



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 12:16 AM EDT

PDB ID : 1R9M
Title : Crystal Structure of Human Dipeptidyl Peptidase IV at 2.1 Ang. Resolution.
Authors : Aertgeerts, K.; Ye, S.; Tennant, M.G.; Collins, B.; Rogers, J.; Sang, B.C.;
Skene, R.J.; Webb, D.R.; Prasad, G.S.
Deposited on : 2003-10-30
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.39

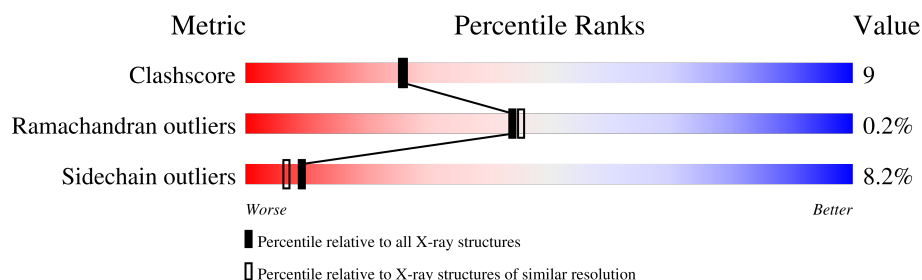
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)





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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	733	71% 23% . .
1	B	733	73% 23% .
1	C	733	74% 22% . .
1	D	733	75% 20% . .
2	E	2	100%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	2	 50% 50%
2	L	2	 50% 50%
3	F	3	 67% 33%
4	K	4	 75% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	I	2	X	-	-	-
4	MAN	K	4	X	-	-	-
5	NAG	A	6851	X	-	-	-
5	NAG	C	1501	X	-	-	-
5	NAG	D	2191	X	-	-	-
5	NAG	D	5201	X	-	-	-
5	NAG	D	6851	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 20 discrepancies between the modelled and reference sequences:

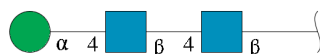
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- Molecule 2 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
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-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	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-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: $C_8H_{15}NO_6$).



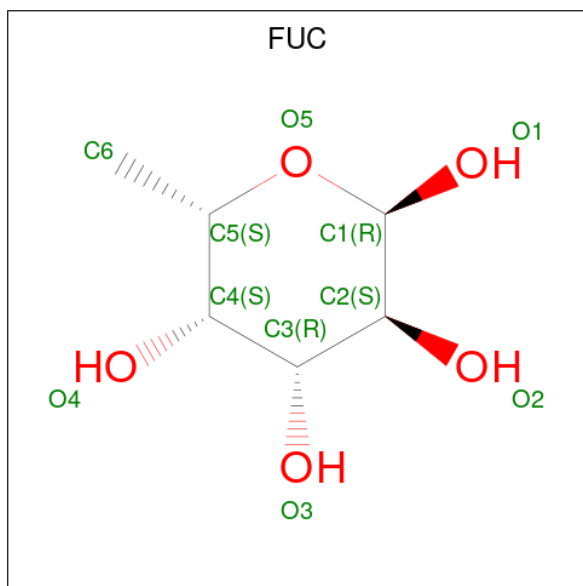
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

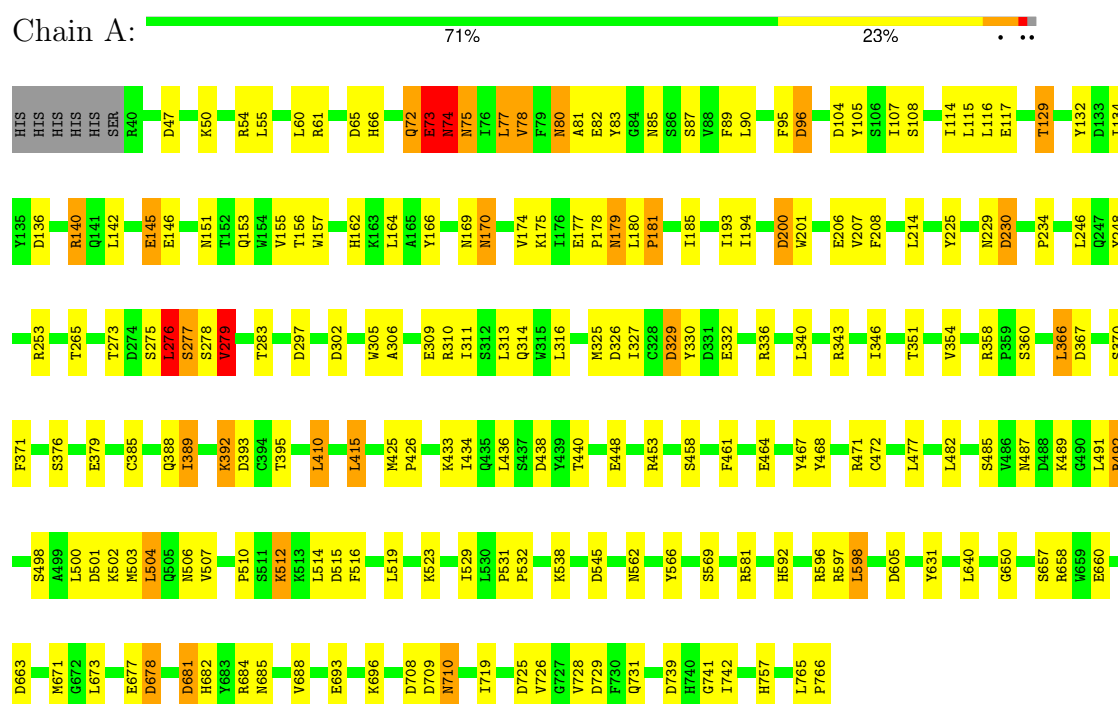
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	466	Total 466	O 466	0	0
7	B	467	Total 467	O 467	0	0
7	C	334	Total 334	O 334	0	0
7	D	411	Total 411	O 411	0	0

