



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2025 – 12:10 PM JST

PDB ID : 8XY9 / pdb\_00008xy9  
Title : Crystal structure of SARS-CoV-2 BF.7 RBD and human ACE2 complex  
Authors : Lan, J.; Wang, C.H.  
Deposited on : 2024-01-19  
Resolution : 3.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	<b>FAILED</b>
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

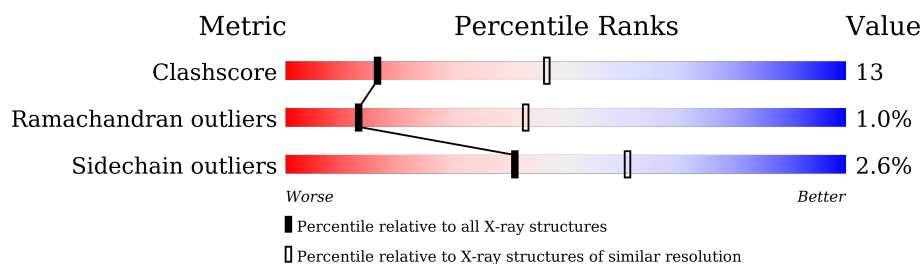
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.64 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))
Clashscore	180529	1046 (3.76-3.52)
Ramachandran outliers	177936	1031 (3.76-3.52)
Sidechain outliers	177891	1029 (3.76-3.52)



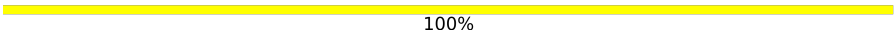

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	597	85% 15%
1	C	597	84% 16% .
2	B	194	50% 45% 5% .
2	D	194	41% 52% 6% .
3	E	3	33% 67%
3	H	3	100%
3	I	3	100%
3	J	3	33% 33% 33%

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Mol	Chain	Length	Quality of chain
4	F	2	 50% 50%
4	G	2	 50% 50%
4	K	2	 100%
4	L	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	F	1	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13154 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	1	0
			4877	3120	808	920	29			
1	C	597	Total	C	N	O	S	0	1	0
			4877	3120	808	920	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	0
			1545	995	259	283	8			
2	D	194	Total	C	N	O	S	0	0	0
			1545	995	259	283	8			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	505	HIS	TYR	variant	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	346	THR	ARG	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	VAL	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2

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



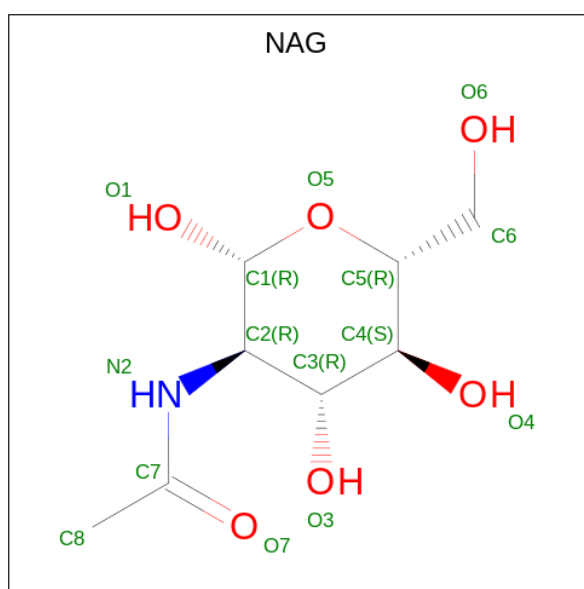
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



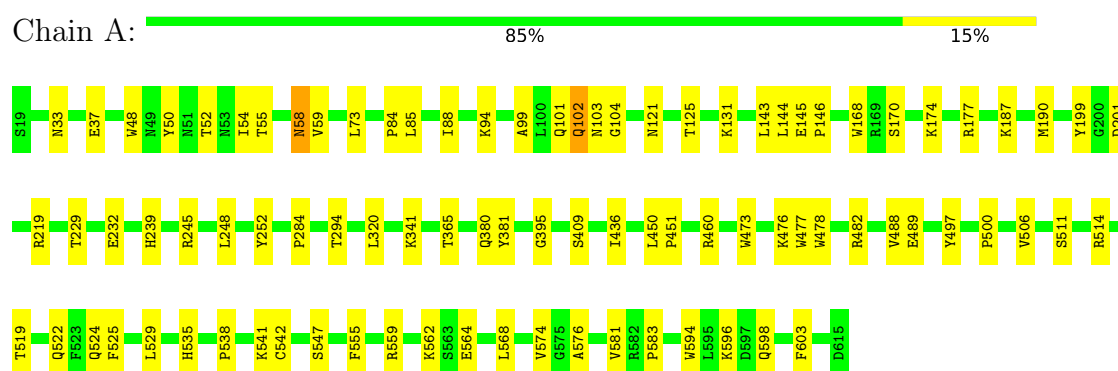
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	14	0
			14	8	1	5		

### 3 Residue-property plots

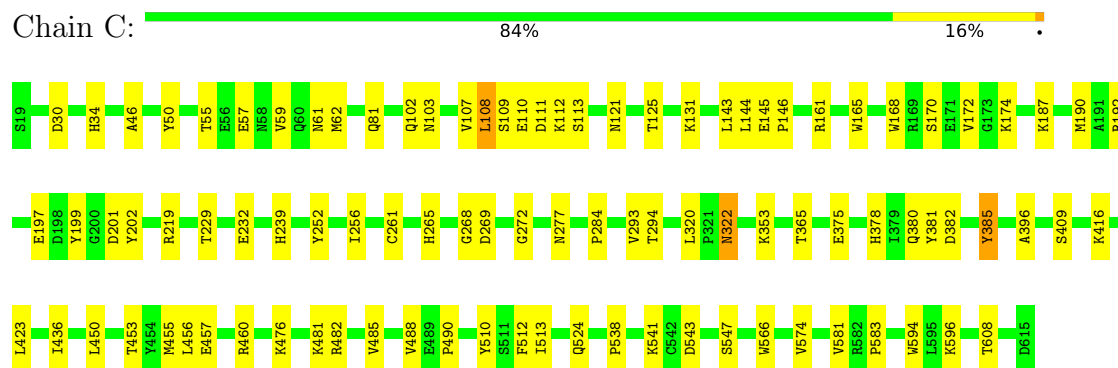
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

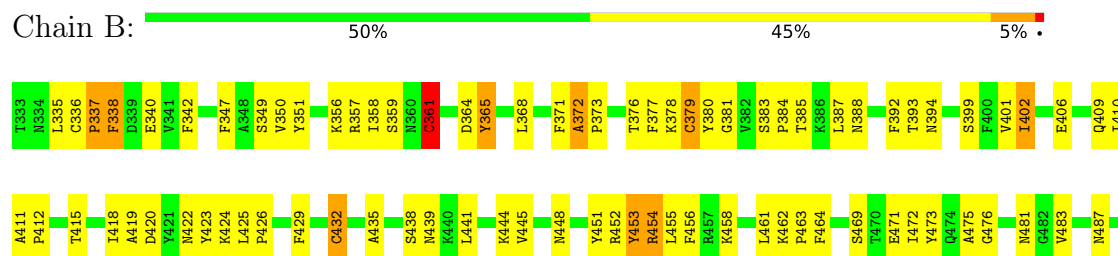
#### • Molecule 1: Processed angiotensin-converting enzyme 2

