



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:38 AM BST

PDB ID : 6CRD  
Title : INFLUENZA VIRUS NEURAMINIDASE SUBTYPE N9 (TERN) with tetra-brachion (TB) domain stalk  
Authors : Streltsov, V.A.; Schmidt, P.; McKimm-Breschkin, J.  
Deposited on : 2018-03-16  
Resolution : 2.57 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

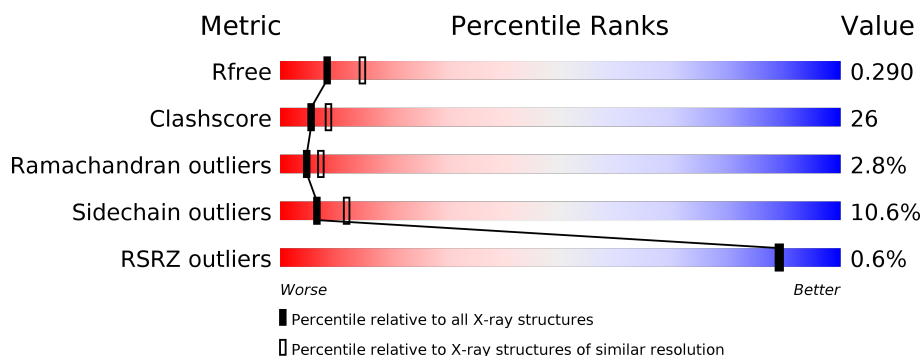
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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.




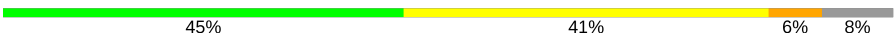
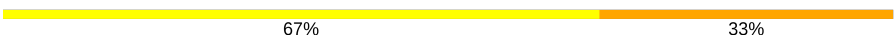


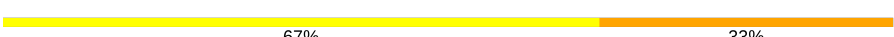
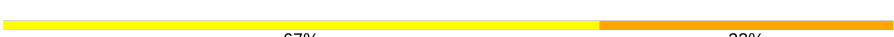

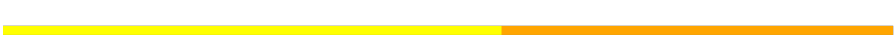

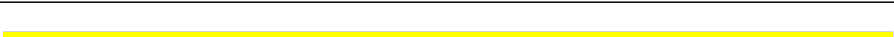


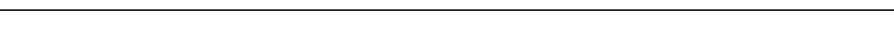


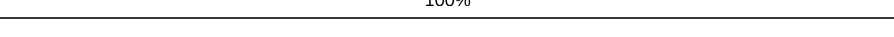


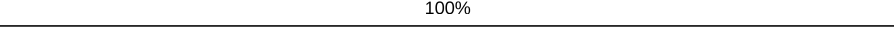
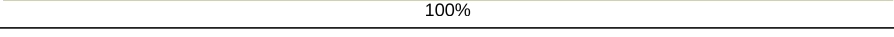
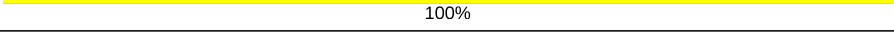
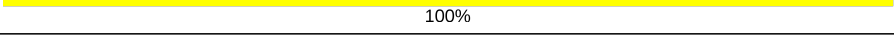
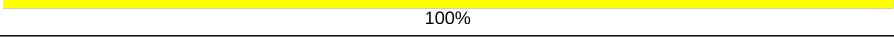
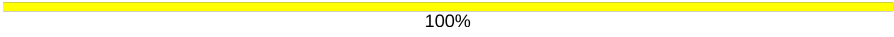
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 on 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	473	
1	B	473	
1	C	473	
1	D	473	
1	E	473	
1	F	473	

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Mol	Chain	Length	Quality of chain
1	G	473	
1	H	473	
2	I	9	
2	L	9	
2	N	9	
2	Q	9	
2	T	9	
2	W	9	
2	Z	9	
2	c	9	
3	J	2	
3	M	2	
3	O	2	
3	P	2	
3	R	2	
3	S	2	
3	U	2	
3	V	2	
3	X	2	
3	Y	2	
3	a	2	
3	b	2	
3	d	2	
3	e	2	
4	K	4	

## 2 Entry composition [i](#)

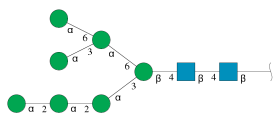
There are 6 unique types of molecules in this entry. The entry contains 29975 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tetrabrachion, Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	B	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	C	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			
1	D	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			
1	E	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	F	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	G	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			
1	H	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			

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



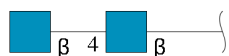
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	L	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	N	9	Total	C	N	O	0	0	0
			105	58	2	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	T	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	W	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	Z	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	c	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

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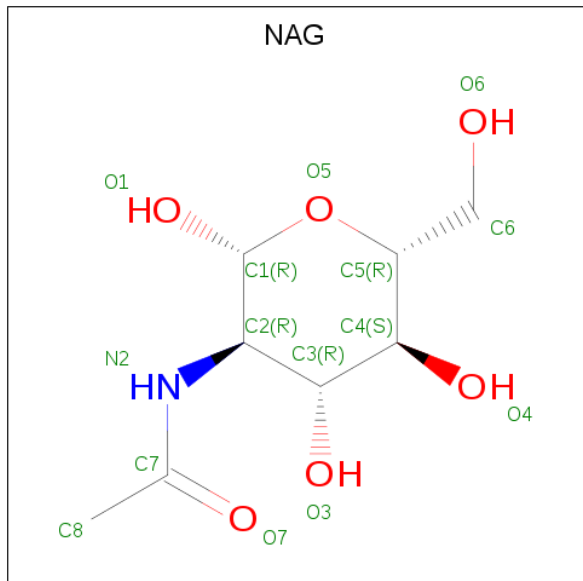
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called 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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

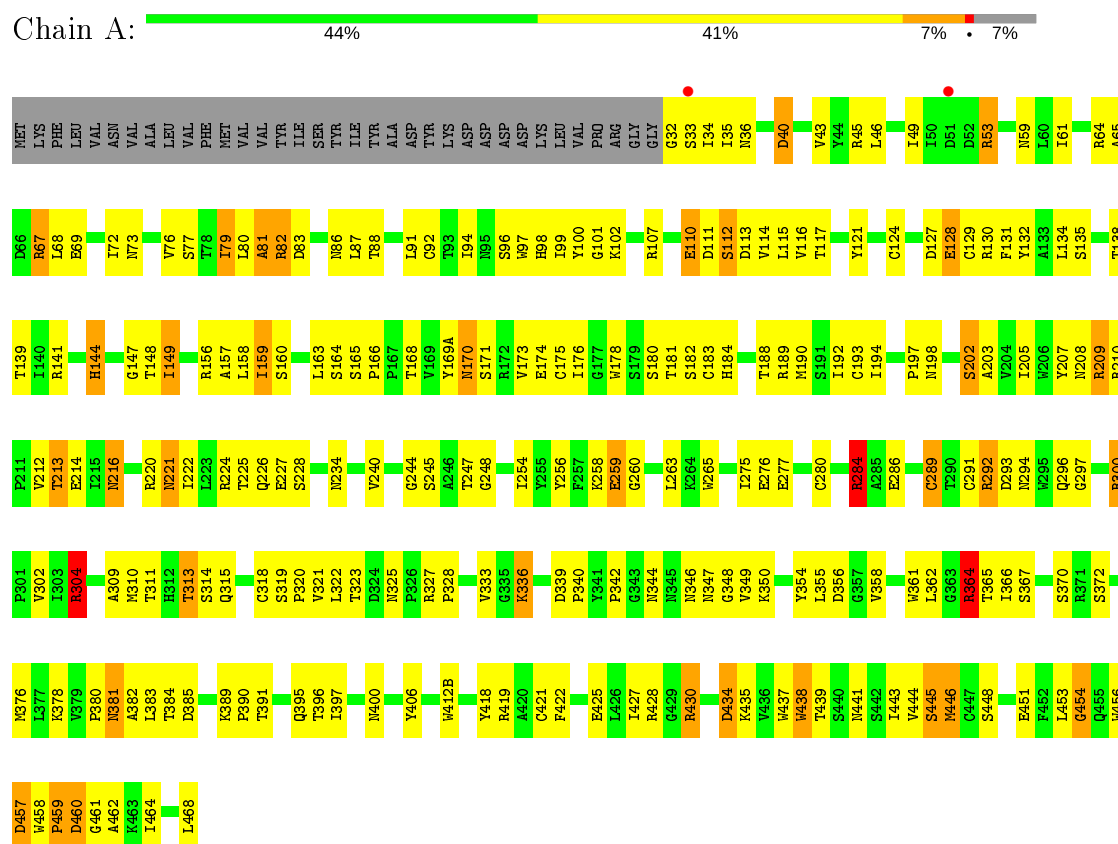
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	122	Total	O	0	0
			122	122		
6	B	111	Total	O	0	0
			111	111		
6	C	103	Total	O	0	0
			103	103		
6	D	122	Total	O	0	0
			122	122		
6	E	124	Total	O	0	0
			124	124		
6	F	111	Total	O	0	0
			111	111		
6	G	98	Total	O	0	0
			98	98		
6	H	142	Total	O	0	0
			142	142		

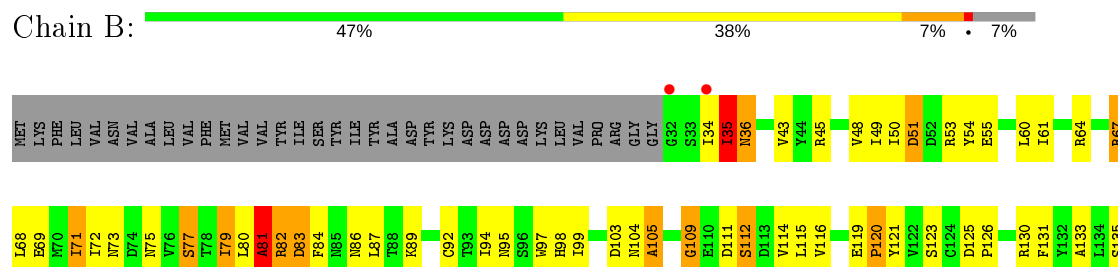
### 3 Residue-property plots

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.

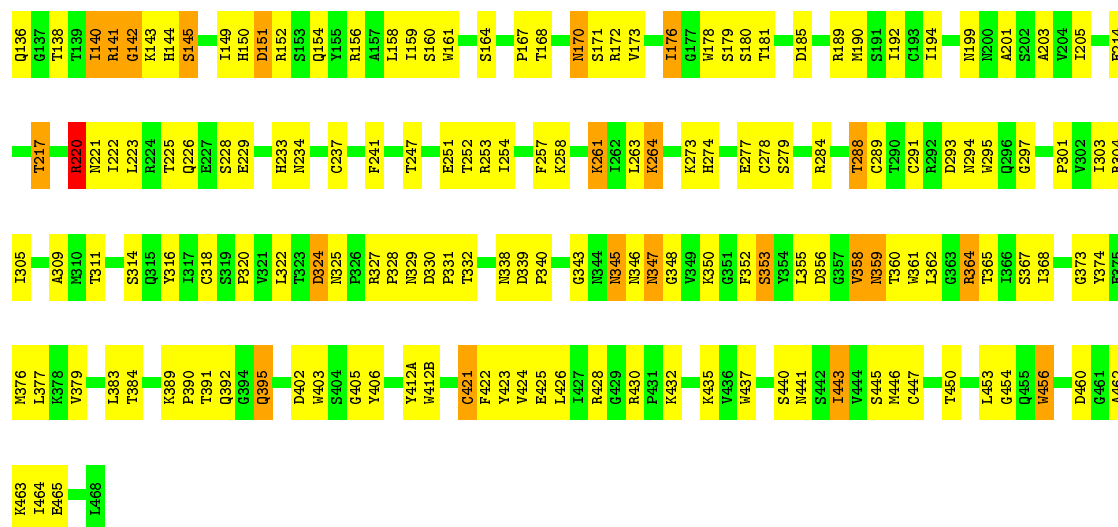
#### • Molecule 1: Tetrabrachion, Neuraminidase



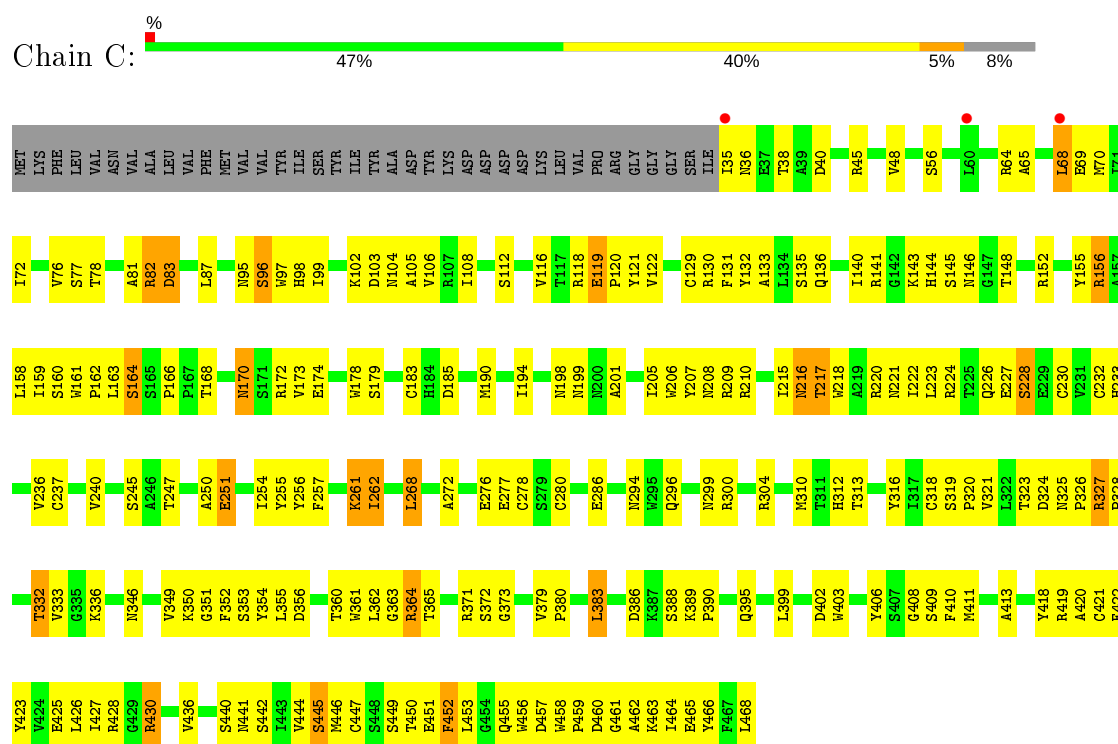
#### • Molecule 1: Tetrabrachion, Neuraminidase



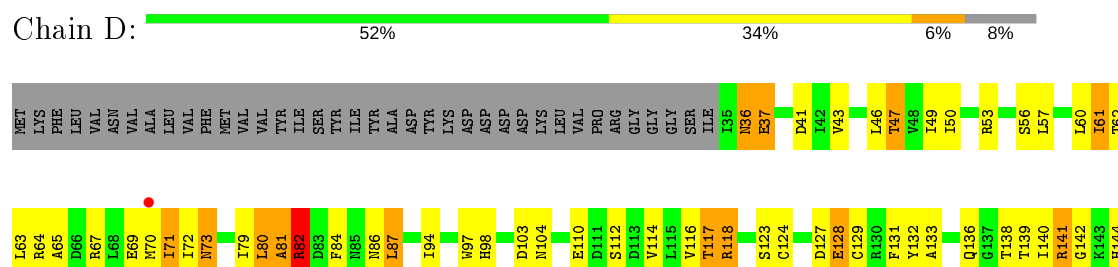


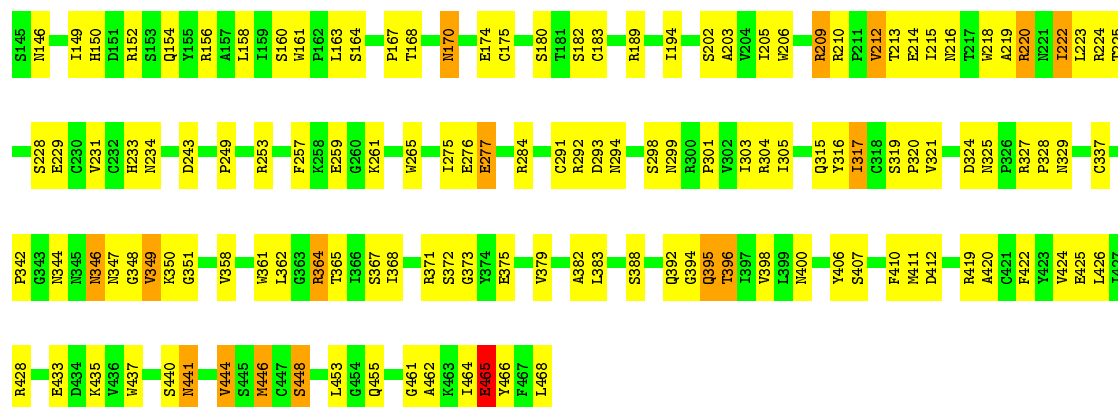


• Molecule 1: Tetrabrachion, Neuraminidase

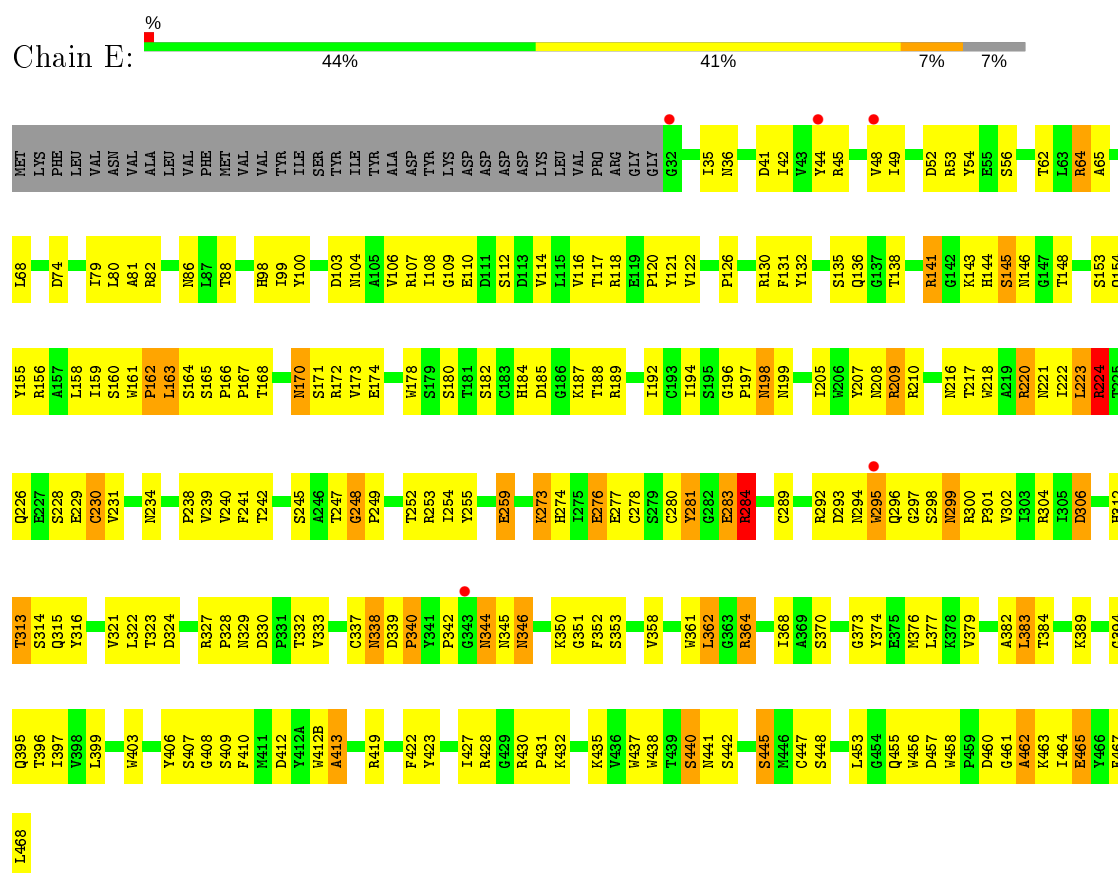


• Molecule 1: Tetrabrachion, Neuraminidase

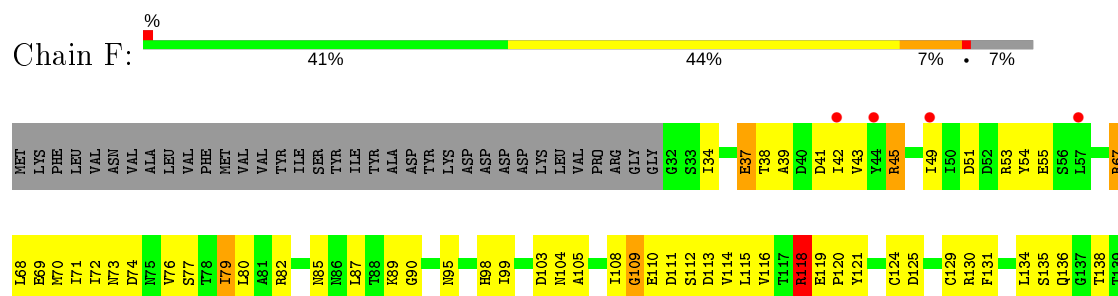


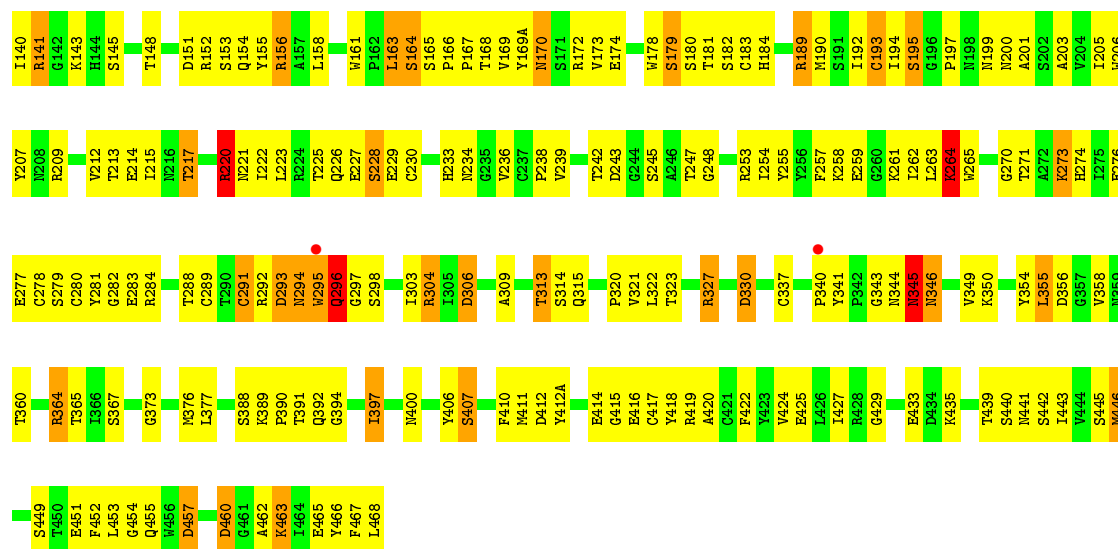


• Molecule 1: Tetrabrachion, Neuraminidase

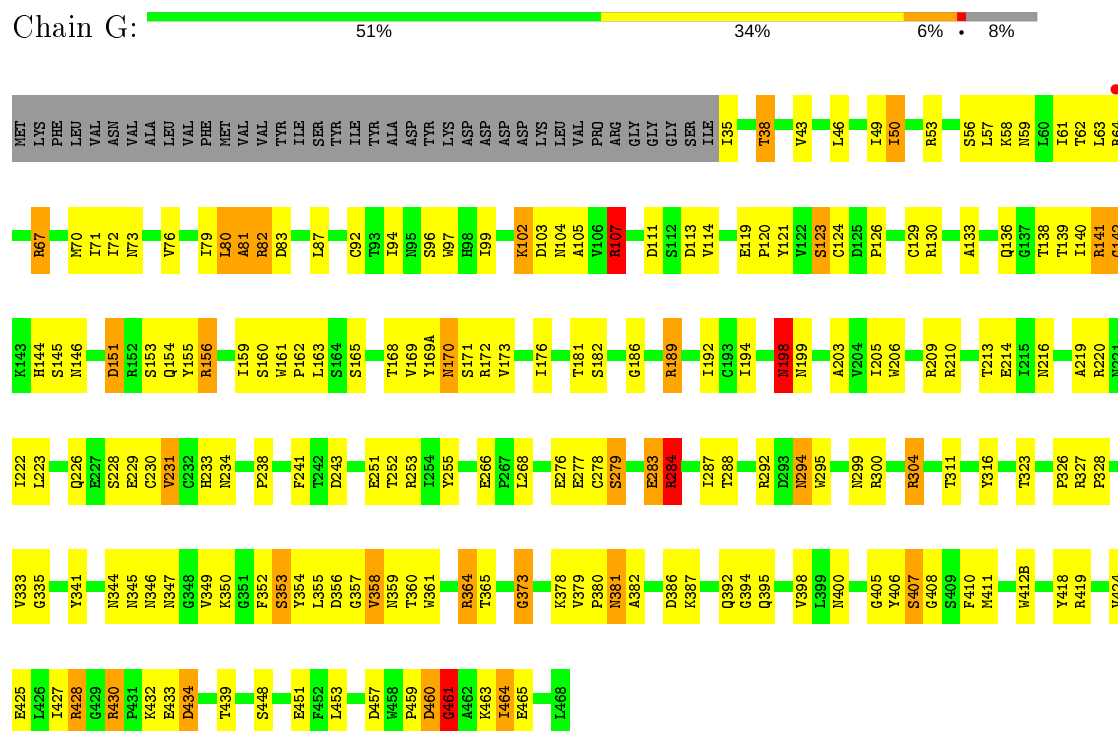


• Molecule 1: Tetrabrachion, Neuraminidase

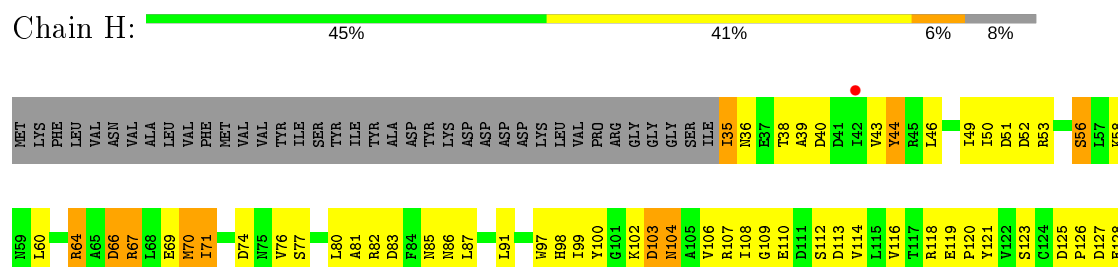


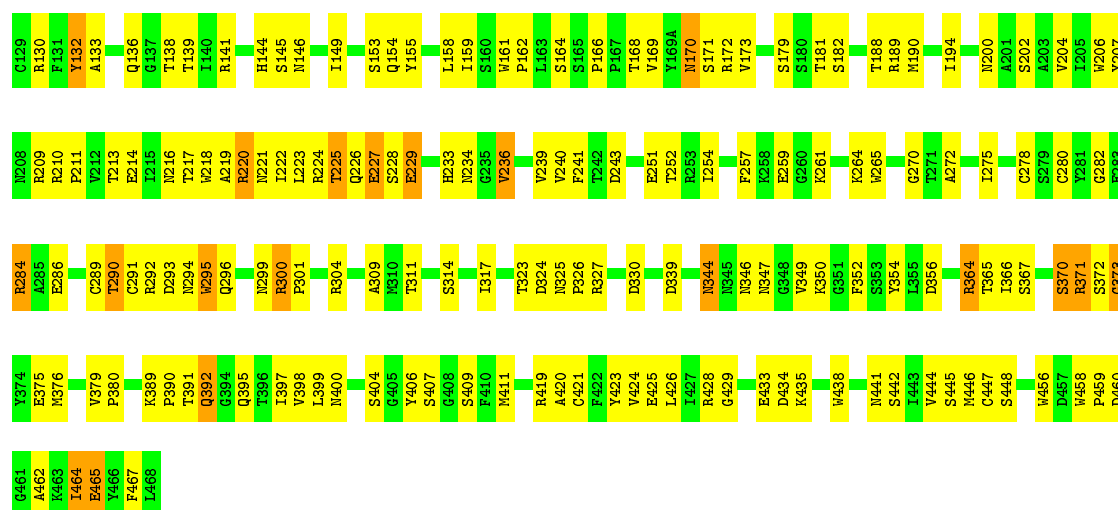


• Molecule 1: Tetrabrachion, Neuraminidase



• Molecule 1: Tetrabrachion, Neuraminidase





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

Chain I:  67% 33%



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

Chain L:  67% 33%



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

Chain N:  78% 22%



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

Chain Q:  67% 33%



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

Chain T:  67% 33%



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

Chain W:  33% 67%

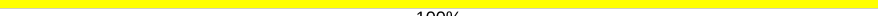


- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  56% 44%



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

Chain c:  100%



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

Chain J:  100%

MAG1  
MAG2

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

Chain M:  50% 50%MAG1  
MAG2

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

Chain O:  100%MAG1  
MAG2

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

Chain P:  100%MAG1  
MAG2

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

Chain R:  50% 50%MAG1  
MAG2

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

Chain S:  100%MAG1  
MAG2

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

Chain U:  50% 50%MAG1  
MAG2

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

Chain V:  50% 50%

NAG1  
NAG2

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

Chain X:  100%

NAG1  
NAG2

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

Chain Y:  100%

NAG1  
NAG2

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

Chain a:  100%

NAG1  
NAG2

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

Chain b:  100%

NAG1  
NAG2

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

Chain d:  100%

NAG1  
NAG2

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

Chain e:  100%

MAG1  
MAG2

- Molecule 4: 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 K:



MAG1  
MAG2  
BMG3  
MAN4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.00Å 142.33Å 163.30Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	40.04 – 2.57 39.45 – 2.59	Depositor EDS
% Data completeness (in resolution range)	77.6 (40.04-2.57) 77.6 (39.45-2.59)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.208 , 0.306 0.210 , 0.290	Depositor DCC
$R_{free}$ test set	5727 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 13.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.165 for h,-k,-l	Xtriage
Reported twinning fraction	0.854 for H, K, L 0.146 for -h,-k,l	Depositor
Outliers	1 of 114357 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	29975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/3550	0.87	3/4834 (0.1%)
1	B	0.42	0/3550	0.86	3/4834 (0.1%)
1	C	0.41	0/3532	0.87	0/4810
1	D	0.41	0/3532	0.83	0/4810
1	E	0.41	0/3550	0.87	1/4834 (0.0%)
1	F	0.39	0/3550	0.85	0/4834
1	G	0.39	0/3532	0.82	1/4810 (0.0%)
1	H	0.43	0/3532	0.87	1/4810 (0.0%)
All	All	0.41	0/28328	0.85	9/38576 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	7
1	D	0	5
1	E	0	9
1	F	0	13
1	G	0	7
1	H	0	7
All	All	0	57

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASP	CB-CA-C	-7.21	95.99	110.40
1	A	289	CYS	CB-CA-C	-5.64	99.12	110.40
1	A	220	ARG	CG-CD-NE	-5.62	99.99	111.80
1	B	220	ARG	CG-CD-NE	5.28	122.89	111.80
1	A	391	THR	CA-CB-OG1	-5.25	97.98	109.00
1	H	83	ASP	CB-CA-C	-5.10	100.20	110.40
1	B	421	CYS	CB-CA-C	-5.06	100.28	110.40
1	E	224	ARG	CB-CG-CD	5.02	124.66	111.60
1	G	198	ASN	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ARG	Sidechain
1	A	304	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	79	ILE	Peptide
1	B	109	GLY	Peptide
1	B	220	ARG	Sidechain
1	B	284	ARG	Sidechain
1	B	81	ALA	Peptide
1	C	141	ARG	Sidechain
1	C	152	ARG	Sidechain
1	C	156	ARG	Sidechain
1	C	209	ARG	Sidechain
1	C	327	ARG	Sidechain
1	C	371	ARG	Sidechain
1	C	81	ALA	Peptide
1	D	141	ARG	Sidechain
1	D	152	ARG	Sidechain
1	D	220	ARG	Sidechain
1	D	225	THR	Peptide
1	D	304	ARG	Sidechain
1	E	141	ARG	Sidechain
1	E	172	ARG	Sidechain
1	E	210	ARG	Sidechain
1	E	224	ARG	Sidechain
1	E	247	THR	Peptide
1	E	248	GLY	Peptide
1	E	344	ASN	Peptide
1	E	430	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	64	ARG	Sidechain
1	F	118	ARG	Sidechain
1	F	130	ARG	Sidechain
1	F	141	ARG	Sidechain
1	F	156	ARG	Sidechain
1	F	189	ARG	Sidechain
1	F	209	ARG	Sidechain
1	F	220	ARG	Sidechain
1	F	248	GLY	Peptide
1	F	296	GLN	Peptide
1	F	327	ARG	Sidechain
1	F	345	ASN	Peptide
1	F	45	ARG	Sidechain
1	F	67	ARG	Sidechain
1	G	107	ARG	Sidechain
1	G	156	ARG	Sidechain
1	G	189	ARG	Sidechain
1	G	279	SER	Peptide
1	G	284	ARG	Sidechain
1	G	428	ARG	Sidechain
1	G	461	GLY	Peptide
1	H	210	ARG	Sidechain
1	H	225	THR	Peptide
1	H	284	ARG	Sidechain
1	H	327	ARG	Sidechain
1	H	371	ARG	Sidechain
1	H	81	ALA	Peptide
1	H	82	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3465	0	3303	212	0
1	B	3465	0	3303	201	0
1	C	3447	0	3284	181	0
1	D	3447	0	3285	170	0
1	E	3465	0	3303	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3465	0	3303	216	0
1	G	3447	0	3284	176	0
1	H	3447	0	3284	195	0
2	I	105	0	88	3	0
2	L	105	0	88	5	0
2	N	105	0	88	6	0
2	Q	105	0	88	2	0
2	T	105	0	88	3	0
2	W	105	0	88	6	0
2	Z	105	0	88	4	0
2	c	105	0	88	0	0
3	J	28	0	25	0	0
3	M	28	0	25	1	0
3	O	28	0	25	2	0
3	P	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	U	28	0	25	2	0
3	V	28	0	25	4	0
3	X	28	0	25	2	0
3	Y	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
4	K	50	0	43	1	0
5	A	14	0	13	0	0
5	B	28	0	26	1	0
5	C	14	0	13	1	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
5	G	14	0	13	1	0
5	H	14	0	13	0	0
6	A	122	0	0	8	0
6	B	111	0	0	13	0
6	C	103	0	0	2	0
6	D	122	0	0	9	1
6	E	124	0	0	5	0
6	F	111	0	0	11	0
6	G	98	0	0	6	0
6	H	142	0	0	6	0
All	All	29975	0	27550	1455	1

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 26.