3 Residue-property plots

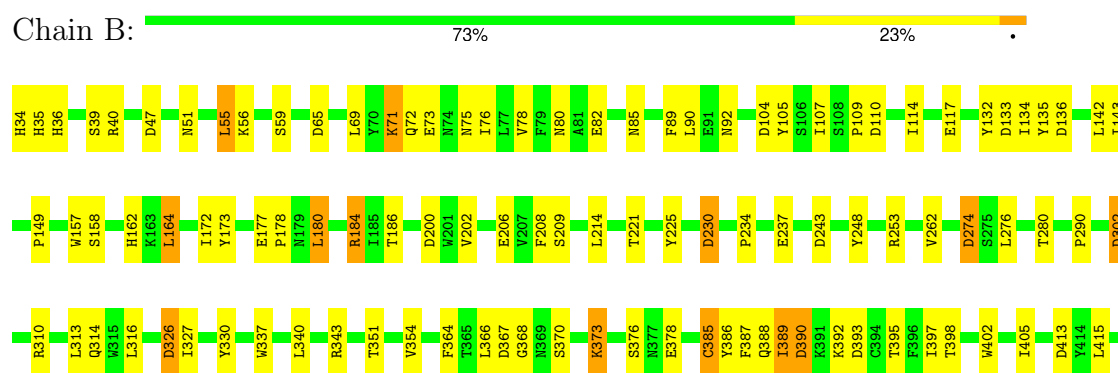
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

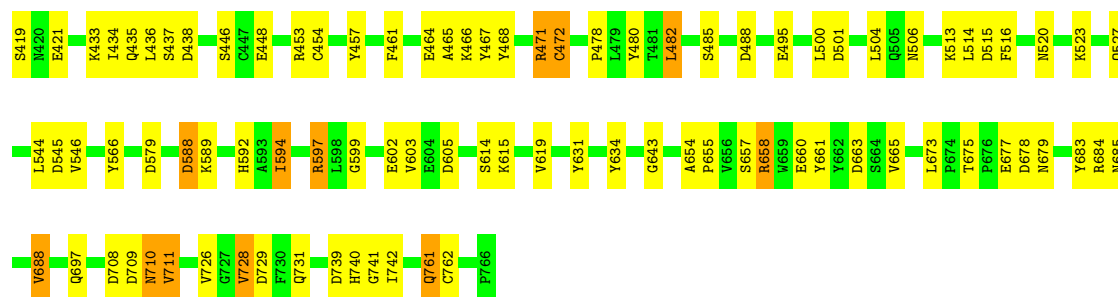
Note EDS was not executed.

• Molecule 1: Dipeptidyl peptidase IV



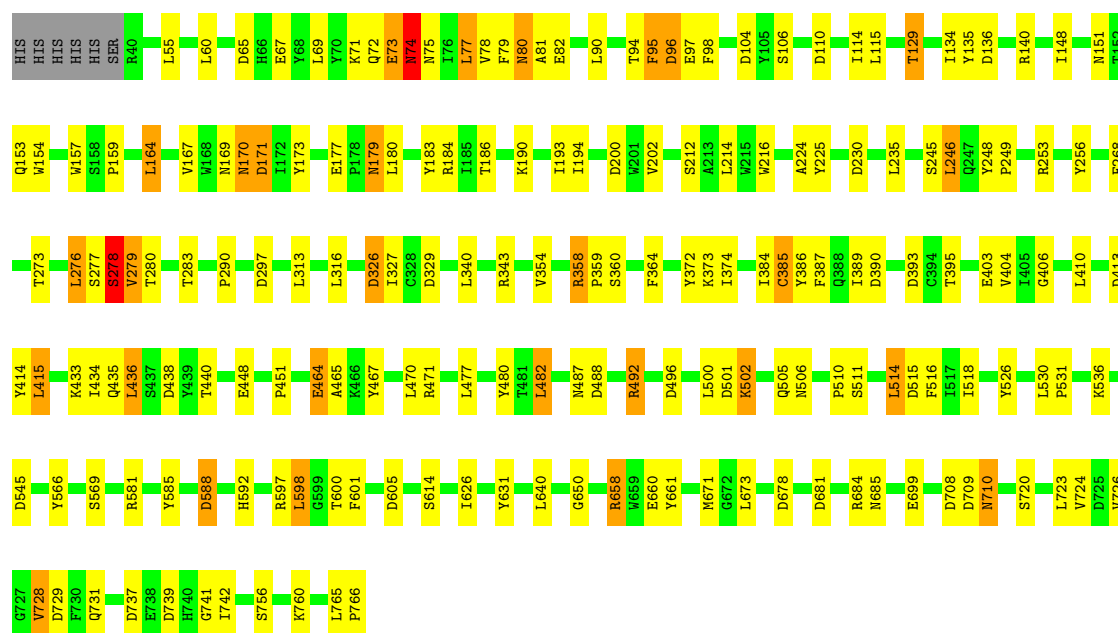
• Molecule 1: Dipeptidyl peptidase IV





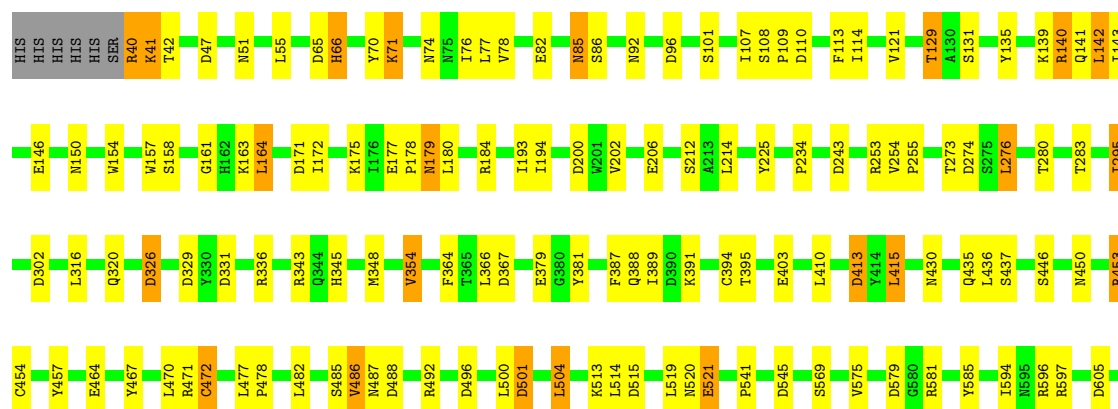
● Molecule 1: Dipeptidyl peptidase IV

Chain C: 74% 22%



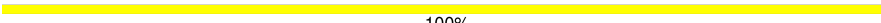
● Molecule 1: Dipeptidyl peptidase IV

Chain D: 75% 20%





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

Chain E:  100%



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

Chain G:  100%



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

Chain H:  50% 50%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain L:  50% 50%




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

Chain F:  67% 33%

MAG1
MAG2
MAN3

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

Chain K:  75% 25%

MAG1
MAG2
MAN3
MAN4

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.82Å 124.06Å 144.49Å 90.00° 114.71° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.218 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26111	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.48	0/6123	0.85	32/8329 (0.4%)
1	B	0.43	0/6190	0.79	25/8419 (0.3%)
1	C	0.41	0/6123	0.85	34/8329 (0.4%)
1	D	0.42	0/6129	0.80	27/8336 (0.3%)
All	All	0.44	0/24565	0.82	118/33413 (0.4%)

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	6
1	C	2	3
All	All	2	9

There are no bond length outliers.