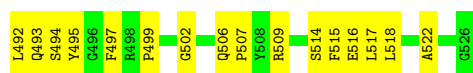


#### • Molecule 1: Processed angiotensin-converting enzyme 2



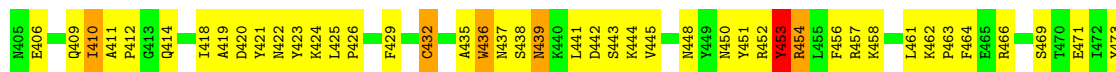
#### • Molecule 2: Spike protein S1





- Molecule 2: Spike protein S1

Chain D: 41% 52% 6%



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

Chain E: 33% 67%



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

Chain H: 100%



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

Chain I: 100%



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

Chain J: 33% 33% 33%



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



Chain F:  50% 50%

MAG1  
MAG2

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

Chain G:  50% 50%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain L:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.47Å 152.68Å 116.69Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	40.30 – 3.64	Depositor
% Data completeness (in resolution range)	98.8 (40.30-3.64)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.66Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, $R_{free}$	0.215 , 0.261	Depositor
Wilson B-factor (Å <sup>2</sup> )	116.4	Xtriage
Anisotropy	0.635	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.28	0/5018	0.49	0/6818
1	C	0.29	0/5018	0.52	1/6818 (0.0%)
2	B	0.35	0/1591	0.66	1/2167 (0.0%)
2	D	0.58	3/1591 (0.2%)	0.76	1/2167 (0.0%)
All	All	0.34	3/13218 (0.0%)	0.56	3/17970 (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	1
2	D	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	374	PHE	CD1-CE1	-8.47	1.22	1.39
2	D	374	PHE	CB-CG	-7.35	1.38	1.51
2	D	436	TRP	CZ3-CH2	-6.86	1.29	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	509	ARG	CG-CD-NE	10.13	133.08	111.80
2	B	361	CYS	CA-CB-SG	8.23	128.82	114.00
1	C	108	LEU	CB-CG-CD1	-7.53	98.21	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ASN	Peptide
2	D	373	PRO	Peptide
2	D	453	TYR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4877	0	4645	54	0
1	C	4877	0	4645	67	0
2	B	1545	0	1466	79	0
2	D	1545	0	1466	129	0
3	E	39	0	34	0	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
3	J	39	0	34	1	0
4	F	28	0	24	7	0
4	G	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
5	A	28	0	26	4	0
5	C	14	0	13	0	0
All	All	13154	0	12496	327	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:VAL:HG11	2:B:451:TYR:HD2	1.31	0.96
1:C:103:ASN:HB2	4:F:1:NAG:H82	1.46	0.95
2:D:445:VAL:HG22	2:D:499:PRO:HG3	1.51	0.92
1:C:103:ASN:HD22	4:F:1:NAG:HN2	1.16	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:CYS:O	2:B:338:PHE:N	2.05	0.90
2:D:380:TYR:CD2	2:D:412:PRO:HD3	2.06	0.90
2:D:380:TYR:HD2	2:D:412:PRO:HD3	1.38	0.87
2:B:454:ARG:NH2	2:B:469:SER:O	2.09	0.85
2:B:453:TYR:CD2	2:B:495:TYR:HE1	1.97	0.83
2:B:401:VAL:HG11	2:B:451:TYR:CD2	2.14	0.82
2:D:422:ASN:HD21	2:D:454:ARG:H	1.25	0.82
2:B:393:THR:HA	2:B:522:ALA:HA	1.61	0.81
2:D:337:PRO:HG2	2:D:358:ILE:HD12	1.61	0.81
2:D:350:VAL:HG11	2:D:418:ILE:HD11	1.62	0.80
2:D:422:ASN:HD21	2:D:454:ARG:N	1.80	0.80
2:B:393:THR:HG21	2:B:518:LEU:HD23	1.62	0.80
2:D:393:THR:HA	2:D:522:ALA:HA	1.65	0.79
1:C:192:ARG:NH1	1:C:197:GLU:O	2.17	0.78
2:D:453:TYR:CD2	2:D:495:TYR:HE1	2.02	0.78
2:B:445:VAL:HG22	2:B:499:PRO:HG3	1.67	0.77
1:C:320:LEU:HD13	1:C:380:GLN:HG2	1.66	0.77
2:D:354:ASN:OD1	2:D:399:SER:OG	2.03	0.75
2:D:442:ASP:O	2:D:448:ASN:ND2	2.16	0.75
2:D:401:VAL:HG11	2:D:451:TYR:CD2	2.22	0.74
2:D:454:ARG:NH2	2:D:469:SER:O	2.20	0.74
1:C:81:GLN:HG2	4:F:1:NAG:C7	2.18	0.74
2:D:374:PHE:CE1	2:D:377:PHE:HB2	2.24	0.73
1:C:57:GLU:O	1:C:61:ASN:ND2	2.22	0.72
2:B:380:TYR:CD2	2:B:412:PRO:HD3	2.25	0.72
2:D:347:PHE:HD1	2:D:509:ARG:NE	1.88	0.72
2:D:436:TRP:HH2	2:D:509:ARG:CG	2.03	0.71
2:B:495:TYR:HD2	2:B:497:PHE:CZ	2.08	0.71
2:D:426:PRO:HB3	2:D:463:PRO:HB3	1.73	0.71
2:D:495:TYR:HD2	2:D:497:PHE:CZ	2.09	0.70
1:C:109:SER:OG	1:C:112:LYS:HG3	1.93	0.69
2:D:374:PHE:CE1	2:D:376:THR:N	2.61	0.69
1:A:229:THR:HB	1:A:581:VAL:HG13	1.75	0.68
2:D:453:TYR:CE1	2:D:493:GLN:HB3	2.29	0.68
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.74	0.68
2:B:444:LYS:HG2	2:B:448:ASN:HB2	1.73	0.68
2:D:374:PHE:CZ	2:D:377:PHE:N	2.62	0.68
2:D:436:TRP:CZ2	2:D:509:ARG:HB2	2.28	0.67
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.30	0.67
2:B:422:ASN:HA	2:B:461:LEU:HD12	1.77	0.67
2:B:438:SER:HB3	2:B:509:ARG:CG	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:LEU:HD21	2:B:364:ASP:HB2	1.75	0.67
2:D:436:TRP:HE3	2:D:437:ASN:N	1.93	0.67
2:B:337:PRO:HG2	2:B:358:ILE:HD12	1.77	0.66
2:B:349:SER:HB2	2:B:452:ARG:H	1.59	0.66
2:B:378:LYS:HB3	2:B:380:TYR:HE1	1.60	0.66
2:D:374:PHE:CD1	2:D:375:PHE:N	2.64	0.66
1:C:455:MET:HE2	1:C:485:VAL:HG21	1.78	0.66
2:D:436:TRP:CH2	2:D:509:ARG:HB2	2.31	0.65
2:D:442:ASP:OD2	2:D:509:ARG:HD2	1.96	0.65
2:B:419:ALA:O	2:B:424:LYS:HD3	1.97	0.65
2:D:371:PHE:C	2:D:373:PRO:HD3	2.18	0.64
2:D:347:PHE:CD1	2:D:509:ARG:NE	2.66	0.64
1:C:108:LEU:HD11	1:C:113:SER:CA	2.27	0.64
2:B:376:THR:HB	2:B:435:ALA:HB3	1.80	0.64
2:B:438:SER:HB3	2:B:509:ARG:HG3	1.80	0.63
2:B:456:PHE:HB3	2:B:473:TYR:CD2	2.33	0.63
2:D:383:SER:O	2:D:387:LEU:HD23	1.99	0.63
2:D:436:TRP:HH2	2:D:509:ARG:HD3	1.63	0.62
1:C:524:GLN:HG2	1:C:583:PRO:HG2	1.81	0.62
1:A:245:ARG:NH2	1:A:603:PHE:O	2.32	0.62
2:B:359:SER:OG	2:B:394:ASN:OD1	2.13	0.61
2:D:350:VAL:HA	2:D:400:PHE:HB2	1.82	0.61
2:B:402:ILE:HA	2:B:495:TYR:HE2	1.66	0.61
1:C:81:GLN:HG2	4:F:1:NAG:O7	2.00	0.60
2:D:435:ALA:HA	2:D:510:VAL:HG12	1.83	0.60
1:C:416:LYS:HD2	1:C:543:ASP:HB3	1.82	0.60
2:D:458:LYS:NZ	2:D:471:GLU:OE2	2.30	0.60
5:A:702:NAG:O7	5:A:702:NAG:O3	2.11	0.60
1:C:538:PRO:HD2	1:C:541:LYS:HD3	1.84	0.59
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.84	0.59
2:B:425:LEU:HD22	2:B:429:PHE:CE2	2.38	0.59
2:B:350:VAL:HG11	2:B:418:ILE:HD11	1.84	0.59
1:C:46:ALA:HB1	1:C:62:MET:HA	1.85	0.59
2:D:423:TYR:HE2	2:D:512:VAL:HG21	1.68	0.58
2:D:436:TRP:CH2	2:D:509:ARG:CG	2.84	0.58
2:B:378:LYS:HB3	2:B:380:TYR:CE1	2.38	0.58
2:D:453:TYR:CD2	2:D:495:TYR:CE1	2.90	0.58
2:B:349:SER:CB	2:B:452:ARG:H	2.17	0.58
2:D:374:PHE:HE1	2:D:376:THR:C	2.08	0.57
2:D:436:TRP:CH2	2:D:509:ARG:CB	2.87	0.57
2:D:357:ARG:HG3	2:D:396:TYR:HE1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:HD22	5:A:701:NAG:C1	2.18	0.56
2:D:418:ILE:O	2:D:422:ASN:N	2.36	0.56
1:A:103:ASN:ND2	5:A:701:NAG:O5	2.39	0.56
2:D:421:TYR:CD1	2:D:457:ARG:HB3	2.41	0.56
1:A:55:THR:OG1	1:A:58:ASN:OD1	2.22	0.56
1:A:564:GLU:HB3	1:A:568:LEU:HD23	1.86	0.56
2:D:353:TRP:NE1	2:D:466:ARG:HG3	2.19	0.56
2:D:374:PHE:CZ	2:D:377:PHE:CB	2.88	0.56
1:C:103:ASN:HB2	4:F:1:NAG:C8	2.27	0.56
2:D:374:PHE:CZ	2:D:377:PHE:HB2	2.39	0.56
1:C:232:GLU:HB2	1:C:581:VAL:HG21	1.87	0.56
1:A:187:LYS:HD2	1:A:199:TYR:CZ	2.40	0.56
1:A:460:ARG:HH21	1:A:506:VAL:HA	1.71	0.56
2:B:409:GLN:O	2:B:411:ALA:N	2.39	0.56
2:D:387:LEU:HD22	2:D:515:PHE:HE2	1.70	0.56
2:D:402:ILE:HB	2:D:406:GLU:HB3	1.88	0.55
2:D:419:ALA:O	2:D:424:LYS:HD3	2.06	0.55
2:B:380:TYR:HD2	2:B:412:PRO:HD3	1.69	0.55
1:C:144:LEU:HB2	1:C:168:TRP:CH2	2.41	0.55
1:C:229:THR:HB	1:C:581:VAL:HG13	1.89	0.55
2:D:436:TRP:HH2	2:D:509:ARG:CD	2.19	0.55
2:B:383:SER:O	2:B:387:LEU:HD23	2.07	0.54
2:D:338:PHE:CE2	2:D:363:ALA:HB1	2.41	0.54
2:D:374:PHE:CE1	2:D:376:THR:C	2.80	0.54
2:D:402:ILE:HA	2:D:495:TYR:HE2	1.71	0.54
1:A:103:ASN:OD1	1:A:104:GLY:N	2.38	0.54
2:B:426:PRO:HB3	2:B:463:PRO:HB3	1.89	0.54
2:B:476:GLY:H	2:B:487:ASN:HB3	1.73	0.54
2:B:476:GLY:N	2:B:487:ASN:HB3	2.23	0.54
1:C:108:LEU:HD11	1:C:113:SER:OG	2.07	0.54
2:D:456:PHE:HB3	2:D:473:TYR:CD2	2.43	0.53
2:B:385:THR:O	2:B:388:ASN:ND2	2.40	0.53
2:B:392:PHE:HD1	2:B:517:LEU:HB2	1.73	0.53
2:B:349:SER:HB3	2:B:451:TYR:HA	1.91	0.53
1:A:294:THR:HG23	1:A:365:THR:HA	1.91	0.53
2:B:502:GLY:O	2:B:506:GLN:HG3	2.08	0.53
1:A:460:ARG:NH2	1:A:506:VAL:HA	2.24	0.52
1:C:187:LYS:HD2	1:C:199:TYR:CZ	2.44	0.52
2:D:336:CYS:HB2	2:D:363:ALA:HA	1.89	0.52
1:C:252:TYR:HB2	1:C:256:ILE:HD12	1.90	0.52
2:D:436:TRP:CH2	2:D:509:ARG:HD3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:476:GLY:H	2:D:487:ASN:HB3	1.74	0.52
2:B:423:TYR:HE1	2:B:425:LEU:HD21	1.75	0.52
2:D:378:LYS:HB3	2:D:380:TYR:CE1	2.45	0.52
2:D:438:SER:O	2:D:438:SER:OG	2.27	0.52
2:D:453:TYR:HE1	2:D:493:GLN:HB3	1.75	0.51
2:D:347:PHE:CD2	2:D:399:SER:HB2	2.45	0.51
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.45	0.51
2:B:335:LEU:HD22	2:B:338:PHE:HD1	1.75	0.51
2:D:374:PHE:CE1	2:D:377:PHE:N	2.78	0.51
2:D:443:SER:HB3	2:D:507:PRO:HG3	1.91	0.51
1:A:538:PRO:HD2	1:A:541:LYS:HD3	1.93	0.51
2:D:498:ARG:HB2	2:D:501:TYR:CE1	2.46	0.51
1:C:261:CYS:HB2	1:C:488:VAL:HB	1.91	0.51
1:C:103:ASN:ND2	4:F:1:NAG:HN2	1.97	0.51
1:C:108:LEU:HD11	1:C:113:SER:N	2.26	0.51
2:D:359:SER:OG	2:D:394:ASN:OD1	2.14	0.51
2:B:337:PRO:HB3	2:B:340:GLU:HB3	1.92	0.51
1:C:457:GLU:HG2	1:C:513:ILE:HB	1.93	0.51
