



Full wwPDB EM Validation Report ⓘ

Mar 15, 2025 – 03:12 pm GMT

PDB ID : 9GXE
EMDB ID : EMD-51659
Title : Structure of the SARS-CoV spike glycoprotein in complex with a homotrimeric Bicycle molecule
Authors : Drulyte, I.; Pellegrino, S.; Harman, M.; Bezerra, G.A.
Deposited on : 2024-09-30
Resolution : 2.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

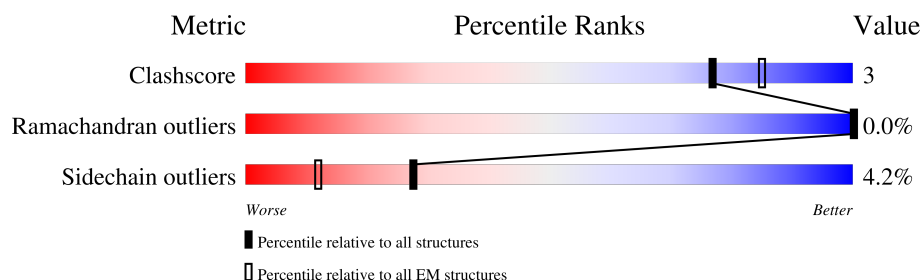
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1133	87% 9% . .
1	B	1133	85% 10% . .
1	C	1133	84% 11% 5%
2	D	16	94% 6%
2	E	16	94% 6%
2	F	16	88% 12%
3	AA	2	50% 50%
3	AB	2	100%
3	AC	2	100%

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Mol	Chain	Length	Quality of chain
3	BA	2	 100%
3	BB	2	 50%50%
3	BC	2	 100%
3	CA	2	 100%
3	CB	2	 100%
3	CC	2	 50%50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26514 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1092	Total	C	N	O	S	0	0
			8542	5450	1426	1626	40		
1	B	1085	Total	C	N	O	S	0	0
			8491	5418	1419	1614	40		
1	C	1075	Total	C	N	O	S	0	0
			8406	5365	1401	1600	40		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Homotrimeric bicycle molecule.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	16	Total	C	N	O	S	0	1
			101	63	18	17	3		
2	E	16	Total	C	N	O	S	0	1
			101	63	18	17	3		
2	F	16	Total	C	N	O	S	0	1
			101	63	18	17	3		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
3	AA	2	Total	C	N	O		0	0
			28	16	2	10			
3	AB	2	Total	C	N	O		0	0
			28	16	2	10			
3	AC	2	Total	C	N	O		0	0
			28	16	2	10			
3	BA	2	Total	C	N	O		0	0
			28	16	2	10			
3	BB	2	Total	C	N	O		0	0
			28	16	2	10			
3	BC	2	Total	C	N	O		0	0
			28	16	2	10			
3	CA	2	Total	C	N	O		0	0
			28	16	2	10			
3	CB	2	Total	C	N	O		0	0
			28	16	2	10			
3	CC	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



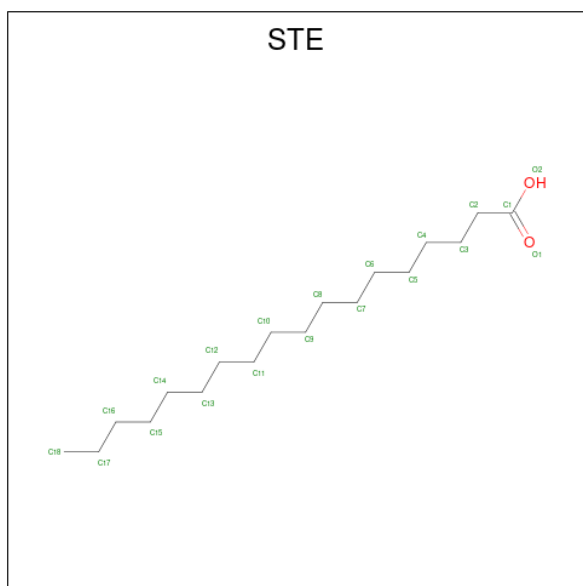
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4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

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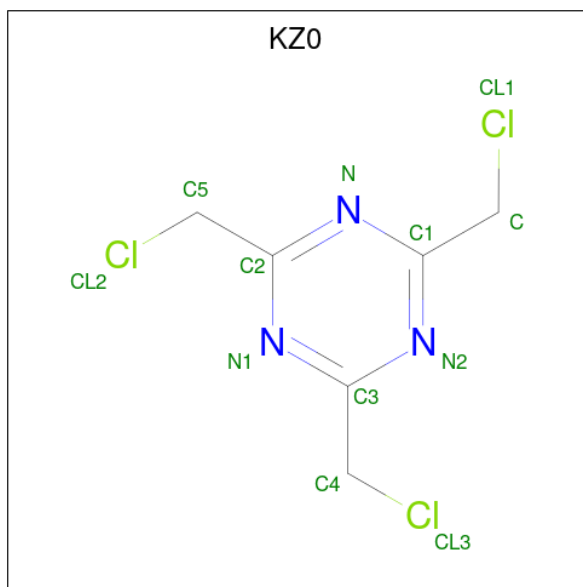
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	C	1	Total	C	O	0
			20	18	2	

- Molecule 6 is 2,4,6-tris(chloromethyl)-1,3,5-triazine (three-letter code: KZ0) (formula: $C_6H_6Cl_3N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	C	N	0
			9	6	3	
6	E	1	Total	C	N	0
			9	6	3	
6	F	1	Total	C	N	0
			9	6	3	

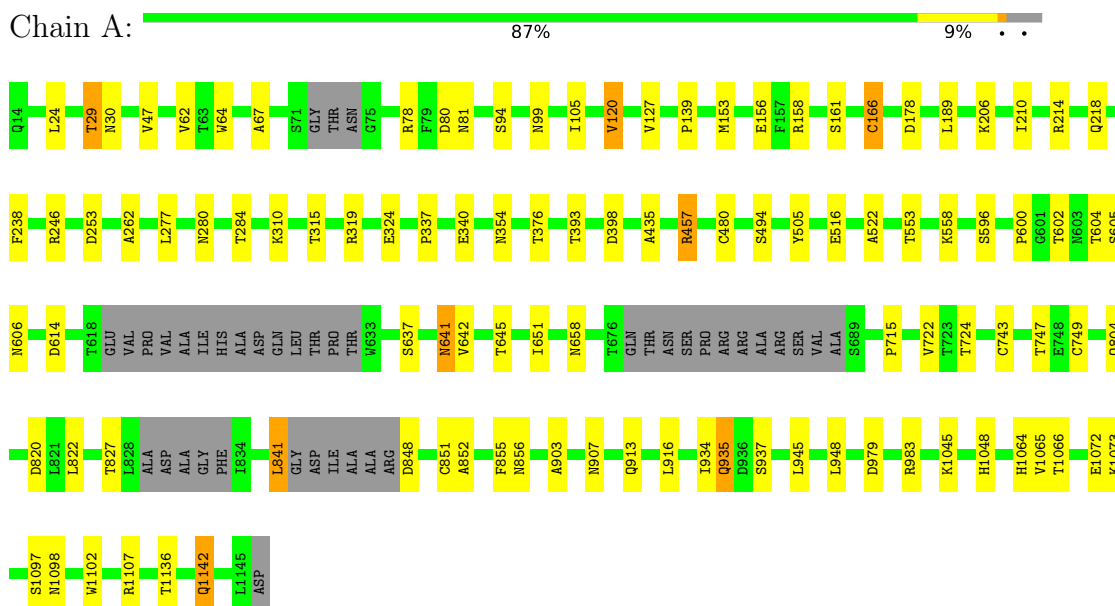
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	45	Total	O	0
			45	45	
7	B	47	Total	O	0
			47	47	
7	C	47	Total	O	0
			47	47	

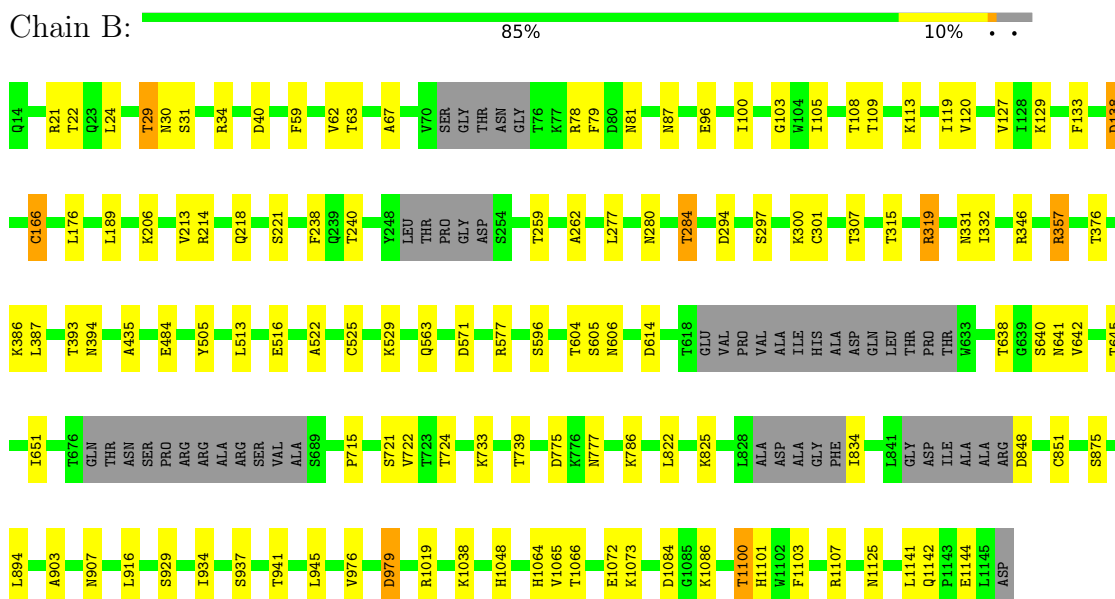
3 Residue-property plots

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.


- Molecule 1: Spike glycoprotein

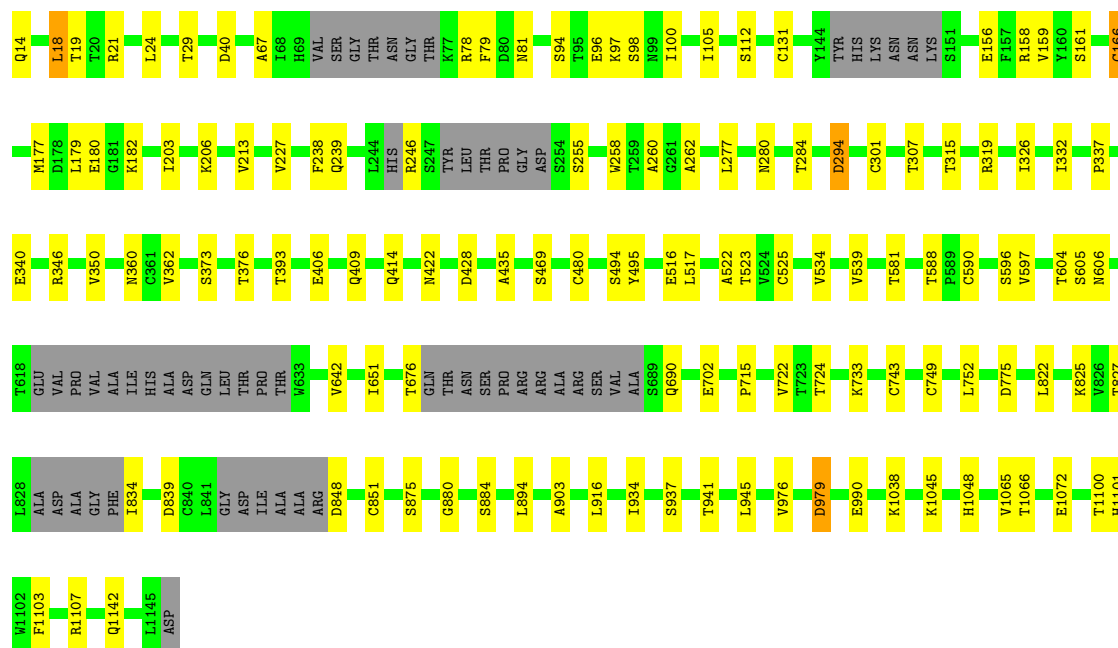


- Molecule 1: Spike glycoprotein



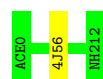
- Molecule 1: Spike glycoprotein

Chain C:  84% 11% 5%



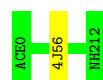
- Molecule 2: Homotrimeric bicycle molecule

