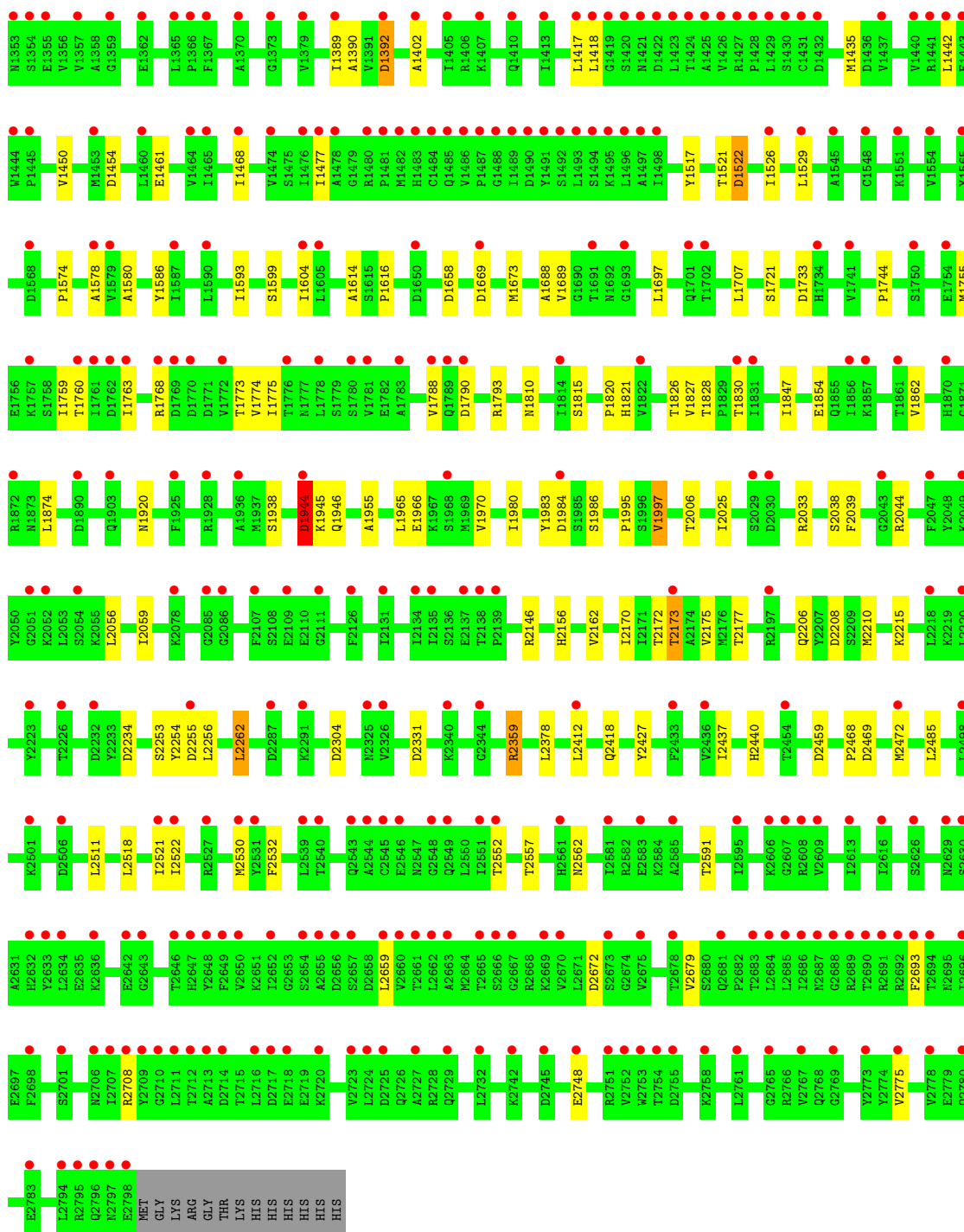




- Molecule 1: Teneurin-2







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

Chain E:

12%

88%



- Molecule 2: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain K:  25% 75%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

- Molecule 2: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Q:  12% 88%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

- Molecule 2: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain W:  25% 75%

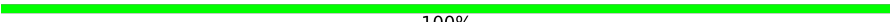
NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

Chain F:  100%

NAG1	NAG2
------	------

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

Chain G:  100%

NAG1	NAG2
------	------

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

Chain H:  50% 50%



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

Chain I:  100%



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

Chain J:  100%



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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain X:  100%



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

Chain Y:  100%



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

Chain Z:  50% 50%



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

Chain a:  50% 50%



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

Chain b:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.56Å 452.56Å 146.36Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	89.38 – 2.38 89.38 – 2.38	Depositor EDS
% Data completeness (in resolution range)	94.3 (89.38-2.38) 94.3 (89.38-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.225 , 0.242 0.245 , 0.262	Depositor DCC
R_{free} test set	21455 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	59451	wwPDB-VP
Average B, all atoms (Å ²)	76.0	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 45.90 % 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 1.2374e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.71	0/14827	1.15	34/20108 (0.2%)
1	B	0.71	0/14827	1.15	36/20108 (0.2%)
1	C	0.71	0/14827	1.15	33/20108 (0.2%)
1	D	0.71	0/14827	1.15	33/20108 (0.2%)
All	All	0.71	0/59308	1.15	136/80432 (0.2%)

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1984	ASP	CA-CB-CG	7.20	119.80	112.60
1	D	2255	ASP	CA-CB-CG	6.96	119.56	112.60
1	B	2255	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	1984	ASP	CA-CB-CG	6.89	119.49	112.60
1	B	2331	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	1669	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	1984	ASP	CA-CB-CG	6.73	119.33	112.60
1	D	2331	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	2331	ASP	CA-CB-CG	6.69	119.29	112.60
1	D	1984	ASP	CA-CB-CG	6.69	119.29	112.60
1	C	2645	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	2255	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	2331	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	1658	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	1658	ASP	CA-CB-CG	6.38	118.98	112.60
1	D	2234	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	1658	ASP	CA-CB-CG	6.29	118.89	112.60
1	C	1522	ASP	N-CA-C	-6.23	105.83	113.50
1	D	1658	ASP	CA-CB-CG	6.23	118.83	112.60
1	D	2304	ASP	CA-CB-CG	6.19	118.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1522	ASP	N-CA-C	-6.18	105.89	113.50
1	A	1522	ASP	N-CA-C	-6.15	105.94	113.50
1	D	1920	ASN	CA-CB-CG	6.08	118.68	112.60
1	D	2208	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	2208	ASP	CA-CB-CG	6.02	118.62	112.60
1	D	2775	VAL	N-CA-C	-5.97	105.31	110.74
1	C	1209	LEU	CA-C-N	5.94	129.73	120.82
1	C	1209	LEU	C-N-CA	5.94	129.73	120.82
1	C	2234	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	2208	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	2208	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	1983	TYR	CA-C-N	5.89	132.97	121.66
1	D	1983	TYR	C-N-CA	5.89	132.97	121.66
1	D	1209	LEU	CA-C-N	5.88	129.65	120.82
1	D	1209	LEU	C-N-CA	5.88	129.65	120.82
1	B	1920	ASN	CA-CB-CG	5.88	118.48	112.60
1	B	1522	ASP	N-CA-C	-5.88	105.94	113.23
1	C	2255	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	1209	LEU	CA-C-N	5.82	129.54	120.82
1	B	1209	LEU	C-N-CA	5.82	129.54	120.82
1	B	1210	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	2398	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	2459	ASP	CA-CB-CG	5.81	118.41	112.60
1	D	1210	ASP	CA-CB-CG	5.81	118.41	112.60
1	D	2459	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	1209	LEU	CA-C-N	5.79	129.50	120.82
1	A	1209	LEU	C-N-CA	5.79	129.50	120.82
1	C	1920	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	1210	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	1210	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	1920	ASN	CA-CB-CG	5.74	118.33	112.60
1	A	1983	TYR	CA-C-N	5.71	132.80	122.02
1	A	1983	TYR	C-N-CA	5.71	132.80	122.02
1	A	1392	ASP	CA-C-N	5.70	127.91	120.28
1	A	1392	ASP	C-N-CA	5.70	127.91	120.28
1	D	1158	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	1158	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	1392	ASP	CA-C-N	5.68	127.90	120.28
1	C	1392	ASP	C-N-CA	5.68	127.90	120.28
1	D	1392	ASP	CA-C-N	5.67	127.88	120.28
1	D	1392	ASP	C-N-CA	5.67	127.88	120.28
1	B	2398	ASP	CA-CB-CG	5.65	118.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1392	ASP	CA-C-N	5.65	127.85	120.28
1	B	1392	ASP	C-N-CA	5.65	127.85	120.28
1	B	2304	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	1158	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	2775	VAL	N-CA-C	-5.58	105.66	110.74
1	A	1158	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	2234	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	2304	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	2775	VAL	N-CA-C	-5.51	105.73	110.74
1	B	2420	THR	N-CA-C	-5.50	103.43	110.53
1	C	1983	TYR	CA-C-N	5.47	133.16	121.45
1	C	1983	TYR	C-N-CA	5.47	133.16	121.45
1	B	1983	TYR	CA-C-N	5.45	132.32	122.02
1	B	1983	TYR	C-N-CA	5.45	132.32	122.02
1	A	2459	ASP	CA-CB-CG	5.40	118.00	112.60
1	D	1276	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	1275	ILE	CA-C-N	5.38	129.82	120.68
1	B	1275	ILE	C-N-CA	5.38	129.82	120.68
1	A	1276	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	2254	TYR	CA-C-N	5.36	131.13	121.06
1	D	2254	TYR	C-N-CA	5.36	131.13	121.06
1	C	1322	ASP	CA-CB-CG	5.30	117.90	112.60
1	D	1322	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	2672	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	2672	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	1322	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	2672	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	2775	VAL	N-CA-C	-5.26	105.96	110.74
1	D	1810	ASN	CA-CB-CG	5.24	117.84	112.60
1	C	2398	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	1276	ASP	CA-CB-CG	5.22	117.82	112.60
1	D	1275	ILE	CA-C-N	5.21	129.54	120.68
1	D	1275	ILE	C-N-CA	5.21	129.54	120.68
1	B	1276	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	1733	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	1322	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	1810	ASN	CA-CB-CG	5.19	117.79	112.60
1	B	2157	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	1733	ASP	CA-CB-CG	5.17	117.78	112.60
1	B	2453	PHE	N-CA-C	-5.17	100.97	109.40
1	A	1275	ILE	CA-C-N	5.17	129.47	120.68
1	A	1275	ILE	C-N-CA	5.17	129.47	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2595	ILE	N-CA-C	-5.17	105.81	110.82
1	B	2595	ILE	N-CA-C	-5.16	105.68	110.53
1	A	1733	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	2672	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	1275	ILE	CA-C-N	5.15	129.44	120.68
1	C	1275	ILE	C-N-CA	5.15	129.44	120.68
1	D	2532	PHE	N-CA-C	-5.14	104.64	112.04
1	A	2277	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	1810	ASN	CA-CB-CG	5.14	117.74	112.60
1	D	1945	LYS	N-CA-C	-5.12	106.29	112.54
1	D	1944	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	1810	ASN	CA-CB-CG	5.11	117.71	112.60
1	B	1945	LYS	N-CA-C	-5.10	106.32	112.54
1	C	2172	THR	CA-C-N	5.08	130.20	121.87
1	C	2172	THR	C-N-CA	5.08	130.20	121.87
1	A	2172	THR	CA-C-N	5.08	130.19	121.87
1	A	2172	THR	C-N-CA	5.08	130.19	121.87
1	A	1945	LYS	N-CA-C	-5.07	106.36	112.54
1	A	2254	TYR	CA-C-N	5.06	130.58	121.06
1	A	2254	TYR	C-N-CA	5.06	130.58	121.06
1	D	2557	THR	CA-C-N	5.06	127.07	120.28
1	D	2557	THR	C-N-CA	5.06	127.07	120.28
1	A	1944	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	2595	ILE	N-CA-C	-5.05	105.78	110.53
1	C	2557	THR	CA-C-N	5.03	127.02	120.28
1	C	2557	THR	C-N-CA	5.03	127.02	120.28
1	D	1733	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	2172	THR	CA-C-N	5.02	130.10	121.87
1	B	2172	THR	C-N-CA	5.02	130.10	121.87
1	A	2532	PHE	N-CA-C	-5.01	104.82	112.04
1	B	2557	THR	CA-C-N	5.01	126.99	120.28
1	B	2557	THR	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14513	0	14253	69	0
1	B	14513	0	14253	72	0
1	C	14513	0	14253	66	0
1	D	14513	0	14253	67	0
2	E	94	0	79	0	0
2	K	94	0	79	0	0
2	Q	94	0	79	0	0
2	W	94	0	79	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
4	A	70	0	65	0	0
4	B	70	0	65	0	0
4	C	70	0	65	0	0
4	D	70	0	65	0	0
5	A	17	0	0	0	0
5	B	29	0	0	0	0
5	C	105	0	0	0	0
5	D	32	0	0	0	0
All	All	59451	0	58088	272	0

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

All (272) 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:C:1821:HIS:HD2	1:C:1830:THR:HG21	1.41	0.85
1:A:1821:HIS:HD2	1:A:1830:THR:HG21	1.41	0.85
1:B:1821:HIS:HD2	1:B:1830:THR:HG21	1.41	0.83
1:D:1821:HIS:HD2	1:D:1830:THR:HG21	1.42	0.82
1:D:982:TYR:HB3	1:D:983:PRO:HD3	1.65	0.79
1:B:982:TYR:HB3	1:B:983:PRO:HD3	1.65	0.78
1:C:982:TYR:HB3	1:C:983:PRO:HD3	1.64	0.78
1:A:982:TYR:HB3	1:A:983:PRO:HD3	1.65	0.76
1:A:2468:PRO:HB3	1:A:2485:LEU:HB3	1.71	0.72
1:B:982:TYR:HB3	1:B:983:PRO:CD	2.20	0.72
1:C:982:TYR:HB3	1:C:983:PRO:CD	2.20	0.71
1:A:982:TYR:HB3	1:A:983:PRO:CD	2.20	0.71
1:D:1821:HIS:CD2	1:D:1830:THR:HG21	2.25	0.71
1:D:982:TYR:HB3	1:D:983:PRO:CD	2.20	0.71
1:D:2468:PRO:HB3	1:D:2485:LEU:HB3	1.73	0.71
1:B:1821:HIS:CD2	1:B:1830:THR:HG21	2.25	0.70
1:C:1821:HIS:CD2	1:C:1830:THR:HG21	2.25	0.70
1:A:1821:HIS:CD2	1:A:1830:THR:HG21	2.25	0.70
1:B:2468:PRO:HB3	1:B:2485:LEU:HB3	1.74	0.69
1:C:2468:PRO:HB3	1:C:2485:LEU:HB3	1.73	0.68
1:C:1201:PRO:HB3	1:C:1214:VAL:HB	1.78	0.65
1:A:1201:PRO:HB3	1:A:1214:VAL:HB	1.79	0.65
1:A:1130:MET:HB2	1:A:1173:SER:HB2	1.80	0.64
1:B:1130:MET:HB2	1:B:1173:SER:HB2	1.79	0.64
1:B:1201:PRO:HB3	1:B:1214:VAL:HB	1.79	0.63
1:D:1201:PRO:HB3	1:D:1214:VAL:HB	1.79	0.63
1:D:1130:MET:HB2	1:D:1173:SER:HB2	1.80	0.63
1:C:1130:MET:HB2	1:C:1173:SER:HB2	1.80	0.63
1:A:1521:THR:HB	1:A:1574:PRO:HD2	1.81	0.62
1:D:1521:THR:HB	1:D:1574:PRO:HD2	1.81	0.62
1:B:1521:THR:HB	1:B:1574:PRO:HD2	1.81	0.61
1:C:1521:THR:HB	1:C:1574:PRO:HD2	1.81	0.61
1:C:1773:THR:HG23	1:C:1788:VAL:HB	1.82	0.60
1:A:2173:THR:HG22	1:A:2175:VAL:H	1.67	0.60
1:B:2173:THR:HG22	1:B:2175:VAL:H	1.67	0.60
1:C:2173:THR:HG22	1:C:2175:VAL:H	1.66	0.60
1:B:1773:THR:HG23	1:B:1788:VAL:HB	1.83	0.59
1:A:1773:THR:HG23	1:A:1788:VAL:HB	1.84	0.59
1:D:1773:THR:HG23	1:D:1788:VAL:HB	1.84	0.59
1:C:1955:ALA:HB3	1:C:2210:MET:HE3	1.85	0.58
1:D:2173:THR:HG22	1:D:2175:VAL:H	1.67	0.58
1:D:1955:ALA:HB3	1:D:2210:MET:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1955:ALA:HB3	1:B:2210:MET:HE3	1.86	0.56
1:C:2359:ARG:HH12	1:C:2530:MET:HE3	1.71	0.56
1:D:1744:PRO:HB2	1:D:2006:THR:HG21	1.87	0.56
1:A:1955:ALA:HB3	1:A:2210:MET:HE3	1.87	0.55
1:B:2359:ARG:HH12	1:B:2530:MET:HE3	1.72	0.55
1:A:1744:PRO:HB2	1:A:2006:THR:HG21	1.88	0.55
1:B:2142:VAL:HG12	1:D:1669:ASP:OD1	2.06	0.55
1:B:2418:GLN:HB2	1:B:2427:TYR:HB3	1.88	0.55
1:C:2290:TYR:CZ	1:C:2301:ARG:HG3	2.42	0.55
1:A:2418:GLN:HB2	1:A:2427:TYR:HB3	1.90	0.54
1:B:1677:LEU:HG	1:B:1687:LEU:HD11	1.89	0.54
1:C:1390:ALA:HB1	1:C:1450:VAL:HG23	1.89	0.54
1:A:1390:ALA:HB1	1:A:1450:VAL:HG23	1.90	0.54
1:D:2418:GLN:HB2	1:D:2427:TYR:HB3	1.90	0.54
1:B:1390:ALA:HB1	1:B:1450:VAL:HG23	1.90	0.53
1:D:1970:VAL:HG22	1:D:1980:ILE:HG12	1.90	0.53
1:D:1390:ALA:HB1	1:D:1450:VAL:HG23	1.90	0.53
1:A:2359:ARG:HH12	1:A:2530:MET:HE3	1.74	0.53
1:B:2290:TYR:CZ	1:B:2301:ARG:HG3	2.44	0.52
1:C:2659:LEU:HD21	1:C:2679:VAL:HG11	1.91	0.52
1:D:2359:ARG:HH12	1:D:2530:MET:HE3	1.73	0.52
1:C:2418:GLN:HB2	1:C:2427:TYR:HB3	1.91	0.52
1:D:2025:ILE:HB	1:D:2038:SER:HB2	1.92	0.52
1:B:2659:LEU:HD21	1:B:2679:VAL:HG11	1.92	0.52
1:C:1854:GLU:HB2	1:C:1862:VAL:HB	1.92	0.52
1:C:1970:VAL:HG22	1:C:1980:ILE:HG12	1.91	0.52
1:A:1854:GLU:HB2	1:A:1862:VAL:HB	1.92	0.52
1:D:1130:MET:HG2	1:D:1139:GLN:HG2	1.92	0.52
1:B:1273:VAL:HG23	1:B:1578:ALA:HB1	1.92	0.52
1:B:972:LEU:HD22	1:B:1012:ARG:HE	1.75	0.52
1:D:1874:LEU:HD13	1:D:2521:ILE:HD12	1.92	0.52
1:B:1874:LEU:HD13	1:B:2521:ILE:HD12	1.92	0.51
1:A:972:LEU:HD22	1:A:1012:ARG:HE	1.75	0.51
1:B:2014:ILE:HG12	1:B:2025:ILE:HG12	1.92	0.51
1:B:1827:VAL:HG13	1:B:1828:THR:HG23	1.92	0.51
1:B:1854:GLU:HB2	1:B:1862:VAL:HB	1.91	0.51
1:C:972:LEU:HD22	1:C:1012:ARG:HE	1.74	0.51
1:C:1827:VAL:HG13	1:C:1828:THR:HG23	1.92	0.51
1:D:1854:GLU:HB2	1:D:1862:VAL:HB	1.92	0.51
1:D:972:LEU:HD22	1:D:1012:ARG:HE	1.75	0.51
1:C:1874:LEU:HD13	1:C:2521:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1130:MET:HG2	1:C:1139:GLN:HG2	1.93	0.51
1:D:1273:VAL:HG23	1:D:1578:ALA:HB1	1.92	0.51
1:D:1827:VAL:HG13	1:D:1828:THR:HG23	1.92	0.51
1:A:1273:VAL:HG23	1:A:1578:ALA:HB1	1.92	0.51
1:B:1130:MET:HG2	1:B:1139:GLN:HG2	1.92	0.51
1:C:1290:ILE:HG12	1:C:1296:VAL:HG22	1.93	0.50
1:A:2469:ASP:HB3	1:A:2472:MET:HE3	1.93	0.50
1:B:1290:ILE:HG12	1:B:1296:VAL:HG22	1.93	0.50
1:D:2469:ASP:HB3	1:D:2472:MET:HE3	1.93	0.50
1:C:1273:VAL:HG23	1:C:1578:ALA:HB1	1.92	0.50
1:A:1522:ASP:HB2	1:A:1526:ILE:HB	1.93	0.50
1:A:2290:TYR:CZ	1:A:2301:ARG:HG3	2.46	0.50
1:D:1290:ILE:HG12	1:D:1296:VAL:HG22	1.93	0.50
1:A:1290:ILE:HG12	1:A:1296:VAL:HG22	1.93	0.50
1:A:1130:MET:HG2	1:A:1139:GLN:HG2	1.92	0.50
1:A:1827:VAL:HG13	1:A:1828:THR:HG23	1.92	0.50
1:B:1274:GLY:HA2	1:B:1321:VAL:HG11	1.94	0.50
1:C:1522:ASP:HB2	1:C:1526:ILE:HB	1.92	0.50
1:A:1874:LEU:HD13	1:A:2521:ILE:HD12	1.93	0.50
1:A:1299:ILE:HD12	1:A:1341:VAL:HG11	1.94	0.49
1:C:2469:ASP:HB3	1:C:2472:MET:HE3	1.94	0.49
1:D:1299:ILE:HD12	1:D:1341:VAL:HG11	1.94	0.49
1:A:2659:LEU:HD21	1:A:2679:VAL:HG11	1.95	0.49
1:B:1522:ASP:HB2	1:B:1526:ILE:HB	1.93	0.49
1:D:1522:ASP:HB2	1:D:1526:ILE:HB	1.92	0.49
1:A:1274:GLY:HA2	1:A:1321:VAL:HG11	1.94	0.49
1:B:1299:ILE:HD12	1:B:1341:VAL:HG11	1.93	0.49
1:D:1274:GLY:HA2	1:D:1321:VAL:HG11	1.95	0.49
1:B:2469:ASP:HB3	1:B:2472:MET:HE3	1.93	0.49
1:D:2659:LEU:HD21	1:D:2679:VAL:HG11	1.95	0.49
1:C:1744:PRO:HB2	1:C:2006:THR:HG21	1.94	0.49
1:C:2039:PHE:HB2	1:C:2044:ARG:HB2	1.95	0.48
1:B:1755:MET:HG3	1:B:1759:ILE:HG12	1.95	0.48
1:C:1299:ILE:HD12	1:C:1341:VAL:HG11	1.94	0.48
1:D:1755:MET:HG3	1:D:1759:ILE:HG12	1.95	0.48
1:A:1755:MET:HG3	1:A:1759:ILE:HG12	1.95	0.48
1:B:2039:PHE:HB2	1:B:2044:ARG:HB2	1.94	0.48
1:C:1755:MET:HG3	1:C:1759:ILE:HG12	1.94	0.48
1:C:1279:LEU:HD23	1:C:1290:ILE:HD12	1.96	0.48
1:B:1995:PRO:HB2	1:B:2256:LEU:HB3	1.96	0.48
1:A:2039:PHE:HB2	1:A:2044:ARG:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1279:LEU:HD23	1:D:1290:ILE:HD12	1.96	0.47
1:D:2039:PHE:HB2	1:D:2044:ARG:HB2	1.94	0.47
1:B:1279:LEU:HD23	1:B:1290:ILE:HD12	1.96	0.47
1:A:1279:LEU:HD23	1:A:1290:ILE:HD12	1.96	0.47
1:C:1274:GLY:HA2	1:C:1321:VAL:HG11	1.95	0.47
1:B:2088:SER:HB3	1:B:2108:SER:HB3	1.96	0.47
1:C:1938:SER:H	1:C:2210:MET:HE1	1.79	0.47
1:A:1938:SER:H	1:A:2210:MET:HE1	1.79	0.47
1:A:1995:PRO:HB2	1:A:2256:LEU:HB3	1.96	0.47
1:B:2261:HIS:HA	1:B:2274:LEU:HB2	1.96	0.47
1:D:1788:VAL:HG22	1:D:1793:ARG:HG2	1.96	0.47
1:A:1442:LEU:HG	1:A:1461:GLU:HG3	1.97	0.47
1:A:1788:VAL:HG22	1:A:1793:ARG:HG2	1.97	0.47
1:C:1788:VAL:HG22	1:C:1793:ARG:HG2	1.96	0.47
1:A:1013:ALA:HB3	1:A:1014:PRO:HD3	1.97	0.47
1:D:1442:LEU:HG	1:D:1461:GLU:HG3	1.97	0.47
1:D:2518:LEU:HB3	1:D:2522:ILE:HD12	1.96	0.47
1:D:1995:PRO:HB2	1:D:2256:LEU:HB3	1.97	0.46
1:B:1938:SER:H	1:B:2210:MET:HE1	1.79	0.46
1:B:2518:LEU:HB3	1:B:2522:ILE:HD12	1.97	0.46
1:D:2172:THR:HG22	1:D:2177:THR:HG22	1.97	0.46
1:C:2518:LEU:HB3	1:C:2522:ILE:HD12	1.97	0.46
1:A:2518:LEU:HB3	1:A:2522:ILE:HD12	1.97	0.46
1:B:1013:ALA:HB3	1:B:1014:PRO:HD3	1.96	0.46
1:B:1788:VAL:HG22	1:B:1793:ARG:HG2	1.97	0.46
1:C:1013:ALA:HB3	1:C:1014:PRO:HD3	1.96	0.46
1:D:1013:ALA:HB3	1:D:1014:PRO:HD3	1.96	0.46
1:C:1442:LEU:HG	1:C:1461:GLU:HG3	1.98	0.46
1:A:2646:THR:HG22	1:A:2704:LEU:HD22	1.97	0.46
1:B:1267:ALA:HB3	1:B:1284:PHE:HB2	1.98	0.46
1:B:2584:LYS:HB3	1:B:2587:HIS:HB2	1.98	0.46
1:A:2402:THR:HG23	1:A:2439:PHE:HA	1.98	0.45
1:B:2172:THR:HG22	1:B:2177:THR:HG22	1.99	0.45
1:C:1995:PRO:HB2	1:C:2256:LEU:HB3	1.98	0.45
1:C:1267:ALA:HB3	1:C:1284:PHE:HB2	1.99	0.45
1:C:956:LEU:HB3	1:C:957:VAL:H	1.63	0.45
1:B:1744:PRO:HB2	1:B:2006:THR:HG21	1.99	0.45
1:D:1267:ALA:HB3	1:D:1284:PHE:HB2	1.98	0.45
1:B:1955:ALA:HB3	1:B:2210:MET:CE	2.46	0.45
1:D:982:TYR:CB	1:D:983:PRO:CD	2.95	0.45
1:B:1442:LEU:HG	1:B:1461:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1955:ALA:HB3	1:A:2210:MET:CE	2.47	0.44
1:D:1955:ALA:HB3	1:D:2210:MET:CE	2.46	0.44
1:A:2199:LEU:HD21	1:A:2202:TRP:CD1	2.52	0.44
1:A:2261:HIS:HA	1:A:2274:LEU:HB2	1.98	0.44
1:B:1517:TYR:HB3	1:B:1529:LEU:HD11	1.99	0.44
1:D:1820:PRO:HB3	1:D:1826:THR:HA	1.99	0.44
1:D:1938:SER:H	1:D:2210:MET:HE1	1.80	0.44
1:A:2056:LEU:HD21	1:A:2059:ILE:HD11	1.99	0.44
1:B:1820:PRO:HB3	1:B:1826:THR:HA	2.00	0.44
1:C:1955:ALA:HB3	1:C:2210:MET:CE	2.46	0.44
1:A:956:LEU:HB3	1:A:957:VAL:H	1.63	0.44
1:A:1267:ALA:HB3	1:A:1284:PHE:HB2	1.98	0.44
1:C:2172:THR:HG22	1:C:2177:THR:HG22	1.99	0.44
1:D:1707:LEU:HB3	1:D:1721:SER:HB2	2.00	0.44
1:A:1820:PRO:HB3	1:A:1826:THR:HA	2.00	0.44
1:B:1970:VAL:HG22	1:B:1980:ILE:HG12	1.99	0.44
1:A:976:ASN:HB3	1:A:1011:GLU:HB2	2.00	0.44
1:A:982:TYR:CB	1:A:983:PRO:CD	2.94	0.44
1:D:2693:PHE:CD2	1:D:2708:ARG:HG3	2.52	0.44
1:A:1970:VAL:HG22	1:A:1980:ILE:HG12	2.00	0.43
1:B:1614:ALA:HB3	1:B:1828:THR:HG21	1.99	0.43
1:C:1614:ALA:HB3	1:C:1828:THR:HG21	2.00	0.43
1:A:1517:TYR:HB3	1:A:1529:LEU:HD11	2.00	0.43
1:A:2206:GLN:HB2	1:A:2215:LYS:HB3	2.01	0.43
1:C:2056:LEU:HD21	1:C:2059:ILE:HD11	1.99	0.43
1:D:976:ASN:HB3	1:D:1011:GLU:HB2	2.00	0.43
1:D:2056:LEU:HD21	1:D:2059:ILE:HD11	1.99	0.43
1:A:2584:LYS:HB3	1:A:2587:HIS:HB2	2.00	0.43
1:D:1768:ARG:HH22	1:D:2033:ARG:HD2	1.84	0.43
1:C:976:ASN:HB3	1:C:1011:GLU:HB2	2.00	0.43
1:A:2172:THR:HG22	1:A:2177:THR:HG22	2.00	0.43
1:B:1072:PRO:HB2	1:B:1087:GLU:HG2	2.01	0.43
1:C:2693:PHE:CD2	1:C:2708:ARG:HG3	2.54	0.43
1:D:1688:ALA:HB3	1:D:1697:LEU:HB3	2.01	0.43
1:B:2018:PRO:HD2	1:B:2279:ARG:HG2	2.00	0.43
1:C:1517:TYR:HB3	1:C:1529:LEU:HD11	2.00	0.43
1:C:1820:PRO:HB3	1:C:1826:THR:HA	2.00	0.43
1:C:1121:PRO:HG2	1:C:1124:LEU:HB2	2.01	0.42
1:D:1517:TYR:HB3	1:D:1529:LEU:HD11	2.00	0.42
1:C:2206:GLN:HB2	1:C:2215:LYS:HB3	2.01	0.42
1:D:1249:ARG:HB3	1:D:1264:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2253:SER:HB3	1:D:2262:LEU:HB2	2.02	0.42
1:A:1616:PRO:HG2	1:A:1830:THR:HG22	2.01	0.42
1:B:1249:ARG:HB3	1:B:1264:LYS:HB3	2.01	0.42
1:B:2056:LEU:HD21	1:B:2059:ILE:HD11	2.00	0.42
1:D:1944:ASP:HB3	1:D:1946:GLN:H	1.85	0.42
1:A:1944:ASP:HB3	1:A:1946:GLN:H	1.84	0.42
1:C:1616:PRO:HG2	1:C:1830:THR:HG22	2.02	0.42
1:A:1768:ARG:HH22	1:A:2033:ARG:HD2	1.85	0.42
1:B:1121:PRO:HG2	1:B:1124:LEU:HB2	2.01	0.42
1:B:2076:VAL:HB	1:B:2095:LYS:HD2	2.02	0.42
1:C:1072:PRO:HB2	1:C:1087:GLU:HG2	2.02	0.42
1:A:1249:ARG:HB3	1:A:1264:LYS:HB3	2.01	0.42
1:B:2139:PRO:HD2	1:D:1689:VAL:O	2.19	0.42
1:C:2436:VAL:HG12	1:C:2437:ILE:HD12	2.00	0.42
1:D:1614:ALA:HB3	1:D:1828:THR:HG21	2.01	0.42
1:D:2206:GLN:HB2	1:D:2215:LYS:HB3	2.01	0.42
1:A:1614:ALA:HB3	1:A:1828:THR:HG21	2.02	0.42
1:B:956:LEU:HB3	1:B:957:VAL:H	1.62	0.42
1:C:1768:ARG:HH22	1:C:2033:ARG:HD2	1.85	0.42
1:B:2199:LEU:HD21	1:B:2202:TRP:CD1	2.54	0.42
1:D:1121:PRO:HG2	1:D:1124:LEU:HB2	2.01	0.42
1:A:2025:ILE:HB	1:A:2038:SER:HB2	2.01	0.41
1:D:1072:PRO:HB2	1:D:1087:GLU:HG2	2.02	0.41
1:C:1944:ASP:HB3	1:C:1946:GLN:H	1.85	0.41
1:A:1707:LEU:HB3	1:A:1721:SER:HB2	2.02	0.41
1:B:1417:LEU:HD21	1:B:1468:ILE:HG21	2.03	0.41
1:B:1768:ARG:HH22	1:B:2033:ARG:HD2	1.85	0.41
1:B:1580:ALA:HB2	1:B:1586:TYR:CE2	2.55	0.41
1:B:1821:HIS:CE1	1:B:1823:LEU:HB2	2.56	0.41
1:B:2206:GLN:HB2	1:B:2215:LYS:HB3	2.01	0.41
1:A:1580:ALA:HB2	1:A:1586:TYR:CE2	2.55	0.41
1:B:1944:ASP:HB3	1:B:1946:GLN:H	1.86	0.41
1:C:2398:ASP:HB3	1:C:2404:LEU:HD11	2.03	0.41
1:A:1821:HIS:CE1	1:A:1823:LEU:HB2	2.56	0.41
1:B:976:ASN:HB3	1:B:1011:GLU:HB2	2.00	0.41
1:B:2162:VAL:HG11	1:B:2378:LEU:HD11	2.03	0.41
1:C:1249:ARG:HB3	1:C:1264:LYS:HB3	2.02	0.41
1:C:2650:VAL:HG12	1:C:2708:ARG:HB3	2.02	0.41
1:D:956:LEU:HB3	1:D:957:VAL:H	1.63	0.41
1:D:1616:PRO:HG2	1:D:1830:THR:HG22	2.02	0.41
1:D:1760:THR:HG22	1:D:1775:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1580:ALA:HB2	1:C:1586:TYR:CE2	2.56	0.41
1:C:1821:HIS:CE1	1:C:1823:LEU:HB2	2.55	0.41
1:D:1580:ALA:HB2	1:D:1586:TYR:CE2	2.55	0.41
1:A:1417:LEU:HD21	1:A:1468:ILE:HG21	2.03	0.41
1:A:2511:LEU:HD13	1:A:2518:LEU:HD11	2.03	0.41
1:D:2146:ARG:HB2	1:D:2156:HIS:HB3	2.03	0.41
1:D:2162:VAL:HG11	1:D:2378:LEU:HD11	2.03	0.41
1:A:2178:LEU:HD13	1:A:2193:TYR:CD1	2.56	0.41
1:B:1616:PRO:HG2	1:B:1830:THR:HG22	2.02	0.41
1:D:1417:LEU:HD21	1:D:1468:ILE:HG21	2.03	0.41
1:A:2088:SER:HB3	1:A:2108:SER:HB3	2.03	0.40
1:A:1012:ARG:HD2	1:A:1015:PHE:HD2	1.86	0.40
1:A:1121:PRO:HG2	1:A:1124:LEU:HB2	2.01	0.40
1:C:2162:VAL:HG11	1:C:2378:LEU:HD11	2.03	0.40
1:D:2511:LEU:HD13	1:D:2518:LEU:HD11	2.03	0.40
1:A:1072:PRO:HB2	1:A:1087:GLU:HG2	2.03	0.40
1:C:1012:ARG:HD2	1:C:1015:PHE:HD2	1.85	0.40
1:C:1417:LEU:HD21	1:C:1468:ILE:HG21	2.02	0.40
1:C:2018:PRO:HD2	1:C:2279:ARG:HG2	2.03	0.40
1:B:982:TYR:CB	1:B:983:PRO:CD	2.94	0.40
1:B:1810:ASN:HA	1:B:2074:THR:HB	2.04	0.40
1:B:2146:ARG:HB2	1:B:2156:HIS:HB3	2.04	0.40
1:B:2192:GLN:HG3	1:B:2199:LEU:HD13	2.03	0.40
1:C:1707:LEU:HD21	1:C:2616:ILE:HG12	2.02	0.40
1:C:2360:VAL:HG21	1:C:2443:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1833/1859 (99%)	1769 (96%)	57 (3%)	7 (0%)	30 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1833/1859 (99%)	1763 (96%)	63 (3%)	7 (0%)	30	40
1	C	1833/1859 (99%)	1768 (96%)	59 (3%)	6 (0%)	36	48
1	D	1833/1859 (99%)	1765 (96%)	61 (3%)	7 (0%)	30	40
All	All	7332/7436 (99%)	7065 (96%)	240 (3%)	27 (0%)	30	40

