



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:55 AM UTC

PDB ID : 7TGY / pdb_00007tgy
EMDB ID : EMD-25889
Title : Prototypic SARS-CoV-2 G614 spike (closed form)
Authors : Ye, G.; Liu, B.; Li, F.
Deposited on : 2022-01-09
Resolution : 3.00 Å (reported)
Based on initial model : 7KRQ

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:

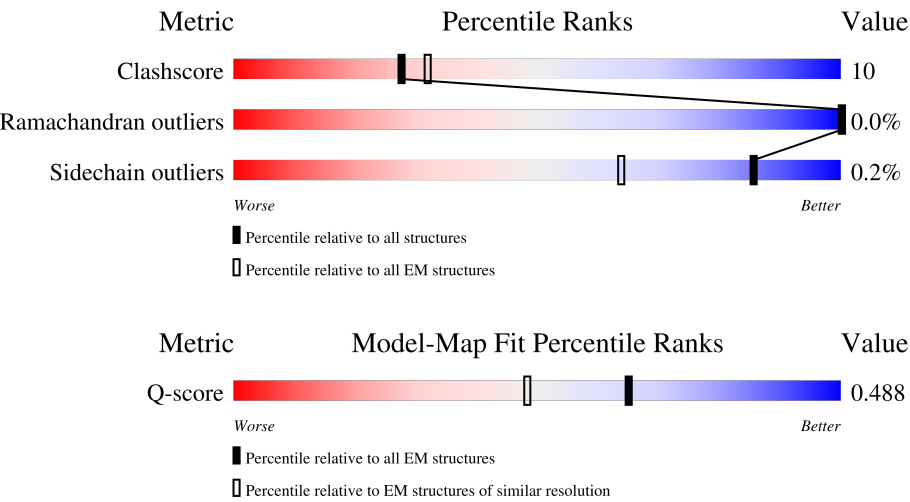
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1234	7% 69% 18% 12%
1	B	1234	7% 72% 16% 12%
1	C	1234	7% 71% 17% 12%
2	K	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	2	50% 50%
2	U	2	100%
2	V	2	100%
2	X	2	50% 50%
2	e	2	50% 100%
2	f	2	50% 50%
2	g	2	50% 50%
2	h	2	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25999 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	1083	Total	C	N	O	S	0	0
			8454	5395	1410	1610	39		
1	B	1084	Total	C	N	O	S	0	0
			8468	5406	1412	1611	39		
1	C	1087	Total	C	N	O	S	0	0
			8489	5419	1415	1616	39		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLY	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLY	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLY	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2

- 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
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

Continued on next page...

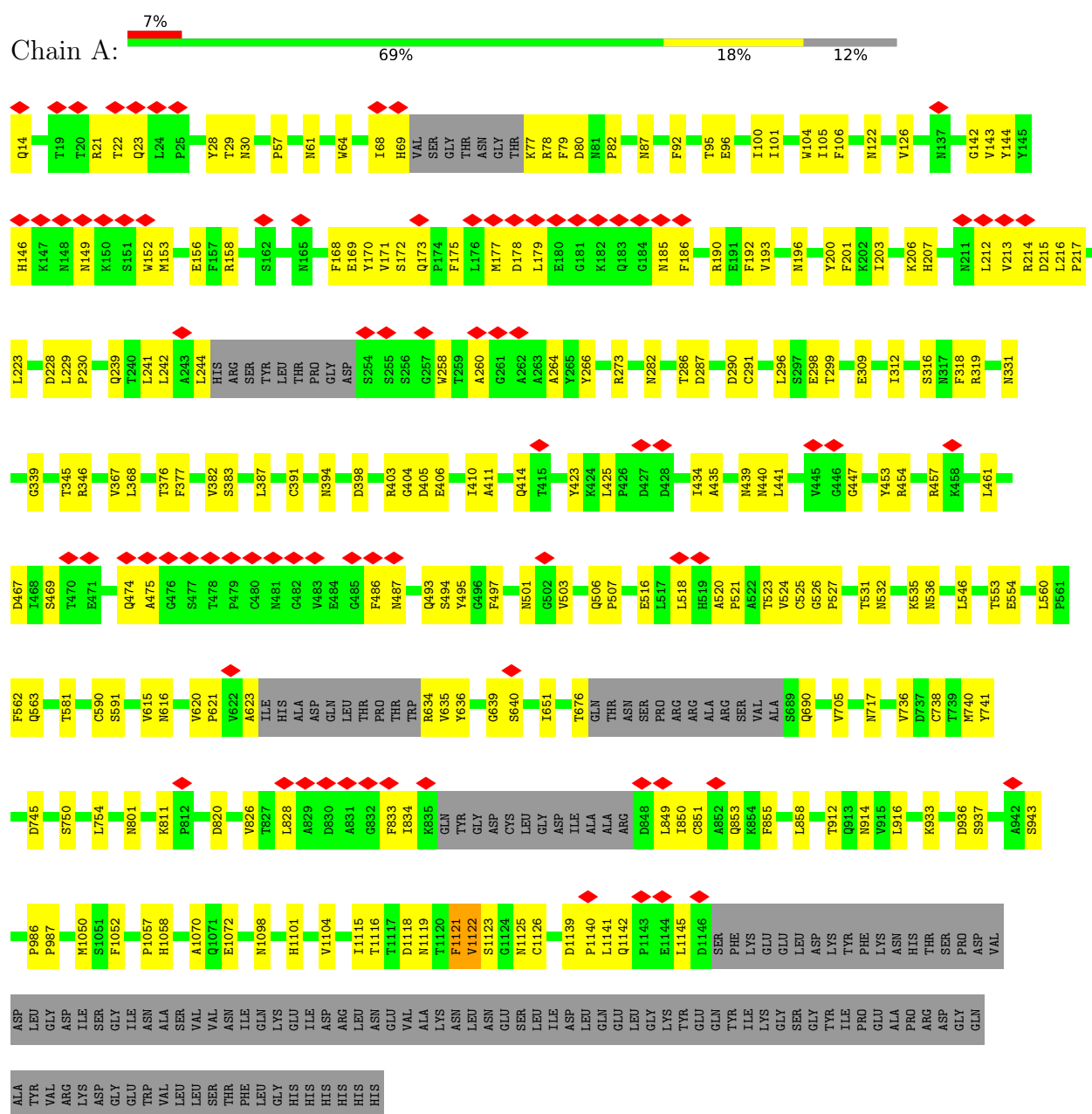
Continued from previous page...

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

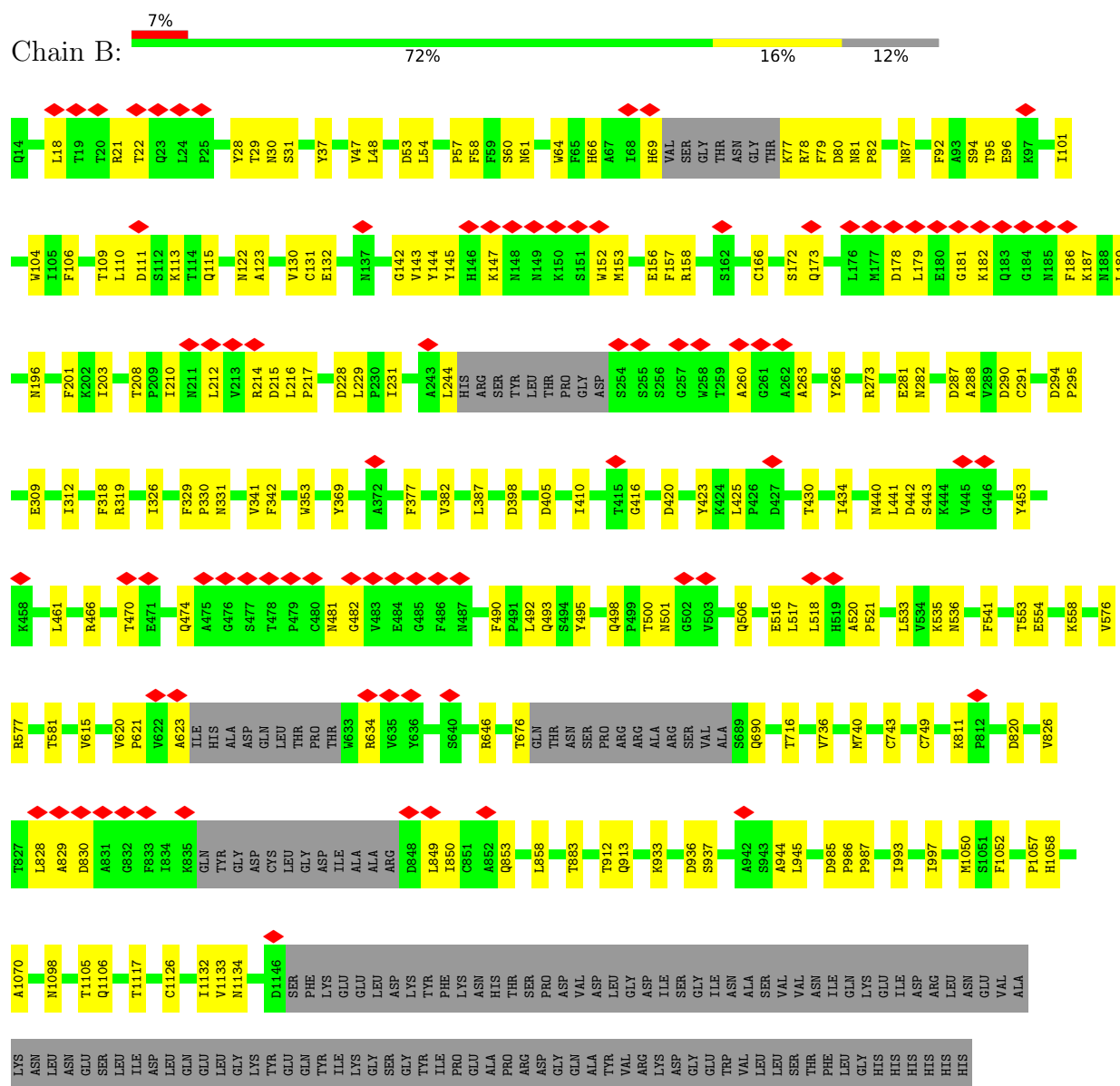
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

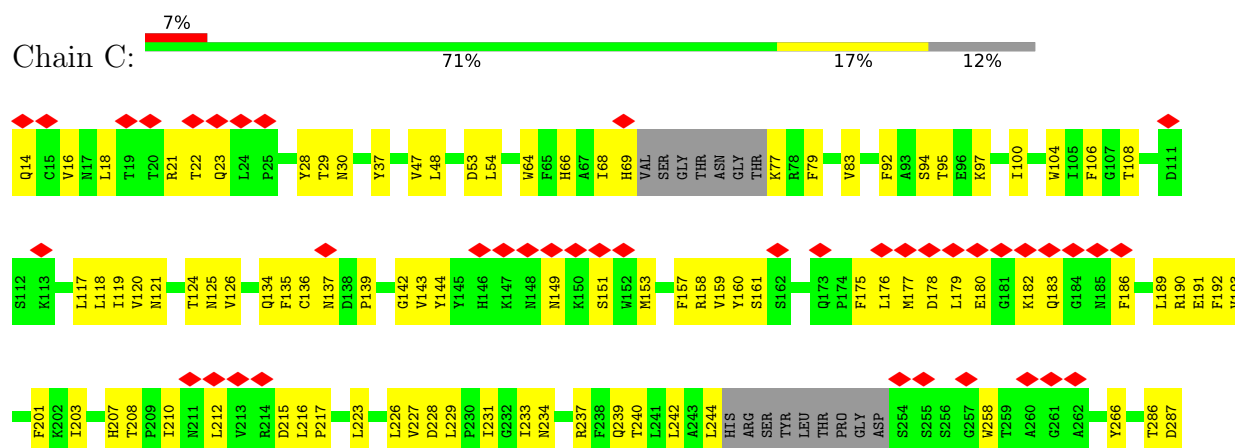
• Molecule 1: Spike glycoprotein

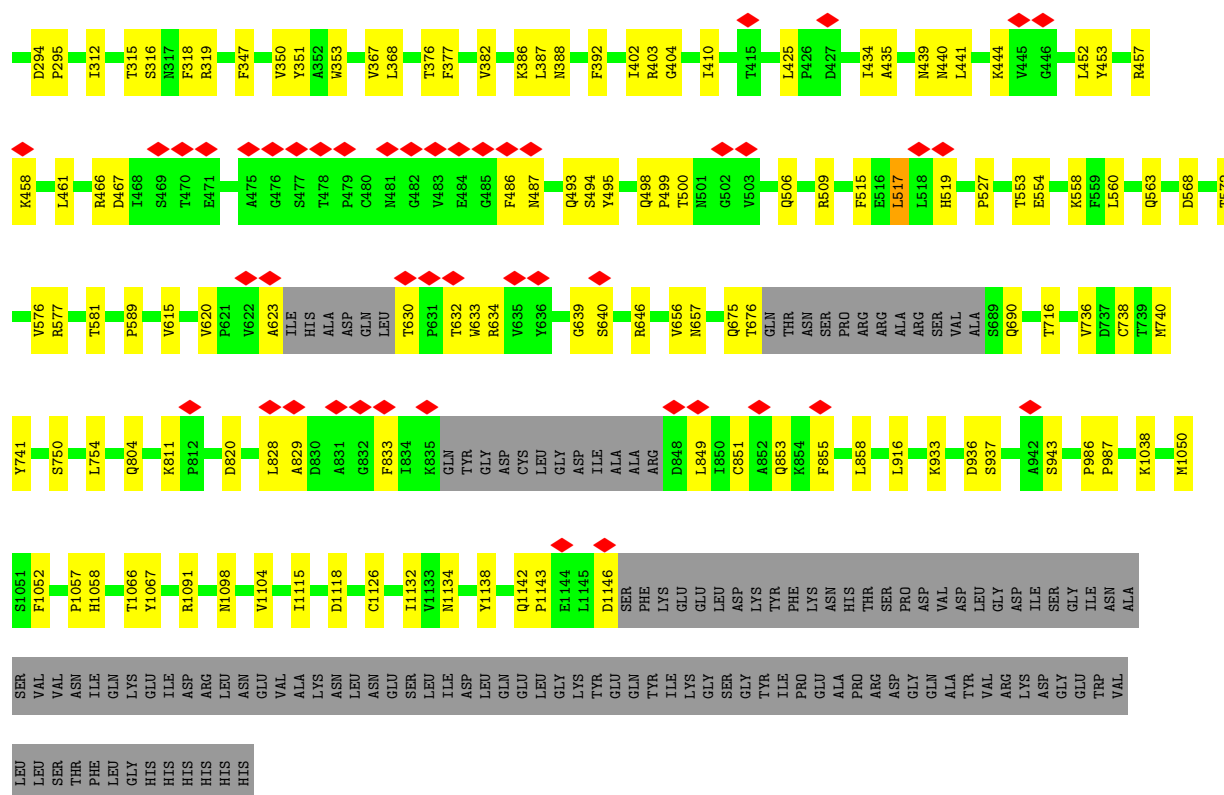


- Molecule 1: Spike glycoprotein

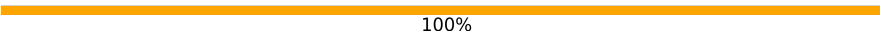


- Molecule 1: Spike glycoprotein





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

Chain K:  100%

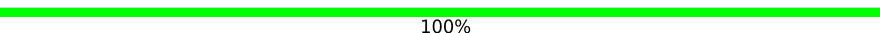
MAG1
MAG2

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

Chain M:  50%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain V:  100%



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

Chain X:  50% 50%



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

Chain e:  50% 100%



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

Chain f:  50% 50%



- 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:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	165708	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.345	Depositor
Minimum map value	-0.508	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	341.76, 341.76, 341.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89000005, 0.89000005, 0.89000005	Depositor

5 Model quality

5.1 Standard geometry

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	0.44	0/8648	0.53	1/11767 (0.0%)
1	B	0.44	0/8664	0.52	0/11790
1	C	0.43	0/8686	0.50	0/11822
All	All	0.44	0/25998	0.52	1/35379 (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	B	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1121	PHE	CB-CA-C	-6.12	103.02	112.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1070	ALA	Peptide
1	B	516	GLU	Peptide
1	C	517	LEU	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	8454	0	8249	176	0
1	B	8468	0	8252	147	0
1	C	8489	0	8276	168	0
2	K	28	0	25	3	0
2	M	28	0	25	2	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	X	28	0	25	0	0
2	e	28	0	25	6	0
2	f	28	0	25	0	0
2	g	28	0	25	1	0
2	h	28	0	25	0	0
3	A	84	0	78	5	0
3	B	140	0	130	2	0
3	C	112	0	104	4	0
All	All	25999	0	25314	495	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 10.

