



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 02:05 pm GMT

PDB ID : 1W1I  
Title : Crystal structure of dipeptidyl peptidase IV (DPPIV or CD26) in complex with adenosine deaminase  
Authors : Weihofen, W.A.; Liu, J.; Reutter, W.; Saenger, W.; Fan, H.  
Deposited on : 2004-06-22  
Resolution : 3.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

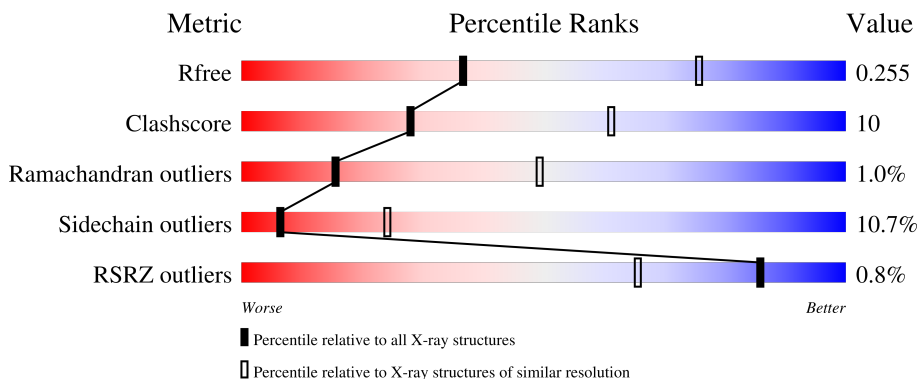
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	 77% 19% .
1	B	728	 79% 17% .
1	C	728	 78% 18% .
1	D	728	 77% 19% .
2	E	357	 4% 60% 32% 5% ..

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Mol	Chain	Length	Quality of chain
2	F	357	
2	G	357	
2	H	357	
3	I	3	
3	Q	3	
4	J	2	
4	K	2	
4	N	2	
4	P	2	
4	R	2	
4	S	2	
4	U	2	
4	W	2	
4	Y	2	
5	L	4	
5	O	4	
5	T	4	
5	X	4	
6	M	2	
6	V	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	I	3	X	-	-	-
3	NAG	Q	2	-	-	-	X
3	FUC	Q	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	J	2	-	-	-	X
4	NAG	R	2	-	-	-	X
4	NAG	U	2	-	-	-	X
6	FUC	M	2	X	-	-	-
6	FUC	V	2	X	-	-	-
7	NAG	A	860	X	-	-	-
7	NAG	A	870	X	-	-	-
7	NAG	B	860	X	-	-	-
7	NAG	C	860	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 35877 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 DIPEPTIDYL PEPTIDASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5963	3827	982	1128	26	0	0	0
1	B	728	5963	3827	982	1128	26	0	0	0
1	C	728	5963	3827	982	1128	26	0	0	0
1	D	728	5963	3827	982	1128	26	0	0	0

- Molecule 2 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	352	2809	1786	473	537	13	0	0	0
2	F	352	2808	1786	472	537	13	0	0	0
2	G	352	2809	1786	473	537	13	0	0	0
2	H	352	2809	1786	473	537	13	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	ASP	ASN	conflict	UNP P56658
E	32	LYS	ARG	conflict	UNP P56658
E	33	ARG	LYS	conflict	UNP P56658
E	47	LEU	GLN	conflict	UNP P56658
E	57	THR	SER	conflict	UNP P56658
E	60	ASP	GLU	conflict	UNP P56658
E	77	ASP	GLU	conflict	UNP P56658
E	79	ILE	VAL	conflict	UNP P56658

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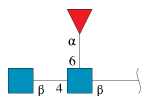
Chain	Residue	Modelled	Actual	Comment	Reference
E	199	GLN	LYS	variant	UNP P56658
E	246	THR	ALA	variant	UNP P56658
E	261	ILE	VAL	conflict	UNP P56658
E	279	ALA	PRO	conflict	UNP P56658
E	281	ILE	VAL	conflict	UNP P56658
E	313	LYS	ASN	conflict	UNP P56658
E	314	ASP	GLU	conflict	UNP P56658
E	352	ARG	GLY	variant	UNP P56658
F	8	ASP	ASN	conflict	UNP P56658
F	32	LYS	ARG	conflict	UNP P56658
F	33	ARG	LYS	conflict	UNP P56658
F	47	LEU	GLN	conflict	UNP P56658
F	57	THR	SER	conflict	UNP P56658
F	60	ASP	GLU	conflict	UNP P56658
F	77	ASP	GLU	conflict	UNP P56658
F	79	ILE	VAL	conflict	UNP P56658
F	199	GLN	LYS	variant	UNP P56658
F	246	THR	ALA	variant	UNP P56658
F	261	ILE	VAL	conflict	UNP P56658
F	279	ALA	PRO	conflict	UNP P56658
F	281	ILE	VAL	conflict	UNP P56658
F	313	LYS	ASN	conflict	UNP P56658
F	314	ASP	GLU	conflict	UNP P56658
F	352	ARG	GLY	variant	UNP P56658
G	8	ASP	ASN	conflict	UNP P56658
G	32	LYS	ARG	conflict	UNP P56658
G	33	ARG	LYS	conflict	UNP P56658
G	47	LEU	GLN	conflict	UNP P56658
G	57	THR	SER	conflict	UNP P56658
G	60	ASP	GLU	conflict	UNP P56658
G	77	ASP	GLU	conflict	UNP P56658
G	79	ILE	VAL	conflict	UNP P56658
G	199	GLN	LYS	variant	UNP P56658
G	246	THR	ALA	variant	UNP P56658
G	261	ILE	VAL	conflict	UNP P56658
G	279	ALA	PRO	conflict	UNP P56658
G	281	ILE	VAL	conflict	UNP P56658
G	313	LYS	ASN	conflict	UNP P56658
G	314	ASP	GLU	conflict	UNP P56658
G	352	ARG	GLY	variant	UNP P56658
H	8	ASP	ASN	conflict	UNP P56658
H	32	LYS	ARG	conflict	UNP P56658

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Chain	Residue	Modelled	Actual	Comment	Reference
H	33	ARG	LYS	conflict	UNP P56658
H	47	LEU	GLN	conflict	UNP P56658
H	57	THR	SER	conflict	UNP P56658
H	60	ASP	GLU	conflict	UNP P56658
H	77	ASP	GLU	conflict	UNP P56658
H	79	ILE	VAL	conflict	UNP P56658
H	199	GLN	LYS	variant	UNP P56658
H	246	THR	ALA	variant	UNP P56658
H	261	ILE	VAL	conflict	UNP P56658
H	279	ALA	PRO	conflict	UNP P56658
H	281	ILE	VAL	conflict	UNP P56658
H	313	LYS	ASN	conflict	UNP P56658
H	314	ASP	GLU	conflict	UNP P56658
H	352	ARG	GLY	variant	UNP P56658

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	3	38	22	2	14	0	0	0
3	Q	3	38	22	2	14	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	J	2	28	16	2	10	0	0	0
4	K	2	28	16	2	10	0	0	0
4	N	2	28	16	2	10	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	P	2	28	16	2	10	0	0	0
4	R	2	28	16	2	10	0	0	0
4	S	2	28	16	2	10	0	0	0
4	U	2	28	16	2	10	0	0	0
4	W	2	28	16	2	10	0	0	0
4	Y	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(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
			Total	C	N	O			
5	L	4	50	28	2	20	0	0	0
5	O	4	50	28	2	20	0	0	0
5	T	4	50	28	2	20	0	0	0
5	X	4	50	28	2	20	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	M	2	24	14	1	9	0	0	0

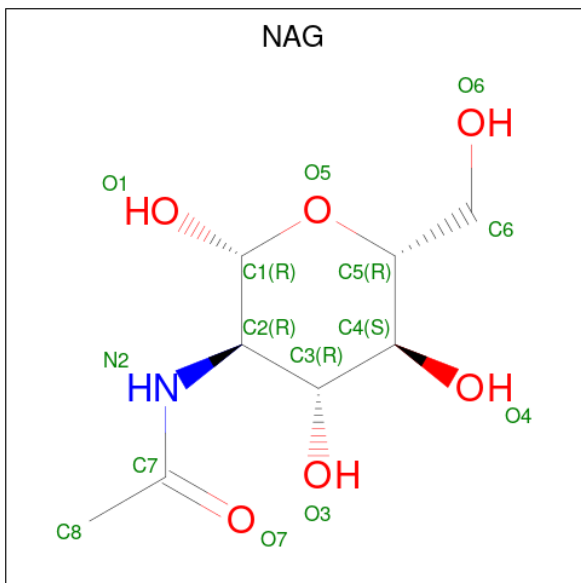
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	V	2	24	14	1	9	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

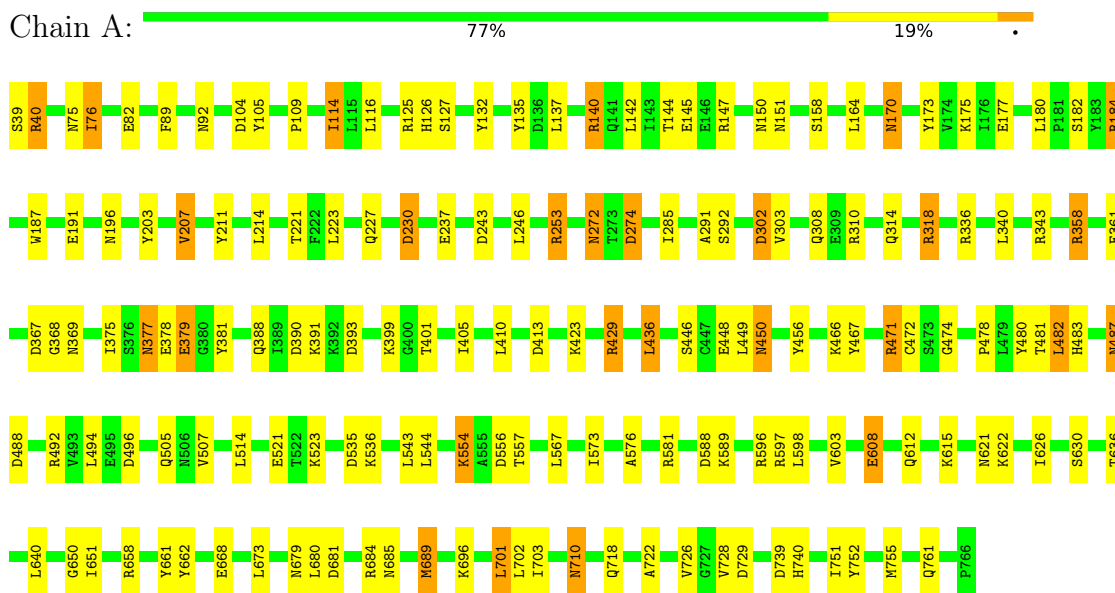
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Zn	0	0
			1	1		
8	F	1	Total	Zn	0	0
			1	1		
8	G	1	Total	Zn	0	0
			1	1		
8	H	1	Total	Zn	0	0
			1	1		

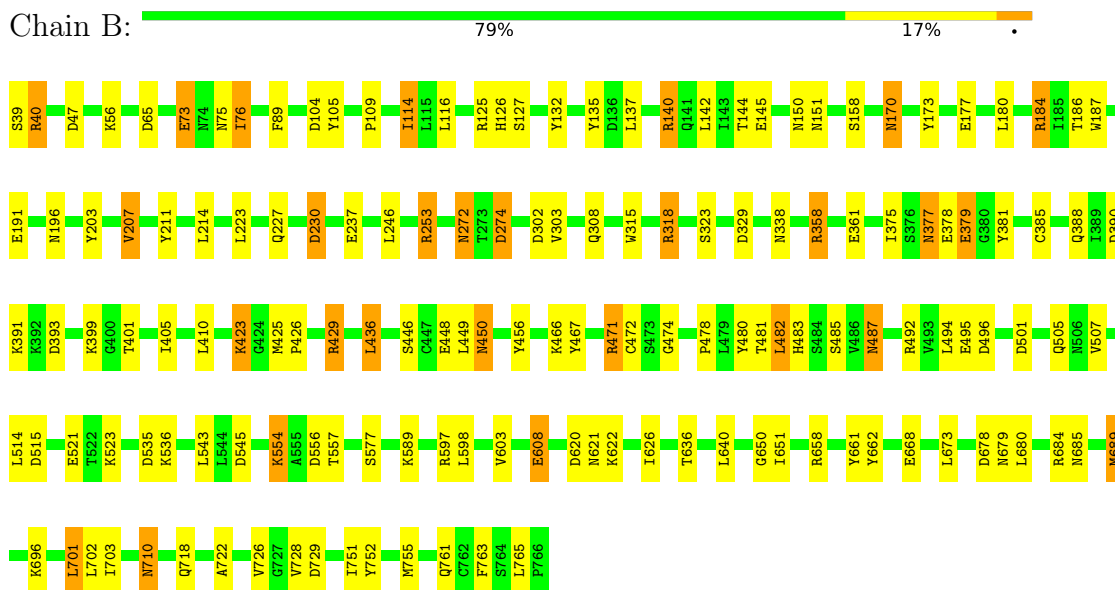
### 3 Residue-property plots

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.

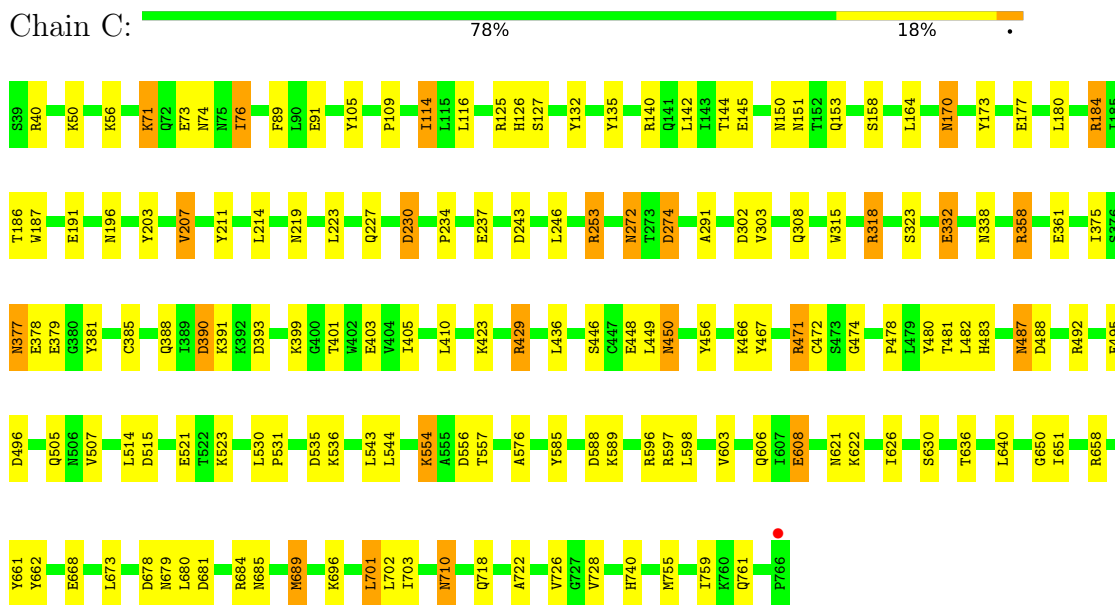
#### • Molecule 1: DIPEPTIDYL PEPTIDASE IV



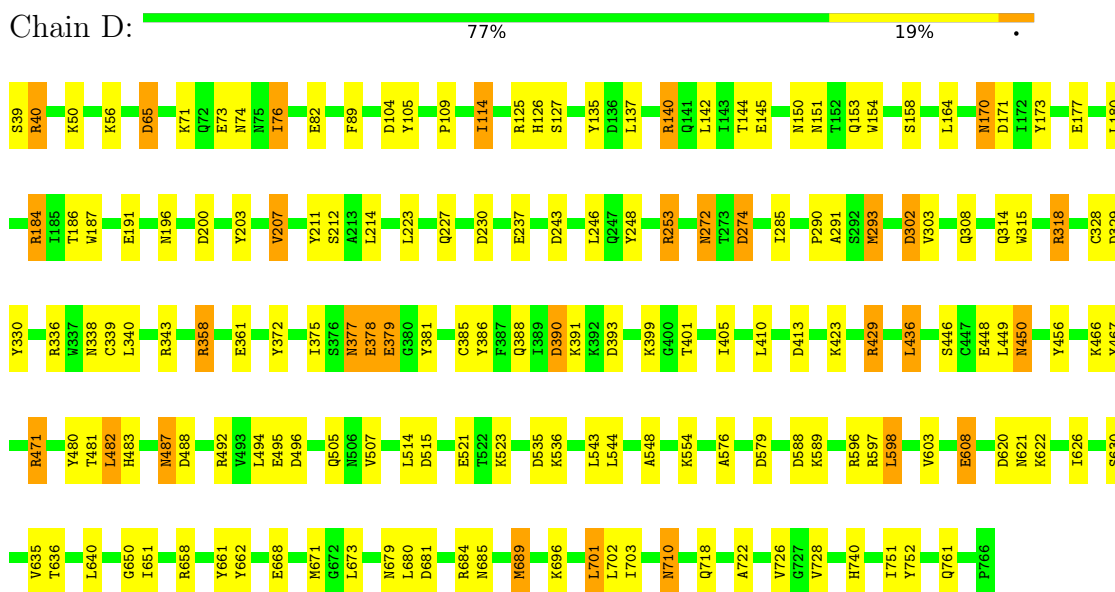
#### • Molecule 1: DIPEPTIDYL PEPTIDASE IV



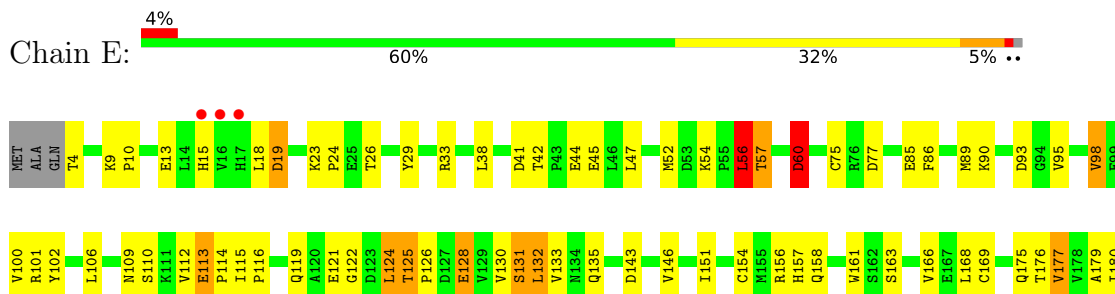
- Molecule 1: DIPEPTIDYL PEPTIDASE IV

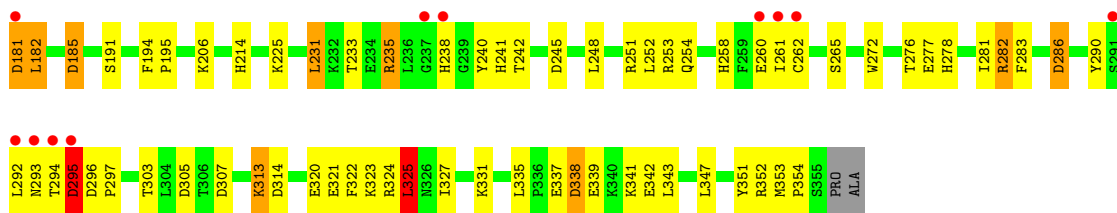


- Molecule 1: DIPEPTIDYL PEPTIDASE IV

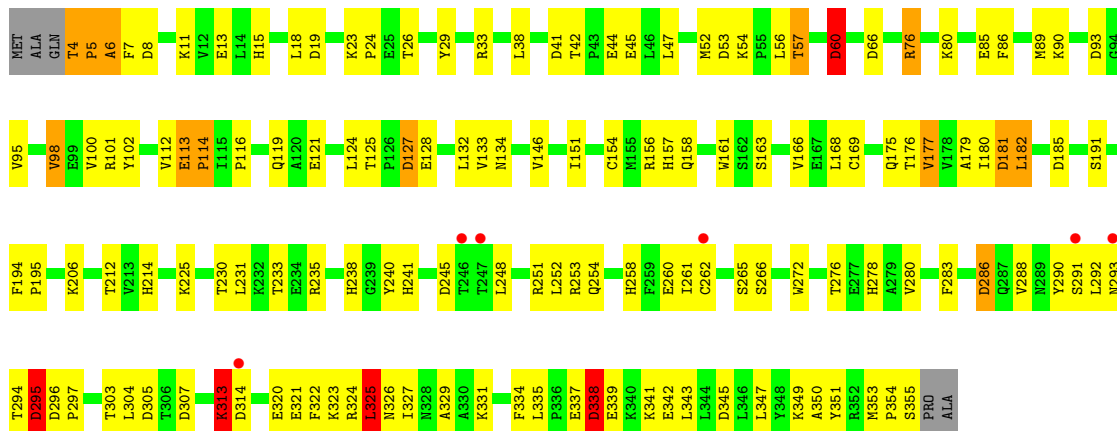


- Molecule 2: ADENOSINE DEAMINASE

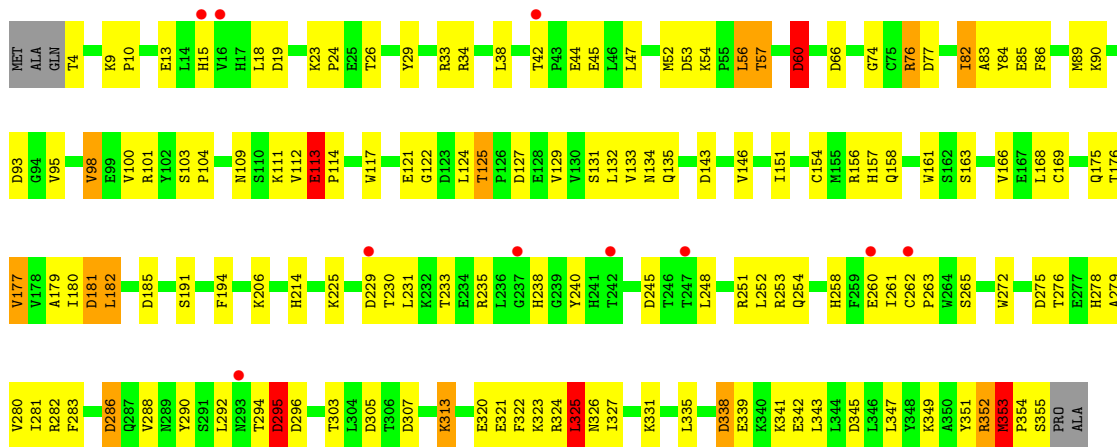




● Molecule 2: ADENOSINE DEAMINASE



● Molecule 2: ADENOSINE DEAMINASE



● Molecule 2: ADENOSINE DEAMINASE





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

Chain I: 33% 67%

MAG1  
MAG2  
FUC3

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

Chain Q: 33% 67%

MAG1  
MAG2  
FUC3

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

Chain J: 50% 50%

MAG1  
MAG2

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

Chain K: 50% 50%


MAG1  
MAG2

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

Chain N: 100%

MAG1  
MAG2

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

Chain P:  100%


MAG1  
MAG2

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

Chain R:  100%

MAG1  
MAG2

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

Chain S:  50% 50%


MAG1  
MAG2

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

Chain U:  100%


MAG1  
MAG2

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

Chain W:  50% 50%

MAG1  
MAG2

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

Chain Y:  100%

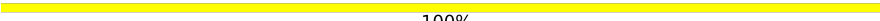
MAG1  
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

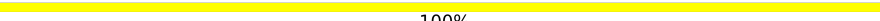
MAG1  
MAG2  
BMA3  
MAV4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

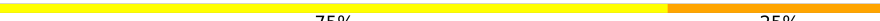
MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

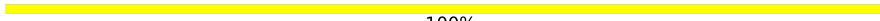
MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  75% 25%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain M:  100%

MAG1  
FUC2

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

Chain V:  100%

MAG1  
FUC2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.06Å 168.50Å 236.84Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	30.00 – 3.03 29.90 – 3.03	Depositor EDS
% Data completeness (in resolution range)	85.5 (30.00-3.03) 85.5 (29.90-3.03)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 3.06Å)	Xtrriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.224 , 0.257 0.224 , 0.255	Depositor DCC
$R_{free}$ test set	2048 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	35877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.39	0/6135	0.75	15/8344 (0.2%)
1	B	0.40	0/6135	0.75	16/8344 (0.2%)
1	C	0.39	0/6135	0.76	14/8344 (0.2%)
1	D	0.40	0/6135	0.75	19/8344 (0.2%)
2	E	0.40	0/2874	0.84	16/3896 (0.4%)
2	F	0.38	0/2872	0.82	17/3891 (0.4%)
2	G	0.36	0/2874	0.83	17/3896 (0.4%)
2	H	0.36	0/2874	0.81	13/3896 (0.3%)
All	All	0.39	0/36034	0.78	127/48955 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	77	ASP	CB-CG-OD2	12.11	129.20	118.30
2	E	77	ASP	CB-CG-OD2	10.17	127.45	118.30
2	H	77	ASP	CB-CG-OD2	8.05	125.54	118.30
2	H	325	LEU	CA-CB-CG	6.80	130.95	115.30
2	F	60	ASP	CB-CG-OD2	6.67	124.30	118.30
2	E	181	ASP	CB-CG-OD2	6.64	124.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	325	LEU	CA-CB-CG	6.56	130.38	115.30
2	E	60	ASP	CB-CG-OD2	6.49	124.14	118.30
1	D	302	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	496	ASP	CB-CG-OD2	6.47	124.12	118.30
2	F	127	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	535	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	302	ASP	CB-CG-OD2	6.37	124.03	118.30
2	G	143	ASP	CB-CG-OD2	6.34	124.00	118.30
2	G	325	LEU	CA-CB-CG	6.32	129.84	115.30
2	G	245	ASP	CB-CG-OD2	6.32	123.99	118.30
2	H	307	ASP	CB-CG-OD2	6.31	123.98	118.30
2	F	181	ASP	CB-CG-OD2	6.21	123.89	118.30
2	E	307	ASP	CB-CG-OD2	6.13	123.82	118.30
2	G	307	ASP	CB-CG-OD2	6.12	123.81	118.30
2	H	60	ASP	CB-CG-OD2	6.12	123.81	118.30
2	F	325	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	230	ASP	CB-CG-OD2	6.10	123.79	118.30
2	H	245	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	496	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	329	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	230	ASP	CB-CG-OD2	6.09	123.78	118.30
2	G	181	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	556	ASP	CB-CG-OD2	6.03	123.73	118.30
2	F	245	ASP	CB-CG-OD2	6.01	123.71	118.30
2	H	295	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	329	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	274	ASP	CB-CG-OD2	5.97	123.68	118.30
2	G	60	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	496	ASP	CB-CG-OD2	5.93	123.63	118.30
1	D	535	ASP	CB-CG-OD2	5.92	123.63	118.30
2	E	245	ASP	CB-CG-OD2	5.91	123.61	118.30
2	F	93	ASP	CB-CG-OD2	5.89	123.60	118.30
2	H	181	ASP	CB-CG-OD2	5.86	123.57	118.30
2	E	143	ASP	CB-CG-OD2	5.85	123.57	118.30
2	G	295	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	104	ASP	CB-CG-OD2	5.80	123.53	118.30
2	E	93	ASP	CB-CG-OD2	5.80	123.52	118.30
2	F	296	ASP	CB-CG-OD2	5.77	123.49	118.30
2	F	53	ASP	CB-CG-OD2	5.76	123.49	118.30
2	F	305	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	681	ASP	CB-CG-OD2	5.71	123.44	118.30
2	E	185	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	307	ASP	CB-CG-OD2	5.71	123.44	118.30
2	F	19	ASP	CB-CG-OD2	5.68	123.41	118.30
2	H	286	ASP	CB-CG-OD2	5.68	123.41	118.30
2	E	19	ASP	CB-CG-OD2	5.67	123.40	118.30
2	H	53	ASP	CB-CG-OD2	5.63	123.37	118.30
2	F	286	ASP	CB-CG-OD2	5.63	123.36	118.30
2	G	305	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	515	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	302	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	535	ASP	CB-CG-OD2	5.61	123.35	118.30
2	H	296	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	496	ASP	CB-CG-OD2	5.60	123.34	118.30
2	F	8	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	104	ASP	CB-CG-OD2	5.58	123.32	118.30
2	E	314	ASP	CB-CG-OD2	5.56	123.30	118.30
1	D	488	ASP	CB-CG-OD2	5.53	123.28	118.30
2	E	295	ASP	CB-CG-OD2	5.52	123.27	118.30
2	G	93	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	393	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	104	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	678	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	390	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	535	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	729	ASP	CB-CG-OD2	5.44	123.19	118.30
2	H	305	ASP	CB-CG-OD2	5.43	123.19	118.30
2	G	296	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	47	ASP	CB-CG-OD2	5.39	123.16	118.30
1	B	393	ASP	CB-CG-OD2	5.39	123.16	118.30
1	D	274	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	588	ASP	CB-CG-OD2	5.39	123.16	118.30
2	G	53	ASP	CB-CG-OD2	5.39	123.15	118.30
2	E	296	ASP	CB-CG-OD2	5.38	123.14	118.30
2	G	286	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	302	ASP	CB-CG-OD2	5.35	123.12	118.30
2	F	295	ASP	CB-CG-OD2	5.35	123.12	118.30
1	D	243	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	556	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	171	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	588	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	678	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	243	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	556	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	274	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	620	ASP	CB-CG-OD2	5.28	123.05	118.30
2	E	305	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	413	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	620	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	488	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	681	ASP	CB-CG-OD2	5.25	123.03	118.30
2	F	66	ASP	CB-CG-OD2	5.25	123.02	118.30
2	F	41	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	393	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	501	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	274	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	243	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	515	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	200	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	390	ASP	CB-CG-OD2	5.21	122.99	118.30
2	G	19	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	729	ASP	CB-CG-OD2	5.18	122.97	118.30
2	G	275	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	579	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	413	ASP	CB-CG-OD2	5.15	122.93	118.30
2	H	41	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	65	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	488	ASP	CB-CG-OD2	5.13	122.92	118.30
2	E	41	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	515	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	588	ASP	CB-CG-OD2	5.11	122.90	118.30
2	G	127	ASP	CB-CG-OD2	5.11	122.90	118.30
2	G	229	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	739	ASP	CB-CG-OD2	5.09	122.88	118.30
2	E	286	ASP	CB-CG-OD2	5.08	122.88	118.30
1	D	393	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	681	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	230	ASP	CB-CG-OD2	5.05	122.84	118.30
2	H	143	ASP	CB-CG-OD2	5.03	122.83	118.30
2	F	314	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	337	GLU	Peptide
2	H	113	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5677	99	0
1	B	5963	0	5677	87	0
1	C	5963	0	5677	86	0
1	D	5963	0	5677	99	0
2	E	2809	0	2767	79	0
2	F	2808	0	2765	85	0
2	G	2809	0	2767	83	0
2	H	2809	0	2767	77	0
3	I	38	0	34	0	0
3	Q	38	0	34	1	0
4	J	28	0	25	1	0
4	K	28	0	25	3	0
4	N	28	0	25	2	0
4	P	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	1	0
4	U	28	0	25	2	0
4	W	28	0	25	2	0
4	Y	28	0	25	0	0
5	L	50	0	43	0	0
5	O	50	0	43	0	0
5	T	50	0	43	0	0
5	X	50	0	43	1	0
6	M	24	0	22	0	0
6	V	24	0	22	0	0
7	A	56	0	52	5	0
7	B	56	0	52	1	0
7	C	42	0	39	3	0
7	D	56	0	52	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1	0	0	0	0
All	All	35877	0	34478	698	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 10.

