



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:04 PM UTC

PDB ID : 9MZI / pdb_00009mzi
EMDB ID : EMD-48757
Title : CryoEM structure of GluK2 bound to glutamate in the deep desensitized state 3
Authors : Chang, P.Z.; Nami, T.
Deposited on : 2025-01-23
Resolution : 3.83 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

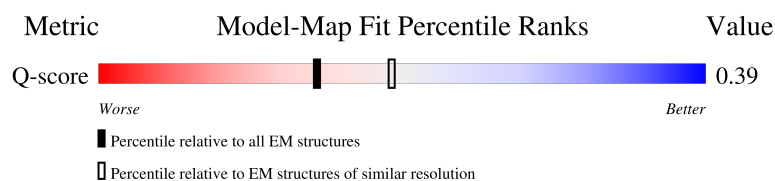
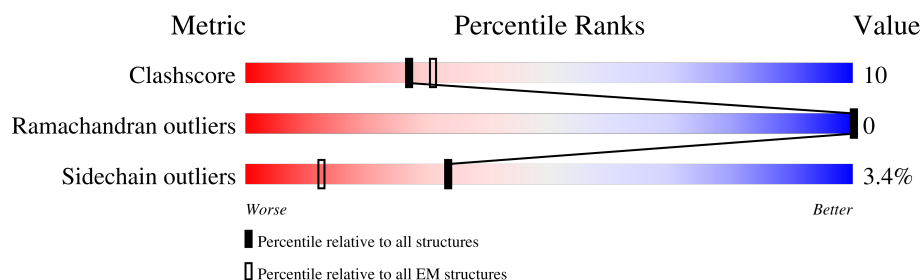
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.83 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.



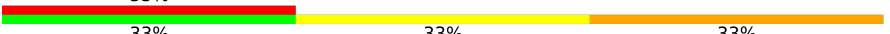
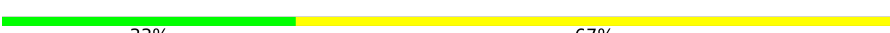
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9087 (3.33 - 4.33)

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	908	 6% 62% 21% 17%
1	B	908	 6% 63% 20% 16%
1	C	908	 6% 61% 22% 16%
1	D	908	 6% 62% 20% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	3	 33% 67%
2	H	3	 100%
2	N	3	 67% 33%
2	R	3	 33% 33% 67%
3	F	3	 33% 33% 33% 33%
4	G	2	 50% 100%
4	I	2	 50% 50%
4	J	2	 50% 50%
4	L	2	 100%
4	M	2	 50% 50%
4	P	2	 50% 50%
4	Q	2	 50% 50%
5	K	2	 50% 50%
6	O	3	 33% 67%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 24582 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.

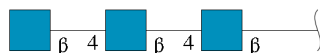
- Molecule 1 is a protein called Glutamate receptor ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	757	Total	C	N	O	S	0	0
			5966	3825	992	1115	34		
1	B	761	Total	C	N	O	S	0	0
			5995	3846	996	1119	34		
1	C	761	Total	C	N	O	S	0	0
			5995	3846	996	1119	34		
1	D	758	Total	C	N	O	S	0	0
			5977	3834	993	1116	34		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	676	CYS	LYS	conflict	UNP P42260
A	802	CYS	ASN	conflict	UNP P42260
B	676	CYS	LYS	conflict	UNP P42260
B	802	CYS	ASN	conflict	UNP P42260
C	676	CYS	LYS	conflict	UNP P42260
C	802	CYS	ASN	conflict	UNP P42260
D	676	CYS	LYS	conflict	UNP P42260
D	802	CYS	ASN	conflict	UNP P42260

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



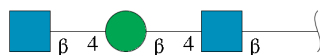
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	3	Total	C	N	O	0	0
			42	24	3	15		
2	H	3	Total	C	N	O	0	0
			42	24	3	15		

Continued on next page...

Continued from previous page...

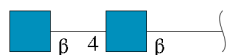
Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	3	Total	C	N	O	0	0
			42	24	3	15		
2	R	3	Total	C	N	O	0	0
			42	24	3	15		

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



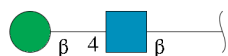
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		

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



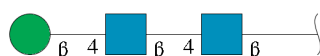
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



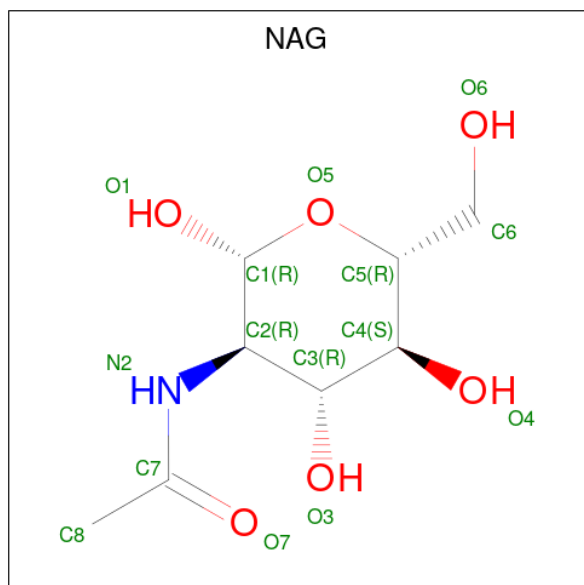
Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 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
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

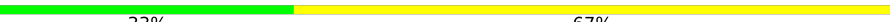
Continued from previous page...

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





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

Chain E:  33% 67%

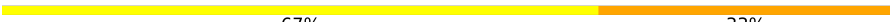


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



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

Chain N:  67% 33%



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

Chain R:  33% 33% 67%



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

Chain F:  33% 33% 33% 33%



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

Chain G:  50% 100%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain L:  100%



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

Chain M:  50% 50%



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  33% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.831	Depositor
Minimum map value	-0.426	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.121	Depositor
Map size (Å)	275.59998, 275.59998, 275.59998	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.10	0/6096	0.28	0/8256
1	B	0.10	0/6126	0.27	0/8297
1	C	0.11	0/6126	0.28	0/8297
1	D	0.11	0/6108	0.31	0/8272
All	All	0.11	0/24456	0.29	0/33122

