



Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 12:14 pm GMT

PDB ID : 9F1R
EMDB ID : EMD-50135
Title : Cryo-EM structure of SV2B-Hc-A1 complex
Authors : Khanppnavar, B.; Leka, O.; Korkhov, V.; Kammerer, R.
Deposited on : 2024-04-20
Resolution : 3.67 Å(reported)
Based on initial models : ., 2vu9

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

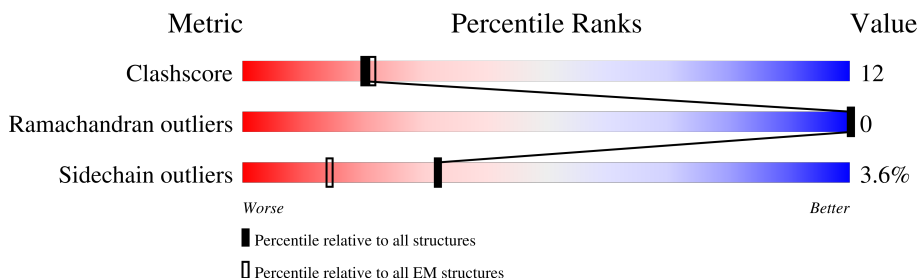
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.67 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	683	56% 23% • 20%
2	B	443	63% 29% 7%
3	C	3	100%
4	D	5	80% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7870 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 Synaptic vesicle glycoprotein 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	547	Total	C	N	O	S	0	0
			4333	2844	695	751	43		

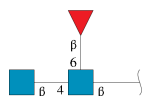
- Molecule 2 is a protein called Botulinum neurotoxin A heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	413	Total	C	N	O	S	2	0
			3425	2184	592	636	13		

There are 17 discrepancies between the modelled and reference sequences:

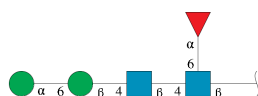
Chain	Residue	Modelled	Actual	Comment	Reference
B	854	MET	-	initiating methionine	UNP P0DPI0
B	855	LYS	-	expression tag	UNP P0DPI0
B	856	LYS	-	expression tag	UNP P0DPI0
B	857	HIS	-	expression tag	UNP P0DPI0
B	858	HIS	-	expression tag	UNP P0DPI0
B	859	HIS	-	expression tag	UNP P0DPI0
B	860	HIS	-	expression tag	UNP P0DPI0
B	861	HIS	-	expression tag	UNP P0DPI0
B	862	HIS	-	expression tag	UNP P0DPI0
B	863	GLY	-	expression tag	UNP P0DPI0
B	864	SER	-	expression tag	UNP P0DPI0
B	865	LEU	-	expression tag	UNP P0DPI0
B	866	VAL	-	expression tag	UNP P0DPI0
B	867	PRO	-	expression tag	UNP P0DPI0
B	868	ARG	-	expression tag	UNP P0DPI0
B	869	GLY	-	expression tag	UNP P0DPI0
B	870	SER	-	expression tag	UNP P0DPI0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



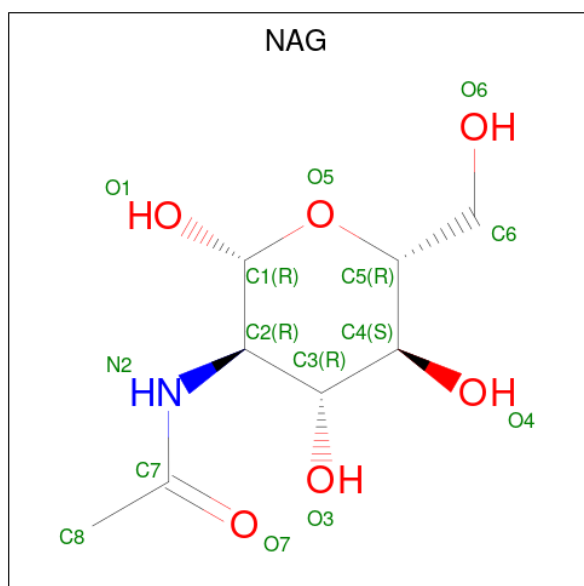
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