Chain D:  94% 6%




- Molecule 2: Homotrimeric bicycle molecule

Chain E:  94% 6%



- Molecule 2: Homotrimeric bicycle molecule

Chain F:  88% 12%



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

Chain AA:  50% 50%



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

Chain AB:  100%



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

Chain AC:  100%



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

Chain BA:  100%



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

Chain BB:  50% 50%



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

Chain BC:  100%



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

Chain CA:  100%



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

Chain CB:  100%

MAG1
MAG2

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

Chain CC:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	429402	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STE, KZ0, DAL, NAG, NH2, 4J5, 0JY, ACE

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	0.30	0/8743	0.53	2/11901 (0.0%)
1	B	0.30	0/8689	0.53	1/11825 (0.0%)
1	C	0.30	0/8599	0.54	3/11700 (0.0%)
2	D	0.70	0/73	0.60	0/97
2	E	0.70	0/73	0.61	0/97
2	F	0.70	0/73	0.60	0/97
All	All	0.30	0/26250	0.54	6/35717 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	166	CYS	CA-CB-SG	6.34	125.42	114.00
1	B	166	CYS	CA-CB-SG	6.28	125.31	114.00
1	C	166	CYS	CA-CB-SG	5.48	123.86	114.00
1	A	153	MET	CB-CG-SD	5.45	128.76	112.40
1	C	428	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1142	GLN	Peptide
1	B	1142	GLN	Peptide
1	C	1142	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8542	0	8323	46	0
1	B	8491	0	8274	55	0
1	C	8406	0	8197	54	0
2	D	101	0	85	0	0
2	E	101	0	85	0	0
2	F	101	0	85	0	0
3	AA	28	0	25	0	0
3	AB	28	0	25	0	0
3	AC	28	0	25	0	0
3	BA	28	0	25	0	0
3	BB	28	0	25	1	0
3	BC	28	0	25	0	0
3	CA	28	0	25	0	0
3	CB	28	0	25	0	0
3	CC	28	0	25	1	0
4	A	98	0	91	0	0
4	B	112	0	104	1	0
4	C	84	0	78	0	0
5	A	20	0	35	2	0
5	B	20	0	35	0	0
5	C	20	0	35	0	0
6	D	9	0	0	0	0
6	E	9	0	0	0	0
6	F	9	0	0	0	0
7	A	45	0	0	0	0
7	B	47	0	0	1	0
7	C	47	0	0	0	0
All	All	26514	0	25652	146	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.

All (146) 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:67:ALA:O	1:C:262:ALA:HA	1.86	0.75
1:A:67:ALA:O	1:A:262:ALA:HA	1.96	0.65
1:C:19:THR:HA	1:C:21:ARG:HH21	1.66	0.61
1:C:180:GLU:HG2	1:C:182:LYS:HG2	1.85	0.59
1:B:825:LYS:NZ	1:B:941:THR:O	2.36	0.59
1:B:24:LEU:HD22	1:B:78:ARG:HD2	1.84	0.58
1:C:332:ILE:HD11	1:C:525:CYS:HB2	1.86	0.58
1:C:24:LEU:HD12	1:C:78:ARG:HH11	1.70	0.57
1:B:563:GLN:O	1:B:577:ARG:NH1	2.39	0.56
1:B:332:ILE:HD11	1:B:525:CYS:HB2	1.88	0.56
1:C:246:ARG:NH2	1:C:255:SER:O	2.38	0.56
1:B:34:ARG:HH12	1:B:189:LEU:HD21	1.69	0.56
1:B:138:ASP:N	1:B:138:ASP:OD1	2.38	0.56
1:A:24:LEU:HG	1:A:78:ARG:HD3	1.88	0.55
1:B:67:ALA:O	1:B:262:ALA:HA	2.06	0.55
1:A:319:ARG:HH22	1:B:739:THR:HB	1.72	0.55
1:C:1103:PHE:HZ	3:CC:1:NAG:H62	1.73	0.55
1:A:29:THR:OG1	1:A:30:ASN:N	2.40	0.54
5:A:1208:STE:H131	1:B:513:LEU:HD13	1.90	0.54
1:C:360:ASN:H	1:C:523:THR:HG22	1.72	0.54
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.39	0.54
1:C:409:GLN:HA	1:C:414:GLN:HG2	1.89	0.54
1:C:825:LYS:NZ	1:C:941:THR:O	2.41	0.54
1:B:22:THR:O	1:B:78:ARG:NH1	2.40	0.54
1:A:848:ASP:HB3	1:A:851:CYS:HB2	1.89	0.54
1:B:31:SER:O	1:B:59:PHE:HA	2.08	0.54
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.90	0.54
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.89	0.53
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.90	0.53
1:C:393:THR:HA	1:C:522:ALA:HA	1.89	0.53
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.90	0.53
1:B:29:THR:OG1	1:B:30:ASN:N	2.41	0.52
1:C:1100:THR:OG1	1:C:1101:HIS:ND1	2.41	0.52
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.91	0.52
1:B:103:GLY:HA3	1:B:119:ILE:O	2.10	0.52
1:C:724:THR:HG23	1:C:934:ILE:HD12	1.91	0.52
1:C:848:ASP:HB3	1:C:851:CYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:VAL:HA	1:C:525:CYS:O	2.10	0.52
1:B:129:LYS:HG3	1:B:133:PHE:HZ	1.75	0.51
1:C:326:ILE:HD12	1:C:539:VAL:HG21	1.92	0.51
1:A:945:LEU:HD23	1:A:948:LEU:HD12	1.93	0.51
1:B:280:ASN:ND2	1:B:284:THR:O	2.43	0.51
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.93	0.51
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.93	0.51
1:B:1100:THR:OG1	1:B:1101:HIS:ND1	2.44	0.50
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.94	0.50
1:B:1103:PHE:HZ	3:BB:1:NAG:H62	1.76	0.50
1:A:105:ILE:O	1:A:238:PHE:HA	2.11	0.50
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.92	0.50
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.94	0.50
1:C:294:ASP:OD1	1:C:294:ASP:N	2.43	0.50
1:A:99:ASN:ND2	1:A:178:ASP:O	2.42	0.49
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.93	0.49
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.92	0.49
1:A:605:SER:OG	1:A:606:ASN:N	2.46	0.49
1:A:337:PRO:HB2	1:A:340:GLU:HB2	1.94	0.49
1:B:29:THR:HG23	1:B:62:VAL:HG23	1.95	0.49
1:B:108:THR:HG23	1:B:109:THR:HG23	1.95	0.48
1:B:294:ASP:N	1:B:294:ASP:OD1	2.46	0.48
1:C:96:GLU:OE1	1:C:100:ILE:N	2.42	0.48
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.95	0.48
1:C:280:ASN:ND2	1:C:284:THR:O	2.47	0.48
1:A:81:ASN:N	1:A:81:ASN:OD1	2.47	0.48
1:B:206:LYS:HA	1:B:206:LYS:HD2	1.67	0.47
1:C:337:PRO:HB2	1:C:340:GLU:HB2	1.96	0.47
1:B:393:THR:HA	1:B:522:ALA:HA	1.96	0.47
1:B:96:GLU:OE1	1:B:100:ILE:N	2.47	0.47
1:C:81:ASN:N	1:C:81:ASN:OD1	2.47	0.47
1:C:105:ILE:O	1:C:238:PHE:HA	2.15	0.47
1:A:280:ASN:ND2	1:A:284:THR:O	2.48	0.47
1:A:642:VAL:HG12	1:A:651:ILE:HG12	1.97	0.47
1:A:907:ASN:HD22	1:C:1107:ARG:HH22	1.62	0.47
1:A:724:THR:HG23	1:A:934:ILE:HD12	1.97	0.46
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.97	0.46
1:A:457:ARG:NH2	4:B:1207:NAG:O7	2.47	0.46
1:B:903:ALA:HB2	1:B:916:LEU:HD22	1.97	0.46
1:C:156:GLU:OE1	1:C:158:ARG:NH1	2.47	0.46
1:A:1073:LYS:HE2	1:A:1073:LYS:HB3	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.98	0.46
1:A:614:ASP:HA	1:B:834:ILE:HG23	1.98	0.46
1:B:81:ASN:OD1	1:B:81:ASN:N	2.48	0.46
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.43	0.46
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.74	0.46
1:C:97:LYS:NZ	1:C:182:LYS:O	2.48	0.46
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.71	0.46
1:C:376:THR:HB	1:C:435:ALA:HB3	1.98	0.46
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.49	0.46
1:B:614:ASP:HA	1:C:834:ILE:HG23	1.98	0.46
1:B:297:SER:HA	1:B:300:LYS:HD2	1.97	0.45
1:C:642:VAL:HG22	1:C:651:ILE:HG13	1.97	0.45
1:B:848:ASP:HB3	1:B:851:CYS:HB2	1.98	0.45
1:B:1073:LYS:HB3	1:B:1073:LYS:HE2	1.76	0.45
1:A:641:ASN:OD1	1:A:641:ASN:N	2.49	0.45
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.99	0.45
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.78	0.45
1:B:376:THR:HB	1:B:435:ALA:HB3	1.98	0.45
1:A:1107:ARG:HH22	1:B:907:ASN:HD22	1.65	0.45
1:B:105:ILE:O	1:B:238:PHE:HA	2.17	0.45
1:A:29:THR:HG23	1:A:62:VAL:HG23	1.98	0.45
1:C:903:ALA:HB2	1:C:916:LEU:HD12	1.99	0.44
1:A:376:THR:HB	1:A:435:ALA:HB3	1.98	0.44
1:B:1107:ARG:NH1	7:B:1307:HOH:O	2.43	0.44
1:B:786:LYS:HA	1:B:786:LYS:HD3	1.67	0.44
1:C:21:ARG:NH1	1:C:79:PHE:O	2.51	0.44
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.99	0.43
1:A:841:LEU:HB2	1:C:588:THR:HG21	2.00	0.43
1:A:983:ARG:HD2	1:C:517:LEU:HD13	1.98	0.43
1:B:357:ARG:HH12	1:B:394:ASN:HB2	1.83	0.43
1:B:976:VAL:HB	1:B:979:ASP:HB3	2.01	0.43
1:C:18:LEU:HD22	1:C:258:TRP:CD1	2.54	0.43
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.64	0.43
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.43
1:C:605:SER:OG	1:C:606:ASN:N	2.52	0.43
1:A:852:ALA:O	1:A:856:ASN:ND2	2.51	0.42
1:C:880:GLY:O	1:C:884:SER:OG	2.34	0.42
1:A:722:VAL:HA	1:A:1064:HIS:O	2.19	0.42
1:C:676:THR:HA	1:C:690:GLN:HA	2.01	0.42
1:B:21:ARG:NH1	1:B:79:PHE:O	2.44	0.42
1:A:139:PRO:HA	1:A:158:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:HH2	1:A:214:ARG:HE	1.68	0.42
1:A:903:ALA:HB1	1:A:913:GLN:HB2	2.02	0.42
1:B:715:PRO:HD3	1:C:894:LEU:HD13	2.01	0.42
1:A:354:ASN:O	1:A:398:ASP:HA	2.20	0.41
1:B:722:VAL:HA	1:B:1064:HIS:O	2.19	0.41
1:A:78:ARG:NH2	1:A:80:ASP:OD2	2.54	0.41
1:A:280:ASN:HD21	1:A:284:THR:HB	1.86	0.41
1:A:120:VAL:HG12	1:A:127:VAL:HB	2.01	0.41
1:C:280:ASN:HD21	1:C:284:THR:HB	1.86	0.41
1:C:976:VAL:HB	1:C:979:ASP:HB3	2.01	0.41
1:B:319:ARG:H	1:B:319:ARG:HG2	1.76	0.41
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.44	0.41
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.03	0.41
5:A:1208:STE:H91	1:B:387:LEU:HD13	2.03	0.41
1:B:642:VAL:HG22	1:B:651:ILE:HG13	2.02	0.41
1:B:605:SER:OG	1:B:606:ASN:N	2.54	0.41
1:C:81:ASN:O	1:C:239:GLN:NE2	2.46	0.40
1:C:258:TRP:HZ3	1:C:260:ALA:HB2	1.86	0.40
1:C:350:VAL:HG22	1:C:422:ASN:HB3	2.03	0.40
1:C:752:LEU:HD11	1:C:990:GLU:HG2	2.03	0.40
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.96	0.40
1:C:203:ILE:HB	1:C:227:VAL:HG12	2.03	0.40
1:A:156:GLU:OE1	1:A:246:ARG:NE	2.45	0.40
1:A:393:THR:HG22	1:A:522:ALA:HB2	2.03	0.40
1:B:386:LYS:HD3	1:B:386:LYS:HA	1.96	0.40
1:C:406:GLU:OE1	1:C:495:TYR:OH	2.32	0.40
1:C:1045:LYS:HE2	1:C:1045:LYS:HB2	1.70	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 PDB entries followed by that with respect to all EM entries.