All (1455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:ASN:HA	6:E:612:HOH:O	1.21	1.32
1:F:169:VAL:HG23	6:F:601:HOH:O	1.26	1.27
1:B:327:ARG:HE	1:B:368:ILE:HG22	1.04	1.18
1:D:321:VAL:HG13	1:D:364:ARG:HH21	1.07	1.12
1:G:304:ARG:HG3	1:G:304:ARG:HH11	1.02	1.12
1:E:108:ILE:HD12	1:E:166:PRO:HG3	1.25	1.10
1:E:293:ASP:HB3	1:E:297:GLY:HA3	1.35	1.07
1:A:188:THR:HG21	1:A:208:ASN:HB2	1.39	1.04
1:D:321:VAL:CG1	1:D:364:ARG:HH21	1.69	1.04
1:C:104:ASN:O	1:C:108:ILE:HG13	1.56	1.03
1:E:98:HIS:HE1	1:E:447:CYS:HB2	1.21	1.03
1:G:373:GLY:HA2	1:G:398:VAL:HG12	1.37	1.02
1:C:103:ASP:OD2	1:C:105:ALA:HB2	1.60	1.01
1:E:98:HIS:CE1	1:E:447:CYS:HB2	1.96	1.00
1:F:169:VAL:CG2	6:F:601:HOH:O	1.92	0.99
1:G:92:CYS:HB2	6:G:616:HOH:O	1.61	0.98
1:A:216:ASN:HD21	1:B:454:GLY:H	0.98	0.97
1:F:118:ARG:HB3	1:F:119:GLU:OE2	1.64	0.96
1:F:258:LYS:CB	1:F:263:LEU:HD11	1.96	0.95
1:G:124:CYS:HB3	6:G:610:HOH:O	1.65	0.95
1:F:270:GLY:HA3	1:F:314:SER:OG	1.67	0.94
1:D:321:VAL:HG13	1:D:364:ARG:NH2	1.81	0.94
1:G:87:LEU:O	1:G:284:ARG:HA	1.67	0.94
1:A:110:GLU:O	1:A:141:ARG:HD2	1.67	0.94
1:C:277:GLU:O	1:C:350:LYS:HD2	1.67	0.93
1:C:45:ARG:NH2	1:F:43:VAL:HG11	1.84	0.93
1:F:295:TRP:O	1:F:345:ASN:HA	1.70	0.92
1:F:72:ILE:O	1:F:76:VAL:HG23	1.69	0.92
1:G:199:ASN:HA	1:G:220:ARG:O	1.68	0.92
3:X:1:NAG:H61	3:X:2:NAG:O7	1.69	0.92
1:E:106:VAL:HG12	1:E:462:ALA:HB2	1.49	0.91
1:A:138:THR:HG21	1:A:144:HIS:O	1.70	0.91
1:G:304:ARG:HG3	1:G:304:ARG:NH1	1.82	0.89
1:F:258:LYS:HB2	1:F:263:LEU:HD11	1.54	0.89
1:B:450:THR:HG21	6:B:687:HOH:O	1.73	0.89
1:H:87:LEU:H	1:H:233:HIS:HD2	1.14	0.89
1:A:454:GLY:H	1:H:216:ASN:HD21	1.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:GLU:OE2	1:E:410:PHE:HB2	1.71	0.88
1:E:376:MET:O	1:E:377:LEU:HD23	1.71	0.88
1:B:144:HIS:HE1	1:E:463:LYS:H	1.21	0.88
1:G:130:ARG:NH2	1:G:160:SER:OG	2.07	0.88
1:E:245:SER:OG	1:E:248:GLY:N	2.07	0.88
1:B:327:ARG:NE	1:B:368:ILE:HG22	1.89	0.87
1:F:134:LEU:HD13	1:F:178:TRP:O	1.73	0.87
1:A:216:ASN:ND2	1:B:454:GLY:H	1.72	0.87
1:F:79:ILE:C	1:F:80:LEU:HD23	1.96	0.87
1:C:280:CYS:O	1:C:409:SER:OG	1.92	0.86
1:A:216:ASN:HD21	1:B:454:GLY:N	1.74	0.86
1:E:65:ALA:HB1	1:H:64:ARG:HH21	1.37	0.86
1:G:304:ARG:HH11	1:G:304:ARG:CG	1.88	0.86
1:G:151:ASP:OD1	1:G:151:ASP:N	2.08	0.86
1:C:324:ASP:O	1:C:327:ARG:HD3	1.77	0.85
1:H:391:THR:O	1:H:392:GLN:HB2	1.77	0.85
1:F:51:ASP:O	1:F:55:GLU:HG2	1.75	0.85
1:D:209:ARG:HG2	1:D:209:ARG:HH11	1.41	0.84
1:E:442:SER:OG	1:E:460:ASP:OD1	1.93	0.84
1:E:109:GLY:HA2	1:E:114:VAL:HG23	1.58	0.84
1:E:49:ILE:HG23	1:E:53:ARG:NH1	1.92	0.84
1:A:297:GLY:O	6:A:601:HOH:O	1.94	0.84
1:A:284:ARG:CG	1:A:284:ARG:HH11	1.91	0.83
1:B:87:LEU:H	1:B:233:HIS:CD2	1.96	0.83
1:C:168:THR:H	1:C:170:ASN:HD21	1.23	0.83
1:G:103:ASP:HB2	1:G:165:SER:O	1.77	0.82
1:E:208:ASN:O	1:E:209:ARG:HB2	1.78	0.82
1:H:300:ARG:NH2	1:H:349:VAL:O	2.12	0.81
1:A:49:ILE:HG23	1:A:53:ARG:NH1	1.95	0.81
1:A:49:ILE:HG23	1:A:53:ARG:HH12	1.46	0.81
1:E:106:VAL:CG1	1:E:462:ALA:HB2	2.09	0.81
1:E:316:TYR:H	1:E:338:ASN:HD21	1.23	0.81
1:H:113:ASP:O	1:H:169:VAL:HG23	1.80	0.81
1:H:217:THR:OG1	1:H:220:ARG:HA	1.80	0.81
1:A:435:LYS:HB3	1:A:468:LEU:HD21	1.61	0.81
1:C:355:LEU:HA	1:C:360:THR:HG23	1.61	0.81
1:B:403:TRP:CH2	1:B:432:LYS:HD2	2.16	0.81
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.44	0.80
1:F:220:ARG:HH11	1:F:220:ARG:HG2	1.45	0.80
1:B:309:ALA:CB	1:B:311:THR:HG23	2.10	0.80
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:VAL:HG11	1:H:278:CYS:SG	2.21	0.80
1:G:465:GLU:CD	1:G:465:GLU:H	1.85	0.80
1:F:134:LEU:CD1	1:F:178:TRP:O	2.29	0.79
1:H:170:ASN:C	1:H:170:ASN:HD22	1.84	0.79
1:B:309:ALA:HB3	1:B:311:THR:HG23	1.65	0.79
1:F:112:SER:HA	1:G:113:ASP:OD2	1.83	0.78
1:A:135:SER:HB2	1:A:159:ILE:HD11	1.64	0.78
1:A:35:ILE:HG21	1:B:34:ILE:HG21	1.65	0.78
1:H:194:ILE:CD1	1:H:224:ARG:HA	2.13	0.78
1:D:41:ASP:OD2	6:D:601:HOH:O	2.00	0.78
1:A:258:LYS:HB2	1:A:263:LEU:HD11	1.66	0.78
1:B:98:HIS:CE1	1:B:447:CYS:HB2	2.19	0.78
1:H:373:GLY:HA2	1:H:399:LEU:O	1.84	0.78
1:H:325:ASN:OD1	1:H:370:SER:O	2.02	0.78
1:E:130:ARG:HH12	1:E:162:PRO:HD3	1.48	0.77
1:C:459:PRO:HD2	1:F:154:GLN:HG2	1.67	0.77
1:B:327:ARG:HH12	1:B:364:ARG:HB2	1.48	0.77
1:G:168:THR:OG1	1:G:170:ASN:ND2	2.17	0.77
1:B:152:ARG:HG2	1:B:178:TRP:CG	2.19	0.77
1:H:170:ASN:HD22	1:H:171:SER:N	1.82	0.77
1:A:100:TYR:HB3	1:A:445:SER:O	1.85	0.77
1:A:168:THR:H	1:A:170:ASN:HD21	1.31	0.77
1:D:315:GLN:HG3	1:D:316:TYR:N	2.00	0.76
1:F:441:ASN:ND2	1:F:442:SER:O	2.17	0.76
1:B:356:ASP:OD2	6:B:601:HOH:O	2.03	0.76
1:D:81:ALA:O	1:D:82:ARG:HG2	1.86	0.76
1:C:456:TRP:CD1	1:F:197:PRO:HD3	2.20	0.76
1:E:109:GLY:HA2	1:E:114:VAL:CG2	2.15	0.76
1:B:43:VAL:HG23	1:E:42:ILE:HG23	1.68	0.76
1:E:441:ASN:ND2	1:E:442:SER:O	2.16	0.76
2:W:7:MAN:H61	2:W:9:MAN:H5	1.68	0.76
1:A:135:SER:HB2	1:A:159:ILE:CD1	2.17	0.76
1:A:212:VAL:HG21	1:A:260:GLY:HA3	1.68	0.75
1:F:454:GLY:H	1:G:216:ASN:ND2	1.84	0.75
1:E:154:GLN:HG2	1:H:459:PRO:HD2	1.66	0.75
1:E:293:ASP:CB	1:E:297:GLY:HA3	2.16	0.75
1:A:192:ILE:HG12	1:A:205:ILE:HG13	1.69	0.74
1:F:367:SER:HB2	1:F:400:ASN:HD21	1.51	0.74
1:C:144:HIS:HE1	1:D:462:ALA:HA	1.52	0.74
1:H:194:ILE:HA	1:H:202:SER:O	1.88	0.74
1:B:98:HIS:HE1	1:B:447:CYS:HB2	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:HIS:O	1:F:446:MET:HB3	1.87	0.74
1:E:316:TYR:N	1:E:338:ASN:HD21	1.86	0.74
1:E:330:ASP:OD2	1:E:364:ARG:NH2	2.21	0.74
1:F:327:ARG:HE	1:F:364:ARG:HH21	1.35	0.74
1:E:106:VAL:HG12	1:E:462:ALA:CB	2.17	0.74
1:A:291:CYS:O	1:A:300:ARG:HG2	1.88	0.73
1:A:72:ILE:O	1:A:76:VAL:HG23	1.88	0.73
1:F:321:VAL:HA	1:F:330:ASP:OD2	1.88	0.73
1:E:108:ILE:HD12	1:E:166:PRO:CG	2.13	0.73
1:G:104:ASN:O	1:G:107:ARG:HB2	1.88	0.73
1:A:294:ASN:HD21	1:A:347:ASN:HA	1.53	0.73
1:E:294:ASN:O	1:E:346:ASN:HA	1.89	0.73
1:E:178:TRP:HE1	1:E:196:GLY:H	1.36	0.73
1:C:240:VAL:HG22	1:C:254:ILE:HG12	1.70	0.73
1:D:168:THR:H	1:D:170:ASN:ND2	1.87	0.73
1:D:315:GLN:HG3	1:D:316:TYR:H	1.54	0.73
1:D:46:LEU:HD12	1:G:46:LEU:HD13	1.71	0.73
1:D:325:ASN:O	1:D:348:GLY:HA2	1.89	0.72
1:C:323:THR:HB	1:C:363:GLY:O	1.90	0.72
1:G:299:ASN:OD1	1:G:341:TYR:CB	2.37	0.72
1:D:98:HIS:CE1	1:D:419:ARG:HH11	2.06	0.72
1:F:236:VAL:HA	1:F:257:PHE:O	1.89	0.71
1:E:168:THR:OG1	1:E:170:ASN:ND2	2.23	0.71
1:D:87:LEU:HG	1:D:233:HIS:HD2	1.56	0.71
1:F:141:ARG:NH2	1:F:467:PHE:HA	2.05	0.71
1:G:379:VAL:HG12	1:G:382:ALA:HB2	1.73	0.71
1:G:392:GLN:NE2	6:G:602:HOH:O	2.21	0.71
1:A:144:HIS:HE1	1:B:463:LYS:H	1.36	0.71
1:A:124:CYS:HB2	1:A:412(B):TRP:HZ3	1.54	0.71
1:B:94:ILE:HB	1:B:361:TRP:NE1	2.04	0.71
1:A:367:SER:CB	1:A:372:SER:HB2	2.21	0.71
1:G:87:LEU:O	1:G:284:ARG:CA	2.39	0.71
1:H:366:ILE:HG21	1:H:400:ASN:HB2	1.71	0.71
1:G:419:ARG:HD3	1:G:448:SER:O	1.90	0.71
1:F:327:ARG:HE	1:F:364:ARG:NH2	1.89	0.71
1:C:256:TYR:CD1	1:C:310:MET:HG2	2.26	0.70
1:B:144:HIS:HE1	1:E:463:LYS:N	1.89	0.70
1:F:293:ASP:OD2	1:F:297:GLY:HA3	1.91	0.70
1:H:204:VAL:HG23	6:H:659:HOH:O	1.90	0.70
1:B:179:SER:HB3	1:B:194:ILE:HB	1.72	0.70
1:D:43:VAL:HA	1:G:46:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:SER:HB2	1:H:438:TRP:HB3	1.74	0.70
1:C:129:CYS:O	1:C:163:LEU:HB2	1.91	0.70
1:E:185:ASP:OD1	1:E:188:THR:N	2.24	0.70
1:F:170:ASN:C	1:F:170:ASN:HD22	1.93	0.70
1:F:205:ILE:HD11	1:F:215:ILE:HD12	1.74	0.70
1:B:460:ASP:OD1	6:B:602:HOH:O	2.10	0.70
1:A:69:GLU:OE1	1:B:64:ARG:NH2	2.24	0.70
1:G:361:TRP:CE2	1:G:378:LYS:HB2	2.27	0.70
1:G:430:ARG:HB2	1:G:439:THR:OG1	1.91	0.70
1:A:180:SER:HB2	1:A:192:ILE:O	1.91	0.70
1:A:318:CYS:SG	1:A:383:LEU:O	2.49	0.70
1:H:442:SER:OG	1:H:460:ASP:OD1	2.05	0.70
1:D:110:GLU:O	1:D:141:ARG:HD2	1.91	0.70
1:G:107:ARG:NH1	1:G:461:GLY:O	2.24	0.70
1:B:294:ASN:O	1:B:346:ASN:HA	1.92	0.69
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.57	0.69
1:E:136:GLN:HG2	1:E:156:ARG:HE	1.57	0.69
1:A:131:PHE:CE1	1:A:163:LEU:HD12	2.27	0.69
1:B:144:HIS:CE1	1:E:463:LYS:H	2.07	0.69
1:C:320:PRO:HG3	1:C:332:THR:O	1.92	0.69
1:H:66:ASP:O	1:H:69:GLU:N	2.25	0.69
1:D:87:LEU:HG	1:D:233:HIS:CD2	2.28	0.69
1:E:437:TRP:HB2	6:E:647:HOH:O	1.92	0.69
1:A:339:ASP:HB3	1:A:340:PRO:HD2	1.75	0.69
1:A:389:LYS:HB3	1:A:390:PRO:HD2	1.74	0.69
1:H:158:LEU:HD12	1:H:159:ILE:O	1.93	0.69
6:D:630:HOH:O	1:G:163:LEU:HD23	1.92	0.69
1:B:199:ASN:ND2	2:L:1:NAG:H81	2.08	0.69
1:H:87:LEU:H	1:H:233:HIS:CD2	2.05	0.68
1:A:158:LEU:HD13	1:A:180:SER:OG	1.94	0.68
1:E:278:CYS:HB3	1:E:289:CYS:HB3	1.75	0.68
1:B:199:ASN:HD21	2:L:1:NAG:H81	1.57	0.68
1:A:99:ILE:HG13	1:A:100:TYR:H	1.58	0.68
1:C:68:LEU:O	1:C:72:ILE:HG13	1.92	0.68
1:A:454:GLY:H	1:H:216:ASN:ND2	1.92	0.68
1:B:131:PHE:CE1	1:B:443:ILE:HG21	2.28	0.68
1:A:437:TRP:CD1	4:K:1:NAG:H82	2.27	0.68
1:B:109:GLY:O	1:B:140:ILE:HD12	1.94	0.68
1:D:168:THR:H	1:D:170:ASN:HD21	1.40	0.68
1:B:168:THR:OG1	1:B:170:ASN:ND2	2.27	0.67
1:D:46:LEU:O	1:D:50:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ALA:O	1:D:69:GLU:HG3	1.93	0.67
1:D:158:LEU:HD23	1:D:174:GLU:HB2	1.77	0.67
1:F:113:ASP:O	6:F:601:HOH:O	2.12	0.67
1:H:280:CYS:O	1:H:409:SER:OG	2.12	0.67
1:F:89:LYS:HE2	1:F:415:GLY:O	1.94	0.67
1:C:144:HIS:CE1	1:D:462:ALA:HA	2.30	0.67
1:D:87:LEU:H	1:D:233:HIS:HD2	1.40	0.67
1:E:295:TRP:O	1:E:296:GLN:HG2	1.95	0.67
1:F:376:MET:HG2	1:F:397:ILE:HD11	1.75	0.67
1:H:46:LEU:O	1:H:50:ILE:HD12	1.94	0.67
1:C:425:GLU:HG3	1:C:441:ASN:HD22	1.58	0.67
1:D:349:VAL:HG23	1:D:371:ARG:NE	2.10	0.67
1:E:465:GLU:CD	1:E:465:GLU:H	1.98	0.67
1:B:135:SER:O	1:B:156:ARG:HA	1.95	0.67
1:C:97:TRP:H	1:C:395:GLN:HE22	1.41	0.67
1:B:152:ARG:HG2	1:B:178:TRP:CD2	2.30	0.67
1:C:155:TYR:OH	1:D:461:GLY:HA2	1.95	0.66
1:G:326:PRO:HD2	1:G:347:ASN:HB3	1.77	0.66
1:E:109:GLY:CA	1:E:114:VAL:CG2	2.73	0.66
1:H:444:VAL:HG21	1:H:458:TRP:HB3	1.75	0.66
1:A:367:SER:HB2	1:A:372:SER:HB2	1.76	0.66
1:B:422:PHE:HE2	1:B:424:VAL:CG2	2.07	0.66
1:C:419:ARG:NH2	1:F:212:VAL:O	2.28	0.66
1:F:350:LYS:HG2	1:F:407:SER:O	1.95	0.66
1:E:188:THR:HG22	1:E:207:TYR:CZ	2.30	0.66
1:F:168:THR:HG21	1:G:169(A):TYR:HD1	1.59	0.66
1:E:108:ILE:CD1	1:E:166:PRO:HG3	2.16	0.66
1:D:103:ASP:HA	1:D:164:SER:O	1.95	0.66
1:D:218:TRP:CZ2	1:D:253:ARG:HG3	2.31	0.66
1:G:114:VAL:HG12	1:G:140:ILE:CD1	2.26	0.65
1:H:293:ASP:O	6:H:602:HOH:O	2.12	0.65
1:F:238:PRO:HA	1:F:255:TYR:O	1.96	0.65
1:G:114:VAL:HG12	1:G:140:ILE:HD11	1.78	0.65
1:A:107:ARG:NH1	1:H:155:TYR:CD2	2.64	0.65
1:B:201:ALA:O	1:B:217:THR:HG22	1.96	0.65
1:B:237:CYS:O	1:B:257:PHE:HB2	1.95	0.65
1:G:358:VAL:HA	1:G:380:PRO:HB3	1.79	0.65
1:F:120:PRO:CB	1:F:443:ILE:HD11	2.26	0.65
1:G:300:ARG:HH22	1:G:349:VAL:HG13	1.62	0.65
1:H:194:ILE:HD13	1:H:224:ARG:HA	1.78	0.65
1:D:329:ASN:HA	2:N:6:MAN:O3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:ILE:O	1:E:457:ASP:HA	1.97	0.65
1:G:299:ASN:OD1	1:G:341:TYR:HB2	1.97	0.65
1:B:143:LYS:HG3	1:E:110:GLU:OE2	1.97	0.65
1:A:327:ARG:HE	1:A:364:ARG:HH21	1.43	0.65
1:D:220:ARG:HG2	1:D:220:ARG:HH11	1.62	0.65
6:F:616:HOH:O	1:G:144:HIS:HD2	1.79	0.65
1:H:373:GLY:CA	1:H:399:LEU:O	2.45	0.64
1:B:103:ASP:OD2	6:B:603:HOH:O	2.13	0.64
1:G:49:ILE:O	1:G:53:ARG:HG2	1.96	0.64
1:A:457:ASP:O	1:H:154:GLN:HG2	1.98	0.64
1:G:57:LEU:O	1:G:61:ILE:HG13	1.97	0.64
1:E:109:GLY:CA	1:E:114:VAL:HG21	2.27	0.64
1:E:130:ARG:NH1	1:E:162:PRO:HD3	2.11	0.64
1:B:87:LEU:H	1:B:233:HIS:HD2	1.45	0.64
1:E:103:ASP:HB2	1:E:165:SER:O	1.98	0.64
1:C:215:ILE:HD13	1:C:255:TYR:CE2	2.32	0.64
1:E:229:GLU:OE2	1:E:410:PHE:CB	2.43	0.64
1:B:73:ASN:O	1:B:77:SER:OG	2.16	0.63
1:C:120:PRO:HD3	1:C:441:ASN:HD21	1.62	0.63
1:B:69:GLU:OE1	1:E:64:ARG:NH2	2.29	0.63
1:D:291:CYS:HB2	1:D:301:PRO:HB2	1.79	0.63
1:H:291:CYS:O	1:H:300:ARG:NH1	2.31	0.63
1:B:379:VAL:HG12	1:B:379:VAL:O	1.98	0.63
1:F:327:ARG:NE	1:F:364:ARG:HH21	1.97	0.63
1:G:327:ARG:HG3	1:G:328:PRO:O	1.99	0.63
1:B:67:ARG:O	1:B:71:ILE:HG13	1.99	0.63
1:C:168:THR:OG1	1:C:170:ASN:ND2	2.31	0.63
1:A:258:LYS:CB	1:A:263:LEU:HD11	2.29	0.63
1:B:203:ALA:O	1:B:214:GLU:HA	1.98	0.63
1:E:322:LEU:CD1	1:E:328:PRO:HG2	2.29	0.63
1:F:138:THR:HG21	1:F:145:SER:HA	1.81	0.63
1:C:325:ASN:HA	1:C:326:PRO:C	2.19	0.63
1:E:122:VAL:HG13	1:E:130:ARG:O	1.99	0.63
1:E:158:LEU:HD23	1:E:174:GLU:HB2	1.81	0.63
1:F:152:ARG:HD3	1:F:222:ILE:HG23	1.79	0.63
1:G:102:LYS:NZ	1:G:460:ASP:O	2.32	0.63
1:F:306:ASP:OD2	1:F:309:ALA:HB3	1.99	0.63
1:A:302:VAL:N	1:A:315:GLN:O	2.29	0.62
1:A:438:TRP:C	1:A:438:TRP:CE3	2.72	0.62
1:F:124:CYS:SG	1:F:412:ASP:HB2	2.39	0.62
1:A:304:ARG:O	1:A:313:THR:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:N	1:C:120:PRO:CD	2.63	0.62
1:C:87:LEU:H	1:C:233:HIS:HD2	1.45	0.62
1:B:329:ASN:ND2	2:I:6:MAN:O2	2.32	0.62
1:B:430:ARG:HE	1:B:437:TRP:HA	1.65	0.62
1:C:183:CYS:HB3	1:C:230:CYS:O	2.00	0.62
1:A:34:ILE:H	1:A:34:ILE:HD12	1.64	0.62
1:C:278:CYS:O	1:C:350:LYS:NZ	2.32	0.62
1:F:163:LEU:O	1:F:164:SER:HB2	1.98	0.62
1:G:194:ILE:HG12	1:G:203:ALA:HB2	1.81	0.62
1:H:225:THR:HG23	1:H:226:GLN:H	1.64	0.62
1:B:293:ASP:HB3	1:B:297:GLY:HA3	1.81	0.62
1:C:245:SER:O	1:C:250:ALA:HB2	2.00	0.62
1:D:435:LYS:HB2	6:D:656:HOH:O	2.00	0.62
1:E:106:VAL:CG1	1:E:462:ALA:CB	2.74	0.62
1:F:364:ARG:NH2	2:Z:6:MAN:O4	2.33	0.62
1:F:67:ARG:O	1:F:71:ILE:HG13	1.99	0.62
1:A:462:ALA:HA	1:H:144:HIS:CE1	2.35	0.62
1:E:352:PHE:CZ	1:E:422:PHE:CG	2.88	0.62
1:B:233:HIS:O	1:B:234:ASN:C	2.38	0.61
1:A:107:ARG:HD2	1:A:461:GLY:HA3	1.81	0.61
1:D:127:ASP:O	1:D:128:GLU:HB3	1.99	0.61
1:H:99:ILE:HD12	1:H:100:TYR:H	1.64	0.61
1:F:199:ASN:OD1	1:F:200:ASN:HB2	1.99	0.61
1:E:412(B):TRP:O	1:E:413:ALA:O	2.17	0.61
1:G:80:LEU:O	1:G:81:ALA:HB3	2.00	0.61
1:E:49:ILE:HD12	1:E:53:ARG:HH12	1.64	0.61
1:F:454:GLY:H	1:G:216:ASN:HD21	1.49	0.61
1:A:182:SER:OG	1:A:189:ARG:NH1	2.32	0.61
1:D:327:ARG:NH2	1:D:364:ARG:HD3	2.15	0.61
1:E:145:SER:O	1:E:438:TRP:HB3	2.01	0.61
1:H:421:CYS:HA	1:H:447:CYS:HA	1.83	0.61
1:A:323:THR:HB	1:A:364:ARG:HB3	1.82	0.61
1:H:86:ASN:OD1	1:H:234:ASN:HB2	2.01	0.61
1:B:151:ASP:O	1:B:156:ARG:HD2	2.01	0.60
1:F:258:LYS:HB3	1:F:263:LEU:HD11	1.80	0.60
1:G:299:ASN:OD1	1:G:341:TYR:N	2.33	0.60
1:G:465:GLU:OE1	1:G:465:GLU:N	2.34	0.60
1:A:116:VAL:HG11	1:A:148:THR:HG21	1.83	0.60
1:A:355:LEU:HD13	1:A:383:LEU:HD13	1.82	0.60
1:B:241:PHE:O	1:B:252:THR:HG23	2.01	0.60
1:B:422:PHE:HE2	1:B:424:VAL:HG23	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:HD22	1:A:170:ASN:H	1.49	0.60
1:A:406:TYR:HB2	1:A:425:GLU:OE1	2.01	0.60
1:D:275:ILE:HD13	1:D:301:PRO:HB3	1.83	0.60
1:A:419:ARG:NH1	1:H:211:PRO:HB2	2.16	0.60
1:E:280:CYS:O	1:E:409:SER:OG	2.06	0.60
1:H:145:SER:O	1:H:146:ASN:C	2.39	0.60
1:E:273:LYS:HE3	1:E:273:LYS:HA	1.83	0.60
1:F:89:LYS:HB3	1:F:417:CYS:HA	1.83	0.60
1:D:116:VAL:CG2	1:D:138:THR:HG23	2.32	0.60
1:F:298:SER:N	1:F:341:TYR:OH	2.33	0.60
1:A:320:PRO:HG2	1:A:389:LYS:HE2	1.82	0.60
1:C:465:GLU:CD	1:C:465:GLU:H	2.05	0.60
1:F:120:PRO:CD	1:F:425:GLU:HG3	2.31	0.60
1:C:121:TYR:CG	1:C:228:SER:HA	2.36	0.60
1:F:194:ILE:HD13	1:F:223:LEU:HG	1.84	0.60
1:D:224:ARG:HH21	1:D:276:GLU:CD	2.03	0.60
1:H:172:ARG:HG2	1:H:173:VAL:N	2.16	0.60
1:D:292:ARG:CZ	1:D:294:ASN:ND2	2.65	0.59
1:G:241:PHE:O	1:G:252:THR:HG23	2.02	0.59
1:G:72:ILE:O	1:G:76:VAL:HG23	2.02	0.59
1:A:147:GLY:HA2	6:A:644:HOH:O	2.01	0.59
1:B:421:CYS:HA	1:B:447:CYS:HA	1.83	0.59
1:F:295:TRP:HA	1:F:346:ASN:HD22	1.66	0.59
1:H:120:PRO:HA	1:H:133:ALA:HA	1.84	0.59
1:H:52:ASP:O	1:H:56:SER:OG	2.20	0.59
1:A:127:ASP:O	1:A:128:GLU:HB2	2.01	0.59
1:A:322:LEU:CD1	1:A:328:PRO:HG2	2.32	0.59
1:A:294:ASN:HD21	1:A:347:ASN:CA	2.15	0.59
1:D:114:VAL:HG22	1:D:168:THR:HG22	1.84	0.59
1:F:169:VAL:CB	6:F:601:HOH:O	2.33	0.59
1:H:106:VAL:HG12	1:H:462:ALA:HB2	1.83	0.59
1:D:116:VAL:HG23	1:D:138:THR:O	2.02	0.59
1:G:459:PRO:O	1:G:460:ASP:O	2.19	0.59
1:C:190:MET:CE	1:C:237:CYS:HB2	2.33	0.59
1:E:229:GLU:O	1:E:229:GLU:HG3	2.02	0.59
1:F:376:MET:O	1:F:377:LEU:HD23	2.02	0.59
1:C:116:VAL:HG12	1:C:136:GLN:HG3	1.83	0.59
1:A:149:ILE:HG22	6:A:644:HOH:O	2.02	0.59
1:A:33:SER:H	1:A:36:ASN:HB2	1.68	0.59
1:D:47:THR:HG23	1:G:49:ILE:HG12	1.85	0.59
1:D:60:LEU:O	1:D:64:ARG:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ALA:O	1:G:82:ARG:HB2	2.03	0.59
1:D:116:VAL:HG21	1:D:138:THR:HG23	1.84	0.59
1:D:154:GLN:HG2	1:G:457:ASP:O	2.03	0.59
2:Q:4:MAN:O3	2:Q:5:MAN:C1	2.51	0.59
1:F:114:VAL:O	1:F:140:ILE:HG13	2.03	0.59
1:B:214:GLU:OE2	1:E:419:ARG:NH1	2.35	0.59
1:C:399:LEU:HG	1:C:457:ASP:HB2	1.83	0.59
1:D:98:HIS:HE1	1:D:419:ARG:HH11	1.51	0.59
1:E:306:ASP:OD1	1:E:306:ASP:C	2.41	0.59
1:F:87:LEU:H	1:F:233:HIS:CD2	2.20	0.59
1:A:202:SER:HB3	1:B:453:LEU:HD22	1.84	0.58
1:E:199:ASN:O	1:E:220:ARG:NH1	2.36	0.58
1:B:86:ASN:HA	1:B:233:HIS:HD2	1.67	0.58
1:C:106:VAL:HG12	1:C:462:ALA:CB	2.33	0.58
1:E:121:TYR:CG	1:E:228:SER:HA	2.38	0.58
1:A:99:ILE:HG13	1:A:100:TYR:N	2.18	0.58
1:B:35:ILE:O	1:B:35:ILE:HG13	2.03	0.58
1:D:118:ARG:HA	1:D:441:ASN:OD1	2.02	0.58
1:F:258:LYS:HB2	1:F:263:LEU:CD1	2.29	0.58
1:H:464:ILE:N	1:H:465:GLU:OE2	2.35	0.58
1:A:438:TRP:HE3	1:A:438:TRP:C	2.07	0.58
1:B:75:ASN:O	1:B:79:ILE:HG12	2.03	0.58
1:D:303:ILE:HG22	1:D:305:ILE:HG13	1.85	0.58
1:H:87:LEU:N	1:H:233:HIS:HD2	1.94	0.58
1:A:293:ASP:HB3	1:A:297:GLY:HA3	1.84	0.58
1:A:322:LEU:HD13	1:A:328:PRO:HG2	1.85	0.58
1:C:199:ASN:HA	1:C:220:ARG:O	2.03	0.58
1:E:328:PRO:HD3	1:E:344:ASN:H	1.68	0.58
1:H:103:ASP:OD1	1:H:442:SER:HB2	2.04	0.58
1:B:327:ARG:HG3	1:B:328:PRO:O	2.04	0.58
1:C:406:TYR:HB2	1:C:425:GLU:OE1	2.03	0.58
1:D:367:SER:HB2	1:D:400:ASN:HD21	1.68	0.58
1:D:98:HIS:HE1	1:D:419:ARG:HD3	1.69	0.58
1:E:116:VAL:HG12	1:E:136:GLN:HB2	1.85	0.58
1:C:76:VAL:C	1:C:78:THR:H	2.05	0.58
1:F:121:TYR:CG	1:F:228:SER:HA	2.39	0.58
1:F:282:GLY:O	1:F:411:MET:HE3	2.04	0.58
1:A:258:LYS:HB2	1:A:263:LEU:CD1	2.32	0.58
1:C:201:ALA:O	1:C:217:THR:HG22	2.04	0.58
1:E:110:GLU:O	1:E:141:ARG:HD2	2.02	0.58
1:F:108:ILE:C	1:F:110:GLU:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PRO:O	1:B:331:PRO:HD2	2.03	0.58
1:B:402:ASP:HB3	6:B:665:HOH:O	2.03	0.58
1:G:355:LEU:HA	1:G:360:THR:HG23	1.85	0.58
1:A:64:ARG:HA	1:A:67:ARG:HB2	1.86	0.57
1:D:79:ILE:O	1:D:80:LEU:HG	2.04	0.57
1:B:86:ASN:HA	1:B:233:HIS:CD2	2.38	0.57
1:C:226:GLN:O	1:C:350:LYS:HE2	2.04	0.57
1:C:365:THR:HA	1:C:373:GLY:O	2.05	0.57
1:F:120:PRO:HB2	1:F:443:ILE:HD11	1.86	0.57
1:A:65:ALA:O	1:A:69:GLU:HG3	2.03	0.57
1:C:206:TRP:HA	1:C:210:ARG:O	2.04	0.57
1:C:456:TRP:CG	1:F:197:PRO:HD3	2.37	0.57
1:E:226:GLN:OE1	1:E:239:VAL:HA	2.04	0.57
1:F:120:PRO:HB3	1:F:443:ILE:HD11	1.86	0.57
1:E:298:SER:HA	1:E:324:ASP:HB3	1.87	0.57
1:G:140:ILE:H	1:G:140:ILE:HD12	1.69	0.57
1:H:465:GLU:OE2	1:H:465:GLU:N	2.34	0.57
1:B:274:HIS:CD2	1:B:295:TRP:HB2	2.40	0.57
1:F:457:ASP:O	1:G:154:GLN:HG2	2.05	0.57
1:H:366:ILE:CG2	1:H:400:ASN:HB2	2.34	0.57
1:B:355:LEU:HA	1:B:360:THR:HG23	1.86	0.57
1:F:110:GLU:O	1:F:141:ARG:HD2	2.05	0.57
1:F:226:GLN:O	1:F:350:LYS:HE2	2.04	0.57
1:F:253:ARG:HD3	1:F:265:TRP:CE3	2.40	0.57
1:A:94:ILE:HG23	1:A:448:SER:HB2	1.86	0.57
1:B:138:THR:HG21	1:B:145:SER:HA	1.87	0.57
1:B:325:ASN:O	1:B:348:GLY:HA2	2.05	0.57
1:E:321:VAL:HG13	1:E:364:ARG:NH2	2.19	0.57
1:G:194:ILE:HD13	1:G:223:LEU:HG	1.87	0.57
1:H:226:GLN:O	1:H:350:LYS:NZ	2.36	0.57
1:A:462:ALA:HA	1:H:144:HIS:HE1	1.68	0.57
1:B:116:VAL:HG13	1:B:440:SER:HB2	1.86	0.57
1:A:284:ARG:NH1	1:A:284:ARG:HG2	2.18	0.57
1:B:159:ILE:HD13	1:B:171:SER:HB3	1.86	0.56
1:B:158:LEU:HD22	1:B:180:SER:HB2	1.87	0.56
1:E:194:ILE:HG21	1:E:223:LEU:HB3	1.85	0.56
1:G:226:GLN:O	1:G:277:GLU:HB3	2.04	0.56
1:G:87:LEU:H	1:G:233:HIS:CD2	2.22	0.56
1:A:45:ARG:HH11	1:H:43:VAL:HG21	1.70	0.56
1:A:367:SER:HB2	1:A:400:ASN:HD21	1.69	0.56
1:B:121:TYR:CG	1:B:228:SER:HA	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LEU:H	1:C:233:HIS:CD2	2.24	0.56
1:G:373:GLY:HA3	1:G:400:ASN:HA	1.87	0.56
1:B:422:PHE:CE2	1:B:424:VAL:HG23	2.40	0.56
1:C:277:GLU:OE2	1:C:406:TYR:OH	2.22	0.56
1:E:192:ILE:HG23	1:E:205:ILE:HG13	1.87	0.56
1:D:411:MET:SD	1:D:420:ALA:HA	2.46	0.56
1:F:109:GLY:HA3	1:F:114:VAL:HB	1.85	0.56
1:B:194:ILE:HD13	1:B:223:LEU:HG	1.88	0.56
1:C:144:HIS:CD2	1:D:466:TYR:HD2	2.24	0.56
1:E:437:TRP:CH2	3:V:1:NAG:H3	2.41	0.56
1:H:35:ILE:HA	1:H:38:THR:HB	1.87	0.56
1:B:201:ALA:H	1:B:217:THR:HG21	1.71	0.56
1:E:299:ASN:ND2	6:E:604:HOH:O	2.36	0.56
1:F:429:GLY:O	1:F:433:GLU:HB2	2.05	0.56
1:H:217:THR:OG1	1:H:220:ARG:CA	2.53	0.56
1:A:110:GLU:OE2	1:A:141:ARG:NH1	2.38	0.56
1:F:108:ILE:O	1:F:110:GLU:N	2.39	0.56
1:H:270:GLY:HA3	1:H:314:SER:H	1.71	0.56
1:G:87:LEU:H	1:G:233:HIS:HD2	1.53	0.56
1:C:451:GLU:HB2	1:C:453:LEU:HD21	1.86	0.56
1:C:422:PHE:CD2	1:C:422:PHE:O	2.59	0.55
1:E:154:GLN:HG2	1:H:459:PRO:CD	2.33	0.55
1:E:180:SER:HA	1:E:192:ILE:O	2.06	0.55
1:F:118:ARG:NH1	1:F:119:GLU:OE2	2.39	0.55
1:B:159:ILE:CD1	1:B:171:SER:HB3	2.35	0.55
1:C:190:MET:HE1	1:C:237:CYS:HB2	1.88	0.55
1:D:249:PRO:HD2	6:D:700:HOH:O	2.06	0.55
1:H:272:ALA:CB	1:H:275:ILE:HD11	2.36	0.55
1:A:132:TYR:HA	1:A:159:ILE:O	2.06	0.55
1:C:159:ILE:HG22	1:C:173:VAL:HG22	1.89	0.55
1:E:107:ARG:HD2	1:E:461:GLY:HA3	1.88	0.55
1:G:198:ASN:H	1:G:198:ASN:HD22	1.52	0.55
1:A:124:CYS:HA	1:A:129:CYS:HA	1.88	0.55
1:F:118:ARG:HB2	1:F:156:ARG:HH22	1.72	0.55
1:A:221:ASN:HB3	1:A:244:GLY:HA2	1.87	0.55
1:A:294:ASN:ND2	1:A:347:ASN:C	2.60	0.55
1:A:336:LYS:HE2	1:A:342:PRO:HD3	1.89	0.55
1:A:300:ARG:HH22	1:A:349:VAL:HG13	1.71	0.55
1:G:136:GLN:HG2	1:G:156:ARG:NE	2.21	0.55
1:G:192:ILE:HG12	1:G:205:ILE:HG13	1.89	0.55
1:B:181:THR:CG2	1:B:192:ILE:HD12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ARG:HB2	1:C:132:TYR:CE1	2.42	0.55
1:G:373:GLY:CA	1:G:398:VAL:HG12	2.24	0.55
1:A:265:TRP:O	1:A:265:TRP:CE3	2.60	0.55
1:D:277:GLU:HB3	1:D:350:LYS:HG3	1.88	0.55
1:D:46:LEU:HD12	1:G:46:LEU:CD1	2.37	0.55
1:G:238:PRO:HA	1:G:255:TYR:O	2.07	0.55
1:A:294:ASN:ND2	1:A:347:ASN:CA	2.70	0.55
1:B:51:ASP:O	1:B:55:GLU:HG2	2.07	0.55
1:E:116:VAL:CG1	1:E:136:GLN:HB2	2.37	0.55
1:E:345:ASN:O	1:E:346:ASN:HB2	2.07	0.55
1:F:120:PRO:HD3	1:F:425:GLU:HG3	1.87	0.55
1:G:357:GLY:O	1:G:381:ASN:N	2.39	0.55
1:A:135:SER:CB	1:A:159:ILE:HD11	2.35	0.54
1:D:222:ILE:HG22	1:D:224:ARG:HD3	1.89	0.54
1:G:81:ALA:O	1:G:82:ARG:CB	2.55	0.54
1:H:97:TRP:H	1:H:395:GLN:HE22	1.55	0.54
1:A:113:ASP:OD2	1:A:169(A):TYR:OH	2.23	0.54
1:E:304:ARG:HB2	1:E:313:THR:HG23	1.89	0.54
1:F:108:ILE:CD1	1:F:166:PRO:HG3	2.37	0.54
1:F:152:ARG:HG3	1:F:152:ARG:HH21	1.72	0.54
1:F:194:ILE:HG12	1:F:203:ALA:HB2	1.89	0.54
1:E:277:GLU:HB3	1:E:350:LYS:HD2	1.89	0.54
1:F:460:ASP:OD2	1:F:462:ALA:N	2.26	0.54
1:H:272:ALA:HB1	1:H:275:ILE:HD11	1.89	0.54
1:A:430:ARG:HE	1:A:437:TRP:HA	1.71	0.54
1:E:144:HIS:C	1:E:146:ASN:H	2.11	0.54
1:E:379:VAL:HG12	1:E:382:ALA:HB2	1.89	0.54
1:F:394:GLY:O	2:Z:2:NAG:H3	2.07	0.54
1:H:188:THR:HG23	1:H:207:TYR:CZ	2.42	0.54
1:H:324:ASP:OD1	1:H:325:ASN:N	2.32	0.54
1:H:98:HIS:CE1	1:H:447:CYS:HB2	2.43	0.54
1:A:76:VAL:HG11	1:B:75:ASN:HB3	1.90	0.54
1:B:120:PRO:HB3	1:B:133:ALA:HB2	1.89	0.54
1:B:309:ALA:HB1	1:B:311:THR:HG23	1.88	0.54
1:E:254:ILE:HD13	1:E:312:HIS:CE1	2.42	0.54
1:F:207:TYR:CZ	1:F:259:GLU:HA	2.43	0.54
1:G:153:SER:C	1:G:155:TYR:H	2.10	0.54
1:H:181:THR:HG21	1:H:239:VAL:CG1	2.38	0.54
1:C:155:TYR:CE1	1:D:461:GLY:HA3	2.43	0.54
1:D:67:ARG:O	1:D:71:ILE:HG13	2.06	0.54
1:H:300:ARG:NH1	1:H:300:ARG:HG2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HE	1:A:364:ARG:NH2	2.05	0.54
1:D:299:ASN:ND2	1:D:316:TYR:HB3	2.23	0.54
1:E:292:ARG:HE	1:E:294:ASN:HD21	1.56	0.54
1:C:300:ARG:NH2	1:C:351:GLY:HA3	2.23	0.54
1:C:425:GLU:HG3	1:C:441:ASN:ND2	2.23	0.54
1:G:103:ASP:OD2	1:G:105:ALA:HB2	2.08	0.54
1:G:123:SER:OG	1:G:189:ARG:NH2	2.40	0.54
6:F:616:HOH:O	1:G:144:HIS:CD2	2.57	0.54
3:O:1:NAG:H62	3:O:2:NAG:C7	2.38	0.54
1:A:102:LYS:HA	1:A:443:ILE:O	2.08	0.54
1:A:111:ASP:O	1:A:112:SER:HB3	2.08	0.54
1:A:319:SER:OG	1:A:321:VAL:HG23	2.08	0.54
1:A:91:LEU:HD12	1:A:356:ASP:HB2	1.89	0.54
1:B:389:LYS:HB3	1:B:390:PRO:CD	2.38	0.54
1:F:199:ASN:ND2	6:F:610:HOH:O	2.38	0.54
1:F:306:ASP:C	1:F:306:ASP:OD1	2.46	0.54
1:A:277:GLU:HB3	1:A:350:LYS:HG3	1.89	0.53
1:B:116:VAL:HG21	1:B:145:SER:HB2	1.90	0.53
1:H:344:ASN:N	1:H:344:ASN:HD22	2.06	0.53
1:B:49:ILE:O	1:B:53:ARG:HG2	2.07	0.53
1:F:134:LEU:HD11	1:F:178:TRP:O	2.08	0.53
1:D:212:VAL:HG12	1:D:213:THR:N	2.23	0.53
1:B:318:CYS:SG	1:B:383:LEU:O	2.66	0.53
1:C:119:GLU:OE1	1:C:156:ARG:NH1	2.38	0.53
1:D:224:ARG:NH2	1:D:276:GLU:OE2	2.20	0.53
1:G:206:TRP:HA	1:G:210:ARG:O	2.09	0.53
1:H:120:PRO:HD3	1:H:441:ASN:ND2	2.24	0.53
1:H:87:LEU:HD13	1:H:282:GLY:HA3	1.90	0.53
1:E:65:ALA:HB1	1:H:64:ARG:HD3	1.90	0.53
1:D:118:ARG:HG2	1:D:425:GLU:OE2	2.08	0.53
2:W:7:MAN:H61	2:W:9:MAN:C5	2.36	0.53
1:A:327:ARG:NE	1:A:364:ARG:HH21	2.05	0.53
1:B:154:GLN:N	1:B:154:GLN:OE1	2.42	0.53
1:C:102:LYS:H	1:C:164:SER:HG	1.57	0.53
1:E:65:ALA:HB1	1:H:64:ARG:CD	2.39	0.53
1:H:429:GLY:O	1:H:433:GLU:N	2.41	0.53
1:A:40:ASP:OD2	1:B:45:ARG:NH1	2.42	0.53
1:B:254:ILE:HG22	1:B:254:ILE:O	2.09	0.53
1:C:217:THR:HG1	1:C:220:ARG:H	1.55	0.53
1:D:219:ALA:HB3	1:D:243:ASP:CG	2.30	0.53
1:E:248:GLY:O	1:E:295:TRP:CD1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:GLU:N	1:F:214:GLU:CD	2.62	0.53
1:C:155:TYR:CZ	1:D:461:GLY:HA3	2.43	0.53
1:C:76:VAL:HG13	1:D:79:ILE:HD11	1.90	0.53
1:C:98:HIS:HD2	1:C:99:ILE:O	1.92	0.53
1:E:135:SER:O	1:E:156:ARG:HA	2.09	0.53
1:E:241:PHE:O	1:E:252:THR:HA	2.09	0.53
1:F:341:TYR:CE1	1:F:343:GLY:HA3	2.45	0.53
1:H:158:LEU:CD1	1:H:159:ILE:O	2.57	0.53
1:B:295:TRP:O	1:B:345:ASN:HB2	2.08	0.52
1:D:87:LEU:H	1:D:233:HIS:CD2	2.25	0.52
1:G:335:GLY:O	1:G:386:ASP:HB2	2.09	0.52
1:H:423:TYR:HA	1:H:445:SER:HB3	1.90	0.52
1:C:136:GLN:HE21	1:C:156:ARG:NH2	2.08	0.52
1:A:94:ILE:HB	1:A:361:TRP:CD1	2.45	0.52
1:C:120:PRO:HD3	1:C:441:ASN:ND2	2.24	0.52
1:D:349:VAL:HG23	1:D:371:ARG:HE	1.74	0.52
1:E:131:PHE:O	1:E:160:SER:HA	2.08	0.52
1:E:170:ASN:C	1:E:170:ASN:HD22	2.11	0.52
1:E:277:GLU:OE1	1:E:292:ARG:NH1	2.38	0.52
1:E:322:LEU:HD13	1:E:328:PRO:HG2	1.90	0.52
1:F:225:THR:OG1	1:F:226:GLN:N	2.42	0.52
1:A:216:ASN:ND2	1:B:453:LEU:HA	2.25	0.52
1:A:94:ILE:HG21	1:A:97:TRP:CZ2	2.45	0.52
1:B:201:ALA:H	1:B:217:THR:CG2	2.21	0.52
1:E:294:ASN:O	1:E:346:ASN:CA	2.57	0.52
1:F:449:SER:C	1:F:451:GLU:H	2.12	0.52
1:F:120:PRO:HB3	6:F:644:HOH:O	2.09	0.52
1:F:220:ARG:NH1	1:F:220:ARG:HG2	2.18	0.52
1:H:106:VAL:CG1	1:H:462:ALA:HB2	2.38	0.52
1:A:286:GLU:OE1	1:A:304:ARG:HB3	2.09	0.52
1:B:247:THR:O	1:C:304:ARG:NH2	2.42	0.52
1:D:275:ILE:CD1	1:D:301:PRO:HB3	2.40	0.52
1:D:379:VAL:HG12	1:D:382:ALA:HB2	1.91	0.52
1:E:130:ARG:NH2	1:E:161:TRP:HA	2.25	0.52
1:E:144:HIS:C	1:E:146:ASN:N	2.63	0.52
1:D:210:ARG:NH2	1:G:126:PRO:O	2.43	0.52
1:A:131:PHE:CE1	1:A:163:LEU:CD1	2.92	0.52
1:B:178:TRP:CE3	1:B:179:SER:HB2	2.45	0.52
1:B:225:THR:OG1	1:B:226:GLN:N	2.43	0.52
1:B:278:CYS:HA	1:B:291:CYS:HA	1.91	0.52
1:D:464:ILE:O	1:D:465:GLU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ASN:OD1	1:D:234:ASN:HB2	2.09	0.52
1:G:80:LEU:O	1:G:81:ALA:CB	2.57	0.52
1:H:429:GLY:O	1:H:433:GLU:HB2	2.09	0.52
1:B:199:ASN:ND2	2:L:1:NAG:C8	2.72	0.52
1:G:457:ASP:OD2	1:G:459:PRO:HD3	2.10	0.52
1:E:197:PRO:O	1:E:199:ASN:N	2.42	0.52
1:H:218:TRP:HE1	1:H:251:GLU:HB3	1.75	0.52
1:A:46:LEU:HG	1:H:43:VAL:HG13	1.92	0.52
1:B:330:ASP:OD1	1:B:364:ARG:NH2	2.43	0.52
1:B:68:LEU:HA	1:B:71:ILE:HD12	1.91	0.52
1:D:97:TRP:N	1:D:395:GLN:HE22	2.08	0.52
1:G:114:VAL:O	1:G:140:ILE:HD12	2.10	0.52
1:G:153:SER:OG	1:G:156:ARG:HG3	2.09	0.52
1:A:194:ILE:HD12	1:A:225:THR:HG22	1.92	0.51
1:C:428:ARG:HH21	1:C:464:ILE:HG12	1.75	0.51
1:F:181:THR:HG22	1:F:192:ILE:HB	1.91	0.51
1:G:465:GLU:CD	1:G:465:GLU:N	2.59	0.51
1:A:346:ASN:O	1:A:347:ASN:HB2	2.09	0.51
1:F:406:TYR:HB2	1:F:425:GLU:OE1	2.09	0.51
1:H:103:ASP:O	1:H:104:ASN:HB2	2.11	0.51
1:H:182:SER:HA	1:H:190:MET:O	2.10	0.51
1:B:123:SER:OG	1:B:189:ARG:NH2	2.35	0.51
1:C:135:SER:OG	1:C:136:GLN:N	2.42	0.51
1:C:161:TRP:HB2	1:C:162:PRO:HD2	1.92	0.51
1:F:124:CYS:HA	1:F:129:CYS:HA	1.91	0.51
1:F:205:ILE:HD12	1:F:213:THR:O	2.10	0.51
1:F:271:THR:OG1	1:F:315:GLN:HA	2.11	0.51
1:G:138:THR:OG1	1:G:144:HIS:HB2	2.10	0.51
1:G:276:GLU:HB2	1:G:292:ARG:HD3	1.91	0.51
1:G:453:LEU:O	2:Q:1:NAG:O6	2.25	0.51
1:H:295:TRP:HD1	1:H:346:ASN:HD21	1.58	0.51
1:H:49:ILE:O	1:H:53:ARG:HG2	2.11	0.51
1:A:129:CYS:O	1:A:163:LEU:HB2	2.09	0.51
1:A:286:GLU:OE1	1:A:304:ARG:HD2	2.10	0.51
1:A:304:ARG:CG	1:A:304:ARG:HH11	2.21	0.51
1:A:40:ASP:CG	1:B:45:ARG:HH12	2.13	0.51
1:C:422:PHE:C	1:C:422:PHE:CD2	2.84	0.51
1:C:95:ASN:O	1:C:96:SER:HB3	2.08	0.51
1:D:319:SER:HB2	1:D:388:SER:OG	2.10	0.51
1:D:62:THR:O	1:D:62:THR:HG22	2.10	0.51
1:F:183:CYS:HB3	1:F:230:CYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:THR:HG22	1:F:243:ASP:N	2.25	0.51
1:F:118:ARG:NH2	1:F:427:ILE:HD11	2.25	0.51
1:F:87:LEU:H	1:F:233:HIS:HD2	1.57	0.51
1:A:86:ASN:OD1	1:A:234:ASN:HB2	2.09	0.51
1:D:325:ASN:O	1:D:348:GLY:CA	2.58	0.51
1:G:428:ARG:NH2	1:G:433:GLU:OE2	2.43	0.51
1:H:188:THR:OG1	1:H:189:ARG:N	2.42	0.51
1:A:276:GLU:HB2	1:A:292:ARG:HG2	1.91	0.51
1:B:288:THR:HG23	1:B:304:ARG:HD2	1.91	0.51
1:C:136:GLN:NE2	1:C:156:ARG:CZ	2.74	0.51
1:E:188:THR:CG2	1:E:207:TYR:CZ	2.93	0.51
1:F:294:ASN:O	1:F:296:GLN:N	2.43	0.51
1:F:161:TRP:CE3	1:F:167:PRO:HB3	2.46	0.51
1:H:465:GLU:CD	1:H:465:GLU:H	2.05	0.51
1:C:268:LEU:HD23	1:C:268:LEU:O	2.11	0.51
5:C:514:NAG:HN2	1:F:73:ASN:ND2	2.08	0.51
1:E:207:TYR:CZ	1:E:259:GLU:HA	2.45	0.51
1:B:309:ALA:HB1	1:B:311:THR:CG2	2.41	0.51
1:E:327:ARG:CG	1:E:368:ILE:HG22	2.41	0.51
1:F:99:ILE:HG13	1:G:176:ILE:HB	1.93	0.51
1:H:181:THR:HG21	1:H:239:VAL:HG13	1.93	0.51
1:H:309:ALA:O	1:H:311:THR:HG23	2.11	0.51
1:E:54:TYR:CD1	1:H:53:ARG:HD2	2.46	0.51
1:B:277:GLU:HB3	1:B:350:LYS:HG3	1.92	0.51
1:D:50:ILE:HD13	1:G:50:ILE:HG12	1.92	0.51
1:D:97:TRP:CE3	1:D:422:PHE:HE1	2.30	0.51
1:E:196:GLY:HA2	1:H:456:TRP:CD2	2.46	0.51
1:E:316:TYR:H	1:E:338:ASN:ND2	2.02	0.51
1:F:320:PRO:HD2	1:F:388:SER:O	2.11	0.51
1:H:116:VAL:HG12	1:H:136:GLN:HG3	1.93	0.51
1:B:277:GLU:O	1:B:350:LYS:NZ	2.44	0.50
1:A:197:PRO:HD3	1:B:456:TRP:CD1	2.46	0.50
1:F:354:TYR:CE2	1:F:420:ALA:HB1	2.46	0.50
1:F:445:SER:O	1:F:446:MET:HG2	2.11	0.50
1:H:39:ALA:O	1:H:43:VAL:HG23	2.12	0.50
1:B:111:ASP:O	1:B:112:SER:HB2	2.10	0.50
1:B:214:GLU:CB	1:E:453:LEU:HD11	2.41	0.50
1:B:392:GLN:NE2	6:B:611:HOH:O	2.43	0.50
1:B:450:THR:HG23	6:B:653:HOH:O	2.11	0.50
1:D:146:ASN:OD1	1:D:437:TRP:HB3	2.10	0.50
1:C:155:TYR:CZ	1:D:461:GLY:CA	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:SER:O	1:F:148:THR:HG23	2.11	0.50
1:F:355:LEU:HA	1:F:360:THR:HG23	1.92	0.50
1:G:124:CYS:CB	6:G:610:HOH:O	2.36	0.50
1:H:188:THR:CG2	1:H:207:TYR:CZ	2.94	0.50
1:H:325:ASN:HA	1:H:326:PRO:C	2.30	0.50
1:C:430:ARG:NE	1:C:436:VAL:O	2.42	0.50
1:C:103:ASP:OD1	1:C:442:SER:HB2	2.12	0.50
1:A:367:SER:HB3	1:A:372:SER:HB2	1.93	0.50
1:B:50:ILE:HG23	6:B:692:HOH:O	2.10	0.50
1:E:41:ASP:OD1	1:E:45:ARG:HD2	2.12	0.50
1:G:153:SER:HB2	1:G:155:TYR:CD2	2.47	0.50
1:G:181:THR:HG22	1:G:192:ILE:HB	1.93	0.50
1:B:423:TYR:C	1:B:423:TYR:CD1	2.85	0.50
1:C:218:TRP:HE1	1:C:251:GLU:HB3	1.76	0.50
1:D:142:GLY:HA2	1:G:111:ASP:HB2	1.93	0.50
1:D:440:SER:OG	1:D:441:ASN:N	2.45	0.50
1:E:104:ASN:O	1:E:107:ARG:HB2	2.12	0.50
1:F:111:ASP:CG	1:G:142:GLY:H	2.14	0.50
1:F:69:GLU:HA	1:F:72:ILE:HD12	1.94	0.50
1:G:139:THR:O	1:G:145:SER:HB3	2.11	0.50
1:H:229:GLU:HG2	6:H:653:HOH:O	2.11	0.50
1:H:282:GLY:O	1:H:411:MET:HE1	2.11	0.50
1:A:61:ILE:HG21	1:B:61:ILE:HG13	1.93	0.50
1:D:209:ARG:HG2	1:D:209:ARG:NH1	2.18	0.50
1:F:422:PHE:HE2	1:F:424:VAL:HG23	1.77	0.50
1:A:76:VAL:HA	1:A:79:ILE:HD12	1.93	0.50
1:A:98:HIS:HD2	1:A:99:ILE:O	1.94	0.50
1:C:97:TRP:N	1:C:395:GLN:HE22	2.10	0.50
1:E:412:ASP:C	1:E:412(B):TRP:H	2.14	0.50
1:H:444:VAL:HG21	1:H:458:TRP:CB	2.42	0.50
1:H:98:HIS:CE1	1:H:419:ARG:HH11	2.30	0.50
1:A:184:HIS:HA	1:A:189:ARG:HA	1.94	0.50
1:A:389:LYS:HB3	1:A:390:PRO:CD	2.42	0.50
1:B:412(A):TYR:HB2	1:B:412(B):TRP:CZ3	2.46	0.50
1:F:164:SER:O	1:G:173:VAL:HG21	2.12	0.50
1:G:326:PRO:HG2	1:G:344:ASN:OD1	2.12	0.50
1:D:36:ASN:HD22	1:G:38:THR:HG23	1.76	0.50
1:A:188:THR:CG2	1:A:208:ASN:HB2	2.26	0.50