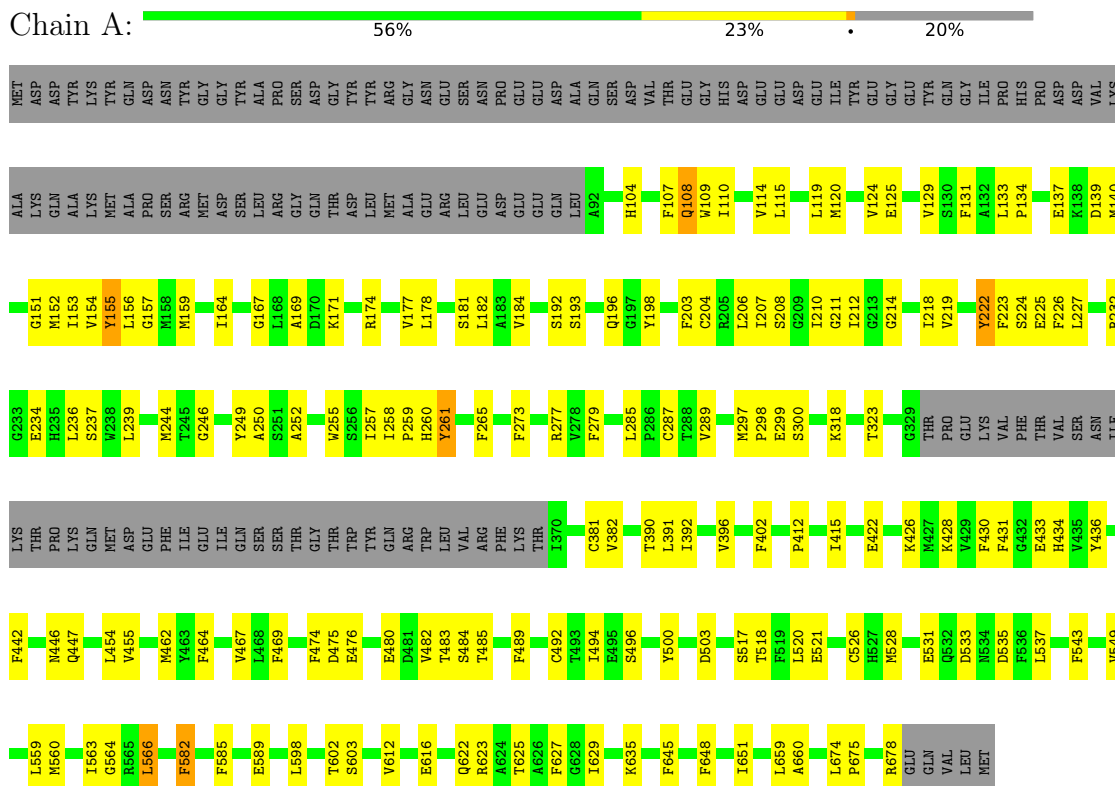


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	

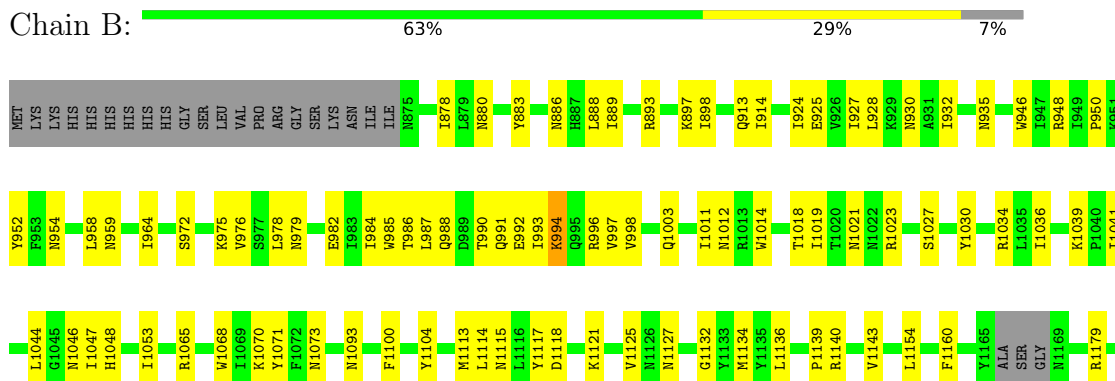
3 Residue-property plots

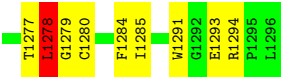
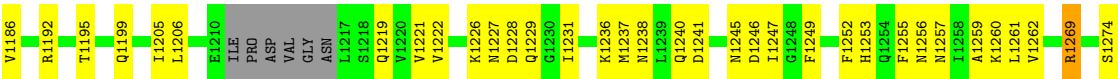
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Synaptic vesicle glycoprotein 2B



• Molecule 2: Botulinum neurotoxin A heavy chain





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%



- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

80%

20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185478	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	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: FUC, FUL, MAN, NAG, BMA

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	0.28	0/4451	0.48	0/6014
2	B	0.26	0/3501	0.49	1/4728 (0.0%)
All	All	0.27	0/7952	0.49	1/10742 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1278	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4333	0	4278	108	0
2	B	3425	0	3390	84	0
3	C	38	0	34	0	0
4	D	60	0	52	0	0
5	A	14	0	13	0	0
All	All	7870	0	7767	189	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 12.

