



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 12:42 PM JST

PDB ID : 7D0D
EMDB ID : EMD-30531
Title : S protein of SARS-CoV-2 in complex bound with P5A-3C12_2B
Authors : Yan, R.H.; Wang, R.K.; Ju, B.; Yu, J.F.; Zhang, Y.Y.; Liu, N.; Wang, H.W.;
Wang, X.Q.; Zhang, L.Q.; Zhou, Q.
Deposited on : 2020-09-09
Resolution : 3.80 Å(reported)

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

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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

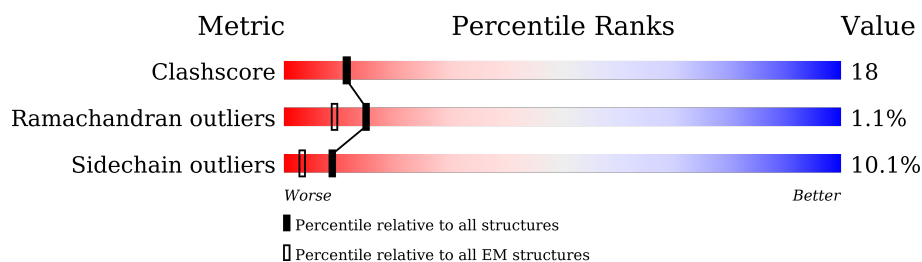
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	1283	
1	B	1283	
1	C	1283	
2	G	226	
2	H	226	
3	F	220	
3	L	220	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	100%
4	I	2	50% 50%
4	J	2	50% 50%
4	K	2	100%
4	M	2	50% 50%
4	N	2	100%
4	O	2	100%
4	P	2	50% 50%
4	Q	2	100%
4	R	2	50% 50%
4	S	2	50% 50%
4	T	2	50% 50%
4	U	2	100%
4	V	2	100%
4	W	2	50% 50%
4	X	2	50% 50%
4	Y	2	50% 50%
4	Z	2	50% 50%
4	a	2	50% 50%
4	b	2	50% 50%
4	c	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28096 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	1004	Total	C	N	O	S	0	0
			7853	5014	1307	1496	36		
1	C	982	Total	C	N	O	S	0	0
			7696	4920	1279	1462	35		
1	B	1006	Total	C	N	O	S	0	0
			7863	5019	1308	1500	36		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

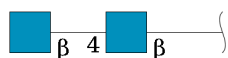
- Molecule 2 is a protein called Heavy chain of P5A-3C12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	125	Total	C	N	O	S	0	0
			972	625	154	189	4		
2	G	125	Total	C	N	O	S	0	0
			972	625	154	189	4		

- Molecule 3 is a protein called Light chain of P5A-3C12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	113	Total	C	N	O	S	0	0
			880	555	145	177	3		
3	F	113	Total	C	N	O	S	0	0
			880	555	145	177	3		

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



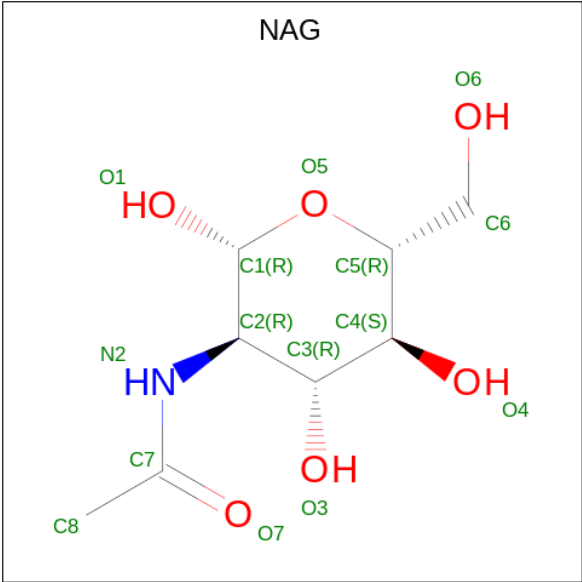
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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	K	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	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	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		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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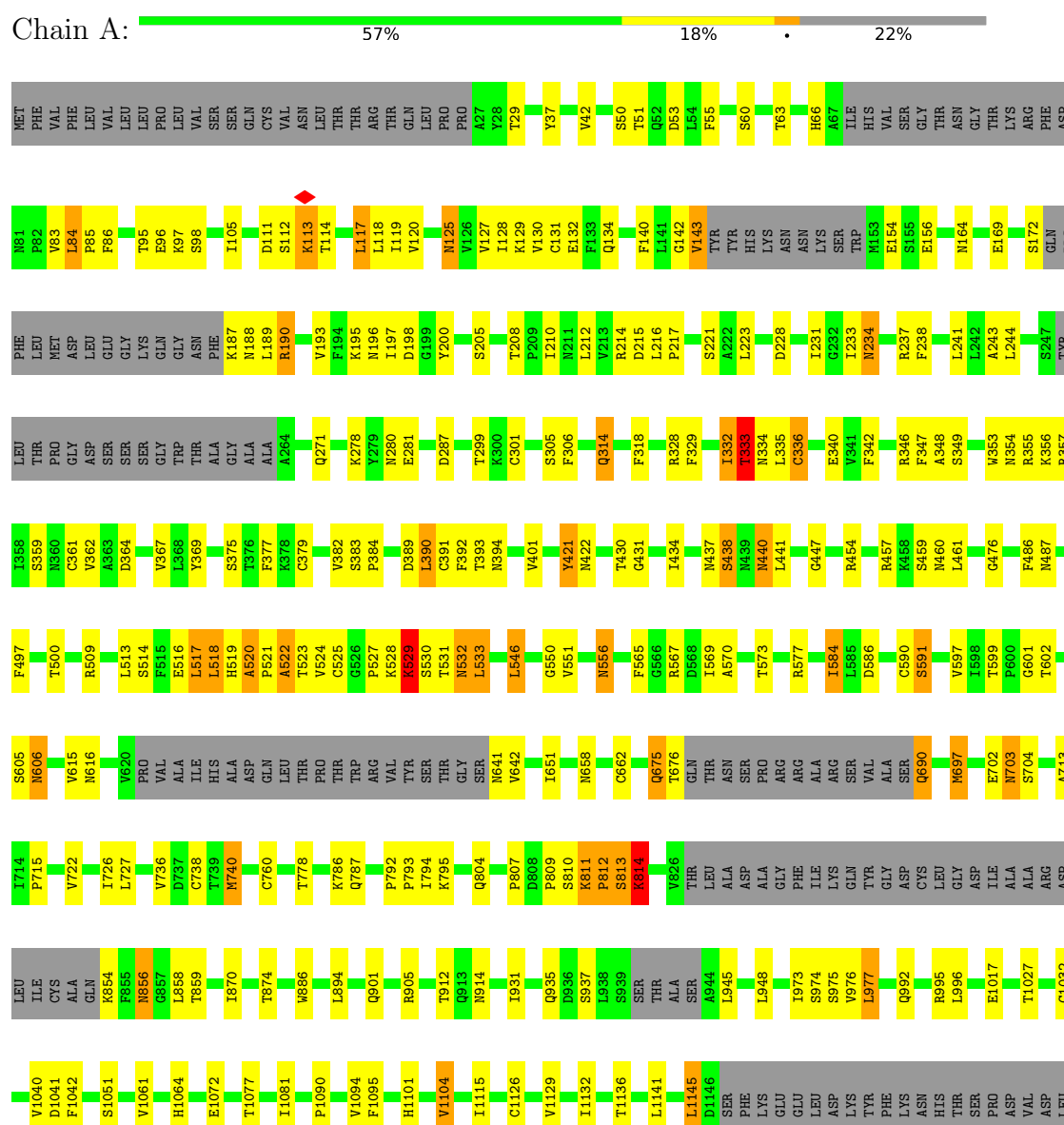
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C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

3 Residue-property plots

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



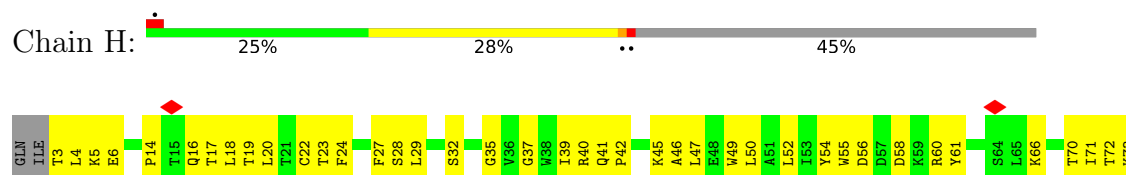
TLE	VAL	MET	MET	VAL	THR	THR	TLE	MET	LEU	CYS	CYS	THR	THR	SER	CYS	CYS	SER	CYS	CYS	LEU	LEU	LYS	GLY	CYS	CYS	CYS	SER	GLY	CYS	CYS	LYS	LYS	PHE	ASP	ASP	GLU	ASP	ASP	ASP	SER	GLU	GLY	PRO	VAL	VAL	LEU	LEU	LYS	GLY	VAL	LYS	VAL	LEU	LEU	HIS	THR	THR	LEU	LEU	LEU	GLU	ASP	ASP	ASP	ASP	LYS	LYS
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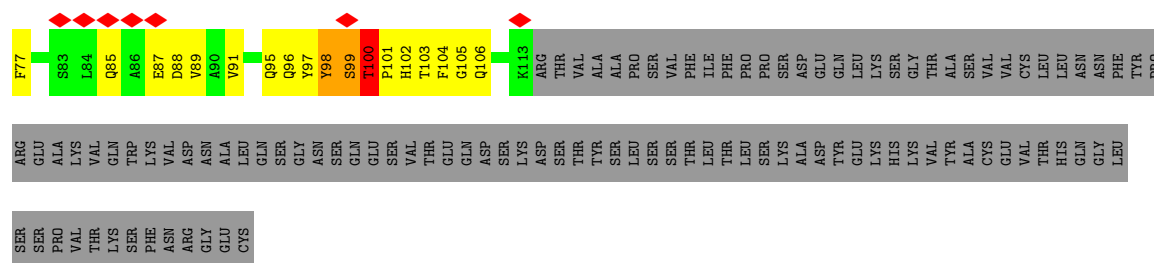
- Molecule 1: Spike glycoprotein



Lys	GLY	ASP	S975	GLY	V674	Q564	Q174	R403	THR	T167	V83	MET
	LEU	VAL	V976	PHE	Q675	R567	A475	G404	ALA	F168	GLY	PHE
	ILE	ASP	L981	ILE	Q676	D568	GLN	D405	GLY	S172	N87	VAL
	ILE	GLY	L981	GLN	THR	I569	THR	E406	ALA	GLN	D88	VAL
	VAL	ASP	L984	TVR	ASN	T573	PRO	R408	ALA	PRO	Y91	VAL
	MET	ILE	L984	GLY	SER	T573	CYS	Q409	GLN	PHE	Y91	VAL
	VAL	SER	E988	ASP	PRO	D574	ASN	CYS	R273	LEU	T95	LEU
	VAL	GLY	Q992	CYS	ARG	A575	GLY	Q415	K278	ASP	E96	PRO
	ILE	ILE	Q992	LEU	ARG	V576	VAL	T415	GLY	MET	K97	LEU
	MET	ASN	L1030	GLY	ALA	B577	GLU	Q416	E281	LEU	S98	VAL
	LEU	ALA	S1030	ASP	ARG	B577	GLY	K417	GLY	GLU	N99	SER
	CYS	SER	E1031	ILE	SER	L582	PHE	I418	T307	GLY	I105	SER
	CYS	VAL	C1032	ALA	VAL	E583	N487	N422	GLN	GLN	CYS	GLN
	MET	VAL	A1032	ALA	ALA	I584	F490	Y423	F318	GLY	T108	VAL
	THR	ASN	S1037	ARG	Q690	V597	F490	K424	R318	GLY	T109	ASN
	SER	ILE	Q690	ASP	SER	V597	A491	K424	V327	ASN	L110	LEU
	GLN	GLN	S691	LEU	S691	P600	L492	Q493	R328	PHE	D111	THR
	CYS	LVS	I692	ILE	I692	P600	S494	S494	N331	K187	D111	THR
	CYS	GLU	K1045	CYS	S698	N603	Y495	G431	N331	E191	K113	ARG
	CYS	ILE	K1045	ALA	S698	N603	G496	V433	T333	D198	S116	THR
	LVS	ARG	S1051	K854	S704	N606	GLN	I434	N334	G199	S116	GLN
	GLY	LEU	S1051	P855	N710	Q607	PRO	N437	V341	S205	V120	LEU
	CYS	ASN	G1059	N856	N710	Q608	THR	S438	F342	K206	N122	PRO
	CYS	GLU	H1064	E868	A713	D614	ASN	S439	V341	S205	N121	PRO
	SER	VAL	GLY	GLY	A713	V615	THR	ASN	F342	K206	N122	ASP
	GLY	ALA	L1074	L878	T719	N616	GLY	N440	T345	H207	T124	T29
	CYS	ASN	N1074	ASN	T719	C617	Y503	I441	T345	T208	T124	T29
	ASN	ASN	V1094	T683	V722	T618	G504	ASP	V350	N211	V127	N30
	LEU	LEU	V1094	ASN	V722	E619	F505	SER	V350	N211	V127	S31
	CYS	ASN	V1104	Q901	V729	V620	P507	LYS	Y351	L212	V130	S45
	LVS	SER	V1104	GLY	V729	V620	GLY	VAL	Y351	L212	V130	S45
	ASP	SER	V1104	ILE	S746	PRO	S514	GLY	W353	R214	C131	L48
	LEU	LEU	I1114	R905	T747	VAL	S514	GLY	W353	R214	C131	L48
	ILE	ILE	I1115	E748	E748	ALA	P521	ASN	I358	D215	E132	H49
	ASP	ASP	C1126	T912	S758	HIS	P521	TYR	S359	L216	F133	S50
	SER	GLN	L1141	L916	S758	ALA	V524	ASN	I358	L216	F133	S50
	GLU	GLU	Q1142	Q926	Q762	ASP	C525	Y451	S359	P217	Q134	T51
	PRO	LEU	P1143	Q926	Q762	ASP	C525	Y453	D364	T231	F135	Q52
	VAL	GLY	P1143	Q935	Q779	GLN	Q525	Y453	D364	T231	G142	D53
	LEU	GLY	P1143	Q935	Q779	LEU	T531	R454	S371	G332	V143	D53
	LEU	TVR	D1146	Q935	Q779	THR	N532	L455	S371	I233	V143	F59
	LVS	TVR	D1146	Q935	Q779	THR	N532	L455	T376	T236	TYR	S60
	GLY	GLU	PHE	S939	K786	THR	N532	L455	F377	T236	TYR	S60
	VAL	GLN	PHE	S939	Q787	THR	N532	L455	F377	T236	TYR	S60
	VAL	GLN	PHE	S939	Q787	THR	N532	L455	F377	T236	TYR	S60
	LVS	TVR	LYS	THR	I788	ARG	F541	S459	C379	Q239	ASN	HIS
	LEU	ILE	GLU	ALA	I788	VAL	N542	N460	G381	T240	LYS	VAL
	HIS	LYS	GLU	SER	K790	TYR	N542	N460	V382	S247	LYS	VAL
	THR	TRP	LEU	A944	T791	SER	L546	K462	V382	TRP	GLY	SER
	THR	TRP	LEU	P792	P792	T638	T547	P463	T385	LEU	M153	THR
	GLU	TRP	LYS	L959	D808	Q639	F464	F464	T385	LEU	M153	THR
	GLU	TVR	TYR	L959	D808	Q639	F464	F464	T385	LEU	M153	THR
	ASP	ILE	PHE	K964	V626	S640	S555	R466	N388	THR	E156	GLY
	THR	TRP	LYS	ASN	V626	R646	S555	R466	N388	THR	E156	GLY
	LVS	LEU	ASN	S968	THR	R646	S557	P463	C391	PRO	F157	THR
	ASP	GLY	HIS	N969	LEU	Q649	K558	I468	C391	GLY	F157	THR
	ASP	PHE	THR	THR	ALA	Q649	K558	I468	C391	GLY	F157	THR
	ASP	PHE	THR	THR	ALA	Q649	K558	I468	C391	GLY	F157	THR
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
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	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E661	L560	S469	Y396	SER	N164	PHE
	ASP	ILE	SER	ASP	ALA	E66						

- Molecule 1: Spike glycoprotein





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

Chain D: 50% 50%

MAG1
MAG2

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

Chain E: 100%

MAG1
MAG2

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

Chain I: 50% 50%

MAG1
MAG2

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

Chain J: 50% 50%

MAG1
MAG2

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

Chain K: 100%

MAG1
MAG2

- 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 N:  100%



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

Chain O:  100%



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

Chain P:  50% 50% 50%



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

Chain Q:  100%



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

Chain R:  50% 50%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  50% 50%



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

Chain X:  50% 50%



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

Chain Y:  50% 50%



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

Chain Z:  50% 50%



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

Chain a:  50% 50%



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

Chain b:  50% 50%



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

Chain c:  50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0087	Depositor
Map size (\AA)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/8028	0.55	0/10919
1	B	0.59	0/8039	0.55	0/10936
1	C	0.49	0/7864	0.55	0/10691
2	G	0.36	0/999	0.68	0/1367
2	H	0.36	0/999	0.68	0/1367
3	F	0.38	0/901	0.59	0/1225
3	L	0.38	0/901	0.60	0/1225
All	All	0.54	0/27731	0.56	0/37730

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	7853	0	7653	203	0
1	B	7863	0	7658	242	0
1	C	7696	0	7514	147	0
2	G	972	0	956	136	0
2	H	972	0	956	141	0
3	F	880	0	849	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	880	0	849	108	0
4	D	28	0	25	0	0
4	E	28	0	25	3	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	1	0
4	N	28	0	25	2	0
4	O	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	3	0
4	X	28	0	25	0	0
4	Y	28	0	25	1	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
5	A	112	0	104	2	0
5	B	126	0	117	4	0
5	C	126	0	117	6	0
All	All	28096	0	27323	981	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 18.