All (698) 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)
2:F:113:GLU:HB2	2:F:161:TRP:HE1	1.10	1.10
2:G:353:MET:HB2	2:G:354:PRO:CD	1.79	1.10
2:E:113:GLU:HB3	2:E:114:PRO:HD3	1.25	1.08
2:E:113:GLU:HB2	2:E:161:TRP:HE1	1.01	1.08
2:G:283:PHE:HD1	2:G:288:VAL:HG11	1.24	1.00
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.59	1.00
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.59	1.00
2:F:113:GLU:HB2	2:F:161:TRP:NE1	1.78	0.97
2:G:113:GLU:HB3	2:G:114:PRO:HD3	1.46	0.94
2:E:240:TYR:O	2:E:242:THR:N	2.01	0.94
2:E:113:GLU:HB2	2:E:161:TRP:NE1	1.84	0.93
2:G:353:MET:HB2	2:G:354:PRO:HD3	1.49	0.92
1:C:253:ARG:HH22	1:D:253:ARG:HH22	0.95	0.90
7:C:870:NAG:H5	7:C:870:NAG:N2	1.85	0.90
2:F:113:GLU:HB3	2:F:114:PRO:HD3	1.54	0.90
2:F:280:VAL:HA	2:F:283:PHE:CD1	2.07	0.88
2:H:76:ARG:HH11	2:H:76:ARG:CG	1.87	0.88
2:E:113:GLU:CB	2:E:114:PRO:HD3	2.02	0.86
2:E:113:GLU:HB3	2:E:114:PRO:CD	2.06	0.85
2:F:240:TYR:HH	2:F:266:SER:HG	1.16	0.83
2:G:283:PHE:CD1	2:G:288:VAL:HG11	2.12	0.82
1:D:39:SER:N	1:D:40:ARG:HH21	1.78	0.81
2:G:109:ASN:O	2:G:122:GLY:HA2	1.81	0.81
2:F:156:ARG:HD2	2:F:185:ASP:O	1.81	0.80
7:A:860:NAG:H83	7:A:860:NAG:H3	1.61	0.80
2:H:156:ARG:HD2	2:H:185:ASP:O	1.80	0.80
2:G:353:MET:HB2	2:G:354:PRO:HD2	1.62	0.80
2:G:156:ARG:HD2	2:G:185:ASP:O	1.81	0.79
2:H:76:ARG:HH11	2:H:76:ARG:HG2	1.47	0.78
2:E:156:ARG:HD2	2:E:185:ASP:O	1.84	0.78
2:F:350:ALA:C	2:F:351:TYR:CA	2.52	0.78
2:E:113:GLU:CB	2:E:114:PRO:CD	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:353:MET:HB2	2:F:354:PRO:HD2	1.63	0.77
2:G:280:VAL:HA	2:G:283:PHE:HD2	1.49	0.77
2:H:4:THR:N	2:H:5:PRO:HD3	2.01	0.75
2:F:15:HIS:CE1	2:F:214:HIS:CE1	2.75	0.75
2:E:323:LYS:HE3	2:E:351:TYR:HB3	1.69	0.74
4:K:1:NAG:H3	4:K:1:NAG:H82	1.69	0.74
2:F:323:LYS:HE3	2:F:351:TYR:HB3	1.71	0.73
2:F:15:HIS:CD2	2:F:295:ASP:OD1	2.42	0.72
2:E:261:ILE:HD11	2:E:283:PHE:HD2	1.54	0.72
2:H:238:HIS:HB3	2:H:240:TYR:CE2	2.23	0.72
2:E:240:TYR:C	2:E:242:THR:H	1.92	0.72
2:G:323:LYS:HE3	2:G:351:TYR:HB3	1.70	0.72
2:H:323:LYS:HE3	2:H:351:TYR:HB3	1.70	0.71
2:E:278:HIS:O	2:E:281:ILE:HG22	1.91	0.71
2:G:42:THR:HB	2:G:45:GLU:HB3	1.72	0.71
1:D:487:ASN:H	1:D:487:ASN:HD22	1.38	0.70
2:F:42:THR:HB	2:F:45:GLU:HB3	1.74	0.70
2:F:90:LYS:HA	2:F:90:LYS:HE2	1.73	0.70
1:D:340:LEU:HD12	1:D:343:ARG:HD2	1.74	0.70
2:F:253:ARG:HH21	2:F:286:ASP:HB3	1.57	0.69
1:A:487:ASN:HD22	1:A:487:ASN:H	1.39	0.69
2:H:42:THR:HB	2:H:45:GLU:HB3	1.73	0.69
2:E:15:HIS:CD2	2:E:295:ASP:OD1	2.45	0.69
2:E:253:ARG:HH21	2:E:286:ASP:HB3	1.57	0.69
2:F:76:ARG:HB3	2:F:132:LEU:HD21	1.74	0.69
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.28	0.69
1:C:253:ARG:NH2	1:D:253:ARG:HH22	1.80	0.68
2:G:15:HIS:CE1	2:G:214:HIS:CE1	2.82	0.68
1:C:487:ASN:HD22	1:C:487:ASN:H	1.41	0.68
2:H:15:HIS:CD2	2:H:295:ASP:OD1	2.46	0.68
2:H:253:ARG:HH21	2:H:286:ASP:HB3	1.59	0.68
2:E:42:THR:HB	2:E:45:GLU:HB3	1.74	0.68
1:B:401:THR:HG22	1:B:401:THR:O	1.94	0.68
1:D:401:THR:O	1:D:401:THR:HG22	1.95	0.67
2:F:15:HIS:HE1	2:F:214:HIS:CE1	2.12	0.67
2:F:112:VAL:HG11	2:F:116:PRO:HD3	1.77	0.67
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.30	0.67
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.09	0.67
2:H:280:VAL:O	2:H:283:PHE:HB2	1.95	0.67
2:G:15:HIS:CD2	2:G:295:ASP:OD1	2.48	0.66
2:G:76:ARG:HB3	2:G:132:LEU:HD21	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:282:ARG:HD3	2:E:286:ASP:OD2	1.94	0.66
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.78	0.66
2:E:15:HIS:CE1	2:E:214:HIS:CE1	2.83	0.66
2:G:253:ARG:HH21	2:G:286:ASP:HB3	1.60	0.66
2:H:15:HIS:CE1	2:H:214:HIS:CE1	2.83	0.66
2:E:115:ILE:HD12	2:E:115:ILE:H	1.61	0.66
2:G:90:LYS:HE2	2:G:90:LYS:HA	1.76	0.66
1:A:401:THR:O	1:A:401:THR:HG22	1.96	0.65
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.60	0.65
2:G:34:ARG:HH12	2:G:74:GLY:HA3	1.61	0.65
2:H:278:HIS:O	2:H:281:ILE:HG22	1.97	0.65
1:B:718:GLN:HA	1:B:718:GLN:NE2	2.12	0.65
1:A:718:GLN:NE2	1:A:718:GLN:HA	2.11	0.64
2:E:131:SER:O	2:E:135:GLN:HG3	1.98	0.64
1:D:173:TYR:CE2	1:D:184:ARG:HG3	2.33	0.64
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.63	0.64
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.33	0.64
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.63	0.63
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.80	0.63
2:H:90:LYS:HE2	2:H:90:LYS:HA	1.79	0.63
2:G:114:PRO:HG2	2:G:158:GLN:NE2	2.12	0.63
2:F:235:ARG:HD2	2:F:260:GLU:OE2	1.99	0.63
2:G:353:MET:CB	2:G:354:PRO:HD3	2.27	0.63
2:E:261:ILE:HD11	2:E:283:PHE:CD2	2.33	0.63
2:G:129:VAL:O	2:G:133:VAL:HG23	1.99	0.63
2:H:113:GLU:HB3	2:H:114:PRO:HD3	1.81	0.63
2:F:23:LYS:HB2	2:F:26:THR:HG23	1.81	0.62
2:H:261:ILE:HD11	2:H:283:PHE:CD2	2.35	0.62
1:B:150:ASN:O	1:B:151:ASN:HB2	2.00	0.62
2:E:90:LYS:HE2	2:E:90:LYS:HA	1.80	0.62
2:H:4:THR:N	2:H:5:PRO:CD	2.63	0.62
2:F:113:GLU:HB3	2:F:114:PRO:CD	2.27	0.62
2:H:261:ILE:HD11	2:H:283:PHE:HD2	1.65	0.62
1:C:401:THR:HG22	1:C:401:THR:O	2.00	0.62
1:D:718:GLN:HA	1:D:718:GLN:NE2	2.15	0.61
1:D:150:ASN:O	1:D:151:ASN:HB2	2.01	0.61
2:H:282:ARG:NH1	2:H:286:ASP:OD2	2.33	0.61
1:D:358:ARG:HH11	1:D:358:ARG:HB3	1.66	0.61
2:H:23:LYS:HB2	2:H:26:THR:HG23	1.82	0.61
1:B:487:ASN:H	1:B:487:ASN:HD22	1.46	0.61
1:A:170:ASN:N	1:A:170:ASN:HD22	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:23:LYS:HB2	2:G:26:THR:HG23	1.83	0.61
2:H:322:PHE:HA	2:H:325:LEU:HD13	1.83	0.61
1:C:170:ASN:N	1:C:170:ASN:HD22	1.99	0.61
2:H:76:ARG:CG	2:H:76:ARG:NH1	2.57	0.61
1:D:170:ASN:N	1:D:170:ASN:HD22	1.99	0.60
2:E:23:LYS:HB2	2:E:26:THR:HG23	1.84	0.60
2:E:322:PHE:HA	2:E:325:LEU:HD13	1.82	0.60
1:A:150:ASN:O	1:A:151:ASN:HB2	2.01	0.60
2:F:322:PHE:HA	2:F:325:LEU:HD13	1.81	0.60
2:G:322:PHE:HA	2:G:325:LEU:HD13	1.82	0.60
2:G:114:PRO:HG2	2:G:158:GLN:HE22	1.67	0.60
2:E:235:ARG:HD2	2:E:260:GLU:OE2	2.01	0.60
7:C:870:NAG:H5	7:C:870:NAG:HN2	1.62	0.60
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.84	0.60
1:A:340:LEU:HB2	1:A:343:ARG:HD2	1.82	0.59
1:B:170:ASN:N	1:B:170:ASN:HD22	2.00	0.59
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.84	0.59
2:E:15:HIS:HE1	2:E:214:HIS:CE1	2.20	0.59
2:E:114:PRO:HG2	2:E:158:GLN:HE22	1.65	0.59
2:G:113:GLU:HB3	2:G:114:PRO:CD	2.27	0.59
2:H:235:ARG:HD2	2:H:260:GLU:OE2	2.02	0.59
1:B:471:ARG:HG3	1:B:480:TYR:CD2	2.37	0.59
2:G:15:HIS:HE1	2:G:214:HIS:CE1	2.19	0.59
2:H:151:ILE:HG12	2:H:179:ALA:HB3	1.85	0.59
1:C:377:ASN:C	1:C:377:ASN:HD22	2.04	0.59
1:C:358:ARG:HB3	1:C:358:ARG:HH11	1.68	0.59
2:H:76:ARG:HH11	2:H:76:ARG:HG3	1.67	0.59
1:A:581:ARG:HH12	7:A:860:NAG:H82	1.67	0.59
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.85	0.59
2:F:283:PHE:HB3	2:F:288:VAL:HG12	1.84	0.58
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.83	0.58
1:D:330:TYR:CE2	4:W:2:NAG:H83	2.38	0.58
2:G:157:HIS:CD2	2:G:158:GLN:HG2	2.38	0.58
1:B:145:GLU:N	1:B:145:GLU:OE2	2.37	0.58
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.67	0.58
2:H:110:SER:HB2	2:H:122:GLY:C	2.24	0.58
2:H:15:HIS:HE1	2:H:214:HIS:CE1	2.20	0.58
1:A:377:ASN:C	1:A:377:ASN:HD22	2.07	0.58
1:A:377:ASN:ND2	1:A:381:TYR:H	2.02	0.58
2:F:114:PRO:HD2	2:F:161:TRP:CZ2	2.38	0.58
2:G:235:ARG:HD2	2:G:260:GLU:OE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:113:GLU:CB	2:F:114:PRO:HD3	2.31	0.57
2:H:157:HIS:CD2	2:H:158:GLN:HG2	2.38	0.57
1:C:718:GLN:HE21	1:C:718:GLN:CA	2.16	0.57
1:D:377:ASN:ND2	1:D:381:TYR:H	2.03	0.57
2:E:277:GLU:OE2	2:E:281:ILE:HG21	2.04	0.57
2:F:76:ARG:NH1	2:F:128:GLU:OE1	2.37	0.57
2:F:280:VAL:HA	2:F:283:PHE:HD1	1.65	0.57
2:G:151:ILE:HG12	2:G:179:ALA:HB3	1.84	0.57
2:E:151:ILE:HG12	2:E:179:ALA:HB3	1.87	0.57
2:F:151:ILE:HG12	2:F:179:ALA:HB3	1.86	0.57
1:A:471:ARG:HG3	1:A:480:TYR:CD2	2.39	0.57
2:F:157:HIS:CD2	2:F:158:GLN:HG2	2.40	0.57
2:H:76:ARG:HG2	2:H:76:ARG:NH1	2.18	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:B:358:ARG:HH11	1:B:358:ARG:HB3	1.70	0.57
1:C:471:ARG:HG3	1:C:480:TYR:CD2	2.39	0.57
2:G:169:CYS:HA	2:G:177:VAL:HG21	1.85	0.57
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.87	0.57
2:E:157:HIS:CD2	2:E:158:GLN:HG2	2.39	0.57
1:D:471:ARG:HG3	1:D:480:TYR:CD2	2.39	0.57
1:A:358:ARG:HB3	1:A:358:ARG:HH11	1.69	0.56
2:H:42:THR:HB	2:H:45:GLU:H	1.70	0.56
2:G:34:ARG:HH22	2:G:74:GLY:H	1.52	0.56
1:A:487:ASN:H	1:A:487:ASN:ND2	2.03	0.56
2:F:169:CYS:HA	2:F:177:VAL:HG21	1.86	0.56
1:C:377:ASN:ND2	1:C:381:TYR:H	2.04	0.56
1:A:651:ILE:HG23	1:A:701:LEU:HB3	1.87	0.56
1:B:377:ASN:C	1:B:377:ASN:HD22	2.09	0.56
2:G:109:ASN:O	2:G:122:GLY:CA	2.52	0.56
2:G:323:LYS:O	2:G:327:ILE:HG12	2.06	0.56
2:F:323:LYS:O	2:F:327:ILE:HG12	2.06	0.56
1:C:150:ASN:O	1:C:151:ASN:HB2	2.04	0.56
1:D:377:ASN:C	1:D:377:ASN:HD22	2.08	0.56
2:E:169:CYS:HA	2:E:177:VAL:HG21	1.88	0.56
1:D:487:ASN:H	1:D:487:ASN:ND2	2.02	0.55
1:D:651:ILE:HG23	1:D:701:LEU:HB3	1.88	0.55
1:C:487:ASN:H	1:C:487:ASN:ND2	2.04	0.55
1:D:73:GLU:O	1:D:74:ASN:HB2	2.05	0.55
2:E:175:GLN:C	2:E:176:THR:HG23	2.26	0.55
2:G:76:ARG:HB3	2:G:132:LEU:CD2	2.35	0.55
2:G:101:ARG:HA	2:G:151:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:CYS:HA	2:H:177:VAL:HG21	1.88	0.55
1:D:446:SER:HA	1:D:449:LEU:HG	1.88	0.55
1:D:710:ASN:C	1:D:710:ASN:HD22	2.10	0.55
1:D:109:PRO:HG2	1:D:158:SER:O	2.07	0.55
2:F:42:THR:HB	2:F:45:GLU:H	1.72	0.55
2:F:113:GLU:CB	2:F:114:PRO:CD	2.84	0.55
1:C:651:ILE:HG23	1:C:701:LEU:HB3	1.88	0.55
1:D:145:GLU:OE2	1:D:145:GLU:N	2.39	0.55
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.90	0.55
2:H:323:LYS:O	2:H:327:ILE:HG12	2.07	0.55
1:B:718:GLN:HE21	1:B:718:GLN:CA	2.18	0.54
1:A:336:ARG:NH2	2:F:127:ASP:OD1	2.37	0.54
1:B:39:SER:OG	1:B:39:SER:O	2.23	0.54
7:C:860:NAG:H61	7:C:860:NAG:H2	1.88	0.54
2:G:42:THR:HB	2:G:45:GLU:H	1.72	0.54
2:G:282:ARG:HH11	2:G:282:ARG:HB3	1.73	0.54
1:B:39:SER:N	1:B:40:ARG:HH21	2.05	0.54
1:A:109:PRO:HG2	1:A:158:SER:O	2.08	0.54
1:C:234:PRO:HG2	1:D:248:TYR:OH	2.08	0.54
1:B:377:ASN:ND2	1:B:381:TYR:H	2.06	0.54
1:C:203:TYR:HA	1:C:207:VAL:HG13	1.89	0.54
1:D:272:ASN:HD22	1:D:274:ASP:H	1.56	0.54
1:A:76:ILE:HG13	1:A:76:ILE:O	2.06	0.54
1:A:145:GLU:OE2	1:A:145:GLU:N	2.42	0.54
2:E:42:THR:HB	2:E:45:GLU:H	1.72	0.54
2:G:95:VAL:HG11	2:G:98:VAL:HG22	1.89	0.53
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.89	0.53
1:C:109:PRO:HG2	1:C:158:SER:O	2.07	0.53
1:C:145:GLU:OE2	1:C:145:GLU:N	2.41	0.53
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.89	0.53
1:A:487:ASN:ND2	1:A:487:ASN:N	2.56	0.53
4:K:1:NAG:H3	4:K:1:NAG:C8	2.38	0.53
1:B:109:PRO:HG2	1:B:158:SER:O	2.09	0.53
1:D:487:ASN:HD22	1:D:487:ASN:N	2.02	0.53
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.90	0.53
2:H:95:VAL:HG11	2:H:98:VAL:HG22	1.90	0.53
1:B:76:ILE:O	1:B:76:ILE:HG13	2.07	0.53
2:F:175:GLN:C	2:F:176:THR:HG23	2.29	0.53
2:H:117:TRP:O	2:H:118:ASN:HB2	2.09	0.53
1:B:487:ASN:H	1:B:487:ASN:ND2	2.06	0.53
2:F:114:PRO:HD2	2:F:161:TRP:HZ2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:GLN:HE21	1:A:718:GLN:CA	2.19	0.53
2:F:26:THR:HG21	2:F:85:GLU:OE1	2.09	0.53
2:F:283:PHE:HB3	2:F:288:VAL:CG1	2.39	0.53
1:B:308:GLN:HA	1:B:308:GLN:OE1	2.08	0.53
2:G:279:ALA:O	2:G:283:PHE:CD2	2.62	0.53
1:A:177:GLU:HB2	1:A:180:LEU:HD13	1.90	0.52
1:C:446:SER:HA	1:C:449:LEU:HG	1.92	0.52
2:H:235:ARG:HG2	2:H:258:HIS:HB3	1.91	0.52
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.39	0.52
1:B:710:ASN:C	1:B:710:ASN:HD22	2.12	0.52
1:D:76:ILE:O	1:D:76:ILE:HG13	2.10	0.52
2:E:277:GLU:HB3	2:E:281:ILE:HG21	1.91	0.52
2:H:261:ILE:HD12	2:H:290:TYR:CD2	2.44	0.52
2:H:65:PHE:HB3	2:H:117:TRP:HH2	1.74	0.52
2:H:339:GLU:HA	2:H:342:GLU:HG2	1.91	0.52
1:A:710:ASN:HD22	1:A:710:ASN:C	2.13	0.52
1:C:177:GLU:HB2	1:C:180:LEU:HD13	1.91	0.52
1:D:487:ASN:ND2	1:D:487:ASN:N	2.56	0.52
1:D:701:LEU:HD13	1:D:703:ILE:HD11	1.92	0.52
2:F:101:ARG:HA	2:F:151:ILE:O	2.09	0.52
1:B:651:ILE:HG23	1:B:701:LEU:HB3	1.91	0.52
1:C:487:ASN:HD22	1:C:487:ASN:N	2.04	0.52
2:H:175:GLN:C	2:H:176:THR:HG23	2.29	0.52
2:E:323:LYS:O	2:E:327:ILE:HG12	2.09	0.52
2:F:114:PRO:HG3	2:F:158:GLN:HE22	1.75	0.52
2:G:235:ARG:HG2	2:G:258:HIS:HB3	1.91	0.52
1:A:726:VAL:HG13	1:A:728:VAL:HG23	1.92	0.52
2:F:235:ARG:HG2	2:F:258:HIS:HB3	1.92	0.52
2:H:138:GLN:HE22	2:H:175:GLN:HG2	1.75	0.52
1:B:446:SER:HA	1:B:449:LEU:HG	1.92	0.52
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.91	0.52
2:E:114:PRO:HG2	2:E:158:GLN:NE2	2.25	0.51
1:D:293:MET:HG2	1:D:315:TRP:HB3	1.92	0.51
1:A:446:SER:HA	1:A:449:LEU:HG	1.91	0.51
1:B:75:ASN:OD1	7:B:870:NAG:O5	2.29	0.51
2:F:95:VAL:HG11	2:F:98:VAL:HG22	1.92	0.51
2:G:175:GLN:C	2:G:176:THR:HG23	2.30	0.51
2:H:65:PHE:HB3	2:H:117:TRP:CH2	2.46	0.51
1:C:487:ASN:ND2	1:C:487:ASN:N	2.57	0.51
1:D:662:TYR:CE1	1:D:710:ASN:ND2	2.78	0.51
2:F:322:PHE:HA	2:F:325:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ASN:HD22	1:D:339:CYS:N	2.08	0.51
2:E:86:PHE:O	2:E:89:MET:HG2	2.10	0.51
2:E:235:ARG:HG2	2:E:258:HIS:HB3	1.92	0.51
2:F:15:HIS:HD2	2:F:295:ASP:OD1	1.88	0.51
1:B:177:GLU:HB2	1:B:180:LEU:HD13	1.93	0.51
1:D:308:GLN:HA	1:D:308:GLN:OE1	2.11	0.51
1:A:39:SER:N	1:A:40:ARG:HH21	2.09	0.51
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.93	0.51
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.93	0.51
2:F:90:LYS:HG3	2:F:98:VAL:HG21	1.92	0.51
2:F:272:TRP:NE1	2:F:278:HIS:HA	2.26	0.51
2:G:339:GLU:HA	2:G:342:GLU:HG2	1.93	0.51
2:H:26:THR:HG21	2:H:85:GLU:OE1	2.11	0.51
1:D:196:ASN:OD1	1:D:227:GLN:HG3	2.11	0.51
2:F:261:ILE:HD12	2:F:290:TYR:CD2	2.46	0.51
1:D:630:SER:OG	1:D:740:HIS:NE2	2.43	0.50
2:E:339:GLU:HA	2:E:342:GLU:HG2	1.94	0.50
2:F:339:GLU:HA	2:F:342:GLU:HG2	1.94	0.50
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.93	0.50
1:C:626:ILE:HG23	1:C:636:THR:HG23	1.94	0.50
2:E:95:VAL:HG11	2:E:98:VAL:HG22	1.93	0.50
1:D:718:GLN:HE21	1:D:718:GLN:CA	2.24	0.50
2:G:352:ARG:O	2:G:352:ARG:HG3	2.10	0.50
1:B:487:ASN:ND2	1:B:487:ASN:N	2.60	0.50
1:C:308:GLN:OE1	1:C:308:GLN:HA	2.11	0.50
2:E:322:PHE:HA	2:E:325:LEU:CD1	2.42	0.50
2:H:233:THR:OG1	2:H:235:ARG:O	2.27	0.50
1:C:272:ASN:HD22	1:C:274:ASP:H	1.59	0.50
1:D:449:LEU:O	1:D:450:ASN:HB2	2.11	0.50
1:D:662:TYR:HE1	1:D:710:ASN:ND2	2.08	0.50
1:D:726:VAL:HG13	1:D:728:VAL:HG23	1.93	0.50
2:G:322:PHE:HA	2:G:325:LEU:CD1	2.41	0.50
2:G:29:TYR:OH	2:G:33:ARG:NH1	2.45	0.50
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.93	0.49
2:G:131:SER:O	2:G:134:ASN:HB2	2.13	0.49
2:H:29:TYR:OH	2:H:33:ARG:NH1	2.45	0.49
1:A:75:ASN:HD21	7:A:870:NAG:H62	1.77	0.49
1:B:142:LEU:HD12	1:B:142:LEU:H	1.77	0.49
1:C:173:TYR:CE2	1:C:184:ARG:CG	2.96	0.49
1:D:177:GLU:HB2	1:D:180:LEU:HD13	1.94	0.49
2:F:225:LYS:HD2	2:F:248:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:261:ILE:HD12	2:G:290:TYR:CD2	2.46	0.49
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.12	0.49
2:F:353:MET:CB	2:F:354:PRO:HD2	2.40	0.49
1:A:487:ASN:HD22	1:A:487:ASN:N	2.02	0.49
1:C:125:ARG:HG2	1:C:126:HIS:NE2	2.28	0.49
1:C:710:ASN:C	1:C:710:ASN:HD22	2.15	0.49
2:E:225:LYS:HD2	2:E:248:LEU:HD13	1.93	0.49
2:G:86:PHE:O	2:G:89:MET:HG2	2.13	0.49
1:D:680:LEU:HD11	1:D:684:ARG:CZ	2.43	0.49
2:E:102:TYR:CE2	2:E:133:VAL:HG11	2.48	0.49
2:H:116:PRO:O	2:H:119:GLN:HG2	2.13	0.49
2:H:321:GLU:OE2	2:H:324:ARG:NH2	2.46	0.49
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.42	0.49
1:D:405:ILE:HG13	1:D:429:ARG:HD3	1.95	0.49
2:E:261:ILE:HD12	2:E:290:TYR:CD2	2.48	0.49
2:H:225:LYS:HD2	2:H:248:LEU:HD13	1.95	0.49
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.95	0.49
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.42	0.49
1:C:105:TYR:HB2	1:C:114:ILE:HD11	1.95	0.49
1:D:328:CYS:HA	1:D:338:ASN:O	2.12	0.49
2:E:29:TYR:OH	2:E:33:ARG:NH1	2.46	0.49
1:B:449:LEU:O	1:B:450:ASN:HB2	2.13	0.49
2:H:79:ILE:O	2:H:82:ILE:HG12	2.13	0.49
2:H:134:ASN:ND2	2:H:175:GLN:O	2.46	0.49
1:A:291:ALA:HB2	2:F:80:LYS:HG2	1.94	0.48
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.13	0.48
1:A:272:ASN:HD22	1:A:274:ASP:H	1.60	0.48
2:H:101:ARG:HA	2:H:151:ILE:O	2.12	0.48
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.28	0.48
1:B:405:ILE:HG13	1:B:429:ARG:HD3	1.94	0.48