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	TYR
1	B	982	TYR
1	C	982	TYR
1	D	982	TYR
1	A	1997	VAL
1	C	1284	PHE
1	C	1997	VAL
1	D	1997	VAL
1	A	1284	PHE
1	B	1284	PHE
1	D	1284	PHE
1	A	1402	ALA
1	A	1790	ASP
1	B	1790	ASP
1	B	1966	GLU
1	B	1997	VAL
1	C	1402	ALA
1	C	1790	ASP
1	D	1402	ALA
1	D	1790	ASP
1	A	1966	GLU
1	B	1402	ALA
1	D	1966	GLU
1	A	1326	GLY
1	B	1326	GLY
1	C	1326	GLY
1	D	1326	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1601/1620 (99%)	1566 (98%)	35 (2%)	45	65
1	B	1601/1620 (99%)	1563 (98%)	38 (2%)	43	63
1	C	1601/1620 (99%)	1565 (98%)	36 (2%)	45	65
1	D	1601/1620 (99%)	1564 (98%)	37 (2%)	44	64
All	All	6404/6480 (99%)	6258 (98%)	146 (2%)	44	64

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	956	LEU
1	A	958	SER
1	A	973	VAL
1	A	1012	ARG
1	A	1112	LYS
1	A	1115	MET
1	A	1116	THR
1	A	1253	CYS
1	A	1389	ILE
1	A	1392	ASP
1	A	1418	LEU
1	A	1435	MET
1	A	1454	ASP
1	A	1477	ILE
1	A	1593	ILE
1	A	1599	SER
1	A	1604	ILE
1	A	1673	MET
1	A	1763	ILE
1	A	1774	VAL
1	A	1847	ILE
1	A	1874	LEU
1	A	1944	ASP
1	A	1965	LEU
1	A	1986	SER
1	A	1997	VAL
1	A	2170	ILE
1	A	2255	ASP
1	A	2359	ARG
1	A	2412	LEU

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Mol	Chain	Res	Type
1	A	2437	ILE
1	A	2440	HIS
1	A	2552	THR
1	A	2591	THR
1	A	2694	THR
1	B	956	LEU
1	B	958	SER
1	B	973	VAL
1	B	1012	ARG
1	B	1112	LYS
1	B	1115	MET
1	B	1116	THR
1	B	1253	CYS
1	B	1389	ILE
1	B	1392	ASP
1	B	1418	LEU
1	B	1435	MET
1	B	1454	ASP
1	B	1459	VAL
1	B	1477	ILE
1	B	1593	ILE
1	B	1599	SER
1	B	1604	ILE
1	B	1669	ASP
1	B	1673	MET
1	B	1763	ILE
1	B	1774	VAL
1	B	1815	SER
1	B	1847	ILE
1	B	1944	ASP
1	B	1965	LEU
1	B	1997	VAL
1	B	2002	MET
1	B	2170	ILE
1	B	2255	ASP
1	B	2303	SER
1	B	2359	ARG
1	B	2412	LEU
1	B	2437	ILE
1	B	2440	HIS
1	B	2552	THR
1	B	2591	THR

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Mol	Chain	Res	Type
1	B	2722	ARG
1	C	956	LEU
1	C	958	SER
1	C	973	VAL
1	C	1012	ARG
1	C	1112	LYS
1	C	1115	MET
1	C	1116	THR
1	C	1253	CYS
1	C	1389	ILE
1	C	1392	ASP
1	C	1418	LEU
1	C	1435	MET
1	C	1454	ASP
1	C	1477	ILE
1	C	1593	ILE
1	C	1599	SER
1	C	1604	ILE
1	C	1673	MET
1	C	1763	ILE
1	C	1774	VAL
1	C	1847	ILE
1	C	1944	ASP
1	C	1965	LEU
1	C	2002	MET
1	C	2088	SER
1	C	2170	ILE
1	C	2173	THR
1	C	2285	LEU
1	C	2359	ARG
1	C	2412	LEU
1	C	2437	ILE
1	C	2440	HIS
1	C	2552	THR
1	C	2591	THR
1	C	2760	GLN
1	C	2784	LEU
1	D	956	LEU
1	D	958	SER
1	D	973	VAL
1	D	1012	ARG
1	D	1112	LYS

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Mol	Chain	Res	Type
1	D	1115	MET
1	D	1116	THR
1	D	1253	CYS
1	D	1389	ILE
1	D	1392	ASP
1	D	1418	LEU
1	D	1435	MET
1	D	1454	ASP
1	D	1477	ILE
1	D	1593	ILE
1	D	1599	SER
1	D	1604	ILE
1	D	1673	MET
1	D	1763	ILE
1	D	1774	VAL
1	D	1815	SER
1	D	1847	ILE
1	D	1944	ASP
1	D	1965	LEU
1	D	1986	SER
1	D	1997	VAL
1	D	2170	ILE
1	D	2173	THR
1	D	2262	LEU
1	D	2359	ARG
1	D	2412	LEU
1	D	2437	ILE
1	D	2440	HIS
1	D	2552	THR
1	D	2562	ASN
1	D	2591	THR
1	D	2748	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1027	ASN
1	A	1285	ASN
1	A	1311	ASN
1	A	1353	ASN
1	A	1473	GLN
1	A	1631	GLN

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Mol	Chain	Res	Type
1	A	1683	GLN
1	A	1701	GLN
1	A	1797	GLN
1	A	1892	HIS
1	A	2156	HIS
1	A	2181	HIS
1	A	2185	HIS
1	A	2206	GLN
1	A	2418	GLN
1	A	2434	GLN
1	A	2440	HIS
1	A	2475	ASN
1	A	2502	ASN
1	A	2549	GLN
1	A	2729	GLN
1	A	2763	ASN
1	B	1001	ASN
1	B	1027	ASN
1	B	1285	ASN
1	B	1311	ASN
1	B	1353	ASN
1	B	1473	GLN
1	B	1631	GLN
1	B	1683	GLN
1	B	1797	GLN
1	B	1892	HIS
1	B	2156	HIS
1	B	2181	HIS
1	B	2206	GLN
1	B	2418	GLN
1	B	2434	GLN
1	B	2475	ASN
1	B	2502	ASN
1	B	2549	GLN
1	B	2681	GLN
1	B	2741	GLN
1	B	2763	ASN
1	C	1027	ASN
1	C	1285	ASN
1	C	1311	ASN
1	C	1353	ASN
1	C	1473	GLN

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Mol	Chain	Res	Type
1	C	1631	GLN
1	C	1683	GLN
1	C	1701	GLN
1	C	1892	HIS
1	C	1978	GLN
1	C	2156	HIS
1	C	2206	GLN
1	C	2238	GLN
1	C	2434	GLN
1	C	2491	ASN
1	C	2502	ASN
1	C	2549	GLN
1	C	2587	HIS
1	C	2681	GLN
1	C	2741	GLN
1	C	2760	GLN
1	C	2763	ASN
1	D	1001	ASN
1	D	1027	ASN
1	D	1263	ASN
1	D	1285	ASN
1	D	1353	ASN
1	D	1473	GLN
1	D	1631	GLN
1	D	1683	GLN
1	D	1892	HIS
1	D	2124	ASN
1	D	2156	HIS
1	D	2181	HIS
1	D	2206	GLN
1	D	2418	GLN
1	D	2434	GLN
1	D	2440	HIS
1	D	2502	ASN
1	D	2549	GLN
1	D	2763	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 ⓘ

72 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.42	0	17,19,21	0.71	1 (5%)
2	NAG	E	2	2	14,14,15	0.43	0	17,19,21	0.89	1 (5%)
2	BMA	E	3	2	11,11,12	0.50	0	15,15,17	0.69	0
2	MAN	E	4	2	11,11,12	0.59	0	15,15,17	0.90	1 (6%)
2	MAN	E	5	2	11,11,12	0.65	0	15,15,17	0.76	1 (6%)
2	MAN	E	6	2	11,11,12	0.61	0	15,15,17	0.88	1 (6%)
2	MAN	E	7	2	11,11,12	0.67	0	15,15,17	1.03	1 (6%)
2	MAN	E	8	2	11,11,12	0.48	0	15,15,17	0.98	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.42	0	17,19,21	0.72	0
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	0.64	0
3	NAG	G	1	1,3	14,14,15	0.43	0	17,19,21	0.61	0
3	NAG	G	2	3	14,14,15	0.45	0	17,19,21	0.70	0
3	NAG	H	1	1,3	14,14,15	0.43	0	17,19,21	0.94	2 (11%)
3	NAG	H	2	3	14,14,15	0.44	0	17,19,21	0.65	0
3	NAG	I	1	1,3	14,14,15	0.44	0	17,19,21	0.82	0
3	NAG	I	2	3	14,14,15	0.43	0	17,19,21	0.59	0
3	NAG	J	1	1,3	14,14,15	0.43	0	17,19,21	0.81	1 (5%)
3	NAG	J	2	3	14,14,15	0.45	0	17,19,21	0.76	1 (5%)
2	NAG	K	1	1,2	14,14,15	0.42	0	17,19,21	0.72	0
2	NAG	K	2	2	14,14,15	0.42	0	17,19,21	0.90	2 (11%)
2	BMA	K	3	2	11,11,12	0.50	0	15,15,17	0.67	0
2	MAN	K	4	2	11,11,12	0.58	0	15,15,17	0.90	1 (6%)
2	MAN	K	5	2	11,11,12	0.63	0	15,15,17	0.77	1 (6%)
2	MAN	K	6	2	11,11,12	0.62	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	K	7	2	11,11,12	0.68	0	15,15,17	1.02	1 (6%)
2	MAN	K	8	2	11,11,12	0.54	0	15,15,17	0.93	2 (13%)
3	NAG	L	1	1,3	14,14,15	0.42	0	17,19,21	0.74	0
3	NAG	L	2	3	14,14,15	0.43	0	17,19,21	0.75	0
3	NAG	M	1	1,3	14,14,15	0.44	0	17,19,21	0.60	0
3	NAG	M	2	3	14,14,15	0.43	0	17,19,21	0.68	0
3	NAG	N	1	1,3	14,14,15	0.42	0	17,19,21	0.91	2 (11%)
3	NAG	N	2	3	14,14,15	0.44	0	17,19,21	0.62	0
3	NAG	O	1	1,3	14,14,15	0.44	0	17,19,21	0.85	1 (5%)
3	NAG	O	2	3	14,14,15	0.44	0	17,19,21	0.59	0
3	NAG	P	1	1,3	14,14,15	0.43	0	17,19,21	0.83	1 (5%)
3	NAG	P	2	3	14,14,15	0.46	0	17,19,21	0.72	1 (5%)
2	NAG	Q	1	1,2	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
2	NAG	Q	2	2	14,14,15	0.43	0	17,19,21	0.88	1 (5%)
2	BMA	Q	3	2	11,11,12	0.49	0	15,15,17	0.68	0
2	MAN	Q	4	2	11,11,12	0.62	0	15,15,17	0.87	1 (6%)
2	MAN	Q	5	2	11,11,12	0.68	0	15,15,17	0.78	1 (6%)
2	MAN	Q	6	2	11,11,12	0.66	0	15,15,17	0.88	1 (6%)
2	MAN	Q	7	2	11,11,12	0.68	0	15,15,17	1.02	1 (6%)
2	MAN	Q	8	2	11,11,12	0.56	0	15,15,17	0.93	2 (13%)
3	NAG	R	1	1,3	14,14,15	0.44	0	17,19,21	0.79	1 (5%)
3	NAG	R	2	3	14,14,15	0.43	0	17,19,21	0.60	0
3	NAG	S	1	1,3	14,14,15	0.42	0	17,19,21	0.60	0
3	NAG	S	2	3	14,14,15	0.43	0	17,19,21	0.67	0
3	NAG	T	1	1,3	14,14,15	0.45	0	17,19,21	0.88	2 (11%)
3	NAG	T	2	3	14,14,15	0.44	0	17,19,21	0.64	0
3	NAG	U	1	1,3	14,14,15	0.45	0	17,19,21	0.87	1 (5%)
3	NAG	U	2	3	14,14,15	0.45	0	17,19,21	0.61	0
3	NAG	V	1	1,3	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
3	NAG	V	2	3	14,14,15	0.45	0	17,19,21	0.80	1 (5%)
2	NAG	W	1	1,2	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
2	NAG	W	2	2	14,14,15	0.41	0	17,19,21	0.86	0
2	BMA	W	3	2	11,11,12	0.54	0	15,15,17	0.65	0
2	MAN	W	4	2	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
2	MAN	W	5	2	11,11,12	0.69	0	15,15,17	0.76	1 (6%)
2	MAN	W	6	2	11,11,12	0.63	0	15,15,17	0.84	1 (6%)
2	MAN	W	7	2	11,11,12	0.66	0	15,15,17	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	W	8	2	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
3	NAG	X	1	1,3	14,14,15	0.44	0	17,19,21	0.74	0
3	NAG	X	2	3	14,14,15	0.45	0	17,19,21	0.65	0
3	NAG	Y	1	1,3	14,14,15	0.44	0	17,19,21	0.62	0
3	NAG	Y	2	3	14,14,15	0.44	0	17,19,21	0.66	0
3	NAG	Z	1	1,3	14,14,15	0.46	0	17,19,21	0.89	2 (11%)
3	NAG	Z	2	3	14,14,15	0.43	0	17,19,21	0.61	0
3	NAG	a	1	1,3	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
3	NAG	a	2	3	14,14,15	0.43	0	17,19,21	0.60	0
3	NAG	b	1	1,3	14,14,15	0.43	0	17,19,21	0.80	0
3	NAG	b	2	3	14,14,15	0.45	0	17,19,21	0.75	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	MAN	E	7	2	-	2/2/19/22	0/1/1/1
2	MAN	E	8	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	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	BMA	K	3	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	0/2/19/22	0/1/1/1
2	MAN	K	6	2	-	0/2/19/22	0/1/1/1
2	MAN	K	7	2	-	2/2/19/22	0/1/1/1
2	MAN	K	8	2	-	2/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	5	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	6	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	7	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	8	2	-	2/2/19/22	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	3/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	BMA	W	3	2	-	2/2/19/22	0/1/1/1
2	MAN	W	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	W	5	2	-	0/2/19/22	0/1/1/1
2	MAN	W	6	2	-	0/2/19/22	0/1/1/1
2	MAN	W	7	2	-	2/2/19/22	0/1/1/1
2	MAN	W	8	2	-	2/2/19/22	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	3/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	MAN	C1-O5-C5	3.36	116.69	112.19
2	K	7	MAN	C1-O5-C5	3.33	116.65	112.19
2	Q	7	MAN	C1-O5-C5	3.28	116.58	112.19
2	W	7	MAN	C1-O5-C5	3.24	116.53	112.19
2	K	4	MAN	C1-O5-C5	2.94	116.12	112.19
2	E	4	MAN	C1-O5-C5	2.93	116.11	112.19
2	W	4	MAN	C1-O5-C5	2.89	116.06	112.19
2	Q	4	MAN	C1-O5-C5	2.85	116.01	112.19
2	Q	5	MAN	C1-O5-C5	2.79	115.93	112.19
2	E	6	MAN	C1-O5-C5	2.78	115.91	112.19
2	K	5	MAN	C1-O5-C5	2.77	115.90	112.19
2	E	5	MAN	C1-O5-C5	2.71	115.82	112.19
2	K	6	MAN	C1-O5-C5	2.70	115.80	112.19
2	Q	6	MAN	C1-O5-C5	2.68	115.77	112.19
2	W	5	MAN	C1-O5-C5	2.65	115.74	112.19
2	W	6	MAN	C1-O5-C5	2.65	115.74	112.19
2	W	8	MAN	C1-C2-C3	2.46	113.23	109.64
2	E	8	MAN	C1-C2-C3	2.41	113.15	109.64
2	Q	8	MAN	C1-C2-C3	2.38	113.11	109.64
3	H	1	NAG	C2-N2-C7	2.38	126.08	122.90
3	Z	1	NAG	C2-N2-C7	2.35	126.05	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	NAG	C2-N2-C7	2.32	126.01	122.90
2	K	8	MAN	C1-C2-C3	2.30	112.99	109.64
3	H	1	NAG	C4-C3-C2	2.24	114.30	111.02
3	U	1	NAG	C2-N2-C7	2.24	125.90	122.90
3	N	1	NAG	C4-C3-C2	2.22	114.28	111.02
3	P	1	NAG	C2-N2-C7	2.21	125.86	122.90
2	E	8	MAN	C1-O5-C5	2.20	115.14	112.19
3	R	1	NAG	C2-N2-C7	2.20	125.85	122.90
3	P	2	NAG	C2-N2-C7	2.19	125.83	122.90
3	T	1	NAG	C2-N2-C7	2.19	125.83	122.90
2	K	8	MAN	C1-O5-C5	2.19	115.12	112.19
3	N	1	NAG	C2-N2-C7	2.18	125.83	122.90
2	W	8	MAN	C1-O5-C5	2.18	115.11	112.19
2	Q	8	MAN	C1-O5-C5	2.15	115.06	112.19
2	Q	2	NAG	C2-N2-C7	2.14	125.77	122.90
3	T	1	NAG	C4-C3-C2	2.12	114.12	111.02
3	a	1	NAG	C2-N2-C7	2.12	125.74	122.90
3	V	2	NAG	C2-N2-C7	2.11	125.73	122.90
2	E	2	NAG	C2-N2-C7	2.09	125.70	122.90
2	W	1	NAG	C1-O5-C5	2.08	114.98	112.19
3	b	2	NAG	C2-N2-C7	2.08	125.69	122.90
3	O	1	NAG	C2-N2-C7	2.08	125.68	122.90
3	J	1	NAG	C2-N2-C7	2.06	125.67	122.90
2	Q	1	NAG	C1-O5-C5	2.06	114.95	112.19
3	Z	1	NAG	C4-C3-C2	2.05	114.02	111.02
2	K	2	NAG	O5-C1-C2	2.04	114.45	111.29
2	K	2	NAG	C2-N2-C7	2.04	125.64	122.90
2	E	1	NAG	C1-O5-C5	2.03	114.91	112.19
3	V	1	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2
2	K	3	BMA	C4-C5-C6-O6
2	Q	3	BMA	C4-C5-C6-O6
2	W	3	BMA	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	W	8	MAN	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	8	MAN	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
2	K	8	MAN	C4-C5-C6-O6
2	Q	8	MAN	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
2	E	8	MAN	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
2	W	8	MAN	O5-C5-C6-O6
2	K	8	MAN	O5-C5-C6-O6
2	Q	8	MAN	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
2	W	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	I	2	NAG	O7-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
2	W	7	MAN	C4-C5-C6-O6
2	E	7	MAN	C4-C5-C6-O6
2	K	7	MAN	C4-C5-C6-O6
2	Q	7	MAN	C4-C5-C6-O6
3	S	2	NAG	C8-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
2	W	7	MAN	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	O7-C7-N2-C2
2	K	7	MAN	O5-C5-C6-O6
2	Q	7	MAN	O5-C5-C6-O6
2	E	7	MAN	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	X	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	X	1	NAG	O7-C7-N2-C2
3	O	2	NAG	C4-C5-C6-O6
3	R	1	NAG	O7-C7-N2-C2
3	U	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C8-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	a	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C1-C2-N2-C7
3	V	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	O	2	NAG	O5-C5-C6-O6

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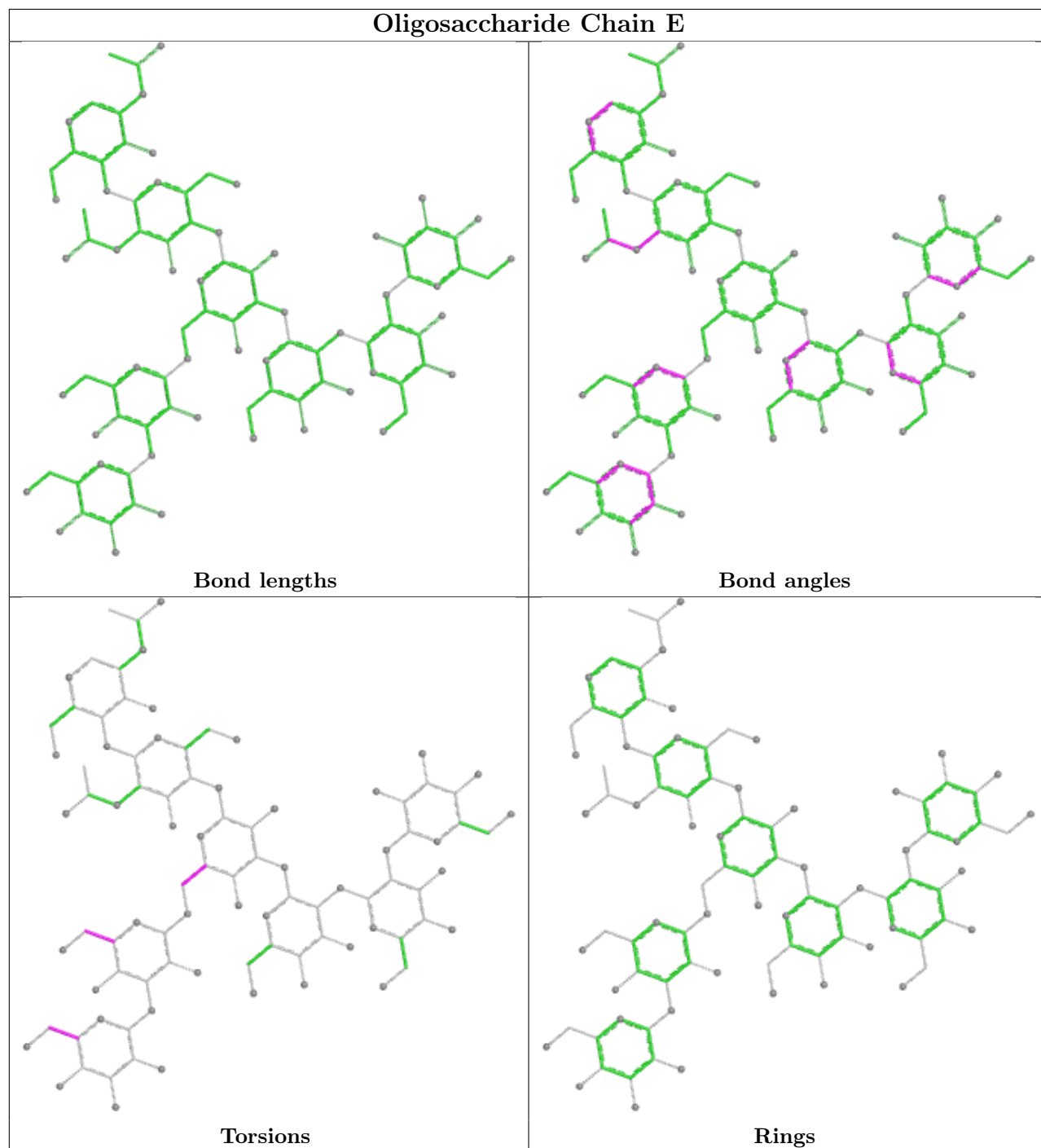
Mol	Chain	Res	Type	Atoms
3	a	1	NAG	O7-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2

There are no ring outliers.

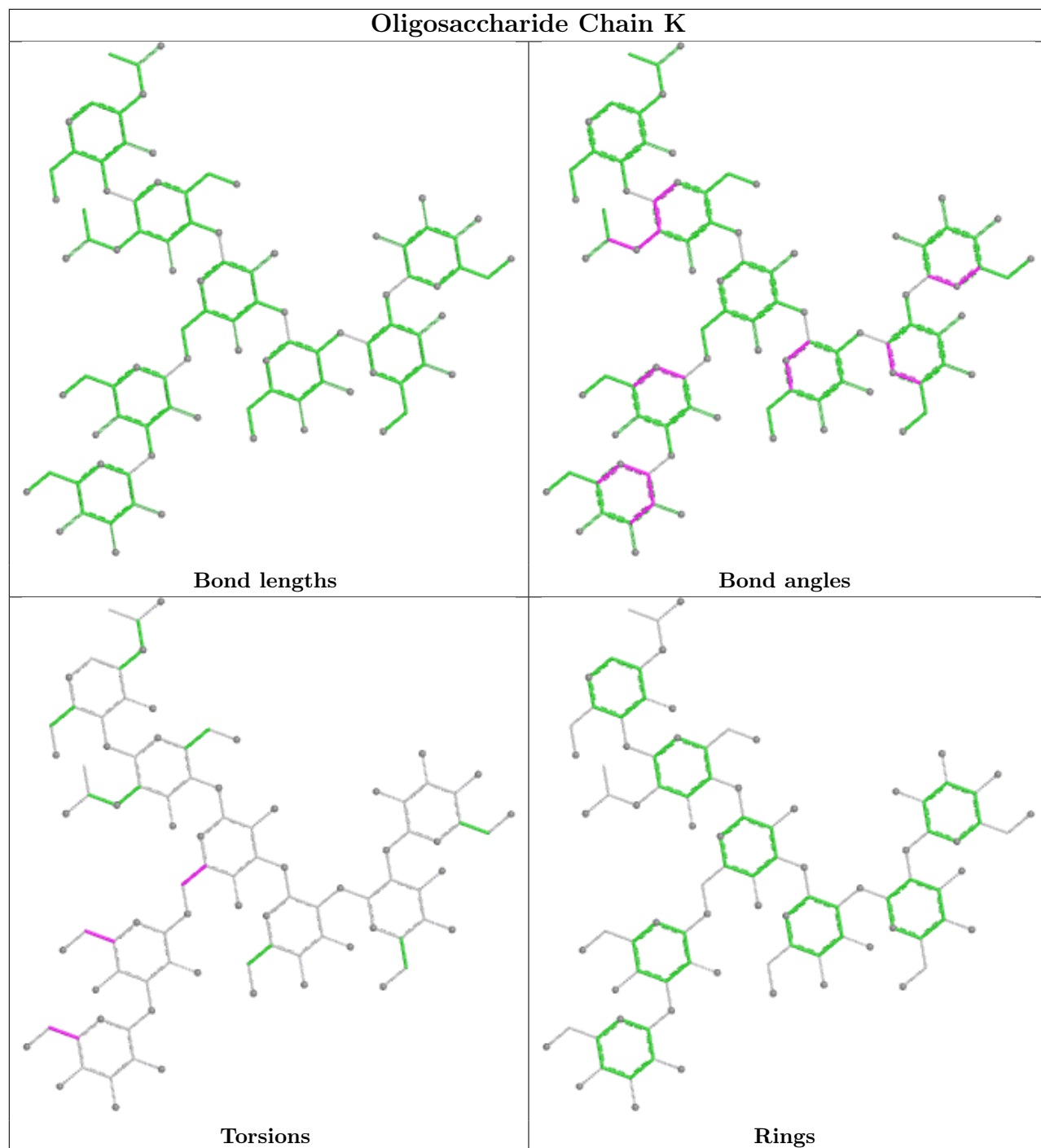
No monomer is involved in short contacts.