All (981) 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:H:113:PRO:HA	2:H:117:TRP:CZ2	1.35	1.59
2:G:113:PRO:HA	2:G:117:TRP:CZ2	1.35	1.58
1:B:329:PHE:CD2	1:B:528:LYS:HG3	1.47	1.47
2:G:111:TRP:HD1	3:F:102:HIS:CE1	1.36	1.44
2:H:111:TRP:HD1	3:L:102:HIS:CE1	1.36	1.42
3:L:7:SER:CB	3:L:22:ASN:H	1.39	1.34
3:F:7:SER:CB	3:F:22:ASN:H	1.39	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLY:CA	1:B:521:PRO:HG3	1.60	1.29
2:G:113:PRO:CA	2:G:117:TRP:HZ2	1.46	1.28
2:H:111:TRP:CD1	3:L:102:HIS:CE1	2.23	1.27
2:H:113:PRO:CA	2:H:117:TRP:HZ2	1.46	1.26
1:C:199:GLY:HA3	1:B:521:PRO:CG	1.64	1.26
2:G:111:TRP:CD1	3:F:102:HIS:CE1	2.23	1.25
2:H:27:PHE:CE2	2:H:116:TYR:CZ	2.28	1.20
2:G:27:PHE:CE2	2:G:116:TYR:CZ	2.28	1.20
1:B:329:PHE:CD2	1:B:528:LYS:CG	2.27	1.16
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
3:F:8:PRO:HG2	3:F:11:LEU:HD11	1.16	1.14
3:L:100:THR:HG23	3:L:101:PRO:HD3	1.30	1.13
3:F:8:PRO:HG3	3:F:20:THR:O	1.48	1.13
1:B:340:GLU:OE2	1:B:356:LYS:HE2	1.47	1.13
2:G:110:SER:O	2:G:111:TRP:CD1	2.02	1.13
2:H:110:SER:O	2:H:111:TRP:CD1	2.02	1.12
3:L:8:PRO:HG2	3:L:11:LEU:HD11	1.16	1.12
3:L:8:PRO:HG3	3:L:20:THR:O	1.48	1.11
2:H:49:TRP:HB3	3:L:102:HIS:HE1	1.15	1.11
2:H:110:SER:O	2:H:111:TRP:CG	2.03	1.11
1:B:523:THR:HG22	1:B:524:VAL:H	0.97	1.10
2:G:110:SER:O	2:G:111:TRP:CG	2.03	1.10
2:H:27:PHE:HE2	2:H:116:TYR:CZ	1.66	1.10
2:H:99:HIS:HB3	2:H:116:TYR:CB	1.82	1.09
1:C:198:ASP:O	1:B:521:PRO:HB3	1.47	1.09
2:G:49:TRP:HB3	3:F:102:HIS:HE1	1.15	1.08
2:G:99:HIS:HB3	2:G:116:TYR:CB	1.82	1.08
2:G:113:PRO:CA	2:G:117:TRP:CZ2	2.28	1.08
1:A:523:THR:HG22	1:A:524:VAL:H	0.97	1.08
3:L:7:SER:HB2	3:L:22:ASN:H	1.18	1.08
1:B:392:PHE:HB3	1:B:517:LEU:HD21	1.35	1.08
2:H:113:PRO:CA	2:H:117:TRP:CZ2	2.28	1.07
3:F:100:THR:HG23	3:F:101:PRO:HD3	1.30	1.07
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.35	1.07
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.06
3:F:7:SER:HB3	3:F:8:PRO:CD	1.85	1.06
2:H:27:PHE:HE2	2:H:116:TYR:CE1	1.73	1.06
3:L:7:SER:HB3	3:L:8:PRO:CD	1.85	1.06
2:H:99:HIS:HB3	2:H:116:TYR:HB2	1.06	1.06
2:G:99:HIS:HB3	2:G:116:TYR:HB2	1.06	1.06
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:SER:HB2	2:H:113:PRO:CG	1.87	1.05
2:G:27:PHE:HE2	2:G:116:TYR:CE1	1.73	1.04
2:G:27:PHE:HE2	2:G:116:TYR:CZ	1.66	1.04
3:F:7:SER:HB2	3:F:22:ASN:H	1.18	1.04
3:F:96:GLN:HE22	3:F:99:SER:CB	1.70	1.04
3:L:7:SER:CB	3:L:22:ASN:N	2.22	1.03
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.03
2:G:109:SER:HB2	2:G:113:PRO:CG	1.87	1.03
3:L:96:GLN:HE22	3:L:99:SER:CB	1.70	1.02
1:B:392:PHE:HB3	1:B:517:LEU:CD2	1.88	1.02
3:F:7:SER:CB	3:F:22:ASN:N	2.22	1.02
1:A:486:PHE:HD1	2:H:103:LEU:HD21	1.24	1.01
1:B:523:THR:HG22	1:B:524:VAL:N	1.72	1.01
3:L:7:SER:HB2	3:L:22:ASN:N	1.75	1.01
3:L:7:SER:HB3	3:L:22:ASN:H	1.24	1.01
1:A:486:PHE:CD1	2:H:103:LEU:HD21	1.96	1.00
1:A:675:GLN:HE21	1:A:675:GLN:HA	1.27	1.00
2:G:49:TRP:HB3	3:F:102:HIS:CE1	1.96	1.00
2:G:103:LEU:HD21	1:B:486:PHE:HD1	1.25	1.00
3:F:7:SER:HB2	3:F:22:ASN:N	1.75	1.00
2:G:103:LEU:HD21	1:B:486:PHE:CD1	1.96	1.00
1:A:811:LYS:HB2	1:A:812:PRO:CD	1.91	0.99
1:A:523:THR:HG22	1:A:524:VAL:N	1.72	0.99
2:H:49:TRP:HB3	3:L:102:HIS:CE1	1.96	0.99
1:A:550:GLY:HA2	1:A:590:CYS:SG	2.01	0.99
3:L:8:PRO:CG	3:L:11:LEU:HD11	1.93	0.99
1:B:392:PHE:CB	1:B:517:LEU:HD21	1.91	0.99
3:F:8:PRO:CG	3:F:11:LEU:HD11	1.93	0.99
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.91	0.98
1:A:523:THR:CG2	1:A:524:VAL:H	1.76	0.98
3:L:6:GLN:NE2	3:L:105:GLY:HA2	1.77	0.98
3:F:7:SER:CB	3:F:8:PRO:CD	2.42	0.97
3:F:6:GLN:NE2	3:F:105:GLY:HA2	1.77	0.97
1:B:523:THR:CG2	1:B:524:VAL:H	1.77	0.97
3:F:7:SER:HB3	3:F:8:PRO:HD2	1.45	0.97
1:B:329:PHE:CE2	1:B:528:LYS:HD2	2.00	0.97
1:A:676:THR:HA	1:A:690:GLN:HB3	1.46	0.96
2:H:99:HIS:CD2	2:H:116:TYR:HD2	1.83	0.96
3:F:7:SER:HB3	3:F:22:ASN:H	1.24	0.96
1:B:346:ARG:NH2	1:B:347:PHE:O	1.98	0.96
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:7:SER:HB3	3:L:8:PRO:HD2	1.45	0.95
2:G:99:HIS:CD2	2:G:116:TYR:HD2	1.83	0.94
3:L:7:SER:CB	3:L:8:PRO:CD	2.42	0.94
3:F:8:PRO:HB2	3:F:11:LEU:HG	1.49	0.94
1:A:811:LYS:HB2	1:A:812:PRO:HD2	1.50	0.94
2:G:111:TRP:CZ2	3:F:100:THR:O	2.21	0.93
2:H:111:TRP:CZ2	3:L:100:THR:O	2.21	0.93
1:C:577:ARG:HH11	1:C:582:LEU:HD13	1.32	0.92
2:G:27:PHE:CE2	2:G:116:TYR:CE2	2.58	0.92
1:B:334:ASN:O	1:B:362:VAL:HB	1.70	0.92
2:H:27:PHE:CE2	2:H:116:TYR:CE2	2.58	0.91
1:C:422:ASN:HD21	1:C:455:LEU:H	1.08	0.91
1:B:334:ASN:HB3	1:B:362:VAL:HG23	1.52	0.91
3:F:96:GLN:NE2	3:F:99:SER:HB2	1.86	0.90
2:H:112:SER:HB2	3:L:95:GLN:HE22	1.36	0.90
3:L:96:GLN:NE2	3:L:99:SER:HB2	1.86	0.90
3:L:8:PRO:HB2	3:L:11:LEU:HG	1.49	0.90
3:L:7:SER:CB	3:L:8:PRO:HD3	2.02	0.90
2:G:109:SER:HB2	2:G:113:PRO:CD	2.02	0.89
2:G:112:SER:HB2	3:F:95:GLN:HE22	1.36	0.89
2:H:109:SER:HB2	2:H:113:PRO:CD	2.02	0.89
1:B:329:PHE:CG	1:B:528:LYS:HG3	2.08	0.89
1:C:199:GLY:HA3	1:B:521:PRO:HG3	0.89	0.88
3:F:7:SER:CB	3:F:8:PRO:HD3	2.02	0.88
2:G:115:ASP:OD1	2:G:116:TYR:N	2.07	0.87
3:L:96:GLN:HE22	3:L:99:SER:HB2	1.40	0.87
3:F:100:THR:CG2	3:F:101:PRO:HD3	2.04	0.87
3:L:100:THR:CG2	3:L:101:PRO:HD3	2.04	0.87
3:F:8:PRO:HB2	3:F:11:LEU:CG	2.04	0.87
2:H:115:ASP:OD1	2:H:116:TYR:N	2.08	0.86
2:G:112:SER:CB	3:F:95:GLN:HE22	1.88	0.86
1:B:336:CYS:SG	1:B:361:CYS:CB	2.63	0.86
3:L:8:PRO:HB2	3:L:11:LEU:CG	2.04	0.86
2:H:112:SER:CB	3:L:95:GLN:HE22	1.88	0.86
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.86
1:B:329:PHE:CE2	1:B:528:LYS:CD	2.58	0.86
1:B:329:PHE:CD2	1:B:528:LYS:HD2	2.11	0.85
3:L:100:THR:HG23	3:L:101:PRO:CD	2.06	0.85
2:G:54:TYR:HH	1:B:486:PHE:HE1	1.24	0.85
1:B:392:PHE:CD2	1:B:517:LEU:HD21	2.11	0.85
1:B:393:THR:O	1:B:523:THR:HG21	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:27:PHE:CD2	2:G:116:TYR:CZ	2.63	0.85
3:F:6:GLN:HE22	3:F:105:GLY:HA2	1.41	0.85
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.57	0.85
1:A:336:CYS:HG	1:A:361:CYS:HG	1.21	0.85
1:A:393:THR:O	1:A:523:THR:HG21	1.76	0.85
1:C:577:ARG:HD3	1:C:582:LEU:CD1	2.07	0.85
3:F:100:THR:HG23	3:F:101:PRO:CD	2.06	0.85
2:H:98:ALA:HB1	2:H:117:TRP:CD1	2.12	0.85
3:F:7:SER:HB2	3:F:22:ASN:CA	2.06	0.85
2:H:27:PHE:CD2	2:H:116:TYR:CZ	2.63	0.84
3:L:7:SER:HB2	3:L:22:ASN:CA	2.06	0.84
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.84
2:H:99:HIS:CD2	2:H:116:TYR:CD2	2.66	0.84
3:F:8:PRO:HD2	3:F:21:ILE:HA	1.60	0.84
2:G:98:ALA:HB1	2:G:117:TRP:CD1	2.12	0.84
1:A:336:CYS:SG	1:A:361:CYS:CB	2.65	0.84
3:L:6:GLN:HE22	3:L:105:GLY:HA2	1.41	0.84
1:A:127:VAL:HG21	5:A:1402:NAG:H5	1.59	0.84
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.06	0.84
2:H:109:SER:OG	2:H:113:PRO:HD2	1.78	0.83
1:B:329:PHE:CD2	1:B:528:LYS:CD	2.61	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
3:L:7:SER:OG	3:L:8:PRO:HD3	1.78	0.83
2:G:99:HIS:CD2	2:G:116:TYR:CD2	2.66	0.83
1:B:516:GLU:O	1:B:517:LEU:HD22	1.78	0.83
2:G:109:SER:OG	2:G:113:PRO:HD2	1.78	0.82
3:L:8:PRO:HD2	3:L:21:ILE:HA	1.59	0.82
3:F:7:SER:OG	3:F:8:PRO:HD3	1.79	0.82
2:H:111:TRP:HD1	3:L:102:HIS:ND1	1.76	0.82
2:G:111:TRP:HD1	3:F:102:HIS:ND1	1.76	0.82
2:H:99:HIS:CB	2:H:116:TYR:HB2	2.02	0.82
2:H:111:TRP:CD1	3:L:102:HIS:ND1	2.48	0.82
1:A:486:PHE:HE1	2:H:54:TYR:HH	1.18	0.82
2:H:109:SER:HB2	2:H:113:PRO:HG2	1.62	0.82
2:G:111:TRP:CD1	3:F:102:HIS:ND1	2.48	0.81
1:B:334:ASN:CB	1:B:362:VAL:HG23	2.09	0.81
1:C:577:ARG:HD3	1:C:582:LEU:HD13	1.61	0.81
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.26	0.81
2:G:109:SER:HB2	2:G:113:PRO:HG2	1.62	0.81
2:G:110:SER:C	2:G:111:TRP:CG	2.52	0.81
1:B:336:CYS:HG	1:B:361:CYS:CB	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:110:SER:C	2:H:111:TRP:CG	2.52	0.80
1:C:214:ARG:H	1:C:214:ARG:HH21	1.29	0.80
3:F:8:PRO:CG	3:F:20:THR:O	2.29	0.80
3:F:96:GLN:NE2	3:F:99:SER:CB	2.45	0.79
2:G:99:HIS:CB	2:G:116:TYR:HB2	2.02	0.79
1:C:452:LEU:HG	1:C:492:LEU:HD22	1.63	0.79
2:G:111:TRP:HE3	3:F:97:TYR:CZ	2.01	0.79
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.27	0.79
2:G:54:TYR:OH	1:B:486:PHE:HE1	1.65	0.79
3:L:8:PRO:CG	3:L:20:THR:O	2.29	0.79
2:G:3:THR:N	2:G:116:TYR:CE1	2.51	0.78
1:A:390:LEU:HD23	1:A:391:CYS:H	1.48	0.78
1:B:392:PHE:O	1:B:523:THR:HB	1.83	0.78
2:H:3:THR:N	2:H:116:TYR:CE1	2.51	0.78
1:A:676:THR:C	1:A:690:GLN:HE21	1.86	0.78
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.78
2:H:111:TRP:HE3	3:L:97:TYR:CZ	2.01	0.78
3:F:96:GLN:HE22	3:F:99:SER:HB2	1.40	0.77
3:L:96:GLN:NE2	3:L:99:SER:CB	2.45	0.77
1:B:390:LEU:HD23	1:B:391:CYS:H	1.48	0.77
1:A:486:PHE:HE1	2:H:54:TYR:OH	1.66	0.77
2:H:100:SER:OG	2:H:114:PHE:CZ	2.37	0.77
3:L:7:SER:HB2	3:L:22:ASN:CB	2.15	0.76
1:B:826:VAL:HG13	1:B:1057:PRO:HG2	1.68	0.76
2:G:113:PRO:C	2:G:117:TRP:HE1	1.89	0.76
3:F:7:SER:HB2	3:F:22:ASN:CB	2.15	0.76
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.76
1:A:529:LYS:O	1:A:530:SER:OG	2.04	0.76
2:H:113:PRO:C	2:H:117:TRP:HE1	1.89	0.76
1:B:422:ASN:HD21	1:B:454:ARG:H	1.32	0.75
1:B:1125:ASN:HD22	1:B:1125:ASN:H	1.33	0.75
2:G:100:SER:OG	2:G:114:PHE:CZ	2.37	0.75
3:L:6:GLN:NE2	3:L:105:GLY:CA	2.51	0.74
1:A:811:LYS:CB	1:A:812:PRO:CD	2.66	0.74
1:C:199:GLY:HA3	1:B:521:PRO:CB	2.17	0.74
2:H:111:TRP:CD1	3:L:102:HIS:NE2	2.55	0.73
1:B:329:PHE:CE2	1:B:528:LYS:CG	2.71	0.73
1:B:335:LEU:O	1:B:337:PRO:HD3	1.88	0.73
1:A:332:ILE:O	1:A:333:THR:HG23	1.88	0.73
2:G:111:TRP:CD1	3:F:102:HIS:NE2	2.55	0.73
1:B:329:PHE:HE2	1:B:528:LYS:HD2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:TRP:HZ2	3:F:100:THR:O	1.70	0.73
1:C:577:ARG:HH11	1:C:582:LEU:CD1	2.01	0.73
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.53	0.73
1:B:527:PRO:HA	1:B:528:LYS:HE2	1.71	0.73
1:A:486:PHE:CE2	2:H:60:ARG:NE	2.57	0.73
2:H:111:TRP:HZ2	3:L:100:THR:O	1.70	0.73
1:B:334:ASN:OD1	1:B:361:CYS:HA	1.89	0.73
1:C:1142:GLN:HG3	1:C:1143:PRO:HD3	1.71	0.72
2:G:60:ARG:NE	1:B:486:PHE:CE2	2.57	0.72
3:F:6:GLN:NE2	3:F:105:GLY:CA	2.51	0.72
2:H:27:PHE:HD2	2:H:116:TYR:HH	1.37	0.72
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.72
2:H:109:SER:CB	2:H:113:PRO:CD	2.67	0.72
3:L:8:PRO:CD	3:L:21:ILE:HA	2.19	0.72
1:C:164:ASN:ND2	5:C:1403:NAG:O6	2.22	0.72
1:B:392:PHE:HD2	1:B:517:LEU:HD21	1.53	0.72
1:C:124:THR:OG1	5:C:1402:NAG:N2	2.22	0.72
2:G:109:SER:CB	2:G:113:PRO:CD	2.67	0.72
1:A:336:CYS:HG	1:A:361:CYS:CB	2.02	0.71
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.53	0.71
3:F:8:PRO:CD	3:F:21:ILE:HA	2.20	0.71
2:G:54:TYR:OH	1:B:486:PHE:CE1	2.42	0.71
1:B:328:ARG:HH11	1:B:533:LEU:HD23	1.53	0.71
1:B:329:PHE:HD2	1:B:528:LYS:HG3	1.45	0.71
1:A:334:ASN:O	1:A:362:VAL:HB	1.92	0.70
2:G:3:THR:N	2:G:116:TYR:HE1	1.89	0.70
2:G:27:PHE:CE2	2:G:116:TYR:CE1	2.65	0.70
1:A:676:THR:C	1:A:690:GLN:NE2	2.45	0.70
1:B:124:THR:HG21	5:B:1402:NAG:HN2	1.56	0.70
1:A:359:SER:O	1:A:524:VAL:CG1	2.39	0.70
2:H:111:TRP:HE3	3:L:97:TYR:CE2	2.10	0.69
2:G:111:TRP:HE1	3:F:102:HIS:CD2	2.09	0.69
1:B:359:SER:O	1:B:524:VAL:CG1	2.39	0.69
1:A:675:GLN:HA	1:A:675:GLN:NE2	1.99	0.69
1:C:391:CYS:HA	1:C:525:CYS:HB2	1.73	0.69
2:G:100:SER:OG	2:G:114:PHE:CE2	2.45	0.69
1:A:233:ILE:HG12	1:A:234:ASN:H	1.58	0.69
1:A:569:ILE:HD12	1:A:569:ILE:H	1.56	0.69
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.74	0.69
1:C:577:ARG:NH1	1:C:582:LEU:HD13	2.07	0.69
2:H:111:TRP:HE1	3:L:102:HIS:CD2	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:N	1:B:212:LEU:O	2.25	0.69
2:H:3:THR:N	2:H:116:TYR:HE1	1.89	0.69
2:G:111:TRP:HE3	3:F:97:TYR:CE2	2.10	0.69
1:C:546:LEU:HD11	1:C:573:THR:HG21	1.74	0.69
1:A:486:PHE:CE1	2:H:54:TYR:OH	2.42	0.68
1:B:340:GLU:OE2	1:B:356:LYS:CE	2.35	0.68
2:H:110:SER:C	2:H:111:TRP:CD2	2.67	0.68
1:B:392:PHE:CG	1:B:517:LEU:HD21	2.29	0.68
1:B:323:THR:C	1:B:324:GLU:HG3	2.14	0.68
1:B:327:VAL:HG12	1:B:328:ARG:N	2.09	0.68
1:C:403:ARG:NH2	1:C:405:ASP:OD2	2.27	0.68
2:G:110:SER:C	2:G:111:TRP:CD2	2.67	0.68
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.27	0.68
1:A:786:LYS:HE3	1:C:1045:LYS:NZ	2.09	0.68
2:G:113:PRO:O	2:G:114:PHE:HB2	1.92	0.68
2:G:113:PRO:HA	2:G:117:TRP:CE2	2.22	0.67
1:B:336:CYS:SG	1:B:361:CYS:HB2	2.34	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:C:97:LYS:H	1:C:97:LYS:HD3	1.60	0.67
1:C:406:GLU:HG3	1:C:418:ILE:HG13	1.75	0.67
2:H:113:PRO:O	2:H:114:PHE:HB2	1.92	0.67
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.59	0.67
2:G:27:PHE:CD2	2:G:116:TYR:OH	2.48	0.66
1:A:702:GLU:OE2	1:B:790:LYS:NZ	2.21	0.66
3:F:8:PRO:HB2	3:F:11:LEU:CD2	2.25	0.66
1:B:336:CYS:HB2	1:B:361:CYS:HB2	1.78	0.66
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.78	0.66
2:H:100:SER:OG	2:H:114:PHE:CE2	2.46	0.66
2:G:27:PHE:HD2	2:G:116:TYR:OH	1.79	0.66
1:B:569:ILE:HD12	1:B:569:ILE:H	1.60	0.66
1:A:85:PRO:HA	1:A:237:ARG:HA	1.78	0.66
1:C:455:LEU:HD21	1:C:457:ARG:HG3	1.78	0.66
2:H:115:ASP:CG	2:H:116:TYR:H	1.99	0.66
1:B:522:ALA:O	1:B:523:THR:OG1	2.14	0.66
1:B:392:PHE:HD2	1:B:517:LEU:CD2	2.09	0.66
1:B:187:LYS:HG2	1:B:213:VAL:HA	1.77	0.65
1:C:691:SER:O	1:C:692:ILE:HG13	1.96	0.65
2:G:98:ALA:CB	2:G:117:TRP:CD1	2.80	0.65
1:B:96:GLU:OE1	1:B:98:SER:N	2.28	0.65
1:C:577:ARG:NH1	1:C:582:LEU:CD1	2.58	0.65
2:H:27:PHE:CE2	2:H:116:TYR:CE1	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HB	1:C:395:VAL:HB	1.79	0.65
3:L:8:PRO:HB2	3:L:11:LEU:CD2	2.25	0.65
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.28	0.65
1:C:719:THR:HA	1:C:926:GLN:HE22	1.60	0.65
2:H:110:SER:O	2:H:111:TRP:CD2	2.49	0.65
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.65
2:H:27:PHE:CD2	2:H:116:TYR:OH	2.48	0.65
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.78	0.65
1:C:883:THR:HG21	1:B:705:VAL:HB	1.78	0.65
2:H:116:TYR:O	2:H:117:TRP:HB2	1.97	0.65
2:G:115:ASP:CG	2:G:116:TYR:H	1.99	0.65
2:G:116:TYR:O	2:G:117:TRP:HB2	1.97	0.65
1:B:334:ASN:HB3	1:B:362:VAL:CG2	2.24	0.65
1:C:472:ILE:HD13	1:C:474:GLN:HB3	1.79	0.64
3:F:8:PRO:HG2	3:F:11:LEU:CD1	2.11	0.64
1:A:521:PRO:HB3	1:B:198:ASP:O	1.97	0.64
1:A:676:THR:HA	1:A:690:GLN:CB	2.25	0.64
1:B:523:THR:HG22	1:B:524:VAL:HG22	1.79	0.64
2:H:98:ALA:CB	2:H:117:TRP:CD1	2.80	0.64
2:G:39:ILE:HB	2:G:96:TYR:HB2	1.79	0.64
1:C:350:VAL:HG22	1:C:453:TYR:HB2	1.79	0.64
1:C:607:GLN:O	1:C:608:VAL:HG23	1.98	0.64
2:H:115:ASP:CG	2:H:116:TYR:N	2.51	0.64
2:G:98:ALA:HB1	2:G:117:TRP:NE1	2.13	0.64
1:C:111:ASP:OD1	1:C:112:SER:N	2.31	0.64
1:C:454:ARG:HH21	1:C:493:GLN:HG3	1.63	0.64
2:H:39:ILE:HA	2:H:49:TRP:HA	1.80	0.64
1:A:523:THR:HG22	1:A:524:VAL:HG22	1.79	0.63
2:H:39:ILE:HB	2:H:96:TYR:HB2	1.79	0.63
2:H:112:SER:CB	3:L:95:GLN:NE2	2.61	0.63
2:G:115:ASP:CG	2:G:116:TYR:N	2.51	0.63
2:G:110:SER:O	2:G:111:TRP:CD2	2.49	0.63
1:B:391:CYS:SG	1:B:523:THR:O	2.56	0.63
3:F:8:PRO:CB	3:F:11:LEU:HD21	2.29	0.63
1:C:108:THR:HA	1:C:236:THR:HG22	1.79	0.63
2:H:98:ALA:HB1	2:H:117:TRP:NE1	2.13	0.63
2:H:29:LEU:HB3	2:H:75:THR:HG22	1.79	0.63
2:H:111:TRP:CZ2	3:L:100:THR:C	2.72	0.63
2:G:39:ILE:HA	2:G:49:TRP:HA	1.80	0.63
1:A:533:LEU:HG	1:A:533:LEU:O	1.98	0.63
2:G:29:LEU:HB3	2:G:75:THR:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:71:ILE:HG13	2:G:82:LEU:HB2	1.81	0.63
2:H:3:THR:N	2:H:116:TYR:CD1	2.66	0.62
2:H:27:PHE:HD2	2:H:116:TYR:OH	1.79	0.62
2:H:71:ILE:HG13	2:H:82:LEU:HB2	1.81	0.62
1:A:391:CYS:SG	1:A:523:THR:O	2.56	0.62
3:L:8:PRO:CB	3:L:11:LEU:HD21	2.29	0.62
2:G:111:TRP:CZ2	3:F:100:THR:C	2.72	0.62
2:G:3:THR:N	2:G:116:TYR:CD1	2.67	0.62
1:B:124:THR:OG1	1:B:125:ASN:N	2.32	0.62
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.79	0.62
1:A:813:SER:O	1:A:814:LYS:HE2	2.00	0.62
1:B:96:GLU:OE1	1:B:97:LYS:N	2.32	0.62
1:B:117:LEU:HD12	1:B:118:LEU:H	1.63	0.62
1:A:786:LYS:HE3	1:C:1045:LYS:HZ2	1.64	0.62
1:C:560:LEU:H	1:C:563:GLN:HE21	1.45	0.62
3:L:44:GLN:HB2	3:L:50:PRO:HG3	1.82	0.62
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.61
3:F:44:GLN:HB2	3:F:50:PRO:HG3	1.82	0.61
1:A:196:ASN:ND2	1:A:200:TYR:O	2.32	0.61
1:A:811:LYS:HB2	1:A:812:PRO:HD3	1.80	0.61
3:F:7:SER:HB3	3:F:22:ASN:N	2.00	0.61
1:B:516:GLU:O	1:B:517:LEU:CD2	2.48	0.61
1:B:808:ASP:HB3	1:B:811:LYS:HD2	1.82	0.61
1:B:457:ARG:NH1	1:B:459:SER:O	2.33	0.61
2:G:112:SER:CB	3:F:95:GLN:NE2	2.61	0.61
3:L:7:SER:HB3	3:L:22:ASN:N	2.00	0.61
1:A:95:THR:HG22	1:A:96:GLU:H	1.66	0.61
1:A:112:SER:HB2	1:A:113:LYS:HD3	1.83	0.61
2:G:27:PHE:CD2	2:G:116:TYR:CE2	2.87	0.61
2:G:111:TRP:HZ2	3:F:100:THR:C	2.04	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.60
2:H:111:TRP:NE1	3:L:102:HIS:CD2	2.69	0.60
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.60
1:B:556:ASN:H	1:B:556:ASN:HD22	1.49	0.60
3:L:8:PRO:HG2	3:L:11:LEU:CD1	2.11	0.60
2:H:111:TRP:HZ2	3:L:100:THR:C	2.04	0.60
1:B:617:CYS:H	1:B:644:GLN:HE22	1.49	0.60
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.60
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.60
1:A:599:THR:HG22	1:A:601:GLY:H	1.67	0.60
2:G:111:TRP:NE1	3:F:102:HIS:CD2	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:113:PRO:O	2:G:114:PHE:CB	2.50	0.60
1:A:336:CYS:SG	1:A:361:CYS:HB2	2.40	0.59
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.84	0.59
1:C:409:GLN:NE2	1:C:416:GLY:HA3	2.17	0.59
2:H:109:SER:CB	2:H:113:PRO:HD2	2.30	0.59
1:B:357:ARG:HH12	1:B:394:ASN:HD21	1.49	0.59
1:B:1077:THR:HG22	1:B:1095:PHE:O	2.01	0.59
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.50	0.59
3:L:7:SER:HB2	3:L:22:ASN:HB3	1.83	0.59
2:G:109:SER:CB	2:G:113:PRO:HD2	2.30	0.59
3:F:7:SER:HB2	3:F:22:ASN:HB3	1.83	0.59
1:B:645:THR:HG22	1:B:647:ALA:H	1.67	0.59
2:H:110:SER:OG	3:L:95:GLN:NE2	2.36	0.59
1:B:164:ASN:OD1	1:B:164:ASN:N	2.35	0.59
1:C:901:GLN:NE2	1:C:905:ARG:HE	1.99	0.59
2:H:27:PHE:CD2	2:H:116:TYR:CE2	2.87	0.59
2:H:113:PRO:O	2:H:114:PHE:CB	2.50	0.59
2:G:110:SER:OG	3:F:95:GLN:NE2	2.36	0.59
1:B:326:ILE:HD12	1:B:326:ILE:O	2.02	0.59
1:B:521:PRO:O	1:B:522:ALA:HB2	2.01	0.59
3:L:9:ASP:O	3:L:11:LEU:N	2.36	0.58
2:G:52:LEU:HB3	2:G:60:ARG:HB2	1.85	0.58
5:B:1405:NAG:H83	5:B:1405:NAG:H3	1.86	0.58
2:H:113:PRO:HB2	3:L:42:TYR:OH	2.04	0.58
1:B:206:LYS:NZ	1:B:221:SER:OG	2.35	0.58
1:A:361:CYS:N	1:A:524:VAL:HG12	2.18	0.58
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.58
1:C:214:ARG:N	1:C:214:ARG:HD3	2.18	0.58
2:G:113:PRO:HB2	3:F:42:TYR:OH	2.04	0.58
3:F:9:ASP:CG	3:F:10:SER:N	2.56	0.58
2:G:41:GLN:NE2	2:G:45:LYS:O	2.36	0.58
1:C:206:LYS:HD2	1:C:207:HIS:H	1.68	0.58
1:C:391:CYS:CA	1:C:525:CYS:HB2	2.30	0.58
1:C:452:LEU:HD21	1:C:492:LEU:HD13	1.85	0.58
2:G:45:LYS:NZ	2:G:46:ALA:O	2.36	0.58
1:B:328:ARG:NH2	1:B:531:THR:O	2.34	0.58
2:H:41:GLN:NE2	2:H:45:LYS:O	2.36	0.58
3:L:9:ASP:CG	3:L:10:SER:N	2.56	0.58
3:F:9:ASP:O	3:F:11:LEU:N	2.36	0.58
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.85	0.58
4:M:2:NAG:H3	4:M:2:NAG:H83	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.85	0.57
1:B:390:LEU:HD23	1:B:391:CYS:N	2.19	0.57
1:B:361:CYS:N	1:B:524:VAL:HG12	2.18	0.57
2:H:52:LEU:HB3	2:H:60:ARG:HB2	1.85	0.57
1:B:336:CYS:CB	1:B:361:CYS:HB2	2.34	0.57
1:A:129:LYS:HZ3	1:A:169:GLU:HG2	1.70	0.57
1:B:722:VAL:HA	1:B:1064:HIS:O	2.03	0.57
1:A:328:ARG:NH1	1:A:531:THR:O	2.30	0.57
1:A:804:GLN:HE21	1:A:935:GLN:HE22	1.52	0.57
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.57
3:F:60:ARG:NH1	3:F:61:GLU:O	2.37	0.57
3:L:60:ARG:NH1	3:L:61:GLU:O	2.37	0.57
1:B:227:VAL:HG12	1:B:228:ASP:N	2.20	0.57
1:C:199:GLY:CA	1:B:521:PRO:CG	2.47	0.57
3:F:9:ASP:CG	3:F:10:SER:H	2.08	0.57
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.56
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.56
1:B:519:HIS:ND1	1:B:519:HIS:O	2.38	0.56
5:C:1405:NAG:H3	5:C:1405:NAG:H83	1.88	0.56
3:L:9:ASP:CG	3:L:10:SER:H	2.08	0.56
1:B:328:ARG:NH1	1:B:533:LEU:HD23	2.19	0.56
3:L:2:ILE:HG23	3:L:27:GLN:H	1.70	0.56
2:G:14:PRO:HA	2:G:87:MET:HB2	1.87	0.56
1:B:663:ASP:OD2	1:B:673:SER:OG	2.22	0.56
3:F:2:ILE:HG23	3:F:27:GLN:H	1.70	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.87	0.56
1:B:563:GLN:O	1:B:577:ARG:NH1	2.38	0.56
1:A:335:LEU:HA	1:A:362:VAL:HB	1.87	0.56
1:B:342:PHE:HB3	4:W:1:NAG:H82	1.88	0.56
1:B:813:SER:O	1:B:813:SER:OG	2.18	0.56
1:C:187:LYS:NZ	1:C:213:VAL:HG13	2.21	0.56
1:C:213:VAL:HB	1:C:214:ARG:HD3	1.87	0.56
2:H:45:LYS:NZ	2:H:46:ALA:O	2.36	0.56
1:B:551:VAL:HB	1:B:588:THR:HG23	1.88	0.55
1:A:332:ILE:HD12	1:A:332:ILE:N	2.20	0.55
5:A:1405:NAG:H3	5:A:1405:NAG:H83	1.88	0.55
2:H:111:TRP:CD1	3:L:102:HIS:CG	2.95	0.55
1:A:391:CYS:SG	1:A:524:VAL:O	2.64	0.55
4:N:2:NAG:H83	4:N:2:NAG:H3	1.87	0.55
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:SER:HB3	3:L:38:TYR:HB3	1.89	0.55
2:G:108:SER:HB3	3:F:38:TYR:HB3	1.88	0.55
1:B:359:SER:O	1:B:524:VAL:HG11	2.06	0.55
1:B:391:CYS:SG	1:B:524:VAL:O	2.64	0.55
1:A:129:LYS:HD3	1:A:131:CYS:SG	2.46	0.55
1:C:105:ILE:HG13	1:C:110:LEU:HD11	1.87	0.55
1:C:165:ASN:OD1	5:C:1403:NAG:N2	2.40	0.55
1:B:556:ASN:HD22	1:B:556:ASN:N	2.05	0.55
1:C:352:ALA:HB2	1:C:468:ILE:HD12	1.88	0.55
2:H:14:PRO:HA	2:H:87:MET:HB2	1.87	0.55
2:G:111:TRP:CD1	3:F:102:HIS:CG	2.95	0.55
1:C:661:GLU:OE2	1:C:698:SER:OG	2.25	0.55
1:A:359:SER:O	1:A:524:VAL:HG11	2.06	0.54
1:C:792:PRO:HG3	1:B:707:TYR:HB3	1.90	0.54
3:L:95:GLN:NE2	3:L:103:THR:O	2.39	0.54
2:H:98:ALA:CB	2:H:117:TRP:NE1	2.70	0.54
2:H:113:PRO:HA	2:H:117:TRP:CE2	2.22	0.54
2:G:40:ARG:HB3	2:G:50:LEU:HD11	1.90	0.54
4:W:1:NAG:H61	4:W:2:NAG:HN2	1.72	0.54
1:A:336:CYS:HB2	1:A:361:CYS:HB2	1.89	0.54
1:A:342:PHE:HB3	4:E:1:NAG:H82	1.88	0.54
1:A:811:LYS:CB	1:A:812:PRO:HD2	2.28	0.54
2:H:99:HIS:CG	2:H:116:TYR:CD2	2.96	0.54
3:F:95:GLN:NE2	3:F:103:THR:O	2.39	0.54
4:Z:2:NAG:H3	4:Z:2:NAG:H83	1.87	0.54
1:A:113:LYS:HD2	1:A:164:ASN:HD21	1.71	0.54
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.54
1:A:1141:LEU:HD11	1:B:1141:LEU:HD12	1.90	0.54
1:C:166:CYS:SG	1:C:167:THR:N	2.81	0.54
2:H:40:ARG:HB3	2:H:50:LEU:HD11	1.90	0.54
3:F:8:PRO:HB2	3:F:11:LEU:HD21	1.90	0.54
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.72	0.54
2:G:98:ALA:CB	2:G:117:TRP:NE1	2.70	0.54
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.42	0.54
1:B:392:PHE:HA	1:B:517:LEU:HD11	1.89	0.54
1:B:886:TRP:HH2	1:B:904:TYR:HD2	1.56	0.54
3:L:96:GLN:HG3	3:L:103:THR:HG21	1.90	0.54
1:B:100:ILE:O	1:B:242:LEU:HA	2.08	0.54
1:B:421:TYR:HA	1:B:461:LEU:HG	1.90	0.54
1:C:333:THR:OG1	1:C:334:ASN:N	2.41	0.54
1:C:408:ARG:O	1:C:414:GLN:NE2	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:CG2	1:B:524:VAL:N	2.45	0.53
