



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 05:07 PM BST

PDB ID : 2BUC  
Title : Crystal Structure Of Porcine Dipeptidyl Peptidase IV (CD26) in Complex with a Tetrahydroisoquinoline Inhibitor  
Authors : Nordhoff, S.; Cerezo-Galvez, S.; Feurer, A.; Hill, O.; Matassa, V.G.; Metz, G.; Rummey, C.; Thiemann, M.; Edwards, P.J.  
Deposited on : 2005-06-09  
Resolution : 2.50 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](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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

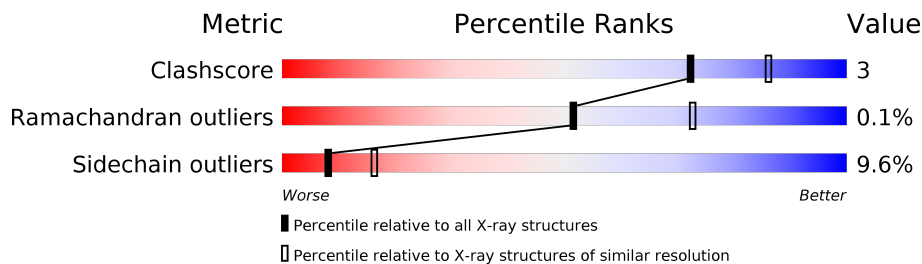
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	
1	C	728	
1	D	728	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%

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	F	1	X	-	-	-
2	NAG	F	2	X	-	-	-
2	NAG	I	2	X	-	-	-
2	NAG	J	1	X	-	-	-
2	NAG	K	1	X	-	-	-
2	NAG	L	2	X	-	-	-
3	NAG	A	1092	X	-	-	-
3	NAG	C	1092	X	-	-	-
3	NAG	D	1085	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DIPEPTIDYL PEPTIDASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5966	3825	986	1132	23	0	0	0
1	B	728	5966	3825	986	1132	23	0	0	0
1	C	728	5966	3825	986	1132	23	0	0	0
1	D	728	5966	3825	986	1132	23	0	0	0

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



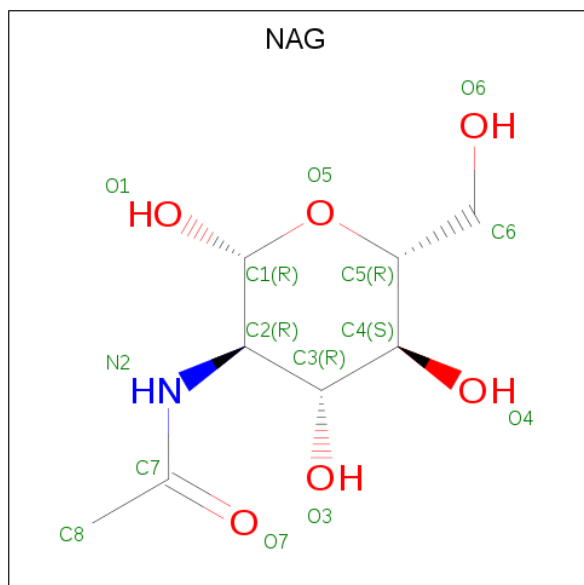
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0
2	G	2	28	16	2	10	0	0	0
2	H	2	28	16	2	10	0	0	0
2	I	2	28	16	2	10	0	0	0
2	J	2	28	16	2	10	0	0	0
2	K	2	28	16	2	10	0	0	0
2	L	2	28	16	2	10	0	0	0

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



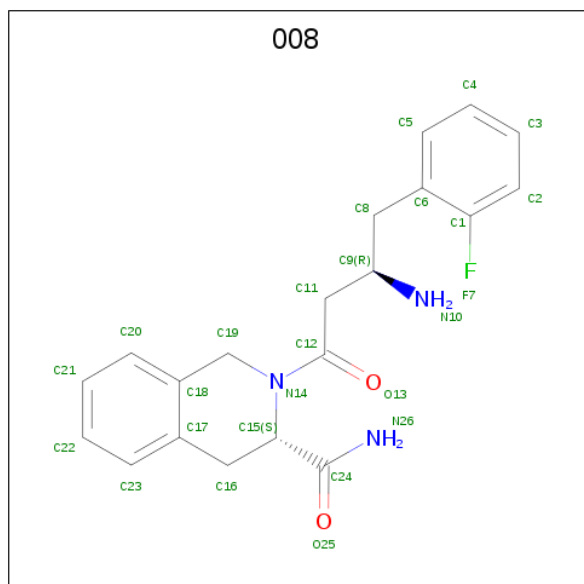
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0

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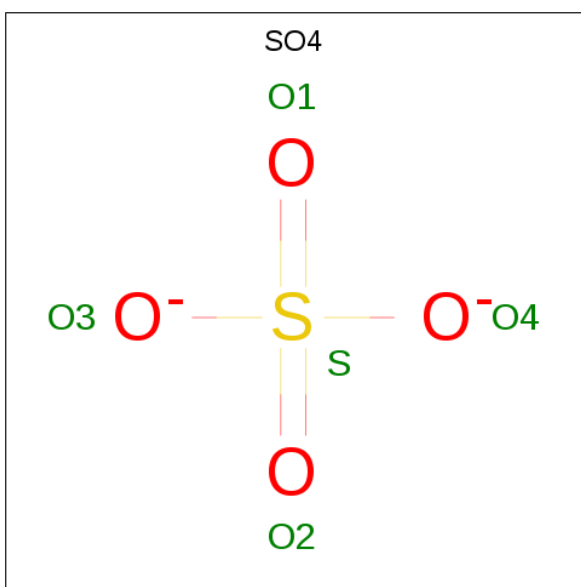
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is (S)-2-[(R)-3-AMINO-4-(2-FLUORO-PHENYL)-BUTYRYL]-1,2,3,4-TETRAHYDRO-ISOQUINOLINE-3-CARBOXYLIC ACID AMIDE (three-letter code: 008) (formula: C<sub>20</sub>H<sub>22</sub>FN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
4	B	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
4	C	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
4	D	1	Total	C	F	N	O	0	0
			26	20	1	3	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

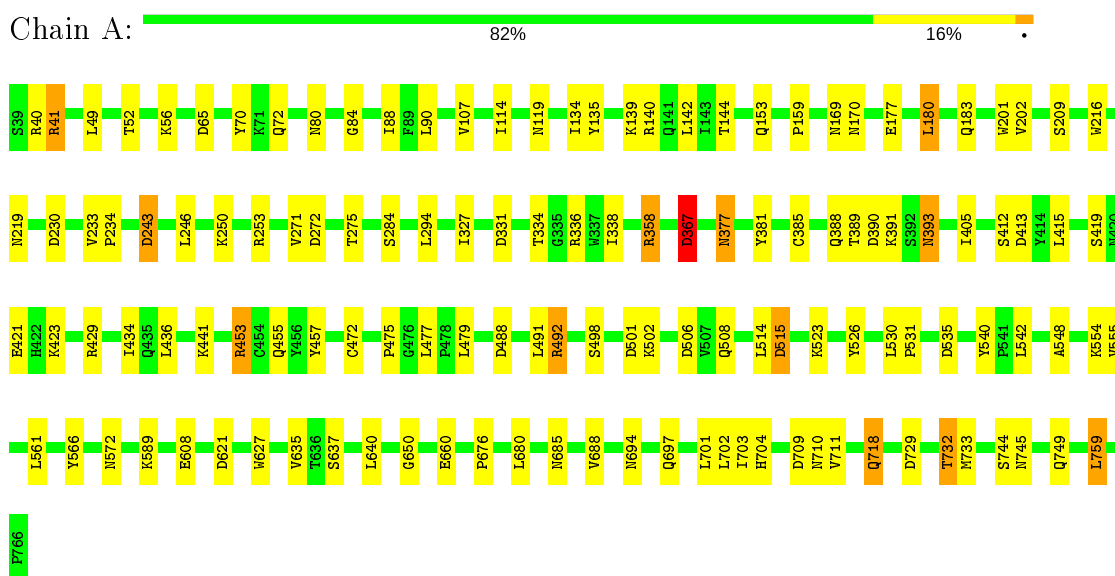
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	242	Total O 242 242	0	0
6	B	248	Total O 248 248	0	0
6	C	228	Total O 228 228	0	0
6	D	233	Total O 233 233	0	0

