



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:07 AM UTC

PDB ID : 2BUC / pdb_00002buc
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 Full wwPDB X-ray Structure Validation 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

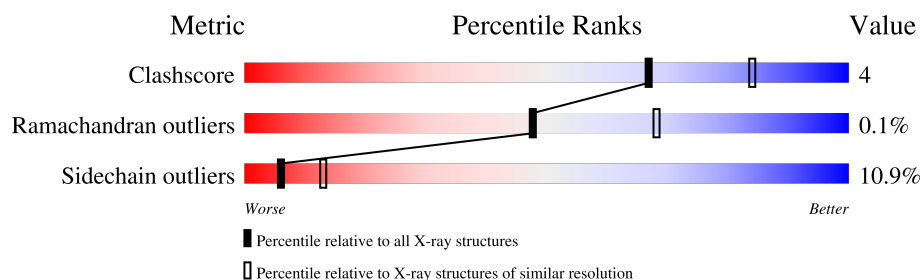
1 Overall quality at a glance

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

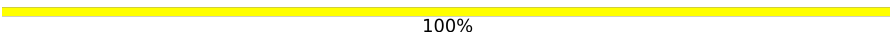
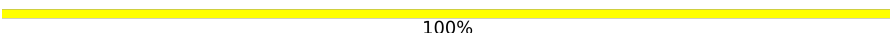
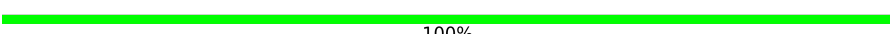
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	728	81% 18% .
1	B	728	82% 17% .
1	C	728	82% 16% .
1	D	728	82% 17% .
2	E	2	100%
2	F	2	100%
2	G	2	50% 50%
2	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	I	2	 50% 50%
2	J	2	 100%
2	K	2	 100%
2	L	2	 50% 50%
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
1	A	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			

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



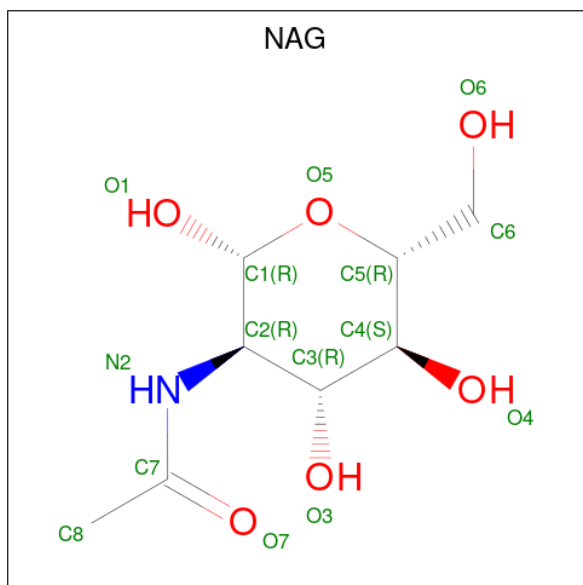
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2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

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

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



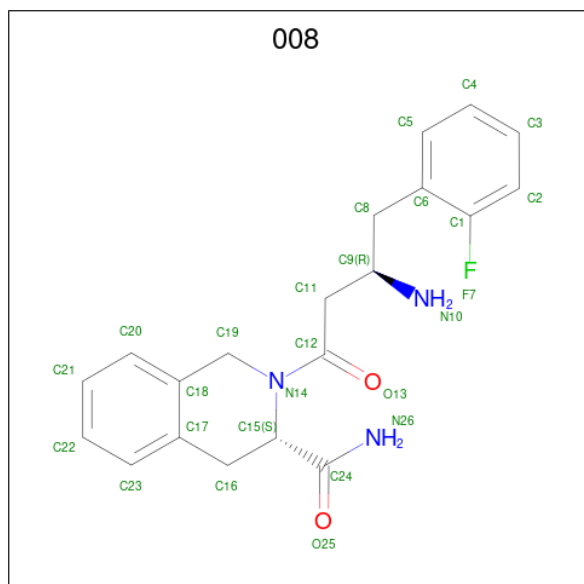
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

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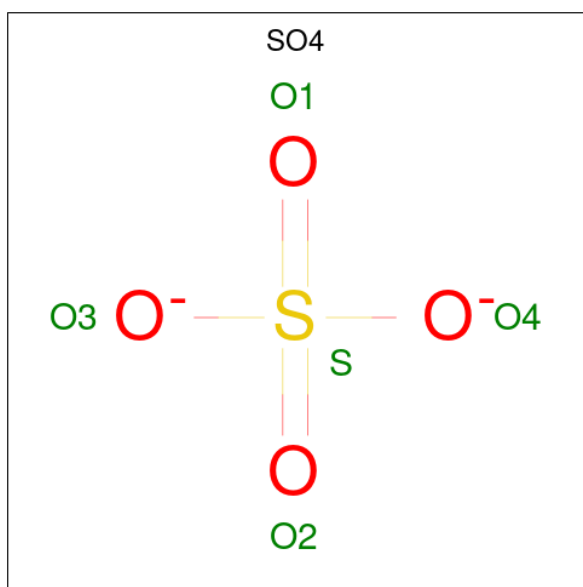
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is (S)-2-[(R)-3-AMINO-4-(2-FLUORO-PHENYL)-BUTYRYL]-1,2,3,4-TETRAHYDRO-ISOQUINOLINE-3-CARBOXYLIC ACID AMIDE (CCD ID: 008) (formula: $C_{20}H_{22}FN_3O_2$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 6 is water.

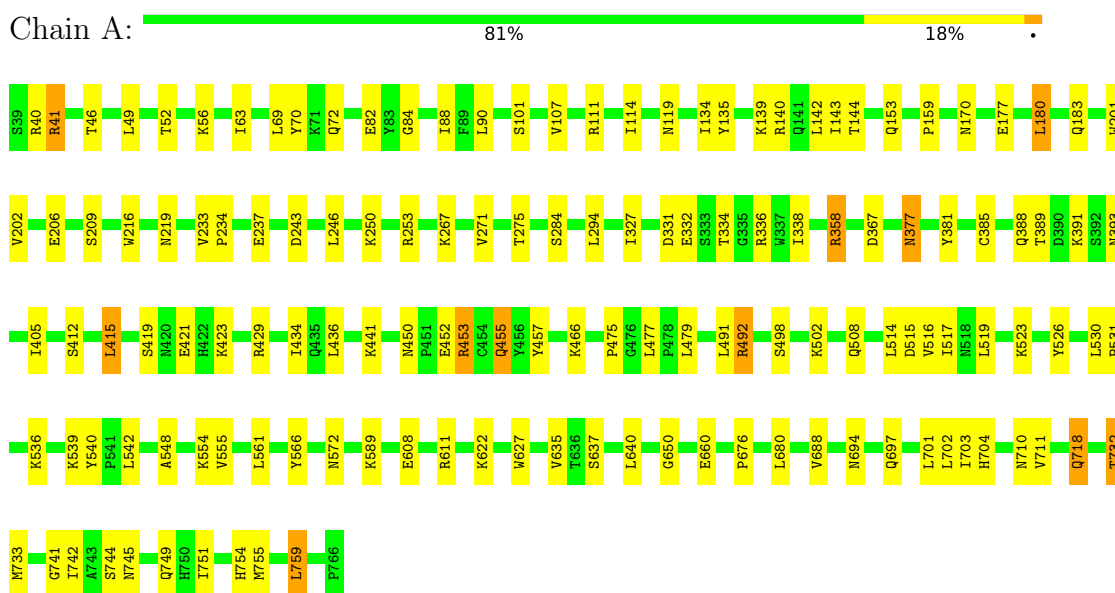
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	242	Total	O	0	0
			242	242		
6	B	248	Total	O	0	0
			248	248		
6	C	228	Total	O	0	0
			228	228		
6	D	233	Total	O	0	0
			233	233		

3 Residue-property plots

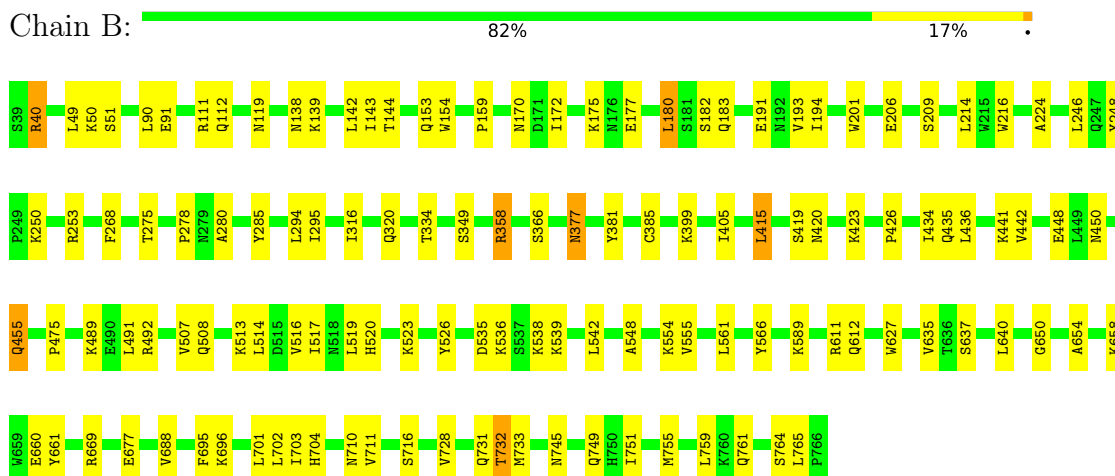
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

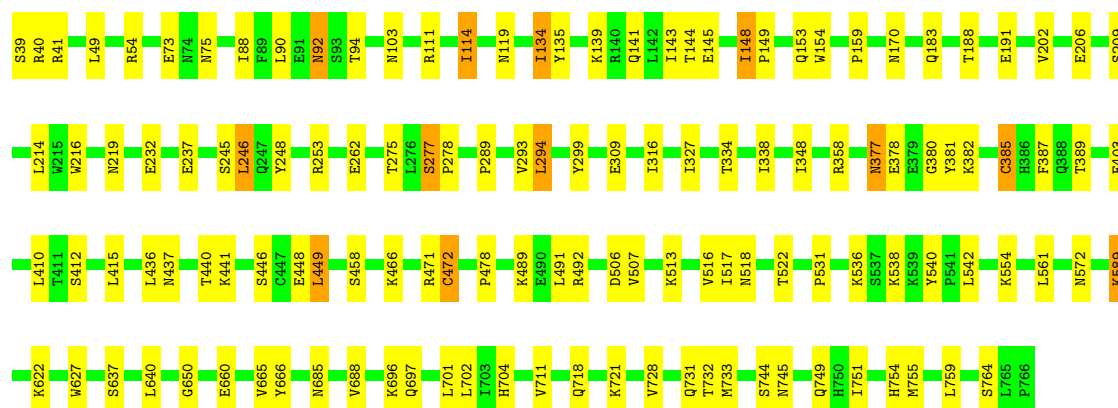


• Molecule 1: DIPEPTIDYL PEPTIDASE IV



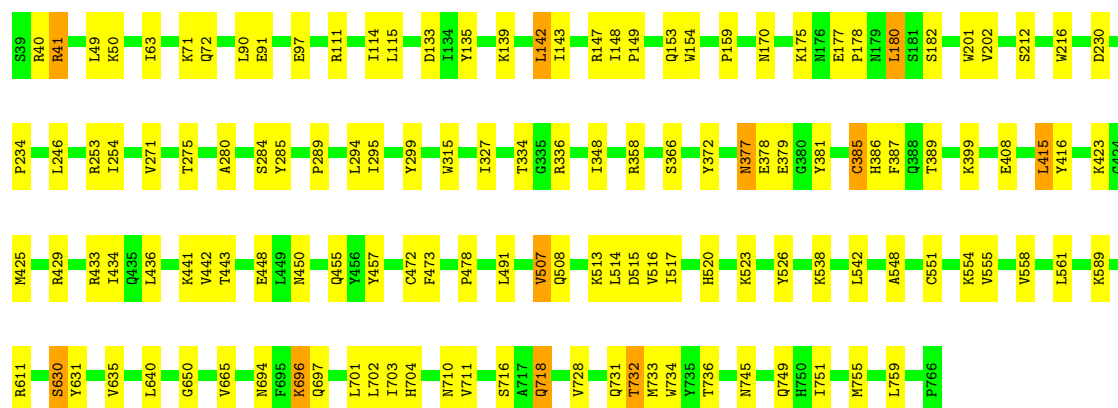
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain C:  82% 16%