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	1080/1133 (95%)	1042 (96%)	38 (4%)	0	100	100
1	B	1071/1133 (94%)	1037 (97%)	34 (3%)	0	100	100
1	C	1057/1133 (93%)	1017 (96%)	40 (4%)	0	100	100
2	D	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	E	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	F	11/16 (69%)	10 (91%)	0	1 (9%)	0	0
All	All	3241/3447 (94%)	3126 (96%)	114 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	11	ALA

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 PDB entries followed by that with respect to all EM entries.

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	957/987 (97%)	919 (96%)	38 (4%)	27	40
1	B	951/987 (96%)	905 (95%)	46 (5%)	21	32
1	C	942/987 (95%)	906 (96%)	36 (4%)	28	42
2	D	8/9 (89%)	8 (100%)	0	100	100
2	E	8/9 (89%)	8 (100%)	0	100	100
2	F	8/9 (89%)	8 (100%)	0	100	100
All	All	2874/2988 (96%)	2754 (96%)	120 (4%)	27	37

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	47	VAL
1	A	94	SER
1	A	120	VAL

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Mol	Chain	Res	Type
1	A	161	SER
1	A	166	CYS
1	A	218	GLN
1	A	253	ASP
1	A	277	LEU
1	A	315	THR
1	A	324	GLU
1	A	457	ARG
1	A	480	CYS
1	A	494	SER
1	A	505	TYR
1	A	516	GLU
1	A	553	THR
1	A	558	LYS
1	A	596	SER
1	A	602	THR
1	A	604	THR
1	A	637	SER
1	A	641	ASN
1	A	645	THR
1	A	658	ASN
1	A	747	THR
1	A	820	ASP
1	A	827	THR
1	A	841	LEU
1	A	855	PHE
1	A	916	LEU
1	A	935	GLN
1	A	937	SER
1	A	979	ASP
1	A	1045	LYS
1	A	1098	ASN
1	A	1136	THR
1	A	1142	GLN
1	B	29	THR
1	B	40	ASP
1	B	63	THR
1	B	87	ASN
1	B	113	LYS
1	B	120	VAL
1	B	127	VAL
1	B	138	ASP

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Mol	Chain	Res	Type
1	B	166	CYS
1	B	176	LEU
1	B	213	VAL
1	B	214	ARG
1	B	218	GLN
1	B	221	SER
1	B	240	THR
1	B	259	THR
1	B	277	LEU
1	B	284	THR
1	B	301	CYS
1	B	307	THR
1	B	315	THR
1	B	319	ARG
1	B	331	ASN
1	B	346	ARG
1	B	357	ARG
1	B	484	GLU
1	B	505	TYR
1	B	516	GLU
1	B	529	LYS
1	B	571	ASP
1	B	596	SER
1	B	604	THR
1	B	638	THR
1	B	640	SER
1	B	641	ASN
1	B	645	THR
1	B	721	SER
1	B	875	SER
1	B	929	SER
1	B	937	SER
1	B	979	ASP
1	B	1038	LYS
1	B	1084	ASP
1	B	1100	THR
1	B	1141	LEU
1	B	1144	GLU
1	C	14	GLN
1	C	29	THR
1	C	40	ASP
1	C	94	SER

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Mol	Chain	Res	Type
1	C	98	SER
1	C	112	SER
1	C	159	VAL
1	C	161	SER
1	C	177	MET
1	C	179	LEU
1	C	213	VAL
1	C	277	LEU
1	C	294	ASP
1	C	301	CYS
1	C	307	THR
1	C	315	THR
1	C	319	ARG
1	C	346	ARG
1	C	373	SER
1	C	469	SER
1	C	480	CYS
1	C	494	SER
1	C	516	GLU
1	C	534	VAL
1	C	581	THR
1	C	590	CYS
1	C	596	SER
1	C	597	VAL
1	C	604	THR
1	C	702	GLU
1	C	827	THR
1	C	839	ASP
1	C	875	SER
1	C	937	SER
1	C	979	ASP
1	C	1038	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	4J5	D	6	2	8,9,10	2.32	2 (25%)	4,10,12	0.48	0
2	4J5	F	6	2	8,9,10	2.31	2 (25%)	4,10,12	0.49	0
2	4J5	E	6	2	8,9,10	2.32	2 (25%)	4,10,12	0.48	0
2	DAL	F	7	2	3,4,5	1.00	0	2,4,6	0.81	0
2	DAL	E	7	2	3,4,5	1.00	0	2,4,6	0.78	0
2	DAL	D	7	2	3,4,5	1.00	0	2,4,6	0.78	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	4J5	D	6	2	-	2/7/8/10	-
2	4J5	F	6	2	-	2/7/8/10	-
2	4J5	E	6	2	-	2/7/8/10	-
2	DAL	F	7	2	-	0/0/2/4	-
2	DAL	E	7	2	-	0/0/2/4	-
2	DAL	D	7	2	-	0/0/2/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	4J5	CE-ND	4.47	1.42	1.33
2	E	6	4J5	CE-ND	4.46	1.42	1.33
2	F	6	4J5	CE-ND	4.43	1.42	1.33
2	D	6	4J5	CE-NH2	3.81	1.47	1.32
2	F	6	4J5	CE-NH2	3.79	1.47	1.32
2	E	6	4J5	CE-NH2	3.78	1.47	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	6	4J5	CA-CB-CG-ND
2	E	6	4J5	CA-CB-CG-ND
2	F	6	4J5	CA-CB-CG-ND
2	D	6	4J5	CB-CG-ND-CE
2	F	6	4J5	CB-CG-ND-CE
2	E	6	4J5	CB-CG-ND-CE

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
3	NAG	AA	1	1,3	14,14,15	0.78	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	AA	2	3	14,14,15	0.32	0	17,19,21	0.56	0
3	NAG	AB	1	1,3	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	AB	2	3	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	AC	1	1,3	14,14,15	0.26	0	17,19,21	0.57	0
3	NAG	AC	2	3	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	BA	1	1,3	14,14,15	0.23	0	17,19,21	0.55	0
3	NAG	BA	2	3	14,14,15	0.27	0	17,19,21	0.48	0
3	NAG	BB	1	1,3	14,14,15	0.34	0	17,19,21	0.52	0
3	NAG	BB	2	3	14,14,15	0.38	0	17,19,21	0.41	0
3	NAG	BC	1	1,3	14,14,15	0.26	0	17,19,21	0.54	0
3	NAG	BC	2	3	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	CA	1	1,3	14,14,15	0.24	0	17,19,21	0.53	0
3	NAG	CA	2	3	14,14,15	0.28	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	CB	1	1,3	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	CB	2	3	14,14,15	0.27	0	17,19,21	0.51	0
3	NAG	CC	1	1,3	14,14,15	0.35	0	17,19,21	0.54	0
3	NAG	CC	2	3	14,14,15	0.37	0	17,19,21	0.41	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
3	NAG	AA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	AA	2	3	-	3/6/23/26	0/1/1/1
3	NAG	AB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	AB	2	3	-	0/6/23/26	0/1/1/1
3	NAG	AC	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	AC	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BA	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BB	2	3	-	2/6/23/26	0/1/1/1
3	NAG	BC	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BC	2	3	-	0/6/23/26	0/1/1/1
3	NAG	CA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	CA	2	3	-	2/6/23/26	0/1/1/1
3	NAG	CB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	CB	2	3	-	2/6/23/26	0/1/1/1
3	NAG	CC	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	CC	2	3	-	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)
3	AA	1	NAG	C1-C2	2.39	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AA	1	NAG	C1-O5-C5	3.04	116.31	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

