



Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 03:04 pm GMT

PDB ID : 8S3O
EMDB ID : EMD-19699
Title : Structure of native human CD109
Authors : Almeida, V.A.; Andersen, G.R.
Deposited on : 2024-02-20
Resolution : 2.99 Å(reported)
Based on initial model : .

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

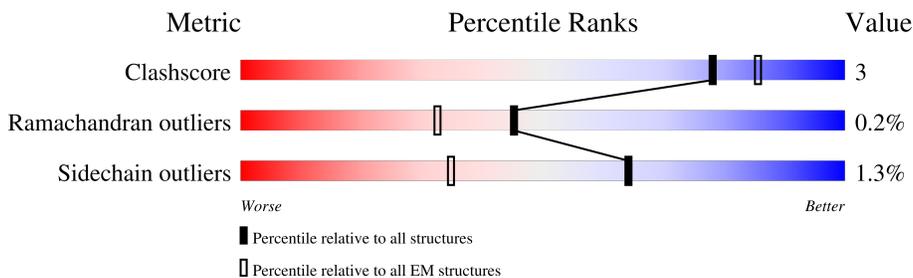
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 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	1447	84% (green), 8% (yellow), 9% (grey)
2	B	2	50% (green), 50% (orange)
2	C	2	100% (green)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21074 atoms, of which 10518 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 CD109 antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	1324	20860	6676	10416	1716	2015	37	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	expression tag	UNP Q6YHK3
A	-19	VAL	-	expression tag	UNP Q6YHK3
A	-18	SER	-	expression tag	UNP Q6YHK3
A	-17	GLY	-	expression tag	UNP Q6YHK3
A	-16	TRP	-	expression tag	UNP Q6YHK3
A	-15	SER	-	expression tag	UNP Q6YHK3
A	-14	HIS	-	expression tag	UNP Q6YHK3
A	-13	PRO	-	expression tag	UNP Q6YHK3
A	-12	GLN	-	expression tag	UNP Q6YHK3
A	-11	PHE	-	expression tag	UNP Q6YHK3
A	-10	GLU	-	expression tag	UNP Q6YHK3
A	-9	LYS	-	expression tag	UNP Q6YHK3
A	-8	GLY	-	expression tag	UNP Q6YHK3
A	-7	GLY	-	expression tag	UNP Q6YHK3
A	-6	GLY	-	expression tag	UNP Q6YHK3
A	-5	SER	-	expression tag	UNP Q6YHK3
A	-4	GLY	-	expression tag	UNP Q6YHK3
A	-3	GLY	-	expression tag	UNP Q6YHK3
A	-2	GLY	-	expression tag	UNP Q6YHK3
A	-1	SER	-	expression tag	UNP Q6YHK3
A	0	GLY	-	expression tag	UNP Q6YHK3
A	1	GLY	-	expression tag	UNP Q6YHK3
A	2	SER	-	expression tag	UNP Q6YHK3
A	3	ALA	-	expression tag	UNP Q6YHK3
A	4	TRP	-	expression tag	UNP Q6YHK3
A	5	SER	-	expression tag	UNP Q6YHK3
A	6	HIS	-	expression tag	UNP Q6YHK3
A	7	PRO	-	expression tag	UNP Q6YHK3

Continued on next page...

Continued from previous page...