All (495) 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:118:LEU:HD21	1:C:120:VAL:HG23	1.42	1.02
3:A:1305:NAG:O7	3:A:1305:NAG:O3	1.95	0.84
1:A:22:THR:O	1:A:78:ARG:NH1	2.09	0.84
1:C:315:THR:HG22	1:C:316:SER:H	1.42	0.82
1:C:517:LEU:O	1:C:519:HIS:ND1	2.13	0.81
1:A:501:ASN:O	1:A:506:GLN:NE2	2.14	0.81
1:A:518:LEU:HD23	1:A:518:LEU:O	1.79	0.81
1:A:21:ARG:NH1	1:A:79:PHE:O	2.16	0.79
1:B:172:SER:OG	1:B:173:GLN:OE1	2.01	0.79
1:C:623:ALA:O	1:C:634:ARG:NH1	2.16	0.79
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.48	0.78
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PHE:HE1	1:C:242:LEU:HD11	1.49	0.77
1:B:95:THR:HG22	1:B:186:PHE:HB2	1.65	0.77
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.50	0.76
1:C:239:GLN:NE2	1:C:240:THR:O	2.18	0.76
1:B:22:THR:O	1:B:78:ARG:NH1	2.20	0.75
1:A:1050:MET:HE2	1:A:1052:PHE:CZ	2.22	0.75
1:B:1050:MET:HE2	1:B:1052:PHE:CZ	2.23	0.73
1:B:490:PHE:O	1:B:493:GLN:NE2	2.21	0.73
2:e:1:NAG:O3	2:e:2:NAG:O5	2.08	0.72
1:B:736:VAL:HG22	1:B:858:LEU:CD2	2.20	0.72
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.19	0.71
1:C:228:ASP:OD1	1:C:229:LEU:N	2.24	0.71
1:A:740:MET:SD	1:C:319:ARG:NH1	2.64	0.70
1:C:1050:MET:HE2	1:C:1052:PHE:CZ	2.25	0.70
1:A:383:SER:OG	1:B:985:ASP:OD2	2.08	0.70
1:A:620:VAL:O	1:A:623:ALA:N	2.24	0.70
1:B:319:ARG:NH2	1:C:740:MET:SD	2.65	0.69
1:A:801:ASN:ND2	2:K:1:NAG:O6	2.26	0.69
1:C:29:THR:HG22	1:C:30:ASN:H	1.57	0.69
2:e:1:NAG:HO3	2:e:2:NAG:HO6	1.37	0.69
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.57	0.69
1:A:1121:PHE:O	1:A:1123:SER:N	2.26	0.69
1:C:118:LEU:CD2	1:C:120:VAL:HG23	2.21	0.68
1:C:736:VAL:HG22	1:C:858:LEU:CD2	2.23	0.68
1:B:29:THR:HG22	1:B:30:ASN:H	1.58	0.68
1:B:37:TYR:OH	1:B:53:ASP:OD2	2.10	0.68
1:A:212:LEU:HD11	1:A:215:ASP:OD1	1.95	0.67
1:C:118:LEU:HD21	1:C:120:VAL:CG2	2.22	0.67
1:A:29:THR:HG22	1:A:30:ASN:H	1.60	0.67
3:C:1304:NAG:H83	3:C:1304:NAG:H3	1.76	0.67
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.29	0.66
1:A:493:GLN:NE2	1:A:494:SER:O	2.28	0.66
1:C:37:TYR:OH	1:C:53:ASP:OD2	2.12	0.66
1:A:318:PHE:CZ	1:A:615:VAL:HG11	2.30	0.66
1:C:66:HIS:CE1	1:C:68:ILE:HD11	2.30	0.66
1:C:149:ASN:ND2	1:C:151:SER:OG	2.28	0.66
1:C:1142:GLN:O	1:C:1146:ASP:N	2.29	0.66
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.78	0.65
2:e:1:NAG:O3	2:e:2:NAG:O6	2.11	0.65
1:B:66:HIS:N	1:B:80:ASP:OD2	2.28	0.65
1:B:142:GLY:HA2	1:B:244:LEU:HB3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:OE2	1:A:100:ILE:N	2.30	0.64
1:A:172:SER:OG	1:A:173:GLN:OE1	2.16	0.64
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.22	0.63
1:B:228:ASP:OD1	1:B:229:LEU:N	2.32	0.63
1:A:936:ASP:OD1	1:A:937:SER:N	2.31	0.63
1:C:804:GLN:OE1	2:g:1:NAG:O6	2.17	0.63
1:C:936:ASP:OD1	1:C:937:SER:N	2.31	0.62
1:C:849:LEU:HD12	1:C:853:GLN:NE2	2.14	0.62
1:B:216:LEU:HD12	1:B:217:PRO:CD	2.29	0.62
1:C:149:ASN:ND2	1:C:151:SER:O	2.31	0.62
1:C:228:ASP:O	1:C:229:LEU:HD12	2.00	0.61
1:A:634:ARG:HG2	1:A:635:VAL:H	1.66	0.61
1:C:353:TRP:O	1:C:466:ARG:NH2	2.34	0.61
1:C:318:PHE:CZ	1:C:615:VAL:HG21	2.34	0.61
1:B:157:PHE:O	1:B:158:ARG:NE	2.34	0.61
1:C:382:VAL:HG21	1:C:387:LEU:HD21	1.83	0.61
1:B:287:ASP:OD1	1:B:288:ALA:N	2.34	0.61
1:C:14:GLN:OE1	1:C:158:ARG:NH2	2.31	0.61
1:A:228:ASP:OD1	1:A:229:LEU:N	2.33	0.60
1:B:143:VAL:HG21	1:B:179:LEU:HD23	1.84	0.60
1:C:229:LEU:HD23	1:C:231:ILE:HD11	1.82	0.60
1:C:493:GLN:NE2	1:C:494:SER:O	2.35	0.60
1:C:736:VAL:HG22	1:C:858:LEU:HD23	1.84	0.60
1:B:131:CYS:HA	1:B:166:CYS:HB3	1.84	0.60
1:B:736:VAL:HG22	1:B:858:LEU:HD23	1.85	0.59
1:B:353:TRP:O	1:B:466:ARG:NH2	2.36	0.59
1:B:212:LEU:HD21	1:B:215:ASP:O	2.02	0.59
1:C:676:THR:N	1:C:690:GLN:OE1	2.34	0.59
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.83	0.59
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.35	0.59
1:C:231:ILE:HG22	1:C:233:ILE:HG23	1.83	0.58
1:A:849:LEU:HD12	1:A:853:GLN:NE2	2.18	0.58
1:B:716:THR:HG22	1:B:716:THR:O	2.02	0.58
1:B:936:ASP:OD1	1:B:937:SER:N	2.36	0.58
1:C:457:ARG:NH2	1:C:467:ASP:OD2	2.36	0.58
1:C:738:CYS:O	1:C:741:TYR:N	2.37	0.58
1:A:1050:MET:HE2	1:A:1052:PHE:CE1	2.39	0.58
1:A:142:GLY:CA	1:A:156:GLU:HB3	2.34	0.58
1:A:1139:ASP:HB2	1:A:1142:GLN:HB2	1.86	0.58
1:C:216:LEU:HD12	1:C:217:PRO:CD	2.34	0.58
1:A:405:ASP:OD2	1:A:406:GLU:N	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:CE1	1:B:260:ALA:HB2	2.40	0.57
1:C:136:CYS:SG	1:C:137:ASN:N	2.76	0.57
1:A:146:HIS:O	1:A:146:HIS:ND1	2.37	0.57
1:B:212:LEU:HD11	1:B:215:ASP:O	2.05	0.57
1:C:828:LEU:HD23	1:C:829:ALA:N	2.20	0.57
1:B:430:THR:HG23	1:B:430:THR:O	2.03	0.57
1:B:581:THR:HG23	1:B:581:THR:O	2.05	0.57
1:C:100:ILE:HG22	1:C:242:LEU:HB2	1.85	0.57
1:A:705:VAL:HG13	1:B:883:THR:HG21	1.86	0.57
1:C:21:ARG:HD3	1:C:79:PHE:HB3	1.86	0.57
1:A:581:THR:HG23	1:A:581:THR:O	2.05	0.57
1:B:64:TRP:CD1	1:B:266:TYR:HE1	2.23	0.57
1:A:258:TRP:HZ3	1:A:260:ALA:HB2	1.69	0.56
1:A:634:ARG:HG2	1:A:635:VAL:N	2.20	0.56
1:B:228:ASP:O	1:B:229:LEU:HD23	2.05	0.56
1:C:441:LEU:HD22	1:C:509:ARG:NH2	2.21	0.56
1:A:142:GLY:N	1:A:156:GLU:HB3	2.20	0.56
1:A:156:GLU:OE2	1:A:158:ARG:HD2	2.06	0.56
1:C:315:THR:HG22	1:C:316:SER:N	2.17	0.56
1:C:486:PHE:O	1:C:487:ASN:OD1	2.23	0.56
1:C:498:GLN:OE1	1:C:500:THR:HG22	2.06	0.56
1:C:159:VAL:HG13	1:C:160:TYR:HD1	1.70	0.56
1:C:22:THR:HG22	1:C:23:GLN:N	2.21	0.55
1:B:620:VAL:HB	1:B:621:PRO:HD3	1.88	0.55
1:A:912:THR:HG22	1:A:914:ASN:H	1.71	0.55
1:C:149:ASN:ND2	1:C:153:MET:HE3	2.20	0.55
1:B:122:ASN:OD1	1:B:123:ALA:N	2.36	0.55
1:B:1117:THR:HG22	1:B:1117:THR:O	2.07	0.55
1:A:1141:LEU:O	1:A:1145:LEU:HB2	2.06	0.55
1:A:296:LEU:O	1:A:299:THR:HG22	2.07	0.55
1:B:95:THR:HG22	1:B:186:PHE:CB	2.34	0.55
1:C:79:PHE:CE1	1:C:242:LEU:HD11	2.37	0.55
1:B:57:PRO:HG3	1:B:273:ARG:HE	1.72	0.55
1:C:95:THR:HG23	1:C:186:PHE:CD2	2.41	0.55
1:C:402:ILE:HG13	1:C:403:ARG:H	1.72	0.55
1:B:501:ASN:O	1:B:506:GLN:NE2	2.40	0.54
1:C:118:LEU:HD23	1:C:118:LEU:C	2.32	0.54
1:A:636:TYR:CE2	1:A:651:ILE:HG22	2.43	0.54
1:C:64:TRP:CD1	1:C:266:TYR:HE1	2.25	0.54
1:C:716:THR:O	1:C:716:THR:HG22	2.07	0.54
1:A:64:TRP:CD1	1:A:266:TYR:HE1	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:SER:HG	1:B:985:ASP:CG	2.16	0.54
1:A:100:ILE:HG22	1:A:242:LEU:CD1	2.38	0.54
1:A:258:TRP:CZ3	1:A:260:ALA:HB2	2.43	0.54
1:C:581:THR:HG23	1:C:581:THR:O	2.08	0.54
1:A:405:ASP:OD2	1:A:405:ASP:C	2.50	0.54
1:A:705:VAL:CG1	1:B:883:THR:HG21	2.38	0.54
1:B:474:GLN:O	1:B:474:GLN:HG2	2.08	0.54
1:A:486:PHE:O	1:A:487:ASN:OD1	2.25	0.53
1:C:143:VAL:HG21	1:C:179:LEU:HD23	1.90	0.53
1:B:131:CYS:HA	1:B:166:CYS:CB	2.38	0.53
1:C:22:THR:HG22	1:C:23:GLN:H	1.73	0.53
1:C:22:THR:N	1:C:77:LYS:O	2.41	0.53
1:C:312:ILE:HG23	1:C:312:ILE:O	2.09	0.53
2:e:1:NAG:O4	2:e:2:NAG:O7	2.26	0.52
1:A:100:ILE:HG22	1:A:242:LEU:HD11	1.91	0.52
1:A:105:ILE:CD1	1:A:241:LEU:HD21	2.39	0.52
1:C:143:VAL:HG23	1:C:153:MET:C	2.34	0.52
1:C:461:LEU:HD23	1:C:461:LEU:H	1.75	0.52
1:C:175:PHE:O	1:C:176:LEU:HD22	2.09	0.52
1:C:675:GLN:NE2	1:C:676:THR:O	2.43	0.52
1:B:143:VAL:HG22	1:B:152:TRP:HB3	1.90	0.52
1:B:405:ASP:OD2	1:B:405:ASP:C	2.53	0.52
1:A:216:LEU:HD12	1:A:217:PRO:CD	2.39	0.52
1:B:830:ASP:HB3	1:B:850:ILE:HD12	1.91	0.52
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.91	0.52
1:B:309:GLU:N	1:B:309:GLU:OE1	2.43	0.52
1:B:470:THR:HG22	1:B:492:LEU:HD11	1.92	0.52
2:K:1:NAG:H4	2:K:2:NAG:O3	2.10	0.52
1:B:1050:MET:HE2	1:B:1052:PHE:CE1	2.45	0.52
1:B:1134:ASN:HB2	3:B:1310:NAG:HN2	1.75	0.52
1:A:676:THR:N	1:A:690:GLN:OE1	2.43	0.52
1:A:172:SER:HG	1:A:173:GLN:H	1.56	0.51
1:A:319:ARG:NH1	1:B:740:MET:SD	2.84	0.51
1:A:738:CYS:O	1:A:740:MET:N	2.43	0.51
1:B:461:LEU:H	1:B:461:LEU:HD23	1.74	0.51
1:B:912:THR:HG22	1:B:913:GLN:H	1.76	0.51
1:A:79:PHE:HB2	1:A:258:TRP:CH2	2.45	0.51
1:A:144:TYR:HB2	1:A:153:MET:SD	2.50	0.51
1:A:461:LEU:HD23	1:A:461:LEU:H	1.76	0.51
1:C:121:ASN:OD1	1:C:177:MET:HE1	2.11	0.51
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.93	0.51
1:B:115:GLN:NE2	1:B:132:GLU:OE1	2.43	0.51
1:B:281:GLU:HG3	1:B:282:ASN:OD1	2.11	0.51
1:A:560:LEU:O	1:A:562:PHE:N	2.43	0.50
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.94	0.50
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.93	0.50
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.93	0.50
1:A:474:GLN:HG3	1:A:474:GLN:O	2.12	0.50
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.27	0.50
1:C:175:PHE:C	1:C:176:LEU:HD22	2.37	0.50
1:A:531:THR:HG22	1:A:532:ASN:N	2.27	0.50
1:C:212:LEU:HD11	1:C:215:ASP:OD1	2.12	0.50
1:C:1050:MET:HE2	1:C:1052:PHE:CE1	2.46	0.50
1:A:168:PHE:CD1	1:A:169:GLU:N	2.80	0.49
1:A:855:PHE:CD1	1:C:589:PRO:HG2	2.47	0.49
1:C:18:LEU:HD12	1:C:258:TRP:HE1	1.76	0.49
1:C:16:VAL:HG12	1:C:18:LEU:HD22	1.93	0.49
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.94	0.49
1:C:738:CYS:O	1:C:740:MET:N	2.45	0.49
1:A:201:PHE:HE2	1:A:203:ILE:HD11	1.77	0.49
1:A:206:LYS:HG3	1:A:207:HIS:N	2.26	0.49
1:B:382:VAL:HG21	1:B:387:LEU:HD21	1.93	0.49
1:C:142:GLY:HA2	1:C:244:LEU:HB3	1.94	0.49
1:A:410:ILE:O	1:A:425:LEU:HD12	2.12	0.49
1:B:558:LYS:O	1:B:558:LYS:HG3	2.11	0.49
1:C:1134:ASN:OD1	3:C:1308:NAG:C1	2.60	0.49
1:A:309:GLU:N	1:A:309:GLU:OE1	2.45	0.49
1:C:560:LEU:N	1:C:563:GLN:OE1	2.38	0.49
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.93	0.48
1:A:1116:THR:HB	1:A:1140:PRO:HD3	1.93	0.48
3:A:1305:NAG:HO3	3:A:1305:NAG:C7	2.07	0.48
1:B:849:LEU:HD12	1:B:853:GLN:NE2	2.28	0.48
1:B:1098:ASN:OD1	1:B:1098:ASN:N	2.43	0.48
1:B:201:PHE:HE2	1:B:203:ILE:HD11	1.78	0.48
1:C:1057:PRO:O	1:C:1058:HIS:HB2	2.12	0.48
1:A:126:VAL:HG23	1:A:175:PHE:CE2	2.48	0.48
1:A:639:GLY:O	1:A:640:SER:HB3	2.13	0.48
1:B:64:TRP:CD1	1:B:266:TYR:CE1	3.02	0.48
1:C:410:ILE:O	1:C:425:LEU:HD12	2.14	0.48
1:A:331:ASN:HB2	3:A:1301:NAG:O5	2.13	0.48
1:B:187:LYS:HD2	1:B:210:ILE:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PRO:HA	1:C:158:ARG:O	2.14	0.48
1:C:191:GLU:N	1:C:191:GLU:OE1	2.47	0.48
1:B:410:ILE:O	1:B:425:LEU:HD12	2.14	0.48
1:A:382:VAL:HG11	1:A:387:LEU:CD2	2.44	0.48
1:A:1057:PRO:O	1:A:1058:HIS:HB2	2.14	0.48
1:A:214:ARG:O	1:A:214:ARG:HG2	2.14	0.47
1:A:849:LEU:HD12	1:A:853:GLN:HE22	1.79	0.47
1:B:440:ASN:OD1	1:B:441:LEU:N	2.47	0.47
1:A:143:VAL:HG11	1:A:179:LEU:HD23	1.96	0.47
1:A:411:ALA:HB3	1:A:414:GLN:NE2	2.29	0.47
1:B:111:ASP:O	1:B:113:LYS:NZ	2.47	0.47
1:A:169:GLU:OE2	1:A:171:VAL:HG23	2.13	0.47
1:A:244:LEU:O	1:A:244:LEU:HD23	2.14	0.47
1:A:376:THR:HG22	1:A:435:ALA:HB3	1.96	0.47
1:B:676:THR:N	1:B:690:GLN:OE1	2.48	0.47
1:C:553:THR:HG22	1:C:554:GLU:N	2.29	0.47
1:A:87:ASN:OD1	1:A:87:ASN:O	2.33	0.47
1:B:1057:PRO:O	1:B:1058:HIS:HB2	2.13	0.47
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.43	0.47
1:A:339:GLY:N	3:A:1302:NAG:H82	2.30	0.47
1:C:315:THR:CG2	1:C:316:SER:H	2.20	0.47
1:C:916:LEU:C	1:C:916:LEU:HD23	2.39	0.47
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.79	0.47
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.48	0.47
1:B:312:ILE:O	1:B:312:ILE:HG23	2.14	0.47
1:C:632:THR:HG23	1:C:633:TRP:N	2.30	0.47
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.50	0.47
1:A:367:VAL:HG23	1:A:368:LEU:HD12	1.96	0.47
1:B:144:TYR:HD1	1:B:147:LYS:HZ3	1.62	0.47
1:A:101:ILE:HD13	1:A:242:LEU:HD13	1.97	0.47
1:A:553:THR:HG22	1:A:554:GLU:N	2.30	0.47
1:A:1141:LEU:O	1:A:1145:LEU:CB	2.63	0.47
1:B:87:ASN:OD1	1:B:87:ASN:O	2.32	0.47
1:B:377:PHE:HD1	1:B:434:ILE:HG12	1.80	0.46
1:C:29:THR:HG22	1:C:30:ASN:N	2.28	0.46
1:C:97:LYS:HD2	1:C:182:LYS:HA	1.96	0.46
1:A:298:GLU:OE2	1:A:316:SER:OG	2.28	0.46
1:A:620:VAL:N	1:A:621:PRO:CD	2.78	0.46
1:A:916:LEU:C	1:A:916:LEU:HD23	2.40	0.46
1:A:1101:HIS:CD2	2:M:1:NAG:H62	2.49	0.46
1:B:986:PRO:N	1:B:987:PRO:HD2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:1:NAG:HO3	2:e:2:NAG:C5	2.27	0.46
1:A:64:TRP:CD1	1:A:266:TYR:CE1	3.03	0.46
1:B:28:TYR:HB3	1:B:61:ASN:OD1	2.14	0.46
1:C:750:SER:O	1:C:754:LEU:HD12	2.16	0.46
1:C:452:LEU:H	1:C:452:LEU:HD23	1.81	0.46
1:A:1121:PHE:O	1:A:1122:VAL:C	2.58	0.46
1:B:18:LEU:H	1:B:18:LEU:HD23	1.79	0.46
1:B:326:ILE:HD11	1:B:533:LEU:HA	1.98	0.46
1:C:620:VAL:HG12	1:C:634:ARG:HH12	1.79	0.46
1:A:152:TRP:O	1:A:179:LEU:HD22	2.15	0.46
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.97	0.46
1:B:31:SER:OG	1:B:60:SER:OG	2.30	0.46
1:B:829:ALA:C	1:B:830:ASP:OD1	2.59	0.46
1:B:1133:VAL:HG22	1:B:1134:ASN:N	2.31	0.46
1:C:376:THR:CG2	1:C:435:ALA:HB3	2.46	0.46
1:B:144:TYR:HB2	1:B:153:MET:SD	2.56	0.46
1:C:92:PHE:HE1	1:C:94:SER:OG	1.99	0.45
1:C:144:TYR:HB2	1:C:153:MET:SD	2.56	0.45
1:C:851:CYS:HB3	1:C:855:PHE:CZ	2.50	0.45
1:A:312:ILE:O	1:A:312:ILE:HG23	2.17	0.45
1:B:829:ALA:O	1:B:830:ASP:OD1	2.34	0.45
1:C:134:GLN:O	1:C:161:SER:N	2.48	0.45
1:C:558:LYS:O	1:C:558:LYS:HG3	2.16	0.45
1:A:750:SER:O	1:A:754:LEU:HD12	2.16	0.45
1:B:178:ASP:C	1:B:179:LEU:HD12	2.42	0.45
1:B:736:VAL:HG22	1:B:858:LEU:HD22	1.98	0.45
1:C:64:TRP:CD1	1:C:266:TYR:CE1	3.04	0.45
1:C:216:LEU:HD12	1:C:217:PRO:HD3	1.97	0.45
1:C:1066:THR:HG22	1:C:1067:TYR:N	2.30	0.45
1:A:105:ILE:HD11	1:A:241:LEU:HD21	1.98	0.45
1:A:943:SER:O	1:A:943:SER:OG	2.30	0.45
1:B:96:GLU:OE2	1:B:101:ILE:HG13	2.17	0.45
1:B:181:GLY:C	1:B:182:LYS:HD2	2.40	0.45
1:C:117:LEU:HD23	1:C:118:LEU:N	2.31	0.45
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.82	0.45
1:A:616:ASN:O	1:A:616:ASN:OD1	2.34	0.45
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.52	0.45
1:A:282:ASN:OD1	1:A:282:ASN:O	2.35	0.45
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.32	0.45
1:B:47:VAL:HG22	1:B:48:LEU:N	2.31	0.45
1:C:440:ASN:OD1	1:C:441:LEU:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:1:NAG:H62	2:e:2:NAG:O7	2.16	0.45
1:A:850:ILE:HD12	1:A:850:ILE:H	1.81	0.45
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.99	0.45
1:B:912:THR:HG22	1:B:913:GLN:N	2.31	0.45
1:B:933:LYS:O	1:B:936:ASP:OD1	2.34	0.45
1:A:28:TYR:HB3	1:A:61:ASN:OD1	2.17	0.45
1:B:214:ARG:HG2	1:B:214:ARG:O	2.16	0.45
1:C:242:LEU:C	1:C:242:LEU:HD12	2.41	0.45
1:C:367:VAL:HG23	1:C:368:LEU:HD22	1.98	0.45
1:C:576:VAL:HG22	1:C:577:ARG:N	2.31	0.45
1:A:345:THR:O	1:A:346:ARG:NH2	2.49	0.45
1:B:29:THR:HG22	1:B:30:ASN:N	2.30	0.45
1:C:377:PHE:HD1	1:C:434:ILE:HG12	1.82	0.45
1:A:185:ASN:ND2	1:A:213:VAL:HG22	2.32	0.45
1:A:535:LYS:O	1:A:536:ASN:HB2	2.18	0.44
1:B:1105:THR:HG22	1:B:1106:GLN:N	2.32	0.44
1:C:319:ARG:O	1:C:630:THR:OG1	2.35	0.44
3:C:1304:NAG:C1	3:C:1304:NAG:H82	2.47	0.44
1:B:22:THR:N	1:B:77:LYS:O	2.49	0.44
1:C:14:GLN:CD	1:C:158:ARG:HE	2.26	0.44
1:A:738:CYS:O	1:A:741:TYR:N	2.50	0.44
1:C:83:VAL:HG23	1:C:83:VAL:O	2.16	0.44
1:A:914:ASN:C	1:A:914:ASN:HD22	2.24	0.44
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.33	0.44
1:A:178:ASP:OD1	1:A:179:LEU:N	2.50	0.44
1:C:125:ASN:OD1	1:C:125:ASN:O	2.36	0.44
1:A:440:ASN:OD1	1:A:441:LEU:N	2.50	0.44
1:A:745:ASP:OD1	1:A:745:ASP:O	2.36	0.44
1:B:331:ASN:HB3	3:B:1301:NAG:HN2	1.82	0.44
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.48	0.44
1:A:68:ILE:O	1:A:77:LYS:HB3	2.17	0.44
1:A:95:THR:HG23	1:A:186:PHE:HD2	1.83	0.44
1:A:122:ASN:O	1:A:177:MET:HE3	2.17	0.44
1:A:1122:VAL:O	1:A:1122:VAL:HG12	2.16	0.44
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.99	0.43
1:B:92:PHE:HE1	1:B:94:SER:OG	2.01	0.43
1:C:441:LEU:O	1:C:441:LEU:HD23	2.17	0.43
1:C:986:PRO:N	1:C:987:PRO:HD2	2.32	0.43
1:A:69:HIS:C	1:A:260:ALA:HB3	2.44	0.43
1:A:149:ASN:HD21	1:A:153:MET:CE	2.31	0.43
1:A:590:CYS:O	1:A:591:SER:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:PHE:C	1:A:1123:SER:H	2.26	0.43
1:B:442:ASP:OD1	1:B:443:SER:N	2.51	0.43
1:B:481:ASN:OD1	1:B:482:GLY:N	2.43	0.43
1:B:634:ARG:HG3	1:B:634:ARG:O	2.18	0.43
1:B:912:THR:OG1	1:B:1106:GLN:OE1	2.30	0.43
1:C:47:VAL:HG22	1:C:48:LEU:N	2.33	0.43
1:C:178:ASP:C	1:C:179:LEU:HD12	2.43	0.43
1:C:286:THR:O	1:C:287:ASP:OD1	2.36	0.43
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.52	0.43
1:B:95:THR:HG21	1:B:212:LEU:HD22	2.01	0.43
1:B:216:LEU:HD12	1:B:217:PRO:HD3	2.01	0.43
1:B:646:ARG:NH2	1:C:833:PHE:CD2	2.87	0.43
1:C:21:ARG:CD	1:C:79:PHE:HB3	2.46	0.43
1:A:851:CYS:O	1:A:855:PHE:CD2	2.72	0.43
1:C:392:PHE:CZ	1:C:515:PHE:CD2	3.06	0.43
1:A:178:ASP:C	1:A:179:LEU:HD12	2.44	0.43
1:A:560:LEU:N	1:A:563:GLN:OE1	2.37	0.43
1:A:634:ARG:O	1:A:635:VAL:HG13	2.18	0.43
1:B:145:TYR:CD2	1:B:145:TYR:O	2.71	0.43
1:B:156:GLU:HA	1:B:156:GLU:OE1	2.18	0.43
1:C:402:ILE:HG13	1:C:403:ARG:N	2.32	0.43
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.54	0.43
1:B:553:THR:HG22	1:B:554:GLU:N	2.33	0.43
1:C:207:HIS:O	1:C:208:THR:OG1	2.34	0.43
1:C:441:LEU:HD23	1:C:441:LEU:C	2.43	0.43
1:A:200:TYR:CD1	1:A:230:PRO:HA	2.54	0.43
1:A:447:GLY:HA2	1:A:497:PHE:O	2.18	0.43
1:B:453:TYR:CD1	1:B:495:TYR:CE2	3.06	0.43
1:C:157:PHE:C	1:C:158:ARG:HD2	2.44	0.43
1:A:833:PHE:CD2	1:C:646:ARG:NH2	2.87	0.43
3:A:1304:NAG:O7	3:A:1304:NAG:O3	2.31	0.43
1:B:623:ALA:C	1:B:634:ARG:HH22	2.26	0.43
2:M:1:NAG:H5	2:M:1:NAG:N2	2.34	0.43
1:B:157:PHE:C	1:B:158:ARG:HE	2.26	0.43
1:B:210:ILE:CD1	1:B:217:PRO:HG3	2.49	0.43
1:C:350:VAL:HG13	1:C:351:TYR:N	2.34	0.43
1:B:81:ASN:N	1:B:82:PRO:CD	2.82	0.43
1:B:517:LEU:HG	1:B:518:LEU:HG	2.00	0.43
1:B:189:LEU:HD22	1:B:217:PRO:HG2	2.01	0.42
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.97	0.42
1:C:149:ASN:OD1	1:C:149:ASN:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:LEU:HD22	1:C:210:ILE:HD13	2.00	0.42
2:K:1:NAG:O6	2:K:1:NAG:C1	2.67	0.42
1:A:1139:ASP:HB2	1:A:1142:GLN:N	2.34	0.42
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.54	0.42
1:B:294:ASP:HB2	1:B:295:PRO:CD	2.49	0.42
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.54	0.42
1:C:388:ASN:OD1	1:C:527:PRO:HD2	2.19	0.42
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.32	0.42
1:C:244:LEU:C	1:C:244:LEU:HD23	2.44	0.42
1:A:92:PHE:CD1	1:A:92:PHE:C	2.97	0.42
1:A:439:ASN:HA	1:A:507:PRO:HG2	2.00	0.42
1:A:454:ARG:NH2	1:A:469:SER:O	2.40	0.42
1:B:216:LEU:CD1	1:B:217:PRO:HD2	2.48	0.42
1:C:124:THR:HA	1:C:175:PHE:O	2.18	0.42
1:C:201:PHE:HE2	1:C:203:ILE:HD11	1.85	0.42
1:A:833:PHE:O	1:A:834:ILE:C	2.63	0.42
1:B:341:VAL:HG13	1:B:342:PHE:N	2.33	0.42
1:B:1133:VAL:HG22	1:B:1134:ASN:H	1.84	0.42
1:A:376:THR:O	1:A:376:THR:HG23	2.20	0.42
1:B:21:ARG:CD	1:B:79:PHE:HB2	2.50	0.42
1:B:326:ILE:CG2	1:B:541:PHE:HA	2.49	0.42
1:A:29:THR:HG22	1:A:30:ASN:N	2.30	0.42
1:A:228:ASP:O	1:A:229:LEU:HD23	2.20	0.42
1:B:53:ASP:CG	1:B:54:LEU:H	2.28	0.42
1:B:158:ARG:NE	1:B:158:ARG:HA	2.35	0.42
1:B:416:GLY:O	1:B:420:ASP:HB2	2.20	0.42
1:C:388:ASN:OD1	1:C:388:ASN:O	2.37	0.42
1:A:523:THR:OG1	1:A:524:VAL:HG23	2.19	0.42
1:B:142:GLY:CA	1:B:244:LEU:HB3	2.49	0.42
1:B:716:THR:O	1:B:716:THR:CG2	2.67	0.42
1:C:193:VAL:HG23	1:C:223:LEU:HD13	2.01	0.42
1:C:347:PHE:CE2	1:C:509:ARG:HD3	2.55	0.42
1:A:291:CYS:O	1:A:291:CYS:SG	2.78	0.42
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.02	0.42
1:C:135:PHE:HA	1:C:160:TYR:HA	2.02	0.42
1:C:227:VAL:HG12	1:C:228:ASP:N	2.34	0.42
1:A:14:GLN:HG3	1:A:158:ARG:HG2	2.02	0.42
1:A:403:ARG:HG2	1:A:404:GLY:N	2.35	0.42
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.55	0.41
1:B:21:ARG:HD3	1:B:79:PHE:HB2	2.00	0.41
1:B:244:LEU:HD23	1:B:244:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:THR:OG1	1:C:234:ASN:O	2.35	0.41
1:C:294:ASP:HB2	1:C:295:PRO:CD	2.50	0.41
1:C:639:GLY:O	1:C:640:SER:HB3	2.20	0.41
1:A:22:THR:HG22	1:A:23:GLN:N	2.36	0.41
1:A:95:THR:HG23	1:A:186:PHE:CD2	2.55	0.41
1:A:717:ASN:HB3	1:A:1070:ALA:HB3	2.02	0.41
1:A:382:VAL:HG12	1:A:383:SER:N	2.36	0.41
1:A:453:TYR:HD1	1:A:495:TYR:CE2	2.39	0.41
1:A:933:LYS:O	1:A:936:ASP:OD1	2.38	0.41
1:B:849:LEU:H	1:B:849:LEU:HD23	1.85	0.41
1:C:178:ASP:OD2	1:C:180:GLU:N	2.51	0.41
1:A:193:VAL:HG23	1:A:223:LEU:HD13	2.02	0.41
1:A:546:LEU:C	1:A:546:LEU:HD23	2.45	0.41
1:B:147:LYS:HG3	1:B:147:LYS:O	2.21	0.41
1:C:1138:TYR:OH	1:C:1143:PRO:HG3	2.20	0.41
1:A:524:VAL:O	1:A:525:CYS:HB3	2.20	0.41
1:B:993:ILE:O	1:B:997:ILE:HG13	2.20	0.41
1:C:126:VAL:HG23	1:C:175:PHE:CE2	2.55	0.41
1:C:376:THR:HG22	1:C:435:ALA:HB3	2.03	0.41
1:C:656:VAL:HG22	1:C:657:ASN:N	2.35	0.41
1:A:239:GLN:OE1	1:A:239:GLN:C	2.63	0.41
1:B:944:ALA:HB3	1:B:945:LEU:HD12	2.03	0.41
1:C:386:LYS:O	1:C:388:ASN:N	2.54	0.41
1:C:403:ARG:HG2	1:C:404:GLY:H	1.84	0.41
1:A:914:ASN:C	1:A:914:ASN:ND2	2.78	0.41
1:B:291:CYS:O	1:B:291:CYS:SG	2.78	0.41
1:A:394:ASN:OD1	1:A:516:GLU:OE1	2.39	0.41
1:A:736:VAL:HG22	1:A:858:LEU:HD22	2.02	0.41
1:A:851:CYS:HB3	1:A:855:PHE:HE2	1.85	0.41
1:A:1118:ASP:OD2	1:A:1140:PRO:CG	2.69	0.41
1:A:1121:PHE:C	1:A:1123:SER:N	2.76	0.41
1:A:1125:ASN:OD1	1:A:1126:CYS:N	2.54	0.41
1:B:109:THR:C	1:B:110:LEU:HD12	2.45	0.41
1:B:498:GLN:OE1	1:B:500:THR:HG22	2.21	0.41
1:B:576:VAL:HG22	1:B:577:ARG:N	2.36	0.41
1:C:28:TYR:HD2	3:C:1301:NAG:O5	2.03	0.41
1:C:97:LYS:HE2	1:C:183:GLN:HB3	2.02	0.41
1:A:286:THR:O	1:A:287:ASP:OD1	2.39	0.41
1:A:376:THR:CG2	1:A:435:ALA:HB3	2.50	0.41
1:A:636:TYR:CD2	1:A:651:ILE:HG22	2.56	0.41
1:A:1119:ASN:O	1:A:1119:ASN:OD1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:TYR:CD1	1:B:377:PHE:CE2	3.09	0.41
1:C:392:PHE:CE2	1:C:515:PHE:CD2	3.09	0.41
1:C:444:LYS:C	1:C:499:PRO:HD3	2.46	0.41
1:C:716:THR:O	1:C:716:THR:CG2	2.69	0.41
1:C:933:LYS:O	1:C:936:ASP:OD1	2.38	0.41
1:A:503:VAL:HA	1:A:506:GLN:HG2	2.03	0.40
1:B:96:GLU:HG2	1:B:263:ALA:HB1	2.03	0.40
1:B:189:LEU:HD23	1:B:208:THR:CG2	2.51	0.40
1:C:66:HIS:HE1	1:C:68:ILE:HD11	1.84	0.40
1:A:273:ARG:NH2	1:A:290:ASP:OD1	2.54	0.40
1:A:526:GLY:N	1:A:527:PRO:CD	2.84	0.40
1:B:95:THR:O	1:B:186:PHE:CD2	2.75	0.40
1:B:453:TYR:HD1	1:B:495:TYR:CE2	2.40	0.40
1:C:118:LEU:HD23	1:C:119:ILE:N	2.36	0.40
1:A:169:GLU:CD	1:A:170:TYR:N	2.80	0.40
1:A:986:PRO:N	1:A:987:PRO:HD2	2.36	0.40
1:B:58:PHE:CD2	1:B:290:ASP:HB2	2.57	0.40
1:B:377:PHE:CD1	1:B:434:ILE:HG12	2.56	0.40
1:B:826:VAL:HG12	1:B:828:LEU:HD12	2.02	0.40
1:C:68:ILE:HG22	1:C:69:HIS:HB2	2.03	0.40
1:A:57:PRO:HG3	1:A:273:ARG:HD3	2.04	0.40
1:A:80:ASP:OD2	1:A:82:PRO:HD3	2.22	0.40
1:A:475:ALA:HB3	1:A:487:ASN:O	2.22	0.40
1:A:826:VAL:HG12	1:A:828:LEU:HD12	2.02	0.40
1:C:53:ASP:CG	1:C:54:LEU:H	2.30	0.40
1:C:83:VAL:HG21	1:C:237:ARG:HH21	1.85	0.40
1:C:568:ASP:HB2	1:C:572:THR:O	2.21	0.40
1:C:943:SER:O	1:C:943:SER:OG	2.36	0.40
1:C:1038:LYS:O	1:C:1038:LYS:HG2	2.22	0.40
1:B:535:LYS:O	1:B:536:ASN:HB2	2.21	0.40
1:C:453:TYR:CD1	1:C:495:TYR:CE2	3.09	0.40
1:C:457:ARG:HG2	1:C:458:LYS:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1071/1234 (87%)	986 (92%)	84 (8%)	1 (0%)	48	80
1	B	1072/1234 (87%)	992 (92%)	80 (8%)	0	100	100
1	C	1075/1234 (87%)	987 (92%)	88 (8%)	0	100	100
All	All	3218/3702 (87%)	2965 (92%)	252 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1122	VAL