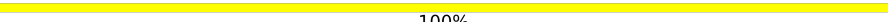


• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain D:  82% 17%

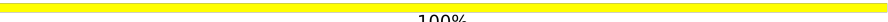


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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%



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

Chain H:  50% 50%

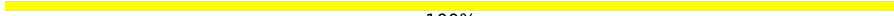


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

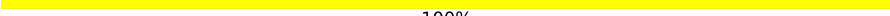


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain M:  100%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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.	Xtriage
Total number of atoms	25421	wwPDB-VP
Average B, all atoms (Å ²)	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: NAG, SO4, 008

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	0.37	0/6141	0.75	0/8353
1	B	0.37	0/6141	0.75	0/8353
1	C	0.38	0/6141	0.76	1/8353 (0.0%)
1	D	0.37	0/6141	0.75	0/8353
All	All	0.37	0/24564	0.75	1/33412 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	531	PRO	O-C-N	5.17	123.69	121.31

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	52	0
1	B	5966	0	5662	47	0
1	C	5966	0	5662	44	0
1	D	5966	0	5660	50	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
4	B	26	0	22	2	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	175	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 4.

All (175) 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
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.91	0.66
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.61	0.65
1:A:453:ARG:HH21	1:A:477:LEU:HB2	1.62	0.64
1:C:751:ILE:HG12	1:C:755:MET:HE2	1.80	0.63
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.81	0.62
1:A:751:ILE:HG12	1:A:755:MET:HE2	1.81	0.62
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.80	0.61
1:B:377:ASN:C	1:B:377:ASN:HD22	2.07	0.61
1:B:285:TYR:HD1	1:D:280:ALA:HB2	1.67	0.58
1:B:377:ASN:ND2	1:B:381:TYR:H	2.01	0.58
1:A:331:ASP:HB2	1:A:338:ILE:HD11	1.86	0.57
1:C:377:ASN:ND2	1:C:381:TYR:H	2.03	0.57
1:B:358:ARG:HG2	4:B:1767:008:H22	1.86	0.57
1:D:751:ILE:HG12	1:D:755:MET:HE2	1.86	0.57
1:D:377:ASN:HD22	1:D:377:ASN:C	2.12	0.57
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.86	0.57
1:A:377:ASN:ND2	1:A:381:TYR:H	2.03	0.56
1:B:751:ILE:HG12	1:B:755:MET:HE2	1.86	0.56
1:A:733:MET:HA	1:B:732:THR:HG22	1.87	0.56
1:A:275:THR:HA	1:C:334:THR:O	2.06	0.56
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.88	0.55
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.89	0.55
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.06	0.54
1:B:637:SER:HB3	1:B:688:VAL:HG11	1.89	0.54
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.89	0.54
1:C:327:ILE:HD13	1:C:389:THR:HG23	1.90	0.54
1:B:704:HIS:HD2	1:B:716:SER:OG	1.90	0.54
1:D:694:ASN:HD22	1:D:697:GLN:HE22	1.54	0.53
1:A:703:ILE:HG12	1:A:733:MET:HB3	1.90	0.53
1:A:540:TYR:HE2	1:A:572:ASN:HD22	1.55	0.53
1:A:429:ARG:HB2	1:A:457:TYR:H	1.74	0.53
1:C:446:SER:HA	1:C:449:LEU:HD12	1.92	0.52
1:A:107:VAL:HG22	1:A:114:ILE:HD12	1.92	0.52
1:A:201:TRP:CZ2	1:A:710:ASN:HA	2.45	0.52
1:A:377:ASN:HD22	1:A:377:ASN:C	2.18	0.52
1:B:703:ILE:HG12	1:B:733:MET:HB3	1.91	0.52
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.92	0.52
1:A:526:TYR:HA	1:A:555:VAL:HG21	1.93	0.51
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.76	0.51
1:C:153:GLN:HE22	1:C:170:ASN:ND2	2.09	0.51
1:D:177:GLU:HB2	1:D:180:LEU:HD23	1.93	0.51
1:B:695:PHE:HB3	1:B:728:VAL:HG11	1.93	0.51
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.93	0.51
1:C:733:MET:HE3	1:C:754:HIS:CE1	2.45	0.51
1:D:696:LYS:HG2	1:D:728:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ILE:HD13	1:A:389:THR:HG23	1.93	0.50
1:A:336:ARG:HD3	1:C:277:SER:OG	2.11	0.50
1:B:696:LYS:HG2	1:B:728:VAL:HG22	1.93	0.50
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.92	0.50
1:C:377:ASN:HD21	1:C:381:TYR:H	1.59	0.50
1:B:193:VAL:HG12	1:B:194:ILE:HG12	1.94	0.50
1:C:377:ASN:C	1:C:377:ASN:HD22	2.20	0.49
1:B:415:LEU:HB3	1:B:434:ILE:HG23	1.94	0.49
1:D:429:ARG:HB2	1:D:457:TYR:H	1.78	0.49
1:D:703:ILE:HG12	1:D:733:MET:HB3	1.94	0.49
1:D:718:GLN:HE21	1:D:718:GLN:HA	1.77	0.49
1:A:732:THR:HG22	1:B:733:MET:HA	1.95	0.49
1:D:416:TYR:CE2	1:D:433:ARG:HD3	2.48	0.49
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.48	0.49
1:A:271:VAL:HG22	1:A:284:SER:HB3	1.96	0.48
1:D:41:ARG:HD3	1:D:507:VAL:HG23	1.95	0.48
1:B:280:ALA:HB2	1:D:285:TYR:HD1	1.79	0.48
1:C:75:ASN:OD1	1:C:92:ASN:HB3	2.14	0.48
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.95	0.48
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.96	0.47
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.96	0.47
1:D:175:LYS:HG3	1:D:182:SER:HB3	1.95	0.47
1:D:704:HIS:HD2	1:D:716:SER:OG	1.97	0.47
1:D:201:TRP:CZ2	1:D:710:ASN:HA	2.49	0.47
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.97	0.46
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.97	0.46
1:A:393:ASN:HD22	1:A:393:ASN:H	1.61	0.46
1:A:334:THR:O	1:C:275:THR:HA	2.15	0.46
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.15	0.46
1:C:733:MET:HA	1:D:732:THR:HG22	1.98	0.46
1:C:232:GLU:HB3	1:C:262:GLU:HG2	1.97	0.46
1:C:380:GLY:HA3	1:C:589:LYS:HE2	1.96	0.46
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.51	0.46
1:C:134:ILE:HD11	1:C:148:ILE:HD12	1.97	0.46
1:C:382:LYS:H	1:C:403:GLU:HG2	1.81	0.46
1:B:658:LYS:HB3	1:B:661:TYR:CD2	2.51	0.46
1:B:704:HIS:CD2	1:B:716:SER:OG	2.69	0.46
1:B:704:HIS:HE1	1:B:711:VAL:O	1.98	0.45
1:C:183:GLN:HE22	1:C:278:PRO:HA	1.81	0.45
1:B:172:ILE:HG12	1:B:214:LEU:HD21	1.97	0.45
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.98	0.45
1:D:271:VAL:HG22	1:D:284:SER:HB3	1.97	0.45
1:A:759:LEU:HD23	1:A:759:LEU:HA	1.86	0.45
1:B:405:ILE:HG12	1:B:419:SER:HA	1.99	0.45
1:C:704:HIS:HE1	1:C:711:VAL:O	1.99	0.45
1:A:694:ASN:HD22	1:A:697:GLN:HE22	1.63	0.45
1:B:526:TYR:HA	1:B:555:VAL:HG21	1.99	0.44
1:D:377:ASN:ND2	1:D:381:TYR:H	2.15	0.44
1:A:367:ASP:HB2	6:A:2125:HOH:O	2.16	0.44
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.98	0.44
1:D:154:TRP:CD2	1:D:212:SER:HB3	2.52	0.44
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.53	0.44
1:D:148:ILE:HA	1:D:149:PRO:HD3	1.90	0.44
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.48	0.44
1:D:704:HIS:HE1	1:D:711:VAL:O	2.00	0.44
1:C:299:TYR:CZ	1:C:665:VAL:HG22	2.53	0.44
1:C:540:TYR:HE2	1:C:572:ASN:HD22	1.66	0.44
1:A:377:ASN:HD21	1:A:381:TYR:H	1.64	0.44
1:B:154:TRP:HD1	1:B:214:LEU:HD12	1.83	0.43
1:D:159:PRO:HD3	1:D:216:TRP:HB3	2.00	0.43
1:C:289:PRO:HG2	1:C:294:LEU:HG	2.00	0.43
1:B:112:GLN:HG2	1:B:138:ASN:HD21	1.83	0.43
1:C:472:CYS:O	1:C:478:PRO:HA	2.19	0.43
1:D:526:TYR:HA	1:D:555:VAL:HG21	2.00	0.43
1:A:732:THR:CG2	1:B:733:MET:HA	2.48	0.43
1:A:741:GLY:O	1:A:742:ILE:C	2.62	0.43
1:B:420:ASN:HB2	1:B:426:PRO:HA	2.00	0.43
1:A:405:ILE:HG12	1:A:419:SER:HA	1.99	0.43
1:B:177:GLU:HB2	1:B:180:LEU:HB2	2.01	0.43
1:B:377:ASN:C	1:B:377:ASN:ND2	2.75	0.43
1:A:733:MET:HA	1:B:732:THR:CG2	2.48	0.43
1:B:206:GLU:CD	4:B:1767:008:H102	2.28	0.42
1:B:377:ASN:HD21	1:B:381:TYR:H	1.66	0.42
1:D:372:TYR:CZ	1:D:386:HIS:HD2	2.37	0.42
1:A:206:GLU:CD	4:A:1767:008:H102	2.27	0.42
1:C:41:ARG:HB3	1:C:507:VAL:HG23	2.00	0.42
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.67	0.42
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.55	0.42
1:A:70:TYR:CE2	1:A:72:GLN:HB2	2.54	0.42
1:A:177:GLU:HB2	1:A:180:LEU:HB2	2.01	0.42
1:A:637:SER:HB3	1:A:688:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.54	0.42
1:C:385:CYS:HB3	1:C:387:PHE:CE1	2.55	0.42
1:C:704:HIS:CE1	1:C:711:VAL:O	2.73	0.42
1:A:41:ARG:H	1:A:41:ARG:HG3	1.57	0.42
1:A:358:ARG:HG2	4:A:1767:008:H22	2.01	0.42
1:A:84:GLY:HA2	1:A:492:ARG:HH12	1.84	0.42
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.54	0.42
1:D:415:LEU:HB3	1:D:434:ILE:HG23	2.01	0.42
1:C:148:ILE:HA	1:C:149:PRO:HD3	1.92	0.41
1:D:630:SER:HB2	1:D:631:TYR:H	1.64	0.41
1:B:275:THR:HA	1:D:334:THR:O	2.19	0.41
1:D:133:ASP:HB3	1:D:142:LEU:HD21	2.02	0.41
1:A:233:VAL:HA	1:A:234:PRO:HD3	1.94	0.41
1:B:316:ILE:HG12	1:B:320:GLN:HA	2.01	0.41
1:B:492:ARG:HD2	6:B:2178:HOH:O	2.19	0.41
1:C:246:LEU:HD13	1:C:248:TYR:O	2.20	0.41
1:D:473:PHE:HB3	1:D:558:VAL:HG13	2.03	0.41
1:D:734:TRP:CD1	1:D:734:TRP:C	2.99	0.41
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.56	0.41
1:A:388:GLN:HB3	1:A:391:LYS:HB2	2.02	0.41
1:A:733:MET:HE3	1:A:754:HIS:CE1	2.56	0.41
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.02	0.41
1:D:472:CYS:O	1:D:478:PRO:HA	2.21	0.41
1:B:201:TRP:CZ2	1:B:710:ASN:HA	2.55	0.41
1:C:154:TRP:HD1	1:C:214:LEU:HD12	1.86	0.41
1:A:49:LEU:HD22	1:A:749:GLN:HA	2.03	0.41
1:A:676:PRO:HD3	1:A:680:LEU:HD22	2.03	0.41
1:A:704:HIS:HE1	1:A:711:VAL:O	2.03	0.41
1:C:637:SER:HB3	1:C:688:VAL:HG11	2.02	0.41
1:A:377:ASN:ND2	1:A:377:ASN:C	2.78	0.41
1:B:548:ALA:HB3	1:B:635:VAL:HG21	2.03	0.41
1:C:721:LYS:HB2	1:D:736:THR:HB	2.03	0.41
1:C:733:MET:HA	1:D:732:THR:CG2	2.51	0.41
1:D:385:CYS:HB3	1:D:387:PHE:CE1	2.56	0.41
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.94	0.40
1:C:206:GLU:CD	1:C:666:TYR:HB2	2.46	0.40
1:C:458:SER:HB3	1:C:471:ARG:HB2	2.02	0.40
1:D:177:GLU:HA	1:D:178:PRO:HD3	1.93	0.40
1:B:153:GLN:HE22	1:B:170:ASN:ND2	2.19	0.40
1:C:589:LYS:N	1:C:589:LYS:HD3	2.36	0.40
1:D:327:ILE:HD13	1:D:389:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:THR:O	1:D:275:THR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/728 (100%)	693 (96%)	32 (4%)	1 (0%)	48	68
1	B	726/728 (100%)	697 (96%)	28 (4%)	1 (0%)	48	68
1	C	726/728 (100%)	696 (96%)	29 (4%)	1 (0%)	48	68
1	D	726/728 (100%)	696 (96%)	29 (4%)	1 (0%)	48	68
All	All	2904/2912 (100%)	2782 (96%)	118 (4%)	4 (0%)	48	68