3:J:1:NAG:O7	3:J:1:NAG:H3	2.10	0.51
2:B:453:TYR:CE1	2:B:493:GLN:HB3	2.46	0.50
1:C:294:THR:HG23	1:C:365:THR:HA	1.92	0.50
2:D:372:ALA:N	2:D:373:PRO:HD3	2.26	0.50
2:D:502:GLY:O	2:D:506:GLN:HG3	2.11	0.50
1:C:268:GLY:O	1:C:277:ASN:ND2	2.33	0.50
2:D:439:ASN:ND2	2:D:506:GLN:HG2	2.27	0.50
1:A:102:GLN:O	1:A:102:GLN:HG3	2.11	0.50
1:C:293:VAL:HB	1:C:423:LEU:HB3	1.92	0.50
2:B:350:VAL:HG22	2:B:422:ASN:HD22	1.77	0.50
2:D:464:PHE:CZ	2:D:514:SER:HB2	2.47	0.50
1:A:121:ASN:O	1:A:125:THR:HG23	2.12	0.49
1:A:239:HIS:CE1	1:A:596:LYS:HG3	2.46	0.49
1:A:525:PHE:O	1:A:529:LEU:HG	2.11	0.49
2:D:401:VAL:HA	2:D:509:ARG:HA	1.93	0.49
2:D:436:TRP:CH2	2:D:509:ARG:HG3	2.47	0.49
2:B:387:LEU:HD22	2:B:515:PHE:HE2	1.76	0.49
2:D:374:PHE:CD1	2:D:374:PHE:C	2.84	0.49
2:B:415:THR:O	2:B:415:THR:OG1	2.29	0.49
2:B:471:GLU:HG3	1:C:197:GLU:HB3	1.94	0.49
2:D:365:TYR:HA	2:D:368:LEU:HB3	1.94	0.49
2:D:379:CYS:C	2:D:381:GLY:H	2.16	0.49
2:B:439:ASN:ND2	2:B:506:GLN:CD	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:TRP:CZ3	1:C:172:VAL:HG21	2.48	0.48
2:D:421:TYR:CE1	2:D:457:ARG:HB3	2.48	0.48
2:D:401:VAL:HG11	2:D:451:TYR:HD2	1.72	0.48
2:B:402:ILE:HB	2:B:406:GLU:HB3	1.95	0.48
2:D:436:TRP:HH2	2:D:509:ARG:HG3	1.78	0.48
2:B:342:PHE:CE2	2:B:368:LEU:HD21	2.48	0.48
2:B:335:LEU:HD22	2:B:338:PHE:CD1	2.48	0.48
2:D:439:ASN:HD22	2:D:506:GLN:CD	2.17	0.48
2:B:393:THR:HG22	2:B:517:LEU:HA	1.93	0.48
1:A:229:THR:HB	1:A:581:VAL:CG1	2.43	0.48
2:D:420:ASP:N	2:D:420:ASP:OD1	2.47	0.48
1:A:478:TRP:CD2	1:A:489:GLU:HB3	2.49	0.47
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.96	0.47
2:D:402:ILE:HA	2:D:495:TYR:CE2	2.48	0.47
1:C:353:LYS:HD3	2:D:501:TYR:CZ	2.49	0.47
2:D:335:LEU:HD21	2:D:364:ASP:HB2	1.96	0.47
2:D:411:ALA:HB3	2:D:414:GLN:HB2	1.96	0.47
1:A:48:TRP:O	1:A:52:THR:HG22	2.15	0.47
1:C:121:ASN:O	1:C:125:THR:HG23	2.14	0.47
1:A:284:PRO:HG2	1:A:436:ILE:HG22	1.96	0.47
2:B:420:ASP:OD1	2:B:420:ASP:N	2.47	0.47
2:D:351:TYR:CE2	2:D:492:LEU:HD21	2.50	0.47
2:B:336:CYS:N	2:B:361:CYS:SG	2.83	0.47
2:D:335:LEU:HD23	2:D:336:CYS:N	2.29	0.47
1:A:54:ILE:O	1:A:55:THR:HG23	2.15	0.47
2:D:404:GLY:N	2:D:504:GLY:O	2.48	0.47
2:D:444:LYS:HG2	2:D:448:ASN:HB2	1.96	0.47
1:C:55:THR:O	1:C:59:VAL:HG23	2.15	0.47
1:C:108:LEU:HD11	1:C:113:SER:HA	1.96	0.47
1:C:455:MET:HE1	1:C:481:LYS:HE2	1.97	0.47
2:B:439:ASN:HD21	2:B:506:GLN:CD	2.19	0.46
1:C:269:ASP:OD1	1:C:272:GLY:N	2.48	0.46
1:A:478:TRP:CE3	1:A:489:GLU:HB3	2.50	0.46
1:C:108:LEU:C	1:C:108:LEU:HD12	2.36	0.46
2:D:436:TRP:HZ3	2:D:438:SER:HB2	1.80	0.46
2:D:452:ARG:HG2	2:D:494:SER:HA	1.96	0.46
2:B:471:GLU:HG3	1:C:197:GLU:CB	2.45	0.46
1:C:34:HIS:ND1	2:D:453:TYR:OH	2.48	0.46
1:A:103:ASN:ND2	5:A:701:NAG:C1	2.77	0.46
2:B:372:ALA:N	2:B:373:PRO:HD3	2.30	0.46
2:D:369:TYR:HB2	2:D:377:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LEU:HG	2:B:371:PHE:CE2	2.50	0.46
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.72	0.46
1:C:131:LYS:HB3	1:C:143:LEU:HD23	1.97	0.46
1:C:30:ASP:O	1:C:34:HIS:HD2	1.99	0.46
1:C:375:GLU:O	1:C:378:HIS:HB2	2.16	0.46
2:B:365:TYR:HE1	2:B:388:ASN:HA	1.80	0.46
1:A:170:SER:O	1:A:174:LYS:HD2	2.16	0.45
1:C:199:TYR:O	1:C:202:TYR:HB3	2.17	0.45
2:D:435:ALA:CB	2:D:510:VAL:HG12	2.46	0.45
2:B:342:PHE:HE2	2:B:368:LEU:HD21	1.82	0.45
1:C:284:PRO:HB3	1:C:594:TRP:CH2	2.50	0.45
1:A:535:HIS:CE1	1:A:542:CYS:HB2	2.52	0.45
1:A:574:VAL:HG23	1:A:576:ALA:H	1.81	0.45
1:A:284:PRO:HB3	1:A:594:TRP:CZ2	2.51	0.45
2:B:419:ALA:O	2:B:424:LYS:HB2	2.17	0.45
1:C:322:ASN:HD22	4:G:1:NAG:C7	2.29	0.45
2:D:349:SER:HB2	2:D:452:ARG:H	1.81	0.45
2:D:350:VAL:O	2:D:353:TRP:HD1	1.98	0.45
2:D:342:PHE:HE1	2:D:511:VAL:HG11	1.81	0.45
2:D:379:CYS:HA	2:D:432:CYS:HA	1.98	0.45
2:D:441:LEU:HD11	2:D:509:ARG:NH1	2.32	0.45
1:A:555:PHE:O	1:A:559:ARG:HG2	2.17	0.45
2:D:374:PHE:HZ	2:D:377:PHE:N	2.11	0.45
2:D:448:ASN:OD1	2:D:450:ASN:HB2	2.18	0.45
1:A:201:ASP:CG	1:A:219:ARG:HE	2.20	0.44
2:B:464:PHE:CZ	2:B:514:SER:HB2	2.53	0.44
1:C:239:HIS:CE1	1:C:596:LYS:HG3	2.52	0.44
1:A:85:LEU:HB3	1:A:94:LYS:HE2	1.99	0.44
2:B:351:TYR:CE2	2:B:492:LEU:HD21	2.52	0.44
1:A:248:LEU:O	1:A:252:TYR:N	2.48	0.44
2:B:475:ALA:HB3	2:B:487:ASN:O	2.18	0.44
1:C:460:ARG:NH2	1:C:510:TYR:O	2.46	0.44
2:D:369:TYR:HB2	2:D:377:PHE:CE2	2.52	0.44
2:D:471:GLU:O	2:D:491:PRO:HG3	2.18	0.44
1:A:395:GLY:O	1:A:562:LYS:HB3	2.17	0.44
2:B:379:CYS:HA	2:B:432:CYS:HA	2.00	0.44
2:D:398:ASP:O	2:D:511:VAL:HA	2.18	0.44
2:D:495:TYR:HD2	2:D:497:PHE:CE2	2.36	0.44
2:D:368:LEU:HA	2:D:371:PHE:HE1	1.83	0.44
2:B:371:PHE:C	2:B:373:PRO:HD3	2.38	0.43
1:C:50:TYR:CE1	1:C:59:VAL:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:SER:O	1:C:174:LYS:HD2	2.18	0.43
1:C:201:ASP:CG	1:C:219:ARG:HE	2.20	0.43
1:C:396:ALA:HB1	1:C:566:TRP:HA	1.98	0.43
2:D:401:VAL:HG23	2:D:509:ARG:N	2.32	0.43
1:A:232:GLU:HB2	1:A:581:VAL:HG21	2.01	0.43
1:A:519:THR:O	1:A:522:GLN:HG2	2.18	0.43
1:A:50:TYR:HE1	1:A:59:VAL:HG22	1.80	0.43
2:D:374:PHE:HE1	2:D:376:THR:N	2.11	0.43
1:C:165:TRP:CH2	1:C:490:PRO:HD2	2.54	0.43
2:D:342:PHE:HE2	2:D:368:LEU:HD21	1.83	0.43
2:D:435:ALA:CA	2:D:510:VAL:HG12	2.48	0.43
1:A:99:ALA:O	1:A:102:GLN:HG2	2.19	0.43
1:C:103:ASN:O	1:C:107:VAL:HG12	2.19	0.43
1:C:375:GLU:OE1	1:C:378:HIS:HD2	2.02	0.43
2:D:409:GLN:OE1	2:D:418:ILE:N	2.47	0.43
1:A:145:GLU:HA	1:A:146:PRO:HA	1.88	0.43
2:B:464:PHE:HZ	2:B:514:SER:HB2	1.83	0.43
1:C:102:GLN:OE1	1:C:102:GLN:HA	2.19	0.42
1:C:453:THR:HG23	1:C:512:PHE:CD2	2.54	0.42
2:D:461:LEU:HA	2:D:461:LEU:HD23	1.73	0.42
2:D:347:PHE:HD1	2:D:509:ARG:HE	1.67	0.42
1:A:84:PRO:O	1:A:88:ILE:HG13	2.19	0.42
1:C:108:LEU:CD1	1:C:113:SER:N	2.82	0.42
2:B:422:ASN:HA	2:B:461:LEU:CD1	2.48	0.42
2:B:453:TYR:CE1	2:B:455:LEU:HB3	2.54	0.42
2:D:364:ASP:O	2:D:368:LEU:HB2	2.19	0.42
2:B:458:LYS:NZ	2:B:471:GLU:OE2	2.38	0.42
2:B:472:ILE:HG21	2:B:483:VAL:O	2.19	0.42
2:D:346:THR:HA	2:D:509:ARG:HH21	1.85	0.42
2:D:353:TRP:HB3	2:D:400:PHE:HB3	2.01	0.42
2:D:438:SER:OG	2:D:442:ASP:HB2	2.20	0.42
2:B:335:LEU:HD23	2:B:336:CYS:H	1.85	0.42
2:B:347:PHE:CE2	2:B:399:SER:HB2	2.55	0.42
1:C:382:ASP:HA	1:C:385:TYR:CZ	2.54	0.42
1:A:177:ARG:HD3	1:A:497:TYR:O	2.20	0.42
1:C:482:ARG:HD3	1:C:608:THR:O	2.20	0.42
2:D:378:LYS:CB	2:D:380:TYR:CE1	3.03	0.42
2:D:411:ALA:O	2:D:425:LEU:HB2	2.20	0.42
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.02	0.42
1:C:81:GLN:HG3	4:F:1:NAG:H81	1.63	0.42
1:A:535:HIS:HE1	1:A:538:PRO:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:SER:OG	2:B:507:PRO:HB2	2.19	0.41
2:D:410:ILE:HD12	2:D:423:TYR:HD2	1.84	0.41
1:A:101:GLN:O	1:A:103:ASN:N	2.53	0.41
2:B:441:LEU:HD11	2:B:509:ARG:NH1	2.35	0.41
2:D:418:ILE:C	2:D:420:ASP:H	2.23	0.41
2:D:436:TRP:O	2:D:508:TYR:CD2	2.73	0.41
1:A:511:SER:O	1:A:514:ARG:HD2	2.20	0.41
1:C:145:GLU:HA	1:C:146:PRO:HA	1.90	0.41
1:C:161:ARG:NE	1:C:265:HIS:O	2.50	0.41
1:C:284:PRO:HG2	1:C:436:ILE:HG22	2.03	0.41
2:D:374:PHE:HZ	2:D:377:PHE:H	1.69	0.41
2:D:398:ASP:OD2	2:D:464:PHE:HE1	2.03	0.41
1:A:594:TRP:CZ2	1:A:598:GLN:HG3	2.56	0.41
2:B:393:THR:CG2	2:B:516:GLU:HG3	2.51	0.41
2:D:425:LEU:HD22	2:D:429:PHE:CE2	2.56	0.41
2:B:336:CYS:O	2:B:338:PHE:HD1	2.03	0.41
2:B:452:ARG:HA	2:B:494:SER:HA	2.03	0.41
1:C:524:GLN:HB3	1:C:574:VAL:HG11	2.02	0.41
2:D:336:CYS:O	2:D:338:PHE:N	2.54	0.41
2:D:368:LEU:HA	2:D:371:PHE:CE1	2.56	0.41
2:D:436:TRP:CE3	2:D:436:TRP:C	2.94	0.41
1:A:144:LEU:HB2	1:A:168:TRP:CH2	2.56	0.41
2:B:453:TYR:HD2	2:B:495:TYR:HE1	1.61	0.41
1:A:54:ILE:HG21	1:A:341:LYS:HB2	2.03	0.40
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.92	0.40
2:D:382:VAL:HG12	2:D:383:SER:N	2.36	0.40
1:A:482:ARG:CZ	1:A:488:VAL:HG23	2.52	0.40
1:C:229:THR:HB	1:C:581:VAL:CG1	2.51	0.40
1:C:456:LEU:HD23	1:C:460:ARG:HD2	2.02	0.40
2:D:380:TYR:HE2	2:D:411:ALA:HA	1.85	0.40
2:D:436:TRP:HE3	2:D:436:TRP:C	2.24	0.40
2:D:436:TRP:CE3	2:D:437:ASN:O	2.75	0.40
2:D:499:PRO:HG2	2:D:500:THR:HG23	2.03	0.40
1:A:33:ASN:O	1:A:37:GLU:HG3	2.22	0.40
2:B:380:TYR:CE2	2:B:412:PRO:HD3	2.56	0.40
1:C:450:LEU:HA	1:C:450:LEU:HD23	1.83	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/597 (100%)	572 (96%)	22 (4%)	2 (0%)	37	66
1	C	596/597 (100%)	571 (96%)	24 (4%)	1 (0%)	44	72
2	B	192/194 (99%)	156 (81%)	28 (15%)	8 (4%)	2	17
2	D	192/194 (99%)	149 (78%)	38 (20%)	5 (3%)	4	25
All	All	1576/1582 (100%)	1448 (92%)	112 (7%)	16 (1%)	13	43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	PRO
2	B	338	PHE
2	B	372	ALA
2	B	481	ASN
2	D	439	ASN
1	A	102	GLN
1	C	110	GLU
2	D	373	PRO
2	D	384	PRO
2	B	410	ILE
1	A	473	TRP
2	B	381	GLY
2	B	384	PRO
2	B	402	ILE
2	D	402	ILE
2	D	410	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	528/527 (100%)	523 (99%)	5 (1%)	75	85
1	C	528/527 (100%)	520 (98%)	8 (2%)	60	76
2	B	167/167 (100%)	157 (94%)	10 (6%)	16	42
2	D	167/167 (100%)	154 (92%)	13 (8%)	10	33
All	All	1390/1388 (100%)	1354 (97%)	36 (3%)	41	61