All (189) 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:125:GLU:HG3	1:A:212:ILE:HG21	1.58	0.85
1:A:222:TYR:OH	1:A:298:PRO:O	2.04	0.76
1:A:119:LEU:HD12	1:A:239:LEU:HD22	1.71	0.72
1:A:560:MET:HE1	1:A:612:VAL:HG21	1.69	0.72
1:A:415:ILE:HD11	1:A:589:GLU:HA	1.73	0.70
1:A:244:MET:HG3	1:A:549:VAL:HG21	1.72	0.70
1:A:232:ARG:HH11	1:A:616:GLU:HG2	1.59	0.68
1:A:428:LYS:HB3	1:A:447:GLN:HE21	1.59	0.67
2:B:1125:VAL:HG23	2:B:1134:MET:HG3	1.76	0.66
1:A:120:MET:HG3	1:A:246:GLY:HA2	1.77	0.66
2:B:1231:ILE:HD13	2:B:1274:SER:HB2	1.78	0.65
1:A:462:MET:HG2	1:A:482:VAL:HG23	1.81	0.63
2:B:897:LYS:HB3	2:B:927:ILE:HB	1.80	0.62
2:B:1121:LYS:HG2	2:B:1136:LEU:HB3	1.81	0.62
2:B:1154:LEU:HD13	2:B:1285:ILE:HD13	1.82	0.62
1:A:257:ILE:HG22	1:A:258:ILE:HG23	1.82	0.61
1:A:426:LYS:O	1:A:446:ASN:ND2	2.33	0.60
2:B:1003:GLN:HA	2:B:1011:ILE:HD11	1.83	0.60
1:A:489:PHE:HB3	1:A:492:CYS:SG	2.43	0.59
1:A:181:SER:OG	1:A:211:GLY:O	2.18	0.58
2:B:1113:MET:O	2:B:1140:ARG:NH2	2.36	0.58
1:A:485:THR:HG22	1:A:528:MET:HG2	1.86	0.58
2:B:1240:GLN:NE2	2:B:1246:ASP:OD1	2.37	0.57
2:B:1241:ASP:OD1	2:B:1245:ASN:N	2.37	0.57
2:B:1195:THR:OG1	2:B:1206:LEU:HA	2.05	0.57
2:B:1117:TYR:CD2	2:B:1278:LEU:HB2	2.40	0.57
2:B:1227:ASN:HB2	2:B:1231:ILE:HB	1.87	0.57
1:A:131:PHE:HE2	1:A:412:PRO:HG2	1.69	0.56
2:B:1014:TRP:CZ3	2:B:1070:LYS:HG2	2.40	0.56
1:A:517:SER:OG	1:A:518:THR:N	2.37	0.55
1:A:151:GLY:O	1:A:154:VAL:HG12	2.07	0.55
1:A:563:ILE:HD12	1:A:563:ILE:H	1.72	0.55
1:A:422:GLU:O	1:A:426:LYS:NZ	2.40	0.55
1:A:433:GLU:N	1:A:433:GLU:OE2	2.40	0.55
1:A:137:GLU:OE2	1:A:198:TYR:OH	2.23	0.55
1:A:225:GLU:OE1	1:A:623:ARG:NH1	2.40	0.55
2:B:952:TYR:HA	2:B:1065:ARG:NH2	2.22	0.54
2:B:1192:ARG:NH1	2:B:1219:GLN:OE1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1206:LEU:HD12	2:B:1261:LEU:HB3	1.89	0.54
2:B:987:LEU:HD22	2:B:1047:ILE:HD13	1.89	0.54
1:A:674:LEU:HD12	1:A:675:PRO:HD2	1.88	0.54
2:B:880:ASN:OD1	2:B:1073:ASN:ND2	2.36	0.54
2:B:948:ARG:HB3	2:B:1068:TRP:HB2	1.89	0.54
2:B:994:LYS:NZ	2:B:996:ARG:HD3	2.21	0.54
2:B:1018:THR:HG22	2:B:1030:TYR:HB2	1.90	0.53
2:B:1093:ASN:ND2	2:B:1104:TYR:OH	2.40	0.53
1:A:496:SER:O	2:B:1294:ARG:NH1	2.41	0.53
2:B:984:ILE:HD13	2:B:996:ARG:HH12	1.74	0.53
1:A:402:PHE:CZ	1:A:659:LEU:HD21	2.44	0.53
1:A:454:LEU:HD22	1:A:474:PHE:HE1	1.74	0.52
1:A:603:SER:OG	1:A:603:SER:O	2.21	0.52
2:B:878:ILE:HD11	2:B:932:ILE:HB	1.91	0.52
1:A:140:MET:HG2	1:A:526:CYS:SG	2.49	0.52
2:B:952:TYR:HA	2:B:1065:ARG:HH22	1.74	0.52
2:B:1274:SER:O	2:B:1274:SER:OG	2.28	0.52
1:A:120:MET:O	1:A:124:VAL:HG13	2.10	0.52
1:A:174:ARG:HG2	1:A:174:ARG:HH11	1.75	0.52
1:A:259:PRO:O	1:A:260:HIS:ND1	2.43	0.52
1:A:120:MET:HG3	1:A:246:GLY:CA	2.40	0.51
1:A:299:GLU:OE1	1:A:300:SER:N	2.30	0.51
1:A:167:GLY:HA2	1:A:625:THR:HA	1.91	0.51
2:B:946:TRP:HB2	2:B:1070:LYS:HG3	1.92	0.50
2:B:984:ILE:HG12	2:B:998:VAL:HG12	1.93	0.50
1:A:625:THR:O	1:A:629:ILE:HG23	2.11	0.50
1:A:412:PRO:O	1:A:415:ILE:HG22	2.11	0.50