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	ASN	O-C-N	-15.46	97.96	122.70
1	C	279	VAL	O-C-N	-10.01	106.68	122.70
1	C	74	ASN	CA-C-O	9.21	139.45	120.10
1	A	279	VAL	O-C-N	-9.17	108.03	122.70
1	A	545	ASP	CB-CG-OD2	8.55	126.00	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	73	GLU	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	C	74	ASN	CA

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Mainchain
1	A	277	SER	Mainchain
1	A	279	VAL	Mainchain
1	A	72	GLN	Peptide
1	A	74	ASN	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5951	0	5660	114	0
1	B	6013	0	5710	110	1
1	C	5951	0	5660	119	0
1	D	5957	0	5673	101	1
2	E	28	0	25	0	0
2	G	28	0	24	0	0
2	H	28	0	25	1	0
2	I	28	0	25	3	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
3	F	39	0	34	2	0
4	K	50	0	41	1	0
5	A	56	0	52	10	0
5	B	84	0	77	9	0
5	C	70	0	65	3	0
5	D	84	0	78	4	0
6	B	10	0	10	3	0
7	A	466	0	0	3	0
7	B	467	0	0	3	0
7	C	334	0	0	0	0
7	D	411	0	0	0	0
All	All	26111	0	23209	442	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 9.

The worst 5 of 442 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:GLN:NE2	1:D:731:GLN:HE22	1.46	1.13
1:A:327:ILE:HD13	1:A:389:ILE:CD1	1.80	1.12
5:B:1501:NAG:O6	6:B:1502:FUC:C1	2.00	1.10
1:C:731:GLN:HE22	1:D:731:GLN:NE2	1.50	1.08
1:C:731:GLN:NE2	1:D:731:GLN:NE2	2.03	1.06

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)
1:B:36:HIS:ND1	1:D:388:GLN:OE1[2_645]	1.96	0.24

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	725/733 (99%)	693 (96%)	29 (4%)	3 (0%)	30	29
1	B	731/733 (100%)	703 (96%)	28 (4%)	0	100	100
1	C	725/733 (99%)	691 (95%)	33 (5%)	1 (0%)	48	51
1	D	725/733 (99%)	693 (96%)	30 (4%)	2 (0%)	37	37
All	All	2906/2932 (99%)	2780 (96%)	120 (4%)	6 (0%)	44	45

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	486	VAL
1	C	73	GLU
1	A	140	ARG
1	D	621	ASN

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	651/658 (99%)	584 (90%)	67 (10%)	6	3
1	B	658/658 (100%)	611 (93%)	47 (7%)	12	10
1	C	651/658 (99%)	601 (92%)	50 (8%)	10	8
1	D	652/658 (99%)	601 (92%)	51 (8%)	10	8
All	All	2612/2632 (99%)	2397 (92%)	215 (8%)	9	7

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	74	ASN
1	C	436	LEU
1	D	482	LEU
1	C	95	PHE
1	C	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	100	HIS
1	C	430	ASN
1	D	430	ASN
1	C	141	GLN
1	C	170	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 ⓘ

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2,1	14,14,15	0.65	0	17,19,21	2.06	4 (23%)
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	1.61	2 (11%)
3	NAG	F	1	3,1	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.62	0
3	MAN	F	3	3	11,11,12	0.33	0	15,15,17	0.87	1 (6%)
2	NAG	G	1	2,1	14,14,15	0.63	0	17,19,21	4.62	9 (52%)
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	1.21	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.44	0	17,19,21	0.95	0
2	NAG	H	2	2	14,14,15	0.52	0	17,19,21	1.08	2 (11%)
2	NAG	I	1	2,1	14,14,15	0.82	1 (7%)	17,19,21	1.25	1 (5%)
2	NAG	I	2	2	14,14,15	1.09	1 (7%)	17,19,21	2.57	6 (35%)
2	NAG	J	1	2,1	14,14,15	0.34	0	17,19,21	1.11	1 (5%)
2	NAG	J	2	2	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	K	1	1,4	14,14,15	0.39	0	17,19,21	1.02	1 (5%)
4	NAG	K	2	4	14,14,15	0.21	0	17,19,21	1.07	3 (17%)
4	MAN	K	3	4	11,11,12	0.42	0	15,15,17	1.98	5 (33%)
4	MAN	K	4	4	11,11,12	0.32	0	15,15,17	1.52	2 (13%)
2	NAG	L	1	2,1	14,14,15	0.30	0	17,19,21	0.92	0
2	NAG	L	2	2	14,14,15	0.35	0	17,19,21	1.23	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
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	2/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	MAN	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	1/1/4/5	2/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	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)
2	I	2	NAG	C1-C2	3.70	1.57	1.52
2	I	1	NAG	O4-C4	2.23	1.48	1.43

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-C2-N2	10.79	127.43	110.43
2	G	1	NAG	C4-C3-C2	-9.64	96.89	111.02
2	G	1	NAG	C2-N2-C7	7.64	133.14	122.90
2	G	1	NAG	O5-C1-C2	-7.52	99.65	111.29
2	I	2	NAG	O5-C1-C2	-6.12	101.82	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	2	NAG	C1
4	K	4	MAN	C1

5 of 30 torsion outliers are listed below:

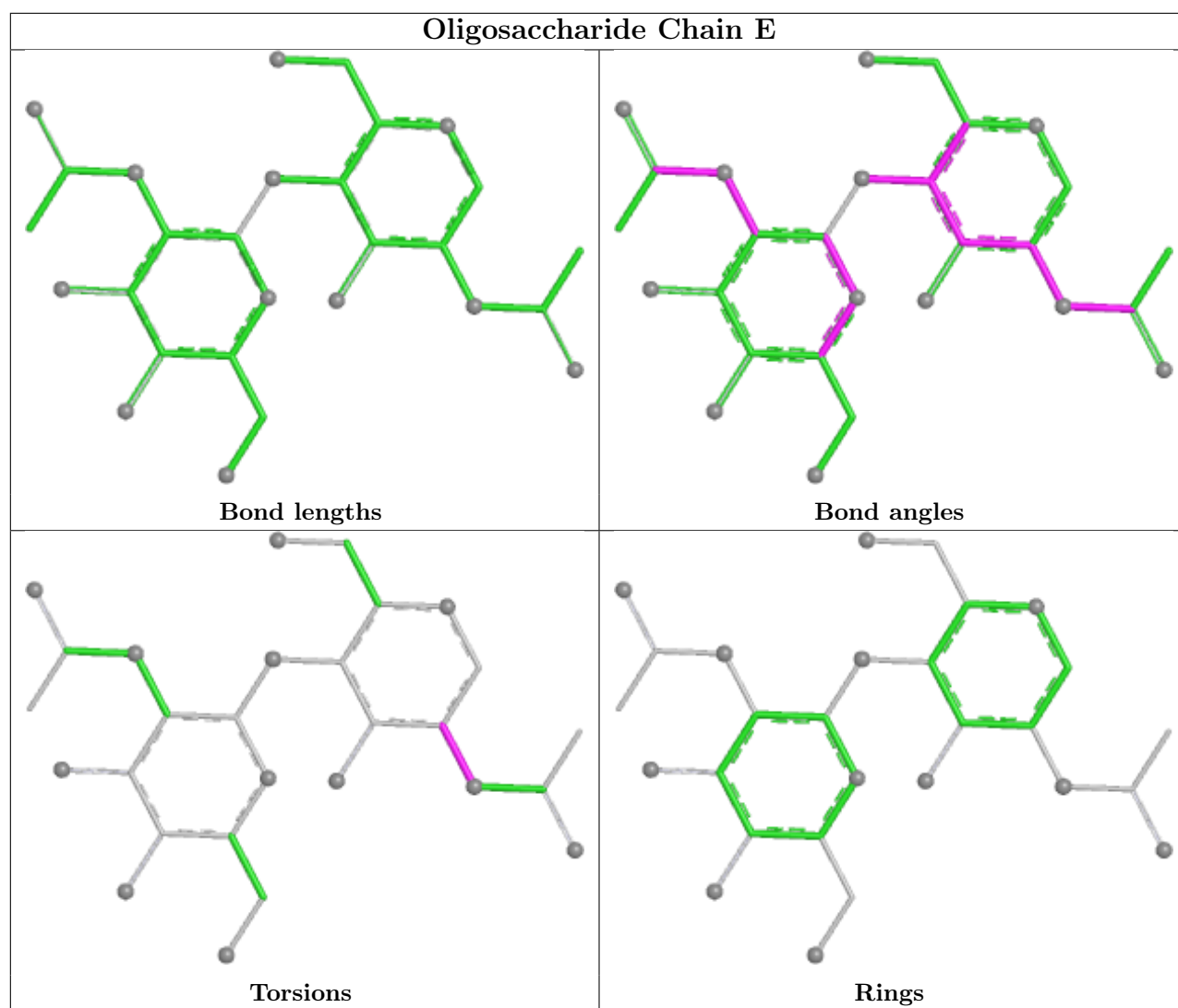
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7

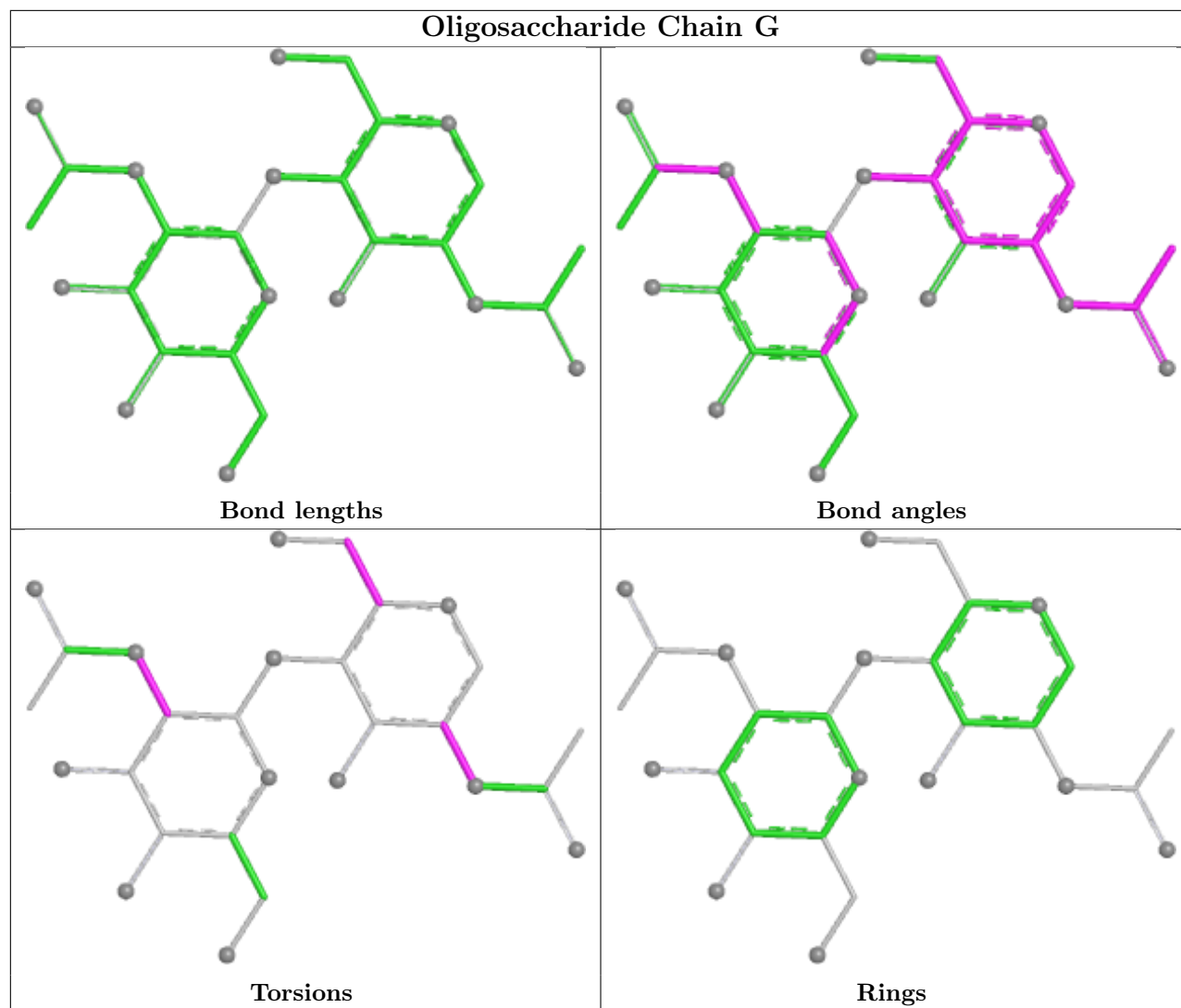
There are no ring outliers.

