



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 10:36 PM JST

PDB ID : 8IFY
EMDB ID : EMD-35426
Title : Cryo-EM structure of SARS-CoV-2 Omicron BA.4/5 spike protein in complex with white-tailed deer ACE2
Authors : Han, P.; Meng, Y.M.; Qi, J.X.
Deposited on : 2023-02-20
Resolution : 2.55 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

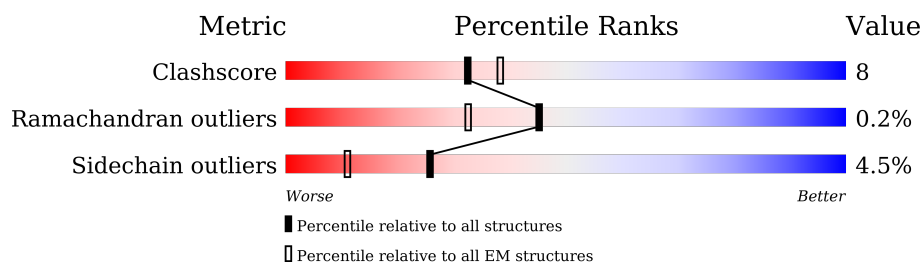
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1127	
1	B	1127	
1	C	1127	
2	E	661	
2	F	661	
3	G	2	
3	H	2	
3	I	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	2	 100%
3	K	2	 100%
3	L	2	 50%50%
3	N	2	 100%
3	O	2	 100%
3	P	2	 50%50%
3	Q	2	 50%50%
3	R	2	 100%
3	S	2	 100%
3	T	2	 50%50%
3	U	2	 50%50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34248 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	1011	Total	C	N	O	S	0	0
			7922	5075	1316	1493	38		
1	B	1006	Total	C	N	O	S	0	0
			7884	5051	1310	1485	38		
1	C	1011	Total	C	N	O	S	0	0
			7922	5075	1316	1493	38		

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLN	-	expression tag	UNP P0DTC2
A	20	CYS	-	expression tag	UNP P0DTC2
A	21	VAL	-	expression tag	UNP P0DTC2
A	22	ASN	-	expression tag	UNP P0DTC2
A	23	LEU	-	expression tag	UNP P0DTC2
A	24	ILE	-	expression tag	UNP P0DTC2
A	25	THR	-	expression tag	UNP P0DTC2
A	26	ARG	-	expression tag	UNP P0DTC2
A	27	THR	-	expression tag	UNP P0DTC2
A	28	GLN	-	expression tag	UNP P0DTC2
A	29	SER	-	expression tag	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	19	GLN	-	expression tag	UNP P0DTC2
B	20	CYS	-	expression tag	UNP P0DTC2
B	21	VAL	-	expression tag	UNP P0DTC2
B	22	ASN	-	expression tag	UNP P0DTC2
B	23	LEU	-	expression tag	UNP P0DTC2
B	24	ILE	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	ARG	-	expression tag	UNP P0DTC2
B	27	THR	-	expression tag	UNP P0DTC2
B	28	GLN	-	expression tag	UNP P0DTC2
B	29	SER	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	19	GLN	-	expression tag	UNP P0DTC2
C	20	CYS	-	expression tag	UNP P0DTC2
C	21	VAL	-	expression tag	UNP P0DTC2
C	22	ASN	-	expression tag	UNP P0DTC2
C	23	LEU	-	expression tag	UNP P0DTC2
C	24	ILE	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	ARG	-	expression tag	UNP P0DTC2
C	27	THR	-	expression tag	UNP P0DTC2
C	28	GLN	-	expression tag	UNP P0DTC2
C	29	SER	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	595	Total	C	N	O	S	0	0
			4888	3123	804	931	30		
2	F	595	Total	C	N	O	S	0	0
			4888	3123	804	931	30		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

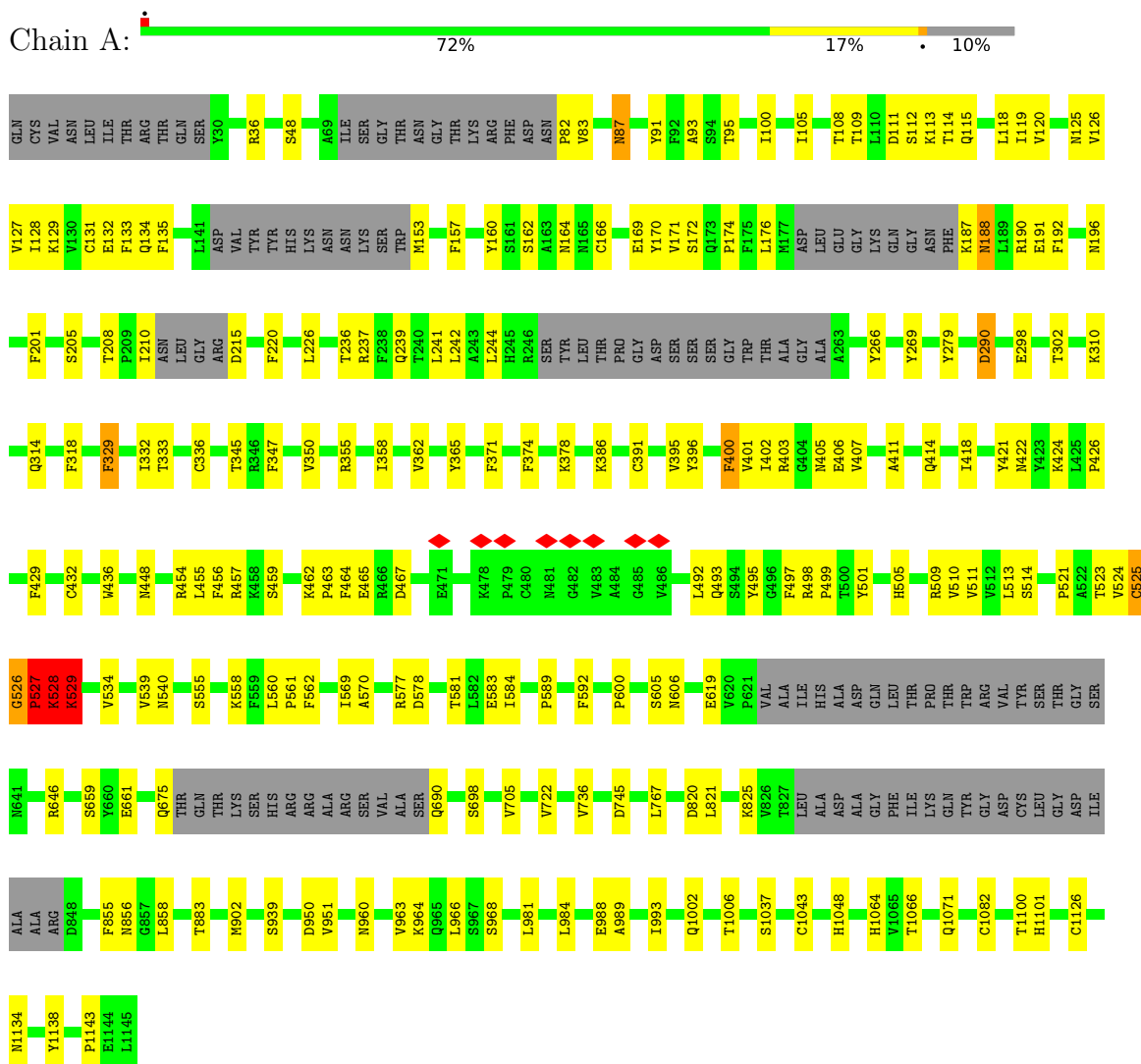
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

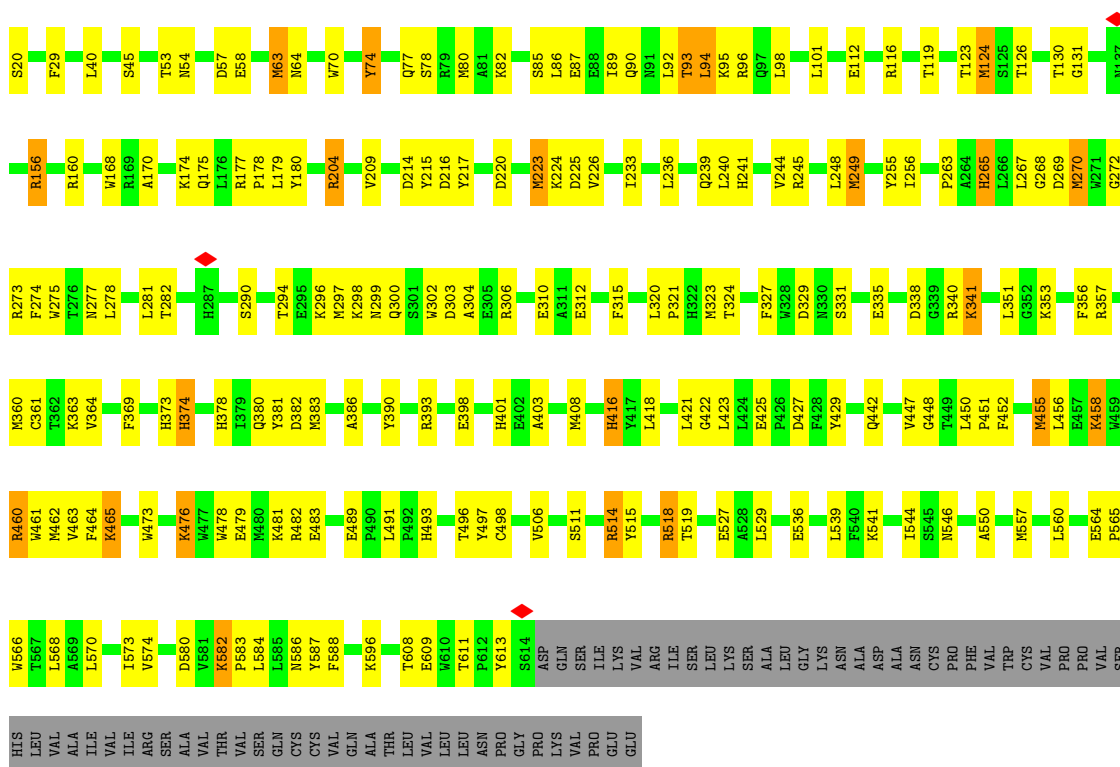




SER	VAL	K528	K529	T430	F347	GLY	V126	GLN
SER	ALA	K529	K530	C432	A348	D215	V127	CYS
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN
SER	SER	K542	K543	V433	V350	D215	I128	ASN

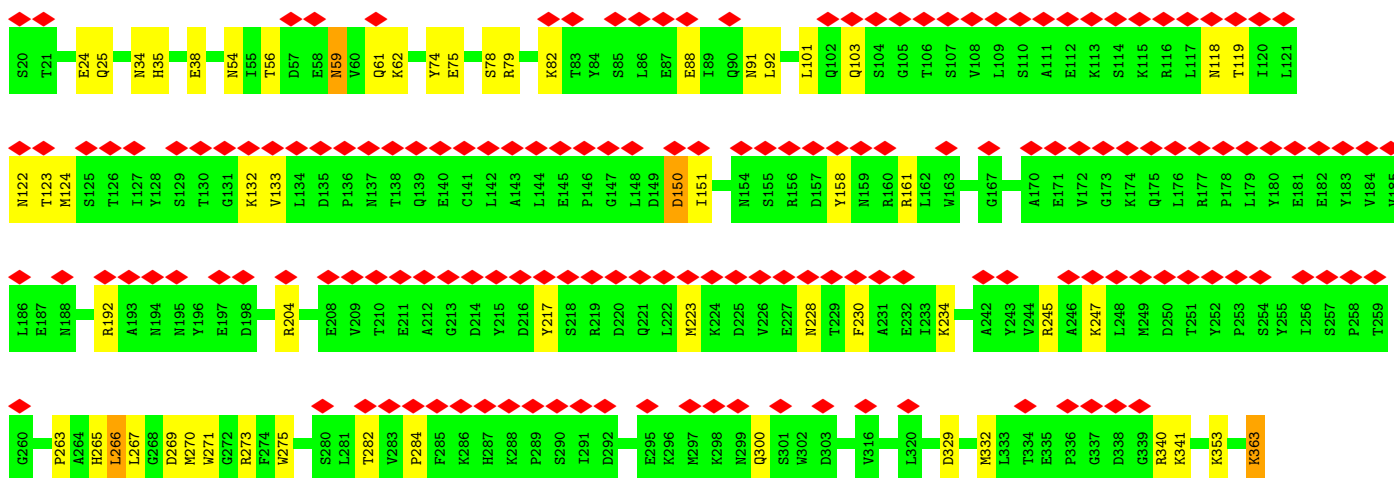
- Molecule 2: Angiotensin-converting enzyme

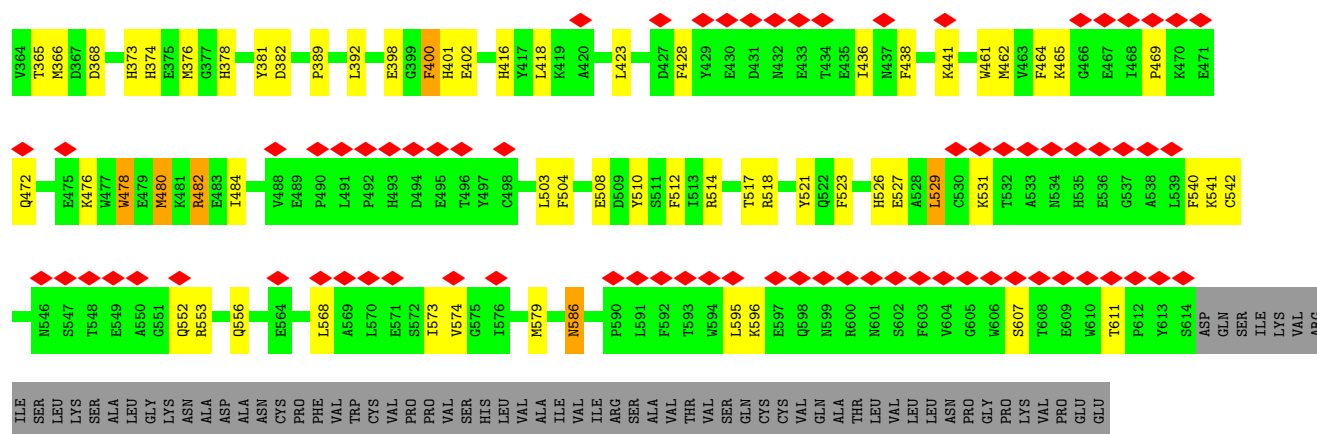
Chain E:  60% 27% 3% 10%



- Molecule 2: Angiotensin-converting enzyme

Chain F:  35% 72% 17% 10%





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

Chain G:  50%



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

Chain H:  100%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  100%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294102	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.412	Depositor
Minimum map value	-0.363	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	457.6, 457.6, 457.6	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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, ZN

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	0.43	13/8108 (0.2%)	0.59	13/11030 (0.1%)
1	B	0.31	0/8067	0.51	0/10971
1	C	0.32	0/8108	0.51	0/11030
2	E	0.28	0/5023	0.50	1/6810 (0.0%)
2	F	0.26	0/5023	0.52	1/6810 (0.0%)
All	All	0.33	13/34329 (0.0%)	0.53	15/46651 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	526	GLY	CA-C	8.74	1.65	1.51
1	A	527	PRO	N-CD	7.96	1.58	1.47
1	A	526	GLY	N-CA	7.85	1.57	1.46
1	A	529	LYS	N-CA	7.63	1.61	1.46
1	A	525	CYS	C-N	7.39	1.46	1.33
1	A	528	LYS	N-CA	7.20	1.60	1.46
1	A	527	PRO	N-CA	6.97	1.59	1.47
1	A	526	GLY	C-N	6.29	1.46	1.34
1	A	527	PRO	CA-C	6.14	1.65	1.52
1	A	524	VAL	C-N	5.45	1.46	1.34
1	A	529	LYS	C-N	5.36	1.46	1.34
1	A	528	LYS	C-N	5.19	1.46	1.34
1	A	527	PRO	C-N	5.15	1.45	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	PRO	CA-N-CD	-14.12	91.73	111.50
1	A	525	CYS	CB-CA-C	-11.62	87.16	110.40
1	A	525	CYS	N-CA-CB	-9.70	93.14	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	CYS	N-CA-C	6.88	129.58	111.00
1	A	528	LYS	N-CA-C	6.53	128.64	111.00
1	A	525	CYS	C-N-CA	6.19	135.29	122.30
1	A	526	GLY	C-N-CD	-6.13	107.11	120.60
1	A	528	LYS	C-N-CA	5.67	135.88	121.70
1	A	525	CYS	CA-C-N	5.58	127.36	116.20
1	A	529	LYS	CA-C-N	5.58	129.47	117.20
1	A	527	PRO	N-CA-C	5.49	126.36	112.10
2	F	266	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	526	GLY	CA-C-O	-5.10	111.42	120.60
2	E	214	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	528	LYS	CA-C-N	5.01	128.22	117.20

There are no chirality outliers.

There are no planarity outliers.

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	7922	0	7760	140	0
1	B	7884	0	7719	113	0
1	C	7922	0	7759	132	0
2	E	4888	0	4655	127	0
2	F	4888	0	4650	62	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	1	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	28	0	25	1	0
3	U	28	0	25	0	0
4	A	70	0	65	0	0
4	B	70	0	65	0	0
4	C	84	0	78	1	0
4	E	56	0	52	8	0
4	F	70	0	65	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	34248	0	33218	559	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 8.