1:A:213:THR:OG1	1:A:260:GLY:O	2.30	0.50
1:A:438:TRP:HE3	1:A:439:THR:N	2.10	0.50
1:B:309:ALA:CB	1:B:311:THR:CG2	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ASN:O	1:C:108:ILE:CG1	2.45	0.50
1:C:130:ARG:HB2	1:C:132:TYR:HE1	1.77	0.50
1:E:350:LYS:HB3	1:E:406:TYR:CG	2.47	0.50
1:F:389:LYS:HB3	1:F:390:PRO:CD	2.41	0.50
1:C:426:LEU:O	1:C:441:ASN:HA	2.12	0.49
1:E:245:SER:OG	1:E:248:GLY:CA	2.60	0.49
1:E:295:TRP:C	1:E:296:GLN:HG2	2.32	0.49
1:A:115:LEU:O	1:A:117:THR:HG23	2.11	0.49
1:B:151:ASP:N	1:B:151:ASP:OD1	2.46	0.49
1:C:444:VAL:HG21	1:C:458:TRP:HB3	1.93	0.49
1:C:45:ARG:NH2	1:F:43:VAL:CG1	2.68	0.49
1:C:464:ILE:O	1:C:465:GLU:C	2.49	0.49
1:D:63:LEU:O	1:D:67:ARG:HG3	2.12	0.49
1:A:96:SER:OG	1:A:451:GLU:O	2.16	0.49
1:D:161:TRP:CE2	1:D:167:PRO:HB3	2.47	0.49
1:G:234:ASN:O	1:G:234:ASN:CG	2.50	0.49
1:G:406:TYR:H	1:G:425:GLU:HB3	1.77	0.49
1:G:76:VAL:O	1:G:79:ILE:HB	2.13	0.49
1:A:208:ASN:O	1:A:209:ARG:HB2	2.12	0.49
1:B:327:ARG:HH12	1:B:364:ARG:CB	2.23	0.49
1:C:158:LEU:HG	1:C:174:GLU:HB2	1.94	0.49
1:H:354:TYR:OH	1:H:421:CYS:O	2.24	0.49
1:H:66:ASP:O	1:H:67:ARG:C	2.51	0.49
1:C:272:ALA:HA	1:C:316:TYR:CE1	2.48	0.49
1:D:325:ASN:ND2	1:D:365:THR:OG1	2.38	0.49
1:F:278:CYS:HB3	1:F:289:CYS:HB3	1.94	0.49
1:G:168:THR:H	1:G:170:ASN:HD21	1.60	0.49
1:B:116:VAL:O	1:B:136:GLN:HB2	2.13	0.49
1:D:320:PRO:HD2	1:D:388:SER:O	2.12	0.49
1:E:273:LYS:HG3	1:E:340:PRO:HG3	1.94	0.49
1:E:281:TYR:C	1:E:281:TYR:CD2	2.86	0.49
1:C:168:THR:HG21	1:F:169(A):TYR:CD1	2.48	0.49
1:G:266:GLU:OE1	1:G:311:THR:HA	2.13	0.49
1:D:205:ILE:HG12	1:D:257:PHE:CE1	2.47	0.49
1:D:253:ARG:HD3	1:D:265:TRP:CZ3	2.48	0.49
1:E:131:PHE:CE1	1:E:163:LEU:HD12	2.47	0.49
1:F:158:LEU:HD13	1:F:180:SER:OG	2.12	0.49
1:F:288:THR:OG1	1:F:304:ARG:HD3	2.13	0.49
1:F:422:PHE:CE2	1:F:424:VAL:HG23	2.48	0.49
1:G:353:SER:OG	1:G:355:LEU:HG	2.13	0.49
1:B:83:ASP:OD1	3:M:2:NAG:O6	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:TRP:H	1:B:395:GLN:NE2	2.10	0.49
1:C:105:ALA:H	1:C:442:SER:HB2	1.78	0.49
1:C:456:TRP:CE2	1:F:154:GLN:NE2	2.81	0.49
1:H:286:GLU:CD	1:H:304:ARG:HE	2.15	0.49
1:H:99:ILE:HG22	6:H:660:HOH:O	2.12	0.49
1:D:149:ILE:HG23	1:D:150:HIS:H	1.77	0.49
1:D:346:ASN:O	1:D:347:ASN:HB2	2.12	0.49
1:E:154:GLN:HB2	1:E:155:TYR:CE1	2.47	0.49
1:E:396:THR:HG21	1:E:399:LEU:HD23	1.95	0.49
1:C:164:SER:O	1:F:173:VAL:HG21	2.13	0.49
1:C:217:THR:OG1	1:C:220:ARG:N	2.43	0.49
1:E:170:ASN:HD22	1:E:171:SER:N	2.11	0.49
1:E:65:ALA:CB	1:H:64:ARG:HD2	2.43	0.49
1:A:459:PRO:O	1:A:460:ASP:O	2.31	0.48
1:F:116:VAL:HG12	1:F:136:GLN:HG3	1.93	0.48
1:H:426:LEU:O	1:H:441:ASN:HA	2.13	0.48
1:B:125:ASP:O	1:B:126:PRO:C	2.52	0.48
1:B:125:ASP:HB3	1:B:126:PRO:HD2	1.95	0.48
1:C:179:SER:HB3	1:C:194:ILE:HB	1.96	0.48
1:C:423:TYR:HA	1:C:445:SER:HB3	1.93	0.48
1:F:183:CYS:HB3	1:F:230:CYS:C	2.34	0.48
1:A:34:ILE:N	1:A:34:ILE:HD12	2.28	0.48
1:B:151:ASP:O	1:B:156:ARG:CD	2.61	0.48
1:C:106:VAL:HG12	1:C:462:ALA:HB2	1.95	0.48
1:D:351:GLY:HA2	1:D:407:SER:OG	2.13	0.48
1:F:135:SER:O	1:F:156:ARG:HA	2.13	0.48
1:H:236:VAL:HA	1:H:257:PHE:O	2.13	0.48
1:H:292:ARG:HA	1:H:300:ARG:HH12	1.79	0.48
1:C:277:GLU:O	1:C:350:LYS:CD	2.52	0.48
1:C:78:THR:O	1:C:78:THR:HG22	2.13	0.48
1:A:309:ALA:O	1:A:311:THR:HG23	2.12	0.48
1:A:438:TRP:O	1:A:438:TRP:CE3	2.67	0.48
1:A:453:LEU:HA	1:H:216:ASN:ND2	2.28	0.48
1:E:218:TRP:CZ2	1:E:253:ARG:HD2	2.48	0.48
1:E:224:ARG:HG3	1:E:242:THR:HB	1.95	0.48
1:E:323:THR:HA	1:E:364:ARG:HB3	1.94	0.48
1:F:169:VAL:HB	6:F:601:HOH:O	2.03	0.48
1:H:159:ILE:HG22	1:H:173:VAL:HG22	1.96	0.48
1:C:210:ARG:NE	1:D:412:ASP:OD2	2.35	0.48
1:E:353:SER:CB	1:E:362:LEU:HB3	2.44	0.48
1:F:465:GLU:O	1:F:468:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:VAL:HG12	1:H:462:ALA:CB	2.43	0.48
1:H:170:ASN:C	1:H:170:ASN:ND2	2.59	0.48
1:H:373:GLY:HA2	1:H:398:VAL:O	2.13	0.48
1:D:229:GLU:OE1	6:D:602:HOH:O	2.19	0.48
1:D:218:TRP:CD1	1:D:253:ARG:NH2	2.82	0.48
1:E:194:ILE:HD11	1:E:241:PHE:HE1	1.78	0.48
1:F:125:ASP:OD1	1:F:184:HIS:CD2	2.67	0.48
1:F:465:GLU:O	1:F:467:PHE:N	2.47	0.48
5:B:513:NAG:H61	6:B:608:HOH:O	2.14	0.48
1:C:143:LYS:HD2	1:D:466:TYR:HB3	1.96	0.48
1:C:76:VAL:C	1:C:78:THR:N	2.65	0.48
1:C:216:ASN:OD1	1:D:453:LEU:HA	2.14	0.48
1:F:95:ASN:HB3	1:F:452:PHE:CE2	2.48	0.48
1:H:206:TRP:CZ3	1:H:211:PRO:HD3	2.48	0.48
1:A:144:HIS:CE1	1:B:462:ALA:HA	2.49	0.48
1:C:185:ASP:HA	1:C:232:CYS:HB2	1.96	0.48
1:D:124:CYS:HA	1:D:129:CYS:HA	1.94	0.48
1:D:131:PHE:CE2	1:D:164:SER:HA	2.48	0.48
1:F:152:ARG:HG3	1:F:152:ARG:NH2	2.28	0.48
1:F:295:TRP:O	1:F:345:ASN:CA	2.53	0.48
1:H:194:ILE:HD12	1:H:224:ARG:HA	1.94	0.48
1:C:83:ASP:HB3	3:O:1:NAG:H83	1.95	0.48
1:C:121:TYR:CD1	1:C:228:SER:HA	2.48	0.48
1:F:115:LEU:HD23	1:F:138:THR:O	2.14	0.48
1:G:124:CYS:HA	1:G:129:CYS:HA	1.96	0.48
1:F:463:LYS:H	1:G:144:HIS:HE1	1.62	0.48
1:E:144:HIS:CD2	1:H:107:ARG:O	2.67	0.48
1:H:225:THR:HG23	1:H:226:GLN:N	2.29	0.48
1:H:91:LEU:HD12	1:H:356:ASP:CB	2.44	0.48
1:A:35:ILE:HG12	1:B:34:ILE:HG22	1.95	0.47
1:F:341:TYR:CD1	1:F:343:GLY:HA3	2.49	0.47
1:C:463:LYS:HA	1:C:463:LYS:HD3	1.75	0.47
1:D:275:ILE:HD13	1:D:301:PRO:CB	2.44	0.47
1:C:419:ARG:NH1	1:F:214:GLU:OE2	2.47	0.47
1:F:226:GLN:O	1:F:350:LYS:CE	2.62	0.47
6:D:658:HOH:O	1:G:99:ILE:HG23	2.13	0.47
1:H:464:ILE:HD13	1:H:464:ILE:HA	1.79	0.47
1:A:111:ASP:O	1:A:112:SER:CB	2.62	0.47
1:A:45:ARG:HH12	1:H:40:ASP:HA	1.80	0.47
1:B:432:LYS:HB2	6:B:643:HOH:O	2.14	0.47
1:D:448:SER:O	6:D:603:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ILE:O	1:D:53:ARG:HG2	2.14	0.47
1:C:461:GLY:HA3	1:F:155:TYR:CE1	2.49	0.47
1:G:299:ASN:HD22	1:G:316:TYR:HB3	1.77	0.47
1:H:367:SER:HB2	1:H:400:ASN:HD21	1.79	0.47
1:H:428:ARG:NH1	1:H:462:ALA:O	2.34	0.47
2:W:4:MAN:O3	2:W:5:MAN:C1	2.62	0.47
1:C:323:THR:HG21	1:C:362:LEU:HB3	1.96	0.47
1:E:163:LEU:O	1:E:164:SER:HB2	2.13	0.47
1:E:428:ARG:NH1	1:E:462:ALA:HB3	2.30	0.47
1:A:98:HIS:CD2	1:A:99:ILE:O	2.67	0.47
1:E:207:TYR:CE2	1:E:259:GLU:HG3	2.48	0.47
1:E:350:LYS:HG3	1:E:351:GLY:H	1.79	0.47
1:F:168:THR:HG21	1:G:169(A):TYR:CD1	2.46	0.47
1:F:193:CYS:O	1:F:203:ALA:HA	2.15	0.47
1:F:277:GLU:CD	1:F:292:ARG:HH11	2.18	0.47
1:G:119:GLU:OE2	6:G:601:HOH:O	2.20	0.47
1:A:132:TYR:CE2	1:A:160:SER:HB3	2.50	0.47
1:B:114:VAL:CG1	1:B:140:ILE:HD11	2.45	0.47
1:C:112:SER:HB2	1:F:169(A):TYR:OH	2.14	0.47
1:E:280:CYS:O	1:E:281:TYR:HB3	2.14	0.47
1:G:392:GLN:HG2	1:G:394:GLY:H	1.80	0.47
1:A:45:ARG:HH11	1:H:43:VAL:CG2	2.28	0.47
1:C:166:PRO:HG2	1:C:168:THR:HG23	1.96	0.47
1:D:368:ILE:C	1:D:368:ILE:HD12	2.35	0.47
1:E:315:GLN:HB2	1:E:338:ASN:HD21	1.78	0.47
1:F:322:LEU:HB2	1:F:327:ARG:HD2	1.97	0.47
1:F:281:TYR:HB2	1:F:411:MET:HE2	1.95	0.47
1:G:278:CYS:O	1:G:350:LYS:NZ	2.48	0.47
1:H:91:LEU:HD12	1:H:356:ASP:HB2	1.96	0.47
1:A:168:THR:O	1:A:171:SER:HB2	2.13	0.47
1:A:434:ASP:O	1:A:435:LYS:C	2.53	0.47
1:A:444:VAL:HG21	1:A:458:TRP:HB3	1.96	0.47
1:C:35:ILE:CG2	1:C:38:THR:HB	2.45	0.47
1:G:206:TRP:CA	1:G:210:ARG:O	2.63	0.47
1:A:168:THR:OG1	1:A:170:ASN:ND2	2.48	0.47
1:A:214:GLU:CB	1:B:453:LEU:HD11	2.45	0.47
1:D:317:ILE:HG23	1:D:383:LEU:HA	1.96	0.47
1:C:144:HIS:NE2	1:D:466:TYR:HD2	2.13	0.47
1:E:234:ASN:ND2	3:U:1:NAG:H5	2.29	0.47
1:E:44:TYR:O	1:E:48:VAL:HG23	2.14	0.47
1:A:127:ASP:N	1:A:127:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLN:C	1:C:228:SER:H	2.18	0.47
1:C:426:LEU:HD13	1:C:460:ASP:HA	1.96	0.47
1:E:352:PHE:CZ	1:E:422:PHE:CD2	3.03	0.47
1:H:114:VAL:O	1:H:139:THR:HA	2.15	0.47
1:A:45:ARG:NH1	1:H:40:ASP:HA	2.29	0.47
1:D:303:ILE:HG22	1:D:305:ILE:CG1	2.44	0.47
1:D:97:TRP:H	1:D:395:GLN:HE22	1.63	0.47
1:E:240:VAL:HG22	1:E:254:ILE:HG13	1.96	0.47
1:F:327:ARG:NE	1:F:364:ARG:NH2	2.59	0.47
1:G:120:PRO:HA	1:G:133:ALA:HA	1.97	0.47
1:G:323:THR:HG22	1:G:364:ARG:HB3	1.97	0.47
1:G:79:ILE:CG2	1:G:79:ILE:O	2.62	0.47
1:E:373:GLY:HA2	1:E:399:LEU:O	2.15	0.46
1:F:229:GLU:OE1	1:F:410:PHE:HB2	2.16	0.46
1:H:290:THR:HG22	1:H:352:PHE:HA	1.96	0.46
1:D:394:GLY:HA3	2:N:3:BMA:O2	2.15	0.46
1:A:256:TYR:CD1	1:A:310:MET:HG2	2.50	0.46
1:B:123:SER:HA	1:B:229:GLU:OE1	2.14	0.46
1:D:292:ARG:NH2	1:D:348:GLY:O	2.41	0.46
1:F:303:ILE:HA	1:F:313:THR:O	2.16	0.46
1:F:411:MET:HB2	1:F:412(A):TYR:CZ	2.50	0.46
1:H:119:GLU:HB3	1:H:227:GLU:HG3	1.95	0.46
1:A:147:GLY:CA	6:A:644:HOH:O	2.61	0.46
1:A:325:ASN:ND2	1:A:367:SER:O	2.48	0.46
1:A:362:LEU:O	1:A:376:MET:HA	2.16	0.46
1:B:277:GLU:O	1:B:350:LYS:HG3	2.15	0.46
1:C:172:ARG:NH1	1:C:174:GLU:OE2	2.48	0.46
1:C:261:LYS:HA	1:C:261:LYS:HD2	1.63	0.46
1:D:364:ARG:HD2	1:D:375:GLU:OE2	2.14	0.46
1:E:299:ASN:OD1	1:E:299:ASN:N	2.47	0.46
1:E:35:ILE:HG22	1:E:36:ASN:N	2.29	0.46
1:F:68:LEU:O	1:F:72:ILE:HG13	2.16	0.46
1:H:465:GLU:CD	1:H:465:GLU:N	2.69	0.46
1:A:240:VAL:HG22	1:A:254:ILE:HG13	1.97	0.46
1:B:82:ARG:HD3	1:B:82:ARG:HA	1.50	0.46
1:C:64:ARG:HD2	1:C:64:ARG:HA	1.75	0.46
1:D:65:ALA:O	1:D:69:GLU:CG	2.62	0.46
1:E:121:TYR:CB	1:E:423:TYR:CE2	2.98	0.46
1:E:301:PRO:HA	1:E:315:GLN:O	2.15	0.46
1:E:121:TYR:HB3	1:E:423:TYR:CE2	2.51	0.46
1:F:108:ILE:HD12	1:F:166:PRO:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:ARG:HH22	1:G:349:VAL:CG1	2.27	0.46
1:G:400:ASN:O	1:G:400:ASN:ND2	2.48	0.46
1:B:261:LYS:HA	1:B:261:LYS:HE3	1.98	0.46
1:B:352:PHE:CZ	1:B:422:PHE:CB	2.98	0.46
1:F:280:CYS:HA	1:F:289:CYS:HA	1.98	0.46
1:F:327:ARG:CZ	1:F:364:ARG:HH21	2.28	0.46
1:G:73:ASN:HA	1:G:73:ASN:HD22	1.55	0.46
1:H:227:GLU:OE1	1:H:227:GLU:HA	2.15	0.46
1:C:224:ARG:NH2	1:C:276:GLU:OE2	2.46	0.46
1:C:268:LEU:HD23	6:C:618:HOH:O	2.14	0.46
1:C:427:ILE:O	1:C:428:ARG:HD2	2.16	0.46
1:C:449:SER:OG	1:C:453:LEU:HD11	2.15	0.46
1:C:459:PRO:HD2	1:F:154:GLN:CG	2.43	0.46
1:D:103:ASP:O	1:D:104:ASN:C	2.53	0.46
1:D:284:ARG:HD2	6:D:692:HOH:O	2.14	0.46
1:D:97:TRP:HB3	1:D:446:MET:HE2	1.98	0.46
1:E:322:LEU:HB2	1:E:327:ARG:HD2	1.98	0.46
1:E:300:ARG:NE	1:E:323:THR:O	2.48	0.46
1:E:389:LYS:HE2	1:E:389:LYS:HA	1.97	0.46
1:G:198:ASN:H	1:G:198:ASN:ND2	2.12	0.46
1:G:451:GLU:OE1	1:G:451:GLU:HA	2.15	0.46
1:B:34:ILE:C	1:B:36:ASN:H	2.19	0.46
1:B:446:MET:HE2	1:B:446:MET:HB3	1.87	0.46
1:C:300:ARG:NE	1:C:323:THR:O	2.49	0.46
1:C:399:LEU:HG	1:C:457:ASP:CB	2.46	0.46
1:C:118:ARG:NE	1:C:425:GLU:OE2	2.36	0.46
1:D:123:SER:HB3	1:D:132:TYR:CE1	2.50	0.46
1:D:61:ILE:C	1:D:63:LEU:H	2.18	0.46
1:E:316:TYR:N	1:E:338:ASN:ND2	2.60	0.46
1:E:437:TRP:CD1	3:V:1:NAG:C8	2.98	0.46
1:H:280:CYS:HA	1:H:289:CYS:HA	1.97	0.46
1:D:364:ARG:HH12	2:N:6:MAN:H5	1.79	0.46
1:C:323:THR:HB	1:C:364:ARG:HB3	1.98	0.46
1:C:466:TYR:CD1	1:F:143:LYS:HB3	2.51	0.46
1:C:168:THR:HG21	1:F:169(A):TYR:CE1	2.50	0.46
1:H:99:ILE:HD12	1:H:445:SER:O	2.15	0.46
1:A:182:SER:HA	1:A:190:MET:O	2.16	0.46
1:C:299:ASN:OD1	1:C:299:ASN:N	2.49	0.46
1:E:65:ALA:CB	1:H:64:ARG:CD	2.94	0.46
1:D:141:ARG:O	1:D:142:GLY:C	2.55	0.46
1:G:87:LEU:O	1:G:284:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:CYS:O	1:A:190:MET:N	2.36	0.45
1:A:381:ASN:O	1:A:382:ALA:C	2.55	0.45
1:C:226:GLN:O	1:C:228:SER:N	2.49	0.45
1:C:318:CYS:SG	1:C:383:LEU:O	2.74	0.45
1:E:145:SER:HA	1:E:148:THR:HG21	1.97	0.45
1:G:97:TRP:H	1:G:395:GLN:HE22	1.63	0.45
1:G:464:ILE:O	1:G:465:GLU:C	2.53	0.45
1:H:222:ILE:O	1:H:224:ARG:HD3	2.16	0.45
1:A:224:ARG:NE	1:A:276:GLU:OE1	2.44	0.45
1:A:80:LEU:O	1:A:81:ALA:CB	2.64	0.45
1:B:114:VAL:O	1:B:140:ILE:HG13	2.16	0.45
1:B:115:LEU:HB2	1:B:167:PRO:O	2.16	0.45
1:C:120:PRO:HA	1:C:133:ALA:HA	1.97	0.45
1:C:352:PHE:CZ	1:C:422:PHE:CG	3.04	0.45
1:D:315:GLN:HG3	1:D:316:TYR:O	2.16	0.45
1:D:327:ARG:HH21	1:D:364:ARG:NH1	2.14	0.45
1:E:185:ASP:OD1	1:E:187:LYS:N	2.45	0.45
1:E:216:ASN:ND2	1:E:217:THR:H	2.14	0.45
1:A:101:GLY:HA2	1:A:164:SER:OG	2.16	0.45
1:B:428:ARG:NH1	1:B:460:ASP:OD2	2.49	0.45
1:D:43:VAL:HA	1:G:46:LEU:CD1	2.44	0.45
1:G:121:TYR:CG	1:G:228:SER:HA	2.51	0.45
1:H:219:ALA:O	1:H:220:ARG:C	2.54	0.45
1:A:300:ARG:NH2	1:A:323:THR:O	2.50	0.45
1:A:296:GLN:O	1:A:340:PRO:HB2	2.16	0.45
1:B:358:VAL:C	1:B:360:THR:H	2.19	0.45
1:D:316:TYR:HB2	1:D:337:CYS:O	2.16	0.45
1:D:465:GLU:CD	1:D:465:GLU:H	2.19	0.45
2:I:4:MAN:O3	2:I:5:MAN:C1	2.64	0.45
1:E:327:ARG:O	1:E:368:ILE:HB	2.16	0.45
1:G:139:THR:HB	6:G:653:HOH:O	2.16	0.45
1:H:70:MET:O	1:H:71:ILE:C	2.54	0.45
1:A:203:ALA:O	1:A:214:GLU:HA	2.16	0.45
1:B:173:VAL:HG21	1:E:164:SER:O	2.16	0.45
1:C:455:GLN:HG2	2:W:1:NAG:O6	2.17	0.45
1:E:144:HIS:O	1:E:146:ASN:N	2.49	0.45
1:G:434:ASP:C	1:G:434:ASP:OD1	2.55	0.45
1:H:141:ARG:NH2	1:H:467:PHE:HA	2.31	0.45
1:A:128:GLU:HA	6:A:646:HOH:O	2.17	0.45
1:F:179:SER:HB3	1:F:194:ILE:HB	1.99	0.45
1:H:294:ASN:O	1:H:346:ASN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:371:ARG:O	1:H:404:SER:N	2.44	0.45
1:A:130:ARG:HE	1:A:160:SER:HB2	1.82	0.45
1:B:94:ILE:HB	1:B:361:TRP:CD1	2.52	0.45
1:C:430:ARG:HH11	1:C:430:ARG:CG	2.29	0.45
1:D:103:ASP:N	6:D:605:HOH:O	2.50	0.45
1:D:410:PHE:O	1:D:411:MET:HG2	2.17	0.45
1:E:161:TRP:HD1	1:E:165:SER:HB2	1.81	0.45
1:E:465:GLU:HA	1:E:468:LEU:HD12	1.98	0.45
1:F:189:ARG:HG2	1:F:190:MET:N	2.32	0.45
1:F:245:SER:HB3	1:F:247:THR:O	2.17	0.45
1:F:276:GLU:O	1:F:291:CYS:HB3	2.16	0.45
1:G:63:LEU:HD13	1:G:64:ARG:HG2	1.98	0.45
1:G:67:ARG:O	1:G:71:ILE:HG13	2.16	0.45
1:B:168:THR:H	1:B:170:ASN:ND2	2.15	0.45
1:B:192:ILE:HG12	1:B:205:ILE:HG13	1.98	0.45
1:B:253:ARG:C	1:B:254:ILE:HD12	2.37	0.45
1:C:354:TYR:OH	1:C:421:CYS:O	2.30	0.45
1:D:292:ARG:HE	1:D:348:GLY:C	2.21	0.45
1:E:54:TYR:CG	1:H:53:ARG:HD2	2.52	0.45
1:F:258:LYS:O	1:F:259:GLU:HB2	2.17	0.45
1:F:226:GLN:HB3	1:F:278:CYS:O	2.16	0.45
1:F:273:LYS:HD3	1:F:295:TRP:HZ3	1.82	0.45
1:G:144:HIS:C	1:G:146:ASN:H	2.19	0.45
1:G:356:ASP:HB3	1:G:359:ASN:HB3	1.99	0.45
1:H:282:GLY:O	1:H:411:MET:CE	2.64	0.45
1:B:87:LEU:N	1:B:233:HIS:CD2	2.76	0.45
1:B:80:LEU:O	1:B:81:ALA:HB2	2.17	0.45
1:C:122:VAL:HB	1:C:410:PHE:CE1	2.51	0.45
1:C:411:MET:HG2	1:C:420:ALA:HA	1.99	0.45
1:D:367:SER:HB2	1:D:372:SER:HB3	1.99	0.45
1:E:427:ILE:O	1:E:428:ARG:HD2	2.17	0.45
1:F:214:GLU:H	1:F:214:GLU:CD	2.20	0.45
1:F:277:GLU:HB3	1:F:350:LYS:HD2	1.98	0.45
1:G:213:THR:HG22	1:G:214:GLU:N	2.31	0.45
1:G:231:VAL:HB	1:G:287:ILE:HG12	1.99	0.45
1:G:299:ASN:OD1	1:G:341:TYR:HB3	2.15	0.45
1:H:344:ASN:ND2	1:H:344:ASN:N	2.65	0.45
1:H:349:VAL:HG23	1:H:406:TYR:CD1	2.52	0.45
1:C:122:VAL:HG22	1:C:131:PHE:CD1	2.51	0.44
1:D:84:PHE:O	3:R:1:NAG:H83	2.17	0.44
1:E:395:GLN:HG3	1:E:455:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:SER:C	1:G:155:TYR:N	2.71	0.44
1:G:162:PRO:O	1:G:165:SER:HB2	2.17	0.44
2:W:3:BMA:H61	2:W:7:MAN:H2	1.81	0.44
1:E:403:TRP:CH2	1:E:432:LYS:HB3	2.52	0.44
1:F:190:MET:HA	1:F:206:TRP:O	2.18	0.44
1:F:298:SER:HB3	1:F:322:LEU:HD13	1.98	0.44
1:H:364:ARG:HD3	1:H:365:THR:O	2.17	0.44
1:E:65:ALA:CB	1:H:64:ARG:HH21	2.20	0.44
1:A:73:ASN:HA	1:A:73:ASN:HD22	1.60	0.44
1:B:168:THR:H	1:B:170:ASN:HD21	1.64	0.44
1:B:325:ASN:ND2	1:B:365:THR:OG1	2.50	0.44
1:C:208:ASN:OD1	1:C:208:ASN:O	2.36	0.44
1:D:98:HIS:O	1:D:446:MET:HE3	2.17	0.44
1:E:383:LEU:HD23	1:E:384:THR:HG23	1.98	0.44
1:A:245:SER:OG	1:A:248:GLY:N	2.46	0.44
1:B:293:ASP:O	6:B:604:HOH:O	2.21	0.44
1:D:424:VAL:HB	1:D:444:VAL:HG13	2.00	0.44
1:D:49:ILE:HG23	1:D:53:ARG:NH2	2.32	0.44
1:E:155:TYR:HE1	1:H:459:PRO:HG2	1.82	0.44
1:F:108:ILE:HD13	1:F:166:PRO:HG3	1.99	0.44
1:F:392:GLN:HG2	2:Z:2:NAG:O3	2.18	0.44
1:H:420:ALA:HB3	1:H:448:SER:HB3	1.99	0.44
2:T:7:MAN:H62	2:T:9:MAN:H2	1.65	0.44
1:H:130:ARG:HB2	1:H:132:TYR:CE1	2.52	0.44
1:H:166:PRO:O	1:H:168:THR:HG23	2.18	0.44
1:H:392:GLN:N	2:T:3:BMA:H61	2.32	0.44
1:A:435:LYS:HD3	1:A:464:ILE:HG21	1.99	0.44
1:B:353:SER:HB3	1:B:362:LEU:HA	1.99	0.44
1:B:34:ILE:O	1:B:36:ASN:N	2.51	0.44
1:G:140:ILE:HD12	1:G:140:ILE:N	2.33	0.44
1:H:161:TRP:HB2	1:H:162:PRO:CD	2.47	0.44
1:H:123:SER:CB	1:H:189:ARG:HH12	2.30	0.44
1:D:293:ASP:OD2	1:D:316:TYR:OH	2.32	0.44
1:D:396:THR:N	1:D:455:GLN:OE1	2.50	0.44
1:F:270:GLY:CA	1:F:314:SER:OG	2.54	0.44
1:G:299:ASN:ND2	1:G:316:TYR:CD2	2.86	0.44
1:H:264:LYS:HG3	1:H:265:TRP:N	2.32	0.44
1:B:329:ASN:HA	2:I:6:MAN:O3	2.17	0.44
1:B:116:VAL:HG12	1:B:136:GLN:HG3	1.99	0.44
1:B:130:ARG:NH2	1:B:160:SER:OG	2.34	0.44
1:C:205:ILE:N	1:C:205:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:THR:HG21	1:D:144:HIS:O	2.18	0.44
1:F:226:GLN:O	1:F:350:LYS:NZ	2.49	0.44
1:F:98:HIS:HD2	1:F:99:ILE:O	2.01	0.44
1:F:453:LEU:HD11	1:G:214:GLU:HG2	2.00	0.44
1:G:294:ASN:HD22	1:G:294:ASN:HA	1.64	0.44
1:A:225:THR:OG1	1:A:226:GLN:N	2.51	0.44
1:A:422:PHE:CZ	1:A:446:MET:HG3	2.53	0.44
1:E:82:ARG:HH21	1:E:126:PRO:HB2	1.83	0.44
1:F:195:SER:O	1:F:201:ALA:HA	2.17	0.44
1:H:194:ILE:HD13	1:H:224:ARG:CA	2.47	0.44
1:A:419:ARG:HH12	1:H:211:PRO:HB2	1.80	0.44
1:H:300:ARG:HH11	1:H:300:ARG:HG2	1.83	0.44
1:H:330:ASP:OD2	1:H:364:ARG:NH2	2.48	0.44
1:H:424:VAL:HG12	1:H:426:LEU:HD23	2.00	0.44
1:H:64:ARG:NH1	1:H:67:ARG:HE	2.16	0.44
1:B:422:PHE:CE2	1:B:424:VAL:CG2	2.94	0.43
1:B:423:TYR:HA	1:B:445:SER:HA	2.00	0.43
1:E:353:SER:HB2	1:E:361:TRP:O	2.18	0.43
1:F:263:LEU:O	1:F:264:LYS:HB2	2.18	0.43
1:A:92:CYS:SG	1:A:418:TYR:O	2.76	0.43
1:C:236:VAL:HA	1:C:257:PHE:O	2.18	0.43
1:E:283:GLU:O	1:E:284:ARG:C	2.56	0.43
1:G:361:TRP:CZ2	1:G:378:LYS:HB2	2.53	0.43
1:G:464:ILE:HA	1:G:464:ILE:HD13	1.78	0.43
1:H:125:ASP:O	1:H:127:ASP:N	2.48	0.43
1:H:219:ALA:C	1:H:243:ASP:OD1	2.57	0.43
1:H:300:ARG:HH11	1:H:300:ARG:CG	2.31	0.43
1:B:291:CYS:HB2	1:B:301:PRO:HG2	1.99	0.43
1:B:289:CYS:HB2	1:B:303:ILE:HB	2.00	0.43
1:C:116:VAL:HG13	1:C:440:SER:HB2	1.99	0.43
1:E:121:TYR:HB3	1:E:423:TYR:CZ	2.53	0.43
1:E:99:ILE:HD13	1:E:458:TRP:CE2	2.53	0.43
1:F:105:ALA:HA	1:F:166:PRO:HB3	1.99	0.43
1:H:97:TRP:H	1:H:395:GLN:NE2	2.16	0.43
1:B:159:ILE:HD12	1:B:161:TRP:HE3	1.82	0.43
1:E:184:HIS:HA	1:E:189:ARG:HA	2.01	0.43
1:D:142:GLY:HA2	1:G:111:ASP:CB	2.48	0.43
1:G:136:GLN:HA	1:G:156:ARG:HG2	2.01	0.43
1:G:365:THR:HA	1:G:373:GLY:O	2.18	0.43
1:A:354:TYR:OH	1:A:421:CYS:O	2.31	0.43
1:B:254:ILE:N	1:B:254:ILE:HD12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LYS:HD3	1:B:432:LYS:HA	1.82	0.43
1:A:197:PRO:HD3	1:B:456:TRP:CG	2.53	0.43
1:E:276:GLU:HB2	1:E:277:GLU:HG3	2.01	0.43
1:E:370:SER:HB2	1:E:432:LYS:HE2	2.01	0.43
1:E:408:GLY:O	1:E:422:PHE:HB2	2.18	0.43
1:F:90:GLY:HA2	1:F:283:GLU:HB2	2.00	0.43
1:C:98:HIS:CE1	1:C:447:CYS:HB2	2.54	0.43
1:C:452:PHE:N	1:C:452:PHE:CD1	2.86	0.43
1:H:278:CYS:HA	1:H:291:CYS:HA	2.00	0.43
1:H:300:ARG:HB2	1:H:317:ILE:HD12	2.00	0.43
1:F:85:ASN:HA	3:X:1:NAG:H82	2.01	0.43
1:A:325:ASN:ND2	1:A:370:SER:O	2.51	0.43
1:B:339:ASP:HB3	1:B:340:PRO:HD2	2.01	0.43
1:C:178:TRP:CZ3	1:C:223:LEU:O	2.72	0.43
1:E:64:ARG:O	1:E:68:LEU:N	2.44	0.43
1:F:306:ASP:CG	1:F:309:ALA:HB3	2.39	0.43
1:H:109:GLY:HA2	1:H:112:SER:HB3	1.99	0.43
1:D:367:SER:HB2	1:D:400:ASN:ND2	2.34	0.43
1:F:449:SER:C	1:F:451:GLU:N	2.72	0.43
1:G:102:LYS:HD3	1:G:104:ASN:OD1	2.19	0.43
1:G:352:PHE:HB3	1:G:408:GLY:HA2	2.00	0.43
1:F:42:ILE:HG23	1:G:43:VAL:HG22	1.99	0.43
1:H:300:ARG:HA	1:H:301:PRO:HD2	1.86	0.43
1:E:394:GLY:HA3	2:L:3:BMA:O2	2.18	0.43
1:D:329:ASN:CA	2:N:6:MAN:O3	2.64	0.43
1:A:135:SER:HB2	1:A:159:ILE:HD13	1.95	0.43
1:A:198:ASN:HB2	6:A:685:HOH:O	2.18	0.43
1:B:141:ARG:O	1:B:142:GLY:C	2.57	0.43
1:B:405:GLY:N	1:B:425:GLU:O	2.52	0.43
1:C:161:TRP:HB2	1:C:162:PRO:CD	2.49	0.43
1:D:324:ASP:OD1	1:D:348:GLY:HA2	2.18	0.43
1:E:302:VAL:O	1:E:314:SER:HA	2.19	0.43
1:E:106:VAL:HG11	1:E:462:ALA:CB	2.49	0.43
1:E:86:ASN:O	1:E:88:THR:N	2.52	0.43
1:A:117:THR:OG1	1:A:441:ASN:OD1	2.32	0.43
1:B:303:ILE:HG22	1:B:305:ILE:HG13	2.01	0.43
1:B:322:LEU:HD12	1:B:328:PRO:O	2.18	0.43
1:B:94:ILE:HB	1:B:361:TRP:HE1	1.80	0.43
1:C:82:ARG:O	1:C:82:ARG:HG3	2.18	0.43
1:E:170:ASN:C	1:E:170:ASN:ND2	2.73	0.43
1:F:120:PRO:O	1:F:121:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:THR:OG1	1:F:220:ARG:HA	2.19	0.43
1:G:161:TRP:N	1:G:161:TRP:CE3	2.86	0.43
1:H:290:THR:CG2	1:H:352:PHE:HA	2.49	0.43
1:H:372:SER:O	1:H:373:GLY:O	2.37	0.43
1:A:121:TYR:N	1:A:132:TYR:O	2.42	0.42
1:A:175:CYS:C	1:A:193:CYS:SG	2.98	0.42
1:A:216:ASN:ND2	1:B:454:GLY:N	2.50	0.42
1:A:427:ILE:O	1:A:428:ARG:HD2	2.18	0.42
1:B:104:ASN:O	1:B:105:ALA:C	2.56	0.42
1:B:294:ASN:O	1:B:346:ASN:CA	2.66	0.42
1:D:203:ALA:O	1:D:214:GLU:HA	2.19	0.42
1:E:161:TRP:CZ3	1:E:167:PRO:HB3	2.54	0.42
1:E:350:LYS:HG3	1:E:351:GLY:N	2.33	0.42
1:F:234:ASN:O	1:F:234:ASN:CG	2.57	0.42
1:F:419:ARG:NH1	1:G:214:GLU:OE2	2.52	0.42
1:G:182:SER:O	1:G:229:GLU:HA	2.19	0.42
1:G:292:ARG:HH21	1:G:294:ASN:ND2	2.16	0.42
1:H:370:SER:HB2	1:H:371:ARG:H	1.63	0.42
1:A:207:TYR:CE2	1:A:259:GLU:HG3	2.54	0.42
1:A:69:GLU:HG2	1:B:68:LEU:HD23	2.01	0.42
1:B:119:GLU:N	1:B:120:PRO:HD3	2.34	0.42
1:B:114:VAL:HG12	1:B:140:ILE:HD11	2.00	0.42
1:A:35:ILE:CG2	1:B:34:ILE:HG21	2.44	0.42
1:D:37:GLU:HG2	1:D:37:GLU:H	1.64	0.42
1:F:446:MET:HB3	1:F:446:MET:HE2	1.71	0.42
1:G:277:GLU:HB2	1:G:350:LYS:HD2	2.00	0.42
1:G:294:ASN:ND2	1:G:347:ASN:C	2.72	0.42
1:G:59:ASN:O	1:G:63:LEU:HB2	2.20	0.42
1:H:97:TRP:HB2	1:H:446:MET:HE2	2.01	0.42
1:C:312:HIS:CD2	1:C:313:THR:N	2.87	0.42
1:C:35:ILE:HG22	1:C:38:THR:HB	2.00	0.42
1:E:374:TYR:OH	1:E:407:SER:CB	2.67	0.42
1:E:100:TYR:HB3	1:E:445:SER:O	2.20	0.42
1:F:114:VAL:HG13	1:F:167:PRO:O	2.19	0.42
1:F:192:ILE:HD12	1:F:239:VAL:HG21	2.01	0.42
1:G:159:ILE:HA	1:G:172:ARG:O	2.18	0.42
1:G:405:GLY:HA3	1:G:427:ILE:HG13	2.01	0.42
1:H:217:THR:CG2	1:H:217:THR:O	2.68	0.42
1:H:241:PHE:O	1:H:252:THR:HA	2.19	0.42
1:C:132:TYR:HD2	1:C:158:LEU:HD11	1.83	0.42
1:C:102:LYS:N	1:C:164:SER:OG	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:VAL:HG21	1:C:390:PRO:HD3	2.01	0.42
1:E:329:ASN:OD1	1:E:368:ILE:HD13	2.19	0.42
1:E:431:PRO:HD2	6:E:699:HOH:O	2.20	0.42
1:E:461:GLY:O	1:E:462:ALA:O	2.38	0.42
1:E:79:ILE:O	1:E:80:LEU:HD23	2.19	0.42
1:F:170:ASN:C	1:F:170:ASN:ND2	2.65	0.42
1:F:194:ILE:HG21	1:F:223:LEU:O	2.20	0.42
1:F:295:TRP:C	1:F:296:GLN:HG2	2.39	0.42
1:G:94:ILE:HG12	1:G:448:SER:CB	2.49	0.42
1:A:284:ARG:NH2	6:A:616:HOH:O	2.50	0.42
1:A:97:TRP:H	1:A:395:GLN:HE22	1.67	0.42
1:B:92:CYS:O	1:B:359:ASN:ND2	2.51	0.42
1:C:299:ASN:ND2	1:C:336:LYS:O	2.52	0.42
1:E:197:PRO:O	1:E:198:ASN:C	2.57	0.42
1:E:207:TYR:CZ	1:E:259:GLU:HG3	2.55	0.42
1:F:254:ILE:HD12	1:F:254:ILE:N	2.34	0.42
1:G:430:ARG:HB2	1:G:439:THR:HG1	1.82	0.42
1:H:85:ASN:O	1:H:234:ASN:N	2.44	0.42
1:C:389:LYS:HD2	2:W:5:MAN:H61	2.01	0.42
1:A:173:VAL:HB	1:B:164:SER:HB2	2.02	0.42
1:B:150:HIS:HB3	6:B:636:HOH:O	2.19	0.42
1:B:159:ILE:HG22	1:B:173:VAL:HA	2.01	0.42
1:C:168:THR:H	1:C:170:ASN:ND2	2.03	0.42
1:F:327:ARG:NH2	1:F:364:ARG:HH21	2.18	0.42
1:F:429:GLY:HA3	1:F:439:THR:HA	2.00	0.42
1:G:219:ALA:HB3	1:G:243:ASP:OD1	2.20	0.42
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.79	0.42
1:A:35:ILE:HG12	1:B:34:ILE:CG2	2.50	0.42
1:A:325:ASN:ND2	1:A:365:THR:OG1	2.47	0.42
1:A:76:VAL:O	1:A:79:ILE:HB	2.19	0.42
1:B:263:LEU:O	1:B:264:LYS:HB2	2.20	0.42
1:C:353:SER:OG	1:C:355:LEU:HD11	2.20	0.42
1:D:259:GLU:O	1:D:261:LYS:HE3	2.19	0.42
1:D:373:GLY:HA2	1:D:398:VAL:O	2.20	0.42
1:F:323:THR:HA	1:F:364:ARG:HB3	2.01	0.42
1:G:276:GLU:CB	1:G:292:ARG:HD3	2.50	0.42
1:H:213:THR:HG22	1:H:214:GLU:N	2.35	0.42
1:H:217:THR:O	1:H:217:THR:HG23	2.20	0.42
1:H:121:TYR:CG	1:H:228:SER:HA	2.54	0.42
1:H:254:ILE:N	1:H:254:ILE:HD12	2.35	0.42
1:H:98:HIS:HE1	1:H:419:ARG:HH11	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:MET:HG3	1:H:74:ASP:OD1	2.20	0.42
1:E:437:TRP:CZ2	3:V:1:NAG:H3	2.55	0.42
1:A:277:GLU:OE1	1:A:292:ARG:NH1	2.53	0.42
1:A:372:SER:HB3	1:A:400:ASN:ND2	2.34	0.42
1:C:300:ARG:CZ	1:C:351:GLY:HA3	2.49	0.42
1:E:241:PHE:C	1:E:242:THR:OG1	2.58	0.42
6:C:649:HOH:O	1:F:172:ARG:HA	2.20	0.42
1:A:86:ASN:HB3	1:A:88:THR:HG23	2.02	0.42
1:B:185:ASP:C	1:B:185:ASP:OD1	2.58	0.42
1:C:403:TRP:O	1:C:426:LEU:HD23	2.19	0.42
1:E:379:VAL:CG1	1:E:382:ALA:HB2	2.49	0.42
1:G:345:ASN:C	1:G:347:ASN:H	2.23	0.42
1:H:141:ARG:NH2	1:H:467:PHE:O	2.53	0.42
1:A:378:LYS:O	1:A:390:PRO:HA	2.19	0.42
1:B:116:VAL:CG2	1:B:140:ILE:HA	2.50	0.42
1:C:352:PHE:HB3	1:C:408:GLY:HA2	2.01	0.42
1:D:212:VAL:O	1:D:214:GLU:OE2	2.38	0.42
1:D:53:ARG:O	1:D:57:LEU:HG	2.19	0.42
1:G:163:LEU:C	1:G:165:SER:H	2.22	0.42
1:G:251:GLU:OE1	1:G:253:ARG:NH2	2.53	0.42
1:G:463:LYS:HB3	1:G:465:GLU:OE1	2.20	0.42
1:H:365:THR:HG23	6:H:616:HOH:O	2.20	0.42
1:A:32:GLY:HA2	1:A:36:ASN:CG	2.40	0.41
1:B:294:ASN:HD22	1:B:347:ASN:C	2.24	0.41
1:B:84:PHE:CE2	1:B:258:LYS:HE3	2.55	0.41
1:C:190:MET:HE2	1:C:237:CYS:HB2	2.00	0.41
1:C:361:TRP:O	1:C:362:LEU:HD23	2.19	0.41
1:D:315:GLN:CG	1:D:316:TYR:H	2.22	0.41
1:G:96:SER:HB2	1:G:395:GLN:HE22	1.85	0.41
1:G:411:MET:SD	1:G:418:TYR:HB3	2.60	0.41
1:G:459:PRO:O	1:G:460:ASP:C	2.58	0.41
1:H:299:ASN:OD1	1:H:299:ASN:N	2.46	0.41
1:A:389:LYS:HA	1:A:389:LYS:HD3	1.89	0.41
1:A:144:HIS:CE1	1:B:463:LYS:H	2.26	0.41
1:C:160:SER:OG	1:C:174:GLU:OE2	2.37	0.41
1:C:379:VAL:O	1:C:380:PRO:C	2.58	0.41
1:D:215:ILE:HG22	1:D:216:ASN:O	2.21	0.41
1:D:292:ARG:HH21	1:D:348:GLY:C	2.23	0.41
1:D:298:SER:CB	1:D:328:PRO:HD3	2.50	0.41
1:D:94:ILE:O	1:D:361:TRP:NE1	2.53	0.41
1:D:98:HIS:C	1:D:446:MET:HE3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:GLN:O	1:E:138:THR:HG22	2.20	0.41
1:E:230:CYS:HB2	1:E:231:VAL:H	1.79	0.41
1:E:117:THR:O	1:E:440:SER:HA	2.20	0.41
1:G:354:TYR:OH	1:G:410:PHE:O	2.38	0.41
1:A:275:ILE:O	1:A:276:GLU:HG2	2.20	0.41
1:B:180:SER:HA	1:B:192:ILE:O	2.20	0.41
1:B:365:THR:HA	1:B:373:GLY:O	2.20	0.41
1:D:194:ILE:HD13	1:D:223:LEU:HG	2.02	0.41
1:D:205:ILE:HD13	1:D:213:THR:HB	2.01	0.41
1:D:406:TYR:HB2	1:D:425:GLU:OE1	2.20	0.41
1:E:327:ARG:HH21	2:L:6:MAN:H62	1.85	0.41
1:F:120:PRO:HB2	1:F:443:ILE:CD1	2.48	0.41
1:F:152:ARG:HG2	1:F:178:TRP:CD2	2.56	0.41
1:H:379:VAL:O	1:H:380:PRO:C	2.56	0.41
1:A:214:GLU:CD	1:A:214:GLU:N	2.74	0.41
1:C:104:ASN:HB2	1:C:108:ILE:HD11	2.02	0.41
1:D:182:SER:O	1:D:183:CYS:HB3	2.20	0.41
1:D:428:ARG:NH2	1:D:433:GLU:OE2	2.41	0.41
1:F:41:ASP:O	1:F:45:ARG:HB2	2.20	0.41
1:H:223:LEU:HB2	1:H:243:ASP:OD2	2.21	0.41
1:H:389:LYS:HD2	2:T:5:MAN:H61	2.03	0.41
1:A:207:TYR:HB2	1:A:212:VAL:HG21	2.02	0.41
1:A:221:ASN:C	1:A:221:ASN:HD22	2.23	0.41
1:A:79:ILE:O	1:A:80:LEU:HD23	2.21	0.41
1:C:262:ILE:HG13	1:C:262:ILE:H	1.42	0.41
1:C:76:VAL:O	1:C:78:THR:N	2.52	0.41
1:E:284:ARG:HB3	1:E:284:ARG:HH11	1.84	0.41
1:D:73:ASN:ND2	5:G:514:NAG:H83	2.35	0.41
1:H:407:SER:HB3	1:H:424:VAL:HG22	2.02	0.41
1:H:102:LYS:HG3	1:H:444:VAL:HG23	2.02	0.41
1:H:44:TYR:C	1:H:44:TYR:CD2	2.94	0.41
1:A:325:ASN:O	1:A:348:GLY:HA2	2.20	0.41
1:B:97:TRP:HE1	1:B:376:MET:HB3	1.85	0.41
1:C:116:VAL:HB	1:C:136:GLN:HB2	2.03	0.41
1:D:133:ALA:HB3	1:D:161:TRP:HH2	1.86	0.41
1:D:182:SER:OG	1:D:189:ARG:HD3	2.19	0.41
1:E:238:PRO:O	1:E:239:VAL:HG23	2.20	0.41
1:E:419:ARG:HD3	1:E:448:SER:O	2.21	0.41
1:F:103:ASP:O	1:F:104:ASN:HB2	2.20	0.41
1:H:106:VAL:CG1	1:H:462:ALA:CB	2.99	0.41
1:H:179:SER:OG	1:H:194:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MET:HE1	1:B:237:CYS:HB2	2.02	0.41
1:C:145:SER:O	1:C:148:THR:HG23	2.20	0.41
1:C:87:LEU:HA	1:C:418:TYR:OH	2.20	0.41
1:E:234:ASN:HD21	3:U:1:NAG:H5	1.85	0.41
1:F:373:GLY:HA3	1:F:400:ASN:HA	2.01	0.41
1:C:45:ARG:CZ	1:F:43:VAL:HG11	2.49	0.41
1:F:455:GLN:O	1:F:455:GLN:HG3	2.20	0.41
1:B:144:HIS:CE1	1:E:462:ALA:HA	2.55	0.41
1:C:463:LYS:HB2	1:C:466:TYR:CD2	2.55	0.41
1:D:117:THR:HG21	1:D:167:PRO:CG	2.51	0.41
1:E:293:ASP:HB2	1:E:301:PRO:HD3	2.02	0.41
1:F:131:PHE:HB2	1:F:161:TRP:CE2	2.56	0.41
1:F:109:GLY:HA3	1:F:140:ILE:HD12	2.03	0.41
1:F:172:ARG:HD2	1:F:174:GLU:OE2	2.21	0.41
1:G:168:THR:H	1:G:170:ASN:ND2	2.19	0.41
1:E:173:VAL:HB	1:H:164:SER:HB2	2.03	0.41
1:A:304:ARG:HG3	1:A:304:ARG:NH1	2.25	0.41
1:B:84:PHE:CZ	1:B:258:LYS:HE3	2.55	0.41
1:B:426:LEU:O	1:B:441:ASN:HB2	2.21	0.41
1:B:95:ASN:HD22	1:B:95:ASN:HA	1.71	0.41
1:D:426:LEU:HD11	1:D:444:VAL:CG1	2.51	0.41
1:D:435:LYS:HB3	1:D:468:LEU:HD11	2.02	0.41
1:E:464:ILE:O	1:E:467:PHE:HB2	2.20	0.41
1:F:274:HIS:O	1:F:293:ASP:HB2	2.21	0.41
1:F:291:CYS:HA	6:F:637:HOH:O	2.21	0.41
1:G:299:ASN:ND2	1:G:316:TYR:CG	2.89	0.41
1:H:364:ARG:HD2	1:H:375:GLU:OE2	2.20	0.41
1:A:165:SER:HB3	1:A:166:PRO:HD3	2.02	0.41
1:A:33:SER:OG	1:A:36:ASN:ND2	2.53	0.41
1:B:159:ILE:HG13	1:B:159:ILE:O	2.20	0.41
1:C:268:LEU:HA	1:C:312:HIS:CE1	2.56	0.41
1:C:406:TYR:O	1:C:425:GLU:HB3	2.20	0.41
1:E:120:PRO:HA	1:E:132:TYR:O	2.20	0.41
1:E:352:PHE:CE2	1:E:422:PHE:HB3	2.55	0.41
1:F:418:TYR:HA	6:F:606:HOH:O	2.19	0.41
1:F:77:SER:O	1:F:80:LEU:HG	2.21	0.41
1:F:95:ASN:HB3	1:F:452:PHE:CZ	2.56	0.41
1:G:283:GLU:O	1:G:284:ARG:C	2.59	0.41
1:G:406:TYR:N	1:G:425:GLU:HB3	2.36	0.41
1:A:458:TRP:O	1:A:459:PRO:O	2.39	0.41
1:B:301:PRO:HA	1:B:316:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:SER:HA	1:C:403:TRP:HA	2.03	0.41
1:D:364:ARG:NH1	2:N:6:MAN:C6	2.84	0.41
1:E:159:ILE:HG22	1:E:173:VAL:HG22	2.03	0.41
1:B:214:GLU:HB3	1:E:453:LEU:HD11	2.02	0.41
1:F:39:ALA:O	1:F:43:VAL:HG23	2.21	0.41
1:F:49:ILE:O	1:F:53:ARG:HG2	2.21	0.41
1:G:114:VAL:HA	1:G:168:THR:HA	2.03	0.41
1:G:407:SER:HB2	1:G:424:VAL:HG22	2.02	0.41
1:H:108:ILE:C	1:H:110:GLU:H	2.24	0.41
1:A:134:LEU:HA	1:A:157:ALA:O	2.21	0.40
1:A:114:VAL:O	1:A:139:THR:HA	2.21	0.40
1:A:181:THR:HG22	1:A:192:ILE:HB	2.02	0.40
1:A:124:CYS:CB	1:A:412(B):TRP:HZ3	2.30	0.40
1:B:324:ASP:O	1:B:325:ASN:HB2	2.21	0.40
1:B:328:PRO:HG3	1:B:343:GLY:HA3	2.03	0.40
1:D:136:GLN:HG2	1:D:156:ARG:HE	1.86	0.40
1:E:143:LYS:HG3	1:H:110:GLU:OE2	2.21	0.40
1:E:408:GLY:HA3	1:E:423:TYR:CE2	2.56	0.40
1:H:376:MET:HG2	1:H:397:ILE:HD11	2.02	0.40
1:A:170:ASN:O	6:A:602:HOH:O	2.21	0.40
1:A:176:ILE:HG21	1:B:99:ILE:HG12	2.03	0.40
1:C:319:SER:HB2	1:C:388:SER:OG	2.21	0.40
1:D:133:ALA:HB3	1:D:161:TRP:CH2	2.56	0.40
1:C:155:TYR:CZ	1:D:461:GLY:HA2	2.56	0.40
1:E:144:HIS:HD2	1:H:107:ARG:O	2.02	0.40
1:E:45:ARG:O	1:E:48:VAL:HB	2.21	0.40
1:F:108:ILE:C	1:F:110:GLU:N	2.74	0.40
1:F:112:SER:OG	1:G:169:VAL:HG21	2.20	0.40
1:F:118:ARG:O	1:F:119:GLU:HB2	2.21	0.40
1:F:262:ILE:HG22	1:F:262:ILE:O	2.20	0.40
1:H:207:TYR:CE2	1:H:259:GLU:HA	2.56	0.40
1:H:67:ARG:O	1:H:71:ILE:HG13	2.22	0.40
1:A:280:CYS:HA	1:A:289:CYS:HA	2.04	0.40
1:B:159:ILE:HD12	1:B:161:TRP:CE3	2.55	0.40
1:B:361:TRP:HA	1:B:377:LEU:O	2.21	0.40
1:C:430:ARG:NH1	1:C:430:ARG:CG	2.85	0.40
1:D:209:ARG:NH1	1:D:209:ARG:CG	2.82	0.40
1:E:238:PRO:HA	1:E:255:TYR:O	2.21	0.40
1:C:56:SER:HB3	1:F:54:TYR:OH	2.21	0.40
1:G:186:GLY:HA2	1:G:412(B):TRP:CZ2	2.56	0.40
1:G:294:ASN:ND2	1:G:346:ASN:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:CB	1:A:390:PRO:HD2	2.47	0.40
1:B:324:ASP:CG	6:B:604:HOH:O	2.59	0.40
1:C:199:ASN:C	1:C:199:ASN:OD1	2.60	0.40
1:D:206:TRP:N	1:D:206:TRP:CD1	2.90	0.40
1:E:273:LYS:CE	1:E:273:LYS:HA	2.51	0.40
1:E:410:PHE:HA	6:E:608:HOH:O	2.21	0.40
1:E:49:ILE:HA	1:E:52:ASP:HB3	2.03	0.40
1:F:182:SER:O	1:F:229:GLU:HA	2.21	0.40
1:G:288:THR:HG23	1:G:304:ARG:HG2	2.03	0.40
1:G:355:LEU:HD23	1:G:360:THR:HG23	2.02	0.40
1:H:217:THR:OG1	1:H:220:ARG:N	2.55	0.40
1:H:347:ASN:O	6:H:602:HOH:O	2.22	0.40
1:A:64:ARG:HH22	1:H:66:ASP:CG	2.25	0.40
1:D:329:ASN:CB	2:N:6:MAN:O3	2.69	0.40
2:Z:4:MAN:O3	2:Z:5:MAN:C1	2.69	0.40
1:B:176:ILE:HA	1:B:176:ILE:HD12	1.96	0.40
1:B:194:ILE:HG12	1:B:203:ALA:HB2	2.03	0.40
1:C:207:TYR:N	1:C:210:ARG:O	2.44	0.40
1:C:65:ALA:O	1:C:69:GLU:HG3	2.22	0.40
1:D:422:PHE:CE1	1:D:446:MET:HB2	2.57	0.40
1:D:71:ILE:H	1:D:71:ILE:HG13	1.55	0.40
1:E:118:ARG:CZ	1:E:427:ILE:HD11	2.52	0.40
1:E:274:HIS:HE1	1:E:276:GLU:OE2	2.04	0.40
1:E:437:TRP:CD1	3:V:1:NAG:H82	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:710:HOH:O	6:D:715:HOH:O[2_443]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/473 (92%)	371 (85%)	51 (12%)	14 (3%)	4	6
1	B	436/473 (92%)	372 (85%)	52 (12%)	12 (3%)	5	7
1	C	433/473 (92%)	372 (86%)	51 (12%)	10 (2%)	6	11
1	D	433/473 (92%)	370 (86%)	52 (12%)	11 (2%)	5	9
1	E	436/473 (92%)	370 (85%)	51 (12%)	15 (3%)	3	5
1	F	436/473 (92%)	367 (84%)	55 (13%)	14 (3%)	4	6
1	G	433/473 (92%)	365 (84%)	58 (13%)	10 (2%)	6	11
1	H	433/473 (92%)	370 (86%)	52 (12%)	11 (2%)	5	9
All	All	3476/3784 (92%)	2957 (85%)	422 (12%)	97 (3%)	5	7