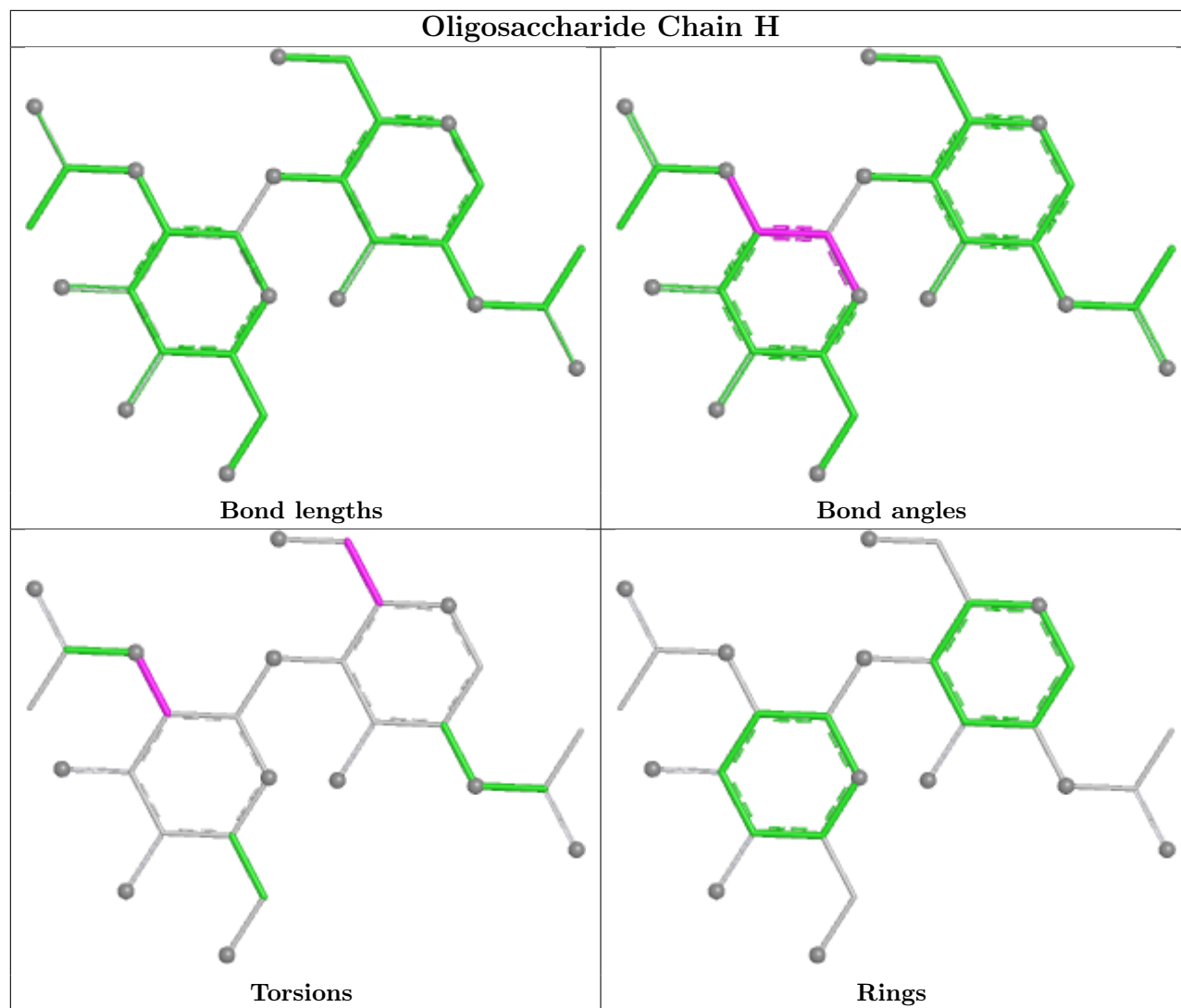
5 monomers are involved in 7 short contacts:

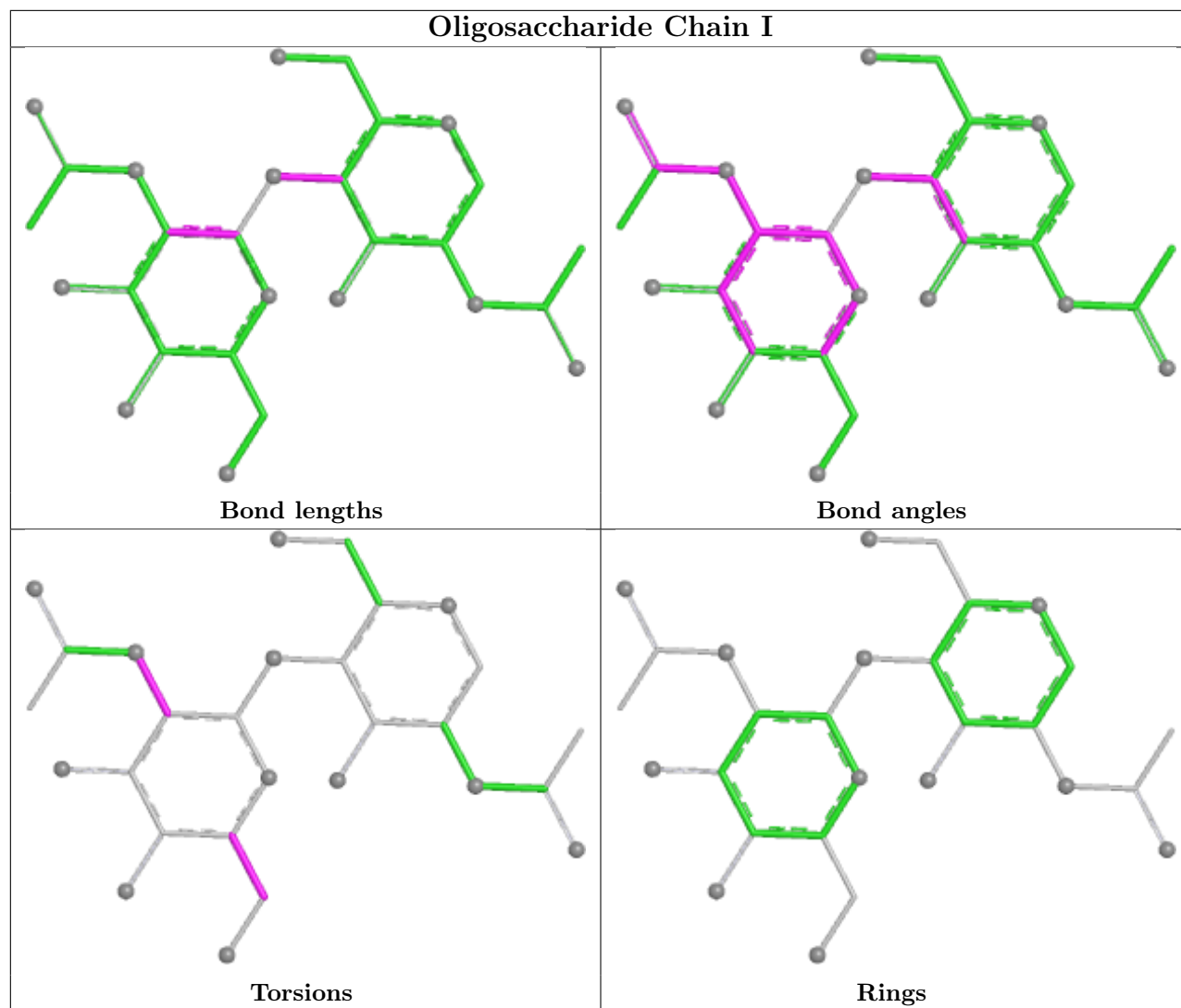
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
2	I	2	NAG	3	0
2	H	2	NAG	1	0
4	K	2	NAG	1	0
3	F	1	NAG	1	0

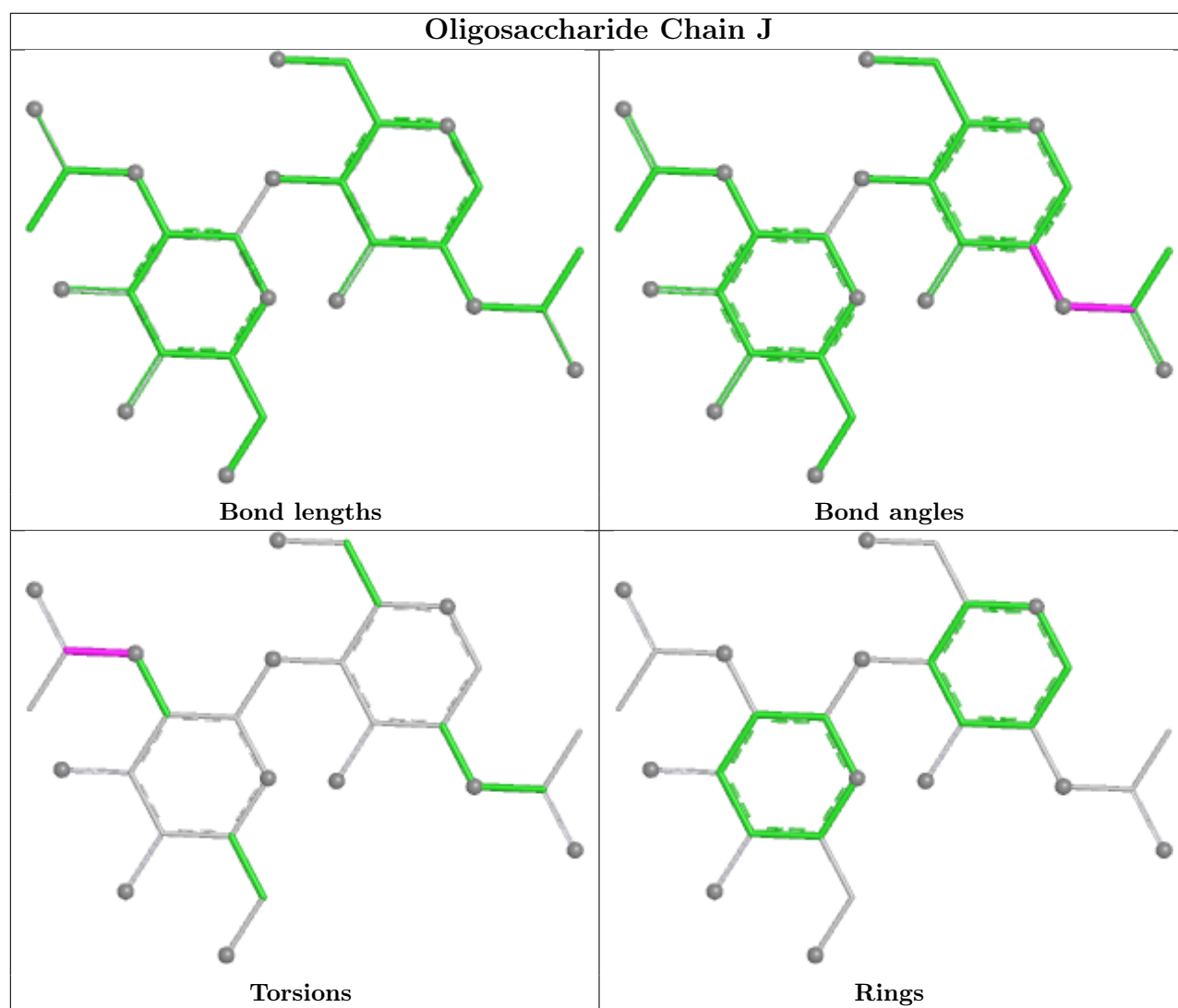
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