### 3 Residue-property plots [i](#)

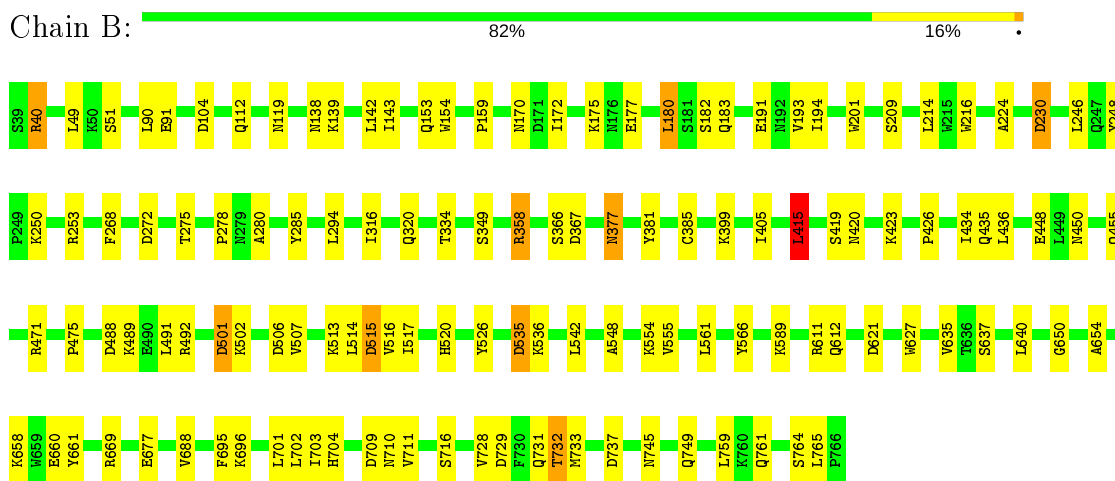
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

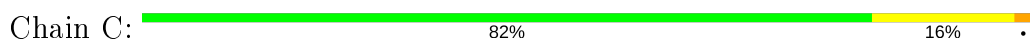
- Molecule 1: DIPEPTIDYL PEPTIDASE IV



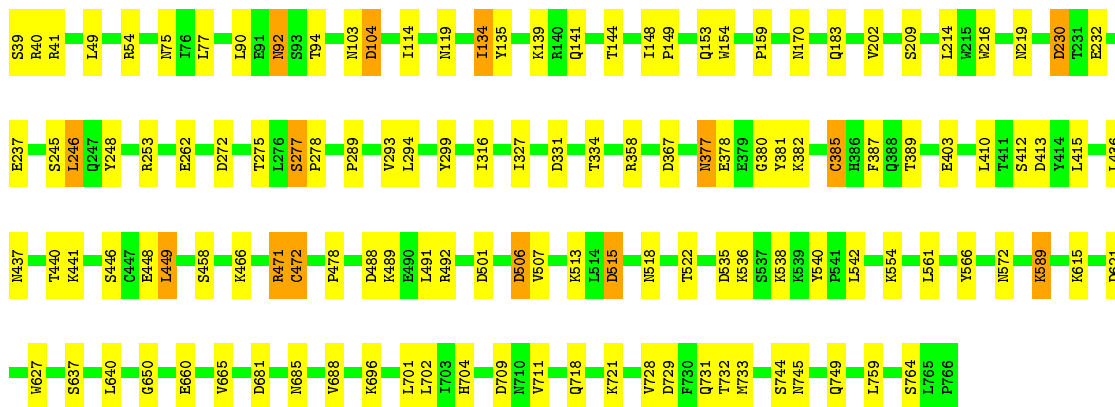
- Molecule 1: DIPEPTIDYL PEPTIDASE IV



- Molecule 1: DIPEPTIDYL PEPTIDASE IV

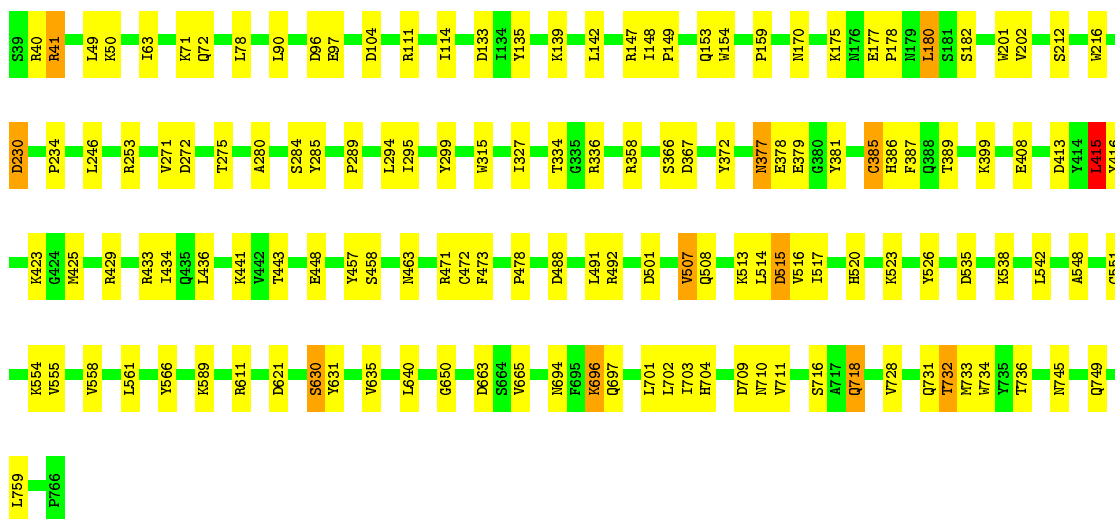






- Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain D: 81% 18%



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

Chain E: 100%

NAG1  
NAG2

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

Chain F: 100%


NAG1  
NAG2

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

Chain G:  50% 50%

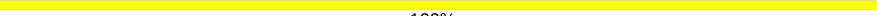
NA01  
NA02

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

Chain H:  100%

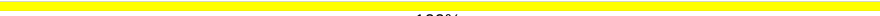
NA01  
NA02

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

Chain I:  100%


NA01  
NA02

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

Chain J:  100%

NA01  
NA02

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

Chain K:  100%

NA01  
NA02

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

Chain L:  100%

NA01  
NA02

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

Chain M:  100%

NA01  
NA02

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.64Å 117.49Å 133.06Å 112.44° 94.72° 91.30°	Depositor
Resolution (Å)	19.28 – 2.50	Depositor
% Data completeness (in resolution range)	100.0 (19.28-2.50)	Depositor
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.221 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	25421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

## 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: 008, NAG, SO4

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	0.31	0/6141	0.65	14/8353 (0.2%)
1	B	0.31	0/6141	0.65	14/8353 (0.2%)
1	C	0.32	0/6141	0.64	15/8353 (0.2%)
1	D	0.31	0/6141	0.64	14/8353 (0.2%)
All	All	0.31	0/24564	0.65	57/33412 (0.2%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	390	ASP	CB-CG-OD2	6.35	124.02	118.30
1	D	535	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	535	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	272	ASP	CB-CG-OD2	6.05	123.74	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5966	0	5661	47	0
1	B	5966	0	5662	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5966	0	5662	41	0
1	D	5966	0	5660	48	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
3	A	56	0	52	0	0
3	B	56	0	52	0	0
3	C	70	0	65	0	0
3	D	28	0	26	0	0
4	A	26	0	22	1	0
4	B	26	0	22	1	0
4	C	26	0	22	0	0
4	D	26	0	22	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	242	0	0	1	0
6	B	248	0	0	1	0
6	C	228	0	0	0	0
6	D	233	0	0	1	0
All	All	25421	0	23153	162	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 3.

The worst 5 of 162 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:D:551:CYS:SG	6:D:2188:HOH:O	2.41	0.78
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.37	0.73
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.71	0.70
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.75	0.68
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.42	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/728 (100%)	693 (96%)	32 (4%)	1 (0%)	51	73
1	B	726/728 (100%)	697 (96%)	28 (4%)	1 (0%)	51	73
1	C	726/728 (100%)	696 (96%)	29 (4%)	1 (0%)	51	73
1	D	726/728 (100%)	696 (96%)	29 (4%)	1 (0%)	51	73
All	All	2904/2912 (100%)	2782 (96%)	118 (4%)	4 (0%)	51	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	B	40	ARG
1	D	40	ARG
1	C	40	ARG

### 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	652/652 (100%)	592 (91%)	60 (9%)	9	18
1	B	652/652 (100%)	590 (90%)	62 (10%)	8	17
1	C	652/652 (100%)	588 (90%)	64 (10%)	8	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	652/652 (100%)	588 (90%)	64 (10%)	8	15
All	All	2608/2608 (100%)	2358 (90%)	250 (10%)	8	16

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	701	LEU
1	C	245	SER
1	D	520	HIS
1	B	732	THR
1	C	92	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	718	GLN
1	C	377	ASN
1	D	694	ASN
1	C	169	ASN
1	C	183	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