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%)	577 (88%)	75 (12%)	5	11
1	B	652/652 (100%)	583 (89%)	69 (11%)	6	14
1	C	652/652 (100%)	578 (89%)	74 (11%)	5	12
1	D	652/652 (100%)	586 (90%)	66 (10%)	7	15
All	All	2608/2608 (100%)	2324 (89%)	284 (11%)	6	13

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	46	THR
1	A	52	THR
1	A	56	LYS
1	A	63	ILE
1	A	69	LEU
1	A	82	GLU
1	A	88	ILE
1	A	90	LEU
1	A	101	SER
1	A	111	ARG
1	A	119	ASN
1	A	134	ILE
1	A	139	LYS
1	A	140	ARG
1	A	142	LEU
1	A	143	ILE
1	A	144	THR
1	A	180	LEU
1	A	183	GLN
1	A	202	VAL
1	A	209	SER
1	A	219	ASN
1	A	237	GLU
1	A	243	ASP
1	A	246	LEU
1	A	250	LYS
1	A	267	LYS
1	A	294	LEU
1	A	332	GLU
1	A	358	ARG
1	A	377	ASN
1	A	385	CYS

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Mol	Chain	Res	Type
1	A	412	SER
1	A	415	LEU
1	A	421	GLU
1	A	423	LYS
1	A	436	LEU
1	A	441	LYS
1	A	450	ASN
1	A	452	GLU
1	A	453	ARG
1	A	455	GLN
1	A	466	LYS
1	A	479	LEU
1	A	491	LEU
1	A	492	ARG
1	A	498	SER
1	A	502	LYS
1	A	508	GLN
1	A	514	LEU
1	A	515	ASP
1	A	516	VAL
1	A	517	ILE
1	A	519	LEU
1	A	523	LYS
1	A	536	LYS
1	A	539	LYS
1	A	542	LEU
1	A	554	LYS
1	A	561	LEU
1	A	566	TYR
1	A	589	LYS
1	A	608	GLU
1	A	611	ARG
1	A	622	LYS
1	A	627	TRP
1	A	660	GLU
1	A	701	LEU
1	A	702	LEU
1	A	718	GLN
1	A	732	THR
1	A	744	SER
1	A	745	ASN
1	A	759	LEU

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Mol	Chain	Res	Type
1	B	40	ARG
1	B	50	LYS
1	B	51	SER
1	B	90	LEU
1	B	91	GLU
1	B	111	ARG
1	B	119	ASN
1	B	139	LYS
1	B	142	LEU
1	B	143	ILE
1	B	144	THR
1	B	175	LYS
1	B	180	LEU
1	B	182	SER
1	B	191	GLU
1	B	209	SER
1	B	246	LEU
1	B	250	LYS
1	B	294	LEU
1	B	295	ILE
1	B	349	SER
1	B	358	ARG
1	B	366	SER
1	B	377	ASN
1	B	385	CYS
1	B	399	LYS
1	B	415	LEU
1	B	423	LYS
1	B	435	GLN
1	B	436	LEU
1	B	441	LYS
1	B	442	VAL
1	B	448	GLU
1	B	450	ASN
1	B	455	GLN
1	B	489	LYS
1	B	491	LEU
1	B	507	VAL
1	B	508	GLN
1	B	513	LYS
1	B	514	LEU
1	B	516	VAL

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Mol	Chain	Res	Type
1	B	517	ILE
1	B	519	LEU
1	B	520	HIS
1	B	523	LYS
1	B	535	ASP
1	B	536	LYS
1	B	538	LYS
1	B	539	LYS
1	B	542	LEU
1	B	554	LYS
1	B	561	LEU
1	B	566	TYR
1	B	589	LYS
1	B	611	ARG
1	B	612	GLN
1	B	627	TRP
1	B	660	GLU
1	B	677	GLU
1	B	701	LEU
1	B	702	LEU
1	B	731	GLN
1	B	732	THR
1	B	745	ASN
1	B	759	LEU
1	B	761	GLN
1	B	764	SER
1	B	765	LEU
1	C	39	SER
1	C	54	ARG
1	C	73	GLU
1	C	88	ILE
1	C	90	LEU
1	C	92	ASN
1	C	94	THR
1	C	103	ASN
1	C	111	ARG
1	C	114	ILE
1	C	119	ASN
1	C	134	ILE
1	C	139	LYS
1	C	141	GLN
1	C	143	ILE

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Mol	Chain	Res	Type
1	C	144	THR
1	C	145	GLU
1	C	148	ILE
1	C	188	THR
1	C	191	GLU
1	C	202	VAL
1	C	209	SER
1	C	219	ASN
1	C	245	SER
1	C	246	LEU
1	C	277	SER
1	C	293	VAL
1	C	294	LEU
1	C	309	GLU
1	C	316	ILE
1	C	338	ILE
1	C	348	ILE
1	C	358	ARG
1	C	377	ASN
1	C	378	GLU
1	C	385	CYS
1	C	412	SER
1	C	436	LEU
1	C	437	ASN
1	C	440	THR
1	C	441	LYS
1	C	448	GLU
1	C	449	LEU
1	C	466	LYS
1	C	472	CYS
1	C	489	LYS
1	C	491	LEU
1	C	492	ARG
1	C	506	ASP
1	C	513	LYS
1	C	516	VAL
1	C	517	ILE
1	C	518	ASN
1	C	522	THR
1	C	536	LYS
1	C	538	LYS
1	C	542	LEU

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Mol	Chain	Res	Type
1	C	554	LYS
1	C	561	LEU
1	C	589	LYS
1	C	622	LYS
1	C	627	TRP
1	C	660	GLU
1	C	685	ASN
1	C	697	GLN
1	C	701	LEU
1	C	702	LEU
1	C	718	GLN
1	C	731	GLN
1	C	732	THR
1	C	744	SER
1	C	745	ASN
1	C	759	LEU
1	C	764	SER
1	D	41	ARG
1	D	50	LYS
1	D	63	ILE
1	D	71	LYS
1	D	72	GLN
1	D	90	LEU
1	D	91	GLU
1	D	97	GLU
1	D	111	ARG
1	D	115	LEU
1	D	139	LYS
1	D	142	LEU
1	D	143	ILE
1	D	147	ARG
1	D	180	LEU
1	D	202	VAL
1	D	230	ASP
1	D	246	LEU
1	D	254	ILE
1	D	294	LEU
1	D	295	ILE
1	D	336	ARG
1	D	348	ILE
1	D	358	ARG
1	D	366	SER

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Mol	Chain	Res	Type
1	D	377	ASN
1	D	378	GLU
1	D	379	GLU
1	D	385	CYS
1	D	399	LYS
1	D	408	GLU
1	D	415	LEU
1	D	423	LYS
1	D	425	MET
1	D	436	LEU
1	D	441	LYS
1	D	442	VAL
1	D	443	THR
1	D	448	GLU
1	D	450	ASN
1	D	455	GLN
1	D	491	LEU
1	D	507	VAL
1	D	508	GLN
1	D	513	LYS
1	D	514	LEU
1	D	515	ASP
1	D	516	VAL
1	D	517	ILE
1	D	520	HIS
1	D	523	LYS
1	D	538	LYS
1	D	542	LEU
1	D	554	LYS
1	D	561	LEU
1	D	589	LYS
1	D	611	ARG
1	D	630	SER
1	D	696	LYS
1	D	701	LEU
1	D	702	LEU
1	D	718	GLN
1	D	731	GLN
1	D	732	THR
1	D	745	ASN
1	D	759	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	141	GLN
1	A	170	ASN
1	A	176	ASN
1	A	192	ASN
1	A	219	ASN
1	A	247	GLN
1	A	369	ASN
1	A	377	ASN
1	A	393	ASN
1	A	435	GLN
1	A	437	ASN
1	A	483	HIS
1	A	572	ASN
1	A	586	GLN
1	A	606	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	B	75	ASN
1	B	80	ASN
1	B	103	ASN
1	B	123	GLN
1	B	138	ASN
1	B	169	ASN
1	B	170	ASN
1	B	183	GLN
1	B	192	ASN
1	B	377	ASN
1	B	393	ASN
1	B	430	ASN
1	B	435	GLN
1	B	483	HIS
1	B	553	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	C	80	ASN
1	C	103	ASN
1	C	123	GLN