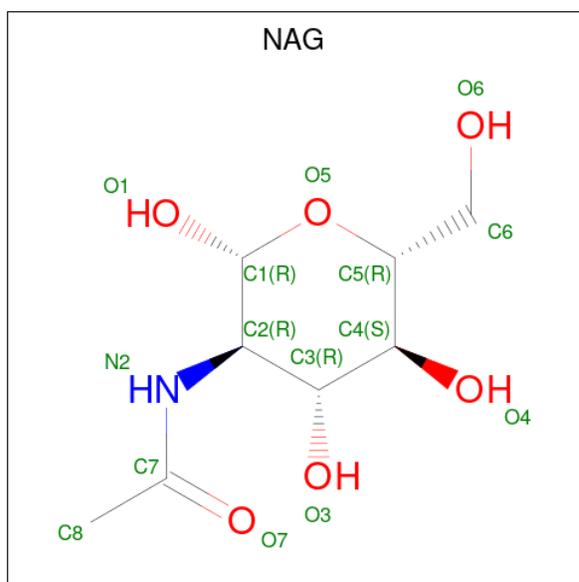
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLN	-	expression tag	UNP Q6YHK3
A	9	PHE	-	expression tag	UNP Q6YHK3
A	10	GLU	-	expression tag	UNP Q6YHK3
A	11	LYS	-	expression tag	UNP Q6YHK3
A	12	GLY	-	expression tag	UNP Q6YHK3
A	13	GLU	-	expression tag	UNP Q6YHK3
A	14	ASN	-	expression tag	UNP Q6YHK3
A	15	LEU	-	expression tag	UNP Q6YHK3
A	16	TYR	-	expression tag	UNP Q6YHK3
A	17	PHE	-	expression tag	UNP Q6YHK3
A	18	GLN	-	expression tag	UNP Q6YHK3
A	19	SER	-	expression tag	UNP Q6YHK3
A	20	GLY	-	expression tag	UNP Q6YHK3
A	21	SER	-	expression tag	UNP Q6YHK3
A	1421	HIS	-	expression tag	UNP Q6YHK3
A	1422	HIS	-	expression tag	UNP Q6YHK3
A	1423	HIS	-	expression tag	UNP Q6YHK3
A	1424	HIS	-	expression tag	UNP Q6YHK3
A	1425	HIS	-	expression tag	UNP Q6YHK3
A	1426	HIS	-	expression tag	UNP Q6YHK3

- 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				AltConf	Trace	
			Total	C	H	N			O
2	B	2	53	16	25	2	10	0	0
2	C	2	53	16	25	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	273564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.9	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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

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	0.29	0/10660	0.55	0/14476

There are no bond length outliers.

There are no bond angle outliers.