18 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all  $Z$  scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	E	1	1,2	14,14,15	0.51	0	17,19,21	0.99	2 (11%)
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	1.10	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.56	0	17,19,21	1.62	3 (17%)
2	NAG	F	2	2	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.60	0	17,19,21	0.98	2 (11%)
2	NAG	G	2	2	14,14,15	0.52	0	17,19,21	0.88	0
2	NAG	H	1	1,2	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.49	0	17,19,21	0.92	1 (5%)
2	NAG	I	2	2	14,14,15	0.48	0	17,19,21	1.20	2 (11%)
2	NAG	J	1	1,2	14,14,15	0.51	0	17,19,21	1.14	2 (11%)
2	NAG	J	2	2	14,14,15	0.50	0	17,19,21	1.08	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.37	0	17,19,21	1.53	2 (11%)
2	NAG	K	2	2	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
2	NAG	L	2	2	14,14,15	0.63	0	17,19,21	1.40	3 (17%)
2	NAG	M	1	1,2	14,14,15	0.51	0	17,19,21	0.77	0
2	NAG	M	2	2	14,14,15	0.51	0	17,19,21	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	F	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C1-O5-C5	5.16	119.18	112.19
2	F	1	NAG	O4-C4-C3	4.01	119.63	110.35
2	L	2	NAG	C1-O5-C5	4.00	117.61	112.19
2	I	2	NAG	C1-O5-C5	3.73	117.24	112.19
2	F	2	NAG	C1-O5-C5	3.51	116.95	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	2	NAG	C1
2	F	1	NAG	C1
2	J	1	NAG	C1
2	I	2	NAG	C1
2	L	2	NAG	C1

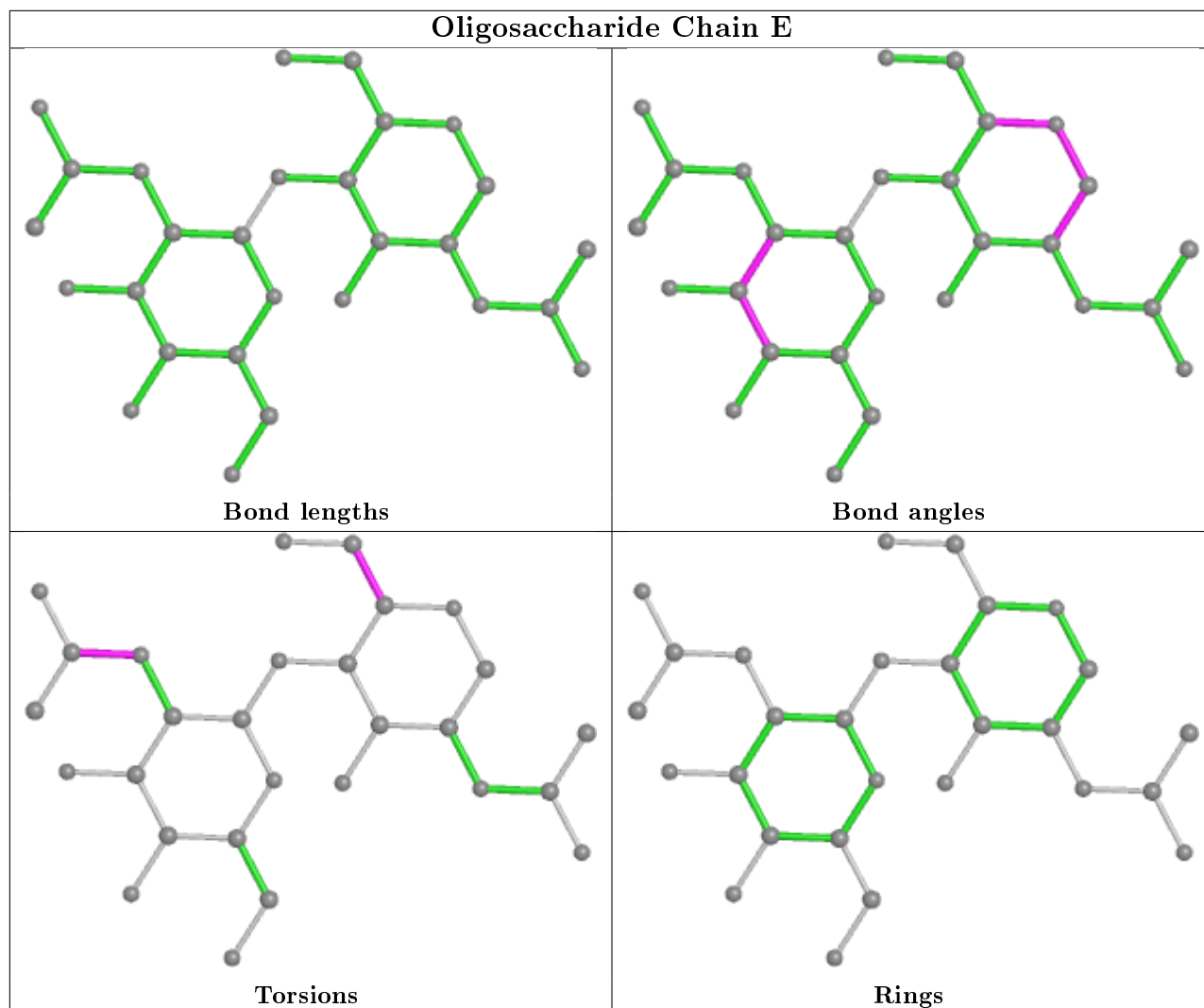
5 of 40 torsion outliers are listed below:

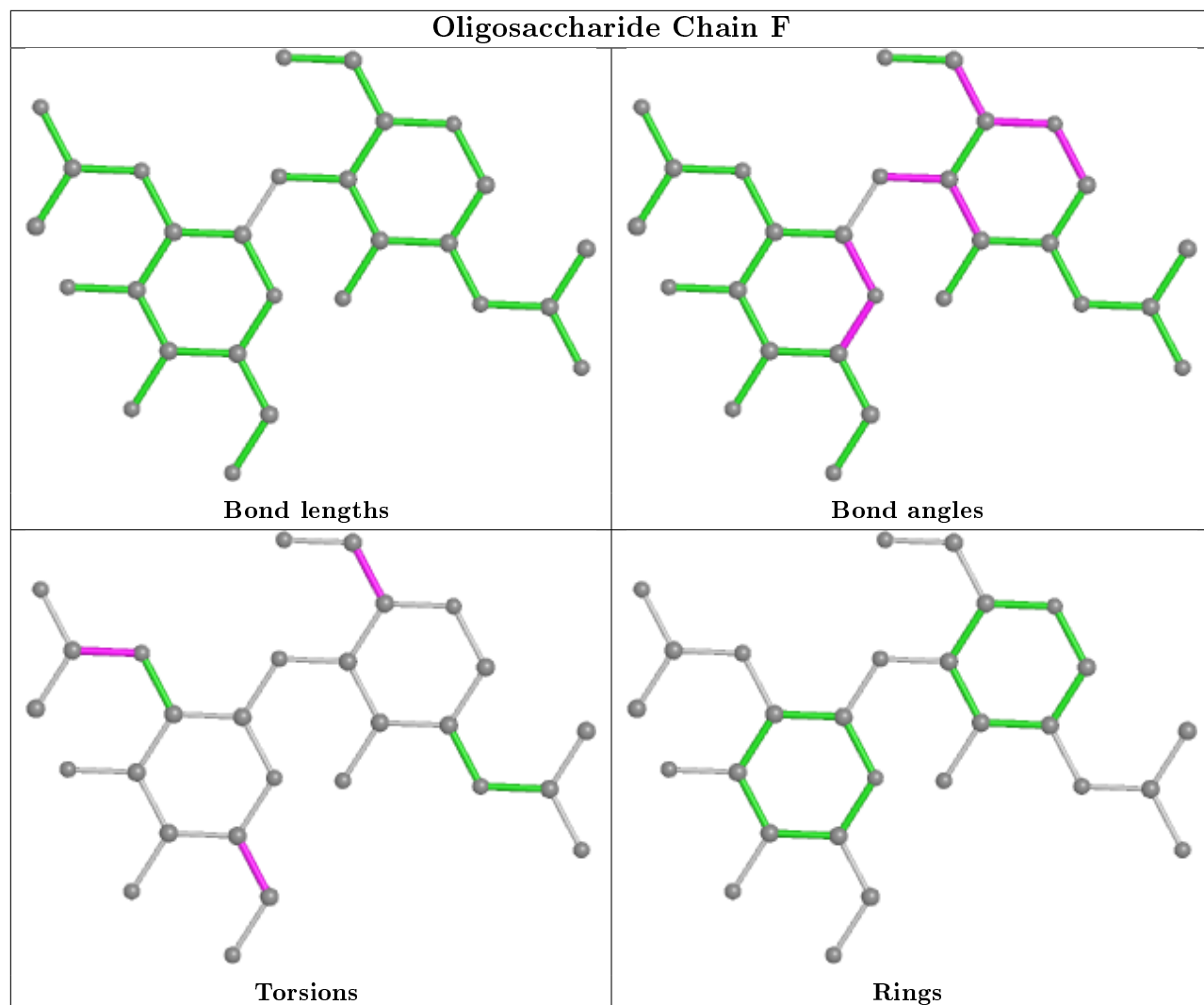
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2