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Mol	Chain	Res	Type
1	C	141	GLN
1	C	169	ASN
1	C	170	ASN
1	C	183	GLN
1	C	192	ASN
1	C	196	ASN
1	C	219	ASN
1	C	227	GLN
1	C	247	GLN
1	C	377	ASN
1	C	393	ASN
1	C	422	HIS
1	C	435	GLN
1	C	463	ASN
1	C	483	HIS
1	C	527	GLN
1	C	572	ASN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	D	75	ASN
1	D	80	ASN
1	D	138	ASN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	192	ASN
1	D	314	GLN
1	D	345	HIS
1	D	377	ASN
1	D	386	HIS
1	D	435	GLN
1	D	450	ASN
1	D	455	GLN
1	D	463	ASN
1	D	483	HIS
1	D	518	ASN
1	D	586	GLN
1	D	679	ASN
1	D	694	ASN

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Mol	Chain	Res	Type
1	D	704	HIS
1	D	718	GLN

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 ⓘ

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	2,1	14,14,15	0.50	0	17,19,21	1.00	2 (11%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	1.05	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.56	0	17,19,21	1.56	2 (11%)
2	NAG	F	2	2	14,14,15	0.63	0	17,19,21	1.10	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.61	0	17,19,21	0.99	2 (11%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	0.83	0
2	NAG	H	1	2,1	14,14,15	0.48	0	17,19,21	0.83	0
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.50	0	17,19,21	0.86	0
2	NAG	I	2	2	14,14,15	0.49	0	17,19,21	1.15	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.51	0	17,19,21	1.16	2 (11%)
2	NAG	J	2	2	14,14,15	0.49	0	17,19,21	1.10	2 (11%)
2	NAG	K	1	2,1	14,14,15	0.37	0	17,19,21	1.55	2 (11%)
2	NAG	K	2	2	14,14,15	0.54	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	1	2,1	14,14,15	0.53	0	17,19,21	0.96	0
2	NAG	L	2	2	14,14,15	0.66	1 (7%)	17,19,21	1.39	3 (17%)
2	NAG	M	1	2,1	14,14,15	0.51	0	17,19,21	0.76	0
2	NAG	M	2	2	14,14,15	0.52	0	17,19,21	0.83	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	2,1	-	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	2,1	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	2,1	-	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	2,1	-	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	2,1	-	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	2,1	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
2	NAG	K	1	2,1	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	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	NAG	C1-C2	2.04	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C1-O5-C5	5.22	119.18	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	NAG	C1-O5-C5	4.04	117.61	112.19
2	F	1	NAG	O4-C4-C3	3.93	119.63	110.38
2	I	2	NAG	C1-O5-C5	3.77	117.24	112.19
2	F	2	NAG	C1-O5-C5	3.55	116.95	112.19
2	F	1	NAG	C1-O5-C5	3.23	116.52	112.19
2	J	1	NAG	O5-C1-C2	-2.95	106.72	111.29
2	J	1	NAG	C1-O5-C5	2.90	116.07	112.19
2	K	1	NAG	O5-C1-C2	2.85	115.70	111.29
2	J	2	NAG	C2-N2-C7	2.80	126.66	122.90
2	E	2	NAG	C4-C3-C2	2.79	115.11	111.02
2	H	2	NAG	C1-O5-C5	2.55	115.61	112.19
2	K	2	NAG	C4-C3-C2	2.35	114.46	111.02
2	L	2	NAG	C4-C3-C2	2.32	114.42	111.02
2	G	1	NAG	O5-C1-C2	-2.30	107.74	111.29
2	L	2	NAG	O5-C1-C2	2.29	114.83	111.29
2	J	2	NAG	C1-O5-C5	2.17	115.10	112.19
2	E	1	NAG	O5-C1-C2	-2.16	107.95	111.29
2	G	1	NAG	C1-O5-C5	2.14	115.05	112.19
2	E	1	NAG	C1-O5-C5	2.13	115.04	112.19

All (6) chirality outliers are listed below:

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

All (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	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	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

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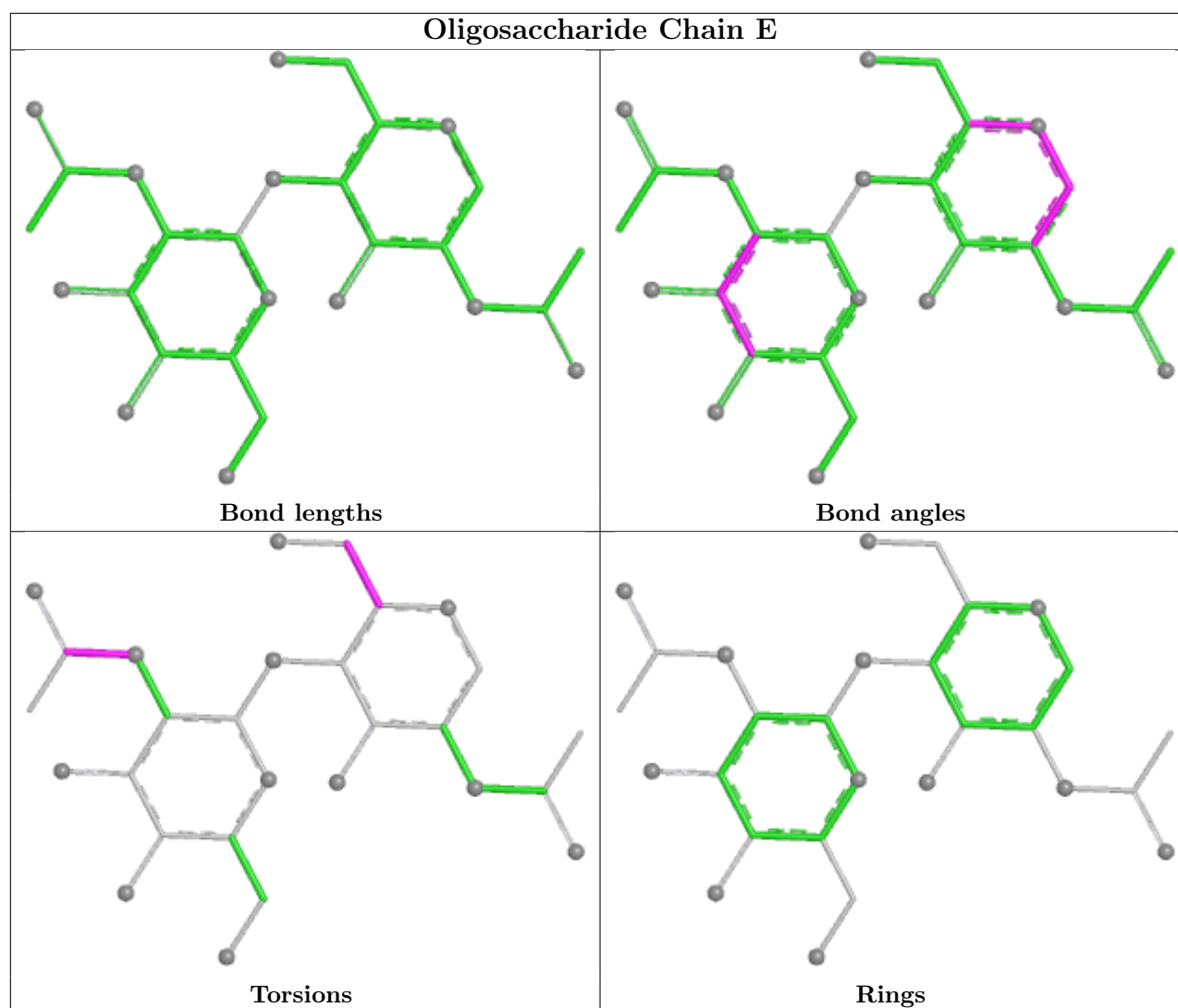
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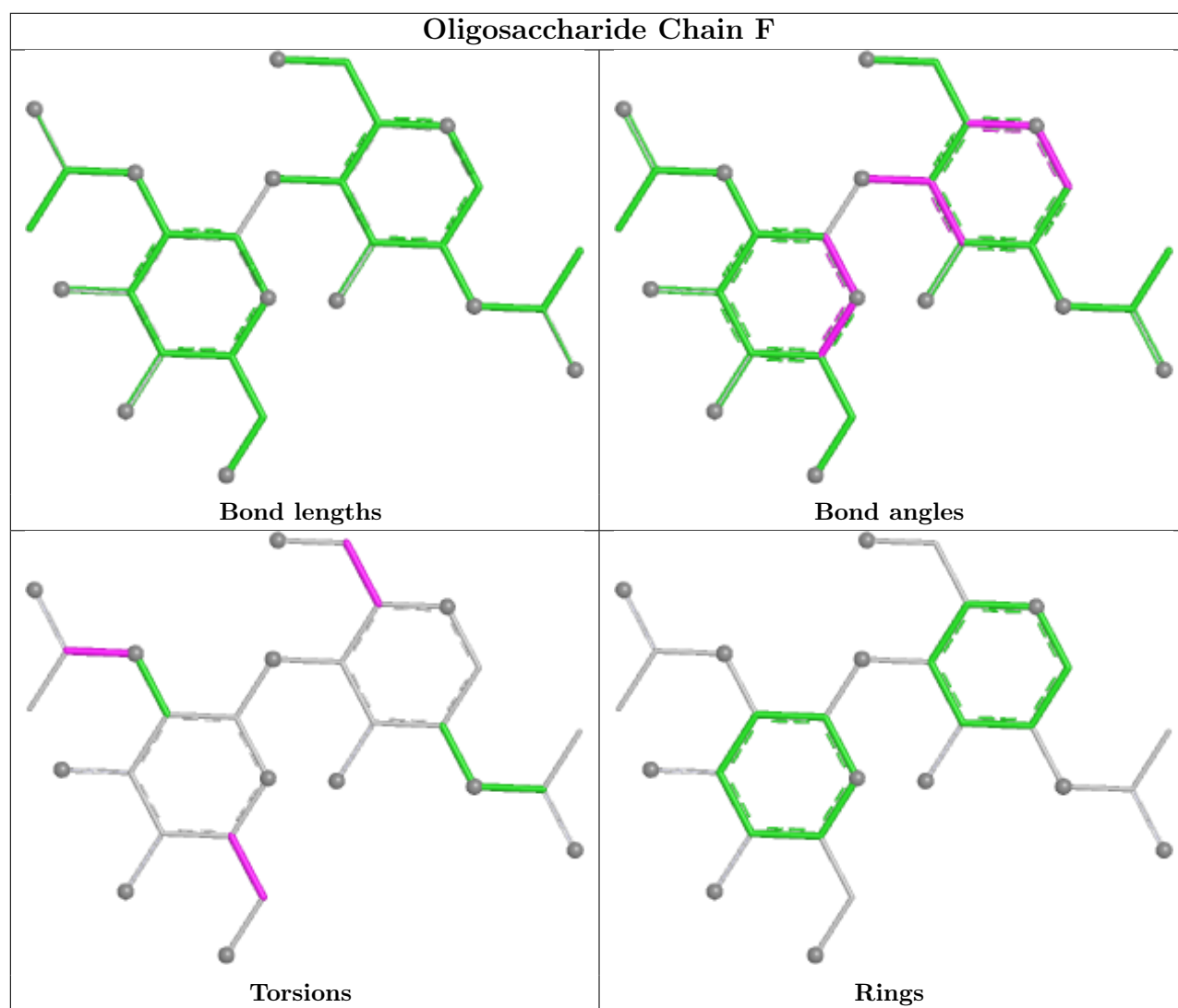
Mol	Chain	Res	Type	Atoms
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2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