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
1	A	82	ARG
1	A	284	ARG
1	A	460	ASP
1	C	222	ILE
1	E	198	ASN
1	E	284	ARG
1	E	413	ALA
1	F	220	ARG
1	F	295	TRP
1	F	344	ASN
1	F	466	TYR
1	G	81	ALA
1	G	82	ARG
1	G	460	ASP
1	H	67	ARG
1	H	392	GLN
1	A	128	GLU
1	A	381	ASN
1	B	112	SER
1	B	406	TYR
1	C	82	ARG
1	C	96	SER
1	C	413	ALA
1	D	82	ARG

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Mol	Chain	Res	Type
1	D	212	VAL
1	D	342	PRO
1	D	465	GLU
1	E	81	ALA
1	E	209	ARG
1	E	281	TYR
1	E	462	ALA
1	F	109	GLY
1	F	164	SER
1	G	142	GLY
1	G	373	GLY
1	H	66	ASP
1	H	373	GLY
1	A	87	LEU
1	A	112	SER
1	A	144	HIS
1	B	105	ALA
1	B	264	LYS
1	B	324	ASP
1	B	359	ASN
1	D	87	LEU
1	E	145	SER
1	E	342	PRO
1	F	284	ARG
1	F	294	ASN
1	G	141	ARG
1	G	295	TRP
1	G	461	GLY
1	H	104	ASN
1	H	126	PRO
1	B	81	ALA
1	C	146	ASN
1	C	332	THR
1	C	356	ASP
1	E	62	THR
1	E	230	CYS
1	E	346	ASN
1	F	217	THR
1	F	346	ASN
1	H	118	ARG
1	H	295	TRP
1	A	380	PRO

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Mol	Chain	Res	Type
1	B	142	GLY
1	C	77	SER
1	C	227	GLU
1	D	70	MET
1	D	277	GLU
1	E	162	PRO
1	E	222	ILE
1	E	340	PRO
1	F	340	PRO
1	F	356	ASP
1	G	222	ILE
1	G	284	ARG
1	H	70	MET
1	H	71	ILE
1	H	200	ASN
1	A	313	THR
1	D	81	ALA
1	D	128	GLU
1	D	346	ASN
1	F	37	GLU
1	F	264	LYS
1	B	35	ILE
1	D	222	ILE
1	A	459	PRO
1	B	71	ILE
1	B	72	ILE
1	C	119	GLU
1	A	222	ILE
1	A	454	GLY
1	B	222	ILE

### 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	387/418 (93%)	341 (88%)	46 (12%)	<b>5</b> <b>9</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	387/418 (93%)	341 (88%)	46 (12%)	5	9
1	C	385/418 (92%)	349 (91%)	36 (9%)	8	16
1	D	385/418 (92%)	347 (90%)	38 (10%)	8	14
1	E	387/418 (93%)	353 (91%)	34 (9%)	10	18
1	F	387/418 (93%)	339 (88%)	48 (12%)	4	8
1	G	385/418 (92%)	347 (90%)	38 (10%)	8	14
1	H	385/418 (92%)	345 (90%)	40 (10%)	7	12
All	All	3088/3344 (92%)	2762 (89%)	326 (11%)	6	12

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	43	VAL
1	A	53	ARG
1	A	59	ASN
1	A	67	ARG
1	A	68	LEU
1	A	77	SER
1	A	82	ARG
1	A	83	ASP
1	A	110	GLU
1	A	149	ILE
1	A	159	ILE
1	A	170	ASN
1	A	174	GLU
1	A	178	TRP
1	A	202	SER
1	A	209	ARG
1	A	210	ARG
1	A	213	THR
1	A	216	ASN
1	A	221	ASN
1	A	227	GLU
1	A	228	SER
1	A	247	THR
1	A	259	GLU
1	A	284	ARG
1	A	292	ARG
1	A	300	ARG

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Mol	Chain	Res	Type
1	A	304	ARG
1	A	314	SER
1	A	333	VAL
1	A	336	LYS
1	A	344	ASN
1	A	358	VAL
1	A	364	ARG
1	A	366	ILE
1	A	384	THR
1	A	385	ASP
1	A	396	THR
1	A	397	ILE
1	A	434	ASP
1	A	438	TRP
1	A	445	SER
1	A	446	MET
1	A	456	TRP
1	A	457	ASP
1	B	35	ILE
1	B	36	ASN
1	B	48	VAL
1	B	51	ASP
1	B	54	TYR
1	B	60	LEU
1	B	67	ARG
1	B	77	SER
1	B	79	ILE
1	B	82	ARG
1	B	89	LYS
1	B	120	PRO
1	B	140	ILE
1	B	141	ARG
1	B	145	SER
1	B	149	ILE
1	B	151	ASP
1	B	170	ASN
1	B	172	ARG
1	B	176	ILE
1	B	217	THR
1	B	220	ARG
1	B	221	ASN
1	B	251	GLU

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Mol	Chain	Res	Type
1	B	261	LYS
1	B	273	LYS
1	B	279	SER
1	B	288	THR
1	B	314	SER
1	B	332	THR
1	B	338	ASN
1	B	345	ASN
1	B	347	ASN
1	B	353	SER
1	B	358	VAL
1	B	364	ARG
1	B	367	SER
1	B	374	TYR
1	B	384	THR
1	B	391	THR
1	B	395	GLN
1	B	435	LYS
1	B	443	ILE
1	B	456	TRP
1	B	464	ILE
1	B	465	GLU
1	C	36	ASN
1	C	40	ASP
1	C	48	VAL
1	C	68	LEU
1	C	70	MET
1	C	83	ASP
1	C	140	ILE
1	C	164	SER
1	C	170	ASN
1	C	198	ASN
1	C	216	ASN
1	C	217	THR
1	C	221	ASN
1	C	228	SER
1	C	247	THR
1	C	251	GLU
1	C	261	LYS
1	C	262	ILE
1	C	268	LEU
1	C	286	GLU

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Mol	Chain	Res	Type
1	C	294	ASN
1	C	296	GLN
1	C	328	PRO
1	C	333	VAL
1	C	346	ASN
1	C	349	VAL
1	C	364	ARG
1	C	383	LEU
1	C	386	ASP
1	C	402	ASP
1	C	430	ARG
1	C	445	SER
1	C	446	MET
1	C	450	THR
1	C	452	PHE
1	C	468	LEU
1	D	36	ASN
1	D	37	GLU
1	D	47	THR
1	D	56	SER
1	D	61	ILE
1	D	71	ILE
1	D	72	ILE
1	D	73	ASN
1	D	80	LEU
1	D	82	ARG
1	D	112	SER
1	D	117	THR
1	D	118	ARG
1	D	139	THR
1	D	140	ILE
1	D	160	SER
1	D	163	LEU
1	D	170	ASN
1	D	175	CYS
1	D	180	SER
1	D	202	SER
1	D	209	ARG
1	D	228	SER
1	D	231	VAL
1	D	317	ILE
1	D	344	ASN

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Mol	Chain	Res	Type
1	D	349	VAL
1	D	358	VAL
1	D	362	LEU
1	D	364	ARG
1	D	392	GLN
1	D	395	GLN
1	D	396	THR
1	D	441	ASN
1	D	444	VAL
1	D	446	MET
1	D	448	SER
1	D	465	GLU
1	E	56	SER
1	E	74	ASP
1	E	112	SER
1	E	153	SER
1	E	163	LEU
1	E	170	ASN
1	E	182	SER
1	E	220	ARG
1	E	221	ASN
1	E	223	LEU
1	E	249	PRO
1	E	259	GLU
1	E	273	LYS
1	E	276	GLU
1	E	283	GLU
1	E	284	ARG
1	E	295	TRP
1	E	299	ASN
1	E	306	ASP
1	E	313	THR
1	E	332	THR
1	E	333	VAL
1	E	337	CYS
1	E	338	ASN
1	E	339	ASP
1	E	358	VAL
1	E	362	LEU
1	E	364	ARG
1	E	383	LEU
1	E	435	LYS

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Mol	Chain	Res	Type
1	E	440	SER
1	E	445	SER
1	E	456	TRP
1	E	465	GLU
1	F	34	ILE
1	F	37	GLU
1	F	38	THR
1	F	70	MET
1	F	74	ASP
1	F	79	ILE
1	F	82	ARG
1	F	118	ARG
1	F	151	ASP
1	F	153	SER
1	F	163	LEU
1	F	165	SER
1	F	170	ASN
1	F	179	SER
1	F	193	CYS
1	F	195	SER
1	F	221	ASN
1	F	227	GLU
1	F	228	SER
1	F	261	LYS
1	F	264	LYS
1	F	273	LYS
1	F	279	SER
1	F	291	CYS
1	F	293	ASP
1	F	296	GLN
1	F	304	ARG
1	F	306	ASP
1	F	313	THR
1	F	330	ASP
1	F	337	CYS
1	F	345	ASN
1	F	349	VAL
1	F	355	LEU
1	F	358	VAL
1	F	364	ARG
1	F	365	THR
1	F	391	THR

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Mol	Chain	Res	Type
1	F	397	ILE
1	F	407	SER
1	F	414	GLU
1	F	416	GLU
1	F	435	LYS
1	F	440	SER
1	F	446	MET
1	F	457	ASP
1	F	460	ASP
1	F	463	LYS
1	G	35	ILE
1	G	38	THR
1	G	50	ILE
1	G	56	SER
1	G	58	LYS
1	G	62	THR
1	G	67	ARG
1	G	70	MET
1	G	80	LEU
1	G	83	ASP
1	G	102	LYS
1	G	107	ARG
1	G	123	SER
1	G	141	ARG
1	G	151	ASP
1	G	170	ASN
1	G	171	SER
1	G	198	ASN
1	G	209	ARG
1	G	230	CYS
1	G	231	VAL
1	G	268	LEU
1	G	279	SER
1	G	283	GLU
1	G	284	ARG
1	G	294	ASN
1	G	304	ARG
1	G	333	VAL
1	G	353	SER
1	G	358	VAL
1	G	364	ARG
1	G	381	ASN

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Mol	Chain	Res	Type
1	G	387	LYS
1	G	407	SER
1	G	430	ARG
1	G	432	LYS
1	G	434	ASP
1	G	464	ILE
1	H	35	ILE
1	H	36	ASN
1	H	44	TYR
1	H	51	ASP
1	H	56	SER
1	H	58	LYS
1	H	60	LEU
1	H	64	ARG
1	H	76	VAL
1	H	77	SER
1	H	80	LEU
1	H	103	ASP
1	H	128	GLU
1	H	132	TYR
1	H	138	THR
1	H	149	ILE
1	H	153	SER
1	H	170	ASN
1	H	209	ARG
1	H	220	ARG
1	H	221	ASN
1	H	227	GLU
1	H	229	GLU
1	H	236	VAL
1	H	261	LYS
1	H	284	ARG
1	H	290	THR
1	H	296	GLN
1	H	300	ARG
1	H	323	THR
1	H	339	ASP
1	H	344	ASN
1	H	364	ARG
1	H	370	SER
1	H	390	PRO
1	H	425	GLU

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Mol	Chain	Res	Type
1	H	434	ASP
1	H	435	LYS
1	H	464	ILE
1	H	465	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	73	ASN
1	A	95	ASN
1	A	98	HIS
1	A	144	HIS
1	A	170	ASN
1	A	216	ASN
1	A	221	ASN
1	A	226	GLN
1	A	294	ASN
1	A	392	GLN
1	A	395	GLN
1	A	400	ASN
1	A	455	GLN
1	B	36	ASN
1	B	95	ASN
1	B	144	HIS
1	B	170	ASN
1	B	216	ASN
1	B	221	ASN
1	B	233	HIS
1	B	274	HIS
1	B	294	ASN
1	B	296	GLN
1	B	325	ASN
1	B	329	ASN
1	B	346	ASN
1	B	392	GLN
1	B	395	GLN
1	B	400	ASN
1	C	95	ASN
1	C	98	HIS
1	C	136	GLN
1	C	170	ASN

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Mol	Chain	Res	Type
1	C	233	HIS
1	C	294	ASN
1	C	344	ASN
1	C	392	GLN
1	C	395	GLN
1	C	400	ASN
1	C	441	ASN
1	D	36	ASN
1	D	73	ASN
1	D	95	ASN
1	D	98	HIS
1	D	144	HIS
1	D	170	ASN
1	D	216	ASN
1	D	226	GLN
1	D	294	ASN
1	D	338	ASN
1	D	346	ASN
1	D	392	GLN
1	D	395	GLN
1	D	400	ASN
1	E	36	ASN
1	E	95	ASN
1	E	144	HIS
1	E	170	ASN
1	E	216	ASN
1	E	221	ASN
1	E	234	ASN
1	E	274	HIS
1	E	294	ASN
1	E	296	GLN
1	E	315	GLN
1	E	338	ASN
1	E	346	ASN
1	E	392	GLN
1	E	400	ASN
1	F	73	ASN
1	F	98	HIS
1	F	170	ASN
1	F	216	ASN
1	F	221	ASN
1	F	233	HIS

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Mol	Chain	Res	Type
1	F	294	ASN
1	F	346	ASN
1	F	395	GLN
1	F	400	ASN
1	G	73	ASN
1	G	95	ASN
1	G	98	HIS
1	G	144	HIS
1	G	170	ASN
1	G	216	ASN
1	G	233	HIS
1	G	294	ASN
1	G	296	GLN
1	G	346	ASN
1	G	395	GLN
1	G	400	ASN
1	H	59	ASN
1	H	95	ASN
1	H	98	HIS
1	H	144	HIS
1	H	170	ASN
1	H	216	ASN
1	H	233	HIS
1	H	294	ASN
1	H	296	GLN
1	H	338	ASN
1	H	344	ASN
1	H	346	ASN
1	H	395	GLN
1	H	400	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