1:A:97:LYS:HB3	1:A:187:LYS:HA	1.89	0.53
1:C:1142:GLN:HG3	1:C:1143:PRO:CD	2.37	0.53
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.41	0.53
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.90	0.53
2:G:99:HIS:CG	2:G:116:TYR:CD2	2.96	0.53
1:B:334:ASN:HB2	1:B:362:VAL:HG23	1.89	0.53
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.53
3:L:8:PRO:HB2	3:L:11:LEU:HD21	1.90	0.53
2:G:23:THR:HA	2:G:79:GLN:HG2	1.91	0.53
1:B:544:ASN:O	1:B:544:ASN:ND2	2.41	0.53
1:A:193:VAL:HG23	1:A:223:LEU:HD23	1.91	0.53
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.53
2:G:54:TYR:HD2	2:G:58:ASP:HB2	1.73	0.53
2:G:109:SER:CB	2:G:113:PRO:HG2	2.37	0.53
1:B:334:ASN:CG	1:B:361:CYS:HA	2.27	0.53
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.91	0.53
2:H:23:THR:HA	2:H:79:GLN:HG2	1.91	0.53
2:H:109:SER:CB	2:H:113:PRO:HG2	2.37	0.53
3:F:44:GLN:N	3:F:91:VAL:O	2.42	0.53
1:B:532:ASN:OD1	1:B:532:ASN:N	2.40	0.53
2:H:28:SER:OG	2:H:29:LEU:N	2.42	0.53
1:A:532:ASN:N	1:A:532:ASN:OD1	2.37	0.52
2:H:54:TYR:HD2	2:H:58:ASP:HB2	1.73	0.52
2:G:111:TRP:CE3	3:F:97:TYR:CZ	2.91	0.52
3:F:96:GLN:NE2	3:F:99:SER:OG	2.31	0.52
1:B:901:GLN:NE2	1:B:905:ARG:HH21	2.07	0.52
3:F:96:GLN:HG3	3:F:103:THR:HG21	1.90	0.52
2:G:27:PHE:HD2	2:G:116:TYR:HH	1.52	0.52
2:G:28:SER:OG	2:G:29:LEU:N	2.42	0.52
1:A:113:LYS:HD3	1:A:113:LYS:N	2.25	0.52
2:H:112:SER:HB3	3:L:95:GLN:NE2	2.24	0.52
1:B:329:PHE:HD2	1:B:528:LYS:CG	2.09	0.52
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.52
1:C:402:ILE:O	1:C:507:PRO:HA	2.09	0.52
1:C:457:ARG:NH2	1:C:469:SER:O	2.43	0.52
1:C:555:SER:OG	1:C:584:ILE:O	2.28	0.52
1:B:327:VAL:HG13	1:B:542:ASN:HB3	1.91	0.52
4:Y:2:NAG:H3	4:Y:2:NAG:H83	1.90	0.52
1:A:105:ILE:HG23	1:A:241:LEU:HD11	1.91	0.52
1:A:1101:HIS:CD2	4:N:1:NAG:H5	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:O	1:C:59:PHE:HA	2.10	0.52
2:G:112:SER:HB3	3:F:95:GLN:NE2	2.24	0.52
1:B:476:GLY:H	1:B:487:ASN:HB3	1.74	0.52
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.52
3:F:44:GLN:HB3	3:F:91:VAL:HB	1.91	0.52
1:B:64:TRP:HD1	1:B:65:PHE:N	2.07	0.52
1:A:83:VAL:HG22	1:A:237:ARG:HD2	1.92	0.52
1:C:403:ARG:HA	1:C:495:TYR:OH	2.10	0.52
1:C:424:LYS:HB3	1:C:463:PRO:HA	1.92	0.52
3:L:44:GLN:N	3:L:91:VAL:O	2.42	0.52
2:G:111:TRP:CD1	3:F:102:HIS:CD2	2.98	0.52
1:B:327:VAL:CG1	1:B:328:ARG:N	2.73	0.52
2:H:112:SER:OG	3:L:104:PHE:CZ	2.55	0.51
1:A:804:GLN:HE21	1:A:935:GLN:NE2	2.08	0.51
1:C:112:SER:O	1:C:113:LYS:HB2	2.10	0.51
1:B:57:PRO:O	1:B:60:SER:OG	2.25	0.51
1:B:348:ALA:HB2	1:B:354:ASN:ND2	2.26	0.51
2:H:92:THR:HG23	2:H:124:THR:HA	1.92	0.51
2:H:111:TRP:CE3	3:L:97:TYR:CZ	2.91	0.51
2:H:113:PRO:HB2	3:L:42:TYR:CZ	2.46	0.51
2:G:113:PRO:HB2	3:F:42:TYR:CZ	2.46	0.51
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.51
1:C:198:ASP:O	1:B:521:PRO:CB	2.40	0.51
1:B:392:PHE:HB3	1:B:517:LEU:HD22	1.82	0.51
1:A:97:LYS:HD3	1:A:187:LYS:HA	1.93	0.51
1:C:577:ARG:CD	1:C:582:LEU:HD13	2.35	0.51
2:H:3:THR:HG23	2:H:116:TYR:HE1	1.74	0.51
1:B:379:CYS:HB3	1:B:382:VAL:O	2.10	0.51
1:A:336:CYS:CB	1:A:361:CYS:HB2	2.41	0.51
1:A:486:PHE:CE1	2:H:103:LEU:HD21	2.43	0.51
4:T:1:NAG:H62	4:T:2:NAG:H2	1.93	0.51
1:C:577:ARG:HD3	1:C:582:LEU:HD11	1.92	0.51
2:H:111:TRP:CD1	3:L:102:HIS:CD2	2.98	0.51
2:H:113:PRO:C	2:H:117:TRP:NE1	2.62	0.51
1:B:438:SER:O	1:B:438:SER:OG	2.21	0.51
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.92	0.51
2:G:3:THR:HG23	2:G:116:TYR:HE1	1.74	0.51
3:L:23:CYS:N	3:L:77:PHE:O	2.43	0.51
3:L:24:LYS:HZ3	3:L:76:ASP:HB2	1.76	0.51
3:L:96:GLN:NE2	3:L:99:SER:OG	2.31	0.51
2:G:103:LEU:HD21	1:B:486:PHE:CE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ALA:CB	1:B:521:PRO:CD	2.79	0.51
1:A:113:LYS:H	1:A:132:GLU:HB3	1.76	0.51
1:C:380:TYR:O	1:C:430:THR:HA	2.11	0.50
1:C:675:GLN:HA	1:C:690:GLN:HG3	1.93	0.50
3:L:44:GLN:HB3	3:L:91:VAL:HB	1.92	0.50
2:G:92:THR:HG23	2:G:124:THR:HA	1.92	0.50
1:B:323:THR:O	1:B:324:GLU:HG3	2.11	0.50
1:B:131:CYS:H	1:B:133:PHE:HE1	1.59	0.50
1:B:327:VAL:HG12	1:B:328:ARG:H	1.75	0.50
2:H:6:GLU:OE1	2:H:120:GLY:N	2.45	0.50
2:G:113:PRO:C	2:G:117:TRP:NE1	2.62	0.50
3:L:45:LYS:NZ	3:L:87:GLU:O	2.43	0.50
2:G:6:GLU:OE1	2:G:120:GLY:N	2.45	0.50
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.93	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.93	0.50
1:A:329:PHE:HB2	1:A:530:SER:OG	2.12	0.50
3:L:67:ARG:NH2	3:L:87:GLU:OE2	2.44	0.50
1:B:735:SER:HB3	1:B:859:THR:HG22	1.94	0.50
1:C:560:LEU:H	1:C:563:GLN:NE2	2.08	0.50
1:A:117:LEU:HB2	1:A:130:VAL:HG22	1.94	0.50
1:A:570:ALA:HA	1:B:964:LYS:HE3	1.93	0.50
1:C:350:VAL:HG23	1:C:422:ASN:HD22	1.77	0.50
1:C:353:TRP:CZ2	1:C:466:ARG:HB3	2.45	0.50
3:F:67:ARG:NH2	3:F:87:GLU:OE2	2.44	0.50
3:F:23:CYS:N	3:F:77:PHE:O	2.43	0.49
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.49
1:A:807:PRO:O	1:A:809:PRO:HD3	2.12	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.93	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.12	0.49
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.47	0.49
3:L:97:TYR:C	3:L:99:SER:H	2.16	0.49
3:F:6:GLN:NE2	3:F:6:GLN:N	2.60	0.49
3:F:97:TYR:C	3:F:99:SER:H	2.16	0.49
1:C:883:THR:HG23	1:B:707:TYR:HB2	1.94	0.49
2:G:4:LEU:HD23	2:G:24:PHE:HB3	1.95	0.49
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.49
1:C:396:TYR:HB2	1:C:514:SER:HB2	1.95	0.49
1:C:576:VAL:O	1:C:584:ILE:HA	2.13	0.49
1:C:616:ASN:HB3	1:C:618:THR:HG22	1.94	0.49
1:C:331:ASN:HD22	4:P:1:NAG:H83	1.78	0.49
1:B:437:ASN:OD1	1:B:438:SER:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:O	1:A:362:VAL:CB	2.60	0.49
1:C:112:SER:N	1:C:133:PHE:O	2.45	0.49
2:H:4:LEU:HD23	2:H:24:PHE:HB3	1.95	0.49
1:B:122:ASN:OD1	1:B:122:ASN:N	2.46	0.49
1:A:334:ASN:ND2	1:A:361:CYS:HA	2.27	0.49
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.49
1:A:675:GLN:NE2	1:A:675:GLN:CA	2.73	0.49
1:B:212:LEU:HD23	1:B:215:ASP:HB2	1.95	0.49
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.12	0.49
1:B:171:VAL:HG12	1:B:172:SER:H	1.78	0.49
1:C:710:ASN:N	1:C:710:ASN:HD22	2.11	0.48
3:F:45:LYS:NZ	3:F:87:GLU:O	2.43	0.48
2:H:109:SER:O	2:H:113:PRO:HD3	2.13	0.48
3:L:6:GLN:NE2	3:L:6:GLN:N	2.60	0.48
1:C:281:GLU:OE2	5:C:1405:NAG:H81	2.14	0.48
2:G:72:THR:N	2:G:81:VAL:O	2.43	0.48
3:F:85:GLN:N	3:F:88:ASP:OD2	2.44	0.48
1:B:129:LYS:HG2	1:B:133:PHE:HZ	1.76	0.48
1:B:886:TRP:CH2	1:B:904:TYR:HD2	2.32	0.48
2:G:4:LEU:O	2:G:118:GLY:HA2	2.14	0.48
1:B:392:PHE:CD2	1:B:517:LEU:CD2	2.85	0.48
1:B:516:GLU:C	1:B:517:LEU:CD2	2.82	0.48
1:B:935:GLN:O	1:B:939:SER:HB3	2.14	0.48
1:A:118:LEU:O	1:A:128:ILE:HA	2.14	0.48
2:G:109:SER:O	2:G:113:PRO:HD3	2.13	0.48
3:F:72:GLY:HA3	3:F:77:PHE:HA	1.96	0.48
1:B:231:ILE:HB	1:B:233:ILE:HG22	1.95	0.48
1:A:200:TYR:HB3	1:A:228:ASP:OD1	2.13	0.48
1:A:530:SER:O	1:A:531:THR:HG22	2.14	0.48
1:C:457:ARG:NH1	1:C:467:ASP:HB3	2.28	0.48
1:C:557:LYS:NZ	1:C:575:ALA:HB2	2.29	0.48
1:B:335:LEU:O	1:B:337:PRO:CD	2.59	0.48
1:B:896:ILE:HG13	1:B:897:PRO:HD2	1.96	0.48
2:G:35:GLY:O	2:G:100:SER:N	2.47	0.48
1:B:45:SER:O	1:B:47:VAL:HG22	2.14	0.48
1:B:336:CYS:SG	1:B:361:CYS:HB3	2.52	0.48
2:H:19:THR:HA	2:H:83:THR:HA	1.95	0.48
1:A:140:PHE:CE2	1:A:244:LEU:HB2	2.49	0.47
1:A:197:ILE:HG22	1:A:198:ASP:H	1.78	0.47
1:B:227:VAL:HG12	1:B:228:ASP:H	1.79	0.47
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:LEU:O	2:H:118:GLY:HA2	2.14	0.47
2:H:71:ILE:HA	2:H:82:LEU:HA	1.96	0.47
2:G:71:ILE:HA	2:G:82:LEU:HA	1.96	0.47
2:G:19:THR:HA	2:G:83:THR:HA	1.95	0.47
1:A:605:SER:OG	1:A:606:ASN:N	2.47	0.47
2:G:111:TRP:CE3	3:F:97:TYR:CE2	2.98	0.47
1:B:326:ILE:HD12	1:B:326:ILE:C	2.34	0.47
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	1.95	0.47
1:C:710:ASN:HD22	1:C:710:ASN:H	1.62	0.47
2:G:29:LEU:HD23	2:G:73:LYS:HB2	1.96	0.47
2:G:112:SER:OG	3:F:104:PHE:CZ	2.55	0.47
3:F:6:GLN:CG	3:F:106:GLN:H	2.28	0.47
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.47
1:A:973:ILE:HG12	1:A:992:GLN:HE21	1.79	0.47
1:C:403:ARG:NH2	1:C:504:GLY:O	2.47	0.47
3:L:6:GLN:CG	3:L:106:GLN:H	2.28	0.47
3:L:72:GLY:HA3	3:L:77:PHE:HA	1.96	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.48	0.47
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.97	0.47
2:G:17:THR:HA	2:G:85:THR:HA	1.97	0.47
1:A:278:LYS:HB2	1:A:306:PHE:CZ	2.50	0.47
2:H:6:GLU:HA	2:H:22:CYS:HA	1.97	0.47
3:L:22:ASN:ND2	3:L:76:ASP:OD1	2.45	0.47
3:L:31:TYR:HD1	3:L:98:TYR:HE1	1.63	0.47
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.50	0.47
1:A:361:CYS:H	1:A:524:VAL:HG12	1.79	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:A:529:LYS:CE	1:A:529:LYS:HA	2.45	0.46
2:H:29:LEU:HD23	2:H:73:LYS:HB2	1.96	0.46
1:A:66:HIS:CE1	1:A:214:ARG:HH22	2.32	0.46
1:C:327:VAL:HG22	1:C:542:ASN:HB3	1.96	0.46
3:F:1:ASP:OD1	3:F:1:ASP:N	2.44	0.46
1:B:364:ASP:O	1:B:367:VAL:HG12	2.15	0.46
1:A:66:HIS:HE1	1:A:214:ARG:HH22	1.62	0.46
1:B:329:PHE:HD2	1:B:528:LYS:CD	2.23	0.46
1:B:1125:ASN:HD22	1:B:1125:ASN:N	2.08	0.46
1:C:122:ASN:OD1	1:C:122:ASN:N	2.48	0.46
1:C:273:ARG:HA	1:C:273:ARG:HD3	1.70	0.46
2:G:112:SER:HB3	3:F:95:GLN:OE1	2.15	0.46
1:B:912:THR:OG1	1:B:914:ASN:ND2	2.48	0.46
1:B:1105:THR:HG22	1:B:1111:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:ASN:ND2	1:C:533:LEU:H	2.14	0.46
1:C:722:VAL:HA	1:C:1064:HIS:O	2.16	0.46
2:H:111:TRP:NE1	3:L:102:HIS:CG	2.83	0.46
2:G:111:TRP:NE1	3:F:102:HIS:CG	2.83	0.46
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.46
1:A:977:LEU:HD12	1:A:996:LEU:HD12	1.98	0.46
2:H:112:SER:HB3	3:L:95:GLN:OE1	2.15	0.46
3:F:18:ARG:NH1	3:F:19:ALA:O	2.49	0.46
3:F:31:TYR:HD1	3:F:98:TYR:HE1	1.63	0.46
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.46
1:C:521:PRO:HG3	1:C:564:GLN:HE21	1.81	0.46
2:H:17:THR:HA	2:H:85:THR:HA	1.97	0.46
2:H:111:TRP:HE1	3:L:102:HIS:CG	2.34	0.46
3:L:18:ARG:NH1	3:L:19:ALA:O	2.49	0.46
3:L:60:ARG:NH1	3:L:64:VAL:O	2.49	0.46
1:A:486:PHE:CD1	2:H:103:LEU:CD2	2.85	0.46
1:C:603:ASN:OD1	5:C:1407:NAG:N2	2.49	0.46
2:H:99:HIS:O	2:H:115:ASP:OD2	2.34	0.46
1:A:1141:LEU:O	1:A:1145:LEU:HD12	2.16	0.46
1:C:729:VAL:HG13	1:C:1059:GLY:HA2	1.97	0.46
1:B:393:THR:HA	1:B:523:THR:HB	1.97	0.46
1:B:447:GLY:HA2	1:B:497:PHE:O	2.16	0.46
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.51	0.46
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.51	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46
1:C:199:GLY:HA3	1:B:521:PRO:HB3	1.97	0.46
1:C:472:ILE:H	1:C:472:ILE:HG13	1.56	0.46
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.16	0.46
2:G:41:GLN:HB2	2:G:47:LEU:HG	1.98	0.46
1:B:560:LEU:O	1:B:562:PHE:N	2.47	0.46
1:B:903:ALA:HB1	1:B:913:GLN:HG2	1.98	0.46
1:C:437:ASN:HD21	1:C:506:GLN:HE21	1.64	0.45
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.51	0.45
1:B:676:THR:HB	1:B:693:ILE:HG21	1.98	0.45
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.78	0.45
1:A:233:ILE:HG12	1:A:234:ASN:N	2.28	0.45
1:A:393:THR:HA	1:A:523:THR:HB	1.97	0.45
1:C:424:LYS:HG3	1:C:461:LEU:O	2.17	0.45
2:H:41:GLN:HB2	2:H:47:LEU:HG	1.98	0.45
1:A:856:ASN:O	1:A:856:ASN:ND2	2.48	0.45
2:H:20:LEU:HD23	2:H:20:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:GLU:HA	2:G:22:CYS:HA	1.97	0.45
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.16	0.45
1:A:804:GLN:HG3	1:A:935:GLN:HE22	1.80	0.45
1:C:439:ASN:HB3	1:C:506:GLN:HB2	1.99	0.45
3:L:60:ARG:HH11	3:L:64:VAL:HB	1.81	0.45
1:B:127:VAL:HG11	5:B:1402:NAG:H61	1.98	0.45
1:B:646:ARG:O	1:B:646:ARG:HG3	2.17	0.45
2:H:109:SER:CB	2:H:113:PRO:CG	2.78	0.45
1:B:29:THR:HG22	1:B:30:ASN:N	2.31	0.45
1:B:329:PHE:HD2	1:B:528:LYS:HD2	1.75	0.45
1:B:1094:VAL:HG22	1:B:1107:ARG:HG2	1.99	0.45
1:A:37:TYR:HA	1:A:223:LEU:H	1.81	0.45
1:A:521:PRO:HG3	1:B:199:GLY:O	2.16	0.45
1:A:676:THR:CA	1:A:690:GLN:HE21	2.29	0.45
1:A:786:LYS:CE	1:C:1045:LYS:NZ	2.79	0.45
3:F:60:ARG:HH11	3:F:64:VAL:HB	1.82	0.45
1:A:1040:VAL:O	1:A:1041:ASP:HB2	2.17	0.45
2:H:35:GLY:O	2:H:100:SER:N	2.47	0.45
2:H:111:TRP:CE3	3:L:97:TYR:CE2	2.98	0.45
2:H:113:PRO:CA	2:H:117:TRP:CE2	2.94	0.45
2:G:99:HIS:O	2:G:115:ASP:OD2	2.34	0.45
1:C:453:TYR:HD1	1:C:453:TYR:H	1.64	0.45
2:G:42:PRO:HD2	2:G:45:LYS:HD3	1.99	0.45
2:G:112:SER:O	2:G:117:TRP:CZ2	2.70	0.45
1:B:153:MET:SD	1:B:153:MET:N	2.90	0.45
1:A:84:LEU:HD13	1:A:238:PHE:CE1	2.52	0.45
1:C:167:THR:HG22	1:C:168:PHE:H	1.82	0.45
2:G:111:TRP:HE1	3:F:102:HIS:CG	2.34	0.45
1:B:440:ASN:ND2	1:B:441:LEU:HG	2.32	0.45
1:C:758:SER:O	1:C:762:GLN:HG3	2.16	0.44
3:F:6:GLN:HE22	3:F:105:GLY:CA	2.20	0.44
3:F:60:ARG:NH1	3:F:64:VAL:O	2.49	0.44
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.44
1:C:364:ASP:N	1:C:364:ASP:OD1	2.50	0.44
2:H:111:TRP:HA	3:L:97:TYR:HE2	1.82	0.44
3:L:45:LYS:HB3	3:L:48:GLN:HB2	1.99	0.44
3:L:98:TYR:O	3:L:98:TYR:CD2	2.71	0.44
1:B:985:ASP:N	1:B:985:ASP:OD1	2.46	0.44
1:C:121:ASN:ND2	1:C:121:ASN:O	2.49	0.44
2:G:39:ILE:O	2:G:96:TYR:N	2.39	0.44
1:B:529:LYS:HA	1:B:529:LYS:HD3	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:VAL:HG21	1:C:231:ILE:HD12	1.98	0.44
1:C:454:ARG:NH2	1:C:456:PHE:HZ	2.16	0.44
2:H:39:ILE:O	2:H:96:TYR:N	2.39	0.44
1:C:521:PRO:HG3	1:C:564:GLN:NE2	2.32	0.44
1:B:521:PRO:O	1:B:522:ALA:CB	2.66	0.44
1:C:376:THR:CG2	1:C:378:LYS:HG3	2.48	0.44
2:H:42:PRO:HD2	2:H:45:LYS:HD3	1.99	0.44
2:H:110:SER:C	2:H:112:SER:H	2.21	0.44
2:G:110:SER:O	2:G:111:TRP:NE1	2.47	0.44
1:B:187:LYS:HE3	1:B:213:VAL:HG12	1.99	0.44
1:B:361:CYS:H	1:B:524:VAL:HG12	1.79	0.44
1:B:527:PRO:CA	1:B:528:LYS:HE2	2.43	0.44
1:A:931:ILE:HD13	1:A:931:ILE:HA	1.86	0.44
2:H:112:SER:O	2:H:117:TRP:CZ2	2.70	0.44
3:F:98:TYR:CD2	3:F:98:TYR:O	2.71	0.44
1:B:140:PHE:CG	1:B:244:LEU:HD11	2.53	0.44
1:C:350:VAL:HG11	1:C:402:ILE:HG23	1.99	0.44
2:H:110:SER:HG	3:L:95:GLN:NE2	2.14	0.44
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.44
1:A:793:PRO:HG2	1:A:794:ILE:HD12	2.00	0.44
1:C:437:ASN:OD1	1:C:438:SER:N	2.51	0.44
2:H:110:SER:HB3	3:L:103:THR:HG22	2.00	0.44
3:L:43:GLN:HB2	3:L:53:LEU:HD11	2.00	0.44
3:L:95:GLN:HG2	3:L:104:PHE:HA	2.00	0.44
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.44
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.44
1:B:327:VAL:CG1	1:B:328:ARG:H	2.30	0.44
1:A:786:LYS:CE	1:C:1045:LYS:HZ2	2.30	0.43
1:C:600:PRO:HB3	1:C:674:TYR:HB2	2.00	0.43
3:L:85:GLN:N	3:L:88:ASP:OD2	2.44	0.43
3:F:45:LYS:HB3	3:F:48:GLN:HB2	1.99	0.43
1:B:134:GLN:HB3	1:B:162:SER:HB2	2.00	0.43
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.53	0.43
2:G:110:SER:HG	3:F:95:GLN:NE2	2.17	0.43
2:G:110:SER:HB3	3:F:103:THR:HG22	2.00	0.43
1:B:795:LYS:HB3	1:B:797:PHE:CE2	2.54	0.43
1:B:1097:SER:HA	1:B:1101:HIS:O	2.18	0.43
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.85	0.43
1:A:530:SER:C	1:A:531:THR:CG2	2.86	0.43
1:A:690:GLN:HB3	1:A:690:GLN:HE21	1.67	0.43
2:G:5:LYS:O	2:G:23:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:22:ASN:ND2	3:F:76:ASP:OD1	2.45	0.43
1:B:99:ASN:O	1:B:102:ARG:NE	2.35	0.43
1:B:967:SER:O	1:B:967:SER:OG	2.24	0.43
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.51	0.43
1:A:336:CYS:CB	1:A:361:CYS:SG	3.05	0.43
1:A:740:MET:HE2	1:A:740:MET:HB2	1.93	0.43
1:C:559:PHE:O	1:C:560:LEU:HD13	2.18	0.43
2:H:5:LYS:O	2:H:23:THR:N	2.52	0.43
2:G:111:TRP:HA	3:F:97:TYR:HE2	1.83	0.43
1:B:127:VAL:HG21	5:B:1402:NAG:H5	2.01	0.43
1:A:142:GLY:H	1:A:243:ALA:HA	1.82	0.43
1:A:550:GLY:CA	1:A:590:CYS:SG	2.90	0.43
2:G:110:SER:C	2:G:112:SER:H	2.21	0.43
3:F:43:GLN:HB2	3:F:53:LEU:HD11	2.00	0.43
1:B:328:ARG:O	1:B:329:PHE:CD1	2.71	0.43
1:B:546:LEU:HD11	1:B:565:PHE:CG	2.53	0.43
1:B:758:SER:O	1:B:762:GLN:HG3	2.19	0.43
1:A:1027:THR:HG22	1:A:1042:PHE:HZ	1.83	0.43
1:C:748:GLU:CD	1:C:981:LEU:HD21	2.39	0.43
1:B:141:LEU:O	1:B:243:ALA:HA	2.18	0.43
1:B:886:TRP:HH2	1:B:904:TYR:CD2	2.35	0.43
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	2.00	0.43
2:H:111:TRP:CH2	3:L:100:THR:O	2.69	0.43
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.18	0.43
1:A:854:LYS:HE2	1:A:854:LYS:HB3	1.88	0.43
1:B:392:PHE:CA	1:B:517:LEU:HD21	2.49	0.43
4:W:1:NAG:H61	4:W:2:NAG:N2	2.33	0.43
1:C:91:TYR:OH	1:C:191:GLU:HG2	2.19	0.42
3:F:95:GLN:HG2	3:F:104:PHE:HA	2.00	0.42
1:B:516:GLU:C	1:B:517:LEU:HD23	2.39	0.42
1:A:119:ILE:HG13	1:A:128:ILE:HG23	2.01	0.42
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.42
3:L:45:LYS:HD2	3:L:45:LYS:HA	1.96	0.42
1:B:933:LYS:HB2	1:B:933:LYS:HE3	1.86	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.42
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.00	0.42
1:B:131:CYS:HB3	1:B:164:ASN:O	2.19	0.42
1:B:329:PHE:HB3	1:B:330:PRO:HD2	2.00	0.42
1:A:722:VAL:HA	1:A:1064:HIS:O	2.19	0.42
2:H:72:THR:N	2:H:81:VAL:O	2.43	0.42
4:E:1:NAG:H61	4:E:2:NAG:N2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:C	1:A:154:GLU:HA	2.39	0.42
1:C:472:ILE:CD1	1:C:474:GLN:HB3	2.47	0.42
1:C:541:PHE:O	1:C:547:THR:HA	2.20	0.42
2:H:18:LEU:HD23	2:H:18:LEU:HA	1.88	0.42
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.42
1:A:42:VAL:HG11	1:C:567:ARG:HG2	2.02	0.42
1:A:188:ASN:HD22	1:A:188:ASN:HA	1.63	0.42
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.81	0.42
1:C:199:GLY:C	1:B:521:PRO:HG3	2.33	0.42
1:C:459:SER:C	1:C:461:LEU:H	2.23	0.42
2:G:110:SER:O	2:G:111:TRP:CE2	2.73	0.42
3:F:96:GLN:HE21	3:F:103:THR:HG21	1.84	0.42
1:A:314:GLN:HE21	1:A:314:GLN:HB2	1.56	0.42
1:A:792:PRO:O	1:A:795:LYS:NZ	2.52	0.42
1:C:341:VAL:HG23	1:C:342:PHE:HD1	1.84	0.42
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.84	0.42
1:A:736:VAL:HG23	1:A:858:LEU:HD23	2.02	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:C:376:THR:O	1:C:434:ILE:HA	2.20	0.42
1:C:462:LYS:H	1:C:462:LYS:HD3	1.84	0.42
2:H:110:SER:O	2:H:111:TRP:NE1	2.47	0.42
3:L:7:SER:HB3	3:L:8:PRO:HD3	1.68	0.42
2:G:109:SER:HB2	2:G:113:PRO:HG3	1.93	0.42
3:F:55:TYR:O	3:F:59:THR:OG1	2.38	0.42
1:A:615:VAL:HG12	1:A:616:ASN:O	2.20	0.42
1:B:112:SER:O	1:B:113:LYS:HB3	2.20	0.42
1:B:332:ILE:HG21	1:B:362:VAL:HG11	2.00	0.42
2:H:70:THR:O	2:H:83:THR:N	2.53	0.42
2:H:110:SER:O	2:H:111:TRP:CE2	2.73	0.42
2:G:114:PHE:N	2:G:117:TRP:HE1	2.17	0.42
3:F:102:HIS:O	3:F:104:PHE:CD2	2.73	0.42
1:C:418:ILE:HD13	1:C:418:ILE:HA	1.88	0.41
2:H:32:SER:HA	2:H:55:TRP:CD1	2.55	0.41
2:H:111:TRP:CZ2	3:L:101:PRO:O	2.73	0.41
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.68	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:A:995:ARG:HE	1:A:995:ARG:HB3	1.66	0.41
1:C:110:LEU:HD12	1:C:110:LEU:HA	1.71	0.41
1:C:379:CYS:HA	1:C:432:CYS:HA	2.02	0.41
2:H:37:GLY:O	2:H:98:ALA:N	2.50	0.41
1:B:295:PRO:HB2	1:B:608:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1:NAG:H83	4:I:1:NAG:H3	2.02	0.41
1:A:738:CYS:HB3	1:A:760:CYS:HB3	1.92	0.41
2:H:56:ASP:OD1	2:H:56:ASP:N	2.39	0.41
1:A:117:LEU:HD22	1:A:231:ILE:HD12	2.03	0.41
1:A:460:ASN:N	1:A:460:ASN:OD1	2.53	0.41
1:C:132:GLU:HG3	1:C:165:ASN:HB2	2.02	0.41
1:C:142:GLY:O	1:C:156:GLU:HG3	2.20	0.41
1:C:964:LYS:HB2	1:C:964:LYS:HE3	1.77	0.41
2:G:18:LEU:HD23	2:G:18:LEU:HA	1.88	0.41
2:G:32:SER:HA	2:G:55:TRP:CD1	2.55	0.41
1:B:460:ASN:N	1:B:460:ASN:OD1	2.53	0.41
1:C:506:GLN:HA	1:C:507:PRO:HD3	1.94	0.41
1:C:959:LEU:HD12	1:C:959:LEU:HA	1.90	0.41
2:H:6:GLU:OE1	2:H:6:GLU:N	2.54	0.41
3:L:6:GLN:CD	3:L:106:GLN:H	2.24	0.41
1:B:538:CYS:HB2	1:B:590:CYS:HB3	1.78	0.41
1:A:703:ASN:C	1:A:703:ASN:HD22	2.24	0.41
2:H:61:TYR:HB2	2:H:66:LYS:HD2	2.03	0.41
3:L:102:HIS:O	3:L:104:PHE:CD2	2.73	0.41
2:G:113:PRO:CA	2:G:117:TRP:CE2	2.94	0.41
1:B:702:GLU:H	1:B:702:GLU:HG2	1.72	0.41
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.55	0.41
1:C:187:LYS:HG2	1:C:212:LEU:O	2.21	0.41
1:C:495:TYR:CZ	1:C:507:PRO:HG3	2.55	0.41
2:H:16:GLN:H	2:H:16:GLN:HG3	1.65	0.41
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.51	0.41
1:B:973:ILE:HG23	1:B:992:GLN:NE2	2.35	0.41
1:A:523:THR:CG2	1:A:524:VAL:N	2.45	0.41
1:C:135:PHE:HE1	1:C:159:VAL:HG12	1.86	0.41
1:C:984:LEU:HD23	1:C:988:GLU:HB3	2.03	0.41
1:B:393:THR:H	1:B:517:LEU:HD22	1.85	0.41
1:A:703:ASN:HD22	1:A:704:SER:N	2.19	0.41
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.21	0.41
2:H:98:ALA:HB1	2:H:114:PHE:HB2	2.03	0.41
2:H:114:PHE:N	2:H:117:TRP:HE1	2.17	0.41
2:G:103:LEU:CD2	1:B:486:PHE:CD1	2.85	0.41
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.78	0.41
1:B:542:ASN:HA	1:B:546:LEU:O	2.21	0.41
1:A:188:ASN:HB2	1:A:190:ARG:HH11	1.86	0.41
1:C:81:ASN:O	1:C:239:GLN:NE2	2.54	0.41
3:L:55:TYR:O	3:L:59:THR:OG1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:96:GLN:HE21	3:L:103:THR:HG21	1.84	0.41
2:G:109:SER:CB	2:G:113:PRO:CG	2.78	0.41
1:B:127:VAL:HG22	1:B:171:VAL:HG13	2.04	0.41
1:B:213:VAL:HG23	1:B:214:ARG:N	2.36	0.41
1:A:642:VAL:HG22	1:A:651:ILE:HG13	2.03	0.40
1:C:199:GLY:HA2	1:B:521:PRO:HG3	1.80	0.40
2:H:108:SER:N	3:L:97:TYR:H	2.19	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:393:THR:O	1:B:523:THR:CG2	2.58	0.40
1:A:125:ASN:HD22	1:A:125:ASN:HA	1.75	0.40
1:A:299:THR:OG1	1:A:597:VAL:HG21	2.21	0.40
1:C:29:THR:OG1	1:C:30:ASN:N	2.50	0.40
1:C:646:ARG:HG3	1:C:646:ARG:O	2.21	0.40
2:G:111:TRP:CZ2	3:F:101:PRO:O	2.73	0.40
2:G:112:SER:HB3	3:F:95:GLN:CD	2.42	0.40
1:B:89:GLY:HA2	1:B:194:PHE:O	2.22	0.40
1:B:328:ARG:HG2	1:B:328:ARG:HH21	1.86	0.40
3:F:6:GLN:CD	3:F:106:GLN:H	2.24	0.40
1:B:1105:THR:HG21	1:B:1110:TYR:CD1	2.57	0.40
1:A:280:ASN:OD1	1:A:281:GLU:N	2.49	0.40
1:A:870:ILE:O	1:A:874:THR:HG23	2.21	0.40
1:C:116:SER:HA	1:C:233:ILE:HD11	2.03	0.40
2:G:7:SER:N	2:G:21:THR:O	2.50	0.40
2:G:56:ASP:OD1	2:G:56:ASP:N	2.39	0.40
1:A:347:PHE:CD1	1:A:509:ARG:HD3	2.56	0.40
1:A:556:ASN:HD22	1:A:556:ASN:HA	1.53	0.40
1:A:577:ARG:HG3	1:A:584:ILE:HG22	2.04	0.40
1:C:424:LYS:CB	1:C:463:PRO:HA	2.51	0.40
1:C:789:TYR:HA	1:B:703:ASN:O	2.22	0.40
2:G:111:TRP:CH2	3:F:100:THR:O	2.69	0.40
1:B:600:PRO:HB3	1:B:674:TYR:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	986/1283 (77%)	891 (90%)	82 (8%)	13 (1%)	10	39
1	B	988/1283 (77%)	889 (90%)	93 (9%)	6 (1%)	22	55
1	C	958/1283 (75%)	868 (91%)	89 (9%)	1 (0%)	48	79
2	G	123/226 (54%)	102 (83%)	18 (15%)	3 (2%)	5	29
2	H	123/226 (54%)	102 (83%)	18 (15%)	3 (2%)	5	29
3	F	111/220 (50%)	92 (83%)	13 (12%)	6 (5%)	1	17
3	L	111/220 (50%)	92 (83%)	13 (12%)	6 (5%)	1	17
All	All	3400/4741 (72%)	3036 (89%)	326 (10%)	38 (1%)	15	42