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	MET
1	A	381	TYR
1	A	409	SER
1	A	476	LYS
1	A	547	SER
2	B	356	LYS
2	B	357	ARG
2	B	361	CYS
2	B	365	TYR
2	B	377	PHE
2	B	379	CYS
2	B	432	CYS
2	B	453	TYR
2	B	454	ARG
2	B	462	LYS
1	C	111	ASP
1	C	190	MET
1	C	322	ASN
1	C	381	TYR
1	C	385	TYR
1	C	409	SER
1	C	476	LYS
1	C	547	SER
2	D	356	LYS
2	D	357	ARG
2	D	365	TYR
2	D	369	TYR
2	D	370	ASN
2	D	374	PHE
2	D	377	PHE

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Mol	Chain	Res	Type
2	D	379	CYS
2	D	432	CYS
2	D	453	TYR
2	D	454	ARG
2	D	462	LYS
2	D	518	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	535	HIS
2	B	422	ASN
2	B	437	ASN
2	B	439	ASN
1	C	103	ASN
2	D	422	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	3,1	14,14,15	0.48	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	2	3	14,14,15	1.11	1 (7%)	17,19,21	1.13	1 (5%)
3	BMA	E	3	3	11,11,12	1.40	1 (9%)	15,15,17	1.20	1 (6%)
4	NAG	F	1	4	14,14,15	1.29	2 (14%)	17,19,21	1.14	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.42	2 (11%)
4	NAG	G	1	4,1	14,14,15	0.43	0	17,19,21	1.01	1 (5%)
4	NAG	G	2	4	14,14,15	1.87	1 (7%)	17,19,21	1.75	3 (17%)
3	NAG	H	1	3,1	14,14,15	0.42	0	17,19,21	1.04	1 (5%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	1.35	2 (11%)
3	BMA	H	3	3	11,11,12	1.64	2 (18%)	15,15,17	2.06	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.39	0	17,19,21	0.54	0
3	NAG	I	2	3	14,14,15	0.41	0	17,19,21	0.32	0
3	BMA	I	3	3	11,11,12	0.23	0	15,15,17	0.54	0
3	NAG	J	1	3,1	14,14,15	0.70	0	17,19,21	1.09	2 (11%)
3	NAG	J	2	3	14,14,15	0.49	0	17,19,21	0.77	0
3	BMA	J	3	3	11,11,12	1.18	2 (18%)	15,15,17	0.88	0
4	NAG	K	1	4,1	14,14,15	1.05	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	K	2	4	14,14,15	0.51	0	17,19,21	0.71	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.50	0	17,19,21	0.78	0
4	NAG	L	2	4	14,14,15	0.88	1 (7%)	17,19,21	1.08	2 (11%)

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

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	NAG	O5-C1	6.43	1.54	1.43
4	F	1	NAG	C1-C2	4.26	1.58	1.52
4	K	1	NAG	C1-C2	3.58	1.57	1.52
3	E	2	NAG	O5-C1	3.52	1.49	1.43
3	H	3	BMA	C1-C2	3.37	1.59	1.52
3	E	3	BMA	O5-C1	3.12	1.48	1.43
3	H	3	BMA	C2-C3	2.90	1.56	1.52
3	J	3	BMA	C1-C2	2.87	1.58	1.52
4	L	2	NAG	C1-C2	2.21	1.55	1.52
3	J	3	BMA	C2-C3	2.06	1.55	1.52
4	F	1	NAG	C3-C2	2.01	1.56	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	-6.63	103.21	112.19
4	G	2	NAG	C2-N2-C7	4.54	129.37	122.90
4	G	2	NAG	C1-O5-C5	4.33	118.06	112.19
4	F	2	NAG	C3-C4-C5	4.04	117.44	110.24
3	H	2	NAG	C3-C4-C5	3.75	116.93	110.24
3	H	1	NAG	C1-O5-C5	3.30	116.66	112.19
4	F	1	NAG	C4-C3-C2	2.98	115.39	111.02
4	L	2	NAG	C4-C3-C2	2.86	115.21	111.02
3	H	3	BMA	O5-C5-C6	2.55	111.21	107.20
3	H	2	NAG	O4-C4-C5	-2.53	103.03	109.30
3	J	1	NAG	C1-O5-C5	2.50	115.58	112.19
3	E	2	NAG	C1-O5-C5	2.40	115.45	112.19
3	J	1	NAG	O4-C4-C3	-2.29	105.05	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C3-C4-C5	2.27	114.28	110.24
4	F	2	NAG	C4-C3-C2	2.26	114.34	111.02
4	G	1	NAG	C3-C4-C5	2.25	114.26	110.24
4	F	1	NAG	C1-O5-C5	-2.17	109.25	112.19
4	K	1	NAG	C4-C3-C2	2.17	114.19	111.02
4	K	2	NAG	C1-O5-C5	2.07	115.00	112.19
3	E	3	BMA	C1-O5-C5	2.03	114.94	112.19
4	G	2	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C8-C7-N2-C2
4	G	2	NAG	C3-C2-N2-C7
3	J	3	BMA	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	H	3	BMA	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C1-C2-N2-C7
4	L	2	NAG	C1-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

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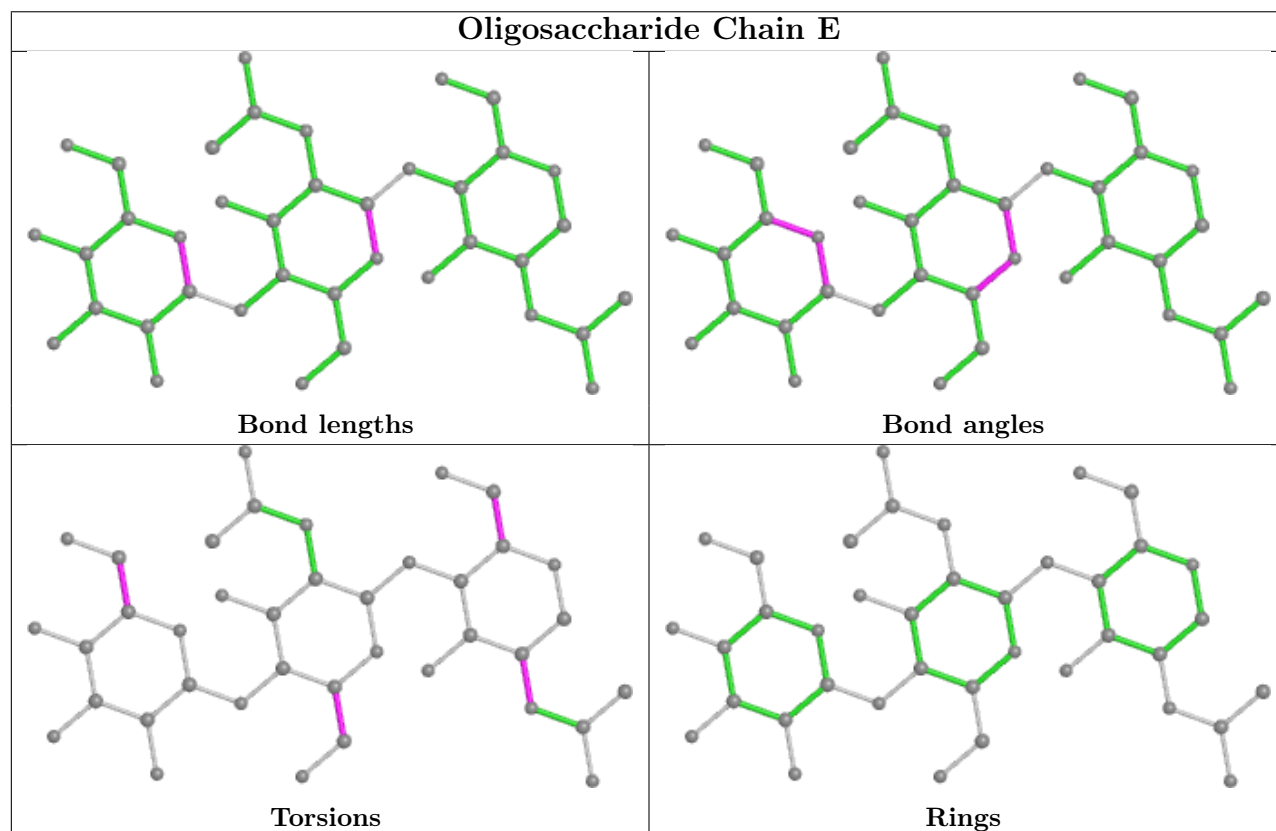
Mol	Chain	Res	Type	Atoms
3	J	1	NAG	C3-C2-N2-C7
3	H	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	H	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C1-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7