104 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	I	1	1,2	14,14,15	0.72	0	17,19,21	1.27	3 (17%)
2	NAG	I	2	2	14,14,15	0.89	1 (7%)	17,19,21	2.42	8 (47%)
2	BMA	I	3	2	11,11,12	0.67	0	15,15,17	2.16	4 (26%)
2	MAN	I	4	2	11,11,12	0.50	0	15,15,17	1.98	3 (20%)
2	MAN	I	5	2	11,11,12	1.10	1 (9%)	15,15,17	1.32	2 (13%)
2	MAN	I	6	2	11,11,12	0.76	0	15,15,17	2.04	6 (40%)
2	MAN	I	7	2	11,11,12	0.87	0	15,15,17	2.32	4 (26%)
2	MAN	I	8	2	11,11,12	1.13	1 (9%)	15,15,17	1.95	6 (40%)
2	MAN	I	9	2	11,11,12	0.97	0	15,15,17	1.64	3 (20%)
3	NAG	J	1	1,3	14,14,15	0.88	0	17,19,21	1.69	6 (35%)
3	NAG	J	2	3	14,14,15	0.57	0	17,19,21	1.58	4 (23%)
4	NAG	K	1	1,4	14,14,15	1.13	2 (14%)	17,19,21	2.35	9 (52%)
4	NAG	K	2	4	14,14,15	0.47	0	17,19,21	2.39	8 (47%)
4	BMA	K	3	4	11,11,12	0.86	0	15,15,17	2.82	6 (40%)
4	MAN	K	4	4	11,11,12	0.83	0	15,15,17	2.81	4 (26%)
2	NAG	L	1	1,2	14,14,15	0.47	0	17,19,21	2.15	4 (23%)
2	NAG	L	2	2	14,14,15	0.70	0	17,19,21	2.06	4 (23%)
2	BMA	L	3	2	11,11,12	0.65	0	15,15,17	1.86	5 (33%)
2	MAN	L	4	2	11,11,12	0.65	0	15,15,17	1.52	4 (26%)
2	MAN	L	5	2	11,11,12	0.69	0	15,15,17	1.79	1 (6%)
2	MAN	L	6	2	11,11,12	0.56	0	15,15,17	1.79	3 (20%)
2	MAN	L	7	2	11,11,12	0.77	0	15,15,17	2.12	6 (40%)
2	MAN	L	8	2	11,11,12	0.79	0	15,15,17	1.16	1 (6%)
2	MAN	L	9	2	11,11,12	0.95	1 (9%)	15,15,17	2.12	4 (26%)
3	NAG	M	1	1,3	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	NAG	M	2	3	14,14,15	0.90	0	17,19,21	1.45	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	N	1	1,2	14,14,15	0.98	0	17,19,21	1.29	2 (11%)
2	NAG	N	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.71	3 (17%)
2	BMA	N	3	2	11,11,12	0.51	0	15,15,17	1.45	2 (13%)
2	MAN	N	4	2	11,11,12	0.74	0	15,15,17	2.26	6 (40%)
2	MAN	N	5	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	N	6	2	11,11,12	0.54	0	15,15,17	2.14	5 (33%)
2	MAN	N	7	2	11,11,12	0.51	0	15,15,17	1.35	1 (6%)
2	MAN	N	8	2	11,11,12	0.55	0	15,15,17	1.55	4 (26%)
2	MAN	N	9	2	11,11,12	0.75	0	15,15,17	1.88	4 (26%)
3	NAG	O	1	1,3	14,14,15	0.65	0	17,19,21	1.97	3 (17%)
3	NAG	O	2	3	14,14,15	1.15	1 (7%)	17,19,21	2.66	4 (23%)
3	NAG	P	1	1,3	14,14,15	0.57	0	17,19,21	1.25	2 (11%)
3	NAG	P	2	3	14,14,15	0.53	0	17,19,21	1.60	5 (29%)
2	NAG	Q	1	1,2	14,14,15	0.73	0	17,19,21	2.65	8 (47%)
2	NAG	Q	2	2	14,14,15	0.90	1 (7%)	17,19,21	1.27	2 (11%)
2	BMA	Q	3	2	11,11,12	0.72	0	15,15,17	1.95	5 (33%)
2	MAN	Q	4	2	11,11,12	0.41	0	15,15,17	1.52	2 (13%)
2	MAN	Q	5	2	11,11,12	0.62	0	15,15,17	1.24	1 (6%)
2	MAN	Q	6	2	11,11,12	0.82	0	15,15,17	1.40	3 (20%)
2	MAN	Q	7	2	11,11,12	0.64	0	15,15,17	1.80	2 (13%)
2	MAN	Q	8	2	11,11,12	0.79	0	15,15,17	2.19	4 (26%)
2	MAN	Q	9	2	11,11,12	1.15	1 (9%)	15,15,17	2.74	7 (46%)
3	NAG	R	1	1,3	14,14,15	0.92	0	17,19,21	2.34	5 (29%)
3	NAG	R	2	3	14,14,15	0.68	0	17,19,21	1.90	2 (11%)
3	NAG	S	1	1,3	14,14,15	0.56	0	17,19,21	1.91	4 (23%)
3	NAG	S	2	3	14,14,15	1.11	1 (7%)	17,19,21	2.46	5 (29%)
2	NAG	T	1	1,2	14,14,15	0.96	0	17,19,21	2.45	7 (41%)
2	NAG	T	2	2	14,14,15	0.68	0	17,19,21	1.97	6 (35%)
2	BMA	T	3	2	11,11,12	0.98	1 (9%)	15,15,17	1.75	4 (26%)
2	MAN	T	4	2	11,11,12	0.42	0	15,15,17	2.16	4 (26%)
2	MAN	T	5	2	11,11,12	0.55	0	15,15,17	1.07	0
2	MAN	T	6	2	11,11,12	1.02	1 (9%)	15,15,17	1.45	2 (13%)
2	MAN	T	7	2	11,11,12	0.75	0	15,15,17	2.20	5 (33%)
2	MAN	T	8	2	11,11,12	0.94	0	15,15,17	1.38	4 (26%)
2	MAN	T	9	2	11,11,12	0.87	0	15,15,17	2.41	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	U	1	1,3	14,14,15	0.64	0	17,19,21	1.55	2 (11%)
3	NAG	U	2	3	14,14,15	0.59	0	17,19,21	2.14	5 (29%)
3	NAG	V	1	1,3	14,14,15	0.68	0	17,19,21	1.48	3 (17%)
3	NAG	V	2	3	14,14,15	0.90	0	17,19,21	1.78	6 (35%)
2	NAG	W	1	1,2	14,14,15	0.77	0	17,19,21	1.85	6 (35%)
2	NAG	W	2	2	14,14,15	0.82	0	17,19,21	2.06	5 (29%)
2	BMA	W	3	2	11,11,12	1.02	0	15,15,17	2.10	5 (33%)
2	MAN	W	4	2	11,11,12	0.81	1 (9%)	15,15,17	2.14	3 (20%)
2	MAN	W	5	2	11,11,12	0.55	0	15,15,17	1.92	4 (26%)
2	MAN	W	6	2	11,11,12	0.67	0	15,15,17	1.47	4 (26%)
2	MAN	W	7	2	11,11,12	0.65	0	15,15,17	2.12	5 (33%)
2	MAN	W	8	2	11,11,12	0.76	0	15,15,17	1.55	2 (13%)
2	MAN	W	9	2	11,11,12	0.79	0	15,15,17	2.07	3 (20%)
3	NAG	X	1	1,3	14,14,15	0.58	0	17,19,21	1.31	1 (5%)
3	NAG	X	2	3	14,14,15	0.70	0	17,19,21	2.01	5 (29%)
3	NAG	Y	1	1,3	14,14,15	0.57	0	17,19,21	1.18	2 (11%)
3	NAG	Y	2	3	14,14,15	1.05	1 (7%)	17,19,21	2.49	4 (23%)
2	NAG	Z	1	1,2	14,14,15	0.71	0	17,19,21	2.00	6 (35%)
2	NAG	Z	2	2	14,14,15	0.56	0	17,19,21	1.71	3 (17%)
2	BMA	Z	3	2	11,11,12	0.69	0	15,15,17	1.57	4 (26%)
2	MAN	Z	4	2	11,11,12	0.75	0	15,15,17	2.06	4 (26%)
2	MAN	Z	5	2	11,11,12	0.47	0	15,15,17	1.92	4 (26%)
2	MAN	Z	6	2	11,11,12	1.10	0	15,15,17	2.84	7 (46%)
2	MAN	Z	7	2	11,11,12	0.84	0	15,15,17	2.49	4 (26%)
2	MAN	Z	8	2	11,11,12	0.64	0	15,15,17	1.68	3 (20%)
2	MAN	Z	9	2	11,11,12	0.77	0	15,15,17	2.23	3 (20%)
3	NAG	a	1	1,3	14,14,15	0.45	0	17,19,21	1.28	2 (11%)
3	NAG	a	2	3	14,14,15	0.66	0	17,19,21	1.42	2 (11%)
3	NAG	b	1	1,3	14,14,15	0.82	0	17,19,21	1.94	7 (41%)
3	NAG	b	2	3	14,14,15	0.85	1 (7%)	17,19,21	1.59	3 (17%)
2	NAG	c	1	1,2	14,14,15	1.11	1 (7%)	17,19,21	2.08	8 (47%)
2	NAG	c	2	2	14,14,15	0.72	0	17,19,21	2.20	3 (17%)
2	BMA	c	3	2	11,11,12	0.50	0	15,15,17	1.83	5 (33%)
2	MAN	c	4	2	11,11,12	0.94	0	15,15,17	1.98	5 (33%)
2	MAN	c	5	2	11,11,12	0.81	0	15,15,17	2.75	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	c	6	2	11,11,12	0.65	0	15,15,17	1.28	2 (13%)
2	MAN	c	7	2	11,11,12	0.58	0	15,15,17	1.84	2 (13%)
2	MAN	c	8	2	11,11,12	0.47	0	15,15,17	1.72	1 (6%)
2	MAN	c	9	2	11,11,12	0.57	0	15,15,17	1.55	4 (26%)
3	NAG	d	1	1,3	14,14,15	1.14	2 (14%)	17,19,21	2.93	7 (41%)
3	NAG	d	2	3	14,14,15	1.13	1 (7%)	17,19,21	1.79	5 (29%)
3	NAG	e	1	1,3	14,14,15	0.54	0	17,19,21	1.79	5 (29%)
3	NAG	e	2	3	14,14,15	1.32	0	17,19,21	2.13	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	0/2/19/22	0/1/1/1
2	MAN	I	6	2	-	0/2/19/22	0/1/1/1
2	MAN	I	7	2	-	0/2/19/22	0/1/1/1
2	MAN	I	8	2	-	0/2/19/22	0/1/1/1
2	MAN	I	9	2	-	2/2/19/22	1/1/1/1
3	NAG	J	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	0/1/1/1
2	MAN	L	5	2	-	0/2/19/22	0/1/1/1
2	MAN	L	6	2	-	2/2/19/22	0/1/1/1
2	MAN	L	7	2	-	2/2/19/22	0/1/1/1
2	MAN	L	8	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	L	9	2	-	2/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
2	MAN	N	4	2	-	0/2/19/22	0/1/1/1
2	MAN	N	5	2	-	0/2/19/22	0/1/1/1
2	MAN	N	6	2	-	2/2/19/22	0/1/1/1
2	MAN	N	7	2	-	2/2/19/22	0/1/1/1
2	MAN	N	8	2	-	2/2/19/22	0/1/1/1
2	MAN	N	9	2	-	0/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	5/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	5	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	6	2	-	1/2/19/22	0/1/1/1
2	MAN	Q	7	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	8	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	9	2	-	0/2/19/22	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	T	2	2	-	5/6/23/26	0/1/1/1
2	BMA	T	3	2	-	0/2/19/22	0/1/1/1
2	MAN	T	4	2	-	0/2/19/22	0/1/1/1
2	MAN	T	5	2	-	0/2/19/22	0/1/1/1
2	MAN	T	6	2	-	0/2/19/22	0/1/1/1
2	MAN	T	7	2	-	1/2/19/22	0/1/1/1
2	MAN	T	8	2	-	0/2/19/22	0/1/1/1
2	MAN	T	9	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	1/6/23/26	0/1/1/1
2	BMA	W	3	2	-	1/2/19/22	0/1/1/1
2	MAN	W	4	2	-	1/2/19/22	0/1/1/1
2	MAN	W	5	2	-	0/2/19/22	0/1/1/1
2	MAN	W	6	2	-	1/2/19/22	0/1/1/1
2	MAN	W	7	2	-	2/2/19/22	0/1/1/1
2	MAN	W	8	2	-	2/2/19/22	0/1/1/1
2	MAN	W	9	2	-	0/2/19/22	0/1/1/1
3	NAG	X	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	4/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	4	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	5	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	6	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	7	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	8	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	9	2	-	0/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	4/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	5/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	BMA	c	3	2	-	0/2/19/22	0/1/1/1
2	MAN	c	4	2	-	2/2/19/22	0/1/1/1
2	MAN	c	5	2	-	0/2/19/22	0/1/1/1
2	MAN	c	6	2	-	2/2/19/22	0/1/1/1
2	MAN	c	7	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	c	8	2	-	0/2/19/22	0/1/1/1
2	MAN	c	9	2	-	1/2/19/22	0/1/1/1
3	NAG	d	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	2	NAG	C1-C2	3.10	1.57	1.52
2	Q	9	MAN	C2-C3	2.65	1.56	1.52
2	I	8	MAN	C2-C3	2.64	1.56	1.52
3	d	2	NAG	C1-C2	2.63	1.56	1.52
2	N	2	NAG	C1-C2	2.57	1.56	1.52
3	d	1	NAG	O5-C1	2.52	1.47	1.43
2	Q	2	NAG	C1-C2	2.50	1.56	1.52
3	b	2	NAG	C1-C2	2.39	1.55	1.52
4	K	1	NAG	C1-C2	2.36	1.55	1.52
2	c	1	NAG	C1-C2	2.35	1.55	1.52
3	S	2	NAG	C3-C2	2.28	1.57	1.52
2	I	2	NAG	C1-C2	2.14	1.55	1.52
4	K	1	NAG	O7-C7	-2.14	1.18	1.23
2	L	9	MAN	C2-C3	2.13	1.55	1.52
2	I	5	MAN	C2-C3	2.12	1.55	1.52
2	T	6	MAN	O3-C3	2.10	1.47	1.43
3	d	1	NAG	O5-C5	2.08	1.47	1.43
2	W	4	MAN	O5-C1	2.07	1.47	1.43
2	T	3	BMA	O5-C1	2.01	1.46	1.43
3	Y	2	NAG	C1-C2	2.01	1.55	1.52

All (413) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	5	MAN	C1-O5-C5	8.70	123.98	112.19
3	Y	2	NAG	C1-O5-C5	8.07	123.13	112.19
2	Q	1	NAG	C1-O5-C5	7.91	122.91	112.19
3	R	1	NAG	C1-O5-C5	7.64	122.55	112.19
2	I	7	MAN	C1-O5-C5	7.53	122.39	112.19
2	L	1	NAG	C2-N2-C7	-7.02	112.91	122.90
3	S	2	NAG	C2-N2-C7	7.01	132.88	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	2	NAG	C1-O5-C5	6.95	121.61	112.19
2	Z	7	MAN	C1-O5-C5	6.82	121.43	112.19
2	c	2	NAG	C1-O5-C5	6.74	121.33	112.19
2	T	9	MAN	C1-O5-C5	6.65	121.20	112.19
4	K	3	BMA	C1-O5-C5	6.63	121.17	112.19
2	T	4	MAN	C1-O5-C5	6.25	120.66	112.19
2	Z	9	MAN	C1-O5-C5	6.16	120.53	112.19
3	d	1	NAG	C4-C3-C2	-6.07	102.12	111.02
2	W	4	MAN	C1-O5-C5	6.05	120.39	112.19
2	L	5	MAN	C1-O5-C5	6.01	120.33	112.19
3	R	2	NAG	C1-O5-C5	5.98	120.29	112.19
2	Q	8	MAN	C1-O5-C5	5.97	120.28	112.19
2	T	7	MAN	C1-O5-C5	5.95	120.25	112.19
2	I	4	MAN	O5-C1-C2	-5.73	101.93	110.77
4	K	4	MAN	C3-C4-C5	-5.64	100.17	110.24
2	Q	9	MAN	O5-C5-C6	5.57	115.94	107.20
2	L	2	NAG	C2-N2-C7	-5.55	115.00	122.90
2	Q	7	MAN	C2-C3-C4	5.54	120.49	110.89
3	d	1	NAG	C1-O5-C5	5.54	119.70	112.19
2	T	1	NAG	C1-O5-C5	5.52	119.67	112.19
2	c	8	MAN	C1-O5-C5	5.50	119.64	112.19
4	K	4	MAN	C1-C2-C3	5.47	116.39	109.67
2	W	7	MAN	C1-C2-C3	5.39	116.29	109.67
2	I	3	BMA	O5-C5-C6	5.38	115.64	107.20
2	L	6	MAN	C1-O5-C5	5.20	119.24	112.19
2	Z	6	MAN	C3-C4-C5	-5.14	101.07	110.24
3	O	2	NAG	C2-N2-C7	5.14	130.22	122.90
4	K	3	BMA	C1-C2-C3	5.12	115.96	109.67
3	U	2	NAG	C1-O5-C5	5.04	119.01	112.19
2	Z	1	NAG	C1-C2-N2	-5.00	101.95	110.49
3	S	1	NAG	C1-O5-C5	4.99	118.96	112.19
4	K	4	MAN	C1-O5-C5	4.97	118.93	112.19
2	Z	4	MAN	C1-O5-C5	4.93	118.87	112.19
2	Z	6	MAN	C1-C2-C3	-4.92	103.62	109.67
3	X	2	NAG	C1-O5-C5	4.91	118.84	112.19
2	W	9	MAN	C1-O5-C5	4.90	118.84	112.19
2	Q	9	MAN	C1-C2-C3	4.90	115.69	109.67
2	L	9	MAN	C1-C2-C3	4.78	115.54	109.67
3	e	2	NAG	O5-C5-C6	4.74	114.64	107.20
3	b	2	NAG	C2-N2-C7	4.70	129.59	122.90
2	N	6	MAN	O5-C1-C2	-4.69	103.53	110.77
3	b	1	NAG	C2-N2-C7	4.68	129.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	8	MAN	C1-O5-C5	4.68	118.53	112.19
2	Z	5	MAN	C1-O5-C5	4.65	118.49	112.19
3	d	1	NAG	C3-C4-C5	-4.65	101.95	110.24
3	O	2	NAG	O5-C1-C2	4.64	118.62	111.29
2	I	9	MAN	O5-C5-C6	4.64	114.48	107.20
3	J	2	NAG	C2-N2-C7	4.60	129.46	122.90
2	L	7	MAN	C1-O5-C5	4.52	118.32	112.19
3	O	1	NAG	C1-O5-C5	-4.51	106.09	112.19
2	c	7	MAN	C1-C2-C3	4.50	115.19	109.67
2	W	2	NAG	O3-C3-C2	4.48	118.74	109.47
2	c	1	NAG	C3-C4-C5	-4.41	102.38	110.24
2	I	6	MAN	O2-C2-C1	4.40	118.15	109.15
4	K	4	MAN	O5-C5-C6	4.40	114.10	107.20
2	N	5	MAN	C1-O5-C5	4.37	118.11	112.19
2	Q	8	MAN	O5-C1-C2	4.35	117.49	110.77
3	U	2	NAG	C3-C4-C5	4.33	117.97	110.24
3	e	1	NAG	C2-N2-C7	-4.33	116.74	122.90
2	W	5	MAN	C1-C2-C3	-4.33	104.34	109.67
2	W	1	NAG	C2-N2-C7	4.30	129.02	122.90
2	I	2	NAG	O3-C3-C2	4.28	118.33	109.47
2	Z	7	MAN	C1-C2-C3	-4.27	104.41	109.67
3	S	2	NAG	O5-C5-C6	4.26	113.88	107.20
3	e	2	NAG	C2-N2-C7	4.23	128.93	122.90
2	I	3	BMA	C6-C5-C4	-4.21	103.15	113.00
2	N	4	MAN	C1-O5-C5	4.18	117.85	112.19
4	K	2	NAG	C1-O5-C5	-4.18	106.53	112.19
2	T	2	NAG	C1-C2-N2	4.18	117.62	110.49
2	I	8	MAN	C2-C3-C4	4.16	118.10	110.89
3	O	1	NAG	O5-C1-C2	-4.15	104.74	111.29
2	W	2	NAG	C1-O5-C5	4.13	117.78	112.19
3	M	1	NAG	O5-C5-C6	4.10	113.63	107.20
3	X	2	NAG	C4-C3-C2	4.10	117.02	111.02
3	U	1	NAG	C1-C2-N2	4.09	117.48	110.49
2	W	3	BMA	O4-C4-C3	-4.09	100.90	110.35
3	R	2	NAG	C2-N2-C7	4.08	128.72	122.90
2	Q	1	NAG	O5-C5-C6	4.07	113.59	107.20
2	I	2	NAG	C3-C4-C5	-4.06	102.99	110.24
2	L	9	MAN	C2-C3-C4	4.05	117.90	110.89
2	Q	9	MAN	C1-O5-C5	4.04	117.67	112.19
3	a	2	NAG	C3-C4-C5	3.99	117.36	110.24
3	d	1	NAG	O3-C3-C2	3.99	117.72	109.47
2	N	2	NAG	C1-O5-C5	-3.98	106.80	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	BMA	C2-C3-C4	3.97	117.77	110.89
2	T	1	NAG	C1-C2-N2	-3.95	103.74	110.49
2	T	3	BMA	O5-C5-C6	3.95	113.39	107.20
4	K	1	NAG	O5-C1-C2	-3.92	105.10	111.29
3	M	2	NAG	C4-C3-C2	3.91	116.75	111.02
2	Z	2	NAG	C1-C2-N2	3.90	117.16	110.49
3	S	1	NAG	C2-N2-C7	-3.90	117.35	122.90
2	Z	6	MAN	O3-C3-C2	3.89	117.45	109.99
3	U	2	NAG	C4-C3-C2	3.89	116.72	111.02
4	K	2	NAG	O4-C4-C3	3.88	119.32	110.35
2	N	4	MAN	O5-C1-C2	-3.82	104.88	110.77
2	Z	6	MAN	O3-C3-C4	3.81	119.17	110.35
2	T	1	NAG	C2-N2-C7	-3.80	117.49	122.90
2	N	4	MAN	O2-C2-C1	-3.78	101.41	109.15
2	Q	9	MAN	C2-C3-C4	3.78	117.44	110.89
2	T	1	NAG	C6-C5-C4	-3.78	104.16	113.00
2	Z	4	MAN	O2-C2-C3	3.76	117.68	110.14
2	I	2	NAG	O5-C1-C2	-3.75	105.36	111.29
2	W	9	MAN	C3-C4-C5	3.71	116.86	110.24
2	L	9	MAN	C3-C4-C5	3.71	116.85	110.24
2	c	4	MAN	C1-O5-C5	3.71	117.22	112.19
2	Q	3	BMA	O2-C2-C3	-3.70	102.72	110.14
4	K	3	BMA	C2-C3-C4	-3.69	104.51	110.89
2	N	9	MAN	C1-O5-C5	-3.69	107.20	112.19
2	W	3	BMA	C6-C5-C4	3.68	121.63	113.00
2	T	9	MAN	C3-C4-C5	3.68	116.81	110.24
2	c	3	BMA	C3-C4-C5	-3.68	103.67	110.24
2	Z	6	MAN	O5-C1-C2	-3.67	105.11	110.77
3	d	2	NAG	C1-O5-C5	3.66	117.14	112.19
2	Q	4	MAN	O5-C5-C6	3.64	112.91	107.20
2	c	2	NAG	O5-C5-C6	-3.63	101.51	107.20
2	T	6	MAN	C1-C2-C3	3.63	114.13	109.67
2	I	8	MAN	C3-C4-C5	3.63	116.71	110.24
2	Z	2	NAG	C3-C4-C5	-3.60	103.82	110.24
3	V	2	NAG	O5-C1-C2	3.56	116.91	111.29
4	K	1	NAG	C8-C7-N2	3.56	122.13	116.10
3	Y	1	NAG	C1-O5-C5	3.52	116.97	112.19
2	c	7	MAN	C1-O5-C5	3.51	116.95	112.19
4	K	3	BMA	O2-C2-C3	-3.50	103.12	110.14
2	I	2	NAG	O3-C3-C4	-3.49	102.28	110.35
2	N	9	MAN	O5-C5-C6	3.48	112.66	107.20
3	V	2	NAG	C1-O5-C5	3.47	116.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	4	MAN	C1-C2-C3	-3.45	105.42	109.67
2	c	1	NAG	C2-N2-C7	-3.44	118.01	122.90
2	N	6	MAN	C1-O5-C5	3.43	116.84	112.19
2	W	4	MAN	O2-C2-C1	-3.41	102.17	109.15
2	W	5	MAN	C1-O5-C5	3.40	116.79	112.19
4	K	1	NAG	C2-N2-C7	-3.39	118.07	122.90
2	L	4	MAN	C3-C4-C5	-3.38	104.20	110.24
3	d	2	NAG	C2-N2-C7	3.37	127.70	122.90
2	Z	6	MAN	C1-O5-C5	3.36	116.74	112.19
2	c	5	MAN	O2-C2-C3	3.35	116.85	110.14
2	Z	9	MAN	C3-C4-C5	3.33	116.18	110.24
2	T	3	BMA	O3-C3-C4	-3.30	102.71	110.35
4	K	1	NAG	O4-C4-C3	-3.30	102.72	110.35
4	K	2	NAG	C2-N2-C7	-3.30	118.21	122.90
2	T	7	MAN	O5-C1-C2	-3.29	105.69	110.77
4	K	2	NAG	O5-C5-C6	3.29	112.36	107.20
2	T	2	NAG	C4-C3-C2	-3.27	106.22	111.02
3	Y	2	NAG	C3-C4-C5	3.26	116.06	110.24
2	N	6	MAN	O5-C5-C6	3.26	112.31	107.20
2	c	9	MAN	C1-O5-C5	3.25	116.60	112.19
3	b	2	NAG	C1-C2-N2	3.25	116.04	110.49
3	X	1	NAG	O5-C1-C2	3.24	116.41	111.29
2	W	8	MAN	C1-O5-C5	3.24	116.58	112.19
3	e	2	NAG	C1-O5-C5	3.24	116.58	112.19
2	N	2	NAG	O3-C3-C2	3.24	116.17	109.47
2	Z	1	NAG	O5-C5-C6	3.24	112.28	107.20
2	Q	3	BMA	O5-C1-C2	-3.23	105.78	110.77
3	V	1	NAG	C2-N2-C7	-3.21	118.33	122.90
3	S	2	NAG	O3-C3-C2	3.20	116.08	109.47
3	V	2	NAG	O5-C5-C6	3.18	112.20	107.20
2	c	5	MAN	C1-C2-C3	-3.18	105.76	109.67
2	N	1	NAG	C4-C3-C2	3.17	115.66	111.02
2	L	2	NAG	C1-O5-C5	-3.17	107.90	112.19
2	L	7	MAN	O3-C3-C2	-3.16	103.94	109.99
2	W	3	BMA	O5-C5-C4	-3.16	103.15	110.83
2	Z	4	MAN	O2-C2-C1	-3.16	102.69	109.15
2	c	4	MAN	O5-C5-C4	3.15	118.49	110.83
2	L	3	BMA	O3-C3-C2	-3.15	103.97	109.99
2	N	8	MAN	C1-O5-C5	3.14	116.45	112.19
2	N	3	BMA	C1-C2-C3	3.14	113.53	109.67
3	d	1	NAG	O5-C5-C4	3.14	118.46	110.83
3	d	2	NAG	O5-C5-C6	3.13	112.12	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	NAG	C2-N2-C7	-3.12	118.46	122.90
4	K	1	NAG	O7-C7-N2	-3.11	116.23	121.95
4	K	1	NAG	C4-C3-C2	3.11	115.57	111.02
2	Z	5	MAN	C1-C2-C3	-3.10	105.85	109.67
2	L	1	NAG	C3-C4-C5	-3.10	104.71	110.24
2	Z	9	MAN	O5-C5-C6	3.10	112.06	107.20
2	Z	1	NAG	C1-O5-C5	3.09	116.38	112.19
2	T	7	MAN	O4-C4-C3	-3.09	103.21	110.35
2	N	8	MAN	C3-C4-C5	3.08	115.74	110.24
2	Z	5	MAN	O5-C1-C2	3.08	115.53	110.77
2	T	2	NAG	O5-C1-C2	-3.07	106.44	111.29
2	W	2	NAG	C1-C2-N2	3.06	115.72	110.49
2	Z	3	BMA	O5-C1-C2	-3.04	106.08	110.77
2	L	3	BMA	C1-C2-C3	3.04	113.40	109.67
2	L	7	MAN	O5-C5-C6	3.03	111.96	107.20
2	W	8	MAN	O5-C1-C2	-3.02	106.11	110.77
2	I	6	MAN	O6-C6-C5	-3.02	100.94	111.29
4	K	2	NAG	C3-C4-C5	-3.02	104.86	110.24
2	W	1	NAG	C4-C3-C2	3.01	115.43	111.02
3	d	1	NAG	O3-C3-C4	2.99	117.27	110.35
2	I	2	NAG	O6-C6-C5	-2.99	101.04	111.29
2	N	6	MAN	O2-C2-C1	-2.98	103.06	109.15
2	N	7	MAN	C1-O5-C5	2.97	116.21	112.19
3	d	2	NAG	C1-C2-N2	2.96	115.55	110.49
3	J	1	NAG	O5-C5-C6	2.96	111.85	107.20
2	W	1	NAG	C1-O5-C5	2.96	116.20	112.19
3	P	2	NAG	C1-C2-N2	-2.94	105.47	110.49
2	Q	5	MAN	C1-C2-C3	-2.93	106.07	109.67
2	N	9	MAN	C1-C2-C3	2.93	113.26	109.67
2	T	4	MAN	C6-C5-C4	-2.91	106.18	113.00
2	Z	7	MAN	O5-C5-C6	2.90	111.75	107.20
2	Q	3	BMA	O5-C5-C6	2.89	111.74	107.20
3	P	2	NAG	C1-O5-C5	2.89	116.11	112.19
3	Y	2	NAG	C1-C2-N2	2.89	115.42	110.49
3	b	1	NAG	C8-C7-N2	2.87	120.95	116.10
3	J	1	NAG	C2-N2-C7	2.85	126.96	122.90
2	W	5	MAN	O5-C1-C2	2.84	115.15	110.77
3	b	1	NAG	C6-C5-C4	2.83	119.64	113.00
3	e	1	NAG	C4-C3-C2	-2.83	106.87	111.02
3	e	1	NAG	C1-O5-C5	2.83	116.03	112.19
3	a	2	NAG	C4-C3-C2	2.83	115.16	111.02
3	P	2	NAG	C2-N2-C7	2.82	126.92	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	NAG	C6-C5-C4	-2.80	106.45	113.00
2	W	3	BMA	C2-C3-C4	2.80	115.73	110.89
3	O	1	NAG	O5-C5-C6	2.78	111.56	107.20
2	Q	6	MAN	C1-O5-C5	2.78	115.95	112.19
2	Z	6	MAN	O4-C4-C5	2.77	116.19	109.30
3	a	1	NAG	C1-O5-C5	2.77	115.94	112.19
3	P	1	NAG	O4-C4-C3	-2.77	103.95	110.35
2	T	9	MAN	O5-C5-C6	2.76	111.54	107.20
2	N	4	MAN	C3-C4-C5	-2.76	105.31	110.24
3	R	1	NAG	C6-C5-C4	-2.75	106.56	113.00
2	c	5	MAN	O5-C1-C2	2.73	114.99	110.77
3	U	1	NAG	O5-C1-C2	-2.73	106.97	111.29
3	S	1	NAG	O5-C1-C2	-2.73	106.97	111.29
2	W	5	MAN	O2-C2-C3	2.72	115.58	110.14
3	X	2	NAG	C6-C5-C4	-2.71	106.66	113.00
3	S	2	NAG	C1-O5-C5	2.70	115.85	112.19
2	c	9	MAN	O5-C1-C2	-2.70	106.61	110.77
2	W	6	MAN	O5-C1-C2	-2.69	106.61	110.77
2	L	7	MAN	O5-C1-C2	-2.69	106.62	110.77
2	c	6	MAN	C1-O5-C5	2.69	115.83	112.19
2	I	5	MAN	C2-C3-C4	2.68	115.53	110.89
2	L	8	MAN	C1-O5-C5	2.68	115.82	112.19
2	T	2	NAG	C2-N2-C7	2.67	126.71	122.90
2	I	8	MAN	O2-C2-C1	2.67	114.62	109.15
2	W	6	MAN	O5-C5-C6	2.67	111.39	107.20
3	e	1	NAG	O3-C3-C2	-2.66	103.96	109.47
3	M	2	NAG	C2-N2-C7	2.66	126.69	122.90
3	Y	2	NAG	C2-N2-C7	2.66	126.68	122.90
3	J	1	NAG	C1-C2-N2	2.65	115.01	110.49
2	c	4	MAN	C2-C3-C4	2.64	115.47	110.89
2	c	4	MAN	C3-C4-C5	2.63	114.94	110.24
4	K	2	NAG	O5-C5-C4	-2.62	104.44	110.83
2	T	6	MAN	O5-C5-C6	2.62	111.31	107.20
3	V	2	NAG	C4-C3-C2	2.62	114.86	111.02
3	V	1	NAG	O5-C1-C2	-2.62	107.15	111.29
3	P	2	NAG	C3-C4-C5	2.61	114.90	110.24
2	W	7	MAN	O5-C5-C4	-2.61	104.47	110.83
2	Q	6	MAN	C1-C2-C3	2.61	112.87	109.67
4	K	3	BMA	O5-C5-C6	2.61	111.29	107.20
2	Q	4	MAN	C3-C4-C5	-2.60	105.60	110.24
2	L	9	MAN	O5-C5-C6	2.60	111.28	107.20
2	Z	3	BMA	O4-C4-C5	2.60	115.75	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2	NAG	C6-C5-C4	-2.59	106.94	113.00
2	I	2	NAG	O4-C4-C3	-2.59	104.37	110.35
3	J	2	NAG	C4-C3-C2	2.57	114.78	111.02
2	Q	9	MAN	O5-C1-C2	2.57	114.73	110.77
4	K	3	BMA	O5-C1-C2	2.56	114.72	110.77
2	N	4	MAN	O2-C2-C3	2.56	115.26	110.14
2	L	4	MAN	O5-C5-C6	2.55	111.21	107.20
4	K	2	NAG	O6-C6-C5	-2.55	102.54	111.29
2	L	4	MAN	O2-C2-C1	-2.55	103.94	109.15
3	e	2	NAG	O7-C7-C8	-2.55	117.33	122.06
2	W	7	MAN	O3-C3-C4	-2.54	104.47	110.35
2	I	6	MAN	C3-C4-C5	-2.54	105.71	110.24
2	L	2	NAG	O4-C4-C3	-2.54	104.48	110.35
2	T	8	MAN	O5-C5-C6	2.54	111.18	107.20
2	c	1	NAG	C8-C7-N2	2.54	120.39	116.10
2	T	1	NAG	O3-C3-C2	-2.53	104.23	109.47
2	I	1	NAG	C1-C2-N2	-2.53	106.17	110.49
2	I	5	MAN	O3-C3-C2	2.53	114.84	109.99
2	T	4	MAN	C1-C2-C3	-2.51	106.58	109.67
2	N	3	BMA	O3-C3-C2	-2.50	105.20	109.99
3	J	1	NAG	C4-C3-C2	-2.50	107.36	111.02
2	W	2	NAG	O7-C7-C8	-2.50	117.42	122.06
3	O	2	NAG	C8-C7-N2	2.49	120.31	116.10
3	e	2	NAG	C1-C2-N2	2.49	114.73	110.49
2	Q	1	NAG	C1-C2-N2	-2.48	106.25	110.49
2	I	4	MAN	O2-C2-C1	-2.48	104.08	109.15
2	W	3	BMA	O5-C1-C2	-2.48	106.95	110.77
2	N	4	MAN	C1-C2-C3	-2.48	106.62	109.67
2	W	7	MAN	O2-C2-C1	-2.45	104.14	109.15
2	I	2	NAG	C1-O5-C5	-2.45	108.88	112.19
2	L	3	BMA	O5-C1-C2	-2.45	107.00	110.77
2	W	6	MAN	O4-C4-C3	-2.44	104.71	110.35
2	c	1	NAG	O7-C7-N2	-2.44	117.47	121.95
2	W	2	NAG	O5-C1-C2	-2.44	107.44	111.29
2	N	1	NAG	O5-C5-C6	2.44	111.02	107.20
3	S	1	NAG	O4-C4-C5	-2.44	103.25	109.30
2	Q	3	BMA	O4-C4-C3	-2.43	104.72	110.35
2	Z	5	MAN	C2-C3-C4	-2.43	106.69	110.89
2	I	9	MAN	C1-O5-C5	-2.41	108.92	112.19
2	c	9	MAN	C3-C4-C5	2.41	114.54	110.24
3	X	2	NAG	O3-C3-C4	-2.40	104.79	110.35
2	Q	2	NAG	O6-C6-C5	-2.40	103.05	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	2	NAG	O3-C3-C4	-2.39	104.83	110.35
3	d	1	NAG	O5-C5-C6	2.38	110.94	107.20
2	Z	8	MAN	C3-C4-C5	-2.38	105.99	110.24
3	a	1	NAG	O4-C4-C3	-2.38	104.84	110.35
2	I	7	MAN	O5-C5-C4	2.38	116.61	110.83
2	I	6	MAN	C6-C5-C4	2.37	118.56	113.00
2	I	9	MAN	O3-C3-C2	2.37	114.53	109.99
3	P	2	NAG	C4-C3-C2	2.37	114.49	111.02
3	b	1	NAG	O5-C5-C6	-2.37	103.49	107.20
2	T	3	BMA	O4-C4-C5	2.36	115.17	109.30
2	T	8	MAN	C1-O5-C5	2.35	115.37	112.19
2	W	6	MAN	O2-C2-C1	2.35	113.95	109.15
2	T	8	MAN	C2-C3-C4	2.34	114.95	110.89
2	I	7	MAN	O6-C6-C5	2.34	119.31	111.29
3	J	1	NAG	O3-C3-C4	2.33	115.75	110.35
4	K	1	NAG	O5-C5-C6	2.33	110.86	107.20
2	T	7	MAN	C2-C3-C4	2.33	114.93	110.89
4	K	1	NAG	O3-C3-C4	-2.33	104.96	110.35
2	I	2	NAG	O5-C5-C4	-2.33	105.16	110.83
2	T	1	NAG	O5-C5-C6	2.33	110.86	107.20
4	K	1	NAG	O3-C3-C2	2.33	114.28	109.47
3	R	1	NAG	O5-C5-C4	2.33	116.48	110.83
2	Z	4	MAN	C2-C3-C4	2.31	114.90	110.89
2	L	3	BMA	C3-C4-C5	2.31	114.36	110.24
2	Q	1	NAG	O3-C3-C4	2.30	115.68	110.35
2	Z	3	BMA	O3-C3-C2	-2.30	105.58	109.99
2	Z	1	NAG	C4-C3-C2	2.30	114.39	111.02
2	T	4	MAN	O2-C2-C3	2.30	114.75	110.14
2	I	8	MAN	O4-C4-C5	-2.30	103.58	109.30
2	c	2	NAG	O4-C4-C3	-2.30	105.03	110.35
3	P	1	NAG	C2-N2-C7	2.30	126.18	122.90
2	Q	6	MAN	O2-C2-C1	2.30	113.85	109.15
2	Q	8	MAN	O3-C3-C2	-2.29	105.60	109.99
3	b	1	NAG	O7-C7-C8	-2.29	117.80	122.06
2	T	7	MAN	O5-C5-C6	-2.29	103.61	107.20
2	L	1	NAG	O5-C5-C4	-2.29	105.27	110.83
3	J	1	NAG	O5-C1-C2	2.28	114.89	111.29
2	I	3	BMA	O5-C1-C2	2.28	114.30	110.77
2	Q	3	BMA	O6-C6-C5	2.28	119.12	111.29
2	W	9	MAN	O3-C3-C2	2.28	114.36	109.99
2	Q	2	NAG	C1-C2-N2	2.28	114.38	110.49
2	I	3	BMA	O4-C4-C5	-2.28	103.64	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	3	BMA	O5-C1-C2	2.28	114.28	110.77
2	N	6	MAN	O2-C2-C3	-2.27	105.58	110.14
2	I	8	MAN	O2-C2-C3	2.27	114.69	110.14
3	J	2	NAG	C3-C4-C5	2.27	114.29	110.24
2	c	1	NAG	C1-C2-N2	2.27	114.36	110.49
3	b	1	NAG	O5-C1-C2	2.27	114.86	111.29
3	b	1	NAG	O4-C4-C5	2.26	114.92	109.30
2	L	6	MAN	O4-C4-C3	-2.25	105.14	110.35
2	T	3	BMA	C2-C3-C4	-2.25	106.99	110.89
2	Z	3	BMA	C3-C4-C5	-2.25	106.23	110.24
2	c	1	NAG	O5-C1-C2	-2.24	107.75	111.29
2	I	6	MAN	C1-O5-C5	-2.24	109.16	112.19
2	L	1	NAG	O5-C5-C6	2.23	110.70	107.20
2	N	8	MAN	C2-C3-C4	2.22	114.74	110.89
2	W	7	MAN	O4-C4-C3	-2.22	105.22	110.35
2	c	1	NAG	O6-C6-C5	-2.21	103.69	111.29
2	L	7	MAN	O2-C2-C1	2.21	113.68	109.15
3	S	2	NAG	O5-C1-C2	2.21	114.78	111.29
3	V	1	NAG	C6-C5-C4	2.21	118.18	113.00
2	W	1	NAG	O5-C5-C6	2.21	110.67	107.20
3	R	1	NAG	O5-C5-C6	2.20	110.66	107.20
2	Q	1	NAG	O4-C4-C5	-2.20	103.83	109.30
2	T	2	NAG	O6-C6-C5	-2.20	103.75	111.29
3	d	2	NAG	O5-C1-C2	-2.18	107.84	111.29
2	T	8	MAN	C3-C4-C5	2.17	114.11	110.24
2	Z	1	NAG	O6-C6-C5	2.17	118.73	111.29
2	L	4	MAN	O6-C6-C5	-2.17	103.85	111.29
2	c	1	NAG	C1-O5-C5	-2.15	109.28	112.19
2	Q	1	NAG	O5-C5-C4	2.15	116.05	110.83
2	Z	2	NAG	O5-C5-C4	-2.14	105.61	110.83
2	c	3	BMA	C1-O5-C5	2.14	115.09	112.19
2	c	3	BMA	O5-C5-C4	-2.14	105.62	110.83
2	Q	9	MAN	O2-C2-C3	2.14	114.42	110.14
3	V	2	NAG	C2-N2-C7	2.14	125.94	122.90
2	L	6	MAN	C1-C2-C3	-2.14	107.04	109.67
2	I	7	MAN	O5-C1-C2	2.13	114.06	110.77
2	T	9	MAN	O3-C3-C4	2.13	115.28	110.35
3	J	2	NAG	C1-C2-N2	-2.13	106.86	110.49
4	K	2	NAG	O3-C3-C2	-2.12	105.07	109.47
3	X	2	NAG	C3-C4-C5	2.12	114.01	110.24
2	L	2	NAG	O5-C1-C2	-2.12	107.95	111.29
2	I	6	MAN	O3-C3-C2	2.11	114.04	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	4	MAN	O3-C3-C2	-2.11	105.95	109.99
3	V	2	NAG	C1-C2-N2	-2.10	106.89	110.49
3	R	1	NAG	C2-N2-C7	2.10	125.90	122.90
2	Q	1	NAG	O5-C1-C2	2.10	114.60	111.29
3	e	1	NAG	C8-C7-N2	2.09	119.64	116.10
2	W	1	NAG	O7-C7-N2	2.07	125.77	121.95
2	W	1	NAG	O3-C3-C4	-2.07	105.56	110.35
3	M	1	NAG	C3-C4-C5	-2.07	106.54	110.24
2	Z	1	NAG	O7-C7-C8	2.07	125.90	122.06
2	c	6	MAN	O3-C3-C2	2.07	113.95	109.99
2	T	1	NAG	C4-C3-C2	2.06	114.03	111.02
2	Q	8	MAN	O3-C3-C4	2.05	115.08	110.35
2	Z	7	MAN	O6-C6-C5	2.05	118.31	111.29
3	b	2	NAG	O5-C5-C6	2.04	110.41	107.20
2	L	7	MAN	C3-C4-C5	2.04	113.88	110.24
2	I	4	MAN	O3-C3-C2	-2.04	106.09	109.99
2	I	8	MAN	O5-C1-C2	-2.04	107.62	110.77
2	T	2	NAG	C8-C7-N2	-2.03	112.66	116.10
2	Q	7	MAN	O2-C2-C1	2.03	113.30	109.15
2	c	3	BMA	C1-C2-C3	2.02	112.15	109.67
2	Z	8	MAN	O4-C4-C3	2.02	115.02	110.35
3	Y	1	NAG	O5-C5-C6	-2.02	104.04	107.20
2	c	9	MAN	C2-C3-C4	2.02	114.39	110.89
2	N	9	MAN	O2-C2-C1	2.02	113.28	109.15
2	Q	9	MAN	C3-C4-C5	2.02	113.84	110.24
2	N	8	MAN	O4-C4-C5	-2.01	104.30	109.30
2	I	1	NAG	O3-C3-C4	-2.01	105.70	110.35
3	U	2	NAG	O5-C5-C4	2.01	115.72	110.83