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	943/1072 (88%)	941 (100%)	2 (0%)	87	92
1	B	944/1072 (88%)	942 (100%)	2 (0%)	87	92
1	C	947/1072 (88%)	946 (100%)	1 (0%)	88	93
All	All	2834/3216 (88%)	2829 (100%)	5 (0%)	85	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	1098	ASN
1	B	69	HIS
1	B	196	ASN
1	C	1098	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	A	450	ASN
1	A	564	GLN
1	A	926	GLN
1	A	1011	GLN
1	A	1058	HIS
1	B	115	GLN
1	B	125	ASN
1	B	487	ASN
1	B	606	ASN
1	B	872	GLN
1	B	926	GLN
1	B	1011	GLN
1	C	125	ASN
1	C	149	ASN
1	C	185	ASN
1	C	439	ASN
1	C	564	GLN
1	C	613	GLN
1	C	901	GLN
1	C	1011	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	K	1	2,1	14,14,15	0.40	0	17,19,21	1.10	1 (5%)
2	NAG	K	2	2	14,14,15	0.81	1 (7%)	17,19,21	0.48	0
2	NAG	M	1	2,1	14,14,15	0.82	0	17,19,21	0.78	1 (5%)
2	NAG	M	2	2	14,14,15	0.46	0	17,19,21	0.55	0
2	NAG	U	1	2,1	14,14,15	0.42	0	17,19,21	0.52	0
2	NAG	U	2	2	14,14,15	0.35	0	17,19,21	0.41	0
2	NAG	V	1	2,1	14,14,15	0.23	0	17,19,21	0.63	0
2	NAG	V	2	2	14,14,15	0.33	0	17,19,21	0.39	0
2	NAG	X	1	2,1	14,14,15	1.94	2 (14%)	17,19,21	1.31	2 (11%)
2	NAG	X	2	2	14,14,15	0.56	0	17,19,21	0.45	0
2	NAG	e	1	2,1	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
2	NAG	e	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.94	1 (5%)
2	NAG	f	1	2,1	14,14,15	0.65	1 (7%)	17,19,21	0.49	0
2	NAG	f	2	2	14,14,15	0.48	0	17,19,21	0.52	0
2	NAG	g	1	2,1	14,14,15	0.45	0	17,19,21	0.50	0
2	NAG	g	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	h	1	2,1	14,14,15	0.29	0	17,19,21	0.41	0
2	NAG	h	2	2	14,14,15	0.22	0	17,19,21	0.52	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	K	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	2/6/23/26	0/1/1/1
2	NAG	e	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	e	2	2	-	4/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	g	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	NAG	h	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	h	2	2	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1	NAG	O5-C1	-6.46	1.32	1.43
2	e	2	NAG	O5-C1	-3.57	1.37	1.43
2	X	1	NAG	C1-C2	-3.08	1.48	1.52
2	e	2	NAG	C1-C2	3.01	1.56	1.52
2	f	1	NAG	O5-C1	-2.26	1.39	1.43
2	K	2	NAG	O5-C1	-2.04	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C1-O5-C5	4.15	117.74	112.19
2	X	1	NAG	C3-C4-C5	3.63	116.82	110.23
2	e	1	NAG	C1-O5-C5	2.88	116.05	112.19
2	e	2	NAG	C4-C3-C2	2.60	114.82	111.02
2	X	1	NAG	C1-O5-C5	-2.32	109.08	112.19
2	M	1	NAG	C1-O5-C5	2.19	115.12	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C1-C2-N2-C7
2	e	2	NAG	C1-C2-N2-C7
2	e	2	NAG	O5-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	g	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

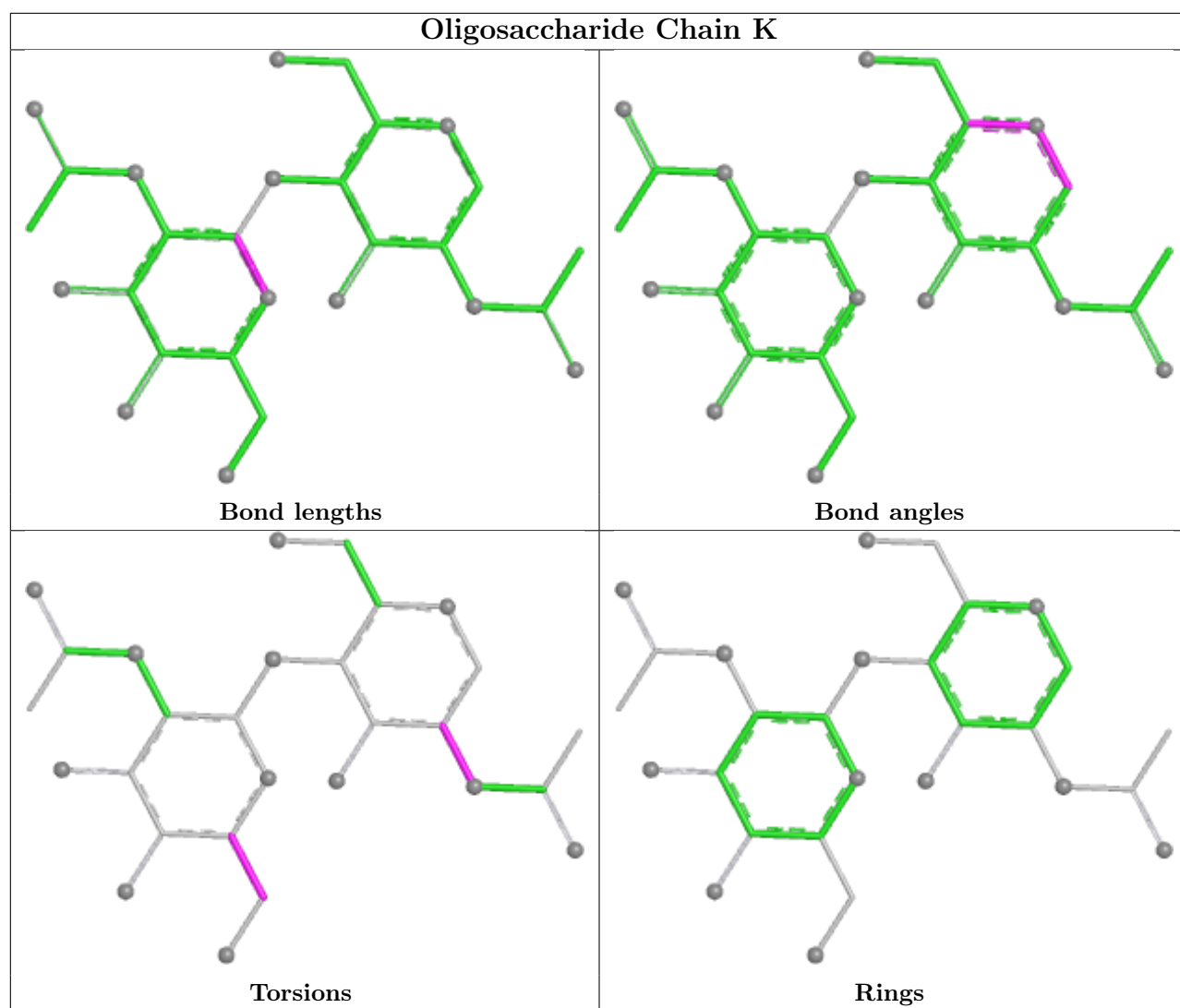
Mol	Chain	Res	Type	Atoms
2	g	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	X	1	NAG	C4-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	e	2	NAG	C3-C2-N2-C7
2	M	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
2	V	1	NAG	C3-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7

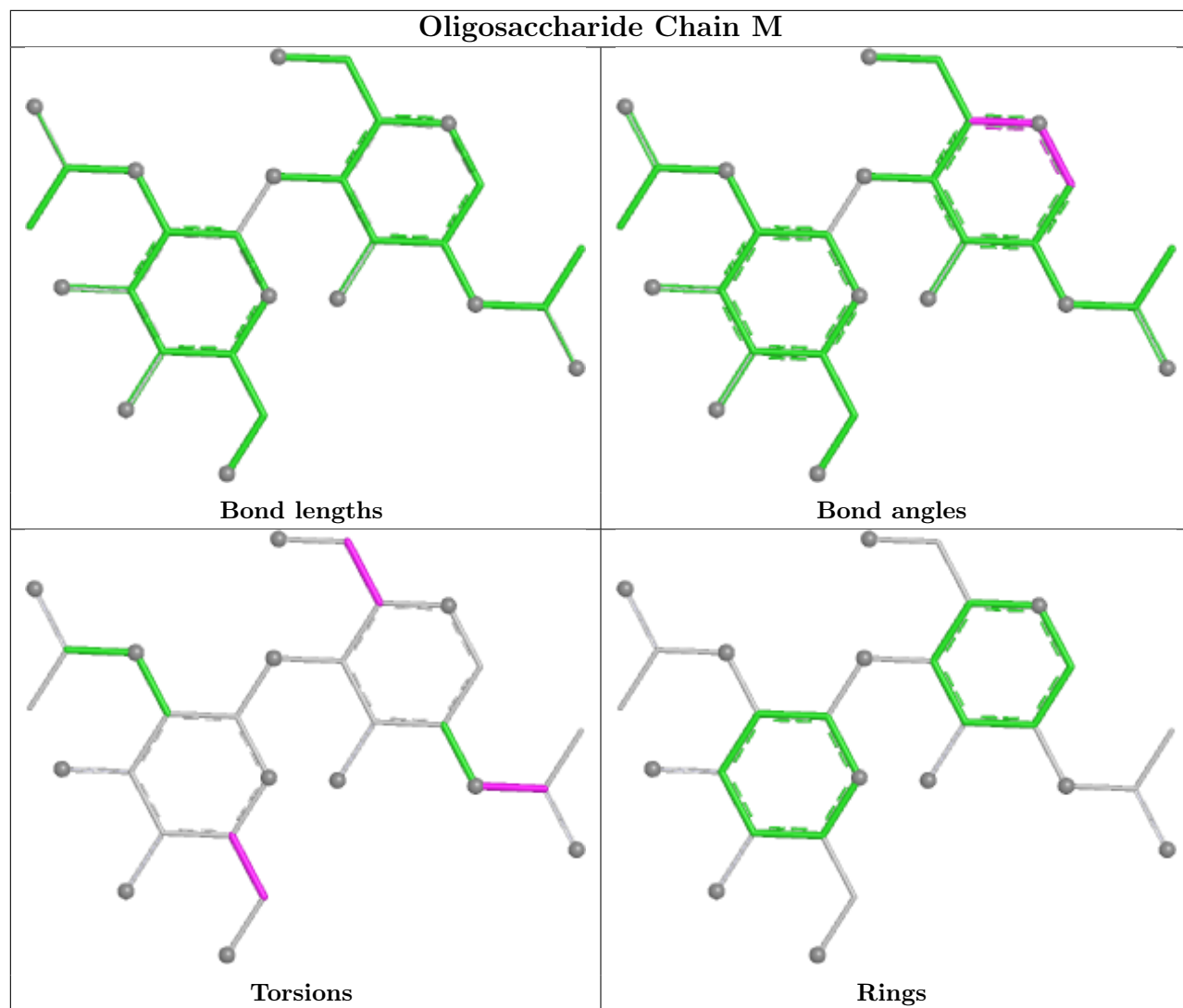
There are no ring outliers.

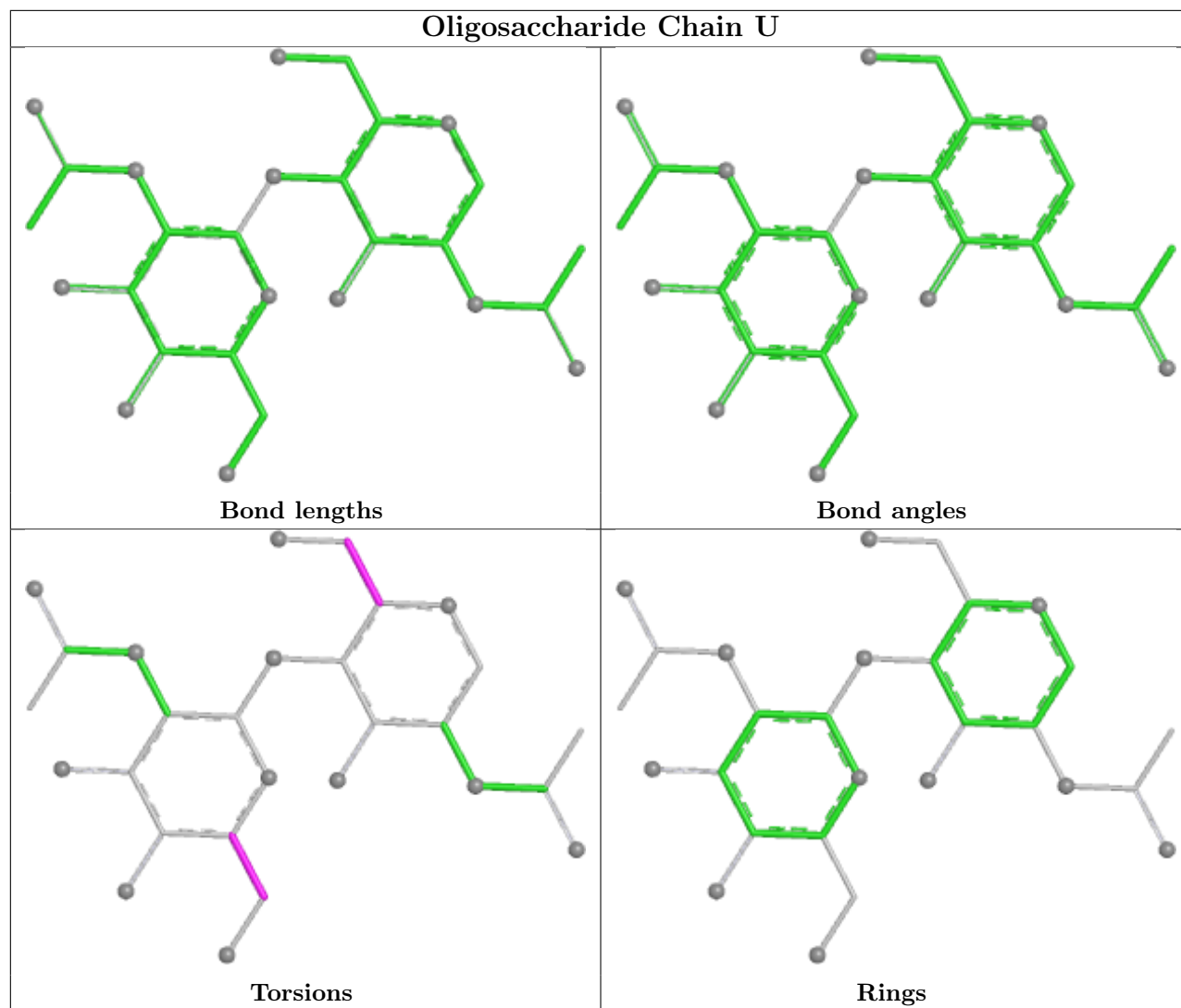
6 monomers are involved in 12 short contacts:

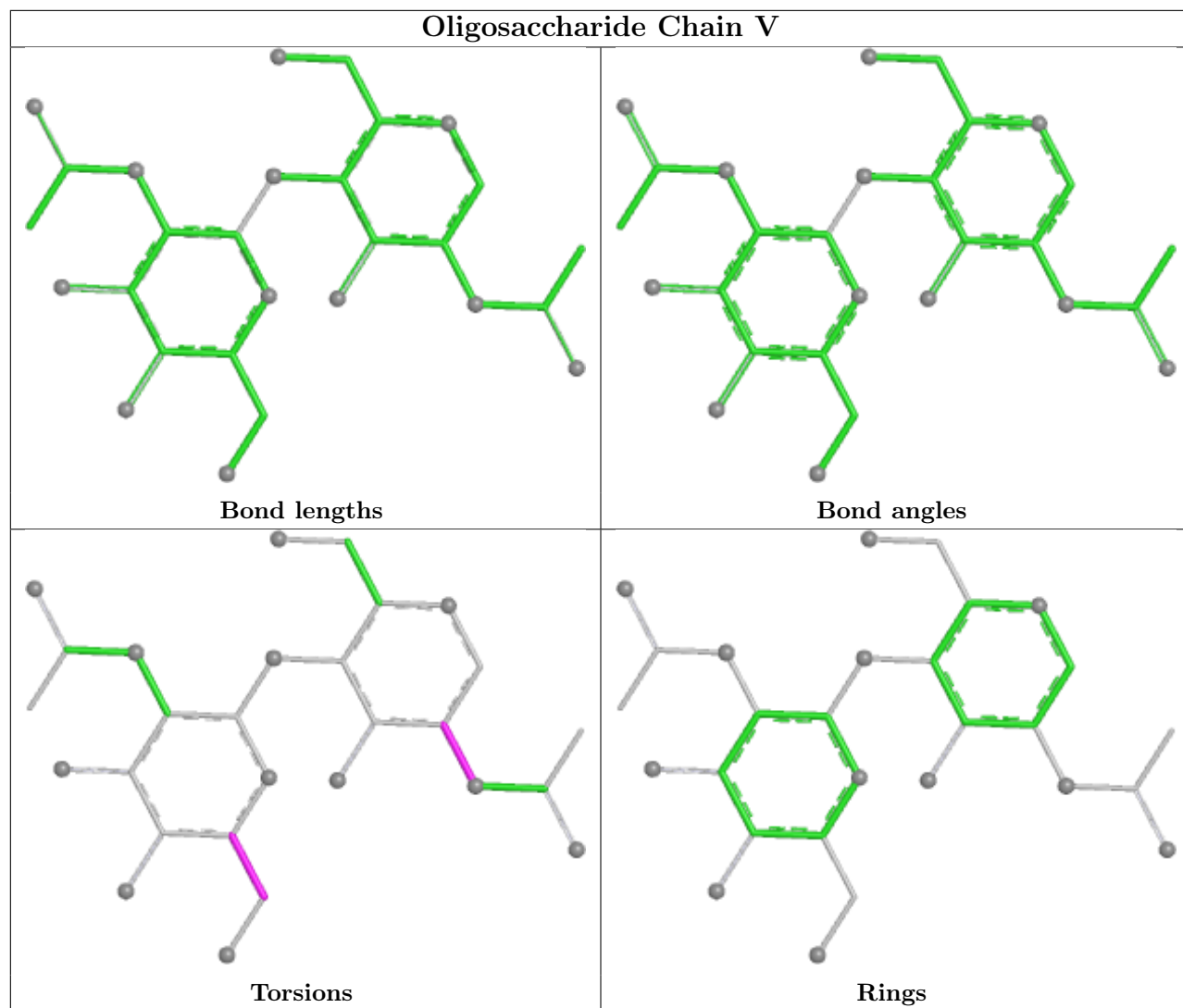
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	3	0
2	e	1	NAG	6	0
2	K	2	NAG	1	0
2	M	1	NAG	2	0
2	g	1	NAG	1	0
2	e	2	NAG	6	0

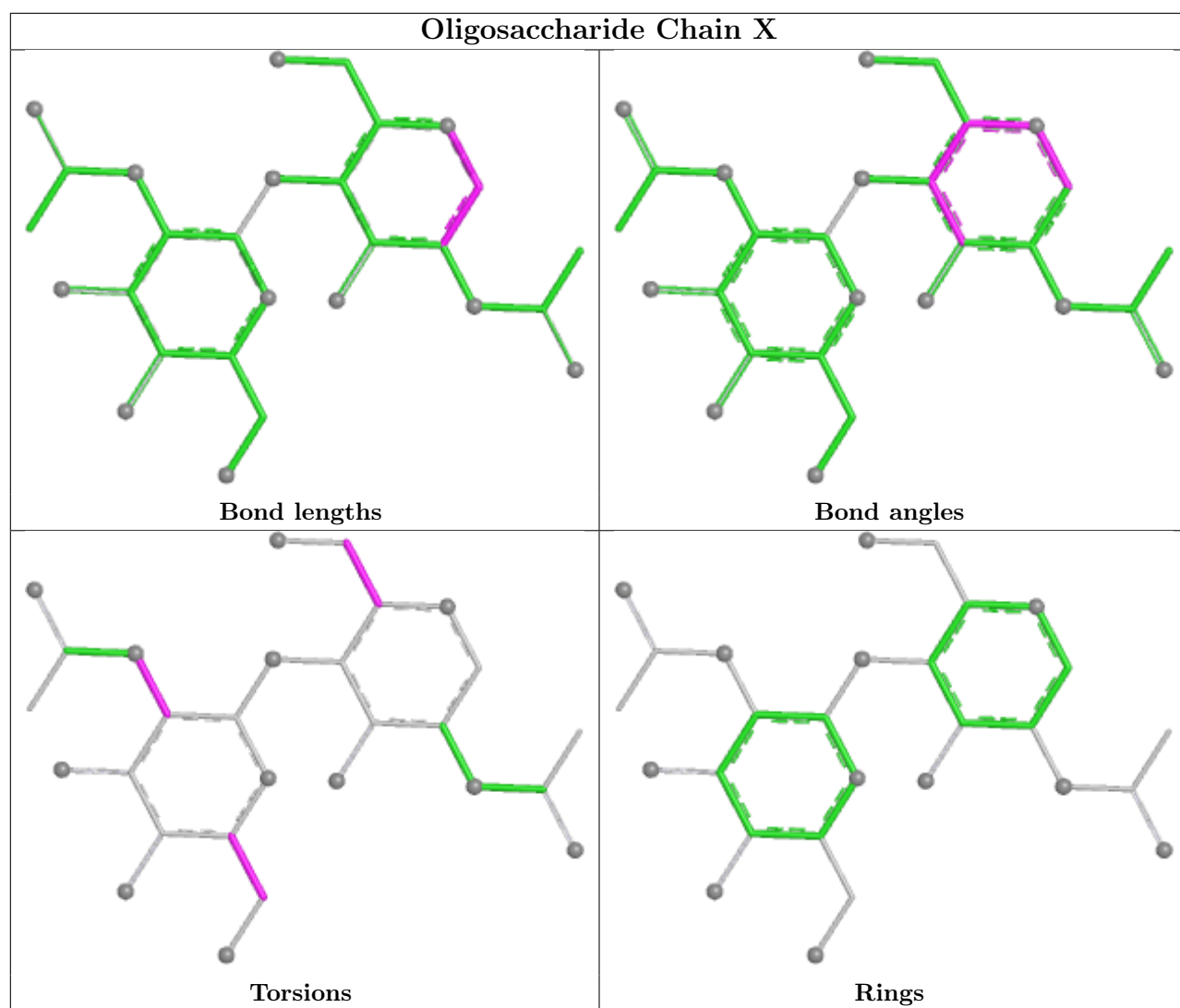
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