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

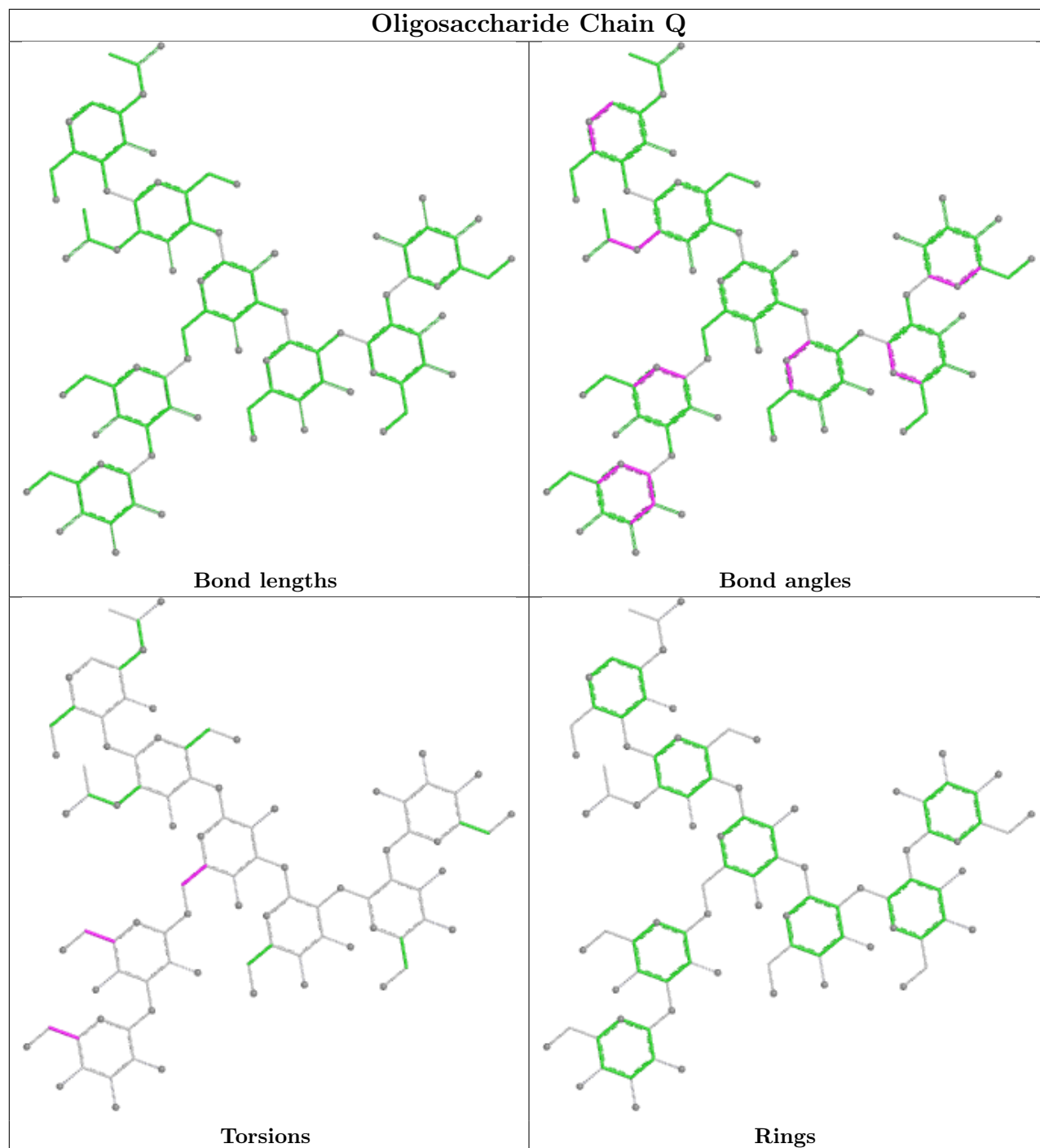
Oligosaccharide Chain E



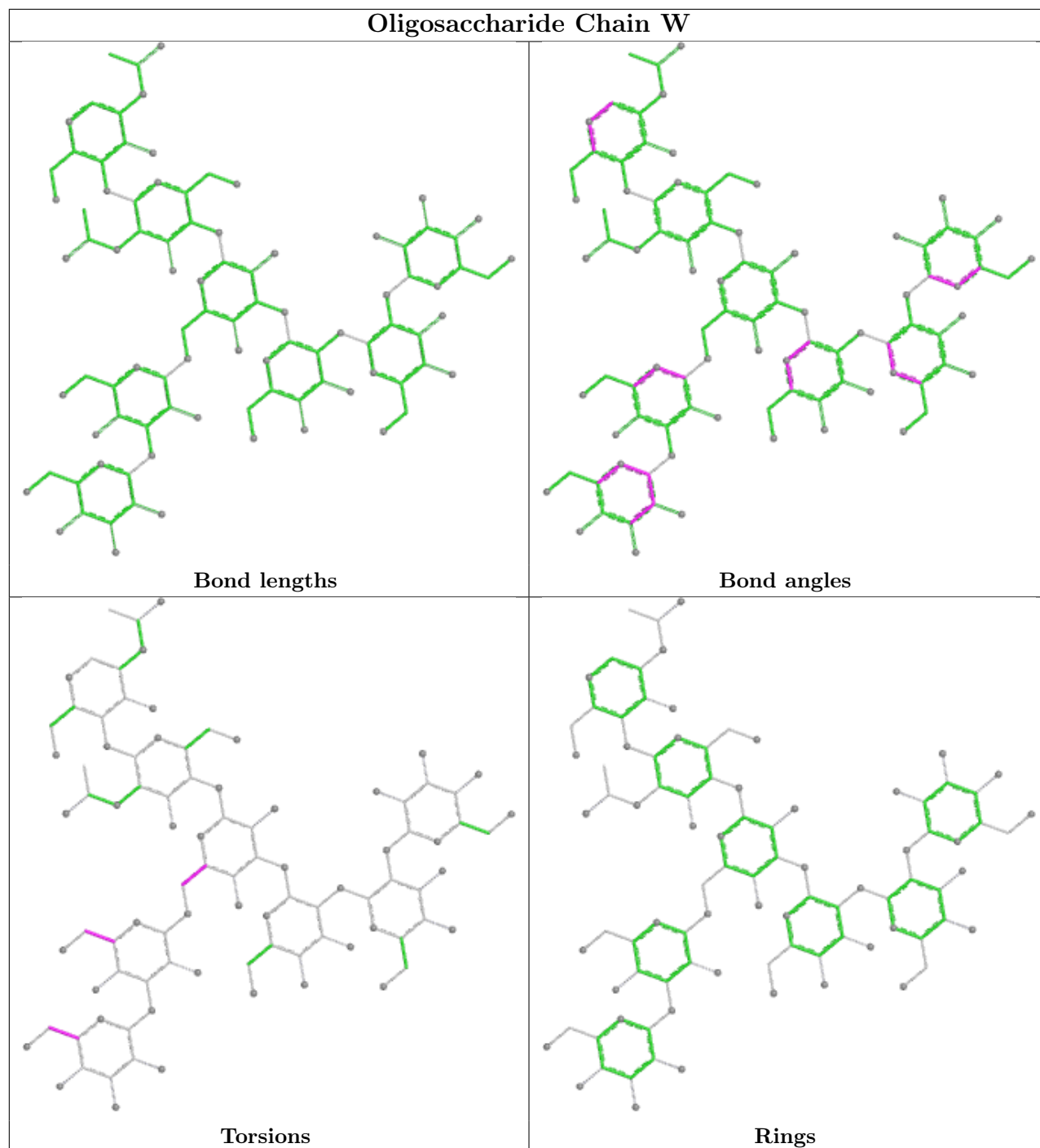
Oligosaccharide Chain K

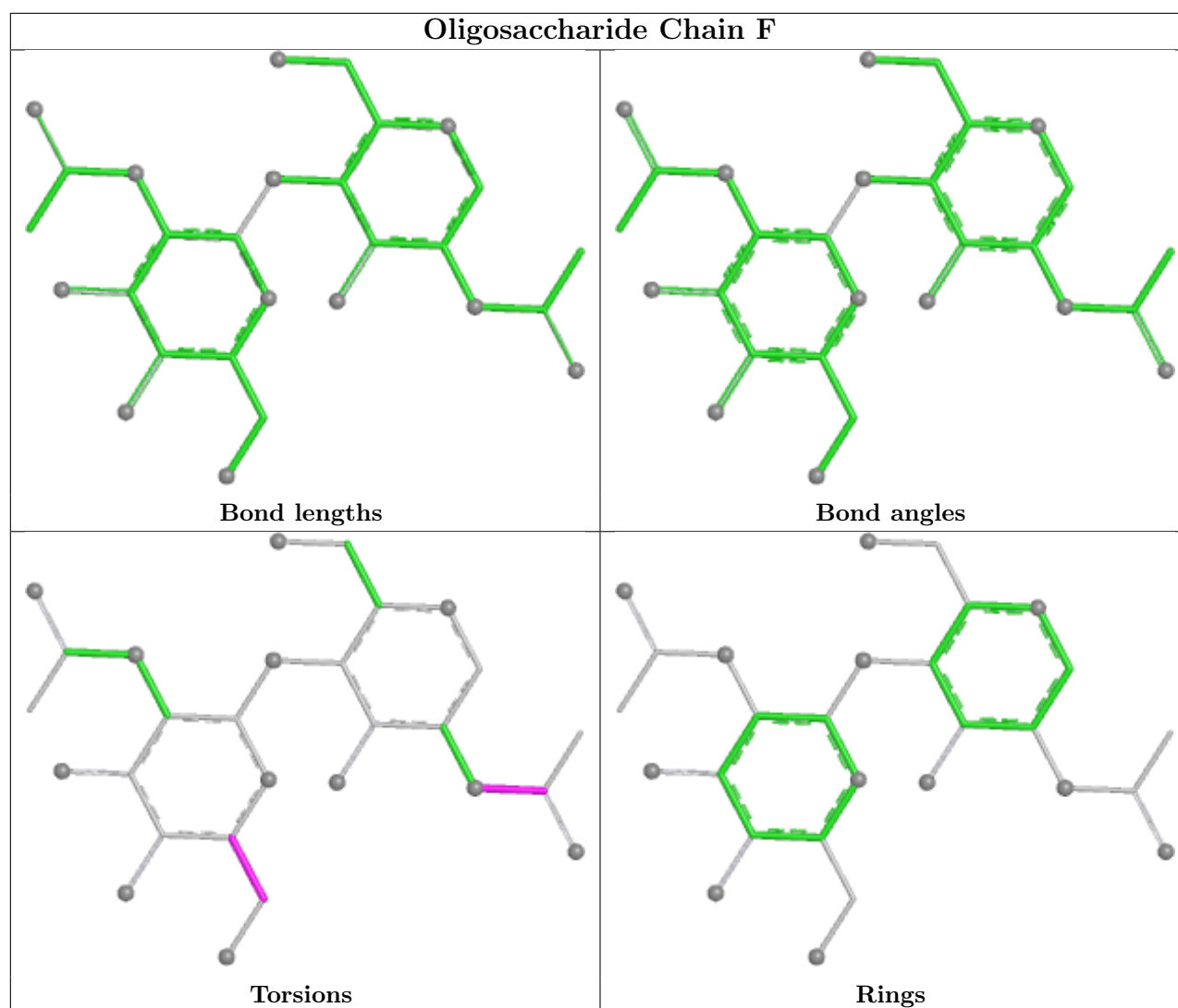


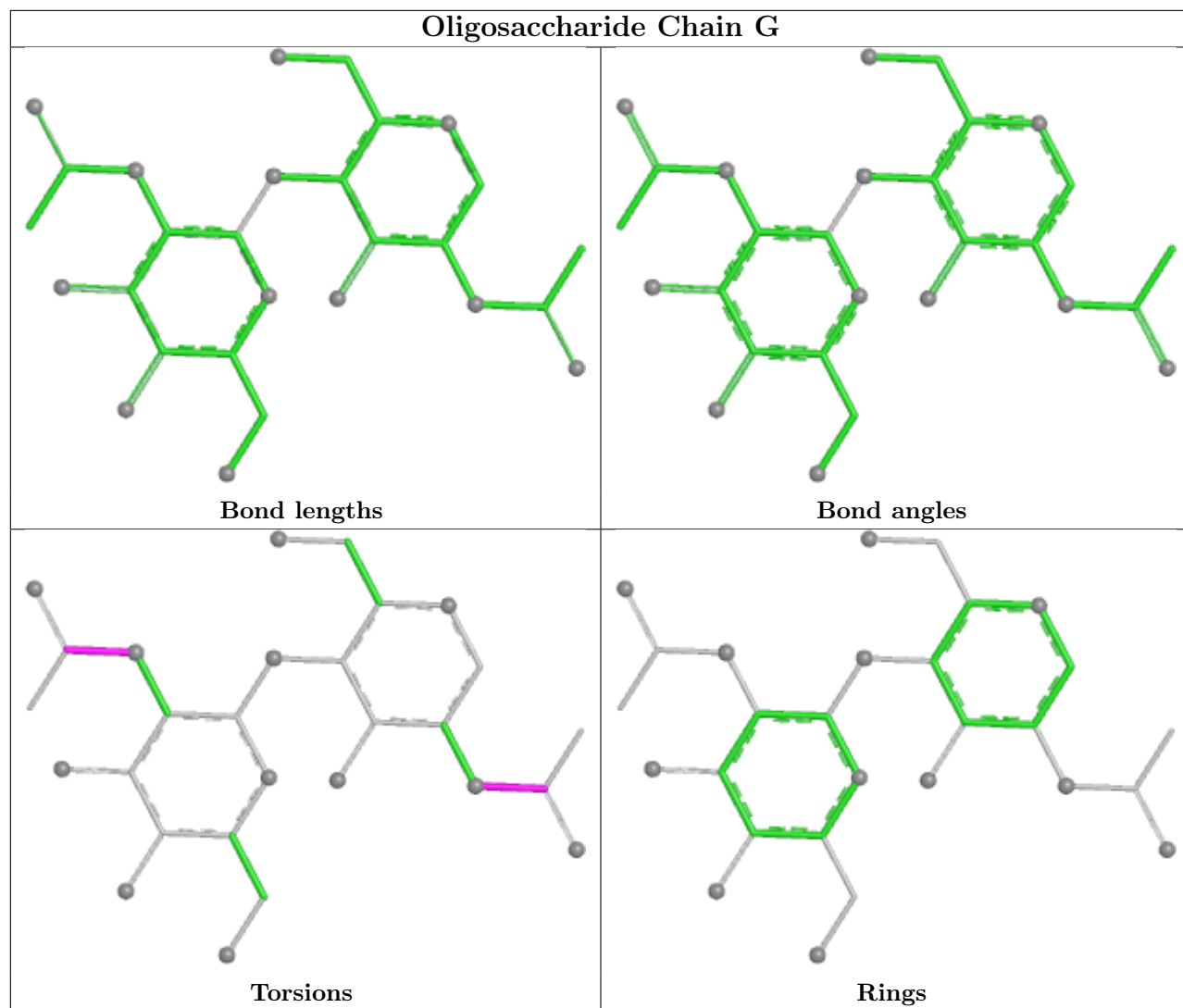
Oligosaccharide Chain Q

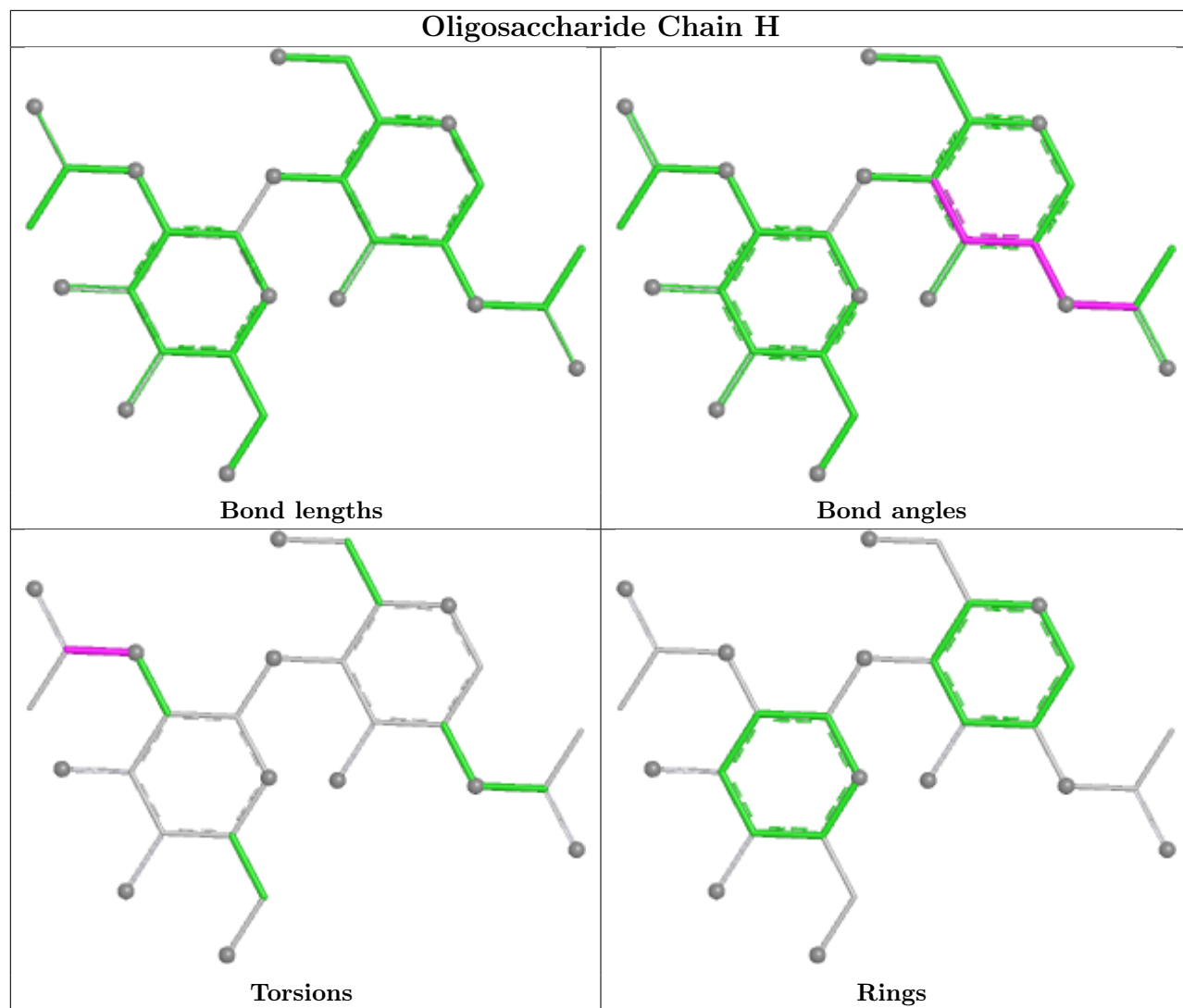


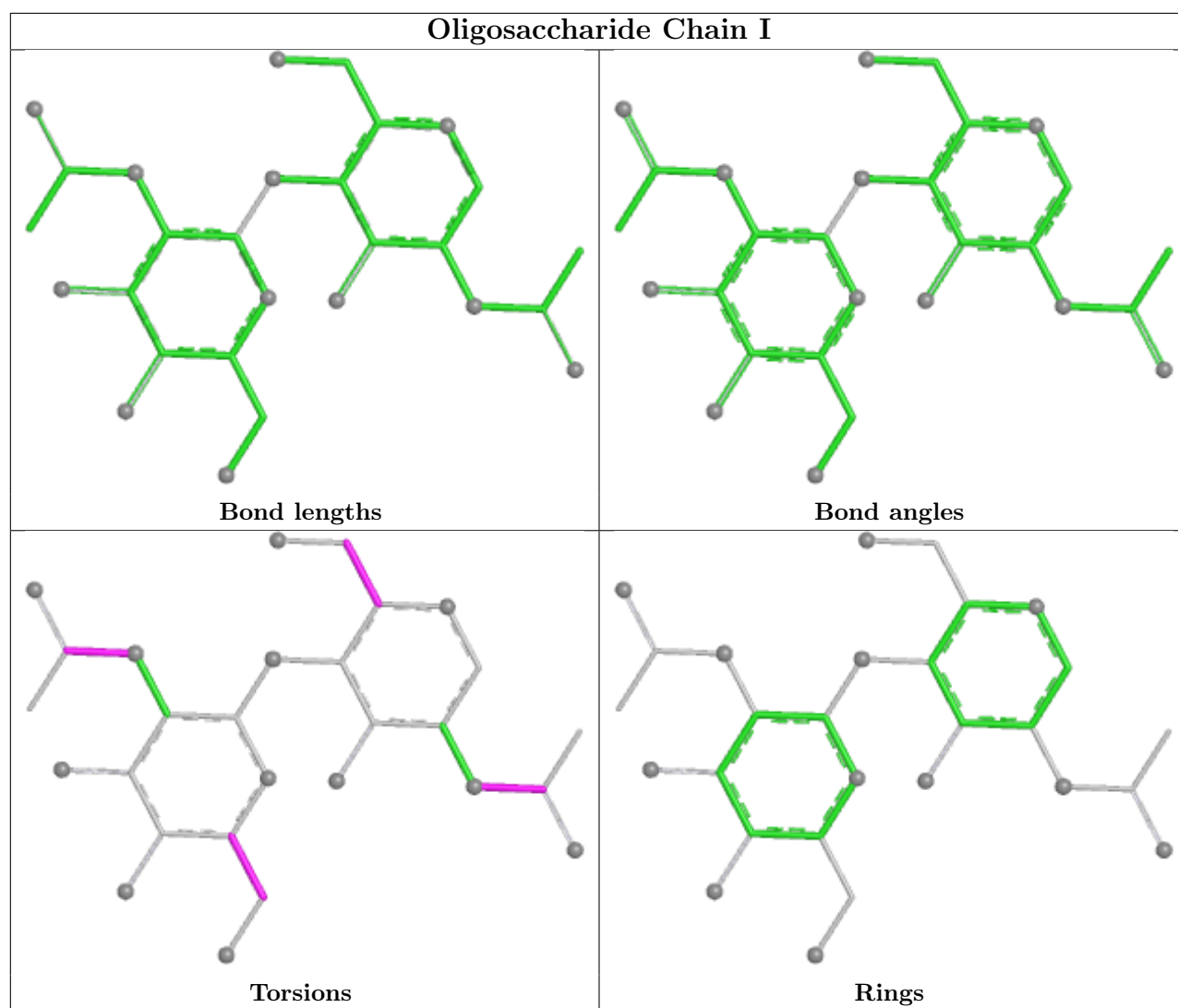
Oligosaccharide Chain W

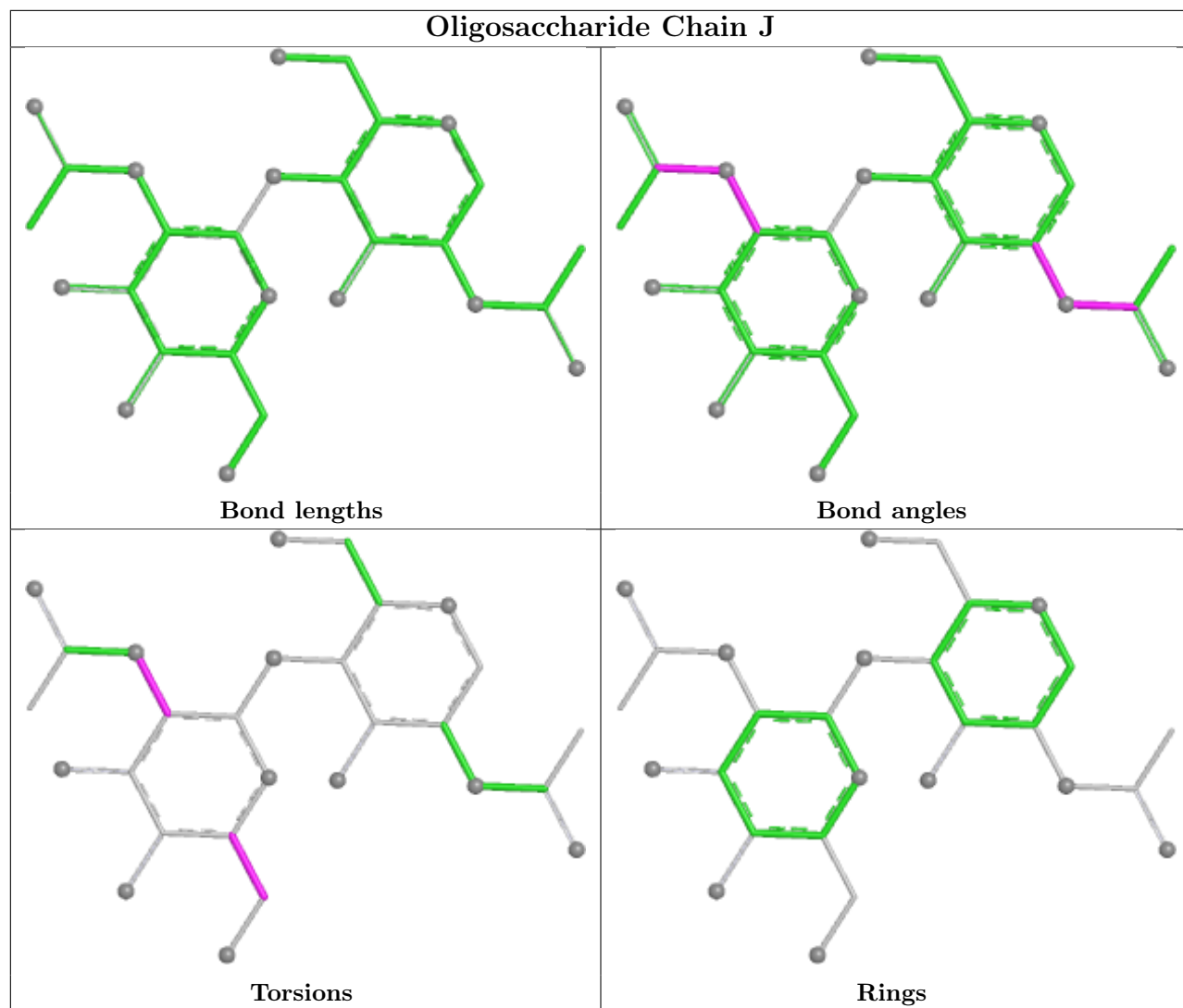


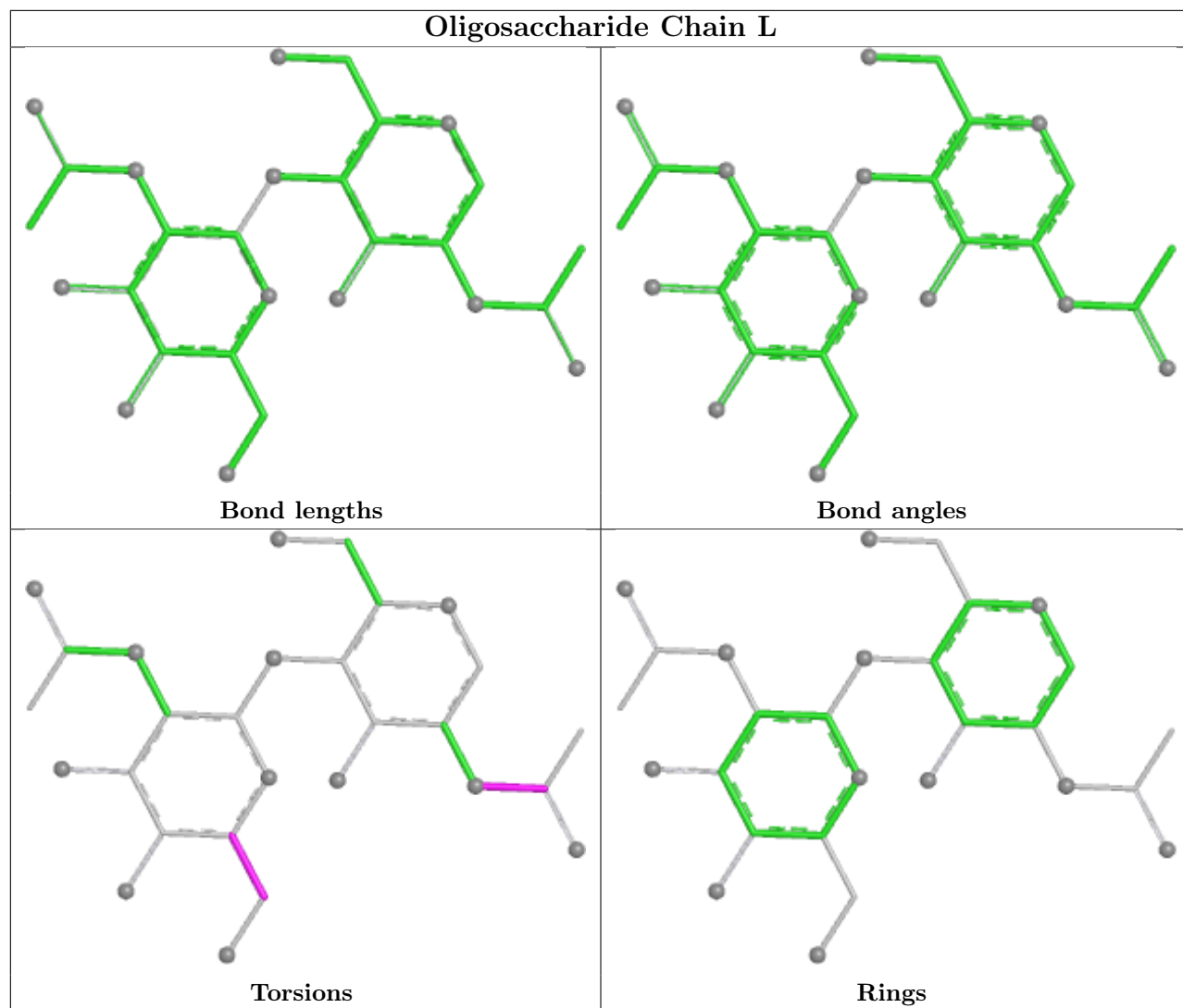


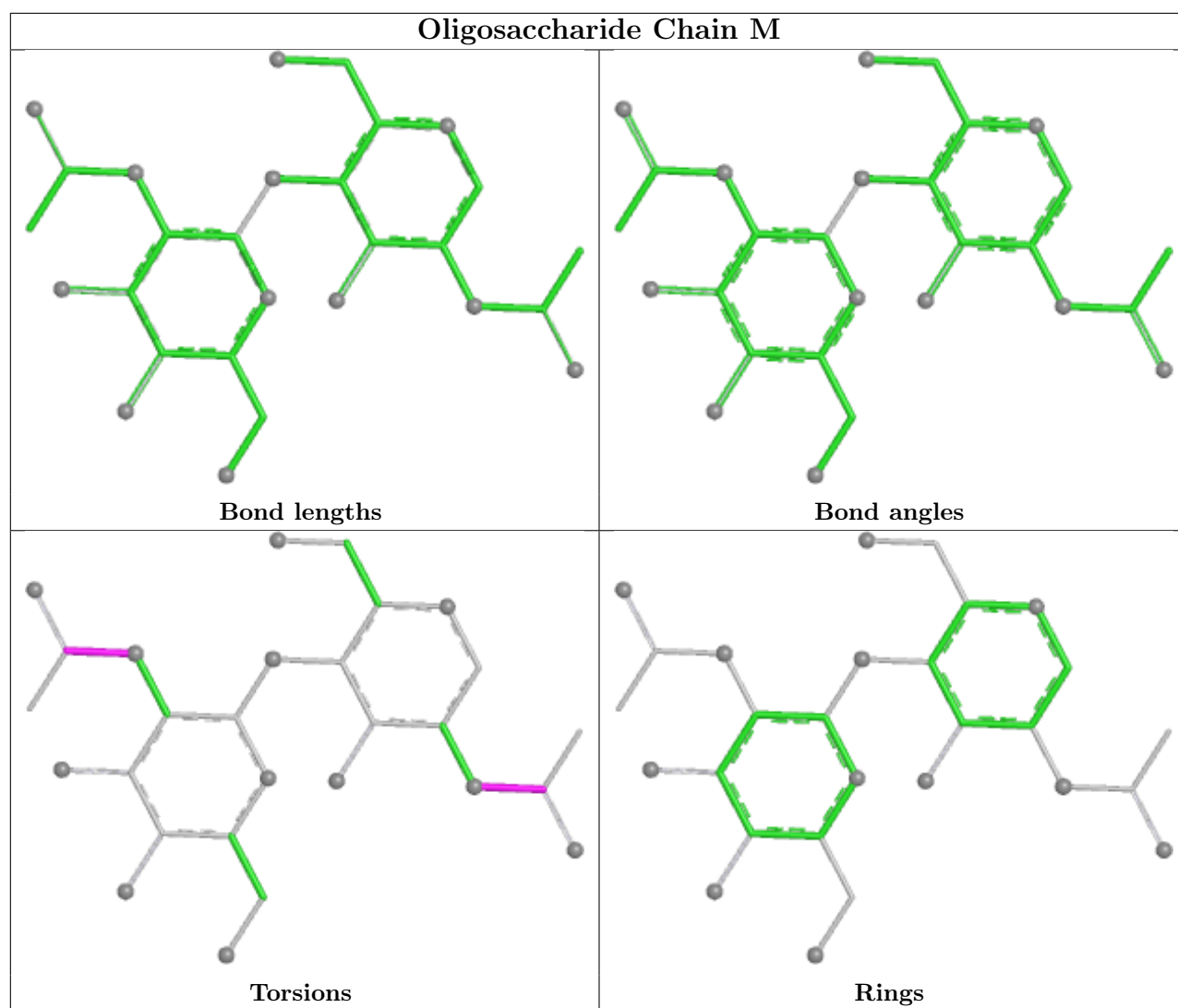


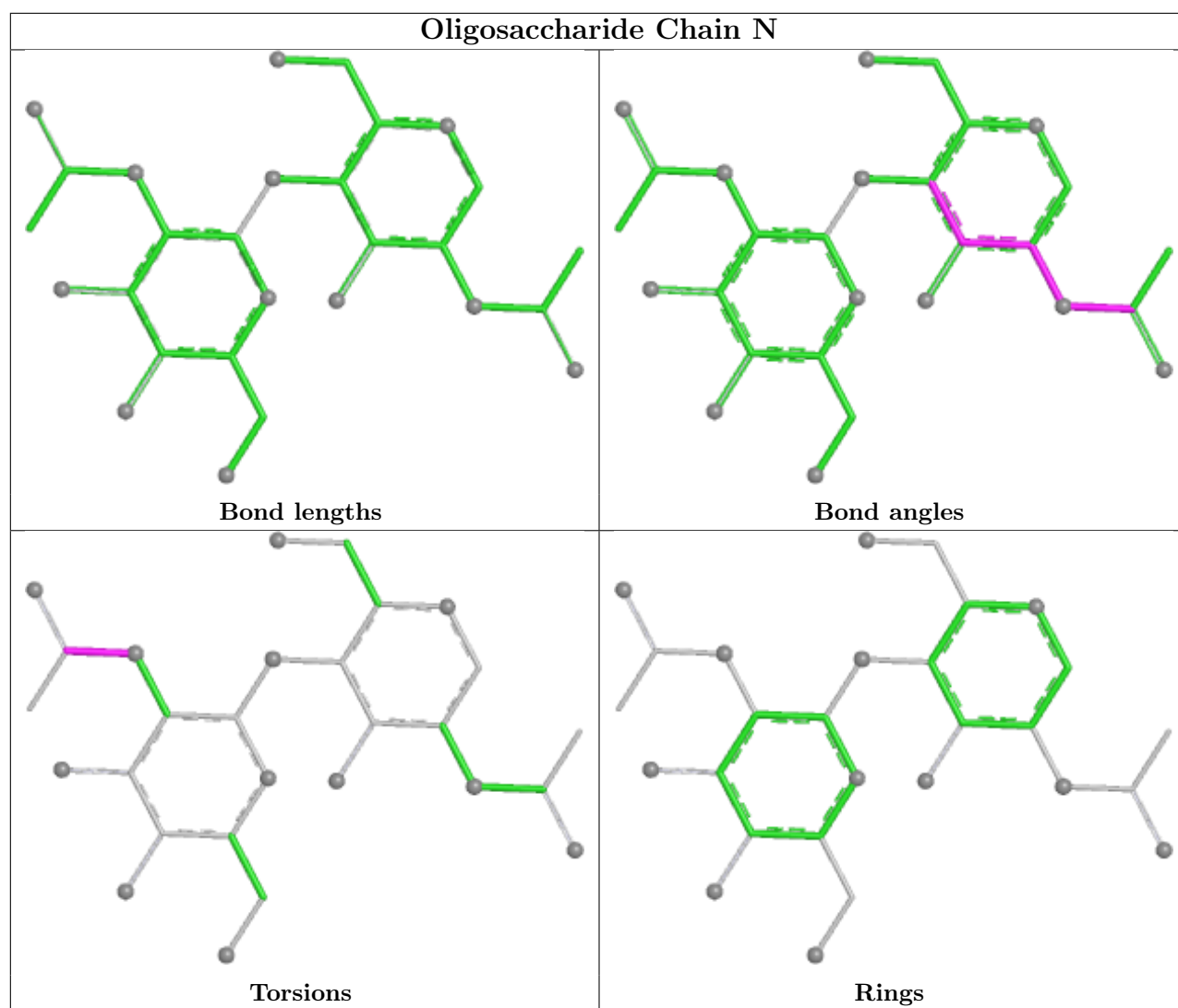


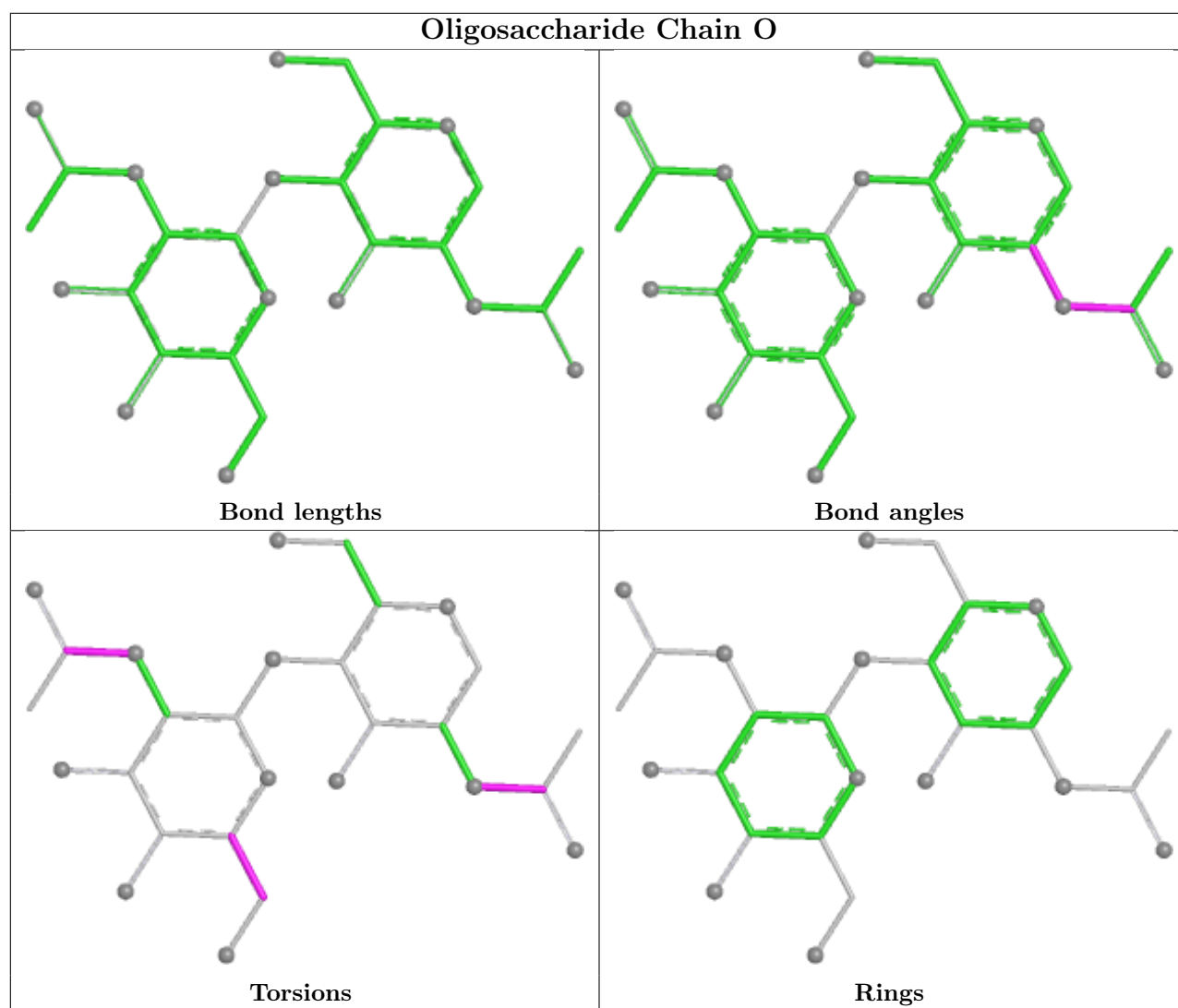


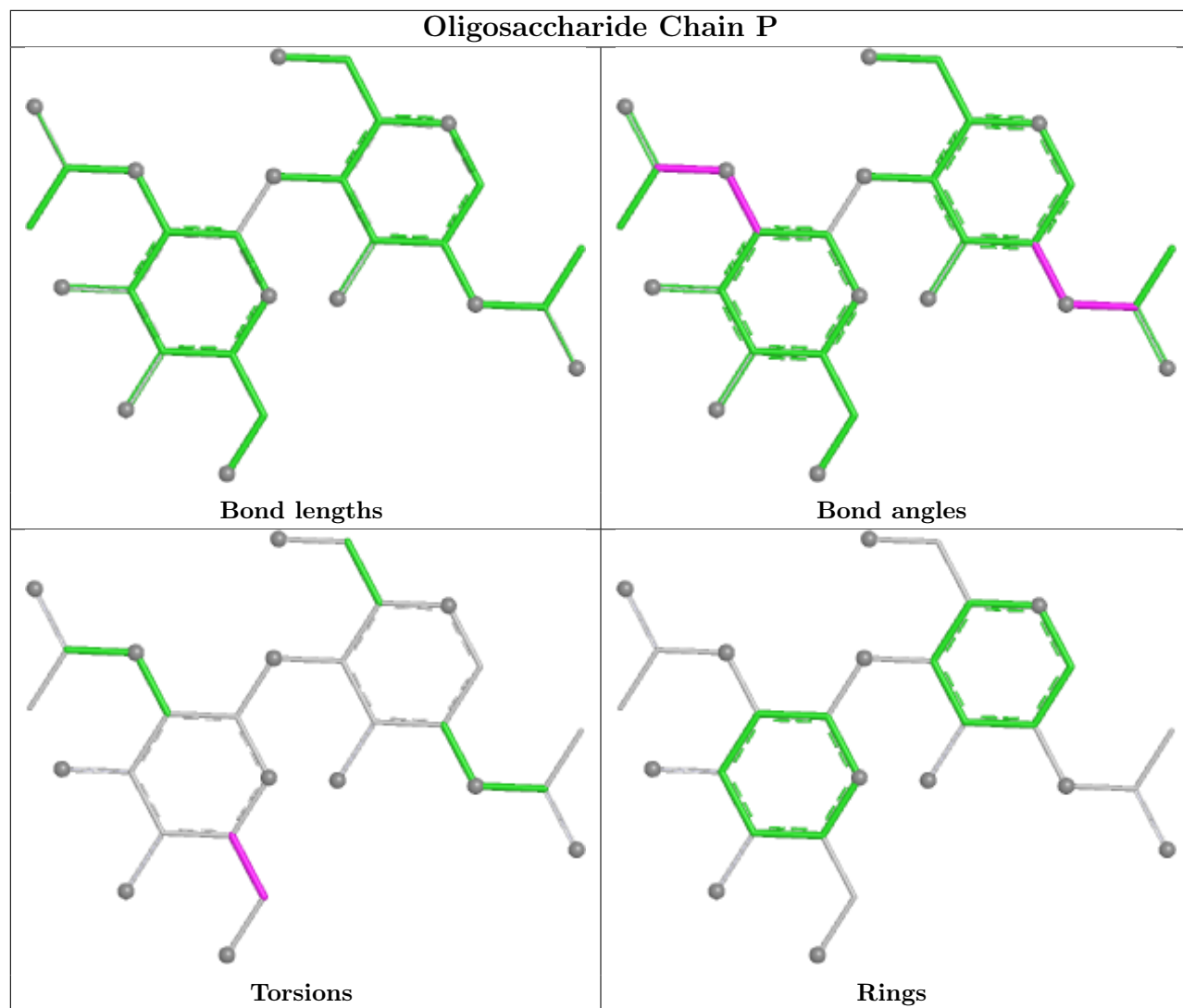


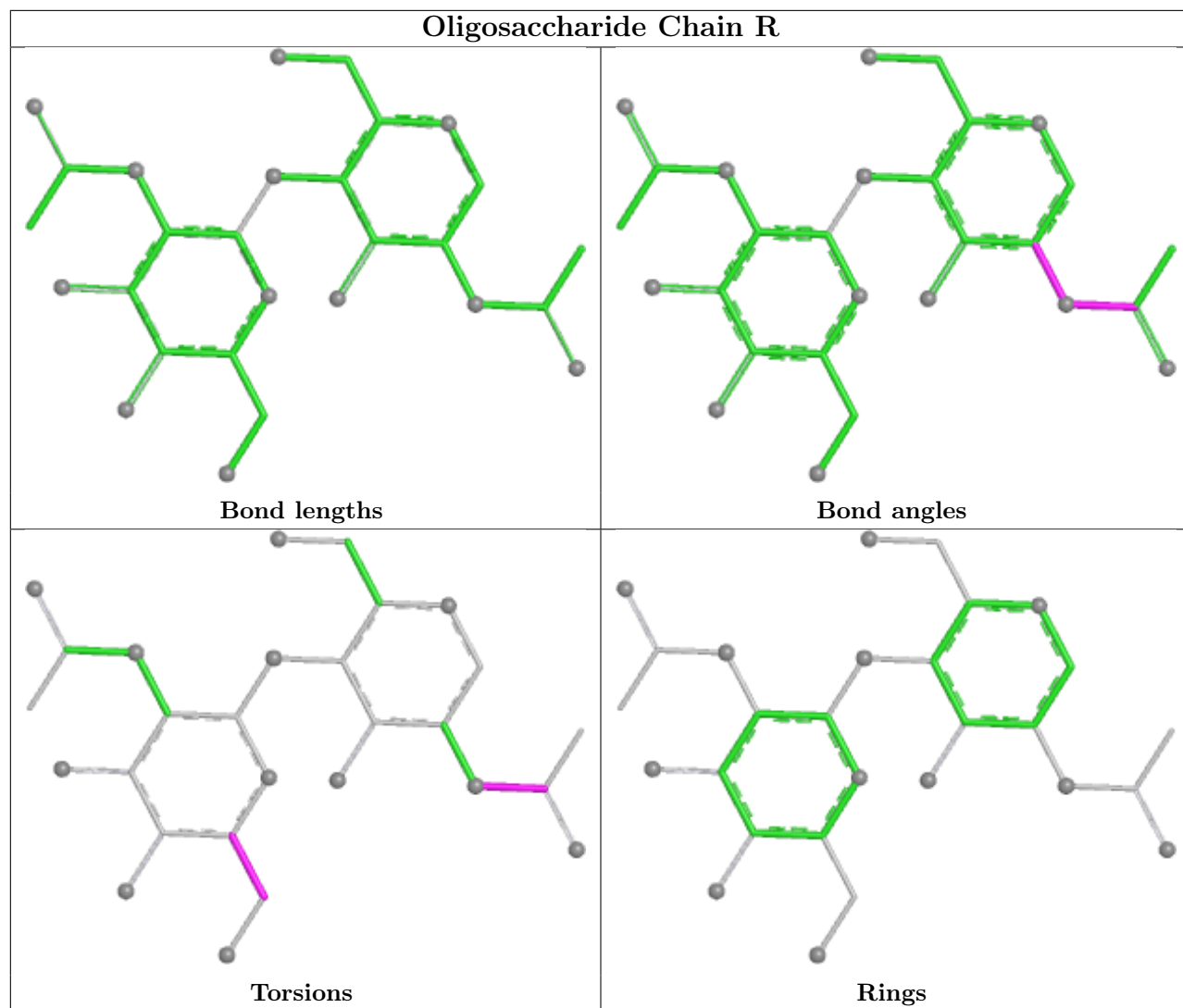


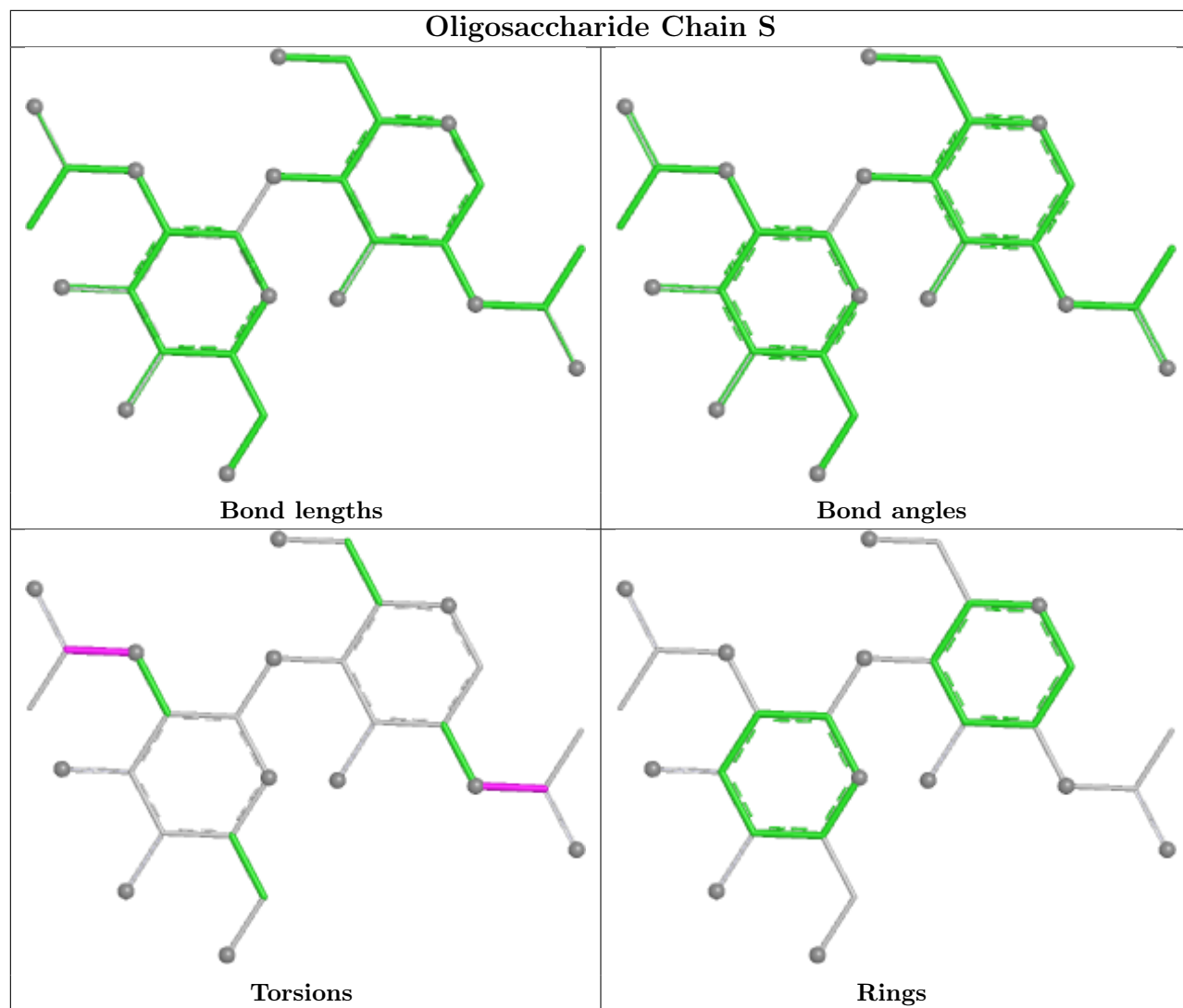


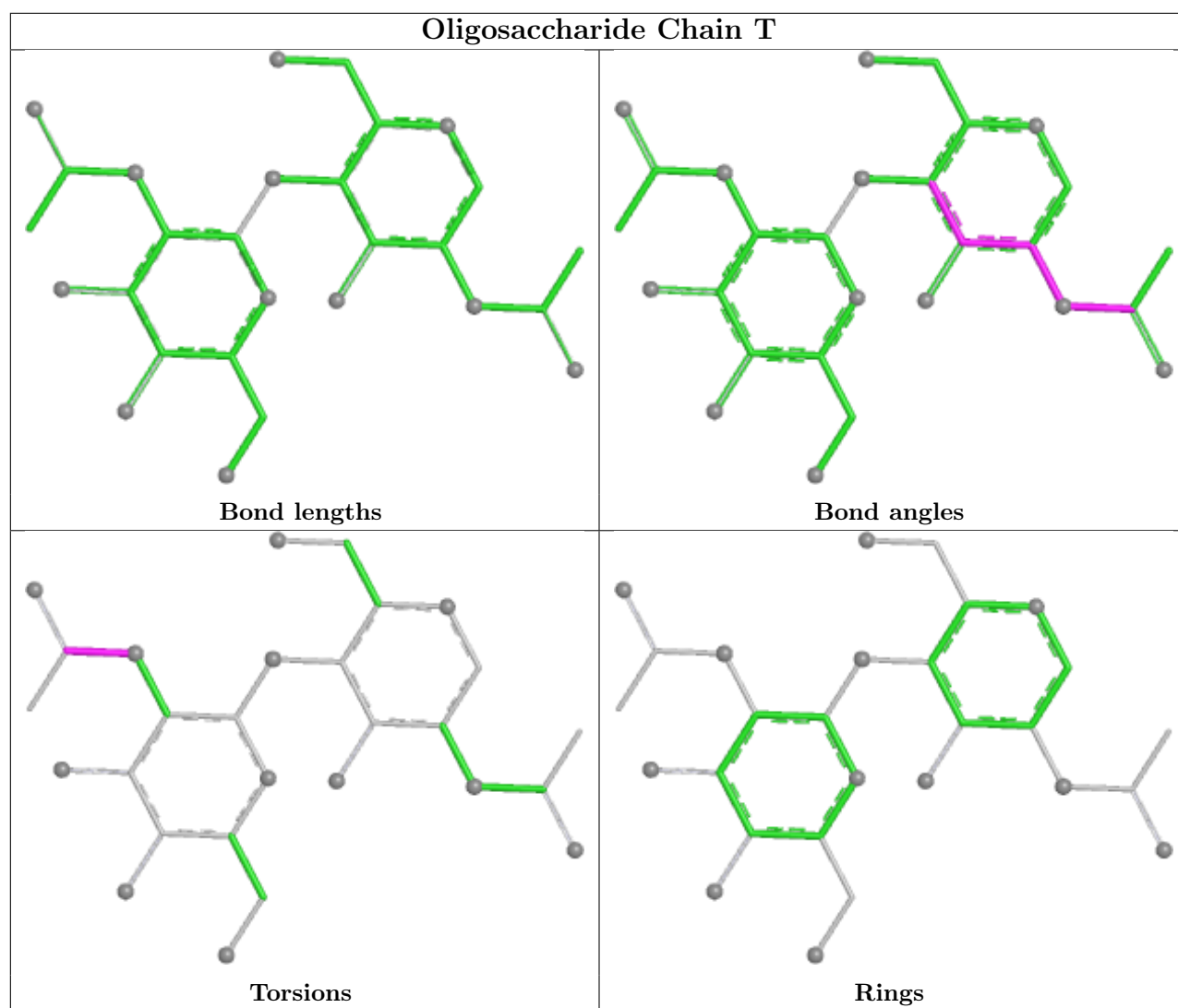


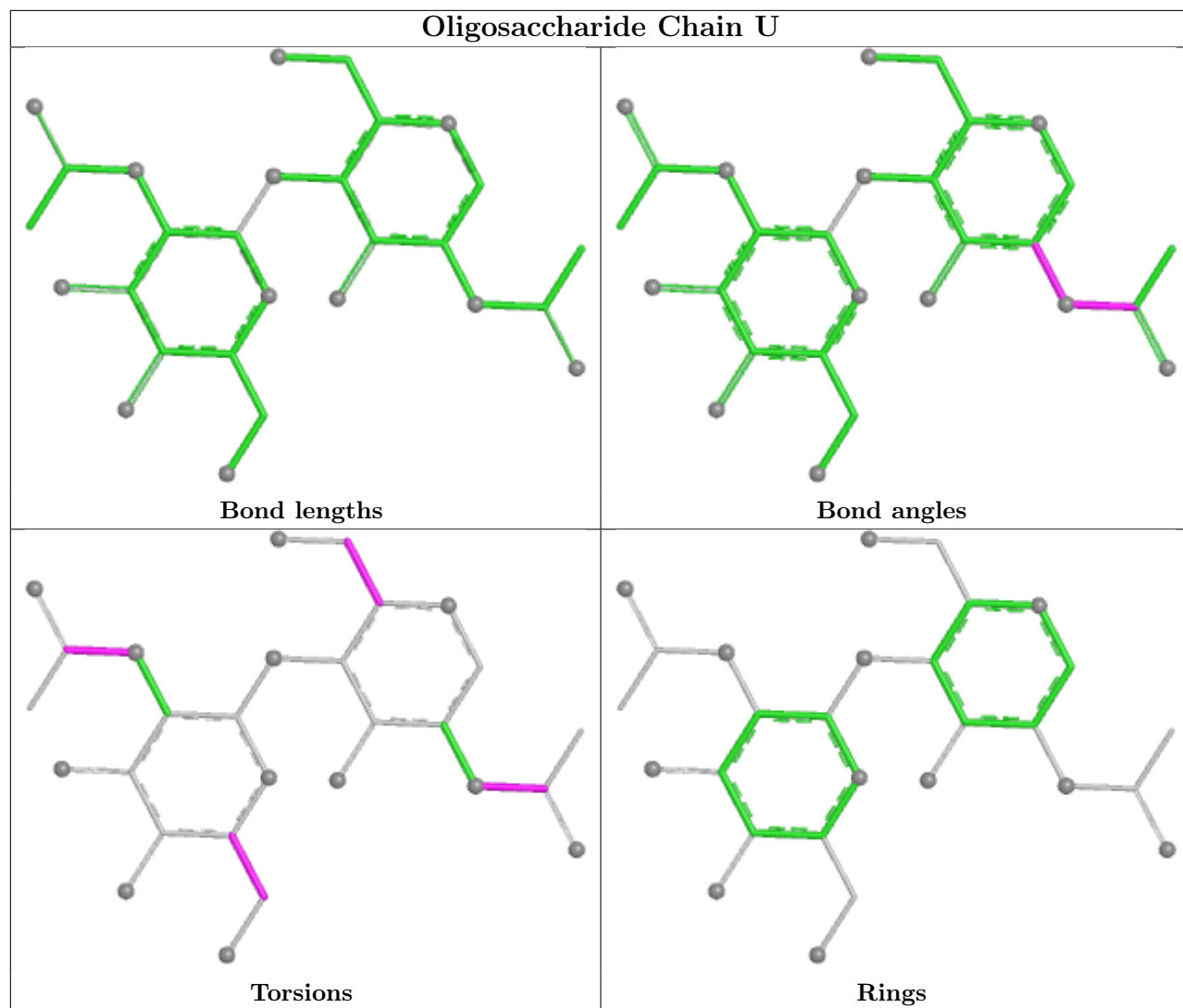


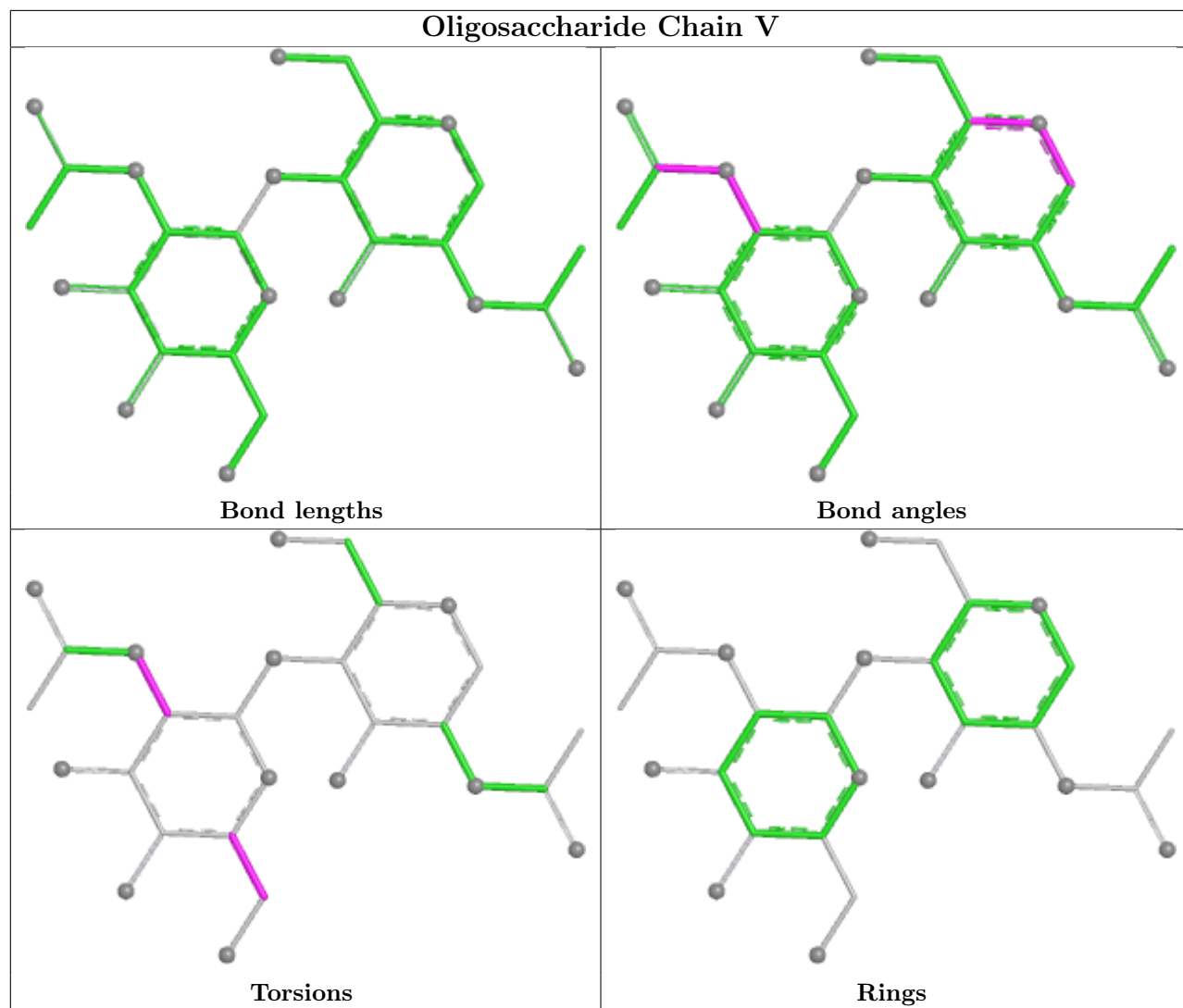


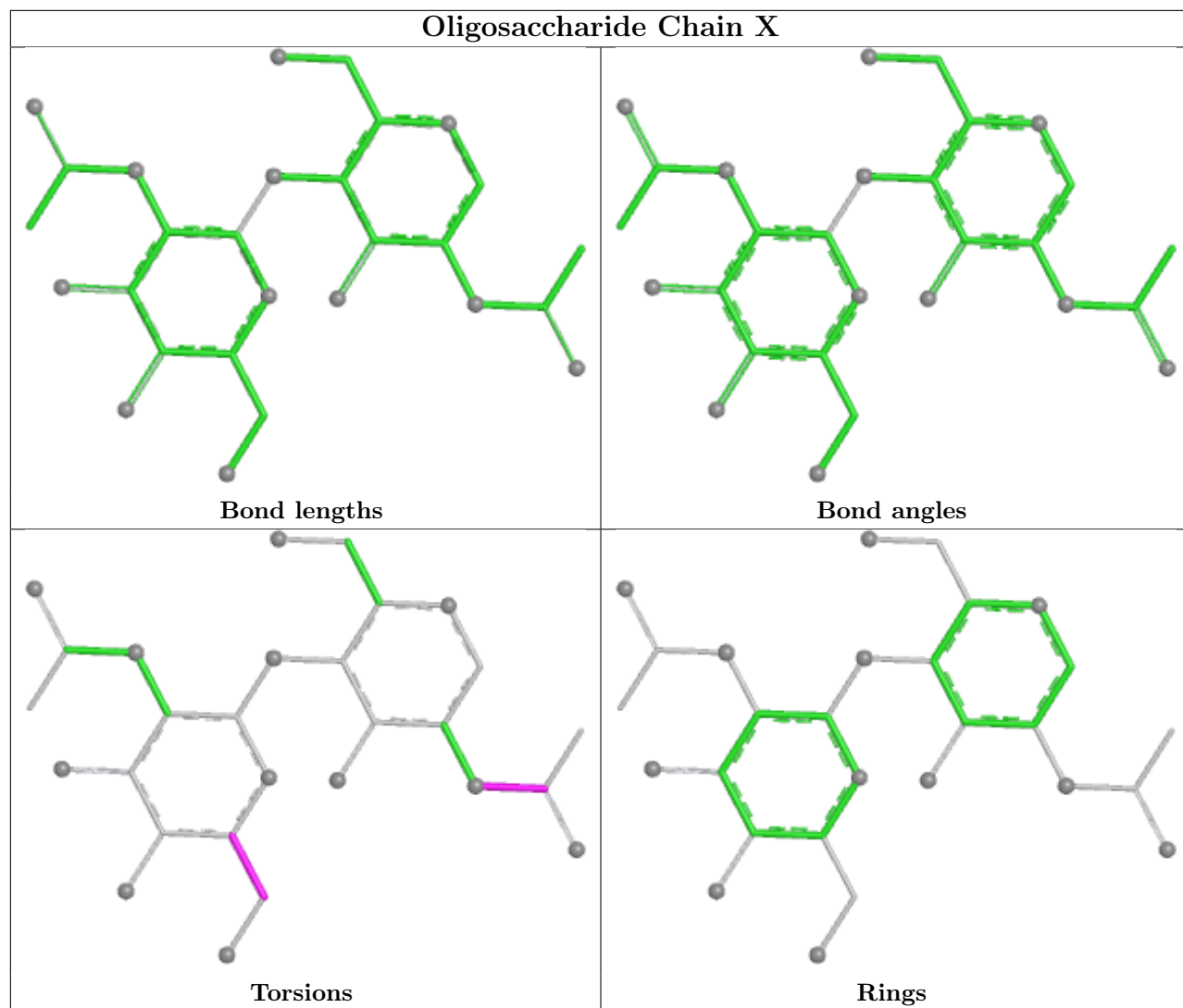


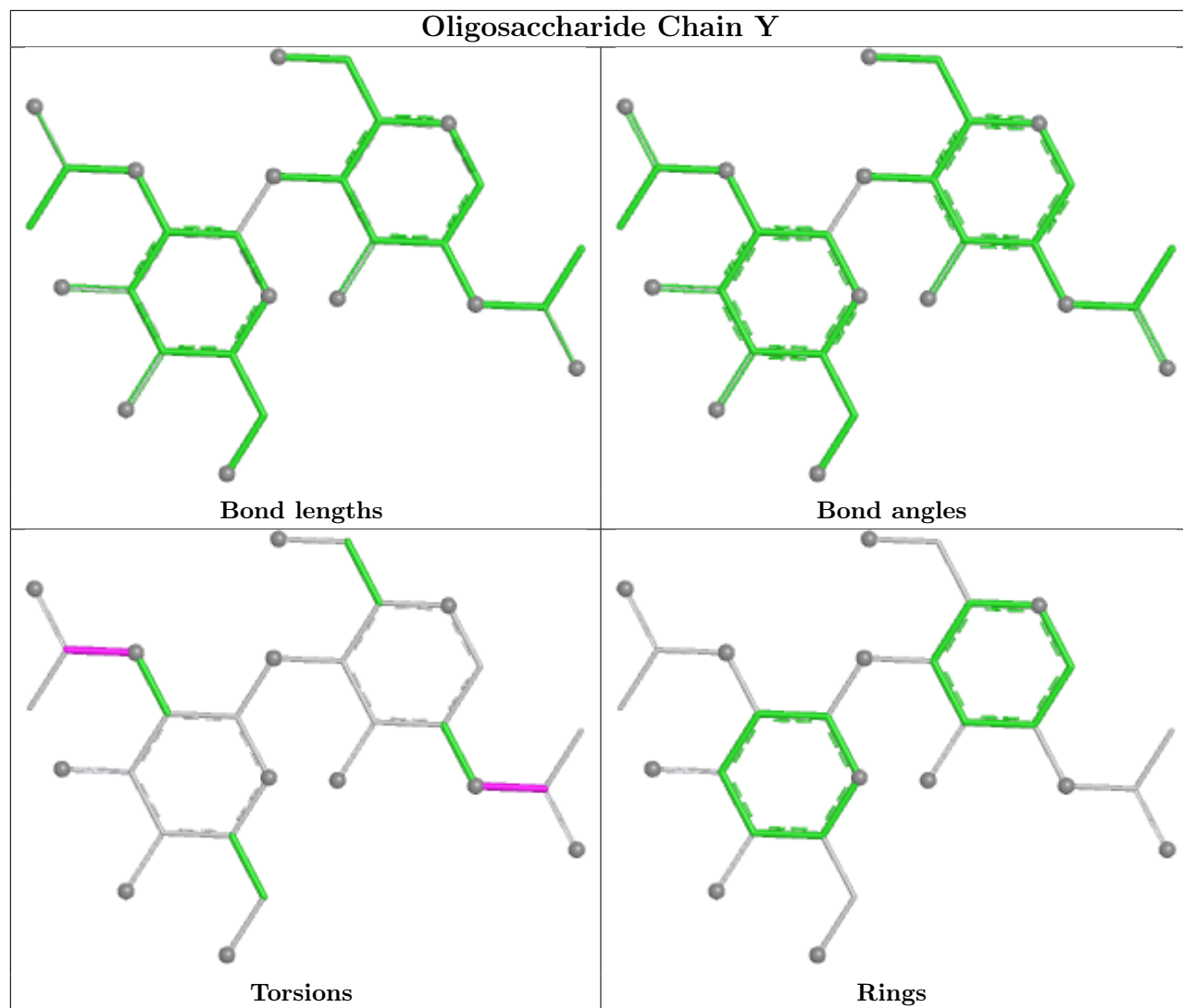


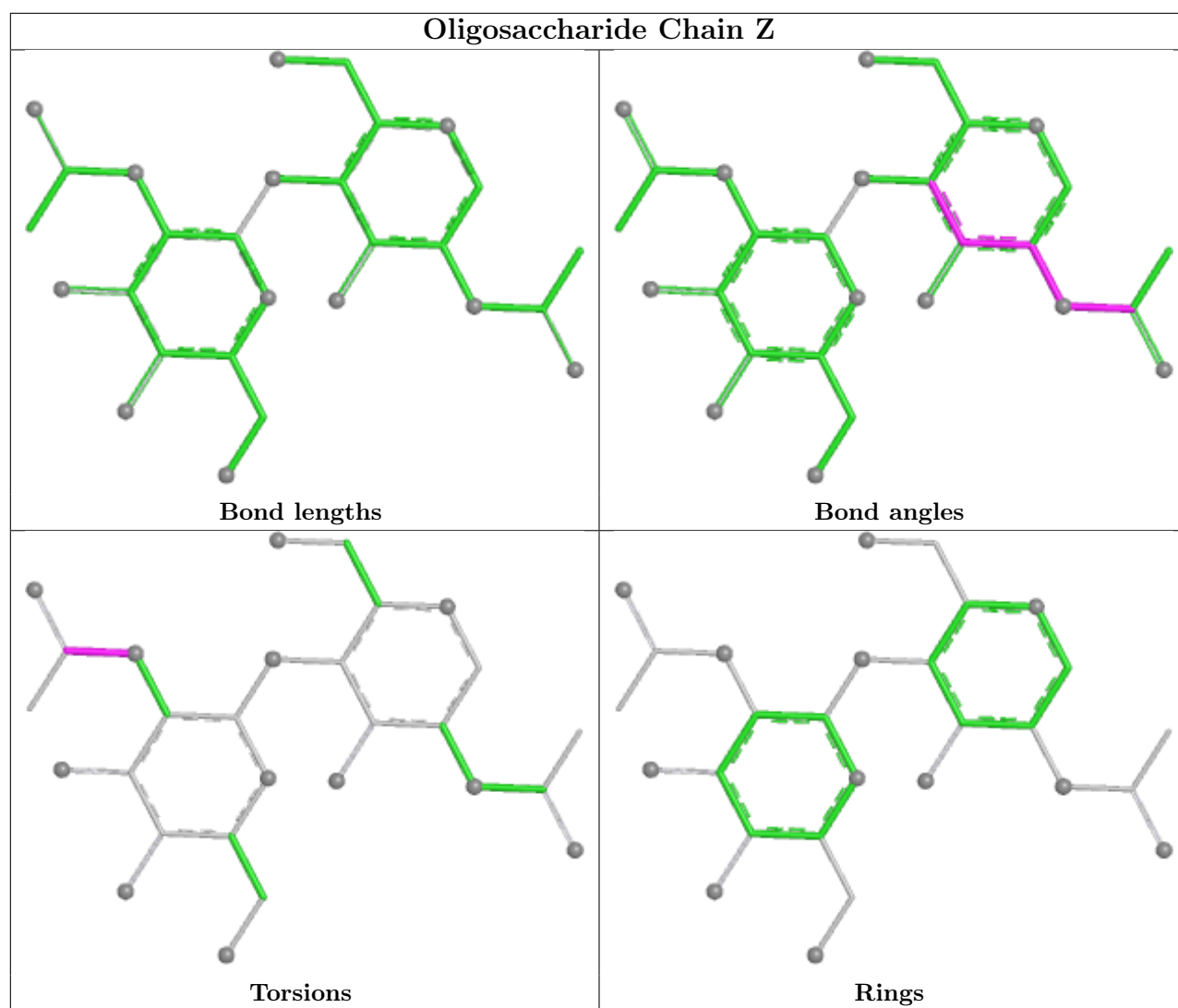


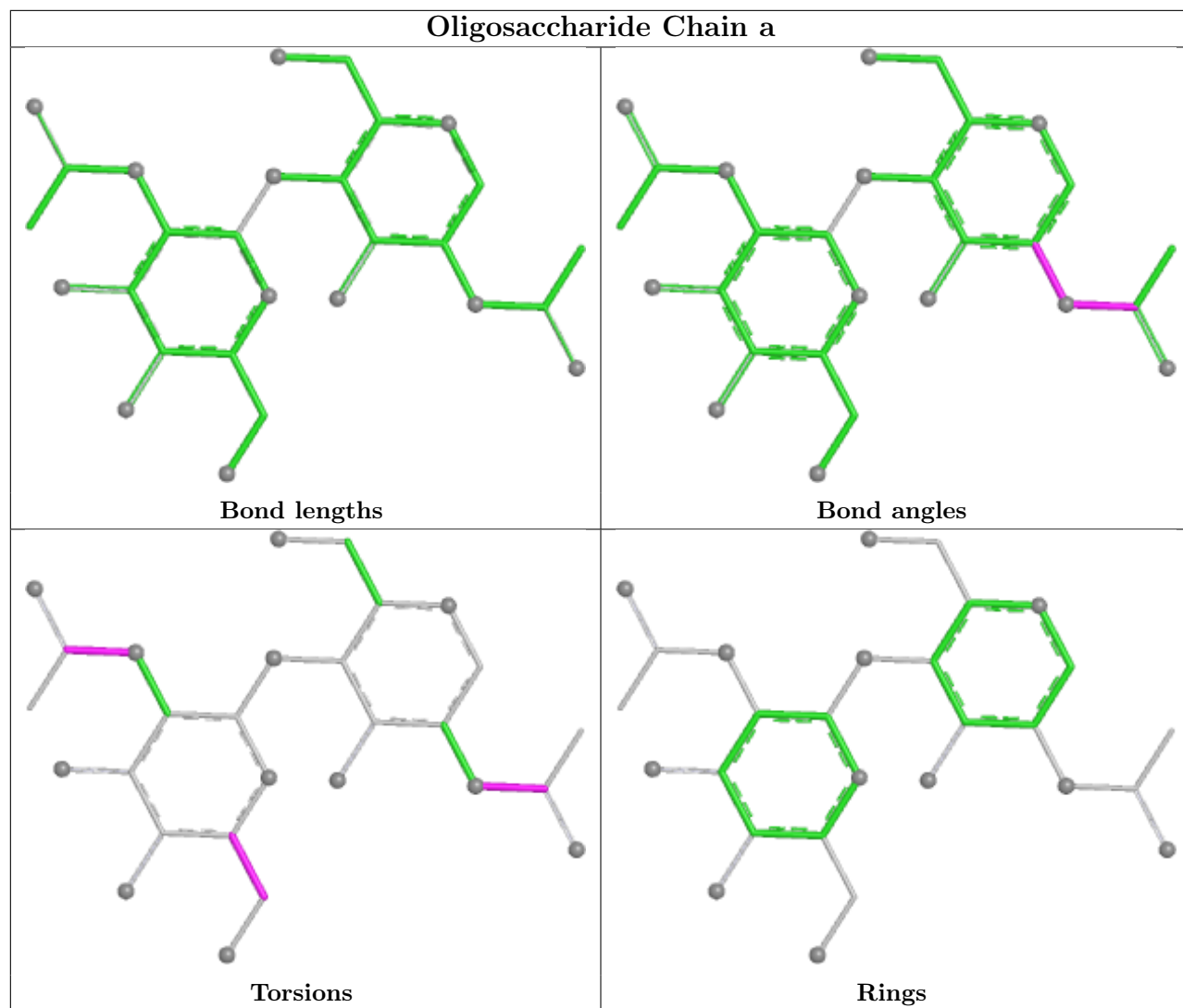


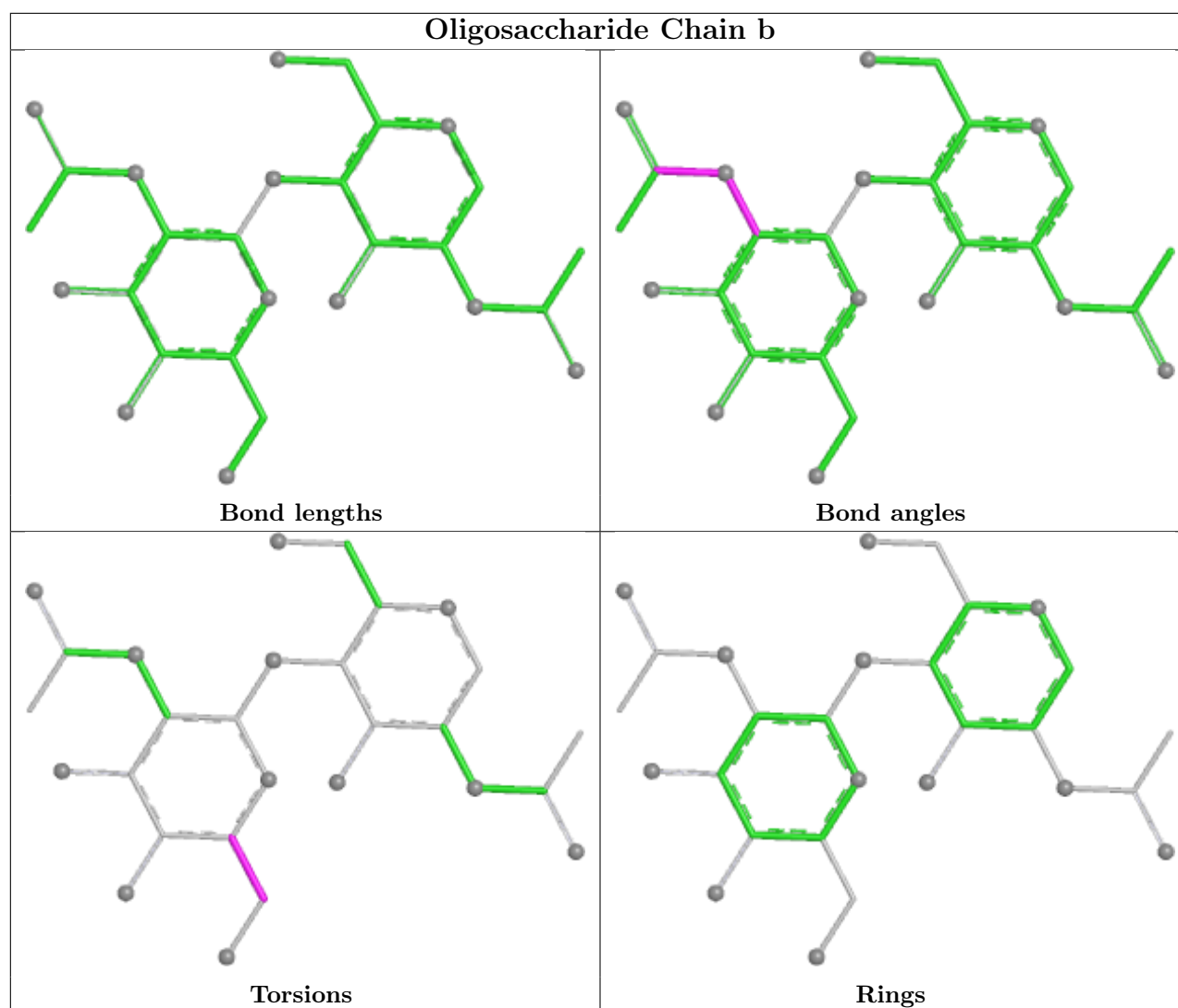












5.6 Ligand geometry [i](#)

20 ligands 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	$\# Z > 2$
4	NAG	B	3011	1	14,14,15	0.44	0	17,19,21	0.73	0
4	NAG	D	3014	1	14,14,15	0.47	0	17,19,21	1.53	3 (17%)
4	NAG	D	3022	1	14,14,15	0.43	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	3014	1	14,14,15	0.47	0	17,19,21	1.51	3 (17%)
4	NAG	C	3019	1	14,14,15	0.43	0	17,19,21	0.70	0
4	NAG	B	3014	1	14,14,15	0.46	0	17,19,21	1.55	3 (17%)
4	NAG	B	3019	1	14,14,15	0.45	0	17,19,21	0.73	0
4	NAG	B	3000	1	14,14,15	0.42	0	17,19,21	1.45	2 (11%)
4	NAG	C	3011	1	14,14,15	0.43	0	17,19,21	0.76	0
4	NAG	A	3022	1	14,14,15	0.44	0	17,19,21	0.71	0
4	NAG	D	3011	1	14,14,15	0.43	0	17,19,21	0.76	0
4	NAG	C	3000	1	14,14,15	0.43	0	17,19,21	1.45	2 (11%)
4	NAG	A	3019	1	14,14,15	0.45	0	17,19,21	0.70	0
4	NAG	C	3022	1	14,14,15	0.43	0	17,19,21	0.74	0
4	NAG	A	3000	1	14,14,15	0.41	0	17,19,21	1.45	2 (11%)
4	NAG	D	3019	1	14,14,15	0.45	0	17,19,21	0.71	0
4	NAG	B	3022	1	14,14,15	0.44	0	17,19,21	0.74	0
4	NAG	D	3000	1	14,14,15	0.42	0	17,19,21	1.44	2 (11%)
4	NAG	A	3014	1	14,14,15	0.47	0	17,19,21	1.55	3 (17%)
4	NAG	A	3011	1	14,14,15	0.43	0	17,19,21	0.75	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
4	NAG	B	3011	1	-	4/6/23/26	0/1/1/1
4	NAG	D	3014	1	-	5/6/23/26	0/1/1/1
4	NAG	D	3022	1	-	2/6/23/26	0/1/1/1
4	NAG	C	3014	1	-	5/6/23/26	0/1/1/1
4	NAG	C	3019	1	-	3/6/23/26	0/1/1/1
4	NAG	B	3014	1	-	5/6/23/26	0/1/1/1
4	NAG	B	3019	1	-	4/6/23/26	0/1/1/1
4	NAG	B	3000	1	-	4/6/23/26	0/1/1/1
4	NAG	C	3011	1	-	4/6/23/26	0/1/1/1
4	NAG	A	3022	1	-	2/6/23/26	0/1/1/1
4	NAG	D	3011	1	-	4/6/23/26	0/1/1/1
4	NAG	C	3000	1	-	4/6/23/26	0/1/1/1
4	NAG	A	3019	1	-	3/6/23/26	0/1/1/1
4	NAG	C	3022	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	3000	1	-	4/6/23/26	0/1/1/1
4	NAG	D	3019	1	-	4/6/23/26	0/1/1/1
4	NAG	B	3022	1	-	2/6/23/26	0/1/1/1
4	NAG	D	3000	1	-	4/6/23/26	0/1/1/1
4	NAG	A	3014	1	-	5/6/23/26	0/1/1/1
4	NAG	A	3011	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3014	NAG	C2-N2-C7	4.43	128.84	122.90