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	V	2	NAG	C8-C7-N2-C2
3	V	2	NAG	O7-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C1-C2-N2-C7
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
2	T	2	NAG	C3-C2-N2-C7
3	b	1	NAG	C8-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C3-C2-N2-C7
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	b	2	NAG	C1-C2-N2-C7
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
2	Q	4	MAN	O5-C5-C6-O6
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	L	6	MAN	O5-C5-C6-O6
2	Z	4	MAN	O5-C5-C6-O6
2	Z	5	MAN	C4-C5-C6-O6
2	T	9	MAN	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
2	Z	7	MAN	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
2	c	6	MAN	C4-C5-C6-O6
2	Z	8	MAN	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	Z	7	MAN	C4-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
2	c	1	NAG	C8-C7-N2-C2
2	c	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	Z	8	MAN	C4-C5-C6-O6
2	Z	4	MAN	C4-C5-C6-O6
2	c	4	MAN	C4-C5-C6-O6
2	Z	5	MAN	O5-C5-C6-O6
2	L	6	MAN	C4-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
2	Z	6	MAN	O5-C5-C6-O6
2	L	9	MAN	O5-C5-C6-O6
2	Q	4	MAN	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
2	T	9	MAN	C4-C5-C6-O6
2	N	8	MAN	C4-C5-C6-O6
4	K	1	NAG	O7-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
2	W	7	MAN	O5-C5-C6-O6
2	c	6	MAN	O5-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
2	W	8	MAN	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	L	7	MAN	O5-C5-C6-O6
3	U	1	NAG	C8-C7-N2-C2
2	T	2	NAG	C8-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
2	N	7	MAN	O5-C5-C6-O6
2	c	4	MAN	O5-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
2	Z	3	BMA	C4-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
2	Q	8	MAN	O5-C5-C6-O6
2	Z	6	MAN	C4-C5-C6-O6
2	Q	7	MAN	O5-C5-C6-O6
2	I	9	MAN	C4-C5-C6-O6
2	N	8	MAN	O5-C5-C6-O6
2	W	7	MAN	C4-C5-C6-O6
2	L	9	MAN	C4-C5-C6-O6
4	K	4	MAN	O5-C5-C6-O6
2	N	7	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	I	9	MAN	O5-C5-C6-O6
2	N	6	MAN	C4-C5-C6-O6
2	Z	3	BMA	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
2	L	8	MAN	C4-C5-C6-O6
3	U	1	NAG	O7-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2
2	Z	1	NAG	C8-C7-N2-C2
3	S	2	NAG	O5-C5-C6-O6
2	Z	1	NAG	O7-C7-N2-C2
2	L	3	BMA	O5-C5-C6-O6
2	W	8	MAN	O5-C5-C6-O6
2	Q	3	BMA	C4-C5-C6-O6
2	T	7	MAN	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	d	1	NAG	C1-C2-N2-C7
3	J	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
2	N	6	MAN	O5-C5-C6-O6
2	T	1	NAG	C8-C7-N2-C2
2	W	3	BMA	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
2	Q	8	MAN	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
2	Q	7	MAN	C4-C5-C6-O6
2	L	7	MAN	C4-C5-C6-O6
2	T	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C4-C5-C6-O6
2	L	8	MAN	O5-C5-C6-O6
2	c	9	MAN	C4-C5-C6-O6
2	Q	6	MAN	C4-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
3	P	2	NAG	C3-C2-N2-C7
3	d	2	NAG	C3-C2-N2-C7
2	T	2	NAG	C1-C2-N2-C7
2	N	1	NAG	C8-C7-N2-C2
3	b	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	1	NAG	O5-C5-C6-O6
2	W	6	MAN	O5-C5-C6-O6
2	W	4	MAN	C4-C5-C6-O6
4	K	4	MAN	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	9	MAN	C1-C2-C3-C4-C5-O5

34 monomers are involved in 42 short contacts:

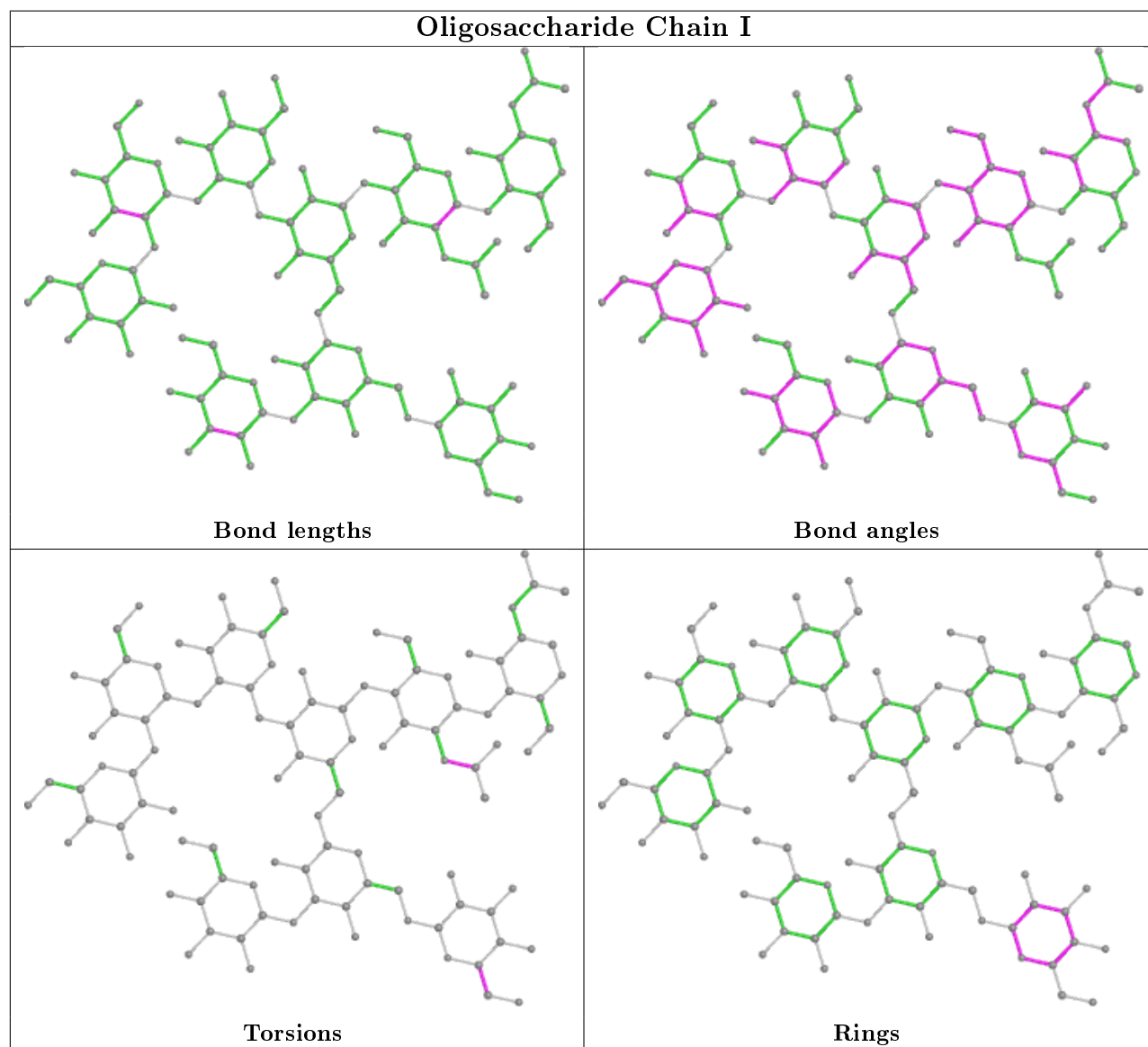
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	1	0
2	Z	2	NAG	2	0
3	M	2	NAG	1	0
2	T	9	MAN	1	0
2	L	6	MAN	1	0
2	T	5	MAN	1	0
2	Z	6	MAN	1	0
3	O	2	NAG	1	0
3	O	1	NAG	2	0
2	I	6	MAN	2	0
3	U	1	NAG	2	0
2	L	3	BMA	1	0
2	W	1	NAG	1	0
3	V	1	NAG	4	0
4	K	1	NAG	1	0
3	R	1	NAG	1	0
2	W	7	MAN	3	0
2	W	5	MAN	2	0
2	W	3	BMA	1	0
2	I	5	MAN	1	0
2	Z	4	MAN	1	0
2	T	3	BMA	1	0
2	Q	4	MAN	1	0
2	N	6	MAN	5	0
2	Q	5	MAN	1	0

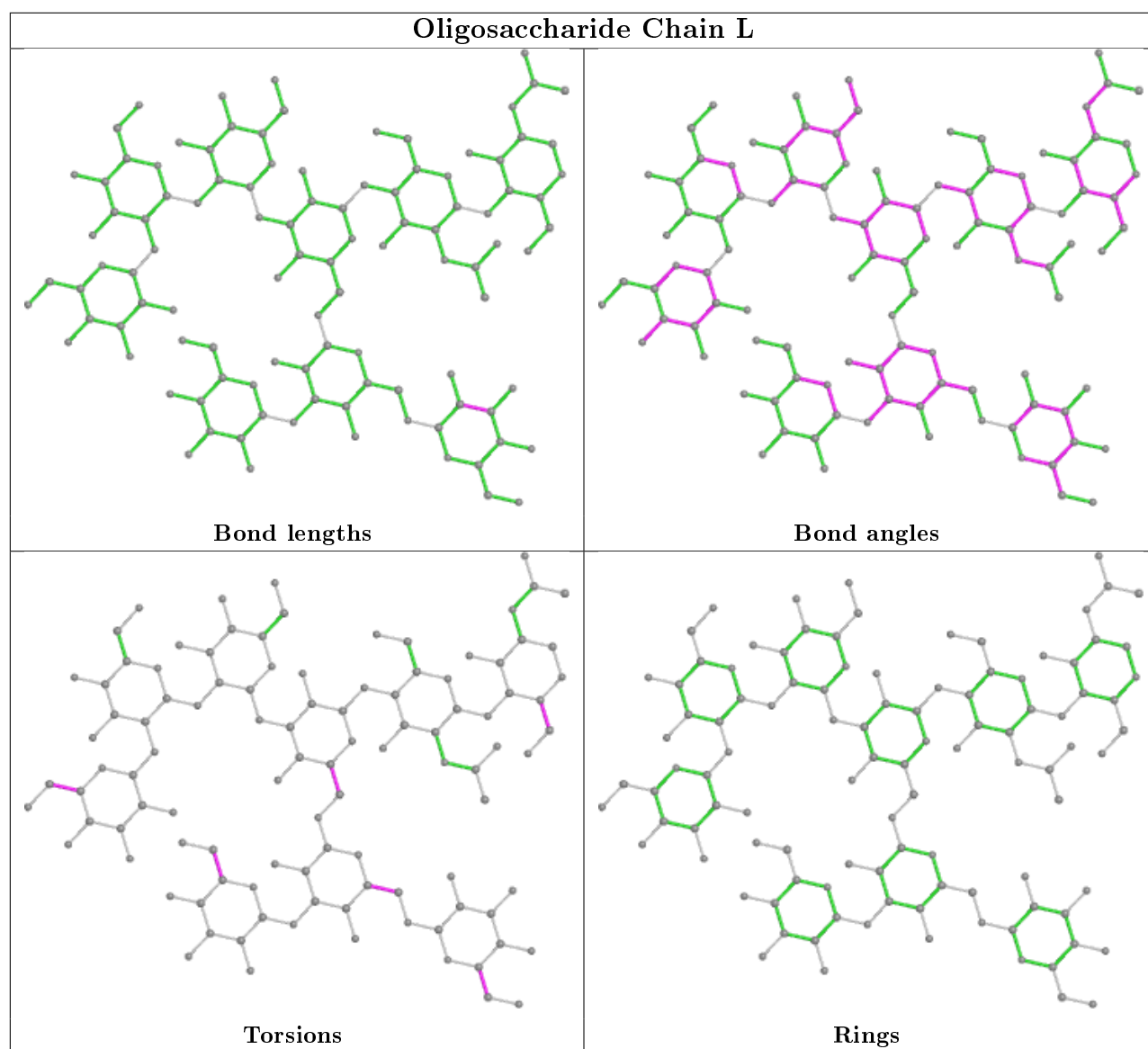
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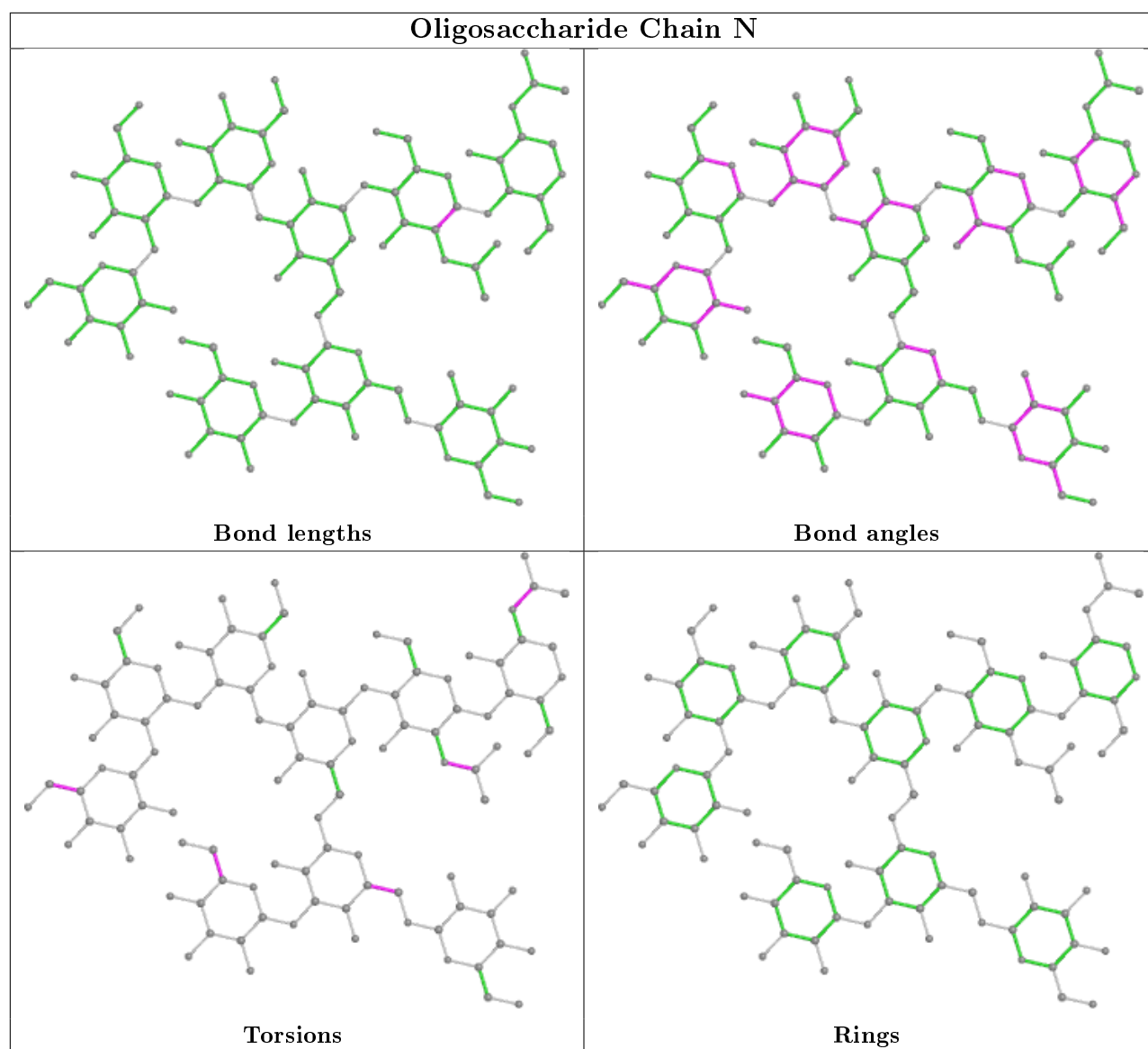
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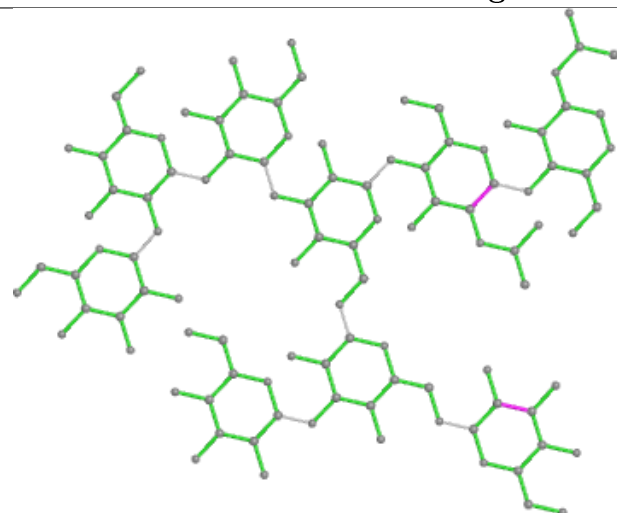
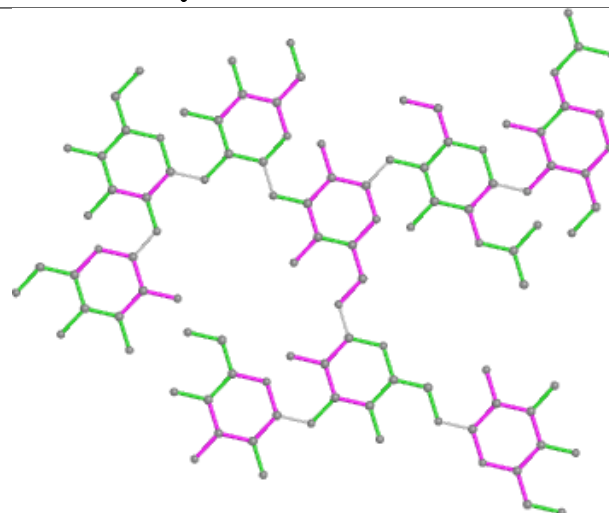
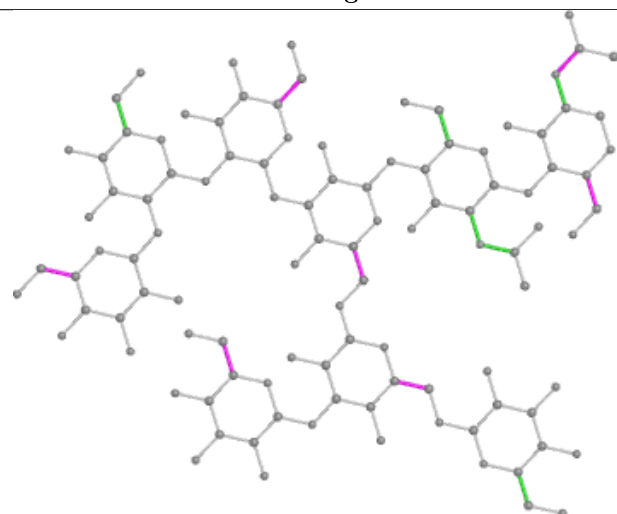
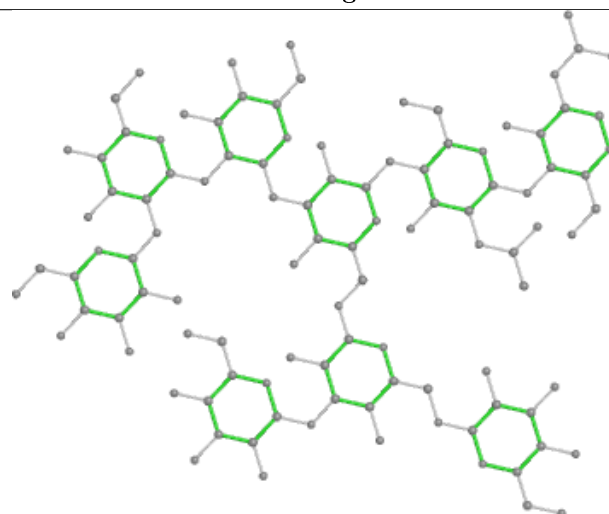
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	1	0
2	W	9	MAN	2	0
2	I	4	MAN	1	0
2	T	7	MAN	1	0
3	X	1	NAG	2	0
2	W	4	MAN	1	0
2	Z	5	MAN	1	0
2	N	3	BMA	1	0
2	L	1	NAG	3	0

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

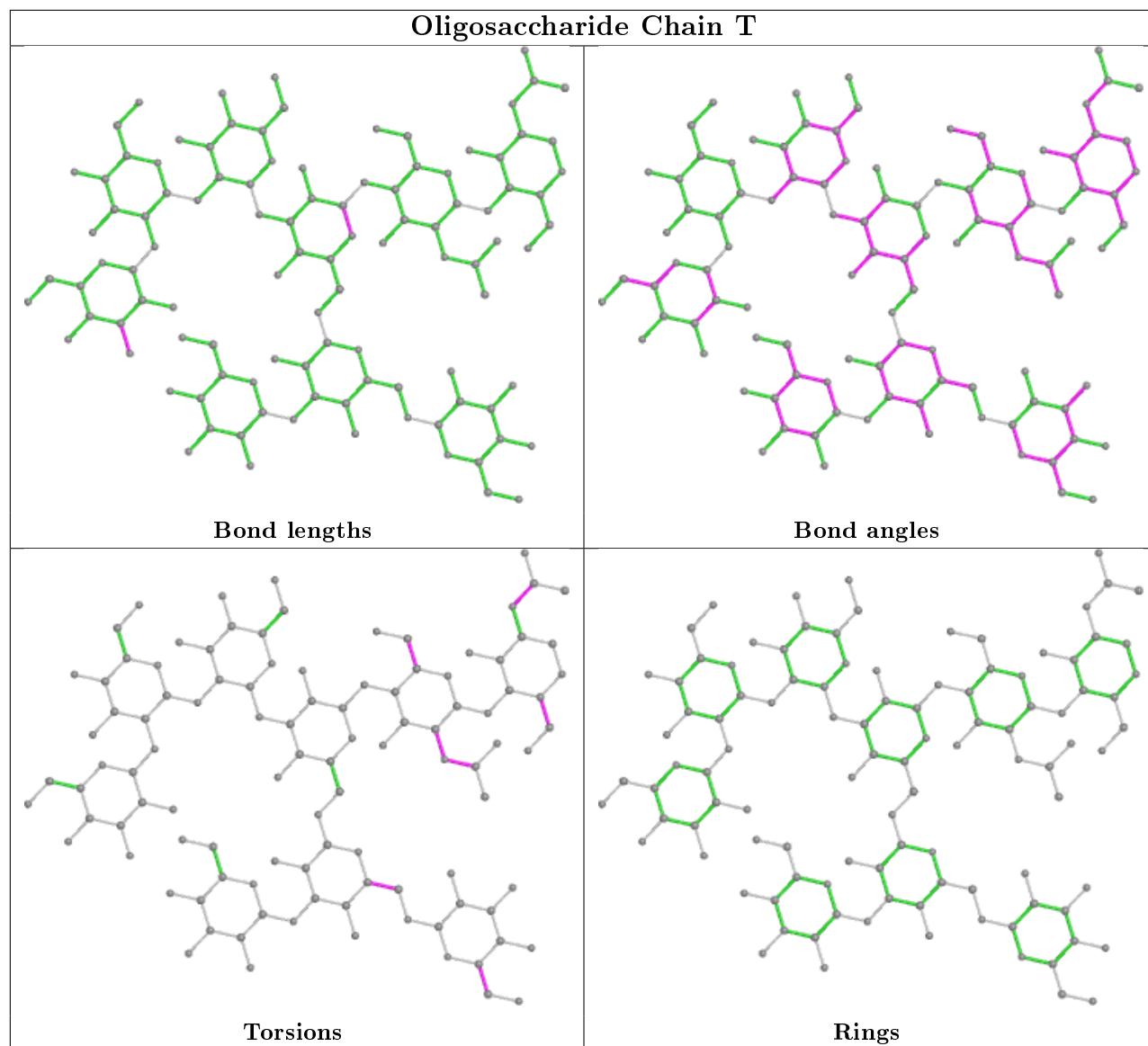


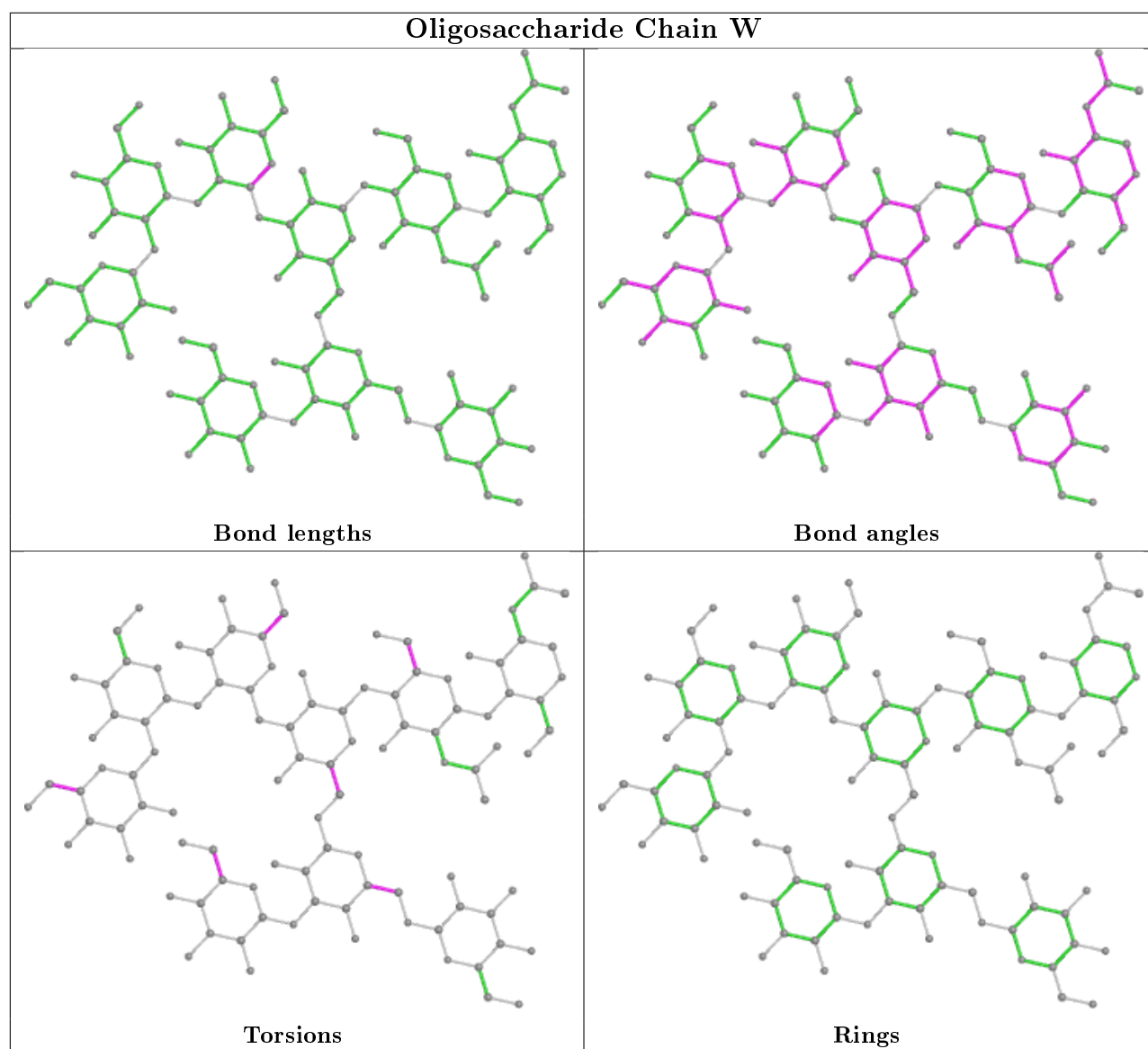


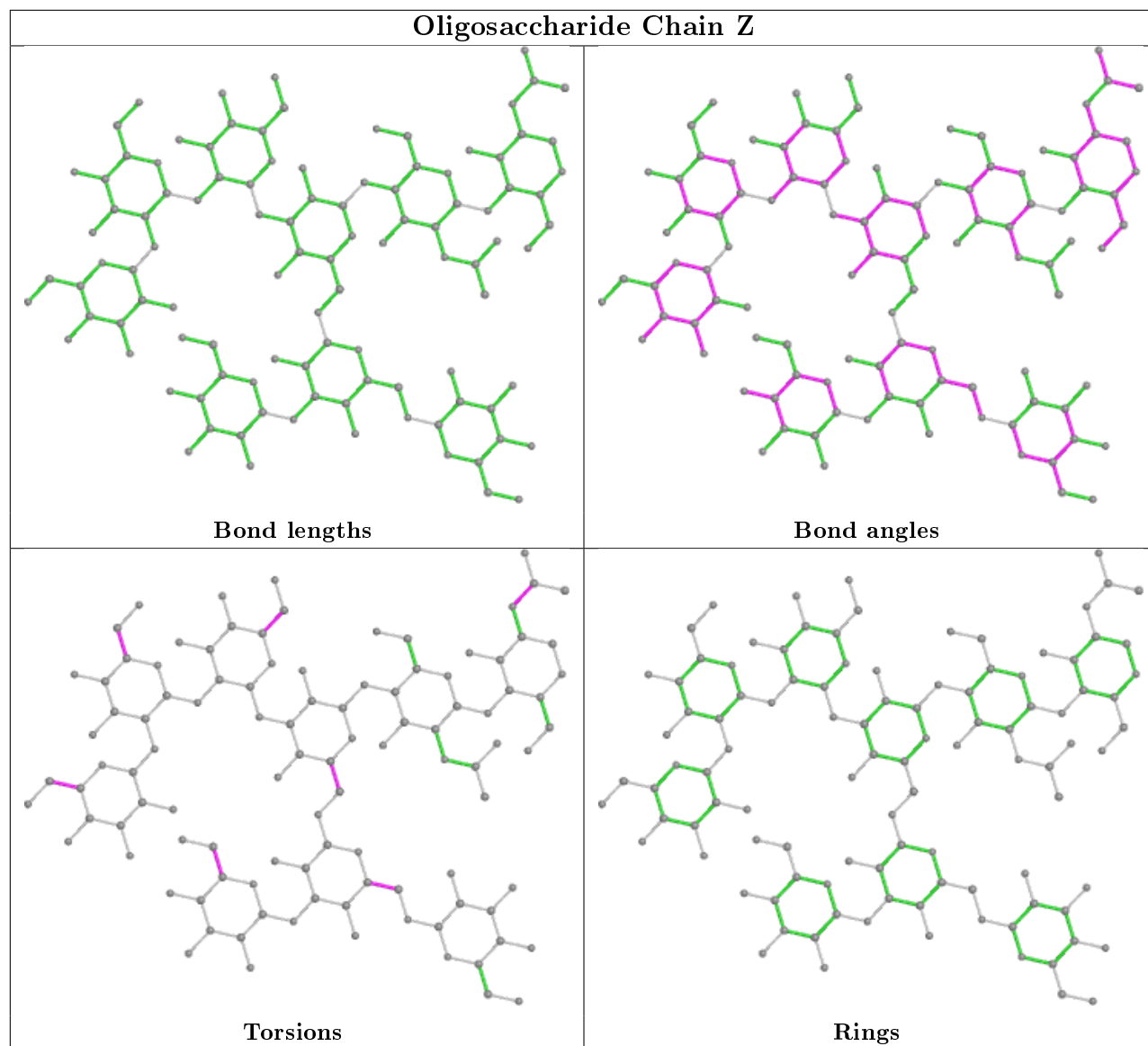


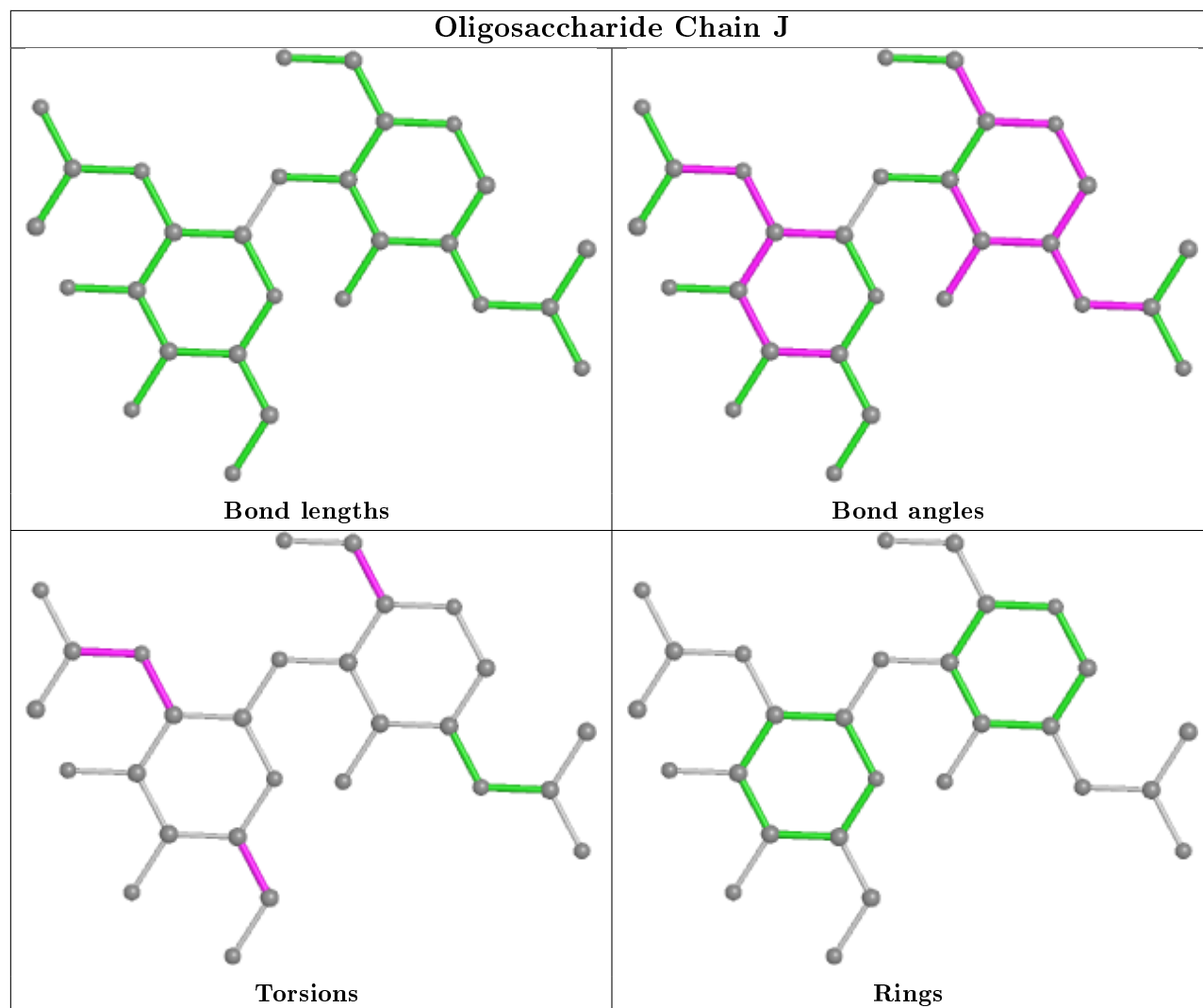
**Oligosaccharide Chain Q****Bond lengths****Bond angles****Torsions****Rings**