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	10444	10416	10420	56	0
2	B	28	25	25	1	0
2	C	28	25	25	0	0
3	A	56	52	52	2	0
All	All	10556	10518	10522	57	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 (57) 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:A:1283:LEU:O	1:A:1393:ARG:NH1	2.28	0.67
1:A:604:ASP:O	1:A:609:ASN:ND2	2.31	0.63
1:A:394:THR:HG23	1:A:415:VAL:HG12	1.82	0.62
1:A:48:LEU:HD11	1:A:56:VAL:HG22	1.82	0.61
1:A:819:LEU:HD12	1:A:1408:SER:HB3	1.85	0.58
1:A:924:GLN:HG2	1:A:1384:TYR:CZ	2.39	0.57
1:A:808:LEU:HD11	1:A:816:ALA:HB1	1.88	0.55
1:A:922:GLY:N	1:A:976:ALA:O	2.40	0.55
1:A:92:SER:N	3:A:1501:NAG:O6	2.41	0.54
1:A:112:ASP:OD1	1:A:113:GLU:N	2.40	0.53
1:A:296:ASP:OD1	1:A:297:GLU:N	2.42	0.53
1:A:970:GLU:OE1	1:A:970:GLU:N	2.40	0.53
1:A:352:GLU:N	1:A:352:GLU:OE1	2.42	0.53
1:A:113:GLU:OE1	1:A:114:ILE:N	2.42	0.52
1:A:109:ARG:NH2	1:A:110:THR:O	2.43	0.52
1:A:902:ASP:OD1	1:A:1227:ARG:NH2	2.42	0.52
1:A:546:VAL:HG23	1:A:632:VAL:HG13	1.91	0.51
1:A:111:GLN:N	1:A:111:GLN:OE1	2.43	0.50
1:A:1089:LEU:HD21	1:A:1110:MET:HG2	1.94	0.50
1:A:371:LYS:NZ	1:A:425:SER:O	2.41	0.50
1:A:927:ILE:HB	1:A:1181:THR:HG23	1.95	0.49
1:A:565:LYS:NZ	1:A:567:LYS:O	2.44	0.49
3:A:1502:NAG:H3	3:A:1502:NAG:H83	1.95	0.48
1:A:416:GLN:NE2	1:A:417:LYS:O	2.46	0.48
1:A:1214:SER:HB2	1:A:1235:LEU:HD22	1.96	0.47
1:A:1116:GLU:OE2	2:B:2:NAG:N2	2.43	0.47
1:A:1201:GLU:OE1	1:A:1201:GLU:N	2.44	0.47
1:A:1279:GLU:OE1	1:A:1393:ARG:NH2	2.47	0.47
1:A:110:THR:OG1	1:A:111:GLN:N	2.47	0.47
1:A:358:THR:O	1:A:458:SER:OG	2.30	0.47
1:A:483:PHE:HE2	1:A:485:LEU:HD21	1.80	0.47
1:A:813:GLU:N	1:A:813:GLU:OE1	2.48	0.47
1:A:557:ASN:OD1	1:A:728:SER:OG	2.28	0.46
1:A:830:ILE:HD12	1:A:851:VAL:HG21	1.96	0.46
1:A:432:PHE:HZ	1:A:441:LEU:HD21	1.81	0.46
1:A:975:SER:OG	1:A:981:ASP:OD2	2.33	0.46
1:A:111:GLN:NE2	1:A:112:ASP:OD2	2.49	0.46
1:A:493:LEU:HD12	1:A:515:THR:HG22	1.98	0.46
1:A:474:ASP:OD1	1:A:475:GLU:N	2.48	0.45
1:A:366:PHE:HB2	1:A:434:ILE:HD11	1.99	0.45
1:A:1183:ASP:OD1	1:A:1184:THR:N	2.50	0.45
1:A:57:THR:HG22	1:A:79:VAL:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:O	1:A:229:PHE:N	2.50	0.44
1:A:594:LYS:HG2	1:A:721:VAL:HG13	1.98	0.44
1:A:776:ASP:N	1:A:776:ASP:OD1	2.51	0.44
1:A:394:THR:OG1	1:A:444:LYS:NZ	2.51	0.43
1:A:1066:ILE:HG22	1:A:1068:VAL:HG13	2.01	0.42
1:A:1274:SER:N	1:A:1282:ASP:OD1	2.53	0.42
1:A:1085:ASP:OD1	1:A:1086:ASN:N	2.53	0.42
1:A:602:SER:O	1:A:609:ASN:ND2	2.53	0.41
1:A:1120:GLY:O	1:A:1166:ARG:NH1	2.53	0.41
1:A:799:ILE:O	1:A:801:ALA:N	2.52	0.41
1:A:1368:ASN:N	1:A:1368:ASN:OD1	2.54	0.41
1:A:1106:GLU:OE1	1:A:1106:GLU:N	2.52	0.40
1:A:271:LEU:HD11	1:A:322:GLU:OE2	2.22	0.40
1:A:770:ILE:H	1:A:816:ALA:HB3	1.86	0.40
1:A:765:ALA:HB1	1:A:819:LEU:HD22	2.03	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	1314/1447 (91%)	1257 (96%)	54 (4%)	3 (0%)	44 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	929	PHE
1	A	228	LYS
1	A	391	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1190/1289 (92%)	1174 (99%)	16 (1%)	65 85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	164	LEU
1	A	344	PHE
1	A	356	TYR
1	A	530	CYS
1	A	557	ASN
1	A	625	MET
1	A	626	PHE
1	A	698	ASP
1	A	753	ASN
1	A	771	PHE
1	A	775	LYS
1	A	872	ARG
1	A	921	CYS
1	A	1288	LYS
1	A	1390	GLN

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

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

4 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	B	1	2,1	14,14,15	0.34	0	17,19,21	0.43	0
2	NAG	B	2	2	14,14,15	0.22	0	17,19,21	0.81	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	C	2	2	14,14,15	0.16	0	17,19,21	0.43	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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C2-N2-C7	2.67	126.71	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