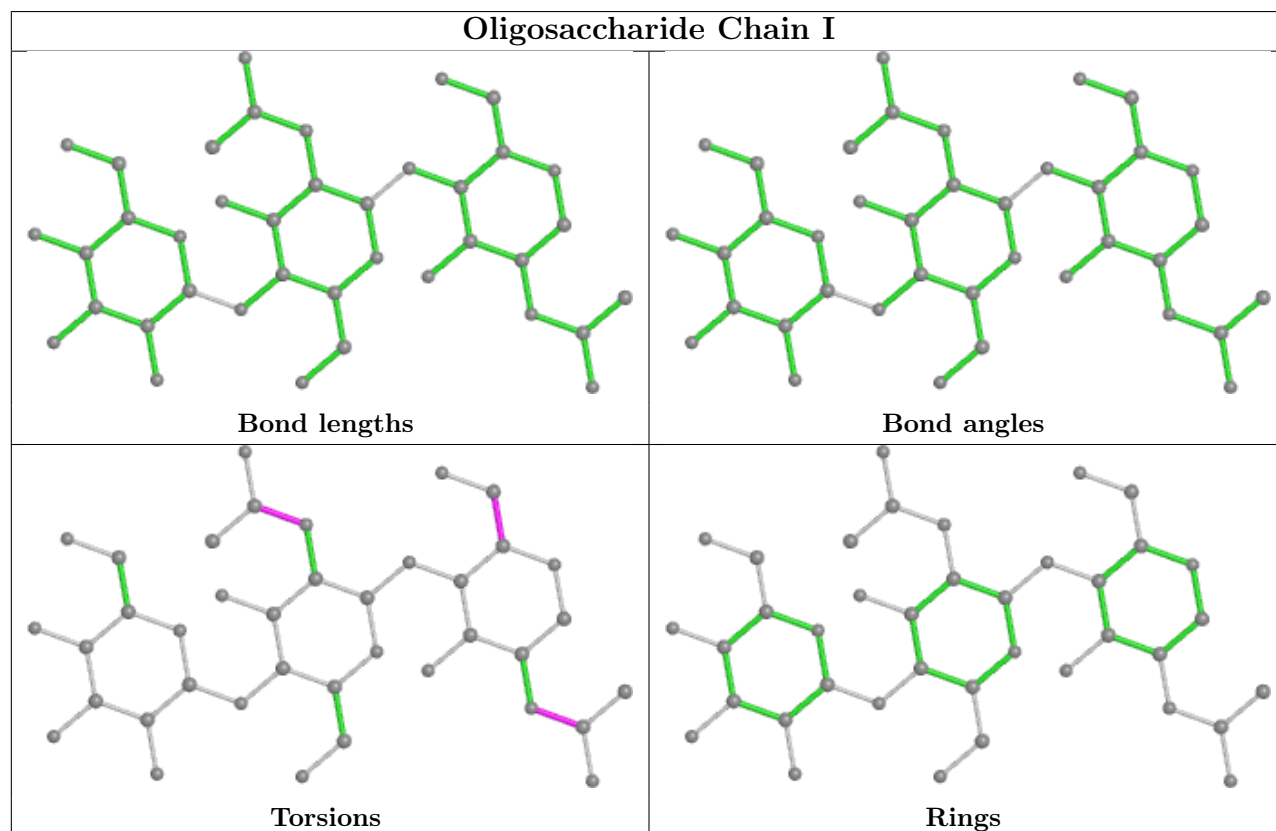
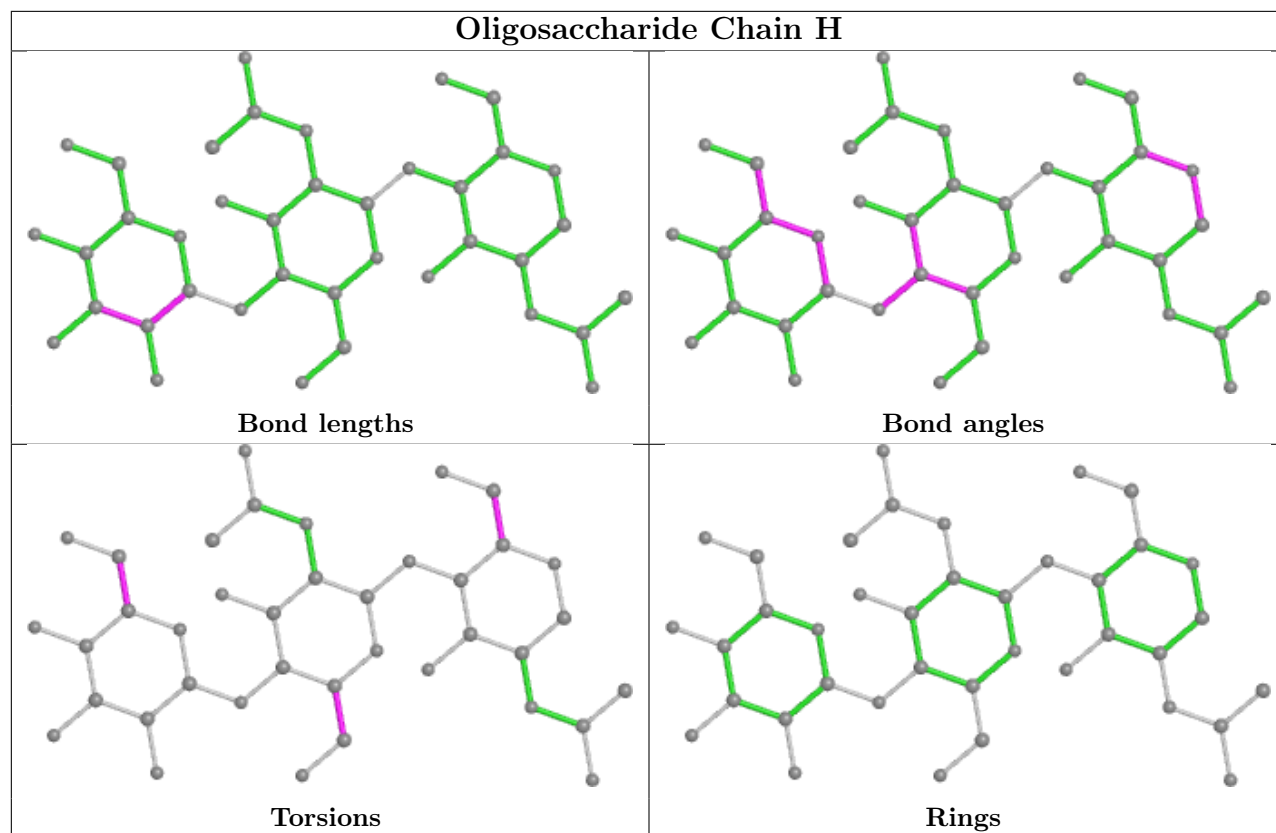
There are no ring outliers.

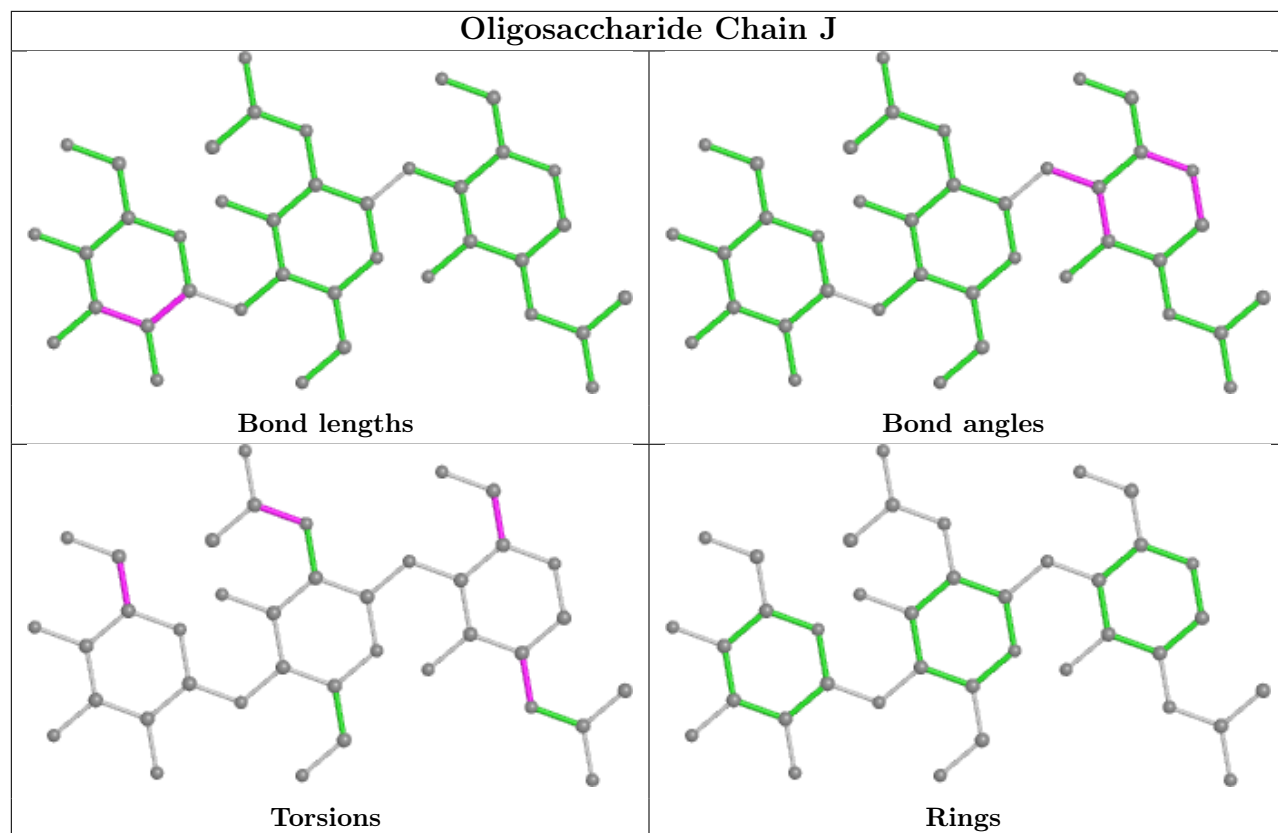
3 monomers are involved in 9 short contacts:

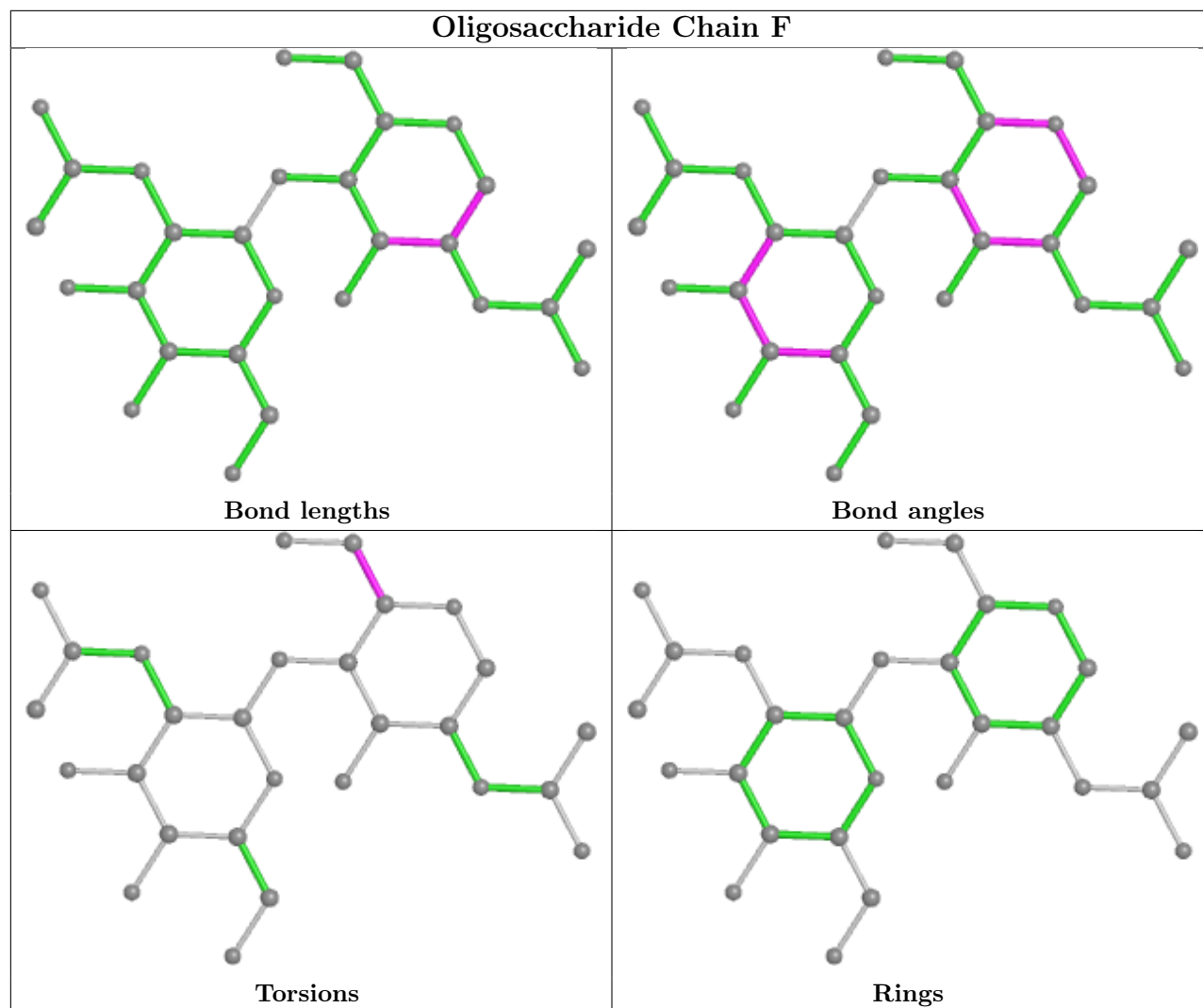
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	7	0
4	G	1	NAG	1	0
3	J	1	NAG	1	0

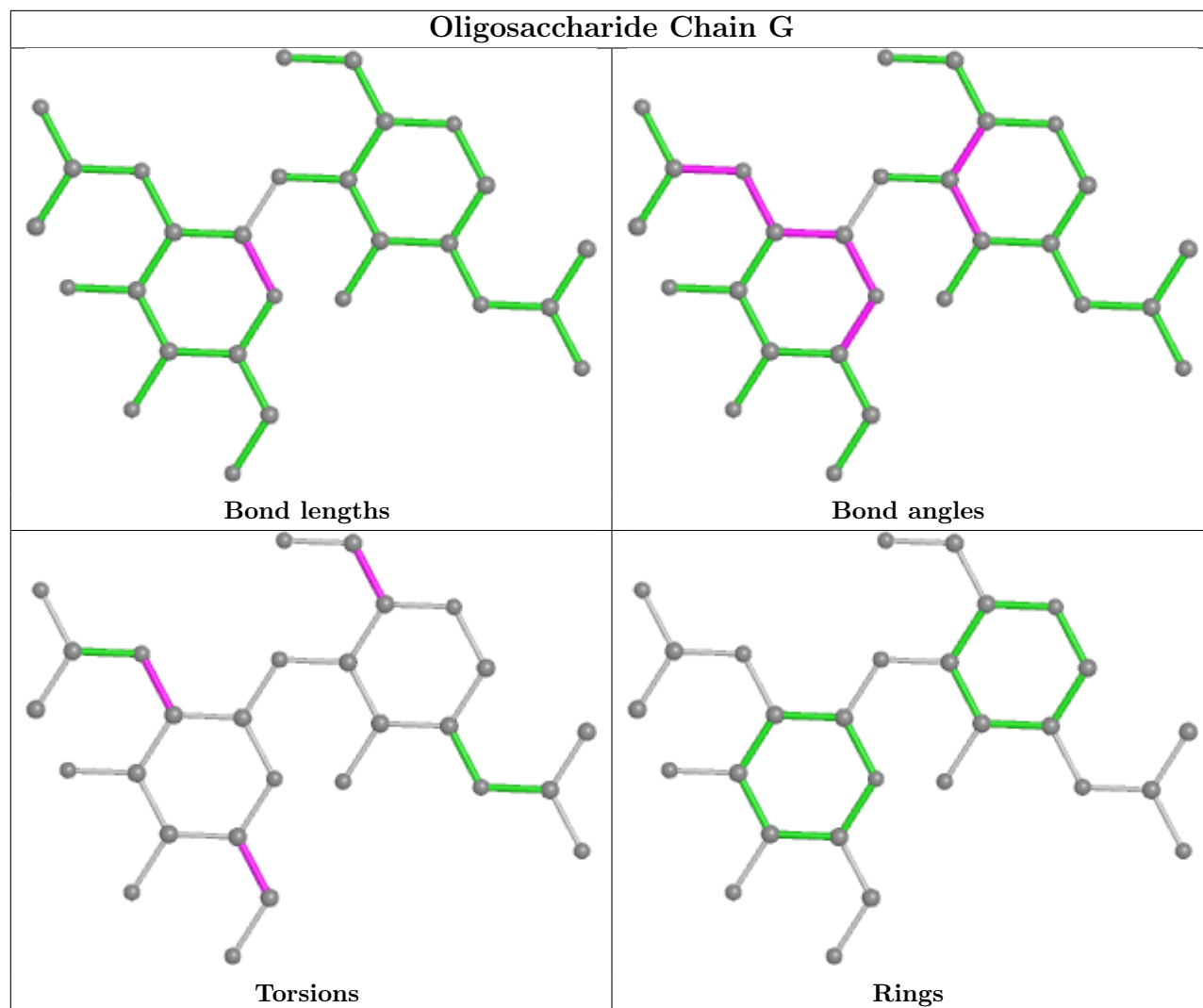
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