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5966	0	5942	127	0
1	B	5995	0	5972	121	0
1	C	5995	0	5971	136	0
1	D	5977	0	5955	127	0
2	E	42	0	37	1	0
2	H	42	0	37	0	0
2	N	42	0	37	3	0
2	R	42	0	37	0	0
3	F	39	0	34	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	2	0
4	M	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
5	K	25	0	22	0	0
6	O	39	0	34	0	0
7	A	42	0	39	1	0
7	B	56	0	52	0	0
7	C	28	0	26	0	0
7	D	56	0	52	0	0
All	All	24582	0	24422	483	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 (483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:GLY:HA3	1:D:413:MET:HA	1.61	0.82
1:D:815:LEU:HD11	1:D:819:ASN:HB3	1.63	0.81
1:D:690:THR:HG21	1:D:737:MET:HA	1.65	0.79
1:C:660:THR:HG22	1:C:664:MET:HE2	1.66	0.76
1:B:533:PHE:HB3	1:B:782:ILE:HD11	1.67	0.76
1:B:266:VAL:HG21	1:B:399:LEU:HD23	1.68	0.75
1:B:96:CYS:HA	1:B:99:LEU:HB2	1.71	0.73
1:D:794:MET:HE3	1:D:794:MET:H	1.53	0.73
1:B:536:LEU:HD11	1:B:738:GLU:HB3	1.71	0.72
1:A:293:ILE:HG23	1:A:316:MET:HG2	1.71	0.72
1:A:814:ALA:HB1	1:A:819:ASN:HD21	1.55	0.72
1:A:215:LEU:HD12	1:A:247:MET:HG3	1.72	0.72
1:A:41:ILE:HG12	1:A:106:ILE:HD11	1.72	0.72
1:D:558:PRO:HB3	1:D:654:ASN:HB3	1.73	0.71
1:B:771:GLY:HA2	1:B:775:ARG:HD3	1.74	0.70
1:A:329:VAL:HG11	1:A:375:ILE:HG21	1.73	0.70
1:A:708:PHE:HB3	1:B:699:ILE:HG21	1.73	0.70
1:C:704:LYS:HG2	1:D:700:SER:HB2	1.74	0.70
1:D:540:ILE:HB	1:D:755:ILE:HB	1.72	0.70
1:D:83:ILE:HD11	1:D:90:GLU:HB3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ILE:HG21	1:A:674:LEU:HD13	1.74	0.69
1:D:337:PHE:HB3	1:D:340:MET:HE1	1.75	0.69
1:D:489:GLY:HA2	1:D:500:GLY:HA3	1.73	0.69
1:B:531:LYS:HG3	1:B:779:THR:HG23	1.75	0.69
1:C:298:MET:HA	1:C:301:LEU:HB2	1.75	0.68
1:B:128:PRO:HB3	1:B:360:MET:HE1	1.75	0.68
1:B:677:GLN:HE22	1:B:680:ILE:H	1.40	0.67
1:A:712:ARG:HG3	1:A:715:SER:HB3	1.77	0.67
1:D:99:LEU:HD11	1:D:127:VAL:HG21	1.75	0.67
1:D:533:PHE:HB3	1:D:764:TYR:HB3	1.76	0.66
1:C:441:GLU:HG2	1:C:442:PRO:HD3	1.76	0.66
1:B:434:ILE:HB	1:B:510:ALA:HA	1.78	0.66
1:B:531:LYS:HZ1	1:B:783:LEU:HG	1.62	0.65
1:A:182:LEU:HD12	1:B:182:LEU:HD23	1.77	0.65
1:B:526:VAL:HG12	1:B:527:ILE:HG13	1.79	0.65
1:C:654:ASN:HD21	1:D:815:LEU:HB3	1.61	0.65
1:B:339:GLN:HE22	1:B:358:ARG:HH21	1.42	0.65
1:C:488:TYR:HB2	1:C:688:GLY:HA2	1.80	0.64
1:D:183:ILE:HD12	1:D:183:ILE:H	1.63	0.64
1:A:336:GLN:HB3	1:A:362:LEU:HD21	1.79	0.64
1:D:215:LEU:HD12	1:D:247:MET:HG3	1.78	0.64
1:D:785:LEU:HB2	1:D:790:LYS:HB3	1.81	0.63
1:A:428:LEU:HD23	1:A:474:LEU:HD13	1.79	0.62
1:D:716:VAL:HA	1:D:727:ARG:HH12	1.65	0.62
1:A:128:PRO:HA	1:A:360:MET:HE1	1.82	0.62
1:B:750:CYS:H	1:B:804:CYS:HB3	1.64	0.61
1:C:43:GLU:HG3	1:C:85:LEU:HD22	1.83	0.61
1:A:437:THR:HG21	1:A:444:VAL:HG11	1.83	0.60
1:A:488:TYR:HE2	1:A:516:PRO:HB2	1.65	0.60
1:C:138:VAL:HG21	1:D:111:HIS:HE1	1.67	0.60
1:A:239:LEU:HD21	1:A:256:PHE:HZ	1.67	0.60
1:D:163:LEU:HD23	1:D:255:ILE:HD13	1.83	0.60
1:C:376:THR:HB	1:C:386:ASP:HB3	1.84	0.59
1:B:44:TYR:HA	1:B:82:LYS:HE2	1.84	0.59
1:C:563:ILE:HD11	1:D:817:VAL:HB	1.83	0.59
1:A:138:VAL:HG11	1:B:111:HIS:HE1	1.68	0.59
1:A:747:GLN:HB3	1:A:801:GLY:HA3	1.84	0.59
1:B:694:PHE:HB3	1:B:706:TRP:HB2	1.83	0.59
1:A:218:MET:HE1	1:A:226:VAL:HG11	1.84	0.59
1:C:121:ILE:HG12	1:D:89:PHE:HB2	1.85	0.59
1:D:292:ILE:HG21	1:D:371:LEU:HD11	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:GLY:HA3	1:B:805:PRO:HB3	1.85	0.58
1:A:45:VAL:HG21	1:A:50:MET:HA	1.85	0.58
1:A:392:ILE:HD12	1:A:399:LEU:HB3	1.84	0.58
1:A:645:LEU:HB3	1:B:648:ILE:HD11	1.84	0.58
1:D:345:LEU:HA	1:D:349:ARG:HH22	1.69	0.58
1:B:824:PHE:HA	1:B:827:LEU:HD12	1.86	0.58
1:D:671:ALA:HB1	1:D:705:MET:HE1	1.85	0.58
1:D:794:MET:HA	1:D:797:LYS:HB2	1.86	0.58
1:A:461:GLY:H	1:A:464:ILE:HB	1.68	0.58
1:B:543:ARG:HD2	1:B:729:LEU:HD13	1.86	0.57
1:B:337:PHE:HD1	1:B:340:MET:HG3	1.70	0.57
1:B:536:LEU:HD12	1:B:740:THR:H	1.69	0.57
1:A:536:LEU:HD11	1:A:762:LYS:HB2	1.86	0.57
1:B:227:ILE:HG12	1:B:255:ILE:HB	1.86	0.57
1:D:551:GLY:HA2	1:D:554:SER:HB2	1.86	0.57
1:D:483:VAL:HG12	1:D:486:GLY:H	1.70	0.57
1:B:138:VAL:HB	1:B:141:ASN:HB2	1.86	0.57
1:B:794:MET:HE3	1:B:794:MET:O	2.04	0.57
1:C:635:ILE:HD12	1:D:833:LEU:HD22	1.87	0.57
1:D:505:LEU:HD21	1:D:513:ALA:HB2	1.87	0.57
1:A:680:ILE:HG13	1:A:682:TYR:HE1	1.70	0.57
1:D:799:TRP:HZ3	1:D:802:CYS:HA	1.70	0.57
1:C:185:LEU:HB3	1:C:188:LEU:HB3	1.87	0.56
1:B:215:LEU:HD21	1:B:238:ILE:HD11	1.87	0.56
1:C:393:SER:HB3	1:C:402:ILE:HG21	1.88	0.56
1:C:444:VAL:HG12	1:C:464:ILE:HG23	1.88	0.56
1:B:256:PHE:HB2	1:B:261:LEU:HD21	1.87	0.56
1:D:564:TRP:HA	1:D:567:ILE:HD12	1.87	0.56
1:C:110:SER:HB2	1:C:133:ARG:HE	1.71	0.55
1:A:210:ASP:HA	1:A:241:GLN:HE22	1.72	0.55
1:B:668:ILE:HG22	1:B:673:ASP:HB3	1.88	0.55
1:B:245:MET:HA	1:D:272:SER:HA	1.89	0.55
1:C:441:GLU:HA	1:C:445:LEU:HD21	1.87	0.55
1:B:487:LYS:HB3	1:B:687:ASP:HB3	1.88	0.55
1:C:439:LEU:HA	1:C:444:VAL:HG23	1.87	0.55
1:D:737:MET:HE2	1:D:738:GLU:N	2.22	0.55
1:C:392:ILE:HG21	1:C:399:LEU:HB3	1.88	0.55
1:B:176:TYR:CZ	1:B:203:GLN:HB2	2.41	0.55
1:B:646:ILE:HG21	1:C:823:ILE:HG13	1.89	0.55
1:A:729:LEU:HD11	1:A:752:LEU:HD21	1.89	0.55
1:C:383:LEU:HB2	2:N:1:NAG:H81	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:GLY:HA2	1:C:824:PHE:HB2	1.89	0.55
1:D:99:LEU:HD12	1:D:345:LEU:HB2	1.88	0.54
1:A:502:VAL:HG22	1:A:527:ILE:HD12	1.88	0.54
1:C:502:VAL:HG22	1:C:527:ILE:HD12	1.90	0.54
1:D:132:THR:HG21	1:D:323:MET:HG3	1.90	0.54
1:D:519:ILE:HG12	1:D:529:PHE:HD2	1.72	0.54
1:A:368:TRP:HH2	3:F:1:NAG:H61	1.73	0.54
1:D:227:ILE:HG12	1:D:255:ILE:HB	1.88	0.54
1:D:204:LEU:HD12	1:D:214:LEU:HD13	1.90	0.53
1:B:110:SER:HB2	1:B:133:ARG:HG3	1.88	0.53
1:C:671:ALA:HB1	1:C:705:MET:HE2	1.90	0.53
1:C:109:PRO:HD2	1:C:118:VAL:HG21	1.89	0.53
1:C:292:ILE:HA	1:C:295:LYS:HZ3	1.73	0.53
1:C:460:GLU:HG2	1:C:798:TRP:HH2	1.73	0.53
1:B:330:VAL:HG22	1:B:363:ILE:HD11	1.89	0.53
1:A:440:GLU:HG3	1:A:442:PRO:HD2	1.90	0.53
1:A:691:MET:HA	1:A:694:PHE:HB2	1.89	0.53
1:C:330:VAL:HG22	1:C:363:ILE:HD11	1.91	0.53
1:A:536:LEU:HD23	1:A:764:TYR:CE2	2.44	0.53
1:B:543:ARG:HH12	1:B:751:ASN:HB3	1.72	0.53
1:A:99:LEU:HD12	1:A:345:LEU:HB2	1.91	0.53
1:B:149:LEU:HB3	1:B:322:LEU:HD12	1.91	0.53
1:C:306:LYS:HE3	1:C:308:ASP:HB3	1.91	0.53
1:D:685:VAL:HG13	1:D:688:GLY:HA3	1.91	0.53
1:C:288:GLN:HG3	4:L:2:NAG:H81	1.91	0.53
1:A:709:MET:HG2	1:A:712:ARG:HH22	1.74	0.52
1:C:643:PHE:O	1:C:647:ILE:HG22	2.09	0.52
1:A:709:MET:HB3	1:A:716:VAL:HG21	1.91	0.52
1:C:497:GLN:HB3	1:C:503:ARG:HH21	1.75	0.52
1:A:439:LEU:HD12	1:A:444:VAL:HG23	1.91	0.52
1:A:531:LYS:HB2	1:A:779:THR:HG23	1.91	0.52
1:C:280:ARG:HB2	1:C:392:ILE:HD11	1.91	0.52
1:D:405:TRP:HD1	1:D:411:LEU:HD23	1.75	0.52
1:A:459:PHE:HB3	1:A:464:ILE:HG13	1.92	0.51
1:C:83:ILE:HD11	1:C:90:GLU:HB3	1.92	0.51
1:C:279:PHE:CG	1:C:389:LEU:HD21	2.44	0.51
1:C:160:ILE:HG13	1:C:257:THR:HG22	1.92	0.51
1:A:227:ILE:HG12	1:A:255:ILE:HB	1.92	0.51
1:B:737:MET:HG3	1:B:742:ILE:HG12	1.93	0.51
1:A:386:ASP:HA	1:A:407:PRO:HG3	1.93	0.51
1:B:230:CYS:HB2	1:B:234:MET:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ALA:HB1	1:D:327:VAL:HG11	1.91	0.51
1:D:111:HIS:NE2	1:D:113:SER:HB3	2.25	0.51
1:D:439:LEU:HA	1:D:444:VAL:HB	1.92	0.51
1:B:153:PHE:HA	1:B:156:LEU:HB3	1.91	0.51
1:D:110:SER:HB3	1:D:133:ARG:HE	1.75	0.51
1:A:735:PHE:CD1	1:A:737:MET:HG2	2.46	0.51
1:D:798:TRP:CD1	1:D:801:GLY:H	2.29	0.51
1:B:390:ASP:HA	1:B:404:THR:HA	1.93	0.50
1:A:145:PHE:CG	1:A:360:MET:HE3	2.47	0.50
1:A:160:ILE:HG22	1:A:188:LEU:HD21	1.94	0.50
1:B:444:VAL:HG13	1:B:463:CYS:HB3	1.93	0.50
1:C:41:ILE:HD12	1:C:83:ILE:HG21	1.93	0.50
1:C:174:VAL:HG12	1:C:227:ILE:HB	1.94	0.50
1:B:162:ASP:HB3	1:B:411:LEU:HD23	1.94	0.50
1:C:234:MET:O	1:C:238:ILE:HG22	2.12	0.50
1:D:437:THR:HB	1:D:480:ILE:HD11	1.92	0.50
1:A:704:LYS:HG3	1:B:700:SER:HB2	1.93	0.50
1:B:61:VAL:HG11	1:B:78:TYR:HB3	1.92	0.50
1:C:122:CYS:SG	1:C:127:VAL:HG13	2.51	0.50
1:B:204:LEU:HD23	1:B:214:LEU:HD13	1.94	0.50
1:C:36:LEU:HD13	1:C:340:MET:HG3	1.92	0.50
1:C:153:PHE:CE2	1:C:184:ARG:HG2	2.46	0.50
1:D:531:LYS:HZ2	1:D:783:LEU:HD23	1.76	0.50
1:A:64:ILE:HG22	1:A:71:LEU:HD22	1.93	0.50
1:B:177:ASP:HB2	1:B:234:MET:HE3	1.93	0.50
1:B:272:SER:HA	1:D:245:MET:HA	1.94	0.50
1:C:668:ILE:HD12	1:C:673:ASP:HB3	1.94	0.50
1:B:85:LEU:HD12	1:B:85:LEU:H	1.76	0.50
1:B:360:MET:HA	1:B:363:ILE:HG22	1.93	0.50
1:C:183:ILE:HD11	1:D:183:ILE:HD11	1.92	0.49
1:A:488:TYR:CE2	1:A:516:PRO:HB2	2.46	0.49
1:C:270:ARG:HD3	1:C:398:GLY:H	1.76	0.49
1:A:706:TRP:HB2	1:A:716:VAL:HG11	1.94	0.49
1:A:34:HIS:HB3	1:A:74:THR:HG22	1.95	0.49
1:B:99:LEU:HD12	1:B:345:LEU:HB2	1.93	0.49
1:C:180:THR:HG22	1:D:136:HIS:HE1	1.77	0.49
1:A:424:ILE:HD13	1:A:780:ILE:HG21	1.93	0.49
1:D:443:TYR:HD2	1:D:516:PRO:HB3	1.77	0.49
1:A:645:LEU:HD22	1:B:648:ILE:HG13	1.94	0.49
1:B:704:LYS:HB3	1:C:700:SER:HB3	1.94	0.49
1:A:451:LYS:HD2	1:A:452:PRO:HD2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:TYR:HA	1:B:777:LYS:HE3	1.94	0.49
1:C:358:ARG:HE	1:C:362:LEU:HD21	1.77	0.49
1:D:682:TYR:CE2	1:D:705:MET:HG2	2.47	0.49
1:A:428:LEU:HD12	1:A:431:ARG:HG3	1.95	0.49
1:B:742:ILE:HA	1:B:745:VAL:HG22	1.95	0.49
1:A:323:MET:HE3	1:A:323:MET:HA	1.94	0.48
1:D:682:TYR:HB3	1:D:734:ALA:HB3	1.95	0.48
1:D:149:LEU:HD21	1:D:329:VAL:HG11	1.93	0.48
1:A:555:PHE:HD2	1:A:564:TRP:HH2	1.61	0.48
1:C:225:HIS:H	1:C:225:HIS:CD2	2.30	0.48
1:C:760:ASP:OD1	1:C:762:LYS:HG2	2.13	0.48
1:D:128:PRO:HA	1:D:360:MET:HE3	1.96	0.48
1:D:776:ASP:HA	1:D:779:THR:HB	1.95	0.48
1:A:169:TRP:HZ2	1:A:253:HIS:CG	2.31	0.48
1:B:499:ASN:HA	1:B:503:ARG:HB2	1.94	0.48
1:B:750:CYS:HB3	1:B:804:CYS:O	2.13	0.48
1:D:330:VAL:O	1:D:334:VAL:HG12	2.14	0.48
1:D:719:LYS:H	1:D:719:LYS:HE2	1.78	0.48
1:C:149:LEU:HG	1:C:377:PHE:HZ	1.78	0.48
1:A:160:ILE:HG13	1:A:257:THR:HG22	1.96	0.48
1:C:538:ILE:HG13	1:C:759:ILE:HB	1.95	0.48
1:B:705:MET:HB3	1:B:705:MET:HE2	1.78	0.48
1:D:359:PHE:O	1:D:363:ILE:HG23	2.13	0.48
1:C:282:LEU:HB3	1:C:284:THR:HG23	1.96	0.48
1:C:563:ILE:HD13	1:C:566:TYR:HD2	1.79	0.48
1:A:483:VAL:HG13	1:A:486:GLY:H	1.79	0.47
1:D:405:TRP:CD1	1:D:411:LEU:HD23	2.49	0.47
1:B:132:THR:HG21	1:B:323:MET:HG2	1.97	0.47
1:C:660:THR:HG22	1:C:664:MET:CE	2.42	0.47
1:A:519:ILE:HG22	1:A:529:PHE:CG	2.49	0.47
1:A:560:SER:HB3	1:A:563:ILE:HG13	1.96	0.47
1:B:392:ILE:HG22	1:B:401:LYS:HA	1.96	0.47
1:B:433:LEU:HD12	1:B:433:LEU:HA	1.77	0.47
1:C:163:LEU:HD22	1:C:255:ILE:HD12	1.96	0.47
1:A:411:LEU:HG	1:A:413:MET:SD	2.54	0.47
1:C:110:SER:HB2	1:C:133:ARG:NE	2.29	0.47
1:C:298:MET:HE3	1:C:298:MET:H	1.78	0.47
1:C:675:ALA:HB2	1:C:705:MET:HG2	1.96	0.47
1:D:322:LEU:HD22	1:D:372:THR:HG21	1.97	0.47
1:D:327:VAL:O	1:D:331:SER:HB3	2.15	0.47
1:D:349:ARG:HG2	1:D:351:LYS:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:ILE:HG23	1:D:510:ALA:HA	1.97	0.47
1:D:516:PRO:HA	1:D:764:TYR:HE1	1.79	0.47
1:A:59:PHE:HA	1:A:62:ASN:HD21	1.80	0.47
1:A:685:VAL:O	1:A:691:MET:HE1	2.14	0.47
1:B:405:TRP:HD1	1:B:411:LEU:HB3	1.80	0.47
1:C:199:LEU:HD21	1:C:201:ILE:HD11	1.96	0.47
1:D:768:THR:HG21	1:D:775:ARG:HB2	1.97	0.47
1:B:682:TYR:CE2	1:B:705:MET:HG2	2.49	0.47
1:B:798:TRP:HA	1:B:800:ARG:HH11	1.80	0.47
1:D:247:MET:HE3	1:D:247:MET:O	2.14	0.47
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.78	0.47
1:B:712:ARG:O	1:B:716:VAL:HG12	2.14	0.47
1:D:163:LEU:HD12	1:D:411:LEU:HD11	1.97	0.47
1:D:498:TRP:HE3	1:D:502:VAL:HG11	1.79	0.47
1:D:666:SER:OG	1:D:667:PRO:HD3	2.15	0.47
1:C:71:LEU:HD22	1:C:331:SER:HB2	1.96	0.46
1:C:140:ASP:OD1	1:C:140:ASP:O	2.33	0.46
1:C:142:LYS:HA	1:C:142:LYS:HD2	1.60	0.46
1:D:406:ASP:HB3	1:D:409:SER:HB2	1.97	0.46
1:D:774:TYR:HA	1:D:777:LYS:HB3	1.96	0.46
1:D:207:ASP:HB2	1:D:210:ASP:OD1	2.16	0.46
1:A:444:VAL:HG12	1:A:464:ILE:HG12	1.97	0.46
1:C:829:ALA:HA	1:C:832:VAL:HG22	1.97	0.46
1:B:254:TYR:HB3	1:B:256:PHE:HE1	1.81	0.46
1:C:643:PHE:HA	1:C:646:ILE:HG22	1.98	0.46
1:D:541:LEU:HB3	1:D:735:PHE:HB3	1.97	0.46
1:A:750:CYS:HB2	7:A:1003:NAG:H82	1.98	0.46
1:B:438:ILE:HG12	1:B:488:TYR:HE1	1.81	0.46
1:A:447:LYS:HE3	1:A:460:GLU:HB3	1.97	0.46
1:A:680:ILE:HG13	1:A:682:TYR:CE1	2.50	0.46
1:B:71:LEU:HD23	1:B:76:LEU:HD11	1.97	0.46
1:C:558:PRO:HB3	1:C:654:ASN:HB3	1.97	0.46
1:D:210:ASP:O	1:D:213:PRO:HD2	2.16	0.46