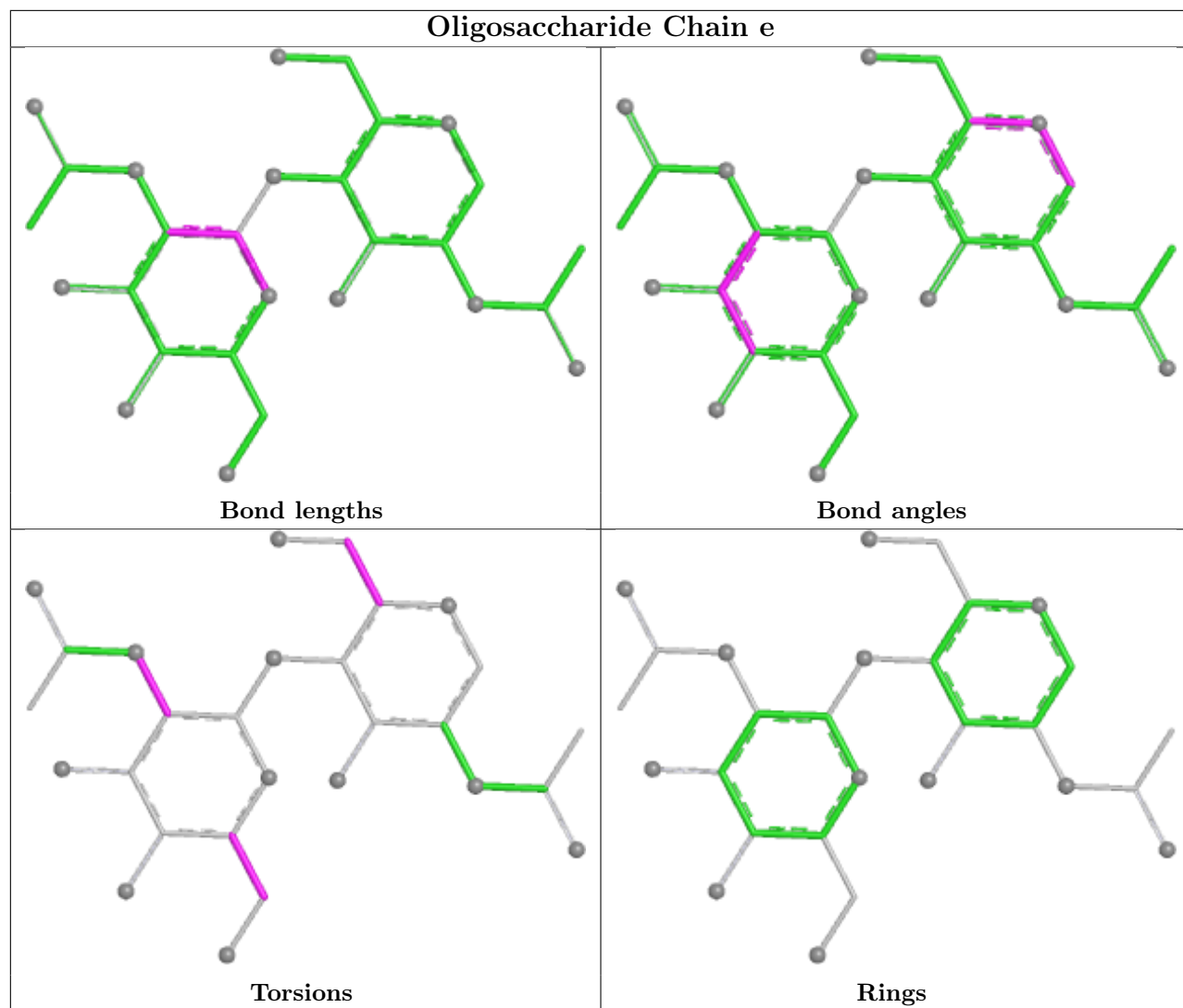


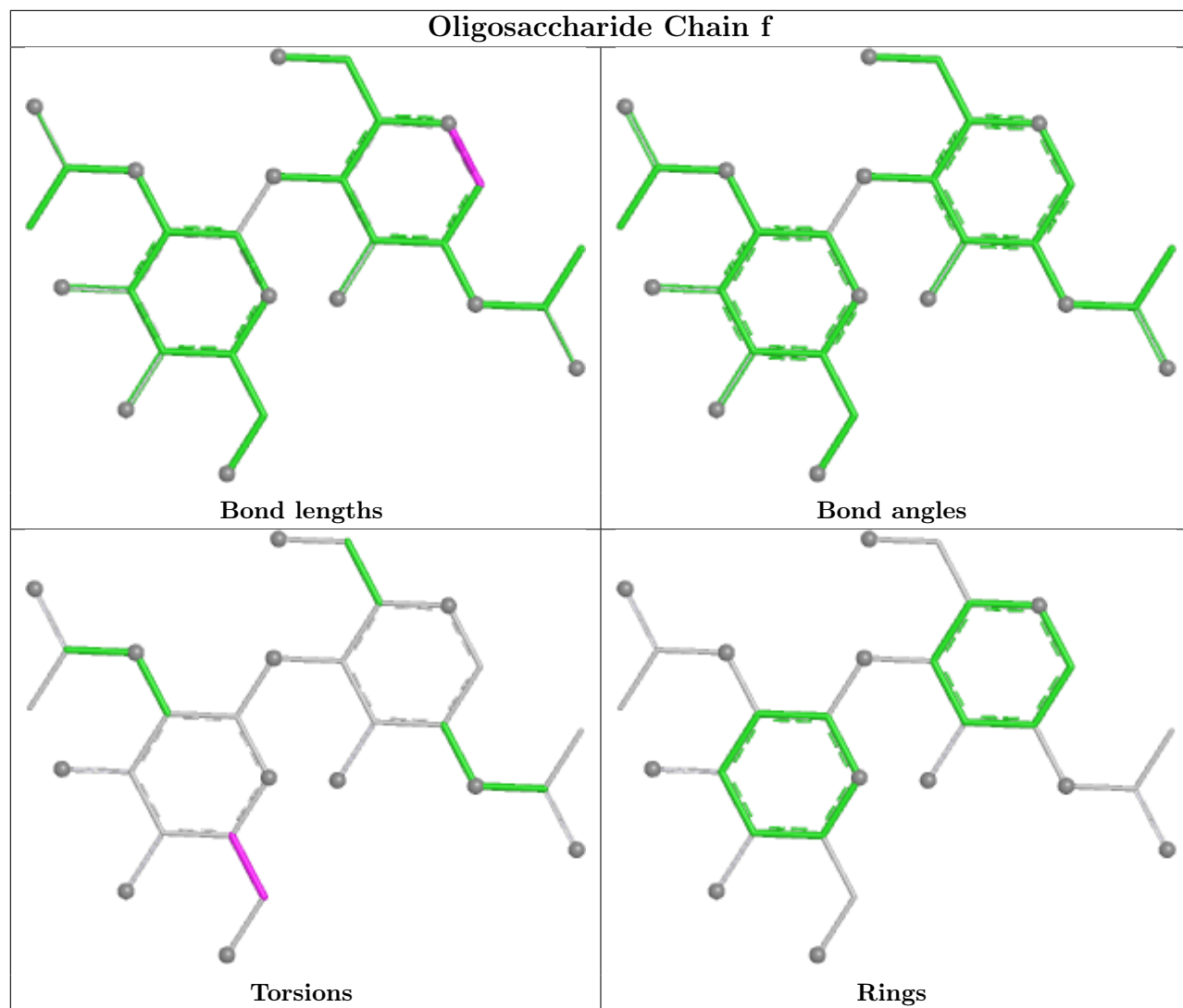


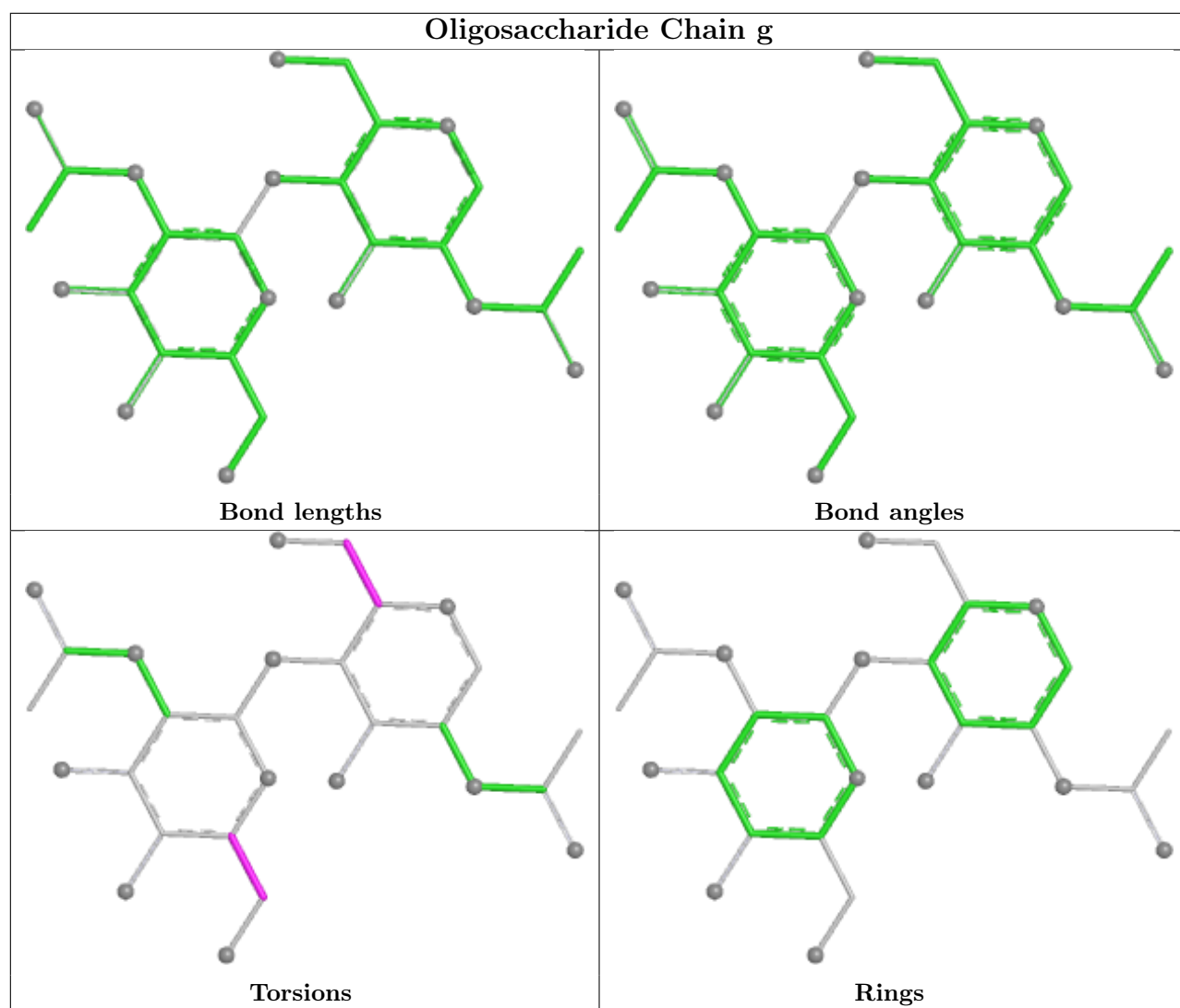


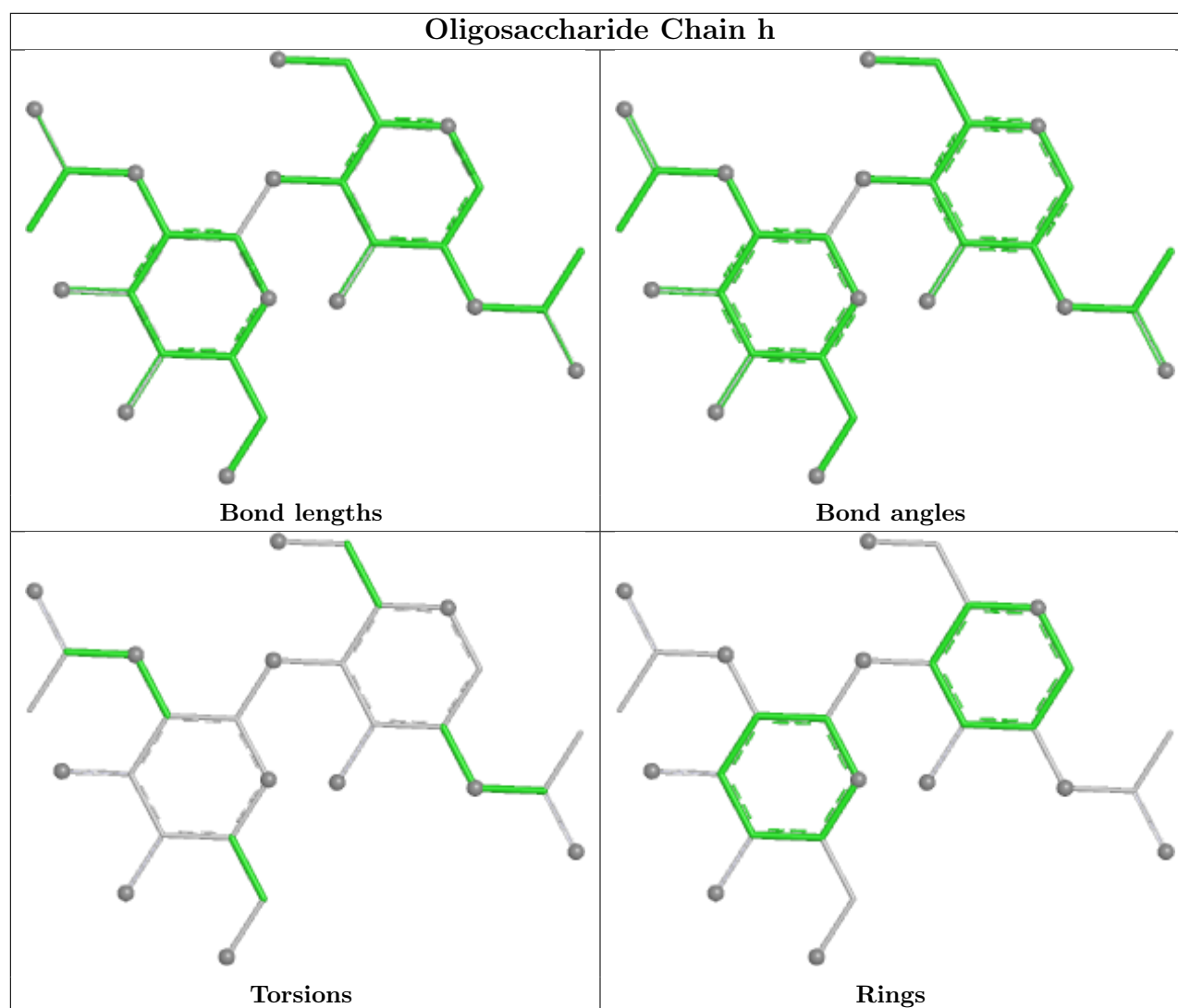












5.6 Ligand geometry [i](#)

24 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	C	1303	1	14,14,15	0.40	0	17,19,21	0.40	0
3	NAG	B	1308	1	14,14,15	0.25	0	17,19,21	0.62	1 (5%)
3	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1302	1	14,14,15	0.28	0	17,19,21	0.42	0
3	NAG	B	1303	1	14,14,15	0.76	1 (7%)	17,19,21	1.06	1 (5%)
3	NAG	B	1304	1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	C	1308	-	14,14,15	0.40	0	17,19,21	0.38	0
3	NAG	B	1310	1	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
3	NAG	B	1306	1	14,14,15	0.23	0	17,19,21	0.37	0
3	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	B	1301	1	14,14,15	0.30	0	17,19,21	0.58	0
3	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.57	0
3	NAG	B	1305	1	14,14,15	0.40	0	17,19,21	0.39	0
3	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.56	0
3	NAG	A	1301	1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	A	1304	-	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	C	1307	1	14,14,15	0.38	0	17,19,21	0.52	0
3	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.42	0
3	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	B	1302	1	14,14,15	0.30	0	17,19,21	0.36	0
3	NAG	B	1307	1	14,14,15	0.70	1 (7%)	17,19,21	0.48	0
3	NAG	C	1304	1	14,14,15	0.38	0	17,19,21	0.94	1 (5%)
3	NAG	A	1305	1	14,14,15	0.64	1 (7%)	17,19,21	0.57	0
3	NAG	C	1306	1	14,14,15	0.20	0	17,19,21	0.44	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	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1303	NAG	O5-C1	2.52	1.47	1.43
3	B	1307	NAG	O5-C1	-2.31	1.39	1.43
3	A	1305	NAG	O5-C1	-2.18	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1303	NAG	C1-O5-C5	4.10	117.68	112.19
3	B	1310	NAG	C1-O5-C5	3.84	117.33	112.19
3	C	1304	NAG	C2-N2-C7	2.76	126.60	122.90
3	B	1308	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1307	NAG	C3-C2-N2-C7
3	C	1308	NAG	C3-C2-N2-C7
3	C	1303	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1303	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	C	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
3	A	1301	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1305	NAG	C3-C2-N2-C7
3	B	1302	NAG	C4-C5-C6-O6
3	B	1307	NAG	C1-C2-N2-C7
3	C	1304	NAG	C1-C2-N2-C7
3	C	1308	NAG	C1-C2-N2-C7
3	A	1303	NAG	O5-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	A	1304	NAG	C3-C2-N2-C7
3	B	1307	NAG	C3-C2-N2-C7
3	C	1304	NAG	C3-C2-N2-C7
3	B	1310	NAG	C4-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 11 short contacts:

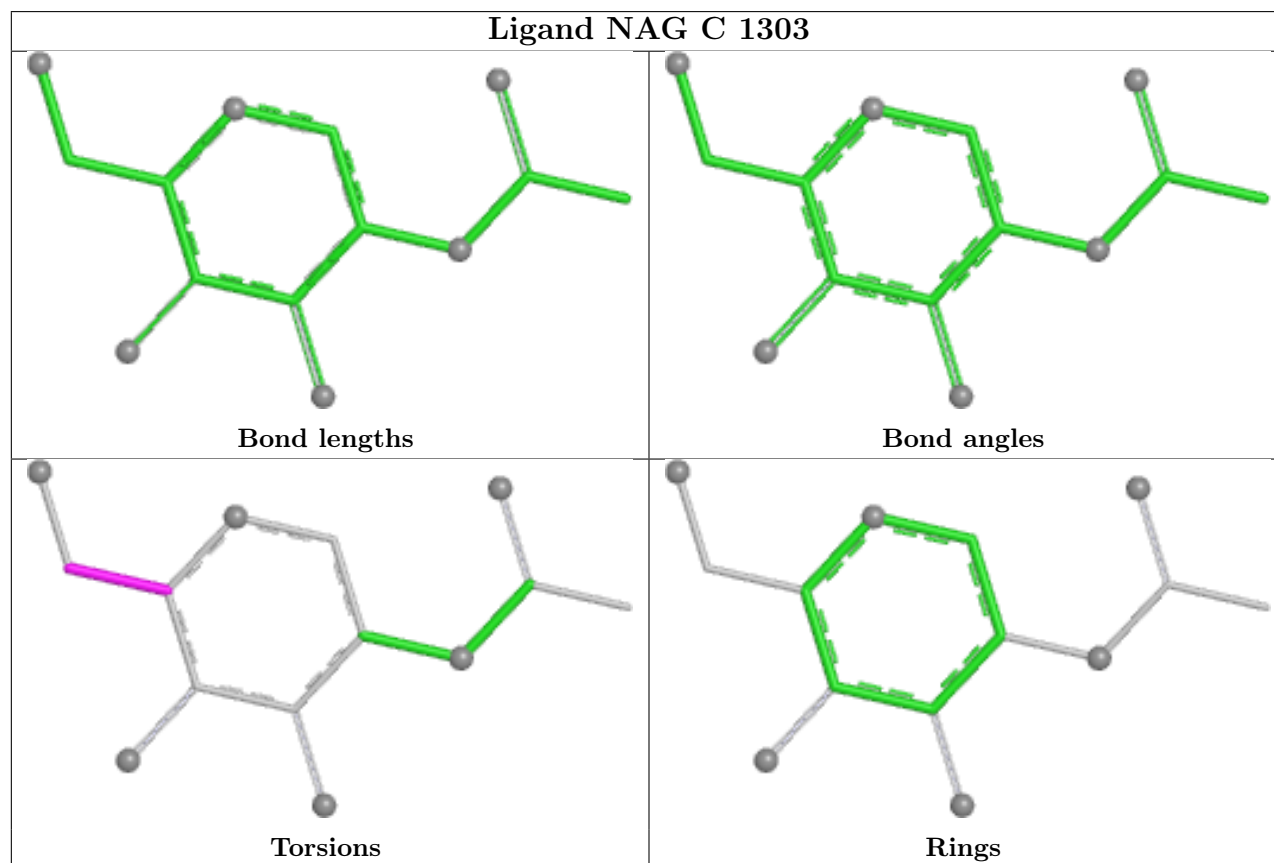
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	NAG	1	0
3	C	1308	NAG	1	0
3	B	1310	NAG	1	0

Continued on next page...

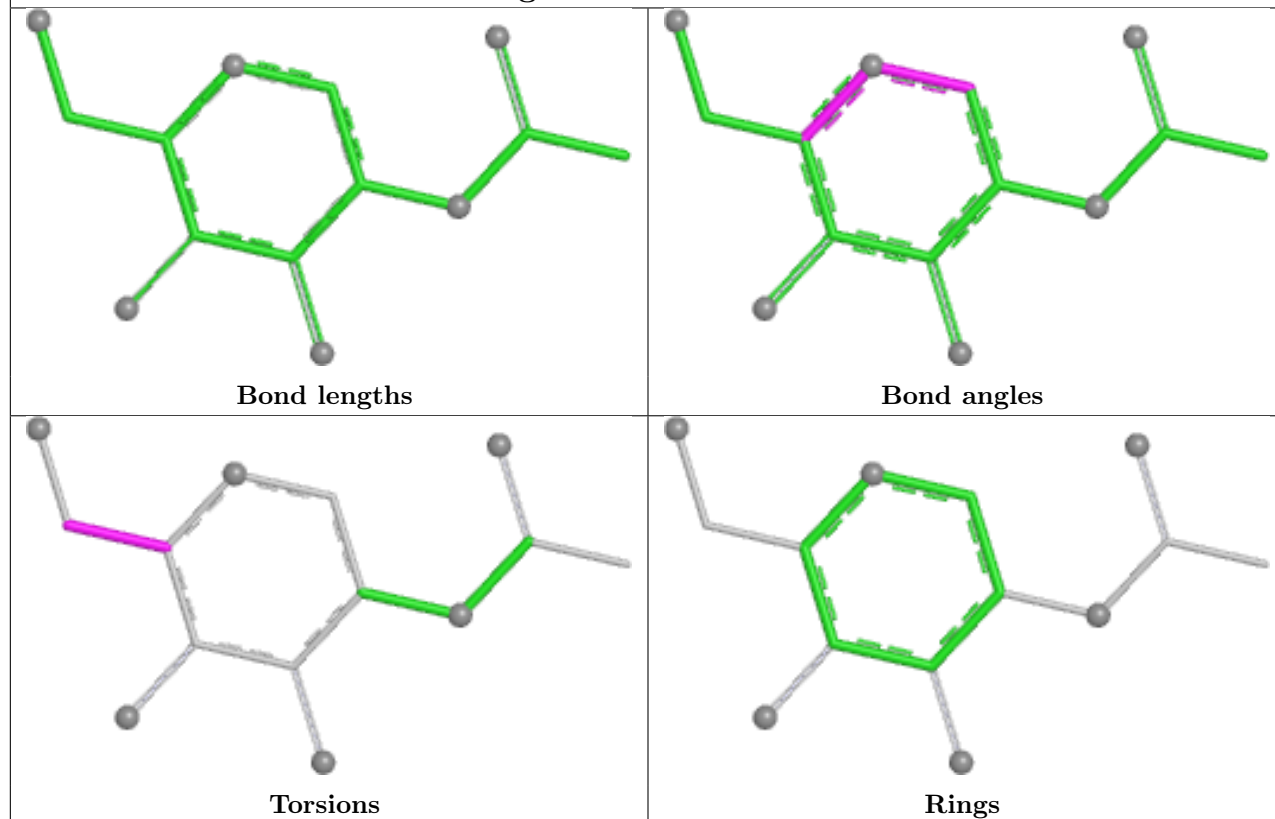
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	NAG	1	0
3	A	1302	NAG	1	0
3	A	1301	NAG	1	0
3	A	1304	NAG	1	0
3	C	1304	NAG	2	0
3	A	1305	NAG	2	0

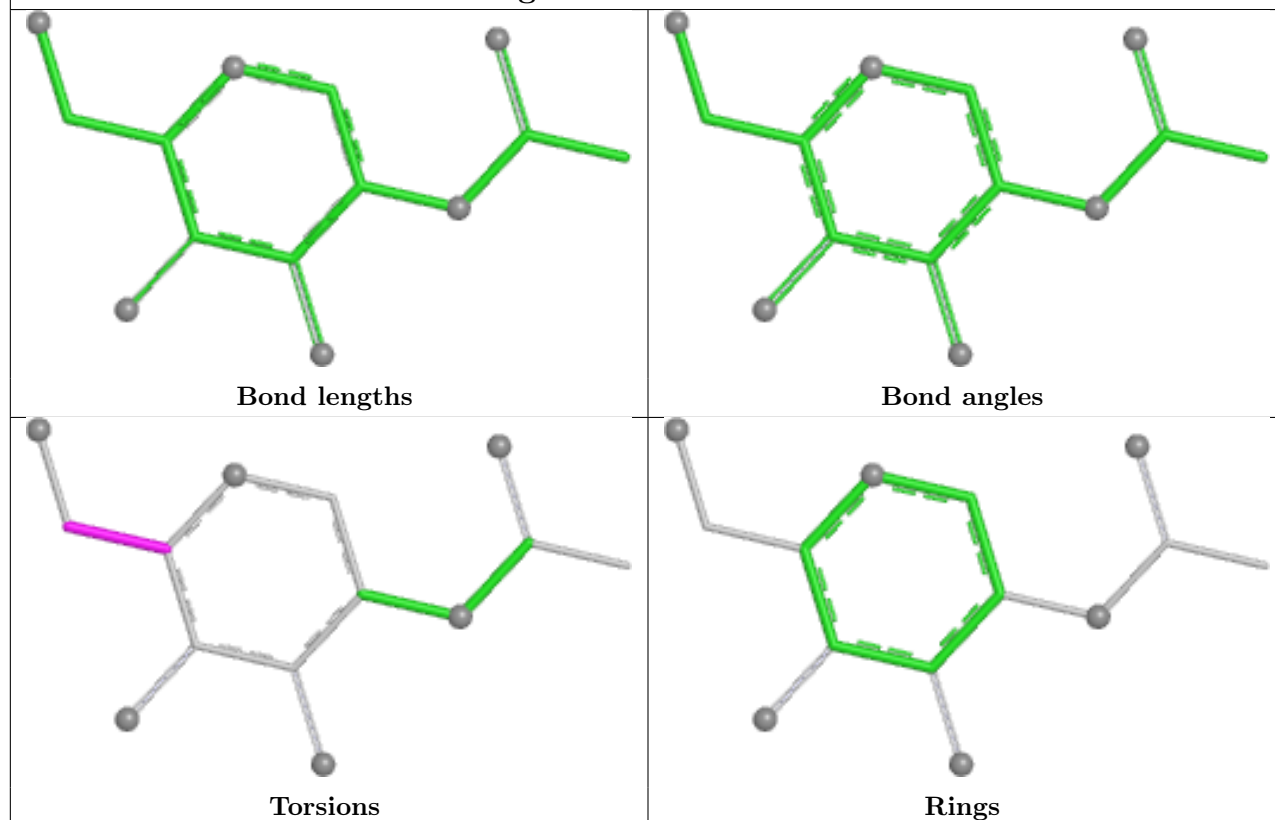
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