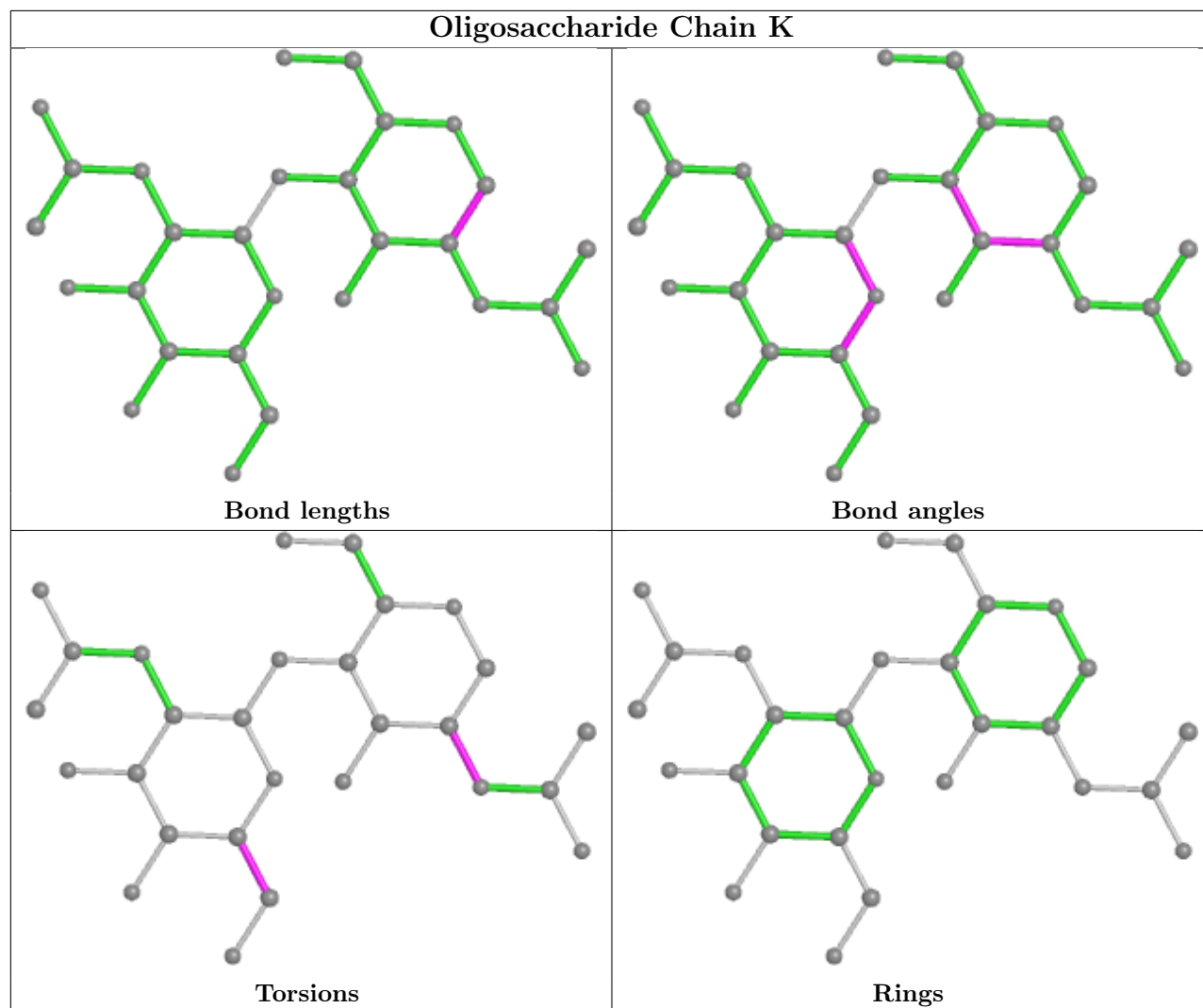




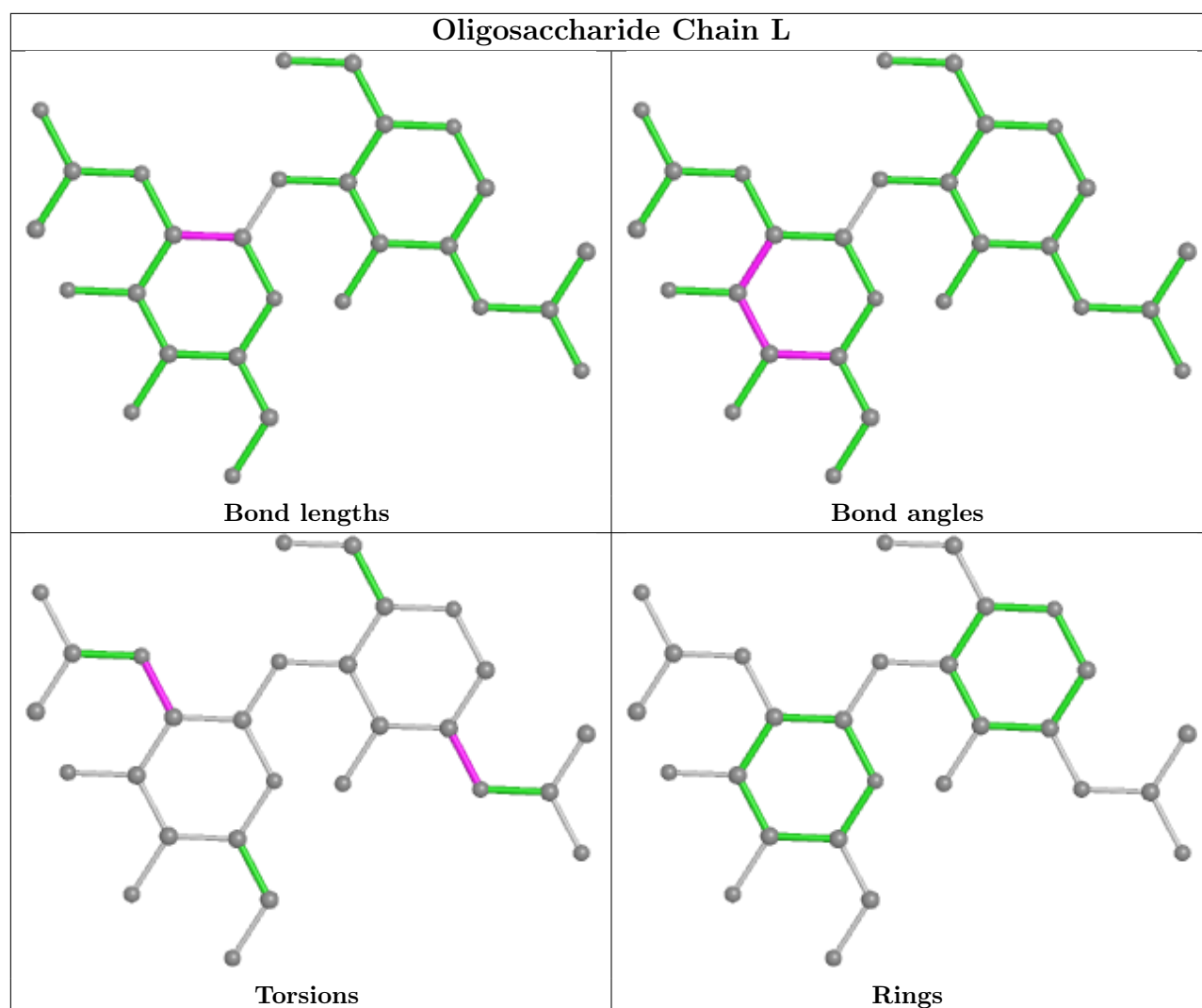












## 5.6 Ligand geometry [i](#)

3 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	C	701	1	14,14,15	0.33	0	17,19,21	0.55	0
5	NAG	A	701	-	14,14,15	0.59	0	17,19,21	1.03	2 (11%)
5	NAG	A	702	1	14,14,15	1.03	2 (14%)	17,19,21	1.17	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	701	1	-	2/6/23/26	0/1/1/1
5	NAG	A	701	-	-	3/6/23/26	0/1/1/1
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	NAG	O5-C1	3.06	1.48	1.43
5	A	702	NAG	C1-C2	2.02	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	NAG	C2-N2-C7	4.07	128.69	122.90
5	A	701	NAG	C2-N2-C7	2.42	126.34	122.90
5	A	701	NAG	C1-O5-C5	-2.08	109.38	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	NAG	C1-C2-N2-C7
5	A	702	NAG	C3-C2-N2-C7
5	C	701	NAG	O5-C5-C6-O6
5	C	701	NAG	C4-C5-C6-O6
5	A	702	NAG	O5-C5-C6-O6
5	A	701	NAG	O5-C5-C6-O6
5	A	701	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	NAG	3	0
5	A	702	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

### 6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

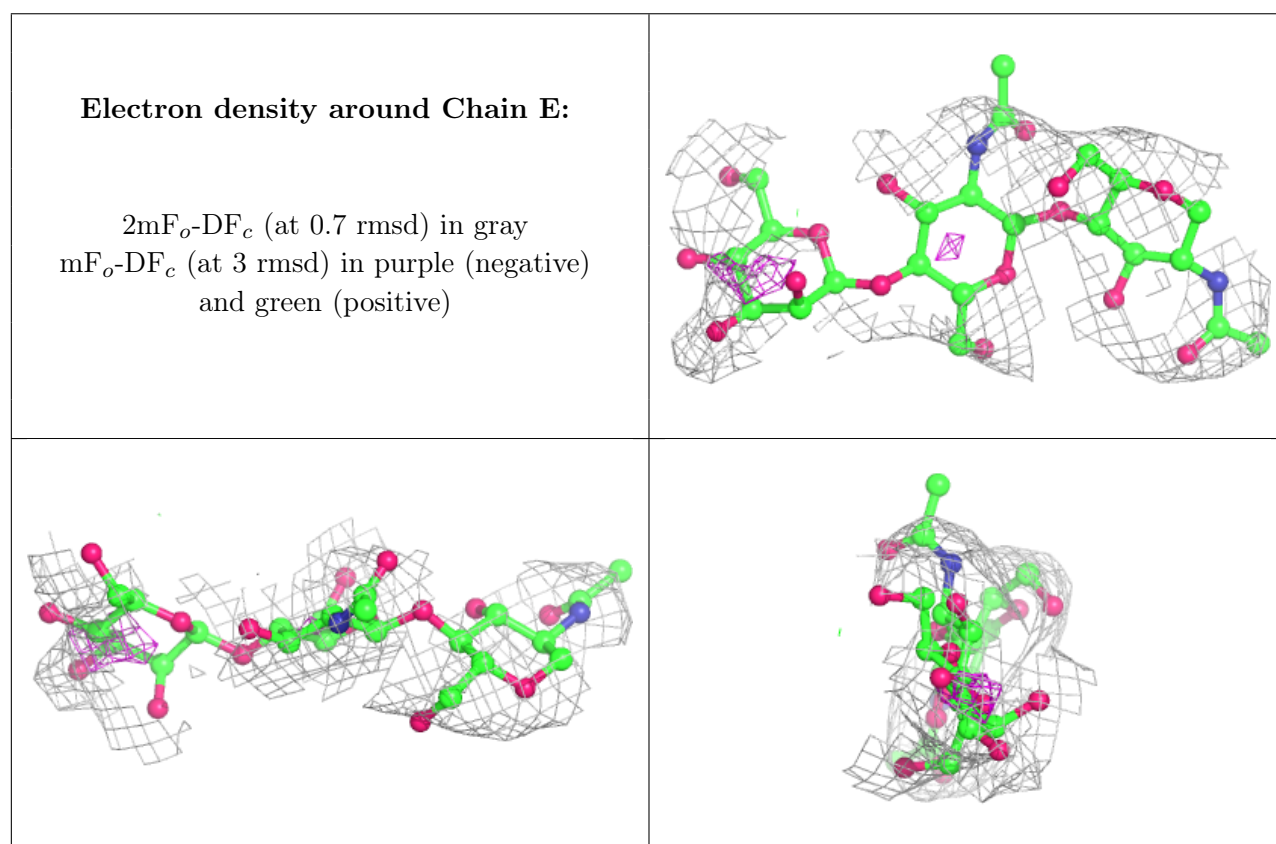
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

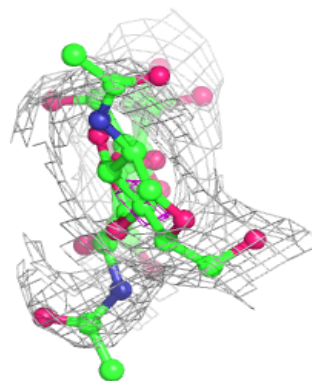
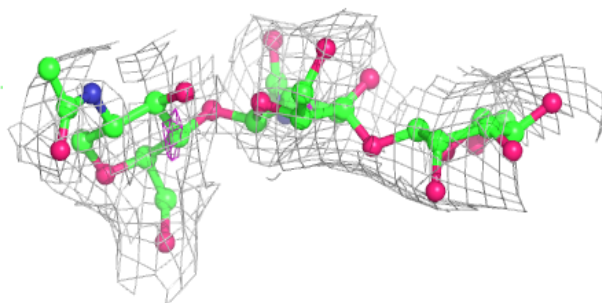
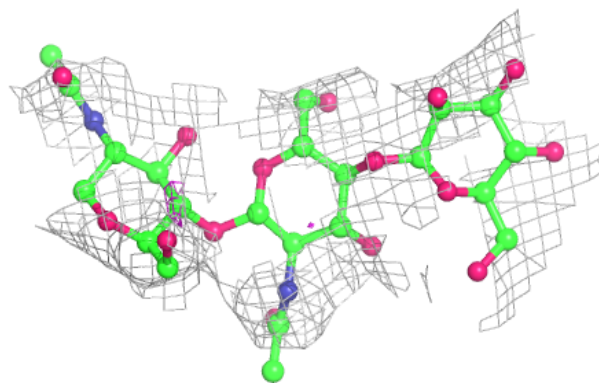
EDS failed to run properly - this section is therefore empty.

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.

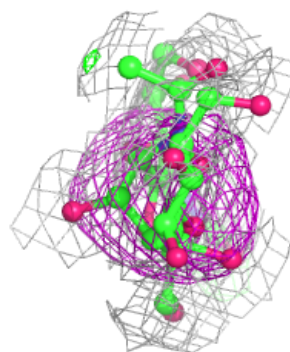
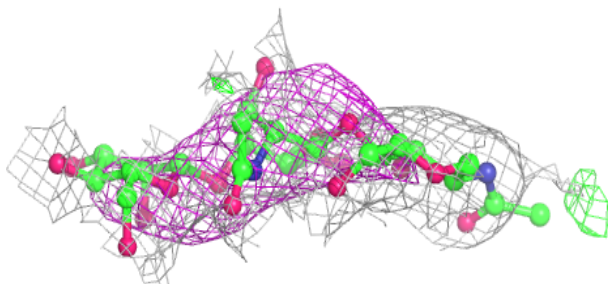
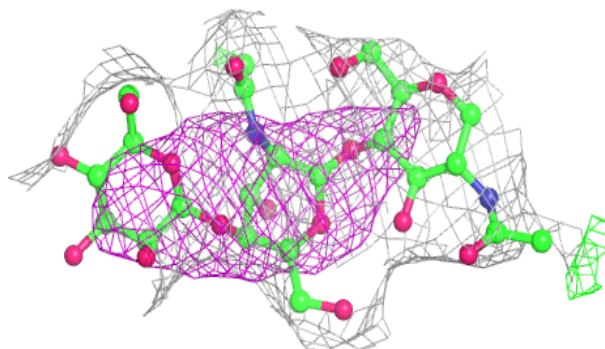