All (559) 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)
2:E:54:ASN:HD22	4:E:701:NAG:C1	1.52	1.21
2:E:422:GLY:O	4:E:703:NAG:O3	1.70	1.06
2:E:299:ASN:HD21	4:E:703:NAG:C1	1.67	1.06
2:E:546:ASN:HD22	4:E:704:NAG:H61	1.25	1.02
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.52	0.92
2:E:54:ASN:ND2	4:E:701:NAG:C1	2.33	0.91
2:E:546:ASN:ND2	4:E:704:NAG:H61	1.89	0.86
1:C:447:GLY:HA2	1:C:498:ARG:HH22	1.42	0.83
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.61	0.81
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.63	0.81
1:B:328:ARG:HH21	1:B:533:LEU:HD23	1.47	0.79
1:B:100:ILE:HG22	1:B:242:LEU:HD11	1.67	0.77
2:F:573:ILE:HG13	2:F:574:VAL:HG13	1.66	0.76
2:E:299:ASN:ND2	4:E:703:NAG:C1	2.47	0.76
1:C:426:PRO:HD3	1:C:463:PRO:HB3	1.68	0.75
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.69	0.75
2:E:124:MET:N	2:E:124:MET:SD	2.59	0.75
1:B:215:ASP:N	1:B:266:TYR:HH	1.85	0.74
1:A:855:PHE:HB3	1:C:589:PRO:HG2	1.69	0.74
2:E:177:ARG:HG2	2:E:498:CYS:HB2	1.69	0.73
2:E:275:TRP:HB2	2:E:448:GLY:HA3	1.68	0.73
2:E:45:SER:HB2	2:E:351:LEU:HD11	1.68	0.73
1:B:125:ASN:ND2	1:B:172:SER:O	2.21	0.72
1:C:357:ARG:HG3	1:C:396:TYR:HE2	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.72	0.72
2:E:220:ASP:O	2:E:223:MET:HB2	1.89	0.72
1:A:332:ILE:H	1:A:333:THR:HA	1.55	0.71
1:B:135:PHE:HA	1:B:160:TYR:HA	1.72	0.71
1:A:527:PRO:C	1:A:528:LYS:HG3	2.10	0.70
1:B:336:CYS:HB3	1:B:363:ALA:HB2	1.74	0.70
2:E:256:ILE:HG12	2:E:263:PRO:HG2	1.74	0.70
1:A:421:TYR:HB3	1:A:457:ARG:H	1.56	0.70
1:A:83:VAL:HG11	1:A:237:ARG:HE	1.56	0.69
2:E:564:GLU:N	2:E:564:GLU:OE1	2.25	0.69
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.74	0.69
2:E:170:ALA:O	2:E:174:LYS:NZ	2.24	0.69
2:E:233:ILE:HG12	2:E:450:LEU:HD13	1.74	0.69
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.26	0.69
2:F:118:ASN:O	2:F:122:ASN:ND2	2.24	0.69
2:E:296:LYS:NZ	2:E:423:LEU:O	2.26	0.69
2:E:361:CYS:O	2:E:363:LYS:NZ	2.25	0.68
2:E:460:ARG:HH22	2:E:506:VAL:HG22	1.59	0.68
1:B:112:SER:HB2	1:B:134:GLN:HB2	1.75	0.68
2:E:78:SER:OG	2:E:101:LEU:O	2.10	0.68
1:C:505:HIS:CE1	2:E:353:LYS:HG2	2.28	0.68
1:A:675:GLN:O	1:A:690:GLN:N	2.27	0.67
1:A:1100:THR:OG1	1:A:1101:HIS:ND1	2.28	0.66
1:C:360:ASN:H	1:C:523:THR:HB	1.60	0.66
2:E:536:GLU:OE1	2:E:536:GLU:N	2.25	0.66
2:F:78:SER:HA	2:F:101:LEU:HG	1.78	0.66
1:C:66:TRP:HE1	1:C:264:ALA:HB1	1.60	0.66
2:E:304:ALA:HB2	2:E:364:VAL:HG22	1.78	0.65
2:E:573:ILE:HG23	2:E:574:VAL:HG13	1.77	0.65
2:E:248:LEU:HD11	2:E:281:LEU:HD22	1.76	0.65
1:A:119:ILE:HD12	1:A:128:ILE:HG13	1.79	0.65
2:E:236:LEU:HD22	2:E:584:LEU:HD21	1.79	0.65
1:C:422:ASN:HA	1:C:454:ARG:HH21	1.62	0.64
1:B:102:ARG:HG3	1:B:243:ALA:HB2	1.80	0.64
2:E:418:LEU:HD13	2:E:421:LEU:HD22	1.77	0.64
1:B:99:ASN:HB2	1:B:102:ARG:HH12	1.62	0.64
2:E:267:LEU:HD13	2:E:278:LEU:HD11	1.80	0.64
1:B:425:LEU:HD12	1:B:426:PRO:HD2	1.80	0.64
1:A:87:ASN:HD21	1:A:269:TYR:HB3	1.63	0.64
1:B:454:ARG:NH1	1:B:467:ASP:OD2	2.31	0.64
1:C:132:GLU:HB2	1:C:164:ASN:HD22	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:CB	1:A:166:CYS:HA	2.29	0.63
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.80	0.63
1:C:336:CYS:HB3	1:C:363:ALA:HA	1.79	0.63
1:C:487:ASN:OD1	2:E:77:GLN:NE2	2.32	0.63
2:E:278:LEU:O	2:E:282:THR:OG1	2.14	0.63
1:A:205:SER:HB3	1:A:226:LEU:HD22	1.81	0.63
1:C:421:TYR:HB3	1:C:457:ARG:HB3	1.81	0.62
1:A:414:GLN:O	1:A:424:LYS:NZ	2.31	0.62
2:E:92:LEU:C	2:E:94:LEU:H	2.03	0.62
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.81	0.62
1:A:675:GLN:OE1	1:A:690:GLN:N	2.32	0.62
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.82	0.62
2:F:553:ARG:O	2:F:553:ARG:NH1	2.32	0.62
2:F:523:PHE:O	2:F:527:GLU:HG2	2.00	0.61
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.33	0.61
2:E:515:TYR:O	2:E:519:THR:OG1	2.18	0.61
2:F:382:ASP:OD1	2:F:401:HIS:NE2	2.33	0.61
1:A:578:ASP:HB3	1:A:581:THR:O	1.99	0.61
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.83	0.61
1:A:345:THR:O	1:A:509:ARG:NH2	2.34	0.61
1:A:457:ARG:NH1	1:A:459:SER:O	2.32	0.61
2:E:82:LYS:HD3	2:E:82:LYS:N	2.15	0.61
2:E:90:GLN:O	2:E:95:LYS:HD3	2.00	0.61
2:E:209:VAL:HG11	2:E:565:PRO:HB3	1.83	0.60
1:A:646:ARG:O	1:A:646:ARG:NH1	2.34	0.60
1:C:659:SER:HB3	1:C:698:SER:HB3	1.83	0.60
1:C:42:ASP:OD2	1:C:46:ARG:NH2	2.33	0.60
1:A:190:ARG:HB3	1:A:192:PHE:HE1	1.67	0.60
1:B:343:ASN:HD21	1:B:371:PHE:HE2	1.49	0.60
1:C:387:LEU:H	1:C:387:LEU:HD23	1.67	0.60
2:F:35:HIS:O	2:F:35:HIS:ND1	2.30	0.60
1:A:856:ASN:HD21	1:A:966:LEU:HD12	1.65	0.60
2:E:341:LYS:HD3	2:E:341:LYS:H	1.67	0.60
2:F:526:HIS:HA	2:F:529:LEU:HD12	1.84	0.60
1:B:131:CYS:HB3	1:B:133:PHE:CE1	2.37	0.60
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.83	0.59
1:A:455:LEU:HD22	2:F:35:HIS:HD2	1.67	0.59
2:E:442:GLN:HB3	2:E:588:PHE:HZ	1.66	0.59
2:F:24:GLU:OE1	2:F:25:GLN:NE2	2.34	0.59
1:A:560:LEU:HD23	1:A:562:PHE:CE1	2.37	0.59
2:E:240:LEU:HD22	2:E:447:VAL:HG11	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:320:LEU:HD13	2:E:380:GLN:HG3	1.82	0.59
1:C:112:SER:HB3	1:C:134:GLN:HB2	1.85	0.59
2:F:552:GLN:O	2:F:556:GLN:NE2	2.25	0.59
1:B:811:LYS:NZ	1:B:815:ARG:O	2.34	0.58
4:C:1203:NAG:H83	4:C:1203:NAG:H3	1.84	0.58
1:A:527:PRO:O	1:A:528:LYS:HG3	2.03	0.58
2:F:282:THR:HG23	2:F:441:LYS:HE2	1.86	0.58
1:A:527:PRO:O	1:A:528:LYS:CG	2.52	0.58
1:B:352:ALA:HB1	1:B:466:ARG:HH21	1.68	0.58
1:B:409:GLN:HA	1:B:414:GLN:HE21	1.69	0.58
1:B:575:ALA:HB1	1:B:584:ILE:HD11	1.85	0.58
1:C:129:LYS:NZ	1:C:166:CYS:SG	2.75	0.58
2:F:38:GLU:OE1	2:F:353:LYS:NZ	2.36	0.58
2:F:541:LYS:O	2:F:541:LYS:HG2	2.03	0.58
2:F:61:GLN:HG3	2:F:62:LYS:HD2	1.85	0.58
1:C:438:SER:OG	1:C:442:ASP:OD2	2.21	0.57
1:C:954:HIS:HB3	1:C:1014:ARG:NH1	2.19	0.57
1:A:170:TYR:HE1	1:A:172:SER:HB2	1.69	0.57
1:A:1134:ASN:OD1	3:L:1:NAG:N2	2.37	0.57
1:B:188:ASN:O	1:B:190:ARG:NH1	2.37	0.57
1:C:752:LEU:HD21	1:C:990:GLU:HG3	1.87	0.57
1:C:375:PHE:HB3	1:C:435:ALA:O	2.05	0.57
1:C:989:ALA:O	1:C:993:ILE:HG12	2.04	0.57
1:A:82:PRO:O	1:A:239:GLN:NE2	2.37	0.57
2:E:478:TRP:HE3	2:E:482:ARG:HH12	1.53	0.57
2:E:240:LEU:O	2:E:244:VAL:HG23	2.04	0.57
2:E:310:GLU:HG2	2:E:421:LEU:HD11	1.86	0.57
1:A:426:PRO:HB3	1:A:463:PRO:HB3	1.87	0.56
4:F:703:NAG:H83	4:F:703:NAG:H3	1.87	0.56
1:C:350:VAL:HA	1:C:400:PHE:HB2	1.87	0.56
2:F:389:PRO:HD2	2:F:392:LEU:HD12	1.87	0.56
1:A:745:ASP:N	1:A:745:ASP:OD1	2.36	0.56
2:F:34:ASN:HA	2:F:389:PRO:HG3	1.87	0.56
2:E:496:THR:HG23	2:E:497:TYR:CD1	2.40	0.56
1:C:403:ARG:NH1	1:C:495:TYR:OH	2.39	0.56
1:A:108:THR:HA	1:A:236:THR:HG22	1.88	0.56
2:E:270:MET:SD	2:E:270:MET:N	2.75	0.56
1:A:883:THR:HG21	1:C:705:VAL:HB	1.88	0.56
1:B:398:ASP:HB2	1:B:512:VAL:HG22	1.88	0.56
1:A:462:LYS:HB2	1:A:465:GLU:HB3	1.87	0.55
2:E:224:LYS:HD3	2:E:224:LYS:N	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:226:VAL:HG11	2:E:458:LYS:HE3	1.88	0.55
2:E:269:ASP:OD2	2:E:274:PHE:N	2.38	0.55
4:E:703:NAG:H3	4:E:703:NAG:H83	1.87	0.55
3:T:1:NAG:H3	3:T:1:NAG:H83	1.88	0.55
1:A:329:PHE:HB2	1:A:529:LYS:O	2.07	0.55
1:B:437:ASN:HB2	1:B:508:TYR:CE2	2.42	0.55
1:B:454:ARG:HG3	1:B:491:PRO:HB2	1.87	0.55
1:A:391:CYS:SG	1:A:526:GLY:N	2.77	0.55
2:E:92:LEU:C	2:E:94:LEU:N	2.59	0.54
2:E:85:SER:C	2:E:87:GLU:H	2.10	0.54
2:E:124:MET:HE1	2:E:179:LEU:HD13	1.90	0.54
2:F:378:HIS:HE1	2:F:402:GLU:HA	1.73	0.54
2:F:418:LEU:HB3	2:F:423:LEU:HD12	1.88	0.54
1:A:1100:THR:HG1	1:A:1101:HIS:CE1	2.26	0.54
2:E:321:PRO:O	2:E:380:GLN:NE2	2.35	0.54
1:A:558:LYS:HZ1	1:A:561:PRO:HD3	1.73	0.54
1:A:661:GLU:N	1:A:661:GLU:OE1	2.37	0.54
1:A:705:VAL:HB	1:B:883:THR:HG21	1.90	0.54
1:C:416:GLY:H	1:C:419:ALA:HB3	1.73	0.54
1:C:776:LYS:O	1:C:780:GLU:HG2	2.08	0.54
2:F:340:ARG:NH1	2:F:341:LYS:O	2.41	0.54
2:E:476:LYS:HA	2:E:479:GLU:HB3	1.90	0.54
1:C:353:TRP:NE1	1:C:466:ARG:HA	2.23	0.54
1:A:455:LEU:HD22	2:F:35:HIS:CD2	2.43	0.53
1:B:357:ARG:CZ	1:C:230:PRO:HB2	2.38	0.53
2:F:482:ARG:O	2:F:482:ARG:NE	2.39	0.53
1:C:392:PHE:CE1	1:C:515:PHE:HB3	2.43	0.53
1:B:434:ILE:HD11	1:B:511:VAL:HG12	1.90	0.53
1:A:436:TRP:HH2	1:A:511:VAL:HG23	1.73	0.53
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.91	0.53
1:C:160:TYR:HE2	1:C:163:ALA:HB2	1.74	0.53
1:C:206:LYS:NZ	1:C:221:SER:OG	2.42	0.53
1:C:358:ILE:HG22	1:C:524:VAL:HG11	1.90	0.53
1:A:605:SER:OG	1:A:606:ASN:N	2.42	0.53
2:E:90:GLN:HE21	2:E:95:LYS:HG2	1.73	0.53
1:A:120:VAL:HB	1:A:127:VAL:HG23	1.91	0.52
2:E:557:MET:HA	2:E:560:LEU:HD12	1.90	0.52
1:C:101:ILE:HG12	1:C:242:LEU:HD13	1.91	0.52
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.09	0.52
2:E:398:GLU:O	2:E:514:ARG:NH2	2.38	0.52
1:A:132:GLU:HB2	1:A:164:ASN:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:483:GLU:HG3	2:E:608:THR:HG21	1.90	0.52
2:F:267:LEU:HD22	2:F:275:TRP:HE1	1.74	0.52
1:B:454:ARG:NH2	1:B:469:SER:O	2.42	0.52
1:A:883:THR:HG23	1:C:707:TYR:HB2	1.89	0.52
1:C:328:ARG:NH1	1:C:578:ASP:OD1	2.42	0.52
1:A:523:THR:HB	1:B:230:PRO:HB2	1.92	0.52
1:C:379:CYS:HA	1:C:432:CYS:HA	1.90	0.52
2:F:373:HIS:HA	2:F:376:MET:HG3	1.90	0.52
1:A:91:TYR:CE2	1:A:93:ALA:HB2	2.45	0.52
1:A:407:VAL:HG21	1:A:510:VAL:HB	1.91	0.52
1:A:984:LEU:HD13	1:A:988:GLU:HG3	1.92	0.52
1:A:534:VAL:HG21	1:A:539:VAL:HG11	1.92	0.52
1:A:100:ILE:HG22	1:A:242:LEU:HD23	1.92	0.52
1:B:153:MET:SD	1:B:155:SER:OG	2.54	0.52
1:C:487:ASN:HA	2:E:77:GLN:HE22	1.75	0.52
1:A:498:ARG:HG2	1:A:499:PRO:HD2	1.91	0.51
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.91	0.51
1:C:447:GLY:HA2	1:C:498:ARG:NH2	2.18	0.51
1:C:454:ARG:NH1	1:C:467:ASP:OD2	2.39	0.51
1:A:196:ASN:HB2	1:A:201:PHE:CD1	2.45	0.51
1:A:365:TYR:OH	1:A:386:LYS:N	2.43	0.51
2:E:369:PHE:O	2:E:373:HIS:ND1	2.43	0.51
1:B:139:PRO:HB2	1:B:159:VAL:HA	1.92	0.51
1:C:373:PRO:HA	1:C:377:PHE:CE1	2.46	0.51
1:B:357:ARG:NH2	1:B:396:TYR:OH	2.45	0.51
2:E:126:THR:O	2:E:130:THR:OG1	2.25	0.51
2:F:573:ILE:HG23	2:F:574:VAL:H	1.76	0.51
1:C:118:LEU:HD21	1:C:120:VAL:HG23	1.93	0.50
2:E:327:PHE:O	2:E:331:SER:OG	2.29	0.50
2:F:234:LYS:HD3	2:F:234:LYS:N	2.25	0.50
2:E:45:SER:O	2:E:357:ARG:NH2	2.45	0.50
2:E:53:THR:O	2:E:341:LYS:NZ	2.39	0.50
2:E:180:TYR:OH	2:E:463:VAL:HG21	2.11	0.50
2:E:297:MET:HG2	2:E:302:TRP:CE3	2.47	0.50
1:B:55:ASP:HB3	1:B:57:PHE:CE2	2.47	0.50
2:E:416:HIS:HE1	2:E:541:LYS:HA	1.76	0.50
1:A:127:VAL:HG12	1:A:171:VAL:HG22	1.92	0.50
1:A:127:VAL:HB	1:A:129:LYS:HZ1	1.77	0.50
1:A:133:PHE:HE1	1:A:160:TYR:HA	1.77	0.50
1:A:493:GLN:HE22	2:F:35:HIS:CE1	2.29	0.50
1:A:555:SER:HB3	1:A:584:ILE:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ILE:HG22	1:C:242:LEU:HD12	1.92	0.50
1:C:452:ARG:HG2	1:C:494:SER:HB3	1.92	0.50
2:E:268:GLY:HA3	2:E:277:ASN:HB2	1.94	0.50
2:E:455:MET:SD	2:E:456:LEU:N	2.84	0.50
1:A:196:ASN:HB2	1:A:201:PHE:HD1	1.76	0.50
1:B:121:ASN:ND2	1:B:176:LEU:HD23	2.26	0.50
2:F:119:THR:O	2:F:123:THR:OG1	2.27	0.50
1:B:36:ARG:NH1	1:B:217:PRO:O	2.45	0.50
1:B:1098:ASN:HD21	3:P:1:NAG:C1	2.24	0.50
1:C:361:CYS:H	1:C:524:VAL:HG12	1.76	0.50
1:A:105:ILE:HG13	1:A:241:LEU:HD11	1.94	0.49
1:A:659:SER:HB3	1:A:698:SER:HB2	1.93	0.49
1:A:821:LEU:HD11	1:A:939:SER:HB3	1.94	0.49
1:C:215:ASP:N	1:C:266:TYR:HH	2.10	0.49
2:F:579:MET:SD	2:F:579:MET:N	2.85	0.49
1:A:358:ILE:N	1:A:395:VAL:O	2.34	0.49
1:B:393:THR:HG22	1:B:522:ALA:HA	1.95	0.49
1:B:1088:HIS:HB3	1:B:1120:THR:HG21	1.95	0.49
2:F:329:ASP:OD1	2:F:329:ASP:N	2.46	0.49
1:B:971:GLY:O	1:B:995:ARG:NH1	2.44	0.49
1:B:391:CYS:SG	1:B:522:ALA:HB1	2.52	0.49
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.93	0.49
1:B:33:SER:HB3	1:B:64:VAL:HG21	1.94	0.49
1:B:134:GLN:HB3	1:B:162:SER:HB3	1.93	0.49
2:E:119:THR:O	2:E:123:THR:OG1	2.27	0.49
2:E:323:MET:HE3	2:E:356:PHE:HB2	1.95	0.49
2:F:586:ASN:O	2:F:586:ASN:ND2	2.46	0.49
2:E:63:MET:SD	2:E:63:MET:N	2.74	0.49
1:A:113:LYS:NZ	1:A:114:THR:HB	2.27	0.49
1:B:328:ARG:HB3	1:B:579:PRO:HD2	1.94	0.49
2:E:442:GLN:HB3	2:E:588:PHE:CZ	2.47	0.49
2:E:539:LEU:HB3	2:E:587:TYR:HD1	1.78	0.49
2:F:461:TRP:O	2:F:465:LYS:NZ	2.44	0.49
1:B:121:ASN:HD21	1:B:176:LEU:H	1.60	0.48
1:B:133:PHE:HA	1:B:162:SER:O	2.12	0.48
1:C:461:LEU:HD11	1:C:467:ASP:HB2	1.94	0.48
2:F:78:SER:OG	2:F:103:GLN:O	2.31	0.48
1:A:400:PHE:HE1	1:A:407:VAL:HG23	1.77	0.48
1:C:163:ALA:O	1:C:164:ASN:OD1	2.32	0.48
1:A:589:PRO:HB2	1:B:855:PHE:HD2	1.77	0.48
1:C:327:VAL:HG12	1:C:542:ASN:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:609:GLU:OE1	2:E:609:GLU:N	2.40	0.48
2:E:338:ASP:HB2	2:E:340:ARG:HG3	1.96	0.48
1:B:470:THR:HG21	1:B:492:LEU:HD22	1.96	0.48
1:B:556:ASN:OD1	1:B:556:ASN:N	2.47	0.47
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.95	0.47
2:E:85:SER:O	2:E:87:GLU:N	2.46	0.47
1:A:83:VAL:HG21	1:A:237:ARG:HH21	1.78	0.47
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.86	0.47
2:F:74:TYR:HB3	2:F:75:GLU:OE2	2.15	0.47
1:A:355:ARG:HH12	1:A:464:PHE:HB3	1.79	0.47
1:A:406:GLU:HB3	1:A:418:ILE:HG21	1.96	0.47
1:A:856:ASN:ND2	1:A:966:LEU:HD12	2.29	0.47
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.95	0.47
1:B:33:SER:O	1:B:61:PHE:HA	2.15	0.47
1:C:55:ASP:HB3	1:C:57:PHE:CE2	2.49	0.47
1:C:498:ARG:HG2	1:C:501:TYR:CE1	2.49	0.47
2:E:489:GLU:N	2:E:489:GLU:OE1	2.47	0.47
1:A:448:ASN:HB2	1:A:497:PHE:HD2	1.78	0.47
1:B:132:GLU:HB2	1:B:164:ASN:HB3	1.96	0.47
2:E:582:LYS:C	2:E:582:LYS:HD2	2.34	0.47
2:E:215:TYR:CZ	2:E:568:LEU:HD13	2.49	0.47
2:E:249:MET:SD	2:E:249:MET:N	2.87	0.47
1:A:577:ARG:HA	1:A:583:GLU:O	2.15	0.47
1:C:38:VAL:HG11	1:C:220:PHE:CE2	2.48	0.47
1:C:350:VAL:HG12	1:C:453:TYR:HB2	1.96	0.47
1:C:868:GLU:OE1	1:C:868:GLU:N	2.45	0.47
2:E:460:ARG:HG2	2:E:464:PHE:CZ	2.50	0.47
1:B:1002:GLN:O	1:B:1006:THR:HG23	2.15	0.47
2:E:269:ASP:HB3	2:E:272:GLY:H	1.79	0.47
2:E:374:HIS:CE1	2:E:378:HIS:HE1	2.33	0.47
2:E:425:GLU:O	2:E:427:ASP:N	2.45	0.47
1:B:1073:LYS:HE2	1:B:1073:LYS:HB3	1.67	0.46
1:C:431:GLY:HA3	1:C:513:LEU:O	2.15	0.46
1:A:569:ILE:HD12	1:A:570:ALA:N	2.30	0.46
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.97	0.46
1:A:589:PRO:HB2	1:B:855:PHE:CD2	2.49	0.46
1:C:505:HIS:ND1	2:E:353:LYS:HE3	2.30	0.46
2:F:88:GLU:N	2:F:88:GLU:OE1	2.48	0.46
1:B:578:ASP:HB3	1:B:581:THR:O	2.15	0.46
2:F:269:ASP:OD1	2:F:270:MET:N	2.48	0.46
1:C:168:PHE:CE1	1:C:170:TYR:HB2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:SER:HB2	1:C:497:PHE:HB3	1.97	0.46
1:C:599:THR:HB	1:C:608:VAL:HG12	1.97	0.46
1:C:703:ASN:OD1	1:C:704:SER:N	2.49	0.46
2:E:226:VAL:HG11	2:E:458:LYS:HB2	1.97	0.46
2:F:56:THR:OG1	2:F:59:ASN:HB2	2.15	0.46
1:A:112:SER:HB3	1:A:134:GLN:HB2	1.98	0.46
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.98	0.46
1:C:206:LYS:HB3	1:C:223:LEU:HD22	1.97	0.46
2:E:329:ASP:OD1	2:E:329:ASP:N	2.48	0.46
2:E:70:TRP:O	2:E:74:TYR:HB2	2.16	0.46
2:E:93:THR:HG23	2:E:96:ARG:HD3	1.98	0.46
2:F:91:ASN:OD1	2:F:92:LEU:N	2.48	0.46
2:F:517:THR:HG22	2:F:521:TYR:HD2	1.81	0.46
1:B:121:ASN:HD22	1:B:176:LEU:HD23	1.81	0.46
1:B:424:LYS:NZ	1:B:425:LEU:O	2.49	0.46
1:C:435:ALA:HB2	1:C:510:VAL:HG22	1.96	0.46
1:C:964:LYS:HE3	1:C:964:LYS:HB3	1.76	0.46
2:F:469:PRO:HD2	2:F:472:GLN:HB2	1.98	0.46
1:A:386:LYS:HA	1:A:386:LYS:HD2	1.69	0.46
1:A:950:ASP:OD1	1:A:951:VAL:N	2.49	0.46
1:C:355:ARG:HD2	1:C:396:TYR:CD1	2.51	0.46
1:C:358:ILE:HB	1:C:395:VAL:HB	1.97	0.46
1:C:398:ASP:O	1:C:511:VAL:HA	2.16	0.46
2:E:390:TYR:HA	2:E:393:ARG:HB2	1.98	0.46
1:C:105:ILE:O	1:C:238:PHE:HA	2.17	0.45
2:E:204:ARG:HH21	2:E:461:TRP:HE1	1.63	0.45
2:E:263:PRO:HB3	2:E:265:HIS:CE1	2.51	0.45
2:F:480:MET:O	2:F:484:ILE:HG22	2.16	0.45
1:A:429:PHE:CE2	1:A:514:SER:HB2	2.51	0.45
1:A:540:ASN:OD1	1:A:540:ASN:N	2.50	0.45
1:B:141:LEU:HB2	1:B:243:ALA:HA	1.98	0.45
2:E:493:HIS:HB3	2:E:497:TYR:HB2	1.98	0.45
1:A:989:ALA:O	1:A:993:ILE:HG12	2.17	0.45
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.49	0.45
1:B:403:ARG:HH11	1:B:495:TYR:HD2	1.63	0.45
1:B:120:VAL:HB	1:B:127:VAL:HG22	1.98	0.45
1:A:454:ARG:NH2	1:A:492:LEU:HD13	2.31	0.45
1:A:562:PHE:HB2	1:B:43:LYS:NZ	2.32	0.45
1:B:101:ILE:HD11	1:B:240:THR:OG1	2.17	0.45
1:B:1088:HIS:HB3	1:B:1120:THR:CG2	2.47	0.45
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:204:ARG:HA	2:E:204:ARG:HD3	1.70	0.45
2:F:150:ASP:OD2	2:F:151:ILE:HG12	2.16	0.45
1:C:605:SER:OG	1:C:606:ASN:N	2.50	0.45
2:E:465:LYS:HD3	2:E:465:LYS:N	2.32	0.45
1:A:48:SER:HA	1:A:279:TYR:O	2.17	0.45
1:C:373:PRO:HD2	1:C:374:PHE:CE1	2.52	0.45
1:C:402:ILE:HD11	1:C:418:ILE:HG13	1.99	0.45
1:C:738:CYS:SG	1:C:739:THR:N	2.89	0.45
1:A:36:ARG:NH2	1:A:191:GLU:OE2	2.41	0.44
1:A:521:PRO:HB2	1:A:523:THR:HG23	1.98	0.44
1:A:1082:CYS:HB2	1:A:1126:CYS:HB2	1.91	0.44
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.53	0.44
2:E:294:THR:O	2:E:298:LYS:HG3	2.16	0.44
2:E:382:ASP:O	2:E:386:ALA:N	2.50	0.44
1:A:95:THR:HG22	1:A:188:ASN:O	2.17	0.44
1:A:1138:TYR:OH	1:A:1143:PRO:HG2	2.17	0.44
1:C:498:ARG:HD2	1:C:498:ARG:N	2.32	0.44
2:E:209:VAL:HG23	2:E:216:ASP:HA	1.99	0.44
1:A:113:LYS:HZ2	1:A:114:THR:HB	1.81	0.44
1:A:176:LEU:HD12	1:A:190:ARG:HD3	2.00	0.44
1:B:342:PHE:HD2	1:B:436:TRP:HZ3	1.66	0.44
1:C:102:ARG:HA	1:C:102:ARG:HD3	1.70	0.44
2:F:478:TRP:CE3	2:F:478:TRP:HA	2.52	0.44
1:A:127:VAL:HB	1:A:129:LYS:NZ	2.32	0.44
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.98	0.44
1:B:448:ASN:H	1:B:497:PHE:HB2	1.82	0.44
1:C:382:VAL:HG21	1:C:515:PHE:HE2	1.82	0.44
2:E:273:ARG:HD2	2:E:452:PHE:CE2	2.52	0.44
1:A:454:ARG:HG2	1:A:456:PHE:O	2.18	0.44
2:F:132:LYS:NZ	2:F:133:VAL:H	2.15	0.44
1:A:187:LYS:O	1:A:210:ILE:HG13	2.17	0.44
1:A:960:ASN:O	1:A:963:VAL:HG12	2.18	0.44
2:E:312:GLU:HA	2:E:315:PHE:HD2	1.80	0.44
2:F:119:THR:HA	2:F:122:ASN:HD21	1.83	0.44
1:A:131:CYS:HB2	1:A:166:CYS:HA	1.99	0.44
1:B:484:ALA:HA	1:B:488:CYS:HB3	1.98	0.44
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.82	0.44
2:E:557:MET:SD	2:E:573:ILE:HB	2.58	0.44
1:A:569:ILE:HD11	1:B:849:LEU:N	2.33	0.43
1:B:868:GLU:O	1:B:872:GLN:HG3	2.18	0.43
1:B:969:LYS:HZ3	1:B:971:GLY:H	1.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:962:LEU:HA	1:C:962:LEU:HD12	1.85	0.43
2:E:452:PHE:HA	2:E:455:MET:HG3	2.00	0.43
2:F:400:PHE:O	2:F:400:PHE:CD1	2.71	0.43
1:A:405:ASN:OD1	1:A:406:GLU:N	2.51	0.43
1:B:340:GLU:OE1	1:B:340:GLU:N	2.47	0.43
1:C:347:PHE:HB2	1:C:509:ARG:NE	2.33	0.43
1:A:215:ASP:N	1:A:266:TYR:HH	2.16	0.43
1:C:48:SER:N	1:C:280:ASN:O	2.46	0.43
2:E:225:ASP:OD1	2:E:225:ASP:N	2.50	0.43
2:E:248:LEU:HD12	2:E:248:LEU:HA	1.71	0.43
2:F:398:GLU:N	2:F:398:GLU:OE1	2.52	0.43
1:A:371:PHE:HB2	1:A:436:TRP:HA	2.01	0.43
1:B:455:LEU:HD12	1:B:455:LEU:HA	1.85	0.43
1:B:434:ILE:HD12	1:B:434:ILE:C	2.39	0.43
1:A:411:ALA:HB3	1:A:414:GLN:HB2	2.01	0.43
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.82	0.43
1:B:439:ASN:HA	1:B:507:PRO:HG2	1.99	0.43
2:E:57:ASP:OD1	2:E:58:GLU:N	2.52	0.43
2:E:302:TRP:HD1	2:E:303:ASP:N	2.17	0.43
2:F:204:ARG:HA	2:F:204:ARG:HD2	1.81	0.43
1:A:290:ASP:N	1:A:290:ASP:OD1	2.52	0.43
1:A:722:VAL:HA	1:A:1064:HIS:O	2.17	0.43
1:B:200:TYR:CZ	1:B:230:PRO:HB3	2.53	0.43
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.01	0.43
1:B:424:LYS:HB3	1:B:463:PRO:HA	2.00	0.43
1:B:439:ASN:O	1:B:443:SER:HB3	2.18	0.43
1:B:576:VAL:O	1:B:584:ILE:HD12	2.19	0.43
1:C:474:GLN:OE1	1:C:485:GLY:HA3	2.18	0.43
1:C:794:ILE:HD12	1:C:794:ILE:O	2.19	0.43
2:E:529:LEU:HD23	2:E:550:ALA:HB1	2.01	0.43
2:F:462:MET:SD	2:F:462:MET:N	2.92	0.43
1:A:125:ASN:HA	1:A:174:PRO:HD3	2.01	0.43
1:B:381:GLY:HA3	1:B:430:THR:HG23	1.99	0.43
1:C:502:GLY:O	1:C:506:GLN:HG3	2.17	0.43
2:E:131:GLY:HA3	2:E:168:TRP:HZ3	1.83	0.43
2:F:436:ILE:HD13	2:F:436:ILE:HA	1.86	0.43
2:E:582:LYS:HG3	2:E:583:PRO:HD3	2.00	0.43
1:B:346:ARG:NE	1:B:451:TYR:OH	2.51	0.42
1:C:452:ARG:HA	1:C:494:SER:HA	2.01	0.42
1:C:599:THR:OG1	1:C:600:PRO:O	2.31	0.42
1:C:1048:HIS:HA	1:C:1066:THR:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:OE1	1:A:170:TYR:N	2.52	0.42
1:A:336:CYS:SG	1:A:362:VAL:HB	2.59	0.42
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.53	0.42
1:C:290:ASP:O	1:C:297:SER:HB3	2.19	0.42
1:C:357:ARG:HB3	1:C:357:ARG:NH1	2.34	0.42
1:C:439:ASN:O	1:C:443:SER:N	2.52	0.42
1:C:505:HIS:ND1	2:E:353:LYS:HG2	2.34	0.42
2:E:335:GLU:HG2	2:E:363:LYS:HA	2.00	0.42
2:E:156:ARG:O	2:E:156:ARG:NH1	2.34	0.42
2:E:160:ARG:HA	2:E:160:ARG:HD3	1.75	0.42
2:E:383:MET:H	2:E:383:MET:HG2	1.68	0.42
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.23	0.42
1:B:444:LYS:HB2	1:B:444:LYS:HE3	1.80	0.42
2:E:236:LEU:HD12	2:E:236:LEU:HA	1.87	0.42
1:A:402:ILE:HG13	1:A:407:VAL:HB	2.01	0.42
1:B:131:CYS:HB3	1:B:133:PHE:CZ	2.54	0.42
1:C:378:LYS:HB3	1:C:378:LYS:HE3	1.90	0.42
2:F:363:LYS:H	2:F:363:LYS:HD3	1.85	0.42
1:B:697:MET:HB2	1:B:697:MET:HE3	1.94	0.42
1:C:108:THR:OG1	1:C:234:ASN:O	2.33	0.42
1:C:429:PHE:HE1	1:C:514:SER:HB2	1.84	0.42
2:F:553:ARG:NH1	2:F:556:GLN:HB2	2.35	0.42
1:B:242:LEU:HD12	1:B:242:LEU:HA	1.85	0.42
2:E:451:PRO:O	2:E:455:MET:HG3	2.19	0.42
1:A:529:LYS:HE2	1:A:529:LYS:HB2	1.66	0.42
1:B:103:GLY:C	1:B:104:TRP:CD1	2.93	0.42
1:C:347:PHE:CG	1:C:509:ARG:HG2	2.54	0.42
1:B:326:ILE:HG12	1:B:539:VAL:HG21	2.02	0.42
1:B:347:PHE:HB2	1:B:401:VAL:HG13	2.01	0.42
1:C:172:SER:OG	1:C:173:GLN:N	2.52	0.42
1:C:376:ALA:O	1:C:434:ILE:HG23	2.20	0.42
1:C:790:LYS:HE2	1:C:790:LYS:HB3	1.90	0.42
1:C:985:ASP:OD1	1:C:988:GLU:HB2	2.20	0.42
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.55	0.42
2:E:175:GLN:O	2:E:178:PRO:HD2	2.20	0.42
2:F:300:GLN:HE21	2:F:300:GLN:HB2	1.65	0.42
1:A:560:LEU:HG	1:A:561:PRO:HD2	2.02	0.42
1:C:392:PHE:CG	1:C:393:THR:N	2.88	0.42
2:F:595:LEU:HD12	2:F:596:LYS:HD3	2.01	0.42
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.82	0.41
1:C:229:LEU:HB3	1:C:231:ILE:HG23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:236:LEU:HG	2:E:447:VAL:HG22	2.01	0.41
2:E:323:MET:HG2	2:E:324:THR:N	2.35	0.41
1:A:83:VAL:HG22	1:A:239:GLN:HE22	1.85	0.41
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.84	0.41
1:B:378:LYS:HB3	1:B:378:LYS:HE2	1.87	0.41
1:C:348:ALA:O	1:C:400:PHE:HA	2.20	0.41
1:C:377:PHE:HA	1:C:434:ILE:HG12	2.02	0.41
1:C:1004:LEU:HD23	1:C:1004:LEU:HA	1.87	0.41
1:A:187:LYS:HD2	1:A:210:ILE:HD11	2.02	0.41
1:B:327:VAL:HG12	1:B:542:ASN:HB3	2.02	0.41
1:C:351:TYR:HB2	1:C:454:ARG:NH1	2.35	0.41
1:C:662:CYS:HB2	1:C:697:MET:HE3	2.03	0.41
2:F:263:PRO:HD2	2:F:266:LEU:HD13	2.02	0.41
1:A:128:ILE:HB	1:A:170:TYR:HB3	2.01	0.41
1:B:344:ALA:HB3	1:B:347:PHE:CE1	2.56	0.41
1:B:855:PHE:CD1	1:B:855:PHE:N	2.88	0.41
1:A:109:THR:OG1	1:A:111:ASP:OD1	2.37	0.41
1:A:619:GLU:H	1:A:619:GLU:HG2	1.68	0.41
1:B:825:LYS:HE2	1:B:825:LYS:HB2	1.74	0.41
2:E:85:SER:C	2:E:87:GLU:N	2.74	0.41
1:A:119:ILE:HD12	1:A:128:ILE:CG1	2.50	0.41
1:A:358:ILE:HD12	1:A:513:LEU:HD11	2.02	0.41
1:A:592:PHE:CE1	1:B:855:PHE:HA	2.56	0.41
1:B:84:LEU:HD22	1:B:84:LEU:H	1.85	0.41
1:B:447:GLY:HA2	1:B:497:PHE:O	2.20	0.41
1:B:1086:LYS:HB2	1:B:1086:LYS:HE3	1.74	0.41
1:C:498:ARG:HG2	1:C:501:TYR:HE1	1.85	0.41
2:F:464:PHE:HB2	2:F:465:LYS:NZ	2.35	0.41
1:B:281:GLU:H	1:B:281:GLU:HG3	1.70	0.41
1:C:351:TYR:CD2	1:C:453:TYR:HA	2.55	0.41
1:C:355:ARG:HD2	1:C:396:TYR:CG	2.56	0.41
1:A:1071:GLN:H	1:A:1071:GLN:HG3	1.57	0.41
1:C:126:VAL:O	1:C:171:VAL:HA	2.20	0.41
2:E:239:GLN:HE22	2:E:596:LYS:NZ	2.19	0.41
2:E:416:HIS:CE1	2:E:541:LYS:HA	2.54	0.41
2:F:503:LEU:HD23	2:F:503:LEU:HA	1.92	0.41
1:A:134:GLN:HB3	1:A:162:SER:HB3	2.03	0.41
1:A:501:TYR:HB3	1:A:505:HIS:CB	2.51	0.41
1:A:501:TYR:HB3	1:A:505:HIS:HB2	2.03	0.41
1:B:215:ASP:N	1:B:266:TYR:OH	2.50	0.41
1:B:358:ILE:HB	1:B:395:VAL:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:SER:HA	1:B:497:PHE:HD2	1.86	0.41
1:B:518:LEU:HD13	1:B:518:LEU:HA	1.94	0.41
1:C:126:VAL:HG12	1:C:128:ILE:HG13	2.03	0.41
1:C:453:TYR:CE1	1:C:495:TYR:HB2	2.56	0.41
1:C:751:ASN:O	1:C:755:GLN:NE2	2.53	0.41
2:E:94:LEU:HD13	2:E:98:LEU:HG	2.03	0.41
2:E:403:ALA:HB2	2:E:518:ARG:HB2	2.03	0.41
2:F:568:LEU:HD12	2:F:568:LEU:HA	1.92	0.41
1:A:298:GLU:O	1:A:302:THR:HG23	2.21	0.41
1:B:529:LYS:HA	1:B:529:LYS:HD3	1.97	0.41
1:C:245:HIS:C	1:C:246:ARG:HD2	2.41	0.41
2:E:560:LEU:HB3	2:E:564:GLU:OE2	2.21	0.41
1:B:764:LYS:HE2	1:B:764:LYS:HB3	1.73	0.40
1:C:713:ALA:HA	1:C:1073:LYS:O	2.21	0.40
2:F:508:GLU:HB3	2:F:510:TYR:CE2	2.56	0.40
1:A:981:LEU:HA	1:A:981:LEU:HD23	1.84	0.40
1:B:1048:HIS:HA	1:B:1066:THR:HG22	2.03	0.40
1:C:357:ARG:HG3	1:C:396:TYR:CE2	2.44	0.40
1:C:365:TYR:CE1	1:C:388:ASN:HA	2.55	0.40
1:C:442:ASP:HA	1:C:451:TYR:CE2	2.56	0.40
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.94	0.40
2:E:566:TRP:CZ3	2:E:570:LEU:HD22	2.56	0.40
1:A:403:ARG:HB2	1:A:406:GLU:OE1	2.21	0.40
1:B:111:ASP:OD1	1:B:113:LYS:N	2.48	0.40
1:B:599:THR:HB	1:B:608:VAL:HG12	2.03	0.40
2:E:300:GLN:CD	2:E:306:ARG:HH12	2.25	0.40
2:E:586:ASN:OD1	2:E:587:TYR:N	2.54	0.40
2:F:363:LYS:HG2	2:F:365:THR:HG23	2.02	0.40
1:A:187:LYS:HD2	1:A:187:LYS:HA	1.87	0.40
1:A:825:LYS:HE3	1:A:825:LYS:HB3	1.90	0.40
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.22	0.40
1:B:294:ASP:N	1:B:294:ASP:OD1	2.55	0.40
1:B:763:LEU:HG	1:B:1008:VAL:HG21	2.04	0.40
1:C:454:ARG:HG3	1:C:491:PRO:O	2.21	0.40
1:C:495:TYR:HB3	1:C:497:PHE:CZ	2.56	0.40
2:F:82:LYS:HA	2:F:82:LYS:HD2	1.94	0.40
1:A:378:LYS:HD3	1:A:378:LYS:HA	1.89	0.40
1:A:964:LYS:HB3	1:A:964:LYS:HE2	1.73	0.40
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.57	0.40
1:B:498:ARG:O	1:B:501:TYR:HB2	2.22	0.40
1:C:190:ARG:HB3	1:C:192:PHE:CE2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LYS:HD2	1:C:386:LYS:HA	1.84	0.40
2:F:245:ARG:HH11	2:F:245:ARG:HG2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	993/1127 (88%)	952 (96%)	38 (4%)	3 (0%)	37	46
1	B	986/1127 (88%)	951 (96%)	35 (4%)	0	100	100
1	C	993/1127 (88%)	955 (96%)	38 (4%)	0	100	100
2	E	593/661 (90%)	563 (95%)	27 (5%)	3 (0%)	25	34
2	F	593/661 (90%)	576 (97%)	16 (3%)	1 (0%)	44	56
All	All	4158/4703 (88%)	3997 (96%)	154 (4%)	7 (0%)	45	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	PRO
2	F	284	PRO
1	A	529	LYS
1	A	528	LYS
2	E	86	LEU
2	E	93	THR
2	E	89	ILE

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	886/980 (90%)	859 (97%)	27 (3%)	36	52
1	B	881/980 (90%)	849 (96%)	32 (4%)	30	44
1	C	886/980 (90%)	867 (98%)	19 (2%)	48	66
2	E	527/585 (90%)	479 (91%)	48 (9%)	7	9
2	F	527/585 (90%)	486 (92%)	41 (8%)	10	13
All	All	3707/4110 (90%)	3540 (96%)	167 (4%)	26	34