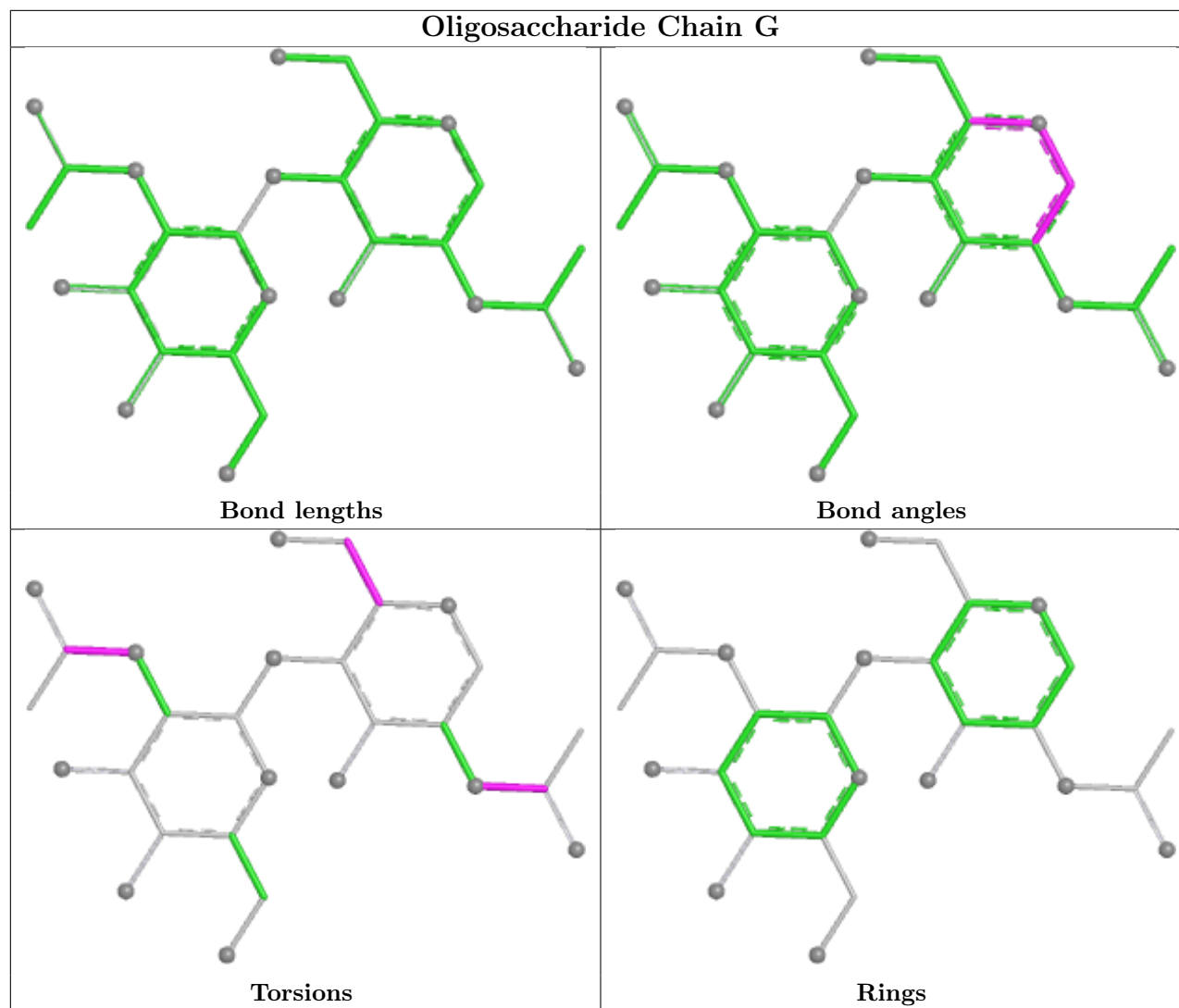
There are no ring outliers.

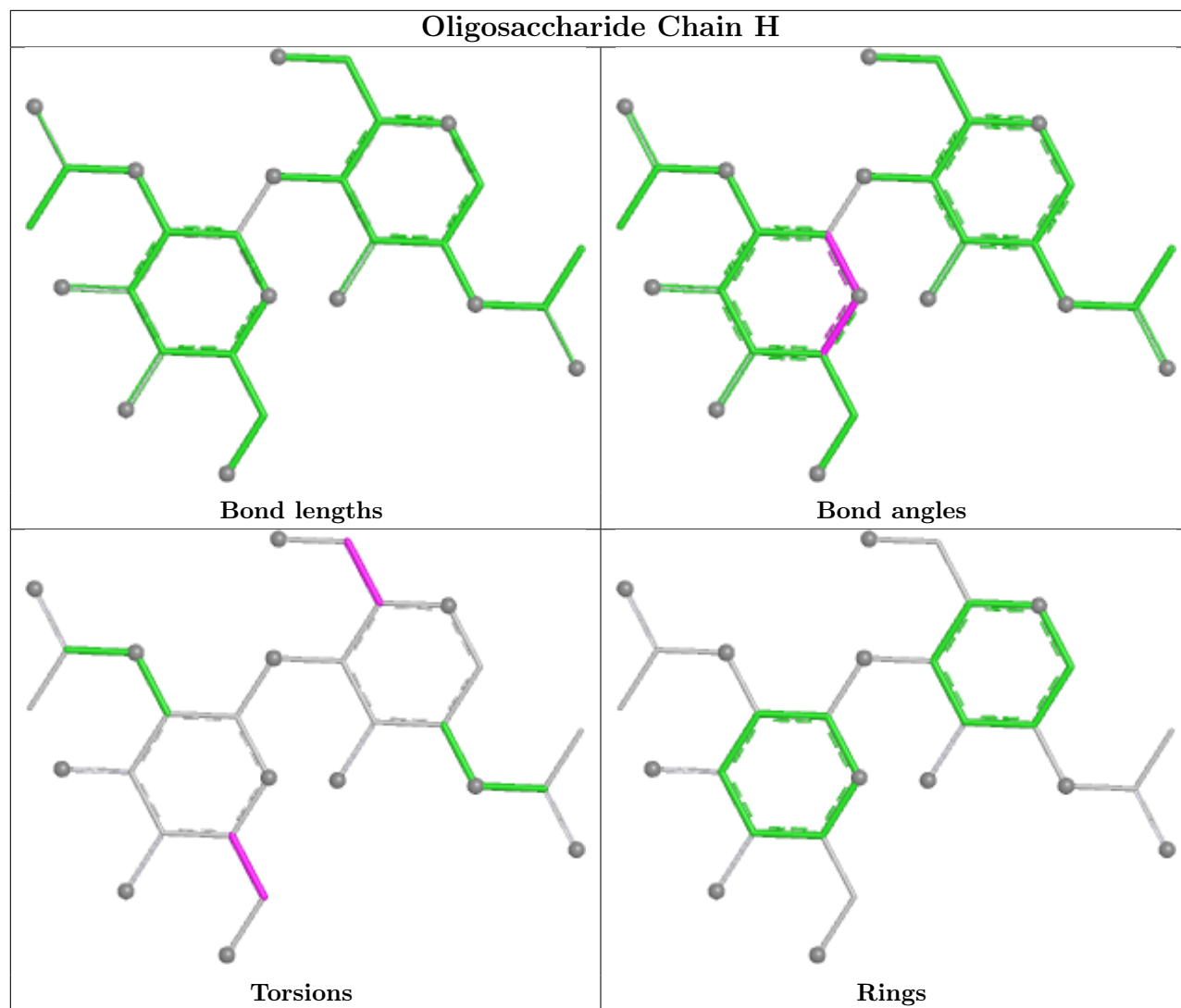
No monomer is involved in short contacts.

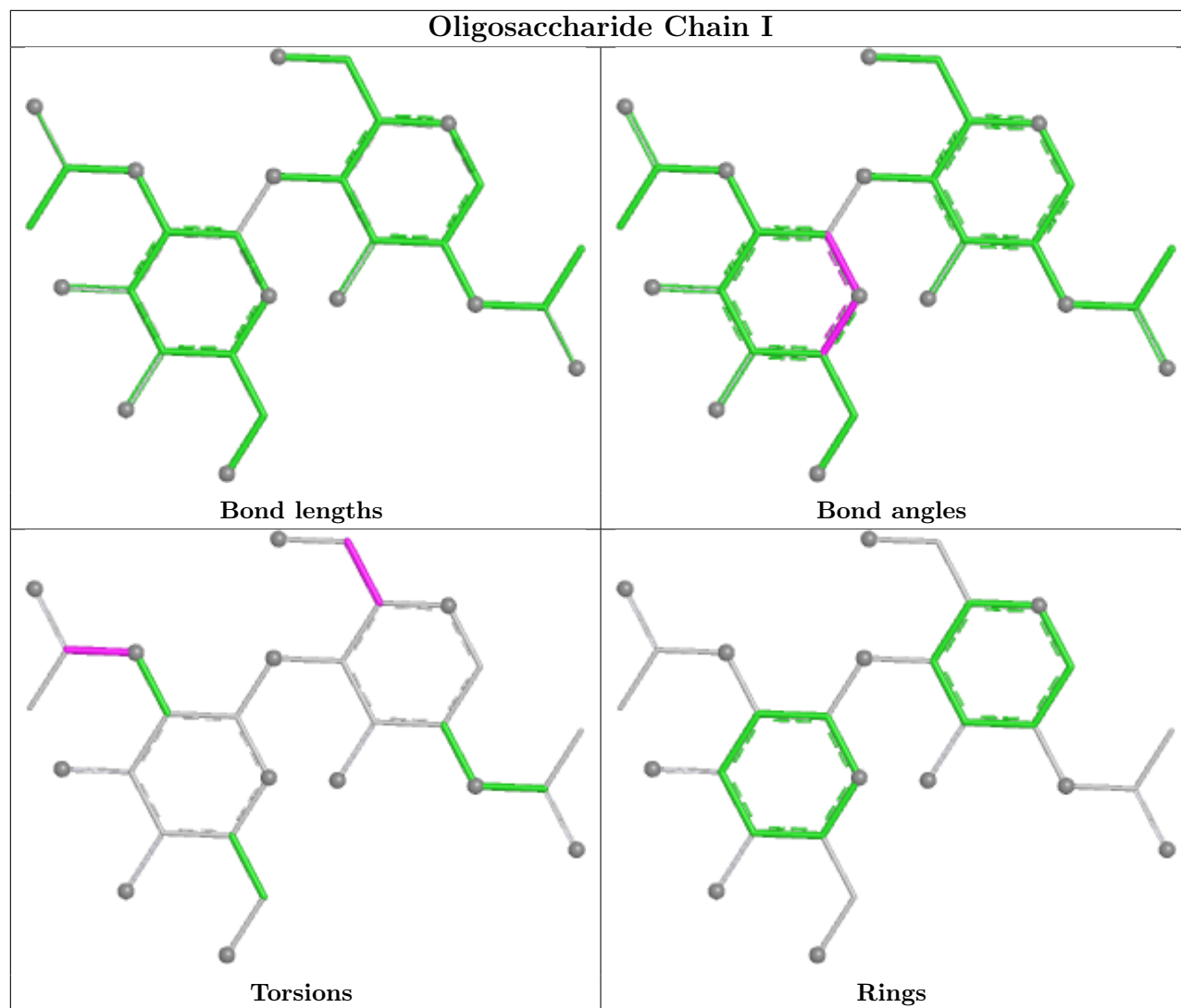
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