1:A:415:ILE:HD11	1:A:589:GLU:HG2	1.93	0.50
2:B:1125:VAL:HG11	2:B:1186:VAL:HG21	1.94	0.50
1:A:464:PHE:HE2	1:A:469:PHE:HE2	1.60	0.50
1:A:115:LEU:HD22	1:A:219:VAL:HG23	1.93	0.49
1:A:521:GLU:HG2	2:B:1139:PRO:HD2	1.94	0.49
2:B:928:LEU:HD11	2:B:1053:ILE:HG13	1.93	0.49
2:B:1241:ASP:HB3	2:B:1247:ILE:HD11	1.94	0.49
1:A:434:HIS:HB3	1:A:436:TYR:CE1	2.46	0.49
1:A:107:PHE:HB2	1:A:323:THR:HG21	1.94	0.49
2:B:1205:ILE:HD13	2:B:1260:LYS:HZ1	1.78	0.49
2:B:889:ILE:HA	2:B:898:ILE:HD13	1.94	0.49
2:B:979:ASN:HB3	2:B:982:GLU:HB2	1.94	0.49
2:B:1179:ARG:HG2	2:B:1222:VAL:HG22	1.94	0.49
2:B:1205:ILE:HG21	2:B:1260:LYS:HZ2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HG21	1:A:297:MET:HG3	1.95	0.48
1:A:110:ILE:O	1:A:114:VAL:HG13	2.13	0.48
2:B:972:SER:OG	2:B:1048:HIS:O	2.30	0.48
2:B:985:TRP:CD2	2:B:1019:ILE:HG21	2.49	0.48
1:A:564:GLY:HA2	1:A:678:ARG:HD2	1.96	0.48
2:B:964:ILE:HG21	2:B:978:LEU:HD13	1.96	0.48
2:B:1134:MET:SD	2:B:1134:MET:N	2.86	0.48
1:A:203:PHE:O	1:A:207:ILE:HG22	2.13	0.48
1:A:261:TYR:H	1:A:261:TYR:HD1	1.62	0.48
2:B:1252:PHE:HD2	2:B:1259:ALA:HB1	1.78	0.48
1:A:434:HIS:HB3	1:A:436:TYR:HE1	1.79	0.47
1:A:442:PHE:O	1:A:462:MET:HB2	2.14	0.47
2:B:988:GLN:NE2	2:B:992:GLU:OE1	2.47	0.47
1:A:125:GLU:HG2	1:A:212:ILE:HD13	1.95	0.47
1:A:483:THR:HA	1:A:503:ASP:OD2	2.15	0.47
1:A:169:ALA:HB2	1:A:177:VAL:HG11	1.95	0.47
1:A:115:LEU:HB3	1:A:219:VAL:HG23	1.97	0.47
1:A:382:VAL:HA	1:A:390:THR:HG21	1.96	0.47
2:B:1115:ASN:ND2	2:B:1118:ASP:H	2.13	0.46
1:A:152:MET:O	1:A:155:TYR:HB2	2.16	0.46
2:B:1236:LYS:HB3	2:B:1280:CYS:HB2	1.98	0.46
2:B:1256:ASN:OD1	2:B:1257:ASN:N	2.41	0.46
2:B:975:LYS:HG2	2:B:986:THR:HB	1.97	0.46
2:B:997:VAL:HG12	2:B:1039:LYS:HB2	1.98	0.46
2:B:1100:PHE:N	2:B:1284:PHE:O	2.46	0.46
2:B:1114:LEU:HB2	2:B:1285:ILE:HD11	1.97	0.46
1:A:645:PHE:HZ	1:A:660:ALA:HB2	1.81	0.46
2:B:954:ASN:OD1	2:B:954:ASN:N	2.41	0.46
2:B:1070:LYS:HD2	2:B:1071:TYR:CD2	2.50	0.46
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.80	0.46
1:A:431:PHE:N	1:A:433:GLU:OE1	2.49	0.46
1:A:428:LYS:HB2	1:A:447:GLN:HG2	1.97	0.45
1:A:500:TYR:HB2	1:A:520:LEU:HD12	1.97	0.45
1:A:559:LEU:HD13	1:A:563:ILE:HD11	1.98	0.45
2:B:1041:ILE:O	2:B:1044:LEU:HB2	2.16	0.45
1:A:104:HIS:HA	1:A:108:GLN:OE1	2.17	0.45
1:A:129:VAL:HG11	1:A:155:TYR:CD1	2.51	0.45
1:A:318:LYS:HE2	1:A:318:LYS:HB3	1.63	0.45
2:B:914:ILE:HG21	2:B:924:ILE:HD11	1.98	0.45
1:A:648:PHE:CG	1:A:651:ILE:HD11	2.52	0.45
2:B:1127:ASN:O	2:B:1132:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LYS:HD3	1:A:635:LYS:HA	1.59	0.44
2:B:1256:ASN:CG	2:B:1257:ASN:H	2.21	0.44
1:A:273:PHE:CD1	1:A:273:PHE:O	2.70	0.44
1:A:566:LEU:HD23	1:A:674:LEU:HB3	2.00	0.44
1:A:645:PHE:CZ	1:A:660:ALA:HB2	2.53	0.44
1:A:223:PHE:O	1:A:227:LEU:HD22	2.18	0.44
2:B:994:LYS:HZ2	2:B:996:ARG:HD3	1.80	0.44
1:A:171:LYS:HD3	1:A:171:LYS:HA	1.70	0.44
2:B:925:GLU:OE2	2:B:927:ILE:HG13	2.18	0.44
1:A:154:VAL:HG23	1:A:206:LEU:HA	1.99	0.44
1:A:124:VAL:HG12	1:A:250:ALA:HB2	1.98	0.43