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	115	GLN
1	A	118	LEU
1	A	135	PHE
1	A	153	MET
1	A	157	PHE
1	A	188	ASN
1	A	208	THR
1	A	220	PHE
1	A	244	LEU
1	A	290	ASP
1	A	314	GLN
1	A	318	PHE
1	A	329	PHE
1	A	347	PHE
1	A	374	PHE
1	A	400	PHE
1	A	432	CYS
1	A	495	TYR
1	A	525	CYS
1	A	528	LYS
1	A	529	LYS
1	A	820	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	902	MET
1	A	968	SER
1	A	1037	SER
1	A	1043	CYS
1	B	53	THR
1	B	68	HIS
1	B	98	SER
1	B	99	ASN
1	B	135	PHE
1	B	153	MET
1	B	160	TYR
1	B	162	SER
1	B	168	PHE
1	B	177	MET
1	B	220	PHE
1	B	238	PHE
1	B	308	VAL
1	B	318	PHE
1	B	351	TYR
1	B	365	TYR
1	B	369	TYR
1	B	375	PHE
1	B	377	PHE
1	B	393	THR
1	B	398	ASP
1	B	428	ASP
1	B	436	TRP
1	B	501	TYR
1	B	519	HIS
1	B	565	PHE
1	B	590	CYS
1	B	698	SER
1	B	820	ASP
1	B	902	MET
1	B	936	ASP
1	B	1005	GLN
1	C	68	HIS
1	C	99	ASN
1	C	131	CYS
1	C	220	PHE
1	C	291	CYS
1	C	314	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	335	LEU
1	C	338	PHE
1	C	365	TYR
1	C	369	TYR
1	C	400	PHE
1	C	498	ARG
1	C	528	LYS
1	C	529	LYS
1	C	553	THR
1	C	588	THR
1	C	617	CYS
1	C	756	TYR
1	C	936	ASP
2	E	20	SER
2	E	29	PHE
2	E	40	LEU
2	E	63	MET
2	E	64	ASN
2	E	74	TYR
2	E	80	MET
2	E	94	LEU
2	E	112	GLU
2	E	116	ARG
2	E	124	MET
2	E	156	ARG
2	E	204	ARG
2	E	217	TYR
2	E	223	MET
2	E	241	HIS
2	E	245	ARG
2	E	249	MET
2	E	255	TYR
2	E	265	HIS
2	E	270	MET
2	E	290	SER
2	E	341	LYS
2	E	360	MET
2	E	374	HIS
2	E	381	TYR
2	E	401	HIS
2	E	408	MET
2	E	416	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	429	TYR
2	E	455	MET
2	E	458	LYS
2	E	460	ARG
2	E	462	MET
2	E	465	LYS
2	E	473	TRP
2	E	476	LYS
2	E	481	LYS
2	E	491	LEU
2	E	511	SER
2	E	514	ARG
2	E	518	ARG
2	E	527	GLU
2	E	544	ILE
2	E	580	ASP
2	E	582	LYS
2	E	611	THR
2	E	613	TYR
2	F	54	ASN
2	F	59	ASN
2	F	79	ARG
2	F	124	MET
2	F	150	ASP
2	F	158	TYR
2	F	161	ARG
2	F	192	ARG
2	F	217	TYR
2	F	223	MET
2	F	228	ASN
2	F	230	PHE
2	F	247	LYS
2	F	265	HIS
2	F	271	TRP
2	F	273	ARG
2	F	332	MET
2	F	363	LYS
2	F	366	MET
2	F	368	ASP
2	F	374	HIS
2	F	381	TYR
2	F	400	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	416	HIS
2	F	428	PHE
2	F	438	PHE
2	F	476	LYS
2	F	478	TRP
2	F	480	MET
2	F	482	ARG
2	F	504	PHE
2	F	512	PHE
2	F	514	ARG
2	F	518	ARG
2	F	529	LEU
2	F	531	LYS
2	F	540	PHE
2	F	542	CYS
2	F	586	ASN
2	F	607	SER
2	F	611	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	331	ASN
1	A	856	ASN
1	B	99	ASN
1	B	394	ASN
1	B	414	GLN
1	B	437	ASN
1	B	954	HIS
1	B	955	ASN
1	B	1098	ASN
1	C	164	ASN
1	C	1134	ASN
2	E	35	HIS
2	E	54	ASN
2	E	77	GLN
2	E	90	GLN
2	E	239	GLN
2	E	299	ASN
2	E	325	GLN
2	E	330	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	416	HIS
2	F	239	GLN
2	F	241	HIS
2	F	300	GLN
2	F	325	GLN
2	F	378	HIS

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 ⓘ

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	G	1	3	14,14,15	0.41	0	17,19,21	0.76	1 (5%)
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	H	1	3	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	H	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	I	1	3	14,14,15	0.52	0	17,19,21	0.35	0
3	NAG	I	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	J	1	3	14,14,15	0.48	0	17,19,21	0.35	0
3	NAG	J	2	3	14,14,15	0.19	0	17,19,21	0.49	0
3	NAG	K	1	3	14,14,15	0.50	0	17,19,21	0.42	0
3	NAG	K	2	3	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	L	1	3	14,14,15	0.75	1 (7%)	17,19,21	0.49	0
3	NAG	L	2	3	14,14,15	0.34	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	3	14,14,15	0.44	0	17,19,21	0.35	0
3	NAG	N	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	O	1	3	14,14,15	0.33	0	17,19,21	0.57	0
3	NAG	O	2	3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	P	1	3	14,14,15	0.50	0	17,19,21	0.40	0
3	NAG	P	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	Q	1	3	14,14,15	0.80	1 (7%)	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.51	0
3	NAG	R	1	3	14,14,15	0.19	0	17,19,21	0.63	0
3	NAG	R	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	S	1	3	14,14,15	0.25	0	17,19,21	0.39	0
3	NAG	S	2	3	14,14,15	0.17	0	17,19,21	0.45	0
3	NAG	T	1	3	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
3	NAG	T	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	U	1	3	14,14,15	0.41	0	17,19,21	1.02	1 (5%)
3	NAG	U	2	3	14,14,15	0.21	0	17,19,21	0.40	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	G	1	3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3	-	4/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	4/6/23/26	0/1/1/1
3	NAG	T	1	3	-	3/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	-2.88	1.39	1.43
3	L	1	NAG	O5-C1	-2.74	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C2-N2-C7	4.29	129.01	122.90
3	U	1	NAG	C1-O5-C5	3.52	116.97	112.19
3	G	1	NAG	C1-O5-C5	2.84	116.04	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O7-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	S	1	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	O	1	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	P	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	T	1	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

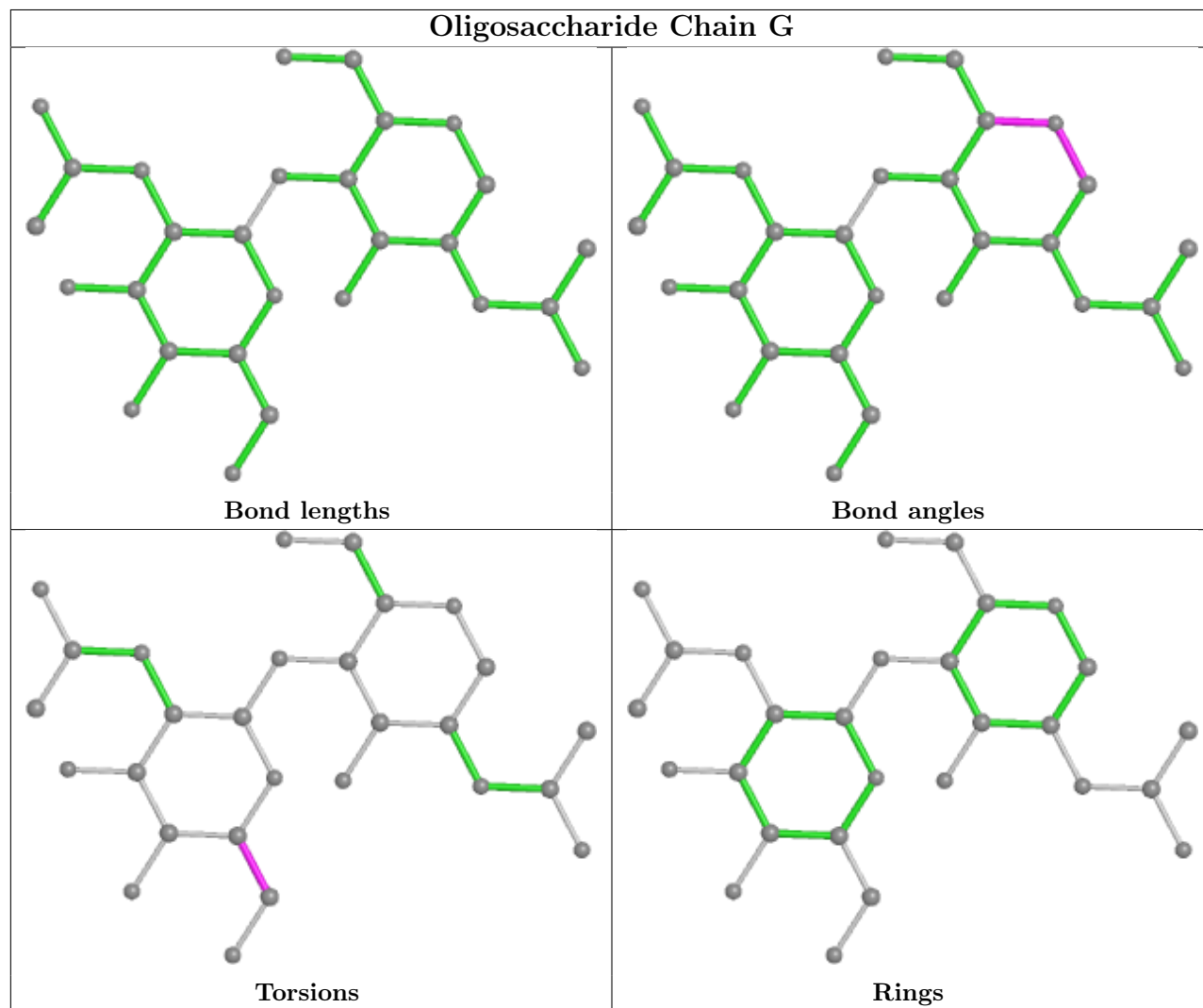
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0
3	L	1	NAG	1	0

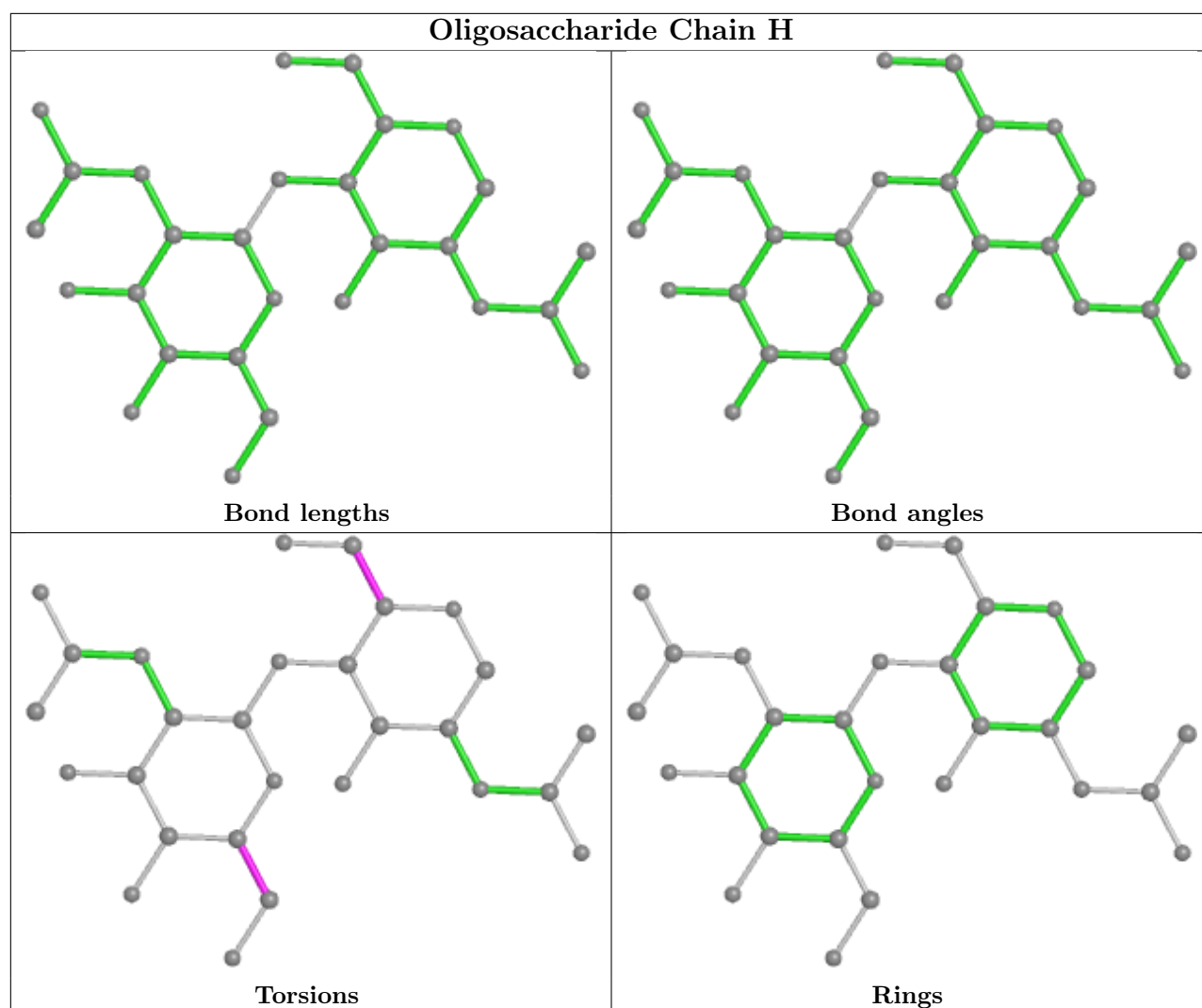
Continued on next page...

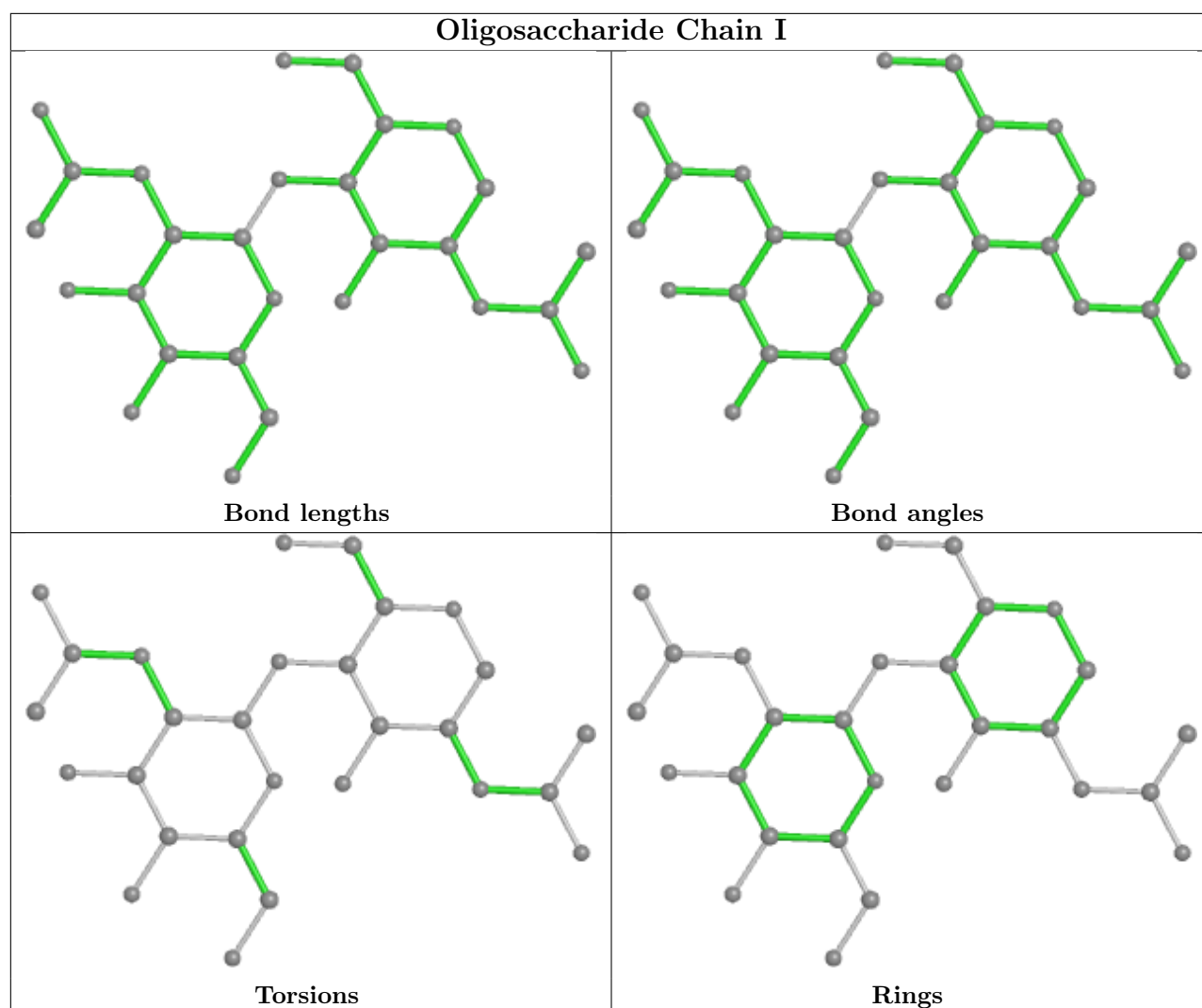
Continued from previous page...

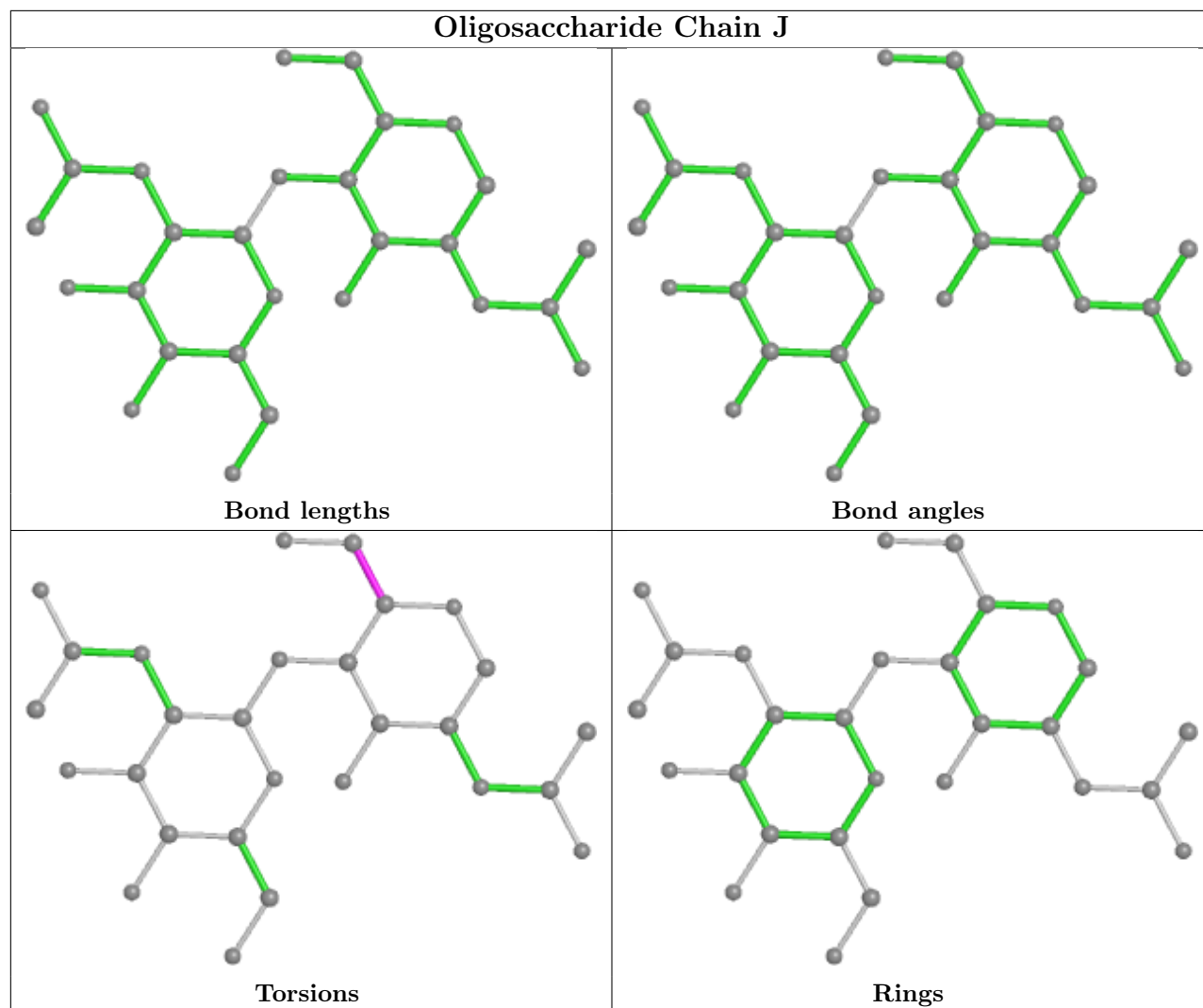
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	1	NAG	1	0

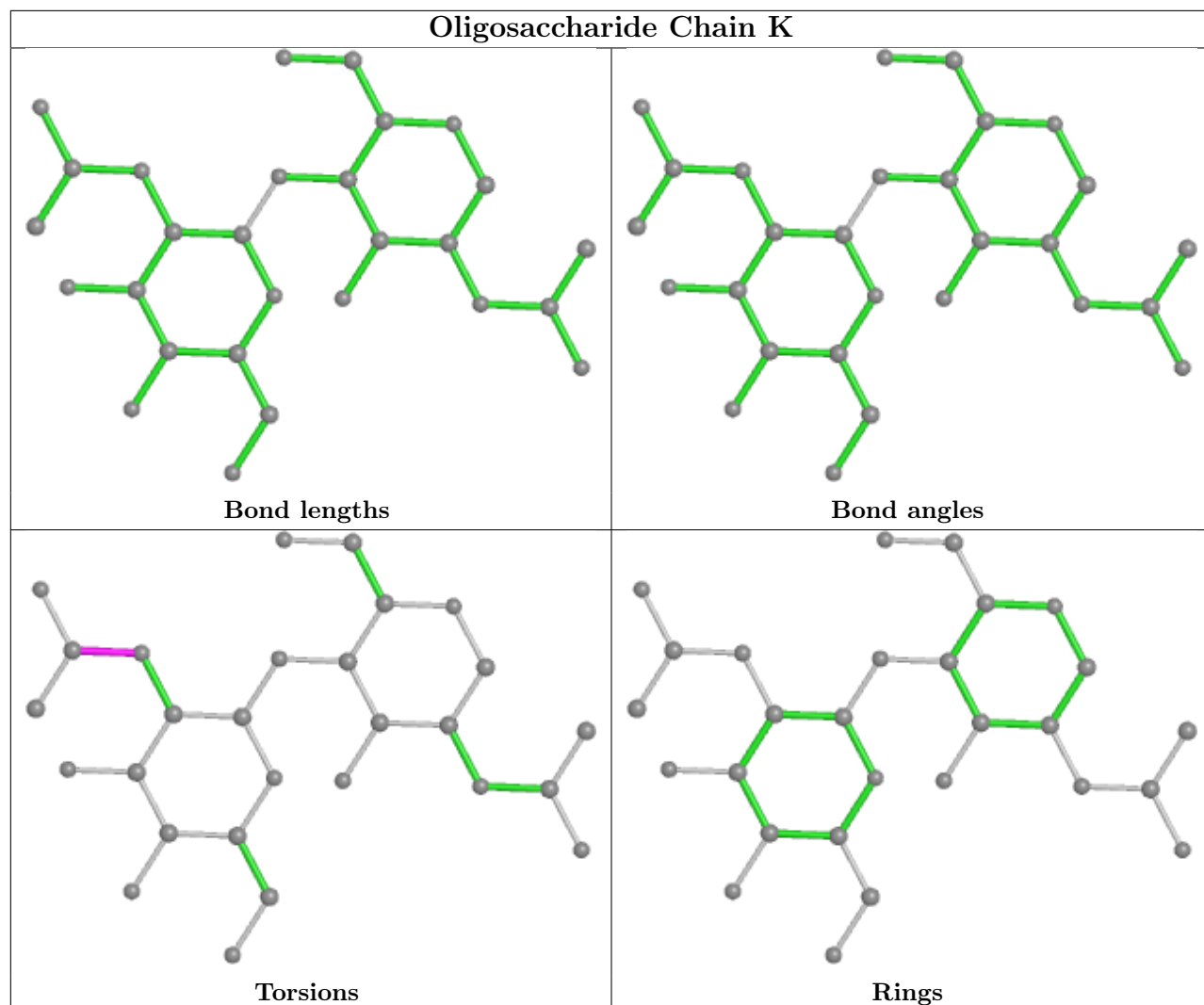
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