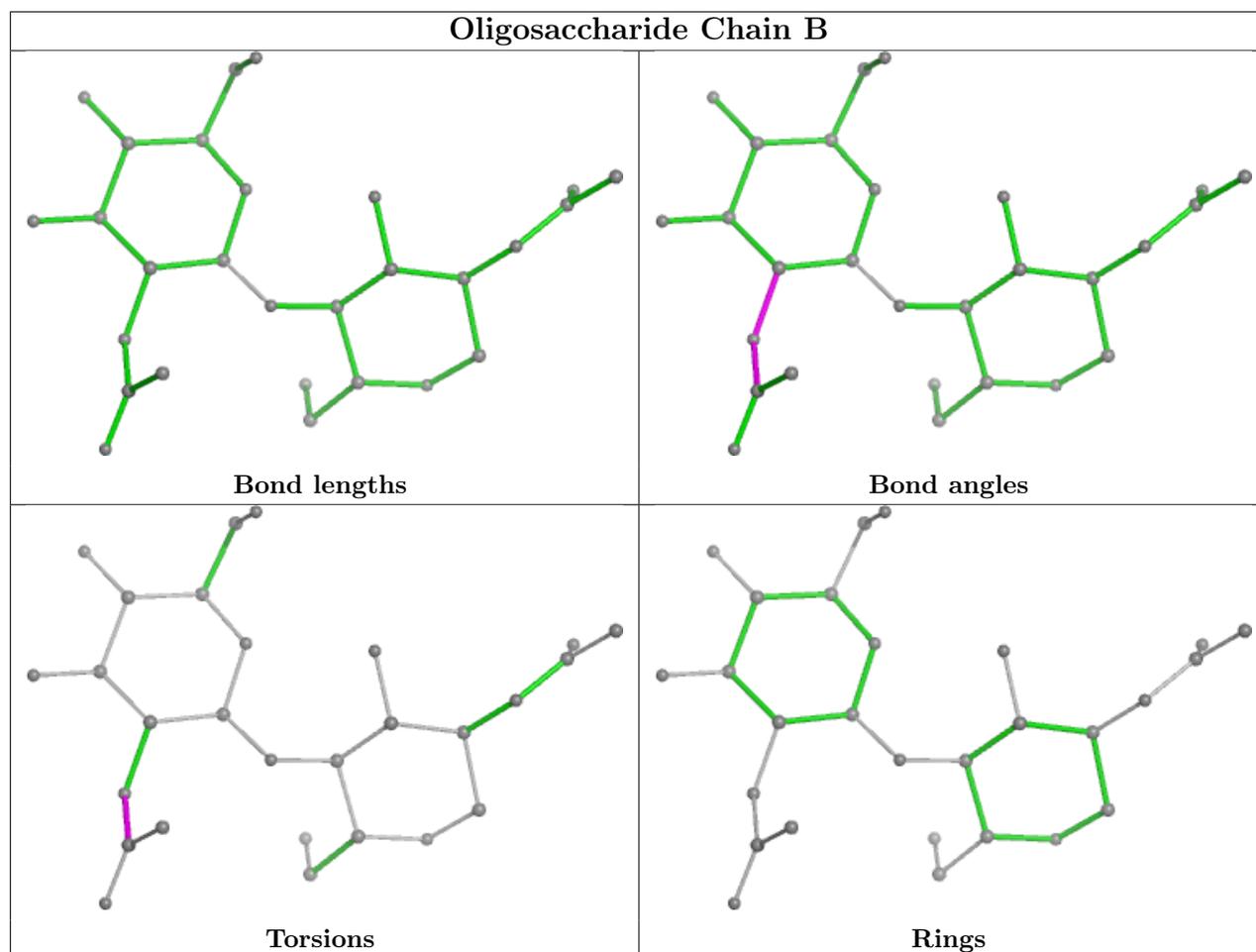
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6