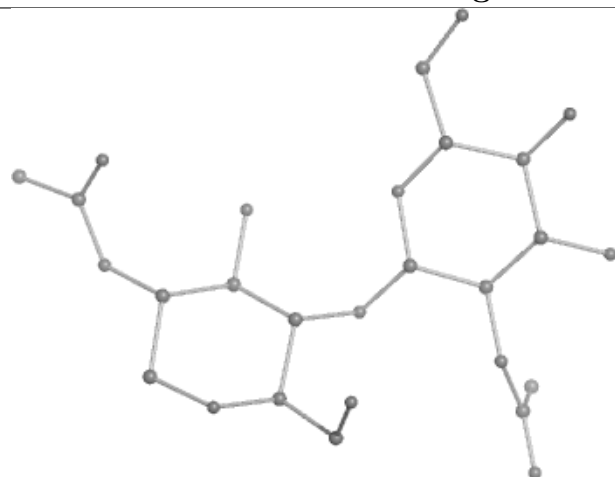
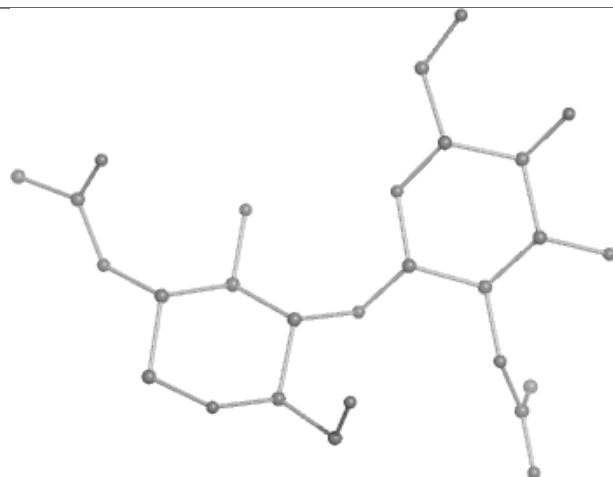
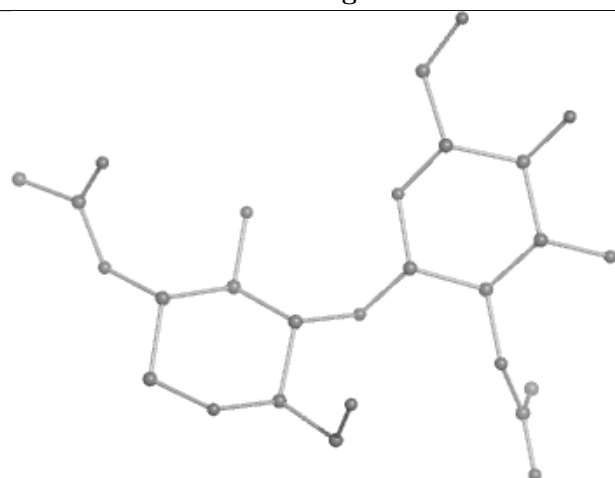
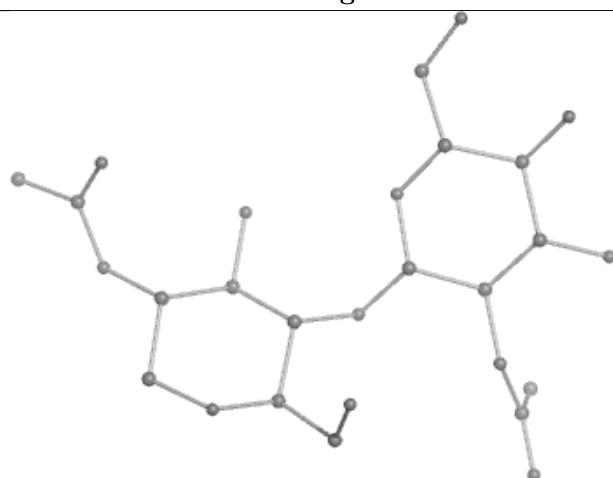
Mol	Chain	Res	Type	Atoms
3	CC	2	NAG	O5-C5-C6-O6
3	BB	2	NAG	O5-C5-C6-O6
3	AA	2	NAG	C8-C7-N2-C2
3	AA	2	NAG	O7-C7-N2-C2
3	BA	2	NAG	O5-C5-C6-O6
3	BB	2	NAG	C4-C5-C6-O6
3	CC	2	NAG	C4-C5-C6-O6
3	BA	2	NAG	C4-C5-C6-O6
3	CA	2	NAG	O5-C5-C6-O6
3	CA	2	NAG	C4-C5-C6-O6
3	AA	2	NAG	O5-C5-C6-O6
3	CA	1	NAG	C4-C5-C6-O6
3	CA	1	NAG	O5-C5-C6-O6
3	CB	2	NAG	C4-C5-C6-O6
3	CB	2	NAG	O5-C5-C6-O6
3	AC	2	NAG	C4-C5-C6-O6
3	AC	2	NAG	O5-C5-C6-O6

There are no ring outliers.

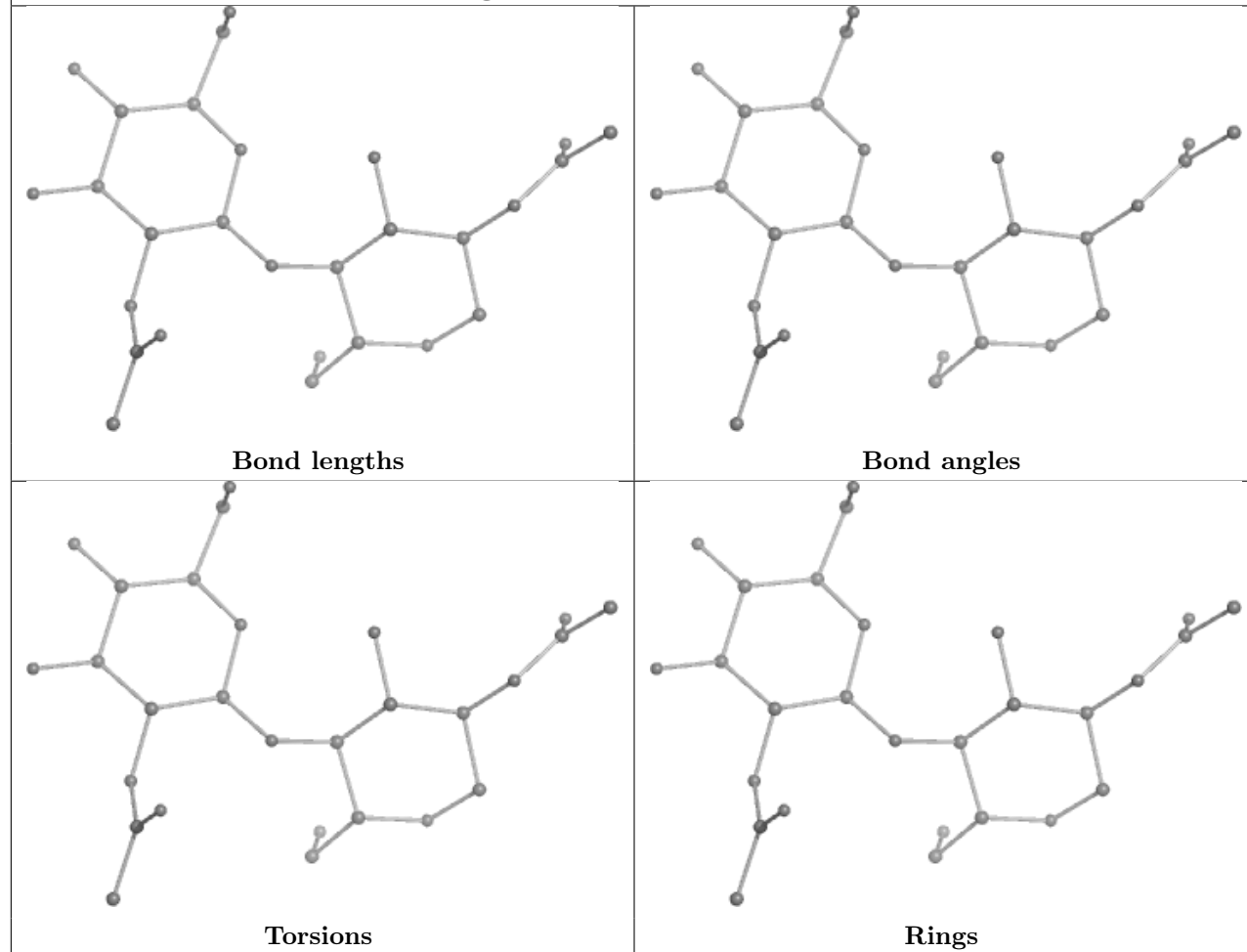
2 monomers are involved in 2 short contacts:

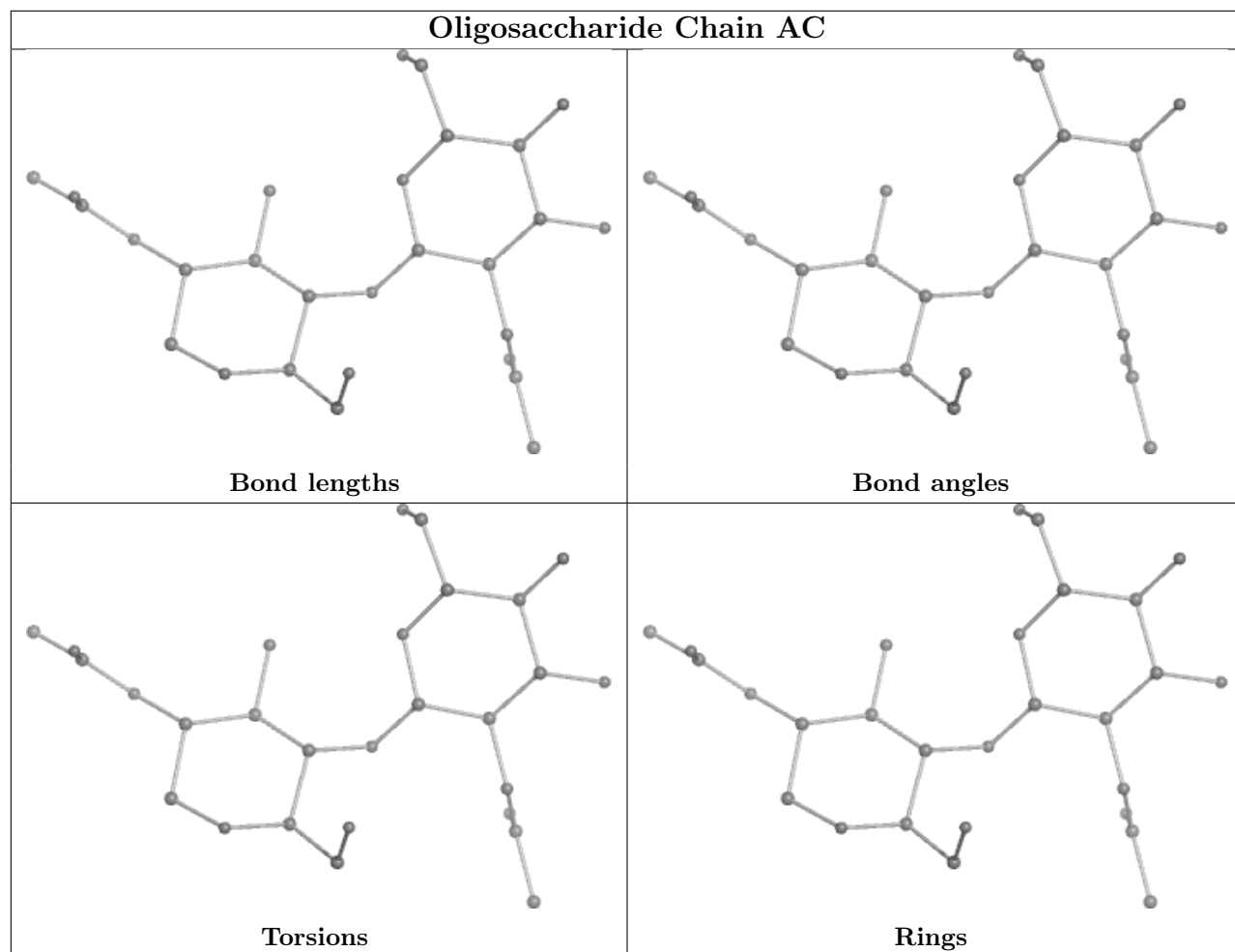
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BB	1	NAG	1	0
3	CC	1	NAG	1	0