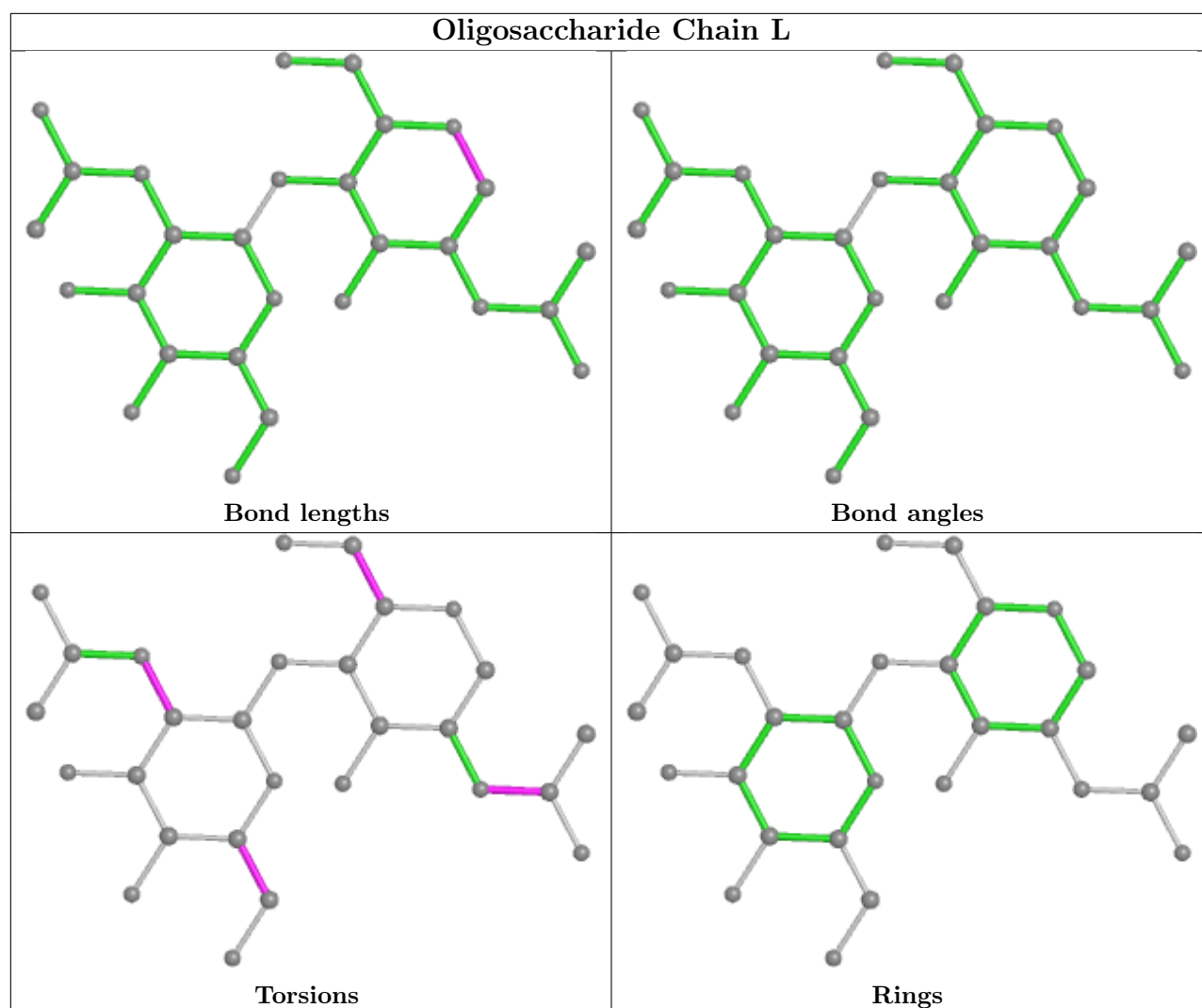


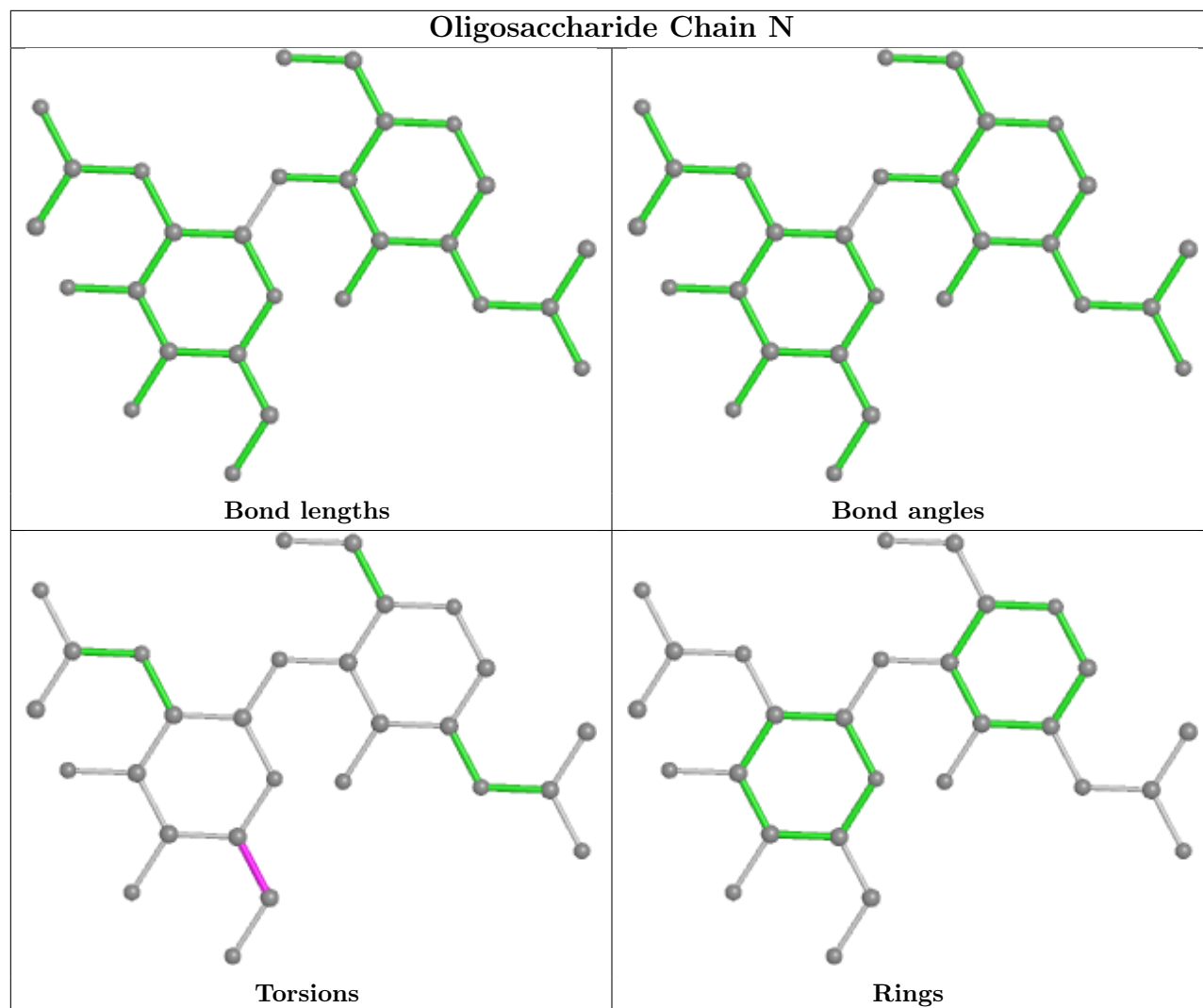


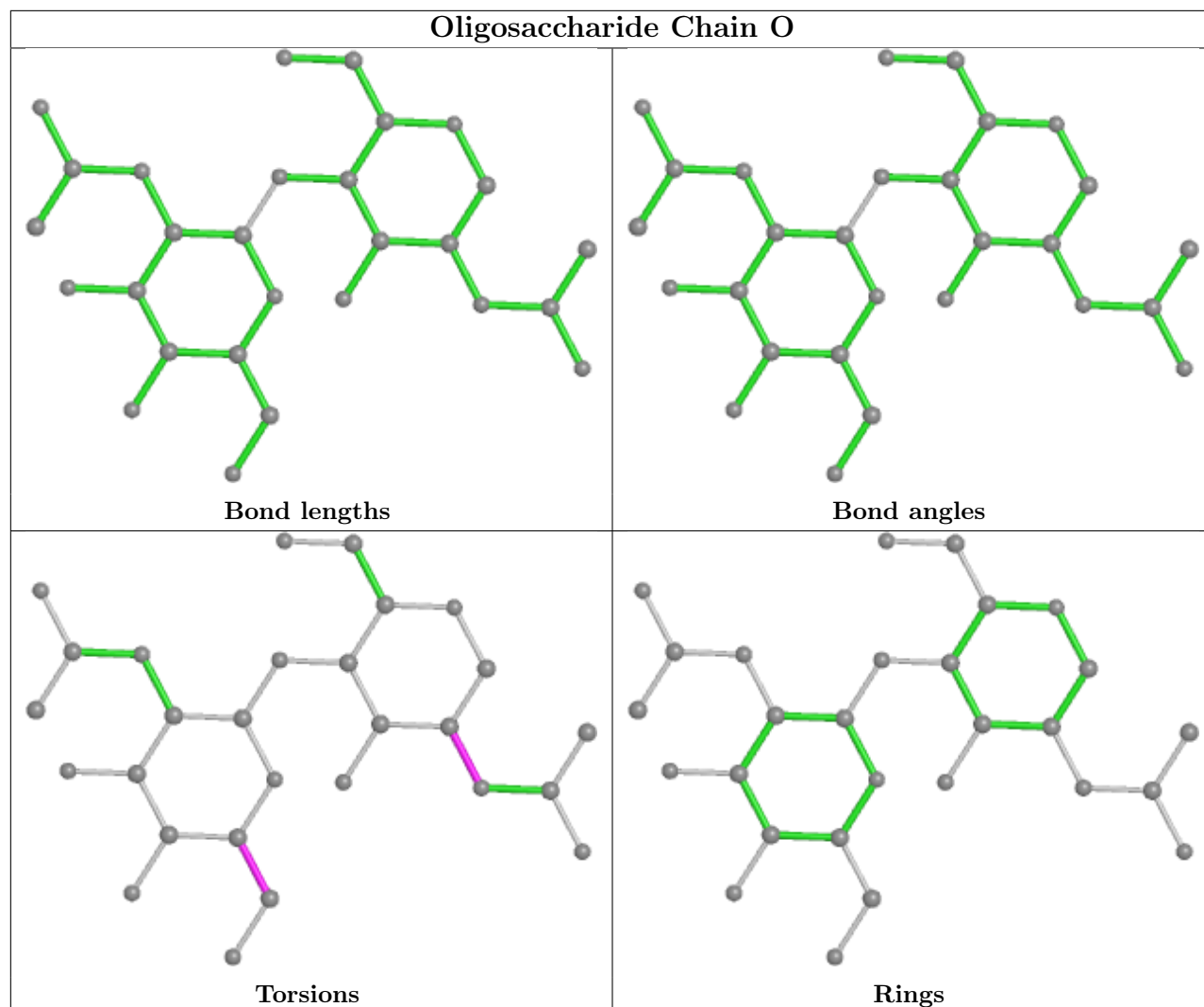


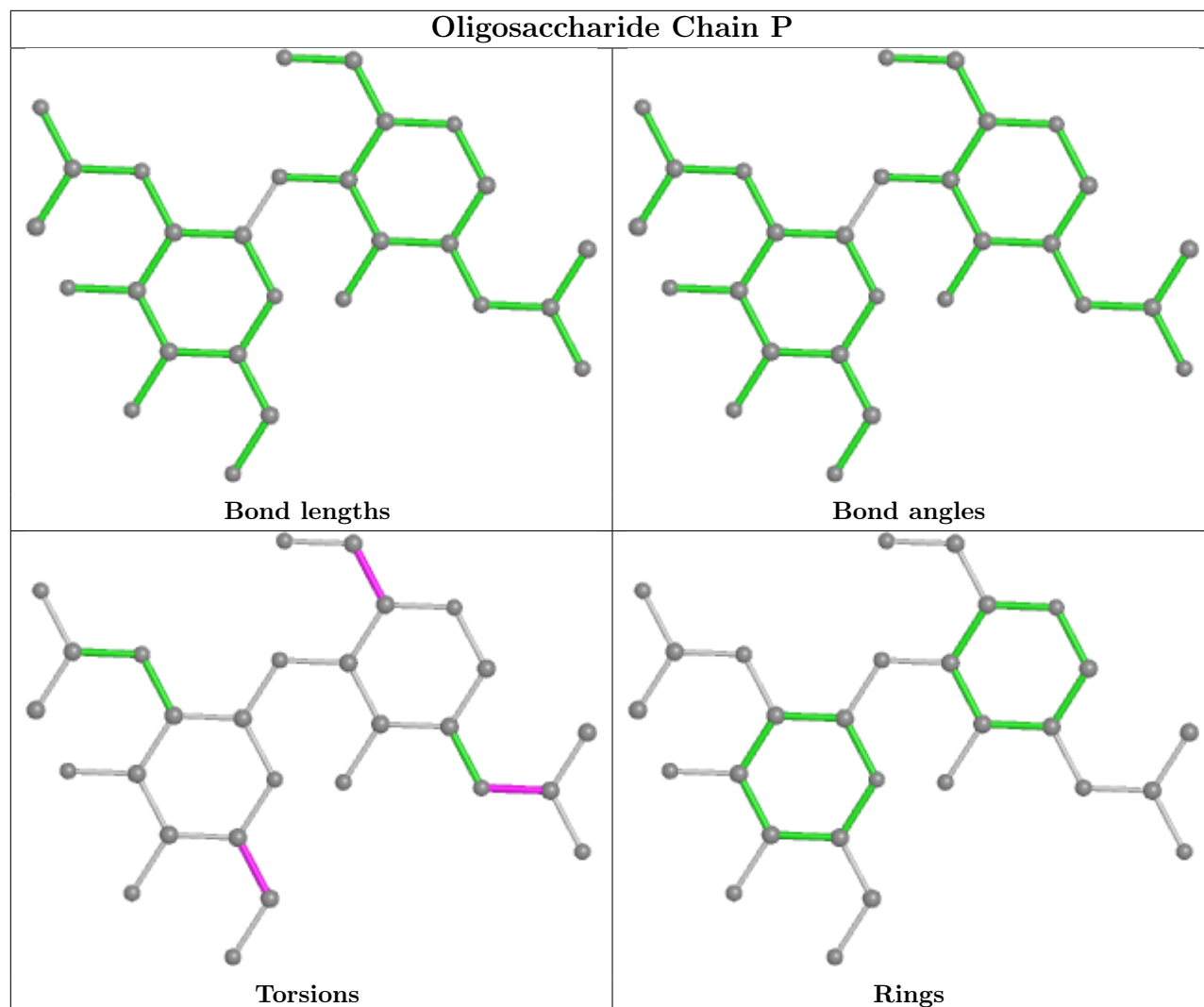


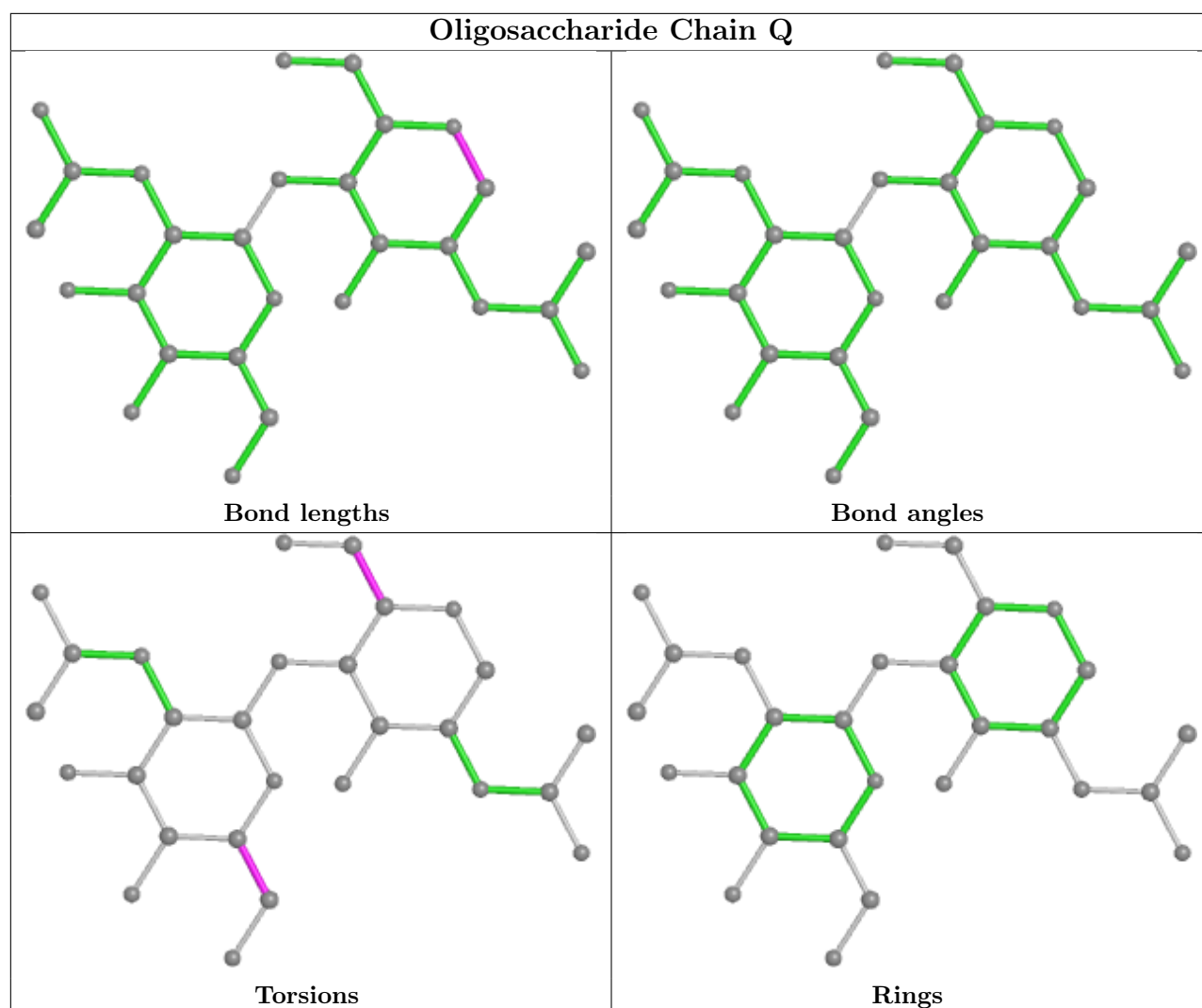


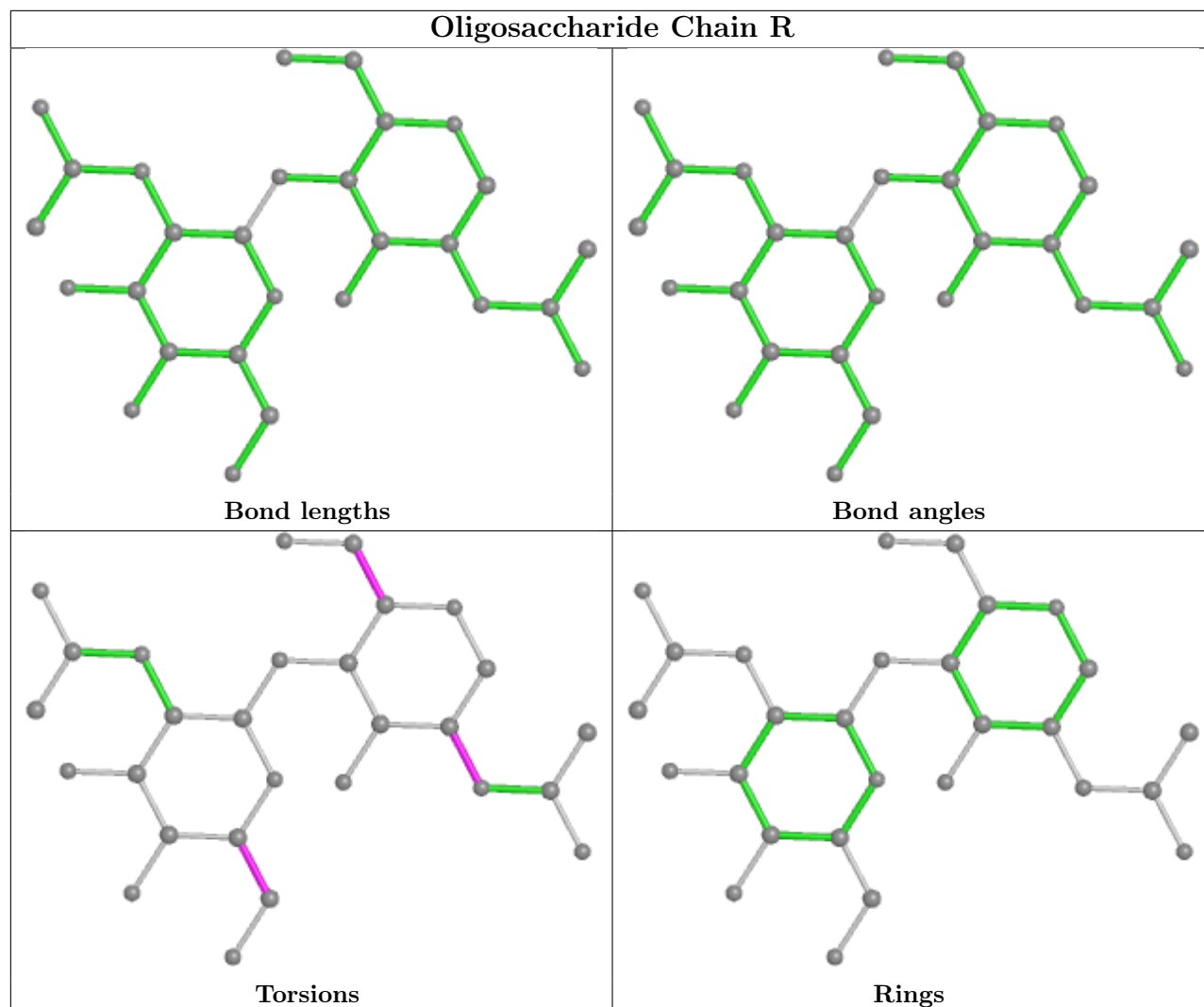


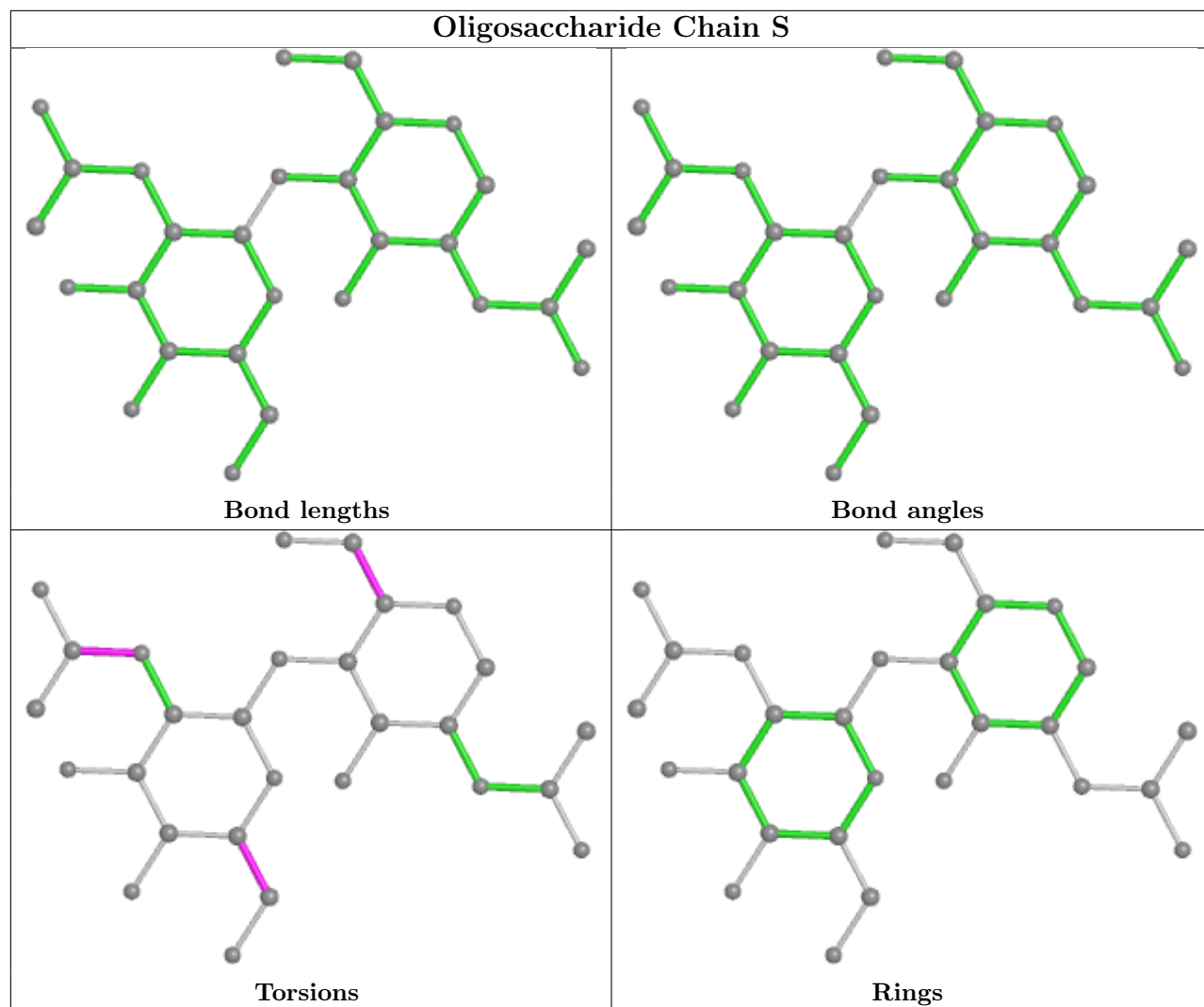


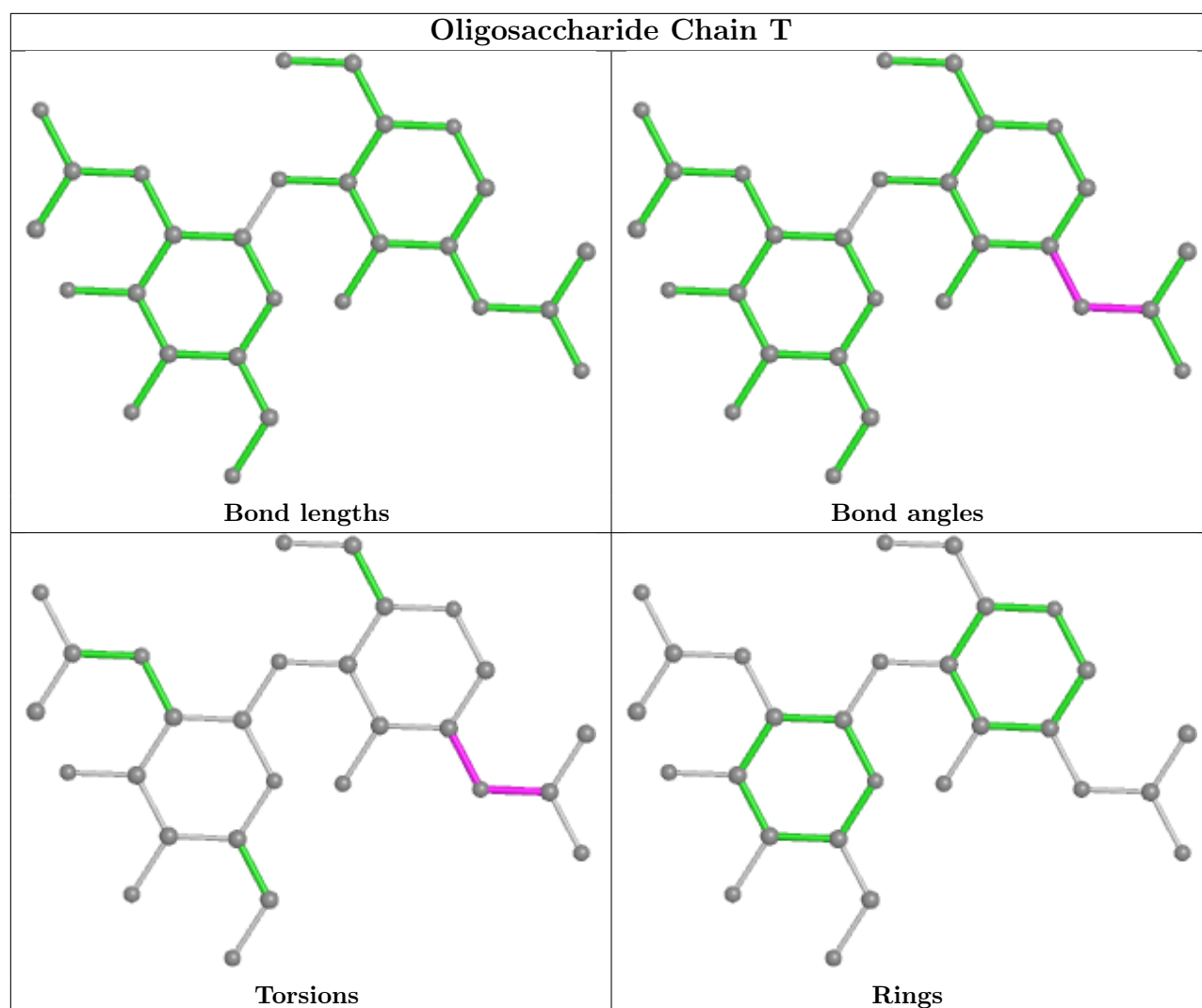


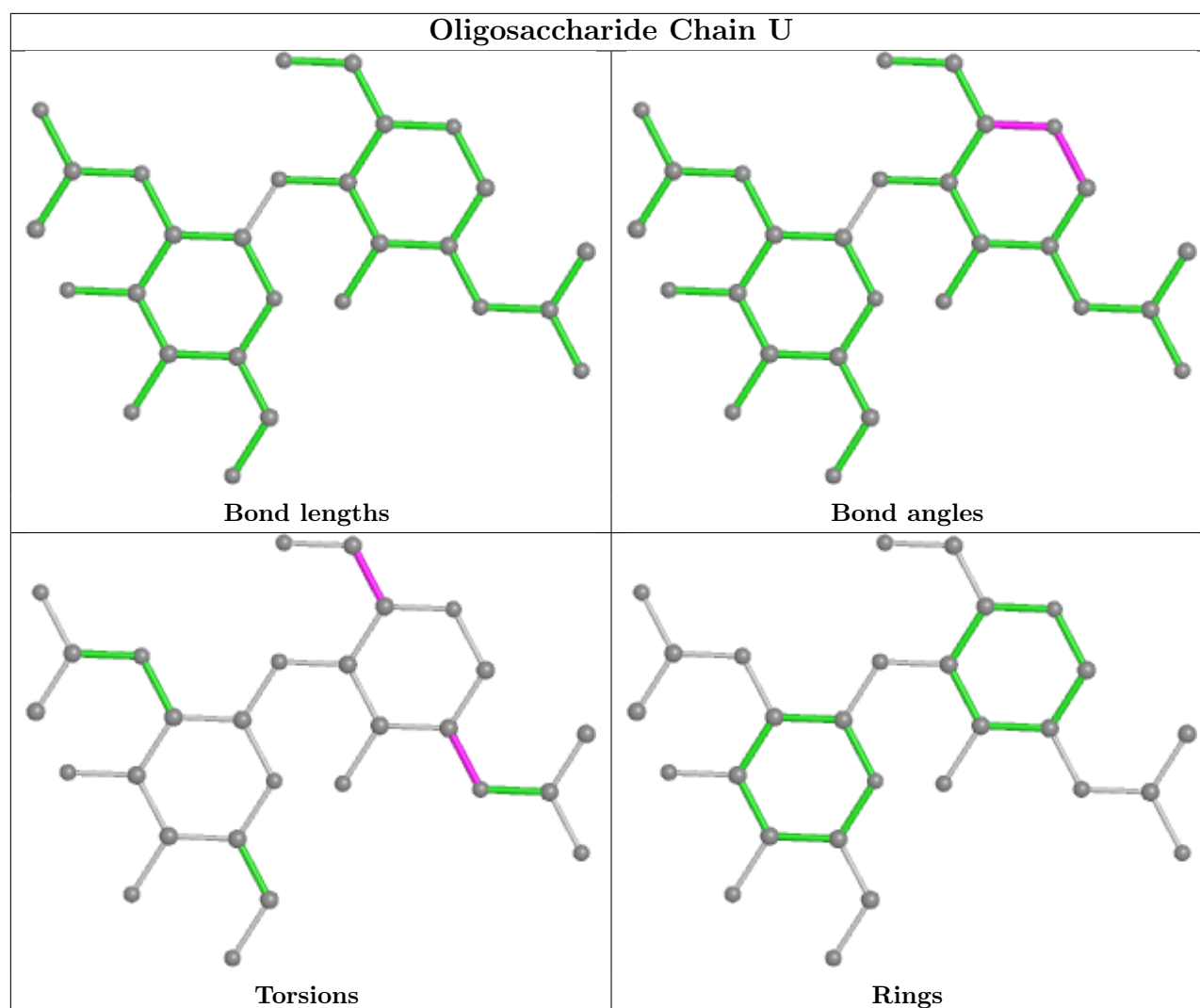












5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 for Mogul analysis.

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	$\# Z > 2$
4	NAG	E	701	-	14,14,15	0.29	0	17,19,21	0.34	0
4	NAG	C	1206	1	14,14,15	0.20	0	17,19,21	0.54	0
4	NAG	E	703	-	14,14,15	0.52	0	17,19,21	1.23	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1202	1	14,14,15	0.20	0	17,19,21	0.38	0
4	NAG	C	1201	1	14,14,15	0.17	0	17,19,21	0.45	0
4	NAG	C	1205	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	A	1202	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	F	705	2	14,14,15	0.33	0	17,19,21	0.62	0
4	NAG	C	1203	1	14,14,15	0.37	0	17,19,21	1.28	2 (11%)
4	NAG	B	1205	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	1205	1	14,14,15	0.46	0	17,19,21	0.46	0
4	NAG	B	1202	1	14,14,15	0.19	0	17,19,21	0.41	0
4	NAG	E	704	2	14,14,15	0.96	1 (7%)	17,19,21	1.23	1 (5%)
4	NAG	A	1204	1	14,14,15	0.54	0	17,19,21	0.42	0
4	NAG	C	1204	1	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	A	1201	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	A	1203	1	14,14,15	0.21	0	17,19,21	0.50	0
4	NAG	F	702	2	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	B	1201	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	B	1204	1	14,14,15	0.14	0	17,19,21	0.47	0
4	NAG	B	1203	1	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	F	701	2	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	F	704	2	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	E	702	2	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	F	703	-	14,14,15	0.53	0	17,19,21	1.25	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	701	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	E	703	-	-	5/6/23/26	0/1/1/1
4	NAG	C	1202	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1201	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1205	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
4	NAG	F	705	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1203	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1205	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1205	1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1202	1	-	0/6/23/26	0/1/1/1
4	NAG	E	704	2	-	3/6/23/26	0/1/1/1
4	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1204	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1201	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1203	1	-	3/6/23/26	0/1/1/1
4	NAG	F	702	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1201	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1204	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1203	1	-	1/6/23/26	0/1/1/1
4	NAG	F	701	2	-	3/6/23/26	0/1/1/1
4	NAG	F	704	2	-	2/6/23/26	0/1/1/1
4	NAG	E	702	2	-	2/6/23/26	0/1/1/1
4	NAG	F	703	-	-	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	E	704	NAG	O5-C1	3.30	1.49	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	704	NAG	C1-O5-C5	4.66	118.50	112.19
4	E	703	NAG	C2-N2-C7	4.31	129.04	122.90
4	C	1203	NAG	C2-N2-C7	4.28	128.99	122.90
4	F	703	NAG	C2-N2-C7	4.27	128.99	122.90
4	C	1203	NAG	C1-C2-N2	2.11	114.10	110.49

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1204	NAG	O5-C5-C6-O6
4	E	703	NAG	C4-C5-C6-O6
4	C	1203	NAG	C4-C5-C6-O6
4	E	702	NAG	O5-C5-C6-O6
4	B	1205	NAG	O5-C5-C6-O6
4	F	702	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	704	NAG	O5-C5-C6-O6
4	A	1203	NAG	O5-C5-C6-O6
4	B	1204	NAG	O5-C5-C6-O6
4	E	701	NAG	O5-C5-C6-O6
4	E	703	NAG	O5-C5-C6-O6
4	C	1203	NAG	O5-C5-C6-O6
4	F	701	NAG	O5-C5-C6-O6
4	E	702	NAG	C4-C5-C6-O6
4	C	1204	NAG	C4-C5-C6-O6
4	F	704	NAG	C4-C5-C6-O6
4	A	1201	NAG	O5-C5-C6-O6
4	E	704	NAG	C4-C5-C6-O6
4	B	1205	NAG	C4-C5-C6-O6
4	B	1204	NAG	C4-C5-C6-O6
4	B	1201	NAG	C8-C7-N2-C2
4	B	1201	NAG	O7-C7-N2-C2
4	B	1204	NAG	C8-C7-N2-C2
4	B	1204	NAG	O7-C7-N2-C2
4	C	1201	NAG	C8-C7-N2-C2
4	C	1201	NAG	O7-C7-N2-C2
4	C	1202	NAG	C8-C7-N2-C2
4	C	1202	NAG	O7-C7-N2-C2
4	C	1203	NAG	C8-C7-N2-C2
4	C	1203	NAG	O7-C7-N2-C2
4	C	1204	NAG	C8-C7-N2-C2
4	C	1204	NAG	O7-C7-N2-C2
4	E	703	NAG	C8-C7-N2-C2
4	E	703	NAG	O7-C7-N2-C2
4	F	702	NAG	C8-C7-N2-C2
4	F	702	NAG	O7-C7-N2-C2
4	F	703	NAG	C8-C7-N2-C2
4	F	703	NAG	O7-C7-N2-C2
4	F	701	NAG	C4-C5-C6-O6
4	C	1201	NAG	O5-C5-C6-O6
4	E	701	NAG	C4-C5-C6-O6
4	C	1201	NAG	C4-C5-C6-O6
4	F	702	NAG	C4-C5-C6-O6
4	A	1203	NAG	C4-C5-C6-O6
4	E	704	NAG	O5-C5-C6-O6
4	C	1206	NAG	O5-C5-C6-O6
4	C	1202	NAG	O5-C5-C6-O6
4	C	1206	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