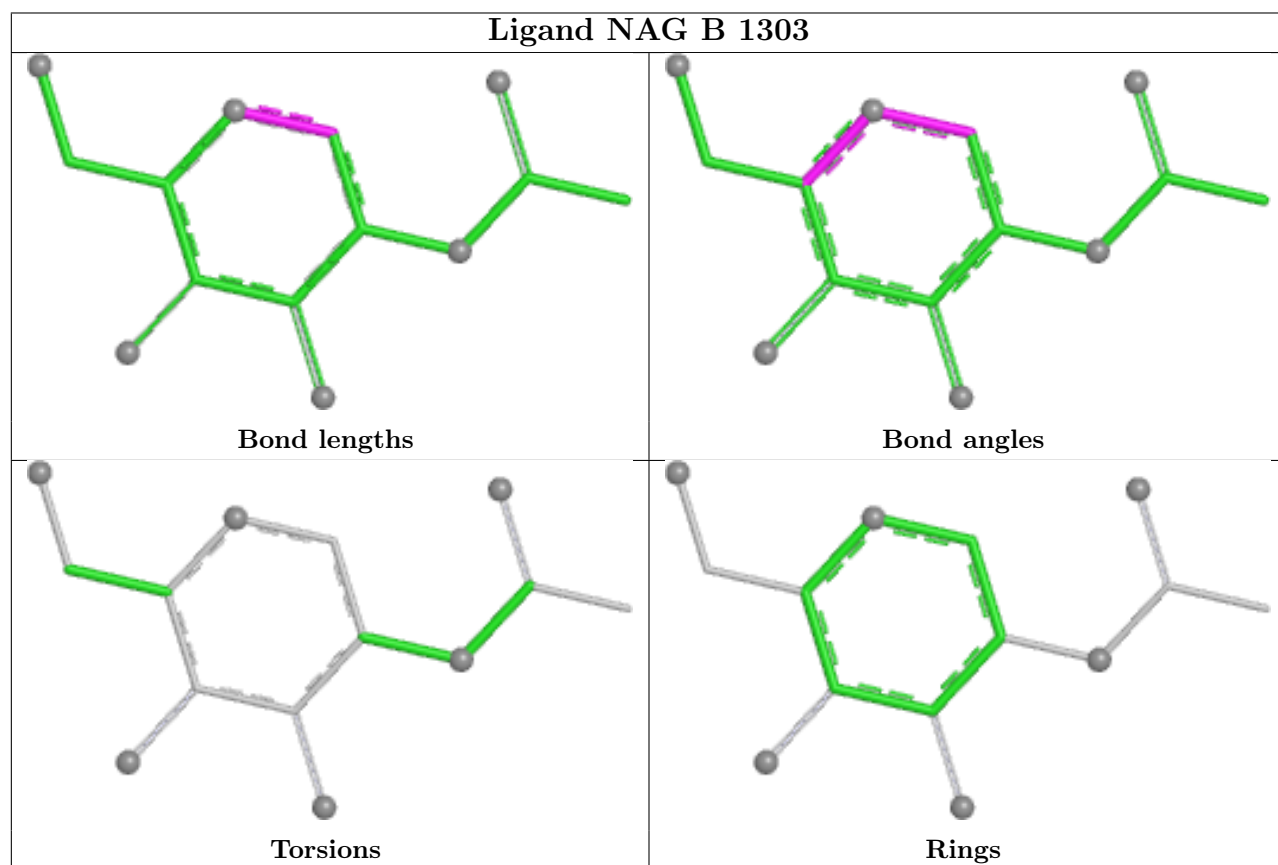
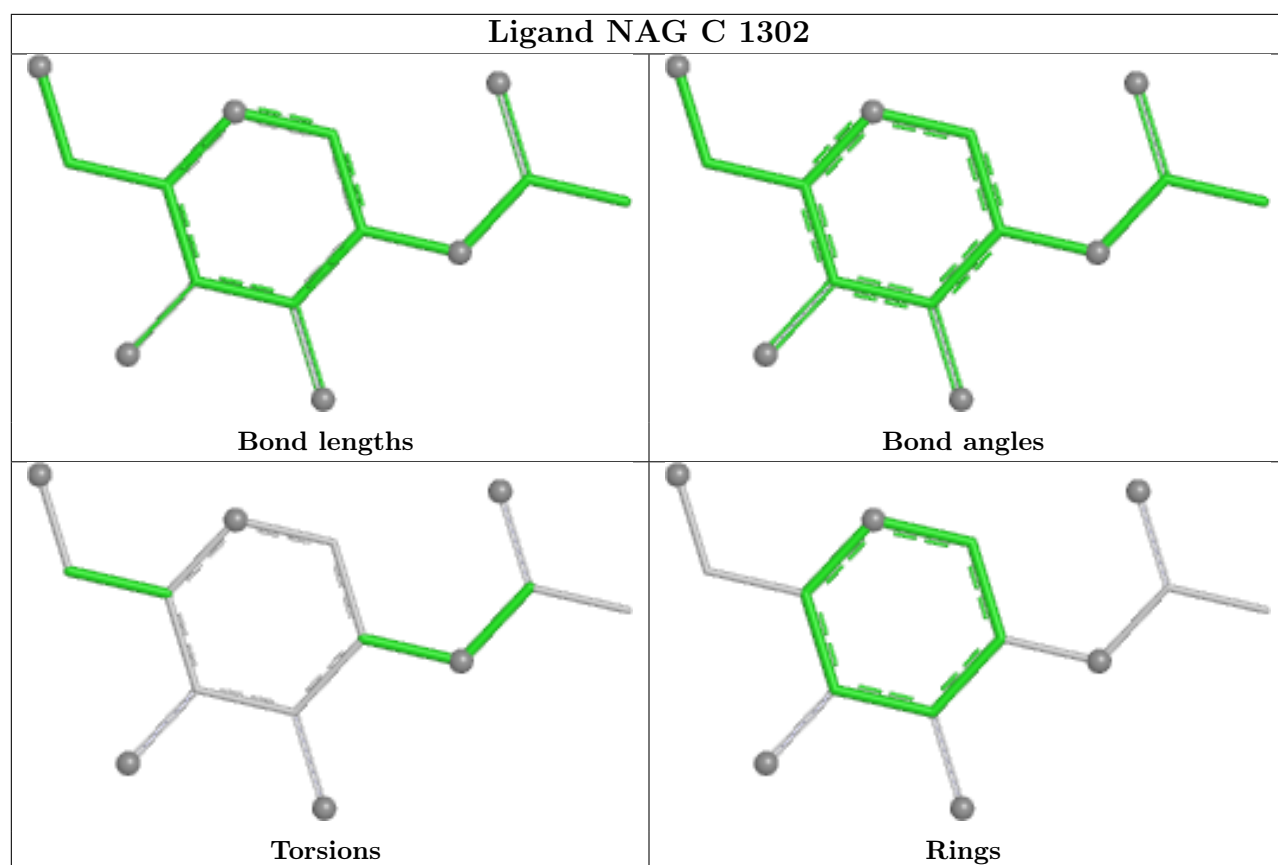


Ligand NAG B 1308

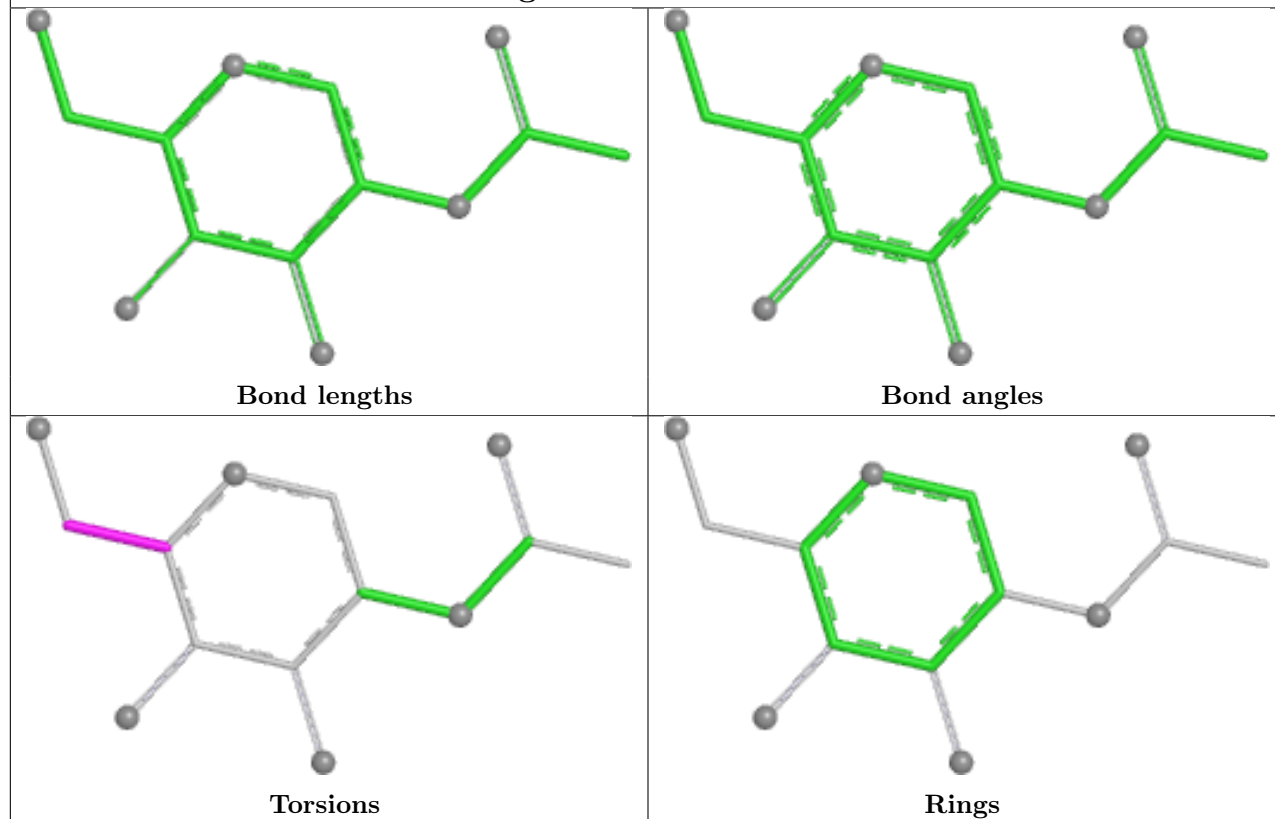


Ligand NAG C 1301

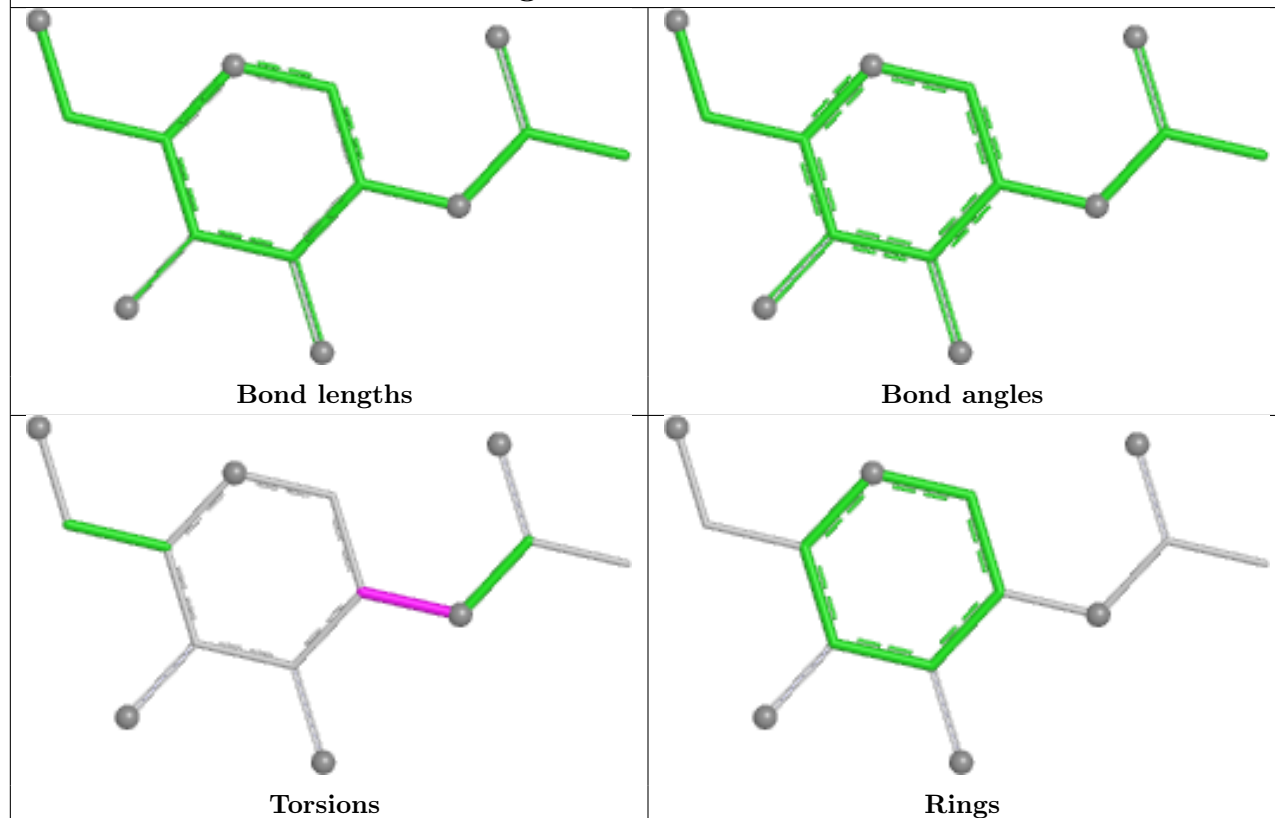




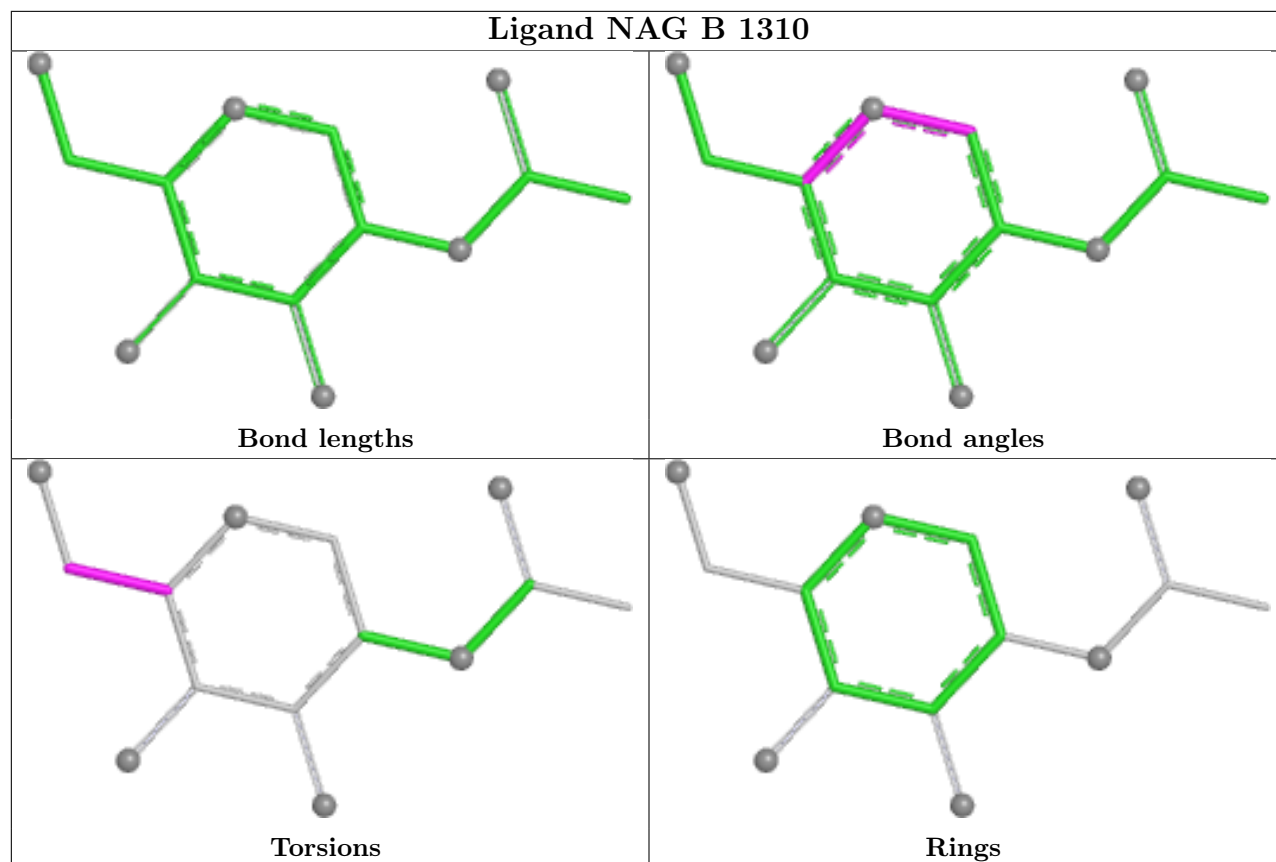
Ligand NAG B 1304



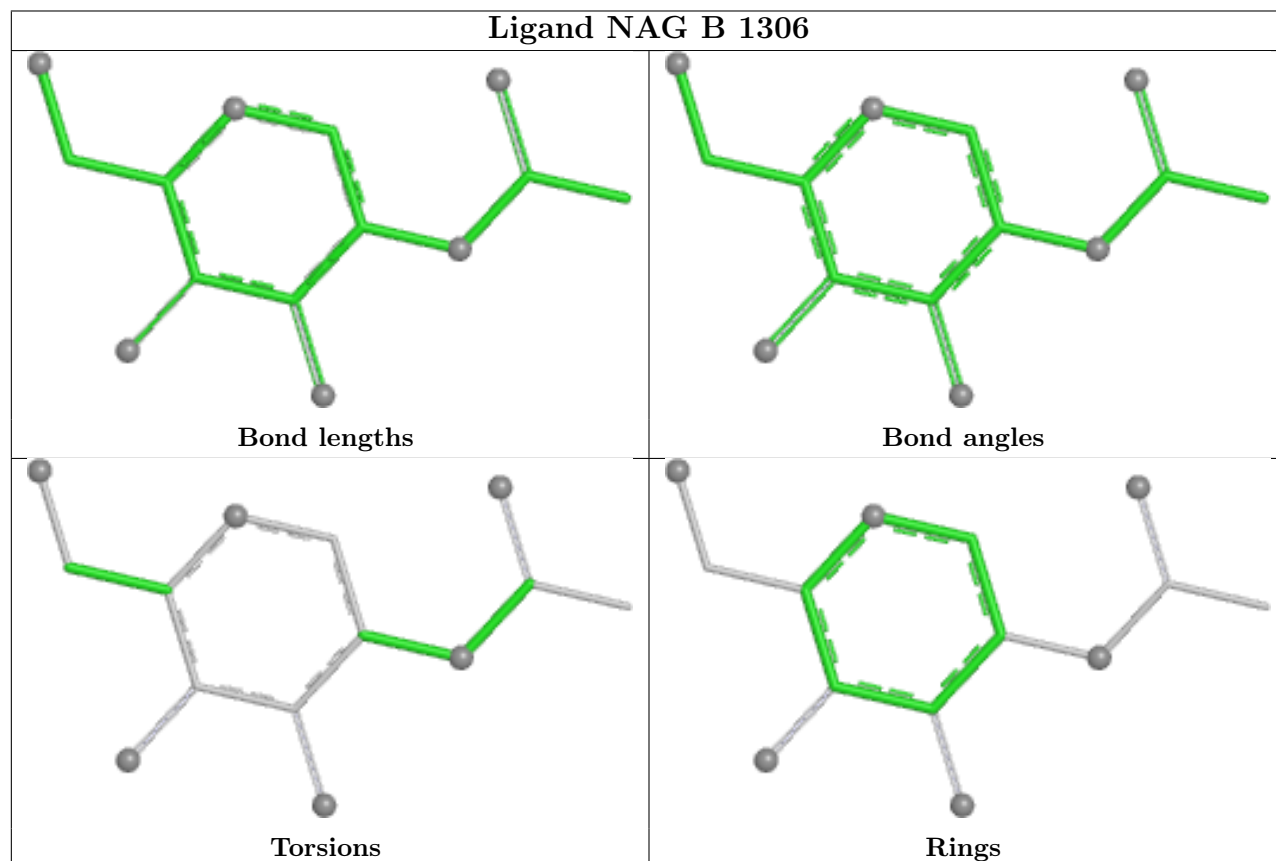
Ligand NAG C 1308

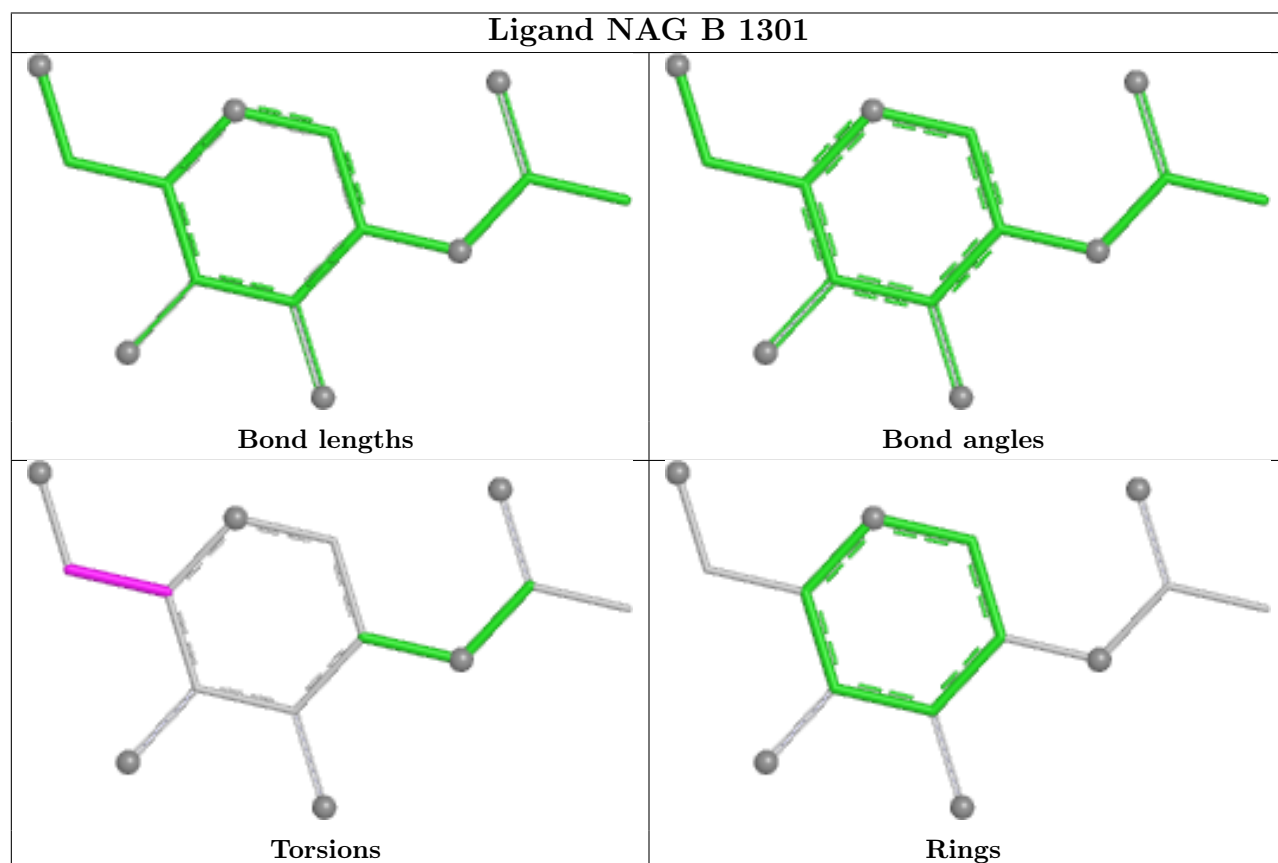
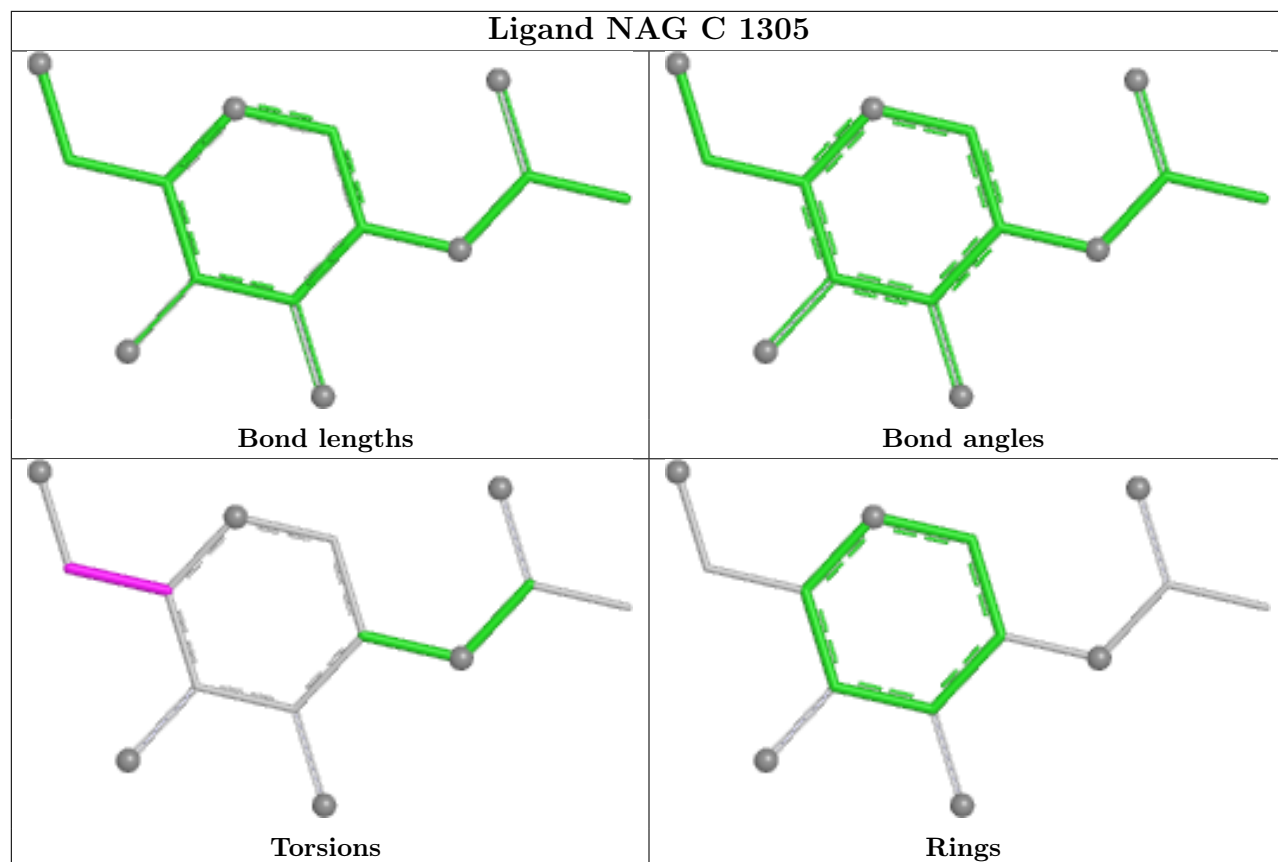