1:C:125:ARG:HG2	1:C:126:HIS:CE1	2.49	0.48
1:C:318:ARG:NH1	1:C:668:GLU:OE2	2.47	0.48
1:C:680:LEU:HD11	1:C:684:ARG:CZ	2.43	0.48
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.95	0.48
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.28	0.48
1:D:125:ARG:HG2	1:D:126:HIS:NE2	2.29	0.48
1:D:378:GLU:CD	1:D:378:GLU:H	2.17	0.48
2:E:126:PRO:O	2:E:130:VAL:HG23	2.12	0.48
1:A:449:LEU:O	1:A:450:ASN:HB2	2.14	0.48
1:B:272:ASN:HD22	1:B:274:ASP:H	1.61	0.48
1:C:662:TYR:CE1	1:C:710:ASN:ND2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:272:TRP:NE1	2:E:278:HIS:HA	2.28	0.48
2:G:34:ARG:NH1	2:G:74:GLY:HA3	2.27	0.48
1:C:726:VAL:HG13	1:C:728:VAL:HG23	1.95	0.48
2:G:90:LYS:HG3	2:G:98:VAL:HG21	1.96	0.48
2:H:102:TYR:CE2	2:H:133:VAL:HG11	2.47	0.48
2:H:272:TRP:NE1	2:H:278:HIS:HA	2.29	0.48
1:B:388:GLN:HB2	1:B:391:LYS:HB2	1.96	0.48
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.44	0.48
2:F:233:THR:OG1	2:F:235:ARG:O	2.28	0.48
2:E:60:ASP:OD2	2:E:60:ASP:N	2.45	0.48
2:F:86:PHE:O	2:F:89:MET:HG2	2.13	0.48
1:A:125:ARG:HG2	1:A:126:HIS:NE2	2.29	0.48
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.96	0.47
1:B:125:ARG:HG2	1:B:126:HIS:NE2	2.29	0.47
1:C:388:GLN:HB2	1:C:391:LYS:HB2	1.95	0.47
1:D:751:ILE:HG23	1:D:752:TYR:N	2.29	0.47
2:E:101:ARG:HA	2:E:151:ILE:O	2.14	0.47
2:E:321:GLU:OE2	2:E:324:ARG:NH2	2.47	0.47
1:C:76:ILE:O	1:C:76:ILE:HG13	2.13	0.47
1:B:701:LEU:HD13	1:B:703:ILE:HD11	1.95	0.47
2:E:26:THR:HG21	2:E:85:GLU:OE1	2.14	0.47
2:G:60:ASP:OD2	2:G:60:ASP:N	2.43	0.47
2:H:86:PHE:O	2:H:89:MET:HG2	2.14	0.47
1:A:76:ILE:HG13	1:A:89:PHE:HB3	1.96	0.47
1:A:318:ARG:NH1	1:A:668:GLU:OE2	2.47	0.47
1:C:114:ILE:CG2	1:C:135:TYR:HB3	2.45	0.47
2:G:154:CYS:SG	2:G:180:ILE:HD11	2.54	0.47
7:A:860:NAG:H3	7:A:860:NAG:C8	2.34	0.47
2:H:322:PHE:HA	2:H:325:LEU:CD1	2.43	0.47
1:B:142:LEU:HD12	1:B:142:LEU:N	2.30	0.47
1:C:76:ILE:HG13	1:C:89:PHE:HB3	1.97	0.47
1:C:378:GLU:H	1:C:378:GLU:CD	2.18	0.47
1:D:290:PRO:HD2	1:D:315:TRP:CD1	2.50	0.47
2:E:56:LEU:HB3	2:E:57:THR:H	1.52	0.47
2:F:29:TYR:OH	2:F:33:ARG:NH1	2.48	0.47
2:G:15:HIS:HD2	2:G:295:ASP:OD1	1.94	0.47
2:F:154:CYS:SG	2:F:180:ILE:HD11	2.55	0.47
2:H:154:CYS:SG	2:H:180:ILE:HD11	2.55	0.47
3:Q:1:NAG:H62	3:Q:3:FUC:O2	2.14	0.47
2:F:240:TYR:CZ	2:F:266:SER:OG	2.60	0.46
1:A:125:ARG:HG2	1:A:126:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HG2	1:D:126:HIS:CE1	2.49	0.46
2:G:225:LYS:HD2	2:G:248:LEU:HD13	1.96	0.46
1:B:40:ARG:H	1:B:40:ARG:HE	1.64	0.46
1:B:308:GLN:HB3	4:N:1:NAG:O6	2.15	0.46
1:C:125:ARG:HG2	1:C:126:HIS:CD2	2.51	0.46
2:E:281:ILE:HG23	2:E:282:ARG:N	2.29	0.46
2:F:321:GLU:OE2	2:F:324:ARG:NH2	2.48	0.46
2:G:272:TRP:NE1	2:G:278:HIS:HA	2.31	0.46
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.44	0.46
1:A:221:THR:OG1	4:K:1:NAG:H5	2.16	0.46
1:A:405:ILE:HG13	1:A:429:ARG:HD3	1.98	0.46
1:B:76:ILE:HG13	1:B:89:PHE:HB3	1.96	0.46
1:B:662:TYR:CE1	1:B:710:ASN:ND2	2.84	0.46
1:B:718:GLN:NE2	1:B:718:GLN:CA	2.76	0.46
1:C:76:ILE:HD11	1:C:89:PHE:CD1	2.50	0.46
2:H:54:LYS:O	2:H:56:LEU:HD22	2.15	0.46
2:H:60:ASP:OD2	2:H:60:ASP:N	2.44	0.46
2:H:114:PRO:HD2	2:H:161:TRP:CZ2	2.51	0.46
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.97	0.46
1:A:608:GLU:OE2	1:A:608:GLU:HA	2.15	0.46
2:E:90:LYS:HG3	2:E:98:VAL:HG21	1.97	0.46
2:E:313:LYS:HD2	2:E:313:LYS:N	2.31	0.46
1:A:630:SER:OG	1:A:740:HIS:NE2	2.41	0.46
1:D:76:ILE:HG13	1:D:89:PHE:HB3	1.96	0.46
2:H:191:SER:HA	2:H:194:PHE:CE2	2.49	0.46
1:C:689:MET:HB3	1:C:722:ALA:HB2	1.97	0.46
1:D:105:TYR:HB2	1:D:114:ILE:HD11	1.97	0.46
1:D:388:GLN:HB2	1:D:391:LYS:HB2	1.97	0.46
1:B:378:GLU:CD	1:B:378:GLU:H	2.18	0.46
2:E:154:CYS:SG	2:E:180:ILE:HD11	2.56	0.46
2:F:181:ASP:CG	2:F:182:LEU:H	2.20	0.45
2:H:90:LYS:HG3	2:H:98:VAL:HG21	1.97	0.45
1:C:291:ALA:HB1	2:G:84:TYR:HB2	1.98	0.45
1:C:630:SER:OG	1:C:740:HIS:NE2	2.44	0.45
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.99	0.45
1:B:125:ARG:HG2	1:B:126:HIS:CE1	2.52	0.45
1:C:219:ASN:HB2	4:S:1:NAG:H82	1.98	0.45
1:C:662:TYR:HE1	1:C:710:ASN:ND2	2.14	0.45
1:D:689:MET:HB3	1:D:722:ALA:HB2	1.99	0.45
1:A:92:ASN:OD1	7:A:870:NAG:O5	2.33	0.45
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.64	0.45
1:A:466:LYS:HB3	1:A:467:TYR:CD2	2.51	0.45
2:H:13:GLU:OE1	2:H:294:THR:HG22	2.17	0.45
1:C:448:GLU:HA	1:C:448:GLU:OE2	2.16	0.45
1:C:449:LEU:O	1:C:450:ASN:HB2	2.15	0.45
2:G:13:GLU:OE1	2:G:294:THR:HG22	2.16	0.45
2:G:111:LYS:HE2	2:G:111:LYS:HB3	1.83	0.45
2:G:233:THR:OG1	2:G:235:ARG:O	2.29	0.45
1:A:689:MET:HB3	1:A:722:ALA:HB2	1.98	0.45
1:C:142:LEU:HD12	1:C:142:LEU:H	1.82	0.45
1:C:544:LEU:HD12	1:C:576:ALA:O	2.15	0.45
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.97	0.45
2:F:5:PRO:O	2:F:7:PHE:N	2.50	0.45
1:A:173:TYR:CE2	1:A:184:ARG:CG	2.97	0.45
2:G:282:ARG:HB3	2:G:282:ARG:NH1	2.31	0.45
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.16	0.45
1:A:429:ARG:HB3	1:A:456:TYR:HA	1.99	0.45
1:B:125:ARG:HG2	1:B:126:HIS:CD2	2.51	0.45
1:C:196:ASN:OD1	1:C:227:GLN:HG3	2.16	0.45
1:C:405:ILE:HG13	1:C:429:ARG:HD3	1.98	0.45
1:C:608:GLU:OE2	1:C:608:GLU:HA	2.16	0.45
2:F:133:VAL:O	2:F:134:ASN:C	2.54	0.45
1:C:466:LYS:HB3	1:C:467:TYR:CD2	2.52	0.45
2:F:13:GLU:OE1	2:F:294:THR:HG22	2.17	0.45
2:G:23:LYS:HA	2:G:24:PRO:HD2	1.78	0.45
2:G:26:THR:HG21	2:G:85:GLU:OE1	2.16	0.45
2:H:261:ILE:HD12	2:H:290:TYR:HD2	1.82	0.45
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.80	0.45
1:A:662:TYR:CE1	1:A:710:ASN:ND2	2.85	0.45
1:B:425:MET:HA	1:B:426:PRO:HD3	1.70	0.45
1:B:662:TYR:HE1	1:B:710:ASN:ND2	2.15	0.45
2:E:116:PRO:O	2:E:119:GLN:HG2	2.17	0.45
2:G:181:ASP:CG	2:G:182:LEU:H	2.20	0.45
2:G:321:GLU:OE2	2:G:324:ARG:NH2	2.50	0.45
1:A:175:LYS:HG3	1:A:182:SER:HB3	2.00	0.44
2:E:191:SER:HA	2:E:194:PHE:CE2	2.51	0.44
2:F:325:LEU:HD22	2:F:326:ASN:N	2.32	0.44
1:A:125:ARG:HG2	1:A:126:HIS:CD2	2.52	0.44
1:A:142:LEU:HD12	1:A:142:LEU:H	1.82	0.44
1:B:173:TYR:CE2	1:B:184:ARG:CG	3.00	0.44
1:B:554:LYS:HE2	1:B:554:LYS:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLU:H	1:A:379:GLU:HG2	1.68	0.44
1:B:184:ARG:NH1	1:B:187:TRP:HA	2.32	0.44
1:D:429:ARG:HB3	1:D:456:TYR:HA	2.00	0.44
2:F:191:SER:HA	2:F:194:PHE:CE2	2.52	0.44
1:A:544:LEU:HD12	1:A:576:ALA:O	2.18	0.44
1:D:125:ARG:HG2	1:D:126:HIS:CD2	2.52	0.44
1:D:318:ARG:NH1	1:D:668:GLU:OE2	2.51	0.44
2:F:262:CYS:CB	2:F:265:SER:HB3	2.46	0.44
2:G:34:ARG:NH2	2:G:74:GLY:H	2.15	0.44
1:D:40:ARG:H	1:D:40:ARG:HE	1.64	0.44
1:D:448:GLU:OE2	1:D:448:GLU:HA	2.17	0.44
1:D:598:LEU:HD22	1:D:671:MET:HG2	2.00	0.44
1:D:608:GLU:OE2	1:D:608:GLU:HA	2.18	0.44
2:E:240:TYR:C	2:E:242:THR:N	2.57	0.44
2:G:191:SER:HA	2:G:194:PHE:CE2	2.53	0.44
1:A:751:ILE:HG23	1:A:752:TYR:N	2.33	0.44
1:B:474:GLY:HA3	1:B:557:THR:O	2.18	0.44
1:D:142:LEU:HD12	1:D:142:LEU:H	1.82	0.44
1:D:184:ARG:HD3	1:D:186:THR:O	2.18	0.44
2:H:11:LYS:HD2	2:H:304:LEU:HD23	1.99	0.44
1:A:378:GLU:CD	1:A:378:GLU:H	2.20	0.44
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.17	0.44
1:C:651:ILE:HG21	1:C:755:MET:HE2	1.99	0.44
2:E:15:HIS:N	2:E:293:ASN:OD1	2.41	0.44
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.52	0.44
1:C:142:LEU:HD12	1:C:142:LEU:N	2.33	0.44
1:D:142:LEU:HD12	1:D:142:LEU:N	2.33	0.44
1:D:302:ASP:HB3	1:D:314:GLN:HB2	2.00	0.44
1:D:661:TYR:OH	1:D:718:GLN:HG3	2.18	0.44
2:F:11:LYS:HD2	2:F:304:LEU:HD23	2.00	0.44
1:C:116:LEU:O	1:C:132:TYR:HA	2.18	0.43
1:B:76:ILE:HD11	1:B:89:PHE:CD1	2.53	0.43
1:B:487:ASN:HD22	1:B:487:ASN:N	2.09	0.43
1:B:608:GLU:OE2	1:B:608:GLU:HA	2.16	0.43
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.99	0.43
1:C:50:LYS:HD3	1:C:50:LYS:HA	1.93	0.43
1:D:76:ILE:HD11	1:D:89:PHE:CD1	2.53	0.43
2:E:233:THR:OG1	2:E:235:ARG:O	2.30	0.43
1:A:474:GLY:HA3	1:A:557:THR:O	2.18	0.43
1:B:689:MET:HB3	1:B:722:ALA:HB2	1.99	0.43
1:D:358:ARG:HB3	1:D:358:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:LYS:HB3	1:D:467:TYR:CD2	2.53	0.43
1:B:358:ARG:HB3	1:B:358:ARG:NH1	2.33	0.43
2:F:240:TYR:N	2:F:240:TYR:CD1	2.87	0.43
2:G:163:SER:O	2:G:166:VAL:HG12	2.18	0.43
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.99	0.43
1:A:701:LEU:HD13	1:A:703:ILE:HD11	1.99	0.43
1:B:651:ILE:HG21	1:B:755:MET:HE2	2.01	0.43
2:E:112:VAL:HG13	2:E:112:VAL:O	2.19	0.43
1:A:310:ARG:NH1	1:A:368:GLY:O	2.49	0.43
1:B:184:ARG:HD3	1:B:186:THR:O	2.17	0.43
1:B:429:ARG:HB3	1:B:456:TYR:HA	1.99	0.43
2:E:132:LEU:HD12	2:E:132:LEU:HA	1.63	0.43
1:B:436:LEU:HD12	1:B:436:LEU:HA	1.83	0.43
2:E:124:LEU:CD2	2:E:128:GLU:HB3	2.49	0.43
2:F:338:ASP:HB3	2:F:339:GLU:H	1.66	0.43
2:H:313:LYS:HD2	2:H:313:LYS:N	2.34	0.43
1:D:338:ASN:ND2	1:D:339:CYS:N	2.66	0.43
2:E:56:LEU:HA	2:E:56:LEU:HD13	1.78	0.43
2:F:116:PRO:O	2:F:119:GLN:HG2	2.18	0.43
1:A:116:LEU:O	1:A:132:TYR:HA	2.19	0.43
2:E:125:THR:HG23	2:E:128:GLU:HB2	2.01	0.43
1:B:315:TRP:O	1:B:323:SER:HB2	2.19	0.43
1:B:626:ILE:HG23	1:B:636:THR:HG23	2.00	0.43
2:F:313:LYS:N	2:F:313:LYS:HD2	2.34	0.43
1:A:567:LEU:HD22	1:A:573:ILE:HD12	2.01	0.42
1:C:56:LYS:HE2	1:C:495:GLU:OE1	2.19	0.42
1:C:429:ARG:HB3	1:C:456:TYR:HA	2.00	0.42
1:C:701:LEU:HD13	1:C:703:ILE:HD11	2.00	0.42
1:D:153:GLN:HE22	1:D:170:ASN:ND2	2.17	0.42
1:D:330:TYR:CD2	4:W:2:NAG:H83	2.54	0.42
2:G:135:GLN:H	2:G:135:GLN:HG2	1.61	0.42
2:G:325:LEU:HD22	2:G:326:ASN:N	2.34	0.42
2:H:243:LEU:HD22	2:H:282:ARG:NH2	2.34	0.42
4:N:1:NAG:H61	4:N:2:NAG:C1	2.49	0.42
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.34	0.42
1:A:367:ASP:CG	1:A:369:ASN:HD22	2.23	0.42
1:C:71:LYS:HZ3	1:C:74:ASN:H	1.66	0.42
1:D:50:LYS:HD3	1:D:50:LYS:HA	1.90	0.42
2:F:349:LYS:HE3	2:F:349:LYS:HB2	1.85	0.42
2:G:82:ILE:HG12	2:G:83:ALA:N	2.34	0.42
2:G:114:PRO:HD2	2:G:161:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:280:VAL:HA	2:G:283:PHE:CD2	2.39	0.42
2:H:163:SER:O	2:H:166:VAL:HG12	2.19	0.42
4:U:1:NAG:H61	4:U:2:NAG:N2	2.34	0.42
1:B:448:GLU:OE2	1:B:448:GLU:HA	2.18	0.42
1:B:466:LYS:HB3	1:B:467:TYR:CD2	2.54	0.42
2:F:26:THR:HG21	2:F:85:GLU:OE2	2.19	0.42
1:A:661:TYR:OH	1:A:718:GLN:HG3	2.19	0.42
2:E:113:GLU:HG3	2:E:161:TRP:CD1	2.54	0.42
2:H:106:LEU:HD23	2:H:106:LEU:HA	1.89	0.42
1:B:125:ARG:O	1:B:125:ARG:HG3	2.19	0.42
1:C:358:ARG:HB3	1:C:358:ARG:NH1	2.33	0.42
1:C:474:GLY:HA3	1:C:557:THR:O	2.20	0.42
1:D:548:ALA:HB3	1:D:635:VAL:HG21	2.01	0.42
2:E:13:GLU:OE1	2:E:294:THR:HG22	2.18	0.42
1:A:142:LEU:HD12	1:A:142:LEU:N	2.34	0.42
1:C:759:ILE:HD13	1:C:759:ILE:HA	1.90	0.42
2:F:194:PHE:HA	2:F:195:PRO:HD3	1.89	0.42
2:H:9:LYS:HB3	2:H:10:PRO:HD2	2.01	0.42
2:H:103:SER:HA	2:H:104:PRO:HD2	1.90	0.42
2:H:181:ASP:CG	2:H:182:LEU:H	2.22	0.42
1:A:285:ILE:HG21	1:A:336:ARG:HA	2.00	0.42
1:A:554:LYS:HE2	1:A:554:LYS:HB3	1.81	0.42
1:C:153:GLN:HE22	1:C:170:ASN:ND2	2.17	0.42
1:D:689:MET:HB3	1:D:722:ALA:CB	2.50	0.42
2:F:261:ILE:HD12	2:F:290:TYR:HD2	1.84	0.42
2:G:103:SER:HA	2:G:104:PRO:HD2	1.89	0.42
2:H:15:HIS:HD2	2:H:295:ASP:OD1	1.92	0.42
1:A:76:ILE:HD11	1:A:89:PHE:CD1	2.54	0.42
1:A:358:ARG:HB3	1:A:358:ARG:NH1	2.34	0.42
1:B:661:TYR:OH	1:B:718:GLN:HG3	2.20	0.42
1:C:127:SER:HB3	1:C:211:TYR:CD1	2.55	0.42
1:C:184:ARG:HD3	1:C:186:THR:O	2.19	0.42
1:C:661:TYR:OH	1:C:718:GLN:HG3	2.20	0.42
1:D:379:GLU:H	1:D:379:GLU:HG2	1.65	0.42
1:D:436:LEU:HD12	1:D:436:LEU:HA	1.86	0.42
2:E:23:LYS:HA	2:E:24:PRO:HD2	1.78	0.42
2:G:9:LYS:HB3	2:G:10:PRO:HD2	2.02	0.42
1:A:662:TYR:HE1	1:A:710:ASN:ND2	2.18	0.42
1:B:318:ARG:NH1	1:B:668:GLU:OE2	2.52	0.42
2:E:15:HIS:HD2	2:E:295:ASP:OD1	1.92	0.42
1:C:554:LYS:HE2	1:C:554:LYS:HB3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:626:ILE:O	1:D:650:GLY:HA2	2.20	0.42
2:F:23:LYS:HA	2:F:24:PRO:HD2	1.78	0.42
2:F:163:SER:O	2:F:166:VAL:HG12	2.20	0.42
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.84	0.41
1:D:272:ASN:ND2	1:D:274:ASP:H	2.18	0.41
2:E:194:PHE:HA	2:E:195:PRO:HD3	1.90	0.41
2:F:56:LEU:HB3	2:F:57:THR:H	1.73	0.41
2:G:125:THR:O	2:G:129:VAL:HG23	2.20	0.41
2:G:313:LYS:HD2	2:G:313:LYS:N	2.34	0.41
1:A:137:LEU:HD23	1:A:140:ARG:HH12	1.85	0.41
1:A:336:ARG:CZ	2:F:128:GLU:HB2	2.50	0.41
2:E:181:ASP:CG	2:E:182:LEU:H	2.23	0.41
4:U:1:NAG:H83	4:U:1:NAG:H3	2.03	0.41
2:F:294:THR:HG23	2:F:297:PRO:HD3	2.02	0.41
1:A:472:CYS:O	1:A:478:PRO:HA	2.20	0.41
1:C:170:ASN:N	1:C:170:ASN:ND2	2.68	0.41
1:D:82:GLU:OE1	1:D:82:GLU:HA	2.20	0.41
1:D:481:THR:OG1	1:D:483:HIS:CE1	2.71	0.41
2:F:4:THR:O	2:F:6:ALA:N	2.54	0.41
2:G:261:ILE:HG22	2:G:263:PRO:HD3	2.02	0.41
2:G:349:LYS:HE3	2:G:349:LYS:HB2	1.85	0.41
2:H:113:GLU:CB	2:H:114:PRO:HD3	2.50	0.41
2:H:116:PRO:HB2	2:H:117:TRP:CD1	2.56	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.87	0.41
2:E:9:LYS:HB3	2:E:10:PRO:HD2	2.03	0.41
1:B:56:LYS:HE2	1:B:495:GLU:OE1	2.20	0.41
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.91	0.41
1:D:173:TYR:CE2	1:D:184:ARG:CG	3.00	0.41
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.03	0.41
1:A:689:MET:HB3	1:A:722:ALA:CB	2.50	0.41
1:B:482:LEU:HD23	1:B:494:LEU:HD11	2.03	0.41
1:D:137:LEU:HD23	1:D:140:ARG:HH12	1.86	0.41
2:E:262:CYS:CB	2:E:265:SER:HB3	2.51	0.41
1:B:763:PHE:HB3	1:B:765:LEU:HD13	2.03	0.41
1:C:315:TRP:O	1:C:323:SER:HB2	2.21	0.41
2:E:294:THR:HG23	2:E:297:PRO:HD3	2.03	0.41
2:H:112:VAL:HG23	2:H:115:ILE:HG12	2.03	0.41
4:R:1:NAG:H61	4:R:2:NAG:H82	2.02	0.41
1:A:147:ARG:CZ	4:J:1:NAG:H83	2.51	0.41
1:A:612:GLN:O	1:A:615:LYS:HB2	2.21	0.41
1:C:472:CYS:O	1:C:478:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:LEU:HD21	1:C:606:GLN:HG3	2.02	0.41
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.56	0.41
1:D:482:LEU:HD23	1:D:494:LEU:HD11	2.03	0.41
2:E:163:SER:O	2:E:166:VAL:HG12	2.21	0.41
2:E:231:LEU:HD12	2:E:231:LEU:HA	1.88	0.41
2:F:60:ASP:OD2	2:F:60:ASP:N	2.44	0.41
2:F:179:ALA:HB2	2:F:334:PHE:CD2	2.56	0.41
2:G:66:ASP:OD2	2:G:117:TRP:HZ3	2.03	0.41
2:G:262:CYS:CB	2:G:265:SER:HB3	2.50	0.41
1:A:127:SER:HB3	1:A:211:TYR:CG	2.56	0.41
1:A:401:THR:O	1:A:401:THR:CG2	2.66	0.41
1:A:482:LEU:HD23	1:A:494:LEU:HD11	2.02	0.41
1:B:377:ASN:ND2	1:B:379:GLU:H	2.19	0.41
1:B:472:CYS:O	1:B:478:PRO:HA	2.20	0.41
1:B:751:ILE:HG23	1:B:752:TYR:N	2.36	0.41
1:D:127:SER:HB3	1:D:211:TYR:CD1	2.56	0.41
2:F:15:HIS:N	2:F:293:ASN:OD1	2.44	0.41
2:F:42:THR:CB	2:F:45:GLU:HB3	2.48	0.41
2:F:291:SER:HB3	2:F:329:ALA:HB2	2.02	0.41
2:F:342:GLU:HA	2:F:345:ASP:HB2	2.03	0.41
2:G:56:LEU:HB3	2:G:57:THR:H	1.61	0.41
2:H:185:ASP:OD2	2:H:188:ILE:HG13	2.20	0.41
1:A:82:GLU:HA	1:A:82:GLU:OE1	2.21	0.40
1:A:448:GLU:OE2	1:A:448:GLU:HA	2.21	0.40
1:A:626:ILE:O	1:A:650:GLY:HA2	2.21	0.40
1:B:545:ASP:HB3	1:B:577:SER:OG	2.20	0.40
1:D:65:ASP:OD2	1:D:466:LYS:HB2	2.22	0.40
1:D:544:LEU:HD12	1:D:576:ALA:O	2.21	0.40
2:E:109:ASN:O	2:E:122:GLY:HA2	2.20	0.40
1:A:651:ILE:HG21	1:A:755:MET:HE2	2.03	0.40
1:C:626:ILE:O	1:C:650:GLY:HA2	2.21	0.40
2:E:106:LEU:HD23	2:E:106:LEU:HA	1.86	0.40
2:H:342:GLU:HA	2:H:345:ASP:HB2	2.03	0.40
5:X:3:BMA:H3	5:X:4:MAN:H2	1.38	0.40
1:B:137:LEU:HD23	1:B:140:ARG:HH12	1.85	0.40
1:D:56:LYS:HE2	1:D:495:GLU:OE1	2.21	0.40
1:D:164:LEU:HD23	1:D:164:LEU:HA	1.90	0.40
1:D:401:THR:O	1:D:401:THR:CG2	2.65	0.40
2:E:23:LYS:HB3	2:E:23:LYS:HE2	1.82	0.40
2:G:283:PHE:HB3	2:G:288:VAL:HG12	2.03	0.40
2:H:110:SER:HB2	2:H:123:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:N	1:A:170:ASN:ND2	2.68	0.40
1:B:116:LEU:O	1:B:132:TYR:HA	2.22	0.40
1:D:291:ALA:HB1	2:H:84:TYR:HB2	2.03	0.40
1:D:372:TYR:CE2	1:D:386:TYR:CD1	3.10	0.40
2:F:102:TYR:CE2	2:F:133:VAL:HG11	2.57	0.40
1:B:150:ASN:O	1:B:151:ASN:CB	2.69	0.40
1:B:423:LYS:HB3	1:B:425:MET:HG2	2.03	0.40
1:C:689:MET:HB3	1:C:722:ALA:CB	2.51	0.40
2:G:23:LYS:HE2	2:G:23:LYS:HB3	1.83	0.40
2:G:342:GLU:HA	2:G:345:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	726/728 (100%)	674 (93%)	49 (7%)	3 (0%)	34 69
1	B	726/728 (100%)	674 (93%)	49 (7%)	3 (0%)	34 69
1	C	726/728 (100%)	670 (92%)	52 (7%)	4 (1%)	25 60
1	D	726/728 (100%)	669 (92%)	54 (7%)	3 (0%)	34 69
2	E	350/357 (98%)	320 (91%)	21 (6%)	9 (3%)	5 24
2	F	348/357 (98%)	311 (89%)	28 (8%)	9 (3%)	5 24
2	G	350/357 (98%)	318 (91%)	26 (7%)	6 (2%)	9 35
2	H	350/357 (98%)	319 (91%)	26 (7%)	5 (1%)	11 40
All	All	4302/4340 (99%)	3955 (92%)	305 (7%)	42 (1%)	15 49