4	A	3000	NAG	C1-C2-N2	4.39	117.36	110.43
4	B	3000	NAG	C1-C2-N2	4.39	117.35	110.43
4	D	3000	NAG	C1-C2-N2	4.38	117.33	110.43
4	C	3000	NAG	C1-C2-N2	4.34	117.28	110.43
4	B	3014	NAG	C2-N2-C7	4.33	128.70	122.90
4	D	3014	NAG	C2-N2-C7	4.33	128.70	122.90
4	C	3014	NAG	C2-N2-C7	4.16	128.47	122.90
4	C	3000	NAG	C2-N2-C7	3.50	127.59	122.90
4	A	3000	NAG	C2-N2-C7	3.46	127.53	122.90
4	D	3000	NAG	C2-N2-C7	3.46	127.53	122.90
4	B	3000	NAG	C2-N2-C7	3.46	127.53	122.90
4	C	3014	NAG	C1-C2-N2	3.33	115.68	110.43
4	B	3014	NAG	C1-C2-N2	3.25	115.55	110.43
4	D	3014	NAG	C1-C2-N2	3.20	115.47	110.43
4	A	3014	NAG	C1-C2-N2	3.17	115.44	110.43
4	A	3014	NAG	O5-C1-C2	2.60	115.31	111.29
4	B	3014	NAG	O5-C1-C2	2.58	115.28	111.29
4	C	3014	NAG	O5-C1-C2	2.56	115.25	111.29
4	D	3014	NAG	O5-C1-C2	2.55	115.24	111.29

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3000	NAG	C8-C7-N2-C2
4	A	3000	NAG	O7-C7-N2-C2
4	A	3014	NAG	C1-C2-N2-C7
4	A	3019	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	3019	NAG	O7-C7-N2-C2
4	A	3022	NAG	O7-C7-N2-C2
4	B	3000	NAG	C8-C7-N2-C2
4	B	3000	NAG	O7-C7-N2-C2
4	B	3014	NAG	C1-C2-N2-C7
4	B	3019	NAG	C8-C7-N2-C2
4	B	3019	NAG	O7-C7-N2-C2
4	B	3022	NAG	O7-C7-N2-C2
4	C	3000	NAG	C8-C7-N2-C2
4	C	3000	NAG	O7-C7-N2-C2
4	C	3014	NAG	C1-C2-N2-C7
4	C	3019	NAG	C8-C7-N2-C2
4	C	3019	NAG	O7-C7-N2-C2
4	C	3022	NAG	O7-C7-N2-C2
4	D	3000	NAG	C8-C7-N2-C2
4	D	3000	NAG	O7-C7-N2-C2
4	D	3014	NAG	C1-C2-N2-C7
4	D	3019	NAG	C8-C7-N2-C2
4	D	3019	NAG	O7-C7-N2-C2
4	D	3022	NAG	O7-C7-N2-C2
4	A	3011	NAG	C8-C7-N2-C2
4	A	3011	NAG	O7-C7-N2-C2
4	A	3022	NAG	C8-C7-N2-C2
4	B	3011	NAG	C8-C7-N2-C2
4	B	3011	NAG	O7-C7-N2-C2
4	B	3022	NAG	C8-C7-N2-C2
4	C	3011	NAG	C8-C7-N2-C2
4	C	3011	NAG	O7-C7-N2-C2
4	C	3022	NAG	C8-C7-N2-C2
4	D	3011	NAG	C8-C7-N2-C2
4	D	3011	NAG	O7-C7-N2-C2
4	D	3022	NAG	C8-C7-N2-C2
4	B	3014	NAG	O5-C5-C6-O6
4	C	3014	NAG	O5-C5-C6-O6
4	D	3014	NAG	O5-C5-C6-O6
4	B	3014	NAG	C8-C7-N2-C2
4	B	3014	NAG	O7-C7-N2-C2
4	C	3014	NAG	C8-C7-N2-C2
4	C	3014	NAG	O7-C7-N2-C2
4	D	3014	NAG	C8-C7-N2-C2
4	D	3014	NAG	O7-C7-N2-C2
4	A	3014	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	3014	NAG	C8-C7-N2-C2
4	A	3014	NAG	O7-C7-N2-C2
4	B	3011	NAG	O5-C5-C6-O6
4	A	3011	NAG	O5-C5-C6-O6
4	C	3011	NAG	O5-C5-C6-O6
4	D	3011	NAG	O5-C5-C6-O6
4	B	3014	NAG	C4-C5-C6-O6
4	C	3014	NAG	C4-C5-C6-O6
4	D	3014	NAG	C4-C5-C6-O6
4	A	3014	NAG	C4-C5-C6-O6
4	B	3011	NAG	C4-C5-C6-O6
4	A	3000	NAG	C3-C2-N2-C7
4	B	3000	NAG	C3-C2-N2-C7
4	C	3000	NAG	C3-C2-N2-C7
4	D	3000	NAG	C3-C2-N2-C7
4	A	3011	NAG	C4-C5-C6-O6
4	C	3011	NAG	C4-C5-C6-O6
4	A	3000	NAG	C1-C2-N2-C7
4	A	3019	NAG	C1-C2-N2-C7
4	B	3000	NAG	C1-C2-N2-C7
4	B	3019	NAG	C1-C2-N2-C7
4	C	3000	NAG	C1-C2-N2-C7
4	C	3019	NAG	C1-C2-N2-C7
4	D	3000	NAG	C1-C2-N2-C7
4	D	3019	NAG	C1-C2-N2-C7
4	D	3011	NAG	C4-C5-C6-O6
4	D	3019	NAG	C4-C5-C6-O6
4	B	3019	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1836/1859 (98%)	1.46	476 (25%) 1 1	22, 80, 142, 183	1 (0%)
1	B	1836/1859 (98%)	1.35	424 (23%) 2 1	28, 74, 129, 163	1 (0%)
1	C	1836/1859 (98%)	0.97	261 (14%) 6 5	21, 57, 103, 143	1 (0%)
1	D	1836/1859 (98%)	1.33	436 (23%) 2 1	28, 72, 136, 176	1 (0%)
All	All	7344/7436 (98%)	1.28	1597 (21%) 2 2	21, 71, 130, 183	4 (0%)