1:A:281:ILE:HD11	1:A:384:ARG:HH22	1.81	0.46
1:A:332:VAL:HG21	1:A:368:TRP:HB2	1.98	0.46
1:A:442:PRO:HB3	1:A:744:PHE:CD2	2.51	0.46
1:C:145:PHE:C	1:C:360:MET:HE1	2.41	0.46
1:D:790:LYS:HA	1:D:793:MET:SD	2.56	0.46
1:B:192:PRO:HG3	1:B:199:LEU:HD13	1.98	0.46
1:C:250:GLU:HB3	1:C:773:PRO:HG3	1.97	0.46
1:C:639:ILE:HD11	1:D:827:LEU:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LEU:HD21	1:D:195:TYR:HE2	1.80	0.46
1:A:703:ASP:HA	1:A:706:TRP:CE2	2.51	0.45
1:B:166:PHE:CE2	1:B:413:MET:HE1	2.51	0.45
1:B:491:GLN:HB2	1:B:498:TRP:CE2	2.51	0.45
1:B:811:GLU:HG3	1:B:814:ALA:HB3	1.97	0.45
1:D:541:LEU:HD22	1:D:742:ILE:HG22	1.99	0.45
1:C:300:ARG:NH2	1:C:305:PRO:HD3	2.31	0.45
1:D:559:LEU:HG	1:D:651:TYR:HD1	1.81	0.45
1:B:781:ALA:O	1:B:784:GLN:HG3	2.16	0.45
1:C:343:SER:HB2	1:C:345:LEU:HD21	1.97	0.45
1:C:256:PHE:HB3	1:C:258:THR:HG22	1.99	0.45
1:C:708:PHE:HD1	1:D:699:ILE:HD13	1.81	0.45
1:D:169:TRP:HZ2	1:D:253:HIS:CG	2.34	0.45
1:B:708:PHE:HA	1:C:699:ILE:HG13	1.97	0.45
1:A:85:LEU:HD12	1:A:111:HIS:HB3	1.99	0.45
1:C:215:LEU:HD22	1:C:247:MET:HE1	1.98	0.45
1:C:817:VAL:HG12	1:C:819:ASN:H	1.82	0.45
1:A:520:THR:HG22	1:A:523:ARG:HD2	1.99	0.45
1:C:70:LEU:HD23	4:L:1:NAG:H5	1.97	0.45
1:C:322:LEU:HD23	1:C:322:LEU:HA	1.85	0.45
1:C:463:CYS:SG	1:C:514:VAL:HG12	2.57	0.45
1:C:43:GLU:HB2	1:C:85:LEU:HD13	1.98	0.44
1:C:123:ASN:HA	1:C:145:PHE:HB2	1.99	0.44
1:D:153:PHE:CG	1:D:184:ARG:HB2	2.52	0.44
1:D:442:PRO:HB3	1:D:748:ARG:HH22	1.82	0.44
1:D:459:PHE:C	1:D:464:ILE:HG13	2.42	0.44
1:B:345:LEU:HD21	1:B:353:TRP:CD1	2.52	0.44
1:C:232:HIS:HB3	1:C:260:ASP:OD1	2.17	0.44
1:C:702:TYR:CZ	1:C:759:ILE:HG23	2.52	0.44
1:C:519:ILE:HG22	1:C:529:PHE:CG	2.52	0.44
1:D:411:LEU:HD23	1:D:411:LEU:HA	1.83	0.44
1:D:556:LEU:HB3	1:D:564:TRP:NE1	2.32	0.44
1:B:261:LEU:HG	1:B:278:GLY:HA3	1.99	0.44
1:C:198:ARG:NH2	1:D:198:ARG:HD2	2.33	0.44
1:B:520:THR:H	1:B:523:ARG:HB2	1.82	0.44
1:D:282:LEU:HD12	1:D:282:LEU:HA	1.84	0.44
1:D:489:GLY:H	1:D:501:MET:HE1	1.82	0.44
1:A:172:VAL:HG13	1:A:199:LEU:HD12	2.00	0.44
1:B:645:LEU:HD21	1:C:648:ILE:HG12	2.00	0.44
1:C:386:ASP:HA	1:C:407:PRO:HG3	2.00	0.44
1:D:346:GLN:HE21	1:D:349:ARG:HB2	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:LYS:O	1:A:794:MET:HG3	2.18	0.44
1:B:833:LEU:HD12	1:B:834:SER:N	2.33	0.44
1:C:691:MET:HE3	1:C:691:MET:HB3	1.90	0.44
1:A:215:LEU:HA	1:A:218:MET:HB2	2.00	0.43
1:B:709:MET:HA	1:B:716:VAL:HG11	2.00	0.43
1:C:180:THR:HG22	1:D:136:HIS:CE1	2.52	0.43
1:C:639:ILE:HD13	1:D:830:GLY:HA3	1.99	0.43
1:C:668:ILE:HD13	1:C:668:ILE:HA	1.85	0.43
1:C:828:ALA:HA	1:C:831:LEU:HD23	2.00	0.43
1:D:527:ILE:HD13	1:D:527:ILE:HA	1.88	0.43
1:A:303:ALA:HB1	1:A:313:ASP:HB2	1.99	0.43
1:A:541:LEU:HB2	1:A:742:ILE:HD12	2.00	0.43
1:B:433:LEU:HD11	1:B:512:LEU:HD23	1.99	0.43
1:C:462:TYR:HB2	1:C:798:TRP:CD1	2.53	0.43
1:A:235:ALA:HB1	1:A:256:PHE:HE2	1.82	0.43
1:A:517:LEU:HD12	1:A:517:LEU:HA	1.85	0.43
1:C:683:GLY:HA2	1:C:709:MET:SD	2.58	0.43
1:D:256:PHE:HB3	1:D:258:THR:HG22	1.99	0.43
1:A:790:LYS:HD3	1:A:790:LYS:HA	1.66	0.43
1:A:800:ARG:NH1	1:A:800:ARG:HA	2.33	0.43
1:B:290:SER:O	1:B:294:GLU:HG2	2.18	0.43
1:C:807:GLU:HG2	1:C:811:GLU:HG3	2.00	0.43
1:D:185:LEU:HD22	1:D:188:LEU:HD23	2.00	0.43
1:A:356:GLY:O	1:A:360:MET:HG2	2.18	0.43
1:A:673:ASP:HB3	1:D:678:THR:HG23	2.01	0.43
1:C:349:ARG:CZ	1:C:351:LYS:HB3	2.48	0.43
1:C:455:GLY:H	1:C:458:ARG:HD3	1.83	0.43
1:C:456:ASN:HB3	1:C:478:TYR:HE1	1.83	0.43
1:C:686:GLU:HG2	1:C:687:ASP:OD1	2.18	0.43
1:C:124:ALA:HB1	1:C:350:HIS:NE2	2.33	0.43
1:C:181:GLY:HA2	1:C:184:ARG:HD2	2.00	0.43
1:D:686:GLU:HA	1:D:717:LEU:HD13	2.00	0.43
1:B:64:ILE:HD12	1:B:76:LEU:HD13	1.99	0.43
1:B:691:MET:O	1:B:695:LYS:HG2	2.19	0.43
1:D:151:PRO:HB3	1:D:387:PHE:CE2	2.54	0.43
1:A:255:ILE:HA	1:A:277:THR:O	2.18	0.43
1:C:270:ARG:CD	1:C:398:GLY:H	2.32	0.43
1:C:768:THR:HA	1:C:769:PRO:HD3	1.89	0.43
1:D:459:PHE:HB2	1:D:464:ILE:HD11	1.99	0.43
2:E:1:NAG:H61	2:E:2:NAG:C7	2.49	0.43
1:A:183:ILE:HD13	1:A:183:ILE:HA	1.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG11	1:A:399:LEU:HD21	2.00	0.43
1:A:306:LYS:HB2	1:A:309:SER:HB3	2.00	0.43
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.86	0.43
1:A:815:LEU:HB3	1:A:819:ASN:HB3	2.00	0.43
1:B:820:ILE:HD12	1:B:820:ILE:H	1.84	0.43
1:C:71:LEU:HG	1:C:74:THR:HB	2.00	0.43
1:C:737:MET:HE2	1:C:742:ILE:HG13	2.00	0.43
1:C:760:ASP:OD1	1:C:760:ASP:C	2.62	0.43
1:C:790:LYS:O	1:C:794:MET:HG2	2.19	0.43
1:A:791:LEU:HD23	1:A:791:LEU:HA	1.81	0.43
1:B:281:ILE:HD13	1:B:389:LEU:HD23	1.99	0.43
1:D:515:ALA:HB3	1:D:517:LEU:HD23	2.01	0.43
1:C:78:TYR:HD2	1:C:80:THR:HG23	1.84	0.42
1:C:448:LYS:HA	1:C:448:LYS:HD3	1.79	0.42
1:C:674:LEU:HB3	1:C:682:TYR:CD2	2.54	0.42
1:D:85:LEU:HD13	1:D:111:HIS:HB2	2.00	0.42
1:D:799:TRP:O	1:D:799:TRP:CG	2.72	0.42
1:A:126:GLY:HA2	1:A:145:PHE:CE2	2.54	0.42
1:A:286:ASN:HB3	1:A:289:VAL:HG22	2.01	0.42
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.93	0.42
1:A:438:ILE:HD11	1:A:488:TYR:CZ	2.54	0.42
1:A:654:ASN:HD22	1:B:815:LEU:HD22	1.83	0.42
1:B:300:ARG:HD2	1:B:300:ARG:HA	1.72	0.42
1:C:42:PHE:CE2	1:C:323:MET:HE3	2.55	0.42
1:C:200:LYS:HE3	1:C:200:LYS:HB2	1.66	0.42
1:C:306:LYS:HG3	1:C:308:ASP:H	1.83	0.42
1:C:677:GLN:HE22	1:C:680:ILE:H	1.65	0.42
1:A:823:ILE:HG13	1:D:646:ILE:HG21	2.01	0.42
1:B:772:SER:O	1:B:775:ARG:HG2	2.19	0.42
1:C:211:ALA:H	1:C:241:GLN:HE22	1.67	0.42
1:D:160:ILE:HG13	1:D:257:THR:HG22	2.01	0.42
1:D:379:LYS:H	1:D:379:LYS:HG2	1.68	0.42
1:D:794:MET:H	1:D:794:MET:CE	2.26	0.42
1:A:698:LYS:HA	1:A:698:LYS:HD3	1.87	0.42
1:B:561:PRO:O	1:B:565:MET:HG2	2.19	0.42
1:B:779:THR:O	1:B:782:ILE:HG22	2.20	0.42
1:C:122:CYS:SG	1:C:129:HIS:HB2	2.59	0.42
1:C:776:ASP:O	1:C:779:THR:HG22	2.20	0.42
1:D:346:GLN:HE22	1:D:348:ASN:HB2	1.85	0.42
1:A:85:LEU:HD11	1:A:109:PRO:HB2	2.01	0.42
1:B:41:ILE:HD11	1:B:106:ILE:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:O	1:B:64:ILE:HG12	2.19	0.42
1:B:64:ILE:HG22	1:B:70:LEU:HD23	2.01	0.42
1:C:385:THR:HB	2:N:1:NAG:H82	2.01	0.42
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.76	0.42
1:A:261:LEU:HD23	1:A:392:ILE:HD11	2.01	0.42
1:B:96:CYS:HB3	1:B:347:CYS:HB3	1.48	0.42
1:C:506:ILE:HD12	1:C:506:ILE:HA	1.83	0.42
1:D:798:TRP:HD1	1:D:801:GLY:H	1.68	0.42
1:A:516:PRO:HA	1:A:764:TYR:CE1	2.54	0.42
1:A:540:ILE:HB	1:A:755:ILE:HB	2.00	0.42
1:B:276:MET:HE3	1:B:394:LEU:HD12	2.00	0.42
1:C:41:ILE:O	1:C:41:ILE:HG13	2.19	0.42
1:C:300:ARG:HA	1:C:302:GLN:HE21	1.84	0.42
1:A:185:LEU:O	1:A:189:ILE:HG12	2.20	0.42
1:D:781:ALA:O	1:D:784:GLN:HG3	2.19	0.42
1:A:260:ASP:HB3	1:A:318:THR:H	1.84	0.42
1:A:543:ARG:HH11	1:A:729:LEU:HA	1.85	0.42
1:B:668:ILE:HD12	1:B:674:LEU:HD13	2.01	0.42
1:B:441:GLU:CD	1:B:442:PRO:HD3	2.44	0.42
1:B:750:CYS:HB3	1:B:804:CYS:HB3	1.73	0.41
1:C:777:LYS:HB3	1:C:777:LYS:HE2	1.84	0.41
1:A:71:LEU:HD21	1:A:75:THR:HA	2.01	0.41
1:B:44:TYR:HA	1:B:82:LYS:HB3	2.02	0.41
1:B:71:LEU:HD12	1:B:71:LEU:HA	1.92	0.41
1:C:83:ILE:HD12	1:C:94:LYS:HG2	2.01	0.41
1:D:538:ILE:HD11	1:D:762:LYS:HE2	2.02	0.41
1:D:747:GLN:O	1:D:803:GLY:HA3	2.20	0.41
1:A:43:GLU:HA	1:A:85:LEU:HD23	2.02	0.41
1:A:239:LEU:HD11	1:A:276:MET:HE1	2.01	0.41
1:B:694:PHE:CZ	1:B:705:MET:HE1	2.54	0.41
1:C:248:MET:HE1	1:C:274:VAL:HG11	2.02	0.41
1:D:177:ASP:OD1	1:D:177:ASP:C	2.62	0.41
1:A:147:VAL:HB	1:A:377:PHE:CE1	2.56	0.41
1:B:678:THR:OG1	1:C:701:THR:HG21	2.20	0.41
1:B:685:VAL:HA	1:B:718:VAL:O	2.20	0.41
1:C:218:MET:HE2	1:C:218:MET:HB2	2.00	0.41
1:A:378:ASN:ND2	1:A:381:ASN:HD21	2.18	0.41
1:A:715:SER:HA	1:A:727:ARG:NH1	2.35	0.41
1:A:829:ALA:O	1:A:833:LEU:HD12	2.20	0.41
1:B:462:TYR:HE2	1:B:533:PHE:HE2	1.68	0.41
1:C:694:PHE:HB3	1:C:706:TRP:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:HD11	1:D:76:LEU:HD11	2.01	0.41
1:D:448:LYS:HD2	1:D:448:LYS:HA	1.85	0.41
2:N:2:NAG:H61	2:N:3:NAG:H82	2.03	0.41
1:A:70:LEU:HD12	1:A:71:LEU:N	2.36	0.41
1:A:463:CYS:HA	1:A:466:LEU:HB3	2.03	0.41
1:B:153:PHE:CG	1:B:184:ARG:HB2	2.54	0.41
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.96	0.41
1:B:420:LYS:HD2	1:B:423:ASN:HB2	2.03	0.41
1:A:94:LYS:HA	1:A:94:LYS:HD2	1.85	0.41
1:A:177:ASP:OD1	1:A:177:ASP:C	2.63	0.41
1:B:282:LEU:HD22	1:B:284:THR:HG22	2.01	0.41
1:B:657:ALA:O	1:B:661:VAL:HG22	2.21	0.41
1:B:684:ALA:H	1:B:717:LEU:HD12	1.85	0.41
1:B:248:MET:SD	1:B:274:VAL:HG11	2.61	0.41
1:C:106:ILE:HD13	1:C:106:ILE:HA	1.88	0.41
1:C:563:ILE:HA	1:C:566:TYR:HB2	2.02	0.41
1:D:298:MET:HE2	1:D:298:MET:C	2.45	0.41
1:A:289:VAL:O	1:A:293:ILE:HG12	2.21	0.41
1:A:639:ILE:HD12	1:A:639:ILE:HA	1.92	0.41
1:A:677:GLN:NE2	1:A:679:LYS:HB3	2.36	0.41
1:B:533:PHE:H	1:B:533:PHE:HD1	1.67	0.41
1:C:191:ALA:HA	1:C:194:ARG:HH12	1.86	0.41
1:C:283:ASN:O	1:C:289:VAL:HG21	2.20	0.41
1:C:685:VAL:HG23	1:C:688:GLY:HA3	2.03	0.41
1:C:742:ILE:HG21	1:C:754:GLN:HG3	2.03	0.41
1:D:98:GLN:HB3	1:D:103:VAL:HG11	2.03	0.41
1:D:329:VAL:HG21	1:D:377:PHE:HE2	1.85	0.41
1:D:664:MET:HE2	1:D:664:MET:HB3	1.70	0.41
1:D:737:MET:SD	1:D:742:ILE:HG23	2.61	0.41
1:B:768:THR:HB	1:B:772:SER:HB2	2.02	0.41
1:D:516:PRO:HA	1:D:764:TYR:CE1	2.56	0.41
1:D:525:LYS:HB2	1:D:525:LYS:HE2	1.89	0.41
1:D:556:LEU:HD22	1:D:564:TRP:CZ2	2.56	0.41
1:A:62:ASN:O	1:A:66:ARG:HG2	2.21	0.40
1:A:126:GLY:HA2	1:A:145:PHE:HE2	1.87	0.40
1:A:534:MET:HE3	1:A:534:MET:HB2	1.78	0.40
1:A:640:TRP:O	1:A:644:THR:HG22	2.21	0.40
1:A:727:ARG:HA	1:A:727:ARG:HD2	1.93	0.40
1:B:742:ILE:H	1:B:742:ILE:HG13	1.62	0.40
1:D:433:LEU:HD12	1:D:476:PHE:HB2	2.02	0.40
1:D:537:GLY:HA3	1:D:758:LEU:HD12	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:SER:HB3	1:B:183:ILE:HG23	2.03	0.40
1:C:222:LYS:HD3	1:C:222:LYS:HA	1.71	0.40
1:D:674:LEU:HA	1:D:677:GLN:HE21	1.87	0.40
1:A:37:ARG:HH21	1:A:102:GLY:H	1.69	0.40
1:A:224:PHE:HA	1:A:252:TYR:HD1	1.86	0.40
1:A:742:ILE:HD13	1:A:742:ILE:HA	1.89	0.40
1:B:541:LEU:HD22	1:B:742:ILE:HG23	2.02	0.40
1:A:420:LYS:HB2	1:A:420:LYS:HE3	1.88	0.40
1:B:531:LYS:NZ	1:B:783:LEU:HG	2.33	0.40
1:B:735:PHE:HD2	1:B:737:MET:HE2	1.86	0.40
1:C:797:LYS:HD2	1:C:798:TRP:NE1	2.36	0.40
1:C:829:ALA:O	1:C:833:LEU:HD23	2.21	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	753/908 (83%)	732 (97%)	21 (3%)	0	100	100
1	B	757/908 (83%)	712 (94%)	45 (6%)	0	100	100
1	C	757/908 (83%)	723 (96%)	34 (4%)	0	100	100
1	D	754/908 (83%)	710 (94%)	44 (6%)	0	100	100
All	All	3021/3632 (83%)	2877 (95%)	144 (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	652/794 (82%)	631 (97%)	21 (3%)	34	56
1	B	655/794 (82%)	631 (96%)	24 (4%)	30	54
1	C	655/794 (82%)	631 (96%)	24 (4%)	30	54
1	D	653/794 (82%)	633 (97%)	20 (3%)	35	57
All	All	2615/3176 (82%)	2526 (97%)	89 (3%)	33	56

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PHE
1	A	83	ILE
1	A	106	ILE
1	A	122	CYS
1	A	171	THR
1	A	172	VAL
1	A	182	LEU
1	A	226	VAL
1	A	258	THR
1	A	259	LEU
1	A	274	VAL
1	A	277	THR
1	A	315	PHE
1	A	391	VAL
1	A	434	ILE
1	A	646	ILE
1	A	664	MET
1	A	676	CYS
1	A	685	VAL
1	A	736	LEU
1	A	835	VAL
1	B	85	LEU
1	B	122	CYS
1	B	127	VAL
1	B	258	THR
1	B	262	PHE
1	B	362	LEU
1	B	391	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	417	GLN
1	B	438	ILE
1	B	440	GLU
1	B	444	VAL
1	B	501	MET
1	B	512	LEU
1	B	538	ILE
1	B	557	ASN
1	B	664	MET
1	B	680	ILE
1	B	705	MET
1	B	715	SER
1	B	742	ILE
1	B	764	TYR
1	B	770	MET
1	B	791	LEU
1	B	820	ILE
1	C	35	VAL
1	C	76	LEU
1	C	172	VAL
1	C	180	THR
1	C	239	LEU
1	C	255	ILE
1	C	262	PHE
1	C	264	LEU
1	C	274	VAL
1	C	302	GLN
1	C	342	VAL
1	C	391	VAL
1	C	505	LEU
1	C	506	ILE
1	C	520	THR
1	C	566	TYR
1	C	705	MET
1	C	716	VAL
1	C	742	ILE
1	C	768	THR
1	C	778	ILE
1	C	779	THR
1	C	791	LEU
1	C	827	LEU
1	D	50	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	106	ILE
1	D	122	CYS
1	D	153	PHE
1	D	226	VAL
1	D	258	THR
1	D	274	VAL
1	D	276	MET
1	D	294	GLU
1	D	327	VAL
1	D	355	PHE
1	D	391	VAL
1	D	399	LEU
1	D	439	LEU
1	D	517	LEU
1	D	664	MET
1	D	665	GLU
1	D	764	TYR
1	D	766	VAL
1	D	833	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	141	ASN
1	A	253	HIS
1	A	346	GLN
1	A	491	GLN
1	A	819	ASN
1	B	111	HIS
1	B	346	GLN
1	B	367	HIS
1	B	677	GLN
1	C	129	HIS
1	C	186	GLN
1	C	423	ASN
1	D	111	HIS
1	D	346	GLN
1	D	348	ASN
1	D	508	HIS
1	D	549	ASN
1	D	747	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 ⓘ