All (42) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	E	56	LEU
2	E	113	GLU
2	E	241	HIS
2	E	338	ASP
2	F	6	ALA
2	F	338	ASP
2	G	338	ASP
2	H	338	ASP
1	A	521	GLU
1	B	521	GLU
1	C	521	GLU
1	D	521	GLU
2	E	354	PRO
2	F	5	PRO
2	F	113	GLU
2	G	56	LEU
1	A	596	ARG
1	B	73	GLU
1	C	332	GLU
1	C	596	ARG
2	F	241	HIS
1	A	450	ASN
1	C	450	ASN
1	D	450	ASN
1	D	596	ARG
2	E	19	ASP
2	E	238	HIS
2	E	295	ASP
2	E	337	GLU
2	F	295	ASP
2	G	238	HIS
2	G	295	ASP
2	H	238	HIS
2	H	295	ASP
1	B	450	ASN
2	F	238	HIS
2	F	313	LYS
2	G	113	GLU
2	G	353	MET
2	H	19	ASP
2	F	114	PRO
2	H	114	PRO

### 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	653/653 (100%)	596 (91%)	57 (9%)	10	34
1	B	653/653 (100%)	593 (91%)	60 (9%)	9	31
1	C	653/653 (100%)	591 (90%)	62 (10%)	8	30
1	D	653/653 (100%)	591 (90%)	62 (10%)	8	30
2	E	307/310 (99%)	262 (85%)	45 (15%)	3	13
2	F	306/310 (99%)	267 (87%)	39 (13%)	4	18
2	G	307/310 (99%)	262 (85%)	45 (15%)	3	13
2	H	307/310 (99%)	265 (86%)	42 (14%)	3	15
All	All	3839/3852 (100%)	3427 (89%)	412 (11%)	6	24

All (412) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	76	ILE
1	A	114	ILE
1	A	140	ARG
1	A	144	THR
1	A	170	ASN
1	A	184	ARG
1	A	191	GLU
1	A	207	VAL
1	A	214	LEU
1	A	223	LEU
1	A	230	ASP
1	A	237	GLU
1	A	246	LEU
1	A	253	ARG
1	A	272	ASN
1	A	292	SER
1	A	303	VAL
1	A	318	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	358	ARG
1	A	361	GLU
1	A	375	ILE
1	A	377	ASN
1	A	379	GLU
1	A	390	ASP
1	A	399	LYS
1	A	410	LEU
1	A	423	LYS
1	A	429	ARG
1	A	436	LEU
1	A	471	ARG
1	A	482	LEU
1	A	487	ASN
1	A	492	ARG
1	A	505	GLN
1	A	507	VAL
1	A	514	LEU
1	A	523	LYS
1	A	536	LYS
1	A	543	LEU
1	A	554	LYS
1	A	589	LYS
1	A	597	ARG
1	A	598	LEU
1	A	603	VAL
1	A	608	GLU
1	A	621	ASN
1	A	622	LYS
1	A	658	ARG
1	A	673	LEU
1	A	679	ASN
1	A	685	ASN
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	710	ASN
1	A	761	GLN
1	B	40	ARG
1	B	73	GLU
1	B	76	ILE
1	B	114	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	140	ARG
1	B	144	THR
1	B	170	ASN
1	B	184	ARG
1	B	191	GLU
1	B	207	VAL
1	B	214	LEU
1	B	223	LEU
1	B	230	ASP
1	B	237	GLU
1	B	246	LEU
1	B	253	ARG
1	B	272	ASN
1	B	303	VAL
1	B	318	ARG
1	B	338	ASN
1	B	358	ARG
1	B	361	GLU
1	B	375	ILE
1	B	377	ASN
1	B	379	GLU
1	B	385	CYS
1	B	390	ASP
1	B	399	LYS
1	B	410	LEU
1	B	423	LYS
1	B	429	ARG
1	B	436	LEU
1	B	471	ARG
1	B	482	LEU
1	B	485	SER
1	B	487	ASN
1	B	492	ARG
1	B	505	GLN
1	B	507	VAL
1	B	514	LEU
1	B	523	LYS
1	B	536	LYS
1	B	543	LEU
1	B	554	LYS
1	B	589	LYS
1	B	597	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	598	LEU
1	B	603	VAL
1	B	608	GLU
1	B	621	ASN
1	B	622	LYS
1	B	658	ARG
1	B	673	LEU
1	B	679	ASN
1	B	685	ASN
1	B	689	MET
1	B	701	LEU
1	B	702	LEU
1	B	710	ASN
1	B	761	GLN
1	C	40	ARG
1	C	71	LYS
1	C	73	GLU
1	C	76	ILE
1	C	91	GLU
1	C	114	ILE
1	C	140	ARG
1	C	144	THR
1	C	170	ASN
1	C	184	ARG
1	C	191	GLU
1	C	207	VAL
1	C	214	LEU
1	C	223	LEU
1	C	230	ASP
1	C	237	GLU
1	C	246	LEU
1	C	253	ARG
1	C	272	ASN
1	C	303	VAL
1	C	318	ARG
1	C	332	GLU
1	C	338	ASN
1	C	358	ARG
1	C	361	GLU
1	C	375	ILE
1	C	377	ASN
1	C	379	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	385	CYS
1	C	390	ASP
1	C	399	LYS
1	C	410	LEU
1	C	423	LYS
1	C	429	ARG
1	C	436	LEU
1	C	471	ARG
1	C	482	LEU
1	C	487	ASN
1	C	492	ARG
1	C	505	GLN
1	C	507	VAL
1	C	514	LEU
1	C	523	LYS
1	C	536	LYS
1	C	543	LEU
1	C	554	LYS
1	C	589	LYS
1	C	597	ARG
1	C	598	LEU
1	C	603	VAL
1	C	608	GLU
1	C	621	ASN
1	C	622	LYS
1	C	658	ARG
1	C	673	LEU
1	C	679	ASN
1	C	685	ASN
1	C	689	MET
1	C	701	LEU
1	C	702	LEU
1	C	710	ASN
1	C	761	GLN
1	D	40	ARG
1	D	71	LYS
1	D	76	ILE
1	D	114	ILE
1	D	140	ARG
1	D	144	THR
1	D	170	ASN
1	D	184	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	191	GLU
1	D	207	VAL
1	D	214	LEU
1	D	223	LEU
1	D	230	ASP
1	D	237	GLU
1	D	246	LEU
1	D	253	ARG
1	D	272	ASN
1	D	285	ILE
1	D	293	MET
1	D	303	VAL
1	D	318	ARG
1	D	336	ARG
1	D	358	ARG
1	D	361	GLU
1	D	375	ILE
1	D	377	ASN
1	D	378	GLU
1	D	379	GLU
1	D	385	CYS
1	D	390	ASP
1	D	399	LYS
1	D	410	LEU
1	D	423	LYS
1	D	429	ARG
1	D	436	LEU
1	D	471	ARG
1	D	482	LEU
1	D	487	ASN
1	D	492	ARG
1	D	505	GLN
1	D	507	VAL
1	D	514	LEU
1	D	523	LYS
1	D	536	LYS
1	D	543	LEU
1	D	554	LYS
1	D	589	LYS
1	D	597	ARG
1	D	598	LEU
1	D	603	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	608	GLU
1	D	621	ASN
1	D	622	LYS
1	D	658	ARG
1	D	673	LEU
1	D	679	ASN
1	D	685	ASN
1	D	689	MET
1	D	701	LEU
1	D	702	LEU
1	D	710	ASN
1	D	761	GLN
2	E	4	THR
2	E	18	LEU
2	E	38	LEU
2	E	44	GLU
2	E	47	LEU
2	E	52	MET
2	E	54	LYS
2	E	56	LEU
2	E	57	THR
2	E	60	ASP
2	E	75	CYS
2	E	98	VAL
2	E	100	VAL
2	E	110	SER
2	E	121	GLU
2	E	124	LEU
2	E	125	THR
2	E	128	GLU
2	E	131	SER
2	E	132	LEU
2	E	146	VAL
2	E	168	LEU
2	E	177	VAL
2	E	182	LEU
2	E	206	LYS
2	E	231	LEU
2	E	235	ARG
2	E	251	ARG
2	E	252	LEU
2	E	254	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	276	THR
2	E	282	ARG
2	E	292	LEU
2	E	303	THR
2	E	313	LYS
2	E	320	GLU
2	E	325	LEU
2	E	331	LYS
2	E	335	LEU
2	E	338	ASP
2	E	341	LYS
2	E	343	LEU
2	E	347	LEU
2	E	352	ARG
2	E	353	MET
2	F	4	THR
2	F	18	LEU
2	F	38	LEU
2	F	44	GLU
2	F	47	LEU
2	F	52	MET
2	F	54	LYS
2	F	57	THR
2	F	60	ASP
2	F	76	ARG
2	F	98	VAL
2	F	100	VAL
2	F	121	GLU
2	F	124	LEU
2	F	125	THR
2	F	146	VAL
2	F	168	LEU
2	F	177	VAL
2	F	182	LEU
2	F	206	LYS
2	F	212	THR
2	F	230	THR
2	F	231	LEU
2	F	251	ARG
2	F	252	LEU
2	F	254	GLN
2	F	276	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	292	LEU
2	F	303	THR
2	F	313	LYS
2	F	320	GLU
2	F	325	LEU
2	F	331	LYS
2	F	335	LEU
2	F	338	ASP
2	F	341	LYS
2	F	343	LEU
2	F	347	LEU
2	F	355	SER
2	G	4	THR
2	G	18	LEU
2	G	38	LEU
2	G	44	GLU
2	G	47	LEU
2	G	52	MET
2	G	54	LYS
2	G	57	THR
2	G	60	ASP
2	G	76	ARG
2	G	82	ILE
2	G	98	VAL
2	G	100	VAL
2	G	112	VAL
2	G	113	GLU
2	G	121	GLU
2	G	124	LEU
2	G	125	THR
2	G	146	VAL
2	G	168	LEU
2	G	177	VAL
2	G	182	LEU
2	G	206	LYS
2	G	230	THR
2	G	231	LEU
2	G	240	TYR
2	G	251	ARG
2	G	252	LEU
2	G	254	GLN
2	G	276	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	281	ILE
2	G	292	LEU
2	G	303	THR
2	G	313	LYS
2	G	320	GLU
2	G	325	LEU
2	G	331	LYS
2	G	335	LEU
2	G	338	ASP
2	G	341	LYS
2	G	343	LEU
2	G	347	LEU
2	G	352	ARG
2	G	353	MET
2	G	355	SER
2	H	4	THR
2	H	18	LEU
2	H	38	LEU
2	H	44	GLU
2	H	47	LEU
2	H	52	MET
2	H	54	LYS
2	H	57	THR
2	H	60	ASP
2	H	76	ARG
2	H	98	VAL
2	H	100	VAL
2	H	111	LYS
2	H	112	VAL
2	H	121	GLU
2	H	124	LEU
2	H	125	THR
2	H	132	LEU
2	H	139	GLU
2	H	146	VAL
2	H	168	LEU
2	H	177	VAL
2	H	182	LEU
2	H	206	LYS
2	H	231	LEU
2	H	251	ARG
2	H	252	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	254	GLN
2	H	276	THR
2	H	283	PHE
2	H	292	LEU
2	H	303	THR
2	H	313	LYS
2	H	320	GLU
2	H	325	LEU
2	H	331	LYS
2	H	335	LEU
2	H	337	GLU
2	H	341	LYS
2	H	343	LEU
2	H	347	LEU
2	H	355	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	51	ASN
1	A	75	ASN
1	A	103	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	377	ASN
1	A	483	HIS
1	A	487	ASN
1	A	505	GLN
1	A	572	ASN
1	A	621	ASN
1	A	679	ASN
1	A	694	ASN
1	A	710	ASN
1	A	718	GLN
1	A	731	GLN
1	B	51	ASN
1	B	74	ASN
1	B	103	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	338	ASN
1	B	345	HIS
1	B	369	ASN
1	B	377	ASN
1	B	483	HIS
1	B	487	ASN
1	B	505	GLN
1	B	572	ASN
1	B	621	ASN
1	B	679	ASN
1	B	694	ASN
1	B	710	ASN
1	B	718	GLN
1	B	731	GLN
1	C	51	ASN
1	C	170	ASN
1	C	247	GLN
1	C	272	ASN
1	C	314	GLN
1	C	338	ASN
1	C	377	ASN
1	C	483	HIS
1	C	487	ASN
1	C	505	GLN
1	C	572	ASN
1	C	621	ASN
1	C	679	ASN
1	C	694	ASN
1	C	710	ASN
1	C	718	GLN
1	C	731	GLN
1	D	51	ASN
1	D	103	ASN
1	D	170	ASN
1	D	272	ASN
1	D	314	GLN
1	D	338	ASN
1	D	369	ASN

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Mol	Chain	Res	Type
1	D	377	ASN
1	D	483	HIS
1	D	487	ASN
1	D	505	GLN
1	D	572	ASN
1	D	621	ASN
1	D	679	ASN
1	D	694	ASN
1	D	710	ASN
1	D	718	GLN
1	D	731	GLN
2	E	48	ASN
2	E	134	ASN
2	E	157	HIS
2	E	158	GLN
2	E	210	HIS
2	E	254	GLN
2	F	48	ASN
2	F	134	ASN
2	F	157	HIS
2	F	158	GLN
2	F	210	HIS
2	F	254	GLN
2	G	48	ASN
2	G	134	ASN
2	G	157	HIS
2	G	158	GLN
2	G	210	HIS
2	G	254	GLN
2	H	48	ASN
2	H	134	ASN
2	H	157	HIS
2	H	210	HIS
2	H	254	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

44 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
3	NAG	I	1	3,1	14,14,15	0.63	0	17,19,21	0.95	0
3	NAG	I	2	3	14,14,15	0.53	0	17,19,21	1.53	3 (17%)
3	FUC	I	3	3	10,10,11	0.60	0	14,14,16	1.65	3 (21%)
4	NAG	J	1	4,1	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
4	NAG	J	2	4	14,14,15	0.60	0	17,19,21	1.99	4 (23%)
4	NAG	K	1	4,1	14,14,15	0.67	0	17,19,21	1.86	7 (41%)
4	NAG	K	2	4	14,14,15	0.56	0	17,19,21	1.71	4 (23%)
5	NAG	L	1	5,1	14,14,15	0.70	0	17,19,21	1.64	3 (17%)
5	NAG	L	2	5	14,14,15	0.79	1 (7%)	17,19,21	1.54	3 (17%)
5	BMA	L	3	5	11,11,12	0.51	0	15,15,17	2.49	6 (40%)
5	MAN	L	4	5	11,11,12	0.70	0	15,15,17	1.72	4 (26%)
6	NAG	M	1	6,1	14,14,15	0.39	0	17,19,21	2.00	2 (11%)
6	FUC	M	2	6	10,10,11	0.73	0	14,14,16	1.34	1 (7%)
4	NAG	N	1	4,1	14,14,15	0.57	0	17,19,21	1.46	4 (23%)
4	NAG	N	2	4	14,14,15	0.63	0	17,19,21	2.14	6 (35%)
5	NAG	O	1	5,1	14,14,15	0.58	0	17,19,21	2.31	6 (35%)
5	NAG	O	2	5	14,14,15	0.63	0	17,19,21	1.38	2 (11%)
5	BMA	O	3	5	11,11,12	0.62	0	15,15,17	1.69	4 (26%)
5	MAN	O	4	5	11,11,12	0.61	0	15,15,17	2.07	6 (40%)
4	NAG	P	1	4,1	14,14,15	0.81	0	17,19,21	2.38	4 (23%)
4	NAG	P	2	4	14,14,15	0.56	0	17,19,21	2.24	3 (17%)
3	NAG	Q	1	3,1	14,14,15	0.51	0	17,19,21	1.13	1 (5%)
3	NAG	Q	2	3	14,14,15	0.66	0	17,19,21	1.55	5 (29%)
3	FUC	Q	3	3	10,10,11	0.59	0	14,14,16	1.43	2 (14%)
4	NAG	R	1	4,1	14,14,15	0.80	0	17,19,21	3.03	7 (41%)
4	NAG	R	2	4	14,14,15	0.62	0	17,19,21	1.59	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	S	1	4,1	14,14,15	0.57	0	17,19,21	1.32	2 (11%)
4	NAG	S	2	4	14,14,15	0.53	0	17,19,21	1.72	4 (23%)
5	NAG	T	1	5,1	14,14,15	0.61	0	17,19,21	1.96	4 (23%)
5	NAG	T	2	5	14,14,15	0.52	0	17,19,21	0.99	1 (5%)
5	BMA	T	3	5	11,11,12	0.63	0	15,15,17	1.76	4 (26%)
5	MAN	T	4	5	11,11,12	0.51	0	15,15,17	2.37	4 (26%)
4	NAG	U	1	4,1	14,14,15	0.65	0	17,19,21	3.03	9 (52%)
4	NAG	U	2	4	14,14,15	0.69	0	17,19,21	3.20	7 (41%)
6	NAG	V	1	6,1	14,14,15	0.57	0	17,19,21	1.72	4 (23%)
6	FUC	V	2	6	10,10,11	0.74	0	14,14,16	1.88	4 (28%)
4	NAG	W	1	4,1	14,14,15	0.52	0	17,19,21	1.63	4 (23%)
4	NAG	W	2	4	14,14,15	0.56	0	17,19,21	1.48	1 (5%)
5	NAG	X	1	5,1	14,14,15	0.54	0	17,19,21	1.80	5 (29%)
5	NAG	X	2	5	14,14,15	0.59	0	17,19,21	1.28	2 (11%)
5	BMA	X	3	5	11,11,12	0.61	0	15,15,17	1.67	3 (20%)
5	MAN	X	4	5	11,11,12	0.61	0	15,15,17	0.97	0
4	NAG	Y	1	4,1	14,14,15	0.67	0	17,19,21	2.21	7 (41%)
4	NAG	Y	2	4	14,14,15	0.59	0	17,19,21	1.92	4 (23%)

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

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2	NAG	O5-C1	-2.05	1.40	1.43

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2	NAG	C1-O5-C5	8.49	123.70	112.19
4	P	2	NAG	C1-O5-C5	7.43	122.26	112.19
4	U	1	NAG	C1-O5-C5	6.97	121.64	112.19
4	P	1	NAG	C2-N2-C7	6.95	132.79	122.90
5	T	4	MAN	C1-O5-C5	6.88	121.51	112.19
6	M	1	NAG	C1-O5-C5	6.68	121.25	112.19
5	O	1	NAG	C1-O5-C5	6.35	120.79	112.19
4	U	2	NAG	C2-N2-C7	6.07	131.55	122.90
4	R	1	NAG	C1-O5-C5	5.97	120.28	112.19
4	N	2	NAG	C1-O5-C5	5.97	120.28	112.19
4	R	1	NAG	C2-N2-C7	5.90	131.30	122.90
4	U	1	NAG	C4-C3-C2	5.41	118.94	111.02
4	R	1	NAG	C4-C3-C2	5.16	118.58	111.02
6	V	1	NAG	C1-O5-C5	4.93	118.87	112.19
4	Y	1	NAG	C1-O5-C5	4.89	118.82	112.19
4	R	2	NAG	C4-C3-C2	4.77	118.01	111.02
4	Y	2	NAG	C2-N2-C7	4.62	129.48	122.90
4	U	1	NAG	C2-N2-C7	4.60	129.45	122.90
5	O	4	MAN	C1-C2-C3	-4.53	104.09	109.67
5	L	3	BMA	O5-C5-C6	4.53	114.31	107.20
5	T	3	BMA	O3-C3-C4	4.51	120.77	110.35
5	T	1	NAG	C1-O5-C5	4.47	118.25	112.19
4	U	2	NAG	O5-C1-C2	4.39	118.21	111.29
6	V	2	FUC	C3-C4-C5	4.35	116.55	109.77
4	W	2	NAG	C4-C3-C2	4.28	117.30	111.02
4	Y	1	NAG	C4-C3-C2	4.27	117.28	111.02
5	L	4	MAN	C1-C2-C3	4.22	114.86	109.67
4	R	1	NAG	C1-C2-N2	4.20	117.67	110.49
5	T	1	NAG	C2-N2-C7	-4.19	116.94	122.90
5	X	1	NAG	C1-O5-C5	-4.17	106.54	112.19
4	J	2	NAG	O5-C1-C2	-4.10	104.81	111.29
5	O	2	NAG	C1-O5-C5	4.01	117.62	112.19
4	W	1	NAG	O5-C1-C2	-4.01	104.96	111.29
5	L	3	BMA	O3-C3-C4	3.97	119.53	110.35
4	R	1	NAG	C3-C4-C5	3.97	117.32	110.24
4	K	1	NAG	C2-N2-C7	3.94	128.51	122.90
5	L	3	BMA	C1-O5-C5	3.93	117.52	112.19
5	T	4	MAN	C3-C4-C5	3.89	117.17	110.24
4	U	1	NAG	C3-C4-C5	3.88	117.17	110.24
4	S	2	NAG	C2-N2-C7	3.88	128.42	122.90
5	L	1	NAG	C3-C4-C5	3.82	117.06	110.24
4	S	1	NAG	C2-N2-C7	-3.76	117.54	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C3-C4-C5	3.72	116.88	110.24
4	K	2	NAG	C3-C4-C5	3.72	116.87	110.24
4	J	2	NAG	C3-C4-C5	3.70	116.84	110.24
4	J	2	NAG	C1-O5-C5	3.57	117.03	112.19
5	L	2	NAG	O5-C5-C4	-3.55	102.20	110.83
5	X	3	BMA	C3-C4-C5	3.52	116.53	110.24
4	Y	2	NAG	O5-C5-C6	3.52	112.72	107.20
4	P	1	NAG	C8-C7-N2	3.49	122.00	116.10
4	U	2	NAG	C8-C7-N2	3.48	122.00	116.10
5	L	3	BMA	O3-C3-C2	3.48	116.66	109.99
6	M	2	FUC	C3-C4-C5	3.47	115.18	109.77
5	X	3	BMA	C1-C2-C3	-3.46	105.41	109.67
5	O	4	MAN	O5-C1-C2	-3.40	105.53	110.77
4	P	2	NAG	O5-C5-C6	3.38	112.50	107.20
4	U	2	NAG	O5-C5-C4	3.34	118.96	110.83
4	W	1	NAG	O5-C5-C6	3.31	112.39	107.20
4	N	2	NAG	C3-C4-C5	3.26	116.06	110.24
5	L	3	BMA	C2-C3-C4	-3.24	105.29	110.89
4	K	1	NAG	C4-C3-C2	3.24	115.77	111.02
3	I	3	FUC	C1-C2-C3	-3.23	105.70	109.67
4	R	1	NAG	C8-C7-N2	3.17	121.47	116.10
4	N	1	NAG	C4-C3-C2	3.15	115.64	111.02
5	X	2	NAG	C2-N2-C7	-3.10	118.50	122.90
6	V	2	FUC	C2-C3-C4	3.08	116.22	110.89
3	Q	3	FUC	C1-O5-C5	3.07	119.73	112.78
4	S	2	NAG	C3-C4-C5	3.06	115.70	110.24
4	J	2	NAG	O5-C5-C4	3.04	118.23	110.83
5	T	4	MAN	O5-C5-C4	3.04	118.22	110.83
6	V	2	FUC	O5-C1-C2	-3.02	106.10	110.77
5	X	1	NAG	O7-C7-C8	-3.02	116.44	122.06
4	K	2	NAG	O5-C1-C2	-3.02	106.53	111.29
5	O	4	MAN	O2-C2-C1	3.01	115.31	109.15
5	T	2	NAG	C1-O5-C5	3.00	116.26	112.19
5	O	3	BMA	O5-C5-C6	2.98	111.88	107.20
4	Y	1	NAG	O3-C3-C4	-2.96	103.50	110.35
4	Y	2	NAG	C1-C2-N2	2.91	115.47	110.49
4	U	1	NAG	O5-C1-C2	2.91	115.89	111.29
3	Q	2	NAG	C2-N2-C7	2.91	127.04	122.90
5	O	3	BMA	C1-O5-C5	2.90	116.13	112.19
5	T	3	BMA	O3-C3-C2	2.90	115.55	109.99
4	P	1	NAG	O7-C7-C8	-2.89	116.69	122.06
4	P	1	NAG	C4-C3-C2	2.87	115.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	3	BMA	C1-O5-C5	2.85	116.06	112.19
4	U	1	NAG	C8-C7-N2	2.85	120.92	116.10
4	N	2	NAG	O5-C1-C2	2.84	115.77	111.29
5	L	4	MAN	O5-C5-C6	2.83	111.63	107.20
5	O	1	NAG	O7-C7-C8	-2.82	116.83	122.06
3	I	3	FUC	O5-C1-C2	-2.78	106.47	110.77
5	L	1	NAG	O5-C1-C2	-2.75	106.95	111.29
4	Y	2	NAG	C4-C3-C2	-2.74	107.00	111.02
5	L	3	BMA	C3-C4-C5	-2.74	105.36	110.24
3	Q	2	NAG	O5-C1-C2	2.73	115.60	111.29
4	R	2	NAG	C3-C4-C5	2.71	115.07	110.24
4	Y	1	NAG	O4-C4-C3	-2.70	104.10	110.35
5	T	1	NAG	O5-C1-C2	-2.70	107.03	111.29
4	P	2	NAG	O5-C5-C4	2.70	117.39	110.83
5	O	1	NAG	C6-C5-C4	-2.69	106.70	113.00
4	W	1	NAG	C2-N2-C7	-2.68	119.09	122.90
4	K	1	NAG	O5-C1-C2	-2.65	107.10	111.29
3	Q	1	NAG	C4-C3-C2	2.65	114.90	111.02
4	K	2	NAG	C1-O5-C5	2.64	115.77	112.19
5	X	1	NAG	C3-C4-C5	-2.64	105.53	110.24
5	T	1	NAG	O3-C3-C4	-2.63	104.27	110.35
3	I	2	NAG	C1-C2-N2	2.62	114.97	110.49
3	Q	2	NAG	C4-C3-C2	2.62	114.86	111.02
4	Y	1	NAG	C3-C4-C5	2.60	114.88	110.24
5	T	3	BMA	C2-C3-C4	-2.59	106.42	110.89
5	O	4	MAN	O5-C5-C6	2.58	111.25	107.20
4	U	2	NAG	C3-C4-C5	2.57	114.82	110.24
4	S	1	NAG	O3-C3-C2	-2.56	104.16	109.47
6	V	1	NAG	C1-C2-N2	2.56	114.86	110.49
4	U	1	NAG	O5-C5-C6	-2.56	103.20	107.20
5	O	1	NAG	C4-C3-C2	2.55	114.75	111.02
6	V	1	NAG	C3-C4-C5	-2.54	105.70	110.24
4	N	1	NAG	O5-C1-C2	-2.54	107.28	111.29
4	U	2	NAG	O7-C7-C8	-2.53	117.36	122.06
6	V	2	FUC	O5-C5-C4	2.53	114.06	109.52
6	M	1	NAG	O4-C4-C5	2.51	115.52	109.30
5	O	3	BMA	O2-C2-C3	-2.50	105.12	110.14
5	L	4	MAN	C1-O5-C5	2.50	115.57	112.19
4	N	1	NAG	C2-N2-C7	-2.49	119.36	122.90
6	V	1	NAG	O5-C5-C6	2.48	111.09	107.20
4	W	1	NAG	C3-C4-C5	-2.47	105.84	110.24
4	N	2	NAG	C4-C3-C2	2.44	114.60	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	1	NAG	O7-C7-C8	-2.41	117.58	122.06
4	K	1	NAG	C8-C7-N2	2.40	120.15	116.10
5	O	1	NAG	O5-C5-C4	2.39	116.64	110.83
5	O	2	NAG	C3-C4-C5	-2.38	105.99	110.24
3	Q	3	FUC	O5-C5-C6	2.37	112.44	107.33
5	T	4	MAN	O2-C2-C1	2.35	113.97	109.15
4	K	1	NAG	C1-O5-C5	2.33	115.36	112.19
4	R	1	NAG	O7-C7-C8	-2.32	117.75	122.06
4	S	2	NAG	O5-C5-C4	2.32	116.47	110.83
4	S	2	NAG	O5-C1-C2	-2.31	107.64	111.29
5	L	2	NAG	O4-C4-C5	2.26	114.91	109.30
5	X	1	NAG	C6-C5-C4	2.26	118.30	113.00
5	O	1	NAG	O5-C5-C6	-2.25	103.68	107.20
4	Y	1	NAG	O4-C4-C5	2.24	114.87	109.30
5	X	2	NAG	O4-C4-C3	-2.24	105.17	110.35
4	J	1	NAG	O5-C5-C6	2.22	110.69	107.20
4	U	1	NAG	O3-C3-C2	-2.22	104.88	109.47
5	L	1	NAG	C2-N2-C7	-2.21	119.75	122.90
4	N	2	NAG	O5-C5-C6	2.20	110.66	107.20
4	J	1	NAG	C4-C3-C2	2.20	114.24	111.02
4	N	1	NAG	O4-C4-C3	-2.19	105.29	110.35
4	N	2	NAG	O7-C7-C8	-2.18	118.01	122.06
4	Y	1	NAG	O5-C5-C6	-2.17	103.80	107.20
3	Q	2	NAG	C1-O5-C5	2.16	115.12	112.19
5	L	2	NAG	C1-O5-C5	-2.16	109.27	112.19
4	K	1	NAG	O7-C7-C8	-2.14	118.09	122.06
5	O	4	MAN	C2-C3-C4	-2.12	107.23	110.89
4	K	1	NAG	C1-C2-N2	2.11	114.10	110.49
5	O	4	MAN	C1-O5-C5	2.09	115.03	112.19
5	O	3	BMA	C2-C3-C4	-2.09	107.28	110.89
5	X	3	BMA	O5-C1-C2	-2.06	107.59	110.77
5	L	4	MAN	O5-C5-C4	-2.06	105.82	110.83
4	K	2	NAG	C4-C3-C2	2.05	114.03	111.02
3	I	3	FUC	C3-C4-C5	2.05	112.97	109.77
3	Q	2	NAG	O5-C5-C6	2.05	110.42	107.20
3	I	2	NAG	O5-C5-C4	2.02	115.73	110.83
5	X	1	NAG	O3-C3-C2	2.01	113.63	109.47