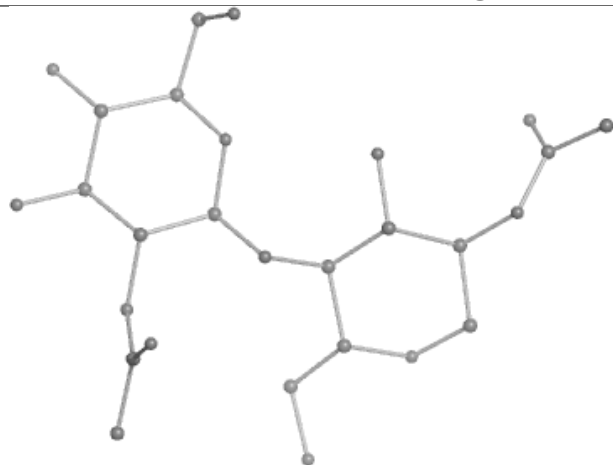
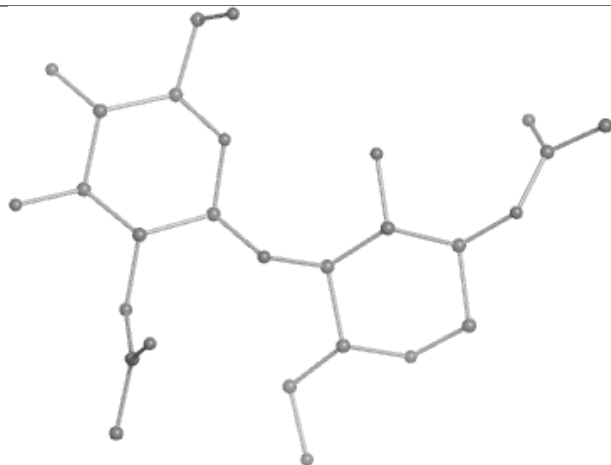
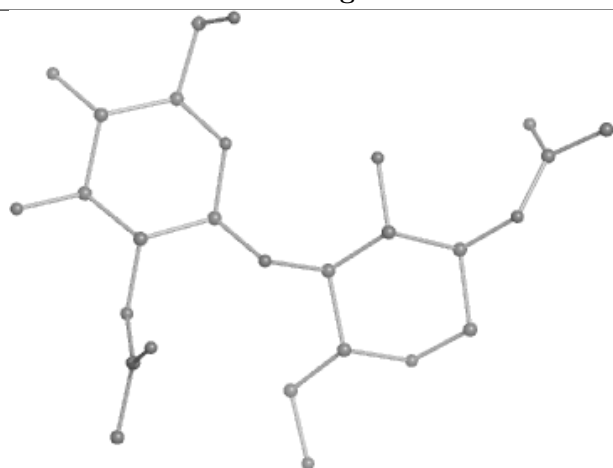
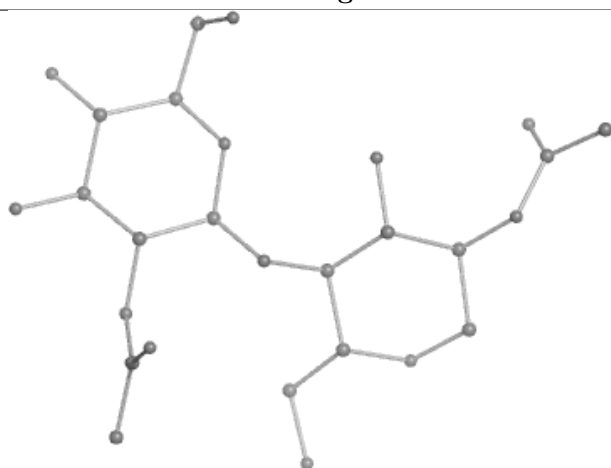
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

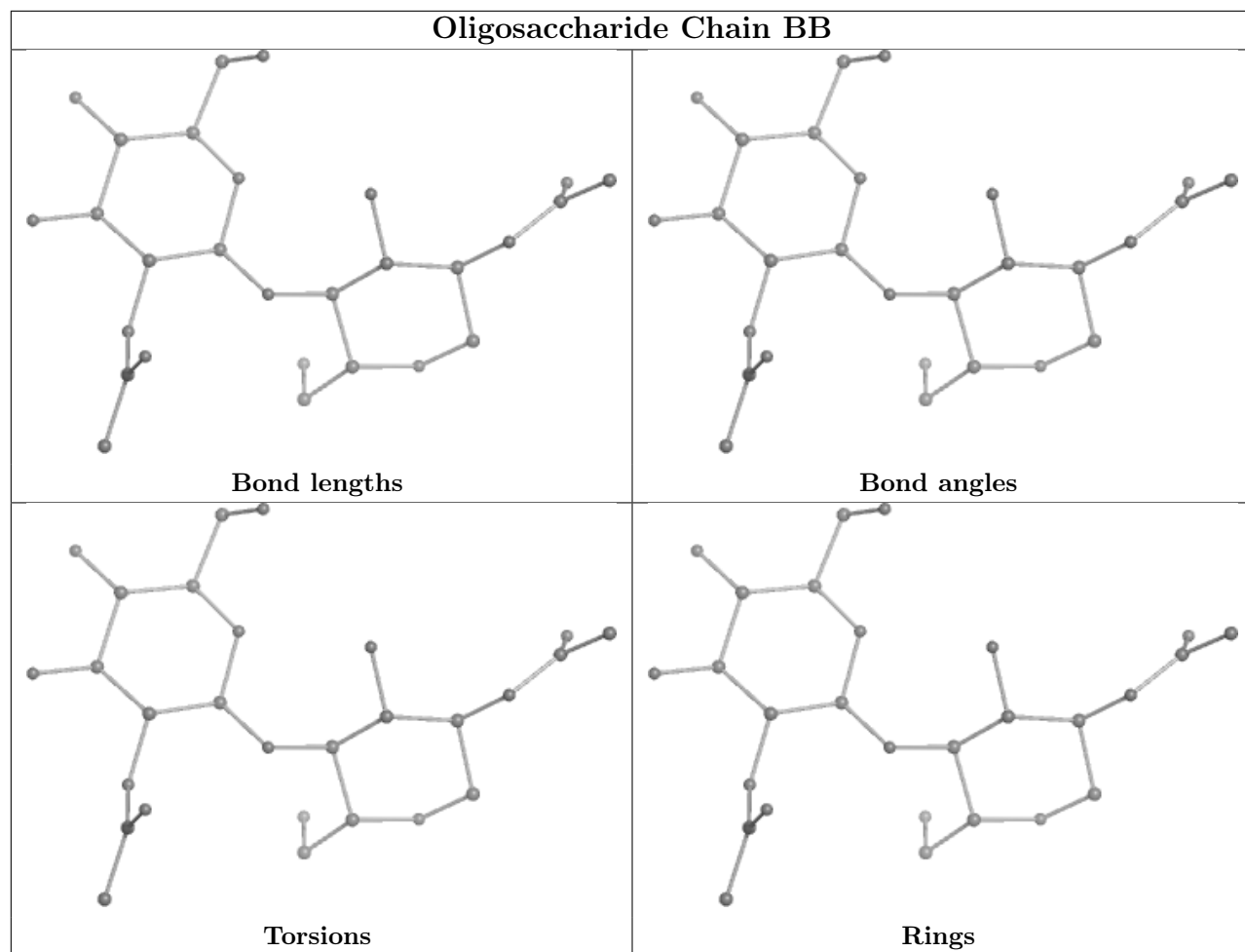
Oligosaccharide Chain AA**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain AB