34 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.76	0	17,19,21	0.94	0
2	NAG	E	2	2	14,14,15	0.67	0	17,19,21	1.03	0
2	NAG	E	3	2	14,14,15	0.74	0	17,19,21	0.87	0
3	NAG	F	1	1,3	14,14,15	0.71	0	17,19,21	1.20	1 (5%)
3	BMA	F	2	3	11,11,12	0.79	0	15,15,17	2.77	5 (33%)
3	NAG	F	3	3	14,14,15	0.71	0	17,19,21	0.88	0
4	NAG	G	1	1,4	14,14,15	0.72	0	17,19,21	0.80	0
4	NAG	G	2	4	14,14,15	0.70	0	17,19,21	0.78	0
2	NAG	H	1	1,2	14,14,15	0.69	0	17,19,21	0.89	0
2	NAG	H	2	2	14,14,15	0.71	0	17,19,21	0.94	0
2	NAG	H	3	2	14,14,15	0.73	0	17,19,21	0.82	0
4	NAG	I	1	1,4	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
4	NAG	I	2	4	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	J	1	1,4	14,14,15	0.74	0	17,19,21	1.00	0
4	NAG	J	2	4	14,14,15	0.74	0	17,19,21	0.85	1 (5%)
5	NAG	K	1	1,5	14,14,15	0.73	0	17,19,21	0.81	0
5	BMA	K	2	5	11,11,12	0.84	0	15,15,17	2.07	3 (20%)
4	NAG	L	1	1,4	14,14,15	0.74	0	17,19,21	1.63	2 (11%)
4	NAG	L	2	4	14,14,15	0.76	1 (7%)	17,19,21	1.99	3 (17%)
4	NAG	M	1	1,4	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
4	NAG	M	2	4	14,14,15	0.72	0	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	N	1	1,2	14,14,15	0.68	0	17,19,21	2.16	4 (23%)
2	NAG	N	2	2	14,14,15	0.72	0	17,19,21	0.97	0
2	NAG	N	3	2	14,14,15	0.73	0	17,19,21	0.88	0
6	NAG	O	1	1,6	14,14,15	0.67	0	17,19,21	1.17	1 (5%)
6	NAG	O	2	6	14,14,15	0.75	0	17,19,21	1.00	0
6	BMA	O	3	6	11,11,12	0.86	0	15,15,17	2.03	3 (20%)
4	NAG	P	1	1,4	14,14,15	0.73	0	17,19,21	1.07	1 (5%)
4	NAG	P	2	4	14,14,15	0.74	0	17,19,21	0.89	0
4	NAG	Q	1	1,4	14,14,15	0.70	0	17,19,21	1.32	2 (11%)
4	NAG	Q	2	4	14,14,15	0.74	0	17,19,21	0.86	0
2	NAG	R	1	1,2	14,14,15	0.72	0	17,19,21	0.84	0
2	NAG	R	2	2	14,14,15	0.71	0	17,19,21	1.35	2 (11%)
2	NAG	R	3	2	14,14,15	0.81	0	17,19,21	1.15	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	3	2	-	1/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	BMA	F	2	3	-	1/2/19/22	0/1/1/1
3	NAG	F	3	3	-	1/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	3	2	-	0/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	BMA	K	2	5	-	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	3	2	-	0/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	3/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	3	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	2	NAG	C1-C2	2.08	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	BMA	C1-O5-C5	8.77	123.94	112.19
2	N	1	NAG	C1-O5-C5	7.09	121.69	112.19
4	L	2	NAG	C1-O5-C5	6.71	121.17	112.19
5	K	2	BMA	C1-O5-C5	6.11	120.38	112.19
6	O	3	BMA	C1-O5-C5	5.90	120.10	112.19
4	L	1	NAG	O5-C1-C2	-3.76	105.47	111.29
3	F	1	NAG	C1-O5-C5	3.66	117.09	112.19
4	L	1	NAG	C2-N2-C7	3.64	127.78	122.90
4	Q	1	NAG	C2-N2-C7	3.22	127.21	122.90
4	P	1	NAG	O5-C1-C2	-3.14	106.44	111.29
2	N	1	NAG	C4-C3-C2	-3.02	106.59	111.02
2	R	3	NAG	C2-N2-C7	2.92	126.81	122.90
2	R	2	NAG	O5-C1-C2	-2.91	106.79	111.29
3	F	2	BMA	C3-C4-C5	2.76	115.23	110.23
3	F	2	BMA	C1-C2-C3	2.71	113.59	109.64
6	O	3	BMA	C3-C4-C5	2.64	115.02	110.23
4	L	2	NAG	C3-C4-C5	-2.60	105.52	110.23
5	K	2	BMA	C3-C4-C5	2.59	114.93	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	2	NAG	O4-C4-C3	-2.58	104.30	110.38
4	M	1	NAG	O5-C1-C2	-2.51	107.41	111.29
3	F	2	BMA	O3-C3-C2	-2.46	105.04	110.05
4	Q	1	NAG	C1-O5-C5	2.45	115.47	112.19
2	N	1	NAG	O5-C1-C2	2.44	115.06	111.29
5	K	2	BMA	C2-C3-C4	2.33	114.96	110.86
6	O	1	NAG	C1-O5-C5	2.27	115.23	112.19
6	O	3	BMA	C2-C3-C4	2.27	114.85	110.86
2	N	1	NAG	O4-C4-C5	2.18	114.70	109.32
3	F	2	BMA	C2-C3-C4	2.14	114.63	110.86
4	L	2	NAG	C2-N2-C7	2.14	125.77	122.90
4	J	2	NAG	O5-C1-C2	-2.11	108.03	111.29
4	I	1	NAG	O5-C1-C2	-2.03	108.14	111.29
2	R	3	NAG	O5-C1-C2	-2.03	108.16	111.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

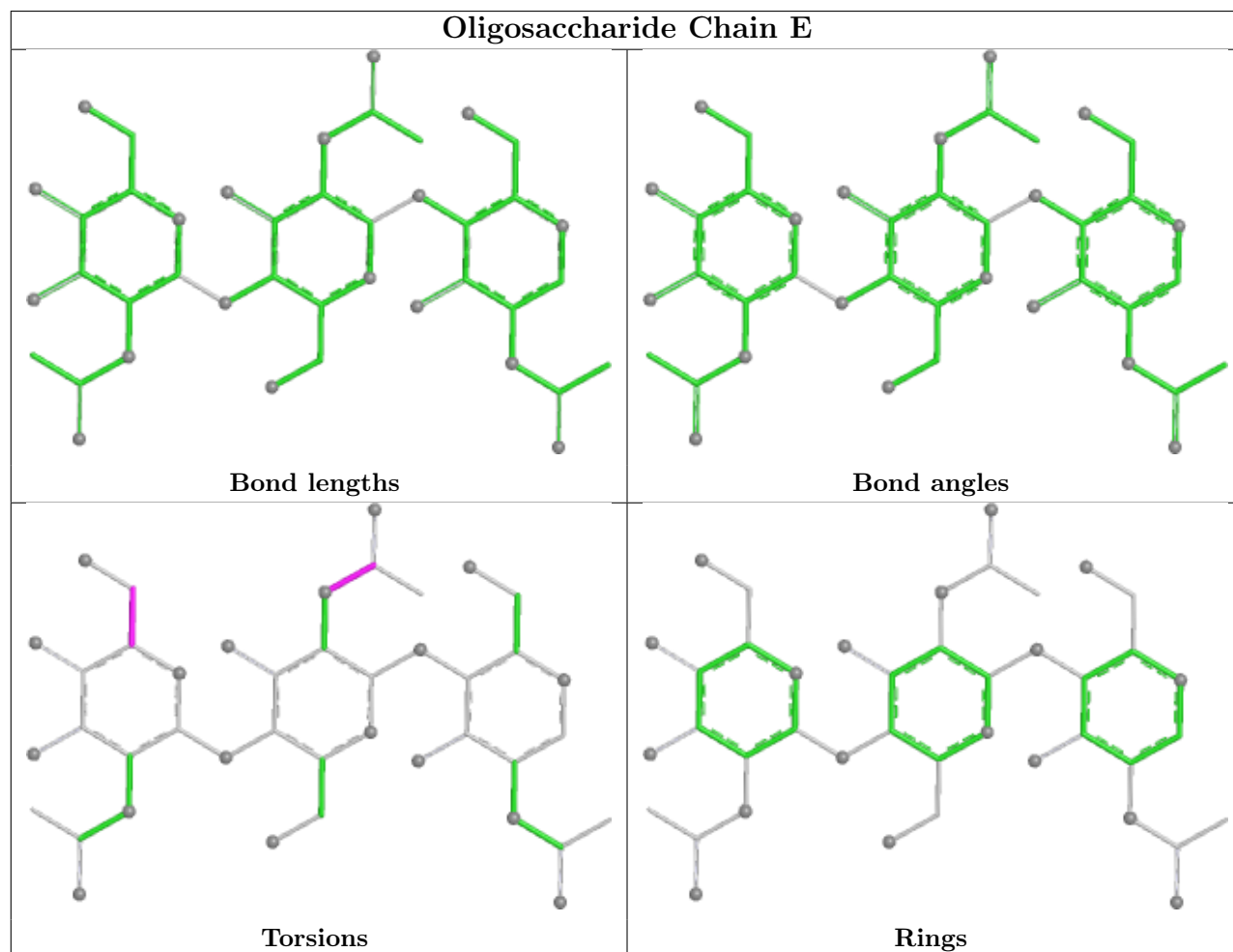
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	R	3	NAG	C8-C7-N2-C2
2	R	3	NAG	O7-C7-N2-C2
6	O	2	NAG	C8-C7-N2-C2
6	O	2	NAG	O7-C7-N2-C2
4	I	1	NAG	O5-C5-C6-O6
2	E	3	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	R	3	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
3	F	2	BMA	C4-C5-C6-O6
3	F	3	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C1-C2-N2-C7
4	Q	1	NAG	C1-C2-N2-C7
4	I	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7

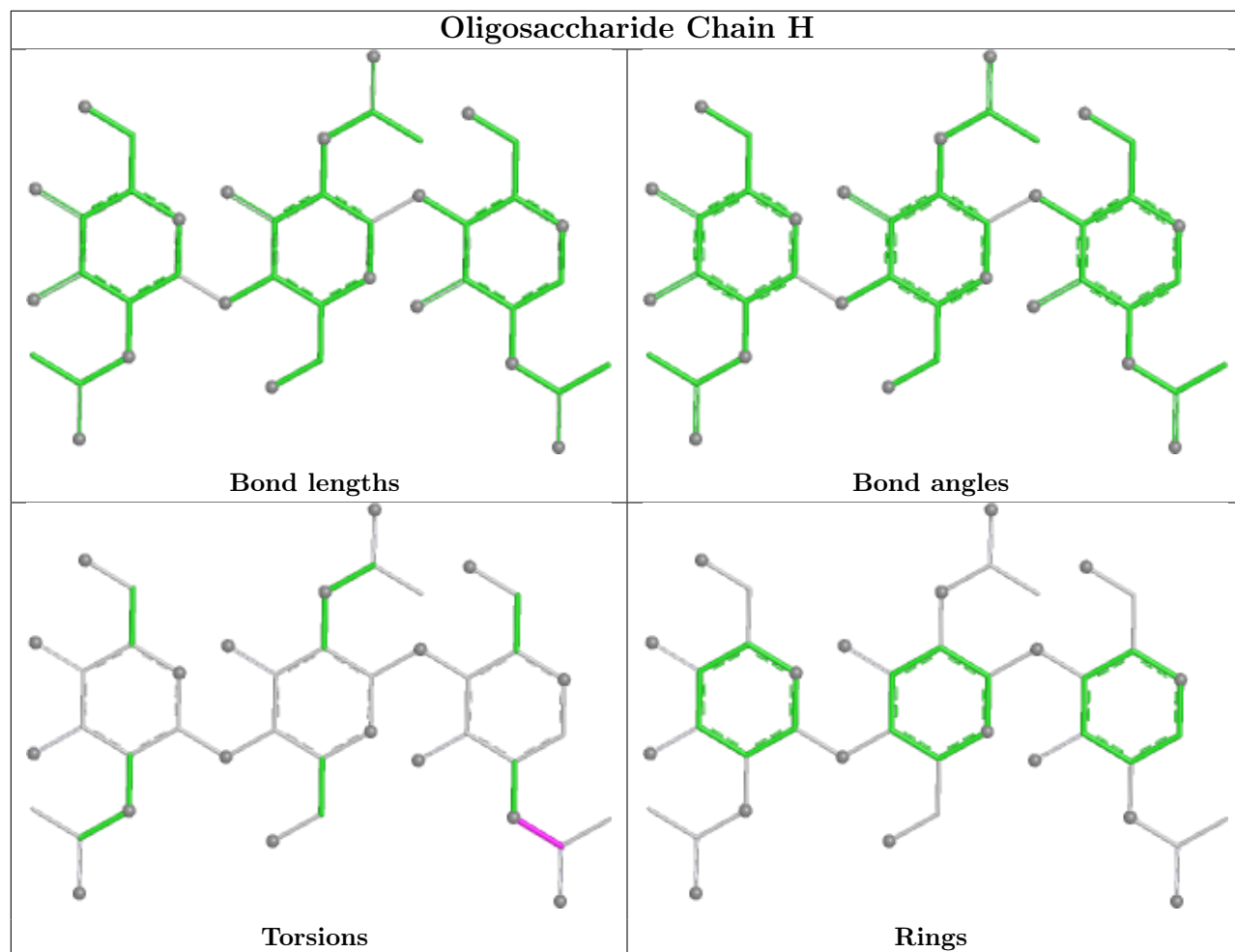
There are no ring outliers.

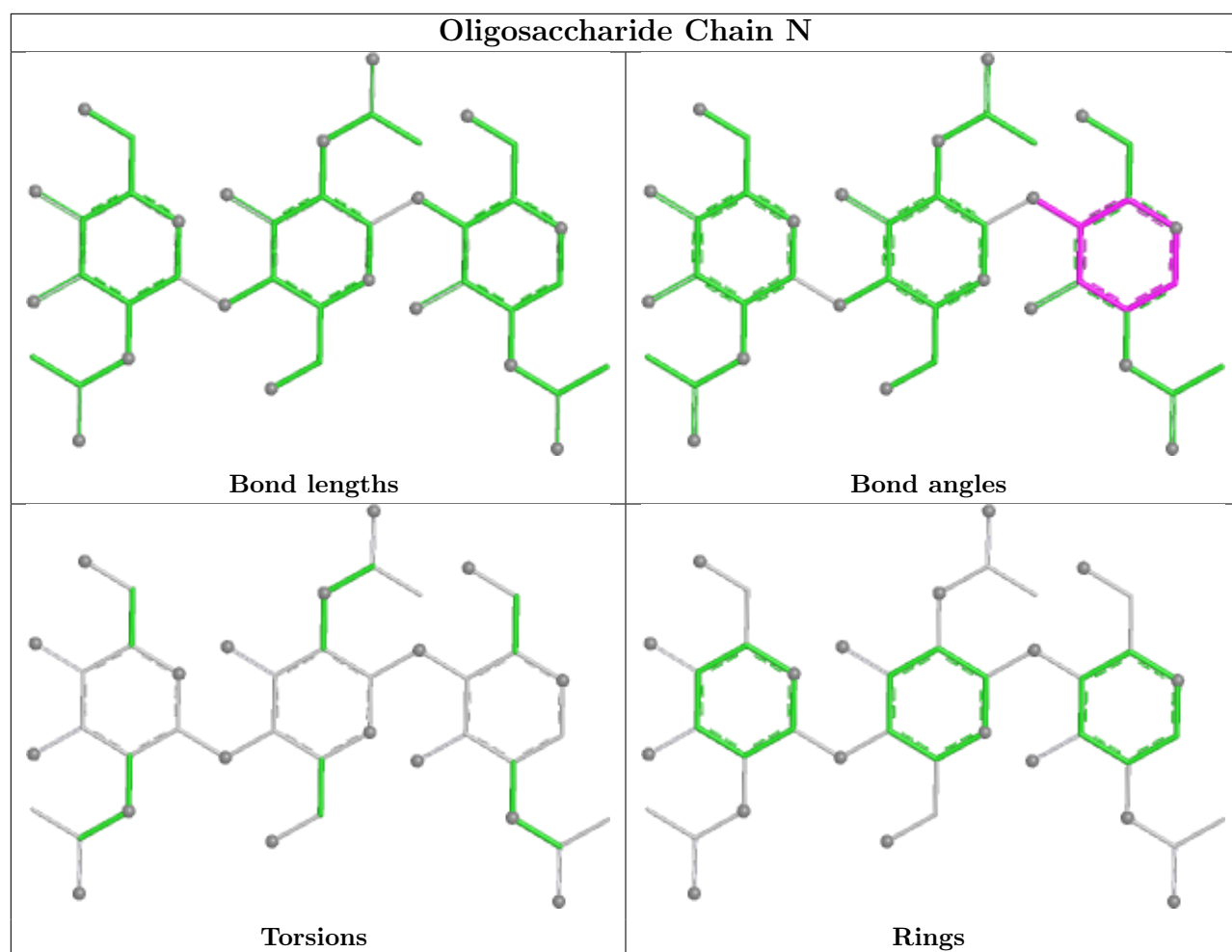
8 monomers are involved in 7 short contacts:

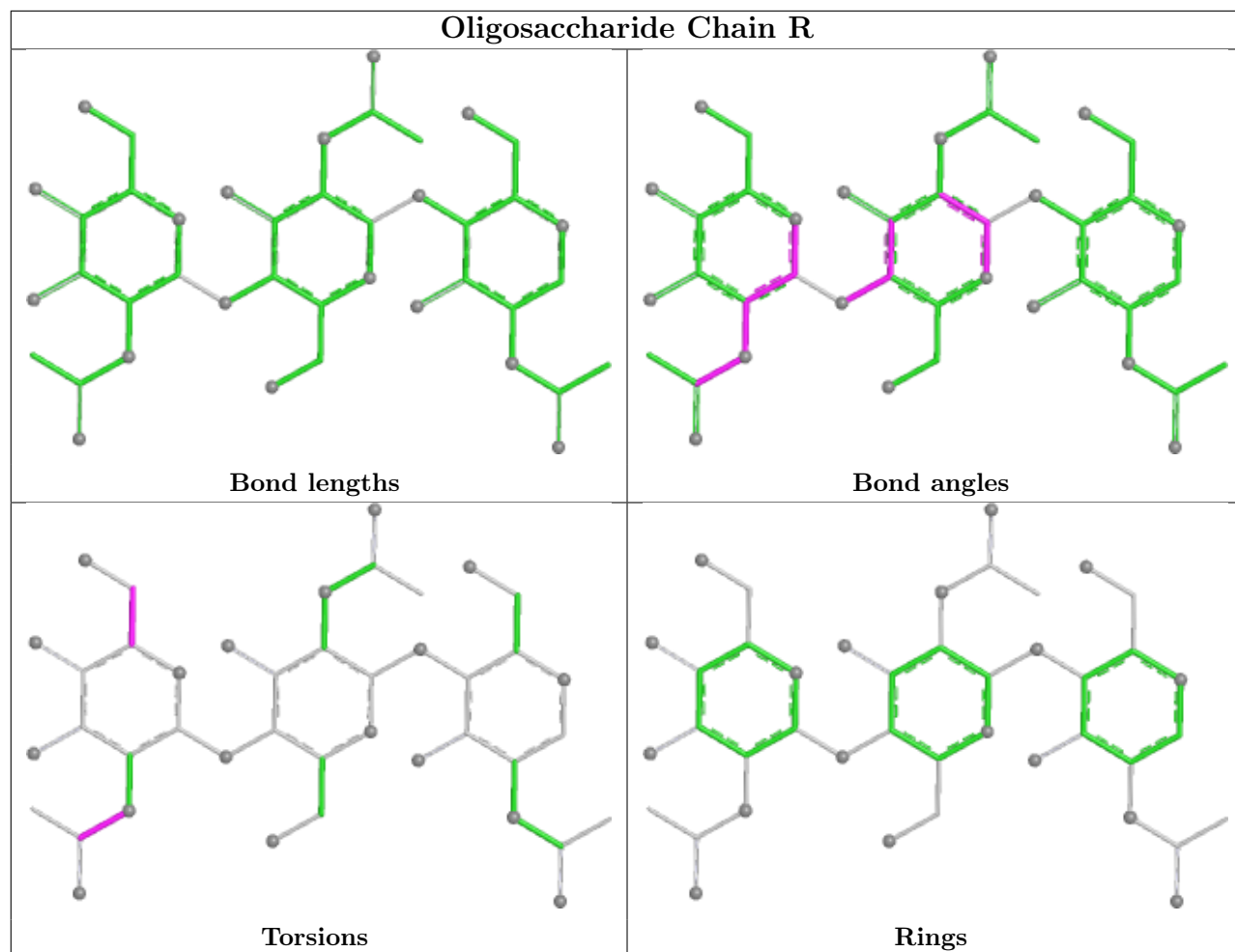
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
4	L	2	NAG	1	0
2	N	1	NAG	2	0
2	N	3	NAG	1	0
2	E	1	NAG	1	0
4	L	1	NAG	1	0
2	N	2	NAG	1	0
3	F	1	NAG	1	0

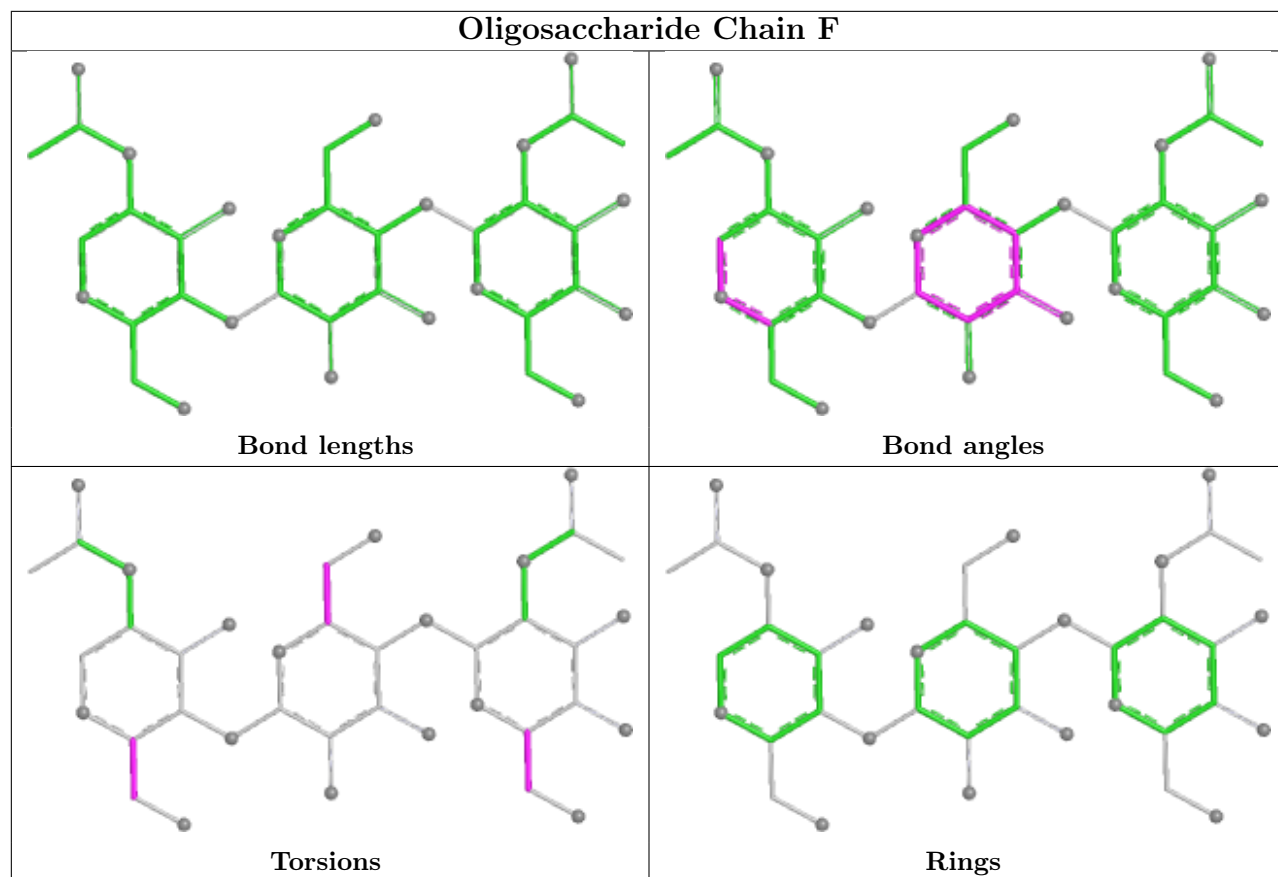
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