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	3	FUC	C1

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Mol	Chain	Res	Type	Atom
3	Q	3	FUC	C1
6	M	2	FUC	C1
6	V	2	FUC	C1

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	C1-C2-N2-C7
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C1-C2-N2-C7
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
6	V	1	NAG	C1-C2-N2-C7
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
4	S	1	NAG	C8-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
4	N	1	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	O	1	NAG	O5-C5-C6-O6
5	T	4	MAN	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C8-C7-N2-C2
4	S	1	NAG	O7-C7-N2-C2
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
4	J	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
5	O	4	MAN	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	T	4	MAN	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	X	4	MAN	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	X	4	MAN	C4-C5-C6-O6
4	N	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
5	O	4	MAN	C4-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
5	X	3	BMA	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
5	X	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	U	2	NAG	O5-C5-C6-O6
5	L	4	MAN	O5-C5-C6-O6
3	I	2	NAG	O7-C7-N2-C2
4	N	2	NAG	O5-C5-C6-O6
4	P	1	NAG	C3-C2-N2-C7
4	U	1	NAG	C3-C2-N2-C7
3	I	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
4	U	2	NAG	C1-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	P	1	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C3-C2-N2-C7
4	S	2	NAG	C1-C2-N2-C7

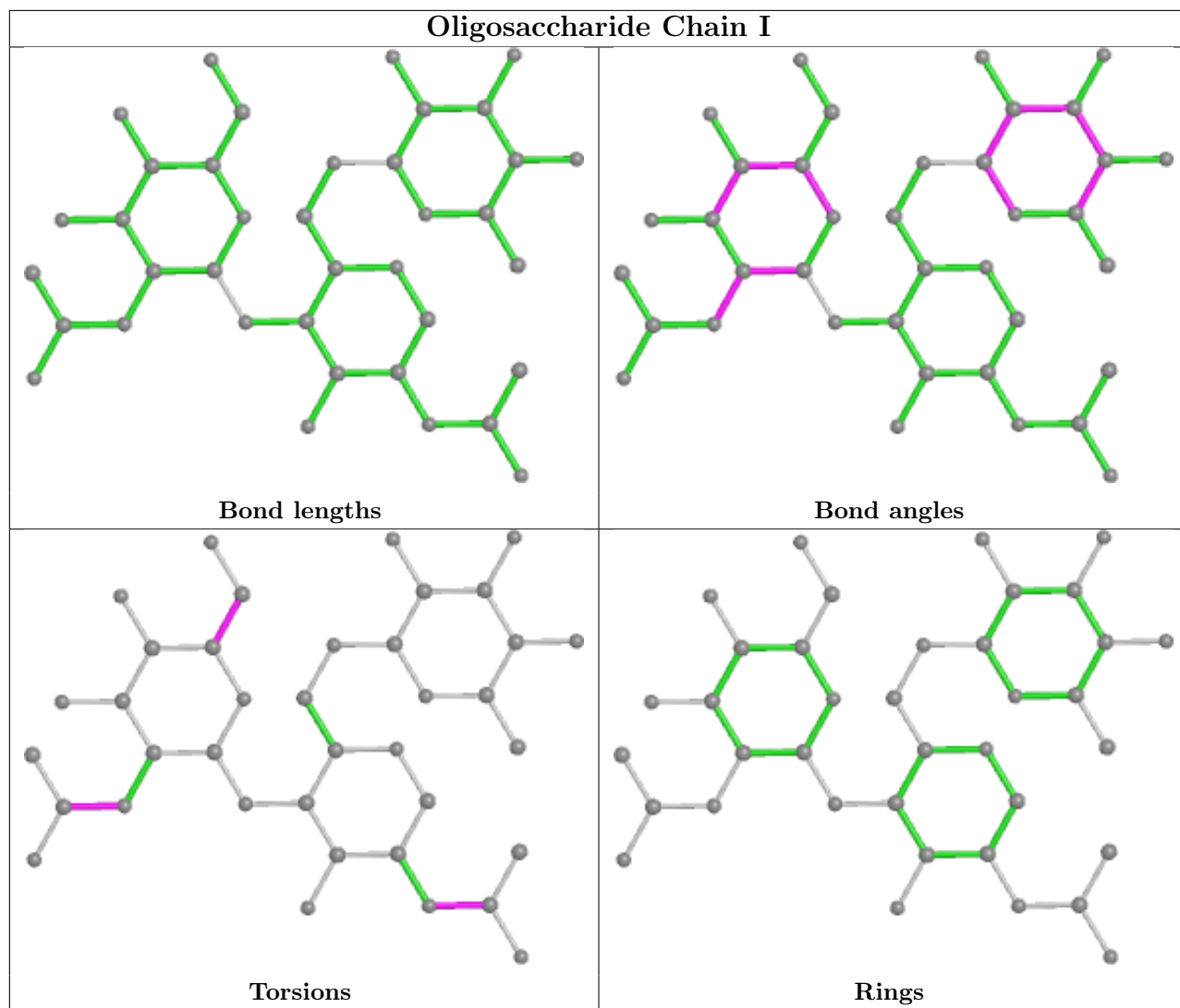
There are no ring outliers.

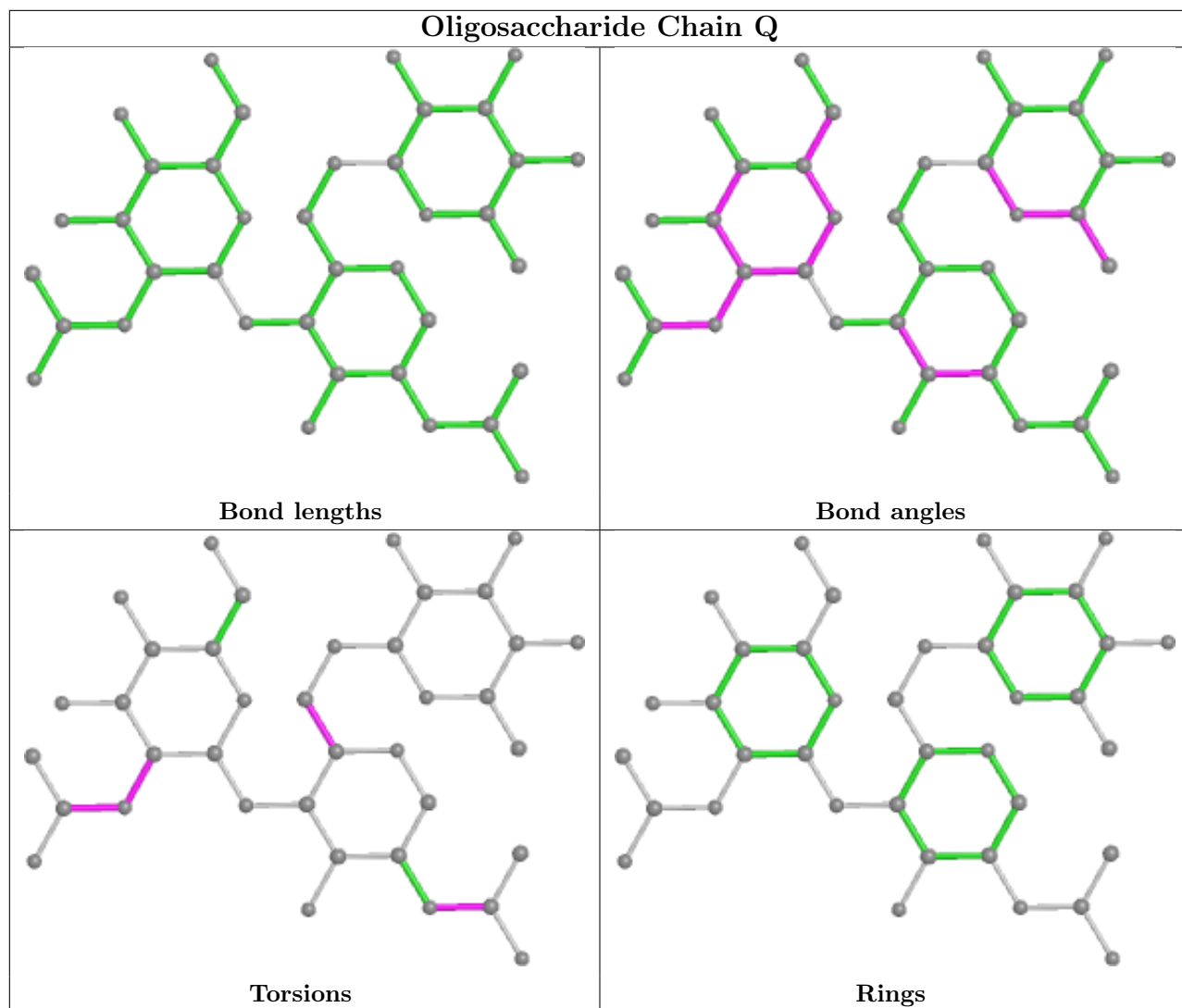
14 monomers are involved in 14 short contacts:

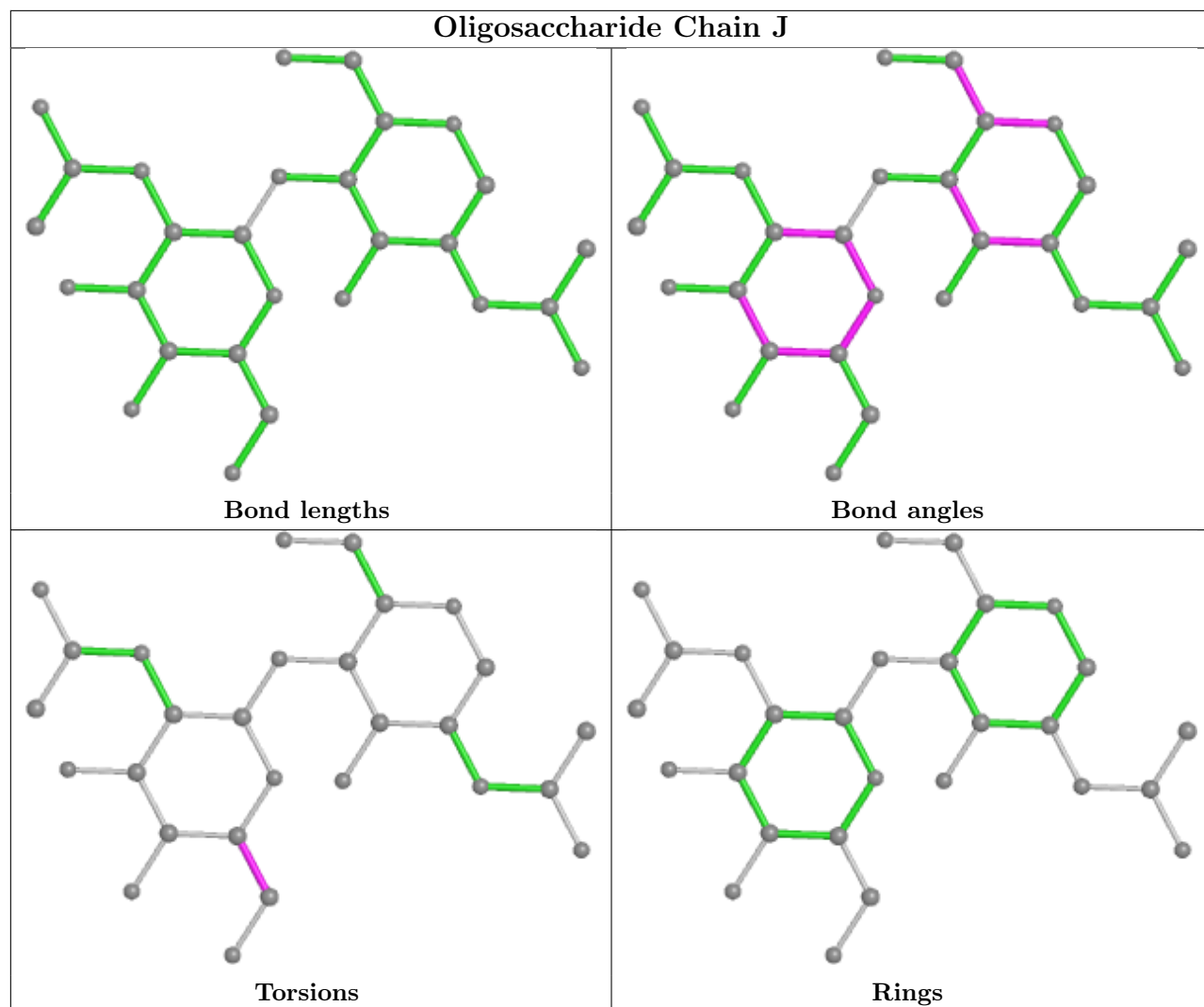
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	2	NAG	1	0
5	X	4	MAN	1	0
4	K	1	NAG	3	0
4	R	1	NAG	1	0
4	J	1	NAG	1	0
3	Q	1	NAG	1	0
3	Q	3	FUC	1	0
4	R	2	NAG	1	0
5	X	3	BMA	1	0
4	W	2	NAG	2	0
4	N	2	NAG	1	0
4	U	1	NAG	2	0
4	N	1	NAG	2	0
4	S	1	NAG	1	0

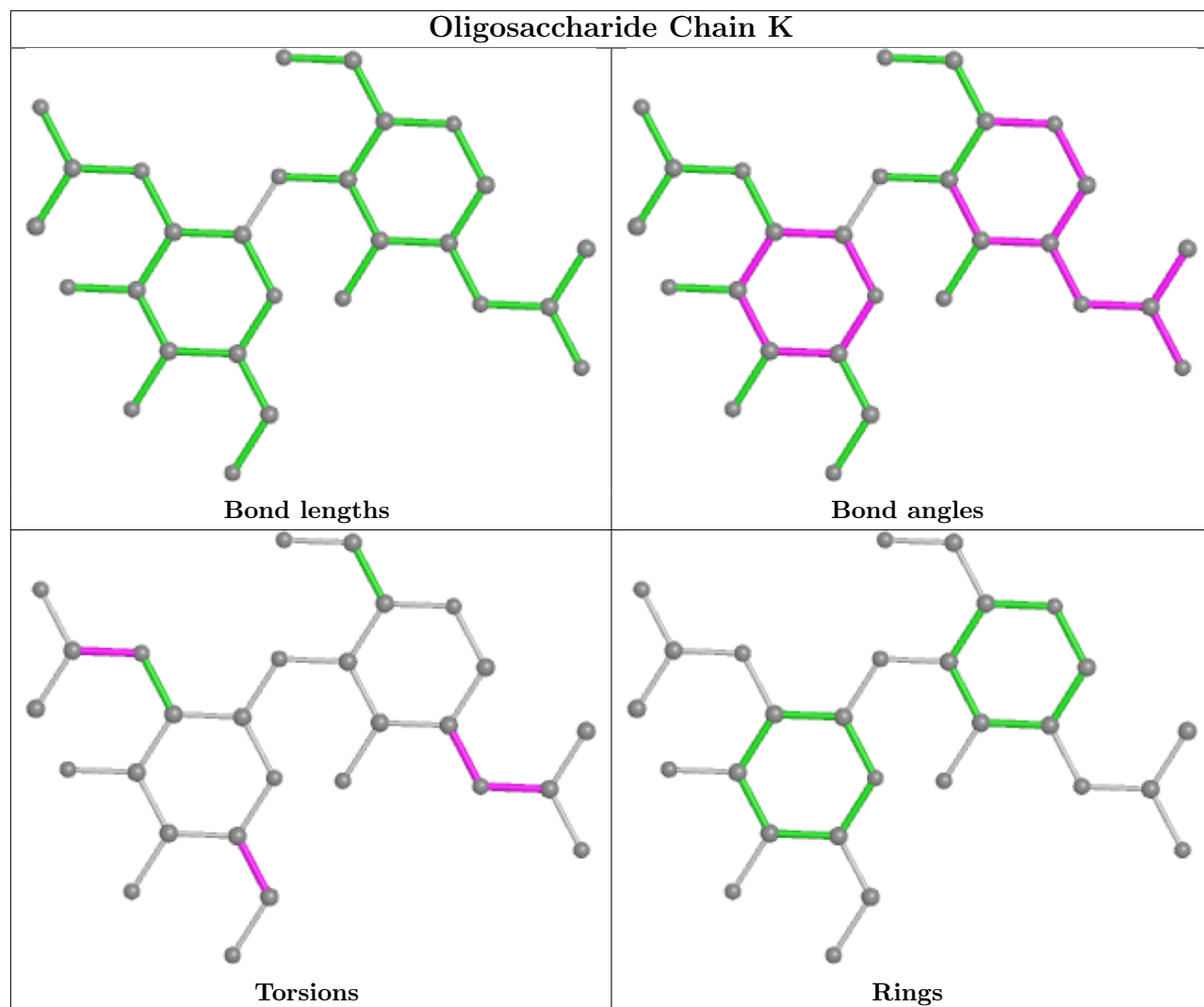
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