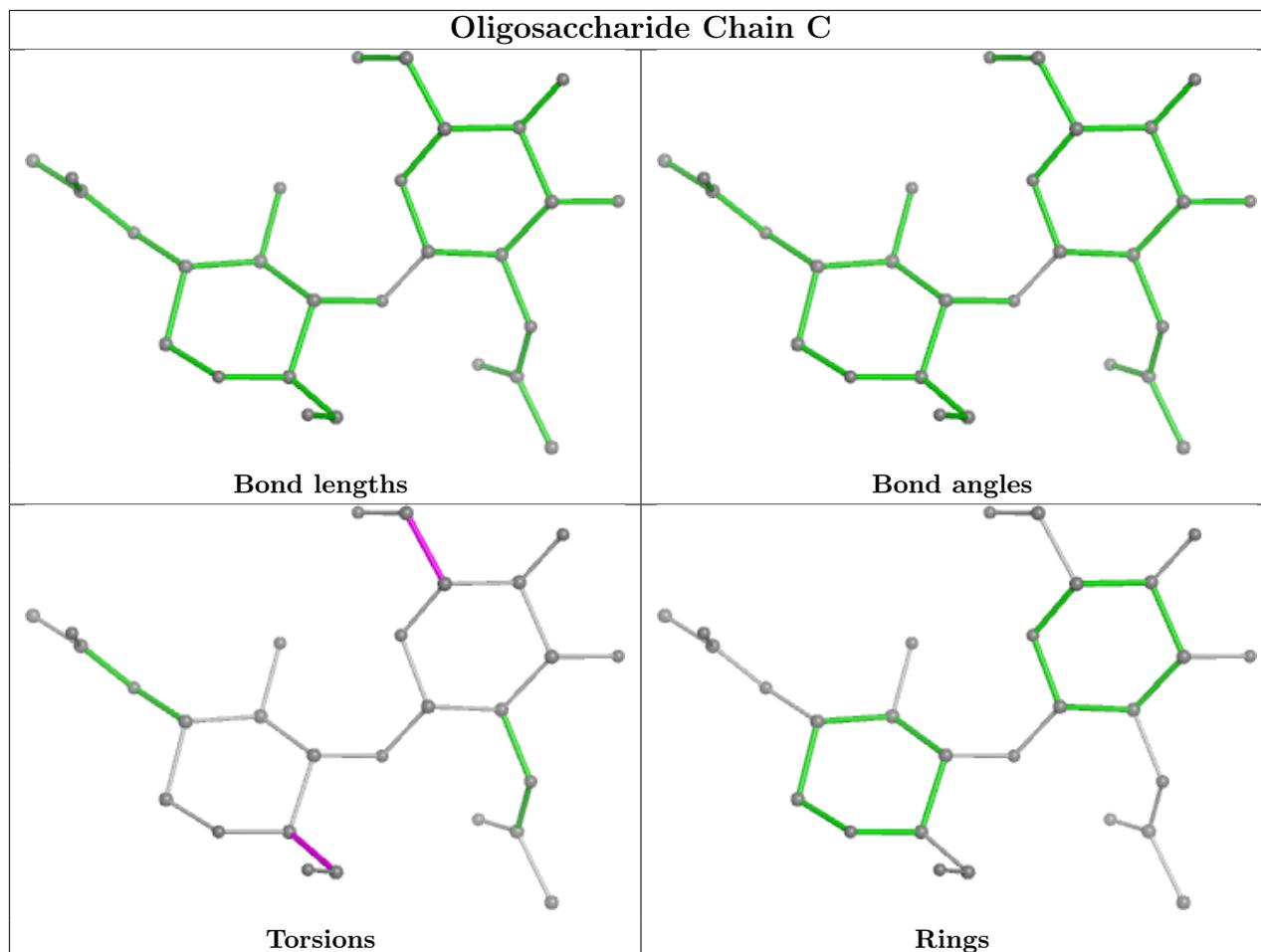
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

4 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	A	1503	1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	A	1502	1	14,14,15	0.24	0	17,19,21	1.32	2 (11%)
3	NAG	A	1504	1	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	A	1501	1	14,14,15	0.20	0	17,19,21	0.46	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	A	1503	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1502	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1504	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1502	NAG	C2-N2-C7	4.47	129.27	122.90
3	A	1502	NAG	C1-C2-N2	2.03	113.96	110.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	NAG	O5-C5-C6-O6
3	A	1502	NAG	C8-C7-N2-C2
3	A	1502	NAG	O7-C7-N2-C2
3	A	1501	NAG	C4-C5-C6-O6
3	A	1502	NAG	C3-C2-N2-C7
3	A	1503	NAG	C4-C5-C6-O6