All (1597) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2202	TRP	8.5
1	B	1493	LEU	7.7
1	A	2220	LEU	7.2
1	A	1493	LEU	7.1
1	C	1486	VAL	7.1
1	C	1493	LEU	6.9
1	D	2686	ILE	6.9
1	C	1045	PRO	6.8
1	B	956	LEU	6.8
1	D	1493	LEU	6.6
1	B	1045	PRO	6.5
1	D	1423	LEU	6.3
1	D	1429	LEU	6.2
1	C	1489	ILE	6.1
1	D	1307	PHE	6.1
1	B	1429	LEU	6.1
1	A	2713	ALA	6.1
1	A	1489	ILE	6.1
1	A	2412	LEU	6.1
1	B	1425	ALA	6.1
1	B	1486	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	1119	LEU	5.9
1	D	1119	LEU	5.9
1	A	1045	PRO	5.9
1	A	1122	LEU	5.8
1	B	1013	ALA	5.8
1	D	1045	PRO	5.8
1	D	1486	VAL	5.8
1	D	974	GLY	5.7
1	C	1423	LEU	5.7
1	D	956	LEU	5.7
1	B	973	VAL	5.7
1	B	1489	ILE	5.7
1	D	1489	ILE	5.6
1	D	2688	GLY	5.6
1	A	956	LEU	5.6
1	A	1423	LEU	5.5
1	B	979	PHE	5.4
1	C	1429	LEU	5.4
1	A	1486	VAL	5.3
1	B	1365	LEU	5.3
1	D	1122	LEU	5.3
1	B	1421	ASN	5.3
1	A	1365	LEU	5.3
1	C	1425	ALA	5.2
1	B	1423	LEU	5.2
1	D	2649	PHE	5.2
1	D	1309	HIS	5.1
1	D	1016	MET	5.1
1	D	2684	LEU	5.1
1	D	2685	LEU	5.0
1	D	2713	ALA	5.0
1	A	2394	TYR	5.0
1	D	983	PRO	5.0
1	A	1307	PHE	5.0
1	A	1184	LEU	5.0
1	B	1491	TYR	5.0
1	C	1013	ALA	5.0
1	D	2716	LEU	4.9
1	A	2221	GLY	4.9
1	C	973	VAL	4.9
1	D	2690	THR	4.9
1	B	982	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	1184	LEU	4.8
1	C	1487	PRO	4.8
1	A	973	VAL	4.8
1	D	973	VAL	4.8
1	D	2752	VAL	4.8
1	A	2711	LEU	4.8
1	B	1122	LEU	4.8
1	C	956	LEU	4.8
1	A	1495	LYS	4.8
1	D	982	TYR	4.7
1	C	1016	MET	4.7
1	B	1496	LEU	4.7
1	A	2531	TYR	4.7
1	B	1016	MET	4.7
1	B	1671	SER	4.7
1	D	1303	ARG	4.7
1	A	1350	LEU	4.7
1	A	1429	LEU	4.7
1	A	1428	PRO	4.7
1	C	1428	PRO	4.7
1	A	2198	SER	4.6
1	B	2498	LEU	4.6
1	C	982	TYR	4.6
1	B	2202	TRP	4.6
1	D	2632	HIS	4.6
1	A	1016	MET	4.6
1	C	1037	MET	4.6
1	A	1180	THR	4.5
1	A	2218	LEU	4.5
1	C	1365	LEU	4.5
1	B	2531	TYR	4.5
1	A	2498	LEU	4.5
1	D	1184	LEU	4.5
1	A	2688	GLY	4.5
1	D	1487	PRO	4.5
1	D	1389	ILE	4.5
1	B	1307	PHE	4.5
1	C	1769	ASP	4.5
1	B	1297	THR	4.4
1	A	1053	VAL	4.4
1	B	1389	ILE	4.4
1	A	1872	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	1367	PHE	4.4
1	A	1037	MET	4.4
1	D	2711	LEU	4.4
1	A	982	TYR	4.4
1	B	1498	ILE	4.4
1	C	1122	LEU	4.4
1	B	1477	ILE	4.4
1	C	985	TYR	4.4
1	A	1013	ALA	4.3
1	D	1037	MET	4.3
1	B	1218	LYS	4.3
1	B	1418	LEU	4.3
1	B	1672	GLY	4.3
1	B	1185	ILE	4.3
1	A	2226	THR	4.3
1	C	1389	ILE	4.3
1	A	1014	PRO	4.2
1	A	1487	PRO	4.2
1	C	1481	PRO	4.2
1	B	1590	LEU	4.2
1	C	1184	LEU	4.2
1	D	1306	GLU	4.2
1	C	1870	HIS	4.2
1	D	985	TYR	4.2
1	B	1367	PHE	4.2
1	B	1487	PRO	4.2
1	B	1419	GLY	4.2
1	D	1310	SER	4.2
1	B	1670	ALA	4.2
1	A	1367	PHE	4.2
1	D	1015	PHE	4.2
1	D	1284	PHE	4.2
1	C	1049	LEU	4.2
1	C	1431	CYS	4.2
1	B	2752	VAL	4.2
1	D	2648	TYR	4.2
1	D	2498	LEU	4.2
1	B	1035	LEU	4.1
1	B	1119	LEU	4.1
1	C	979	PHE	4.1
1	D	1442	LEU	4.1
1	D	2710	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	1255	SER	4.1
1	D	1349	ASP	4.1
1	B	1366	PRO	4.1
1	C	983	PRO	4.1
1	D	2531	TYR	4.1
1	A	2173	THR	4.1
1	B	1769	ASP	4.1
1	B	2686	ILE	4.1
1	B	2687	ASN	4.1
1	D	1114	ILE	4.1
1	C	1015	PHE	4.1
1	A	2174	ALA	4.0
1	D	1590	LEU	4.0
1	A	985	TYR	4.0
1	B	1422	ASP	4.0
1	D	979	PHE	4.0
1	B	1444	TRP	4.0
1	A	980	VAL	4.0
1	B	1431	CYS	4.0
1	A	1370	ALA	4.0
1	A	2199	LEU	4.0
1	D	1701	GLN	4.0
1	B	1604	ILE	4.0
1	B	2689	ARG	4.0
1	C	1418	LEU	4.0
1	D	1365	LEU	4.0
1	A	2052	LYS	3.9
1	A	1054	ARG	3.9
1	A	2752	VAL	3.9
1	D	1053	VAL	3.9
1	D	2712	THR	3.9
1	D	1925	PHE	3.9
1	A	2755	ASP	3.9
1	D	2755	ASP	3.9
1	B	1348	LYS	3.9
1	B	1299	ILE	3.9
1	D	1143	LEU	3.9
1	C	974	GLY	3.9
1	A	2409	ILE	3.9
1	B	1856	ILE	3.9
1	A	1425	ALA	3.9
1	A	983	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	1498	ILE	3.9
1	D	2652	ILE	3.9
1	A	1296	VAL	3.9
1	A	2175	VAL	3.9
1	B	980	VAL	3.9
1	B	2052	LYS	3.9
1	A	1498	ILE	3.8
1	D	1185	ILE	3.8
1	A	984	LYS	3.8
1	D	2720	LYS	3.8
1	B	1120	VAL	3.8
1	B	1186	LEU	3.8
1	D	1259	LEU	3.8
1	D	1496	LEU	3.8
1	C	1303	ARG	3.8
1	C	1444	TRP	3.8
1	D	1367	PHE	3.8
1	C	1182	PRO	3.8
1	C	1366	PRO	3.8
1	A	2176	MET	3.8
1	A	974	GLY	3.8
1	D	1023	TRP	3.8
1	A	2383	PHE	3.8
1	B	1037	MET	3.8
1	B	1492	SER	3.8
1	C	1014	PRO	3.8
1	D	2052	LYS	3.8
1	A	1125	ILE	3.8
1	A	1491	TYR	3.8
1	D	1120	VAL	3.8
1	D	2660	VAL	3.8
1	A	2690	THR	3.8
1	B	1476	ILE	3.8
1	C	1442	LEU	3.8
1	A	2201	TYR	3.7
1	D	975	VAL	3.8
1	D	2665	THR	3.7
1	A	1405	ILE	3.7
1	B	1405	ILE	3.7
1	A	1496	LEU	3.7
1	B	984	LYS	3.7
1	B	1424	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1481	PRO	3.7
1	B	1014	PRO	3.7
1	B	1428	PRO	3.7
1	C	1780	SER	3.7
1	A	2686	ILE	3.7
1	C	1419	GLY	3.7
1	A	1424	THR	3.7
1	A	2223	TYR	3.7
1	D	1180	THR	3.7
1	D	2661	THR	3.7
1	D	2773	TYR	3.7
1	D	2691	ARG	3.7
1	D	2692	ARG	3.7
1	A	2222	PRO	3.7
1	B	1015	PHE	3.7
1	A	1143	LEU	3.7
1	C	972	LEU	3.7
1	A	2200	MET	3.7
1	B	1341	VAL	3.7
1	A	1255	SER	3.7
1	A	1389	ILE	3.6
1	A	1413	ILE	3.6
1	B	1593	ILE	3.6
1	B	1872	ARG	3.6
1	D	1872	ARG	3.6
1	C	2752	VAL	3.6
1	A	2224	ALA	3.6
1	B	987	TYR	3.6
1	C	2052	LYS	3.6
1	A	2652	ILE	3.6
1	A	1366	PRO	3.6
1	D	984	LYS	3.6
1	D	1481	PRO	3.6
1	B	985	TYR	3.6
1	A	1488	GLY	3.6
1	A	1418	LEU	3.6
1	B	2685	LEU	3.6
1	D	1049	LEU	3.6
1	B	1253	CYS	3.6
1	C	1422	ASP	3.6
1	A	1333	THR	3.6
1	C	1007	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1757	LYS	3.6
1	D	1444	TRP	3.6
1	B	1182	PRO	3.6
1	B	1578	ALA	3.6
1	A	2140	LEU	3.6
1	B	1350	LEU	3.6
1	B	1285	ASN	3.6
1	D	1495	LYS	3.6
1	A	1269	VAL	3.6
1	B	1296	VAL	3.6
1	D	1296	VAL	3.6
1	D	1428	PRO	3.6
1	A	2648	TYR	3.5
1	C	1496	LEU	3.5
1	D	1407	LYS	3.5
1	A	1309	HIS	3.5
1	B	1483	HIS	3.5
1	A	964	VAL	3.5
1	A	1400	VAL	3.5
1	B	983	PRO	3.5
1	B	1440	VAL	3.5
1	A	2689	ARG	3.5
1	D	2049	LYS	3.5
1	A	1476	ILE	3.5
1	C	1125	ILE	3.5
1	D	1059	ILE	3.5
1	D	2086	GLY	3.5
1	D	998	LEU	3.5
1	C	1424	THR	3.5
1	A	1303	ARG	3.5
1	A	1453	MET	3.5
1	A	1482	MET	3.5
1	A	1023	TRP	3.5
1	A	2219	LYS	3.5
1	B	1286	TYR	3.5
1	C	2531	TYR	3.5
1	D	1286	TYR	3.5
1	D	1491	TYR	3.5
1	B	2616	ILE	3.5
1	A	1460	LEU	3.5
1	B	1143	LEU	3.5
1	A	1182	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1515	VAL	3.5
1	B	2472	MET	3.5
1	C	1488	GLY	3.5
1	D	1498	ILE	3.5
1	D	1422	ASP	3.5
1	A	2665	THR	3.4
1	A	1189	LYS	3.4
1	B	1426	VAL	3.4
1	C	1296	VAL	3.4
1	D	1314	ALA	3.4
1	B	1181	CYS	3.4
1	A	1251	ILE	3.4
1	A	1518	ILE	3.4
1	B	1020	ARG	3.4
1	A	1286	TYR	3.4
1	B	1417	LEU	3.4
1	D	1350	LEU	3.4
1	A	1052	PHE	3.4
1	B	1007	THR	3.4
1	A	1554	VAL	3.4
1	D	1269	VAL	3.4
1	A	2408	SER	3.4
1	A	2691	ARG	3.4
1	D	1020	ARG	3.4
1	D	2751	ARG	3.4
1	A	1590	LEU	3.4
1	D	1312	ASN	3.4
1	D	2696	ILE	3.4
1	B	1316	LYS	3.4
1	B	1394	TYR	3.4
1	A	1029	PHE	3.4
1	B	1010	PHE	3.4
1	C	1284	PHE	3.4
1	C	1307	PHE	3.4
1	D	1366	PRO	3.4
1	C	1255	SER	3.4
1	A	1754	GLU	3.4
1	C	2642	GLU	3.4
1	C	1181	CYS	3.4
1	D	1285	ASN	3.4
1	D	1052	PHE	3.4
1	D	2683	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1036	VAL	3.4
1	D	980	VAL	3.4
1	C	1054	ARG	3.4
1	A	2051	GLY	3.4
1	A	2545	CYS	3.4
1	D	1431	CYS	3.4
1	A	1422	ASP	3.4
1	A	2135	ILE	3.3
1	A	2371	ILE	3.3
1	B	959	LEU	3.3
1	C	989	ILE	3.3
1	D	1186	LEU	3.3
1	A	979	PHE	3.3
1	A	2646	THR	3.3
1	B	2690	THR	3.3
1	C	1491	TYR	3.3
1	A	2434	GLN	3.3
1	C	1373	GLY	3.3
1	A	2687	ASN	3.3
1	D	1200	ASP	3.3
1	D	1769	ASP	3.3
1	B	1049	LEU	3.3
1	C	2498	LEU	3.3
1	D	1417	LEU	3.3
1	A	2139	PRO	3.3
1	A	1444	TRP	3.3
1	A	2270	ARG	3.3
1	B	2683	THR	3.3
1	B	1870	HIS	3.3
1	D	2636	LYS	3.3
1	A	1341	VAL	3.3
1	B	1822	VAL	3.3
1	A	1359	GLY	3.3
1	A	2716	LEU	3.3
1	C	1119	LEU	3.3
1	D	2218	LEU	3.3
1	A	1185	ILE	3.3
1	B	1413	ILE	3.3
1	B	1883	ILE	3.3
1	D	2694	THR	3.3
1	A	1217	VAL	3.3
1	B	1453	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	2769	GLY	3.3
1	C	1392	ASP	3.3
1	A	1442	LEU	3.3
1	A	2382	LEU	3.3
1	C	1323	PRO	3.3
1	A	2391	GLU	3.3
1	B	1495	LYS	3.3
1	C	1495	LYS	3.3
1	A	967	THR	3.3
1	C	1023	TRP	3.3
1	A	1120	VAL	3.3
1	B	977	VAL	3.3
1	C	977	VAL	3.3
1	D	999	VAL	3.3
1	D	1036	VAL	3.3
1	B	1482	MET	3.2
1	C	1285	ASN	3.2
1	B	1448	LEU	3.2
1	C	2616	ILE	3.2
1	D	2669	LYS	3.2
1	A	1047	CYS	3.2
1	A	1015	PHE	3.2
1	A	1925	PHE	3.2
1	A	1310	SER	3.2
1	B	2223	TYR	3.2
1	A	2008	VAL	3.2
1	B	1359	GLY	3.2
1	A	1769	ASP	3.2
1	B	2620	ASP	3.2
1	D	1210	ASP	3.2
1	D	1551	LYS	3.2
1	A	1049	LEU	3.2
1	A	1870	HIS	3.2
1	A	988	THR	3.2
1	A	2712	THR	3.2
1	D	1420	SER	3.2
1	B	1458	TYR	3.2
1	C	980	VAL	3.2
1	C	1426	VAL	3.2
1	D	2633	TYR	3.2
1	A	1547	ASP	3.2
1	C	2687	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	2755	ASP	3.2
1	D	1490	ASP	3.2
1	B	1778	LEU	3.2
1	C	1405	ILE	3.2
1	A	1256	CYS	3.2
1	D	1012	ARG	3.2
1	D	1050	SER	3.2
1	D	2657	SER	3.2
1	A	977	VAL	3.2
1	D	2344	GLY	3.2
1	D	1315	HIS	3.2
1	B	1023	TRP	3.2
1	A	2685	LEU	3.2
1	A	2197	ARG	3.1
1	A	2751	ARG	3.1
1	A	1126	LYS	3.1
1	B	2051	GLY	3.1
1	A	2191	VAL	3.1
1	B	1053	VAL	3.1
1	A	1186	LEU	3.1
1	B	1396	LEU	3.1
1	B	2220	LEU	3.1
1	D	1014	PRO	3.1
1	A	2131	ILE	3.1
1	A	2195	MET	3.1
1	B	1032	MET	3.1
1	A	1151	THR	3.1
1	A	1142	PHE	3.1
1	C	1004	SER	3.1
1	B	1669	ASP	3.1
1	B	2174	ALA	3.1
1	A	965	VAL	3.1
1	B	965	VAL	3.1
1	B	1474	VAL	3.1
1	B	972	LEU	3.1
1	B	1329	TYR	3.1
1	B	2218	LEU	3.1
1	D	972	LEU	3.1
1	D	1418	LEU	3.1
1	B	1494	SER	3.1
1	B	1142	PHE	3.1
1	A	1210	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	2755	ASP	3.1
1	D	1311	ASN	3.1
1	D	2643	GLY	3.1
1	B	1501	ALA	3.1
1	A	1427	ARG	3.1
1	C	984	LYS	3.1
1	C	1482	MET	3.1
1	C	2546	GLU	3.1
1	D	2138	THR	3.1
1	A	1284	PHE	3.1
1	A	2407	PHE	3.1
1	A	1349	ASP	3.1
1	C	1210	ASP	3.1
1	D	1484	CYS	3.1
1	D	1568	ASP	3.1
1	C	1020	ARG	3.1
1	C	1053	VAL	3.1
1	A	1059	ILE	3.0
1	B	1251	ILE	3.0
1	B	1831	ILE	3.0
1	D	1831	ILE	3.0
1	D	1347	THR	3.0
1	B	1315	HIS	3.0
1	A	1354	SER	3.0
1	B	1420	SER	3.0
1	B	1169	ASP	3.0
1	B	2688	GLY	3.0
1	C	1454	ASP	3.0
1	C	1845	ASN	3.0
1	B	1054	ARG	3.0
1	C	1047	CYS	3.0
1	B	2585	ALA	3.0
1	D	1182	PRO	3.0
1	B	999	VAL	3.0
1	D	1426	VAL	3.0
1	A	2364	TYR	3.0
1	D	1477	ILE	3.0
1	D	1187	TRP	3.0
1	B	1427	ARG	3.0
1	C	1696	LYS	3.0
1	A	2225	ASN	3.0
1	C	1332	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1432	ASP	3.0
1	D	1488	GLY	3.0
1	B	2383	PHE	3.0
1	D	996	PHE	3.0
1	A	1484	CYS	3.0
1	B	1370	ALA	3.0
1	B	1484	CYS	3.0
1	D	2472	MET	3.0
1	C	1120	VAL	3.0
1	C	1590	LEU	3.0
1	D	964	VAL	3.0
1	D	989	ILE	3.0
1	D	1870	HIS	3.0
1	C	1861	THR	3.0
1	A	2720	LYS	3.0
1	C	1337	ARG	3.0
1	D	1348	LYS	3.0
1	D	2689	ARG	3.0
1	A	1005	SER	3.0
1	A	1494	SER	3.0
1	A	1419	GLY	3.0
1	D	2706	ASN	3.0
1	A	2546	GLU	3.0
1	A	1259	LEU	3.0
1	C	1256	CYS	3.0
1	D	1047	CYS	3.0
1	A	1459	VAL	3.0
1	D	1148	LEU	3.0
1	D	1772	VAL	3.0
1	D	2634	LEU	3.0
1	D	1125	ILE	3.0
1	D	2131	ILE	3.0
1	B	1371	ARG	3.0
1	B	1945	LYS	3.0
1	C	1310	SER	3.0
1	A	1392	ASP	3.0
1	B	1373	GLY	3.0
1	C	1421	ASN	3.0
1	D	1669	ASP	3.0
1	A	2472	MET	3.0
1	A	2798	GLU	3.0
1	B	1201	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	2585	ALA	2.9
1	A	2436	VAL	2.9
1	B	1309	HIS	2.9
1	C	975	VAL	2.9
1	D	977	VAL	2.9
1	A	1894	LYS	2.9
1	A	2501	LYS	2.9
1	A	2669	LYS	2.9
1	B	1393	LYS	2.9
1	B	2529	LYS	2.9
1	A	1760	THR	2.9
1	B	1347	THR	2.9
1	A	2393	TYR	2.9
1	A	1373	GLY	2.9
1	B	986	GLY	2.9
1	B	1770	ASP	2.9
1	D	1115	MET	2.9
1	D	1419	GLY	2.9
1	A	1121	PRO	2.9
1	B	1442	LEU	2.9
1	B	1571	LEU	2.9
1	B	1664	LEU	2.9
1	D	1265	LEU	2.9
1	A	1348	LYS	2.9
1	C	1348	LYS	2.9
1	A	2692	ARG	2.9
1	D	1554	VAL	2.9
1	C	1484	CYS	2.9
1	D	2545	CYS	2.9
1	C	1185	ILE	2.9
1	D	1405	ILE	2.9
1	A	2683	THR	2.9
1	B	1638	THR	2.9
1	C	1420	SER	2.9
1	D	1005	SER	2.9
1	D	2630	SER	2.9
1	D	2718	GLU	2.9
1	A	1669	ASP	2.9
1	A	1770	ASP	2.9
1	A	2410	ASN	2.9
1	A	1417	LEU	2.9
1	A	2544	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	2731	ALA	2.9
1	B	1925	PHE	2.9
1	C	1010	PHE	2.9
1	B	1667	ARG	2.9
1	B	2576	ARG	2.9
1	C	1074	ARG	2.9
1	D	1013	ALA	2.9
1	A	2137	GLU	2.9
1	A	2392	GLU	2.9
1	B	2173	THR	2.9
1	D	1691	THR	2.9
1	A	1374	ASP	2.9
1	A	1421	ASN	2.9
1	A	1780	SER	2.9
1	A	2630	SER	2.9
1	B	1611	TYR	2.9
1	C	987	TYR	2.9
1	D	2223	TYR	2.9
1	D	971	PRO	2.9
1	D	1121	PRO	2.9
1	B	1303	ARG	2.9
1	D	1054	ARG	2.9
1	A	2649	PHE	2.9
1	B	1402	ALA	2.9
1	B	2224	ALA	2.9
1	D	2549	GLN	2.9
1	D	2732	LEU	2.9
1	A	1187	TRP	2.9
1	D	965	VAL	2.9
1	B	2545	CYS	2.9
1	D	1256	CYS	2.9
1	A	2616	ILE	2.9
1	B	1403	THR	2.9
1	C	1180	THR	2.9
1	A	978	SER	2.8
1	B	1210	ASP	2.9
1	D	1252	SER	2.8
1	D	1421	ASN	2.9
1	D	2717	ASP	2.9
1	A	1308	LYS	2.8
1	D	1768	ARG	2.8
1	A	2117	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	1578	ALA	2.8
1	D	2693	PHE	2.8
1	C	1116	THR	2.8
1	C	1477	ILE	2.8
1	D	1548	CYS	2.8
1	A	1490	ASP	2.8
1	A	2287	ASP	2.8
1	A	2063	SER	2.8
1	B	1441	ARG	2.8
1	C	978	SER	2.8
1	D	1693	GLY	2.8
1	A	2647	HIS	2.8
1	B	1317	TYR	2.8
1	B	1460	LEU	2.8
1	B	1703	LEU	2.8
1	B	2412	LEU	2.8
1	A	1578	ALA	2.8
1	B	2544	ALA	2.8
1	C	1052	PHE	2.8
1	D	1425	ALA	2.8
1	D	2798	GLU	2.8
1	B	1379	VAL	2.8
1	C	1441	ARG	2.8
1	C	2545	CYS	2.8
1	C	2751	ARG	2.8
1	D	1181	CYS	2.8
1	B	1048	ASP	2.8
1	D	1984	ASP	2.8
1	B	1628	GLY	2.8
1	A	1150	TYR	2.8
1	A	2374	LEU	2.8
1	B	998	LEU	2.8
1	B	1189	LYS	2.8
1	D	1482	MET	2.8
1	A	2363	VAL	2.8
1	B	1330	VAL	2.8
1	B	2660	VAL	2.8
1	D	1788	VAL	2.8
1	B	1180	THR	2.8
1	B	1861	THR	2.8
1	D	1007	THR	2.8
1	A	2797	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	2325	ASN	2.8
1	D	2725	ASP	2.8
1	A	2192	GLN	2.8
1	A	2344	GLY	2.8
1	B	1255	SER	2.8
1	B	1310	SER	2.8
1	B	1313	PRO	2.8
1	A	1383	LEU	2.8
1	B	1344	LEU	2.8
1	B	2716	LEU	2.8
1	A	2384	ALA	2.8
1	B	1478	ALA	2.8
1	B	2713	ALA	2.8
1	C	2472	MET	2.8
1	D	2530	MET	2.8
1	D	1427	ARG	2.8
1	A	1437	VAL	2.8
1	A	2650	VAL	2.8
1	B	1450	VAL	2.8
1	C	1309	HIS	2.7
1	A	1776	THR	2.7
1	B	989	ILE	2.7
1	D	1048	ASP	2.7
1	D	1290	ILE	2.7
1	A	1701	GLN	2.7
1	D	1650	ASP	2.7
1	B	1479	GLY	2.7
1	D	2051	GLY	2.7
1	A	1431	CYS	2.7
1	B	1481	PRO	2.7
1	A	1302	LEU	2.7
1	C	1319	LEU	2.7
1	D	1302	LEU	2.7
1	A	1358	ALA	2.7
1	A	975	VAL	2.7
1	B	1036	VAL	2.7
1	B	1437	VAL	2.7
1	B	2572	VAL	2.7
1	A	2455	GLN	2.7
1	A	989	ILE	2.7
1	B	1414	ILE	2.7
1	D	2714	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1326	GLY	2.7
1	A	2086	GLY	2.7
1	B	1252	SER	2.7
1	C	1046	SER	2.7
1	B	1187	TRP	2.7
1	C	2529	LYS	2.7
1	B	1404	MET	2.7
1	B	1673	MET	2.7
1	C	1370	ALA	2.7
1	A	1483	HIS	2.7
1	A	2632	HIS	2.7
1	A	2196	PHE	2.7
1	B	1138	PHE	2.7
1	B	964	VAL	2.7
1	D	2650	VAL	2.7
1	A	2232	ASP	2.7
1	A	2717	ASP	2.7
1	C	1522	ASP	2.7
1	A	2551	ILE	2.7
1	B	2041	GLY	2.7
1	D	2607	GLY	2.7
1	A	1268	PRO	2.7
1	A	2657	SER	2.7
1	B	978	SER	2.7
1	B	1331	SER	2.7
1	C	1012	ARG	2.7
1	D	2708	ARG	2.7
1	A	1129	LEU	2.7
1	A	1148	LEU	2.7
1	A	1540	LEU	2.7
1	C	1302	LEU	2.7
1	C	1417	LEU	2.7
1	A	2721	ALA	2.7
1	D	2543	GLN	2.7
1	D	2729	GLN	2.7
1	D	1010	PHE	2.7
1	A	2113	VAL	2.7
1	A	1347	THR	2.7
1	A	2656	ASP	2.7
1	B	1490	ASP	2.7
1	C	1440	VAL	2.7
1	C	1554	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	1172	VAL	2.7
1	C	1189	LYS	2.7
1	C	1702	THR	2.7
1	D	1257	ASN	2.7
1	D	1316	LYS	2.7
1	D	1424	THR	2.7
1	D	2232	ASP	2.7
1	A	1461	GLU	2.7
1	A	2642	GLU	2.7
1	D	1754	GLU	2.7
1	D	2137	GLU	2.7
1	D	2646	THR	2.7
1	D	2748	GLU	2.7
1	A	1585	ILE	2.7
1	B	1847	ILE	2.7
1	B	2749	GLY	2.7
1	C	1479	GLY	2.7
1	C	1186	LEU	2.7
1	A	1315	HIS	2.6
1	B	2632	HIS	2.6
1	A	1314	ALA	2.6
1	D	2681	GLN	2.6
1	A	1010	PHE	2.6
1	A	2529	LYS	2.6
1	D	1308	LYS	2.6
1	A	1362	GLU	2.6
1	A	1774	VAL	2.6
1	A	1873	ASN	2.6
1	B	1459	VAL	2.6
1	A	2138	THR	2.6
1	A	1441	ARG	2.6
1	A	1477	ILE	2.6
1	A	1570	ILE	2.6
1	A	2521	ILE	2.6
1	A	2769	GLY	2.6
1	B	2691	ARG	2.6
1	A	2750	SER	2.6
1	B	1434	SER	2.6
1	B	1780	SER	2.6
1	C	1494	SER	2.6
1	D	1046	SER	2.6
1	A	2404	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	2435	LEU	2.6
1	B	1874	LEU	2.6
1	B	1916	LEU	2.6
1	D	1129	LEU	2.6
1	D	1460	LEU	2.6
1	B	1701	GLN	2.6
1	B	981	LYS	2.6
1	A	1317	TYR	2.6
1	A	1480	ARG	2.6
1	B	1398	TYR	2.6
1	D	1432	ASP	2.6
1	D	2745	ASP	2.6
1	B	2751	ARG	2.6
1	D	1480	ARG	2.6
1	A	999	VAL	2.6
1	A	1375	GLY	2.6
1	B	1360	THR	2.6
1	C	1036	VAL	2.6
1	D	967	THR	2.6
1	D	1151	THR	2.6
1	D	2609	VAL	2.6
1	D	2675	VAL	2.6
1	A	1046	SER	2.6
1	A	1856	ILE	2.6
1	B	1433	SER	2.6
1	C	1604	ILE	2.6
1	D	1492	SER	2.6
1	A	2724	LEU	2.6
1	C	1407	LYS	2.6
1	B	1461	GLU	2.6
1	B	1754	GLU	2.6
1	C	1480	ARG	2.6
1	C	1770	ASP	2.6
1	A	1379	VAL	2.6
1	A	1398	TYR	2.6
1	A	2205	VAL	2.6
1	B	1416	THR	2.6
1	B	2764	THR	2.6
1	B	2767	VAL	2.6