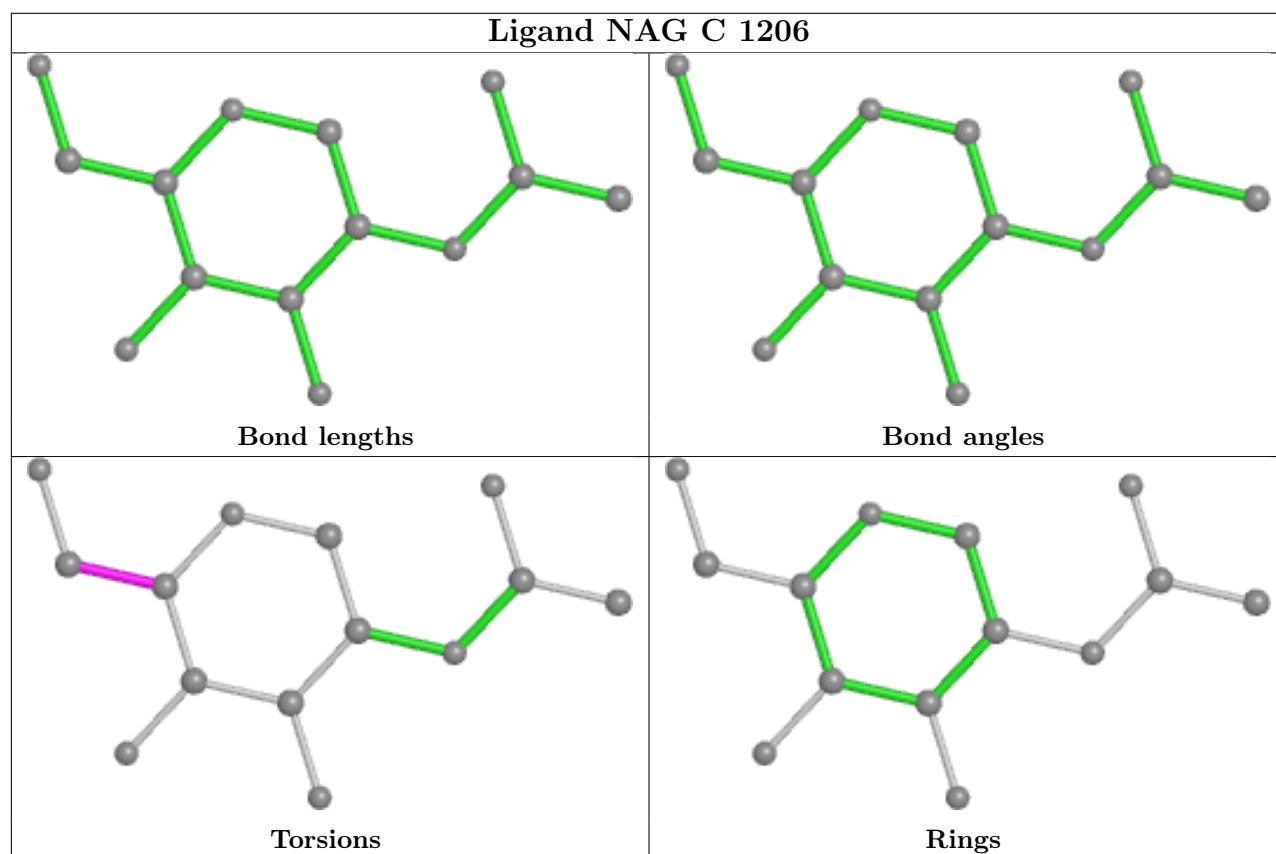
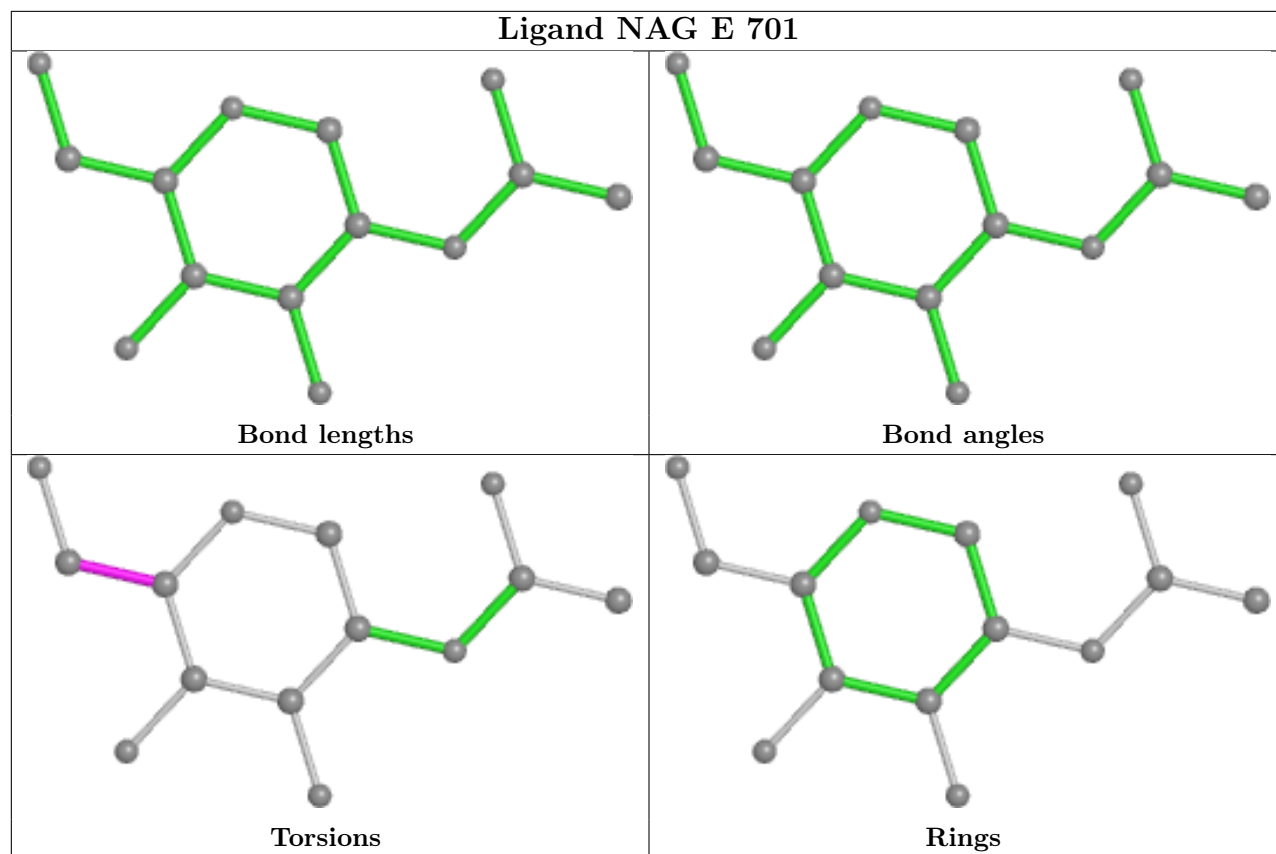
Mol	Chain	Res	Type	Atoms
4	A	1201	NAG	C4-C5-C6-O6
4	A	1203	NAG	C3-C2-N2-C7
4	B	1203	NAG	C3-C2-N2-C7
4	C	1203	NAG	C3-C2-N2-C7
4	E	704	NAG	C3-C2-N2-C7
4	F	701	NAG	C3-C2-N2-C7
4	F	705	NAG	C3-C2-N2-C7
4	A	1205	NAG	O5-C5-C6-O6
4	F	705	NAG	C4-C5-C6-O6
4	C	1205	NAG	C1-C2-N2-C7
4	F	705	NAG	O5-C5-C6-O6
4	A	1201	NAG	C3-C2-N2-C7
4	A	1205	NAG	C3-C2-N2-C7
4	E	703	NAG	C3-C2-N2-C7
4	F	703	NAG	C3-C2-N2-C7
4	A	1205	NAG	C1-C2-N2-C7
4	A	1201	NAG	C1-C2-N2-C7

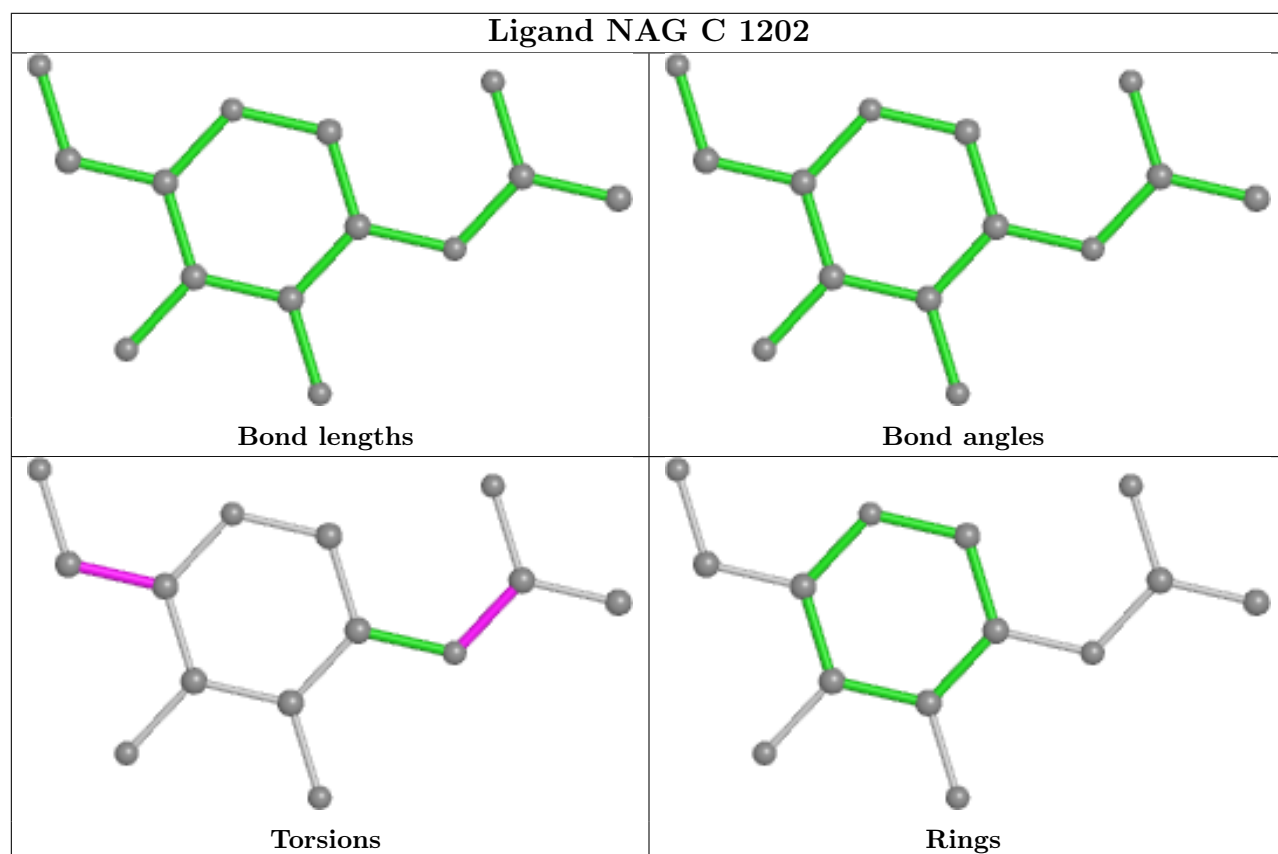
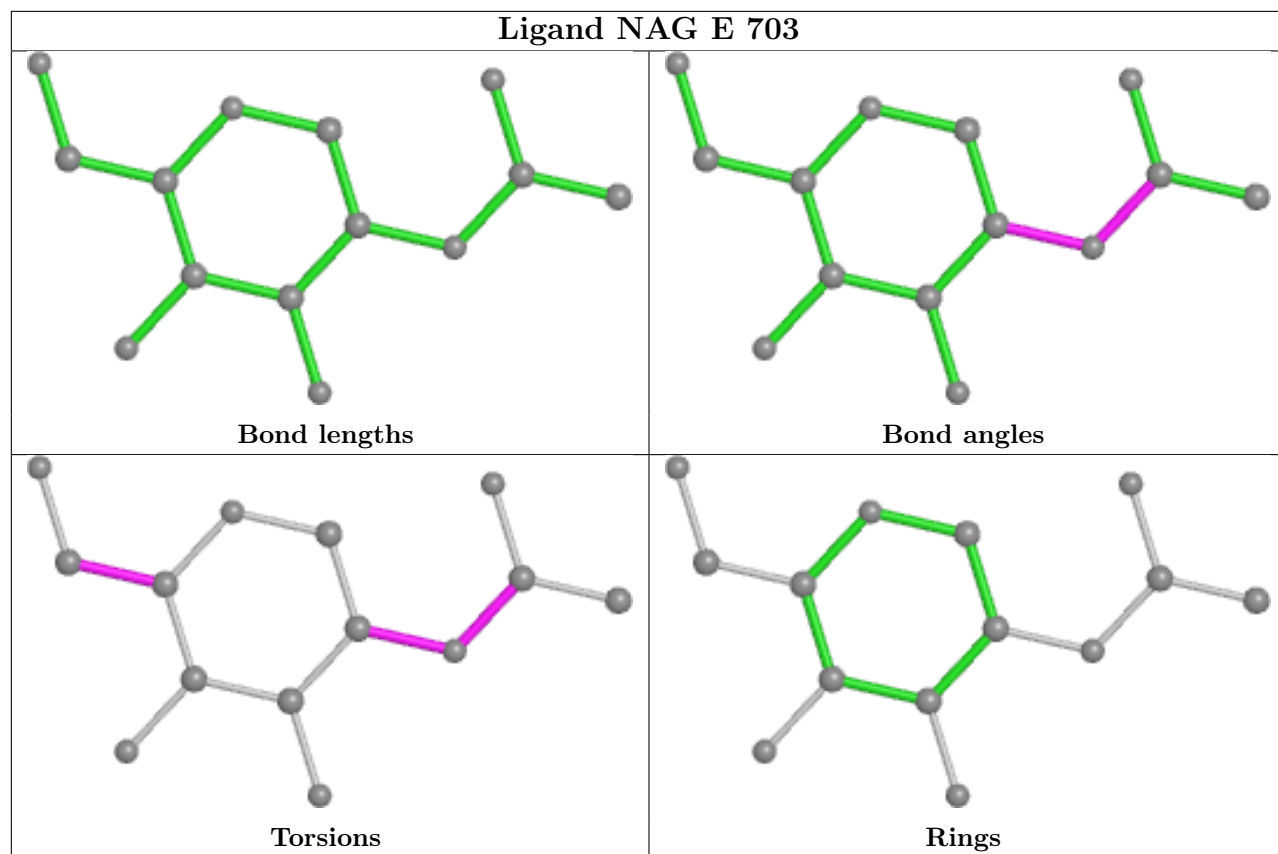
There are no ring outliers.

5 monomers are involved in 10 short contacts:

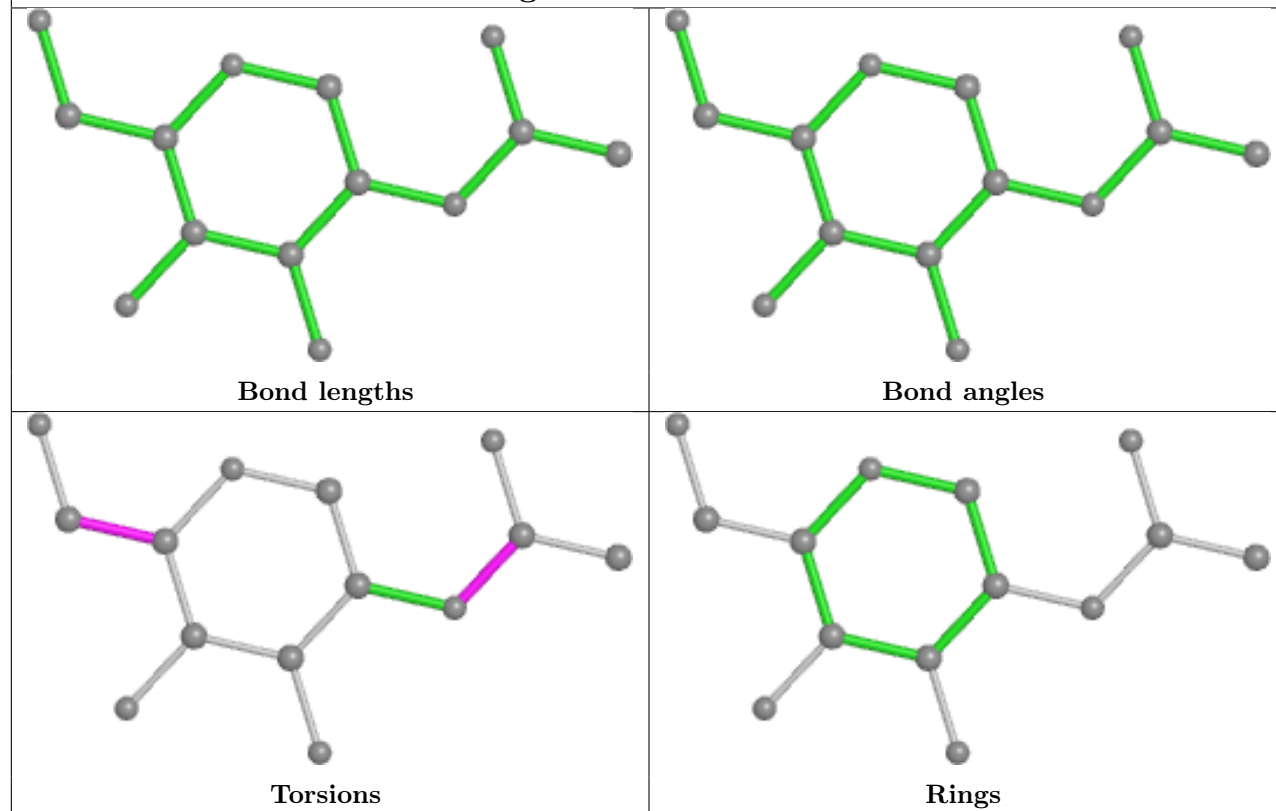
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	701	NAG	2	0
4	E	703	NAG	4	0
4	C	1203	NAG	1	0
4	E	704	NAG	2	0
4	F	703	NAG	1	0

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.

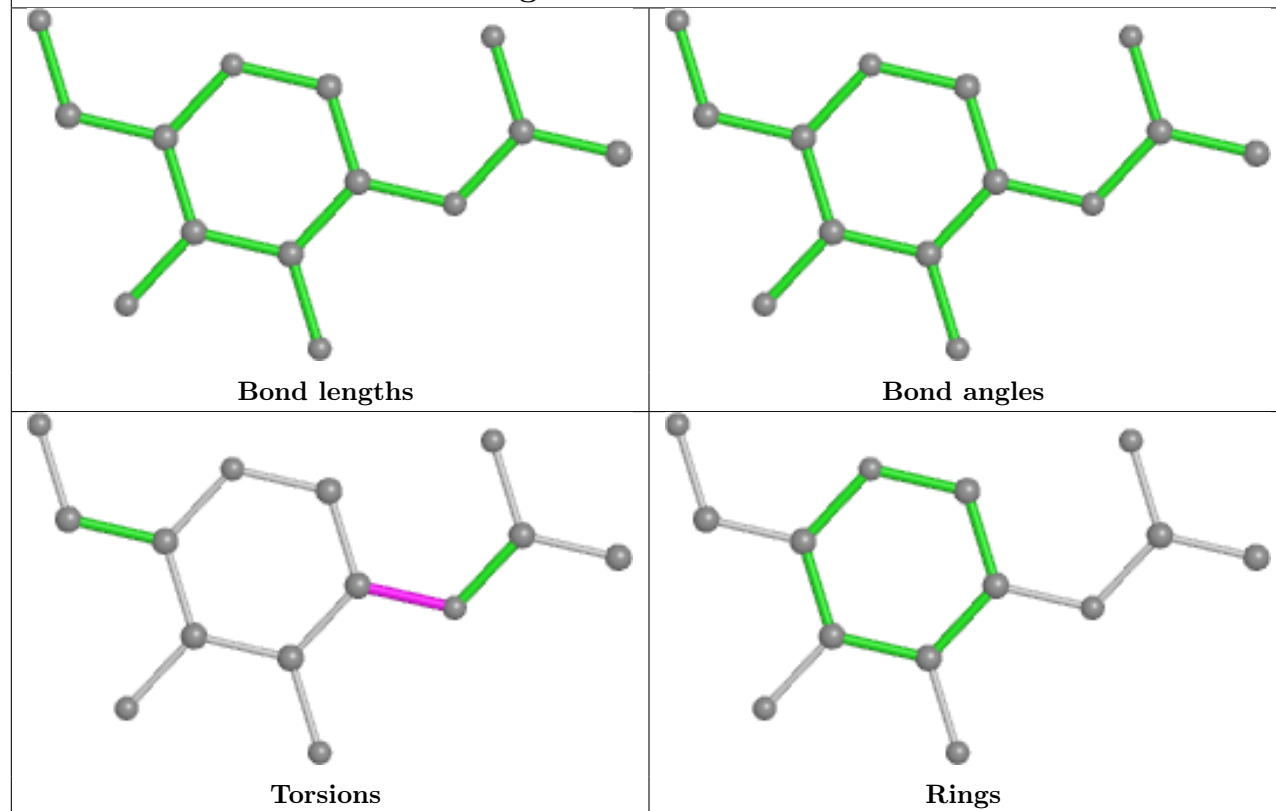


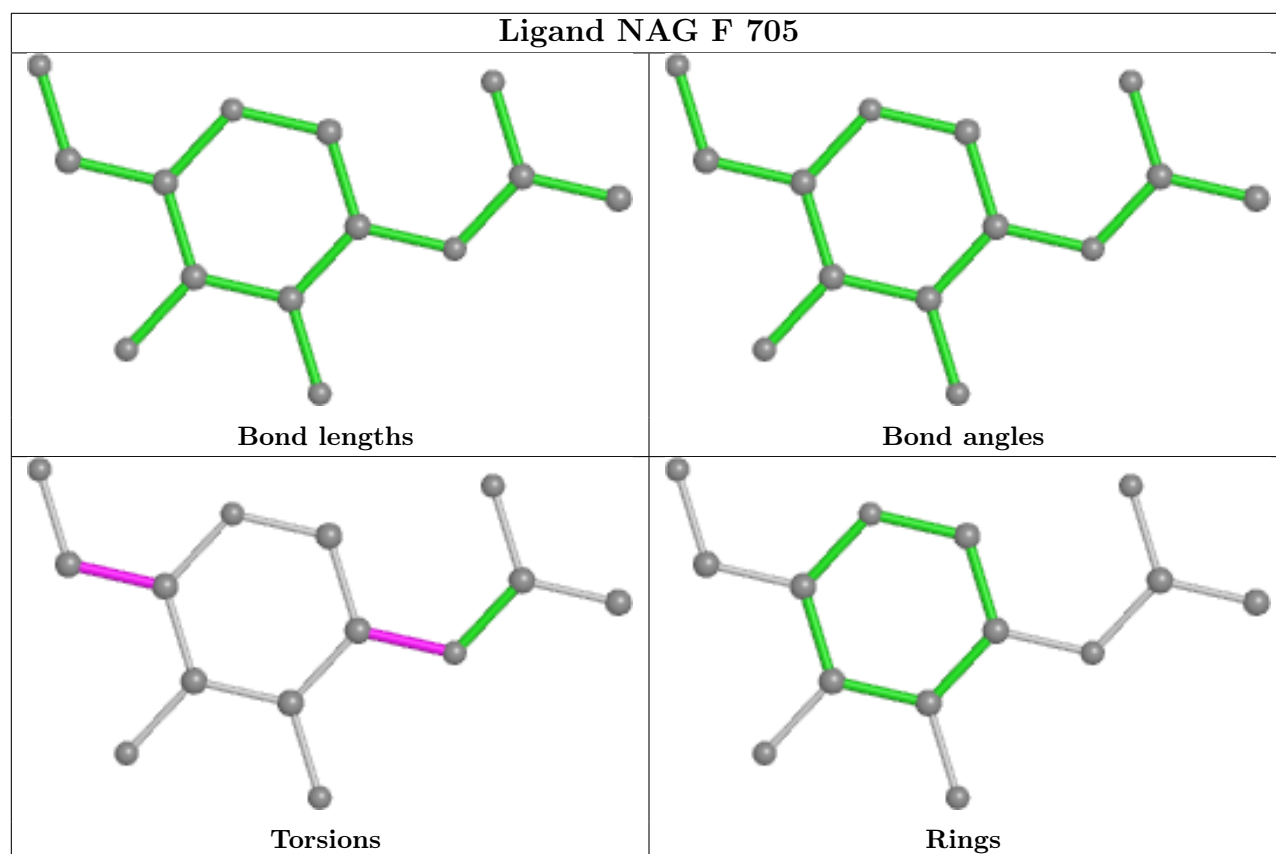
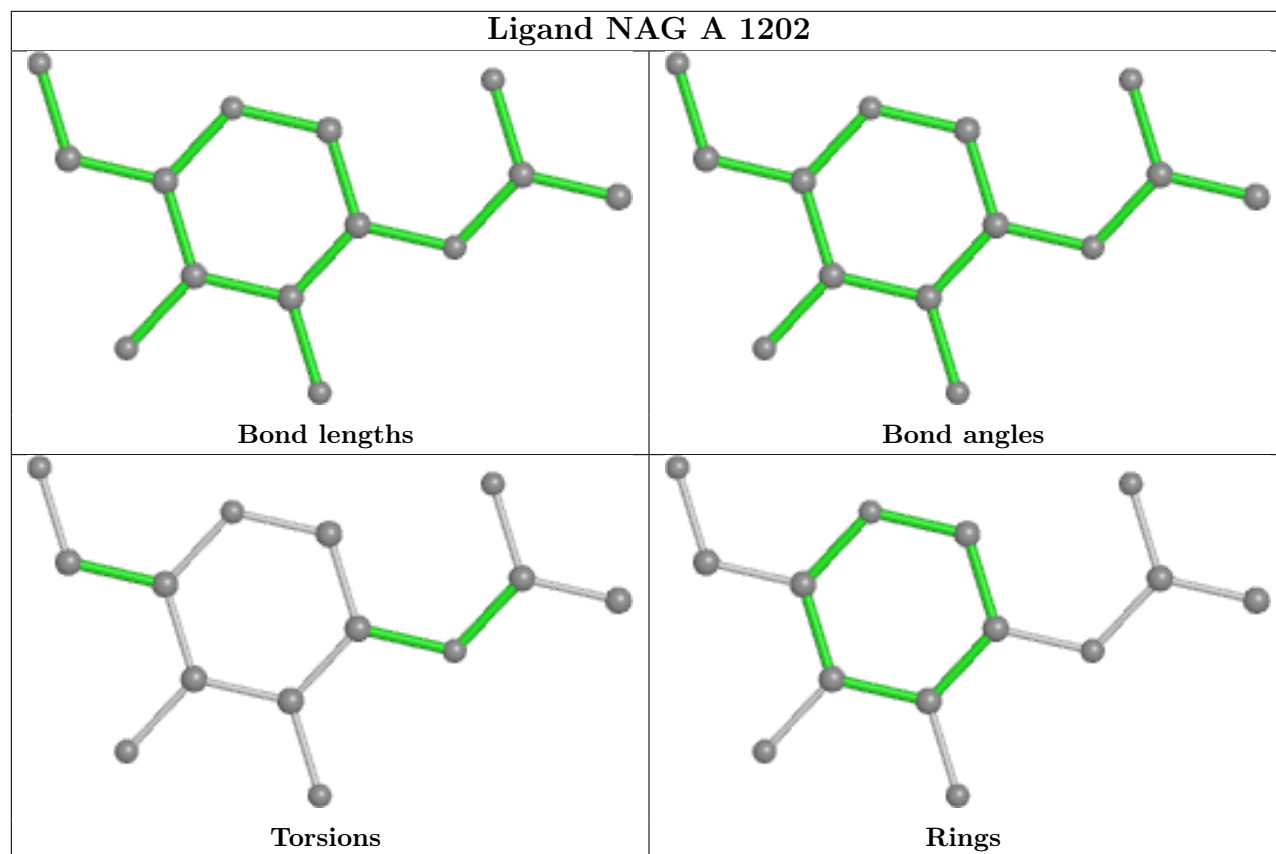