1:A:381:CYS:SG	1:A:622:GLN:HB3	2.57	0.43
1:A:182:LEU:HD22	1:A:287:CYS:HB2	2.00	0.43
2:B:976:VAL:HG22	2:B:985:TRP:HE3	1.83	0.43
2:B:948:ARG:HD3	2:B:1014:TRP:CD1	2.53	0.43
1:A:115:LEU:HB3	1:A:219:VAL:CG2	2.48	0.43
1:A:455:VAL:HA	1:A:475:ASP:HB3	2.01	0.43
2:B:985:TRP:HB3	2:B:997:VAL:HG23	2.01	0.43
2:B:1221:VAL:CG1	2:B:1237:MET:HB3	2.49	0.43
1:A:157:GLY:O	1:A:210:ILE:HD13	2.19	0.43
1:A:559:LEU:O	1:A:563:ILE:HD12	2.18	0.43
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.88	0.43
1:A:156:LEU:O	1:A:159:MET:HB3	2.19	0.43
1:A:164:ILE:HD13	1:A:164:ILE:HA	1.88	0.43
1:A:109:TRP:HA	1:A:109:TRP:CE3	2.54	0.42
1:A:537:LEU:HD23	1:A:537:LEU:HA	1.92	0.42
1:A:178:LEU:HB2	1:A:218:ILE:HG21	2.01	0.42
1:A:474:PHE:HD2	1:A:494:ILE:HG12	1.85	0.42
1:A:153:ILE:HA	1:A:156:LEU:HD12	2.01	0.42
1:A:193:SER:O	1:A:277:ARG:HG2	2.19	0.42
1:A:447:GLN:O	1:A:467:VAL:HA	2.19	0.42
1:A:392:ILE:O	1:A:396:VAL:HG23	2.19	0.42
2:B:990:THR:HG23	2:B:1046:ASN:O	2.20	0.42
2:B:1021:ASN:OD1	2:B:1027:SER:HB2	2.20	0.42
1:A:234:GLU:O	1:A:237:SER:OG	2.26	0.41
2:B:1226:LYS:HE3	2:B:1226:LYS:HB2	1.79	0.41
1:A:182:LEU:HA	1:A:182:LEU:HD23	1.85	0.41
1:A:181:SER:O	1:A:184:VAL:HG12	2.20	0.41
1:A:517:SER:O	2:B:1143:VAL:HG23	2.21	0.41
2:B:1253:HIS:HB2	2:B:1262:VAL:HG21	2.02	0.41
1:A:252:ALA:HB2	1:A:543:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:883:TYR:CE2	2:B:886:ASN:HA	2.55	0.41
2:B:1034:ARG:NH1	2:B:1036:ILE:HD11	2.36	0.41
2:B:1199:GLN:H	2:B:1199:GLN:HG3	1.70	0.41
1:A:214:GLY:O	1:A:218:ILE:HG12	2.21	0.41
1:A:476:GLU:HA	1:A:496:SER:O	2.21	0.41
2:B:1117:TYR:HD2	2:B:1278:LEU:HB2	1.84	0.41
2:B:913:GLN:HA	2:B:1070:LYS:HB3	2.01	0.41
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.86	0.41
2:B:1023:ARG:HA	2:B:1041:ILE:HD11	2.03	0.41
2:B:1238:ASN:HB2	2:B:1249:PHE:CE1	2.55	0.41
1:A:192:SER:HB3	1:A:204:CYS:HB3	2.03	0.41
1:A:598:LEU:O	1:A:602:THR:HG23	2.21	0.41
2:B:1113:MET:HE3	2:B:1160:PHE:CD2	2.56	0.41
2:B:1291:TRP:HD1	2:B:1293:GLU:HB3	1.86	0.41
1:A:133:LEU:HB2	1:A:134:PRO:HD3	2.03	0.41
1:A:208:SER:O	1:A:212:ILE:HG22	2.21	0.41
1:A:285:LEU:O	1:A:289:VAL:HG23	2.21	0.40
1:A:297:MET:N	1:A:297:MET:SD	2.93	0.40
2:B:883:TYR:HD1	2:B:888:LEU:HD13	1.87	0.40
2:B:958:LEU:O	2:B:959:ASN:ND2	2.53	0.40
2:B:1277:THR:C	2:B:1279:GLY:H	2.24	0.40
1:A:257:ILE:HG21	1:A:279:PHE:HB2	2.03	0.40
1:A:582:PHE:O	1:A:582:PHE:HD1	2.04	0.40
2:B:948:ARG:NH1	2:B:1012:ASN:O	2.38	0.40
2:B:1269:ARG:HD3	2:B:1269:ARG:HA	1.80	0.40
2:B:950:PRO:HG2	2:B:1065:ARG:HH11	1.86	0.40
1:A:227:LEU:H	1:A:227:LEU:HD23	1.86	0.40
2:B:991:GLN:HB2	2:B:993:ILE:HD12	2.04	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	543/683 (80%)	521 (96%)	22 (4%)	0	100	100
2	B	409/443 (92%)	387 (95%)	22 (5%)	0	100	100
All	All	952/1126 (84%)	908 (95%)	44 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	459/580 (79%)	438 (95%)	21 (5%)	23	48
2	B	384/408 (94%)	375 (98%)	9 (2%)	45	64
All	All	843/988 (85%)	813 (96%)	30 (4%)	32	55