**Electron density around Chain H:**

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

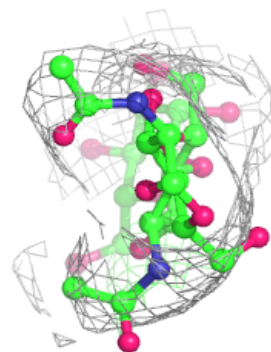
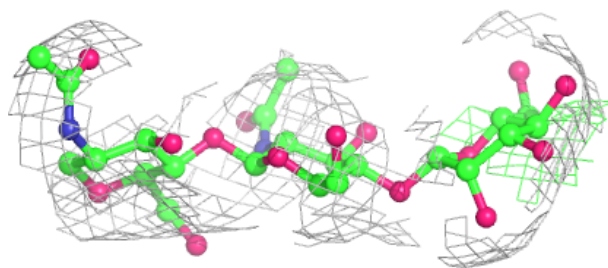
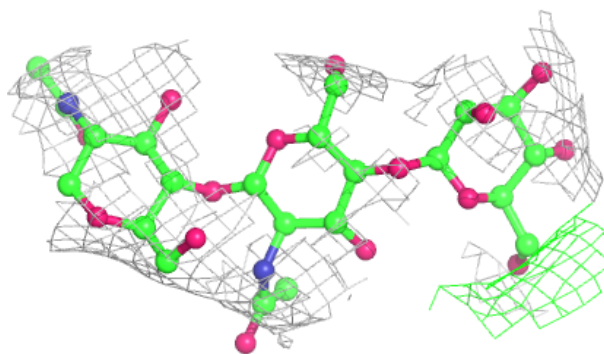
**Electron density around Chain I:**

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



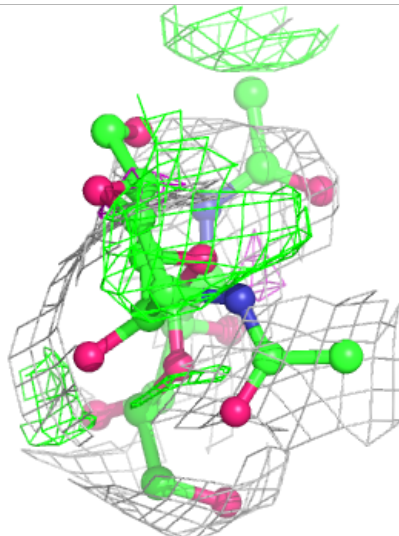
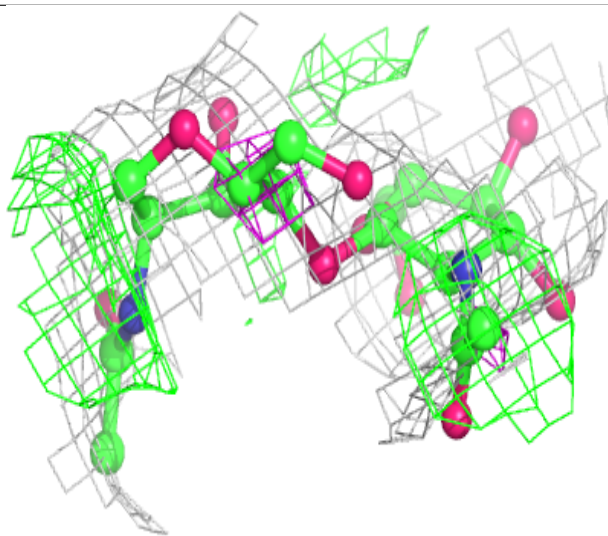
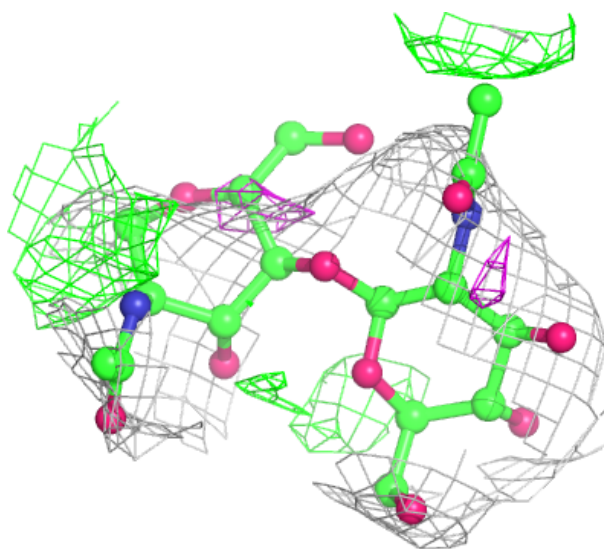
**Electron density around Chain J:**

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



**Electron density around Chain F:**

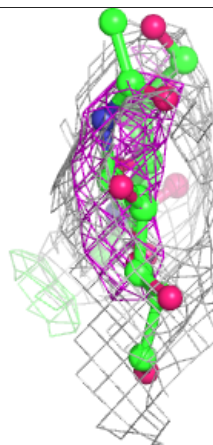
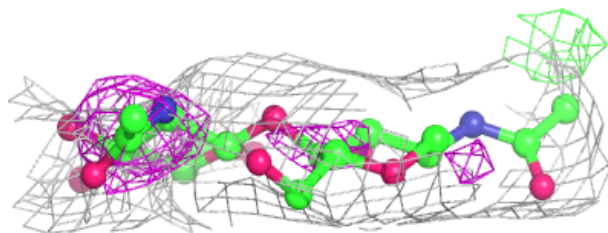
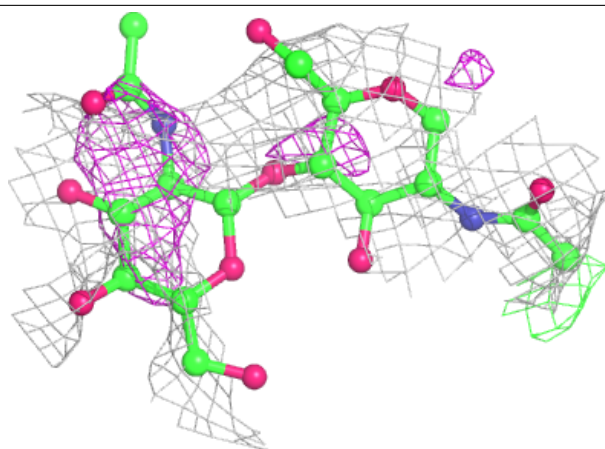
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain G:**

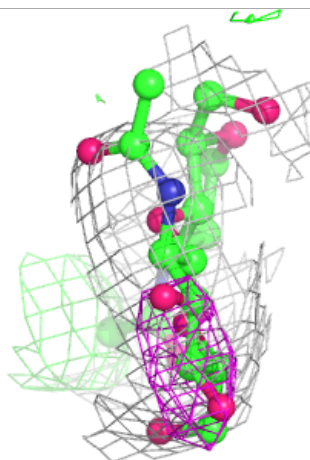
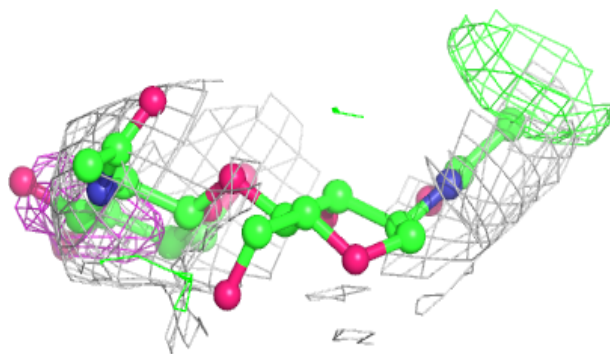
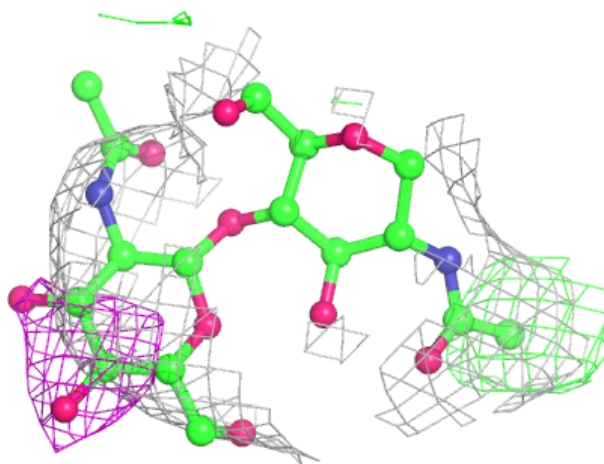
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

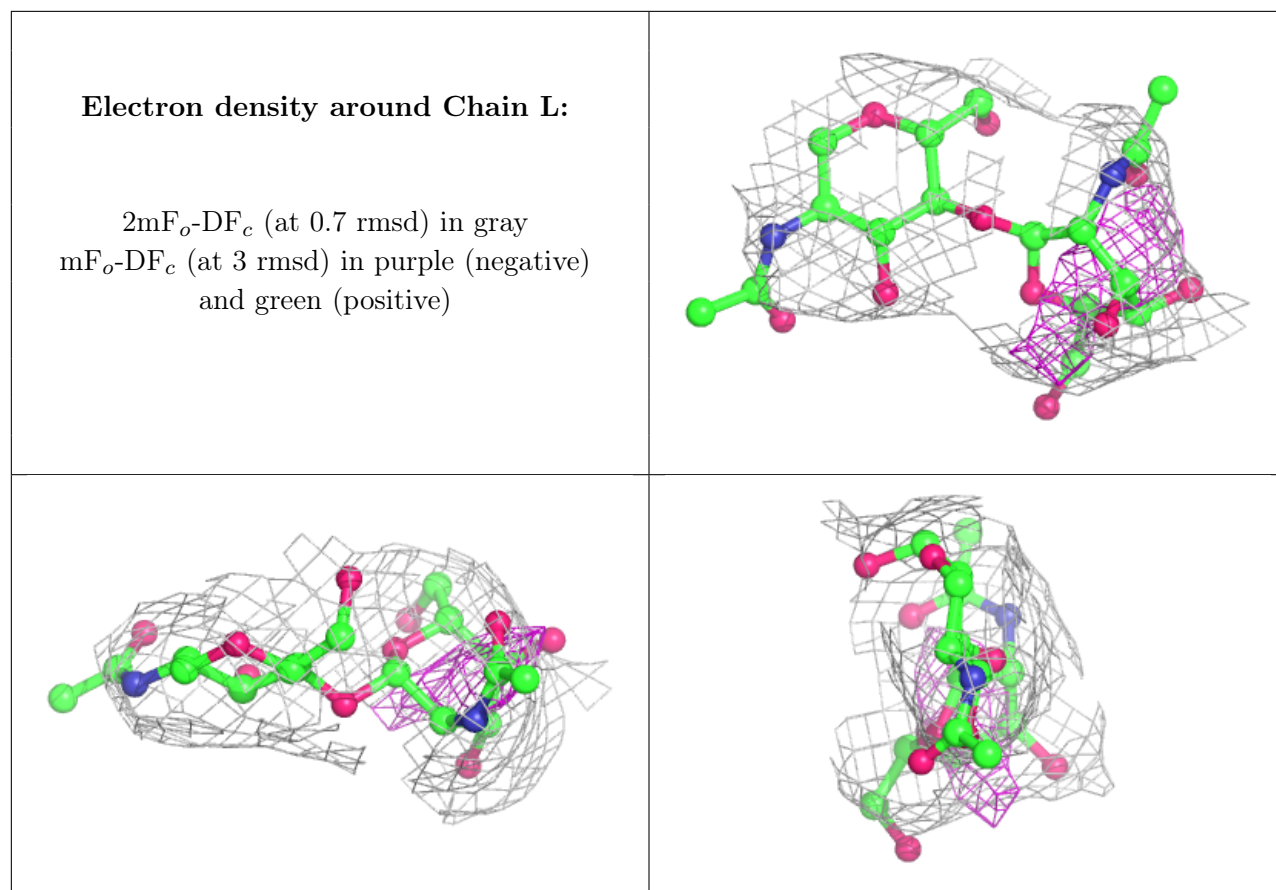




**Electron density around Chain K:**

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





## 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

## 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.