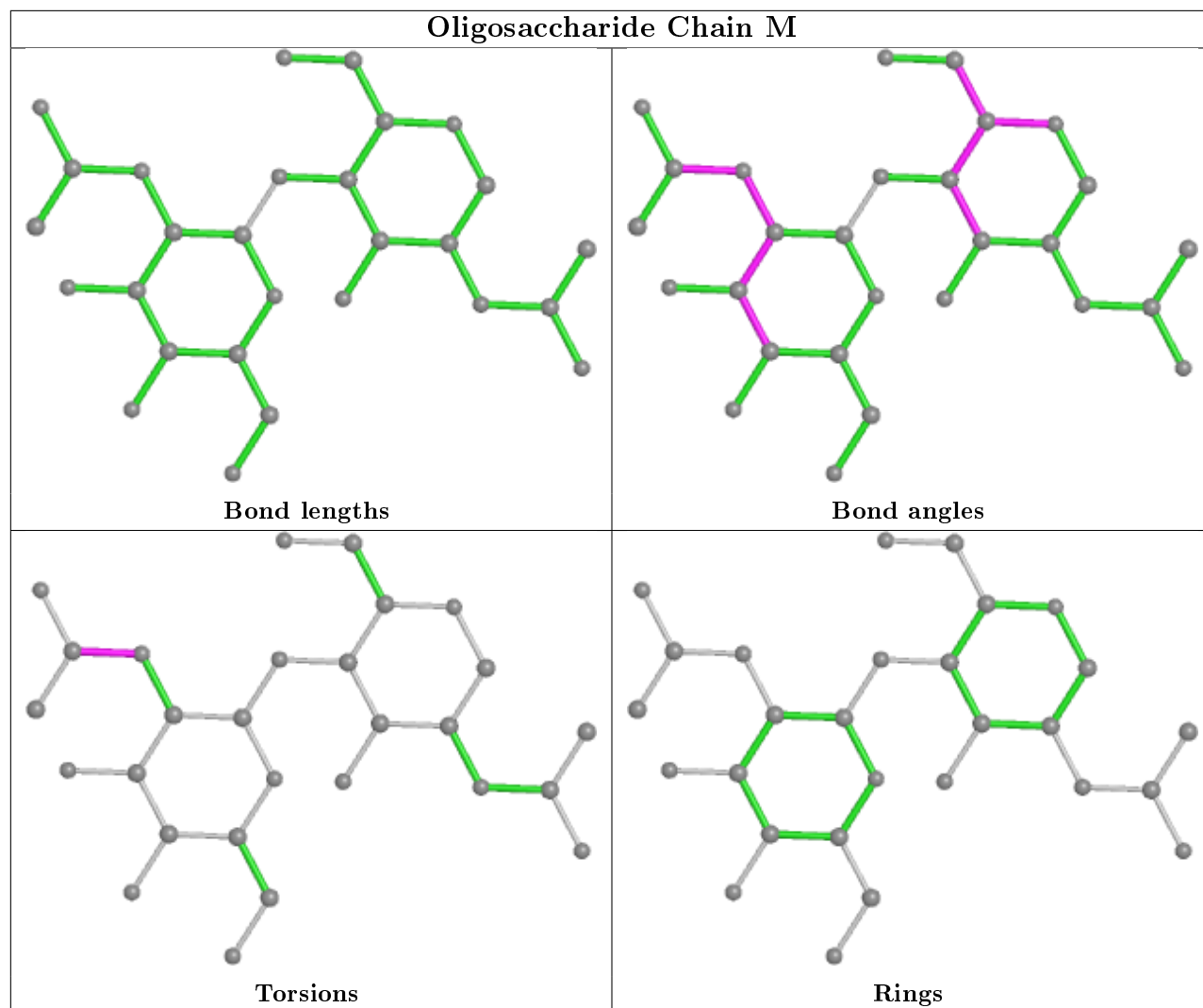


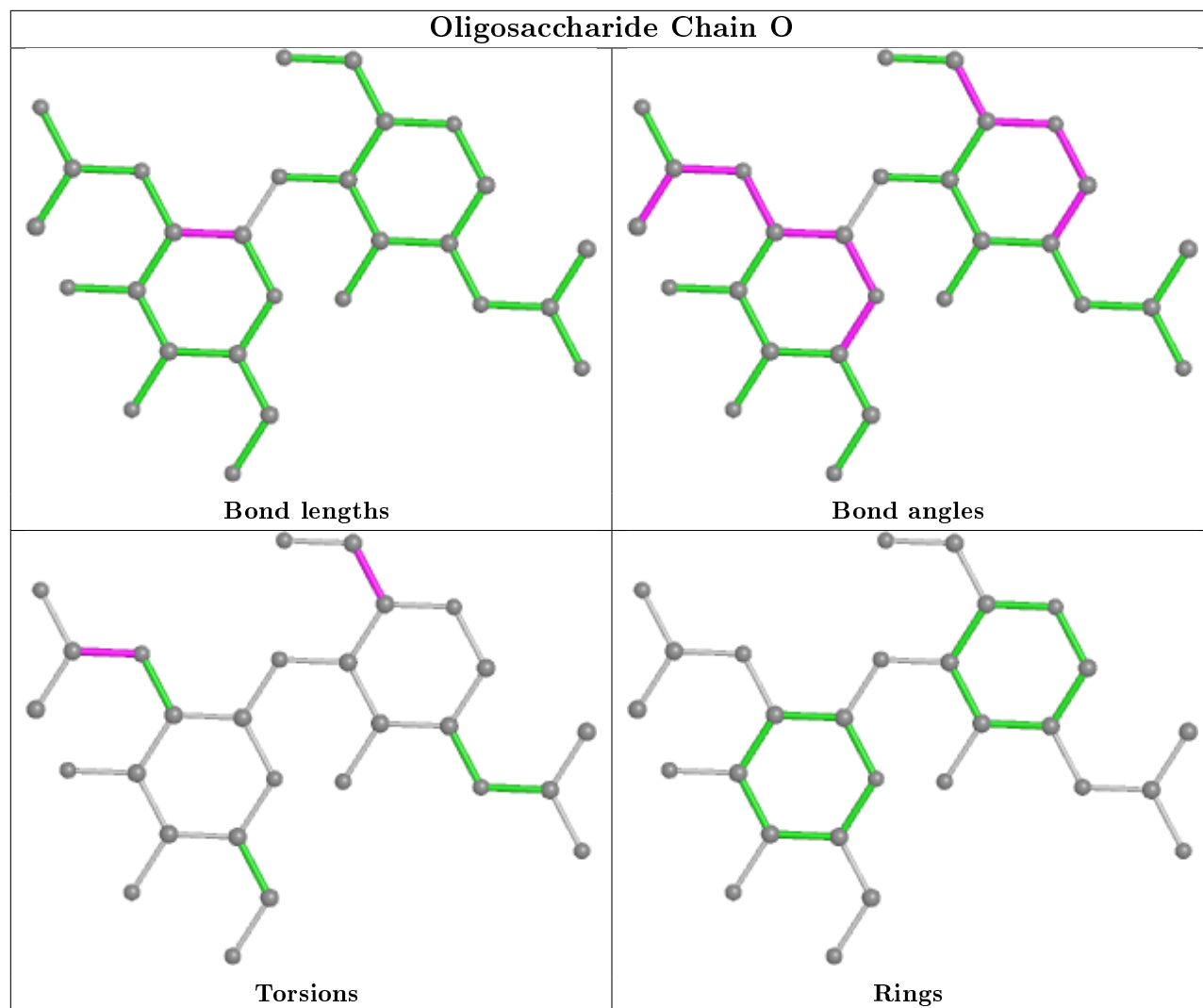


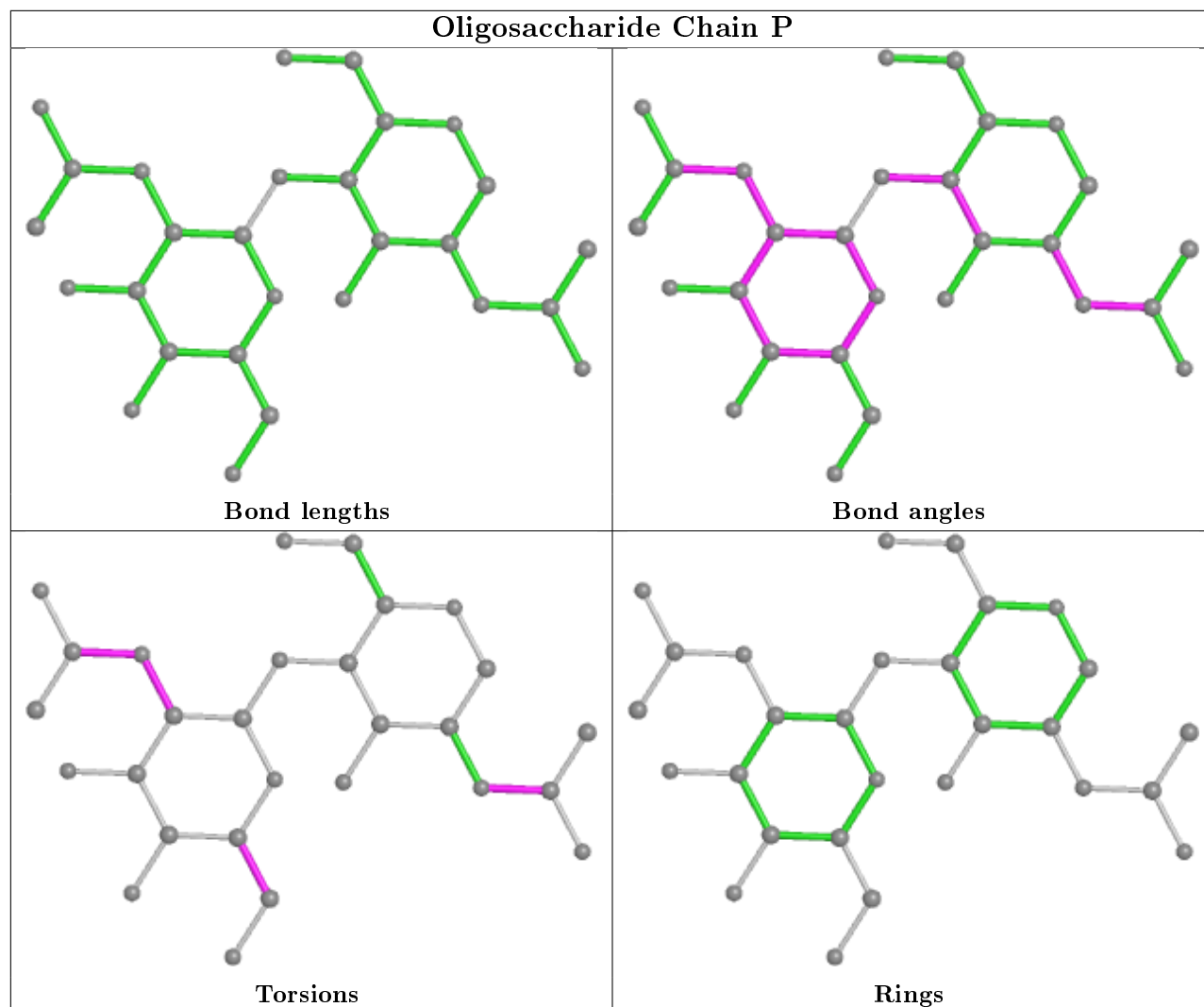


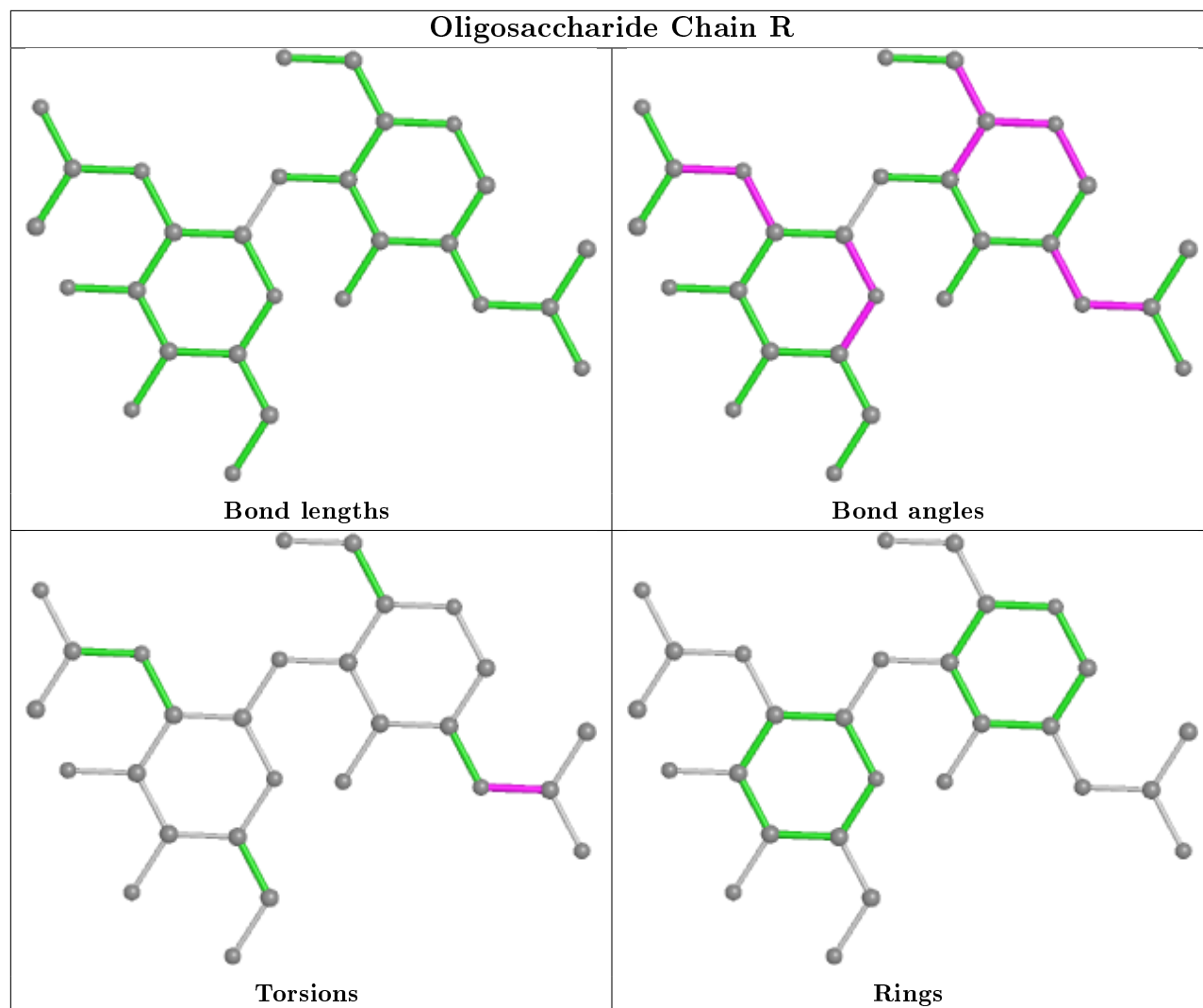




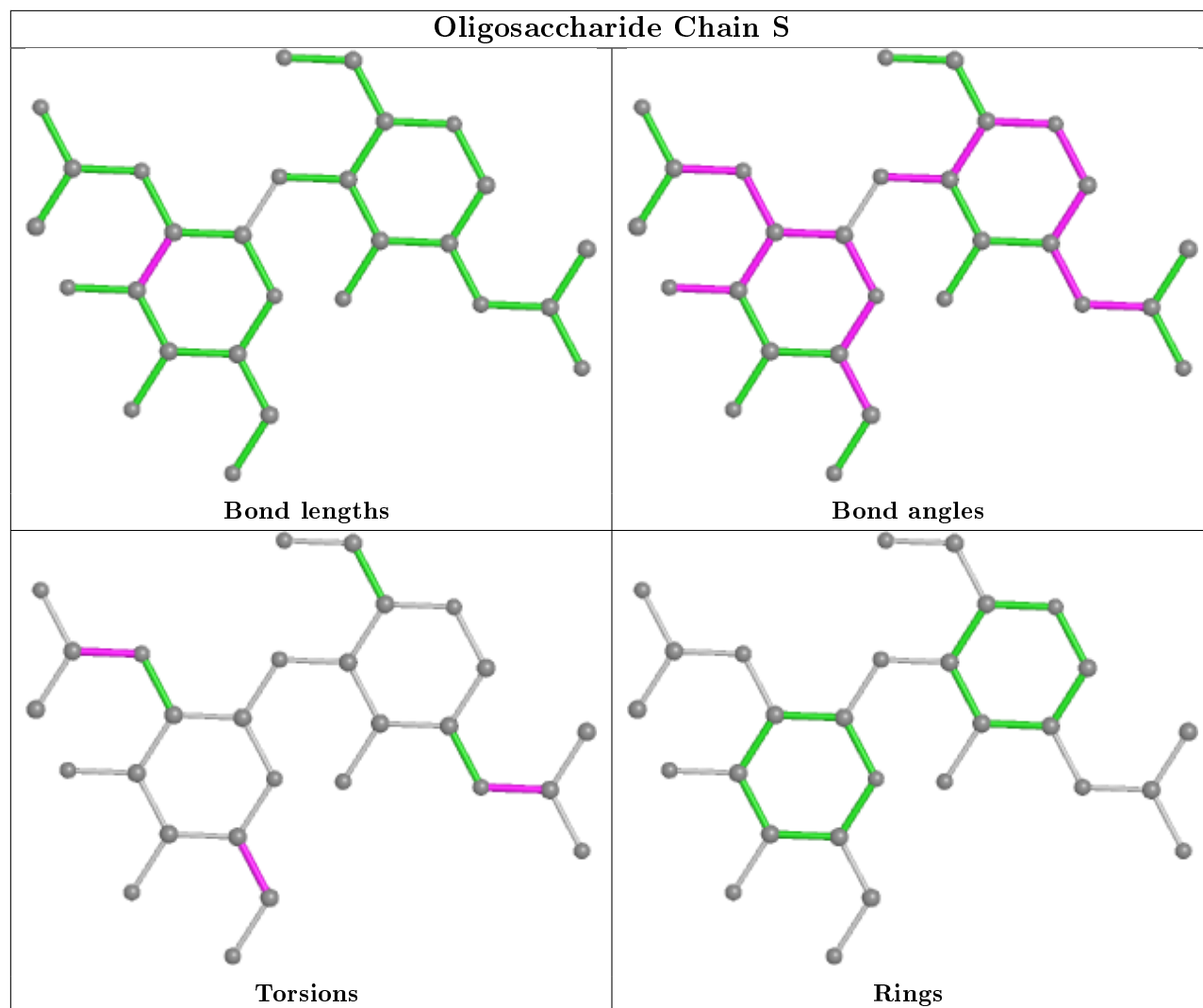


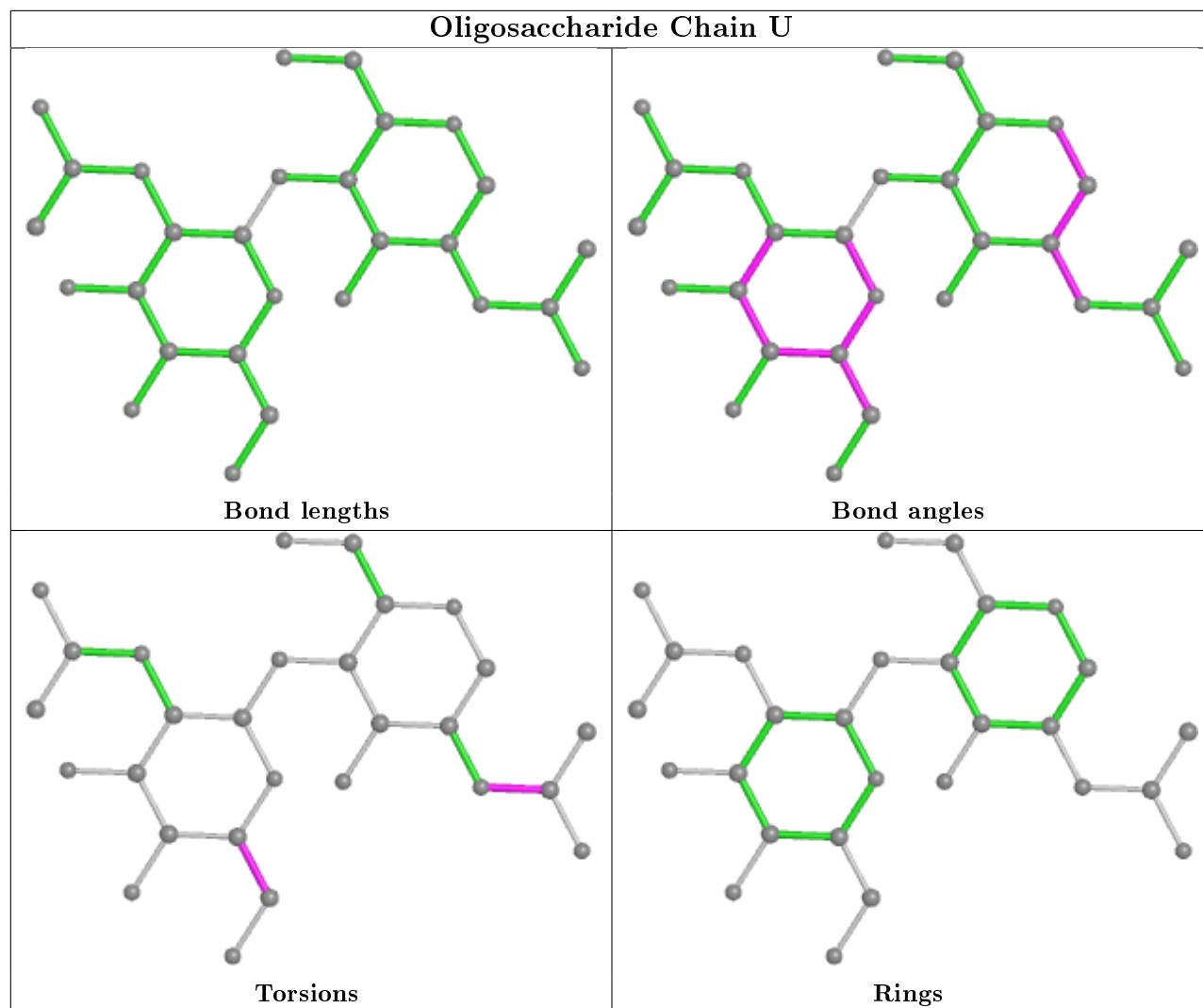


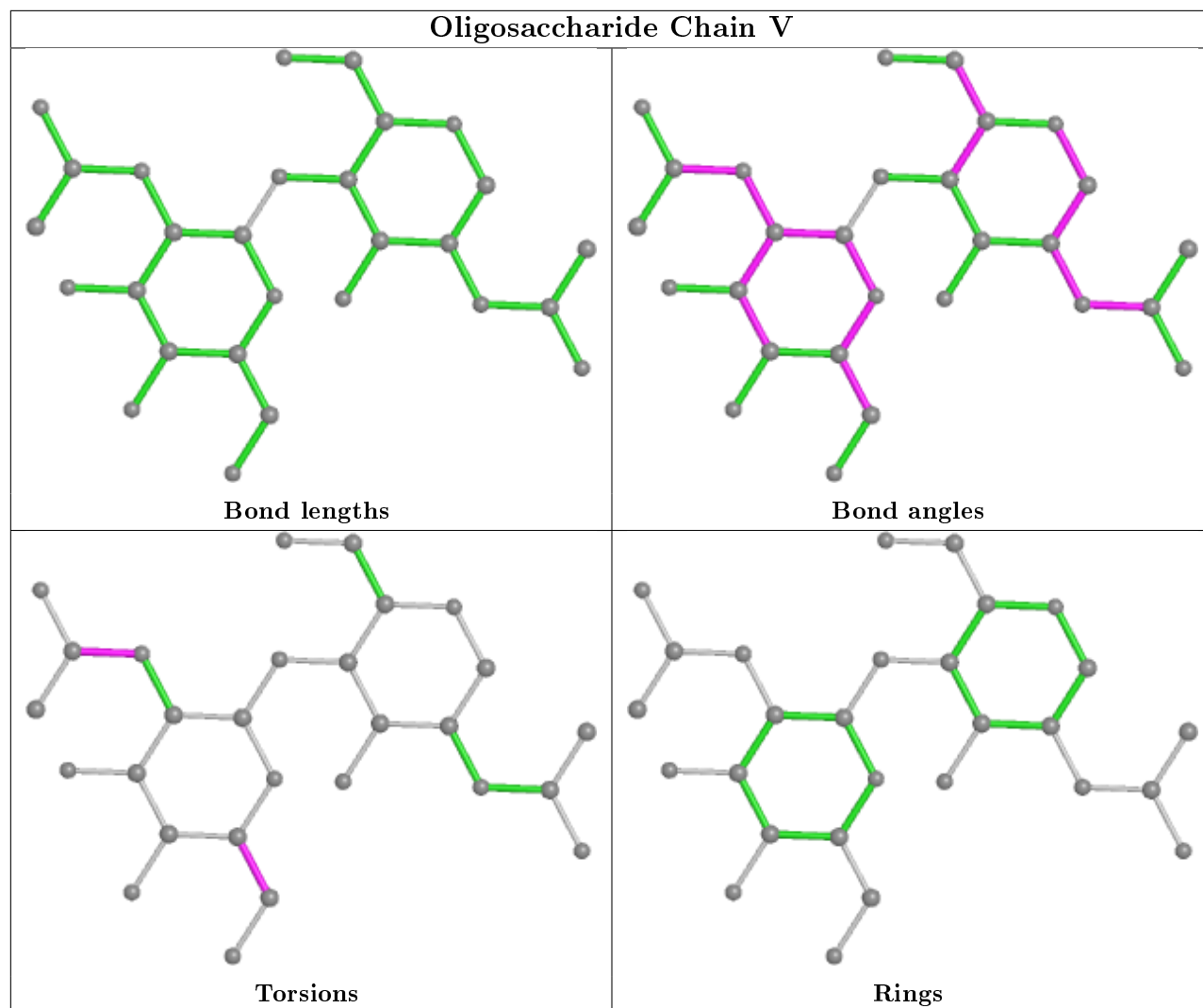


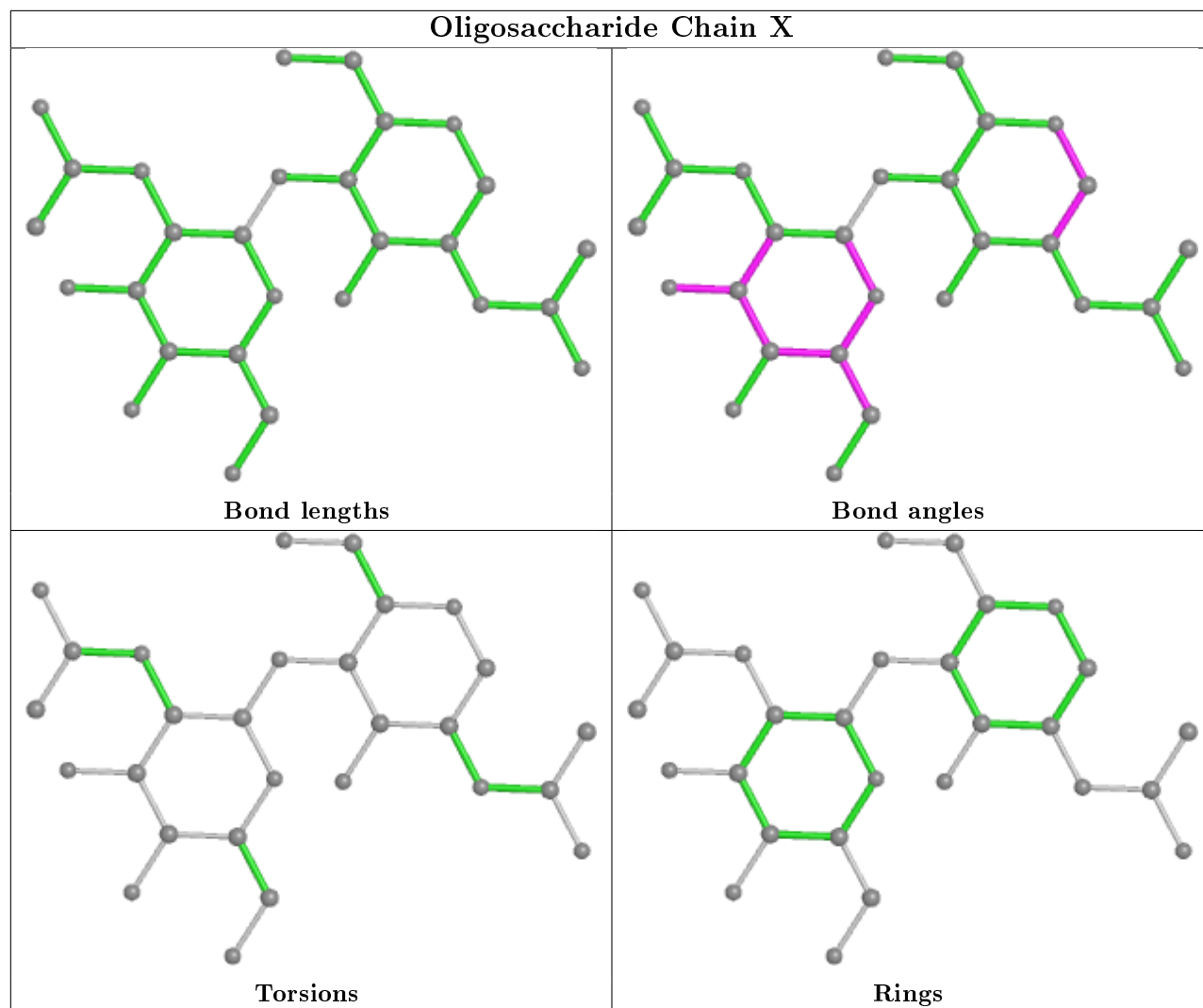




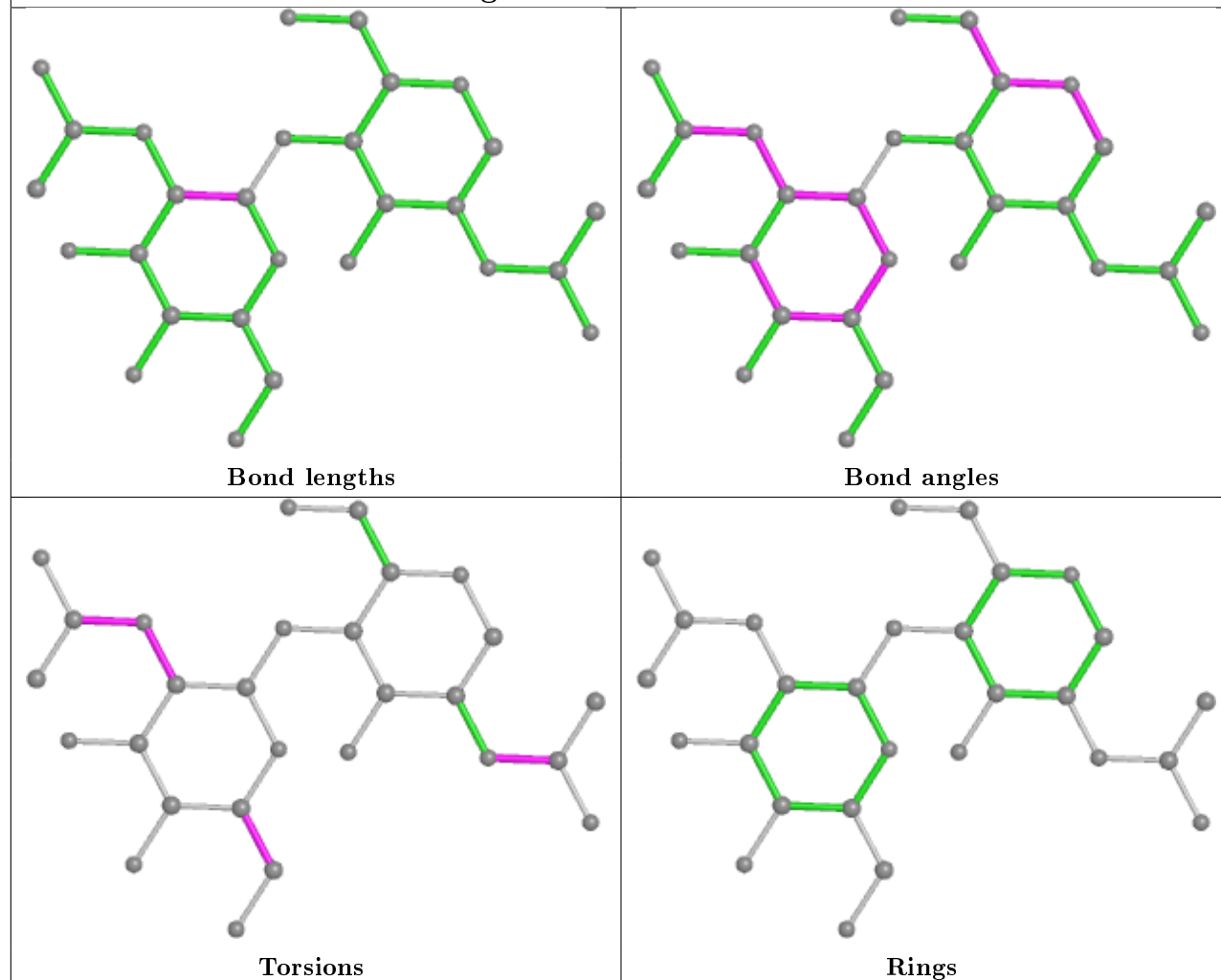




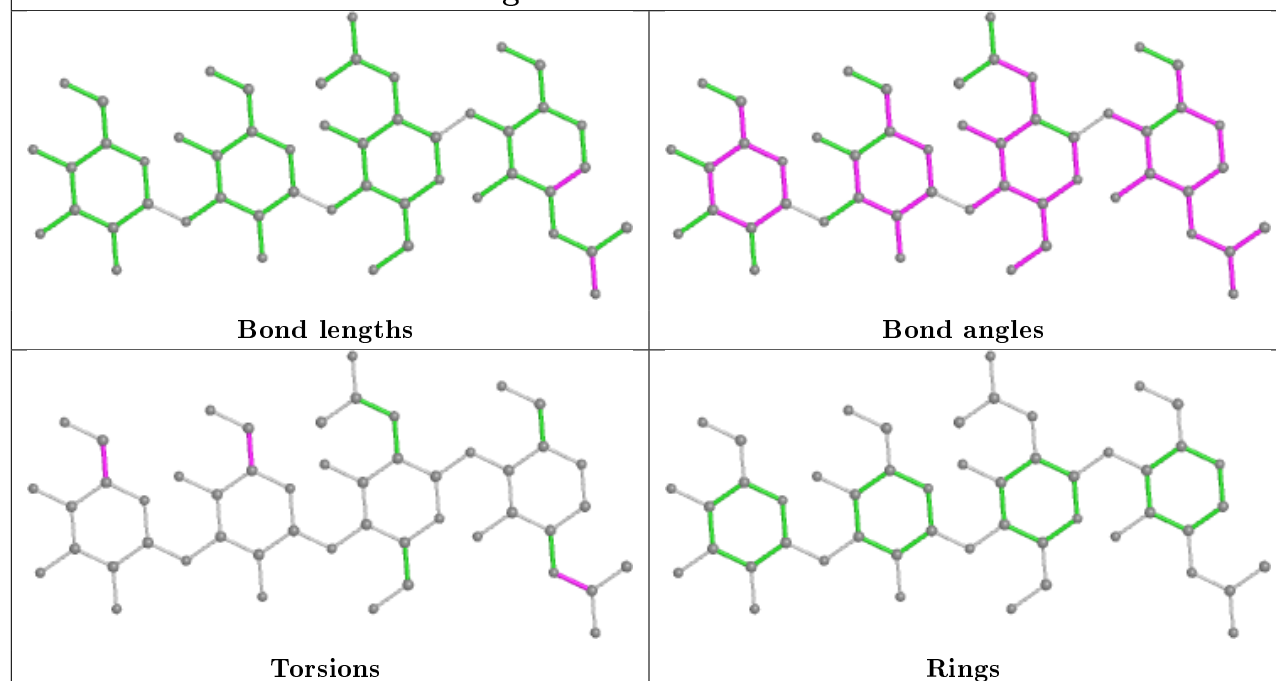




## Oligosaccharide Chain Y



## Oligosaccharide Chain K



## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	514	1	14,14,15	0.74	1 (7%)	17,19,21	1.68	2 (11%)
5	NAG	B	512	1	14,14,15	1.04	1 (7%)	17,19,21	2.28	4 (23%)
5	NAG	A	516	1	14,14,15	0.73	0	17,19,21	1.53	3 (17%)
5	NAG	H	514	1	14,14,15	0.86	1 (7%)	17,19,21	1.73	3 (17%)
5	NAG	F	514	1	14,14,15	0.91	1 (7%)	17,19,21	1.50	4 (23%)
5	NAG	G	514	1	14,14,15	0.91	1 (7%)	17,19,21	1.84	2 (11%)
5	NAG	B	513	1	14,14,15	0.71	0	17,19,21	1.66	3 (17%)
5	NAG	C	514	1	14,14,15	0.76	0	17,19,21	2.76	5 (29%)

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
5	NAG	E	514	1	-	2/6/23/26	0/1/1/1
5	NAG	B	512	1	-	3/6/23/26	0/1/1/1
5	NAG	A	516	1	-	1/6/23/26	0/1/1/1
5	NAG	H	514	1	-	6/6/23/26	0/1/1/1
5	NAG	F	514	1	-	3/6/23/26	0/1/1/1
5	NAG	G	514	1	-	4/6/23/26	0/1/1/1
5	NAG	B	513	1	-	4/6/23/26	0/1/1/1
5	NAG	C	514	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	512	NAG	C1-C2	2.69	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	514	NAG	C1-C2	2.46	1.56	1.52
5	F	514	NAG	C1-C2	2.32	1.55	1.52
5	H	514	NAG	C3-C2	2.17	1.57	1.52
5	E	514	NAG	C1-C2	2.12	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	512	NAG	C1-O5-C5	7.68	122.60	112.19
5	C	514	NAG	C2-N2-C7	6.84	132.65	122.90
5	C	514	NAG	C1-O5-C5	6.22	120.61	112.19
5	E	514	NAG	C1-O5-C5	5.45	119.58	112.19
5	A	516	NAG	C4-C3-C2	4.71	117.92	111.02
5	G	514	NAG	C4-C3-C2	4.46	117.55	111.02
5	H	514	NAG	O3-C3-C2	3.88	117.50	109.47
5	C	514	NAG	O7-C7-N2	3.86	129.05	121.95
5	H	514	NAG	O5-C5-C6	3.74	113.06	107.20
5	G	514	NAG	O5-C1-C2	-3.71	105.44	111.29
5	B	513	NAG	C4-C3-C2	3.53	116.19	111.02
5	B	513	NAG	C3-C4-C5	3.12	115.81	110.24
5	F	514	NAG	O3-C3-C4	-2.76	103.97	110.35
5	A	516	NAG	C3-C4-C5	2.75	115.15	110.24
5	C	514	NAG	O5-C1-C2	2.69	115.53	111.29
5	H	514	NAG	C2-N2-C7	-2.59	119.21	122.90
5	F	514	NAG	O3-C3-C2	2.53	114.70	109.47
5	B	512	NAG	C6-C5-C4	-2.51	107.13	113.00
5	F	514	NAG	C1-O5-C5	2.40	115.44	112.19
5	B	512	NAG	O5-C1-C2	-2.35	107.58	111.29
5	A	516	NAG	O4-C4-C3	-2.32	104.99	110.35
5	F	514	NAG	O4-C4-C5	2.27	114.94	109.30
5	B	513	NAG	C1-O5-C5	2.22	115.20	112.19
5	C	514	NAG	O7-C7-C8	-2.16	118.04	122.06
5	B	512	NAG	O5-C5-C6	2.10	110.49	107.20
5	E	514	NAG	O3-C3-C4	-2.00	105.72	110.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	514	NAG	C1-C2-N2-C7
5	G	514	NAG	C8-C7-N2-C2
5	G	514	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	B	513	NAG	C8-C7-N2-C2
5	B	513	NAG	O7-C7-N2-C2
5	C	514	NAG	O5-C5-C6-O6
5	C	514	NAG	C4-C5-C6-O6
5	H	514	NAG	C8-C7-N2-C2
5	G	514	NAG	C4-C5-C6-O6
5	H	514	NAG	O7-C7-N2-C2
5	F	514	NAG	C8-C7-N2-C2
5	F	514	NAG	O7-C7-N2-C2
5	E	514	NAG	O5-C5-C6-O6
5	B	513	NAG	O5-C5-C6-O6
5	G	514	NAG	O5-C5-C6-O6
5	B	513	NAG	C4-C5-C6-O6
5	B	512	NAG	C8-C7-N2-C2
5	E	514	NAG	C4-C5-C6-O6
5	A	516	NAG	O5-C5-C6-O6
5	B	512	NAG	O7-C7-N2-C2
5	F	514	NAG	O5-C5-C6-O6
5	H	514	NAG	O5-C5-C6-O6
5	H	514	NAG	C3-C2-N2-C7
5	B	512	NAG	C4-C5-C6-O6
5	H	514	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	514	NAG	1	0
5	B	513	NAG	1	0
5	C	514	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	438/473 (92%)	-0.43	2 (0%) 91 90	8, 18, 40, 69	0
1	B	438/473 (92%)	-0.47	2 (0%) 91 90	9, 18, 36, 68	0
1	C	435/473 (91%)	-0.44	3 (0%) 87 86	10, 20, 42, 71	0
1	D	435/473 (91%)	-0.38	1 (0%) 95 95	8, 20, 40, 63	0
1	E	438/473 (92%)	-0.42	5 (1%) 80 79	6, 19, 45, 79	0
1	F	438/473 (92%)	-0.29	6 (1%) 75 73	11, 23, 50, 78	0
1	G	435/473 (91%)	-0.37	1 (0%) 95 95	13, 24, 43, 74	0
1	H	435/473 (91%)	-0.51	1 (0%) 95 95	9, 16, 36, 57	0
All	All	3492/3784 (92%)	-0.41	21 (0%) 89 89	6, 20, 43, 79	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	295	TRP	5.1
1	B	34	ILE	4.2
1	E	295	TRP	3.5
1	F	340	PRO	3.5
1	F	44	TYR	3.3
1	E	32	GLY	3.3
1	G	64	ARG	3.0
1	E	44	TYR	2.8
1	B	32	GLY	2.6
1	A	33	SER	2.6
1	D	70	MET	2.5
1	E	343	GLY	2.5
1	H	42	ILE	2.5
1	C	35	ILE	2.3
1	E	48	VAL	2.3
1	F	49	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	60	LEU	2.1
1	A	51	ASP	2.1
1	F	57	LEU	2.1
1	C	68	LEU	2.1
1	F	42	ILE	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
2	MAN	L	9	11/12	0.77	0.23	72,75,77,78	0
2	MAN	Q	9	11/12	0.79	0.22	42,55,57,57	0
3	NAG	Y	2	14/15	0.80	0.25	45,57,59,63	0
3	NAG	J	2	14/15	0.81	0.22	54,69,77,80	0
3	NAG	O	2	14/15	0.82	0.27	58,62,66,66	0
3	NAG	V	2	14/15	0.83	0.20	45,52,58,59	0
3	NAG	P	2	14/15	0.84	0.21	58,64,71,72	0
2	MAN	I	9	11/12	0.84	0.16	37,39,43,44	0
3	NAG	R	2	14/15	0.84	0.23	40,58,61,64	0
3	NAG	b	2	14/15	0.84	0.31	75,81,83,86	0
3	NAG	J	1	14/15	0.85	0.23	53,57,65,71	0
3	NAG	a	2	14/15	0.86	0.30	45,55,64,71	0
3	NAG	b	1	14/15	0.86	0.20	41,52,61,73	0
2	MAN	c	9	11/12	0.87	0.15	33,37,39,39	0
3	NAG	e	2	14/15	0.87	0.21	29,34,35,35	0
3	NAG	d	2	14/15	0.87	0.24	37,45,47,50	0
2	MAN	N	9	11/12	0.88	0.13	36,50,53,58	0
2	MAN	N	4	11/12	0.88	0.17	25,29,32,32	0
3	NAG	X	2	14/15	0.89	0.26	47,63,71,71	0
4	MAN	K	4	11/12	0.89	0.16	41,44,52,52	0
3	NAG	M	1	14/15	0.89	0.20	40,46,50,57	0
3	NAG	O	1	14/15	0.90	0.17	36,45,51,60	0
2	MAN	W	8	11/12	0.90	0.19	42,44,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	X	1	14/15	0.91	0.15	33,44,53,55	0
3	NAG	M	2	14/15	0.91	0.33	49,57,61,61	0
2	MAN	Z	9	11/12	0.91	0.13	43,51,51,57	0
3	NAG	V	1	14/15	0.91	0.15	31,42,48,52	0
2	MAN	T	9	11/12	0.92	0.18	32,37,45,45	0
3	NAG	P	1	14/15	0.92	0.13	35,41,49,57	0
3	NAG	S	2	14/15	0.92	0.12	27,31,35,36	0
2	MAN	Q	8	11/12	0.92	0.15	36,41,44,45	0
3	NAG	U	2	14/15	0.92	0.20	43,48,52,54	0
2	MAN	c	8	11/12	0.93	0.11	29,37,38,41	0
4	BMA	K	3	11/12	0.93	0.13	37,42,46,47	0
2	MAN	N	8	11/12	0.93	0.16	39,43,45,45	0
3	NAG	R	1	14/15	0.93	0.21	42,46,52,61	0
2	MAN	Q	7	11/12	0.93	0.11	38,43,46,51	0
2	BMA	L	3	11/12	0.93	0.14	28,31,37,39	0
2	MAN	W	9	11/12	0.93	0.15	42,46,50,55	0
2	MAN	I	8	11/12	0.93	0.14	23,26,28,29	0
3	NAG	d	1	14/15	0.94	0.14	25,31,34,40	0
2	MAN	L	7	11/12	0.94	0.11	35,38,47,60	0
2	MAN	L	8	11/12	0.94	0.11	28,33,40,41	0
3	NAG	Y	1	14/15	0.94	0.12	37,41,45,51	0
2	MAN	Z	6	11/12	0.94	0.12	22,25,28,29	0
2	MAN	N	5	11/12	0.94	0.15	25,27,29,32	0
2	MAN	I	5	11/12	0.94	0.15	20,23,26,26	0
2	NAG	L	2	14/15	0.94	0.12	23,25,27,31	0
2	BMA	Q	3	11/12	0.94	0.16	26,29,36,40	0
3	NAG	a	1	14/15	0.94	0.20	44,52,56,57	0
2	MAN	T	8	11/12	0.94	0.12	30,34,37,37	0
2	MAN	T	6	11/12	0.95	0.12	23,26,28,32	0
2	BMA	W	3	11/12	0.95	0.10	26,28,31,31	0
4	NAG	K	2	14/15	0.95	0.12	29,32,40,45	0
3	NAG	U	1	14/15	0.95	0.14	23,29,34,36	0
2	MAN	W	7	11/12	0.95	0.13	30,33,39,45	0
2	MAN	I	6	11/12	0.95	0.11	13,16,17,17	0
2	MAN	Z	5	11/12	0.95	0.13	25,27,29,29	0
2	NAG	N	1	14/15	0.95	0.13	25,29,36,37	0
2	MAN	Z	8	11/12	0.95	0.10	37,41,44,45	0
2	MAN	I	7	11/12	0.95	0.11	25,30,36,39	0
2	NAG	Q	1	14/15	0.95	0.12	18,19,21,21	0
2	MAN	Z	4	11/12	0.95	0.13	29,31,34,36	0
2	BMA	T	3	11/12	0.95	0.11	21,22,24,25	0
2	MAN	T	7	11/12	0.96	0.11	24,27,31,33	0

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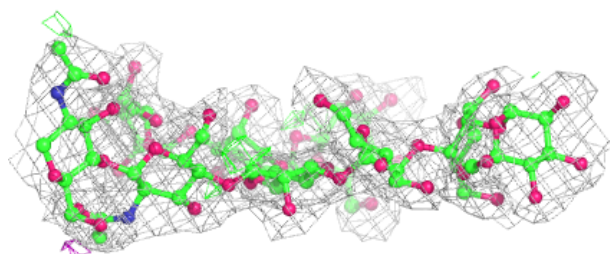
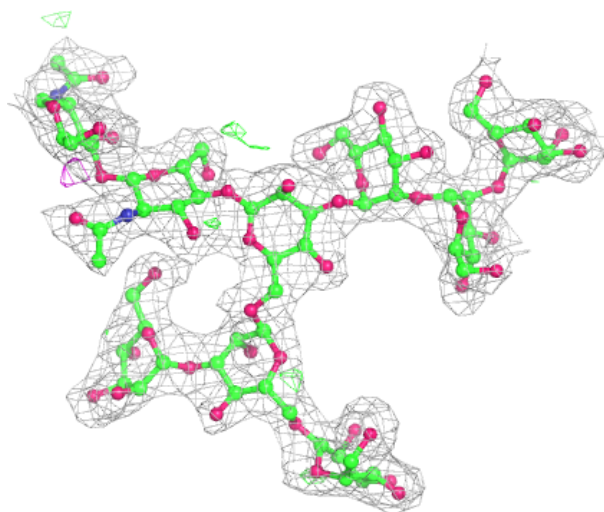
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	T	2	14/15	0.96	0.12	15,19,21,23	0
2	BMA	Z	3	11/12	0.96	0.09	23,25,30,34	0
2	NAG	I	1	14/15	0.96	0.11	14,17,18,18	0
2	MAN	N	6	11/12	0.96	0.09	19,23,24,24	0
4	NAG	K	1	14/15	0.96	0.11	15,20,22,28	0
2	MAN	W	4	11/12	0.96	0.13	25,26,28,29	0
2	MAN	c	7	11/12	0.96	0.12	29,34,38,39	0
2	MAN	Q	6	11/12	0.96	0.10	27,31,32,33	0
3	NAG	e	1	14/15	0.96	0.12	20,25,31,35	0
2	MAN	c	4	11/12	0.96	0.15	20,22,24,24	0
2	MAN	L	6	11/12	0.96	0.16	25,26,28,29	0
2	BMA	N	3	11/12	0.96	0.11	27,28,30,37	0
2	MAN	Z	7	11/12	0.96	0.10	37,40,49,50	0
2	NAG	Z	1	14/15	0.96	0.12	23,24,27,29	0
2	MAN	L	5	11/12	0.96	0.13	26,26,29,29	0
2	MAN	W	6	11/12	0.96	0.12	17,20,24,27	0
2	NAG	I	2	14/15	0.96	0.14	18,19,22,23	0
3	NAG	S	1	14/15	0.97	0.11	26,28,30,30	0
2	MAN	Q	5	11/12	0.97	0.13	28,32,35,36	0
2	NAG	W	2	14/15	0.97	0.10	20,26,30,32	0
2	NAG	T	1	14/15	0.97	0.14	17,18,19,19	0
2	MAN	T	5	11/12	0.97	0.10	27,28,31,36	0
2	MAN	Q	4	11/12	0.97	0.13	28,30,32,34	0
2	NAG	N	2	14/15	0.97	0.10	24,27,30,31	0
2	NAG	Z	2	14/15	0.97	0.13	19,21,24,24	0
2	MAN	I	4	11/12	0.97	0.10	19,20,20,23	0
2	NAG	Q	2	14/15	0.97	0.11	15,18,19,23	0
2	NAG	c	1	14/15	0.97	0.10	15,17,21,21	0
2	MAN	L	4	11/12	0.97	0.12	22,26,28,28	0
2	BMA	I	3	11/12	0.97	0.10	17,19,23,26	0
2	NAG	W	1	14/15	0.97	0.11	23,25,26,26	0
2	MAN	N	7	11/12	0.97	0.08	35,38,42,49	0
2	MAN	c	5	11/12	0.98	0.09	17,19,20,22	0
2	MAN	c	6	11/12	0.98	0.12	13,15,15,17	0
2	MAN	W	5	11/12	0.98	0.09	21,24,26,26	0
2	NAG	L	1	14/15	0.98	0.10	17,21,22,24	0
2	BMA	c	3	11/12	0.98	0.10	18,20,22,26	0
2	MAN	T	4	11/12	0.98	0.09	24,26,28,29	0
2	NAG	c	2	14/15	0.98	0.09	14,17,19,19	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.