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	139	ASP
1	A	155	TYR
1	A	196	GLN
1	A	222	TYR
1	A	224	SER
1	A	226	PHE
1	A	249	TYR
1	A	255	TRP
1	A	261	TYR
1	A	265	PHE
1	A	430	PHE
1	A	480	GLU
1	A	484	SER
1	A	531	GLU
1	A	533	ASP
1	A	535	ASP
1	A	566	LEU

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Mol	Chain	Res	Type
1	A	582	PHE
1	A	585	PHE
1	A	627	PHE
2	B	893	ARG
2	B	930	ASN
2	B	935	ASN
2	B	994	LYS
2	B	1228	ASP
2	B	1229	GLN
2	B	1255	PHE
2	B	1269	ARG
2	B	1278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	446	ASN
1	A	447	GLN
1	A	553	ASN
1	A	642	ASN
2	B	913	GLN
2	B	935	ASN
2	B	959	ASN
2	B	1026	ASN
2	B	1046	ASN
2	B	1093	ASN
2	B	1115	ASN
2	B	1270	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 ⓘ

8 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	C	1	3,1	14,14,15	0.38	0	17,19,21	0.61	0
3	NAG	C	2	3	14,14,15	0.40	0	17,19,21	0.45	0
3	FUL	C	3	3	10,10,11	0.47	0	14,14,16	0.39	0
4	NAG	D	1	4,1	14,14,15	0.35	0	17,19,21	0.58	0
4	NAG	D	2	4	14,14,15	0.20	0	17,19,21	0.41	0
4	BMA	D	3	4	11,11,12	0.57	0	15,15,17	0.83	0
4	MAN	D	4	4	11,11,12	0.67	0	15,15,17	0.95	2 (13%)
4	FUC	D	5	4	10,10,11	0.81	0	14,14,16	0.98	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	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	FUL	C	3	3	-	-	0/1/1/1
4	NAG	D	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	FUC	D	5	4	-	-	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(°)
4	D	4	MAN	O2-C2-C3	-2.24	105.65	110.14
4	D	4	MAN	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