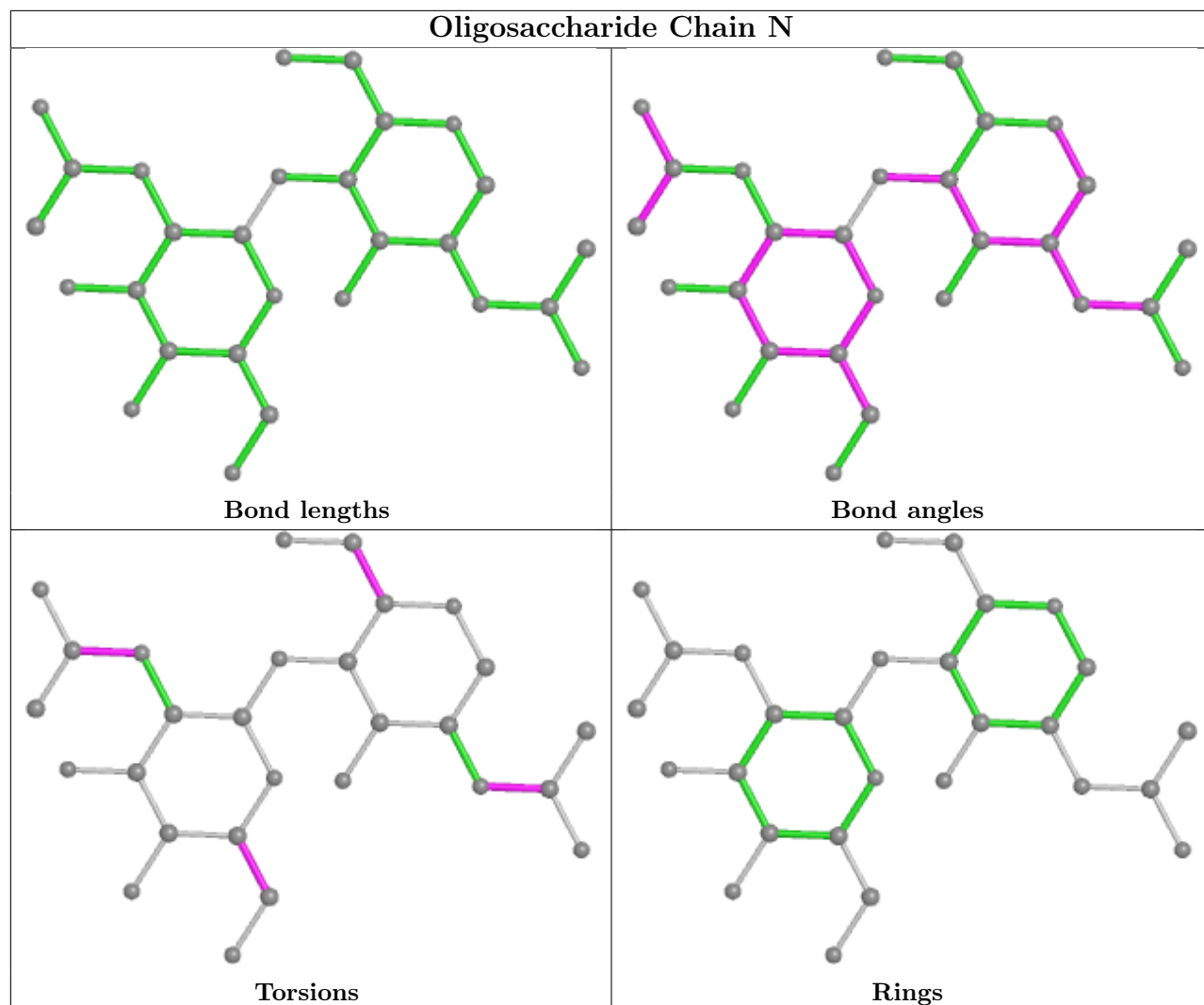


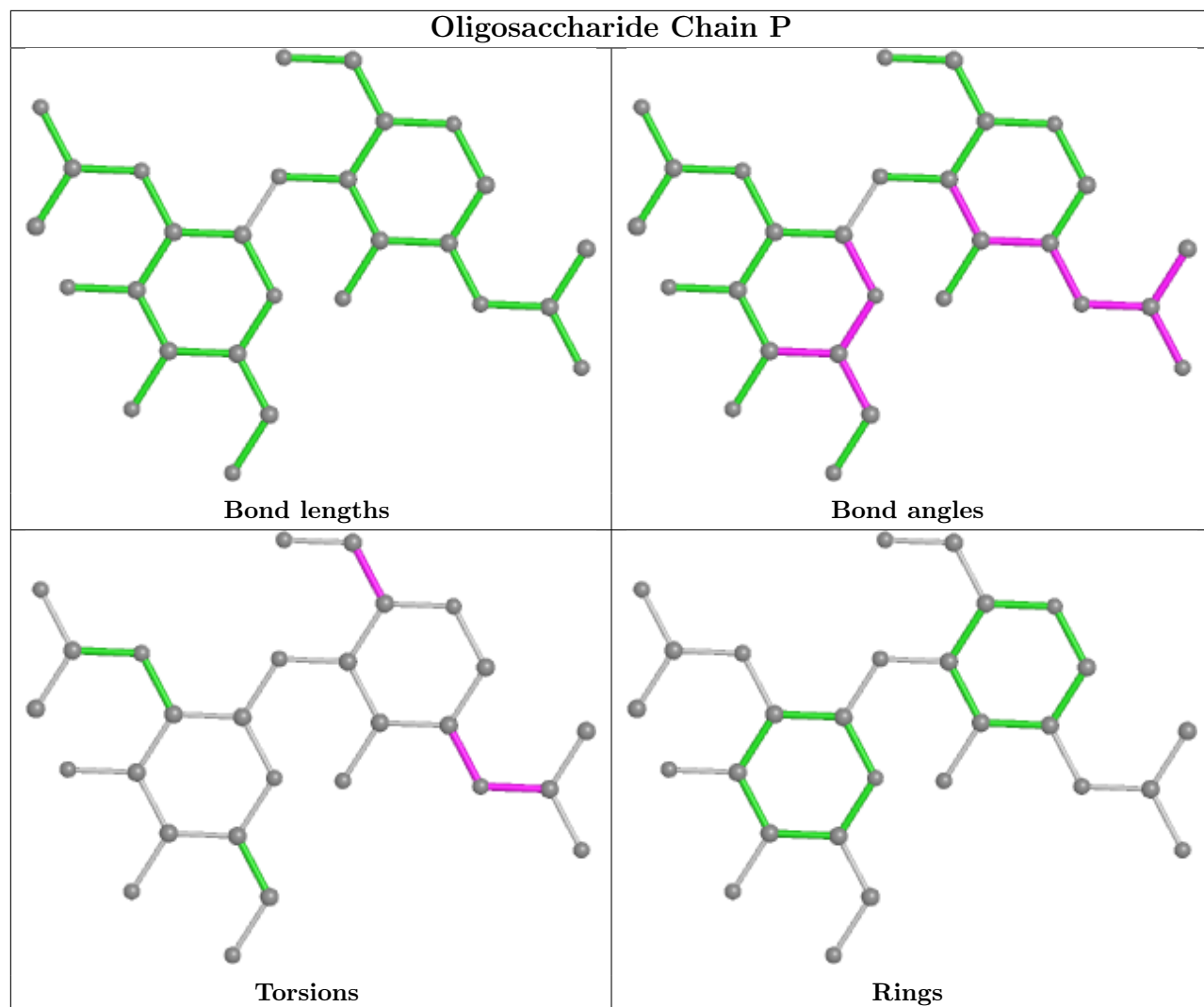


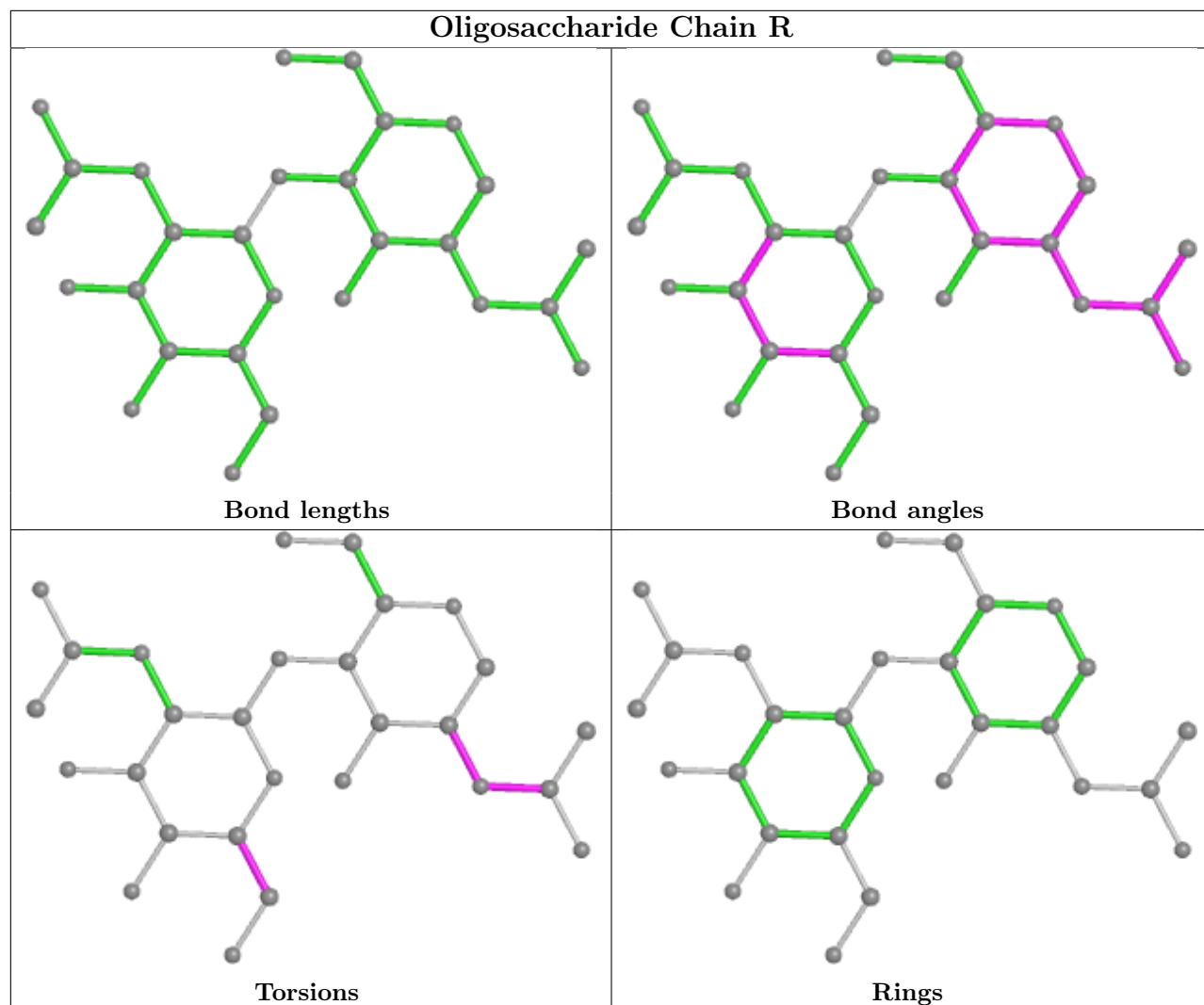


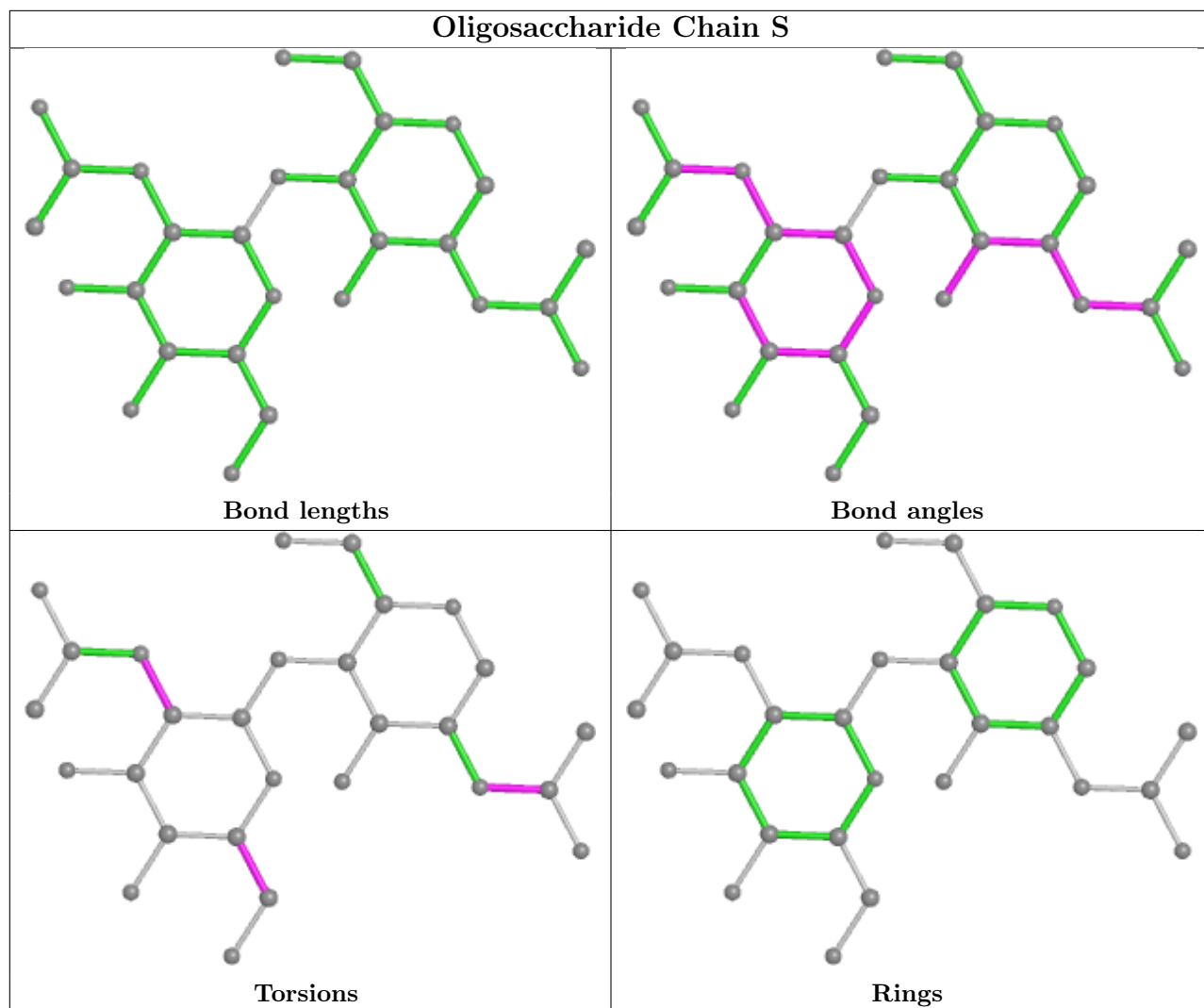




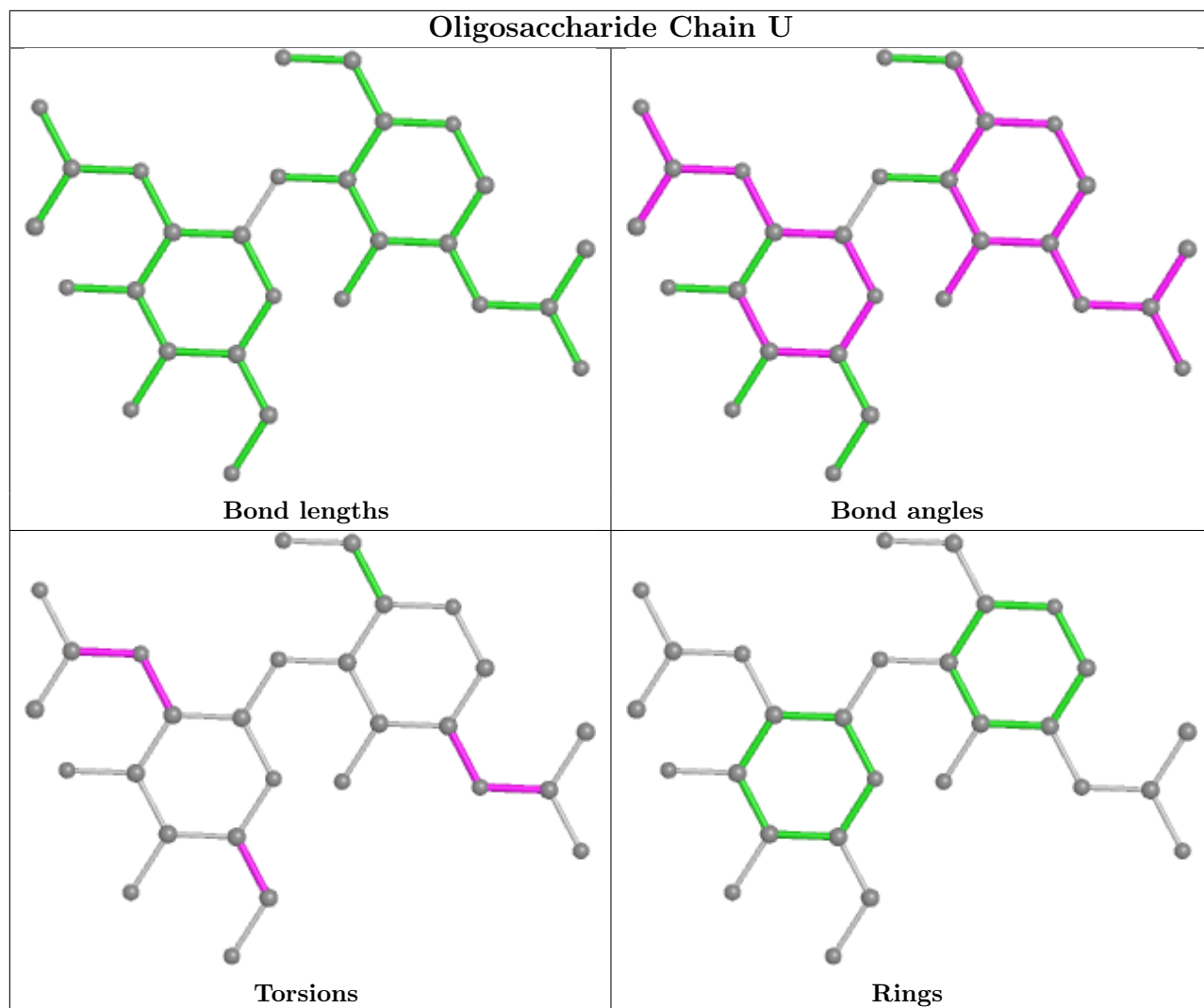


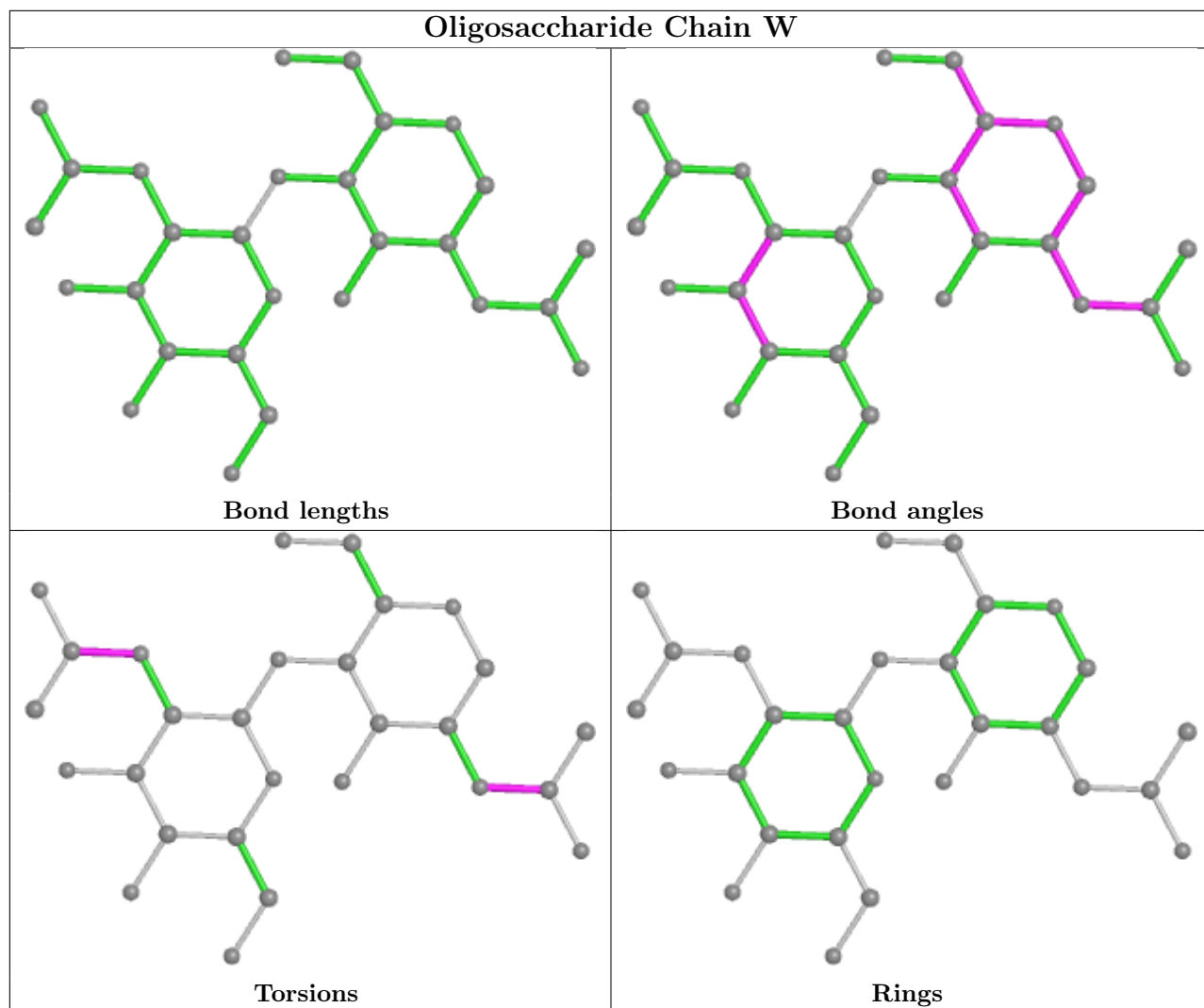


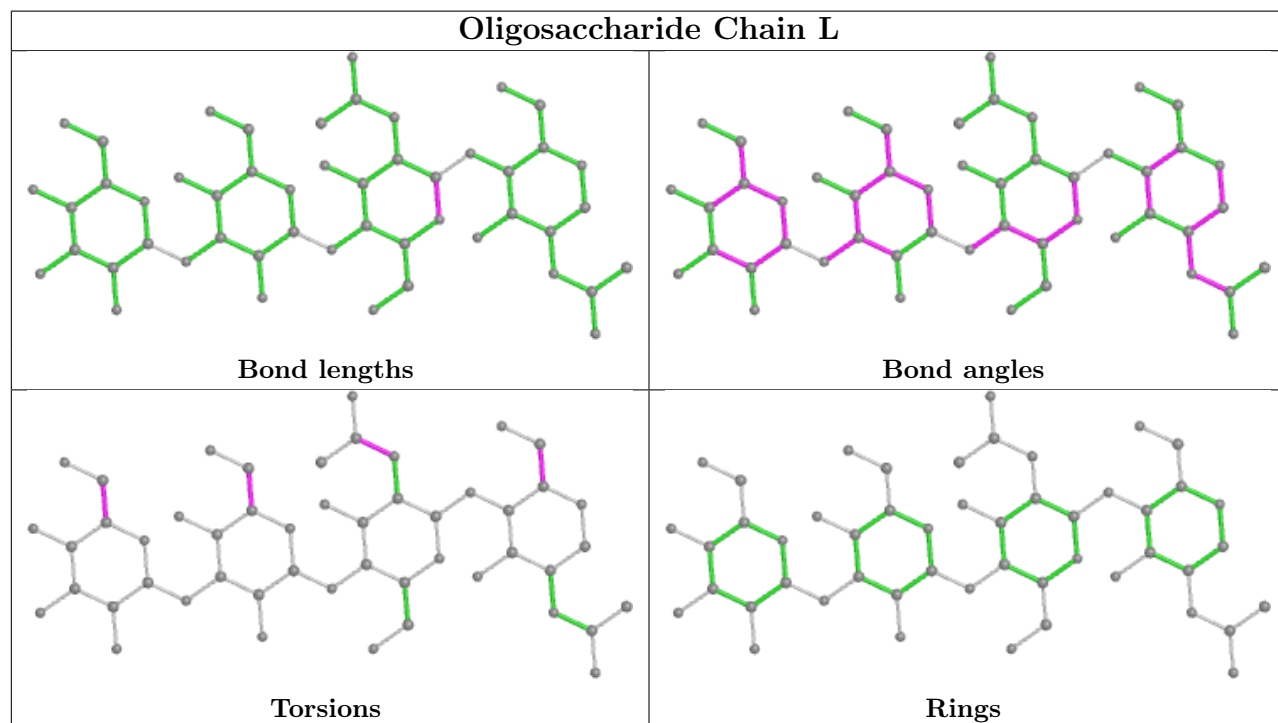
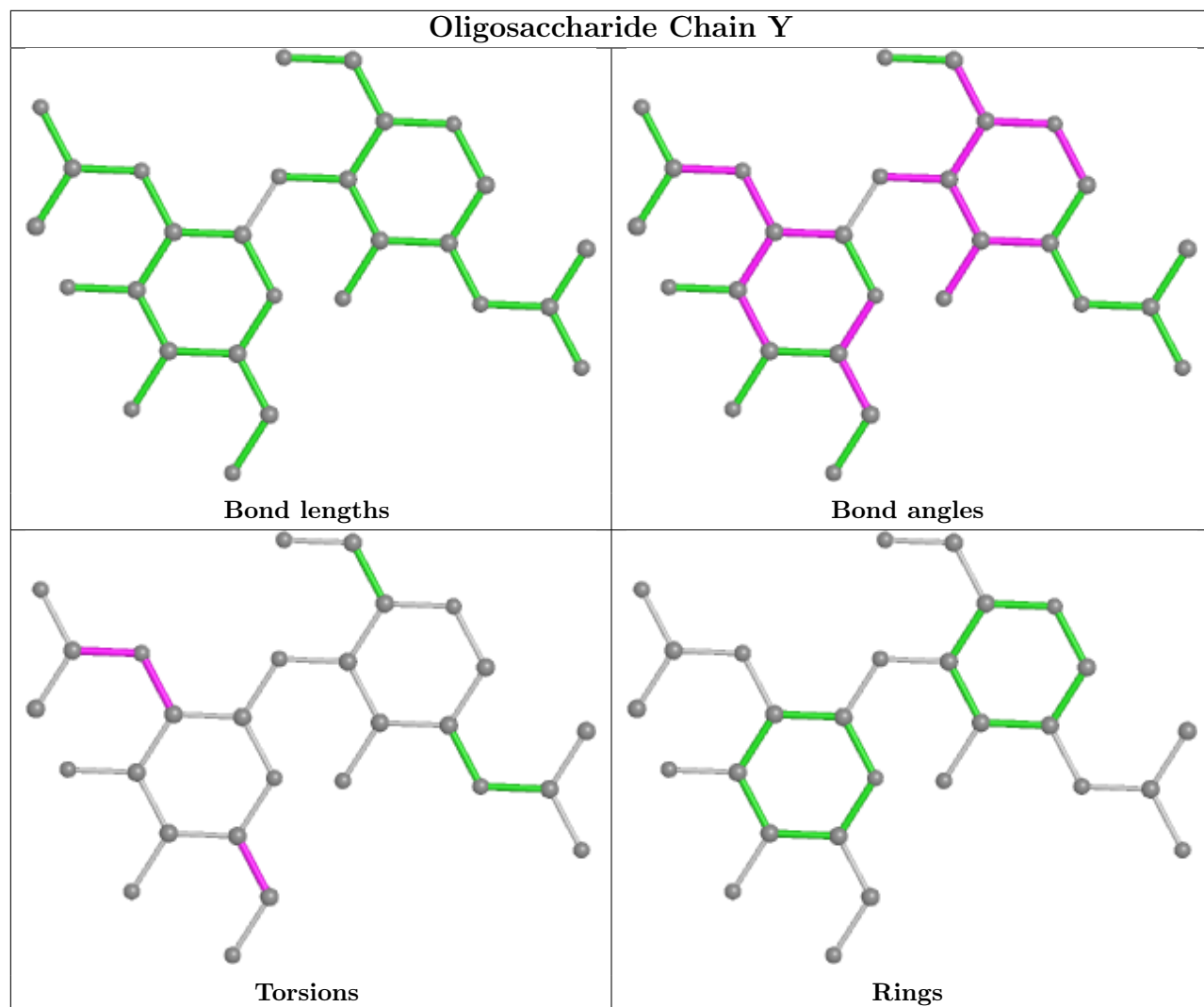