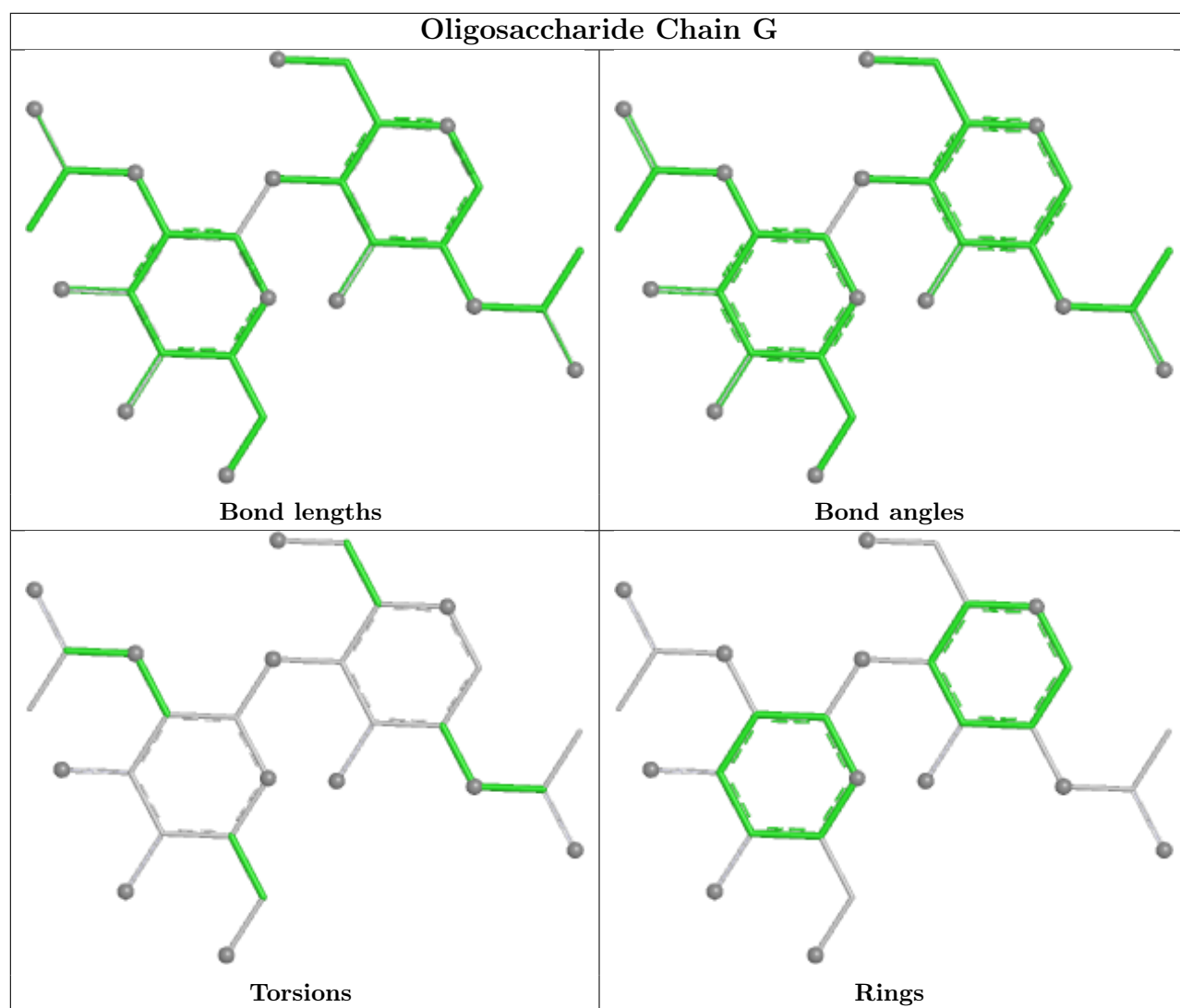


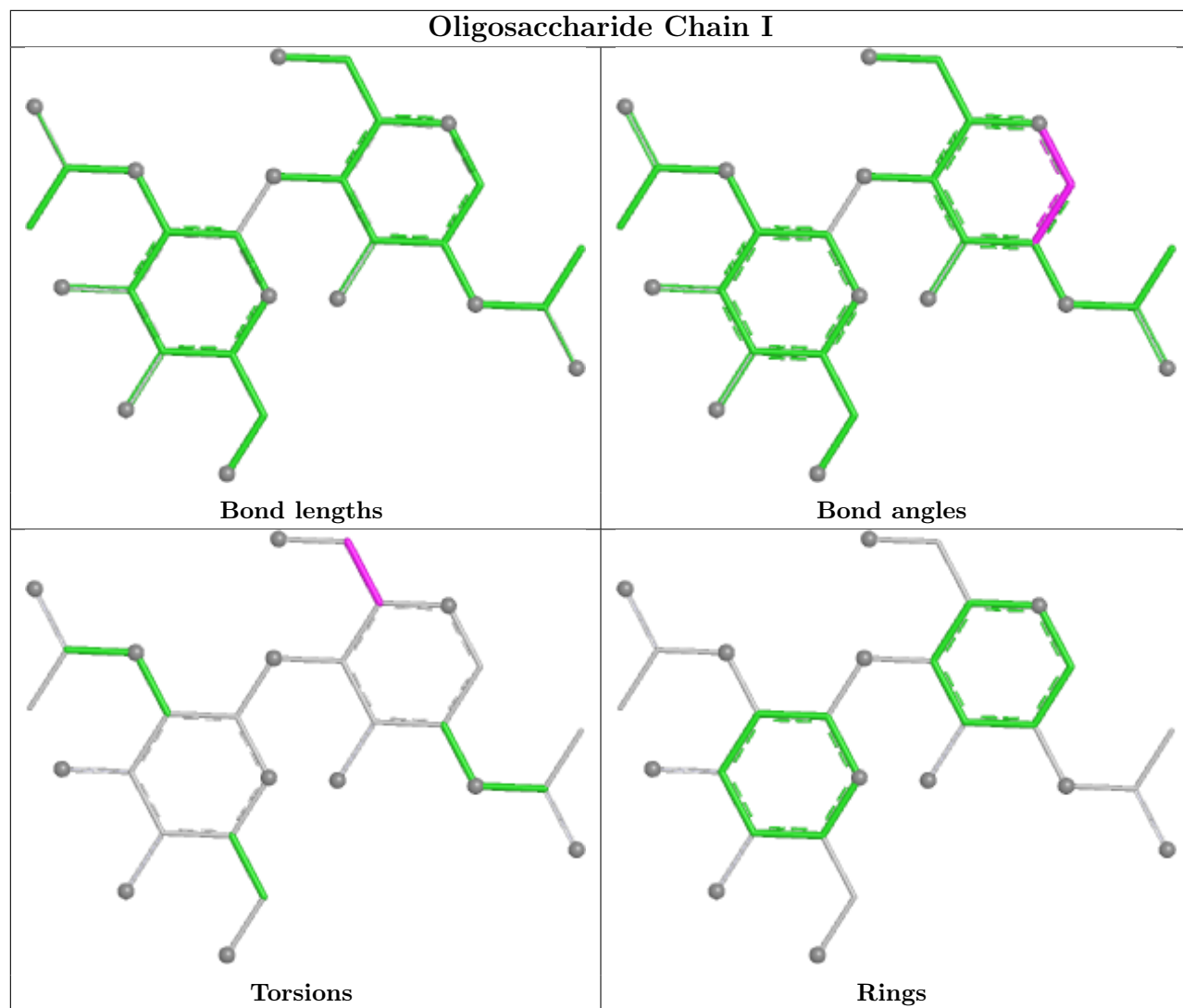


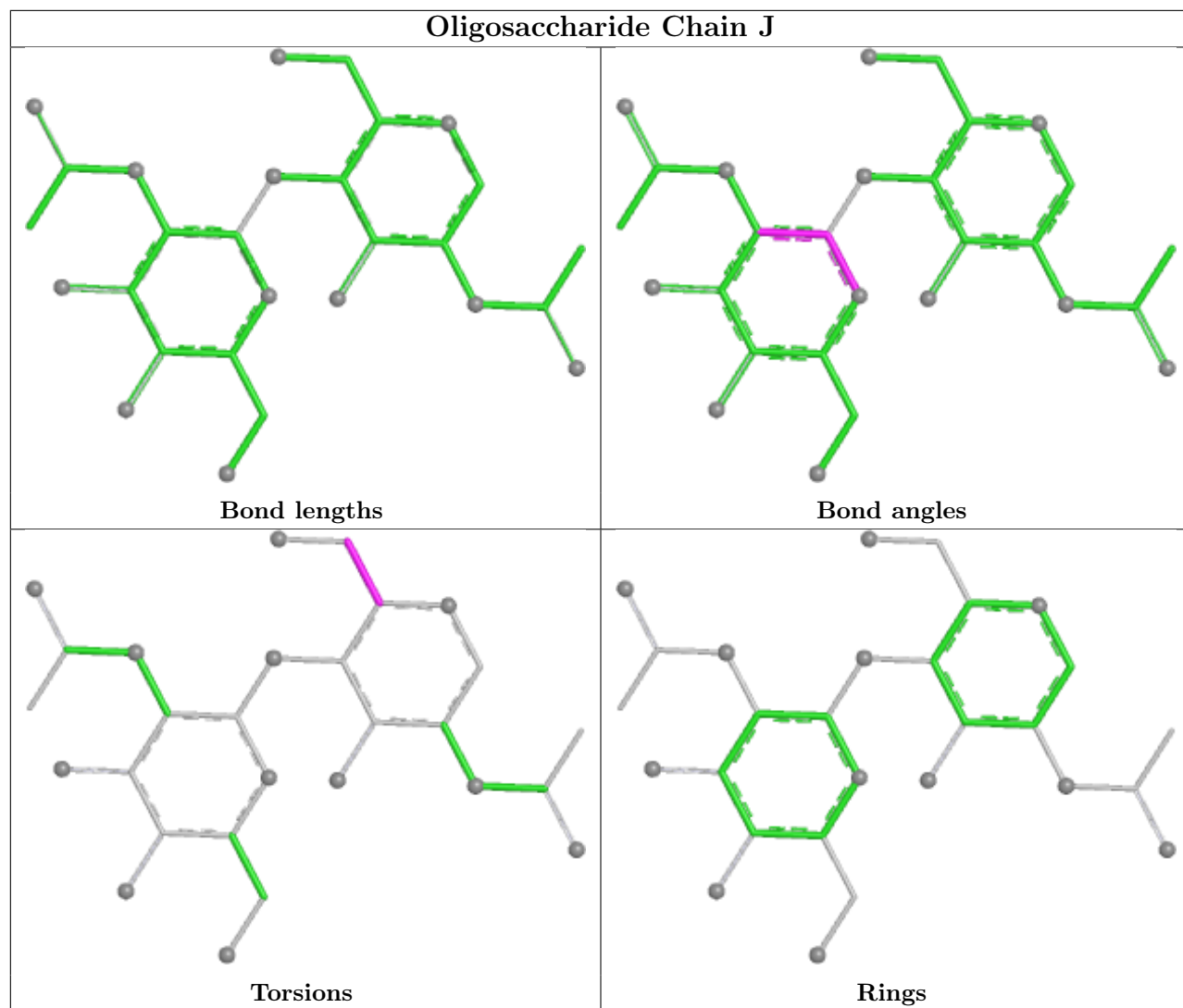


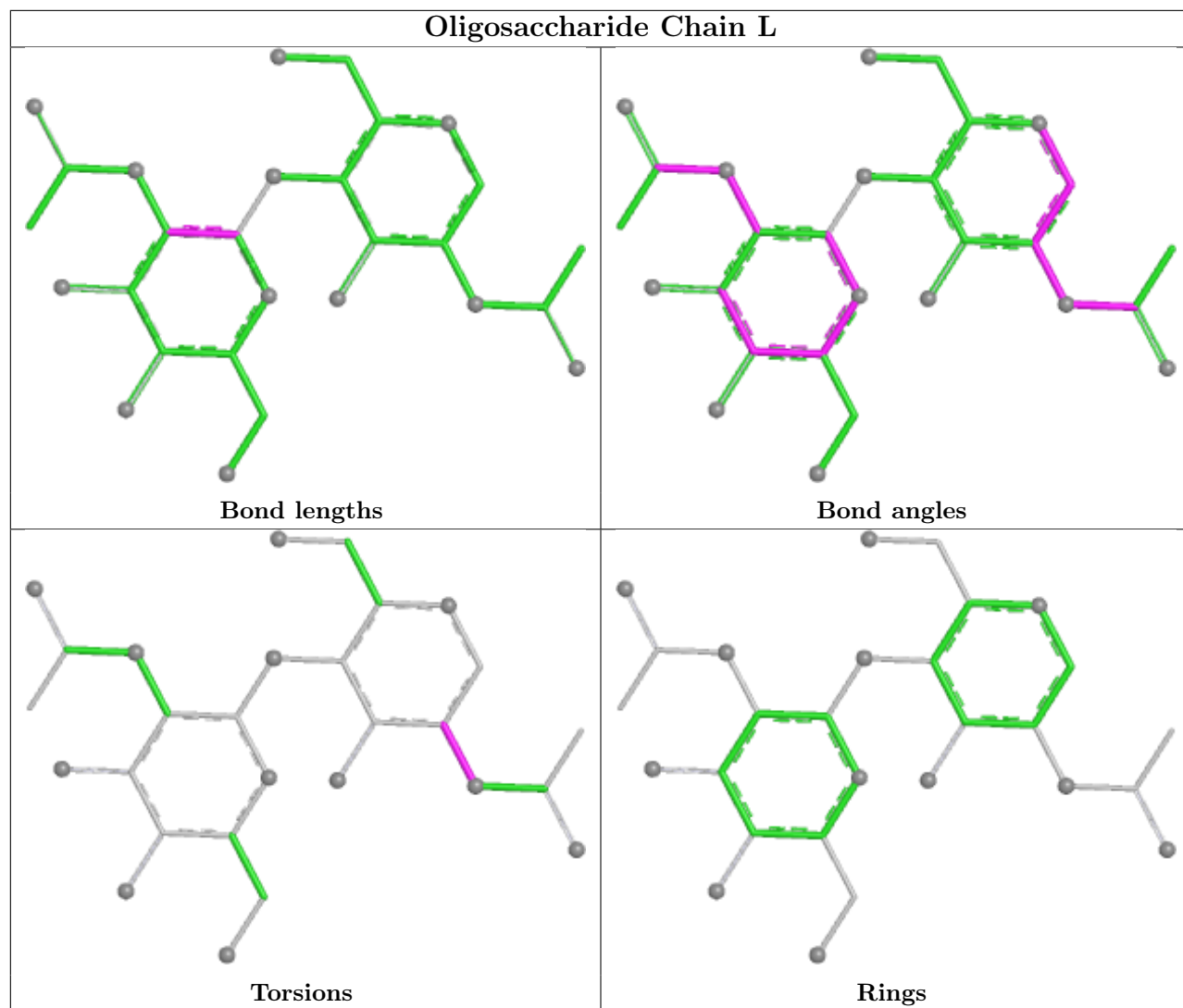


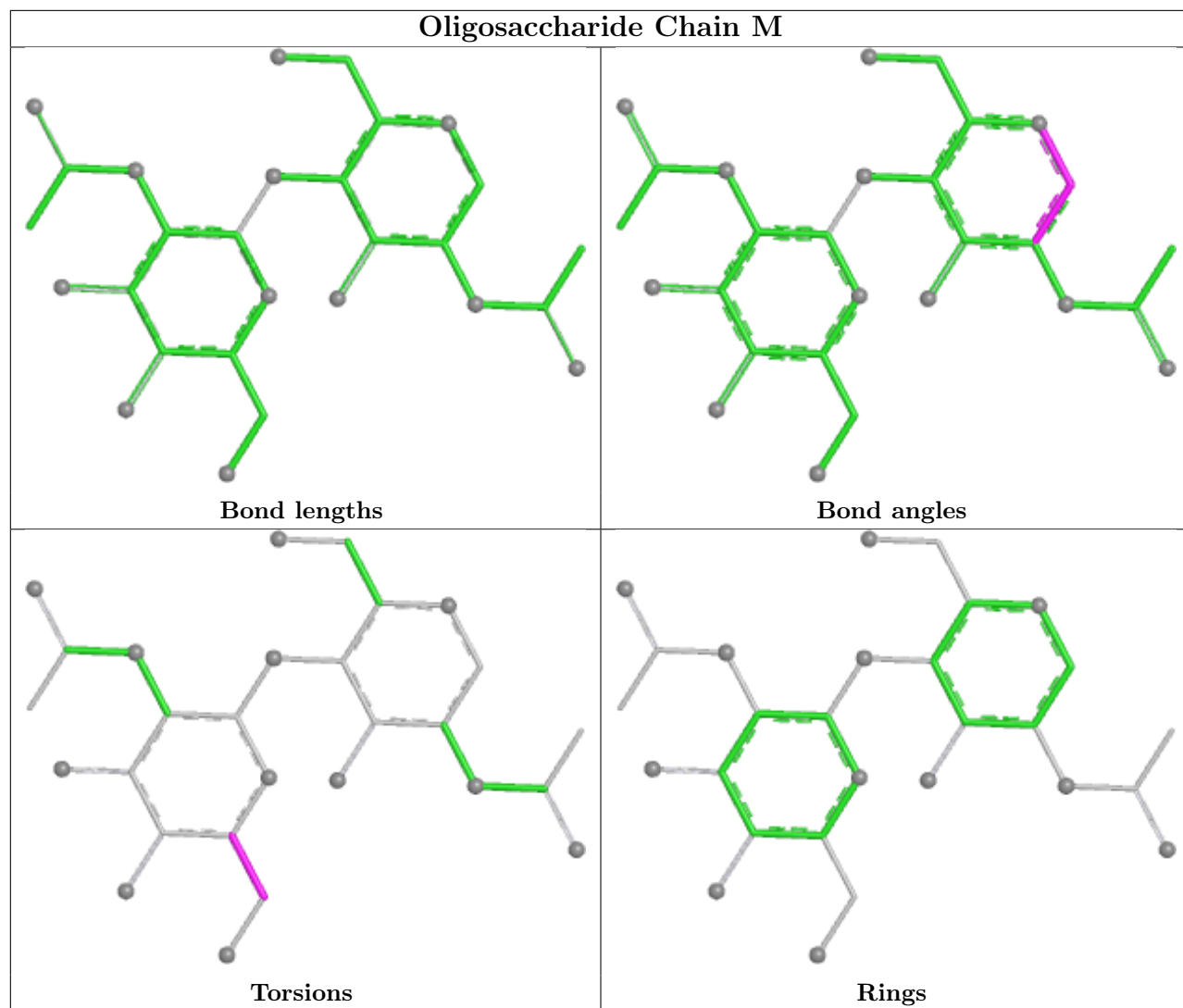


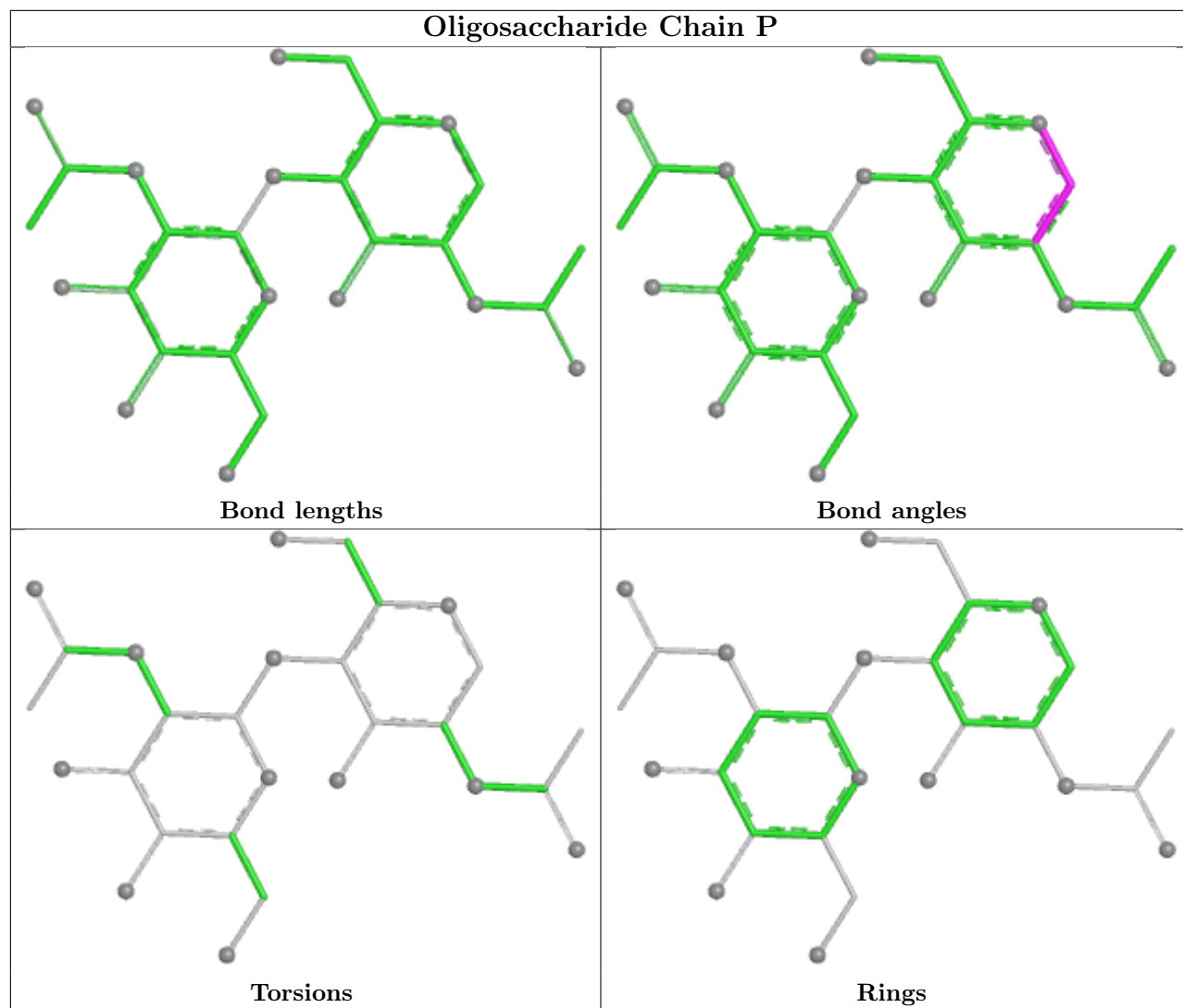


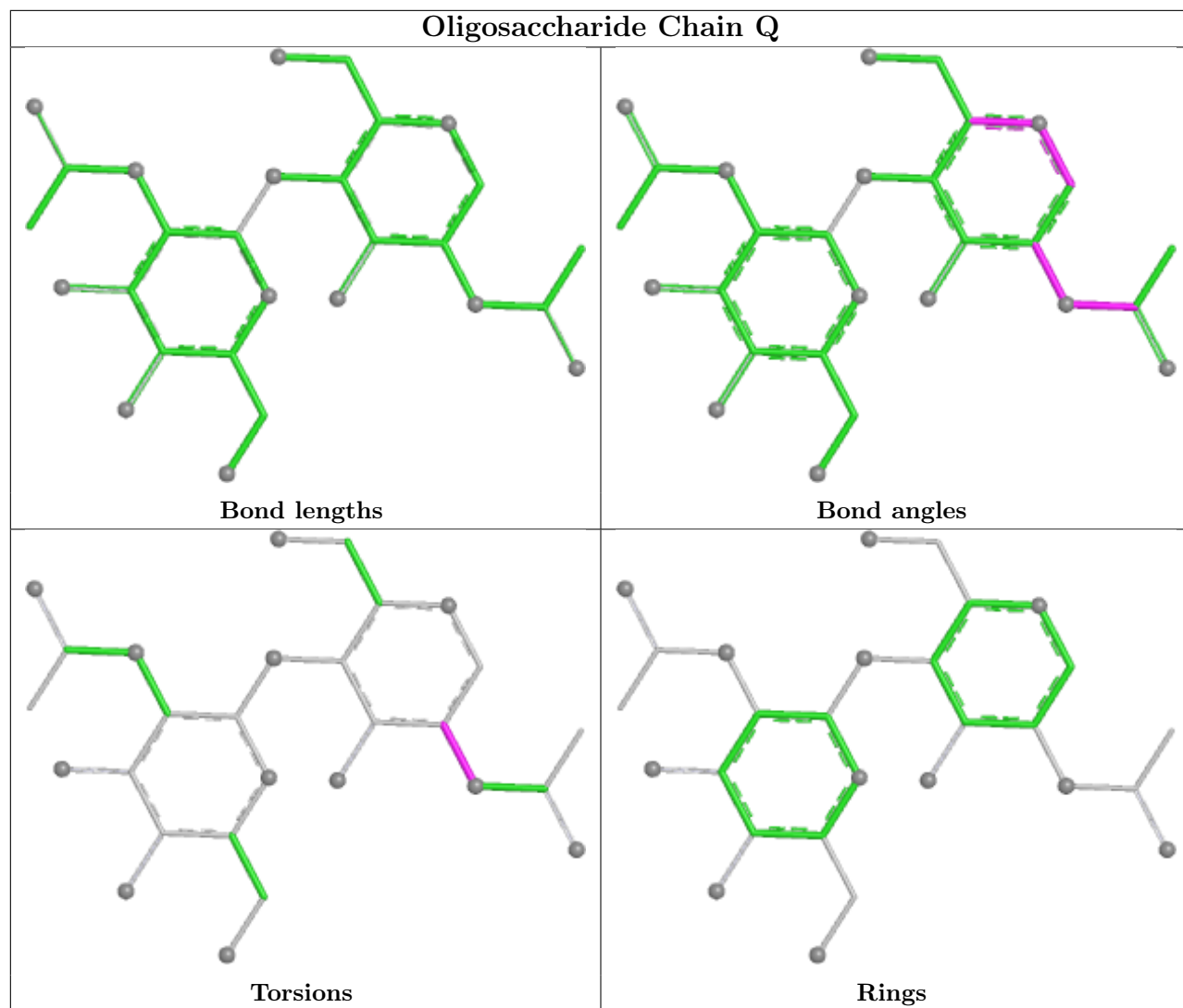


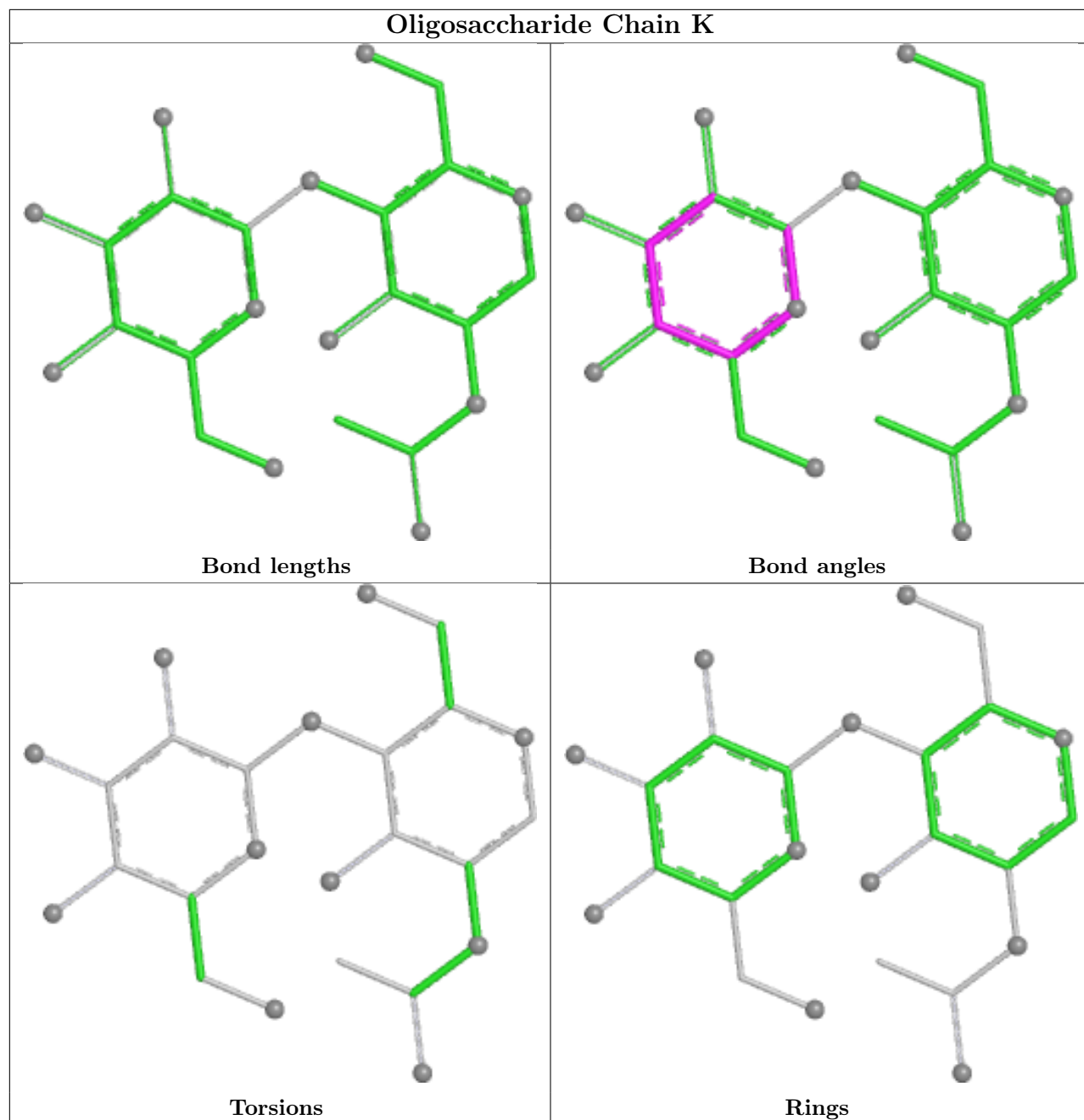


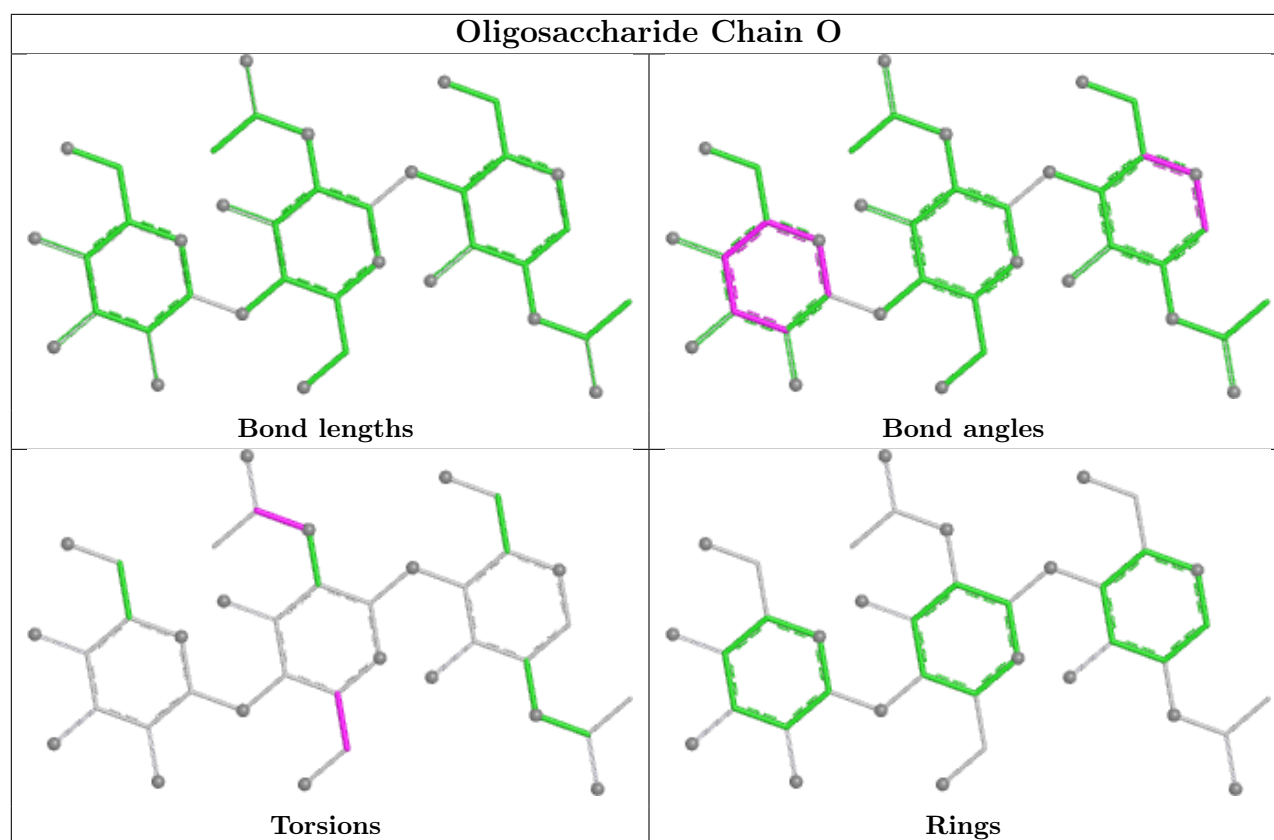












5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
7	NAG	D	1001	1	14,14,15	0.73	0	17,19,21	0.86	0
7	NAG	D	1002	1	14,14,15	0.76	0	17,19,21	0.95	1 (5%)
7	NAG	C	1001	1	14,14,15	0.74	0	17,19,21	0.91	0
7	NAG	A	1003	1	14,14,15	0.74	0	17,19,21	0.86	0
7	NAG	B	1004	1	14,14,15	0.72	0	17,19,21	0.77	0
7	NAG	B	1001	1	14,14,15	0.73	0	17,19,21	0.82	0
7	NAG	B	1002	1	14,14,15	0.71	0	17,19,21	0.85	0
7	NAG	D	1003	1	14,14,15	0.73	0	17,19,21	0.79	0
7	NAG	A	1002	1	14,14,15	0.71	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	D	1004	1	14,14,15	0.72	0	17,19,21	0.75	0
7	NAG	B	1003	1	14,14,15	0.74	0	17,19,21	0.74	0
7	NAG	A	1001	1	14,14,15	0.71	0	17,19,21	0.78	0
7	NAG	C	1002	1	14,14,15	0.71	0	17,19,21	0.79	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
7	NAG	D	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1002	1	-	2/6/23/26	0/1/1/1
7	NAG	D	1003	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1003	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1002	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1002	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1002	NAG	C8-C7-N2-C2
7	B	1002	NAG	O7-C7-N2-C2
7	C	1001	NAG	C8-C7-N2-C2
7	C	1001	NAG	O7-C7-N2-C2
7	D	1001	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	D	1001	NAG	O7-C7-N2-C2
7	B	1001	NAG	O5-C5-C6-O6
7	A	1001	NAG	O5-C5-C6-O6
7	B	1003	NAG	O5-C5-C6-O6
7	B	1001	NAG	C1-C2-N2-C7

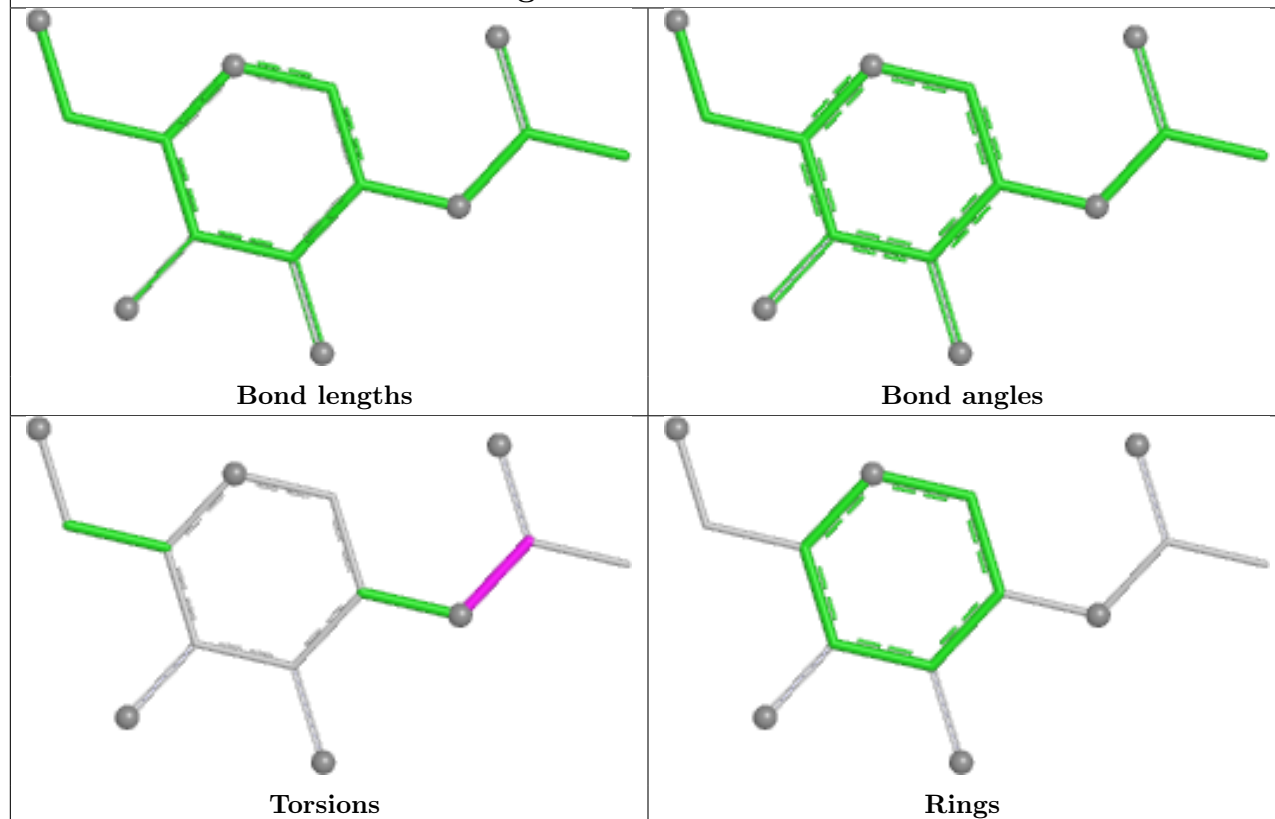
There are no ring outliers.

1 monomer is involved in 1 short contact:

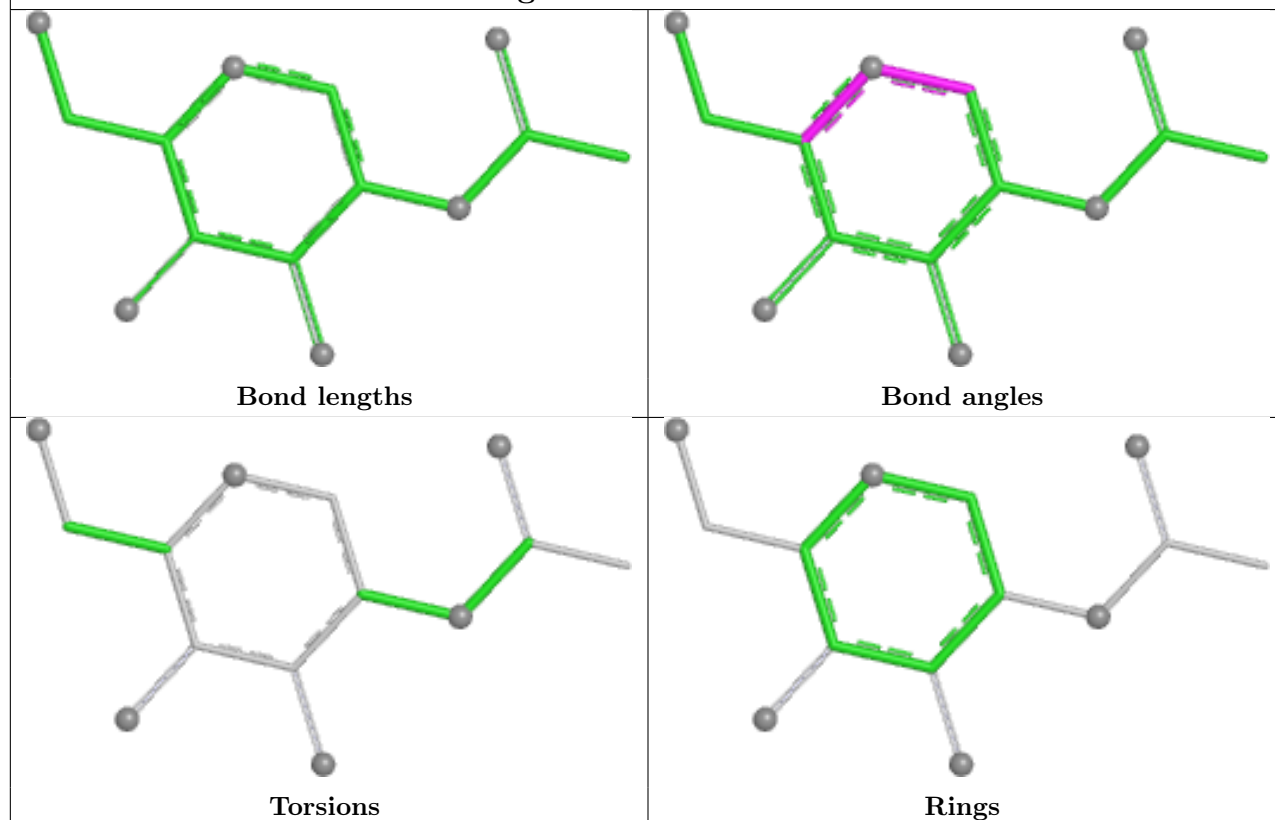
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1003	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