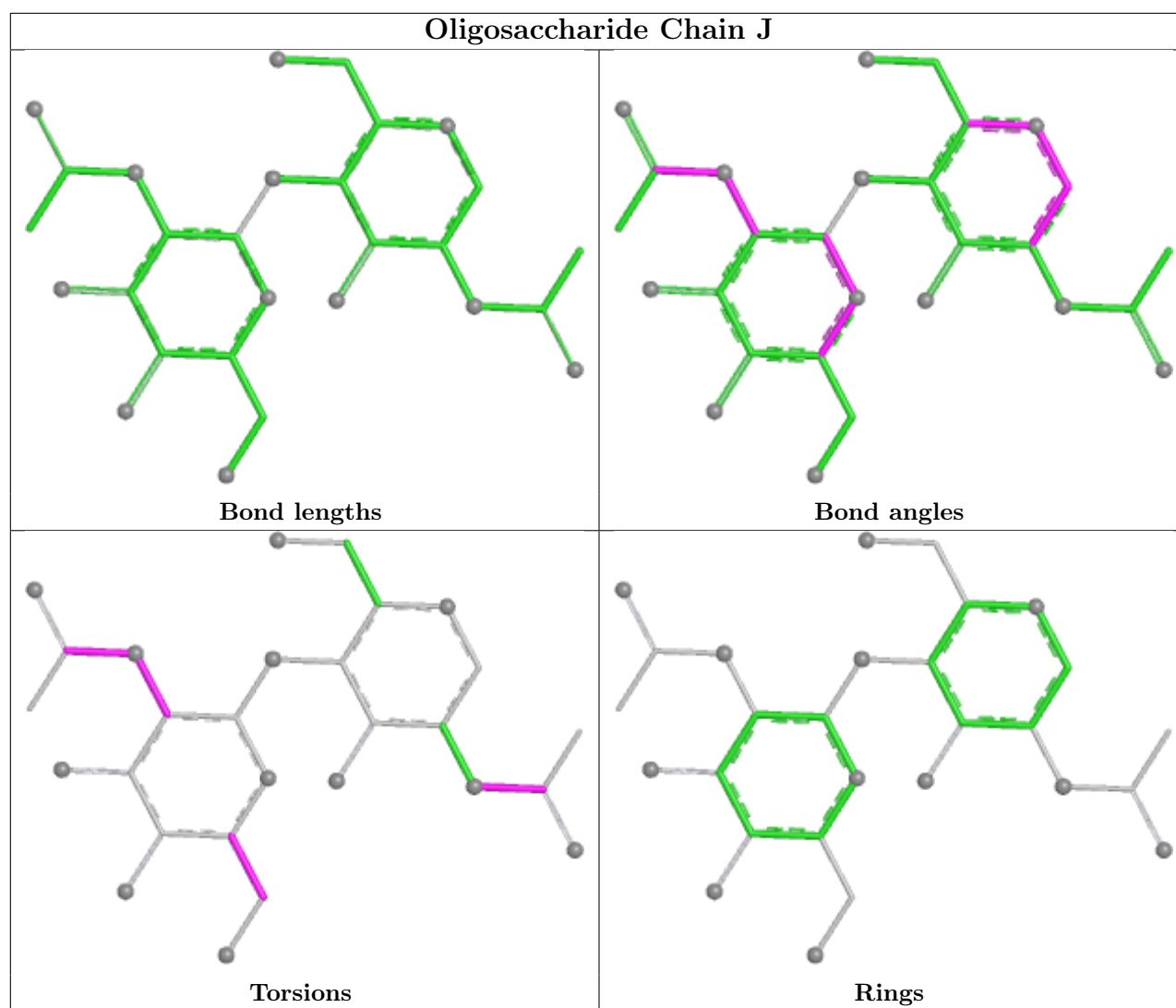


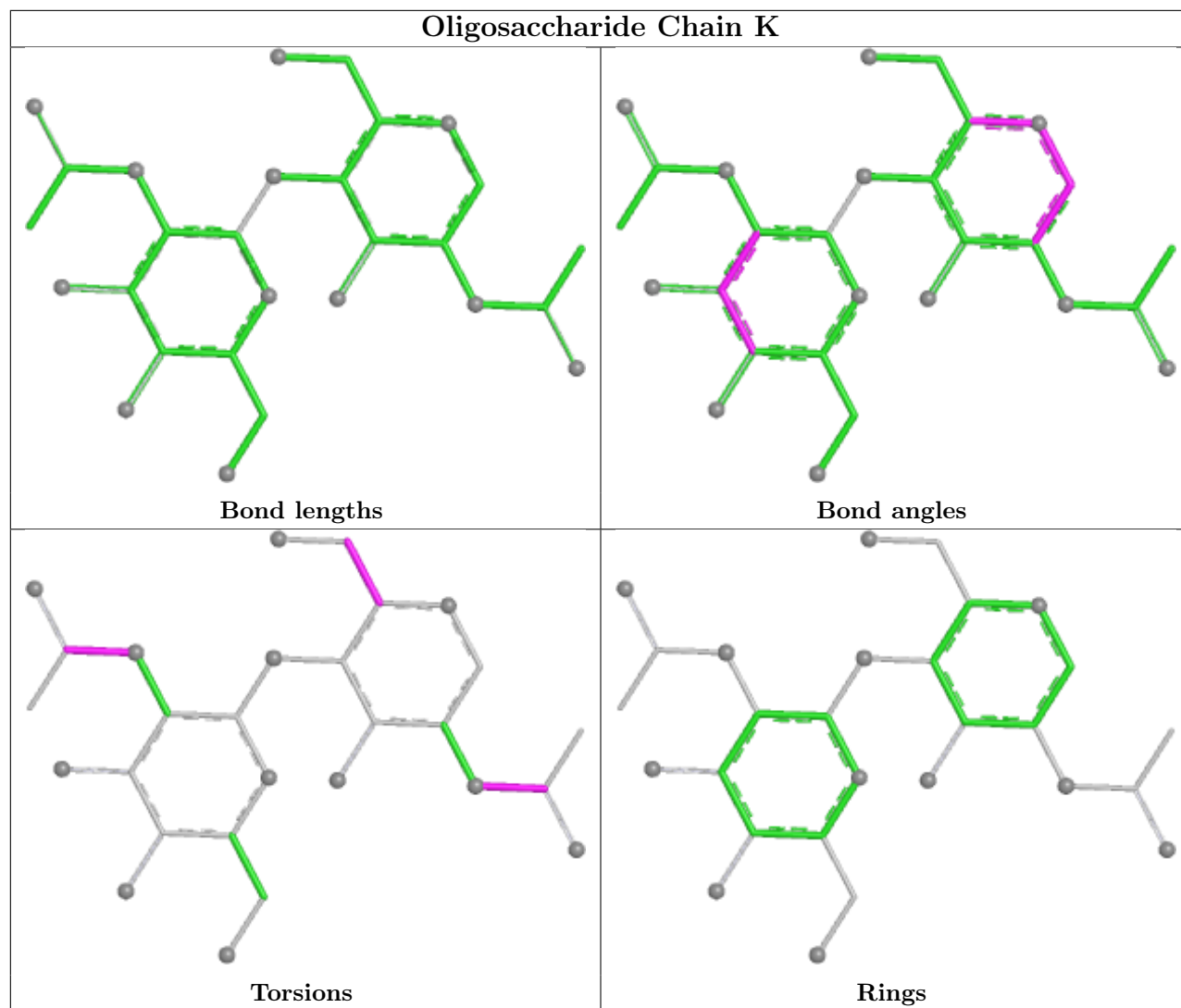


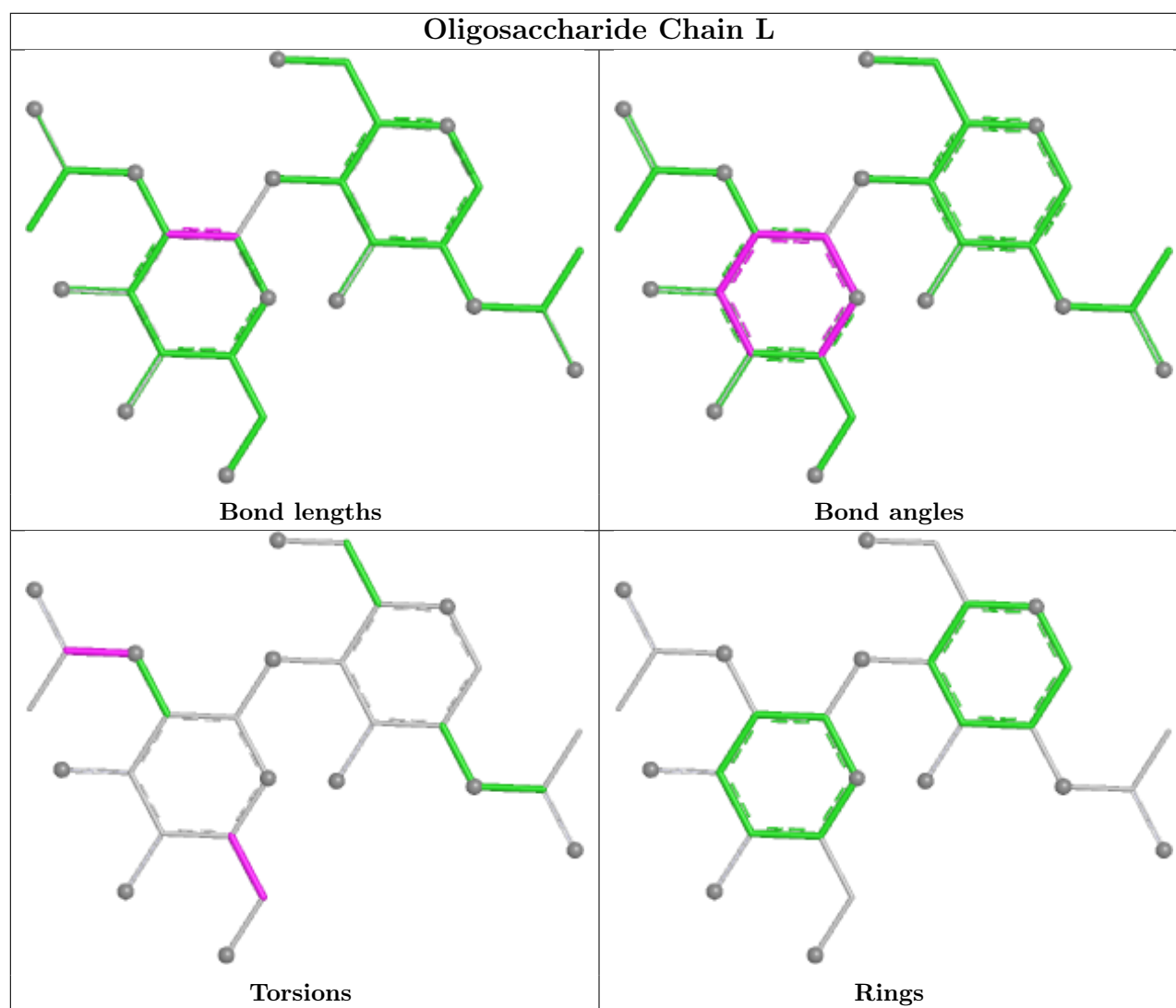


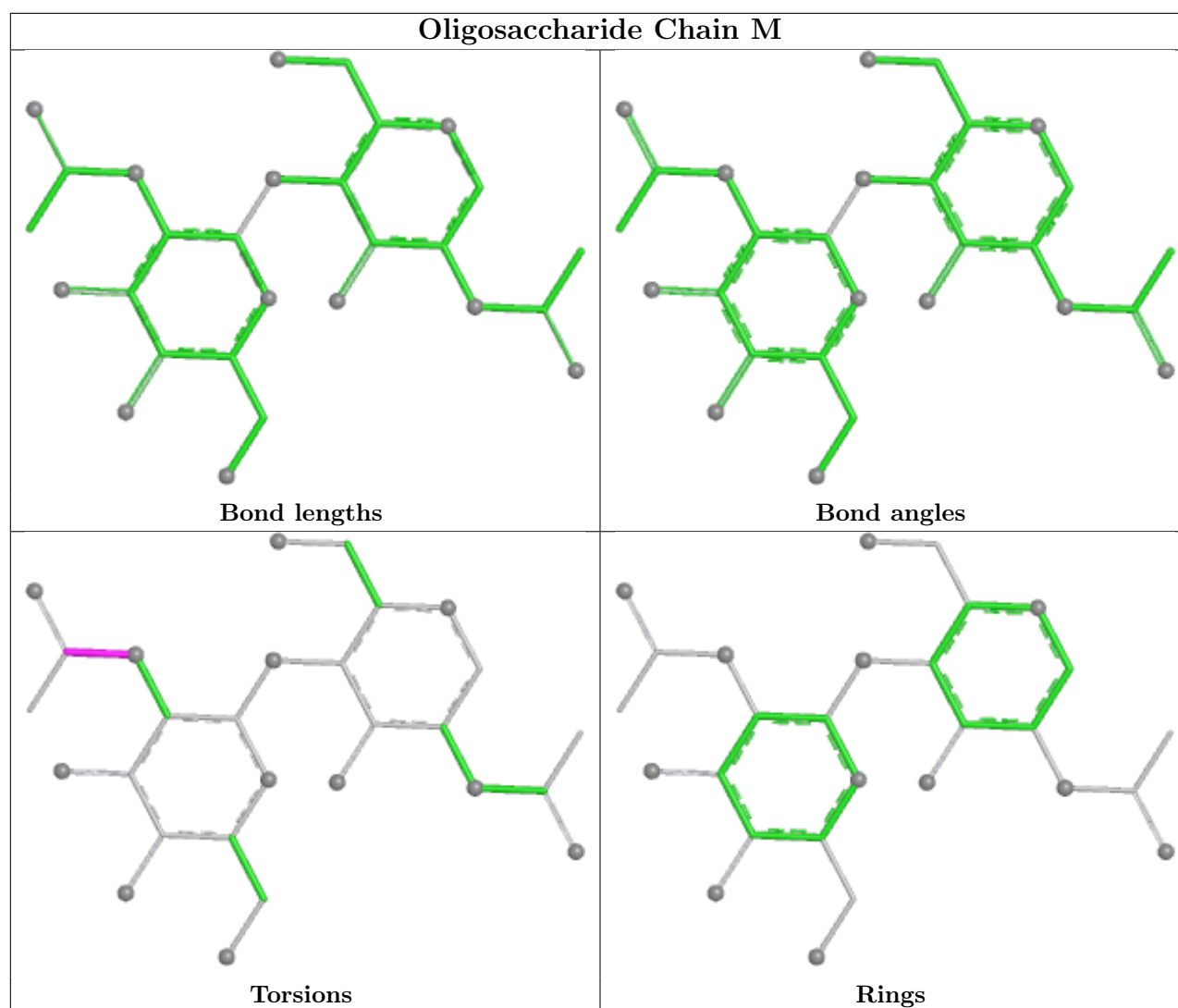












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NAG	B	1229	1	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
5	SO4	B	1769	-	4,4,4	0.24	0	6,6,6	0.11	0
3	NAG	A	1321	1	14,14,15	0.49	0	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	1768	-	4,4,4	0.24	0	6,6,6	0.07	0
4	008	A	1767	-	28,28,28	0.61	0	32,39,39	1.31	2 (6%)
3	NAG	B	1085	1	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
5	SO4	C	1768	-	4,4,4	0.25	0	6,6,6	0.17	0
3	NAG	A	1092	1	14,14,15	0.61	0	17,19,21	1.01	1 (5%)
3	NAG	A	1085	1	14,14,15	0.53	0	17,19,21	0.68	0
3	NAG	C	1279	1	14,14,15	0.44	0	17,19,21	1.07	1 (5%)
5	SO4	D	1769	-	4,4,4	0.24	0	6,6,6	0.05	0
3	NAG	C	1092	1	14,14,15	0.50	0	17,19,21	0.75	0
3	NAG	C	1229	1	14,14,15	0.47	0	17,19,21	1.12	1 (5%)
4	008	D	1767	-	28,28,28	0.60	0	32,39,39	1.28	4 (12%)
3	NAG	B	1321	1	14,14,15	0.52	0	17,19,21	0.77	0
5	SO4	A	1769	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	B	1768	-	4,4,4	0.25	0	6,6,6	0.11	0
3	NAG	B	1279	1	14,14,15	0.51	0	17,19,21	0.79	0
3	NAG	C	1085	1	14,14,15	0.51	0	17,19,21	0.74	0
3	NAG	A	1279	1	14,14,15	0.52	0	17,19,21	0.81	0
3	NAG	D	1279	1	14,14,15	0.49	0	17,19,21	0.71	0
5	SO4	C	1769	-	4,4,4	0.23	0	6,6,6	0.06	0
3	NAG	C	1321	1	14,14,15	0.51	0	17,19,21	0.67	0
4	008	B	1767	-	28,28,28	0.59	0	32,39,39	1.30	4 (12%)
5	SO4	D	1768	-	4,4,4	0.25	0	6,6,6	0.08	0
3	NAG	D	1085	1	14,14,15	0.53	0	17,19,21	1.41	3 (17%)
4	008	C	1767	-	28,28,28	0.57	0	32,39,39	1.19	2 (6%)

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	B	1229	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1321	1	-	0/6/23/26	0/1/1/1
4	008	A	1767	-	-	1/15/28/28	0/3/3/3
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	A	1085	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1279	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1092	1	1/1/5/7	3/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1767	008	C16-C15-N14	4.22	114.21	109.86