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	LEU
1	A	529	LYS
1	A	814	LYS
2	H	113	PRO
2	H	114	PHE
2	H	116	TYR
3	L	6	GLN
3	L	7	SER
2	G	113	PRO
2	G	114	PHE
2	G	116	TYR
3	F	6	GLN
3	F	7	SER
1	B	518	LEU
1	A	333	THR
1	A	591	SER
1	A	810	SER
3	L	9	ASP
3	L	10	SER
3	F	9	ASP
3	F	10	SER
1	A	522	ALA
1	A	527	PRO
1	B	324	GLU
1	B	325	SER
1	B	522	ALA

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Mol	Chain	Res	Type
1	A	349	SER
1	A	520	ALA
1	A	813	SER
1	B	349	SER
1	B	520	ALA
1	A	812	PRO
1	C	88	ASP
3	L	98	TYR
3	L	100	THR
3	F	98	TYR
3	F	100	THR
1	A	811	LYS

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	879/1122 (78%)	789 (90%)	90 (10%)	6	24
1	B	881/1122 (78%)	783 (89%)	98 (11%)	5	21
1	C	862/1122 (77%)	762 (88%)	100 (12%)	4	21
2	G	112/199 (56%)	107 (96%)	5 (4%)	23	47
2	H	112/199 (56%)	107 (96%)	5 (4%)	23	47
3	F	99/195 (51%)	95 (96%)	4 (4%)	27	50
3	L	99/195 (51%)	95 (96%)	4 (4%)	27	50
All	All	3044/4154 (73%)	2738 (90%)	306 (10%)	9	24

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	50	SER
1	A	51	THR
1	A	60	SER
1	A	63	THR

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Mol	Chain	Res	Type
1	A	84	LEU
1	A	86	PHE
1	A	98	SER
1	A	113	LYS
1	A	114	THR
1	A	117	LEU
1	A	120	VAL
1	A	125	ASN
1	A	143	VAL
1	A	156	GLU
1	A	172	SER
1	A	190	ARG
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	212	LEU
1	A	215	ASP
1	A	221	SER
1	A	234	ASN
1	A	271	GLN
1	A	287	ASP
1	A	301	CYS
1	A	305	SER
1	A	314	GLN
1	A	318	PHE
1	A	332	ILE
1	A	333	THR
1	A	336	CYS
1	A	353	TRP
1	A	355	ARG
1	A	375	SER
1	A	383	SER
1	A	389	ASP
1	A	390	LEU
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	440	ASN
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU

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Mol	Chain	Res	Type
1	A	525	CYS
1	A	528	LYS
1	A	529	LYS
1	A	532	ASN
1	A	533	LEU
1	A	546	LEU
1	A	551	VAL
1	A	556	ASN
1	A	567	ARG
1	A	573	THR
1	A	584	ILE
1	A	586	ASP
1	A	591	SER
1	A	602	THR
1	A	606	ASN
1	A	641	ASN
1	A	658	ASN
1	A	675	GLN
1	A	690	GLN
1	A	697	MET
1	A	703	ASN
1	A	727	LEU
1	A	740	MET
1	A	778	THR
1	A	787	GLN
1	A	814	LYS
1	A	856	ASN
1	A	859	THR
1	A	886	TRP
1	A	937	SER
1	A	974	SER
1	A	975	SER
1	A	976	VAL
1	A	977	LEU
1	A	1017	GLU
1	A	1077	THR
1	A	1094	VAL
1	A	1104	VAL
1	A	1126	CYS
1	A	1129	VAL
1	A	1132	ILE
1	A	1136	THR

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Mol	Chain	Res	Type
1	A	1145	LEU
1	C	45	SER
1	C	48	LEU
1	C	50	SER
1	C	51	THR
1	C	52	GLN
1	C	53	ASP
1	C	60	SER
1	C	87	ASN
1	C	88	ASP
1	C	95	THR
1	C	97	LYS
1	C	99	ASN
1	C	108	THR
1	C	109	THR
1	C	112	SER
1	C	113	LYS
1	C	116	SER
1	C	120	VAL
1	C	127	VAL
1	C	158	ARG
1	C	164	ASN
1	C	205	SER
1	C	207	HIS
1	C	208	THR
1	C	214	ARG
1	C	240	THR
1	C	278	LYS
1	C	307	THR
1	C	318	PHE
1	C	328	ARG
1	C	345	THR
1	C	359	SER
1	C	371	SER
1	C	382	VAL
1	C	385	THR
1	C	388	ASN
1	C	402	ILE
1	C	403	ARG
1	C	409	GLN
1	C	417	LYS
1	C	430	THR

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Mol	Chain	Res	Type
1	C	453	TYR
1	C	462	LYS
1	C	464	PHE
1	C	467	ASP
1	C	473	TYR
1	C	487	ASN
1	C	490	PHE
1	C	494	SER
1	C	495	TYR
1	C	506	GLN
1	C	514	SER
1	C	525	CYS
1	C	531	THR
1	C	532	ASN
1	C	533	LEU
1	C	534	VAL
1	C	567	ARG
1	C	569	ILE
1	C	576	VAL
1	C	582	LEU
1	C	597	VAL
1	C	606	ASN
1	C	607	GLN
1	C	614	ASP
1	C	615	VAL
1	C	617	CYS
1	C	640	SER
1	C	649	CYS
1	C	676	THR
1	C	704	SER
1	C	710	ASN
1	C	746	SER
1	C	779	GLN
1	C	786	LYS
1	C	787	GLN
1	C	791	THR
1	C	808	ASP
1	C	854	LYS
1	C	855	PHE
1	C	856	ASN
1	C	868	GLU
1	C	878	LEU

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Mol	Chain	Res	Type
1	C	912	THR
1	C	916	LEU
1	C	935	GLN
1	C	964	LYS
1	C	968	SER
1	C	969	ASN
1	C	974	SER
1	C	976	VAL
1	C	1030	SER
1	C	1037	SER
1	C	1045	LYS
1	C	1074	ASN
1	C	1094	VAL
1	C	1104	VAL
1	C	1114	ILE
1	C	1126	CYS
1	C	1141	LEU
2	H	111	TRP
2	H	114	PHE
2	H	116	TYR
2	H	119	GLN
2	H	121	THR
3	L	18	ARG
3	L	89	VAL
3	L	99	SER
3	L	100	THR
2	G	111	TRP
2	G	114	PHE
2	G	116	TYR
2	G	119	GLN
2	G	121	THR
3	F	18	ARG
3	F	89	VAL
3	F	99	SER
3	F	100	THR
1	B	45	SER
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	137	ASN

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Mol	Chain	Res	Type
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	282	ASN
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	314	GLN
1	B	315	THR
1	B	318	PHE
1	B	328	ARG
1	B	333	THR
1	B	334	ASN
1	B	335	LEU
1	B	336	CYS
1	B	353	TRP
1	B	355	ARG
1	B	375	SER
1	B	383	SER
1	B	389	ASP
1	B	390	LEU
1	B	421	TYR
1	B	430	THR
1	B	438	SER
1	B	440	ASN
1	B	500	THR
1	B	514	SER
1	B	517	LEU
1	B	518	LEU
1	B	525	CYS
1	B	528	LYS
1	B	530	SER
1	B	532	ASN
1	B	540	ASN
1	B	546	LEU
1	B	553	THR

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Mol	Chain	Res	Type
1	B	554	GLU
1	B	556	ASN
1	B	558	LYS
1	B	576	VAL
1	B	583	GLU
1	B	588	THR
1	B	590	CYS
1	B	599	THR
1	B	602	THR
1	B	646	ARG
1	B	673	SER
1	B	698	SER
1	B	703	ASN
1	B	722	VAL
1	B	727	LEU
1	B	729	VAL
1	B	738	CYS
1	B	746	SER
1	B	773	GLU
1	B	785	VAL
1	B	787	GLN
1	B	791	THR
1	B	826	VAL
1	B	868	GLU
1	B	878	LEU
1	B	883	THR
1	B	902	MET
1	B	916	LEU
1	B	929	SER
1	B	937	SER
1	B	939	SER
1	B	951	VAL
1	B	967	SER
1	B	982	SER
1	B	994	ASP
1	B	1005	GLN
1	B	1074	ASN
1	B	1076	THR
1	B	1077	THR
1	B	1092	GLU
1	B	1094	VAL
1	B	1100	THR

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Mol	Chain	Res	Type
1	B	1104	VAL
1	B	1123	SER
1	B	1125	ASN
1	B	1132	ILE
1	B	1141	LEU
1	B	1142	GLN
1	B	1144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	188	ASN
1	A	207	HIS
1	A	271	GLN
1	A	314	GLN
1	A	321	GLN
1	A	354	ASN
1	A	360	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	498	GLN
1	A	556	ASN
1	A	606	ASN
1	A	641	ASN
1	A	675	GLN
1	A	690	GLN
1	A	703	ASN
1	A	784	GLN
1	A	804	GLN
1	A	901	GLN
1	A	907	ASN
1	A	914	ASN
1	A	926	GLN
1	A	935	GLN
1	A	969	ASN
1	A	992	GLN
1	A	1010	GLN
1	A	1071	GLN
1	A	1101	HIS
1	A	1106	GLN

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Mol	Chain	Res	Type
1	C	115	GLN
1	C	134	GLN
1	C	164	ASN
1	C	188	ASN
1	C	245	HIS
1	C	422	ASN
1	C	487	ASN
1	C	506	GLN
1	C	532	ASN
1	C	540	ASN
1	C	563	GLN
1	C	606	ASN
1	C	607	GLN
1	C	710	ASN
1	C	804	GLN
1	C	901	GLN
1	C	914	ASN
1	C	919	ASN
1	C	920	GLN
1	C	926	GLN
1	C	992	GLN
1	C	1054	GLN
2	H	41	GLN
3	L	6	GLN
3	L	95	GLN
3	L	96	GLN
3	L	102	HIS
2	G	41	GLN
3	F	6	GLN
3	F	95	GLN
3	F	96	GLN
3	F	102	HIS
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	239	GLN
1	B	360	ASN
1	B	394	ASN
1	B	422	ASN
1	B	440	ASN
1	B	498	GLN
1	B	540	ASN

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Mol	Chain	Res	Type
1	B	556	ASN
1	B	644	GLN
1	B	658	ASN
1	B	690	GLN
1	B	703	ASN
1	B	762	GLN
1	B	787	GLN
1	B	856	ASN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	926	GLN
1	B	955	ASN
1	B	969	ASN
1	B	992	GLN
1	B	1125	ASN
1	B	1142	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 ⓘ

44 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.41	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.57	0	17,19,21	0.57	0
4	NAG	E	2	4	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	I	1	1,4	14,14,15	0.23	0	17,19,21	1.35	1 (5%)
4	NAG	I	2	4	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	J	1	1,4	14,14,15	0.52	0	17,19,21	0.70	1 (5%)
4	NAG	J	2	4	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	K	1	1,4	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	K	2	4	14,14,15	0.20	0	17,19,21	0.73	0
4	NAG	M	1	1,4	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.57	0	17,19,21	1.32	1 (5%)
4	NAG	N	1	1,4	14,14,15	0.65	1 (7%)	17,19,21	0.44	0
4	NAG	N	2	4	14,14,15	0.31	0	17,19,21	1.36	2 (11%)
4	NAG	O	1	1,4	14,14,15	0.42	0	17,19,21	0.43	0
4	NAG	O	2	4	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	P	1	1,4	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	P	2	4	14,14,15	0.16	0	17,19,21	0.48	0
4	NAG	Q	1	1,4	14,14,15	0.32	0	17,19,21	0.40	0
4	NAG	Q	2	4	14,14,15	0.37	0	17,19,21	0.36	0
4	NAG	R	1	1,4	14,14,15	0.35	0	17,19,21	1.11	1 (5%)
4	NAG	R	2	4	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	S	1	1,4	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
4	NAG	S	2	4	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	T	1	1,4	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	T	2	4	14,14,15	0.29	0	17,19,21	0.68	0
4	NAG	U	1	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	U	2	4	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	V	1	1,4	14,14,15	0.52	0	17,19,21	0.50	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.59	0
4	NAG	W	1	1,4	14,14,15	0.59	1 (7%)	17,19,21	0.56	0
4	NAG	W	2	4	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	X	1	1,4	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
4	NAG	X	2	4	14,14,15	0.52	0	17,19,21	0.46	0
4	NAG	Y	1	1,4	14,14,15	0.38	0	17,19,21	0.72	0
4	NAG	Y	2	4	14,14,15	0.30	0	17,19,21	1.31	2 (11%)
4	NAG	Z	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.69	0
4	NAG	Z	2	4	14,14,15	0.40	0	17,19,21	1.40	3 (17%)
4	NAG	a	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	a	2	4	14,14,15	0.30	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	b	1	1,4	14,14,15	0.24	0	17,19,21	0.69	1 (5%)
4	NAG	b	2	4	14,14,15	0.16	0	17,19,21	0.46	0
4	NAG	c	1	1,4	14,14,15	0.40	0	17,19,21	1.16	2 (11%)
4	NAG	c	2	4	14,14,15	0.34	0	17,19,21	0.41	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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	5/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	3/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	4/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	3/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	5/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	3/6/23/26	0/1/1/1
4	NAG	b	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	NAG	c	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	O5-C1	-2.69	1.39	1.43
4	a	1	NAG	O5-C1	-2.55	1.39	1.43
4	Z	1	NAG	O5-C1	-2.36	1.39	1.43
4	N	1	NAG	O5-C1	-2.19	1.40	1.43
4	W	1	NAG	O5-C1	-2.06	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C2-N2-C7	4.64	129.51	122.90
4	Z	2	NAG	C2-N2-C7	4.37	129.13	122.90
4	N	2	NAG	C2-N2-C7	4.36	129.12	122.90
4	M	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	Y	2	NAG	C2-N2-C7	4.34	129.09	122.90
4	R	1	NAG	C1-O5-C5	3.23	116.56	112.19
4	Z	2	NAG	C1-C2-N2	2.40	114.59	110.49
4	T	1	NAG	O4-C4-C3	-2.39	104.83	110.35
4	c	1	NAG	C8-C7-N2	2.33	120.05	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	1	NAG	C1-O5-C5	2.27	115.27	112.19
4	N	2	NAG	C1-C2-N2	2.25	114.33	110.49
4	Y	2	NAG	C1-C2-N2	2.25	114.33	110.49
4	J	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	b	1	NAG	C1-O5-C5	2.16	115.12	112.19
4	Z	2	NAG	C1-O5-C5	2.09	115.03	112.19
4	D	2	NAG	C1-O5-C5	2.09	115.02	112.19
4	X	1	NAG	C1-O5-C5	2.03	114.94	112.19
4	c	1	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	U	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	W	2	NAG	C1-C2-N2-C7
4	N	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7