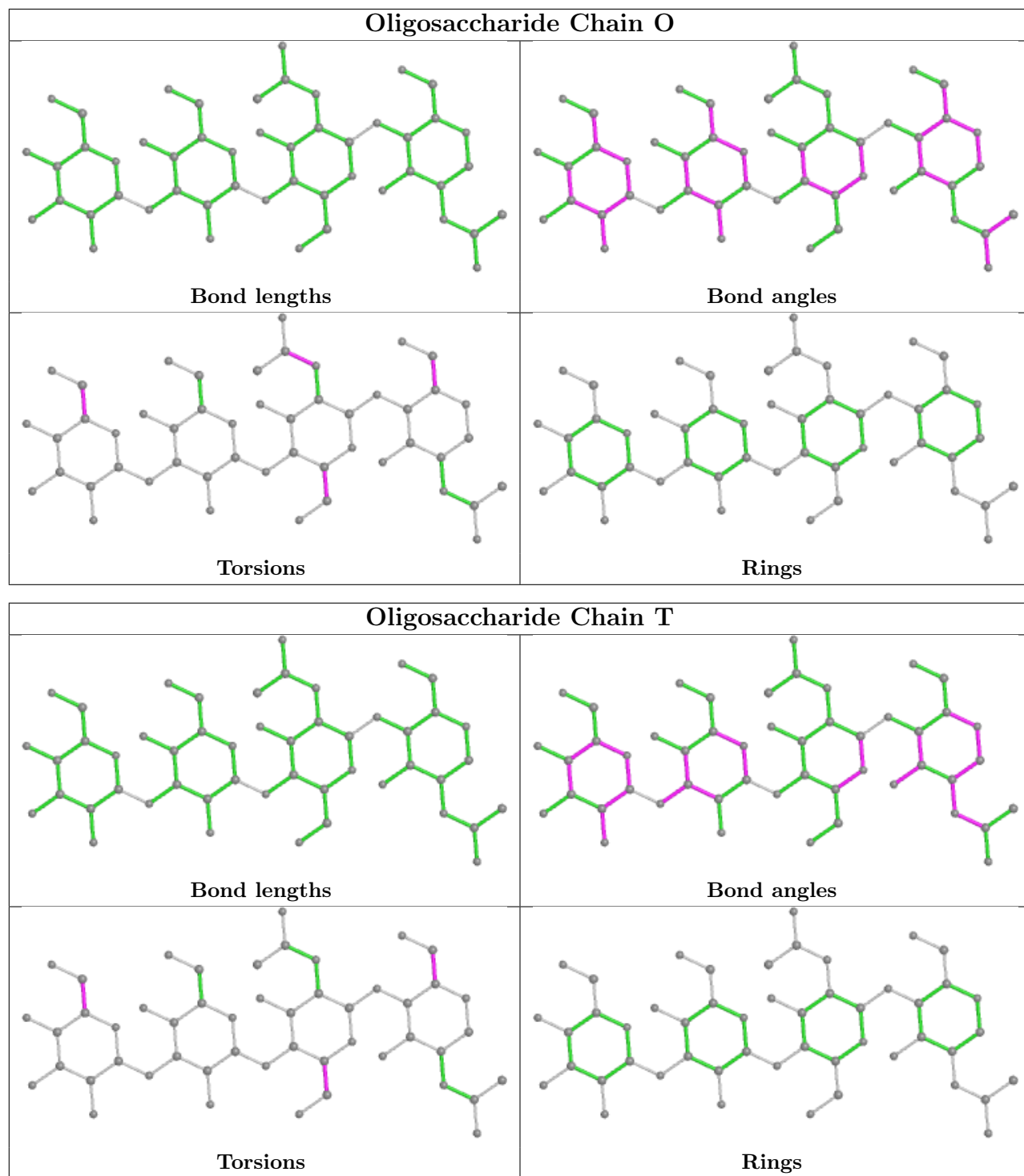


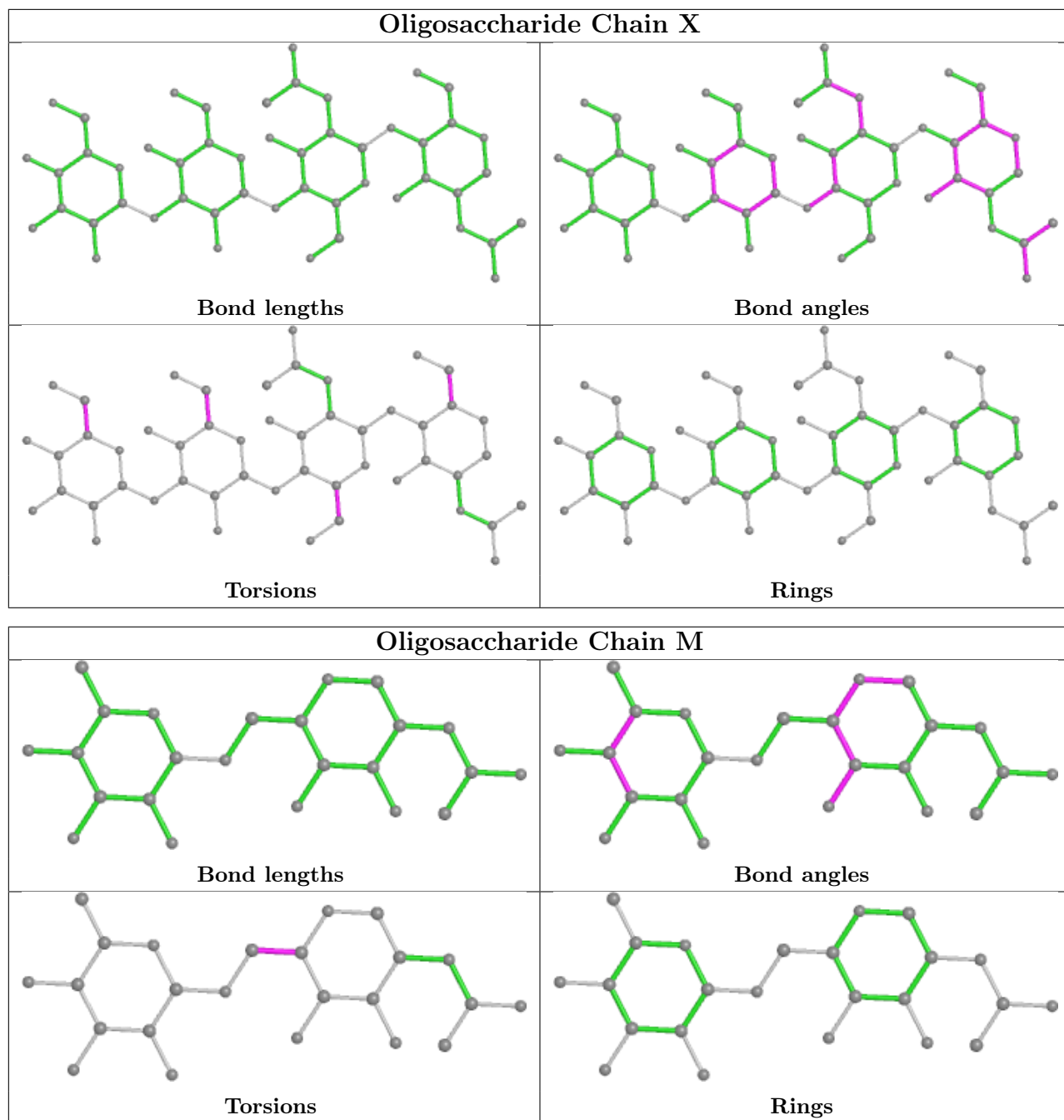


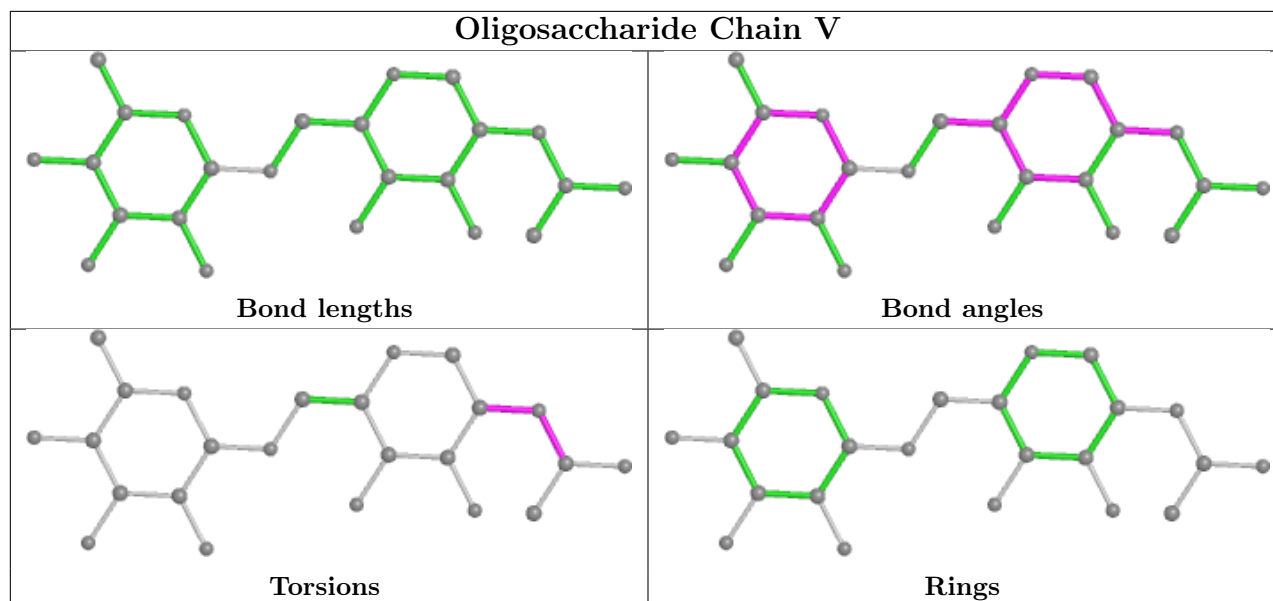












## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	NAG	A	840	1	14,14,15	0.45	0	17,19,21	2.02	5 (29%)
7	NAG	D	840	1	14,14,15	0.74	0	17,19,21	2.40	5 (29%)
7	NAG	B	810	1	14,14,15	0.63	0	17,19,21	2.88	6 (35%)
7	NAG	D	870	1	14,14,15	0.82	0	17,19,21	1.76	4 (23%)
7	NAG	C	870	1	14,14,15	0.63	0	17,19,21	2.42	4 (23%)
7	NAG	B	870	1	14,14,15	0.37	0	17,19,21	2.88	6 (35%)
7	NAG	C	840	1	14,14,15	0.46	0	17,19,21	1.91	5 (29%)
7	NAG	D	860	1	14,14,15	0.37	0	17,19,21	2.14	4 (23%)
7	NAG	C	860	1	14,14,15	0.77	1 (7%)	17,19,21	2.17	5 (29%)
7	NAG	B	860	1	14,14,15	0.64	0	17,19,21	2.02	5 (29%)
7	NAG	B	840	1	14,14,15	0.57	0	17,19,21	2.46	5 (29%)
7	NAG	A	870	1	14,14,15	0.46	0	17,19,21	1.56	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	850	1	14,14,15	0.58	0	17,19,21	1.73	3 (17%)
7	NAG	D	810	1	14,14,15	0.53	0	17,19,21	2.02	6 (35%)
7	NAG	A	860	1	14,14,15	0.64	0	17,19,21	2.16	7 (41%)

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
7	NAG	A	840	1	-	2/6/23/26	0/1/1/1
7	NAG	D	840	1	-	2/6/23/26	0/1/1/1
7	NAG	B	810	1	-	3/6/23/26	0/1/1/1
7	NAG	D	870	1	-	5/6/23/26	0/1/1/1
7	NAG	C	870	1	-	3/6/23/26	0/1/1/1
7	NAG	B	870	1	-	4/6/23/26	0/1/1/1
7	NAG	C	840	1	-	0/6/23/26	0/1/1/1
7	NAG	D	860	1	-	4/6/23/26	0/1/1/1
7	NAG	C	860	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	B	860	1	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	B	840	1	-	4/6/23/26	0/1/1/1
7	NAG	A	870	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	850	1	-	0/6/23/26	0/1/1/1
7	NAG	D	810	1	-	2/6/23/26	0/1/1/1
7	NAG	A	860	1	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	860	NAG	C1-C2	2.21	1.55	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	870	NAG	O5-C1-C2	-7.74	99.06	111.29
7	D	840	NAG	C1-O5-C5	7.20	121.95	112.19
7	B	840	NAG	C1-O5-C5	6.69	121.25	112.19
7	B	810	NAG	C1-O5-C5	6.48	120.97	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	870	NAG	C2-N2-C7	6.15	131.67	122.90
7	C	870	NAG	O5-C5-C6	6.06	116.71	107.20
7	A	840	NAG	C1-O5-C5	5.99	120.31	112.19
7	B	860	NAG	C2-N2-C7	5.77	131.11	122.90
7	B	810	NAG	C1-C2-N2	5.64	120.13	110.49
7	C	840	NAG	C1-O5-C5	5.48	119.62	112.19
7	B	870	NAG	C1-O5-C5	5.41	119.52	112.19
7	A	860	NAG	C2-N2-C7	5.36	130.54	122.90
7	D	860	NAG	C1-O5-C5	5.34	119.43	112.19
7	B	810	NAG	C2-N2-C7	5.27	130.41	122.90
7	B	870	NAG	C4-C3-C2	-4.98	103.72	111.02
7	C	860	NAG	C1-O5-C5	4.94	118.89	112.19
7	D	860	NAG	C4-C3-C2	-4.76	104.03	111.02
7	D	870	NAG	C2-N2-C7	4.54	129.37	122.90
7	C	860	NAG	C1-C2-N2	4.48	118.15	110.49
7	D	810	NAG	C1-O5-C5	4.27	117.98	112.19
7	A	870	NAG	C1-O5-C5	4.12	117.77	112.19
7	B	840	NAG	C2-N2-C7	3.98	128.57	122.90
7	D	840	NAG	C2-N2-C7	3.70	128.18	122.90
7	D	810	NAG	C3-C4-C5	-3.68	103.67	110.24
7	B	810	NAG	C4-C3-C2	-3.47	105.93	111.02
7	A	850	NAG	C4-C3-C2	3.46	116.09	111.02
7	A	850	NAG	C3-C4-C5	3.45	116.39	110.24
7	D	810	NAG	O5-C5-C6	3.41	112.55	107.20
7	B	810	NAG	C3-C4-C5	-3.41	104.16	110.24
7	A	850	NAG	C1-O5-C5	3.32	116.69	112.19
7	B	840	NAG	C1-C2-N2	3.17	115.90	110.49
7	D	840	NAG	C4-C3-C2	3.16	115.64	111.02
7	C	870	NAG	C1-C2-N2	3.12	115.82	110.49
7	A	860	NAG	C8-C7-N2	3.11	121.37	116.10
7	C	860	NAG	O5-C5-C6	3.08	112.03	107.20
7	A	840	NAG	O5-C5-C6	2.94	111.81	107.20
7	D	860	NAG	C2-N2-C7	-2.77	118.96	122.90
7	A	870	NAG	O5-C1-C2	-2.75	106.95	111.29
7	D	810	NAG	C4-C3-C2	-2.75	107.00	111.02
7	B	860	NAG	O5-C1-C2	2.71	115.56	111.29
7	C	840	NAG	C4-C3-C2	-2.69	107.07	111.02
7	B	870	NAG	C1-C2-N2	2.65	115.02	110.49
7	C	870	NAG	C3-C4-C5	-2.64	105.53	110.24
7	C	860	NAG	C4-C3-C2	-2.63	107.16	111.02
7	D	870	NAG	C4-C3-C2	2.61	114.85	111.02
7	B	860	NAG	C1-C2-N2	2.57	114.88	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	860	NAG	O7-C7-C8	-2.57	117.28	122.06
7	D	840	NAG	O5-C1-C2	2.57	115.34	111.29
7	A	860	NAG	C3-C4-C5	-2.50	105.78	110.24
7	B	840	NAG	O5-C5-C6	2.48	111.09	107.20
7	B	870	NAG	O3-C3-C2	2.43	114.49	109.47
7	A	840	NAG	C3-C4-C5	-2.41	105.93	110.24
7	B	810	NAG	O4-C4-C5	2.40	115.27	109.30
7	C	840	NAG	O4-C4-C5	2.39	115.24	109.30
7	A	860	NAG	O4-C4-C5	2.37	115.18	109.30
7	C	840	NAG	C8-C7-N2	2.33	120.05	116.10
7	A	840	NAG	O7-C7-C8	-2.32	117.75	122.06
7	C	860	NAG	O7-C7-C8	-2.29	117.80	122.06
7	D	870	NAG	O5-C1-C2	2.29	114.91	111.29
7	B	860	NAG	C3-C4-C5	2.26	114.27	110.24
7	B	870	NAG	C2-N2-C7	-2.25	119.70	122.90
7	A	860	NAG	O3-C3-C2	2.24	114.10	109.47
7	D	810	NAG	O3-C3-C2	2.23	114.08	109.47
7	D	810	NAG	O4-C4-C5	2.22	114.80	109.30
7	C	840	NAG	O7-C7-C8	-2.17	118.03	122.06
7	D	870	NAG	C1-O5-C5	2.14	115.09	112.19
7	D	840	NAG	C6-C5-C4	-2.12	108.05	113.00
7	B	840	NAG	O4-C4-C5	2.09	114.50	109.30
7	D	860	NAG	O5-C5-C6	2.07	110.45	107.20
7	B	860	NAG	C1-O5-C5	2.05	114.97	112.19
7	A	860	NAG	C1-O5-C5	2.04	114.96	112.19
7	A	840	NAG	C6-C5-C4	-2.04	108.23	113.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	860	NAG	C1
7	A	870	NAG	C1
7	B	860	NAG	C1
7	C	860	NAG	C1

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	860	NAG	C3-C2-N2-C7
7	A	860	NAG	C8-C7-N2-C2
7	A	860	NAG	O7-C7-N2-C2
7	A	870	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	870	NAG	O7-C7-N2-C2
7	B	810	NAG	C1-C2-N2-C7
7	B	810	NAG	C8-C7-N2-C2
7	B	810	NAG	O7-C7-N2-C2
7	B	860	NAG	C3-C2-N2-C7
7	C	860	NAG	C8-C7-N2-C2
7	C	860	NAG	O7-C7-N2-C2
7	C	870	NAG	C8-C7-N2-C2
7	C	870	NAG	O7-C7-N2-C2
7	D	840	NAG	C8-C7-N2-C2
7	D	840	NAG	O7-C7-N2-C2
7	D	870	NAG	C8-C7-N2-C2
7	D	870	NAG	O7-C7-N2-C2
7	B	840	NAG	C8-C7-N2-C2
7	B	840	NAG	O7-C7-N2-C2
7	B	860	NAG	C4-C5-C6-O6
7	D	870	NAG	O5-C5-C6-O6
7	D	870	NAG	C4-C5-C6-O6
7	D	860	NAG	O5-C5-C6-O6
7	B	860	NAG	O5-C5-C6-O6
7	B	870	NAG	O5-C5-C6-O6
7	D	860	NAG	C4-C5-C6-O6
7	D	860	NAG	C8-C7-N2-C2
7	B	870	NAG	C4-C5-C6-O6
7	A	870	NAG	O5-C5-C6-O6
7	B	840	NAG	C1-C2-N2-C7
7	B	870	NAG	C8-C7-N2-C2
7	D	860	NAG	O7-C7-N2-C2
7	A	840	NAG	C4-C5-C6-O6
7	A	840	NAG	O5-C5-C6-O6
7	C	870	NAG	O5-C5-C6-O6
7	A	870	NAG	C4-C5-C6-O6
7	B	870	NAG	O7-C7-N2-C2
7	A	860	NAG	O5-C5-C6-O6
7	D	870	NAG	C3-C2-N2-C7
7	D	810	NAG	C8-C7-N2-C2
7	D	810	NAG	O7-C7-N2-C2
7	B	840	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	870	NAG	2	0
7	B	870	NAG	1	0
7	C	860	NAG	1	0
7	A	870	NAG	2	0
7	A	860	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	728/728 (100%)	-0.51	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	25, 42, 71, 86	0
1	B	728/728 (100%)	-0.46	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	17, 42, 71, 86	0
1	C	728/728 (100%)	-0.49	1 (0%) <span style="border: 1px solid blue; padding: 2px;">95</span> <span style="border: 1px solid blue; padding: 2px;">89</span>	25, 43, 71, 86	0
1	D	728/728 (100%)	-0.52	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	25, 43, 71, 86	0
2	E	352/357 (98%)	0.09	14 (3%) <span style="border: 1px solid red; padding: 2px;">38</span> <span style="border: 1px solid red; padding: 2px;">16</span>	21, 66, 82, 88	0
2	F	352/357 (98%)	0.10	6 (1%) <span style="border: 1px solid blue; padding: 2px;">70</span> <span style="border: 1px solid blue; padding: 2px;">42</span>	40, 67, 84, 88	0
2	G	352/357 (98%)	0.00	10 (2%) <span style="border: 1px solid blue; padding: 2px;">53</span> <span style="border: 1px solid red; padding: 2px;">24</span>	36, 67, 83, 88	0
2	H	352/357 (98%)	-0.03	2 (0%) <span style="border: 1px solid blue; padding: 2px;">89</span> <span style="border: 1px solid blue; padding: 2px;">72</span>	40, 67, 84, 88	0
All	All	4320/4340 (99%)	-0.32	33 (0%) <span style="border: 1px solid blue; padding: 2px;">86</span> <span style="border: 1px solid blue; padding: 2px;">65</span>	17, 49, 79, 88	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	293	ASN	4.0
2	E	262	CYS	3.9
2	G	293	ASN	3.4
2	E	15	HIS	3.3
2	G	247	THR	3.3
2	G	242	THR	3.0
2	E	295	ASP	2.9
2	E	294	THR	2.9
2	G	262	CYS	2.8
2	E	291	SER	2.8
2	E	237	GLY	2.8
2	F	314	ASP	2.7
2	G	229	ASP	2.6
2	G	237	GLY	2.6
2	G	42	THR	2.6
2	F	262	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	260	GLU	2.5
2	E	17	HIS	2.3
2	G	260	GLU	2.3
2	H	219	GLY	2.3
2	F	246	THR	2.2
2	H	54	LYS	2.2
2	E	261	ILE	2.1
2	E	238	HIS	2.1
1	C	766	PRO	2.1
2	F	293	ASN	2.1
2	G	15	HIS	2.1
2	E	16	VAL	2.0
2	G	16	VAL	2.0
2	F	291	SER	2.0
2	E	181	ASP	2.0
2	F	247	THR	2.0
2	E	292	LEU	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	Q	2	14/15	0.69	0.45	90,91,92,92	0
4	NAG	J	2	14/15	0.75	0.46	78,79,80,80	0
4	NAG	R	2	14/15	0.76	0.45	78,79,80,80	0
4	NAG	U	2	14/15	0.79	0.43	67,69,71,71	0
5	MAN	O	4	11/12	0.80	0.29	48,49,50,50	0
4	NAG	Y	2	14/15	0.82	0.39	61,62,64,64	0
4	NAG	P	2	14/15	0.82	0.39	58,60,60,60	0
5	MAN	T	4	11/12	0.84	0.37	70,71,72,72	0
4	NAG	R	1	14/15	0.85	0.29	70,73,74,76	0
4	NAG	N	2	14/15	0.85	0.32	60,61,62,62	0
5	BMA	X	3	11/12	0.85	0.27	64,65,66,68	0

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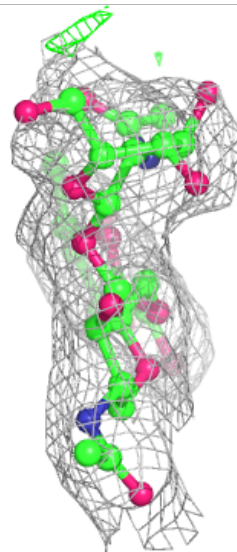
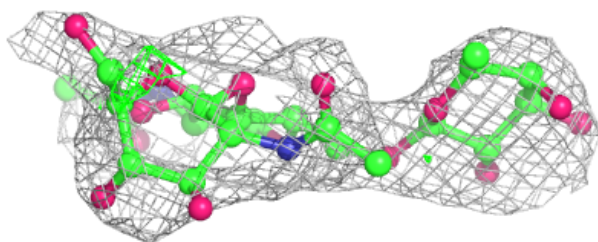
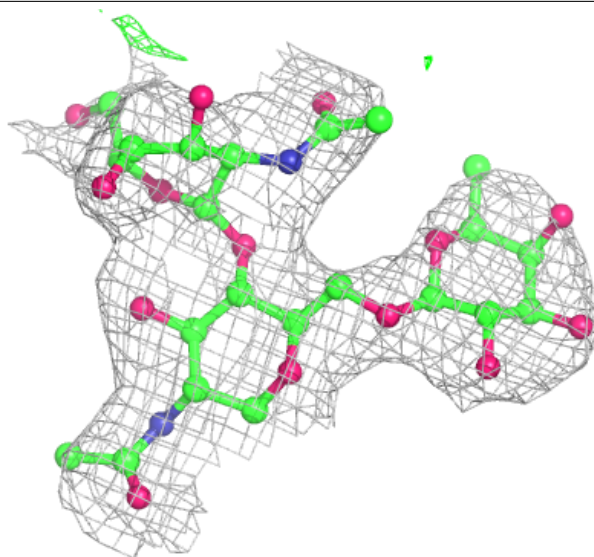
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	I	2	14/15	0.86	0.42	81,82,82,83	0
3	FUC	Q	3	10/11	0.86	0.43	86,86,87,87	0
5	MAN	L	4	11/12	0.87	0.24	58,59,60,61	0
5	MAN	X	4	11/12	0.87	0.31	69,69,70,71	0
6	FUC	M	2	10/11	0.87	0.28	73,74,75,75	0
6	NAG	V	1	14/15	0.87	0.29	81,83,84,86	0
4	NAG	J	1	14/15	0.88	0.23	67,70,72,75	0
4	NAG	W	2	14/15	0.88	0.33	62,65,66,66	0
6	FUC	V	2	10/11	0.88	0.32	85,86,86,86	0
6	NAG	M	1	14/15	0.89	0.25	74,75,76,76	0
4	NAG	S	2	14/15	0.89	0.36	66,68,68,69	0
3	FUC	I	3	10/11	0.89	0.40	79,80,80,80	0
5	BMA	T	3	11/12	0.89	0.27	62,64,65,68	0
4	NAG	Y	1	14/15	0.90	0.27	53,56,58,60	0
4	NAG	S	1	14/15	0.90	0.28	59,61,62,64	0
4	NAG	K	1	14/15	0.90	0.28	57,60,62,62	0
3	NAG	Q	1	14/15	0.90	0.23	82,84,86,88	0
4	NAG	W	1	14/15	0.90	0.28	58,60,61,63	0
4	NAG	P	1	14/15	0.90	0.25	50,53,55,56	0
4	NAG	K	2	14/15	0.91	0.32	62,64,66,66	0
3	NAG	I	1	14/15	0.92	0.25	74,77,80,80	0
5	NAG	L	2	14/15	0.92	0.23	52,54,54,56	0
4	NAG	N	1	14/15	0.93	0.27	55,57,58,59	0
5	NAG	X	2	14/15	0.93	0.20	55,56,59,62	0
5	NAG	L	1	14/15	0.93	0.16	42,43,46,49	0
4	NAG	U	1	14/15	0.93	0.20	54,57,60,64	0
5	NAG	O	2	14/15	0.94	0.21	35,37,38,39	0
5	BMA	O	3	11/12	0.94	0.18	41,43,45,46	0
5	NAG	X	1	14/15	0.94	0.18	42,45,48,52	0
5	BMA	L	3	11/12	0.94	0.28	56,58,58,58	0
5	NAG	T	2	14/15	0.94	0.21	52,54,57,60	0
5	NAG	T	1	14/15	0.95	0.12	41,42,47,49	0
5	NAG	O	1	14/15	0.97	0.15	30,31,33,33	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.

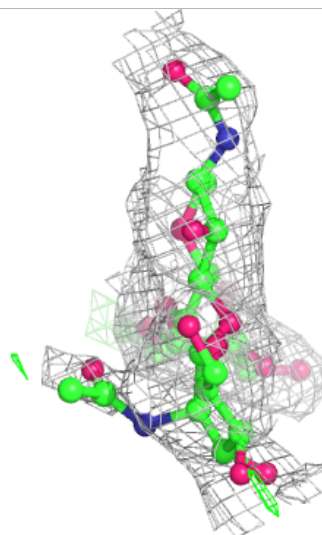
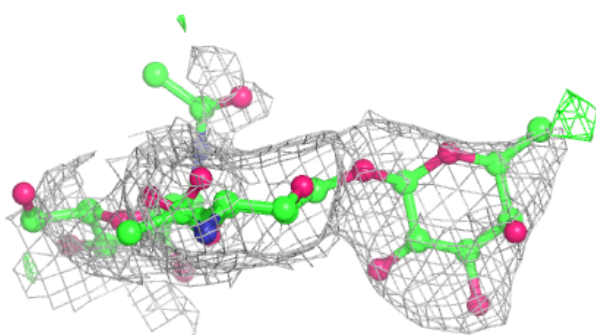
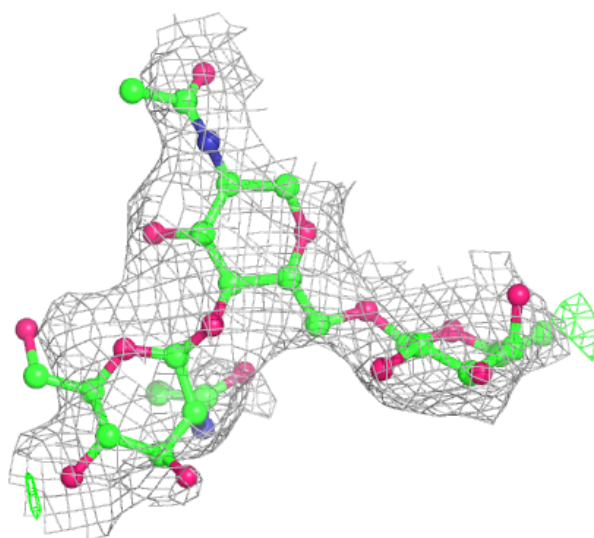
**Electron density around Chain I:**

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



**Electron density around Chain Q:**

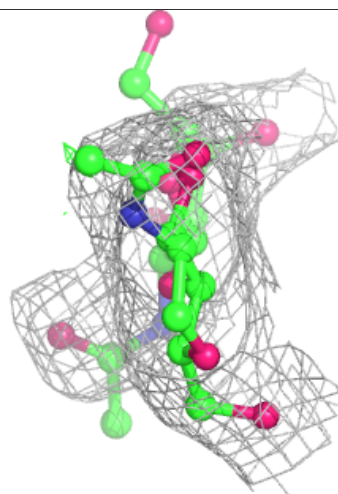
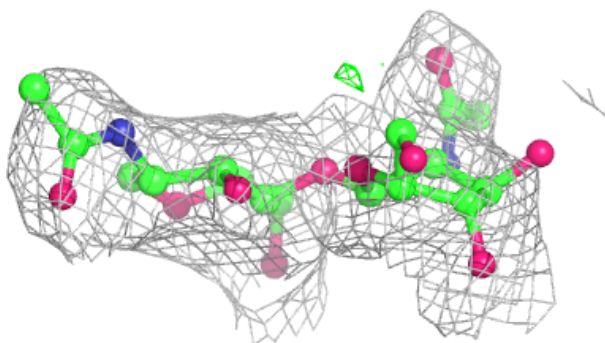
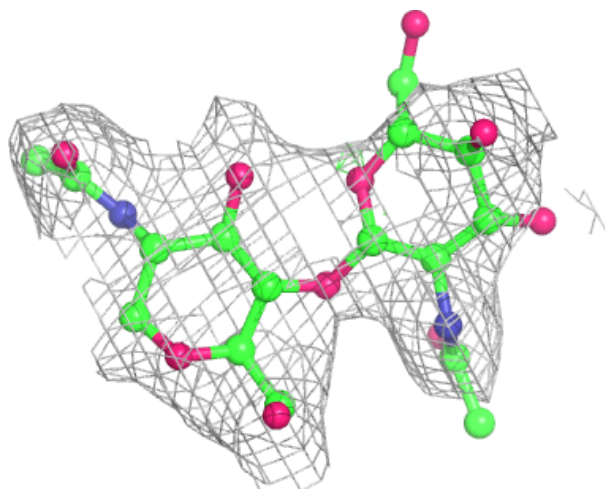
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





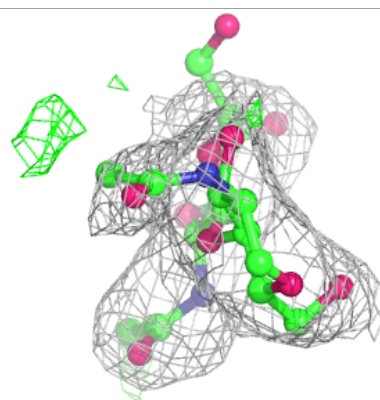
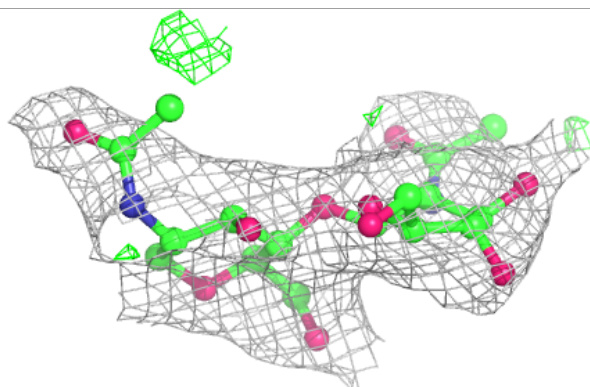
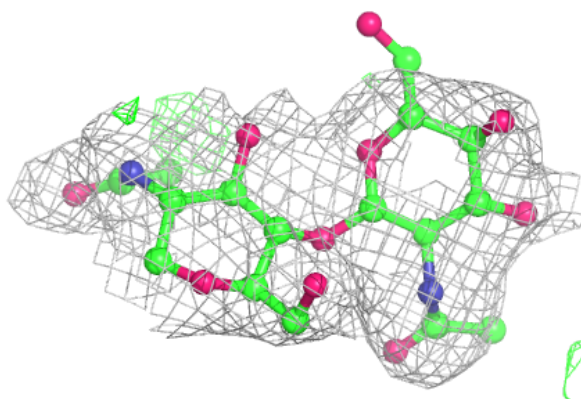
**Electron density around Chain J:**