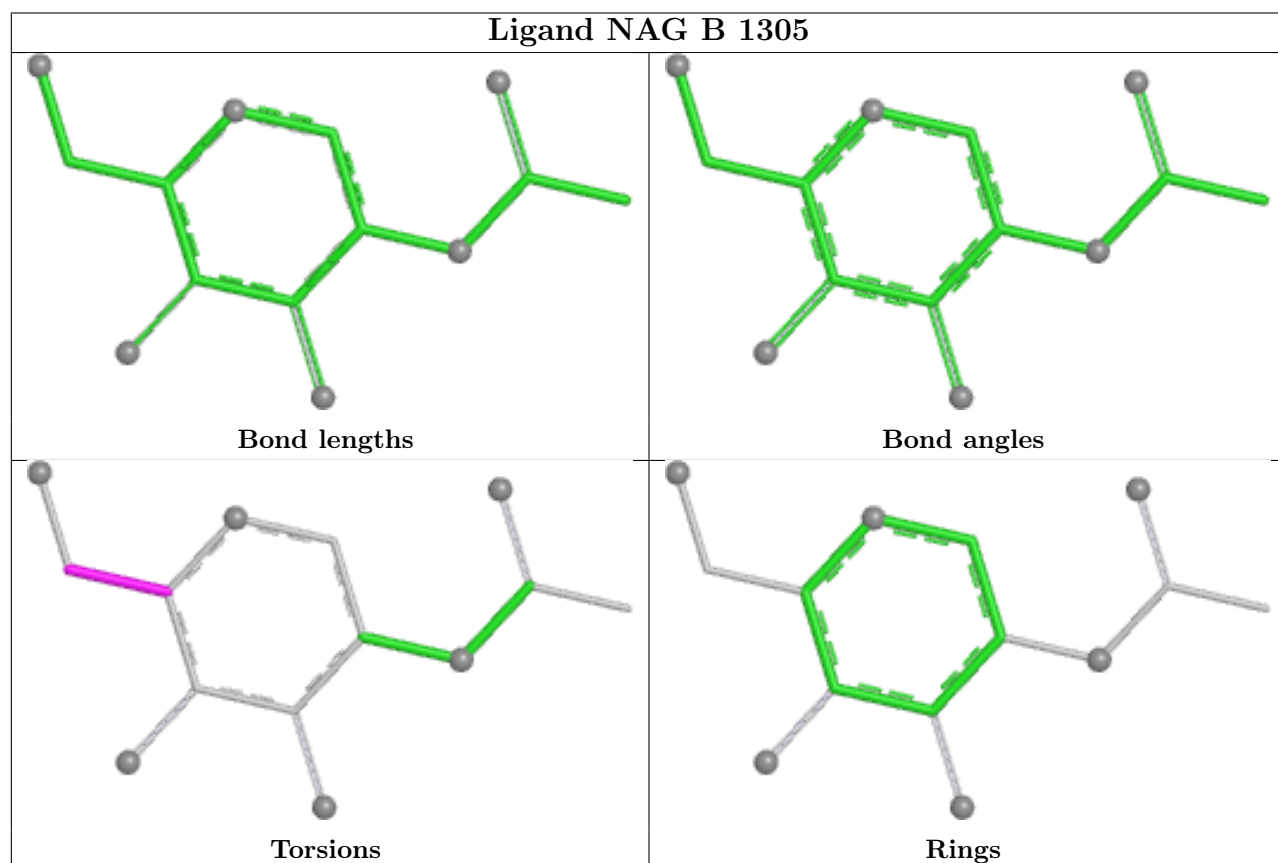
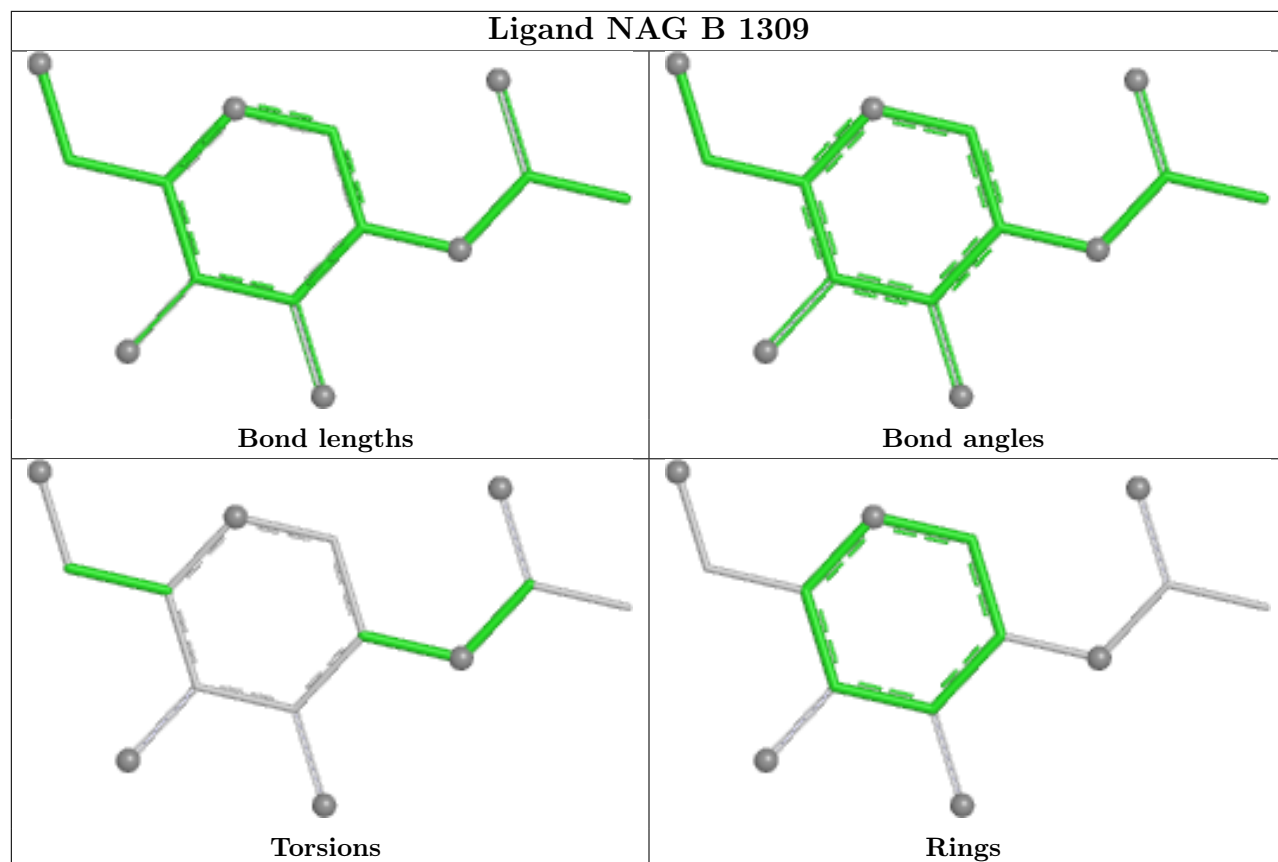
Ligand NAG B 1310