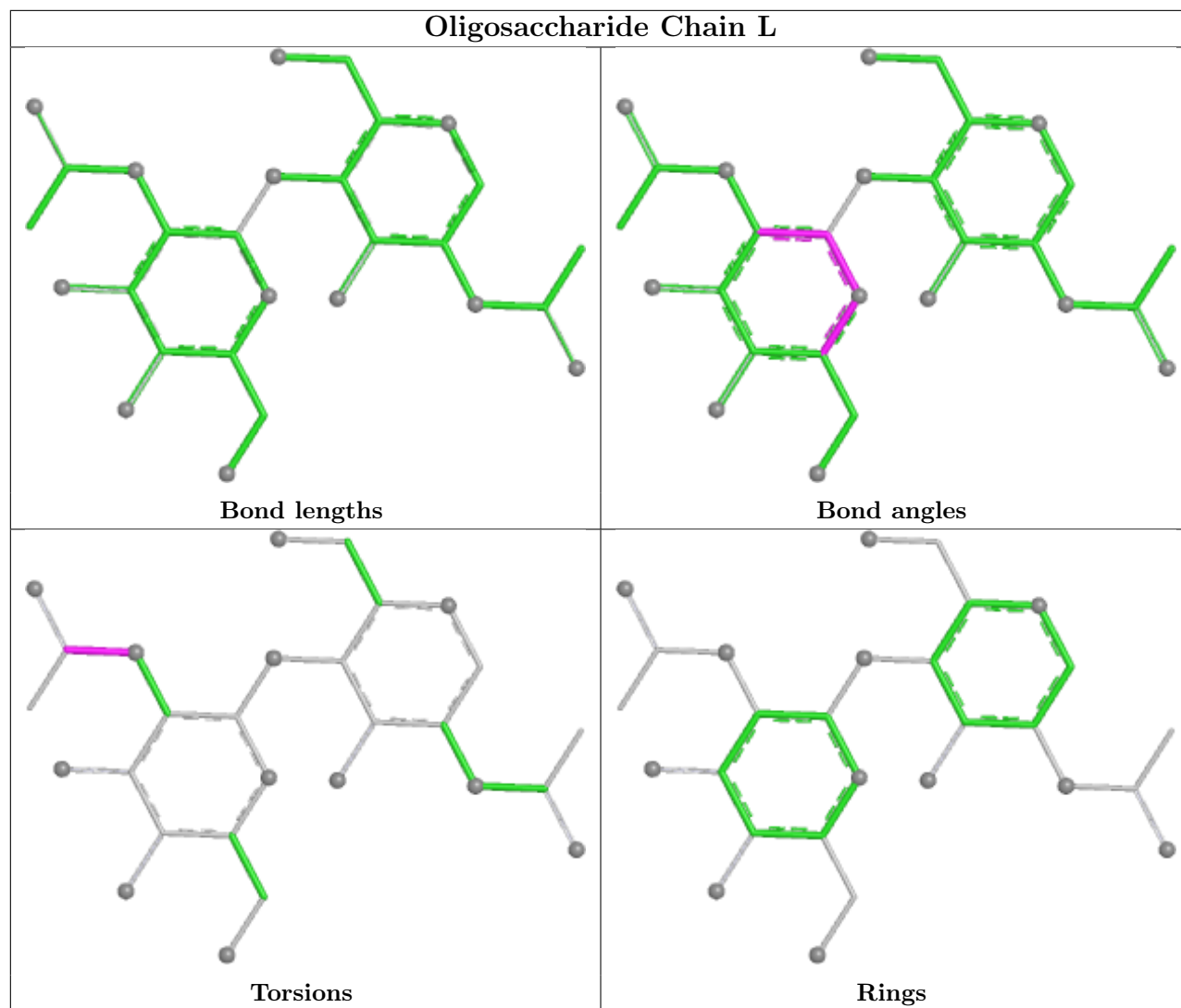


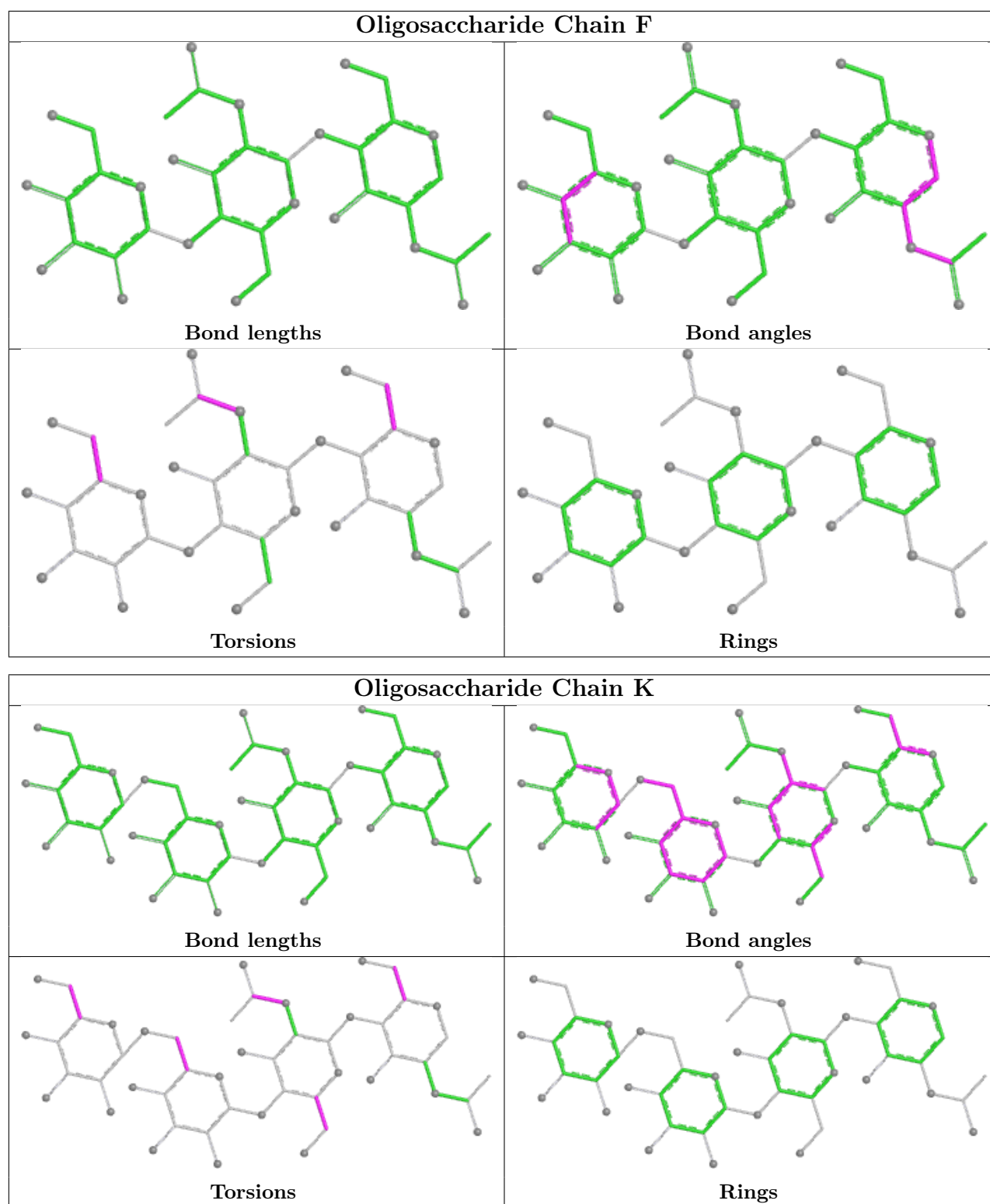












5.6 Ligand geometry [i](#)

22 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	2811	1	14,14,15	0.37	0	17,19,21	0.97	1 (5%)
5	NAG	D	6851	1	14,14,15	0.43	0	17,19,21	1.62	3 (17%)
5	NAG	A	6851	1	14,14,15	0.38	0	17,19,21	1.82	3 (17%)
5	NAG	D	2811	1	14,14,15	0.35	0	17,19,21	0.77	0
5	NAG	C	1501	1	14,14,15	0.38	0	17,19,21	0.88	1 (5%)
5	NAG	B	5201	1	14,14,15	0.50	0	17,19,21	3.87	6 (35%)
5	NAG	A	5201	1	14,14,15	0.38	0	17,19,21	1.93	5 (29%)
5	NAG	D	5201	1	14,14,15	0.33	0	17,19,21	1.38	1 (5%)
5	NAG	C	2191	1	14,14,15	0.29	0	17,19,21	0.82	0
5	NAG	B	2811	1	14,14,15	0.34	0	17,19,21	0.83	0
5	NAG	B	1501	1	14,14,15	0.40	0	17,19,21	1.27	2 (11%)
5	NAG	B	3211	1	14,14,15	0.32	0	17,19,21	1.10	2 (11%)
5	NAG	B	851	1	14,14,15	0.32	0	17,19,21	1.23	2 (11%)
5	NAG	A	851	1	14,14,15	0.30	0	17,19,21	2.51	5 (29%)
5	NAG	D	2191	1	14,14,15	0.34	0	17,19,21	0.58	0
5	NAG	D	3211	1	14,14,15	0.27	0	17,19,21	1.30	3 (17%)
5	NAG	A	2191	1	14,14,15	0.28	0	17,19,21	1.92	2 (11%)
6	FUC	B	1502	-	10,10,11	0.41	0	14,14,16	1.14	1 (7%)
5	NAG	D	1501	1	14,14,15	0.35	0	17,19,21	1.24	2 (11%)
5	NAG	C	3211	1	14,14,15	0.40	0	17,19,21	1.10	1 (5%)
5	NAG	C	5201	1	14,14,15	0.53	0	17,19,21	1.57	3 (17%)
5	NAG	B	6851	1	14,14,15	0.30	0	17,19,21	1.05	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
5	NAG	C	2811	1	-	2/6/23/26	0/1/1/1
5	NAG	D	6851	1	1/1/5/7	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	6851	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	C	1501	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	D	2811	1	-	0/6/23/26	0/1/1/1