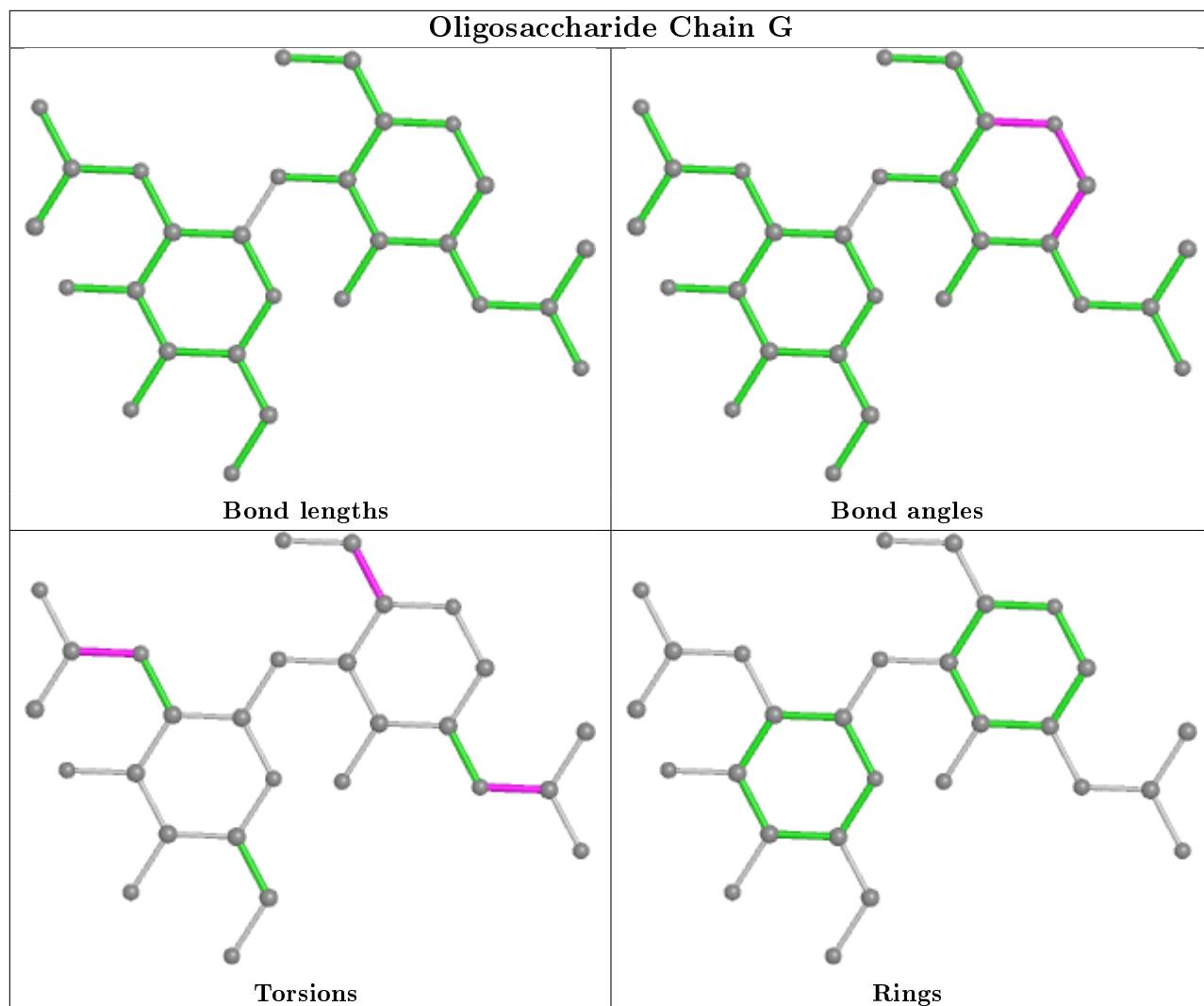
There are no ring outliers.

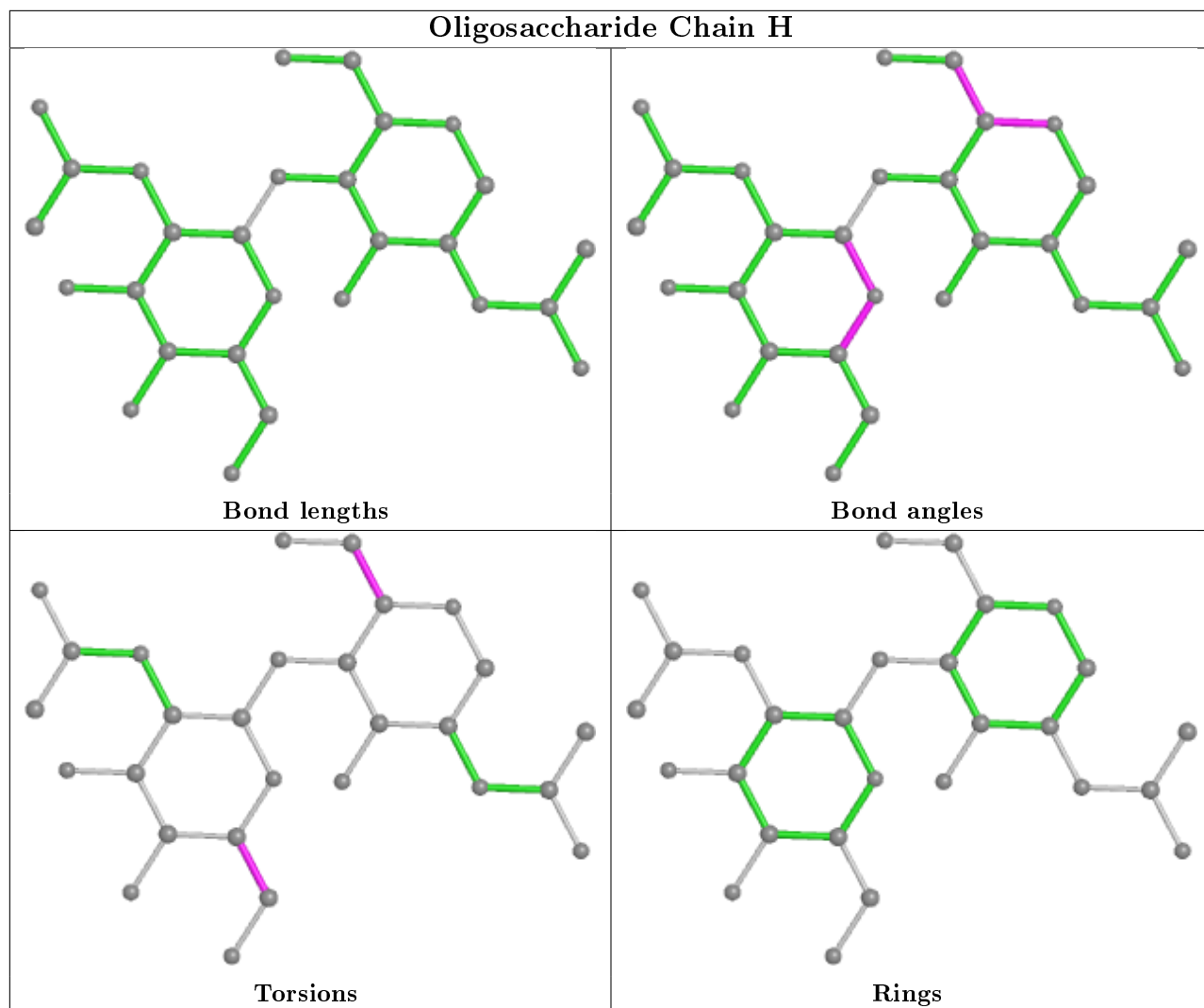
No monomer is involved in short contacts.