1	C	1341	VAL	2.6
1	C	1347	THR	2.6
1	D	1565	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1413	ILE	2.6
1	D	2616	ILE	2.6
1	C	1315	HIS	2.6
1	A	1551	LYS	2.6
1	A	972	LEU	2.6
1	A	1529	LEU	2.6
1	D	2546	GLU	2.6
1	D	2583	GLU	2.6
1	A	1181	CYS	2.6
1	D	2608	ARG	2.6
1	B	1260	ALA	2.6
1	C	1358	ALA	2.6
1	D	2544	ALA	2.6
1	A	1944	ASP	2.6
1	C	2797	ASN	2.6
1	A	1116	THR	2.6
1	A	2433	PHE	2.6
1	B	1176	PHE	2.6
1	B	1284	PHE	2.6
1	B	1702	THR	2.6
1	D	970	THR	2.6
1	D	1142	PHE	2.6
1	A	1414	ILE	2.6
1	A	1430	SER	2.6
1	B	1125	ILE	2.6
1	D	978	SER	2.6
1	D	2613	ILE	2.6
1	D	2707	ILE	2.6
1	C	998	LEU	2.5
1	C	1754	GLU	2.5
1	D	1301	GLU	2.5
1	D	2220	LEU	2.5
1	A	1200	ASP	2.5
1	A	1984	ASP	2.5
1	A	2101	ASP	2.5
1	B	1311	ASN	2.5
1	B	2195	MET	2.5
1	D	2255	ASP	2.5
1	A	2694	THR	2.5
1	B	967	THR	2.5
1	D	1313	PRO	2.5
1	A	1357	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1407	LYS	2.5
1	A	1420	SER	2.5
1	B	957	VAL	2.5
1	A	1604	ILE	2.5
1	C	2519	SER	2.5
1	D	1145	SER	2.5
1	A	2633	TYR	2.5
1	C	2455	GLN	2.5
1	A	998	LEU	2.5
1	A	1265	LEU	2.5
1	B	1457	LEU	2.5
1	D	1778	LEU	2.5
1	C	2530	MET	2.5
1	D	1453	MET	2.5
1	A	1332	ASP	2.5
1	B	1682	ASN	2.5
1	C	1200	ASP	2.5
1	A	2636	LYS	2.5
1	B	1887	LYS	2.5
1	B	2548	GLY	2.5
1	D	1292	PRO	2.5
1	A	1638	THR	2.5
1	A	2754	THR	2.5
1	C	1638	THR	2.5
1	D	988	THR	2.5
1	B	1280	PHE	2.5
1	A	1492	SER	2.5
1	A	2775	VAL	2.5
1	C	1217	VAL	2.5
1	D	1430	SER	2.5
1	A	2427	TYR	2.5
1	C	1872	ARG	2.5
1	C	1460	LEU	2.5
1	D	1266	LEU	2.5
1	D	2794	LEU	2.5
1	A	2530	MET	2.5
1	B	993	ASP	2.5
1	C	1308	LYS	2.5
1	D	1218	LYS	2.5
1	D	1276	ASP	2.5
1	D	2742	LYS	2.5
1	A	969	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1047	CYS	2.5
1	B	1361	GLY	2.5
1	C	1253	CYS	2.5
1	A	1702	THR	2.5
1	B	1034	THR	2.5
1	B	1885	THR	2.5
1	B	2454	THR	2.5
1	D	1702	THR	2.5
1	A	2693	PHE	2.5
1	B	1152	PHE	2.5
1	C	1269	VAL	2.5
1	C	1433	SER	2.5
1	D	1138	PHE	2.5
1	A	2679	VAL	2.5
1	B	1391	VAL	2.5
1	C	1437	VAL	2.5
1	D	1587	ILE	2.5
1	D	2670	VAL	2.5
1	D	2753	TRP	2.5
1	B	1339	TYR	2.5
1	C	1703	LEU	2.5
1	A	1140	LYS	2.5
1	B	1308	LYS	2.5
1	D	1189	LYS	2.5
1	A	1762	ASP	2.5
1	B	1312	ASN	2.5
1	A	1824	ALA	2.5
1	D	1128	HIS	2.5
1	D	1545	ALA	2.5
1	A	2085	GLY	2.5
1	A	1548	CYS	2.4
1	A	2247	ARG	2.4
1	D	1179	GLU	2.4
1	D	2642	GLU	2.4
1	A	2654	SER	2.4
1	B	2519	SER	2.4
1	A	1299	ILE	2.4
1	A	2437	ILE	2.4
1	B	2436	VAL	2.4
1	B	2522	ILE	2.4
1	B	2652	ILE	2.4
1	C	1379	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	2521	ILE	2.4
1	D	1058	VAL	2.4
1	D	1321	VAL	2.4
1	D	2326	VAL	2.4
1	C	1187	TRP	2.4
1	A	1344	LEU	2.4
1	B	2518	LEU	2.4
1	C	1344	LEU	2.4
1	D	1344	LEU	2.4
1	B	2584	LYS	2.4
1	C	1404	MET	2.4
1	C	1551	LYS	2.4
1	C	2501	LYS	2.4
1	A	1285	ASN	2.4
1	B	1027	ASN	2.4
1	C	1048	ASP	2.4
1	D	1790	ASP	2.4
1	A	2517	GLN	2.4
1	A	1313	PRO	2.4
1	C	1427	ARG	2.4
1	D	1268	PRO	2.4
1	D	1370	ALA	2.4
1	B	1161	GLY	2.4
1	B	1282	GLY	2.4
1	B	1333	THR	2.4
1	B	2665	THR	2.4
1	D	2454	THR	2.4
1	B	1004	SER	2.4
1	B	1354	SER	2.4
1	A	1847	ILE	2.4
1	A	2134	ILE	2.4
1	A	2360	VAL	2.4
1	B	1052	PHE	2.4
1	B	1464	VAL	2.4
1	B	2551	ILE	2.4
1	B	2501	LYS	2.4
1	D	2291	LYS	2.4
1	A	1115	MET	2.4
1	B	1243	MET	2.4
1	B	1259	LEU	2.4
1	A	1458	TYR	2.4
1	A	2193	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	2632	HIS	2.4
1	B	1018	GLN	2.4
1	C	1371	ARG	2.4
1	C	1490	ASP	2.4
1	C	1701	GLN	2.4
1	D	1485	GLN	2.4
1	D	1770	ASP	2.4
1	D	2687	ASN	2.4
1	D	2780	GLN	2.4
1	A	1292	PRO	2.4
1	A	2570	GLY	2.4
1	B	1277	GLY	2.4
1	D	2111	GLY	2.4
1	B	2646	THR	2.4
1	D	1861	THR	2.4
1	A	1438	SER	2.4
1	B	1183	SER	2.4
1	B	1430	SER	2.4
1	C	1252	SER	2.4
1	A	1316	LYS	2.4
1	A	2126	PHE	2.4
1	A	2627	VAL	2.4
1	B	996	PHE	2.4
1	D	1857	LYS	2.4
1	D	2758	LYS	2.4
1	B	1400	VAL	2.4
1	D	2436	VAL	2.4
1	A	1130	MET	2.4
1	B	1300	LEU	2.4
1	B	992	GLN	2.4
1	B	1643	TYR	2.4
1	C	1483	HIS	2.4
1	C	2689	ARG	2.4
1	D	1317	TYR	2.4
1	A	2745	ASP	2.4
1	C	2325	ASN	2.4
1	B	1003	GLY	2.4
1	B	1561	GLY	2.4
1	B	2111	GLY	2.4
1	C	1003	GLY	2.4
1	D	1359	GLY	2.4
1	D	1497	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	2667	GLY	2.4
1	A	981	LYS	2.4
1	C	2173	THR	2.4
1	D	2701	SER	2.4
1	A	2150	ILE	2.4
1	A	2581	ILE	2.4
1	A	2613	ILE	2.4
1	B	1579	VAL	2.4
1	C	1822	VAL	2.4
1	D	1856	ILE	2.4
1	D	2135	ILE	2.4
1	A	2518	LEU	2.4
1	B	2762	LEU	2.4
1	D	2724	LEU	2.4
1	B	2197	ARG	2.4
1	D	2647	HIS	2.4
1	A	2780	GLN	2.4
1	B	2391	GLU	2.4
1	B	1651	ASN	2.3
1	C	2255	ASP	2.3
1	D	1339	TYR	2.3
1	D	2325	ASN	2.3
1	A	971	PRO	2.3
1	A	994	GLY	2.3
1	A	2078	LYS	2.3
1	A	2411	GLY	2.3
1	B	1488	GLY	2.3
1	A	2317	ALA	2.3
1	A	2663	ALA	2.3
1	B	1497	ALA	2.3
1	A	2715	THR	2.3
1	D	1830	THR	2.3
1	D	2754	THR	2.3
1	A	2389	SER	2.3
1	B	2367	SER	2.3
1	D	2666	SER	2.3
1	A	1426	VAL	2.3
1	A	1788	VAL	2.3
1	A	2675	VAL	2.3
1	B	1217	VAL	2.3
1	B	1238	VAL	2.3
1	B	1595	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2521	ILE	2.3
1	D	2126	PHE	2.3
1	D	2134	ILE	2.3
1	D	2723	VAL	2.3
1	D	1441	ARG	2.3
1	A	2040	LEU	2.3
1	A	2082	LEU	2.3
1	A	2684	LEU	2.3
1	B	1319	LEU	2.3
1	B	2796	GLN	2.3
1	C	1362	GLU	2.3
1	B	1845	ASN	2.3
1	C	1669	ASP	2.3
1	A	1264	LYS	2.3
1	A	1339	TYR	2.3
1	A	1394	TYR	2.3
1	B	1026	TRP	2.3
1	B	1126	LYS	2.3
1	C	971	PRO	2.3
1	C	1126	LYS	2.3
1	D	1201	PRO	2.3
1	D	2709	TYR	2.3
1	D	1346	GLY	2.3
1	A	2785	ALA	2.3
1	A	1384	MET	2.3
1	A	1403	THR	2.3
1	B	988	THR	2.3
1	C	1034	THR	2.3
1	B	2630	SER	2.3
1	D	1494	SER	2.3
1	B	1074	ARG	2.3
1	A	2696	ILE	2.3
1	D	1604	ILE	2.3
1	A	1117	GLN	2.3
1	A	2609	VAL	2.3
1	A	2796	GLN	2.3
1	C	2109	GLU	2.3
1	C	2565	PHE	2.3
1	D	1174	VAL	2.3
1	A	1266	LEU	2.3
1	A	1396	LEU	2.3
1	A	1457	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1571	LEU	2.3
1	D	2662	LEU	2.3
1	B	2255	ASP	2.3
1	C	981	LYS	2.3
1	C	1123	ASN	2.3
1	C	1547	ASP	2.3
1	D	1304	ASN	2.3
1	A	1445	PRO	2.3
1	A	1543	GLY	2.3
1	A	2165	TYR	2.3
1	B	1160	TYR	2.3
1	B	2085	GLY	2.3
1	C	2223	TYR	2.3
1	D	2548	GLY	2.3
1	A	2316	ARG	2.3
1	B	1118	SER	2.3
1	C	1768	ARG	2.3
1	D	1294	ARG	2.3
1	D	2029	SER	2.3
1	D	2654	SER	2.3
1	D	1483	HIS	2.3
1	A	2543	GLN	2.3
1	D	2796	GLN	2.3
1	A	1060	ILE	2.3
1	D	1761	ILE	2.3
1	B	1029	PHE	2.3
1	D	2767	VAL	2.3
1	A	1008	LEU	2.3
1	A	2447	LEU	2.3
1	B	1540	LEU	2.3
1	B	1696	LYS	2.3
1	B	2758	LYS	2.3
1	C	1316	LYS	2.3
1	D	1757	LYS	2.3
1	C	1548	CYS	2.3
1	A	1070	ASP	2.3
1	B	1553	ASP	2.3
1	C	1276	ASP	2.3
1	C	1277	GLY	2.3
1	D	2085	GLY	2.3
1	A	1402	ALA	2.3
1	C	1824	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	2202	TRP	2.3
1	C	2544	ALA	2.3
1	C	2713	ALA	2.3
1	D	2197	ARG	2.3
1	A	1830	THR	2.3
1	B	1686	THR	2.3
1	A	1385	SER	2.3
1	B	1301	GLU	2.3
1	B	1946	GLN	2.3
1	A	1465	ILE	2.3
1	A	2132	LYS	2.3
1	B	1059	ILE	2.3
1	B	2581	ILE	2.3
1	C	1856	ILE	2.3
1	C	2584	LYS	2.3
1	A	1798	LEU	2.2
1	A	2659	LEU	2.2
1	B	1281	VAL	2.3
1	B	1328	LEU	2.2
1	B	1875	LEU	2.2
1	C	965	VAL	2.3
1	C	1778	LEU	2.2
1	D	1324	VAL	2.3
1	D	1357	VAL	2.3
1	D	1822	VAL	2.3
1	D	2539	LEU	2.2
1	D	2698	PHE	2.2
1	A	1311	ASN	2.2
1	B	1200	ASP	2.2
1	D	2506	ASP	2.2
1	D	1445	PRO	2.2
1	D	2139	PRO	2.2
1	A	1247	ARG	2.2
1	A	1768	ARG	2.2
1	B	1346	GLY	2.2
1	B	1953	MET	2.2
1	C	986	GLY	2.2
1	D	1928	ARG	2.2
1	D	2765	GLY	2.2
1	A	2349	TYR	2.2
1	D	2727	ALA	2.2
1	A	2792	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1116	THR	2.2
1	C	1018	GLN	2.2
1	C	1297	THR	2.2
1	C	1438	SER	2.2
1	C	1485	GLN	2.2
1	C	2646	THR	2.2
1	D	990	THR	2.2
1	D	1116	THR	2.2
1	D	1776	THR	2.2
1	D	2173	THR	2.2
1	D	2552	THR	2.2
1	D	2783	GLU	2.2
1	C	1094	SER	2.2
1	C	1183	SER	2.2
1	C	2389	SER	2.2
1	D	2673	SER	2.2
1	D	2340	LYS	2.2
1	A	1275	ILE	2.2
1	A	2414	ILE	2.2
1	B	1242	ILE	2.2
1	C	2131	ILE	2.2
1	D	2522	ILE	2.2
1	A	1174	VAL	2.2
1	A	1703	LEU	2.2
1	A	2142	VAL	2.2
1	B	1324	VAL	2.2
1	B	2711	LEU	2.2
1	C	996	PHE	2.2
1	D	1131	VAL	2.2
1	D	1474	VAL	2.2
1	A	1552	ASN	2.2
1	B	1263	ASN	2.2
1	D	1944	ASP	2.2
1	A	1020	ARG	2.2
1	A	1201	PRO	2.2
1	B	1012	ARG	2.2
1	B	1467	ARG	2.2
1	C	1032	MET	2.2
1	C	1121	PRO	2.2
1	A	2041	GLY	2.2
1	B	1355	GLU	2.2
1	B	2583	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2642	GLU	2.2
1	B	1485	GLN	2.2
1	A	1034	THR	2.2
1	A	1297	THR	2.2
1	B	1446	THR	2.2
1	B	1626	ALA	2.2
1	C	1578	ALA	2.2
1	D	1402	ALA	2.2
1	D	1478	ALA	2.2
1	D	2663	ALA	2.2
1	A	1004	SER	2.2
1	C	1492	SER	2.2
1	C	1818	SER	2.2
1	D	1250	SER	2.2
1	A	1114	ILE	2.2
1	B	1518	ILE	2.2
1	C	1060	ILE	2.2
1	A	1279	LEU	2.2
1	A	1300	LEU	2.2
1	A	1516	LEU	2.2
1	D	1529	LEU	2.2
1	D	2761	LEU	2.2
1	A	1058	VAL	2.2
1	A	1869	VAL	2.2
1	B	1269	VAL	2.2
1	B	1399	PHE	2.2
1	A	1447	ASP	2.2
1	A	2747	ARG	2.2
1	B	1374	ASP	2.2
1	D	1337	ARG	2.2
1	D	1762	ASP	2.2
1	D	2656	ASP	2.2
1	A	986	GLY	2.2
1	B	974	GLY	2.2
1	A	1945	LYS	2.2
1	B	1340	LYS	2.2
1	B	1894	LYS	2.2
1	B	2543	GLN	2.2
1	C	992	GLN	2.2
1	D	2078	LYS	2.2
1	A	1478	ALA	2.2
1	A	1783	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2227	THR	2.2
1	B	2654	SER	2.2
1	B	2666	SER	2.2
1	D	1354	SER	2.2
1	D	1968	SER	2.2
1	D	2054	SER	2.2
1	D	2540	THR	2.2
1	B	2773	TYR	2.2
1	A	2104	ILE	2.2
1	B	1516	LEU	2.2
1	B	1888	ILE	2.2
1	C	1383	LEU	2.2
1	C	1526	ILE	2.2
1	D	1476	ILE	2.2
1	A	2146	ARG	2.2
1	D	2659	LEU	2.2
1	A	2660	VAL	2.2
1	B	1357	VAL	2.2
1	B	1432	ASP	2.2
1	B	1555	ASN	2.2
1	B	1563	ASP	2.2
1	B	1656	VAL	2.2
1	B	2530	MET	2.2
1	C	1070	ASP	2.2
1	C	1650	ASP	2.2
1	D	1070	ASP	2.2
1	B	1268	PRO	2.2
1	A	1887	LYS	2.2
1	C	1757	LYS	2.2
1	D	1305	LYS	2.2
1	A	1485	GLN	2.2
1	A	2043	GLY	2.2
1	A	2653	GLY	2.2
1	C	1230	GLN	2.2
1	C	1359	GLY	2.2
1	C	1364	CYS	2.2
1	A	1298	SER	2.2
1	A	2564	ALA	2.2
1	B	1575	SER	2.2
1	C	1403	THR	2.2
1	C	1478	ALA	2.2
1	D	1760	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2774	TYR	2.1
1	D	2527	ARG	2.1
1	D	2795	ARG	2.1
1	A	2577	LEU	2.1
1	B	1129	LEU	2.1
1	B	2613	ILE	2.1
1	B	2662	LEU	2.1
1	C	1265	LEU	2.1
1	C	1465	ILE	2.1
1	D	1242	ILE	2.1
1	D	1299	ILE	2.1
1	D	1300	LEU	2.1
1	D	1763	ILE	2.1
1	D	1814	ILE	2.1
1	D	2595	ILE	2.1
1	D	1026	TRP	2.1
1	A	1432	ASP	2.1
1	A	1440	VAL	2.1
1	A	1454	ASP	2.1
1	A	2143	ASP	2.1
1	A	2255	ASP	2.1
1	A	2723	VAL	2.1
1	B	1408	VAL	2.1
1	B	1568	ASP	2.1
1	B	1873	ASN	2.1
1	D	1379	VAL	2.1
1	D	1437	VAL	2.1
1	D	1781	VAL	2.1
1	A	1443	GLU	2.1
1	B	1551	LYS	2.1
1	D	1029	PHE	2.1
1	D	1126	LYS	2.1
1	A	2141	PRO	2.1
1	C	2796	GLN	2.1
1	A	1390	ALA	2.1
1	A	1416	THR	2.1
1	A	1497	ALA	2.1
1	A	2367	SER	2.1
1	B	1151	THR	2.1
1	B	1298	SER	2.1
1	B	1438	SER	2.1
1	D	1750	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2527	ARG	2.1
1	A	1329	TYR	2.1
1	A	2385	MET	2.1
1	A	2584	LYS	2.1
1	D	1060	ILE	2.1
1	D	1113	ILE	2.1
1	D	1140	LYS	2.1
1	D	2551	ILE	2.1
1	A	1436	ASP	2.1
1	B	1011	GLU	2.1
1	B	1447	ASP	2.1
1	B	2287	ASP	2.1
1	C	1443	GLU	2.1
1	C	2798	GLU	2.1
1	D	1443	GLU	2.1
1	D	1890	ASP	2.1
1	D	2109	GLU	2.1
1	D	2287	ASP	2.1
1	D	2629	ASN	2.1
1	A	1356	VAL	2.1
1	A	1734	HIS	2.1
1	B	1164	VAL	2.1
1	B	1554	VAL	2.1
1	B	1666	VAL	2.1
1	B	2269	VAL	2.1
1	A	996	PHE	2.1
1	B	1903	GLN	2.1
1	C	1029	PHE	2.1
1	D	2107	PHE	2.1
1	A	2266	GLY	2.1
1	A	1007	THR	2.1
1	A	2251	ARG	2.1
1	B	1256	CYS	2.1
1	B	1675	ARG	2.1
1	A	2369	SER	2.1
1	A	2373	SER	2.1
1	B	2042	THR	2.1
1	C	1360	THR	2.1
1	C	2454	THR	2.1
1	D	1297	THR	2.1
1	D	1780	SER	2.1
1	D	1936	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1857	LYS	2.1
1	A	1859	LYS	2.1
1	A	2758	LYS	2.1
1	B	1407	LYS	2.1
1	C	1945	LYS	2.1
1	D	2501	LYS	2.1
1	A	2539	LEU	2.1
1	B	1110	LEU	2.1
1	B	1302	LEU	2.1
1	B	1362	GLU	2.1
1	B	2546	GLU	2.1
1	B	2761	LEU	2.1
1	C	1369	GLU	2.1
1	C	1396	LEU	2.1
1	D	1362	GLU	2.1
1	A	1276	ASP	2.1
1	A	1845	ASN	2.1
1	A	2096	ILE	2.1
1	B	1056	ASP	2.1
1	B	1454	ASP	2.1
1	B	1589	ASP	2.1
1	C	1762	ASP	2.1
1	C	1890	ASP	2.1
1	D	1526	ILE	2.1
1	B	1139	GLN	2.1
1	B	2578	HIS	2.1
1	D	1734	HIS	2.1
1	D	1903	GLN	2.1
1	C	1324	VAL	2.1
1	D	1341	VAL	2.1
1	D	2775	VAL	2.1
1	A	1026	TRP	2.1
1	A	1138	PHE	2.1
1	D	2047	PHE	2.1
1	D	1326	GLY	2.1
1	A	1012	ARG	2.1
1	B	2247	ARG	2.1
1	A	1343	SER	2.1
1	B	1145	SER	2.1
1	B	1511	SER	2.1
1	B	2712	THR	2.1
1	C	2665	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	2678	THR	2.1
1	A	2606	LYS	2.1
1	C	1260	ALA	2.1
1	C	2585	ALA	2.1
1	D	2606	LYS	2.1
1	B	2200	MET	2.1
1	A	1179	GLU	2.1
1	D	1123	ASN	2.1
1	D	1353	ASN	2.1
1	D	2561	HIS	2.1
1	B	1060	ILE	2.1
1	B	1275	ILE	2.1
1	C	1593	ILE	2.1
1	C	2150	ILE	2.1
1	C	2551	ILE	2.1
1	D	1465	ILE	2.1
1	D	2521	ILE	2.1
1	A	987	TYR	2.1
1	A	2526	PRO	2.1
1	C	1292	PRO	2.1
1	B	975	VAL	2.1
1	B	1058	VAL	2.1
1	D	1217	VAL	2.1
1	D	1440	VAL	2.1
1	D	1464	VAL	2.1
1	D	1741	VAL	2.1
1	A	2756	GLY	2.1
1	B	1639	GLY	2.1
1	B	2126	PHE	2.1
1	C	2769	GLY	2.1
1	D	2043	GLY	2.1
1	D	2433	PHE	2.1
1	D	991	ARG	2.1
1	D	1074	ARG	2.1
1	D	1325	SER	2.0
1	D	1333	THR	2.0
1	D	2226	THR	2.0
1	C	1011	GLU	2.0
1	C	2299	CYS	2.0
1	C	2321	ALA	2.0
1	D	1783	ALA	2.0
1	B	1789	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1024	LEU	2.0
1	A	1965	LEU	2.0
1	B	1265	LEU	2.0
1	C	1541	LEU	2.0
1	D	1008	LEU	2.0
1	D	1332	ASP	2.0
1	D	1392	ASP	2.0
1	D	2030	ASP	2.0
1	D	2797	ASN	2.0
1	B	1877	ILE	2.0
1	C	1414	ILE	2.0
1	D	1468	ILE	2.0
1	B	1674	PRO	2.0
1	D	1025	PRO	2.0
1	B	1517	TYR	2.0
1	C	1458	TYR	2.0
1	A	1127	VAL	2.0
1	A	2778	VAL	2.0
1	B	1387	ARG	2.0
1	B	1623	VAL	2.0
1	B	1774	VAL	2.0
1	B	1781	VAL	2.0
1	B	1928	ARG	2.0
1	C	2582	ARG	2.0
1	D	1579	VAL	2.0
1	D	2778	VAL	2.0
1	A	1871	GLY	2.0
1	B	1206	GLY	2.0
1	D	1373	GLY	2.0
1	B	1608	PHE	2.0
1	B	1924	PHE	2.0
1	A	1218	LYS	2.0
1	C	2324	TRP	2.0
1	A	1966	GLU	2.0
1	B	1830	THR	2.0
1	B	1968	SER	2.0
1	B	2226	THR	2.0
1	B	2370	GLU	2.0
1	C	2370	GLU	2.0
1	D	966	THR	2.0
1	D	1298	SER	2.0
1	D	1355	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	2626	SER	2.0
1	D	2655	ALA	2.0
1	A	1472	HIS	2.0
1	A	2089	CYS	2.0
1	B	1117	GLN	2.0
1	D	1410	GLN	2.0
1	D	1789	GLN	2.0
1	A	1874	LEU	2.0
1	A	2658	ASP	2.0
1	A	2762	LEU	2.0
1	B	2659	LEU	2.0
1	C	1035	LEU	2.0
1	D	1605	LEU	2.0
1	D	2412	LEU	2.0
1	B	1768	ARG	2.0
1	C	2523	PRO	2.0
1	D	1275	ILE	2.0
1	D	2581	ILE	2.0
1	B	1600	LYS	2.0
1	B	1967	LYS	2.0
1	B	2720	LYS	2.0
1	C	1967	LYS	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	MAN	E	6	11/12	0.09	0.20	182,185,186,186	0
2	MAN	E	8	11/12	0.26	0.21	175,176,176,176	0
2	MAN	E	7	11/12	0.28	0.17	172,175,175,176	0
2	MAN	W	8	11/12	0.33	0.19	137,141,146,147	0
2	MAN	K	7	11/12	0.34	0.18	117,122,127,129	0
3	NAG	N	2	14/15	0.38	0.20	128,132,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	W	7	11/12	0.39	0.17	120,124,130,133	0
2	MAN	Q	7	11/12	0.44	0.18	103,109,113,113	0
2	MAN	W	6	11/12	0.47	0.18	114,116,119,120	0
3	NAG	Y	2	14/15	0.56	0.20	111,114,116,117	0
2	MAN	Q	8	11/12	0.58	0.15	116,119,122,122	0
3	NAG	O	2	14/15	0.58	0.17	104,107,110,111	0
3	NAG	T	2	14/15	0.58	0.16	91,94,97,98	0
2	MAN	K	8	11/12	0.58	0.15	132,135,139,140	0
2	MAN	K	6	11/12	0.59	0.17	118,121,123,123	0
3	NAG	Z	2	14/15	0.60	0.15	100,107,109,110	0
3	NAG	U	2	14/15	0.62	0.16	91,93,96,97	0
2	MAN	Q	6	11/12	0.64	0.20	92,95,98,99	0
3	NAG	G	2	14/15	0.64	0.19	110,112,117,118	0
3	NAG	F	2	14/15	0.65	0.18	91,95,100,102	0
3	NAG	H	2	14/15	0.66	0.15	104,109,113,114	0
3	NAG	S	2	14/15	0.66	0.17	93,95,97,97	0
3	NAG	L	2	14/15	0.67	0.18	119,122,127,129	0
3	NAG	J	2	14/15	0.69	0.16	93,94,97,99	0
3	NAG	M	2	14/15	0.70	0.17	103,105,108,108	0
3	NAG	I	2	14/15	0.70	0.14	104,107,112,113	0
2	MAN	E	5	11/12	0.73	0.16	173,173,176,179	0
3	NAG	P	2	14/15	0.77	0.15	86,89,92,92	0
3	NAG	X	2	14/15	0.77	0.16	93,98,103,105	0
3	NAG	L	1	14/15	0.78	0.15	106,110,112,115	0
2	NAG	E	1	14/15	0.78	0.22	109,116,126,126	0
3	NAG	R	2	14/15	0.78	0.15	85,89,92,92	0
2	MAN	W	5	11/12	0.80	0.15	100,102,107,110	0
3	NAG	V	2	14/15	0.81	0.14	72,76,79,79	0
2	MAN	E	4	11/12	0.81	0.22	164,166,168,171	0
2	BMA	E	3	11/12	0.82	0.15	156,161,165,168	0
2	MAN	K	5	11/12	0.84	0.14	104,107,111,114	0
3	NAG	I	1	14/15	0.86	0.13	82,90,96,100	0
3	NAG	F	1	14/15	0.86	0.12	77,80,84,87	0
3	NAG	J	1	14/15	0.86	0.12	78,87,93,93	0
3	NAG	X	1	14/15	0.87	0.13	83,85,88,91	0
3	NAG	N	1	14/15	0.87	0.13	100,110,116,122	0
2	MAN	K	4	11/12	0.88	0.14	96,102,107,108	0
2	BMA	Q	3	11/12	0.88	0.10	76,77,90,97	0
3	NAG	Z	1	14/15	0.88	0.12	59,77,86,92	0
3	NAG	R	1	14/15	0.88	0.12	70,73,76,81	0
3	NAG	O	1	14/15	0.89	0.12	81,90,95,99	0
2	BMA	W	3	11/12	0.89	0.12	96,99,108,114	0