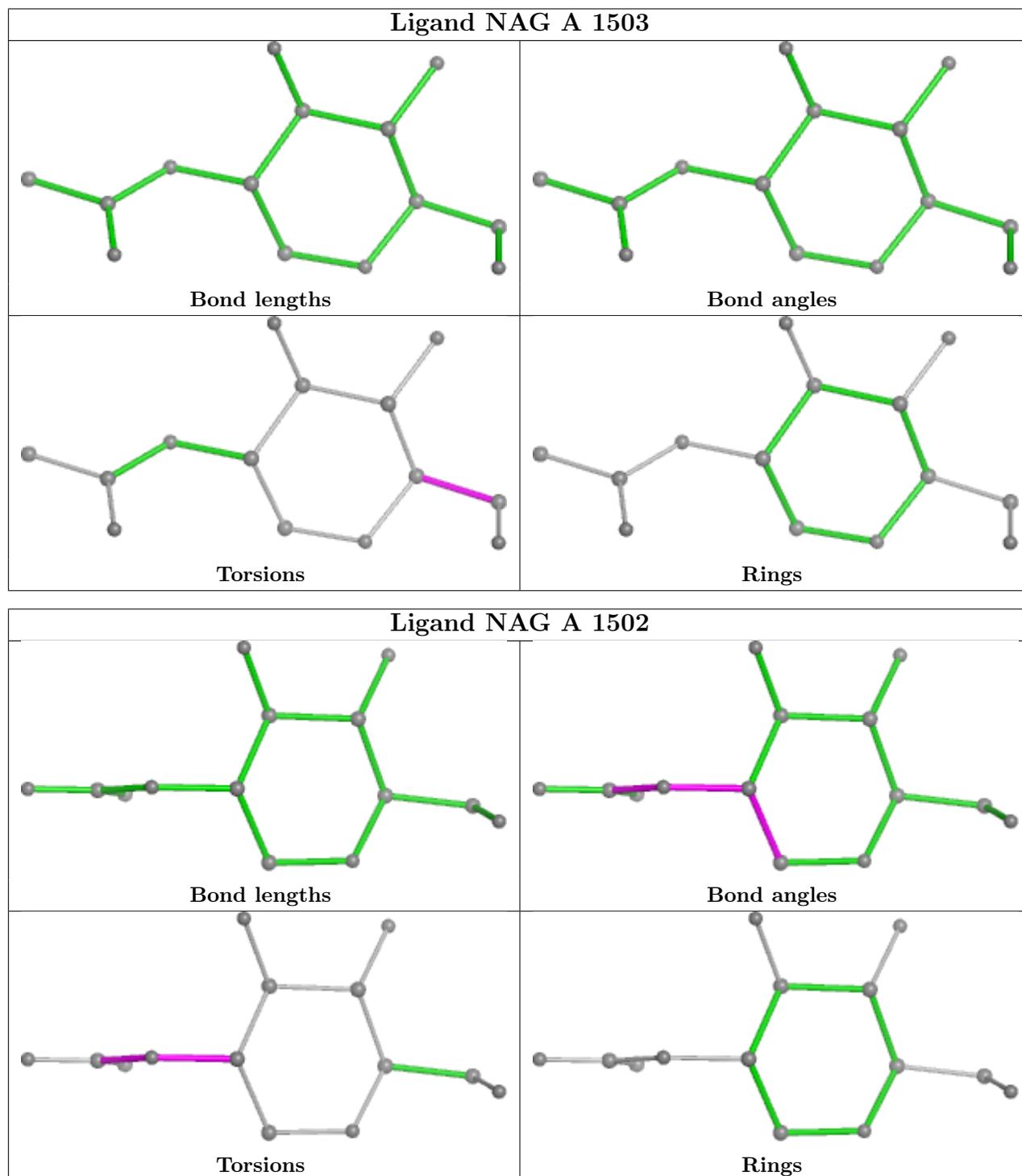
There are no ring outliers.