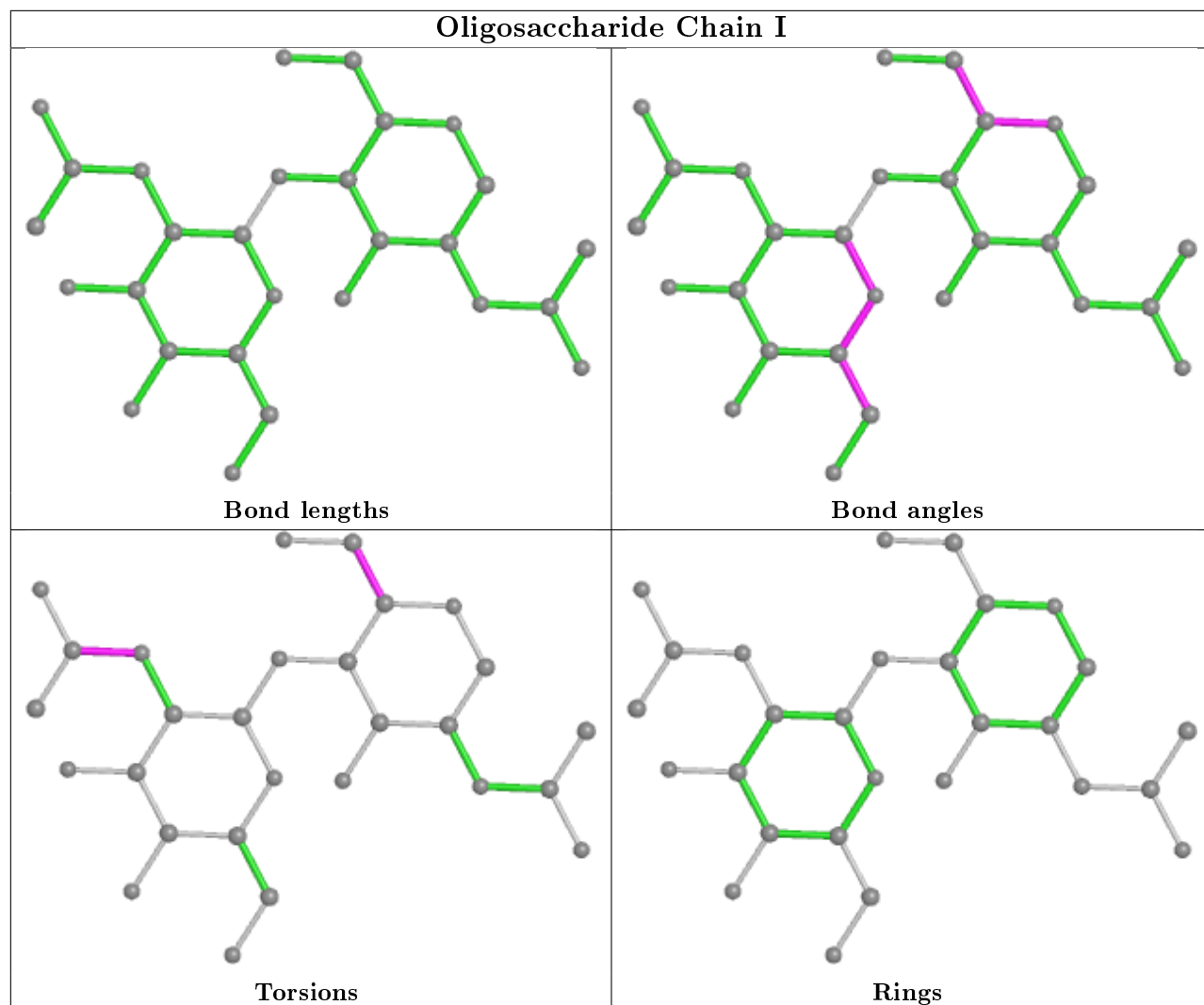
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