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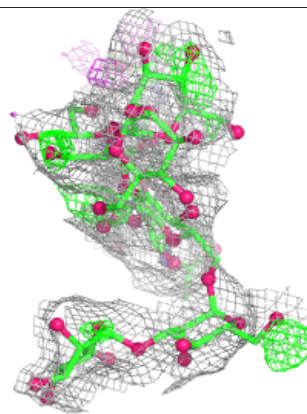
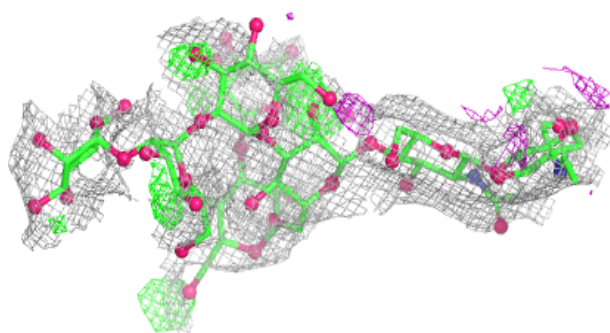
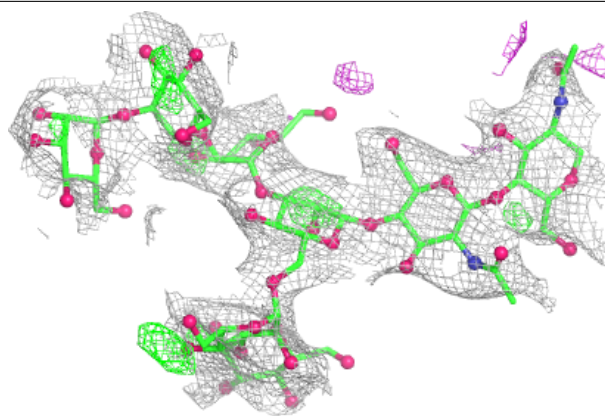
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	H	1	14/15	0.89	0.11	76,89,97,100	0
3	NAG	T	1	14/15	0.89	0.11	61,73,81,86	0
2	NAG	Q	2	14/15	0.90	0.12	61,63,67,72	0
2	BMA	K	3	11/12	0.90	0.10	92,98,106,112	0
2	MAN	Q	4	11/12	0.90	0.11	67,72,75,78	0
2	NAG	E	2	14/15	0.90	0.16	129,136,140,150	0
2	NAG	Q	1	14/15	0.91	0.12	47,52,56,57	0
3	NAG	G	1	14/15	0.91	0.14	93,96,100,105	0
3	NAG	U	1	14/15	0.91	0.10	69,79,83,86	0
2	NAG	K	1	14/15	0.91	0.13	55,63,69,70	0
2	MAN	Q	5	11/12	0.91	0.10	79,80,83,87	0
3	NAG	Y	1	14/15	0.92	0.13	96,99,103,107	0
3	NAG	S	1	14/15	0.92	0.13	79,81,85,88	0
2	NAG	W	1	14/15	0.92	0.13	67,73,78,80	0
2	MAN	W	4	11/12	0.92	0.10	87,97,101,102	0
3	NAG	V	1	14/15	0.93	0.09	46,54,58,65	0
3	NAG	M	1	14/15	0.93	0.12	91,92,96,99	0
2	NAG	W	2	14/15	0.93	0.12	83,89,93,93	0
3	NAG	P	1	14/15	0.93	0.09	69,77,80,83	0
2	NAG	K	2	14/15	0.94	0.10	72,74,78,85	0
3	NAG	a	1	14/15	-	-	87,95,102,104	0
3	NAG	a	2	14/15	-	-	107,111,116,117	0
3	NAG	b	1	14/15	-	-	89,99,102,102	0
3	NAG	b	2	14/15	-	-	96,102,107,110	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.

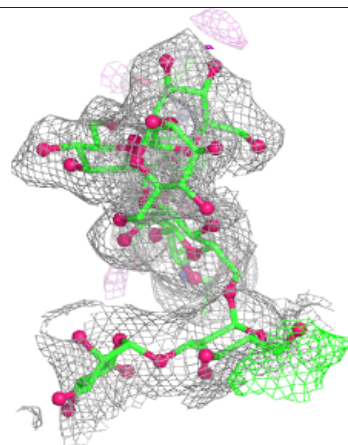
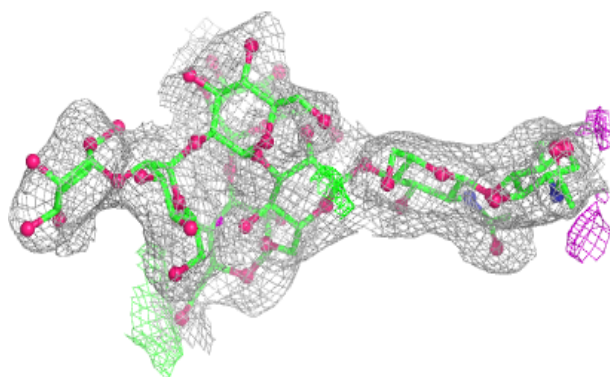
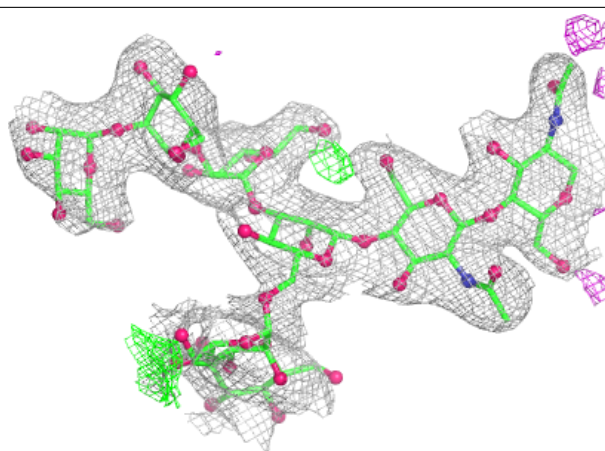
Electron density around Chain E:

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



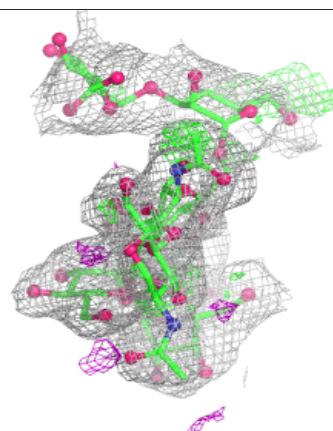
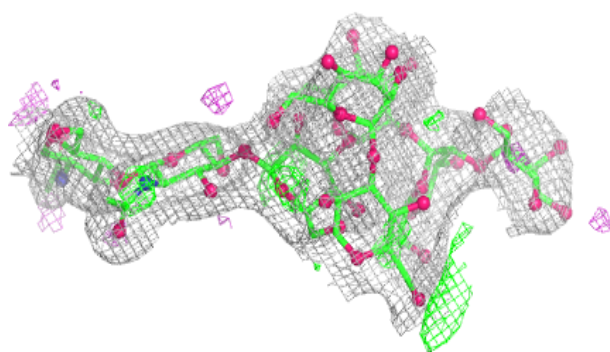
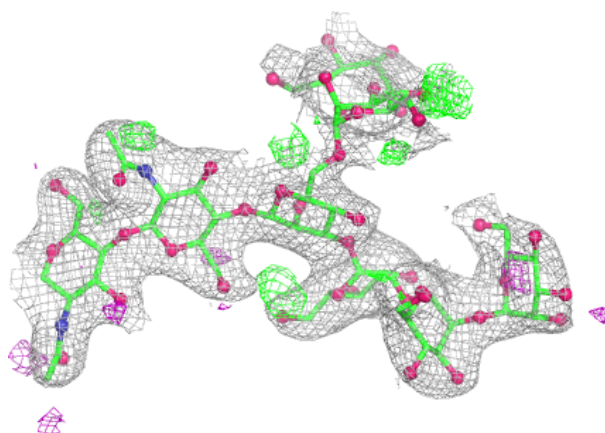
Electron density around Chain K:

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



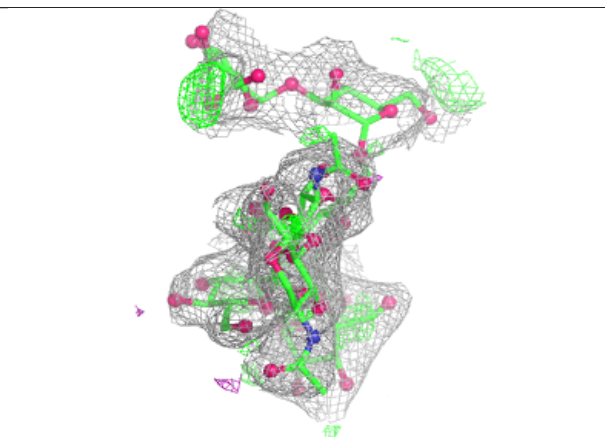
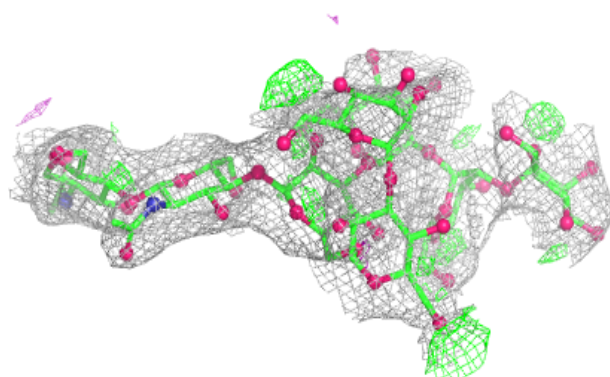
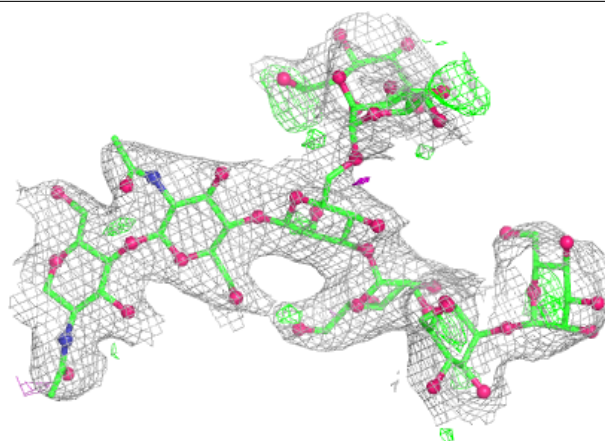
Electron density around Chain Q:

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

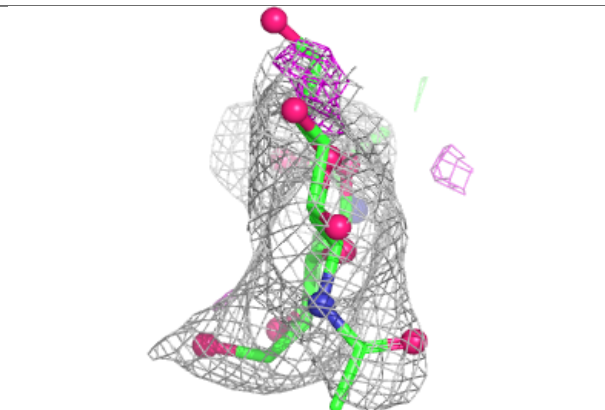
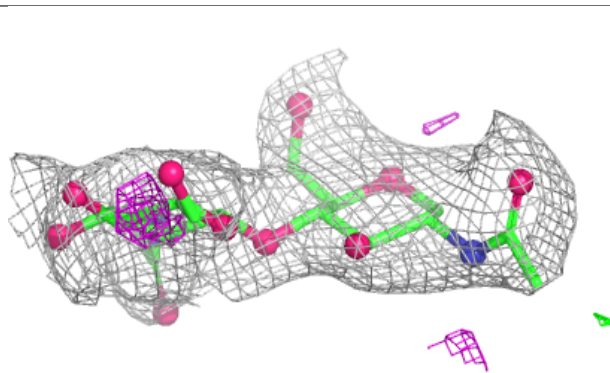
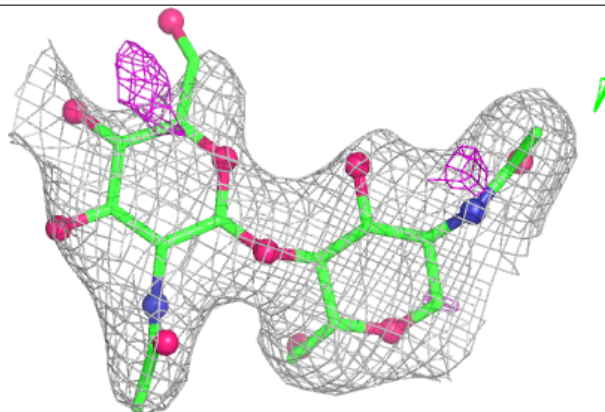


Electron density around Chain W:

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

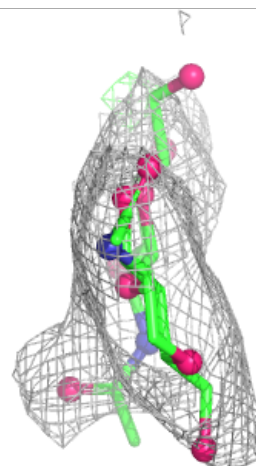
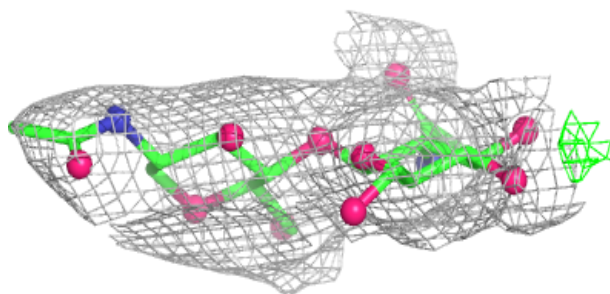
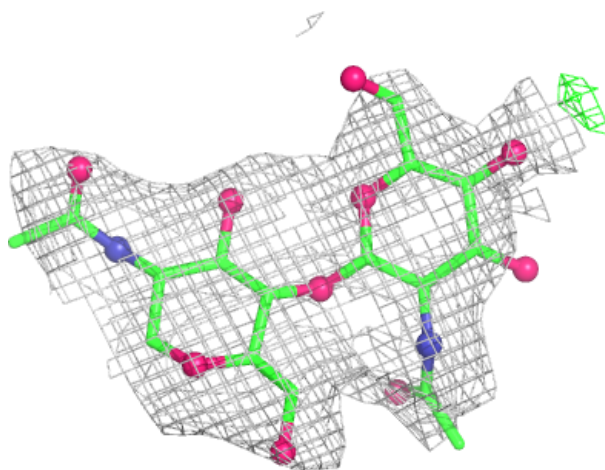
**Electron density around Chain F:**

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



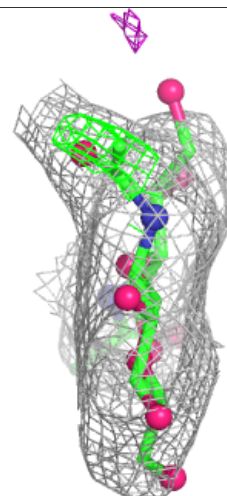
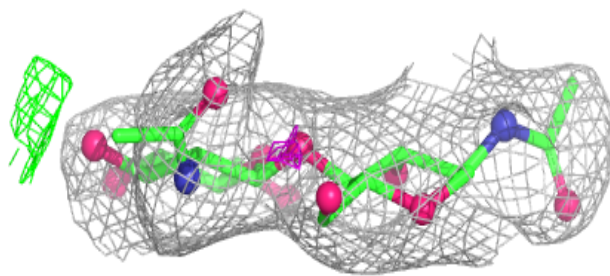
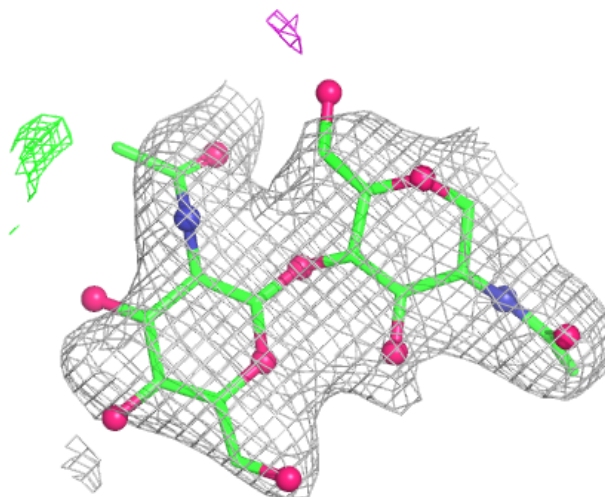
Electron density around Chain G:

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



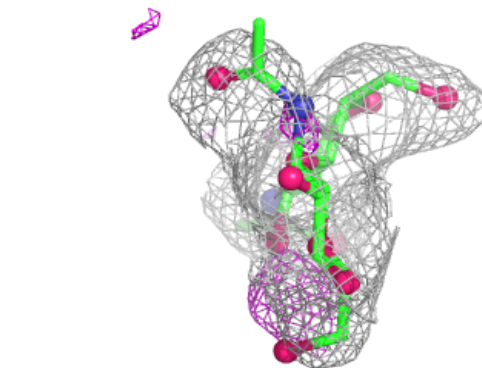
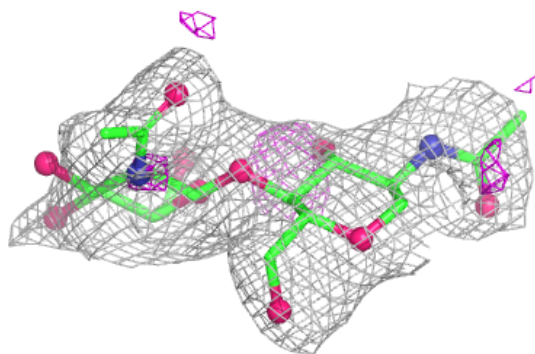
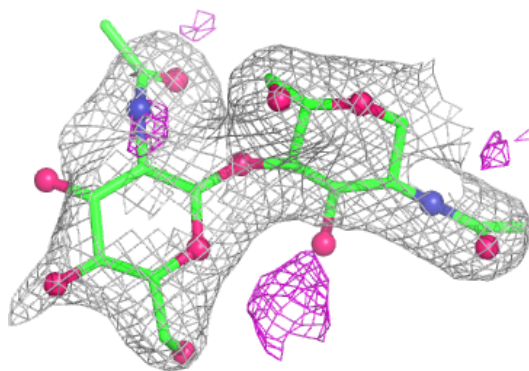
Electron density around Chain H:

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

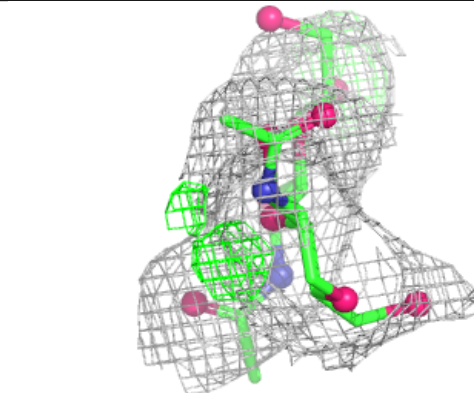
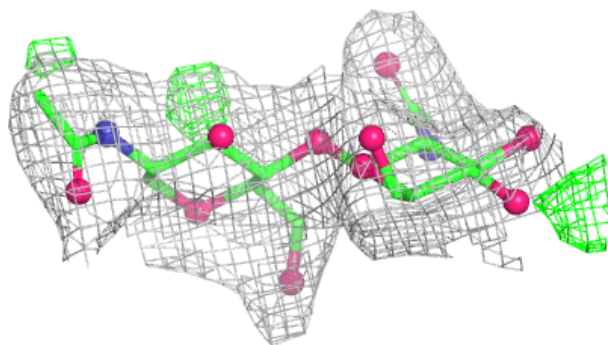
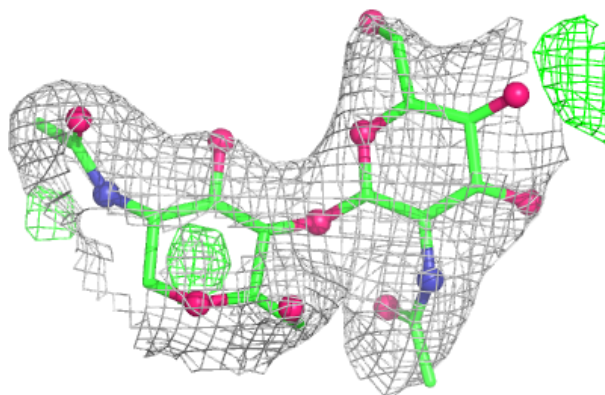


Electron density around Chain I:

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

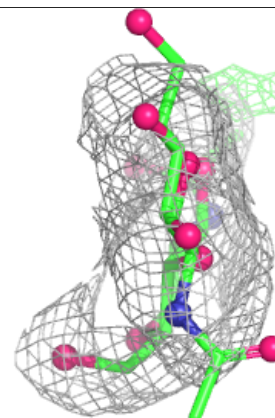
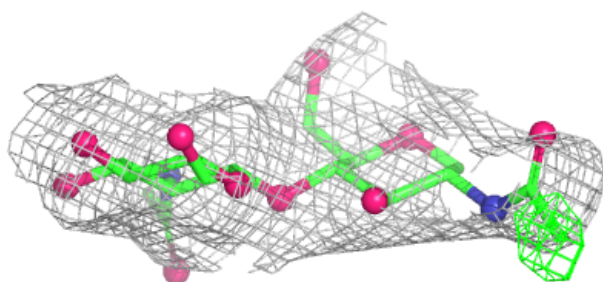
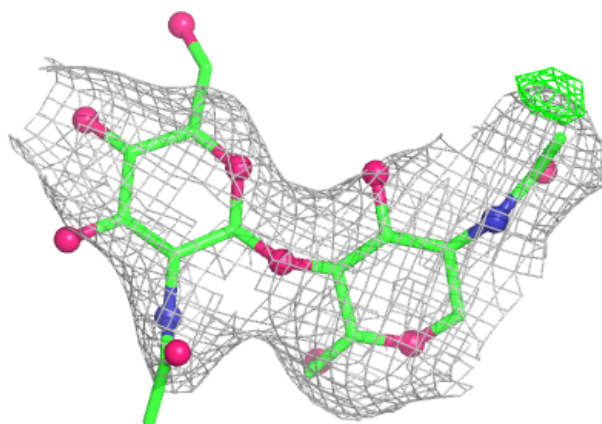
**Electron density around Chain J:**

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



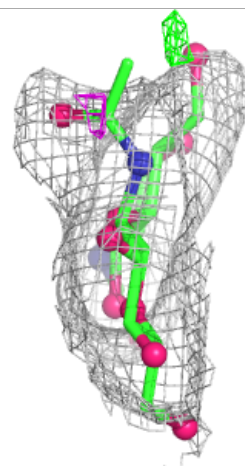
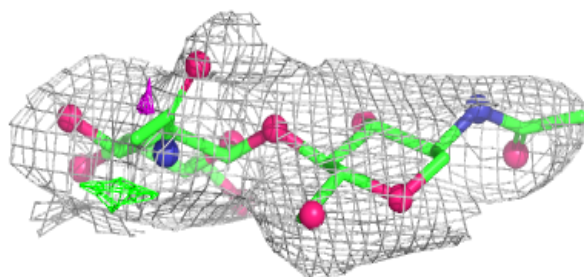
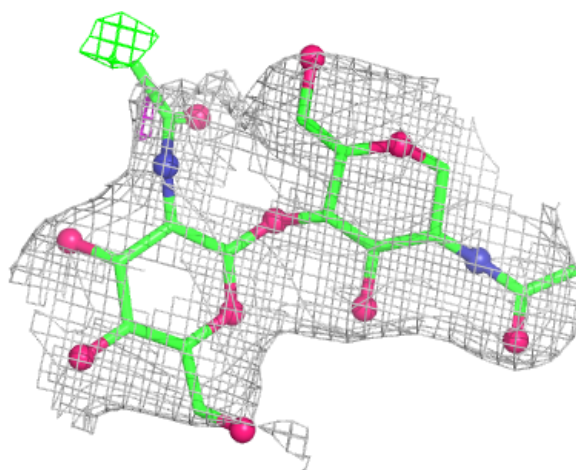
Electron density around Chain L:

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



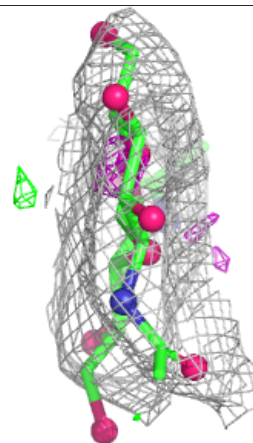
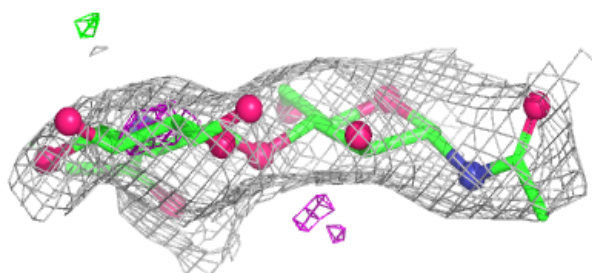
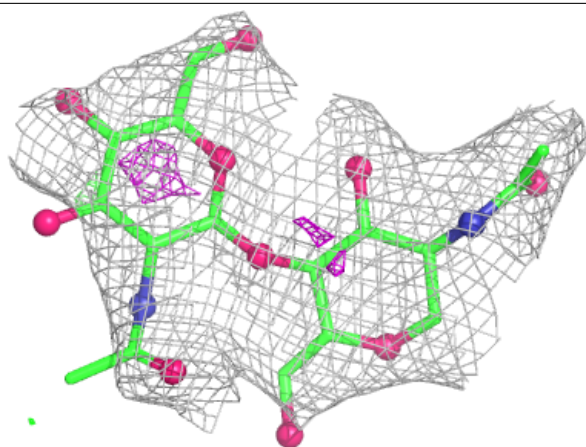
Electron density around Chain M:

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



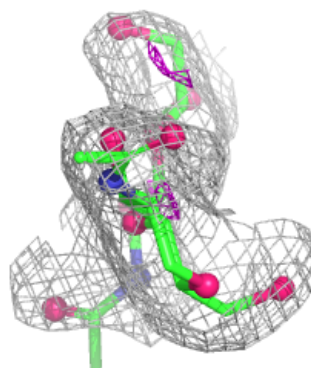
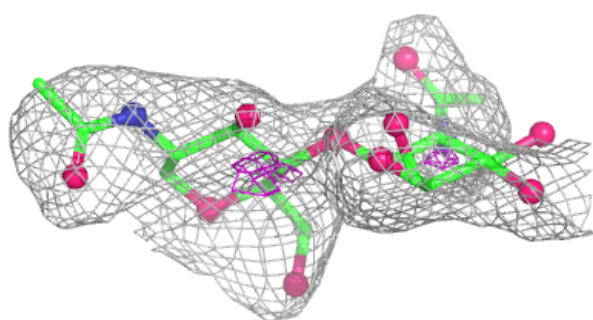
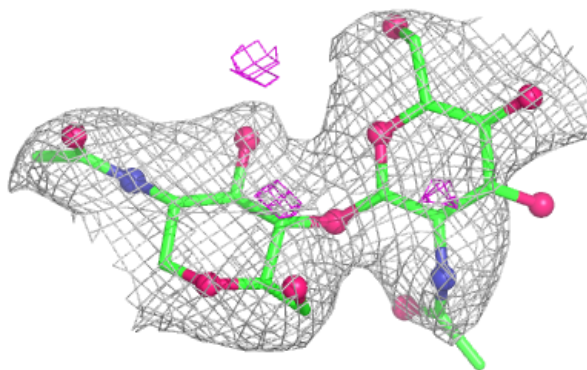
Electron density around Chain N:

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

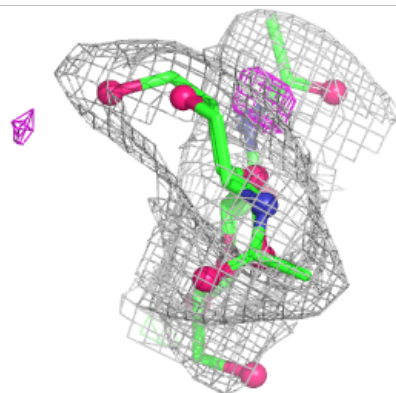
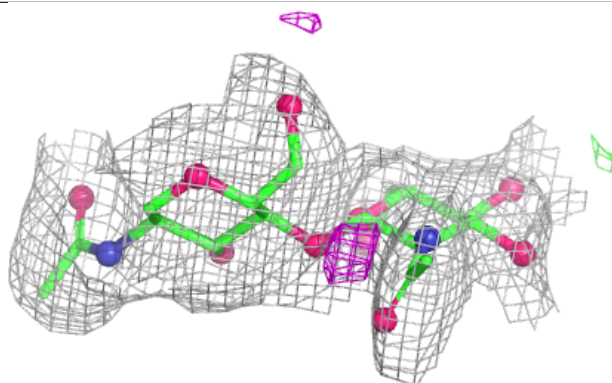
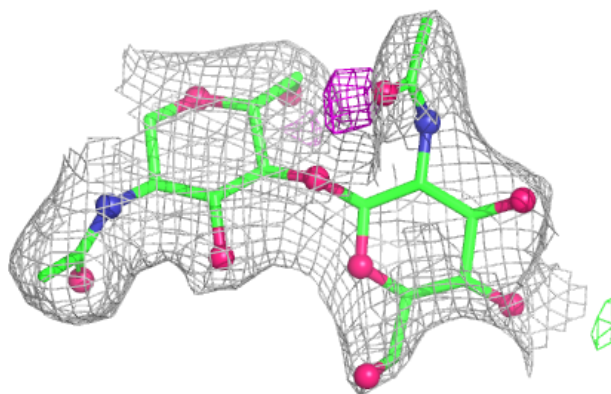


Electron density around Chain O:

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

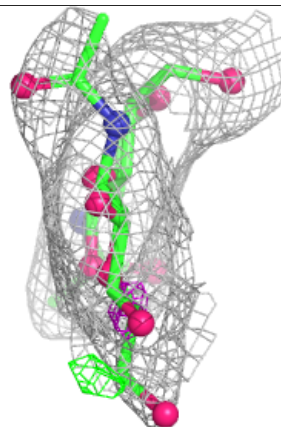
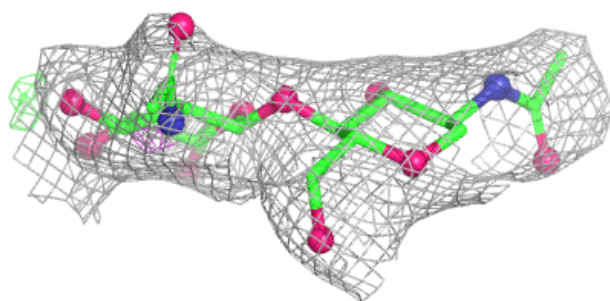
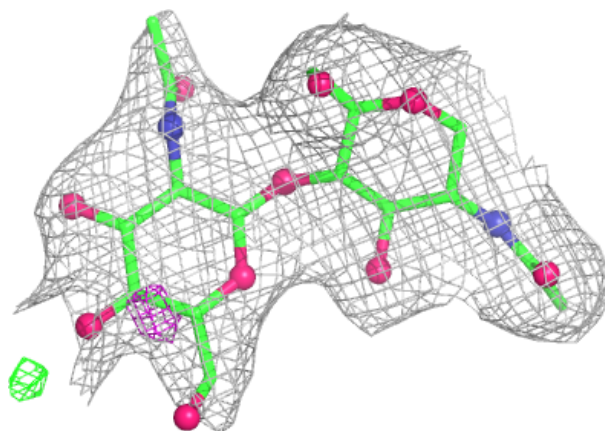
**Electron density around Chain P:**

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



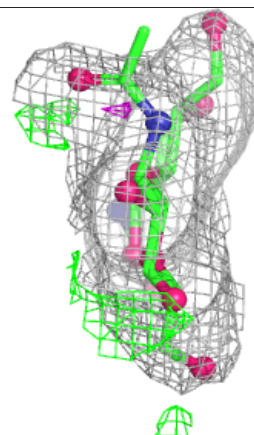
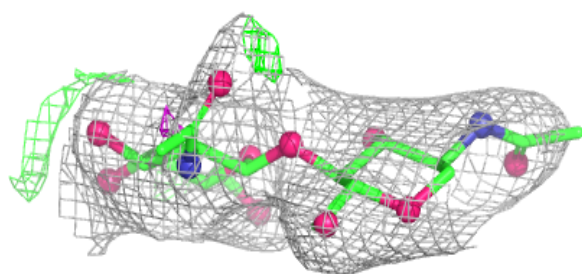
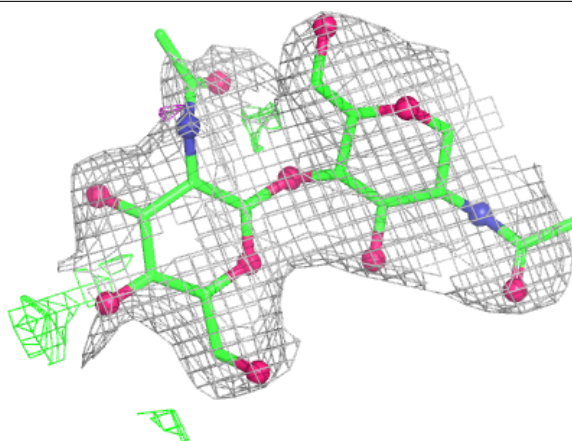
Electron density around Chain R:

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



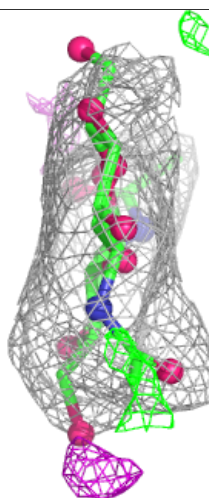
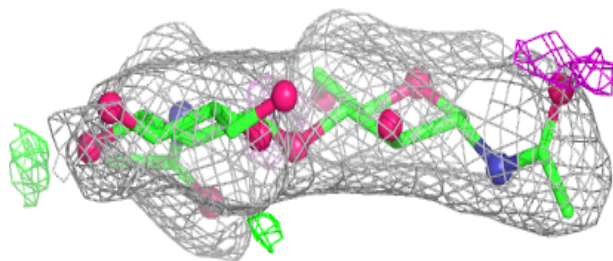
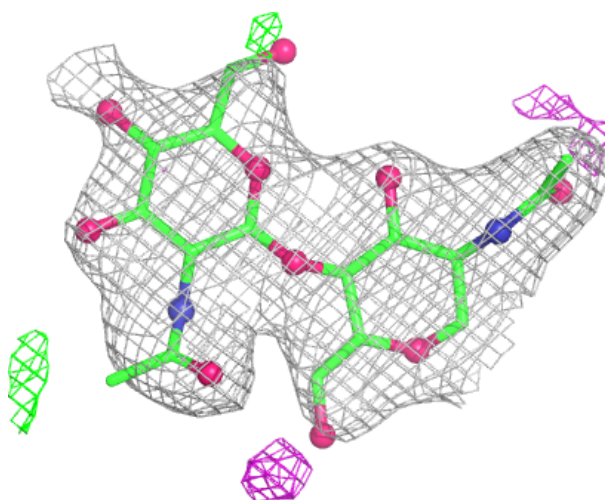
Electron density around Chain S:

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



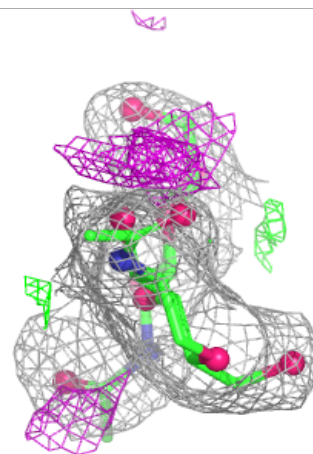
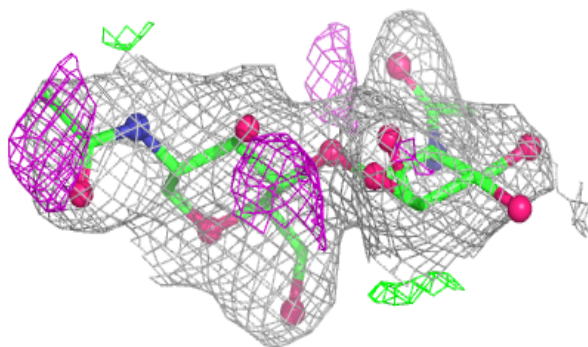
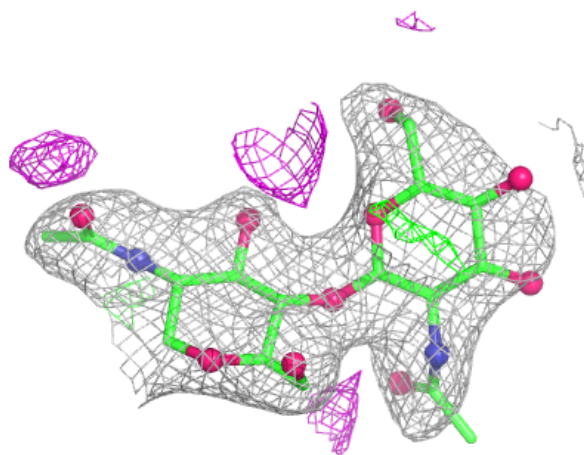
Electron density around Chain T:

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



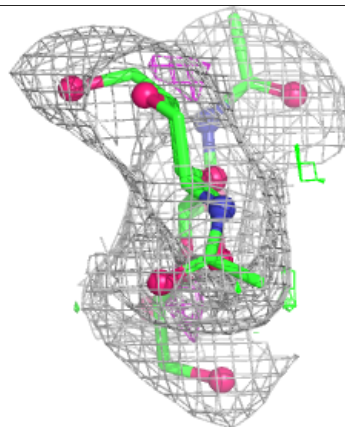
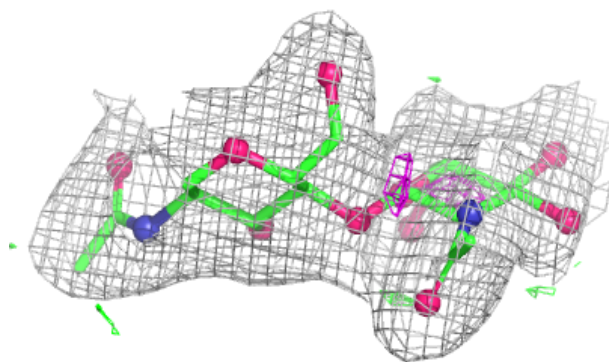
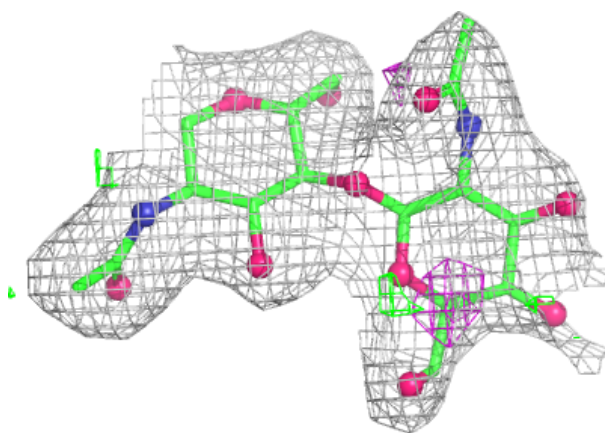
Electron density around Chain U:

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

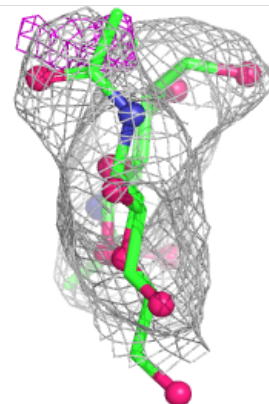
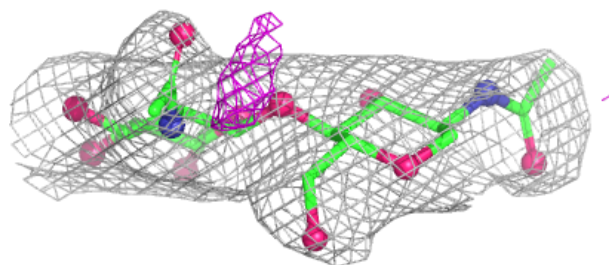
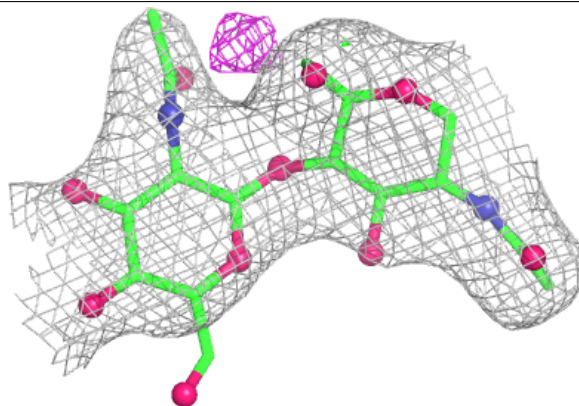


Electron density around Chain V:

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

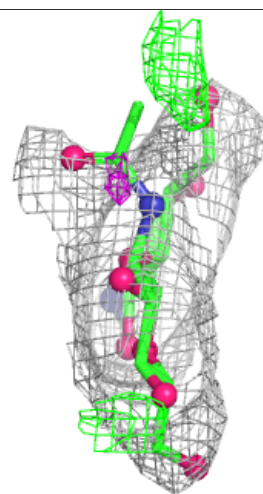
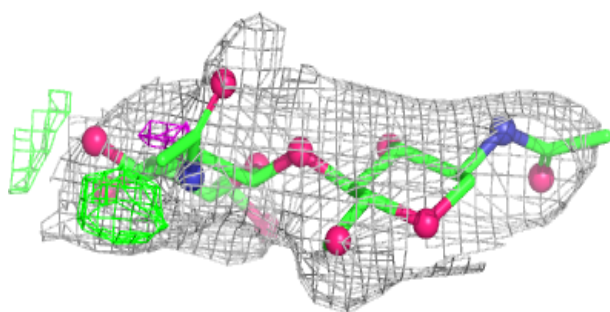
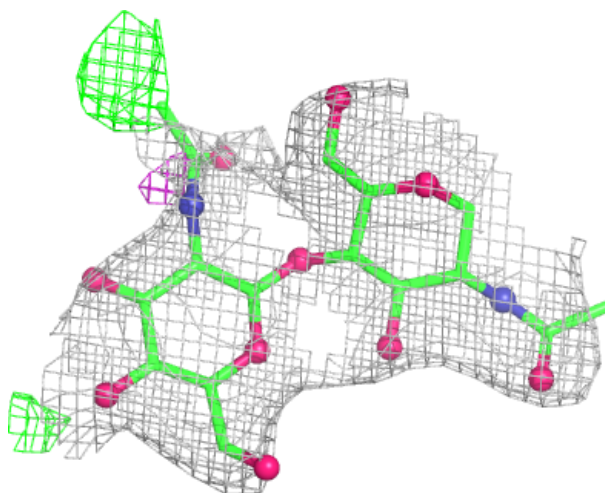
**Electron density around Chain X:**

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



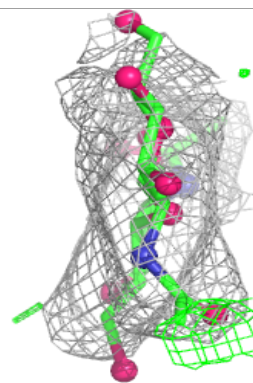
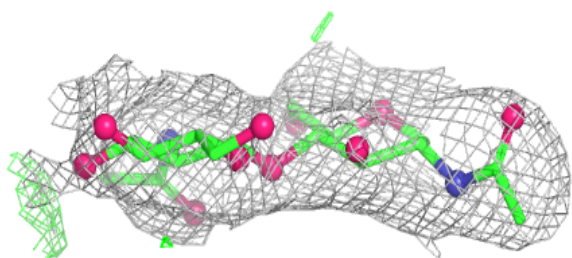
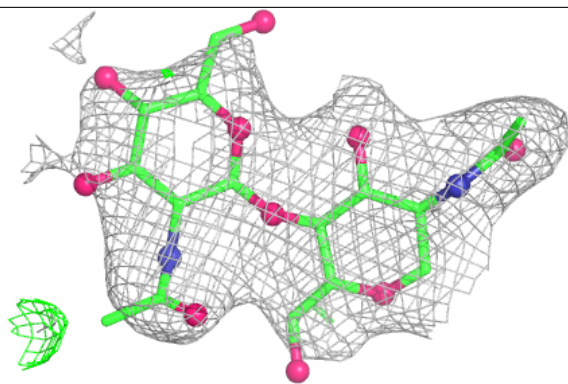
Electron density around Chain Y:

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

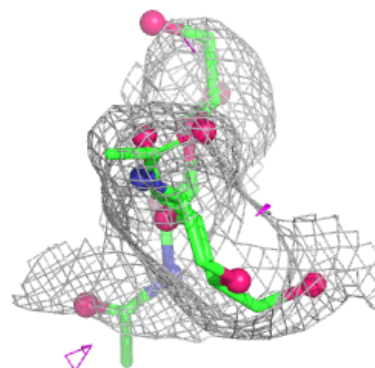
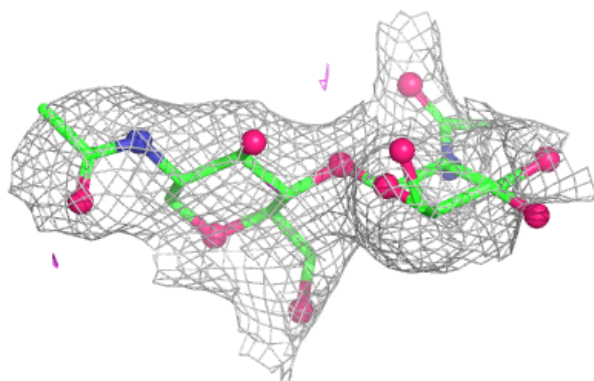
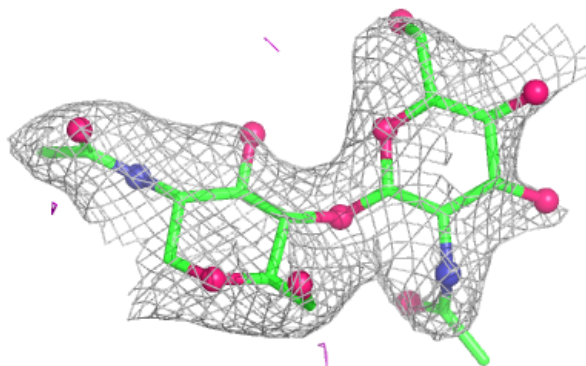


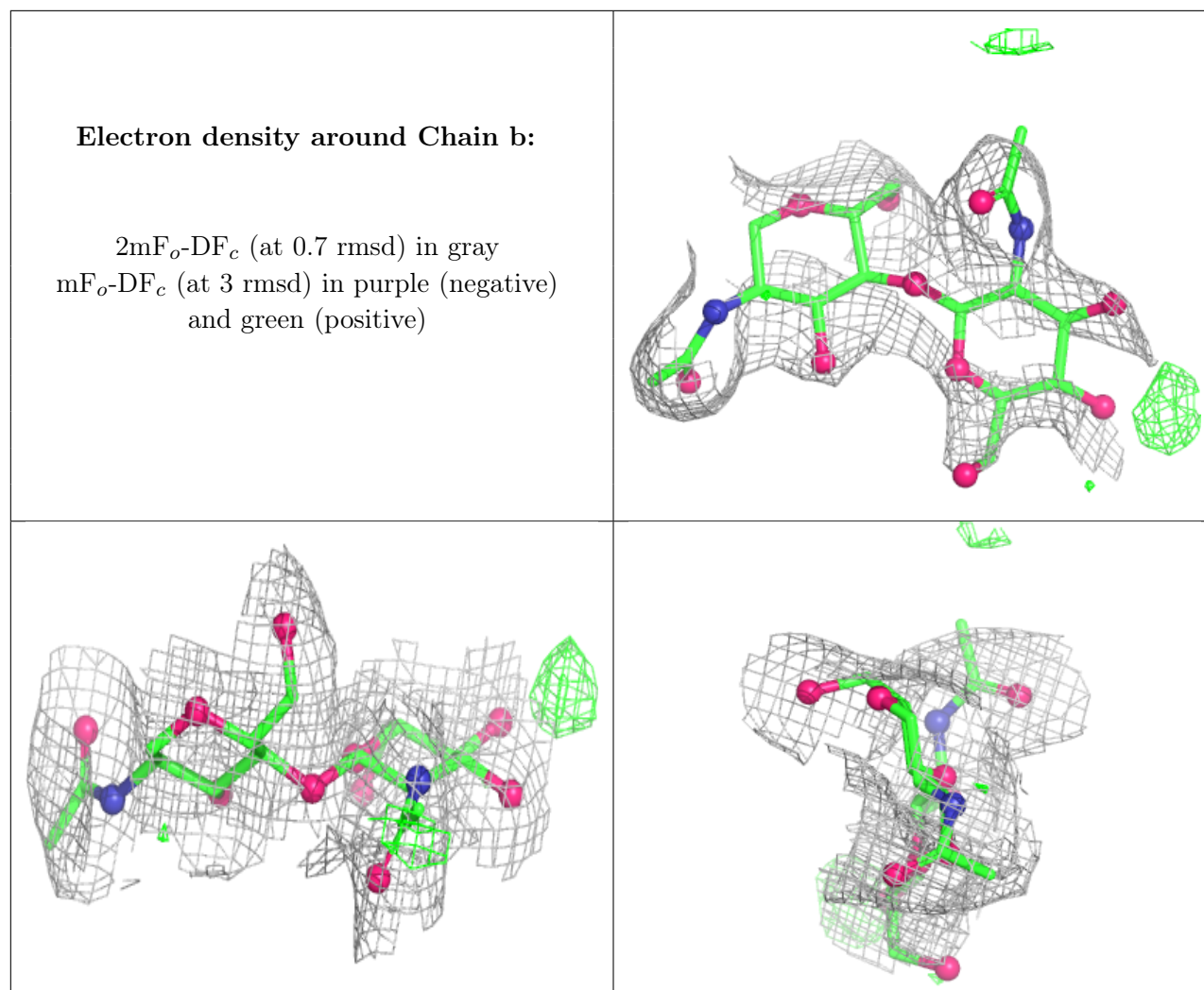
Electron density around Chain Z:

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

**Electron density around Chain a:**

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





6.4 Ligands ⓘ

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
4	NAG	A	3019	14/15	0.42	0.19	183,185,186,186	0
4	NAG	B	3019	14/15	0.49	0.17	128,131,135,135	0
4	NAG	D	3019	14/15	0.50	0.19	123,126,128,130	0
4	NAG	C	3019	14/15	0.53	0.18	116,118,120,121	0
4	NAG	A	3014	14/15	0.64	0.21	110,113,116,116	0
4	NAG	B	3022	14/15	0.64	0.16	145,148,152,152	0
4	NAG	B	3011	14/15	0.65	0.22	106,109,111,112	0
4	NAG	B	3014	14/15	0.66	0.19	91,95,100,102	0
4	NAG	C	3014	14/15	0.67	0.20	92,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	3011	14/15	0.68	0.20	87,92,93,95	0
4	NAG	A	3000	14/15	0.69	0.19	184,187,188,188	0
4	NAG	A	3022	14/15	0.69	0.16	134,137,139,139	0
4	NAG	B	3000	14/15	0.70	0.19	166,170,173,174	0
4	NAG	C	3000	14/15	0.70	0.18	121,122,124,124	0
4	NAG	D	3000	14/15	0.70	0.18	150,156,159,160	0
4	NAG	D	3014	14/15	0.70	0.18	96,100,101,102	0
4	NAG	A	3011	14/15	0.70	0.18	98,103,107,108	0
4	NAG	D	3022	14/15	0.75	0.14	124,127,128,128	0
4	NAG	D	3011	14/15	0.77	0.17	117,120,124,125	0
4	NAG	C	3022	14/15	0.78	0.13	111,113,114,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.