Ligand NAG C 1201

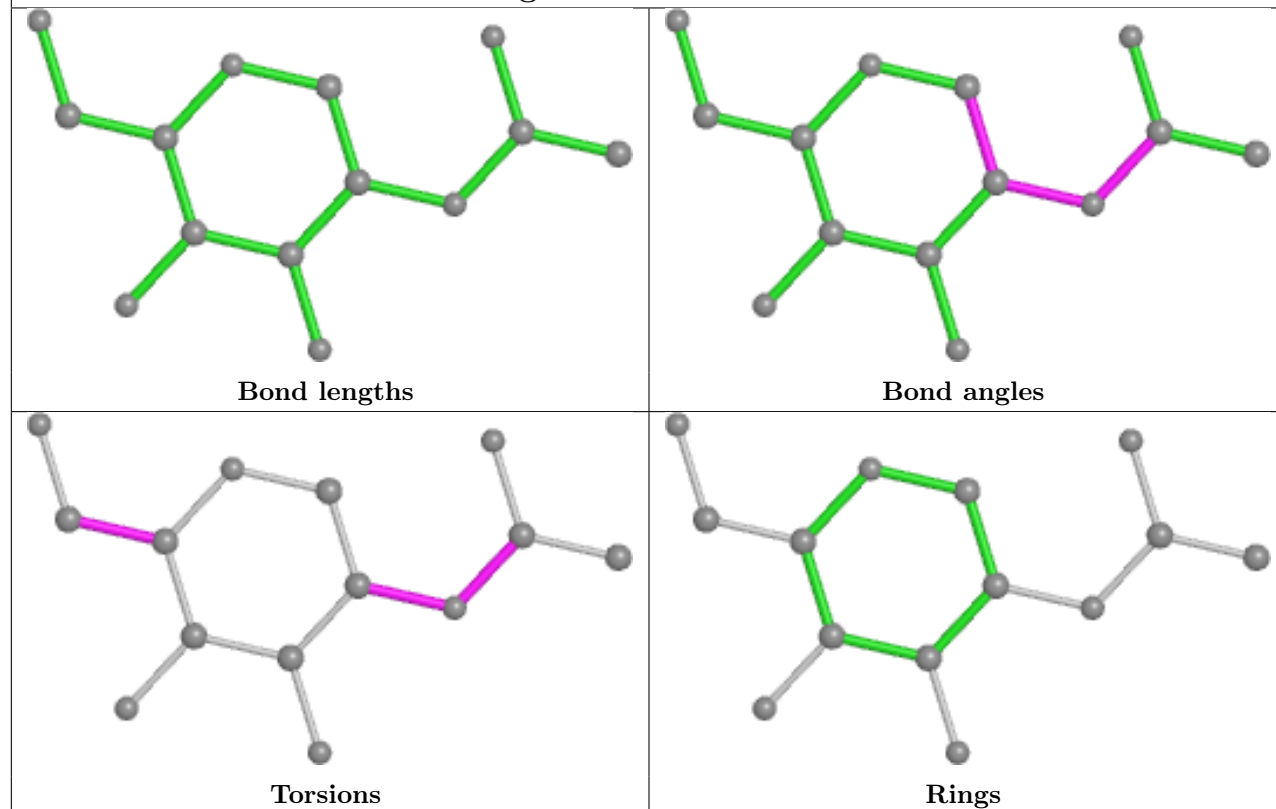


Ligand NAG C 1205

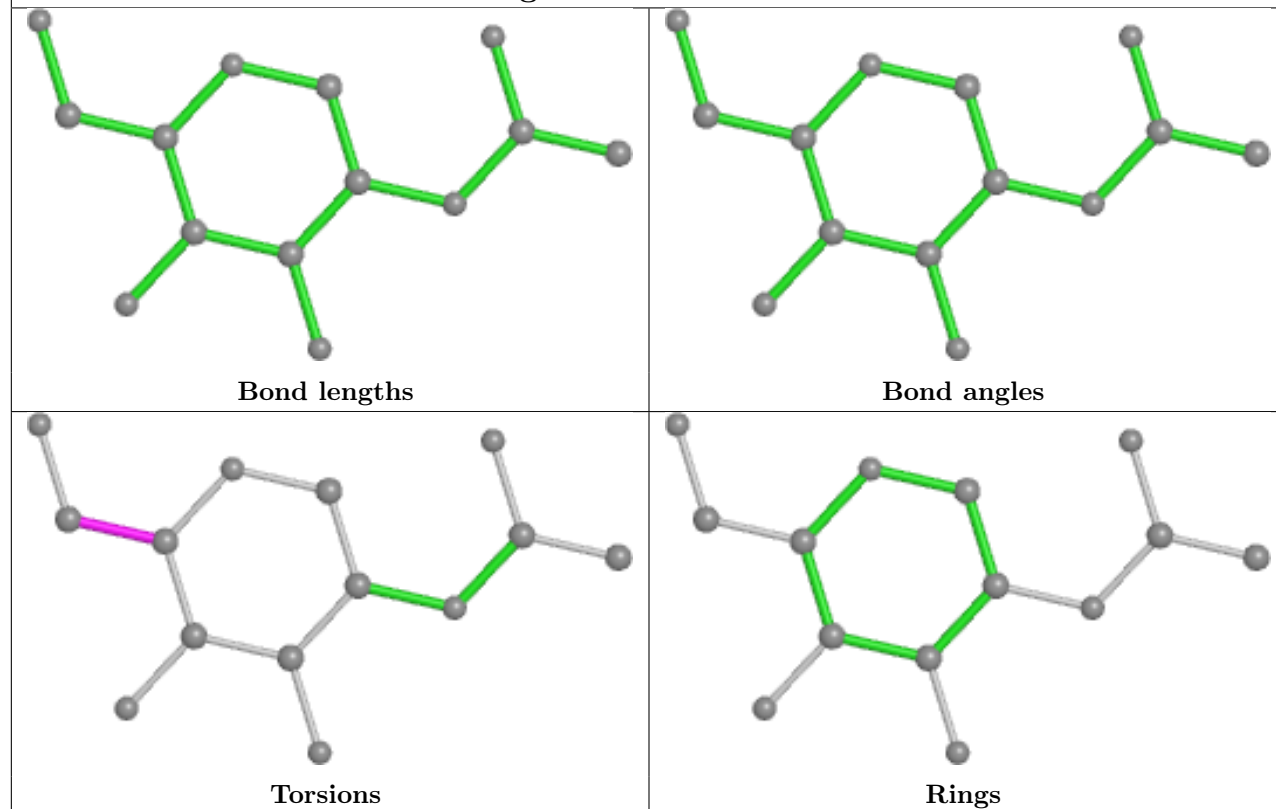




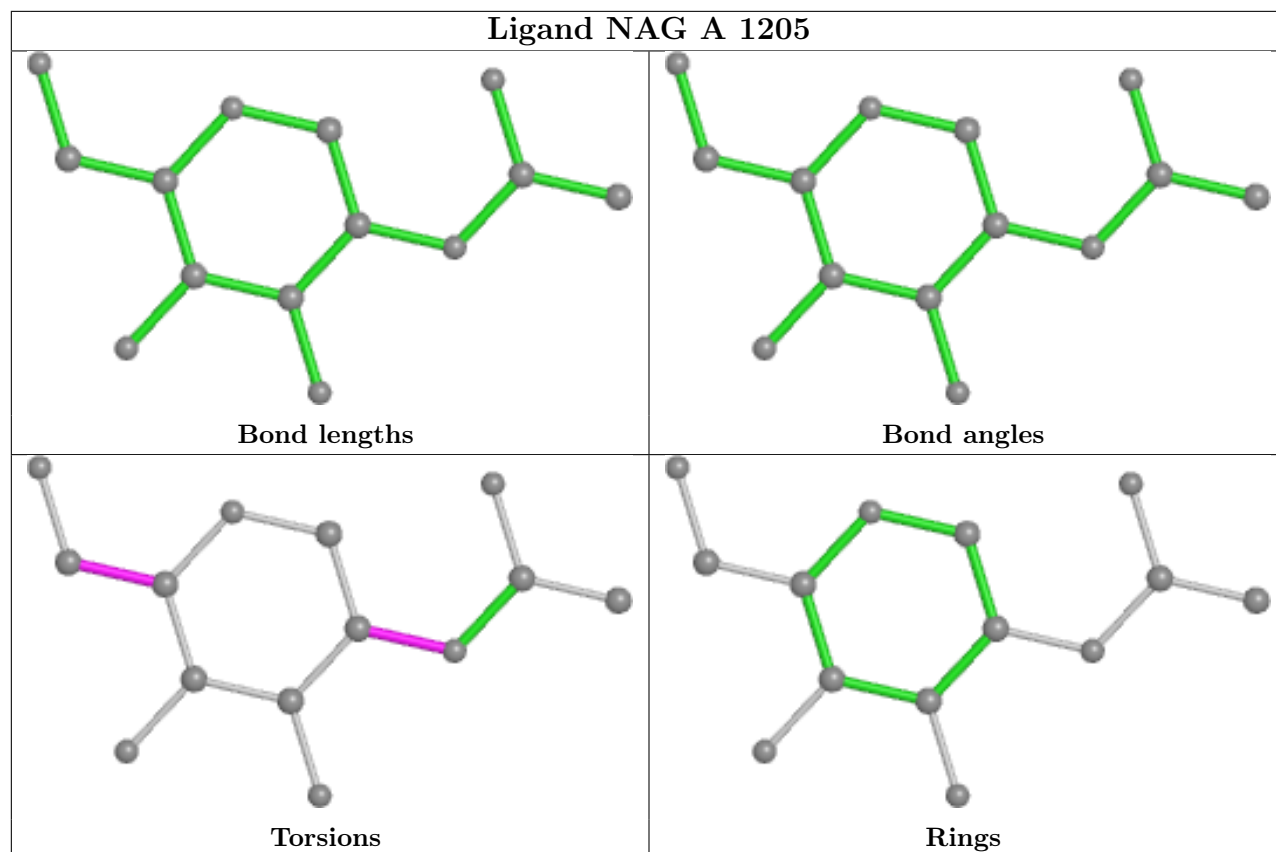
Ligand NAG C 1203



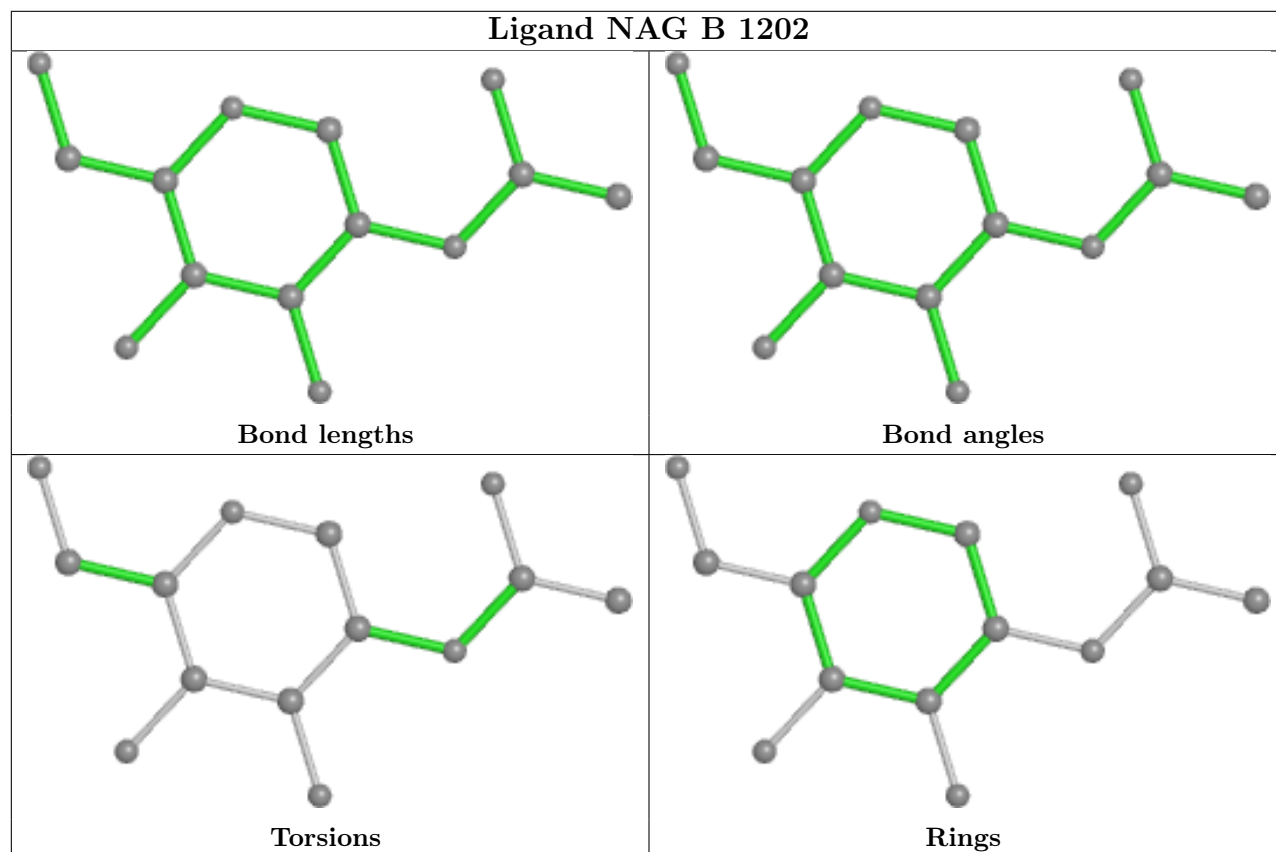
Ligand NAG B 1205

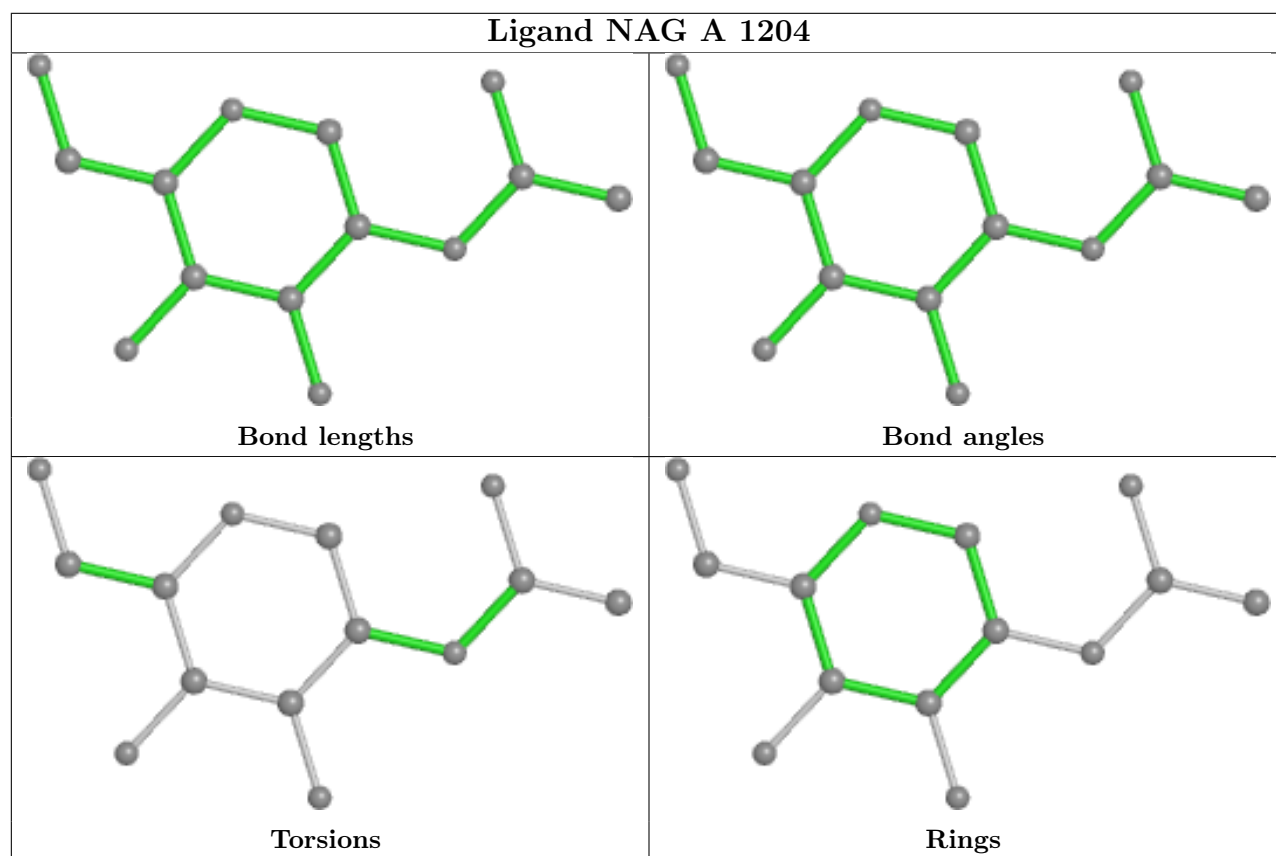
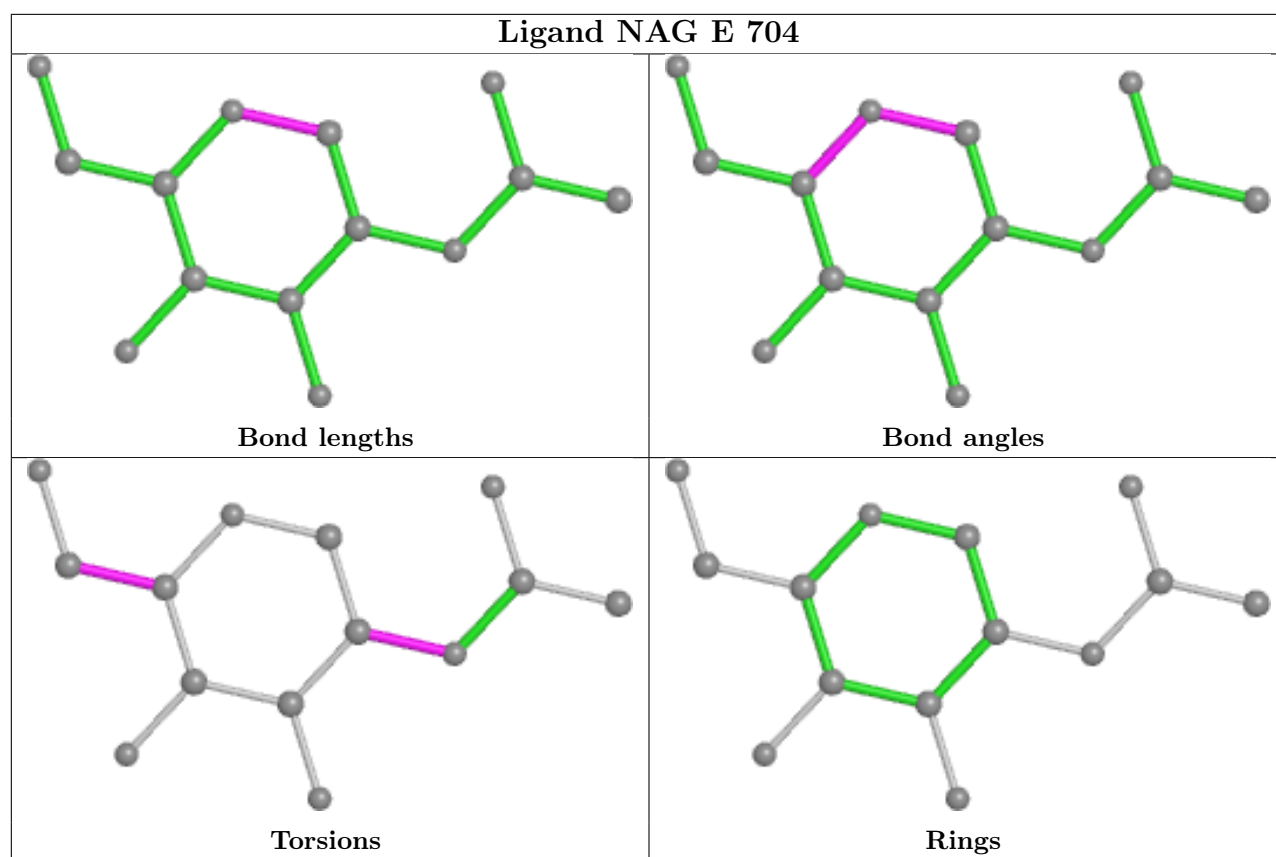


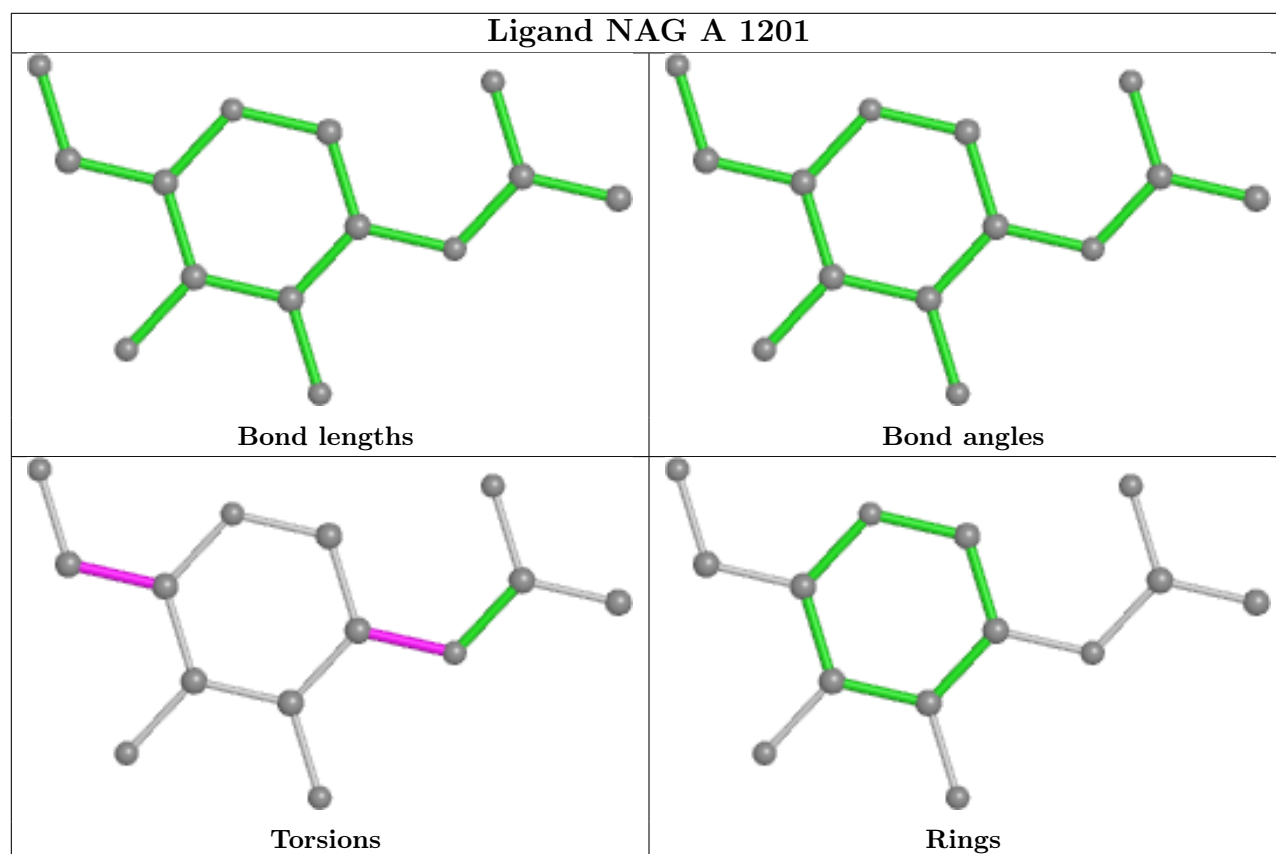
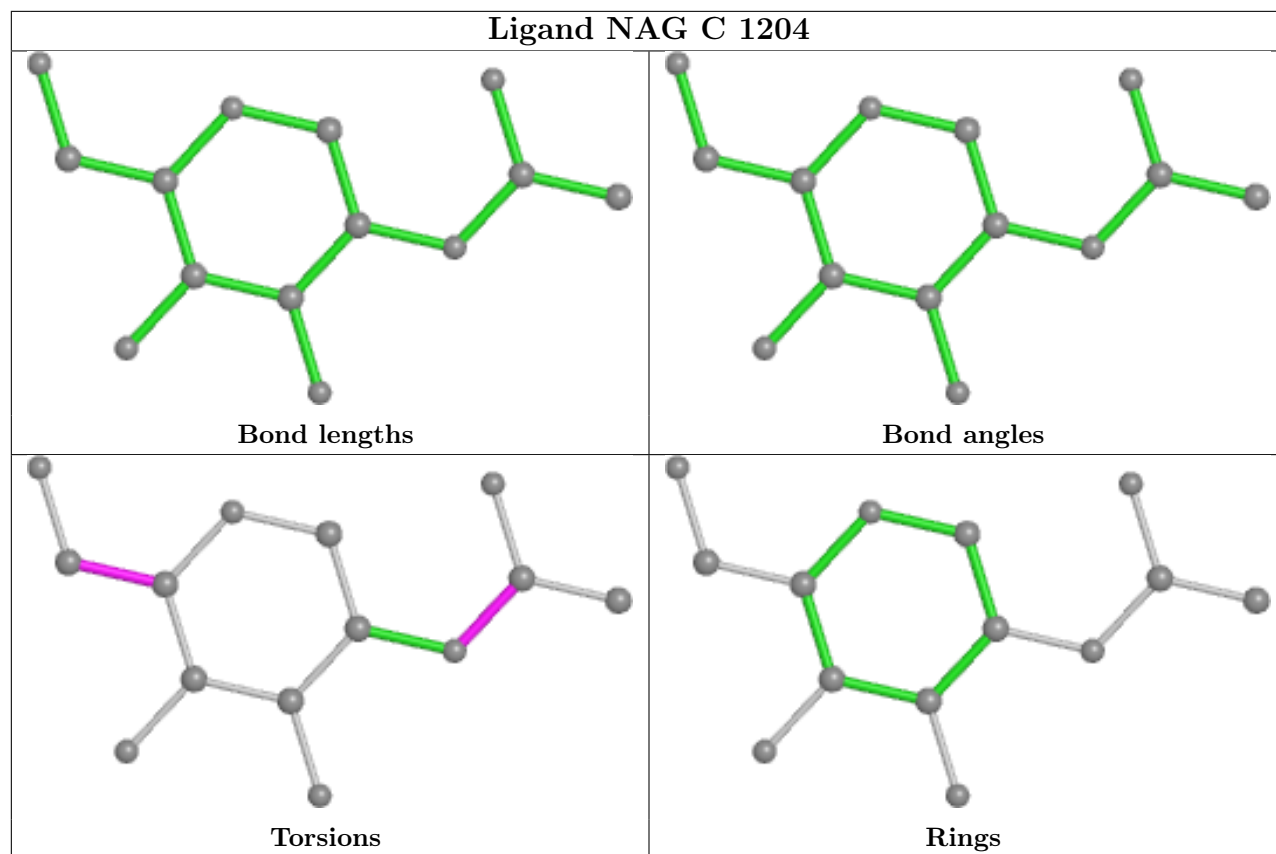
Ligand NAG A 1205

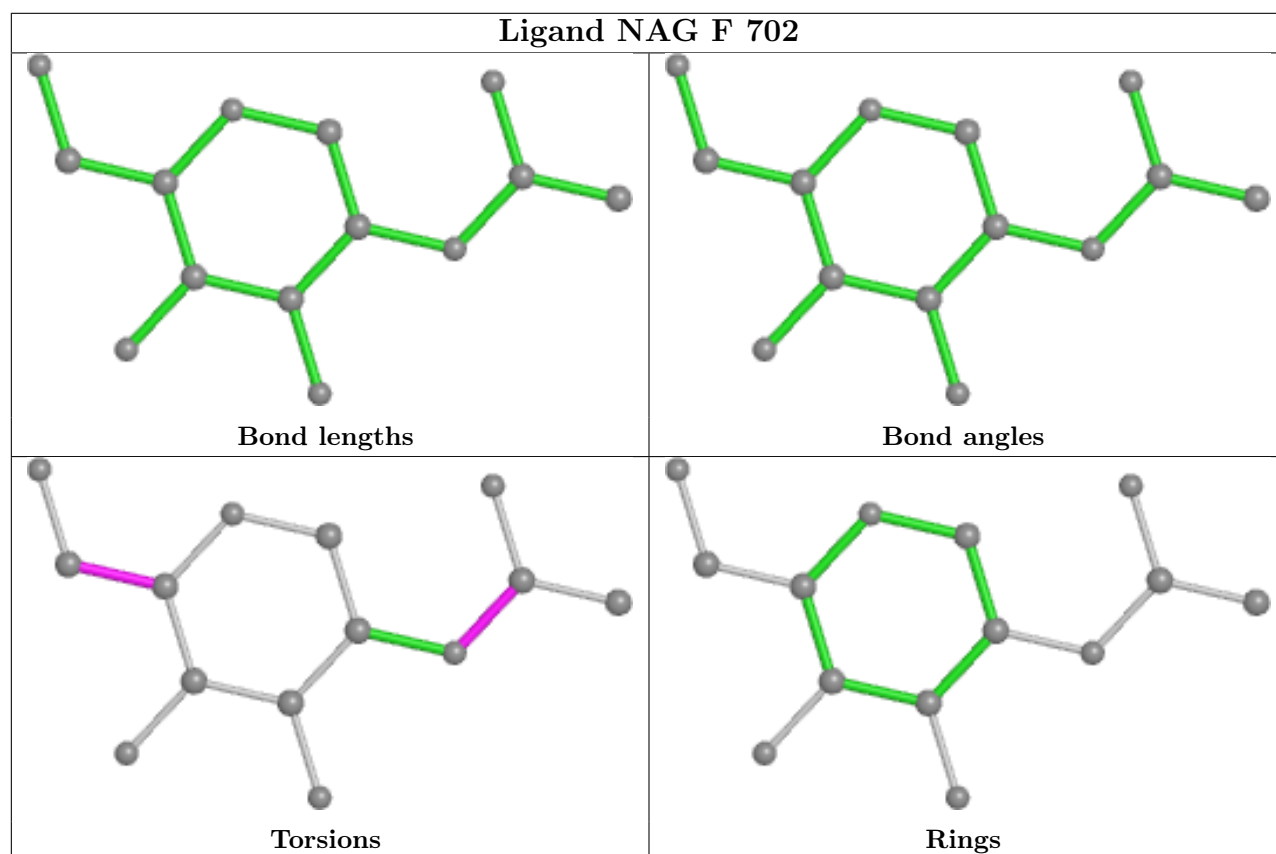
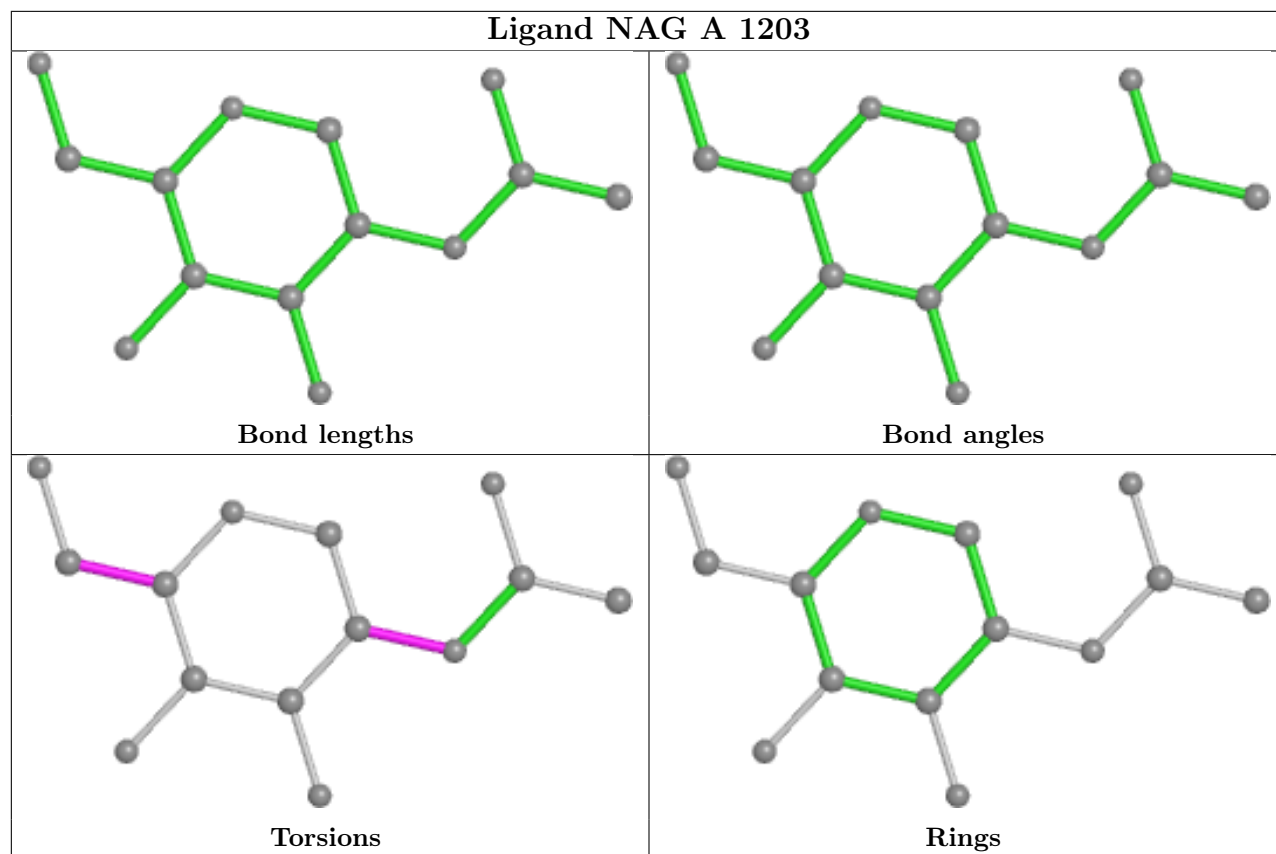