5	NAG	B	5201	1	-	1/6/23/26	0/1/1/1
5	NAG	A	5201	1	-	2/6/23/26	0/1/1/1
5	NAG	D	5201	1	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	C	2191	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2811	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1501	1	-	4/6/23/26	0/1/1/1
5	NAG	B	3211	1	-	0/6/23/26	0/1/1/1
5	NAG	B	851	1	-	2/6/23/26	0/1/1/1
5	NAG	A	851	1	-	3/6/23/26	0/1/1/1
5	NAG	D	2191	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	D	3211	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2191	1	-	4/6/23/26	0/1/1/1
6	FUC	B	1502	-	-	-	0/1/1/1
5	NAG	D	1501	1	-	4/6/23/26	0/1/1/1
5	NAG	C	3211	1	-	2/6/23/26	0/1/1/1
5	NAG	C	5201	1	-	1/6/23/26	0/1/1/1
5	NAG	B	6851	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5201	NAG	C2-N2-C7	12.29	139.37	122.90
5	B	5201	NAG	C1-C2-N2	5.91	119.74	110.43
5	A	2191	NAG	C4-C3-C2	-5.72	102.63	111.02
5	A	851	NAG	C4-C3-C2	-5.72	102.64	111.02
5	A	851	NAG	C1-C2-N2	5.54	119.17	110.43

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	6851	NAG	C1
5	C	1501	NAG	C1
5	D	2191	NAG	C1
5	D	5201	NAG	C1
5	D	6851	NAG	C1

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	851	NAG	C1-C2-N2-C7
5	A	5201	NAG	C3-C2-N2-C7
5	A	6851	NAG	C3-C2-N2-C7
5	B	1501	NAG	C1-C2-N2-C7
5	B	5201	NAG	C1-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6851	NAG	2	0
5	B	5201	NAG	1	0
5	A	5201	NAG	2	0
5	D	5201	NAG	4	0
5	C	2191	NAG	2	0
5	B	1501	NAG	4	0
5	B	851	NAG	2	0
5	A	851	NAG	5	0
5	A	2191	NAG	1	0
6	B	1502	FUC	3	0
5	C	5201	NAG	1	0
5	B	6851	NAG	2	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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.