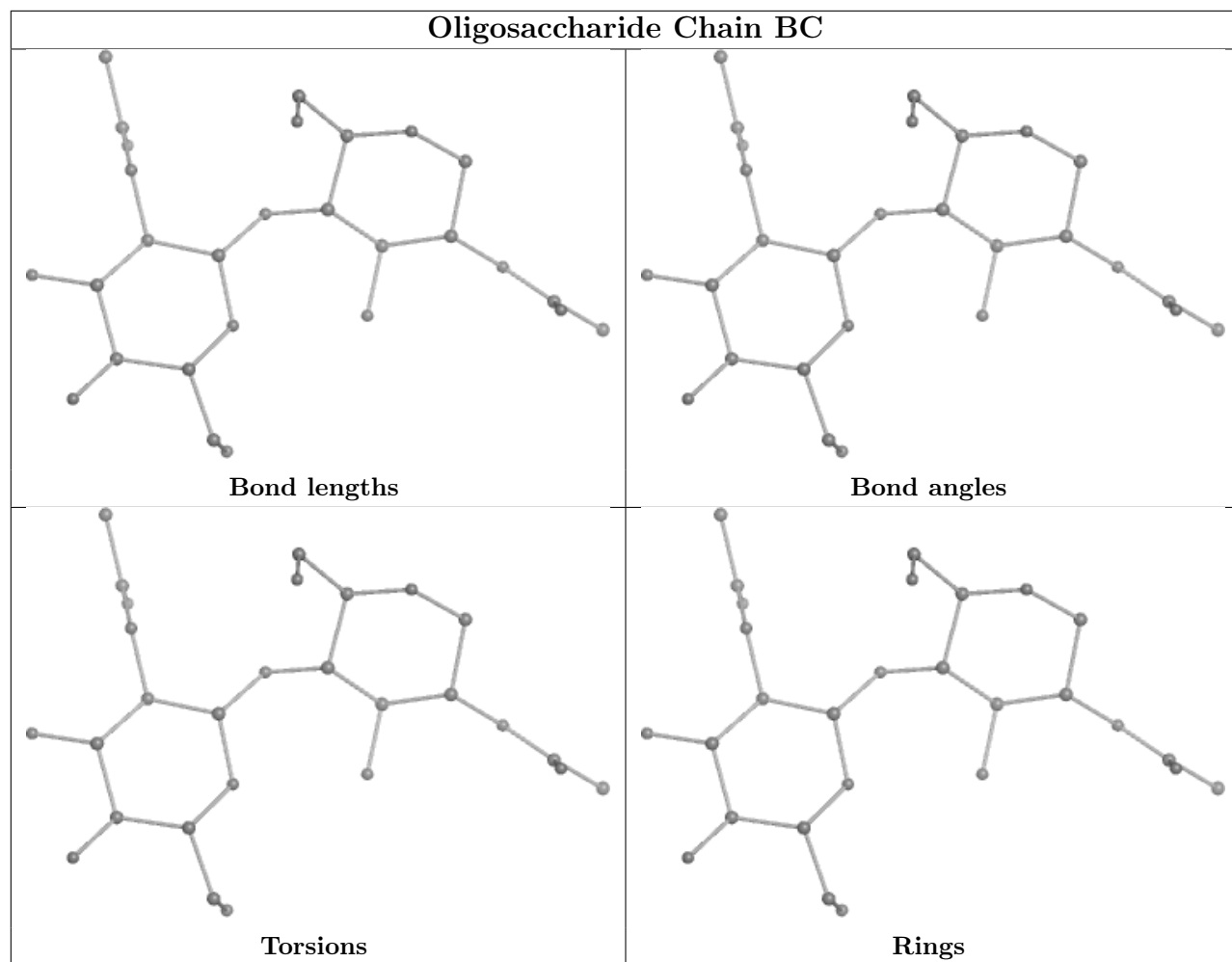


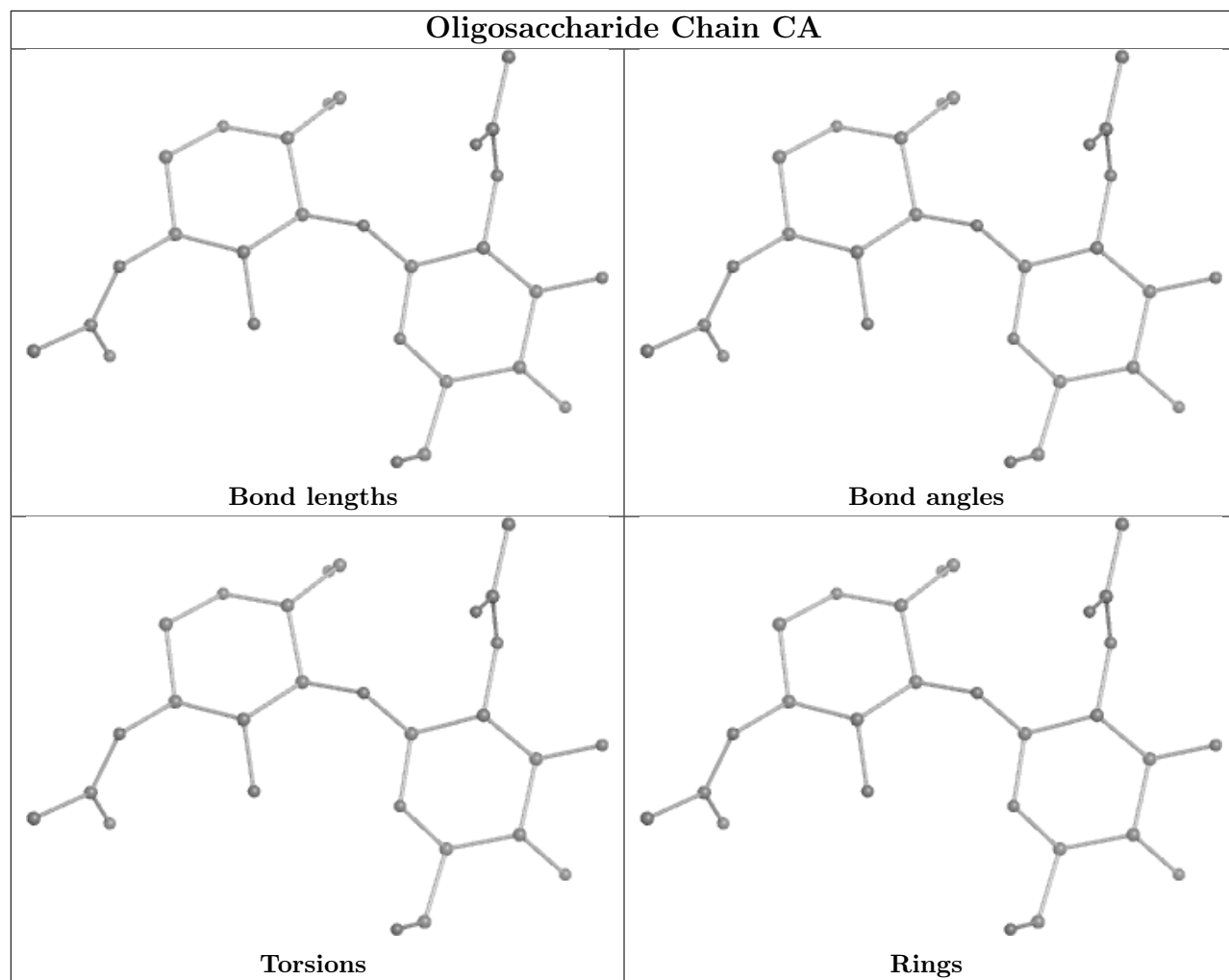


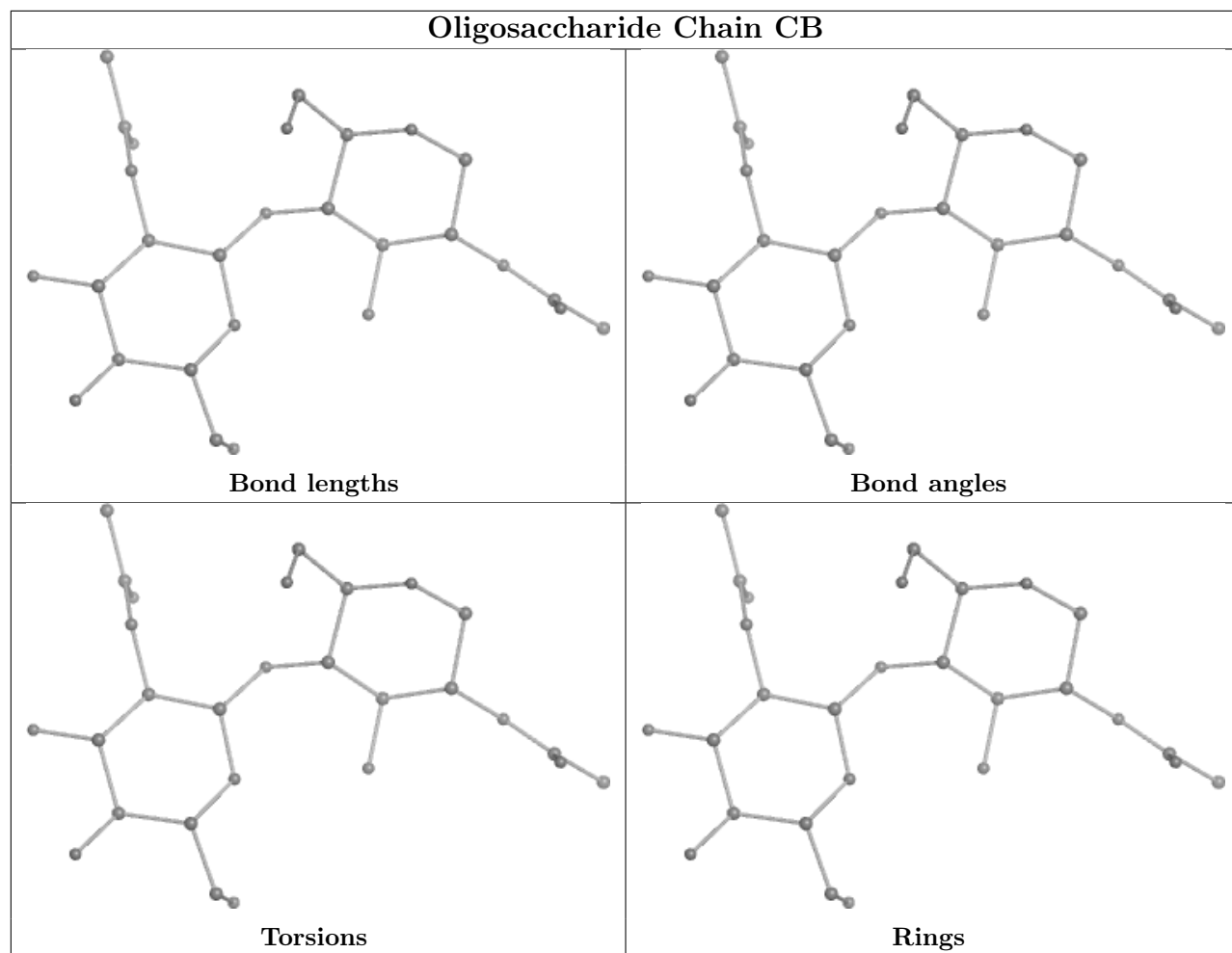
Oligosaccharide Chain BA**Bond lengths****Bond angles****Torsions****Rings**