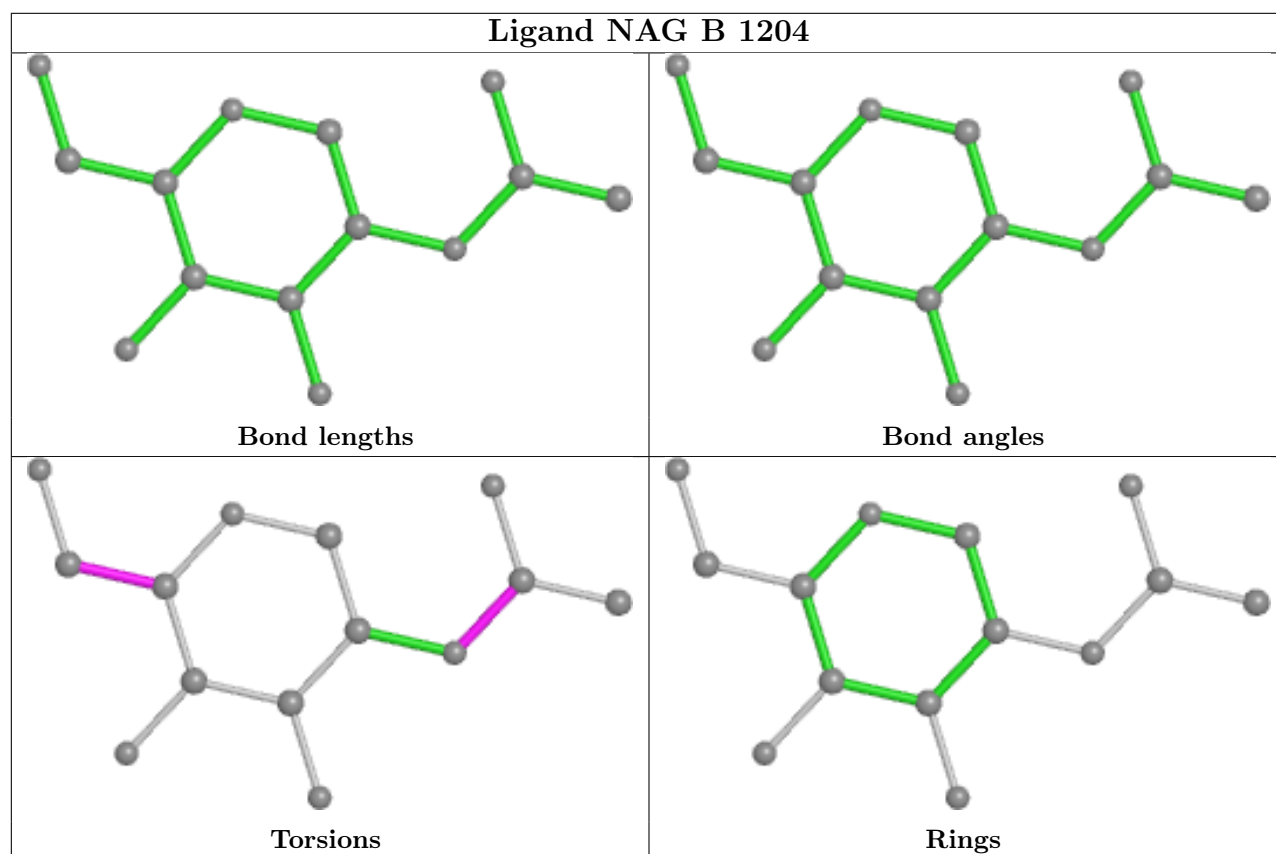
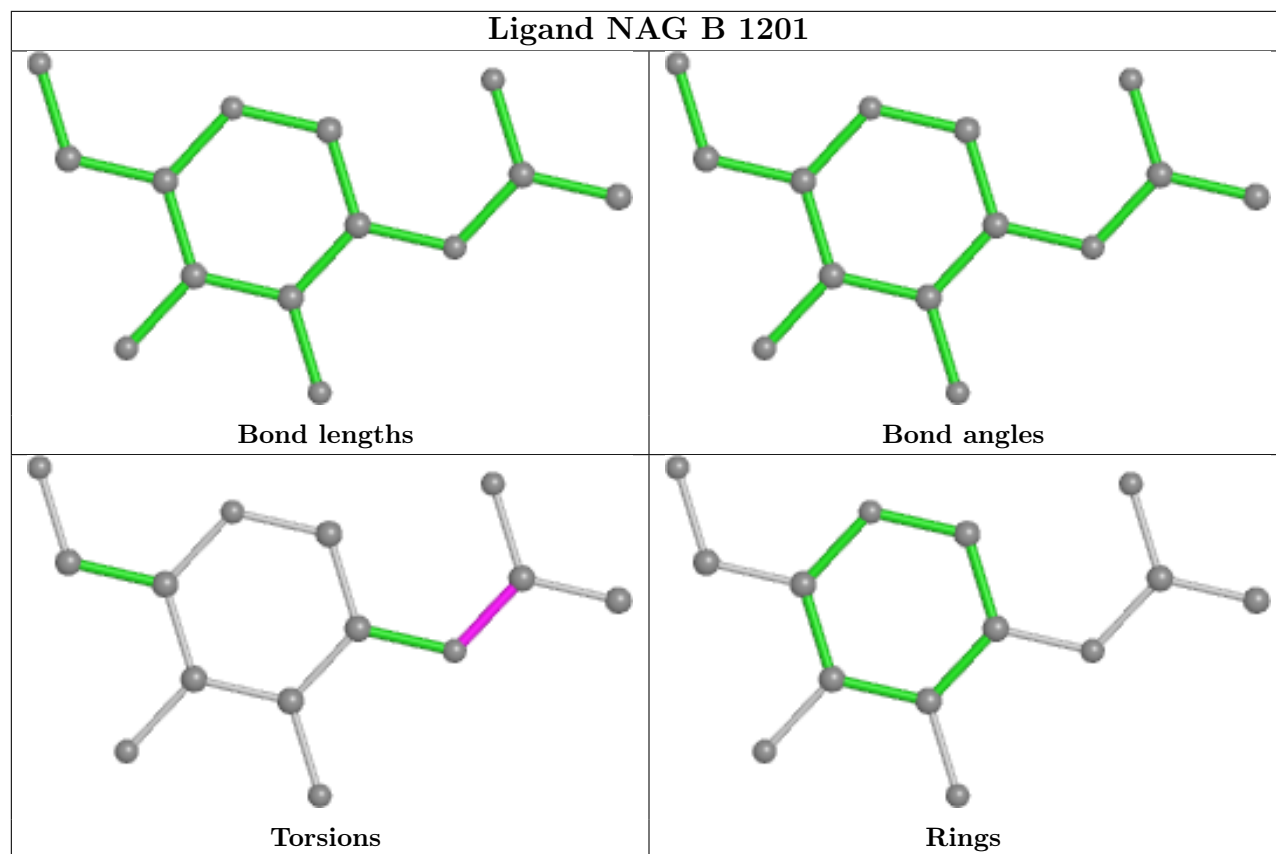
Ligand NAG B 1202

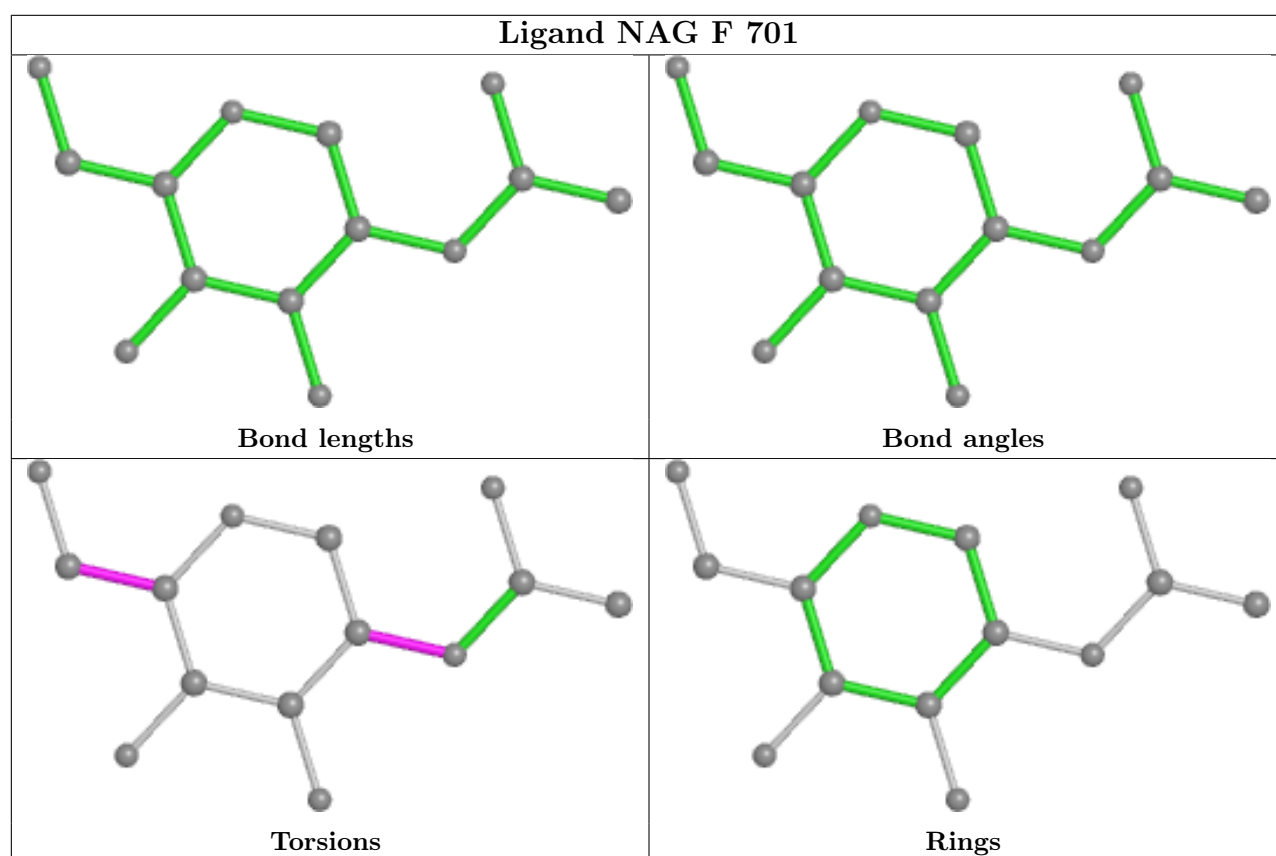
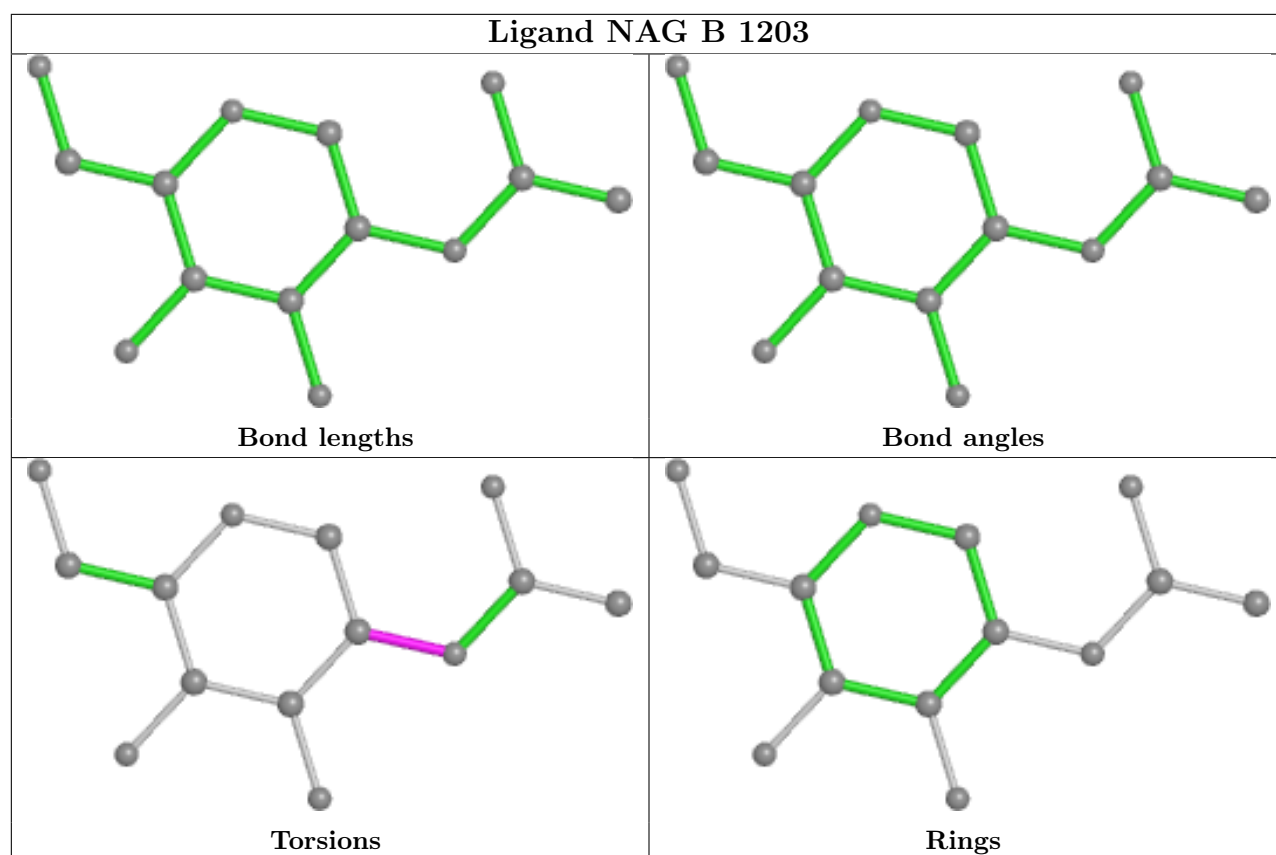


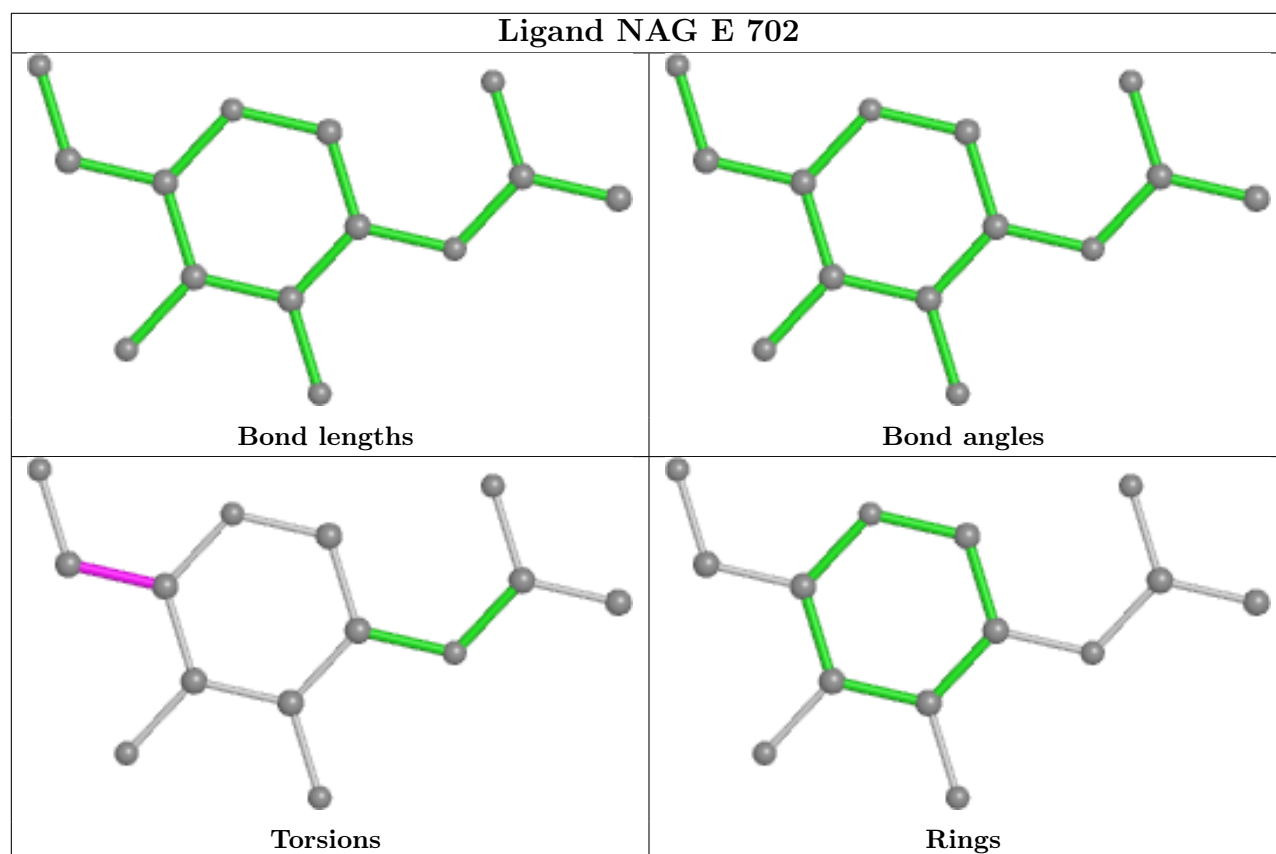
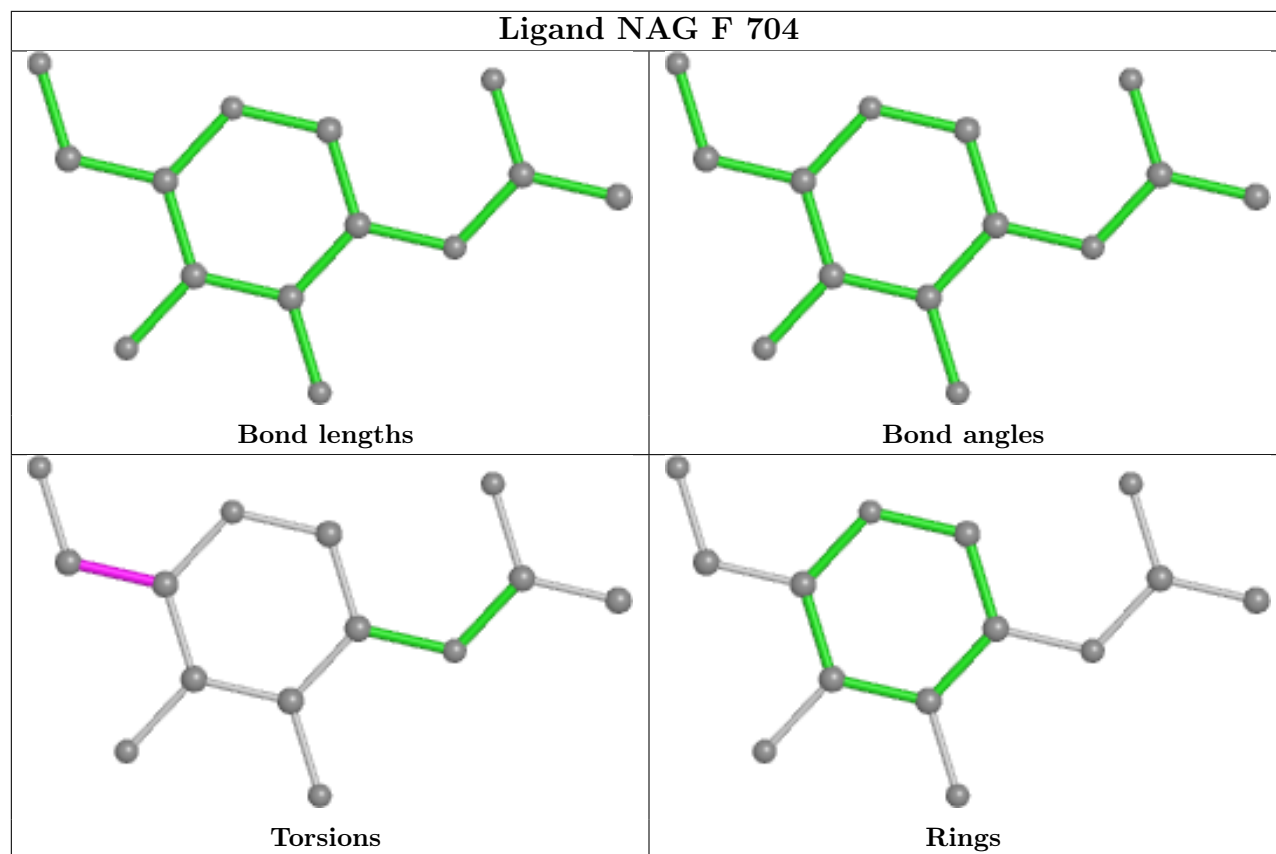


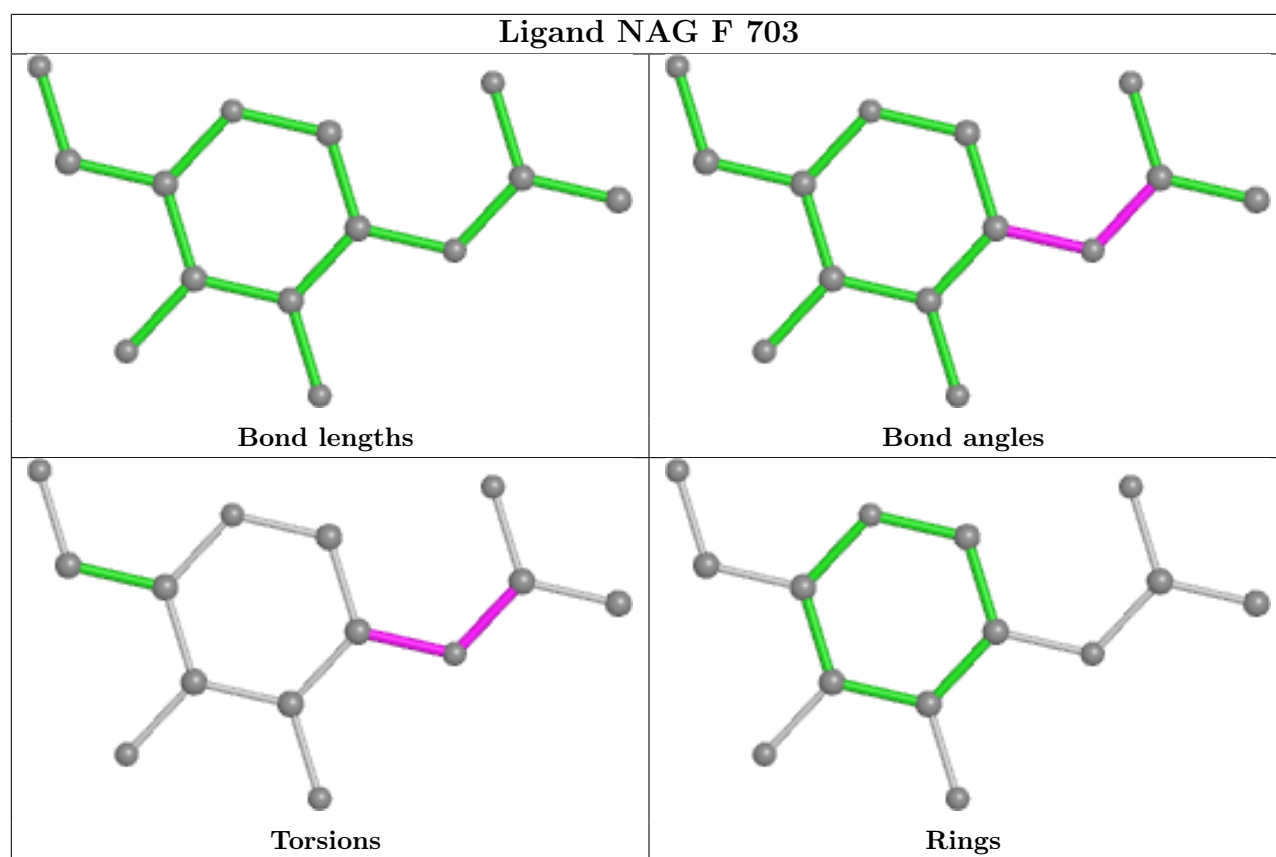












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

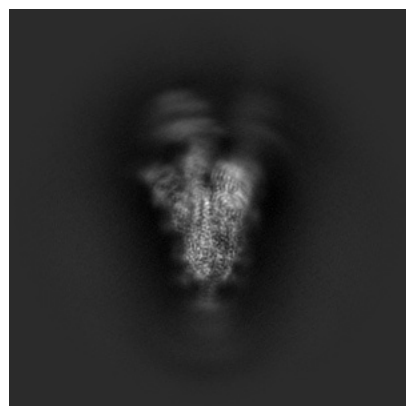
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35426. These allow visual inspection of the internal detail of the map and identification of artifacts.

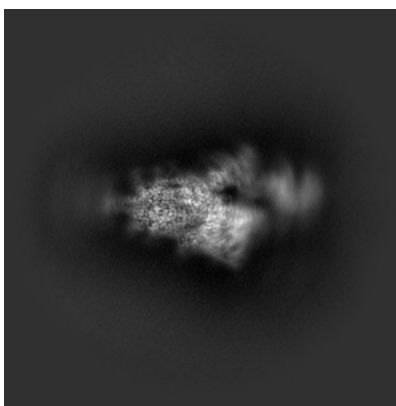
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

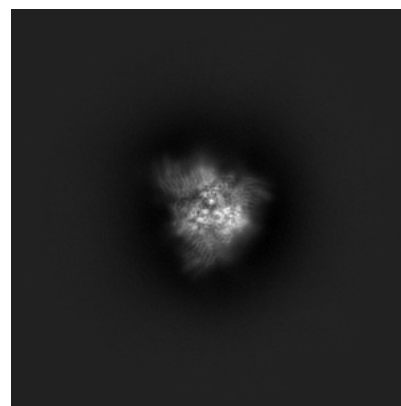
6.1.1 Primary map



X

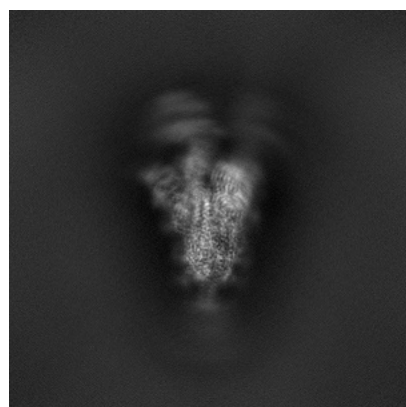


Y

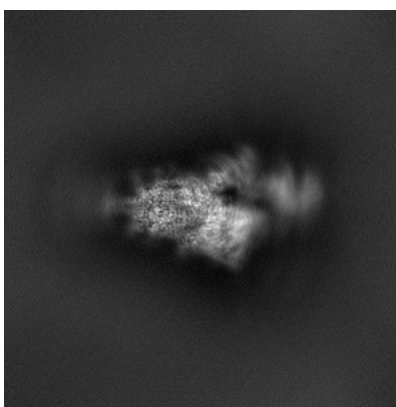


Z

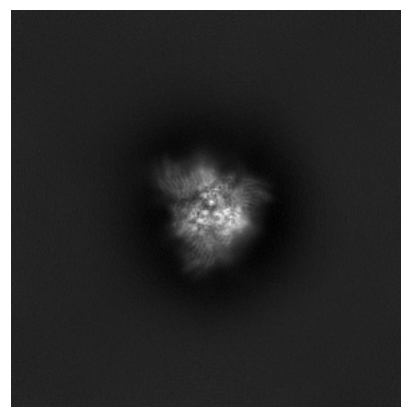
6.1.2 Raw map



X



Y

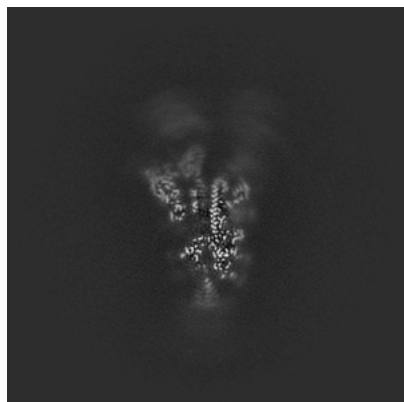


Z

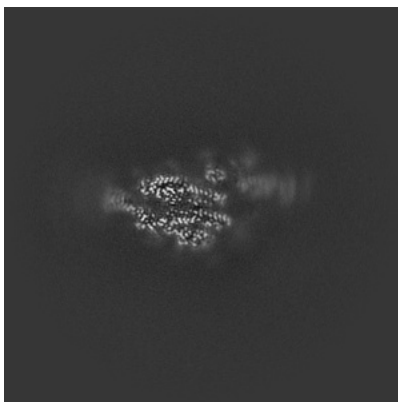
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

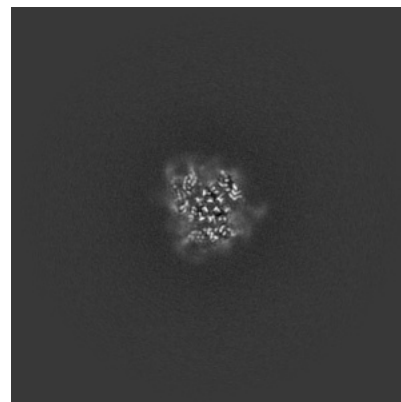
6.2.1 Primary map



X Index: 260

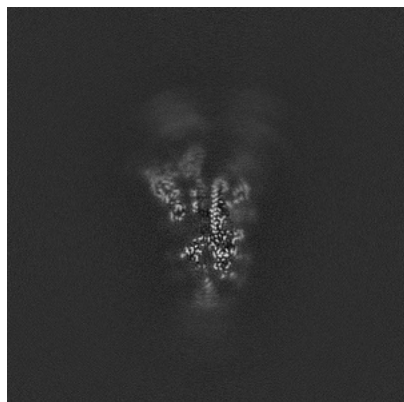


Y Index: 260

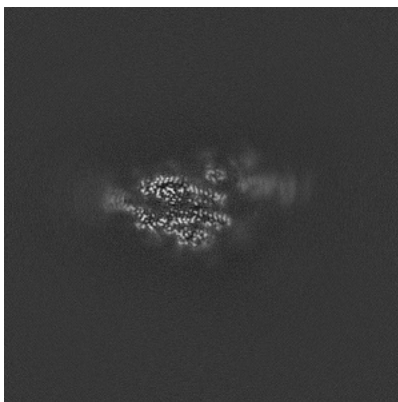


Z Index: 260

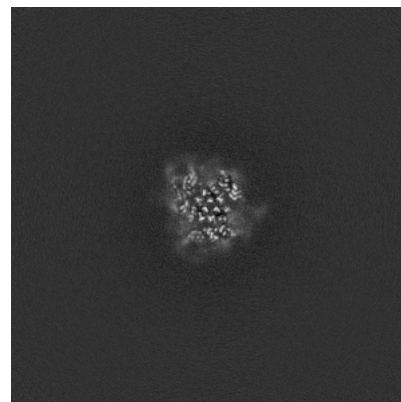
6.2.2 Raw map



X Index: 260



Y Index: 260



Z Index: 260

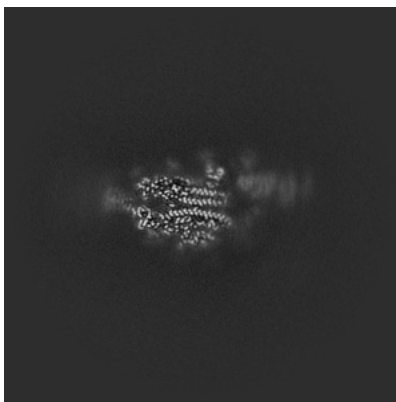
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

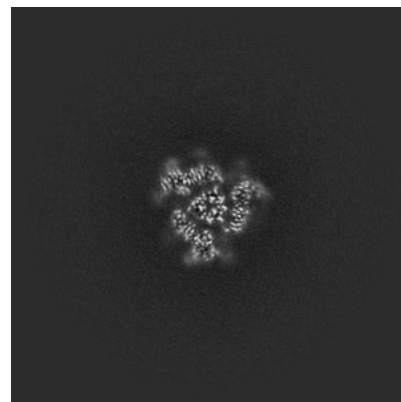
6.3.1 Primary map



X Index: 252

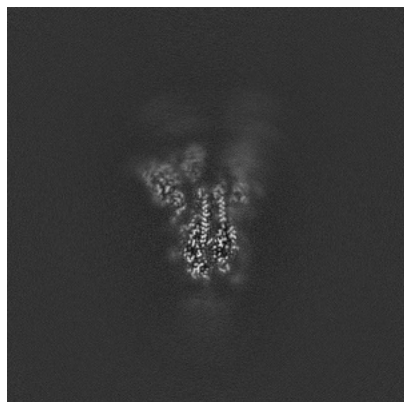


Y Index: 257



Z Index: 275

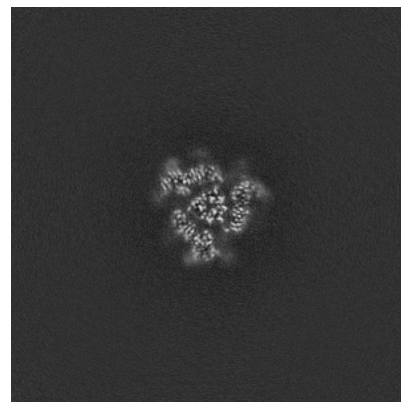
6.3.2 Raw map



X Index: 252



Y Index: 254



Z Index: 275

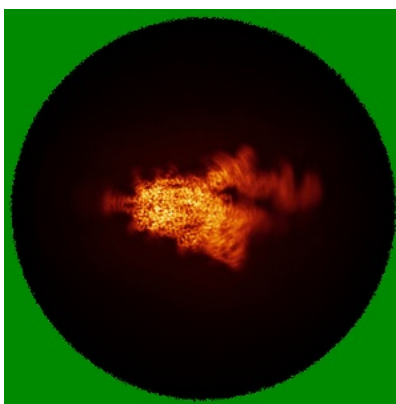
The images above show the largest variance slices of the map in three orthogonal directions.