4	B	1767	008	C16-C15-N14	3.67	113.65	109.86
4	C	1767	008	C16-C15-N14	3.27	113.23	109.86
3	D	1085	NAG	C1-O5-C5	3.20	116.48	112.19
3	D	1085	NAG	C3-C4-C5	2.95	115.58	110.23
4	D	1767	008	C16-C15-N14	2.88	112.83	109.86
3	C	1229	NAG	C1-O5-C5	2.84	116.00	112.19
4	D	1767	008	C19-C18-C17	-2.35	116.07	120.68
3	D	1085	NAG	C4-C3-C2	2.34	114.45	111.02
3	A	1092	NAG	O5-C1-C2	-2.25	107.81	111.29
3	B	1085	NAG	C1-O5-C5	2.22	115.16	112.19
4	D	1767	008	C18-C19-N14	-2.21	108.38	111.94
4	B	1767	008	C16-C15-C24	-2.20	107.15	110.63
4	D	1767	008	C16-C15-C24	-2.09	107.33	110.63
3	C	1279	NAG	C3-C4-C5	2.08	114.01	110.23
4	C	1767	008	C19-C18-C17	-2.05	116.66	120.68
4	A	1767	008	C18-C19-N14	-2.04	108.65	111.94
4	B	1767	008	C18-C19-N14	-2.04	108.65	111.94
3	B	1229	NAG	C1-O5-C5	2.03	114.91	112.19
4	B	1767	008	C19-C18-C17	-2.01	116.73	120.68

All (3) chirality outliers are listed below:

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

All (33) torsion outliers are listed below:

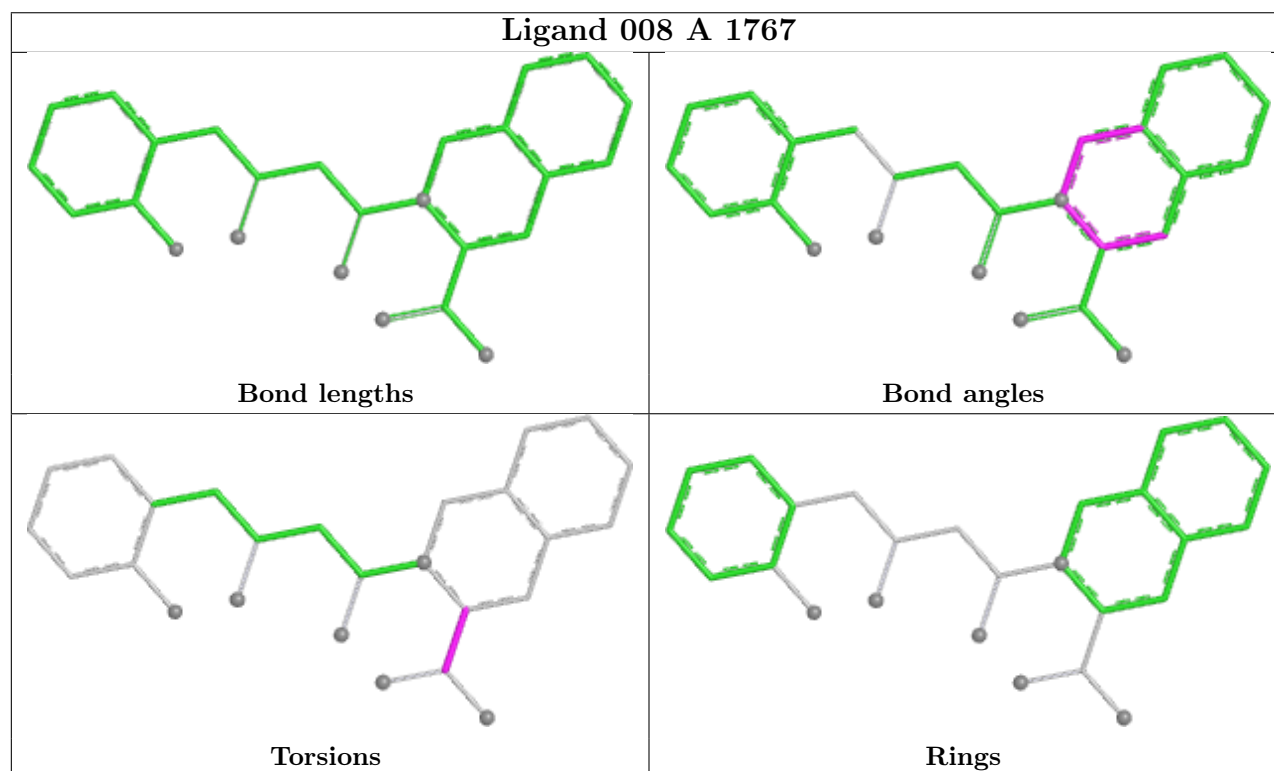
Mol	Chain	Res	Type	Atoms
3	A	1085	NAG	C8-C7-N2-C2
3	A	1085	NAG	O7-C7-N2-C2
3	A	1092	NAG	C8-C7-N2-C2
3	A	1092	NAG	O7-C7-N2-C2
3	B	1085	NAG	C8-C7-N2-C2
3	B	1085	NAG	O7-C7-N2-C2
3	C	1085	NAG	C8-C7-N2-C2
3	C	1085	NAG	O7-C7-N2-C2
3	C	1092	NAG	C8-C7-N2-C2
3	C	1092	NAG	O7-C7-N2-C2
3	C	1321	NAG	C8-C7-N2-C2
3	C	1321	NAG	O7-C7-N2-C2
3	D	1085	NAG	C8-C7-N2-C2
3	D	1085	NAG	O7-C7-N2-C2
3	D	1279	NAG	C8-C7-N2-C2
3	D	1279	NAG	O7-C7-N2-C2
3	A	1085	NAG	O5-C5-C6-O6
3	A	1279	NAG	O5-C5-C6-O6
3	A	1279	NAG	C4-C5-C6-O6
3	B	1085	NAG	O5-C5-C6-O6
3	C	1321	NAG	O5-C5-C6-O6
3	A	1085	NAG	C4-C5-C6-O6
3	D	1279	NAG	O5-C5-C6-O6
3	B	1279	NAG	C4-C5-C6-O6
3	B	1279	NAG	O5-C5-C6-O6
3	C	1321	NAG	C4-C5-C6-O6
3	B	1085	NAG	C4-C5-C6-O6
3	C	1229	NAG	C8-C7-N2-C2
3	C	1092	NAG	C4-C5-C6-O6
3	D	1279	NAG	C4-C5-C6-O6
3	C	1229	NAG	O7-C7-N2-C2
3	A	1085	NAG	C1-C2-N2-C7
4	A	1767	008	N14-C15-C24-O25