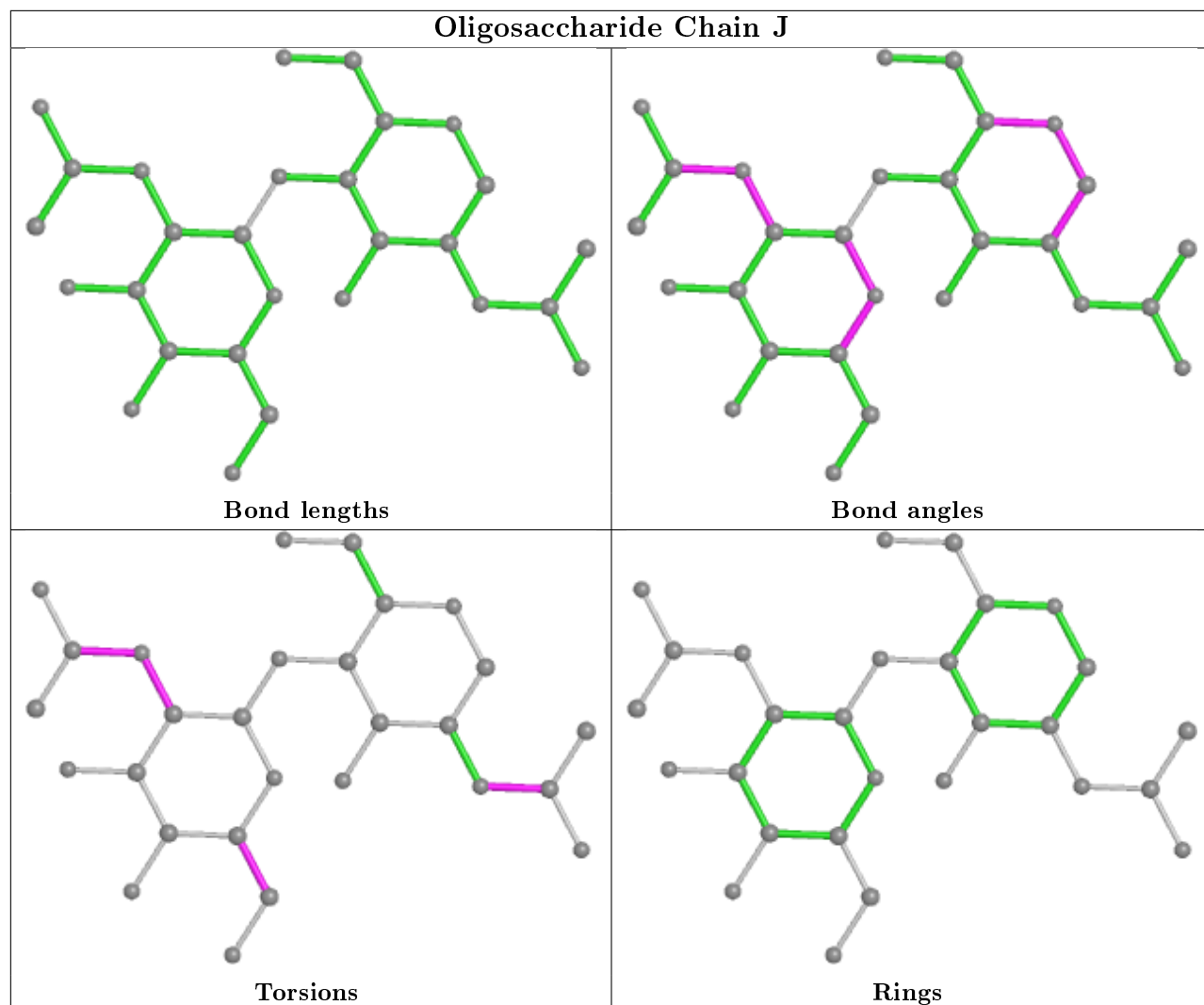




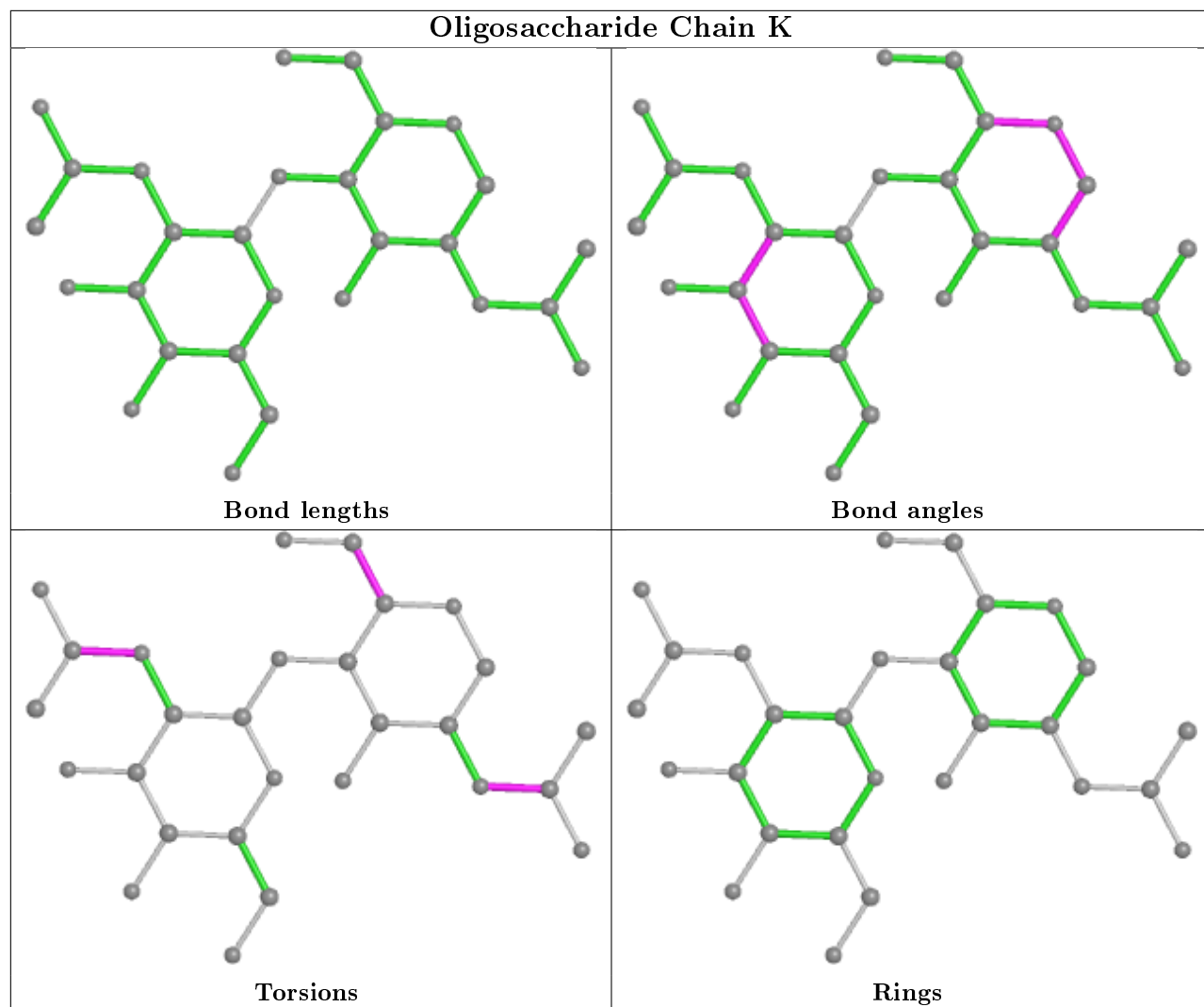


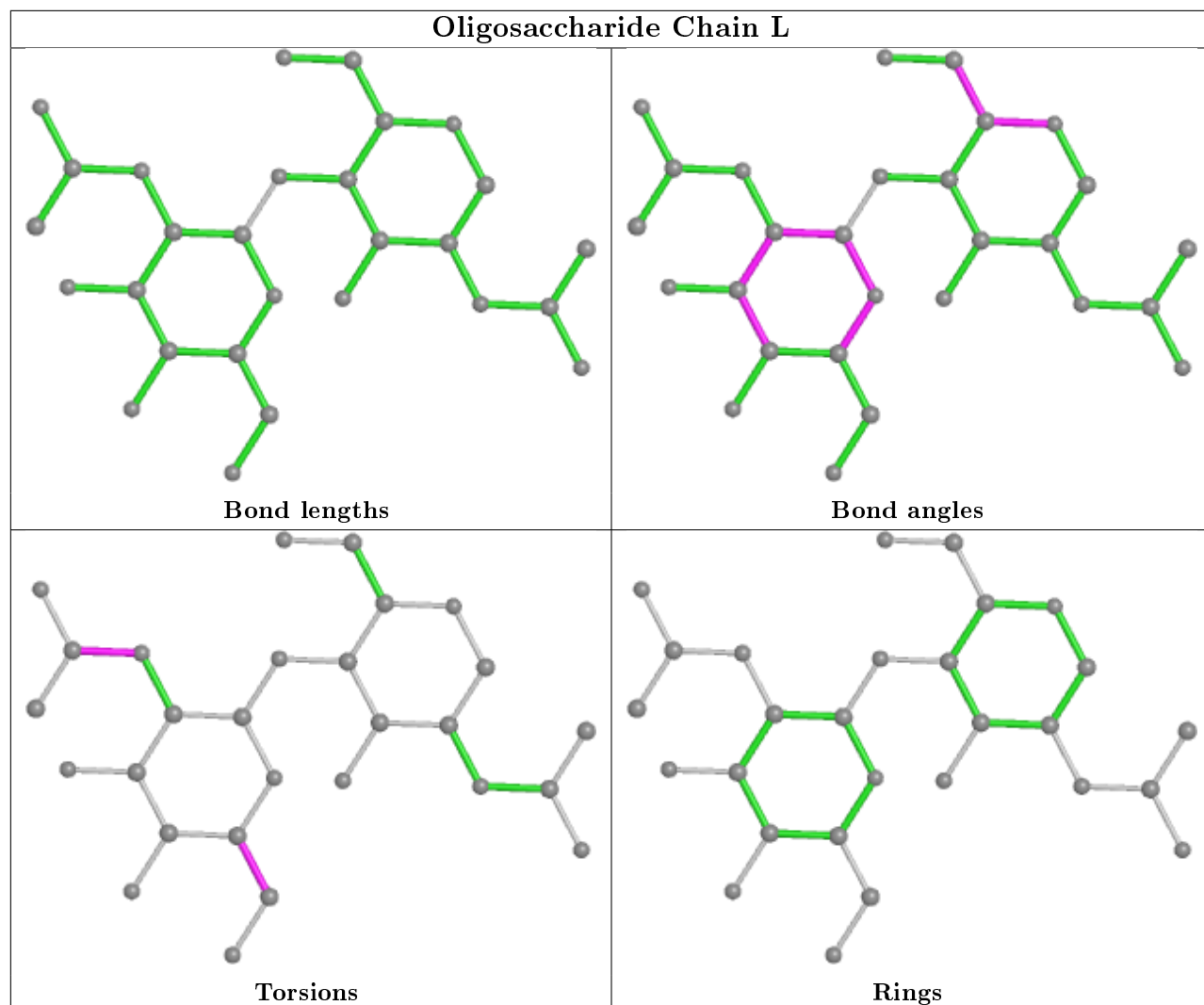


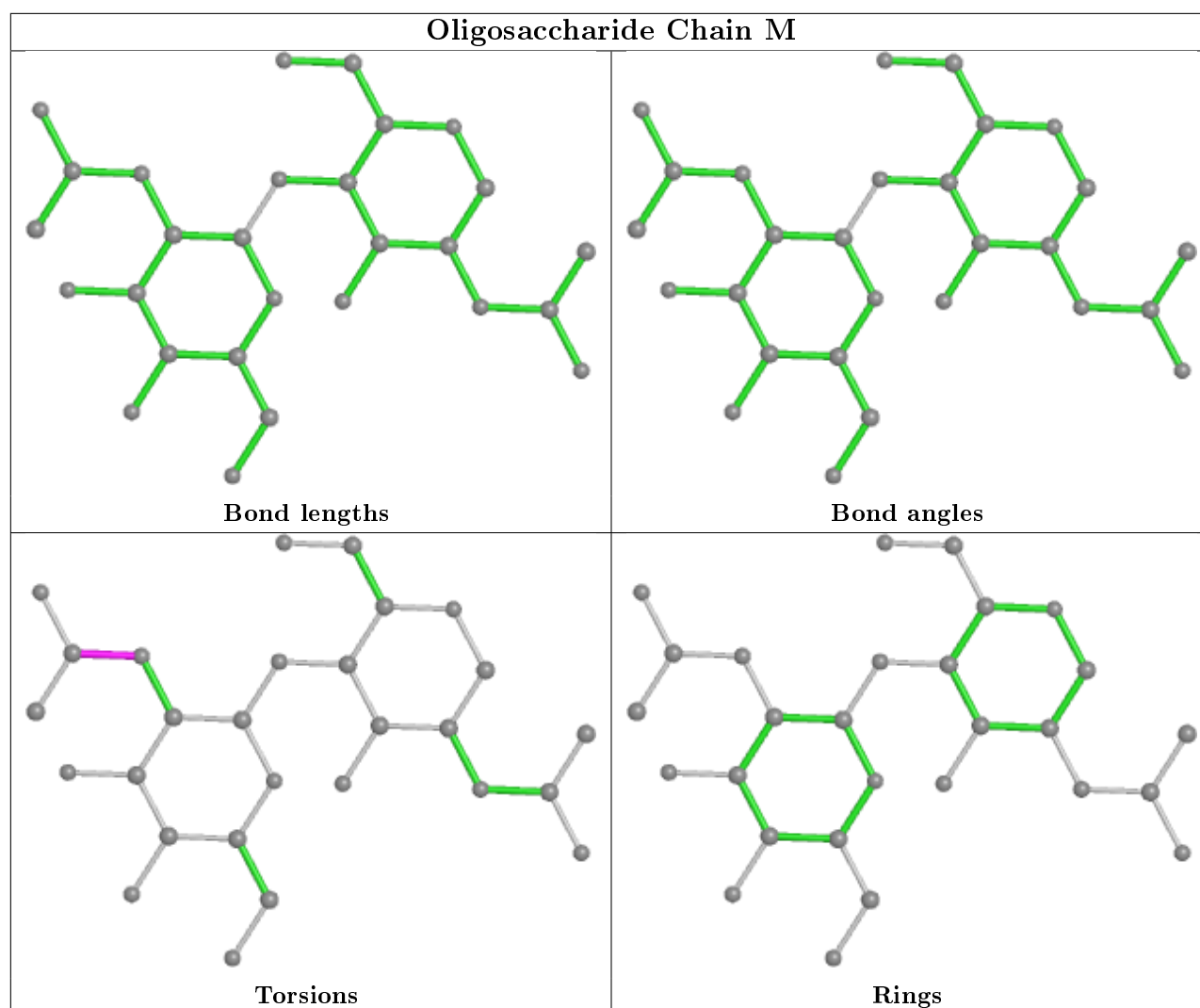












## 5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	008	A	1767	-	28,28,28	0.59	0	30,39,39	1.31	1 (3%)
3	NAG	D	1279	1	14,14,15	0.50	0	17,19,21	0.74	0
5	SO4	B	1768	-	4,4,4	0.15	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	1769	-	4,4,4	0.14	0	6,6,6	0.11	0
3	NAG	C	1279	1	14,14,15	0.44	0	17,19,21	1.10	1 (5%)
5	SO4	A	1768	-	4,4,4	0.14	0	6,6,6	0.06	0
4	008	B	1767	-	28,28,28	0.58	0	30,39,39	1.31	2 (6%)
4	008	C	1767	-	28,28,28	0.55	0	30,39,39	1.18	1 (3%)
3	NAG	A	1321	1	14,14,15	0.49	0	17,19,21	0.89	0
3	NAG	A	1092	1	14,14,15	0.60	0	17,19,21	1.03	1 (5%)
3	NAG	B	1321	1	14,14,15	0.51	0	17,19,21	0.84	1 (5%)
3	NAG	C	1321	1	14,14,15	0.51	0	17,19,21	0.70	0
5	SO4	A	1769	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	D	1768	-	4,4,4	0.15	0	6,6,6	0.06	0
3	NAG	A	1279	1	14,14,15	0.52	0	17,19,21	0.91	1 (5%)
3	NAG	A	1085	1	14,14,15	0.53	0	17,19,21	0.72	0
3	NAG	C	1229	1	14,14,15	0.48	0	17,19,21	1.13	1 (5%)
5	SO4	C	1769	-	4,4,4	0.13	0	6,6,6	0.06	0
3	NAG	B	1229	1	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
3	NAG	B	1085	1	14,14,15	0.47	0	17,19,21	0.78	1 (5%)
3	NAG	C	1085	1	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
3	NAG	B	1279	1	14,14,15	0.51	0	17,19,21	0.86	1 (5%)
3	NAG	D	1085	1	14,14,15	0.54	0	17,19,21	1.47	4 (23%)
3	NAG	C	1092	1	14,14,15	0.50	0	17,19,21	0.77	0
5	SO4	D	1769	-	4,4,4	0.13	0	6,6,6	0.07	0
4	008	D	1767	-	28,28,28	0.58	0	30,39,39	1.27	4 (13%)