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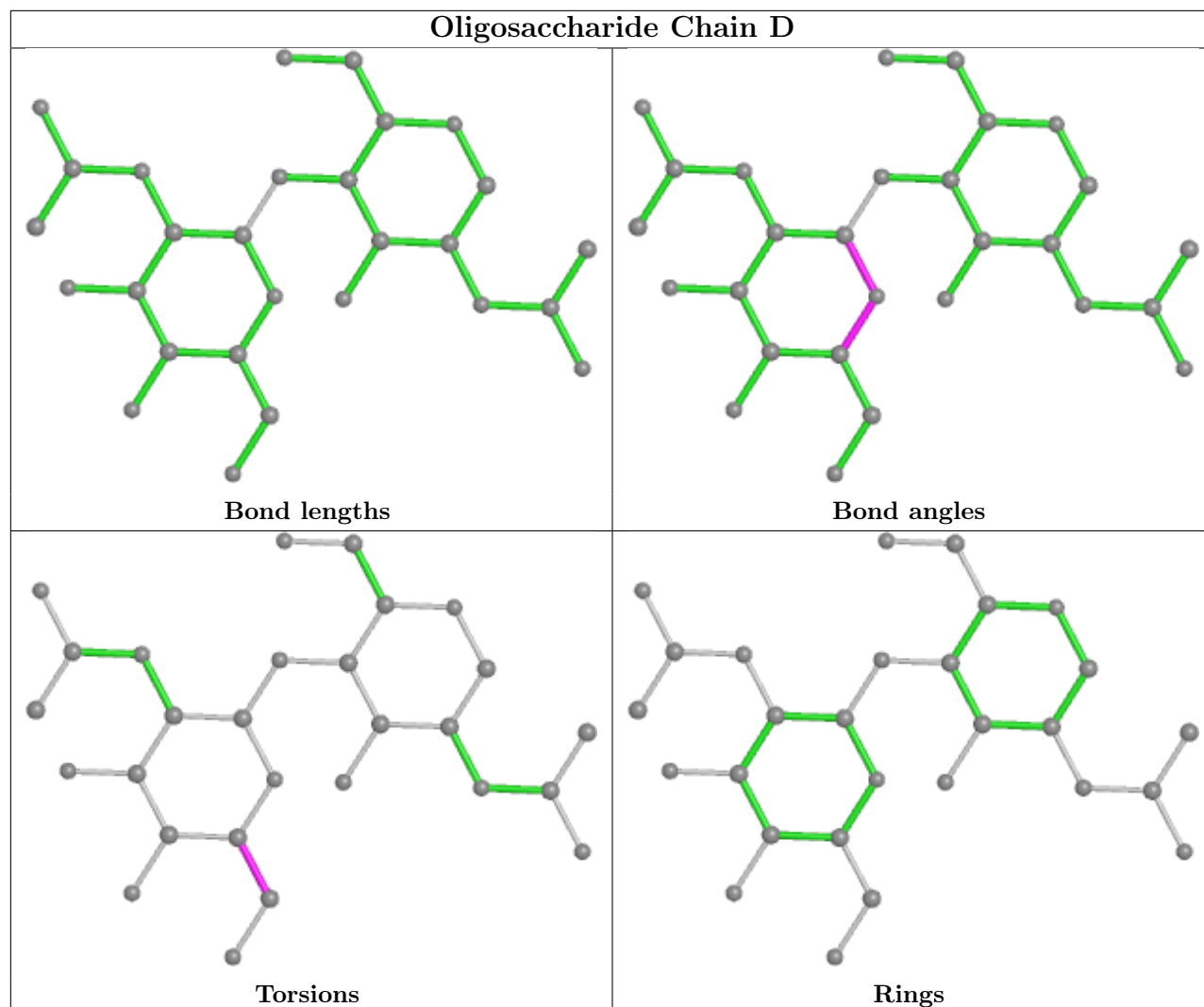
Mol	Chain	Res	Type	Atoms
4	Z	2	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C1-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
4	M	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
4	W	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	Z	2	NAG	C3-C2-N2-C7
4	W	2	NAG	O5-C5-C6-O6

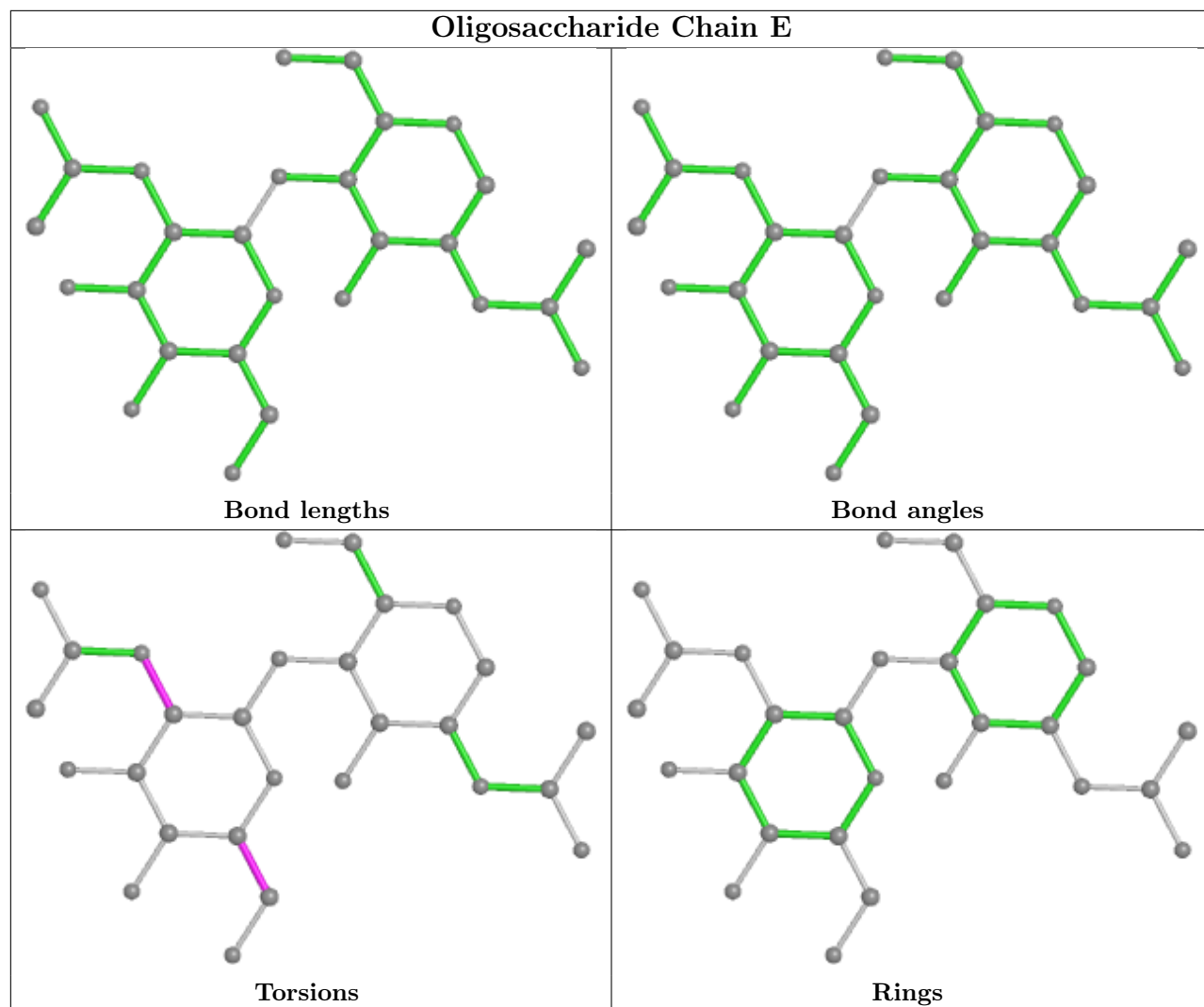
There are no ring outliers.

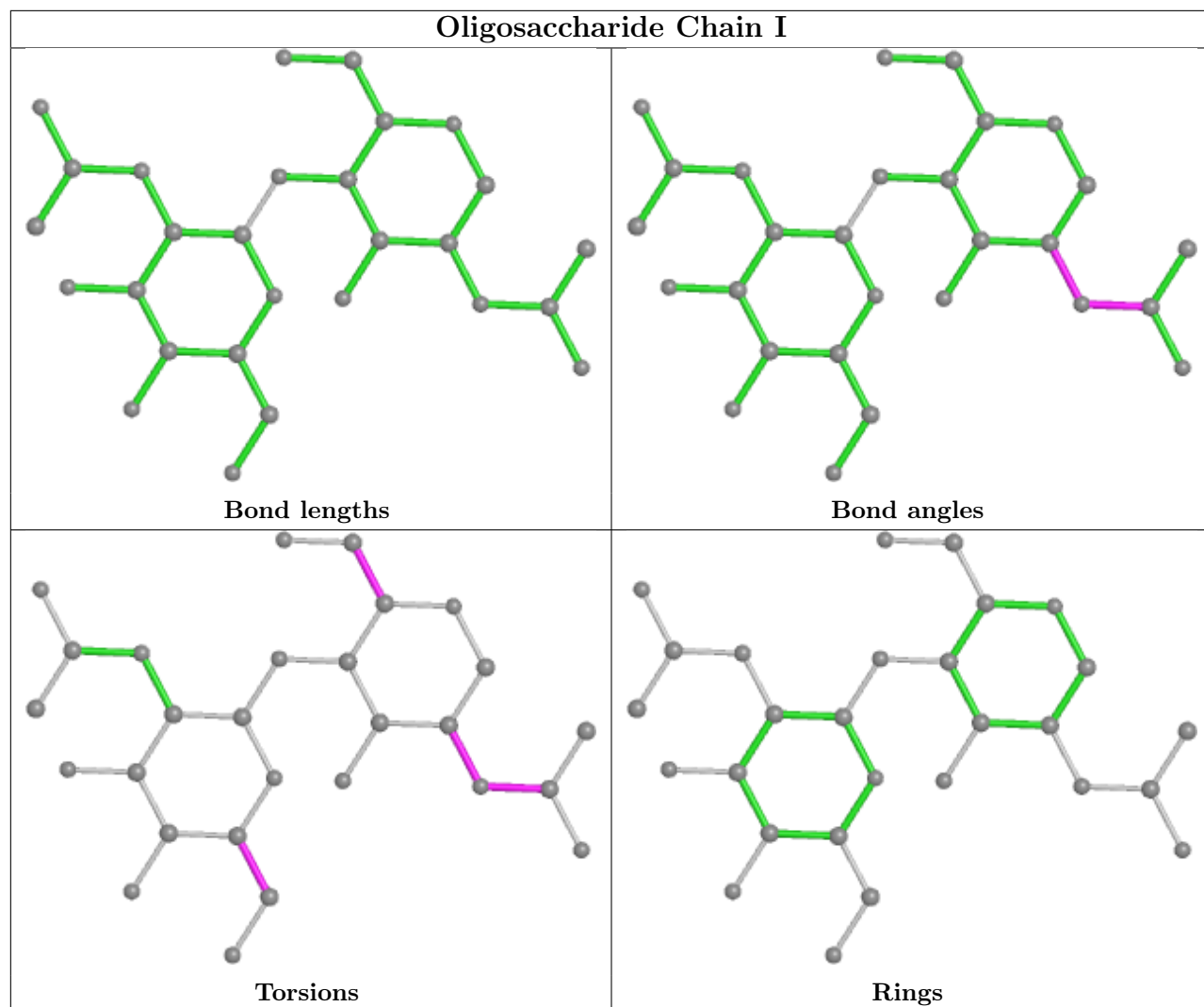
13 monomers are involved in 14 short contacts:

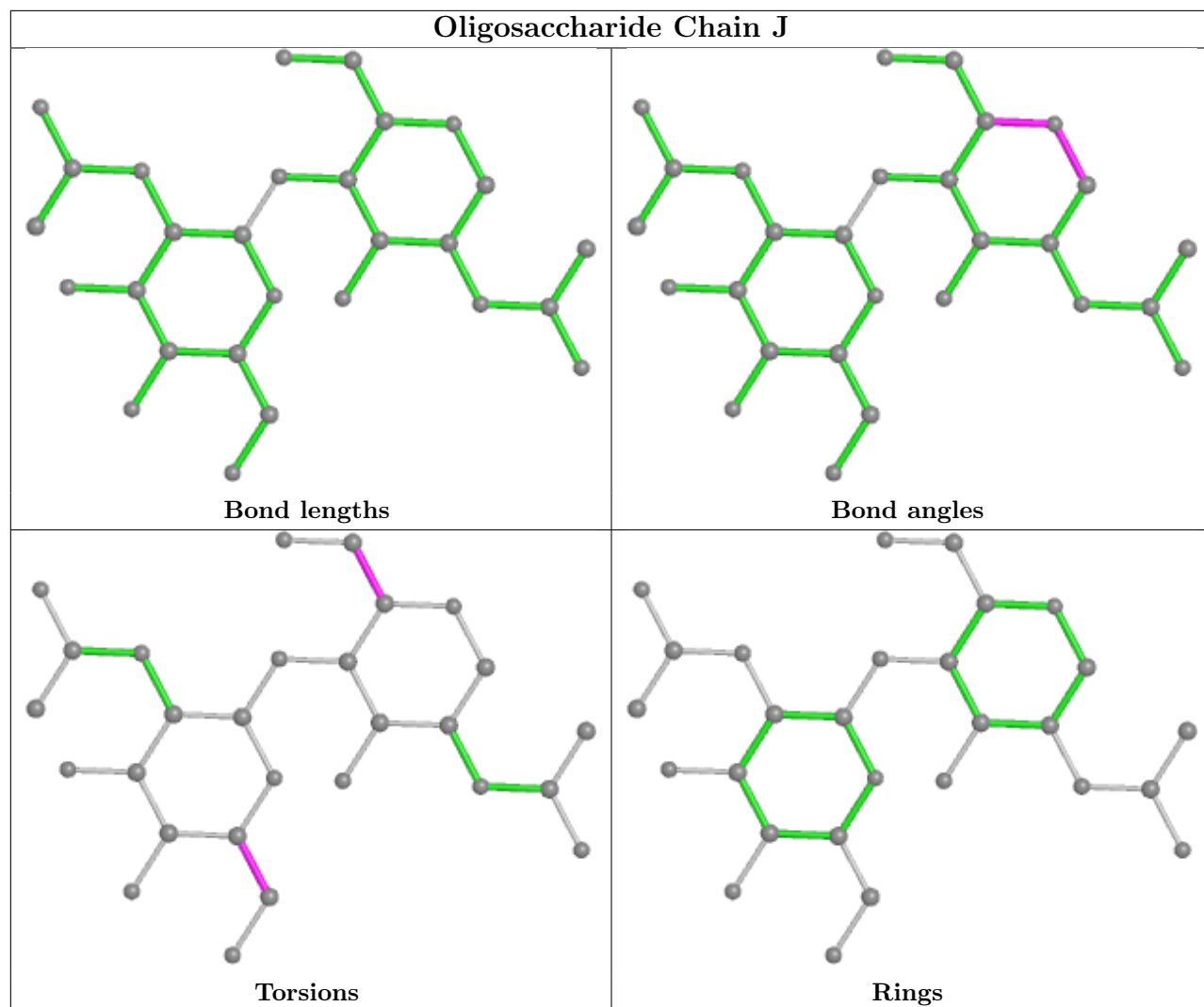
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	1	NAG	3	0
4	P	1	NAG	1	0
4	N	1	NAG	1	0
4	Y	2	NAG	1	0
4	E	1	NAG	3	0
4	E	2	NAG	2	0
4	I	1	NAG	1	0
4	T	2	NAG	1	0
4	N	2	NAG	1	0
4	W	2	NAG	2	0
4	T	1	NAG	1	0
4	M	2	NAG	1	0
4	Z	2	NAG	1	0

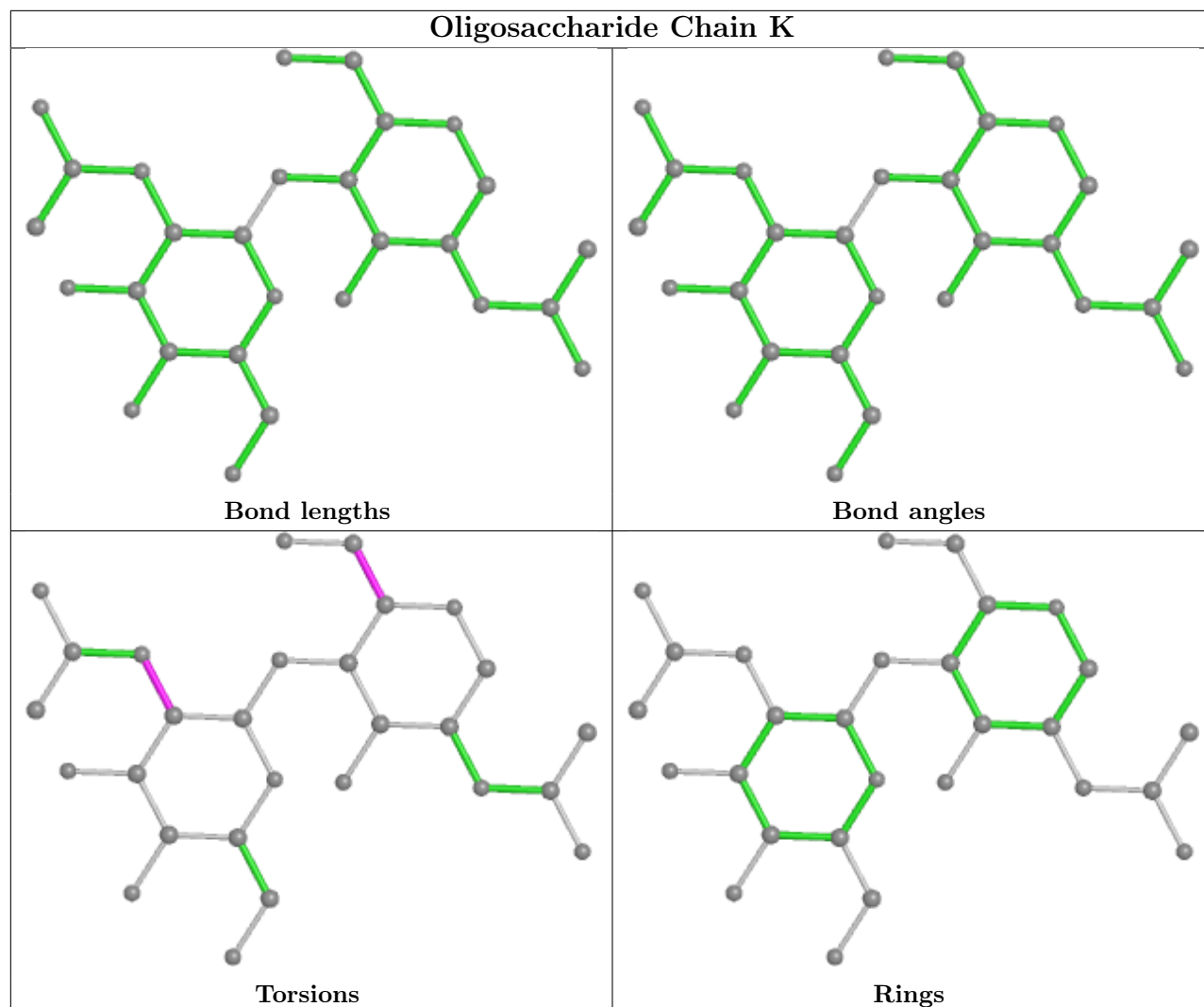
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