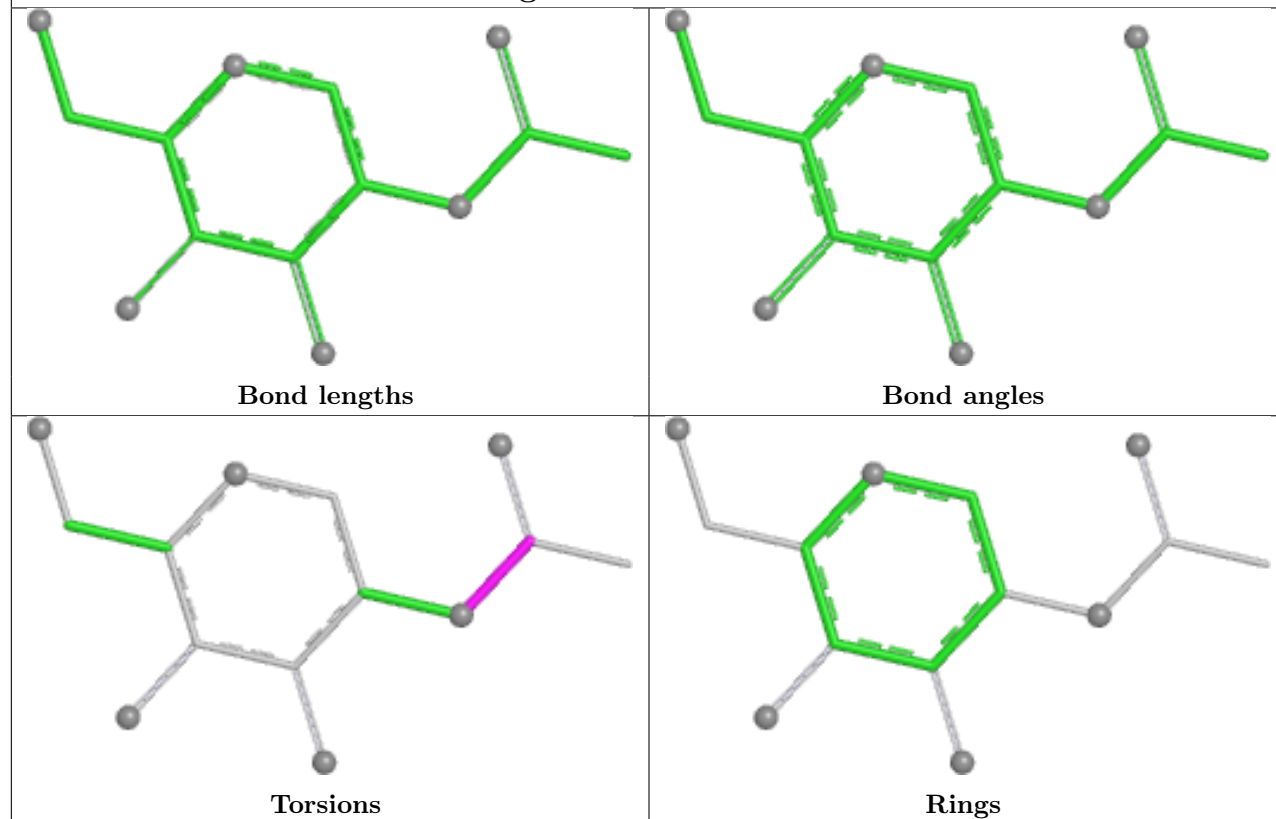
Ligand NAG D 1001



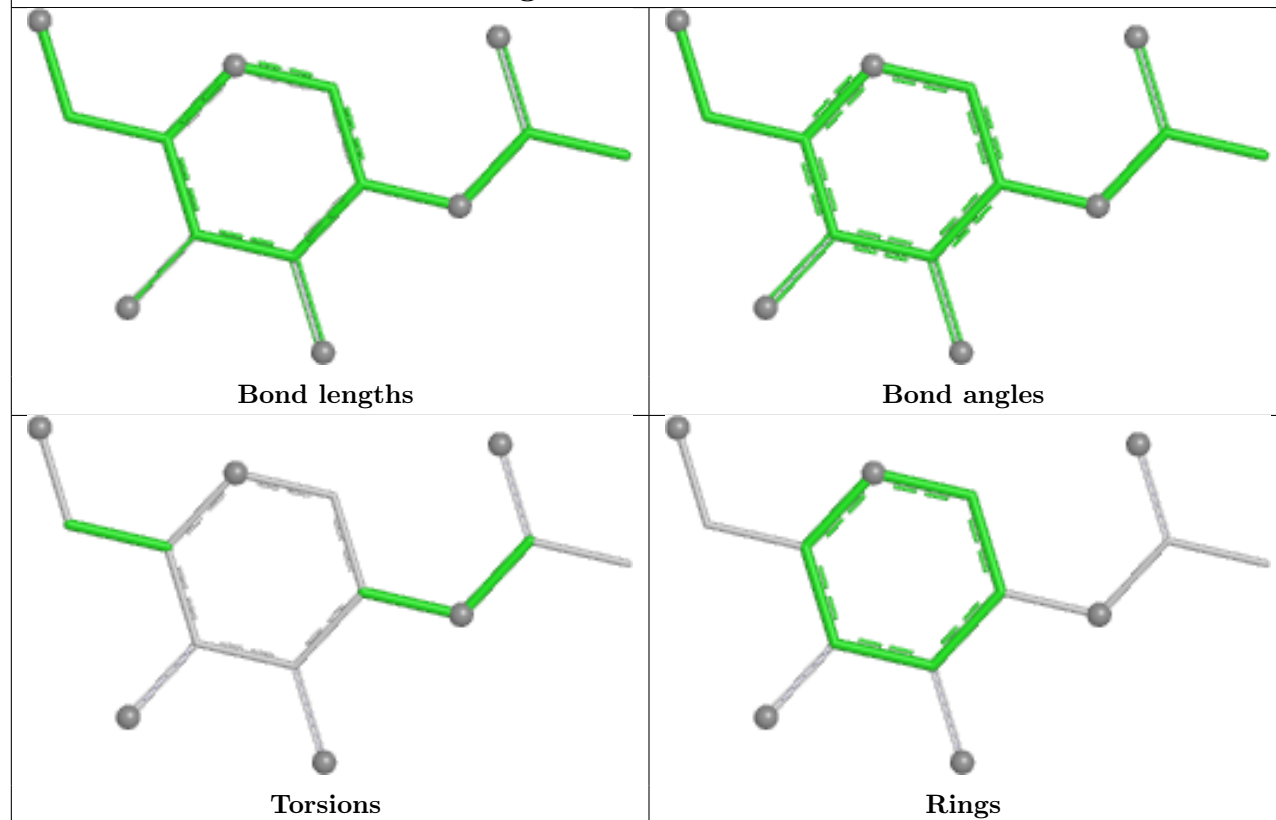
Ligand NAG D 1002

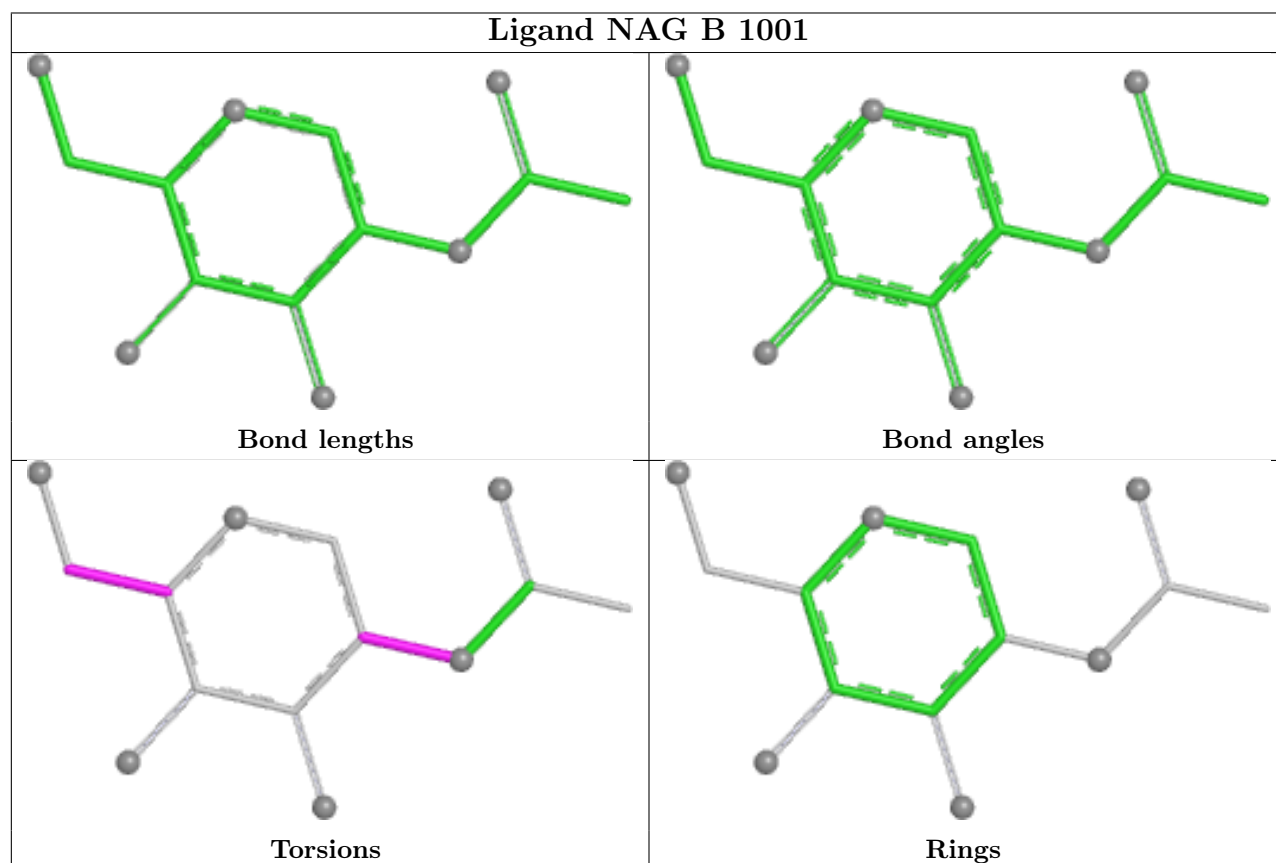
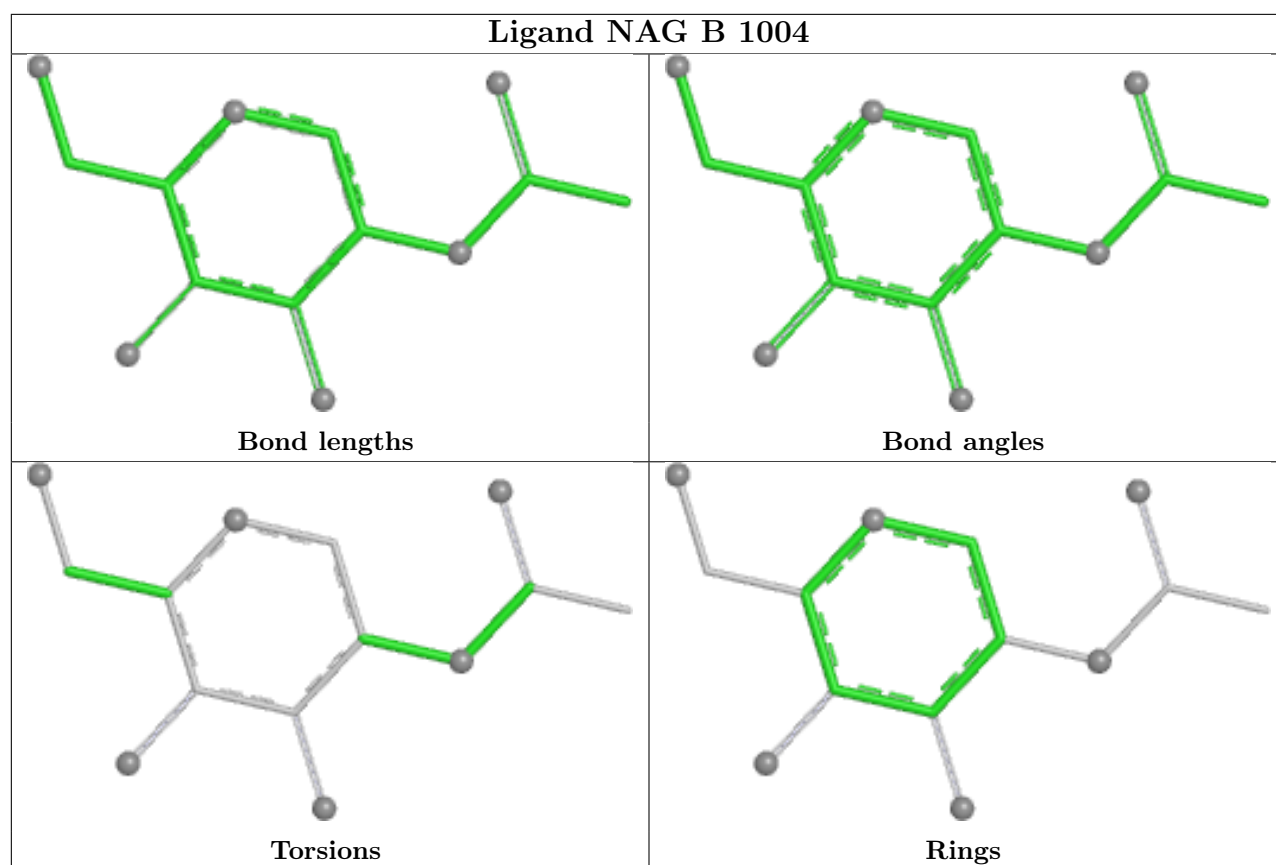