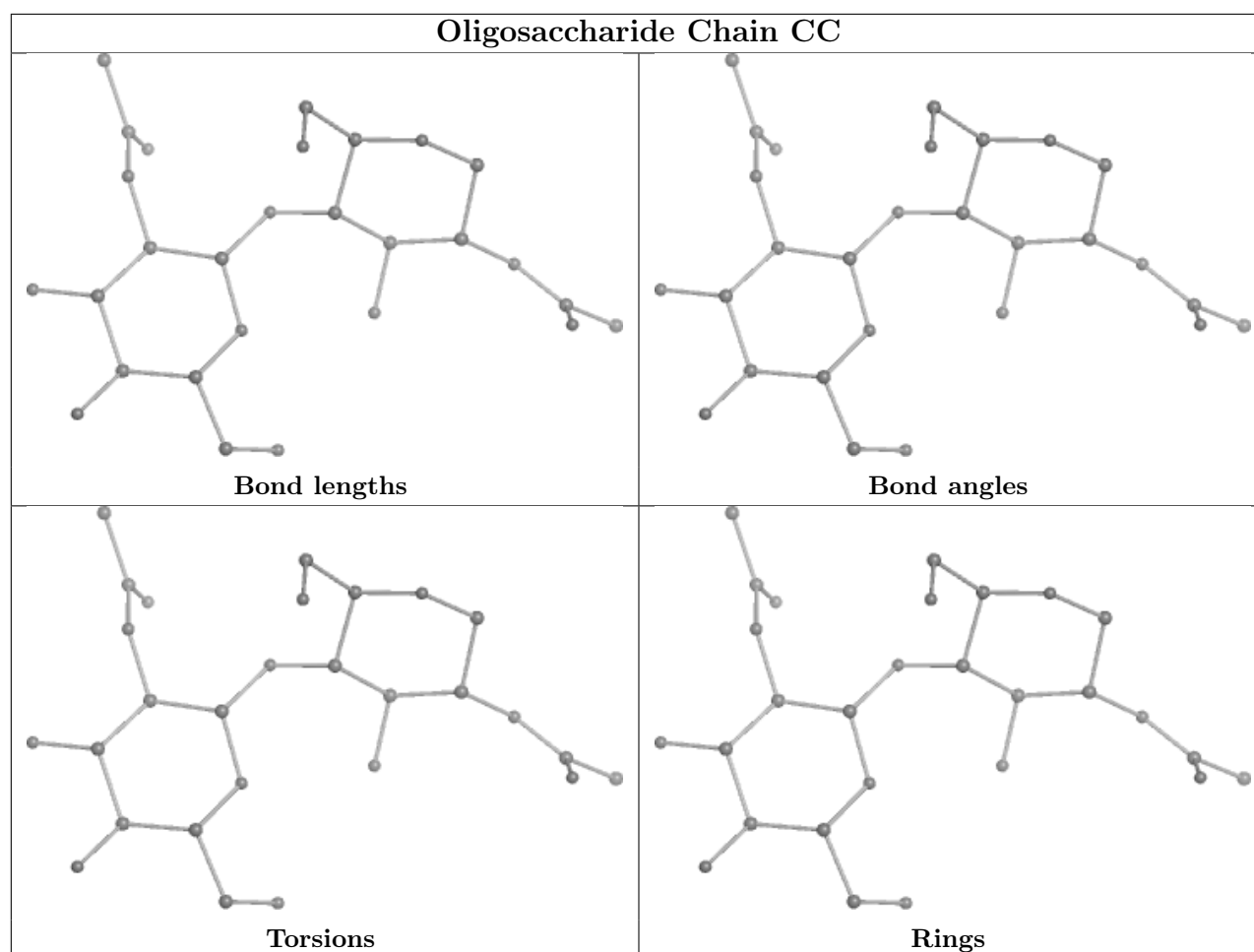


Oligosaccharide Chain BC









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	$\# Z > 2$
6	KZ0	F	101	2	9,9,12	1.01	0	12,12,15	3.87	6 (50%)
4	NAG	B	1208	1	14,14,15	0.41	0	17,19,21	0.54	0
4	NAG	A	1205	1	14,14,15	0.32	0	17,19,21	0.58	0
6	KZ0	D	101	2	9,9,12	1.02	0	12,12,15	3.85	6 (50%)
4	NAG	C	1203	1	14,14,15	0.31	0	17,19,21	0.55	0
5	STE	C	1207	-	19,19,19	0.57	0	19,19,19	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1207	1	14,14,15	0.37	0	17,19,21	0.59	1 (5%)
6	KZ0	E	101	2	9,9,12	1.02	0	12,12,15	3.84	6 (50%)
4	NAG	A	1206	1	14,14,15	0.43	0	17,19,21	0.52	0
4	NAG	C	1204	1	14,14,15	0.35	0	17,19,21	0.59	1 (5%)
4	NAG	C	1201	1	14,14,15	0.26	0	17,19,21	0.43	0
5	STE	A	1208	-	19,19,19	0.58	0	19,19,19	0.54	0
4	NAG	A	1202	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	B	1206	1	14,14,15	0.38	0	17,19,21	0.52	0
4	NAG	B	1205	1	14,14,15	0.30	0	17,19,21	0.57	0
4	NAG	C	1205	1	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	A	1204	1	14,14,15	0.36	0	17,19,21	0.59	1 (5%)
4	NAG	B	1207	1	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	B	1202	1	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	C	1206	1	14,14,15	0.39	0	17,19,21	0.59	1 (5%)
4	NAG	B	1204	1	14,14,15	0.33	0	17,19,21	0.58	1 (5%)
4	NAG	B	1201	1	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	A	1203	1	14,14,15	0.32	0	17,19,21	0.56	0
4	NAG	A	1201	1	14,14,15	0.24	0	17,19,21	0.45	0
5	STE	B	1209	-	19,19,19	0.57	0	19,19,19	0.55	0
4	NAG	B	1203	1	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
4	NAG	C	1202	1	14,14,15	0.39	0	17,19,21	0.58	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	KZ0	F	101	2	-	-	0/1/1/1
4	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1205	1	-	0/6/23/26	0/1/1/1
6	KZ0	D	101	2	-	-	0/1/1/1
4	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
5	STE	C	1207	-	-	10/17/17/17	-
4	NAG	A	1207	1	-	2/6/23/26	0/1/1/1
6	KZ0	E	101	2	-	-	0/1/1/1
4	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1204	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1201	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	STE	A	1208	-	-	6/17/17/17	-
4	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1205	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1206	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1204	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1201	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
5	STE	B	1209	-	-	5/17/17/17	-
4	NAG	B	1203	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1202	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	KZ0	C3-N1-C2	6.63	119.99	115.13
6	F	101	KZ0	C3-N2-C1	6.61	119.98	115.13
6	F	101	KZ0	C2-N-C1	6.60	119.97	115.13
6	E	101	KZ0	C3-N2-C1	6.58	119.96	115.13
6	D	101	KZ0	C3-N1-C2	6.58	119.96	115.13
6	D	101	KZ0	C3-N2-C1	6.58	119.96	115.13
6	E	101	KZ0	C2-N-C1	6.55	119.94	115.13
6	D	101	KZ0	C2-N-C1	6.55	119.94	115.13
6	E	101	KZ0	C3-N1-C2	6.54	119.93	115.13
6	F	101	KZ0	N2-C3-N1	-3.12	119.98	125.72
6	F	101	KZ0	N2-C1-N	-3.11	120.00	125.72
6	E	101	KZ0	N2-C1-N	-3.10	120.02	125.72
6	D	101	KZ0	N-C2-N1	-3.10	120.03	125.72
6	E	101	KZ0	N2-C3-N1	-3.09	120.04	125.72
6	D	101	KZ0	N2-C1-N	-3.08	120.06	125.72
6	F	101	KZ0	N-C2-N1	-3.08	120.06	125.72
6	D	101	KZ0	N2-C3-N1	-3.08	120.06	125.72
4	B	1203	NAG	C2-N2-C7	3.07	127.27	122.90
6	E	101	KZ0	N-C2-N1	-3.05	120.11	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1204	NAG	C1-O5-C5	2.08	115.00	112.19
4	A	1204	NAG	C1-O5-C5	2.07	115.00	112.19
4	C	1206	NAG	C1-O5-C5	2.06	114.98	112.19
4	A	1207	NAG	C1-O5-C5	2.05	114.97	112.19
4	B	1204	NAG	C1-O5-C5	2.03	114.94	112.19
4	C	1202	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1207	NAG	O5-C5-C6-O6
4	A	1206	NAG	C4-C5-C6-O6
4	B	1208	NAG	C4-C5-C6-O6
4	C	1202	NAG	O5-C5-C6-O6
4	B	1206	NAG	O5-C5-C6-O6
4	B	1204	NAG	O5-C5-C6-O6
4	B	1206	NAG	C4-C5-C6-O6
4	A	1207	NAG	C4-C5-C6-O6
4	A	1202	NAG	O5-C5-C6-O6
4	B	1204	NAG	C4-C5-C6-O6
4	C	1202	NAG	C4-C5-C6-O6
4	B	1208	NAG	O5-C5-C6-O6
4	A	1206	NAG	O5-C5-C6-O6
4	A	1202	NAG	C4-C5-C6-O6
4	B	1203	NAG	O5-C5-C6-O6
4	B	1203	NAG	C4-C5-C6-O6
5	C	1207	STE	C10-C11-C12-C13
5	A	1208	STE	C14-C15-C16-C17
5	B	1209	STE	C6-C7-C8-C9
4	B	1202	NAG	O5-C5-C6-O6
5	B	1209	STE	C1-C2-C3-C4
4	B	1202	NAG	C4-C5-C6-O6
5	C	1207	STE	C11-C12-C13-C14
5	C	1207	STE	C3-C4-C5-C6
5	C	1207	STE	C9-C10-C11-C12
5	C	1207	STE	C14-C15-C16-C17
5	B	1209	STE	C12-C13-C14-C15
5	A	1208	STE	C7-C8-C9-C10
4	C	1205	NAG	C4-C5-C6-O6
4	C	1205	NAG	O5-C5-C6-O6
4	A	1204	NAG	O5-C5-C6-O6

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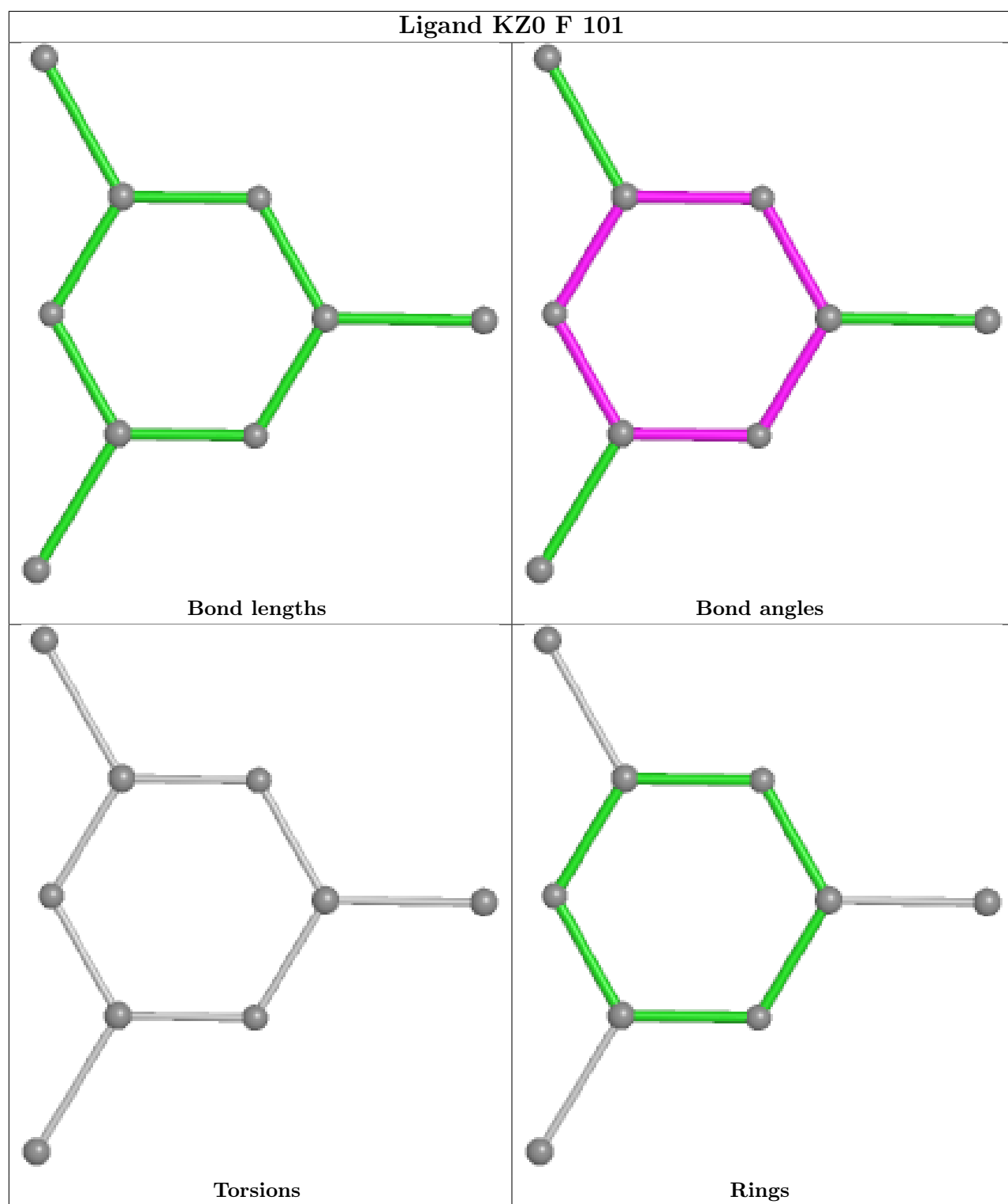
Mol	Chain	Res	Type	Atoms
5	B	1209	STE	C10-C11-C12-C13
4	A	1204	NAG	C4-C5-C6-O6
5	C	1207	STE	C4-C5-C6-C7
4	C	1204	NAG	C4-C5-C6-O6
4	C	1204	NAG	O5-C5-C6-O6
5	C	1207	STE	O1-C1-C2-C3
5	A	1208	STE	O1-C1-C2-C3
5	C	1207	STE	C11-C10-C9-C8
5	A	1208	STE	O2-C1-C2-C3
5	C	1207	STE	C6-C7-C8-C9
5	C	1207	STE	O2-C1-C2-C3
5	A	1208	STE	C4-C5-C6-C7
5	A	1208	STE	C11-C10-C9-C8
5	B	1209	STE	C7-C8-C9-C10
4	B	1203	NAG	C3-C2-N2-C7

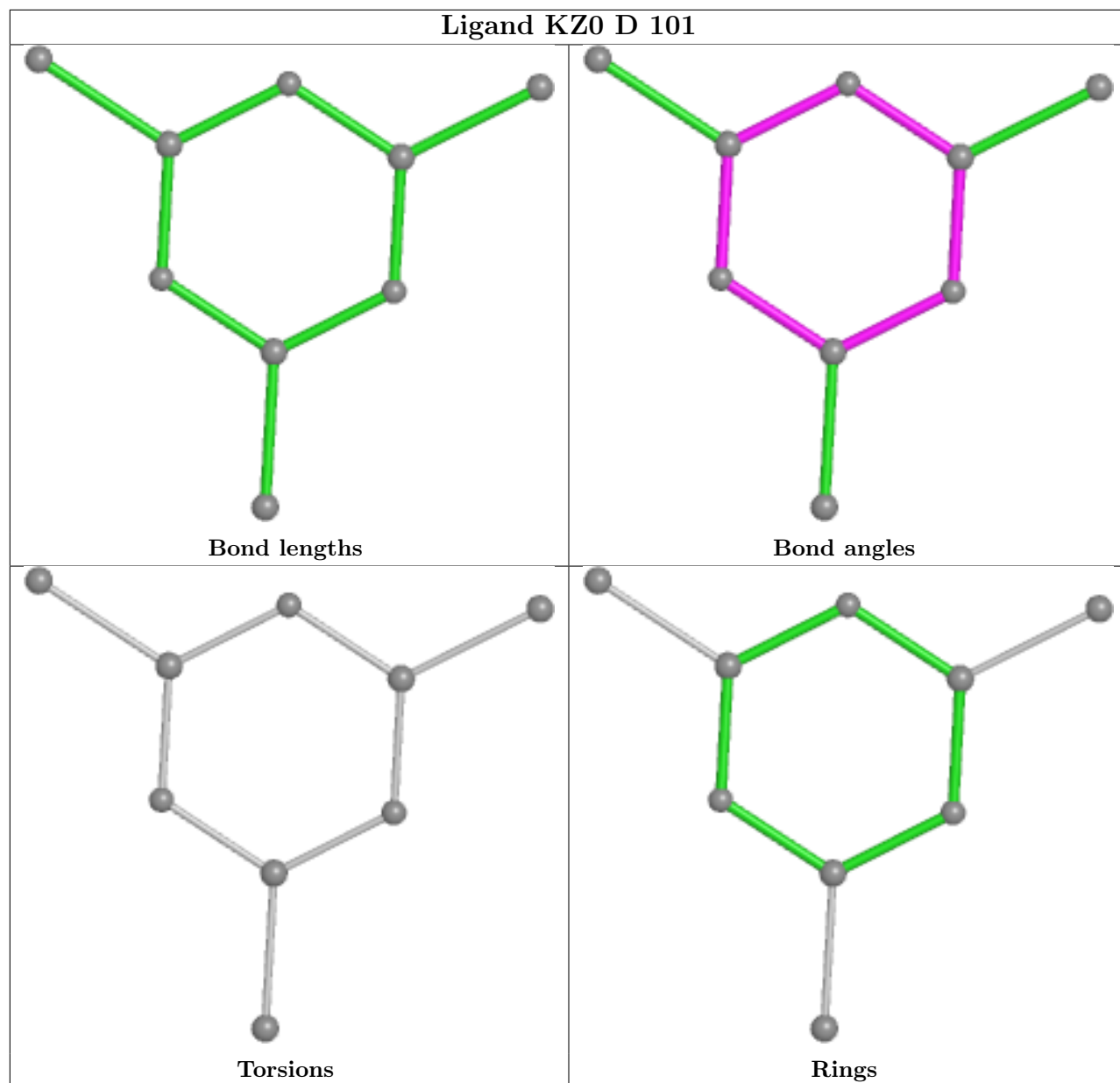
There are no ring outliers.