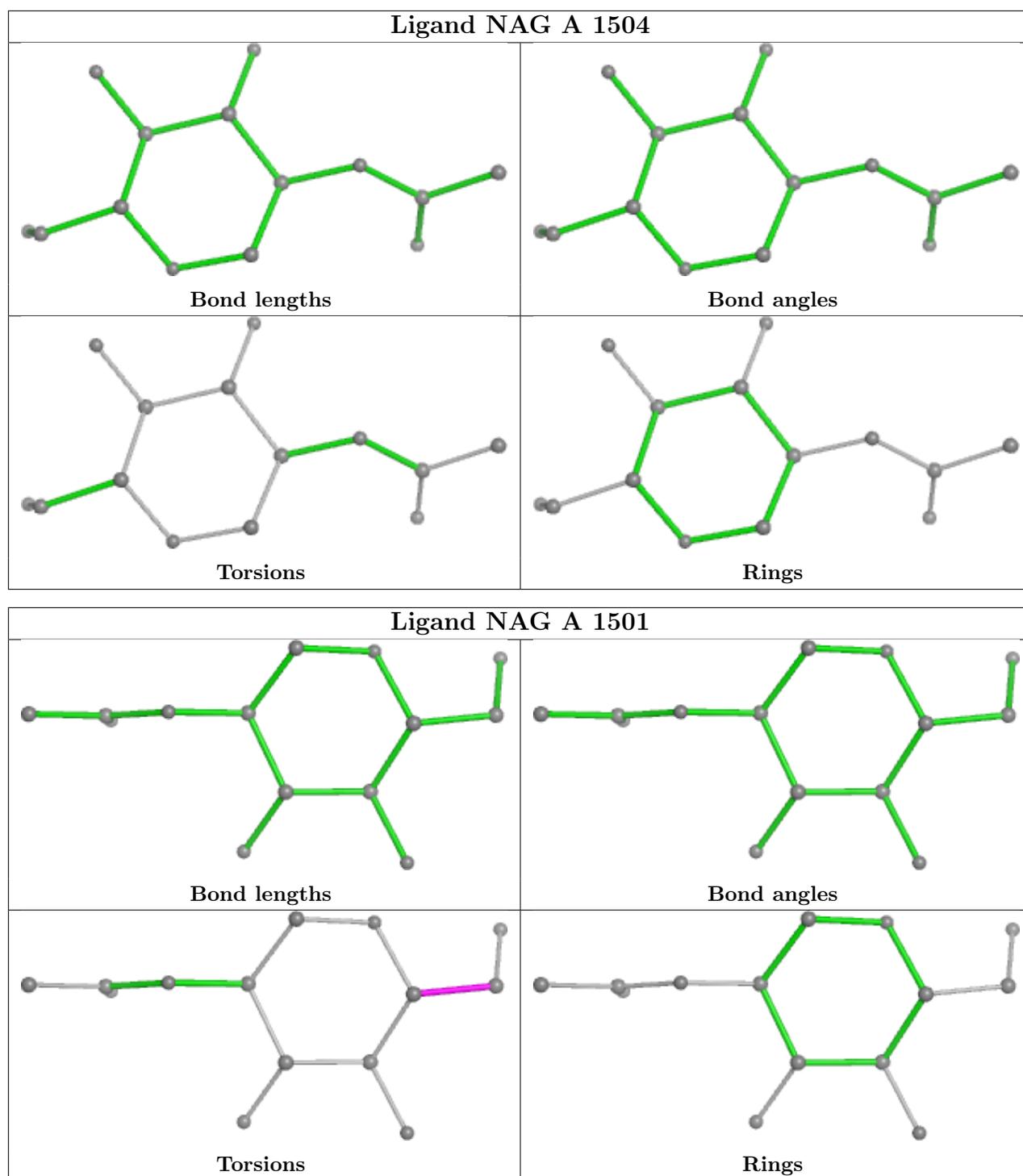
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	NAG	1	0
3	A	1501	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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.