Ligand NAG C 1001

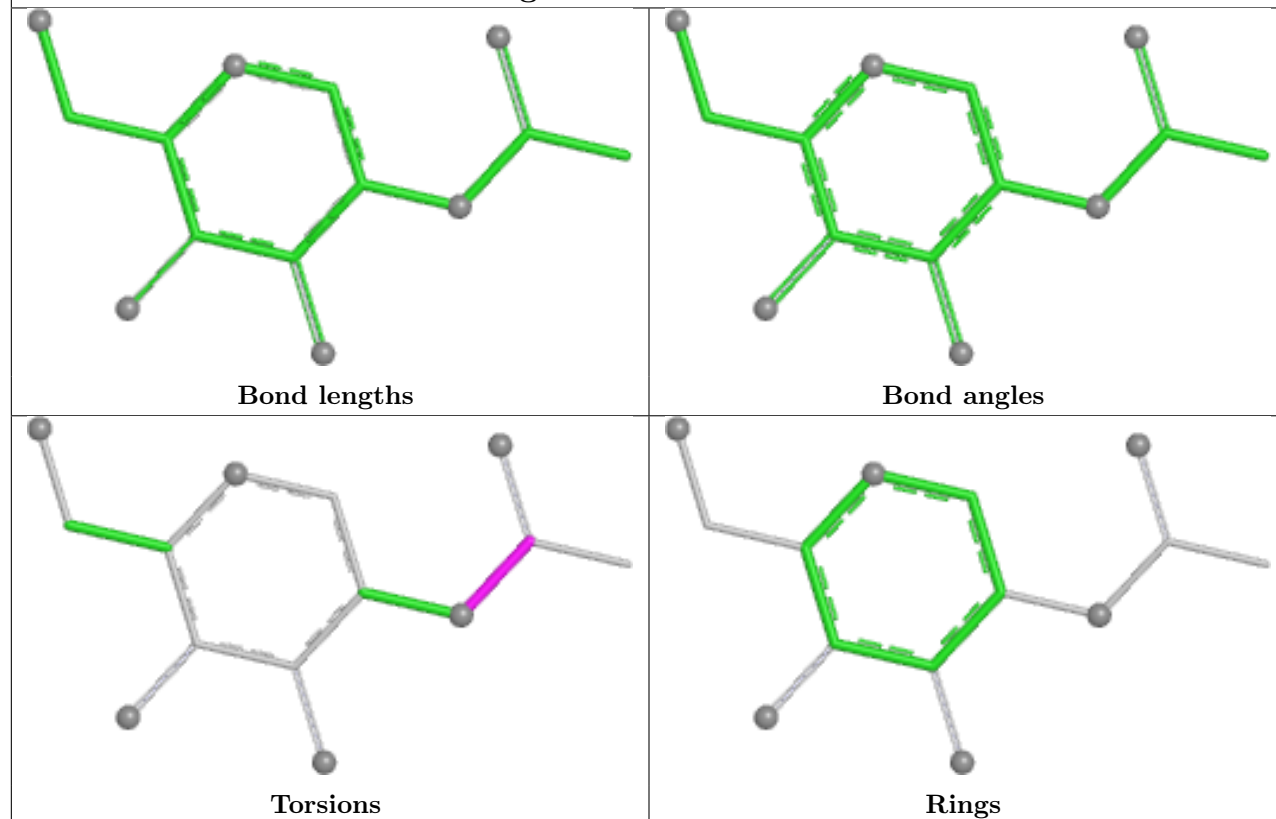


Ligand NAG A 1003

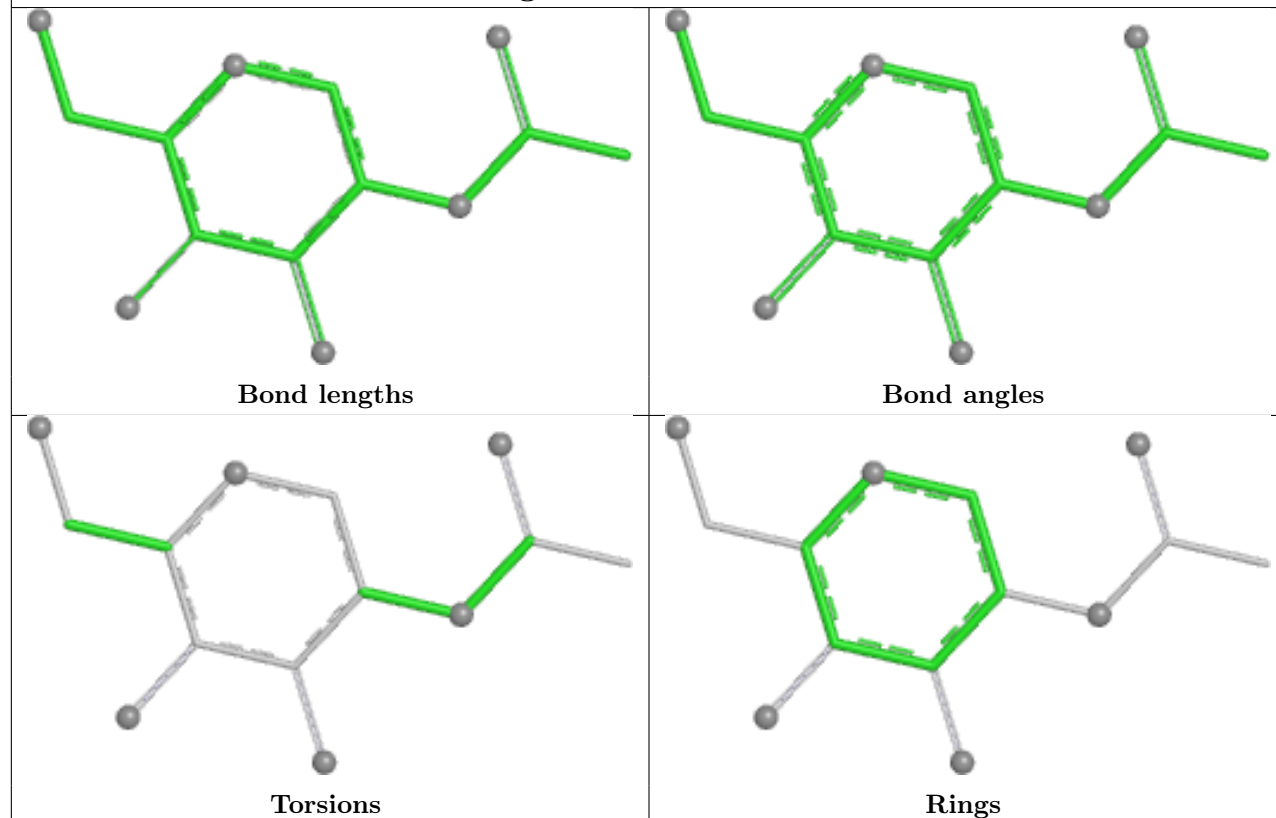




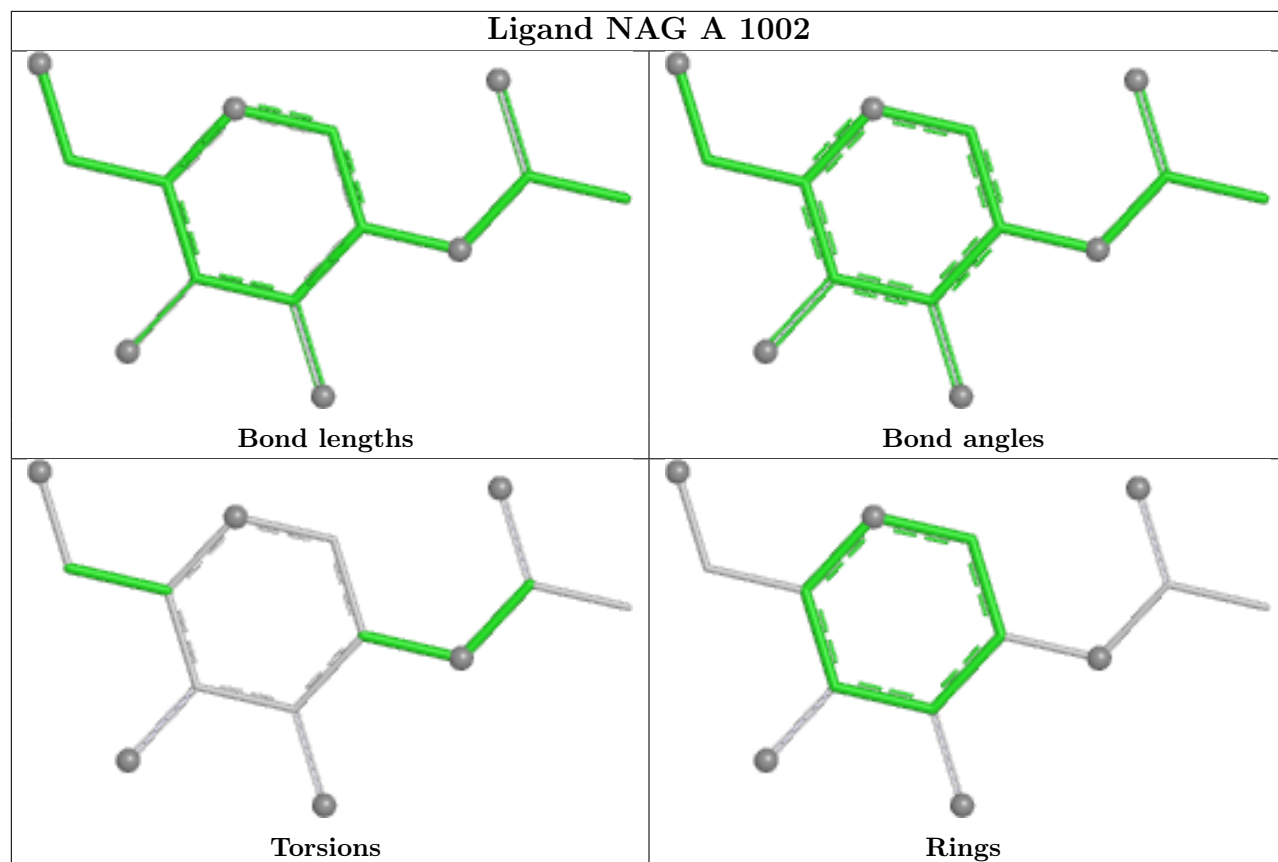
Ligand NAG B 1002



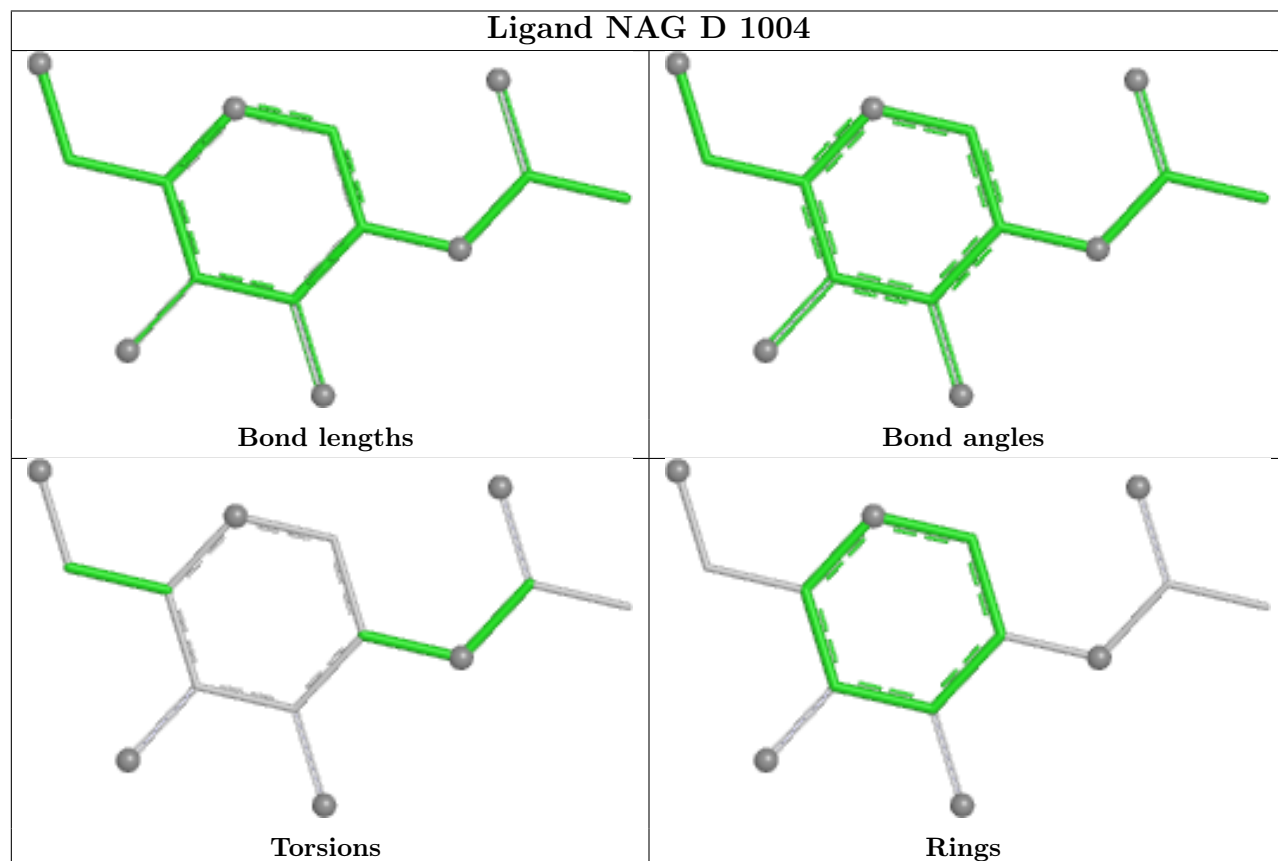
Ligand NAG D 1003

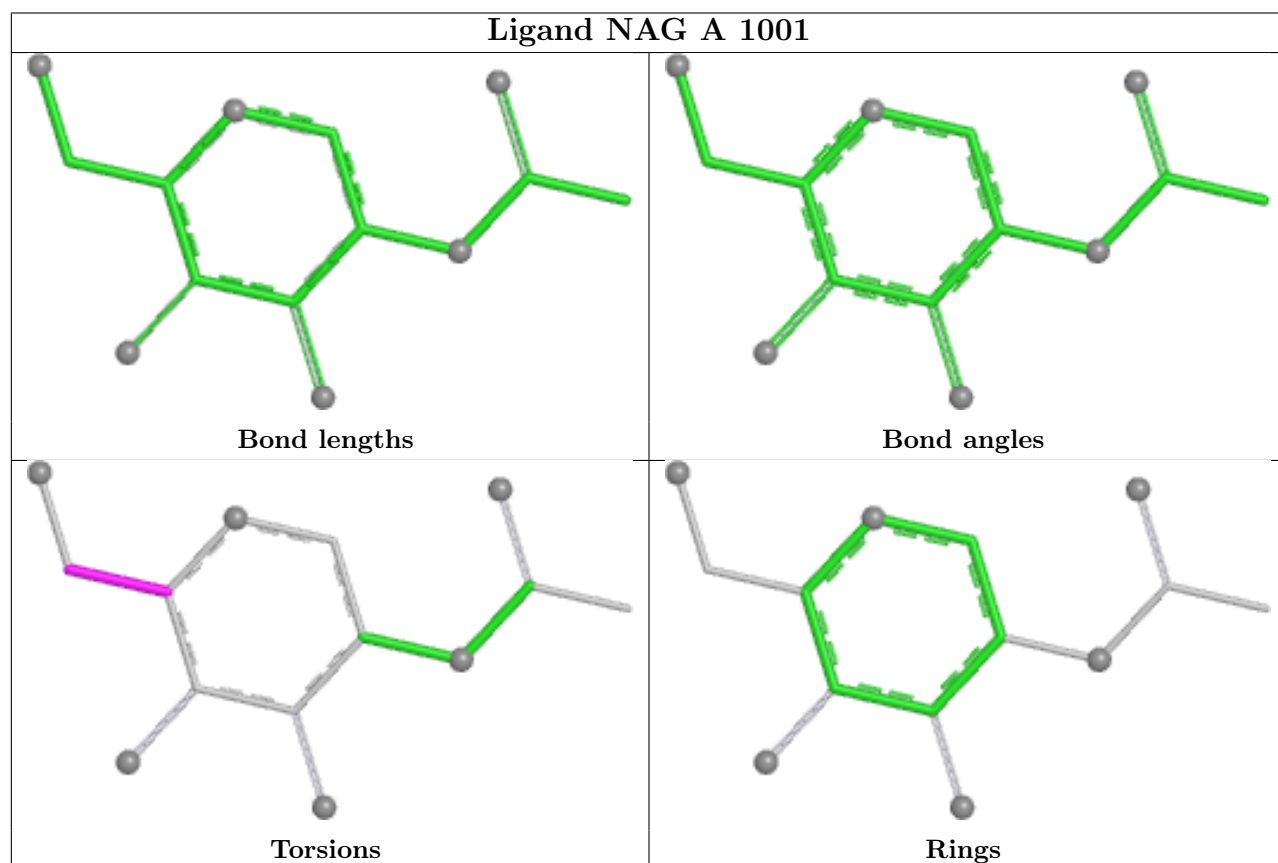
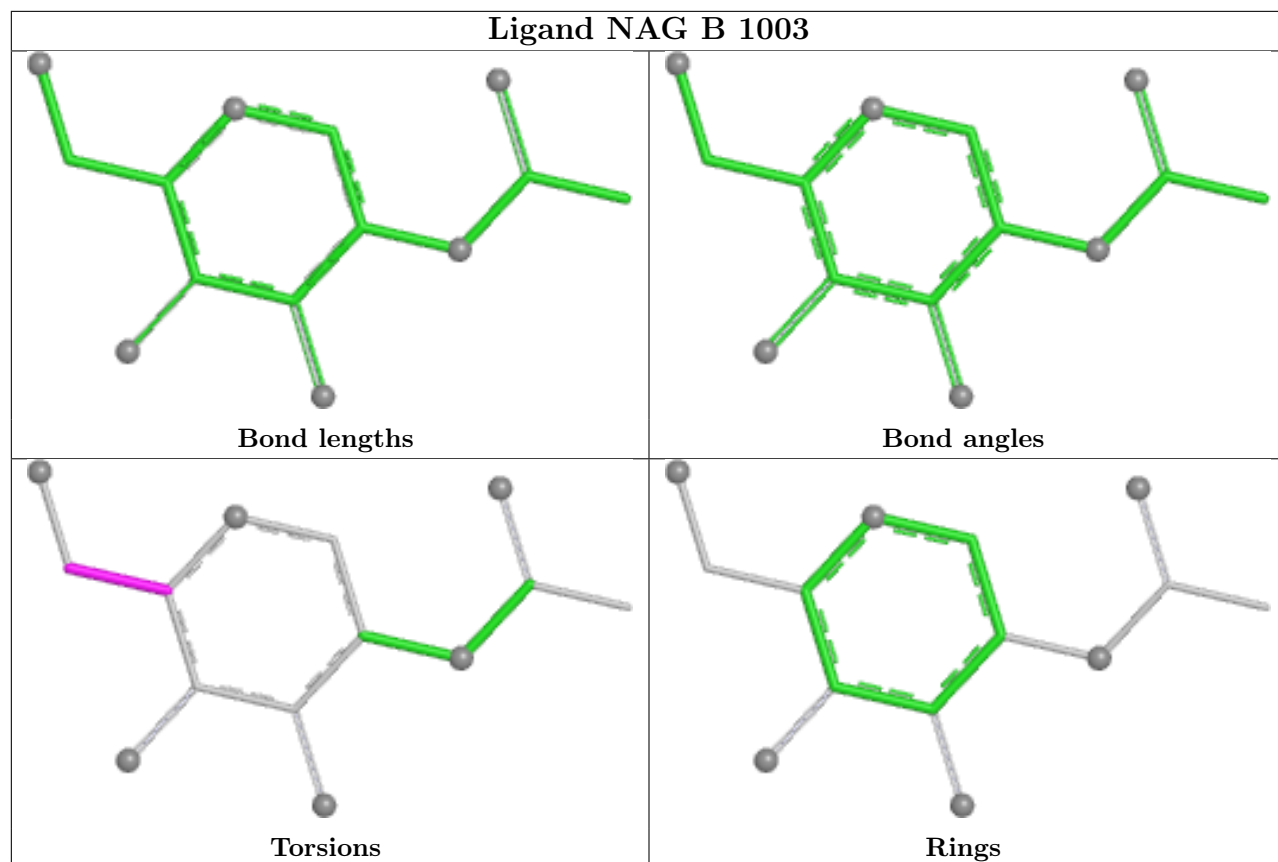


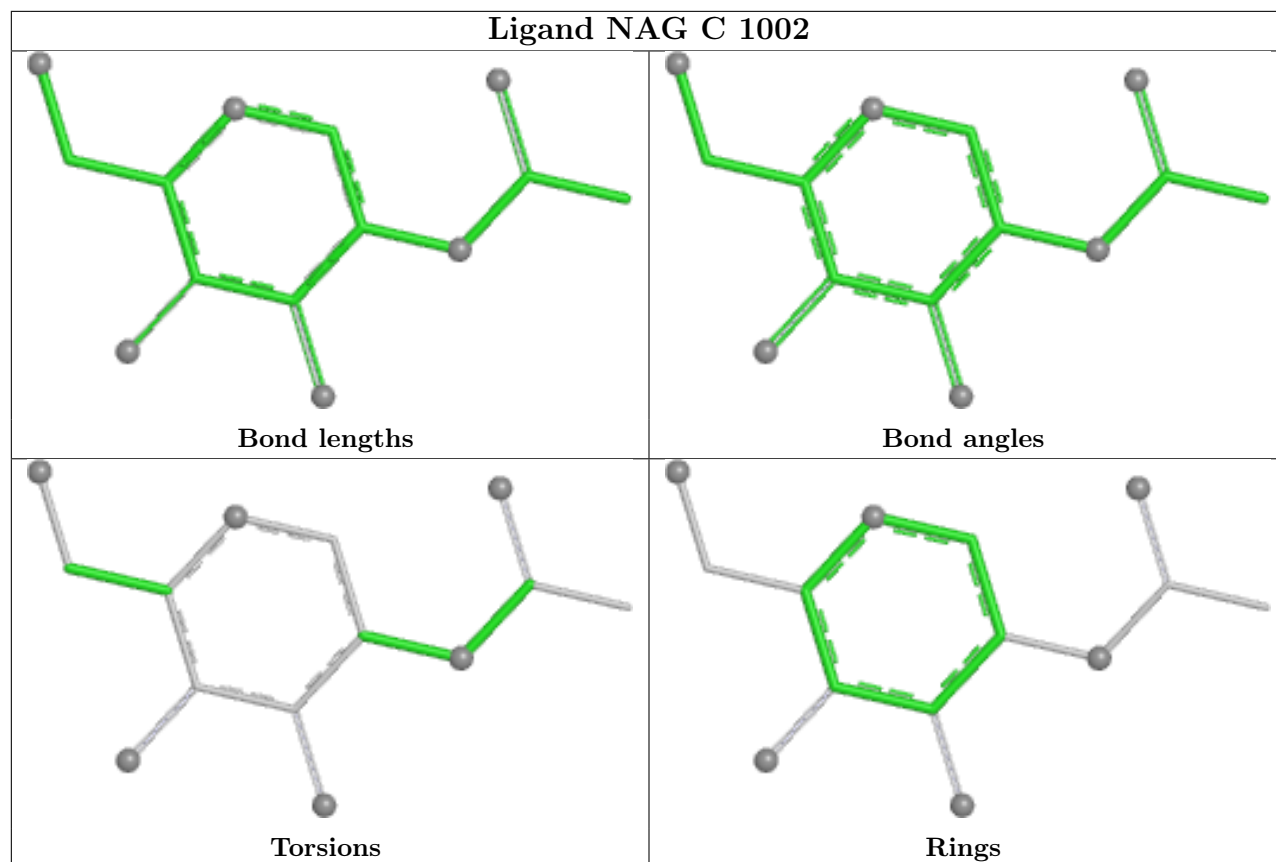
Ligand NAG A 1002



Ligand NAG D 1004







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.

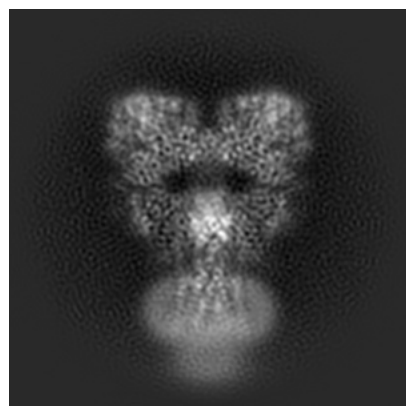
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48757. These allow visual inspection of the internal detail of the map and identification of artifacts.

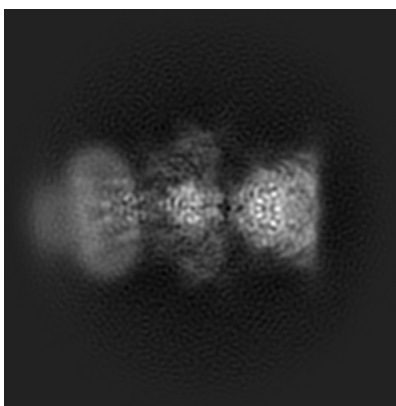
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

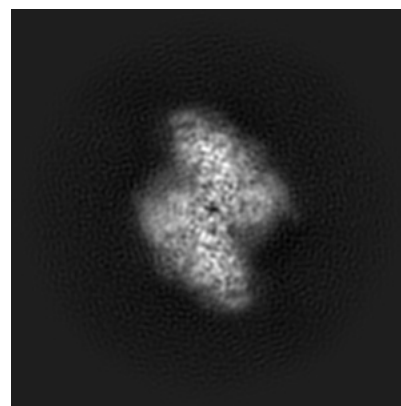
6.1.1 Primary map



X

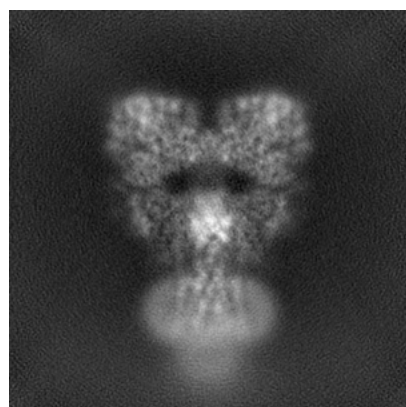


Y

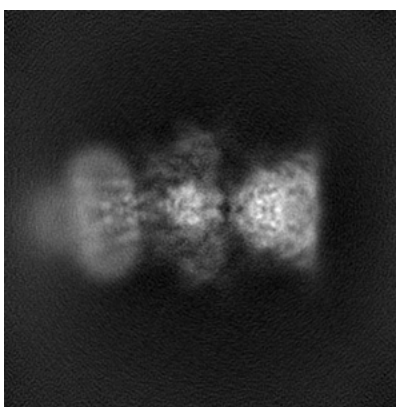


Z

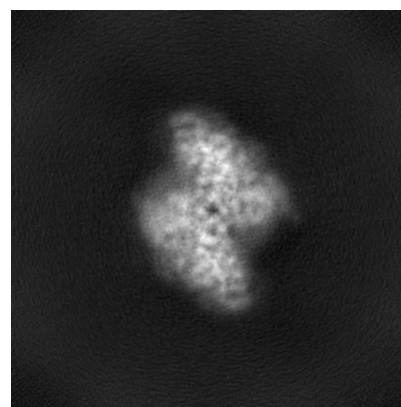
6.1.2 Raw map



X



Y

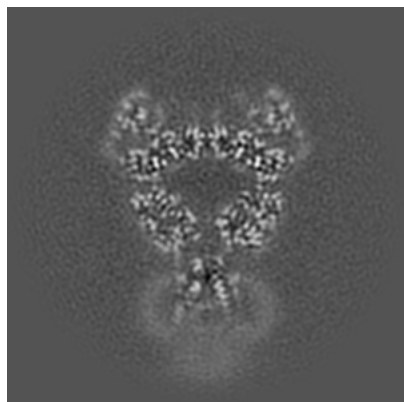


Z

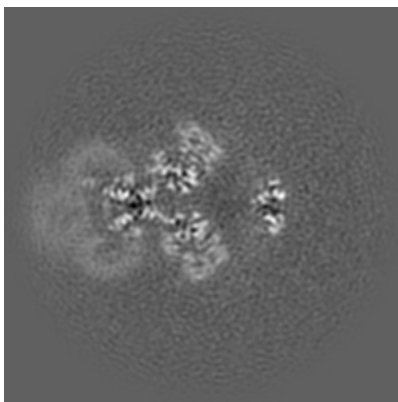
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

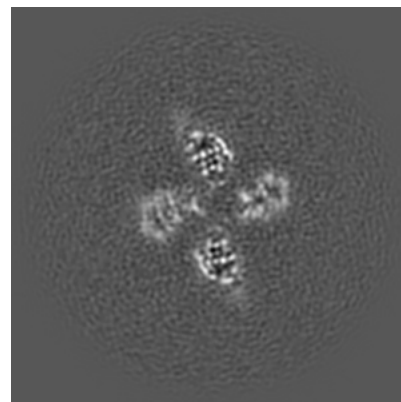
6.2.1 Primary map



X Index: 130

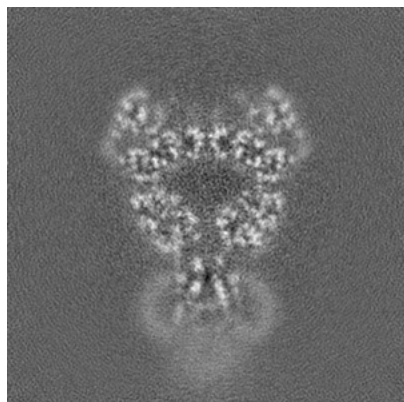


Y Index: 130

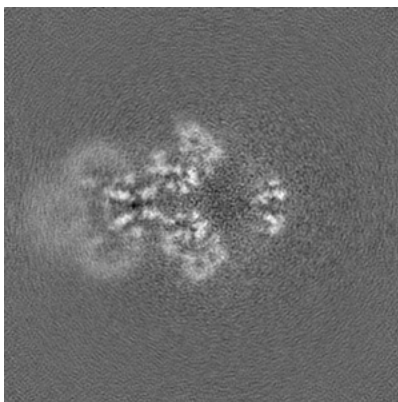


Z Index: 130

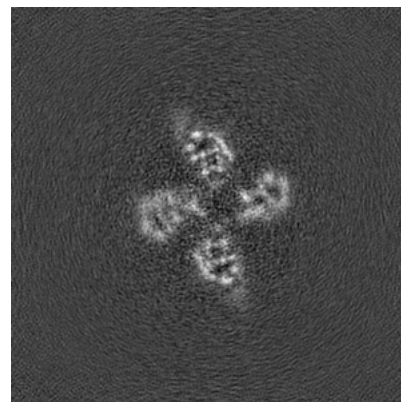
6.2.2 Raw map



X Index: 130



Y Index: 130

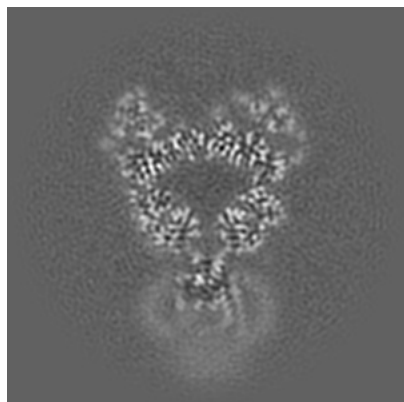


Z Index: 130

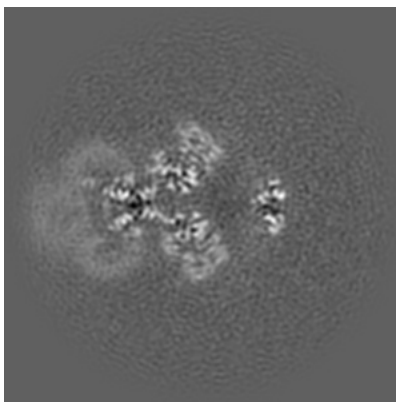
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

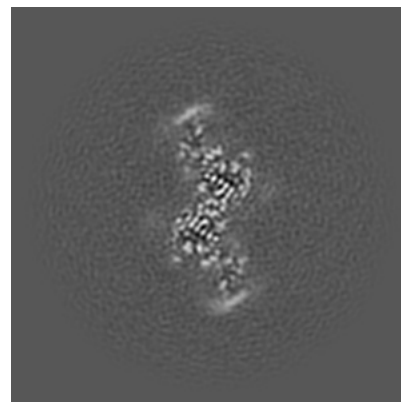
6.3.1 Primary map



X Index: 133

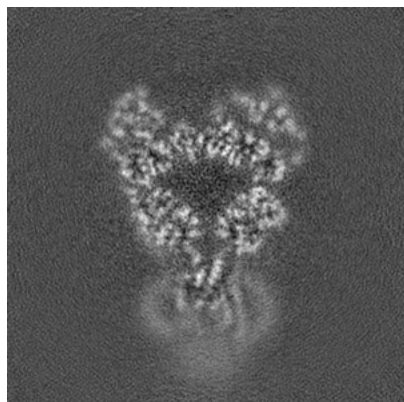


Y Index: 130

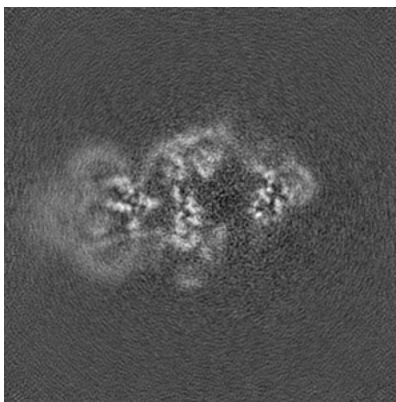


Z Index: 171

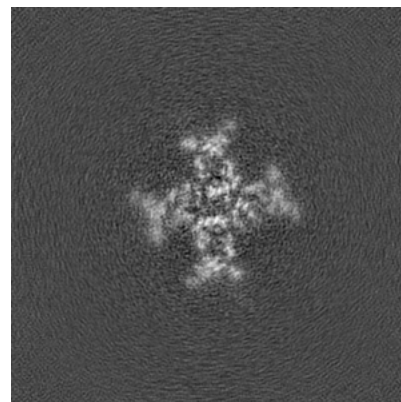
6.3.2 Raw map



X Index: 134



Y Index: 138

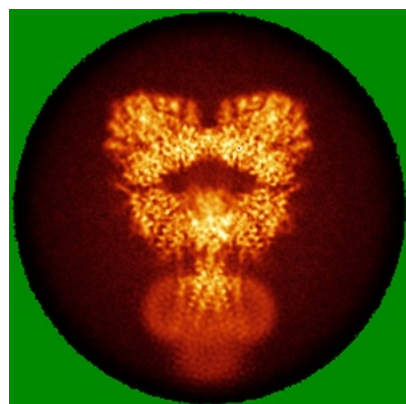


Z Index: 120

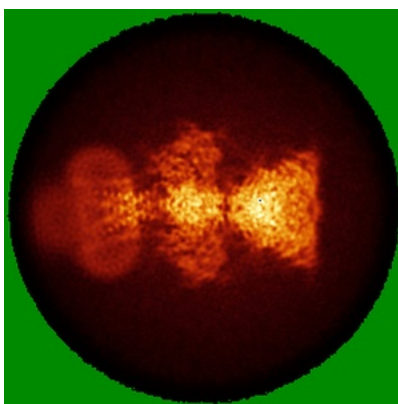
The images above show the largest variance slices of the map in three orthogonal directions.

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

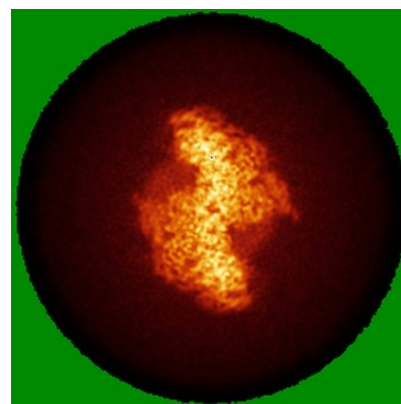
6.4.1 Primary map



X

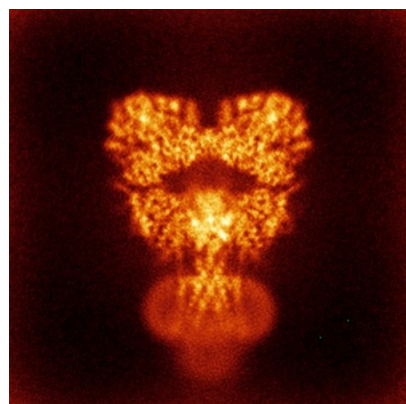


Y

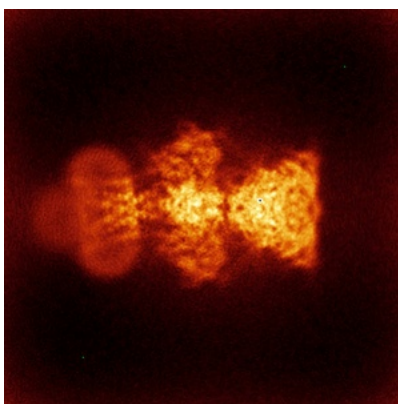


Z

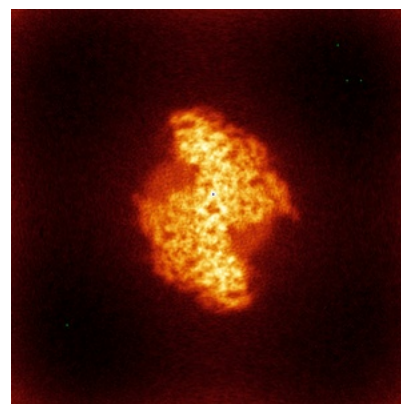
6.4.2 Raw map



X



Y

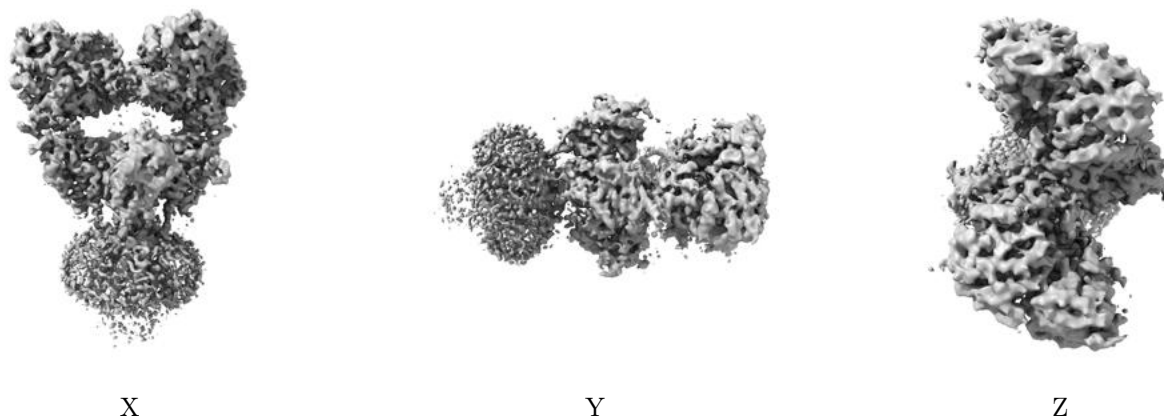


Z

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.