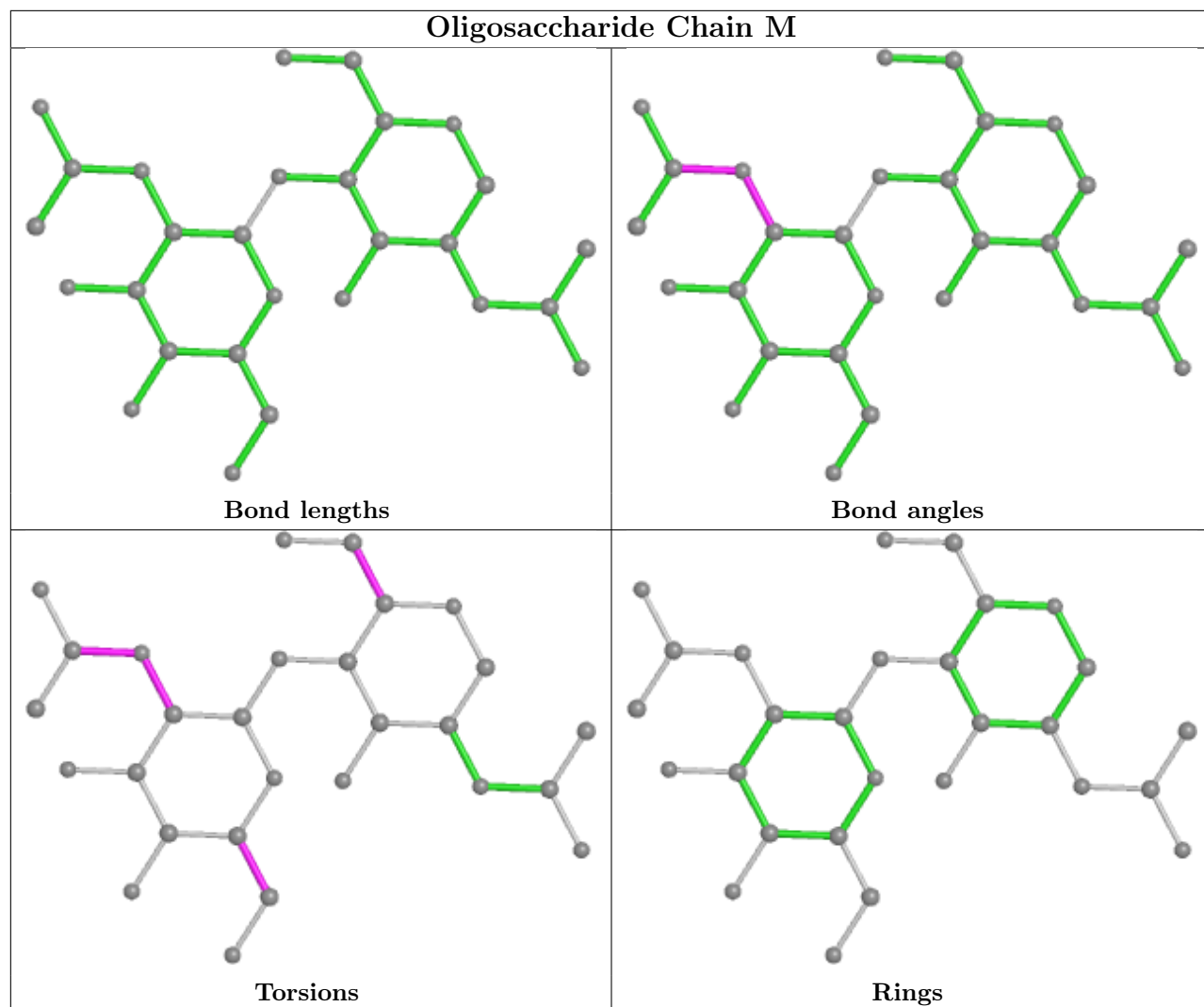


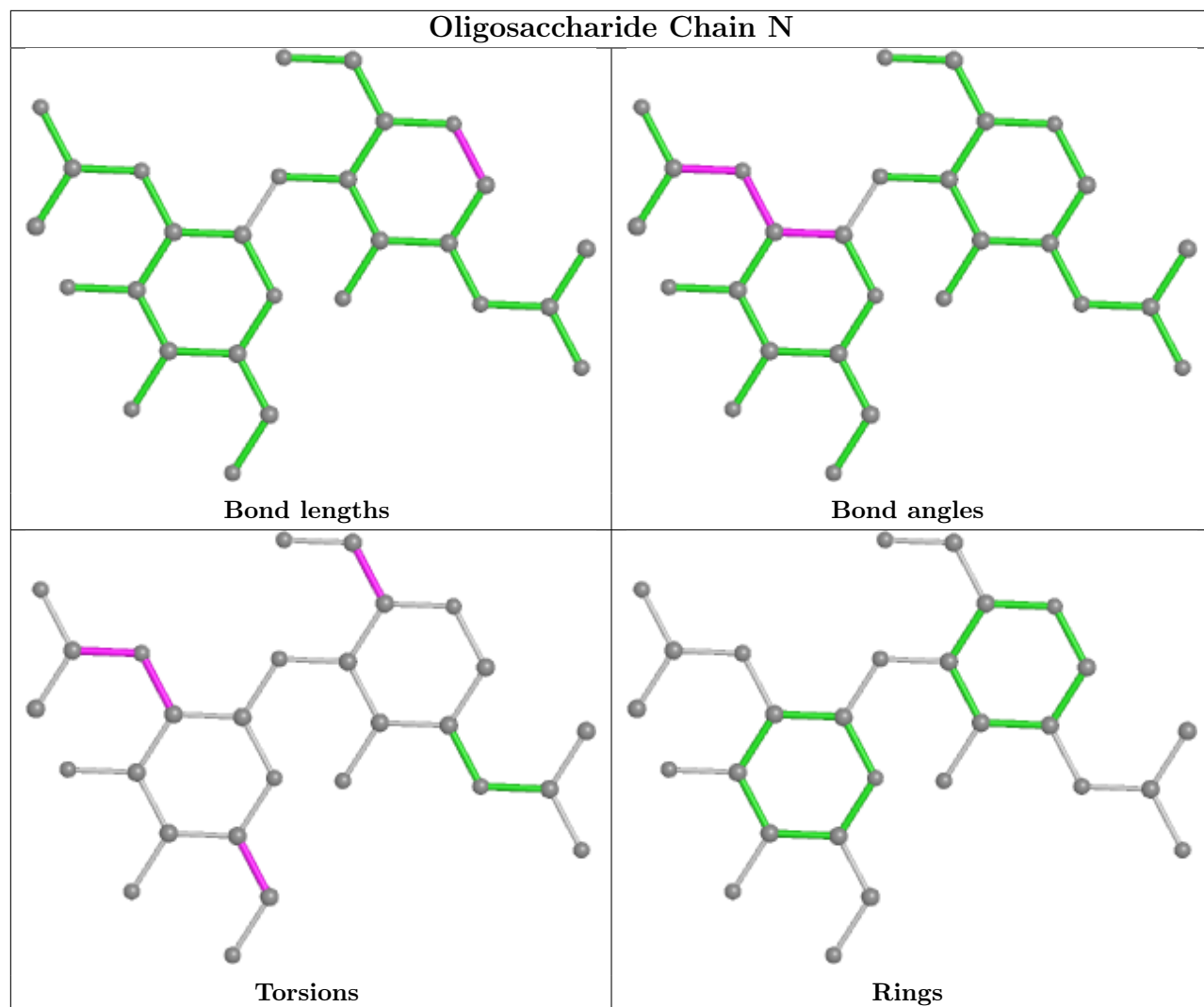


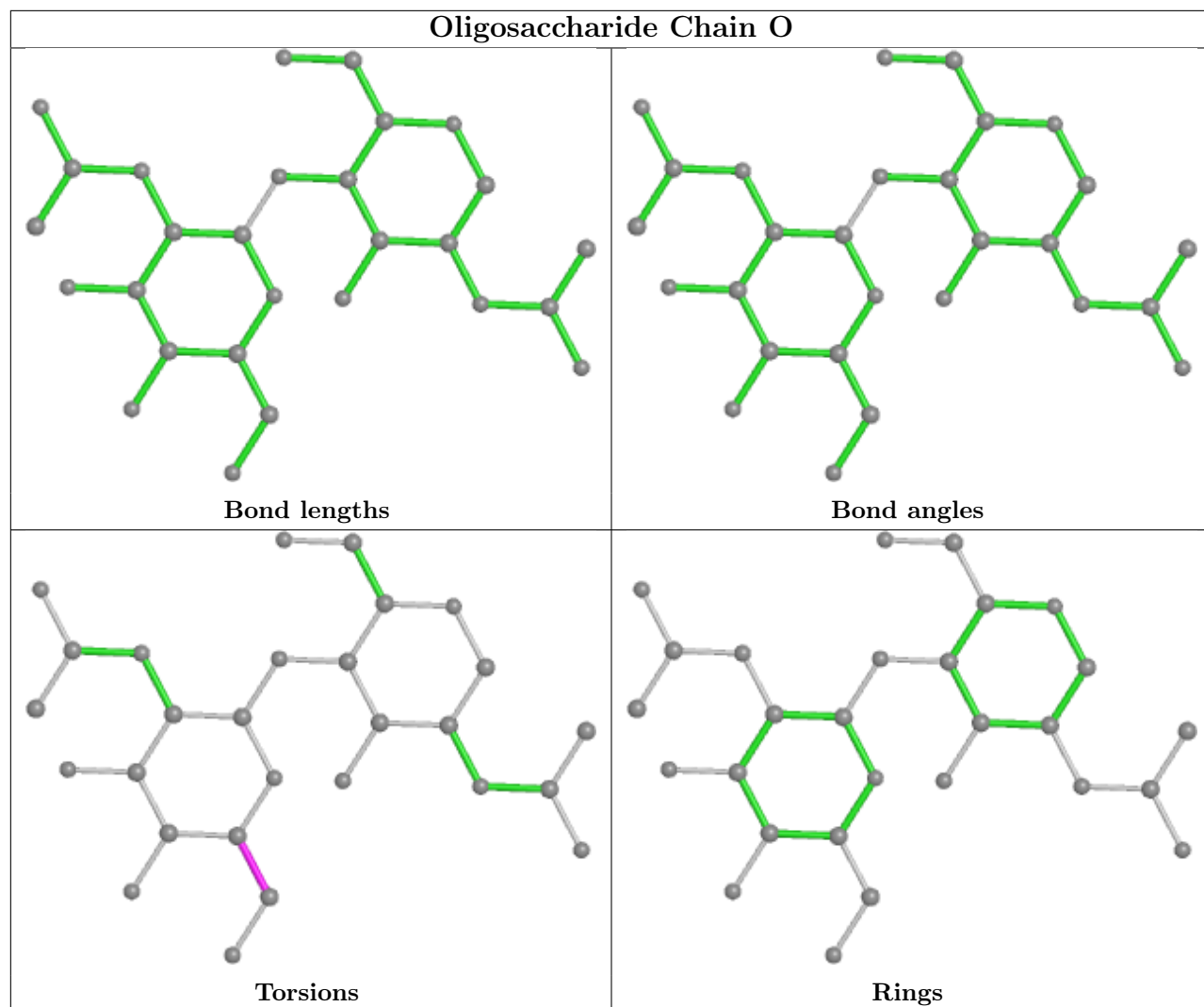


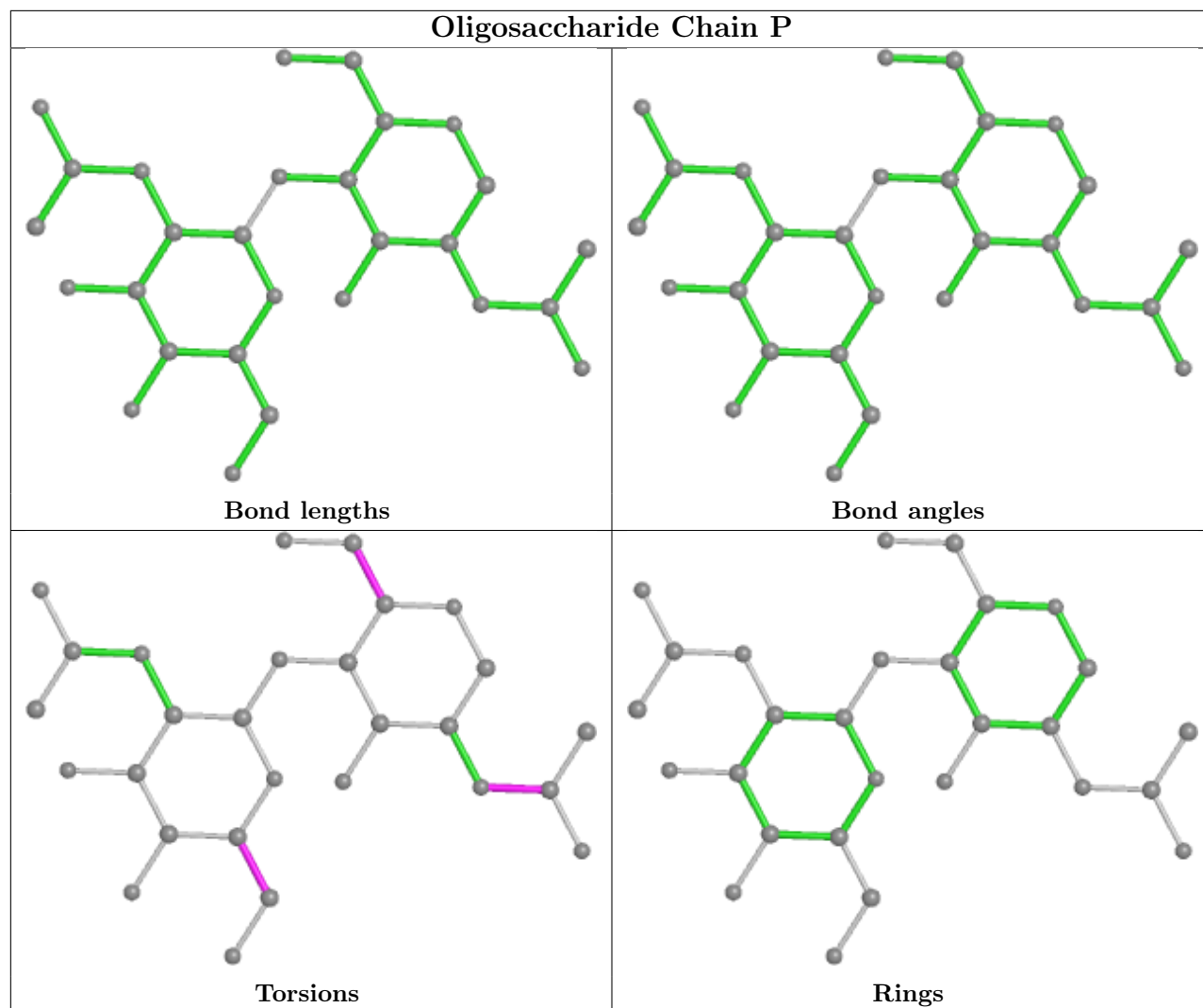


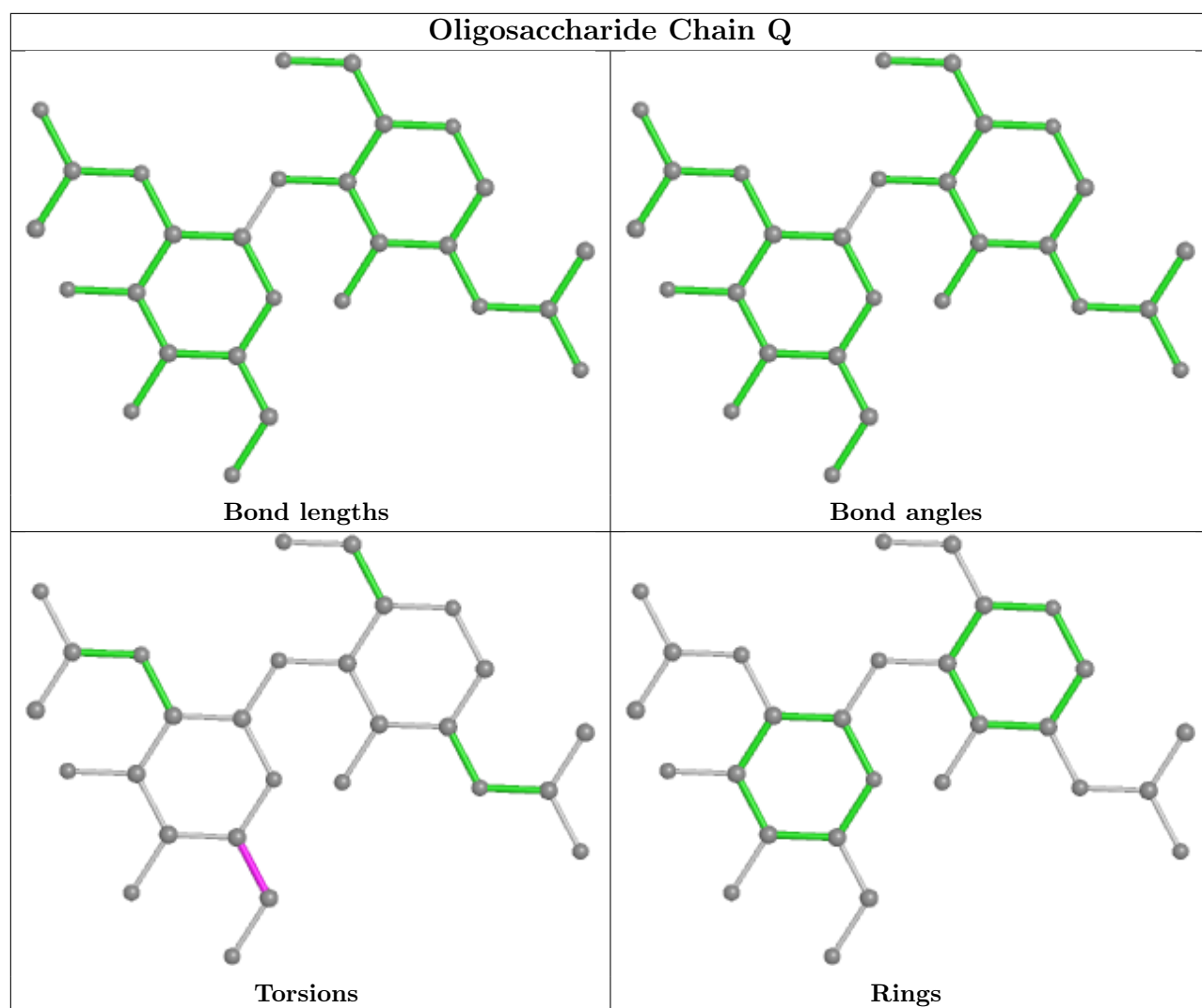


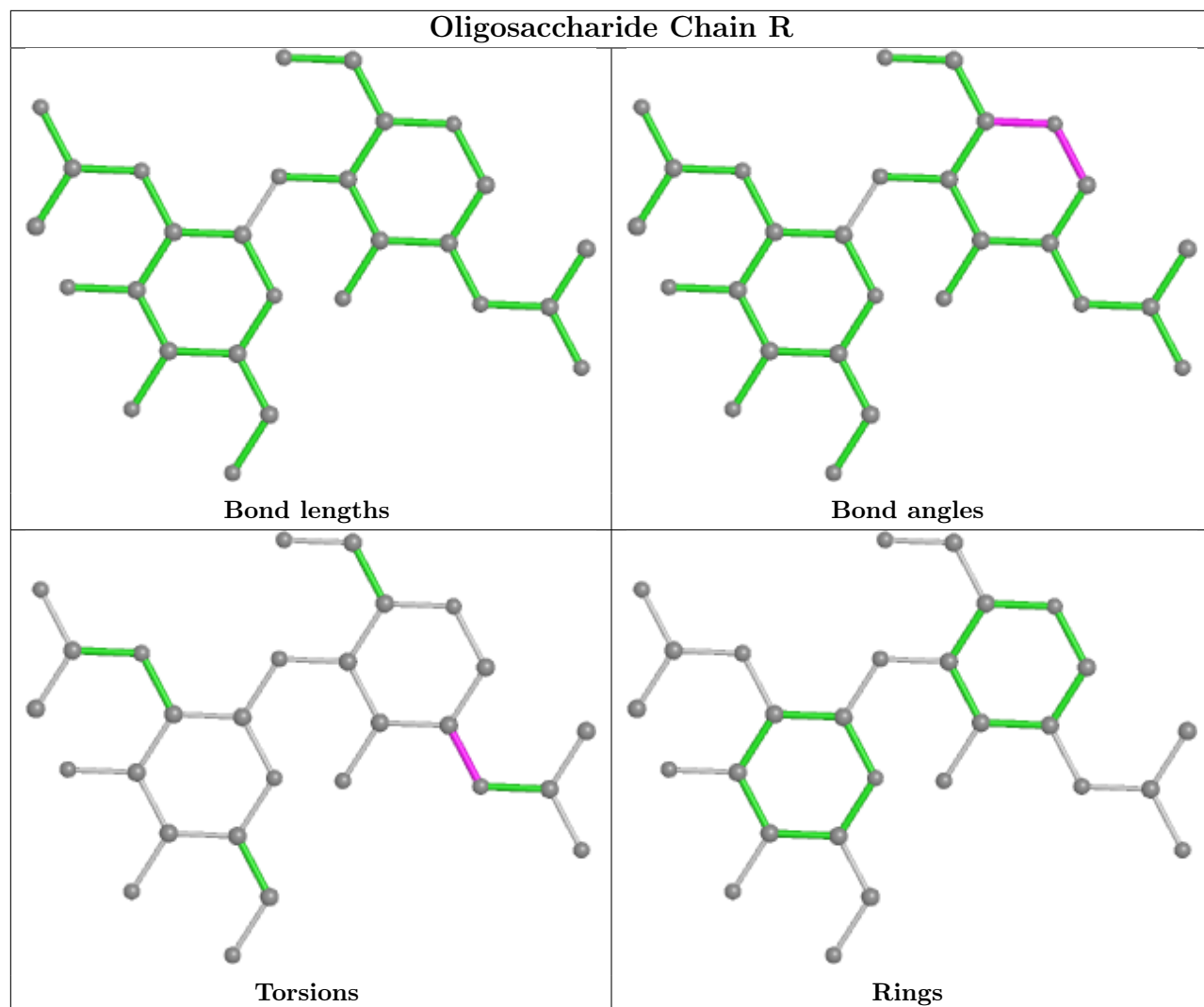


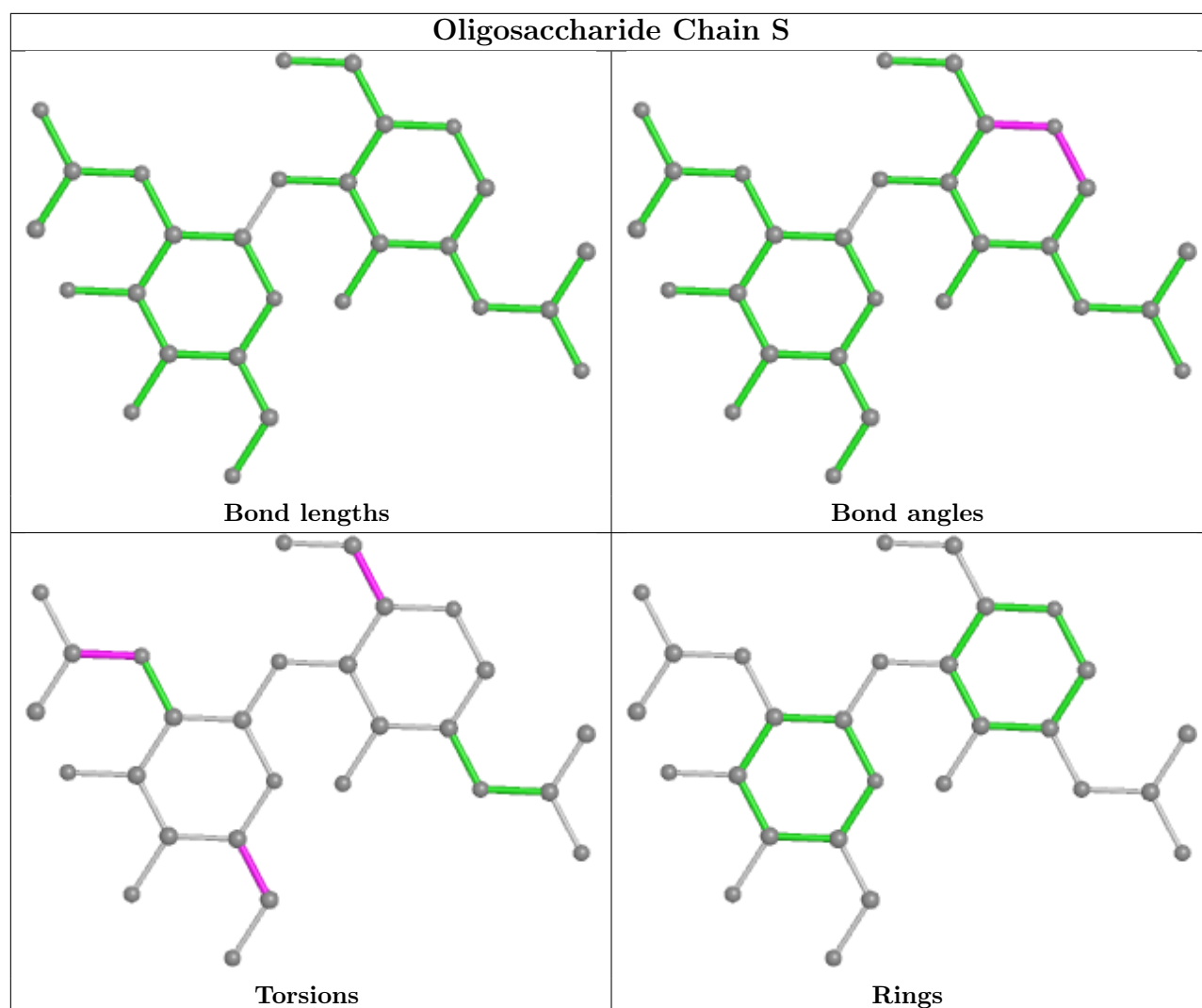


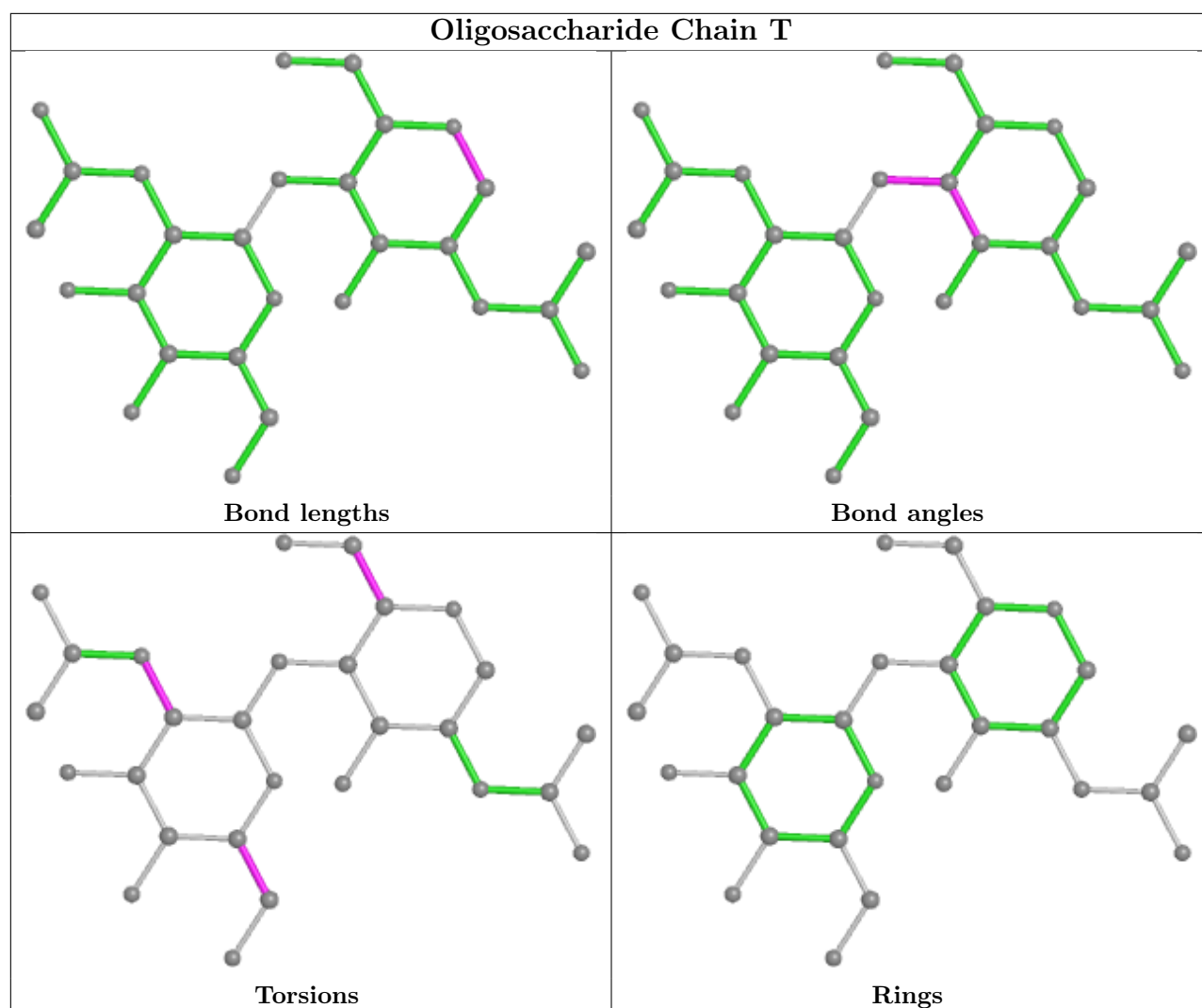


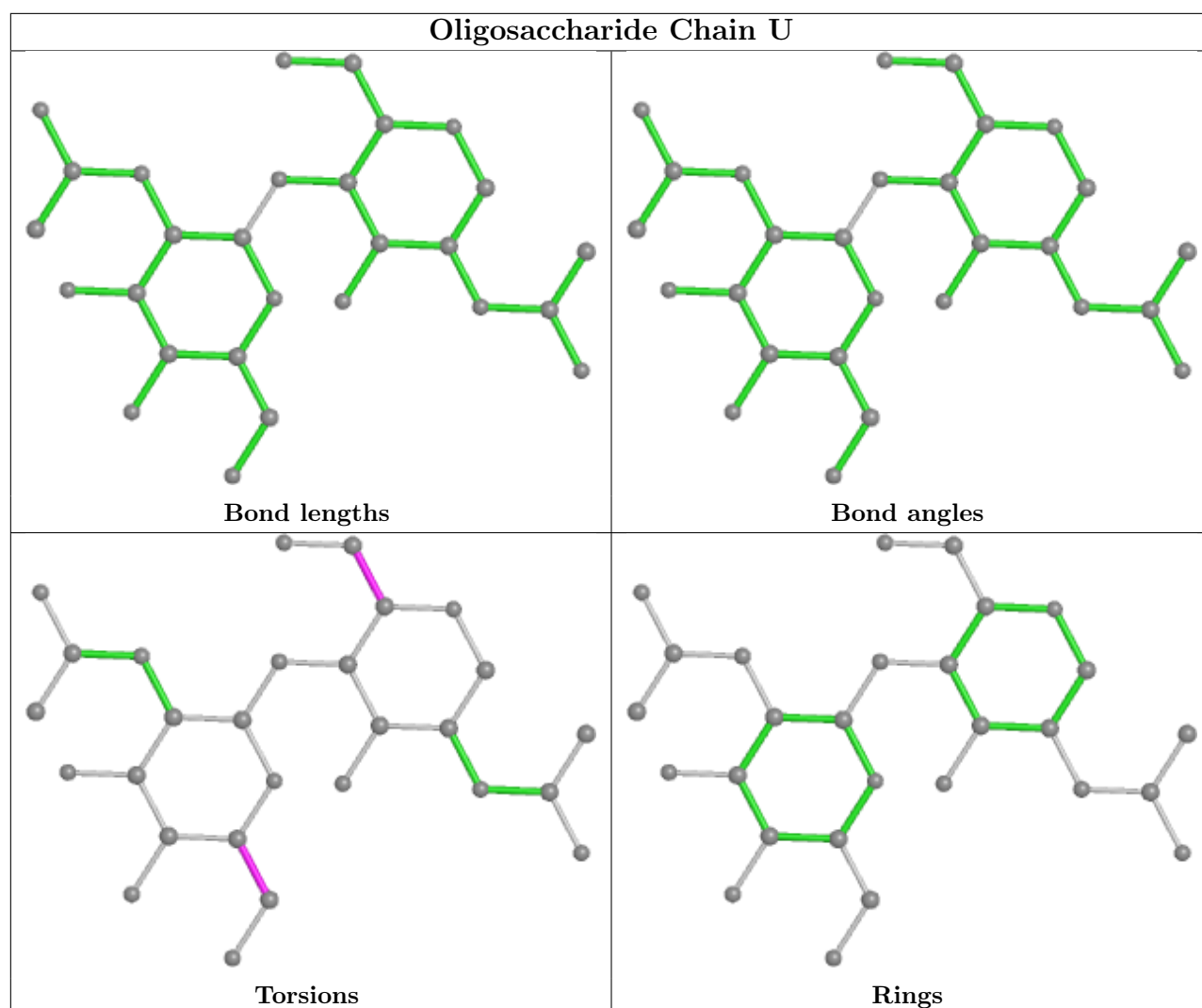


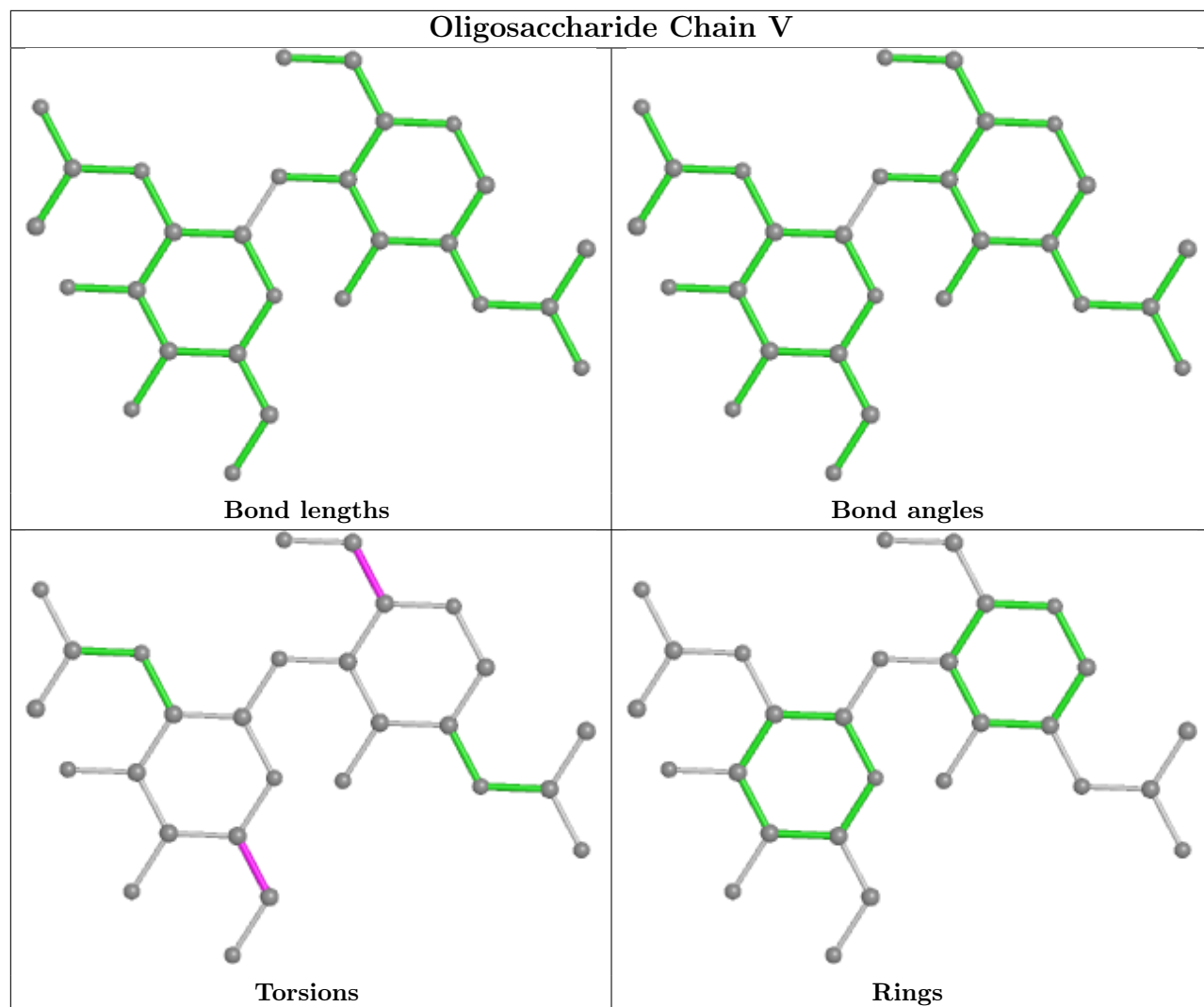


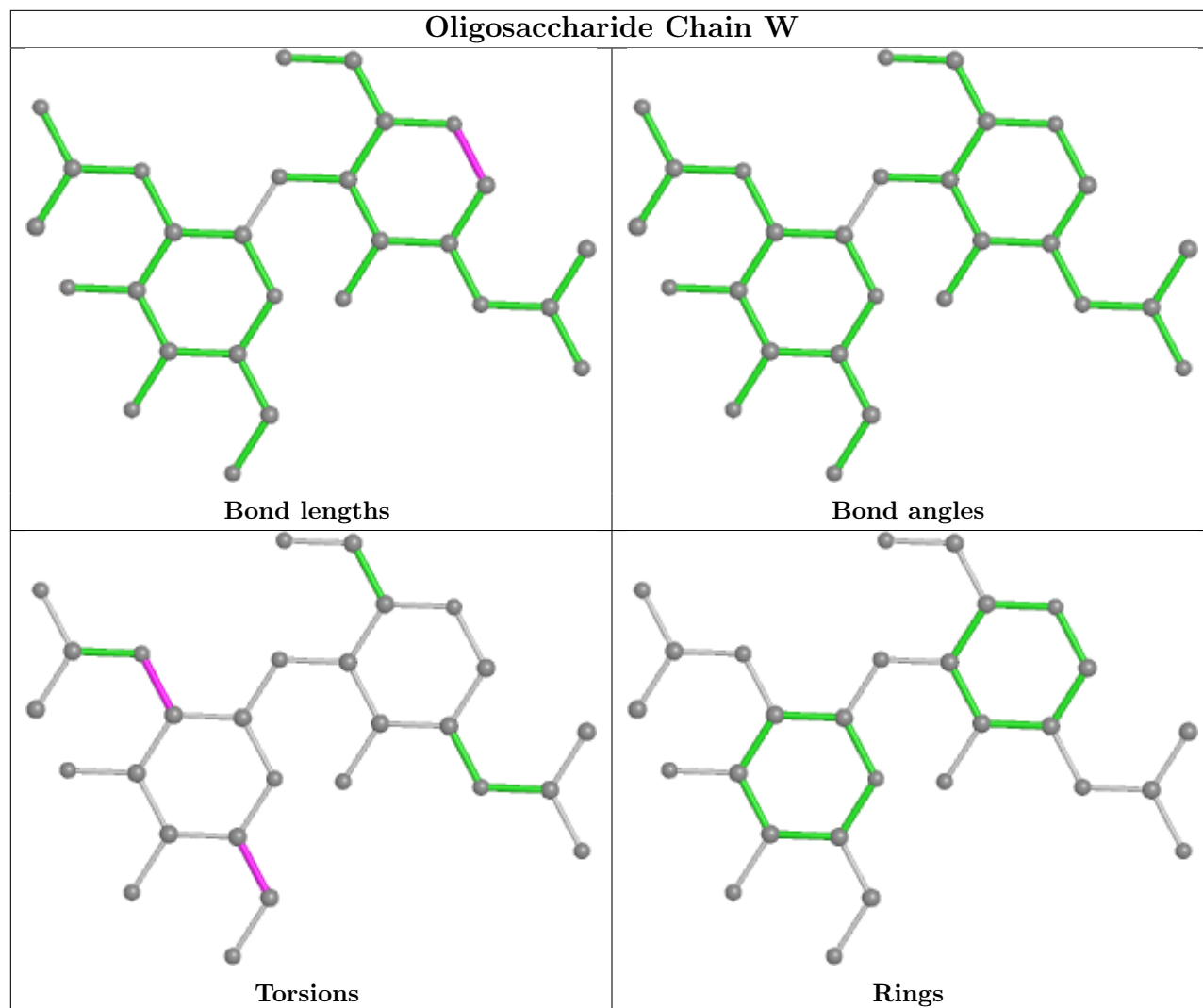


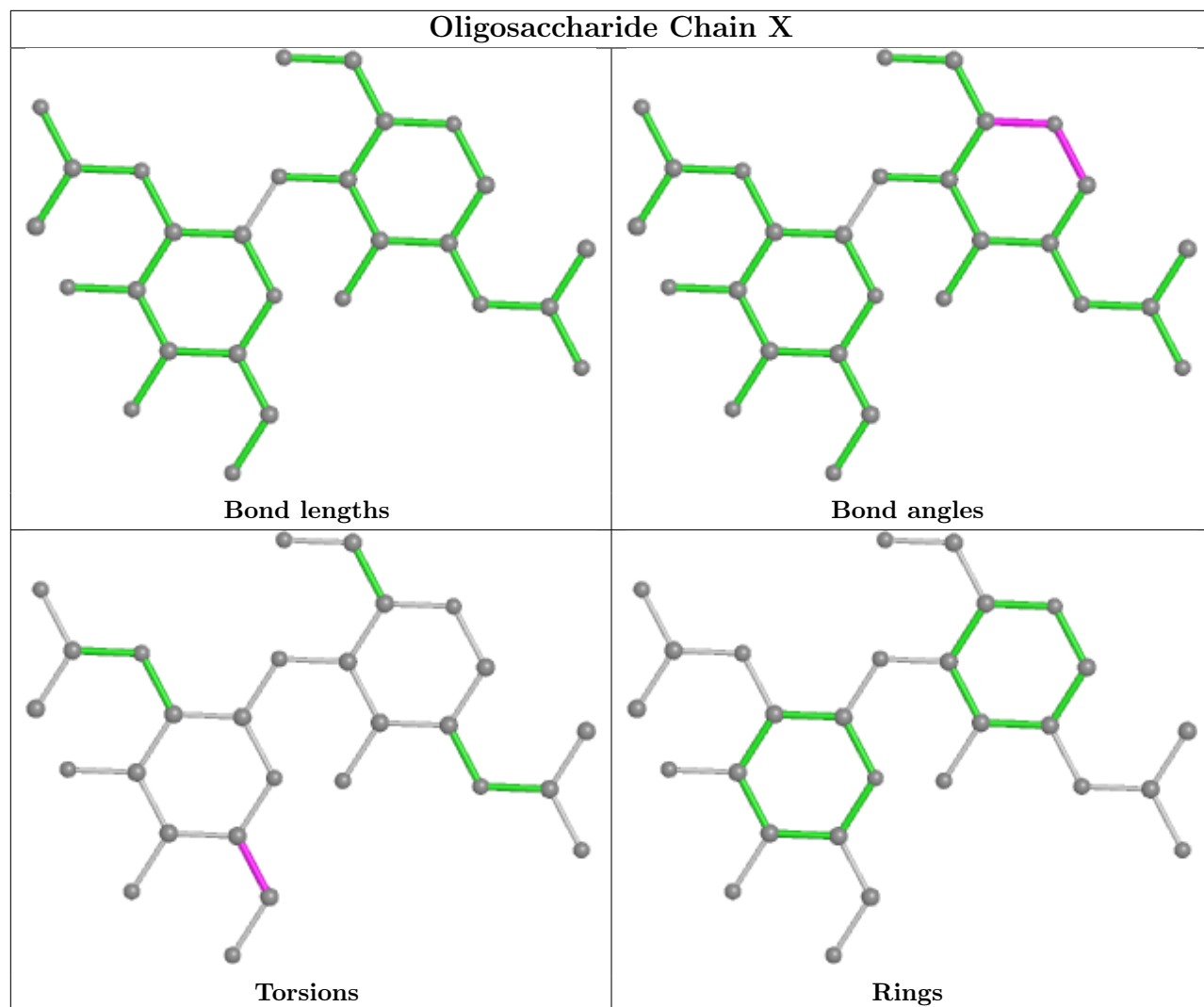


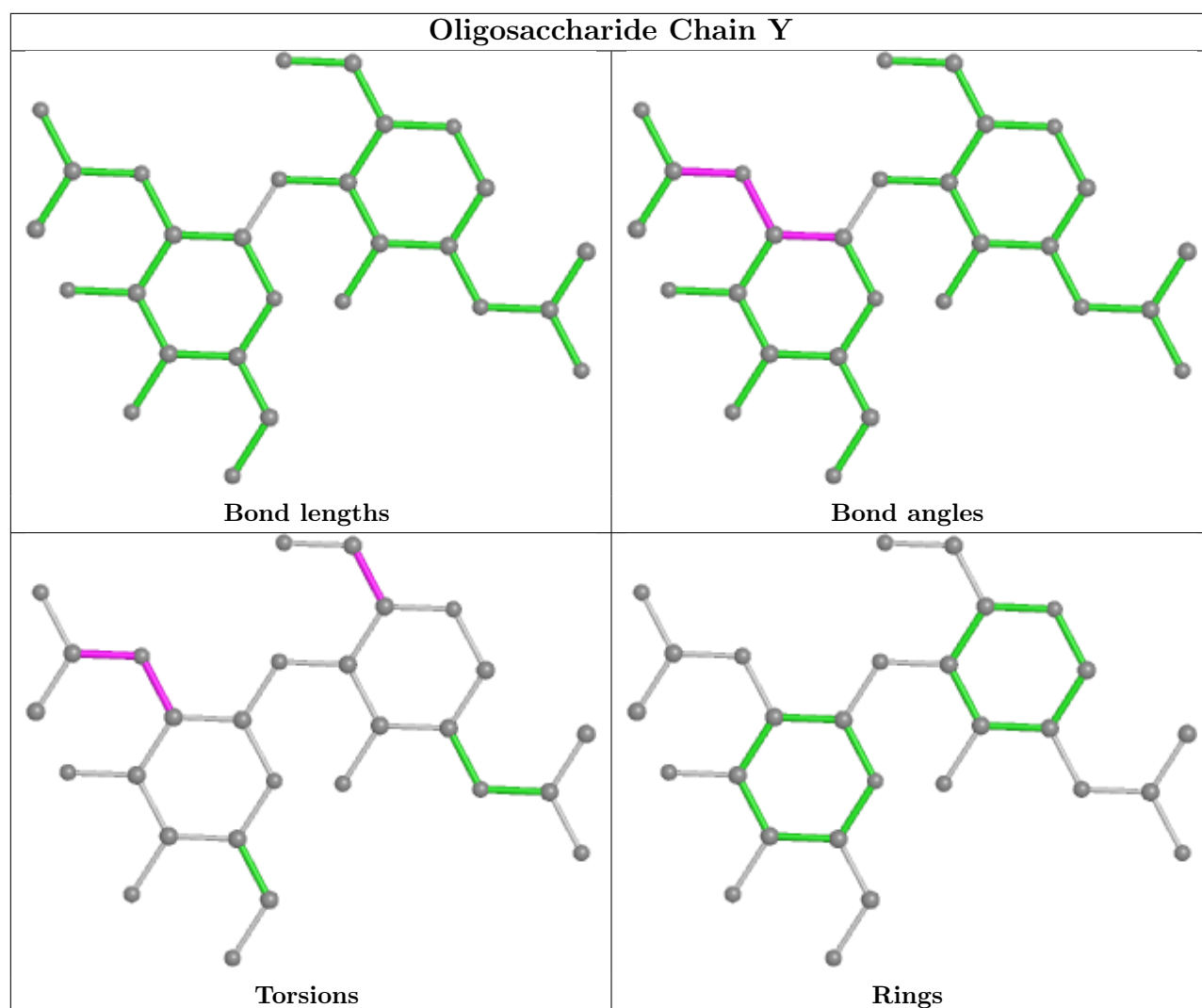


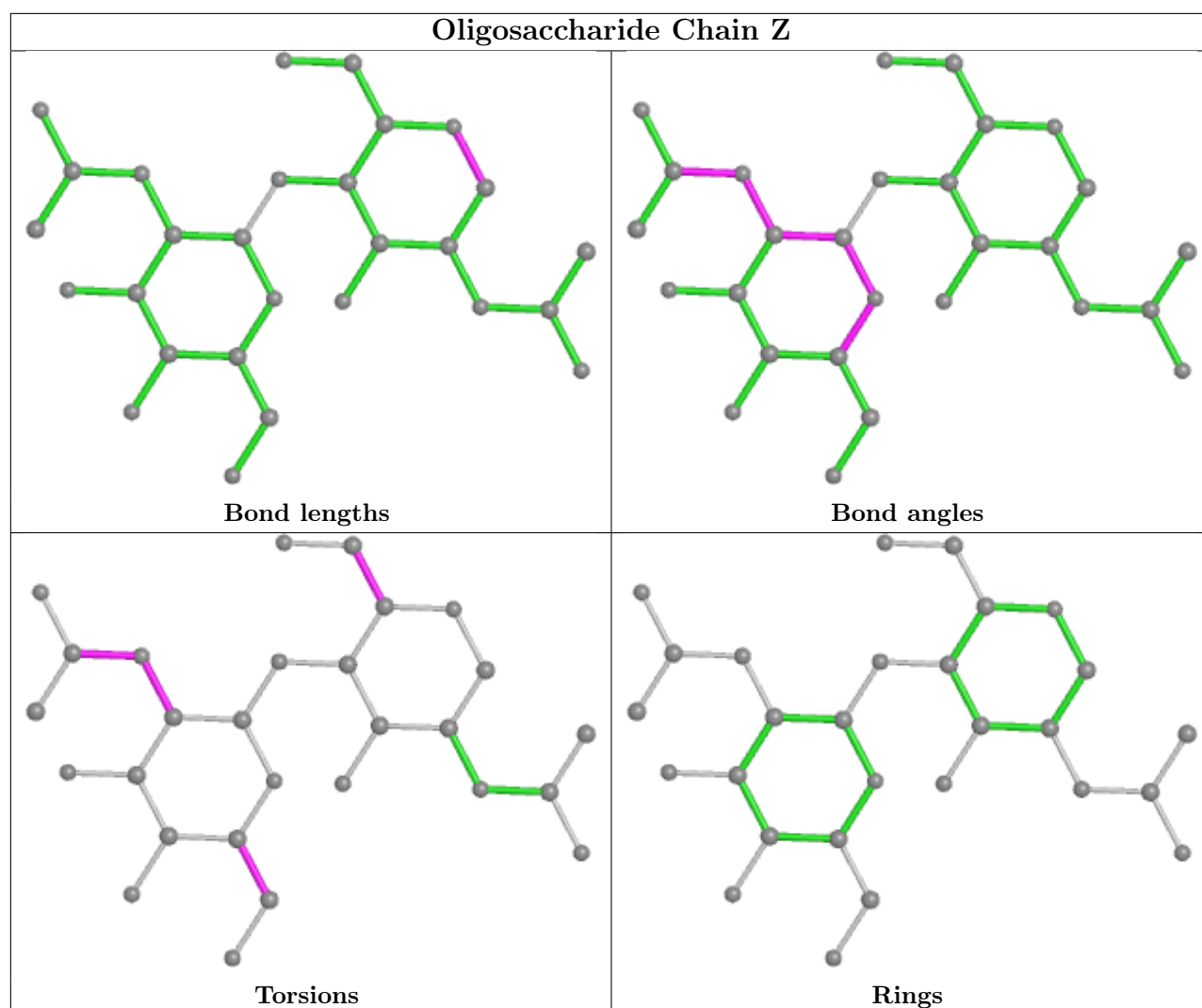


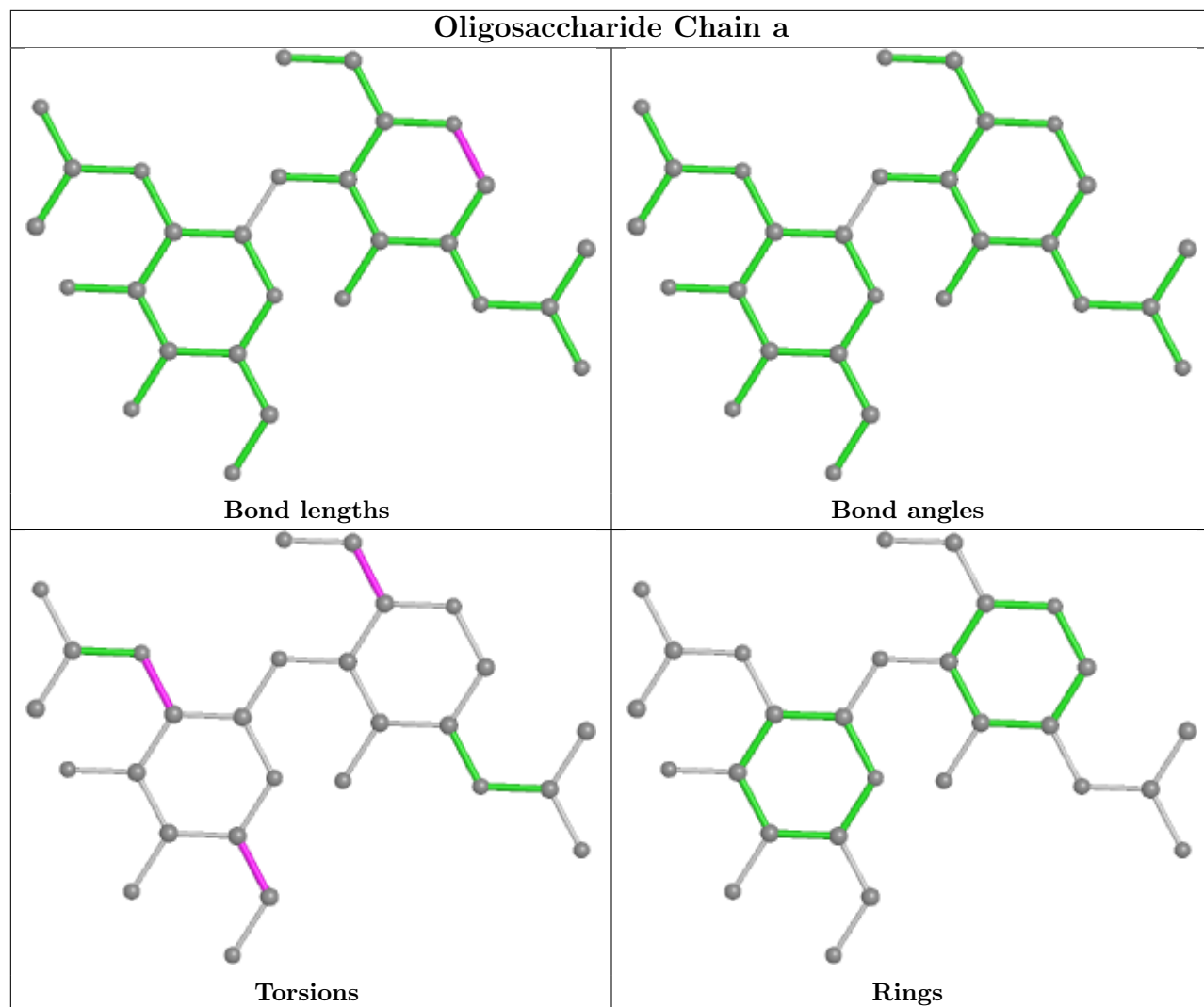


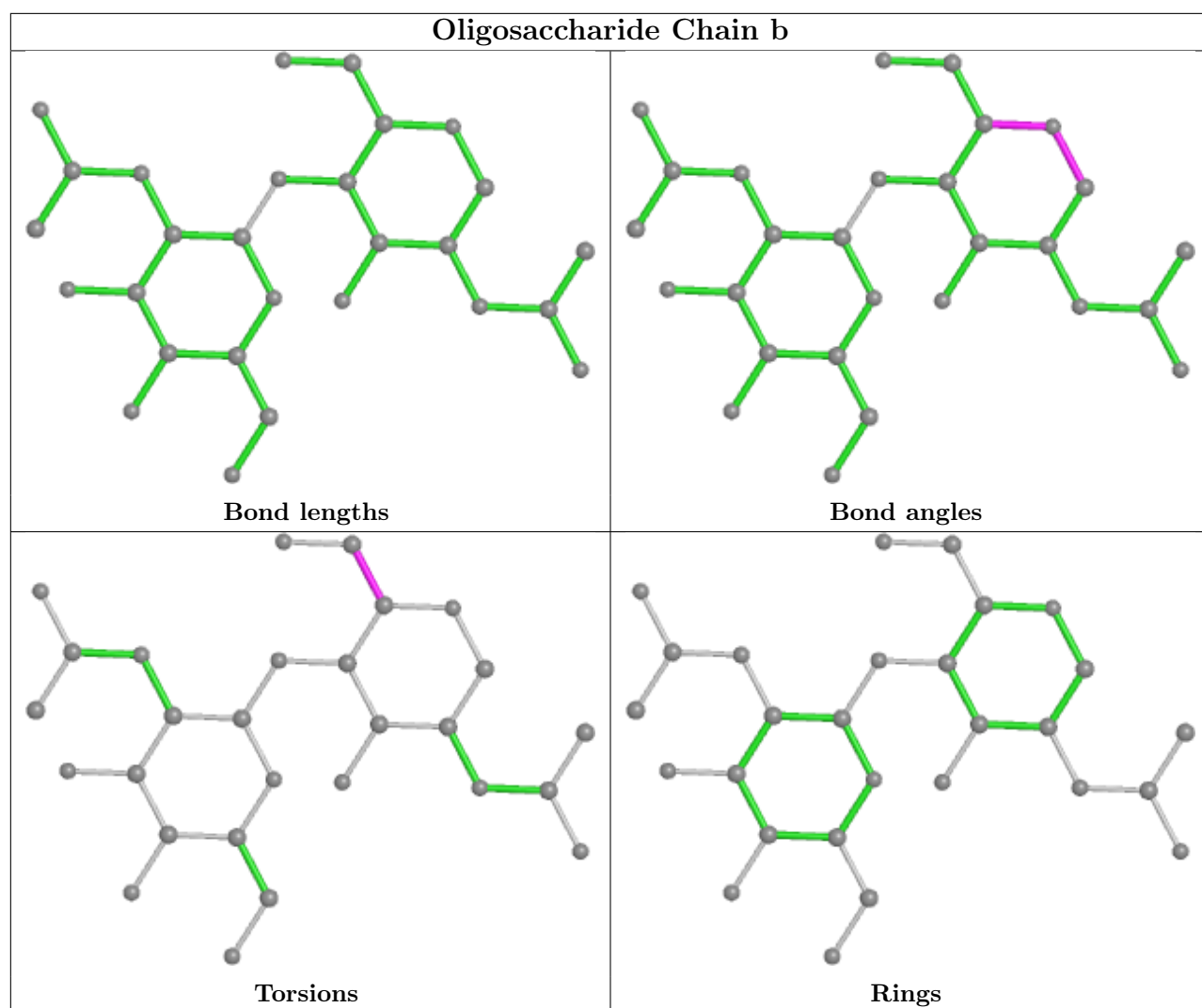


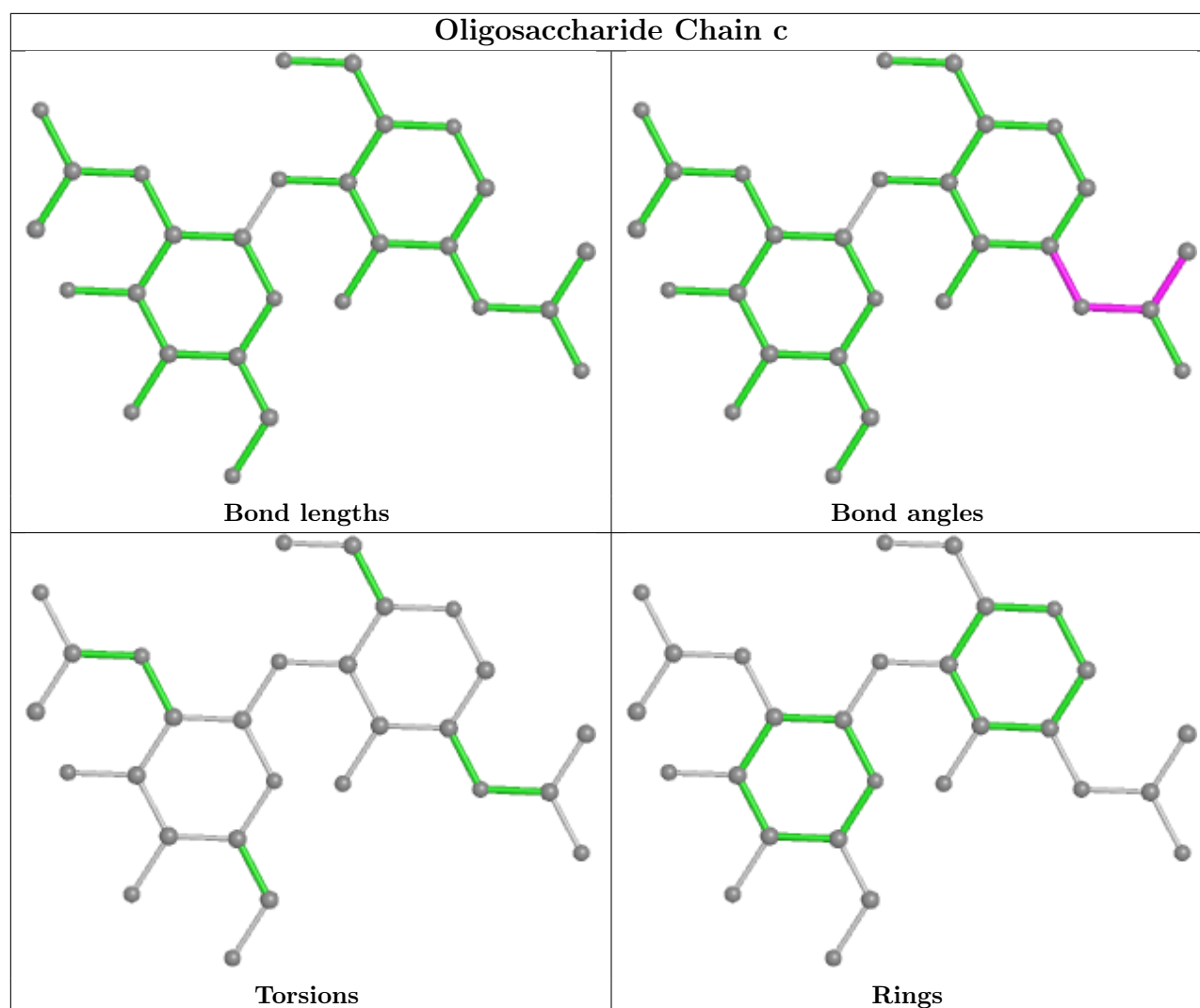












5.6 Ligand geometry [i](#)

26 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	$\# Z > 2$
5	NAG	A	1404	1	14,14,15	0.30	0	17,19,21	0.37	0
5	NAG	C	1406	1	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
5	NAG	C	1402	1	14,14,15	0.34	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1401	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
5	NAG	C	1403	1	14,14,15	0.30	0	17,19,21	0.40	0
5	NAG	C	1404	1	14,14,15	0.33	0	17,19,21	0.59	0
5	NAG	A	1406	1	14,14,15	0.21	0	17,19,21	0.37	0
5	NAG	A	1407	1	14,14,15	0.36	0	17,19,21	0.63	0
5	NAG	B	1404	1	14,14,15	0.44	0	17,19,21	0.54	0
5	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	C	1405	1	14,14,15	0.37	0	17,19,21	1.28	2 (11%)
5	NAG	A	1408	1	14,14,15	0.17	0	17,19,21	0.56	0
5	NAG	B	1401	1	14,14,15	0.29	0	17,19,21	0.34	0