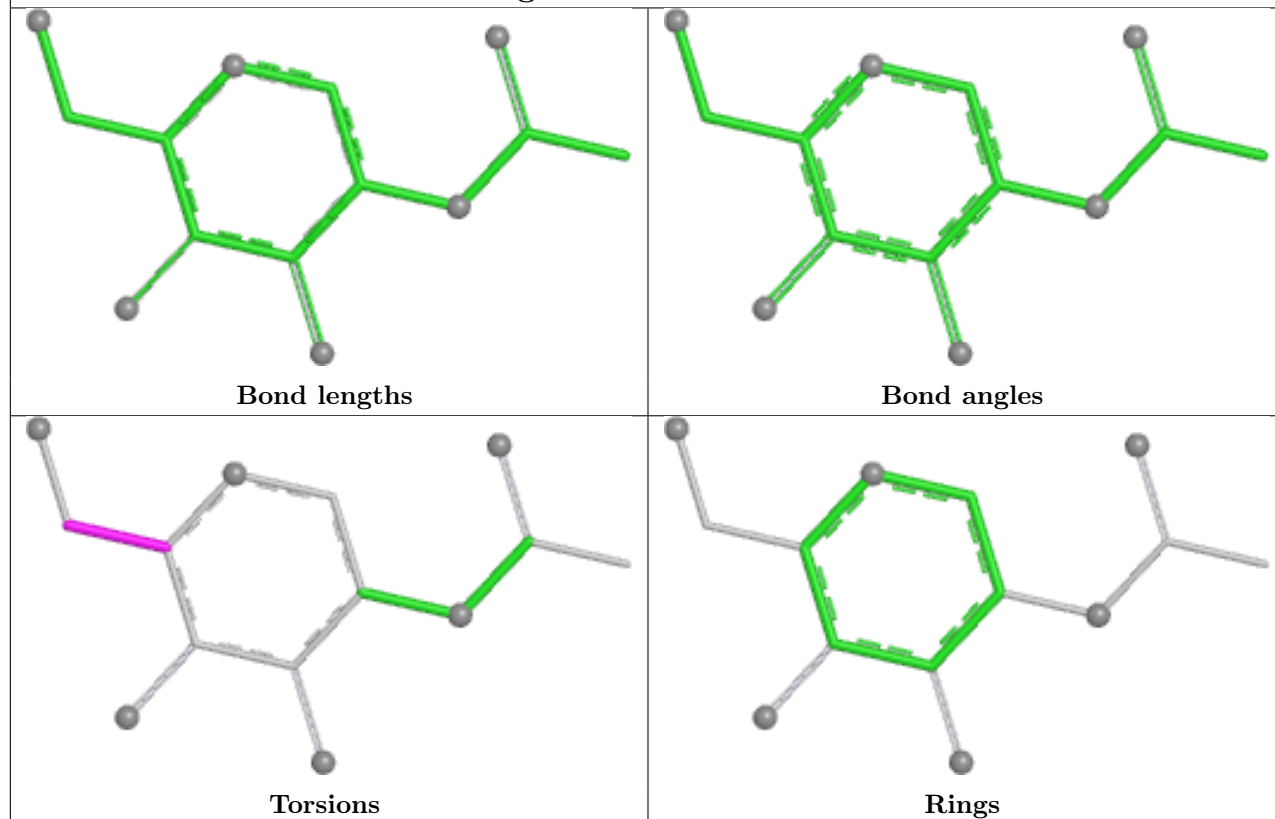
Ligand NAG B 1306



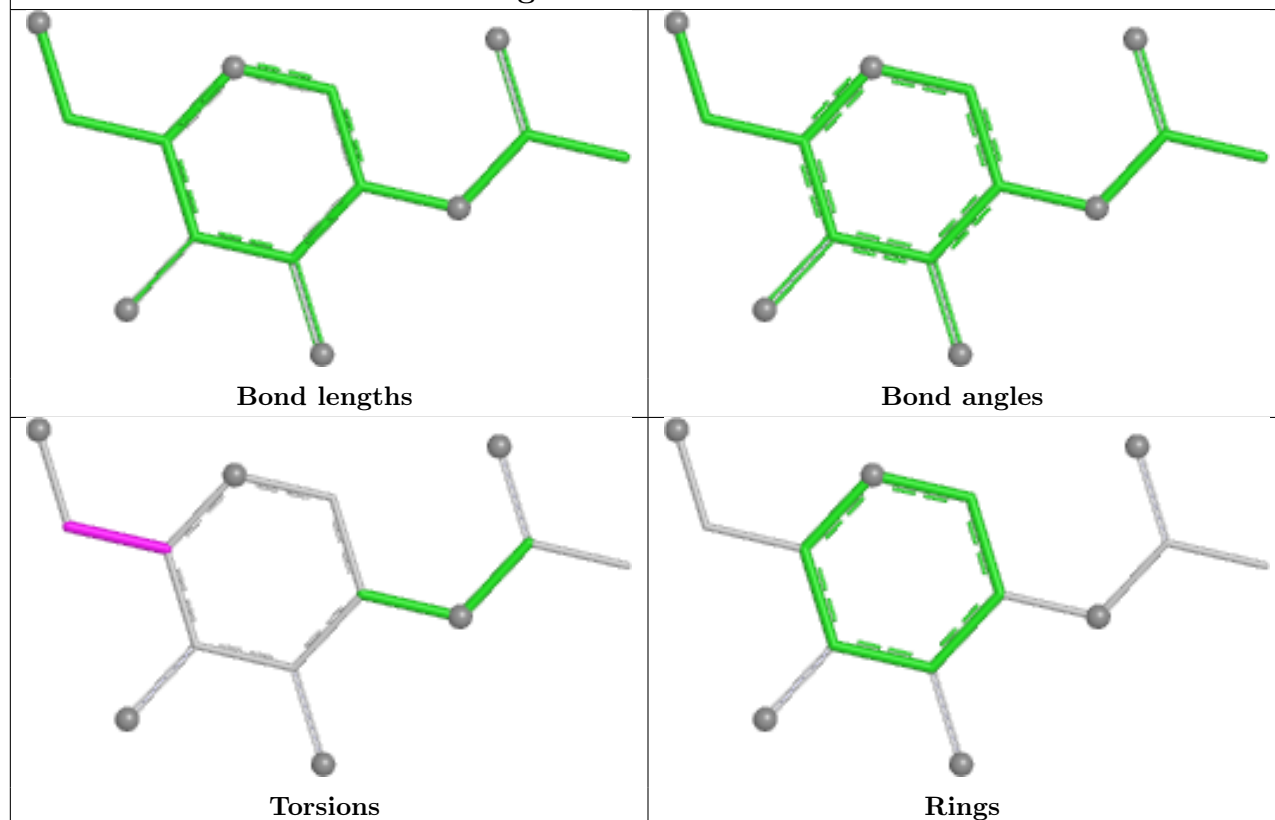




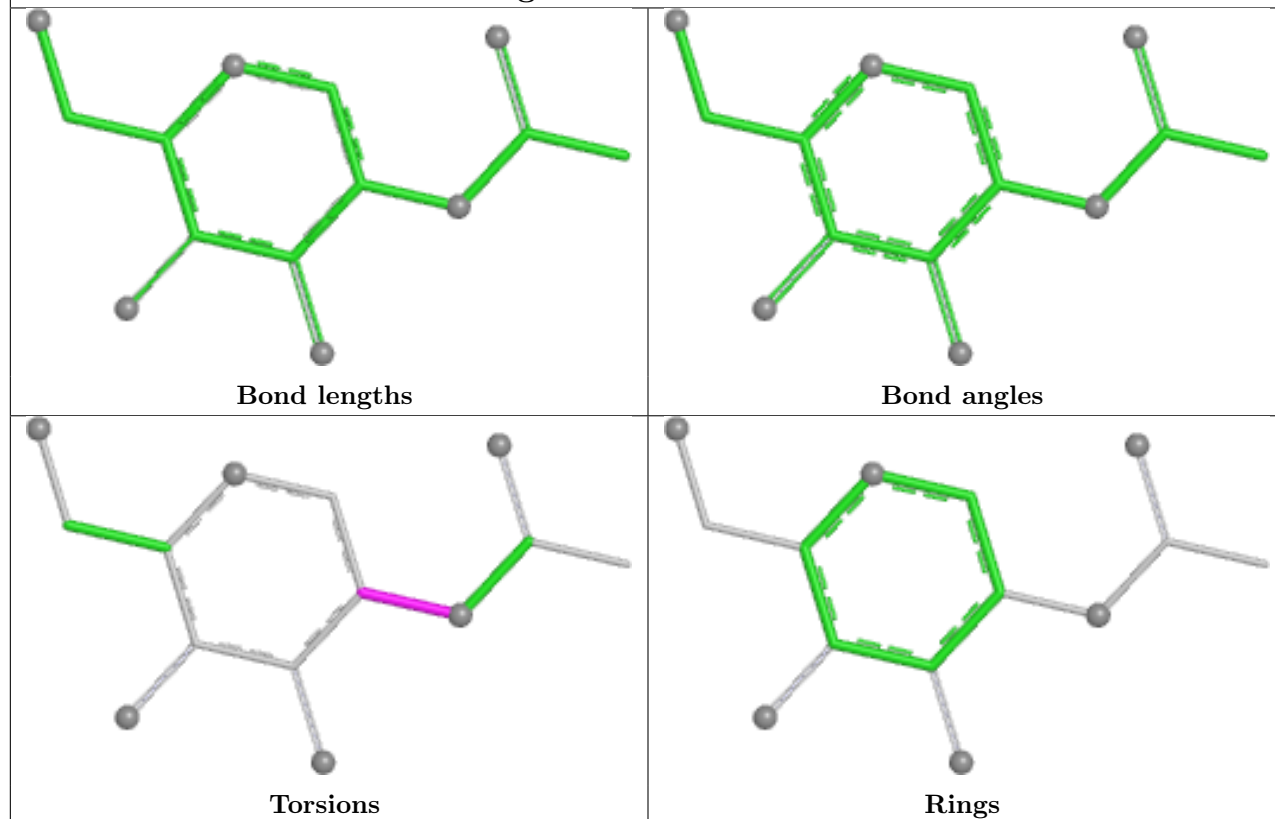
Ligand NAG A 1302



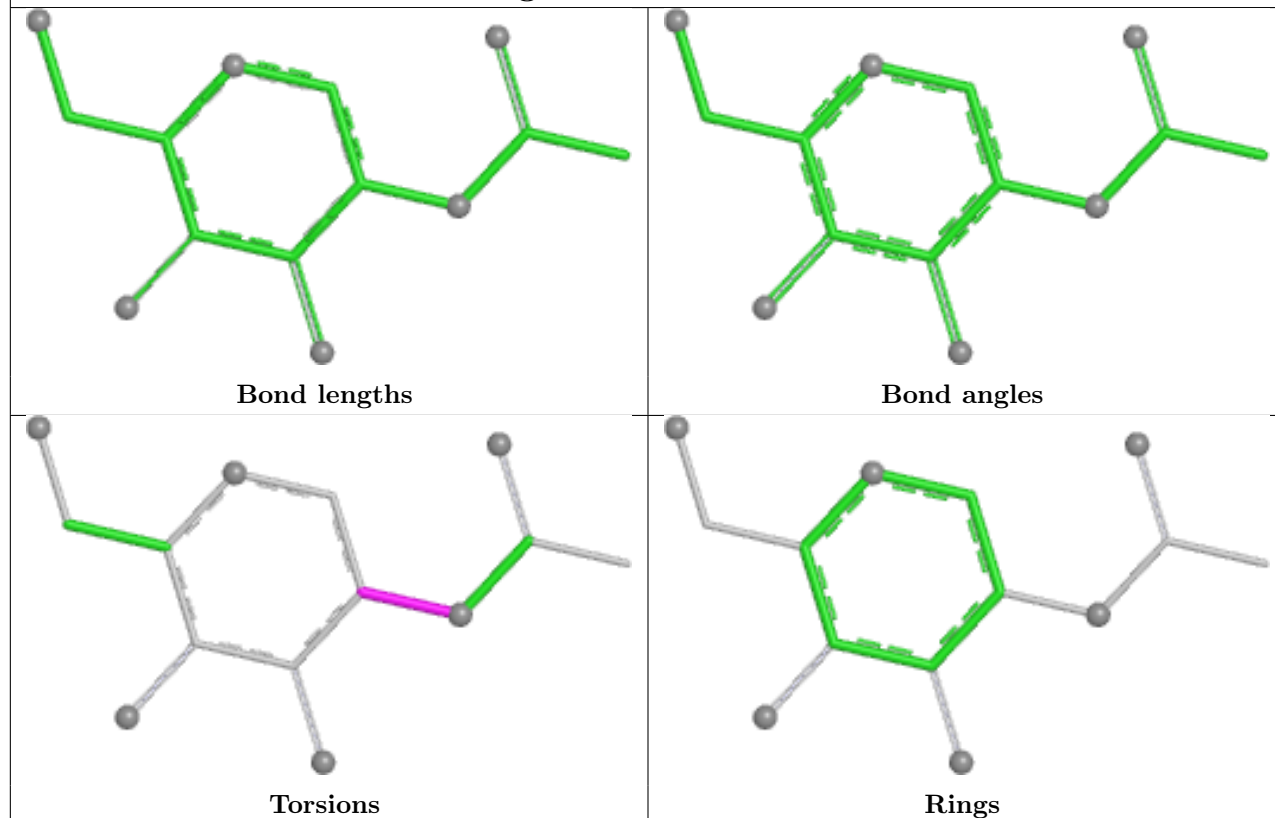
Ligand NAG A 1301



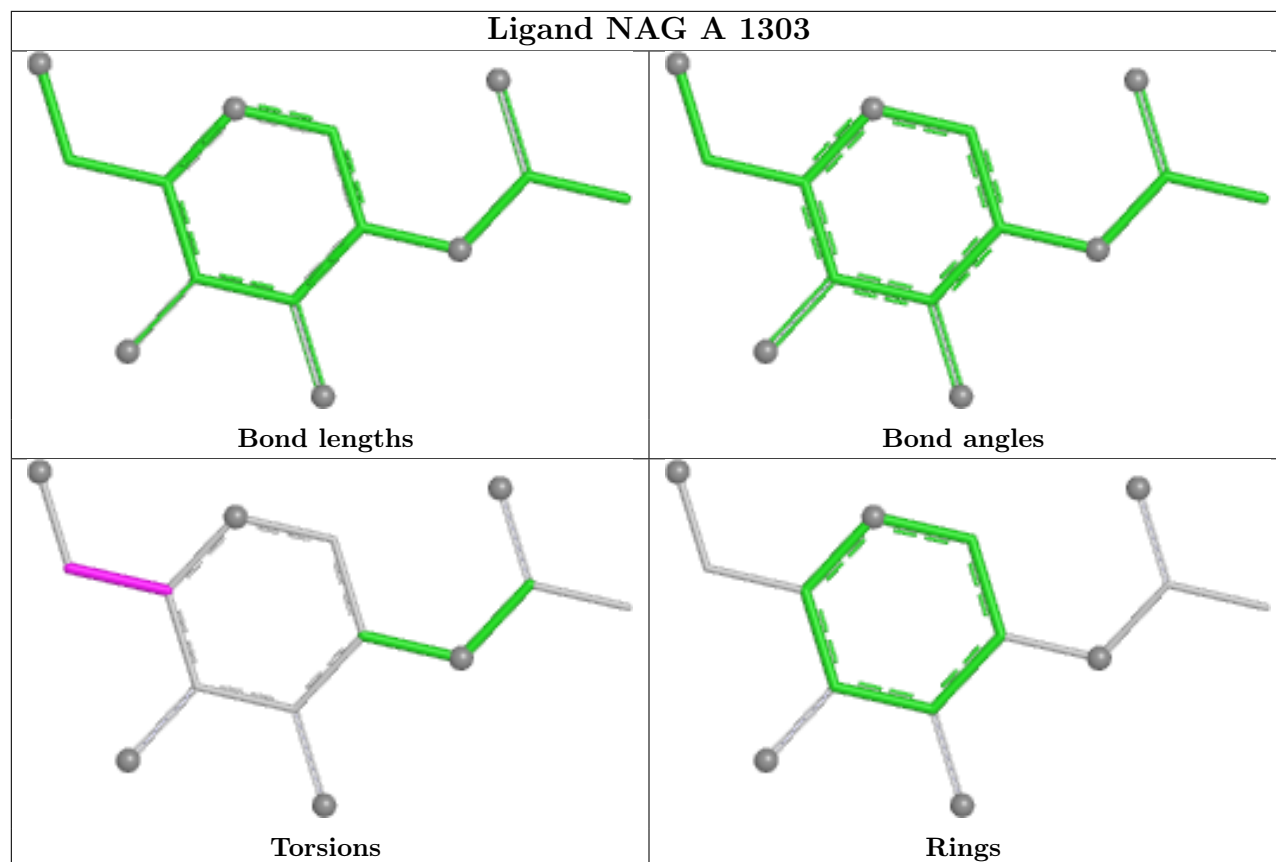
Ligand NAG A 1304



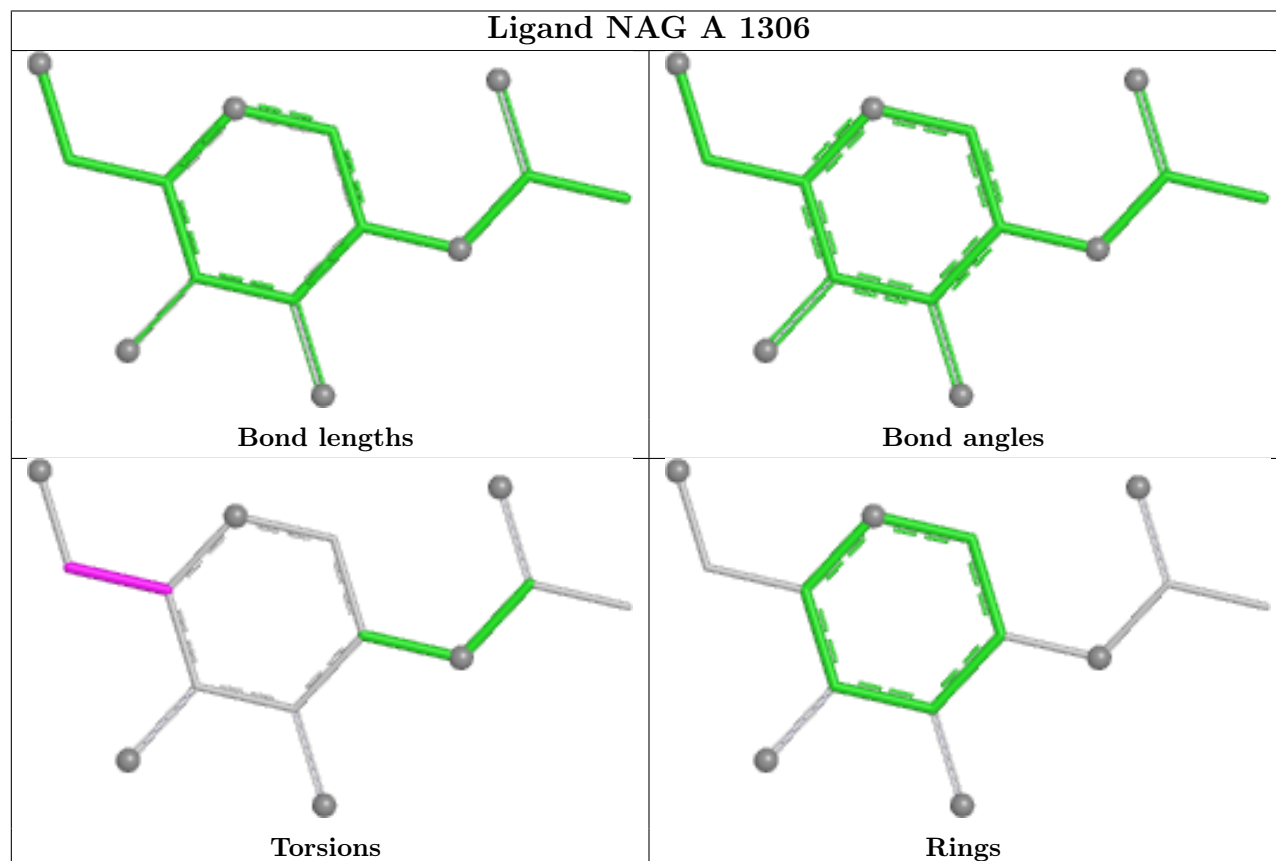
Ligand NAG C 1307

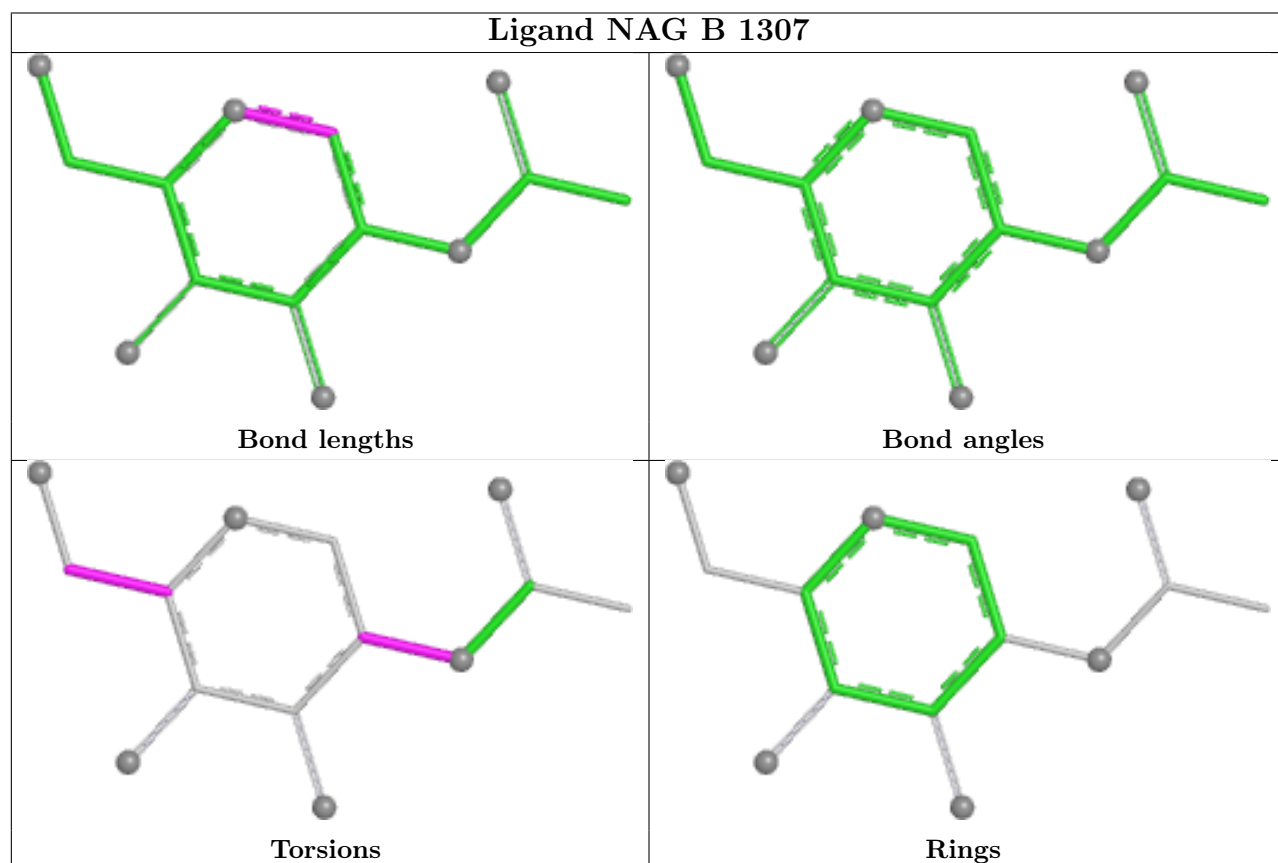
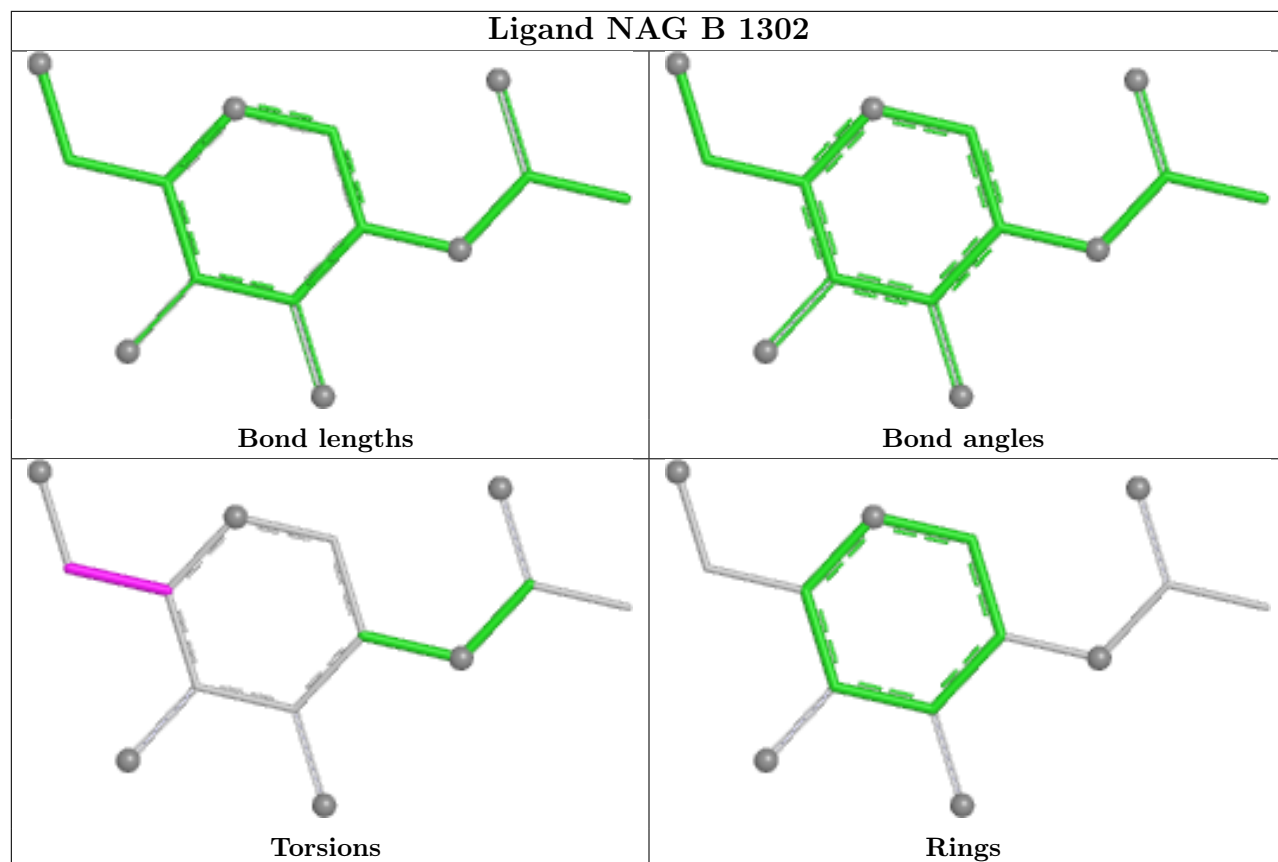


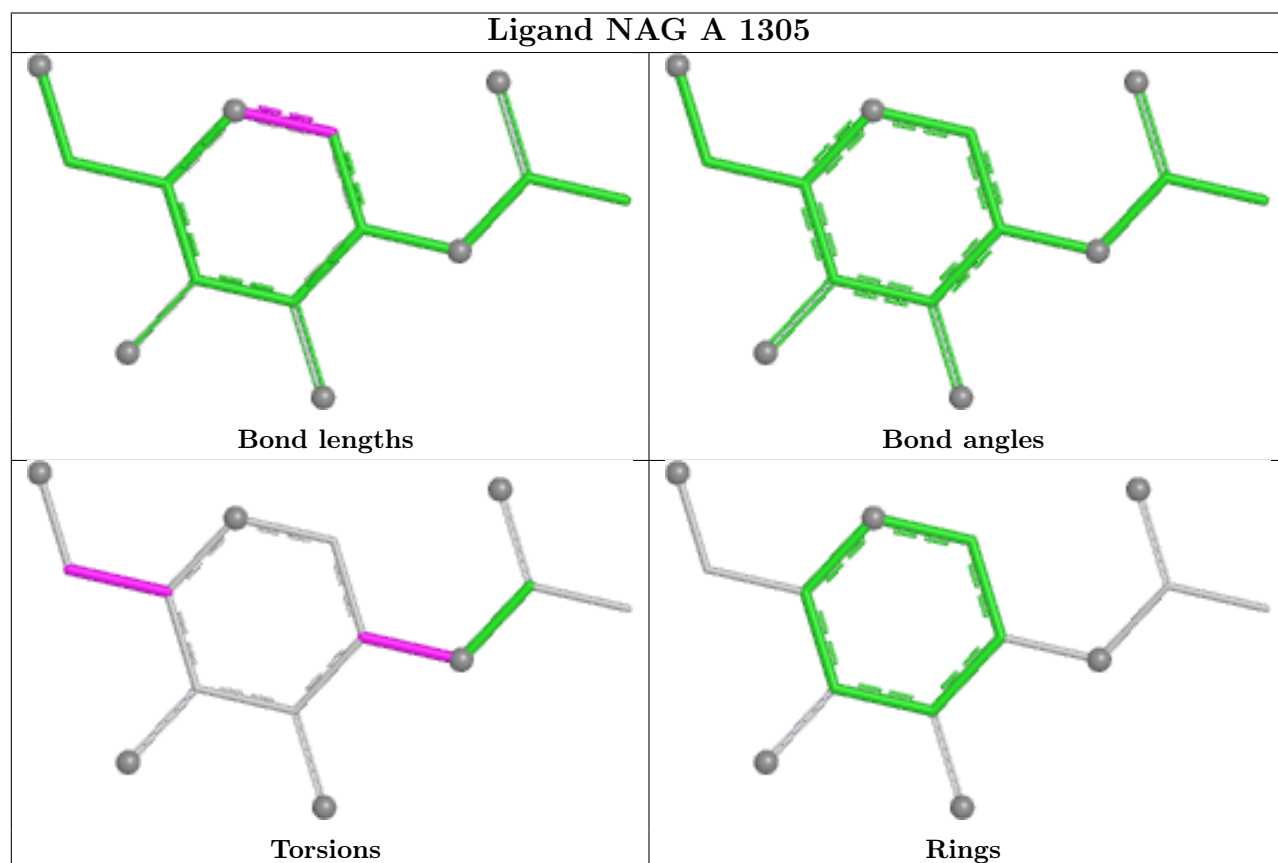
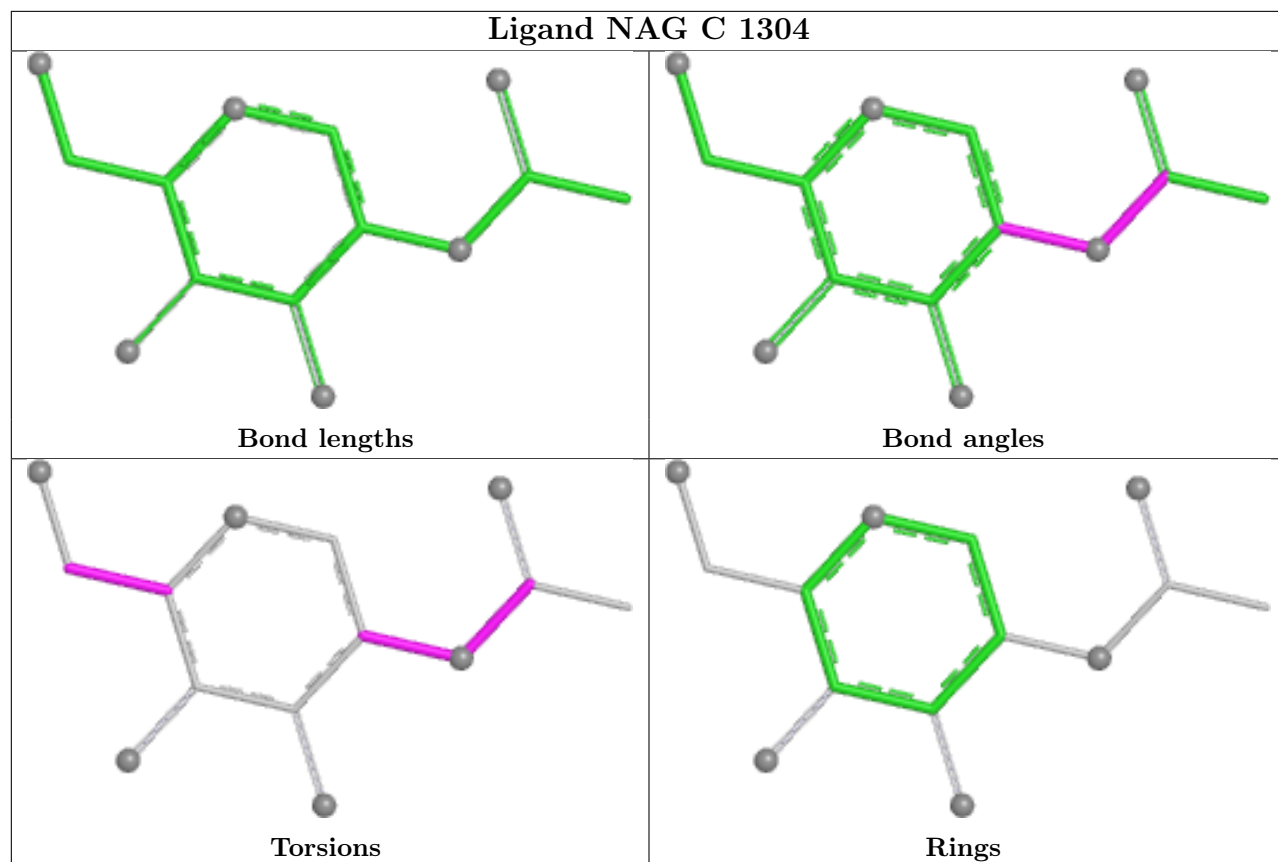
Ligand NAG A 1303

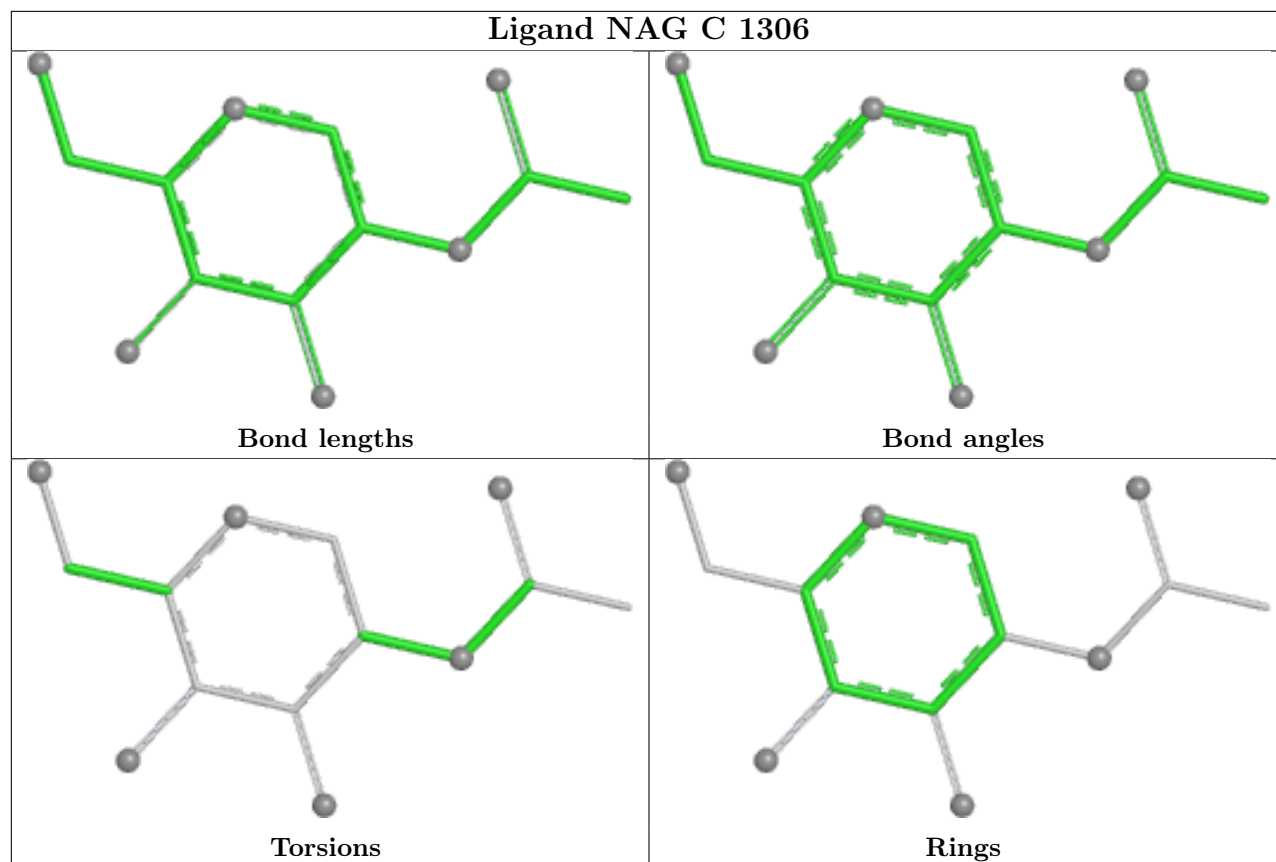


Ligand NAG A 1306









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.

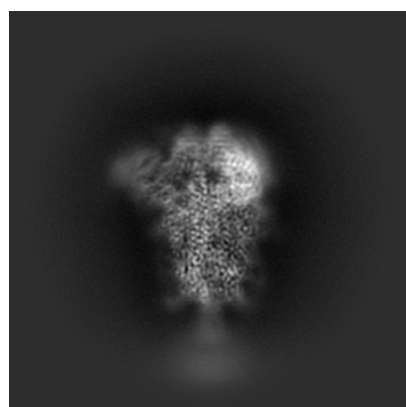
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25889. These allow visual inspection of the internal detail of the map and identification of artifacts.

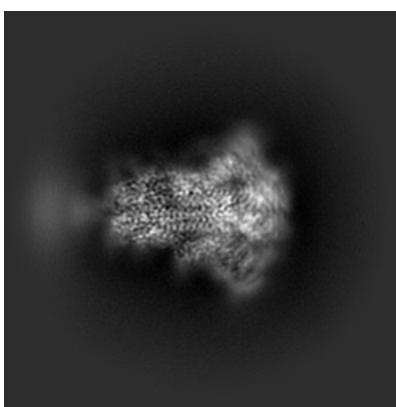
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

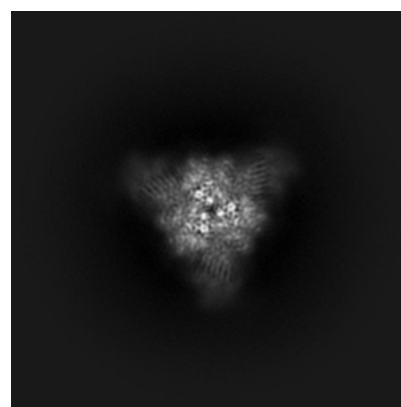
6.1.1 Primary map



X



Y

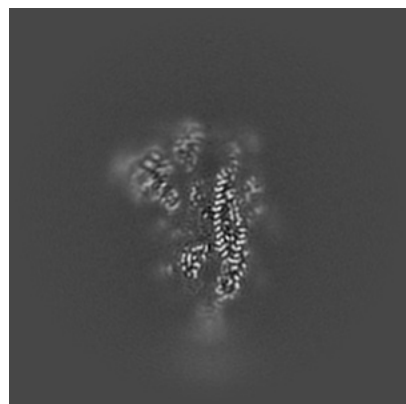


Z

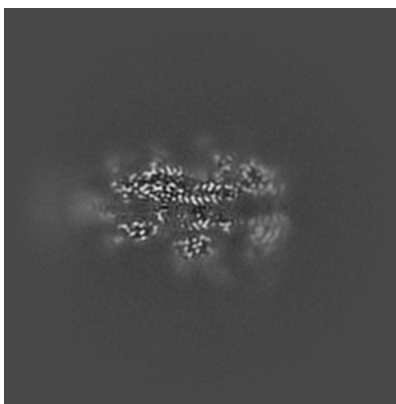
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

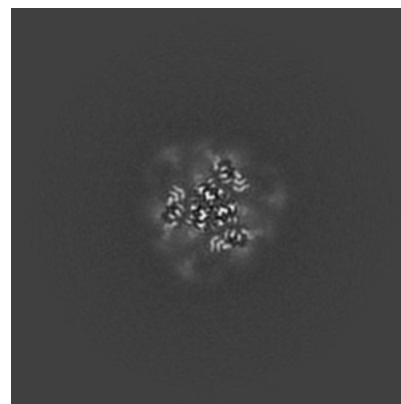
6.2.1 Primary map



X Index: 192



Y Index: 192

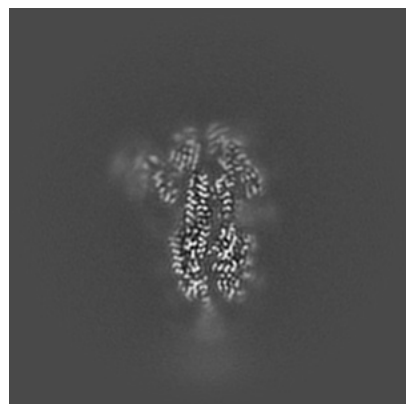


Z Index: 192

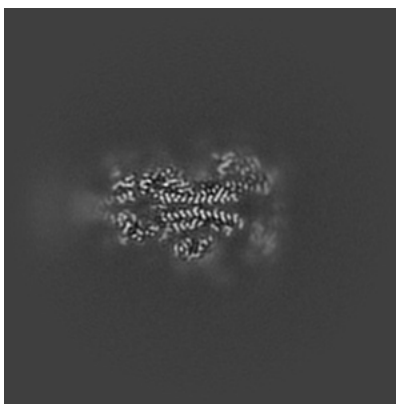
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

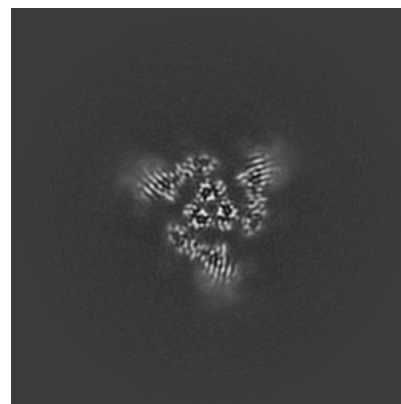
6.3.1 Primary map



X Index: 183



Y Index: 188

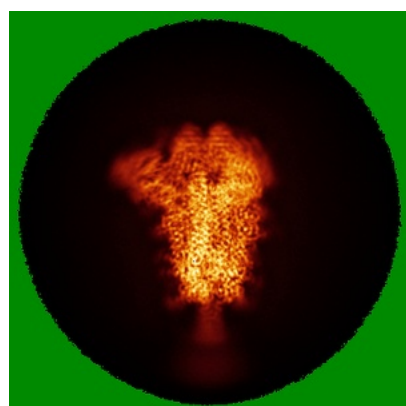


Z Index: 215

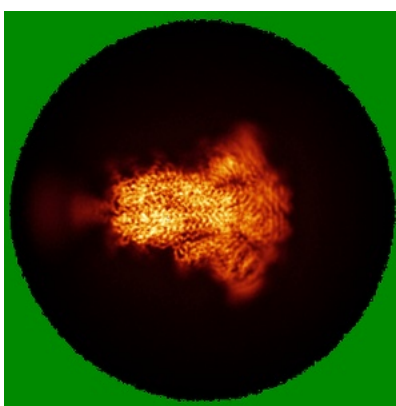
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