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

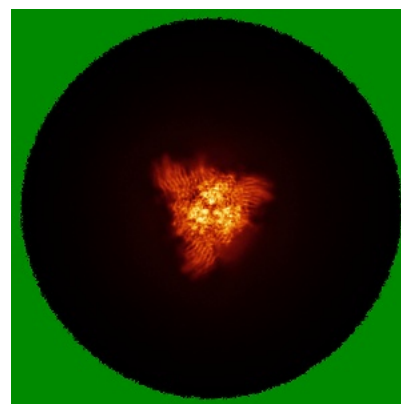
6.4.1 Primary map



X



Y

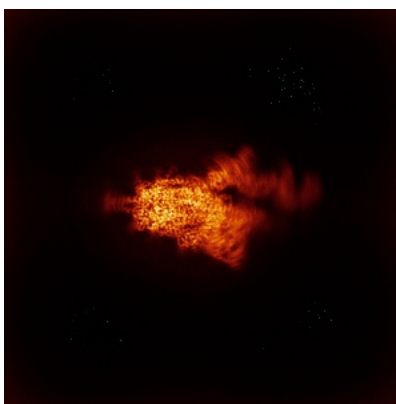


Z

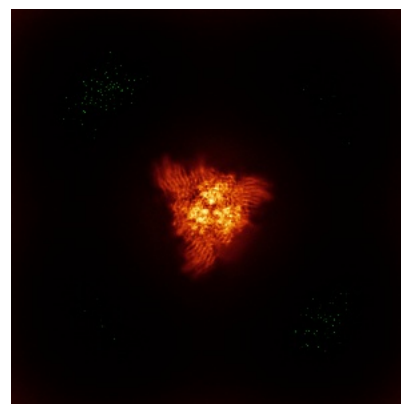
6.4.2 Raw map



X



Y

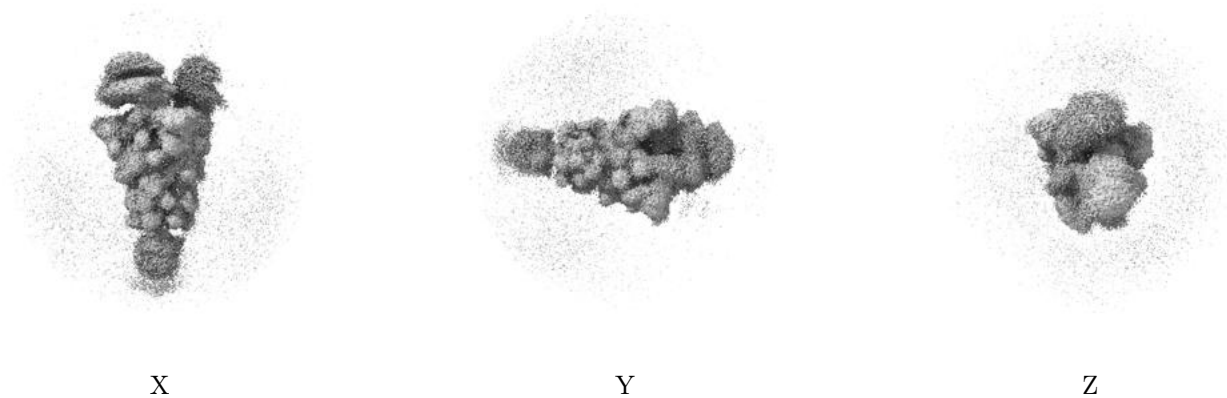


Z

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.

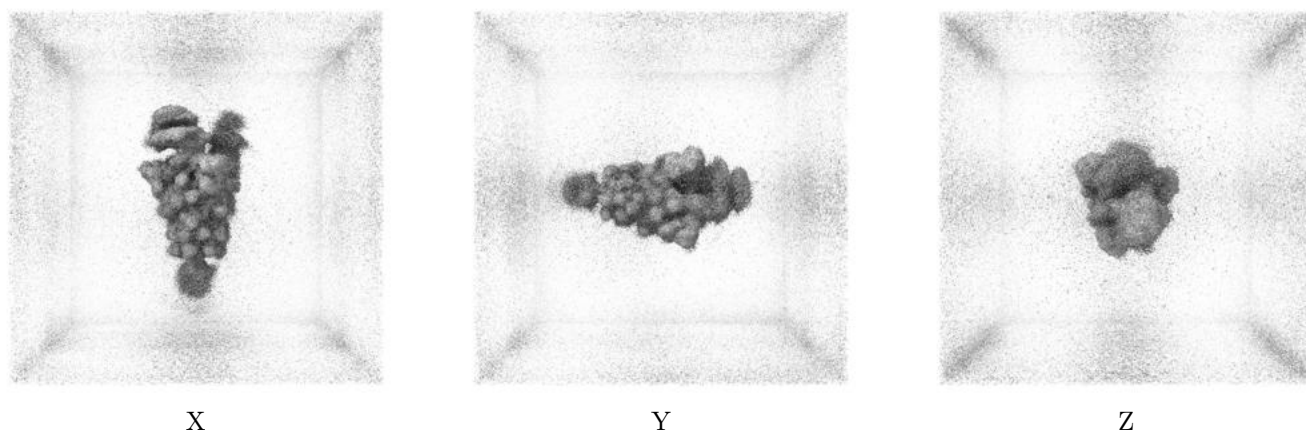
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

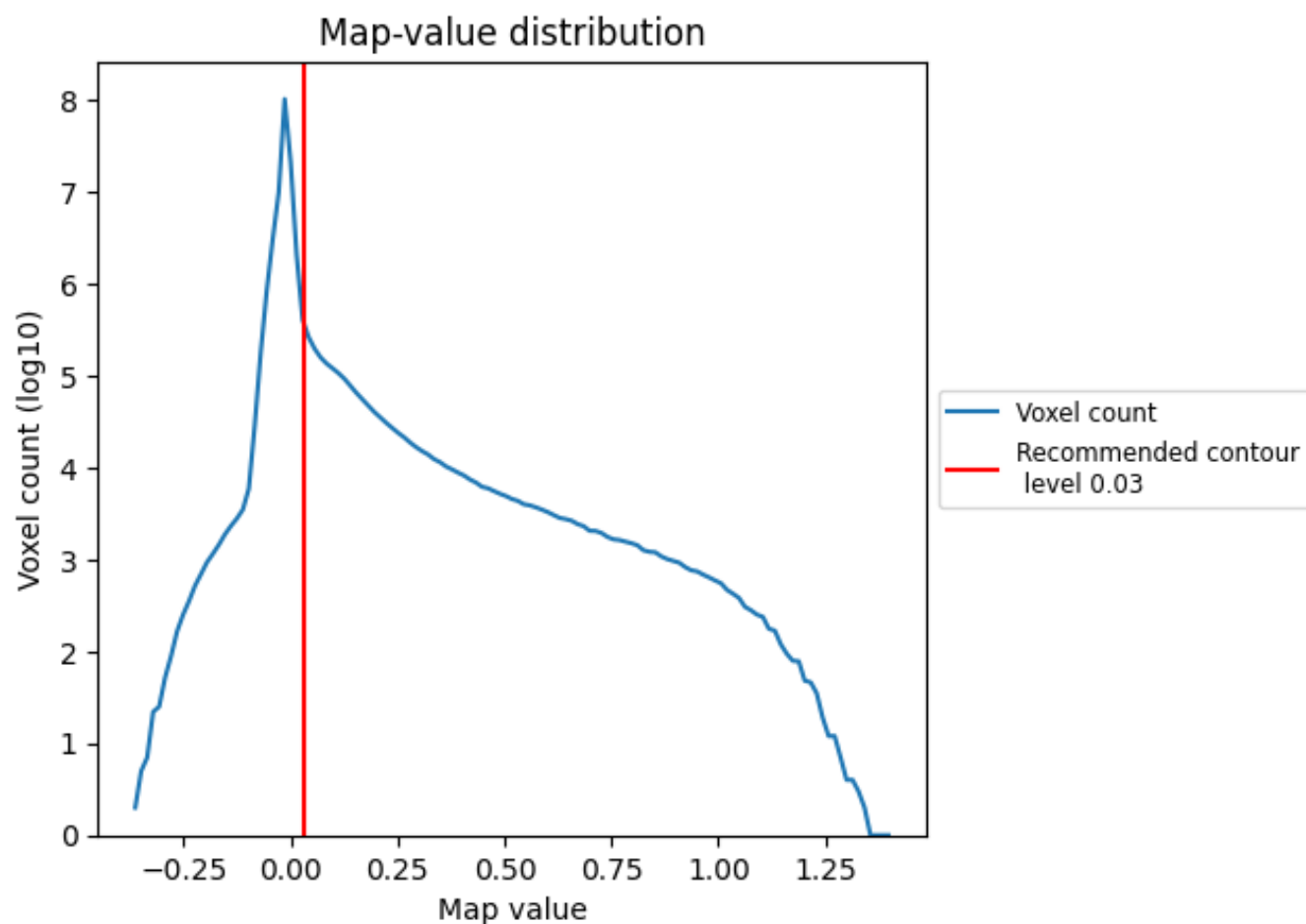
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

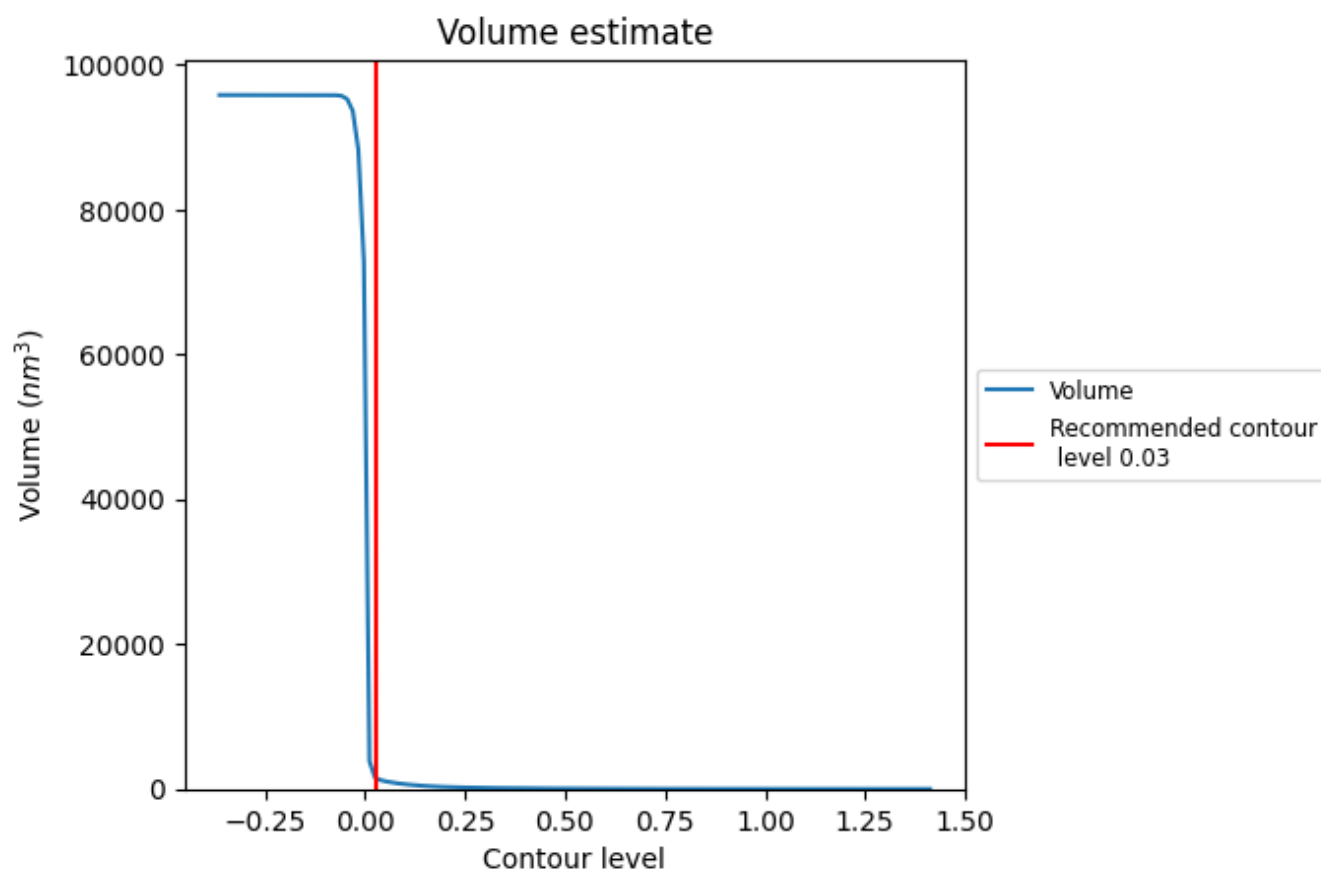
This section contains the results of statistical analysis of the map.

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.

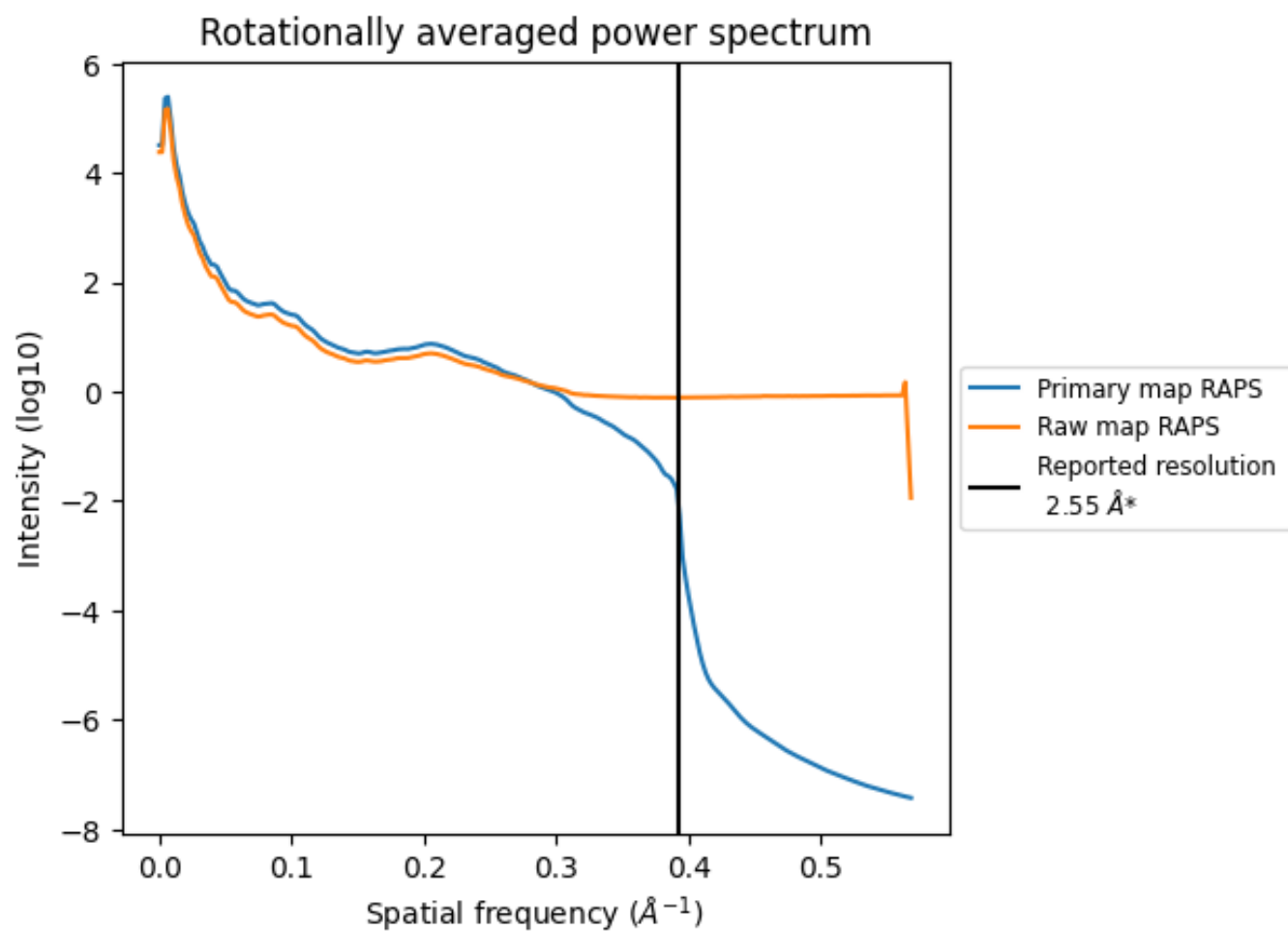
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1446 nm^3 ; this corresponds to an approximate mass of 1306 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 ⓘ

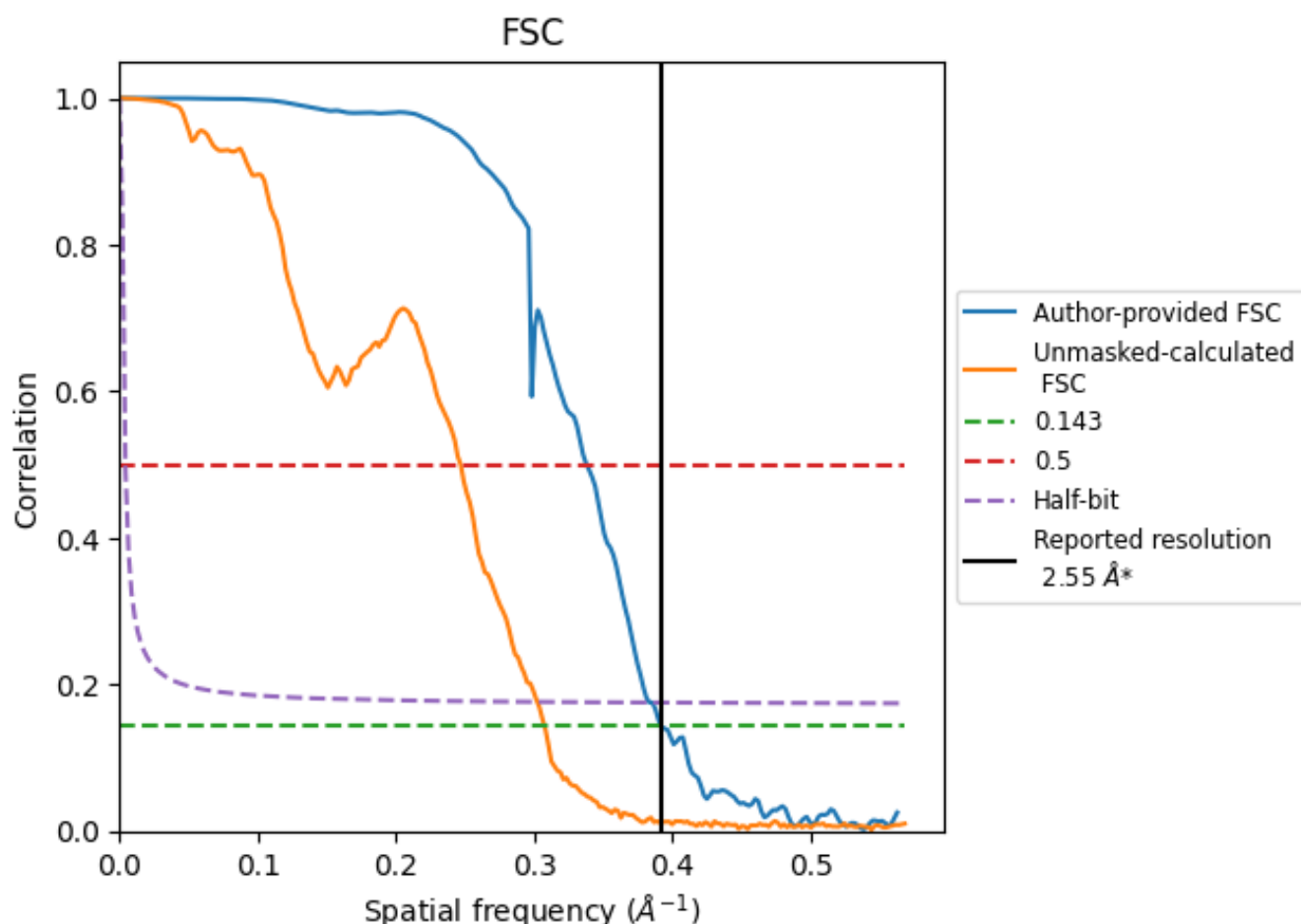


*Reported resolution corresponds to spatial frequency of 0.392 \AA^{-1}

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 0.392 \AA^{-1}

8.2 Resolution estimates [i](#)

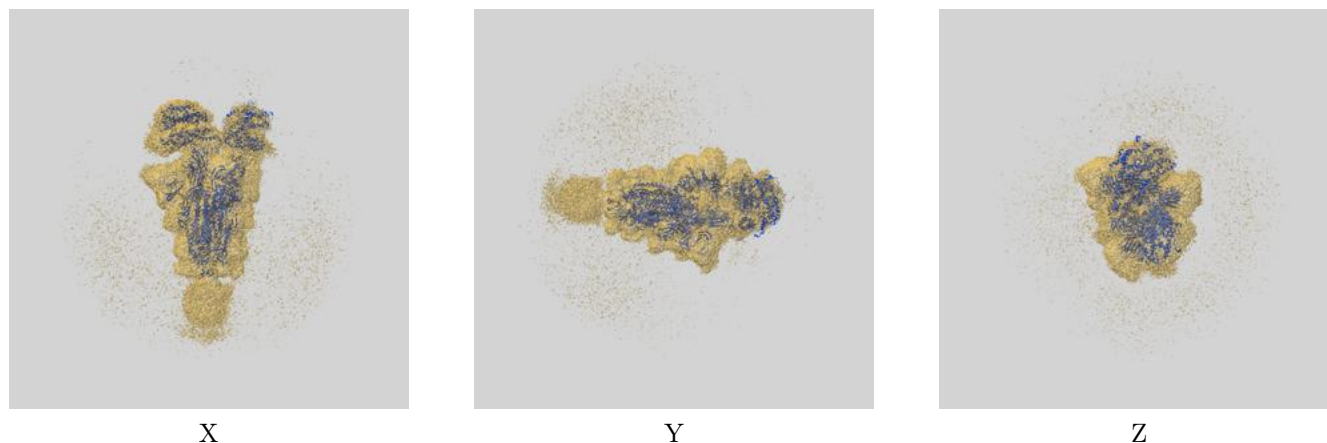
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.96	2.61
Unmasked-calculated*	3.25	4.05	3.31

*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 3.25 differs from the reported value 2.55 by more than 10 %

9 Map-model fit [i](#)

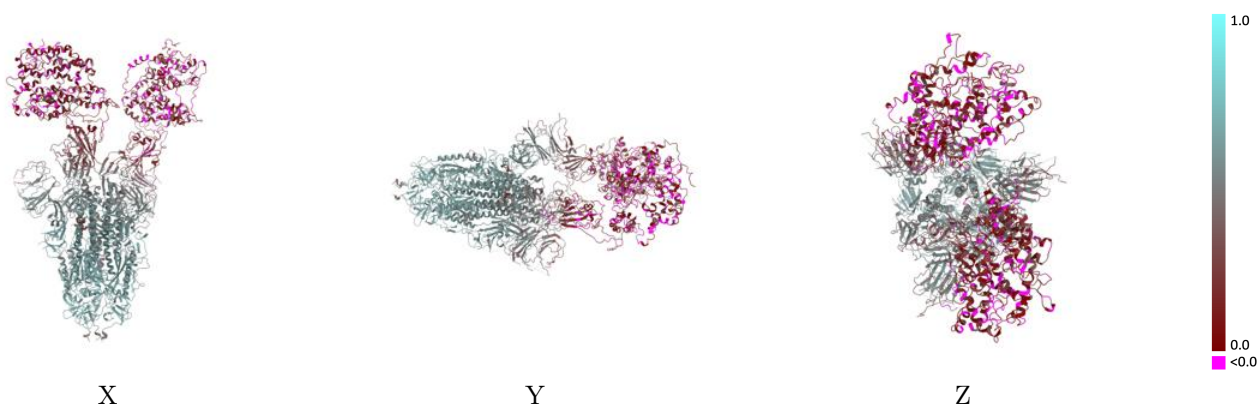
This section contains information regarding the fit between EMDB map EMD-35426 and PDB model 8IFY. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



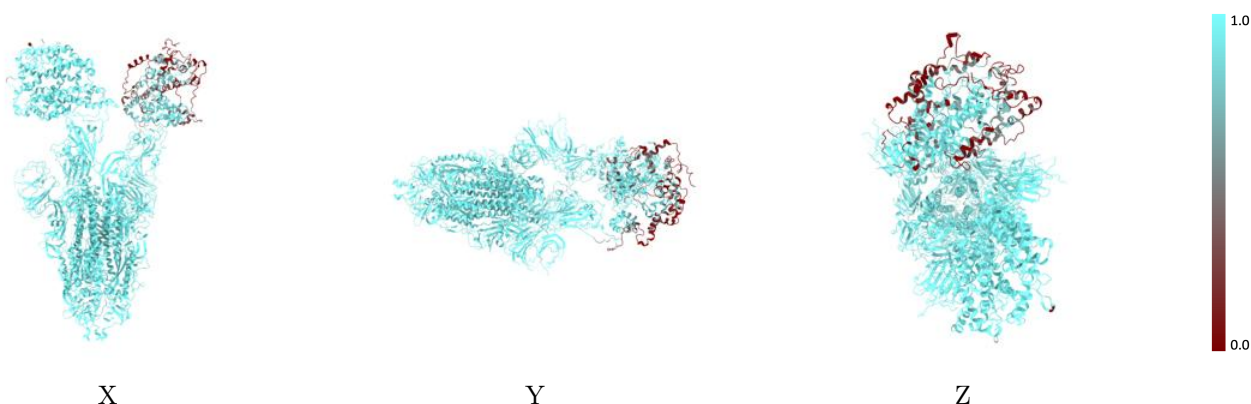
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



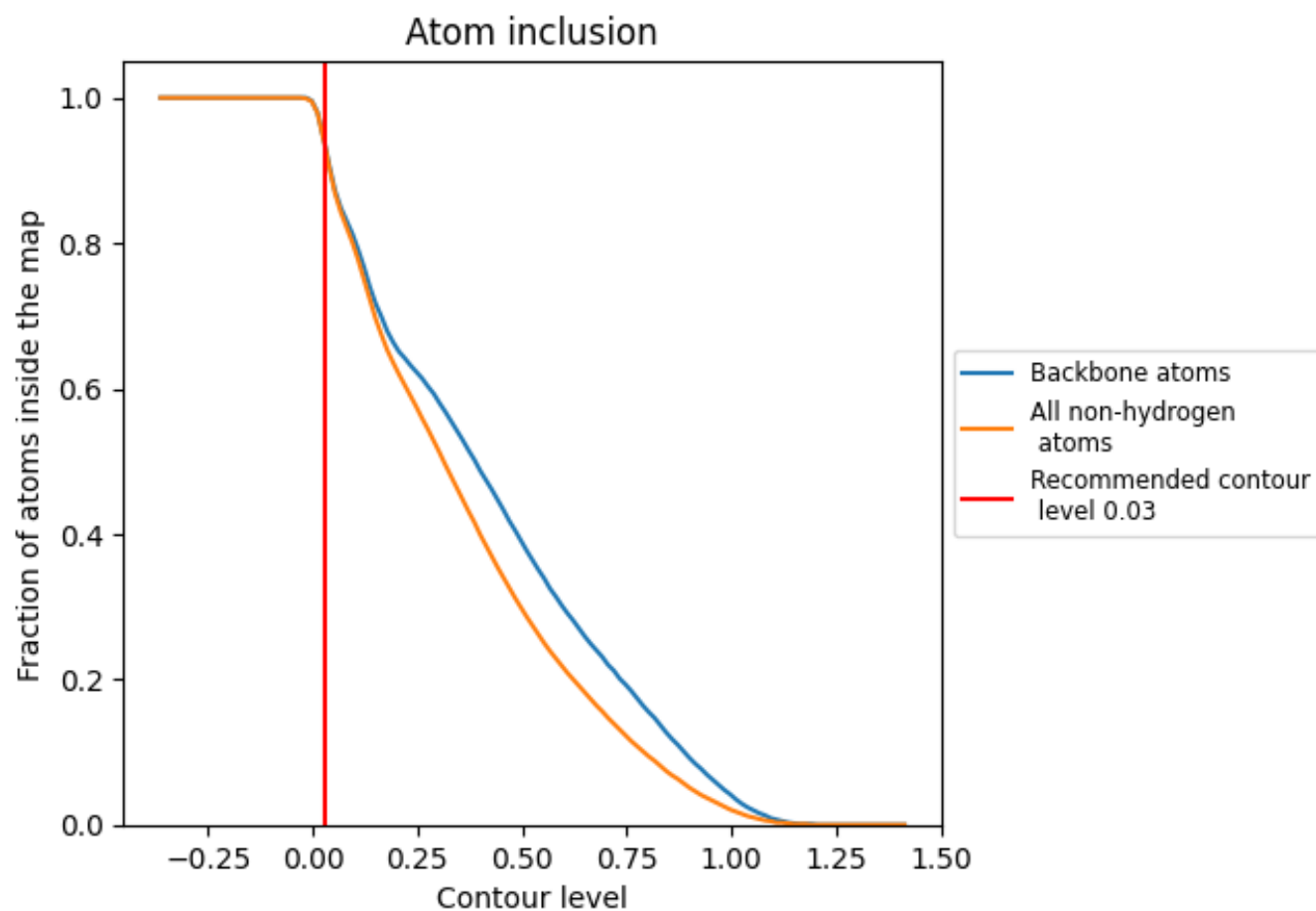
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.3820
A	 0.9900	 0.4640
B	 1.0000	 0.5070
C	 1.0000	 0.4980
E	 0.9890	 0.1230
F	 0.5540	 0.1090
G	 1.0000	 0.3950
H	 1.0000	 0.5350
I	 1.0000	 0.5350
J	 1.0000	 0.5030
K	 1.0000	 0.5280
L	 1.0000	 0.3960
N	 1.0000	 0.5270
O	 1.0000	 0.5220
P	 1.0000	 0.5150
Q	 1.0000	 0.4200
R	 1.0000	 0.5150
S	 1.0000	 0.5220
T	 1.0000	 0.5110
U	 1.0000	 0.4130