5	SO4	C	1768	-	4,4,4	0.15	0	6,6,6	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	008	A	1767	-	-	0/15/28/28	0/3/3/3
3	NAG	A	1321	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1229	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1279	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1085	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1092	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	1085	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1279	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1085	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	1092	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	1279	1	-	2/6/23/26	0/1/1/1
4	008	C	1767	-	-	0/15/28/28	0/3/3/3
3	NAG	C	1279	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1321	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1085	1	-	4/6/23/26	0/1/1/1
4	008	D	1767	-	-	0/15/28/28	0/3/3/3
4	008	B	1767	-	-	0/15/28/28	0/3/3/3
3	NAG	C	1321	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1229	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1767	008	C16-C15-N14	4.33	114.21	109.91
4	B	1767	008	C16-C15-N14	3.76	113.65	109.91
4	C	1767	008	C16-C15-N14	3.35	113.23	109.91
3	D	1085	NAG	C1-O5-C5	3.16	116.48	112.19
3	D	1085	NAG	C3-C4-C5	2.99	115.58	110.24

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1092	NAG	C1
3	D	1085	NAG	C1
3	C	1092	NAG	C1

5 of 31 torsion outliers are listed below:

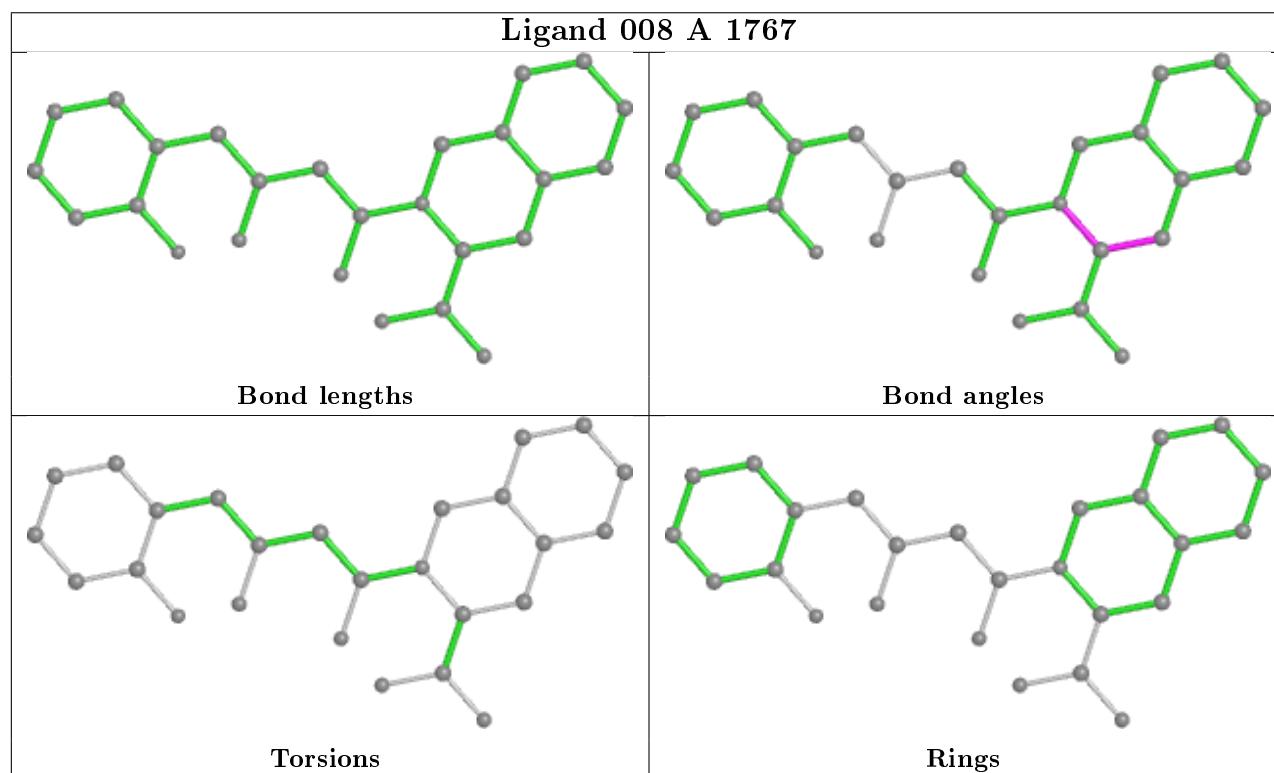
Mol	Chain	Res	Type	Atoms
3	D	1279	NAG	C8-C7-N2-C2
3	D	1279	NAG	O7-C7-N2-C2
3	A	1092	NAG	C8-C7-N2-C2
3	A	1092	NAG	O7-C7-N2-C2
3	C	1321	NAG	C8-C7-N2-C2