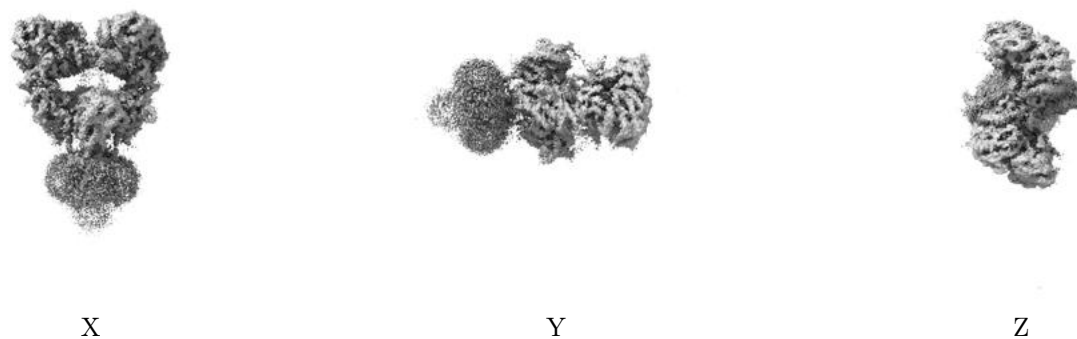
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.121. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

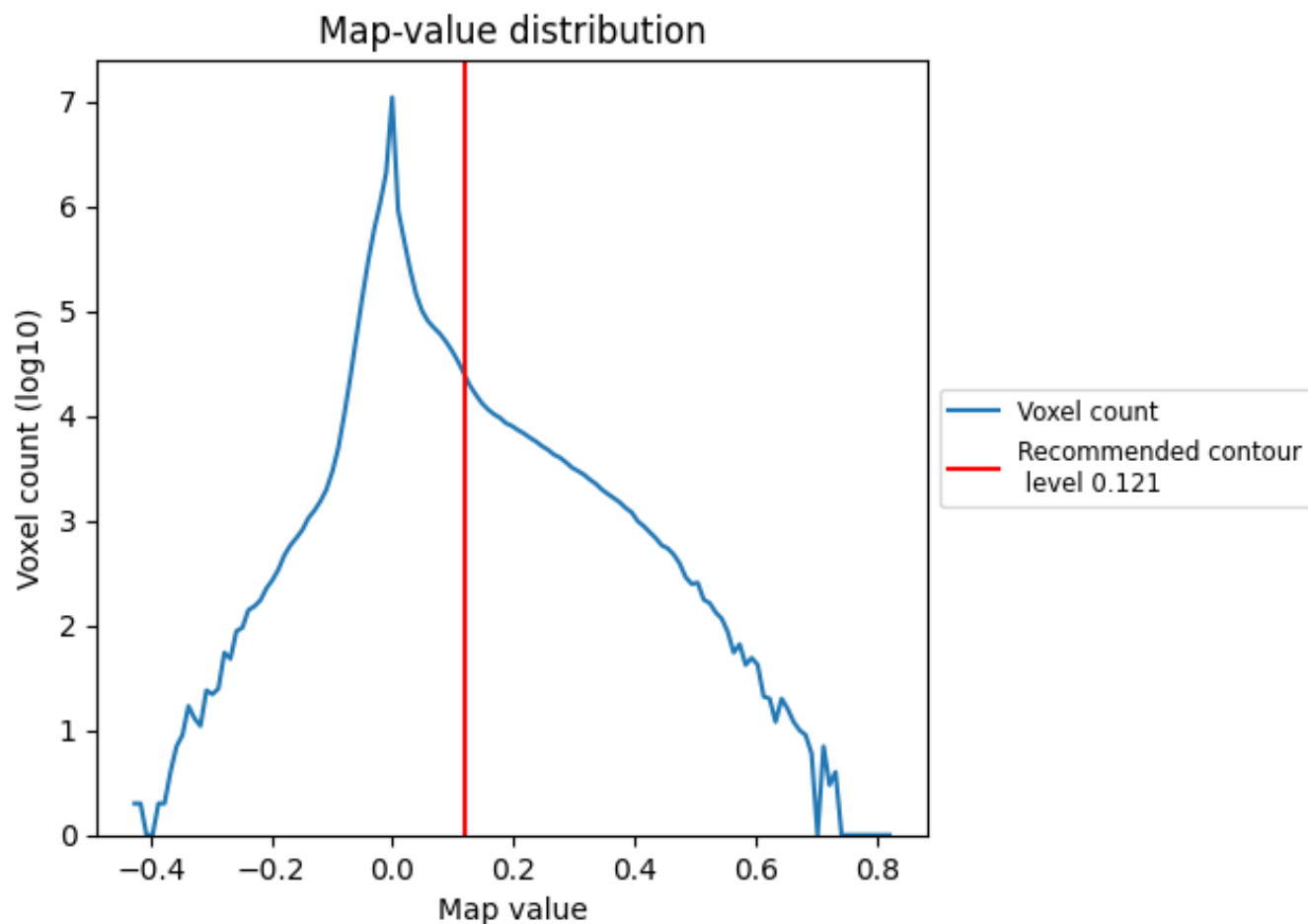
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

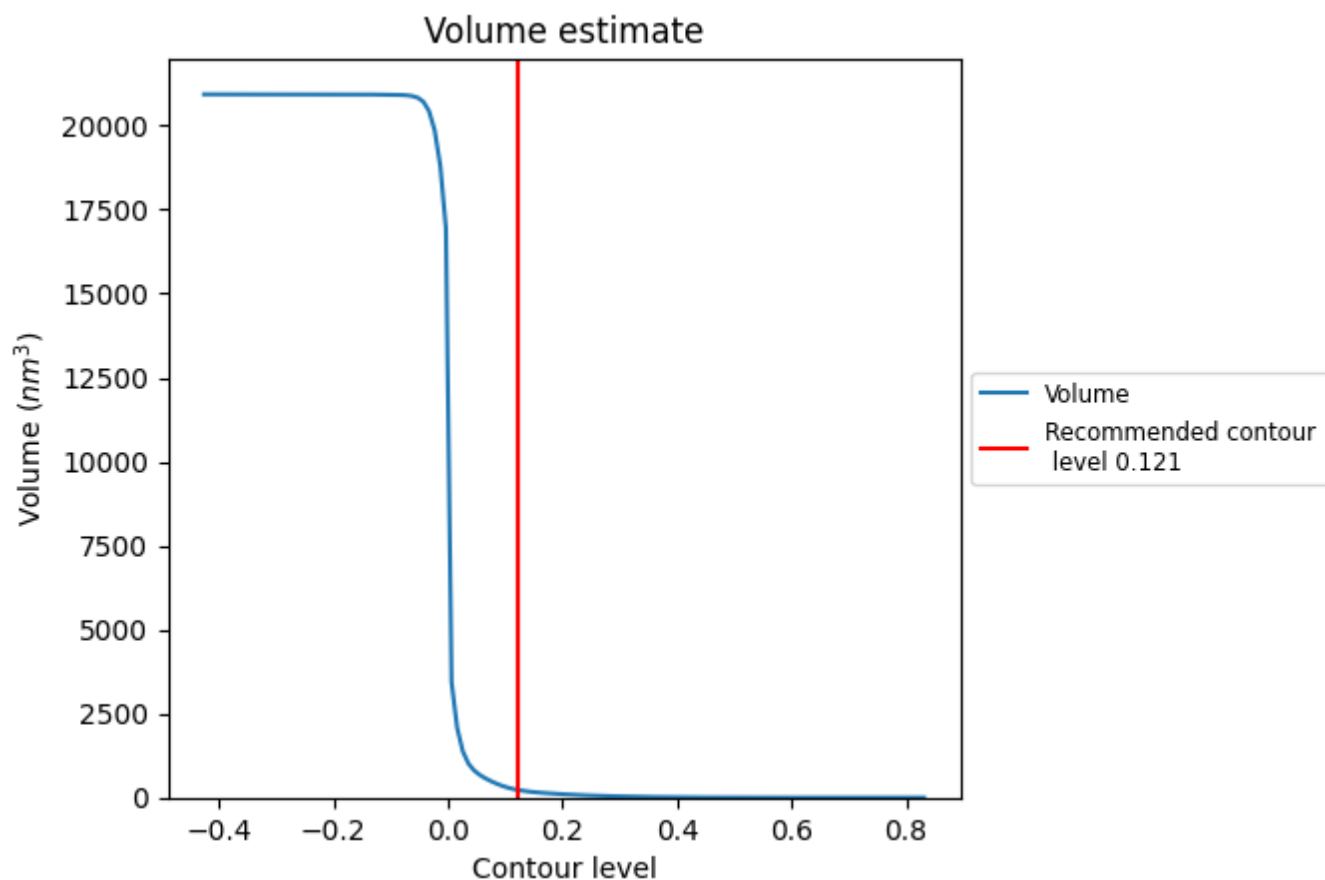
This section contains the results of statistical analysis of the map.

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.

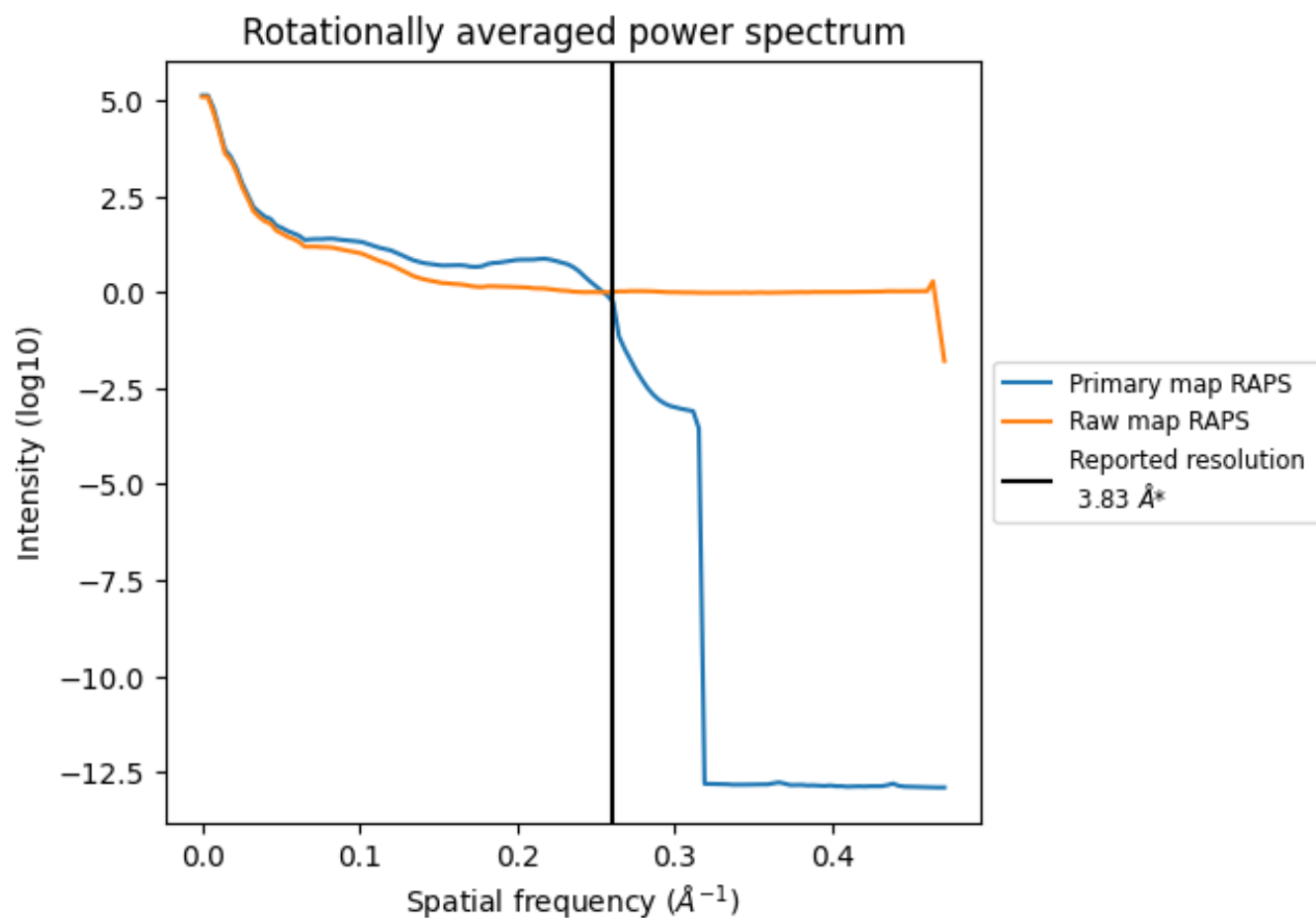
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm³; this corresponds to an approximate mass of 206 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 ⓘ

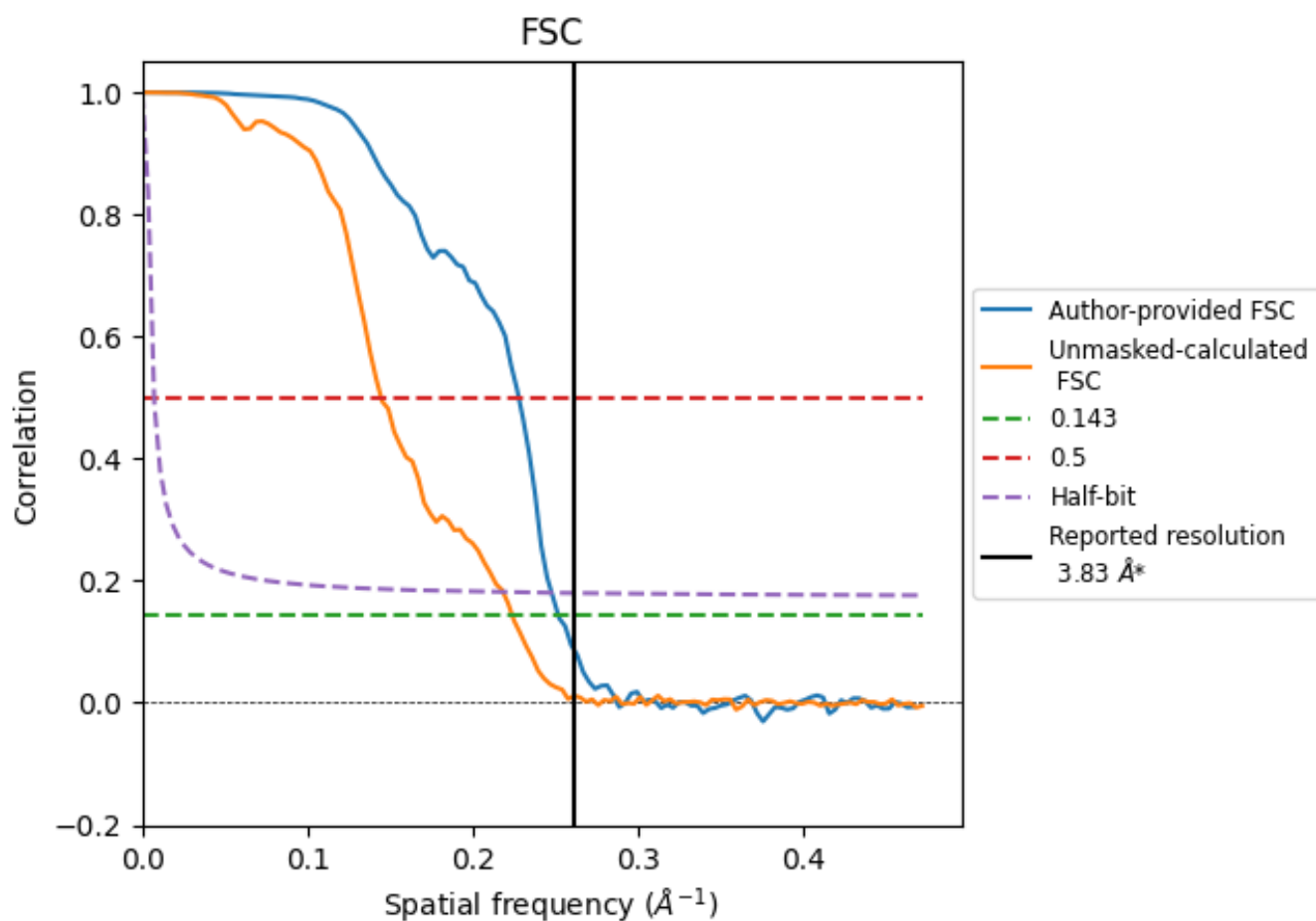


*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

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 0.261 Å⁻¹

8.2 Resolution estimates [i](#)

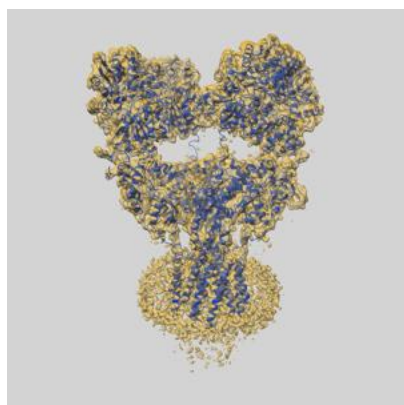
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	3.97	4.39	4.04
Unmasked-calculated*	4.47	6.92	4.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.47 differs from the reported value 3.83 by more than 10 %

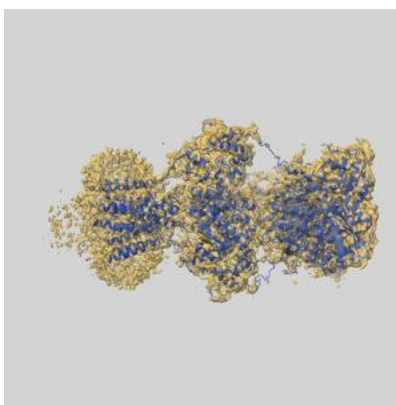
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48757 and PDB model 9MZI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

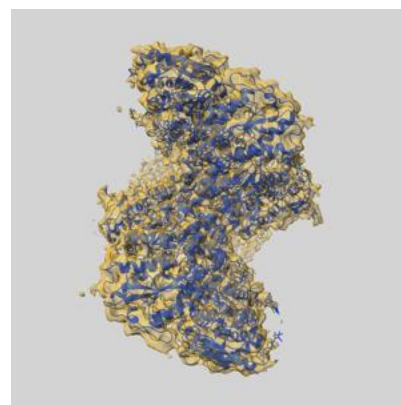
9.1 Map-model overlay [i](#)



X



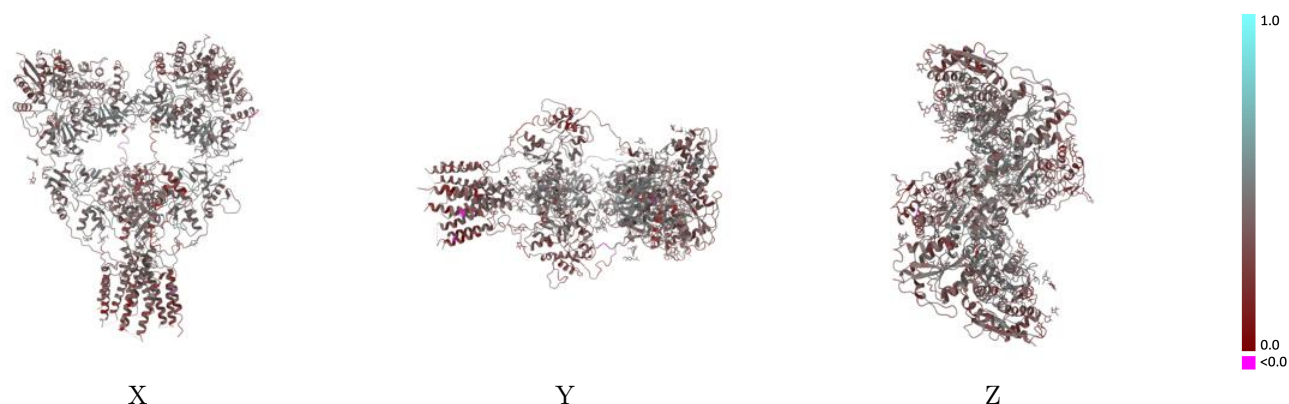
Y



Z

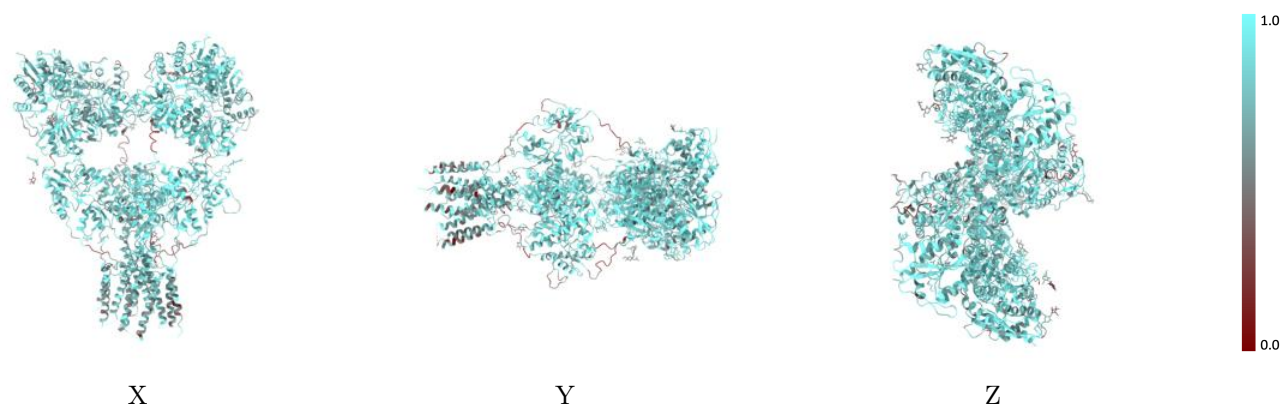
The images above show the 3D surface view of the map at the recommended contour level 0.121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



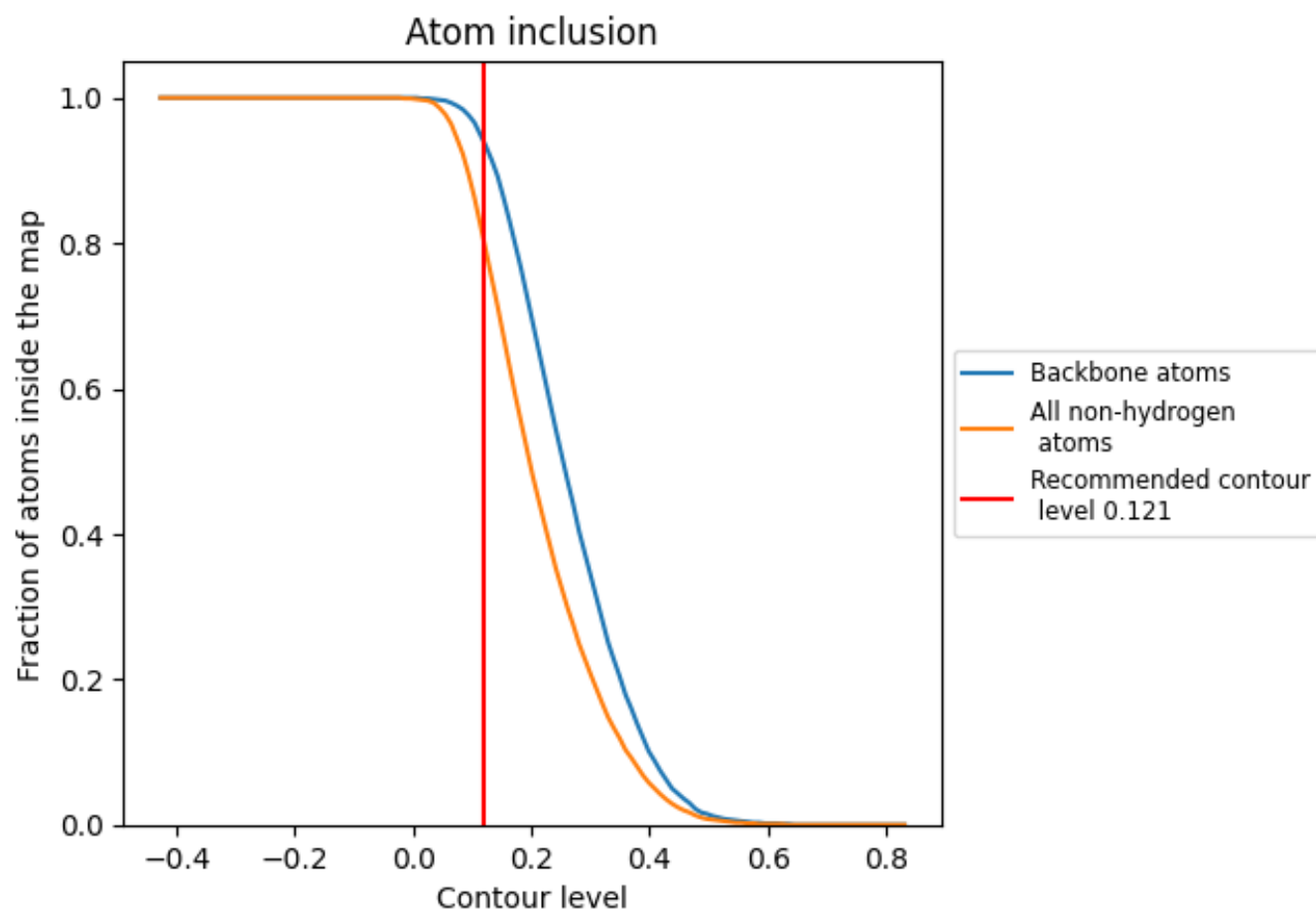
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.121).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.3900
A	 0.8060	 0.3980
B	 0.7780	 0.3710
C	 0.8180	 0.4020
D	 0.8070	 0.3880
E	 0.6910	 0.3720
F	 0.5640	 0.3560
G	 0.4290	 0.3660
H	 0.8330	 0.4650
I	 0.7500	 0.3750
J	 0.6790	 0.3900
K	 0.8400	 0.4060
L	 0.6070	 0.3380
M	 0.5000	 0.3910
N	 0.7380	 0.3530
O	 0.7690	 0.4550
P	 0.8210	 0.4190
Q	 0.7860	 0.4030
R	 0.6430	 0.3290