There are no ring outliers.

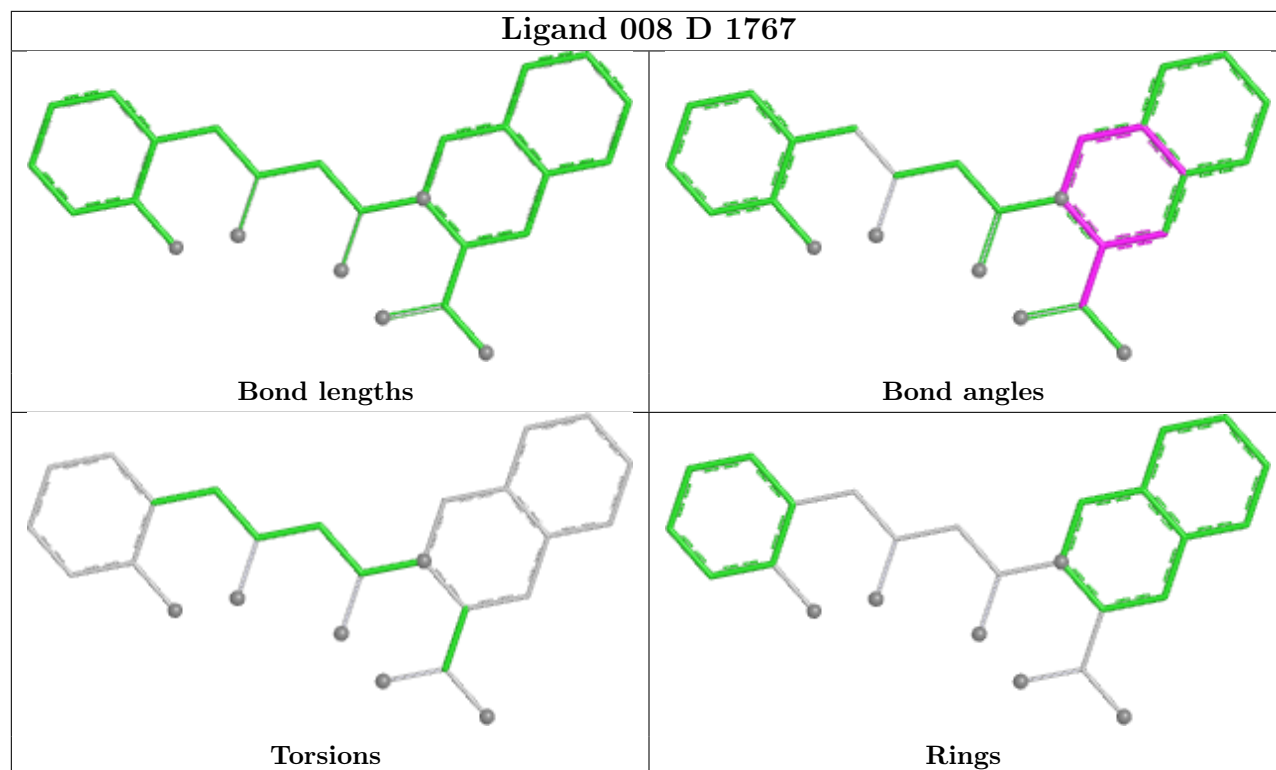
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1767	008	2	0
4	B	1767	008	2	0

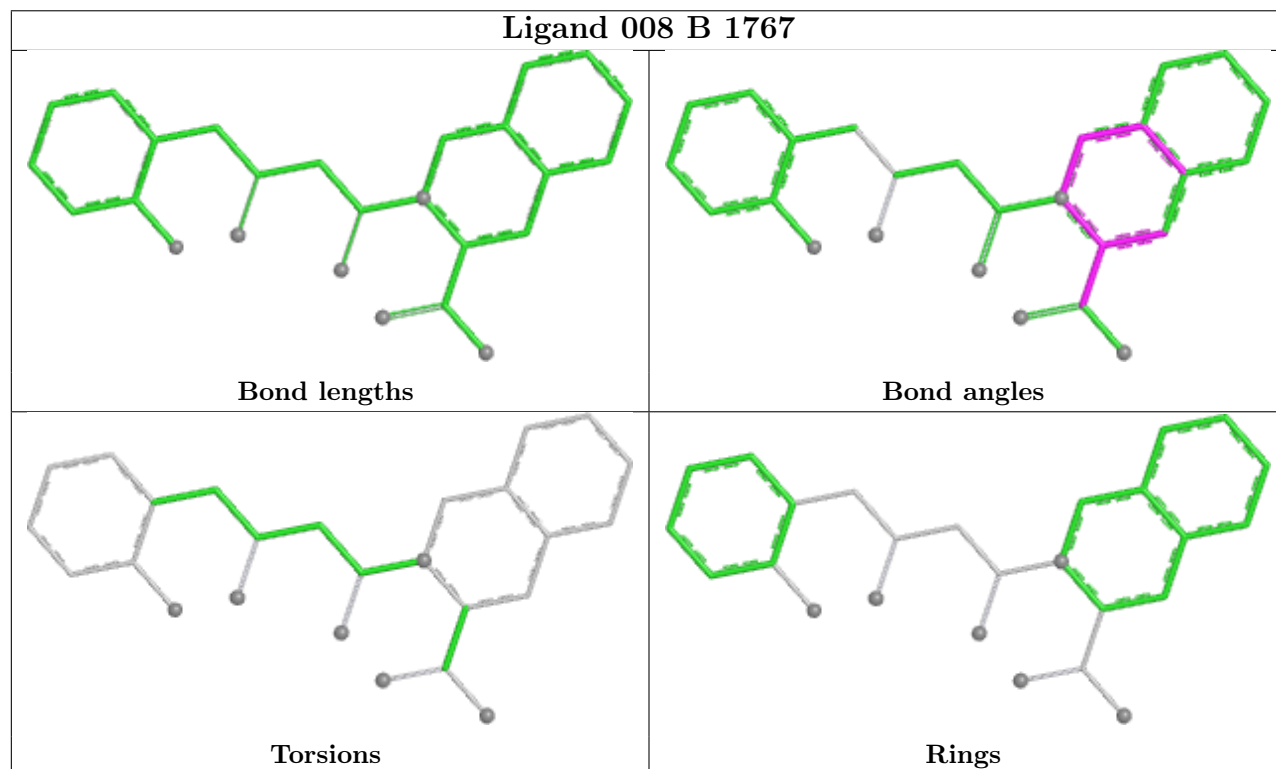
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

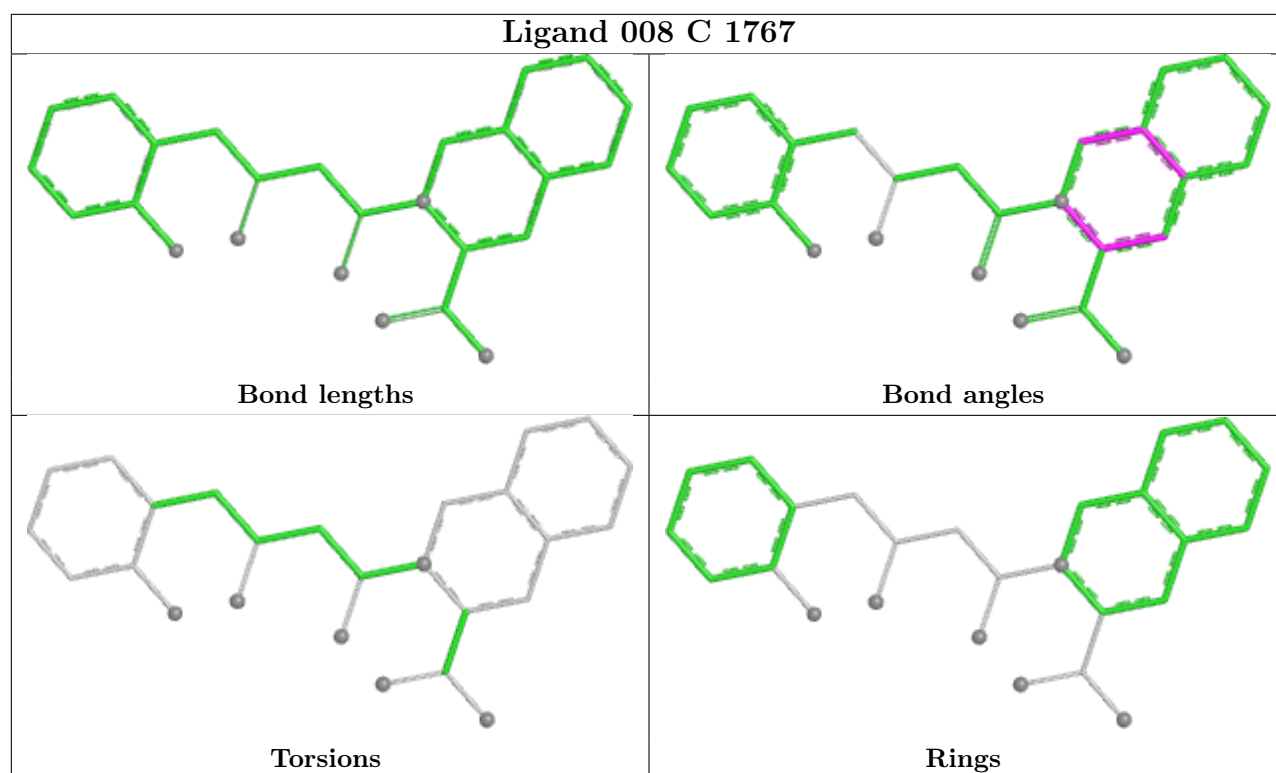


Ligand 008 D 1767



Ligand 008 B 1767





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.