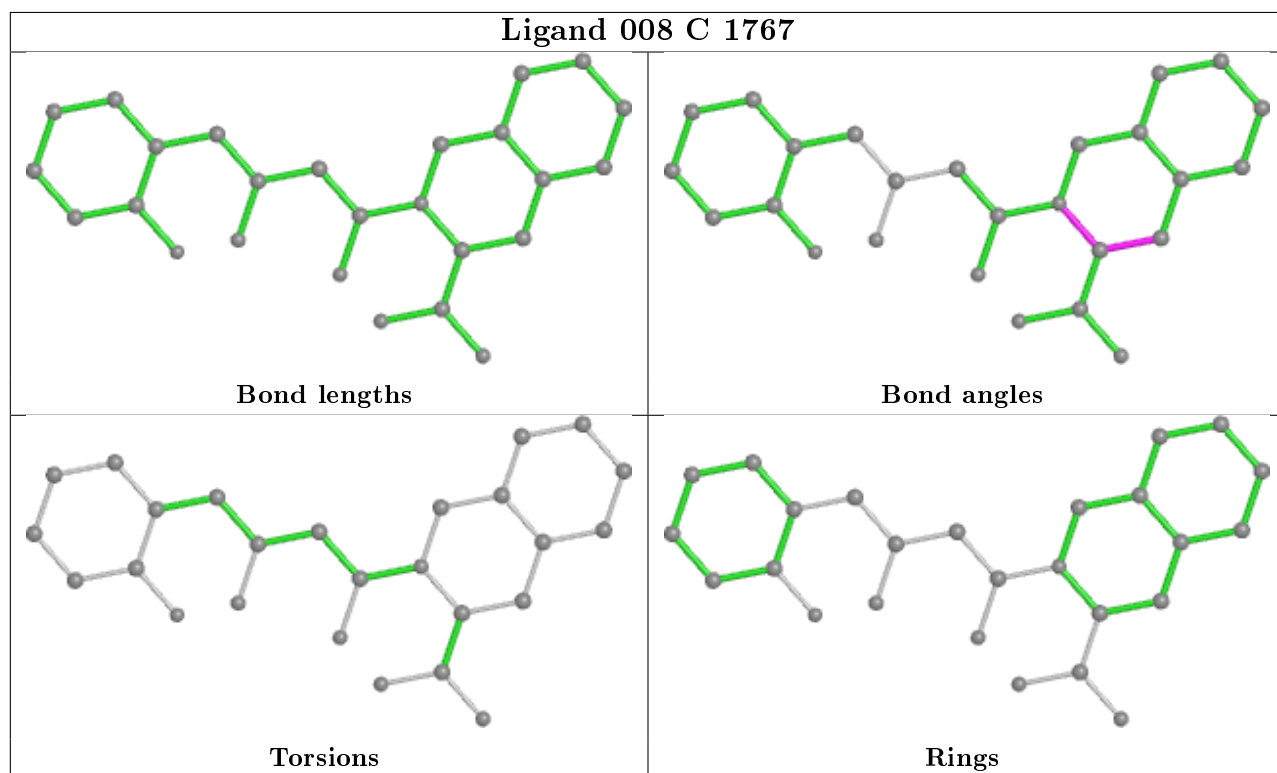
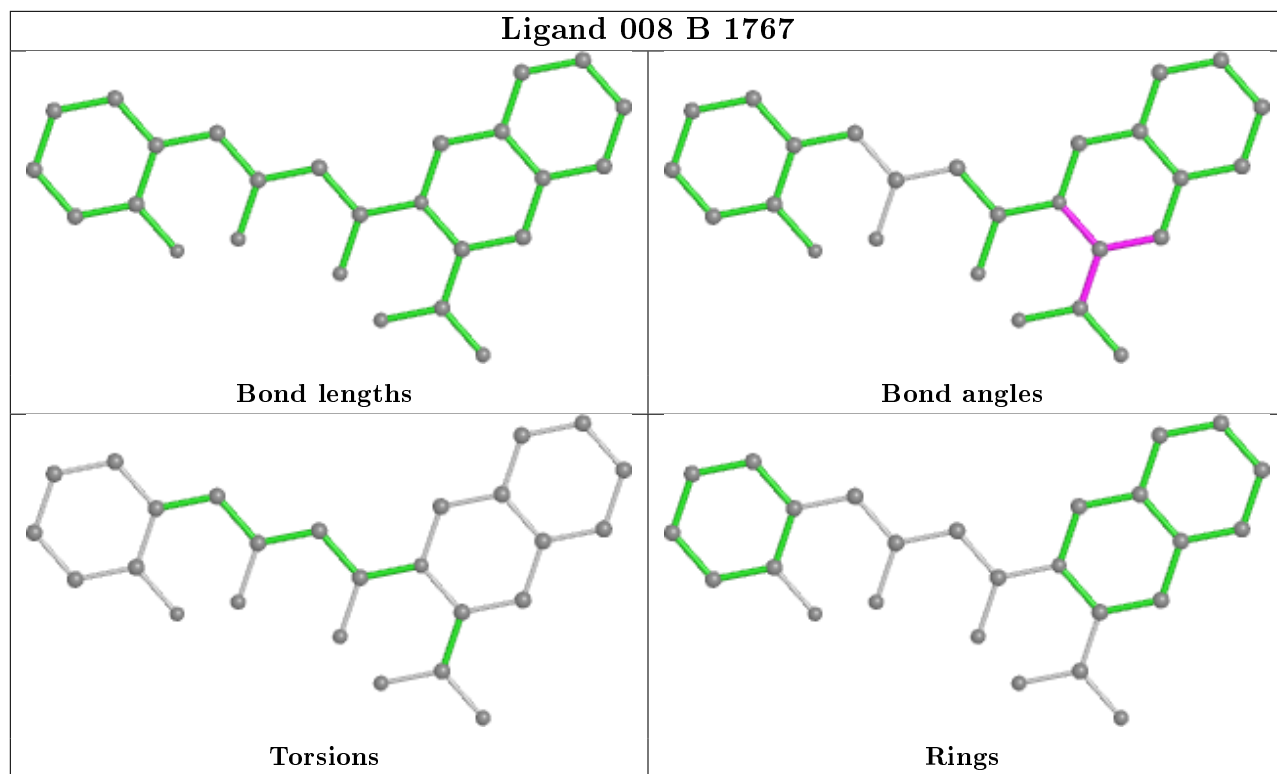
There are no ring outliers.

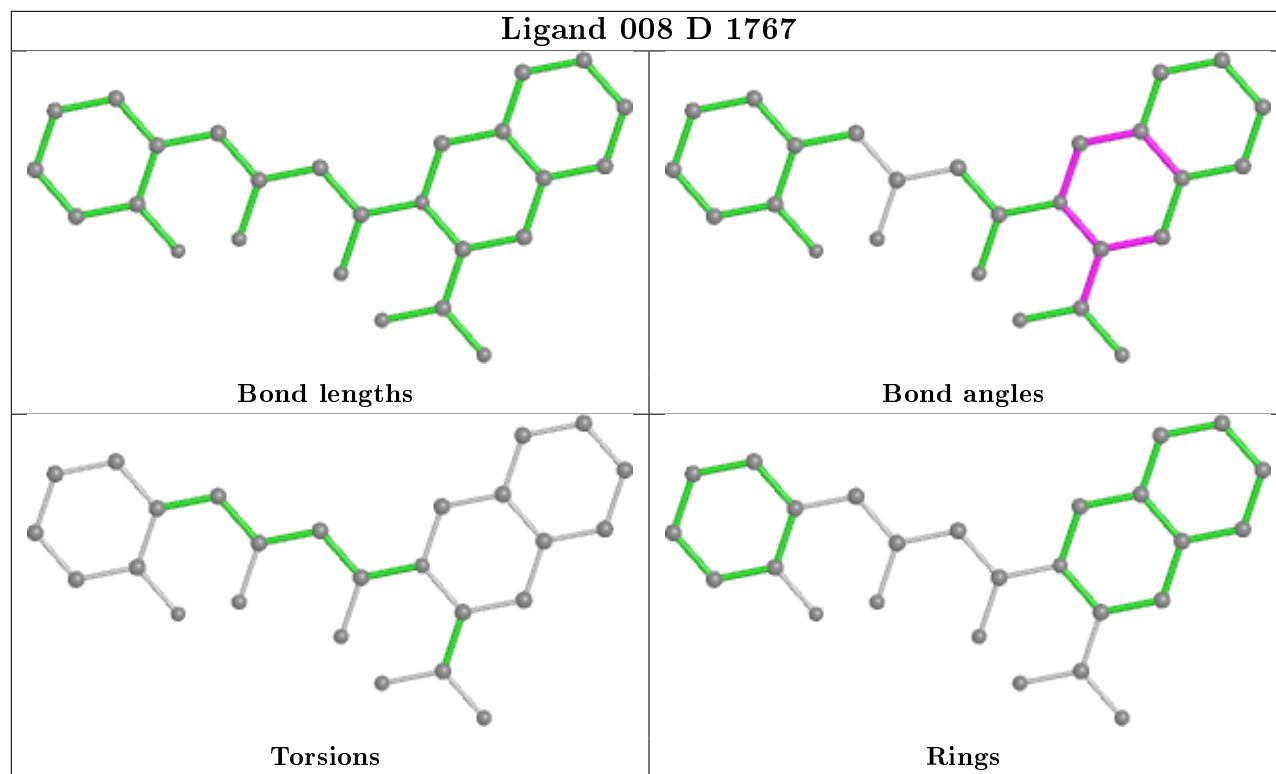
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1767	008	1	0
4	B	1767	008	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.