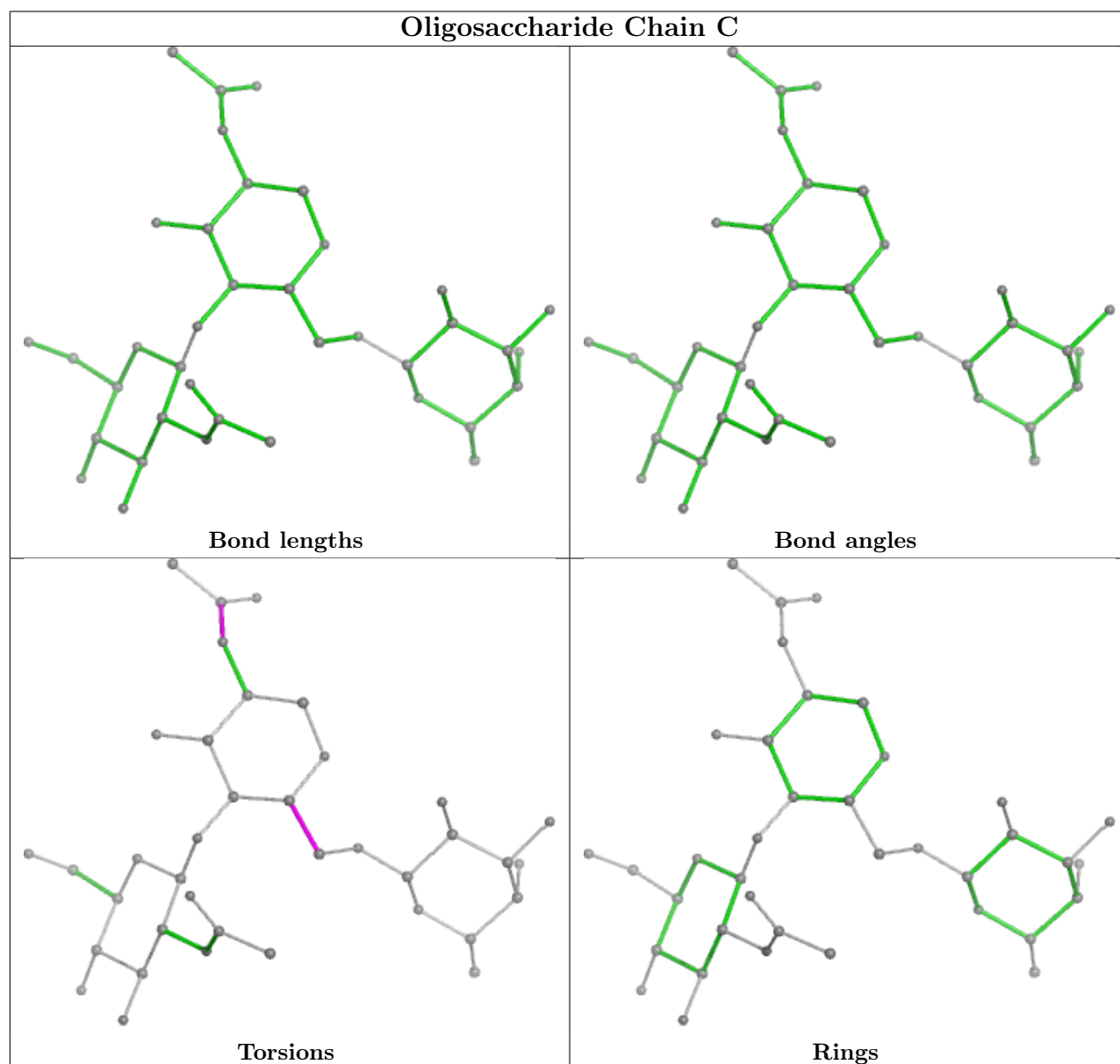
All (7) torsion outliers are listed below:

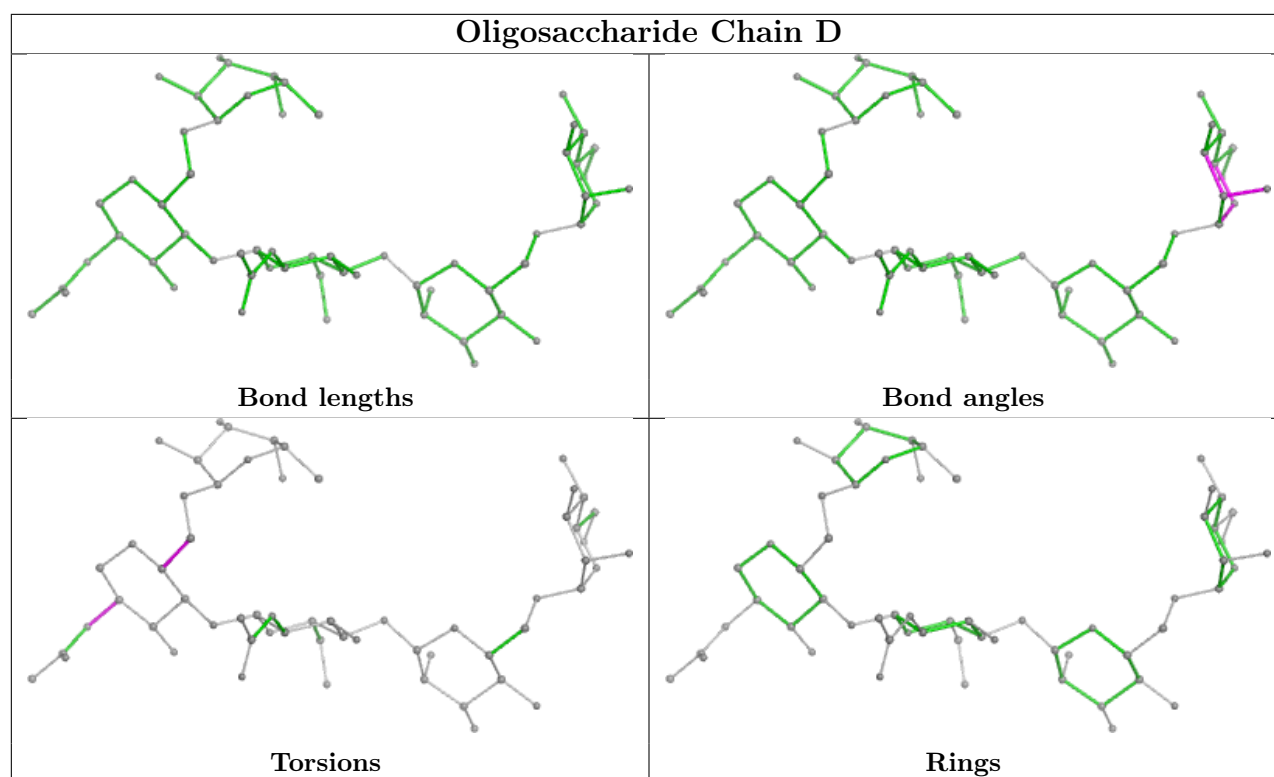
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C3-C2-N2-C7

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	701	1	14,14,15	0.24	0	17,19,21	0.36	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
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

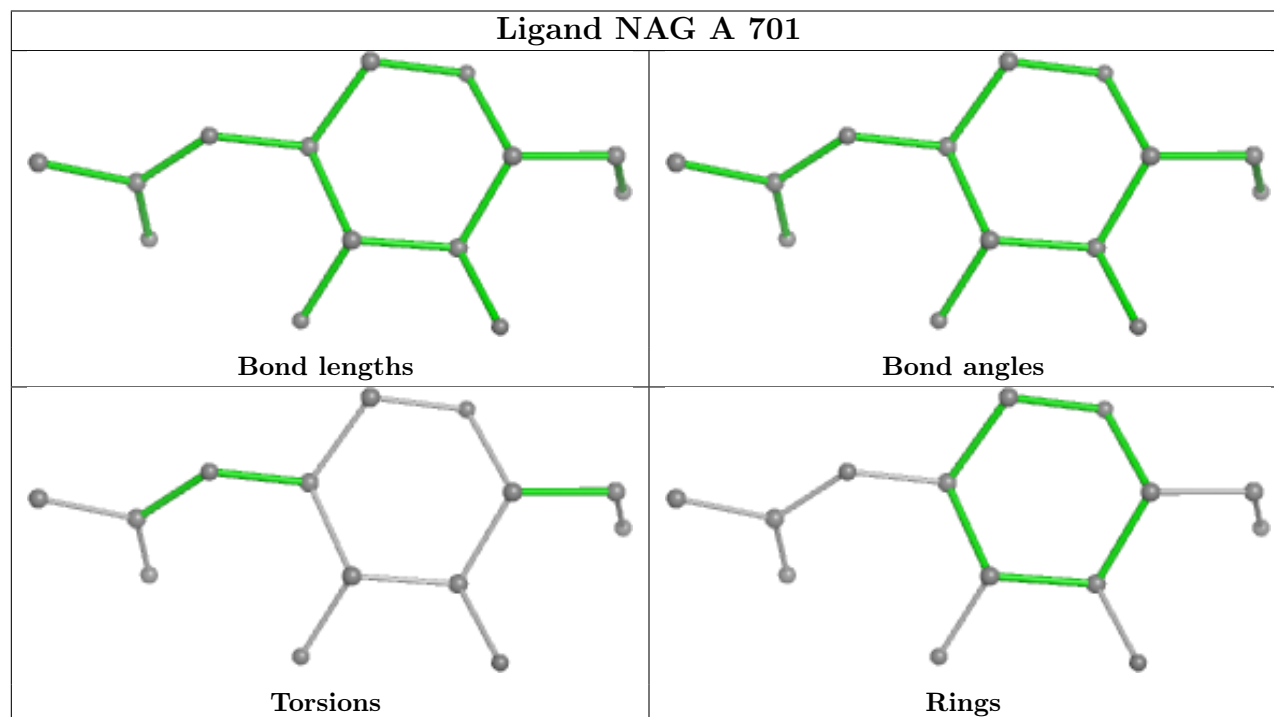
There are no chirality outliers.

There are no torsion outliers.

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 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.