5	NAG	B	1403	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	B	1409	1	14,14,15	0.49	0	17,19,21	0.36	0
5	NAG	A	1403	1	14,14,15	0.55	0	17,19,21	0.45	0
5	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.63	0
5	NAG	A	1402	1	14,14,15	0.46	0	17,19,21	0.57	0
5	NAG	C	1407	1	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
5	NAG	C	1408	1	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	B	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1401	1	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	B	1406	1	14,14,15	0.29	0	17,19,21	0.39	0
5	NAG	C	1409	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	B	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
5	NAG	A	1405	1	14,14,15	0.36	0	17,19,21	1.29	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
5	NAG	A	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1405	NAG	C2-N2-C7	4.31	129.05	122.90
5	A	1405	NAG	C2-N2-C7	4.29	129.02	122.90
5	C	1405	NAG	C2-N2-C7	4.15	128.81	122.90
5	A	1401	NAG	C1-O5-C5	2.88	116.09	112.19
5	C	1406	NAG	C1-O5-C5	2.57	115.67	112.19
5	C	1407	NAG	C1-O5-C5	2.40	115.44	112.19
5	A	1405	NAG	C1-C2-N2	2.22	114.28	110.49
5	C	1405	NAG	C1-C2-N2	2.11	114.09	110.49

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1408	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1406	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	B	1409	NAG	C4-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	B	1408	NAG	O5-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	C	1404	NAG	C4-C5-C6-O6
5	C	1407	NAG	O5-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	A	1405	NAG	C8-C7-N2-C2