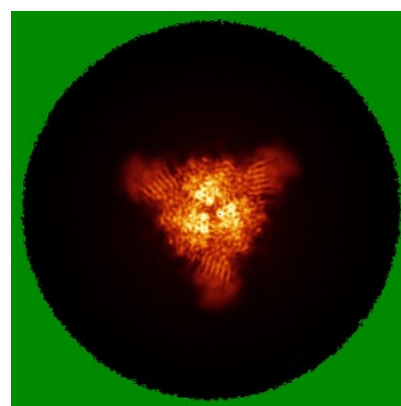
6.4.1 Primary map



X



Y

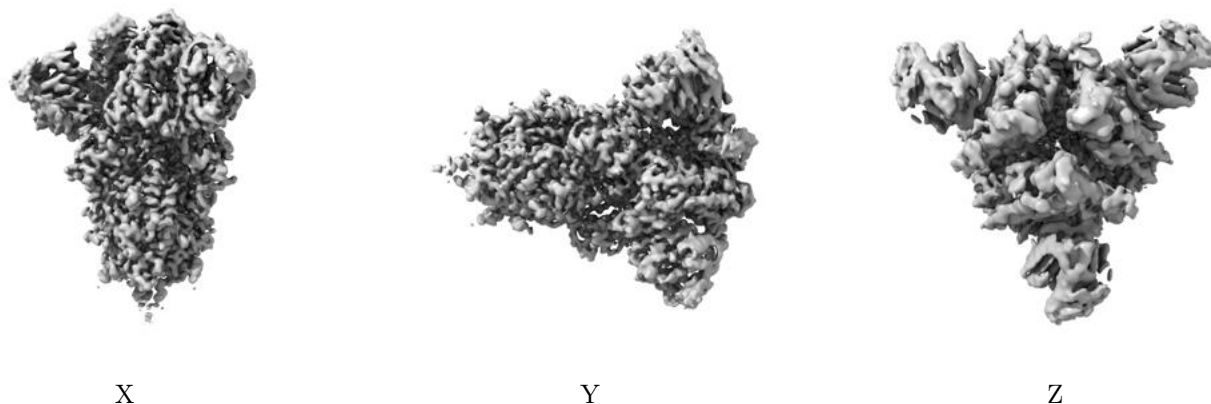


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

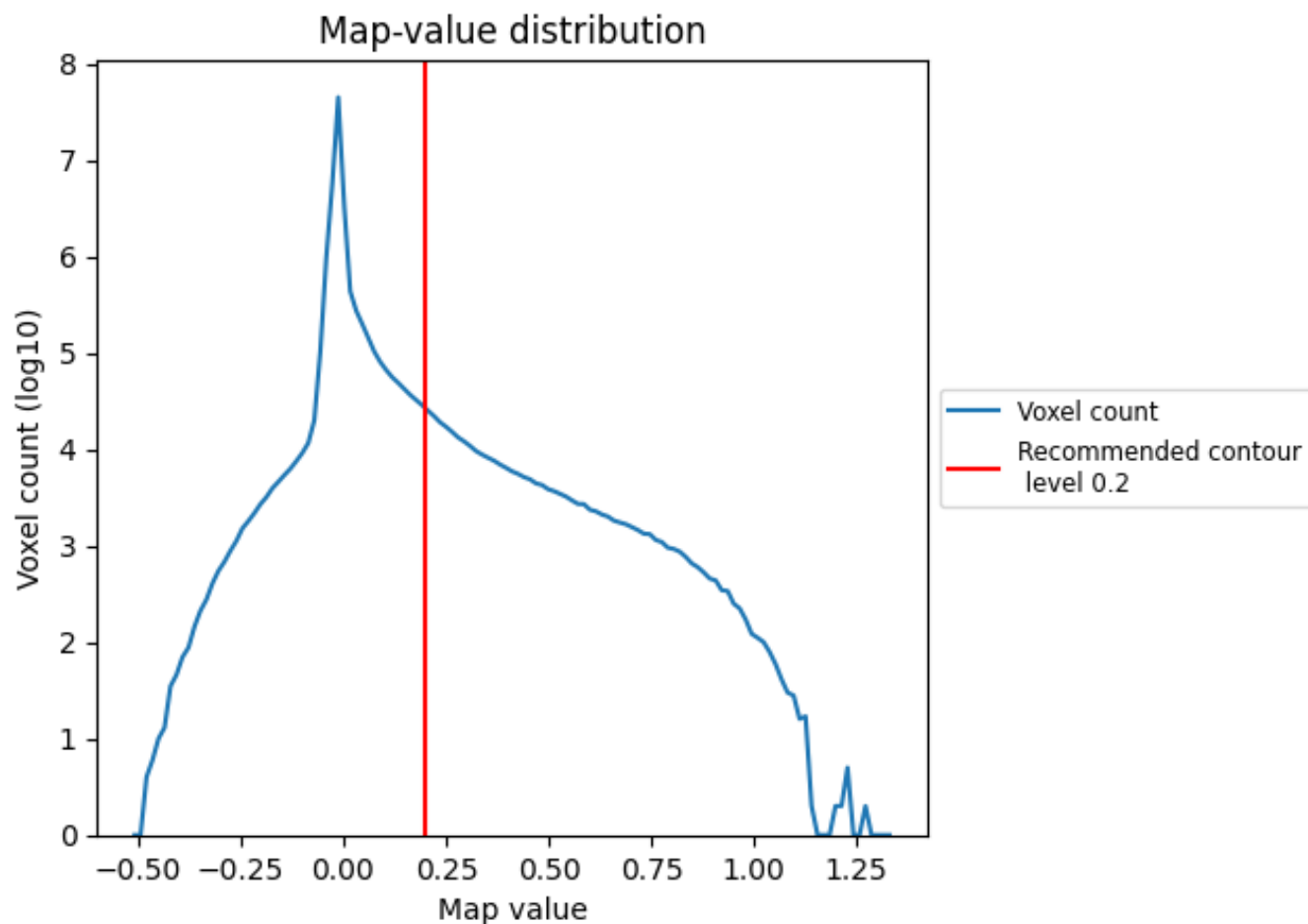
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

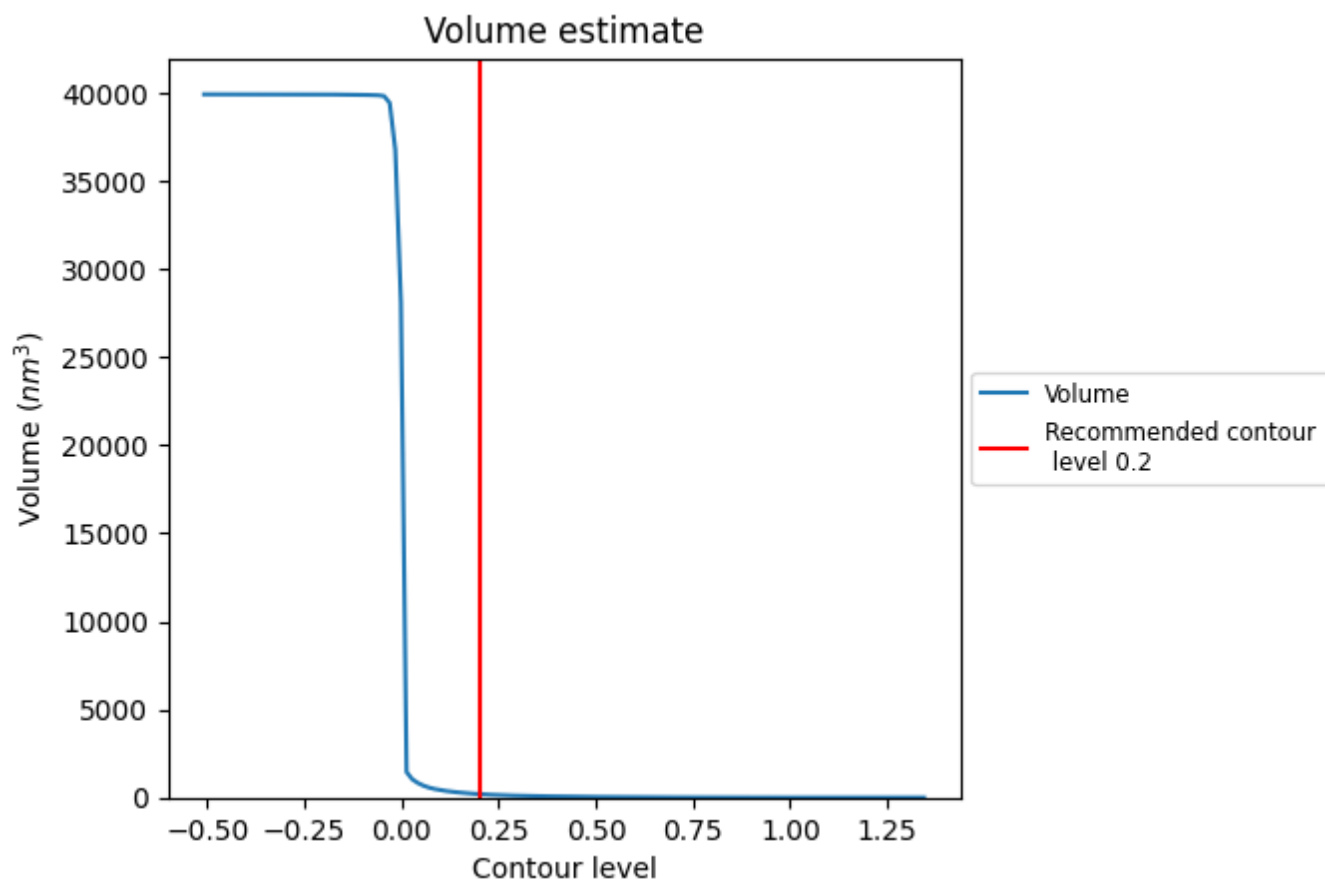
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

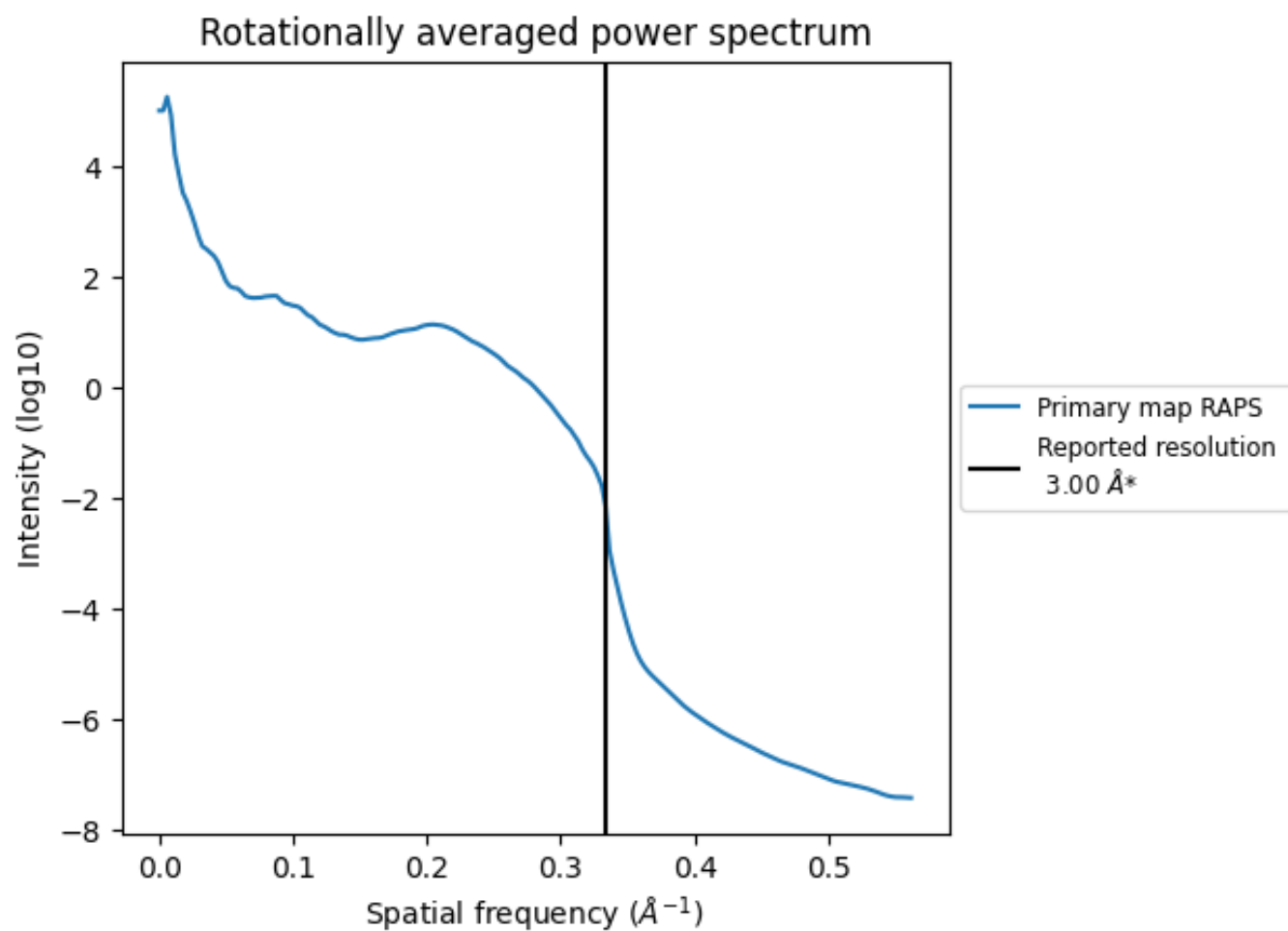
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

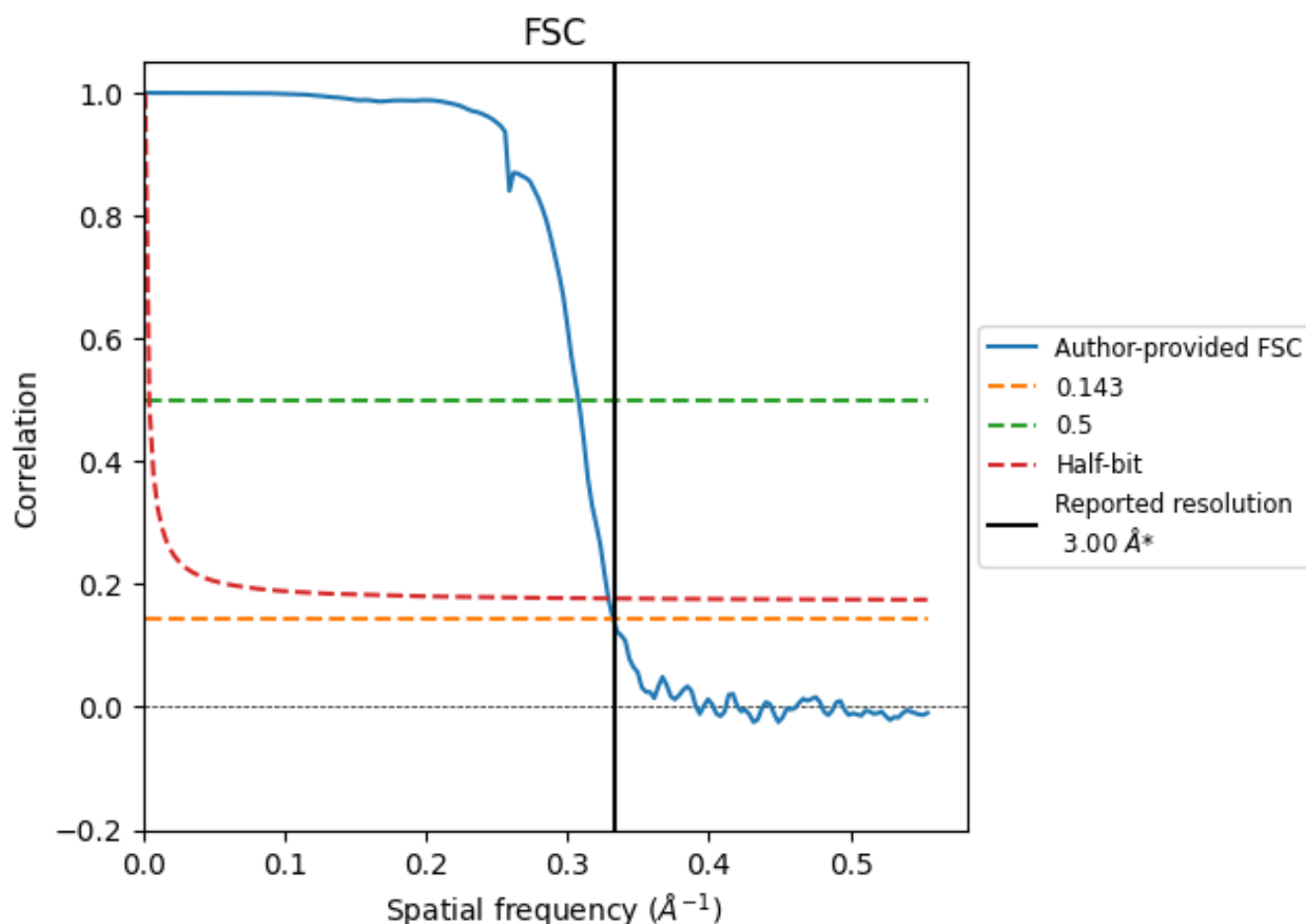


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

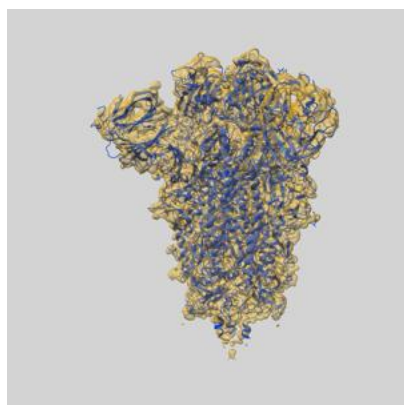
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.25	3.04
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

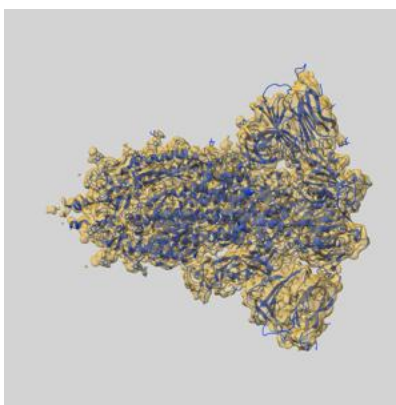
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25889 and PDB model 7TGY. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

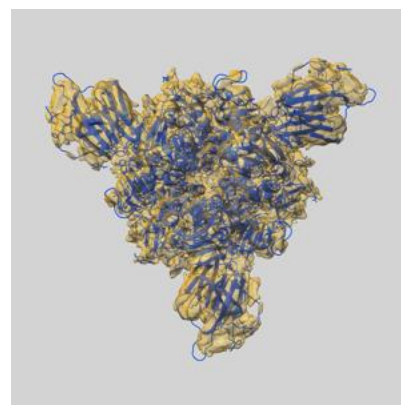
9.1 Map-model overlay [i](#)



X



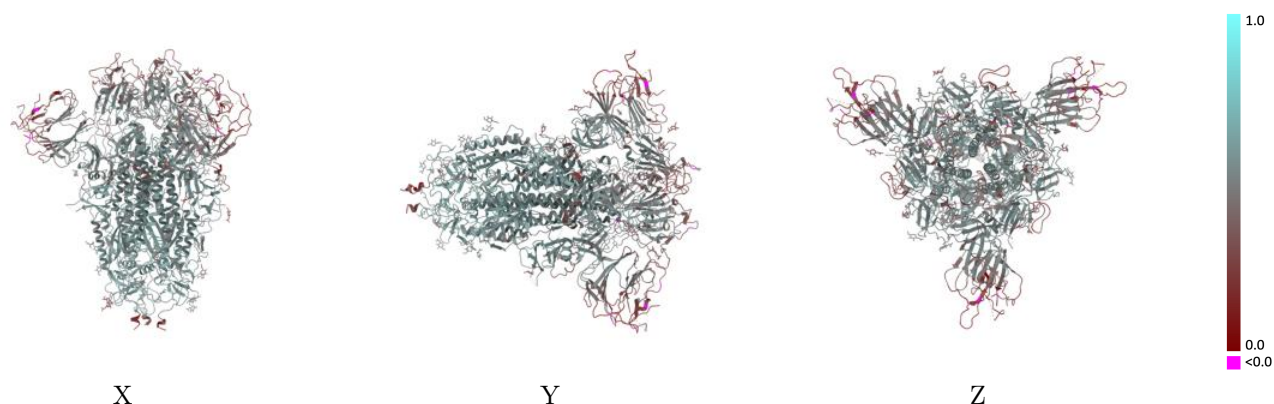
Y



Z

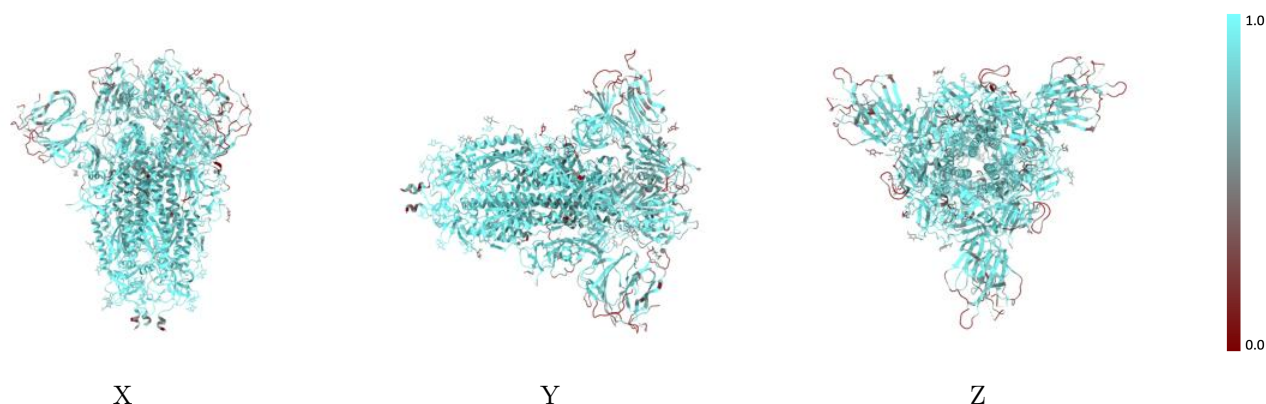
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



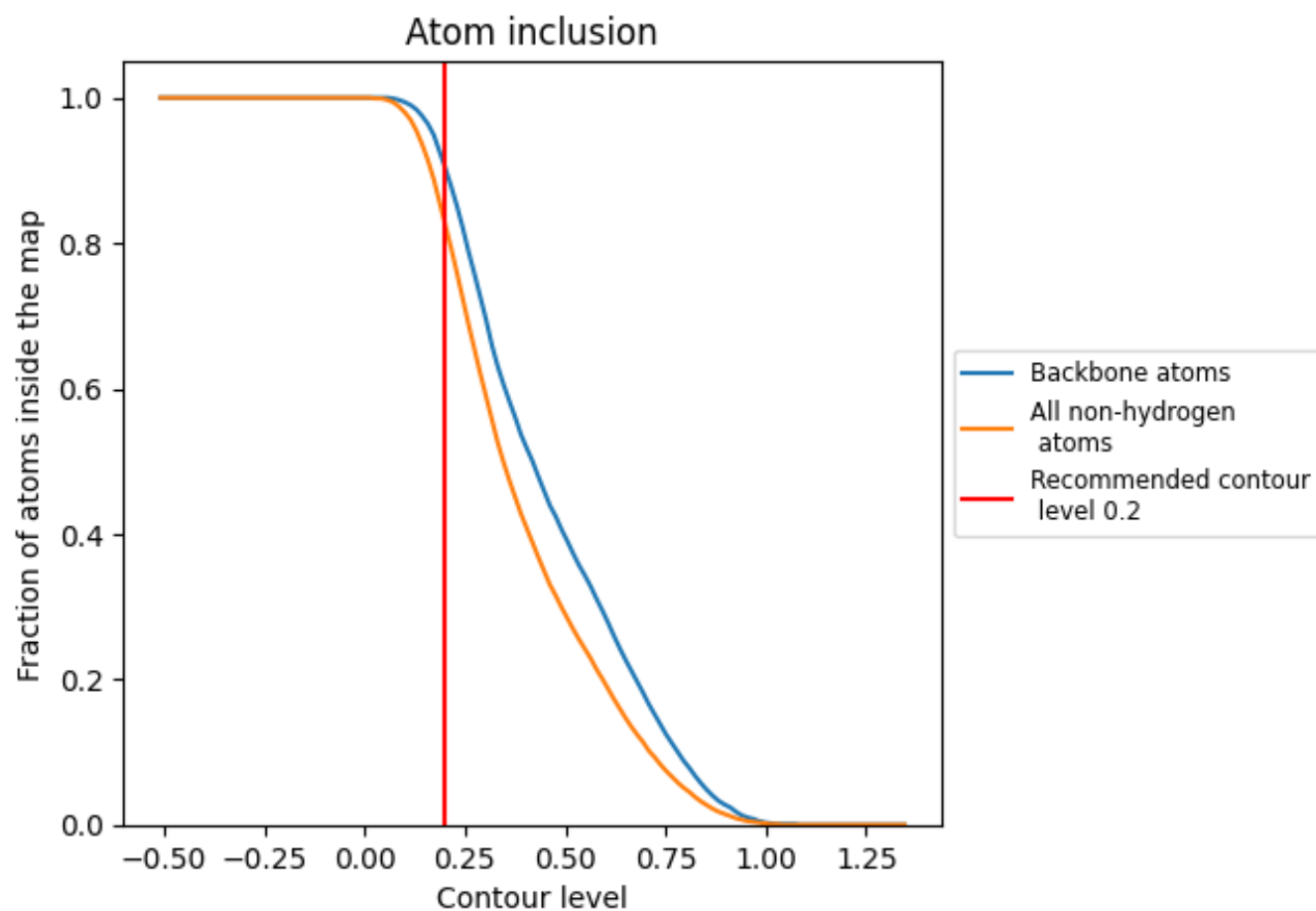
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.4880
A	0.8310	0.4900
B	0.8260	0.4870
C	0.8300	0.4890
K	0.7860	0.4370
M	0.7140	0.3020
U	0.7140	0.4810
V	0.7860	0.4520
X	0.8570	0.4860
e	0.4290	0.3330
f	0.8570	0.5100
g	0.8210	0.4880
h	0.6790	0.5480

1.0

0.0

<0.0