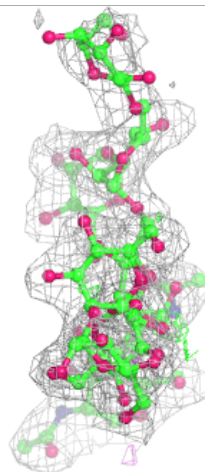
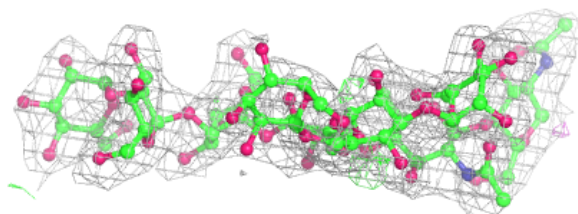
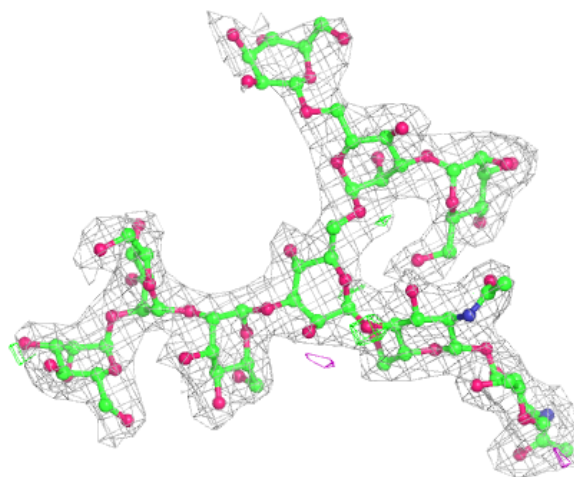
**Electron density around Chain I:**

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



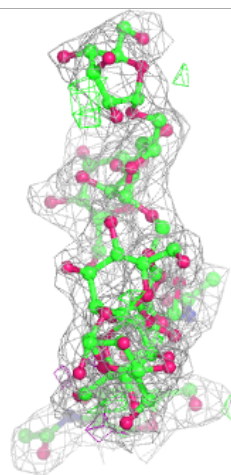
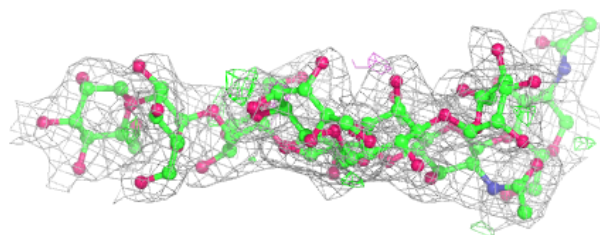
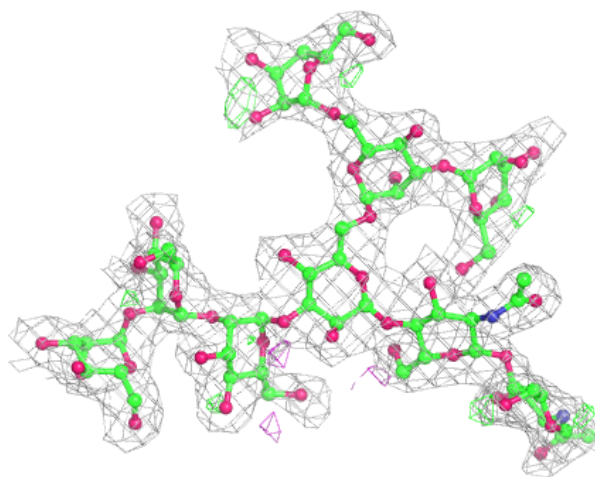
**Electron density around Chain L:**

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



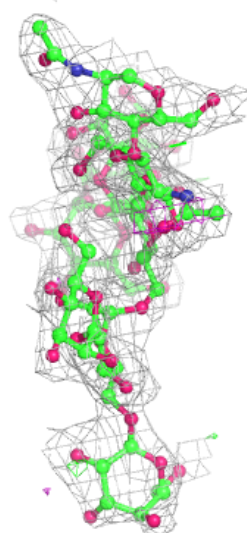
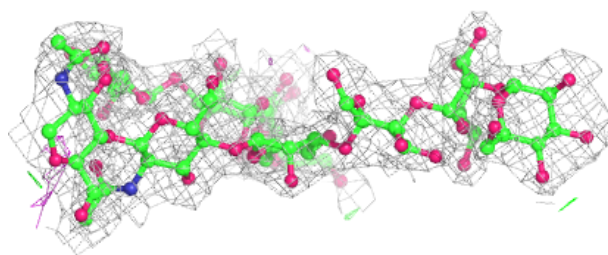
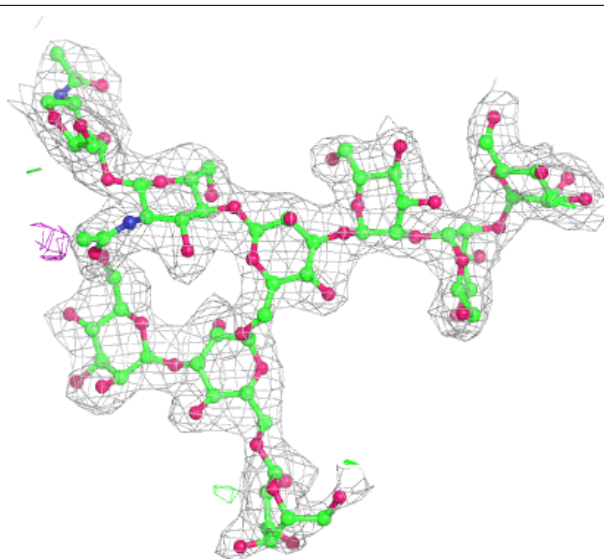
**Electron density around Chain N:**

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



**Electron density around Chain Q:**

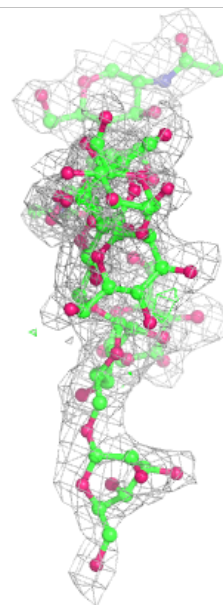
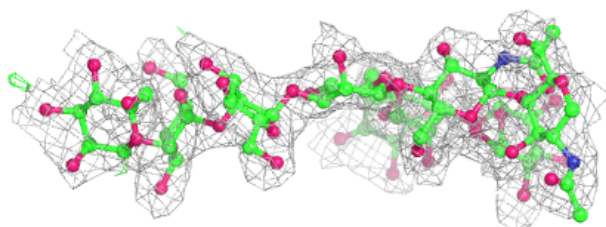
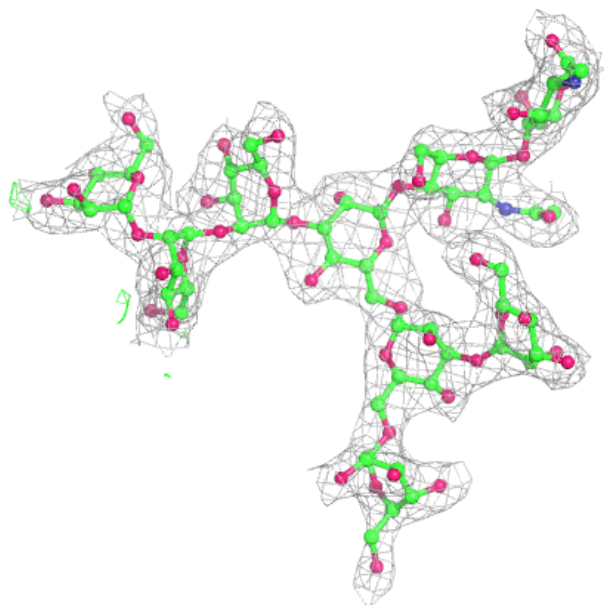
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





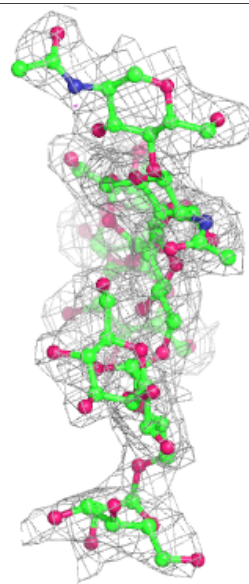
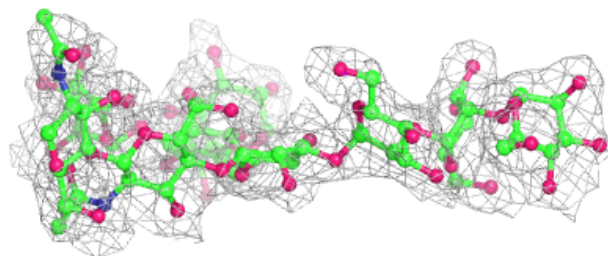
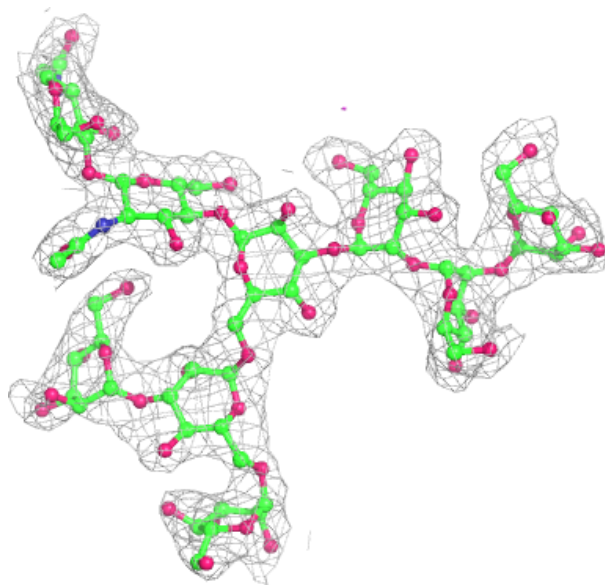
**Electron density around Chain T:**

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



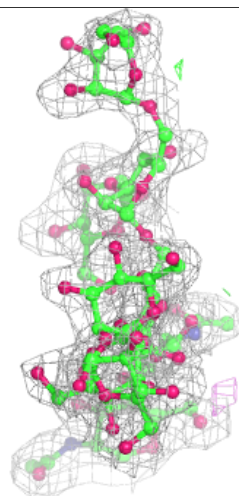
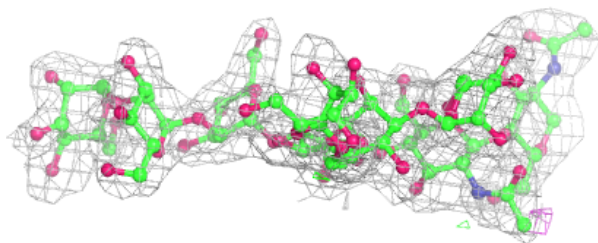
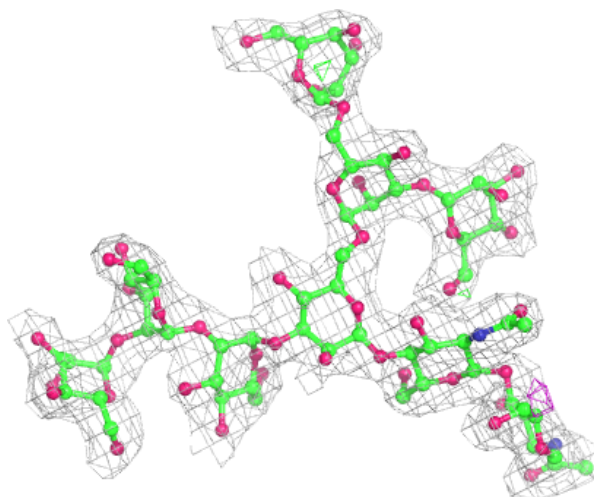
**Electron density around Chain W:**

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



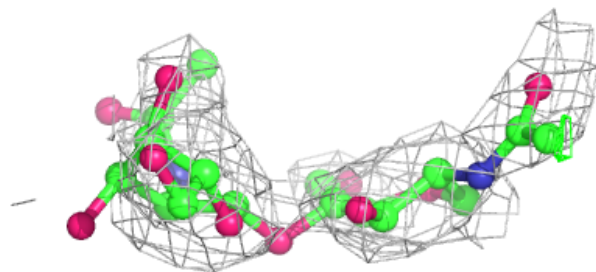
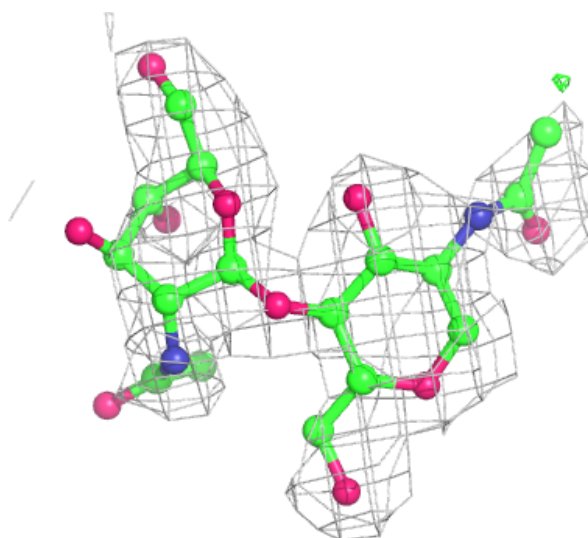
**Electron density around Chain Z:**

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



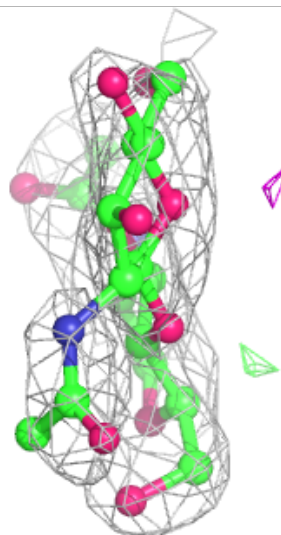
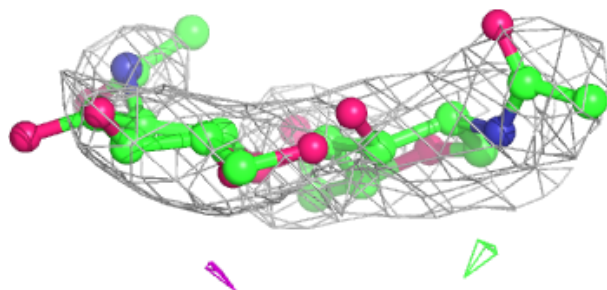
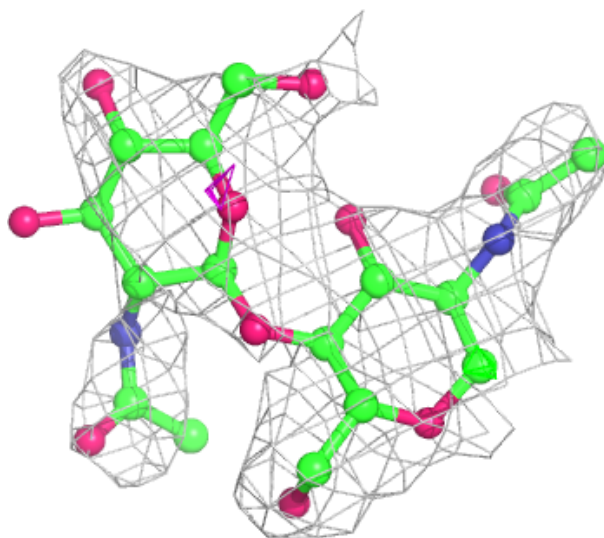
**Electron density around Chain J:**

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



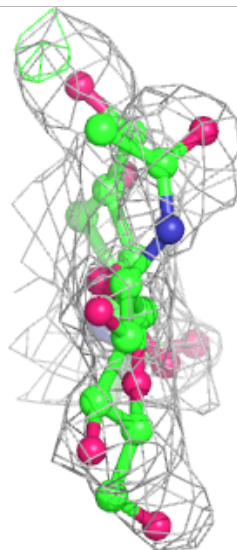
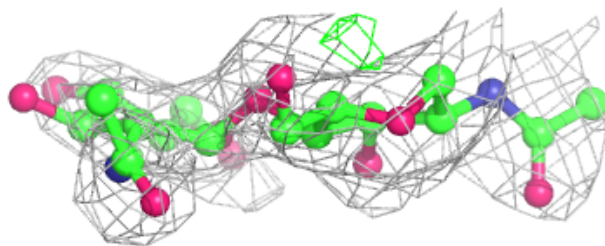
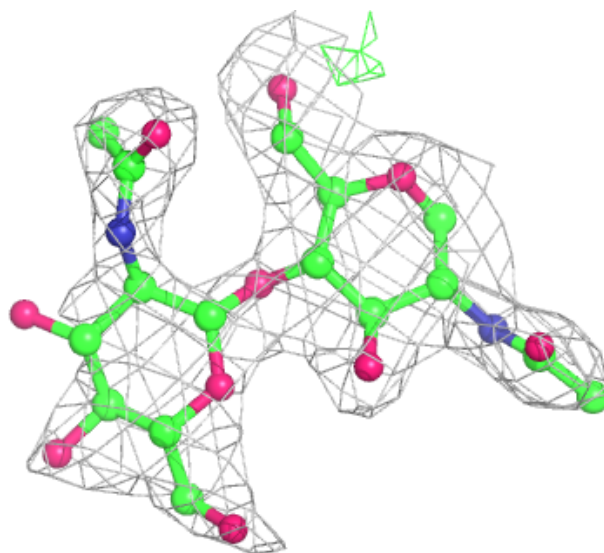
**Electron density around Chain M:**

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



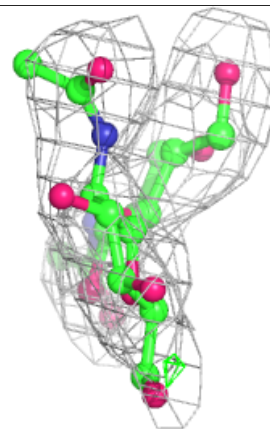
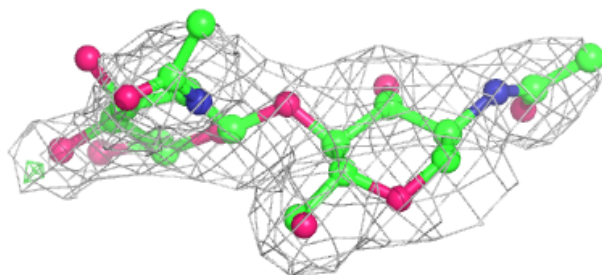
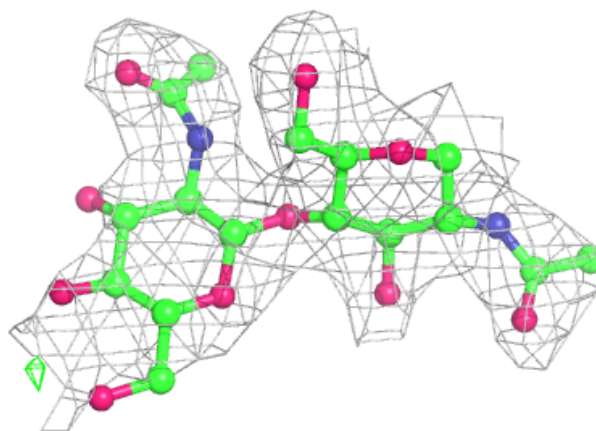
**Electron density around Chain O:**

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



**Electron density around Chain P:**

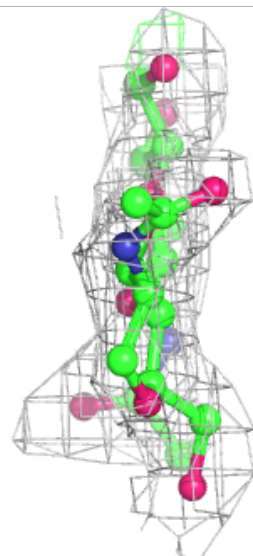
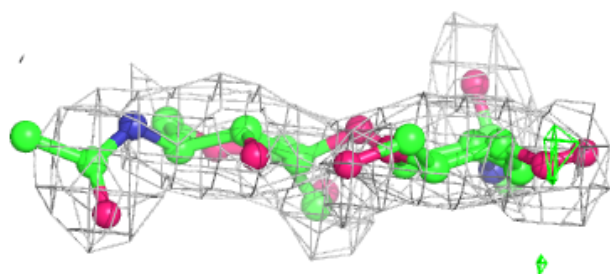
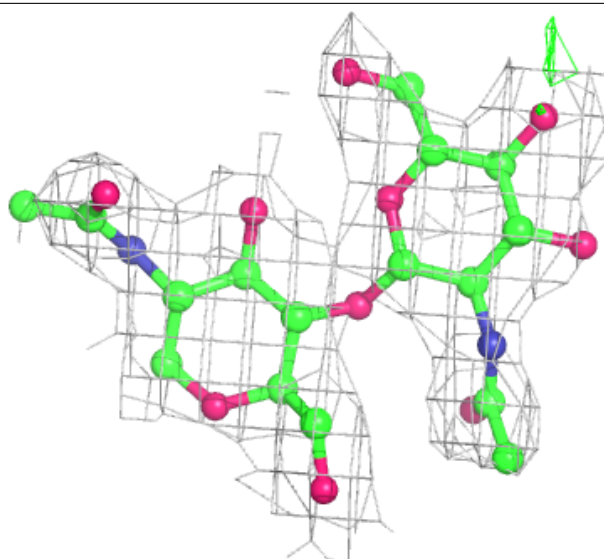
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain R:**

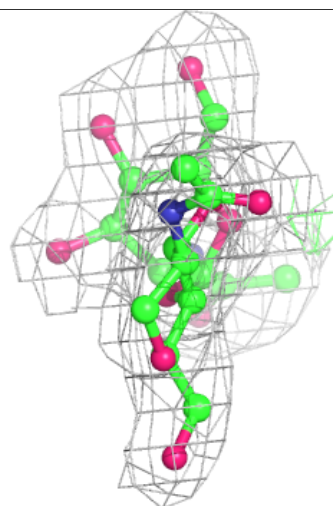
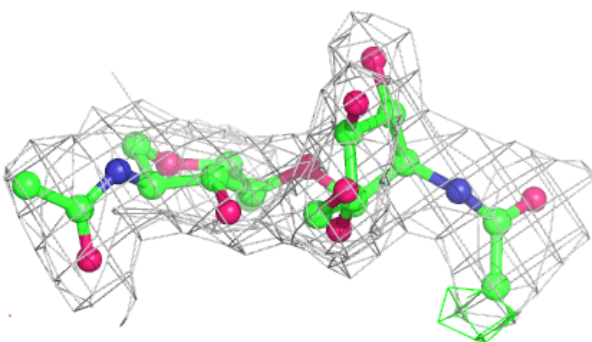
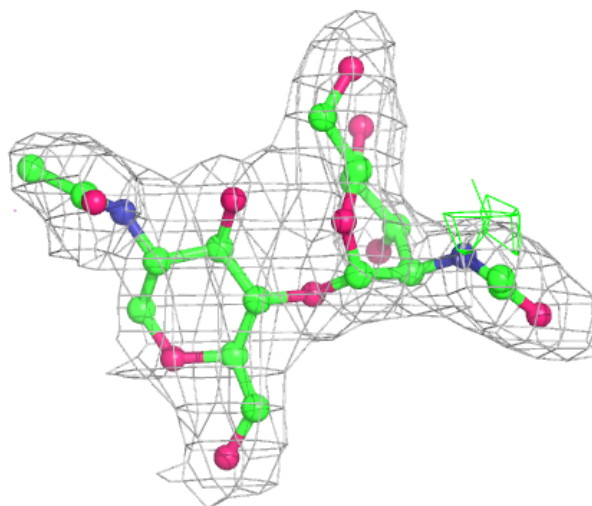
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
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and green (positive)





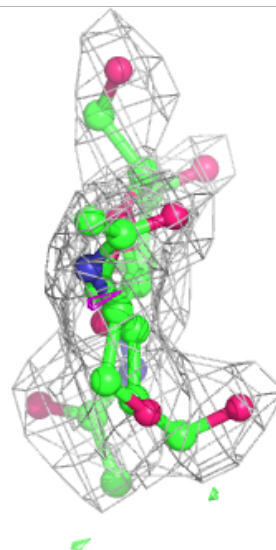
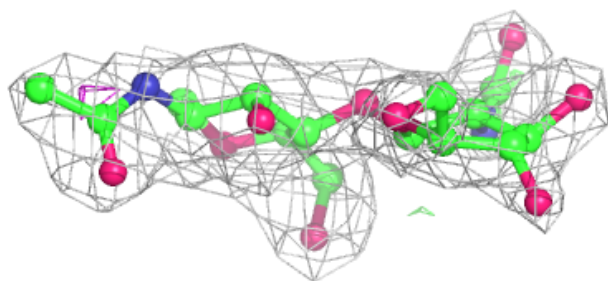
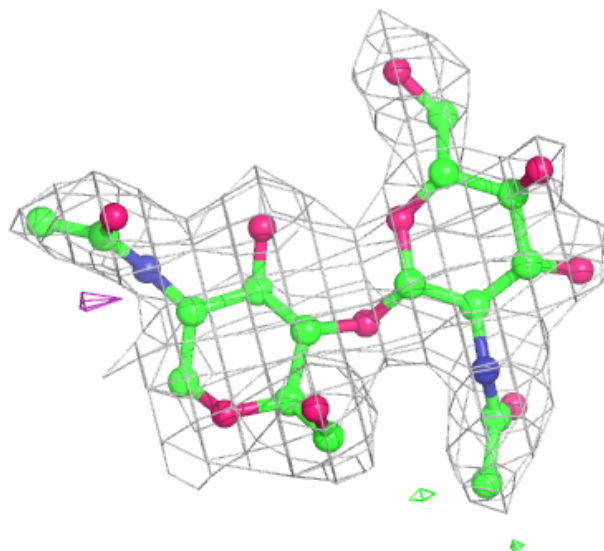
**Electron density around Chain S:**

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



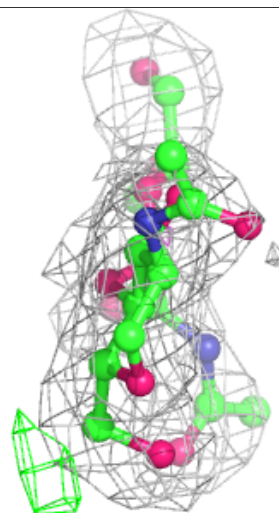
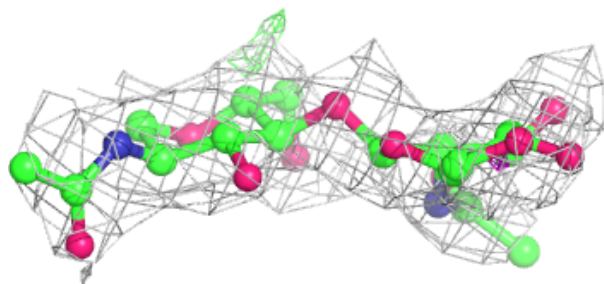
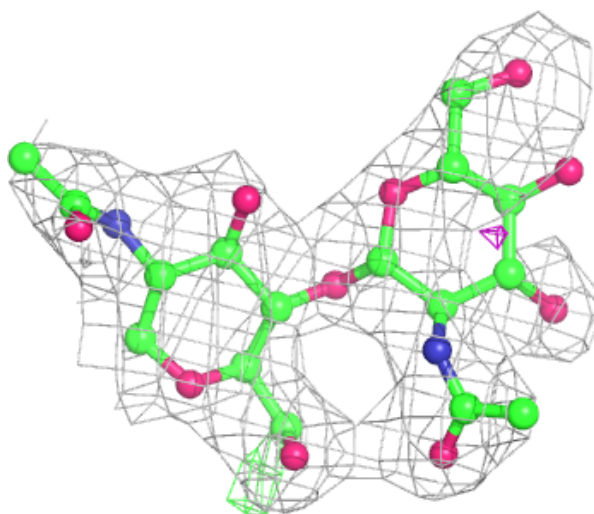
**Electron density around Chain U:**

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



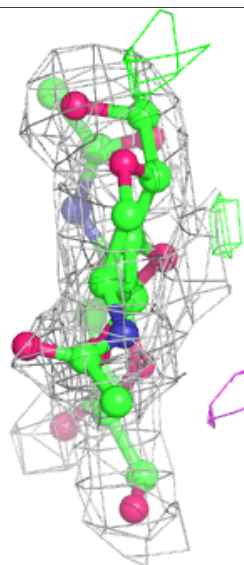
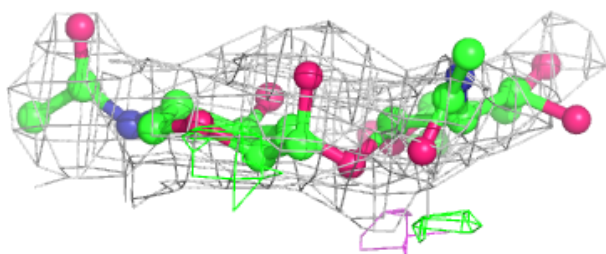
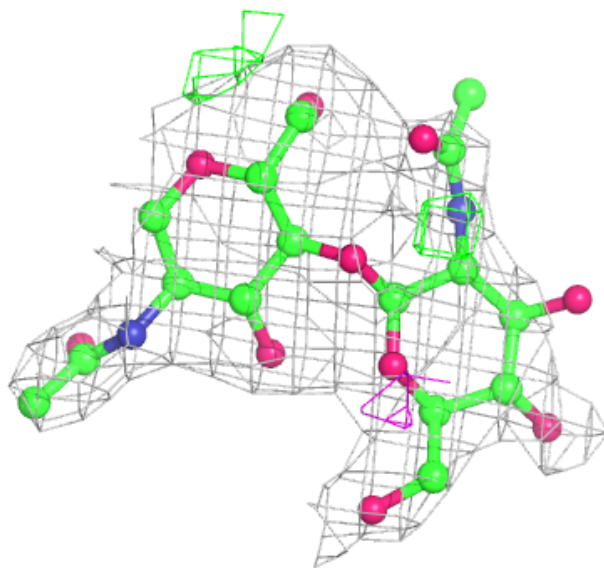
**Electron density around Chain V:**

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



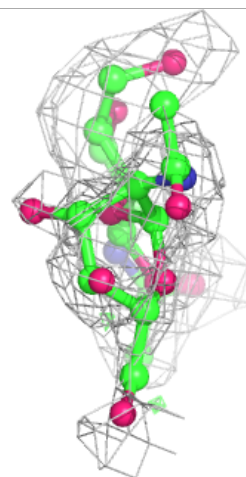
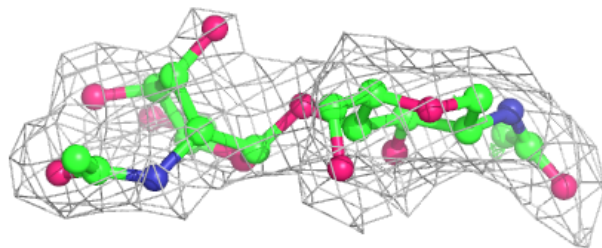
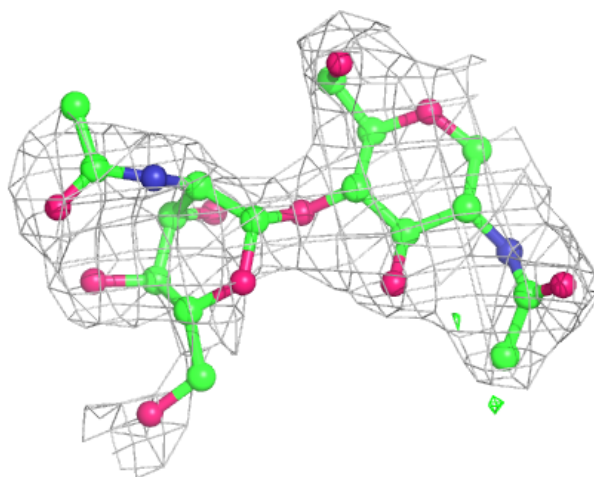
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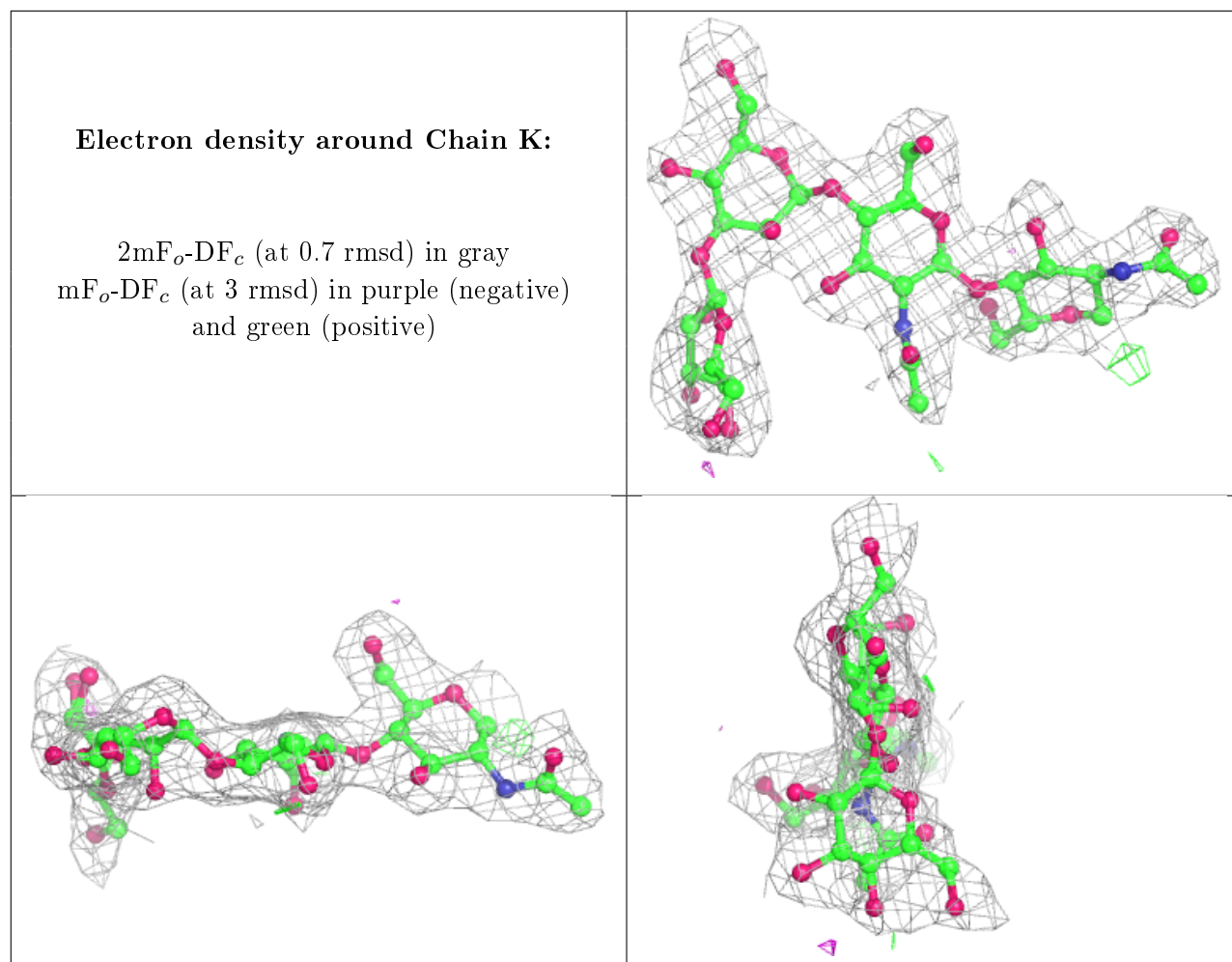
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
5	NAG	F	514	14/15	0.86	0.16	42,48,55,58	0
5	NAG	H	514	14/15	0.89	0.16	33,36,39,42	0
5	NAG	G	514	14/15	0.89	0.13	36,42,45,45	0
5	NAG	B	513	14/15	0.90	0.15	37,42,44,44	0
5	NAG	E	514	14/15	0.91	0.15	31,35,39,42	0
5	NAG	B	512	14/15	0.93	0.15	39,47,51,51	0
5	NAG	A	516	14/15	0.94	0.11	39,42,47,48	0
5	NAG	C	514	14/15	0.94	0.12	32,37,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.