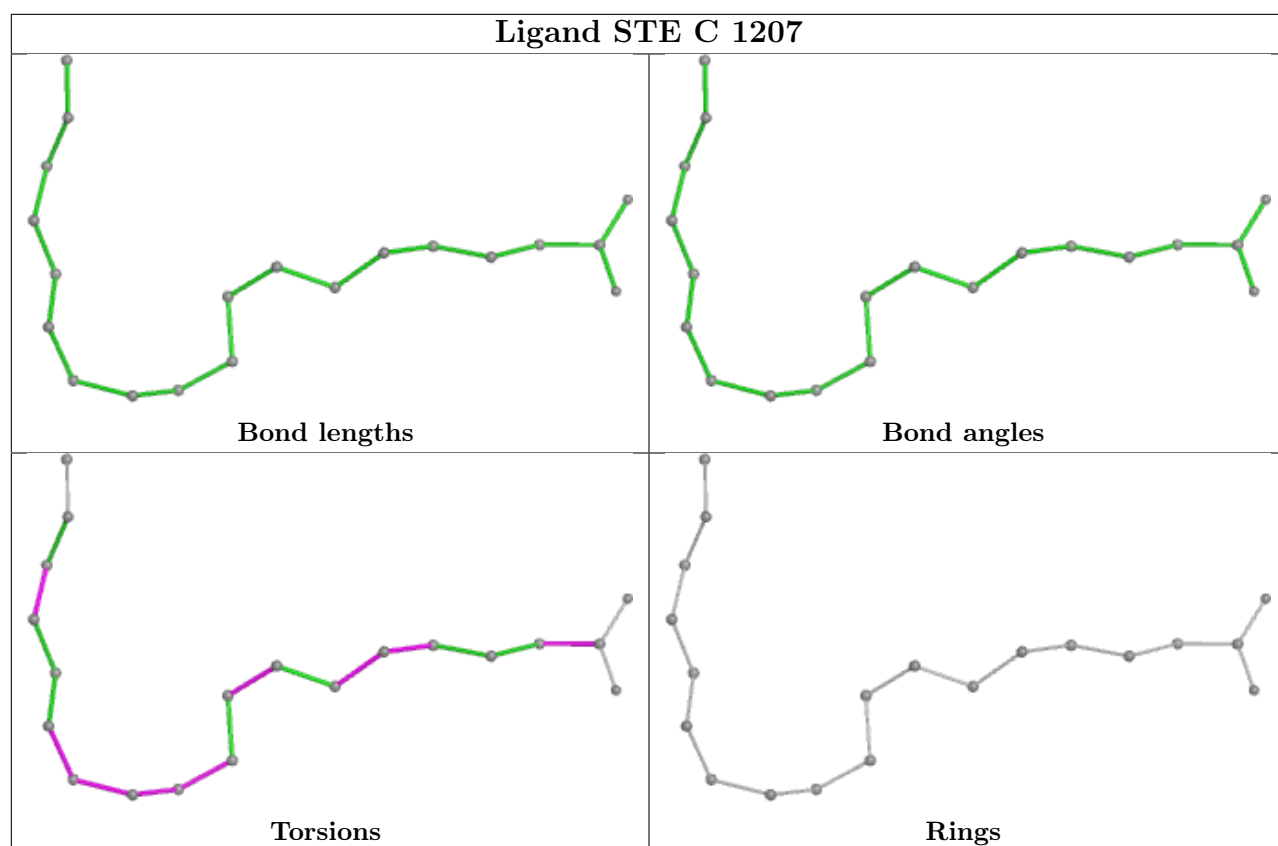
2 monomers are involved in 3 short contacts:

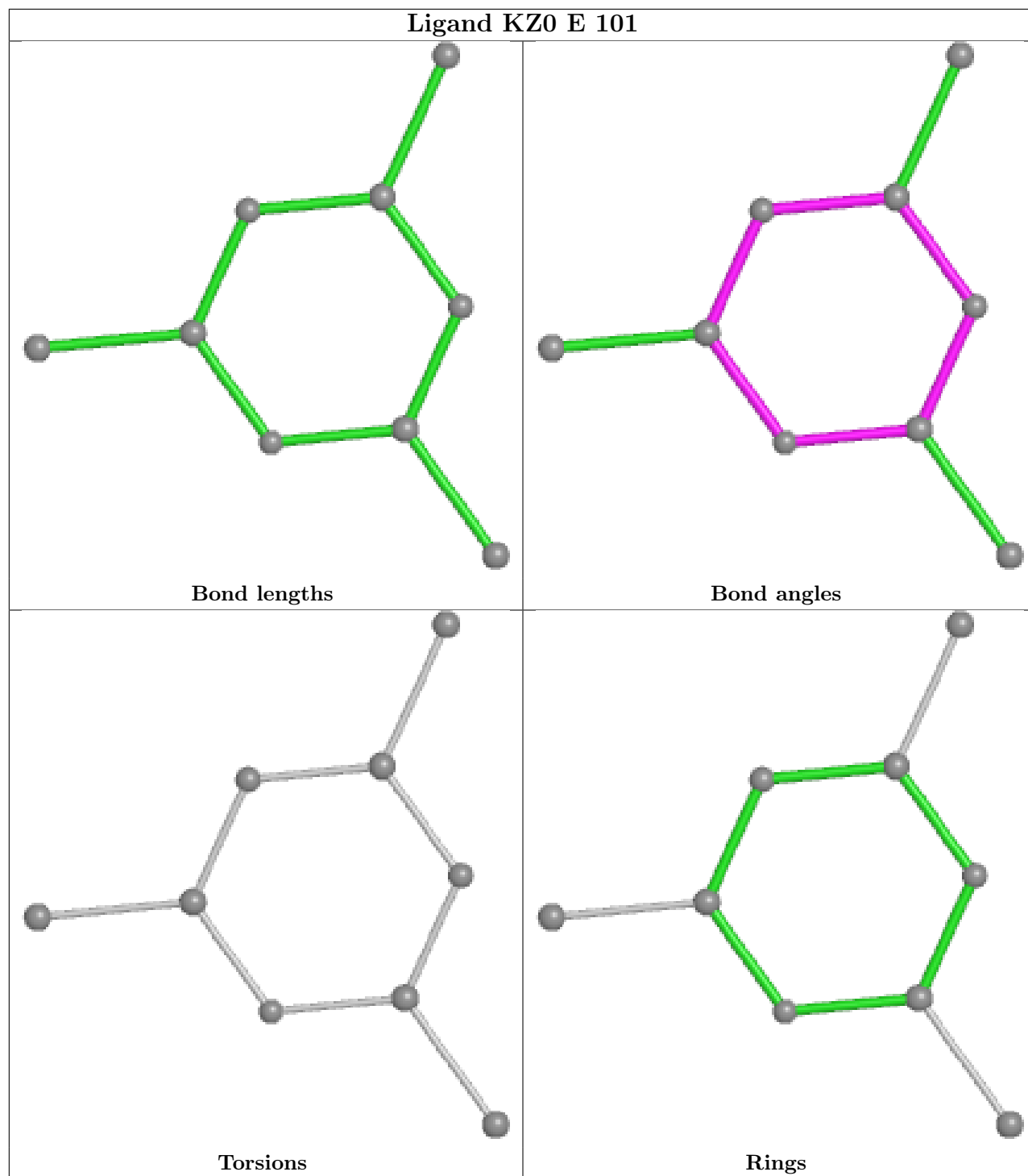
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1208	STE	2	0
4	B	1207	NAG	1	0

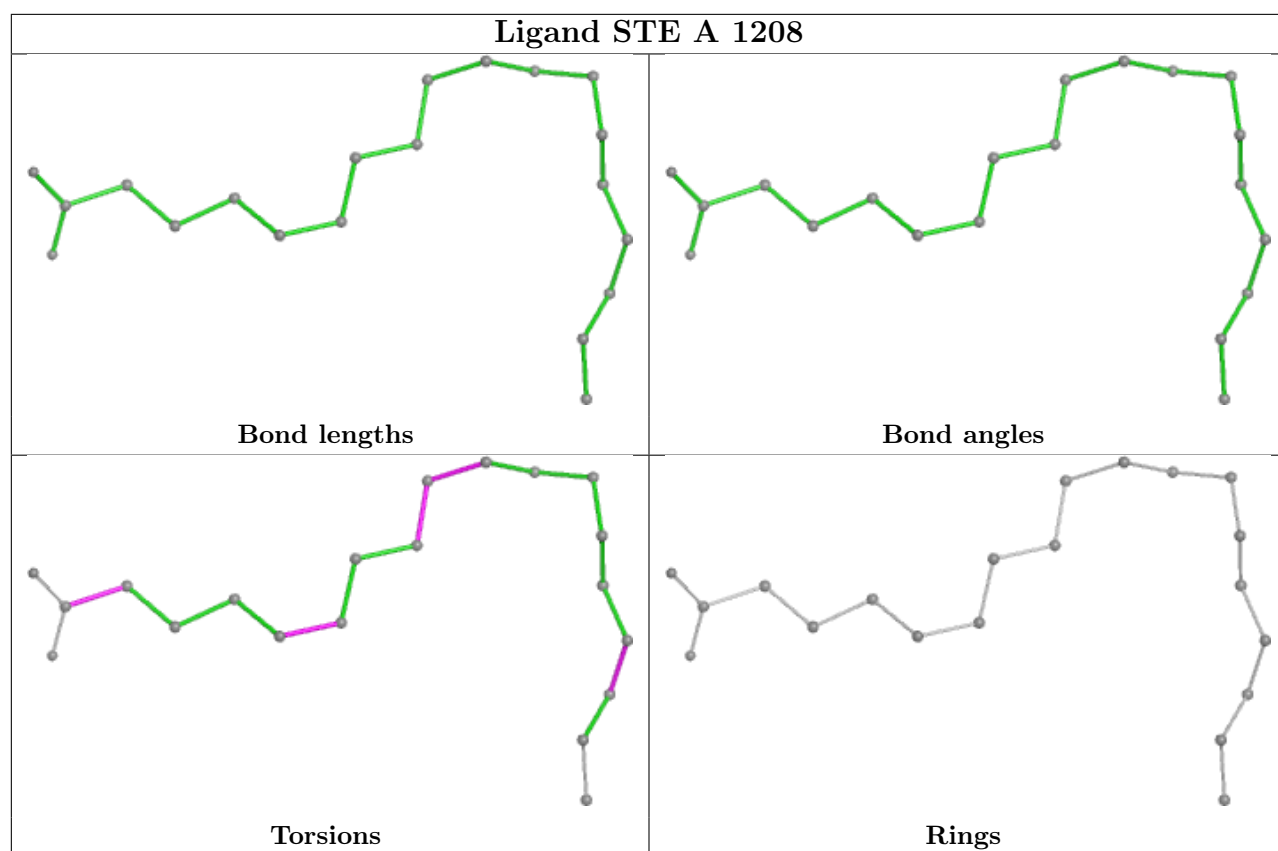
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.