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

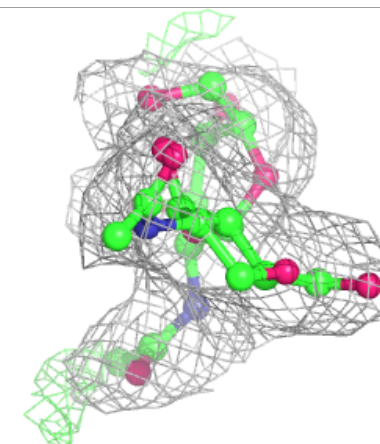
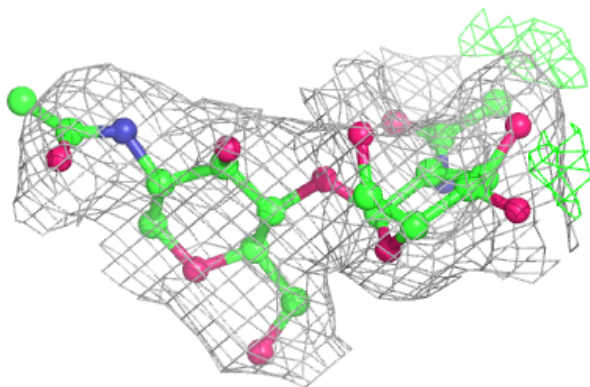
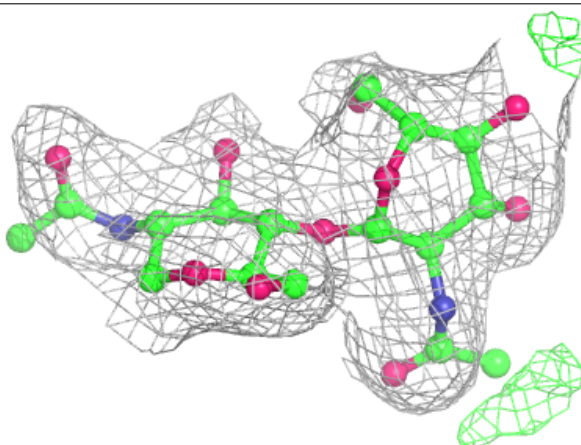


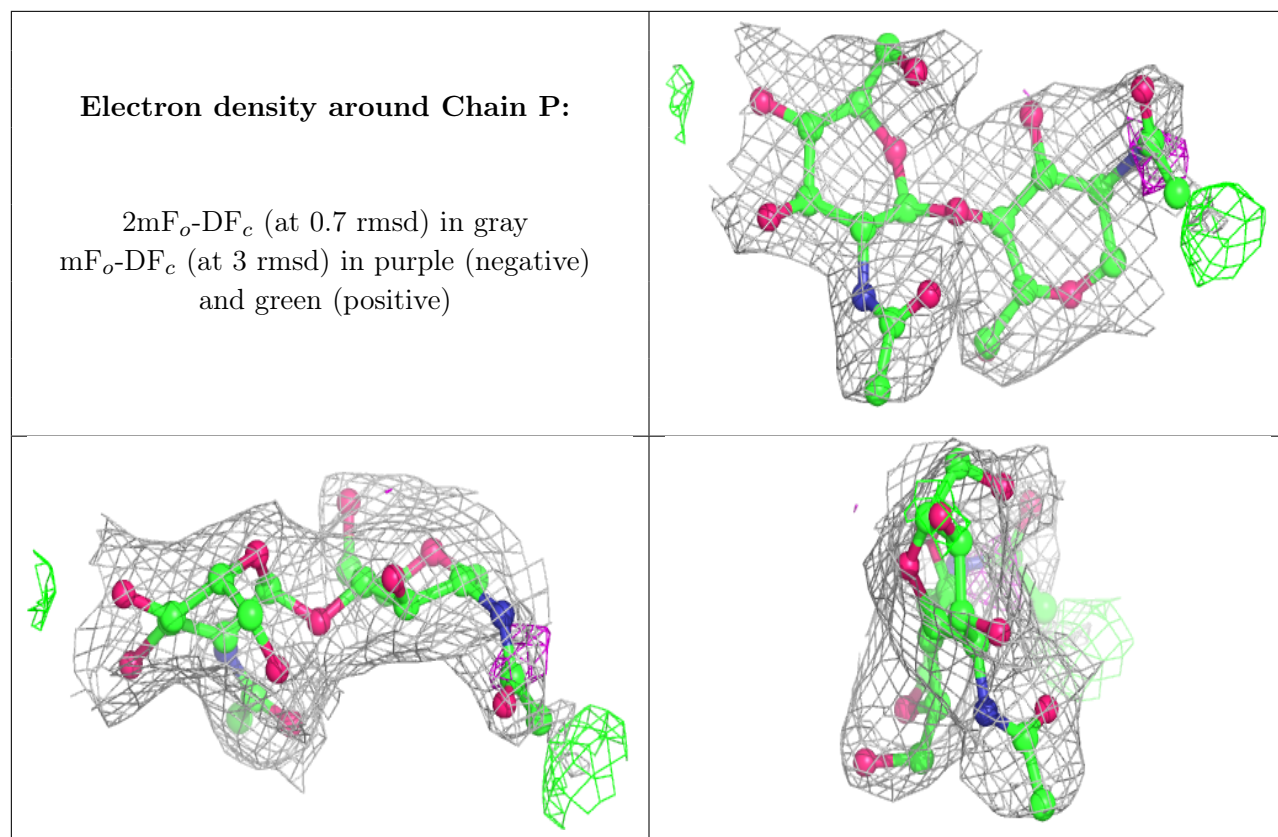
**Electron density around Chain K:**

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

**Electron density around Chain N:**

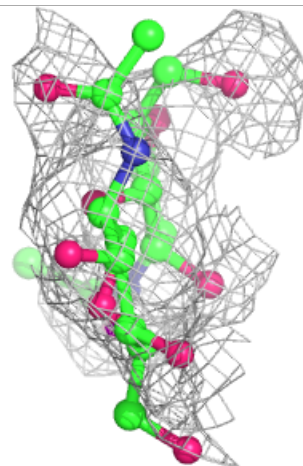
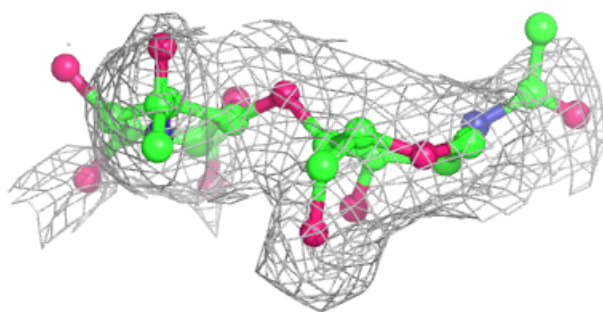
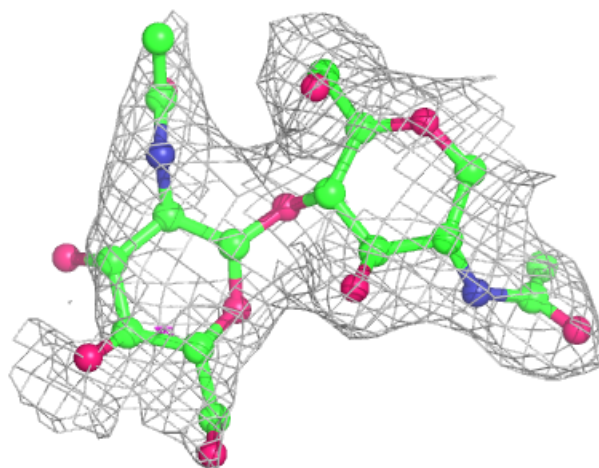
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





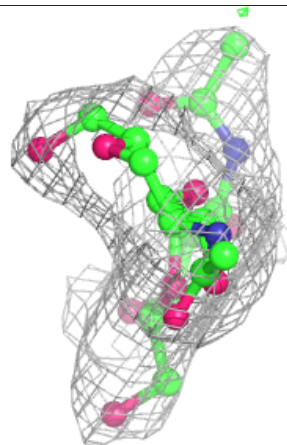
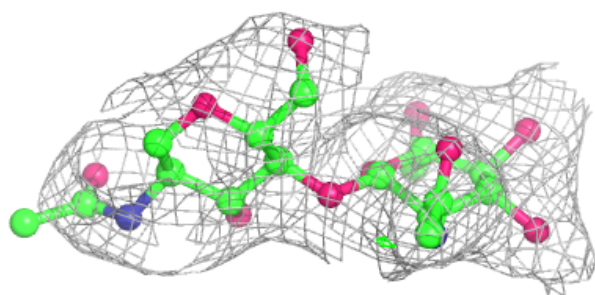
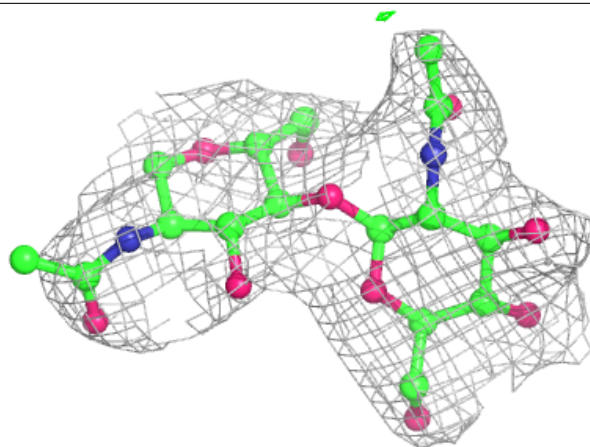
**Electron density around Chain R:**

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



**Electron density around Chain S:**

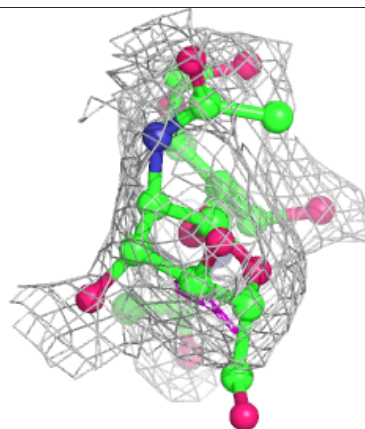
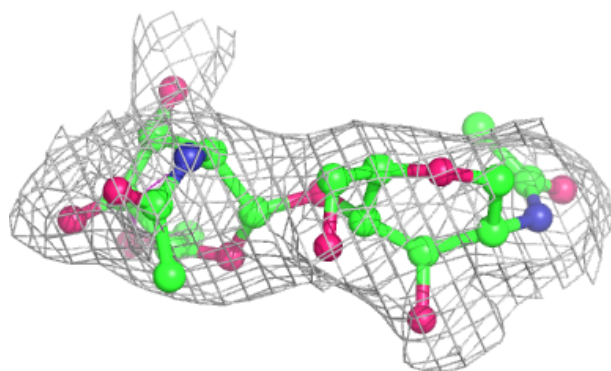
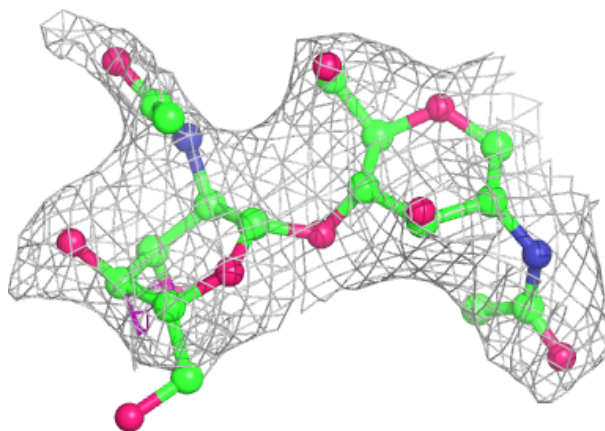
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





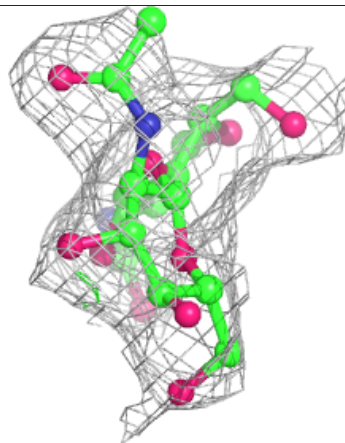
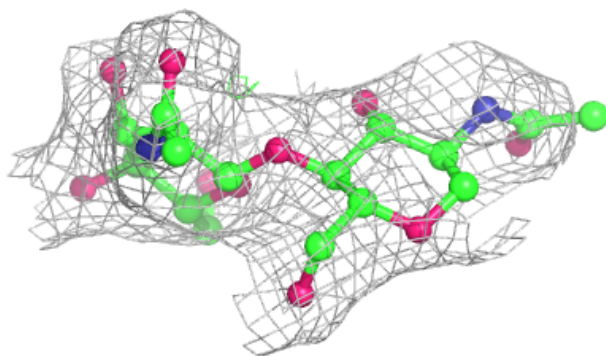
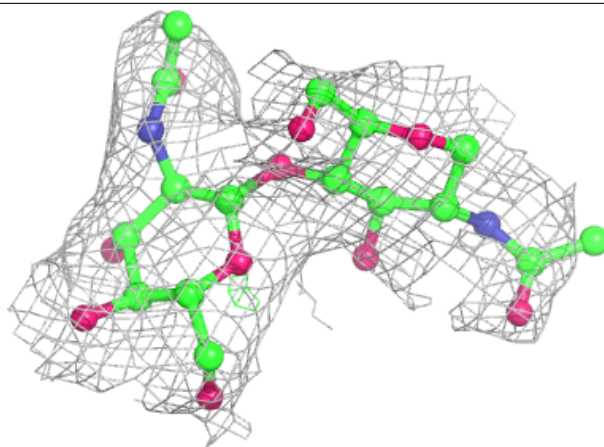
**Electron density around Chain U:**

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



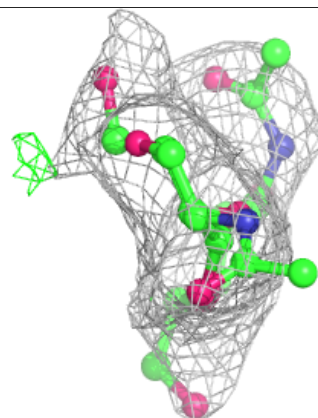
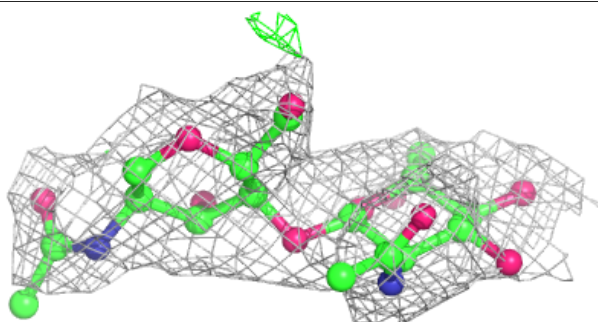
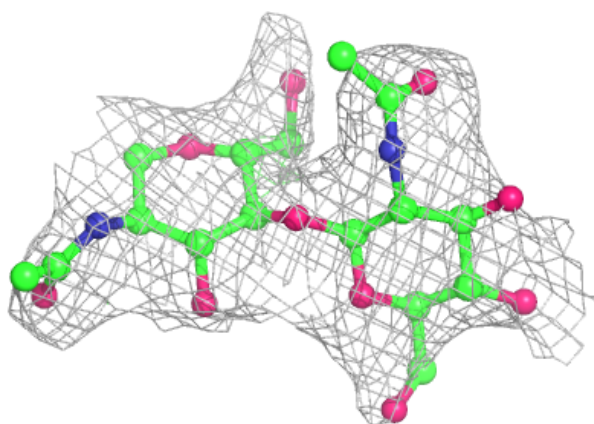
**Electron density around Chain W:**

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

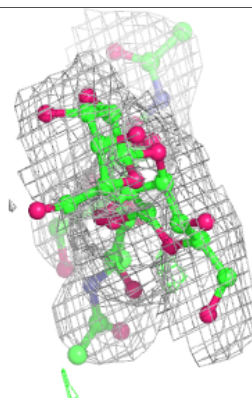
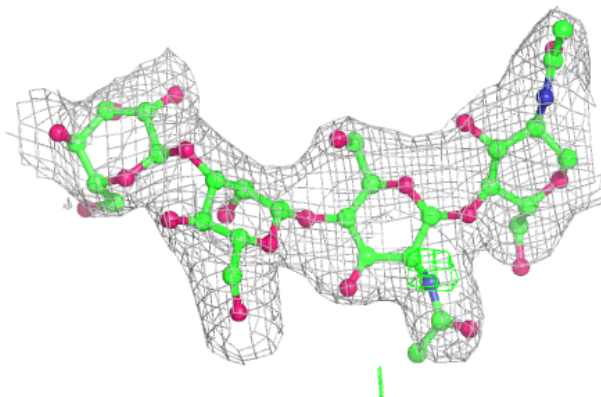


**Electron density around Chain Y:**

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

**Electron density around Chain L:**

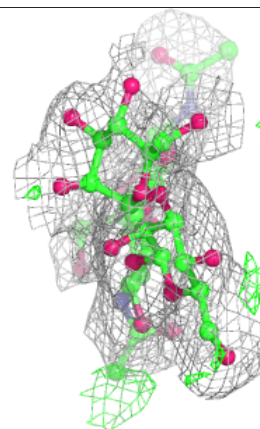
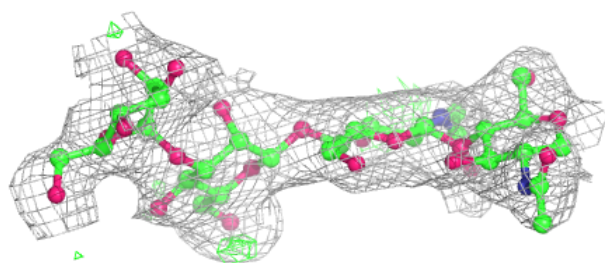
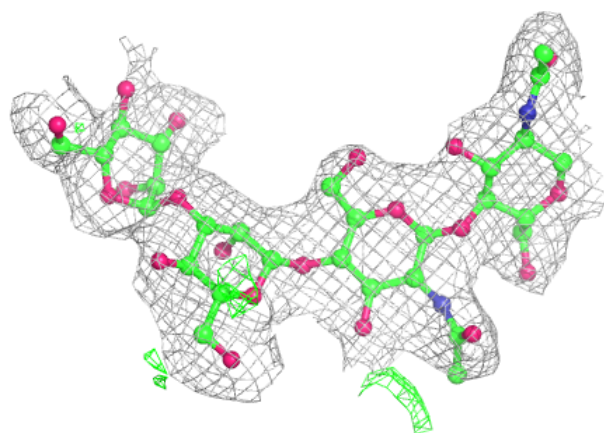
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



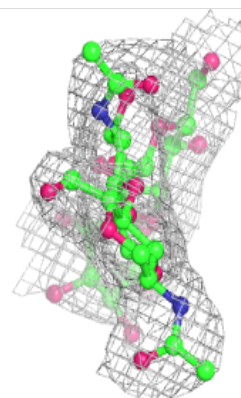
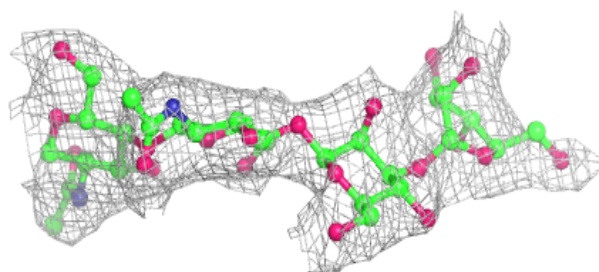
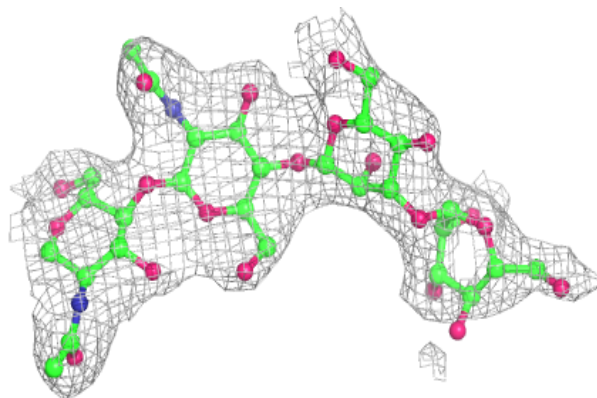


**Electron density around Chain O:**

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

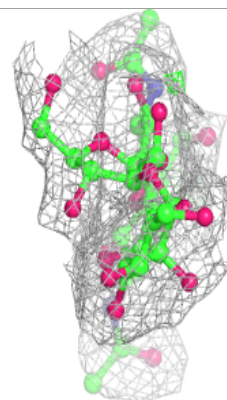
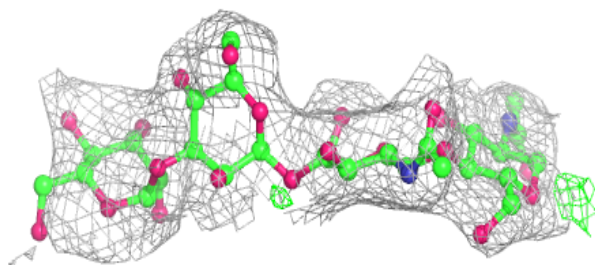
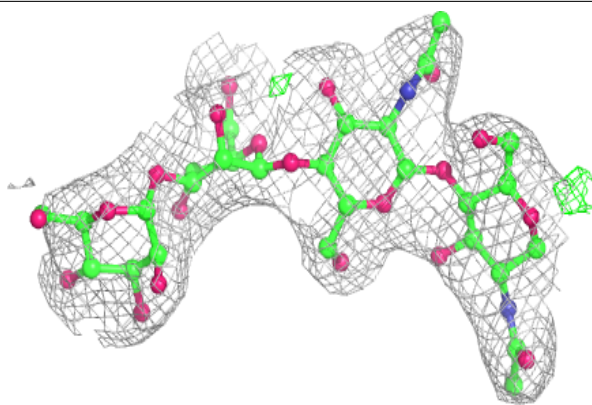
**Electron density around Chain T:**

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

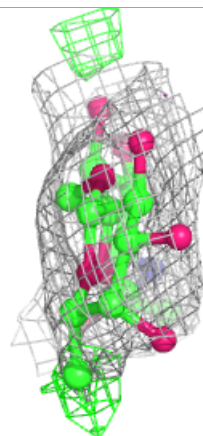
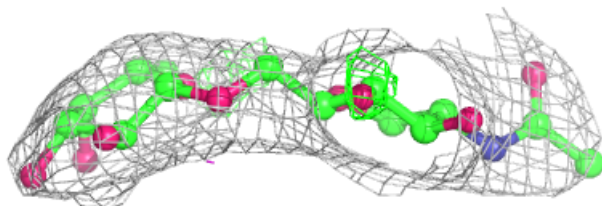
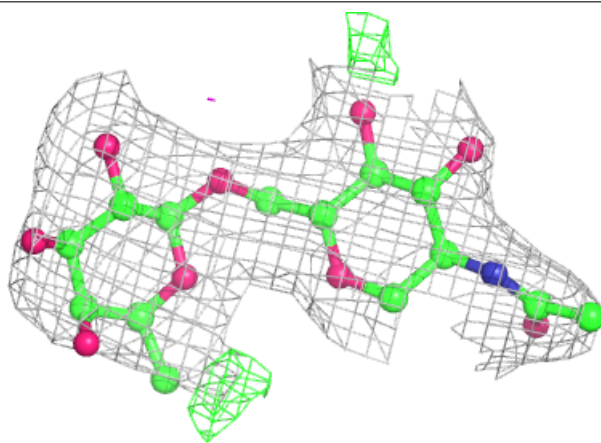


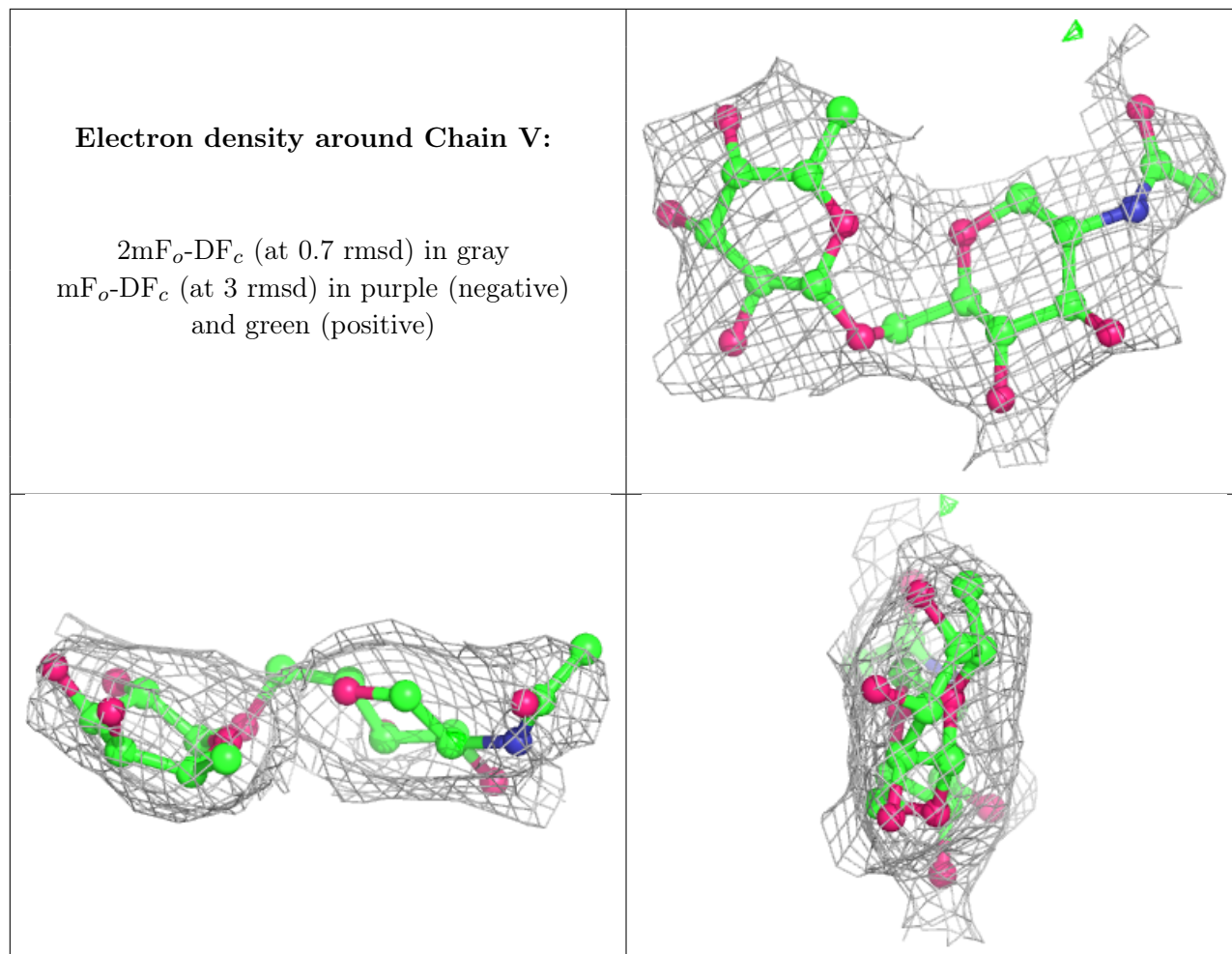
**Electron density around Chain X:**

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

**Electron density around Chain M:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	D	870	14/15	0.65	0.38	90,91,93,93	0
7	NAG	C	870	14/15	0.76	0.31	88,89,90,90	0
7	NAG	A	870	14/15	0.78	0.33	88,88,90,90	0
7	NAG	A	860	14/15	0.79	0.30	67,68,71,71	0
7	NAG	C	860	14/15	0.80	0.38	68,69,71,71	0
7	NAG	B	870	14/15	0.81	0.24	87,88,88,89	0
7	NAG	D	810	14/15	0.83	0.34	69,71,72,72	0
7	NAG	D	840	14/15	0.86	0.19	48,50,51,51	0
7	NAG	B	860	14/15	0.86	0.31	64,65,66,66	0
7	NAG	D	860	14/15	0.87	0.30	63,66,67,67	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	F	501	1/1	0.87	0.10	62,62,62,62	0
7	NAG	B	810	14/15	0.88	0.27	64,65,66,66	0
7	NAG	B	840	14/15	0.90	0.16	46,48,49,49	0
7	NAG	A	850	14/15	0.92	0.21	52,54,57,60	0
7	NAG	C	840	14/15	0.93	0.26	51,54,55,55	0
7	NAG	A	840	14/15	0.96	0.21	48,50,50,50	0
8	ZN	H	501	1/1	0.96	0.19	58,58,58,58	0
8	ZN	G	501	1/1	0.98	0.23	58,58,58,58	0
8	ZN	E	501	1/1	0.99	0.33	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.