5	A	1405	NAG	O7-C7-N2-C2
5	A	1406	NAG	C8-C7-N2-C2
5	A	1406	NAG	O7-C7-N2-C2
5	C	1405	NAG	C8-C7-N2-C2
5	C	1405	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	B	1409	NAG	O5-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	C	1407	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	C	1405	NAG	O5-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	A	1407	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	C	1409	NAG	C4-C5-C6-O6
5	A	1403	NAG	C1-C2-N2-C7
5	B	1408	NAG	C4-C5-C6-O6
5	C	1406	NAG	C4-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1407	NAG	O5-C5-C6-O6
5	C	1409	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	C	1405	NAG	C4-C5-C6-O6
5	C	1406	NAG	O5-C5-C6-O6
5	B	1407	NAG	C1-C2-N2-C7
5	A	1407	NAG	C3-C2-N2-C7
5	C	1406	NAG	C3-C2-N2-C7
5	C	1407	NAG	C3-C2-N2-C7
5	A	1403	NAG	C3-C2-N2-C7
5	A	1405	NAG	C3-C2-N2-C7
5	C	1405	NAG	C3-C2-N2-C7
5	B	1405	NAG	C3-C2-N2-C7

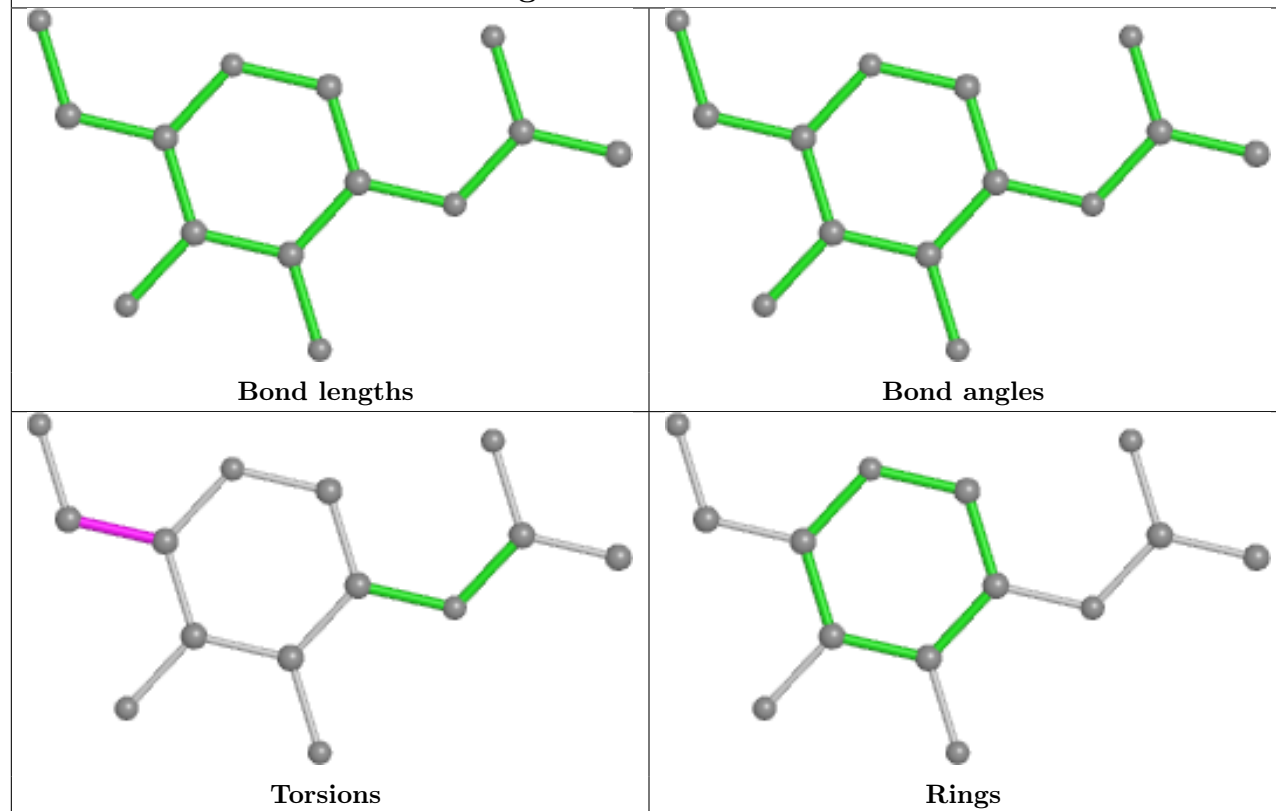
There are no ring outliers.

8 monomers are involved in 12 short contacts:

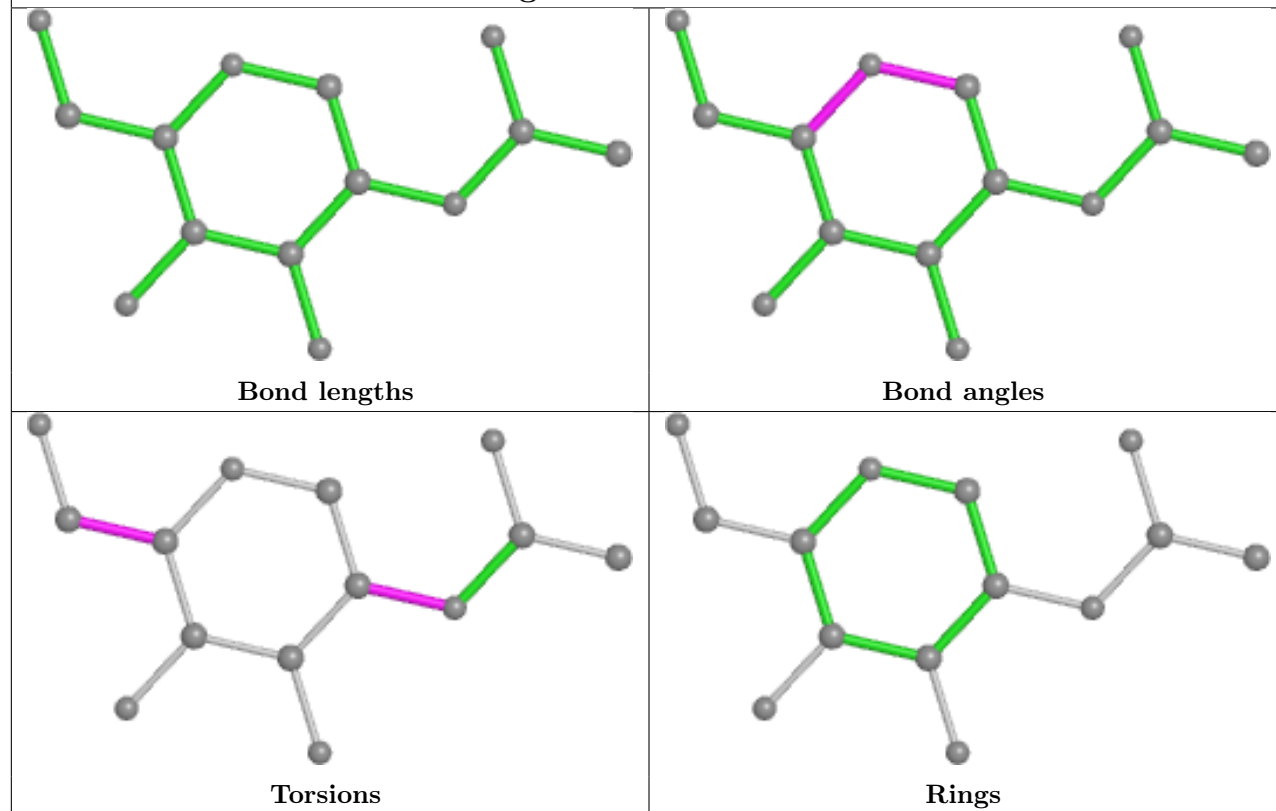
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1402	NAG	1	0
5	C	1403	NAG	2	0
5	C	1405	NAG	2	0
5	B	1402	NAG	3	0
5	A	1402	NAG	1	0
5	C	1407	NAG	1	0
5	B	1405	NAG	1	0
5	A	1405	NAG	1	0

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 A 1404



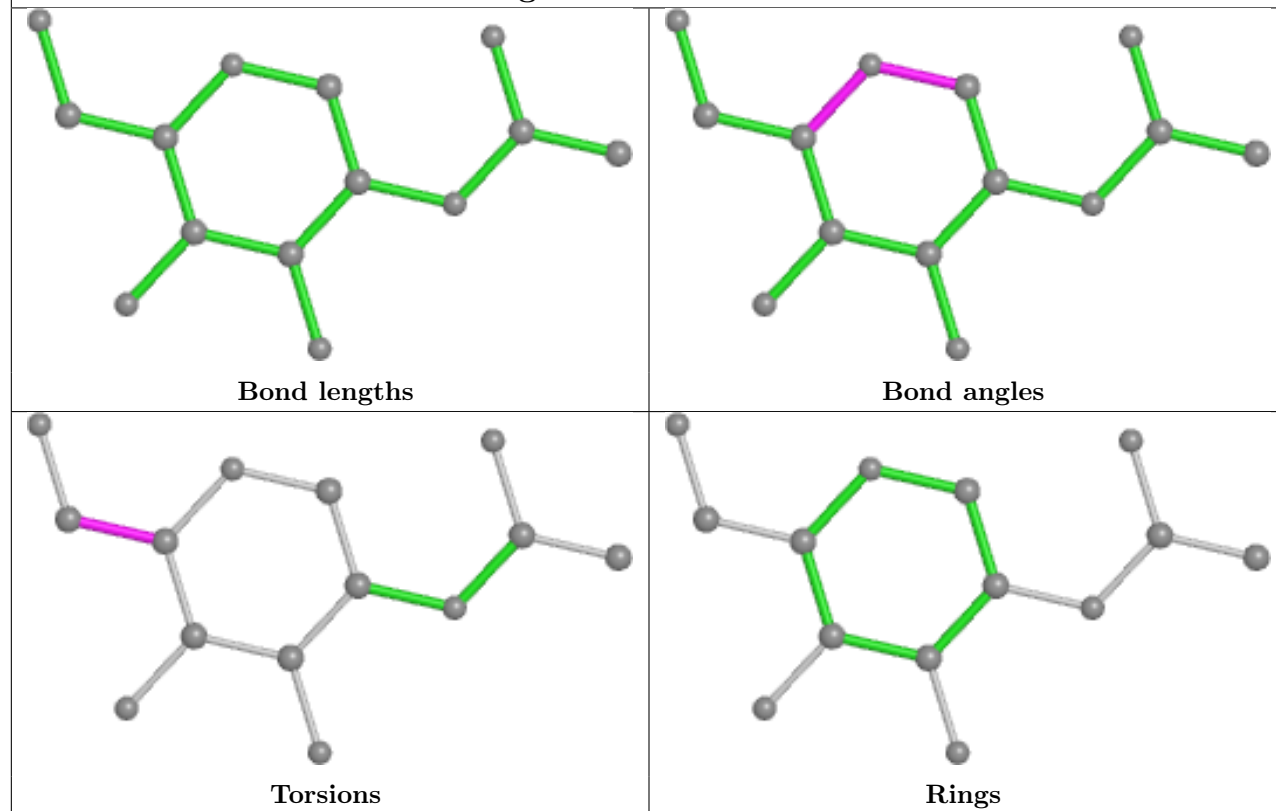
Ligand NAG C 1406



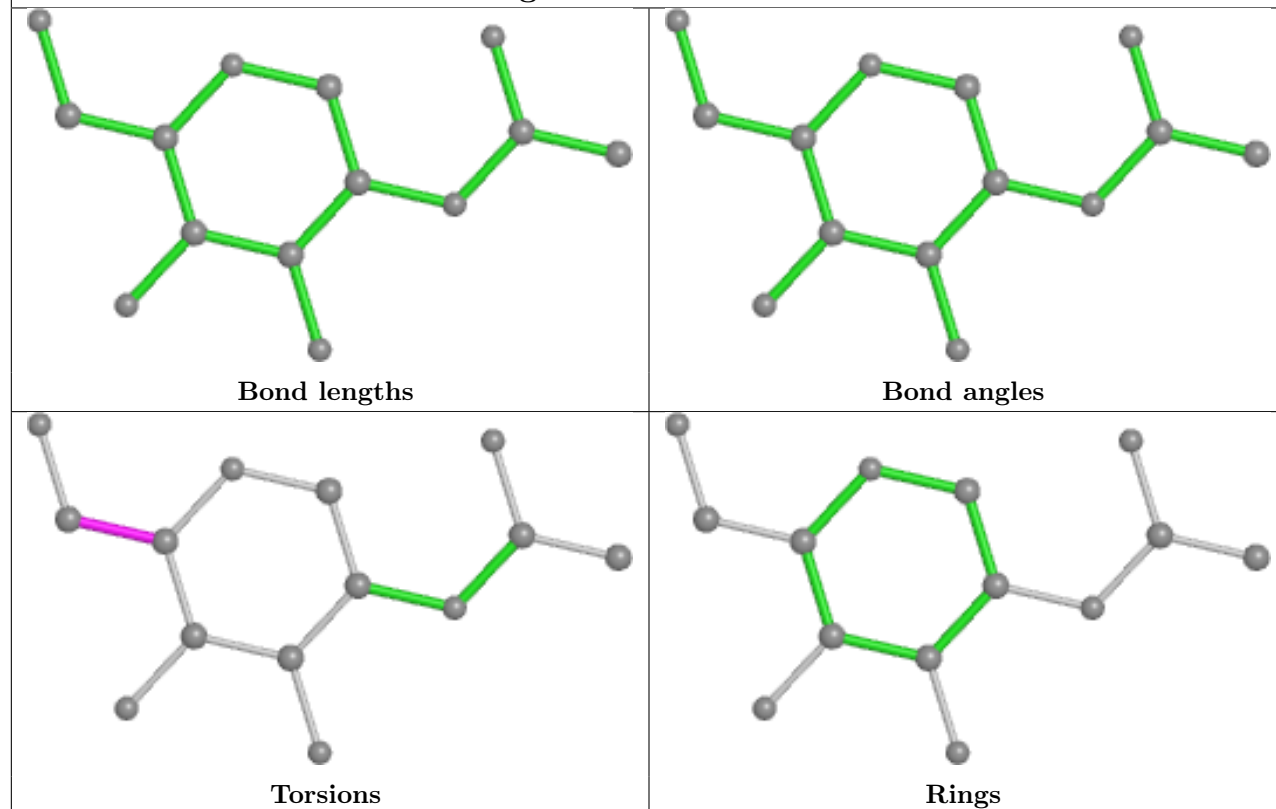
Ligand NAG C 1402



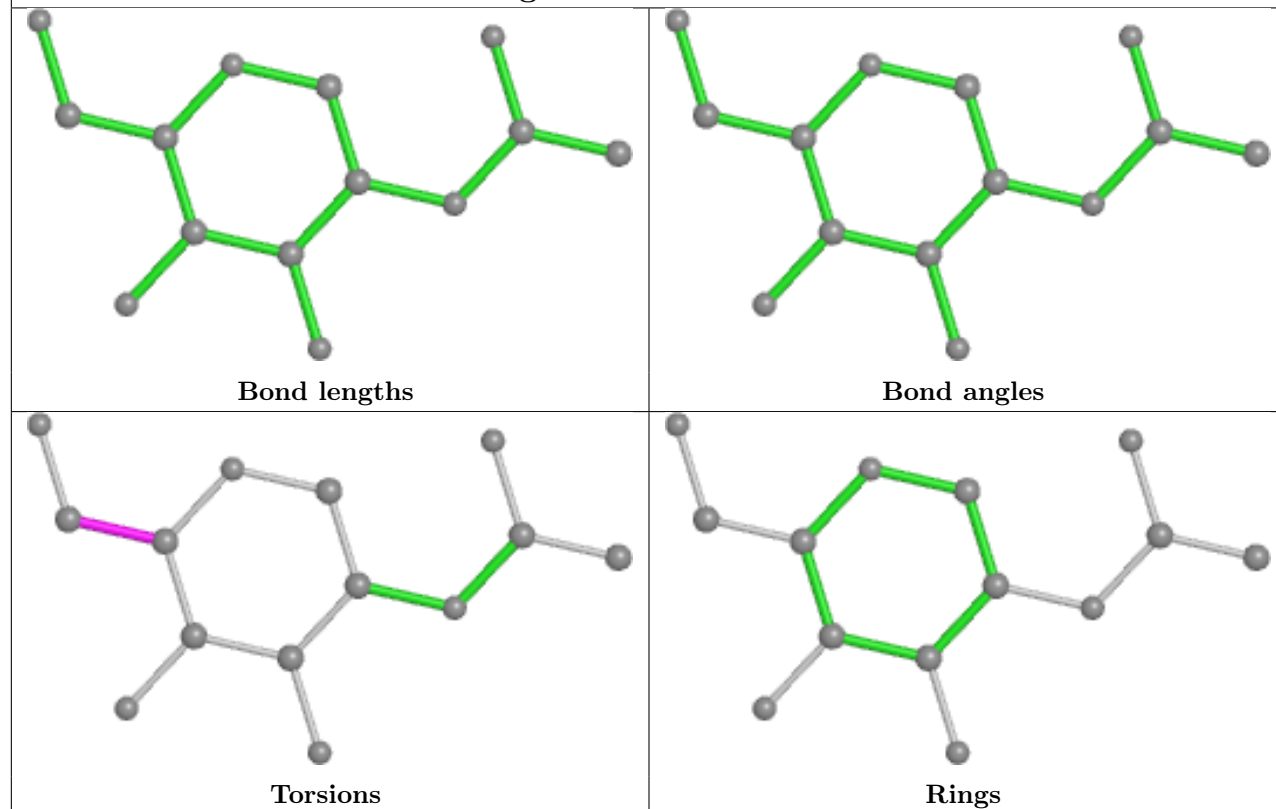
Ligand NAG A 1401



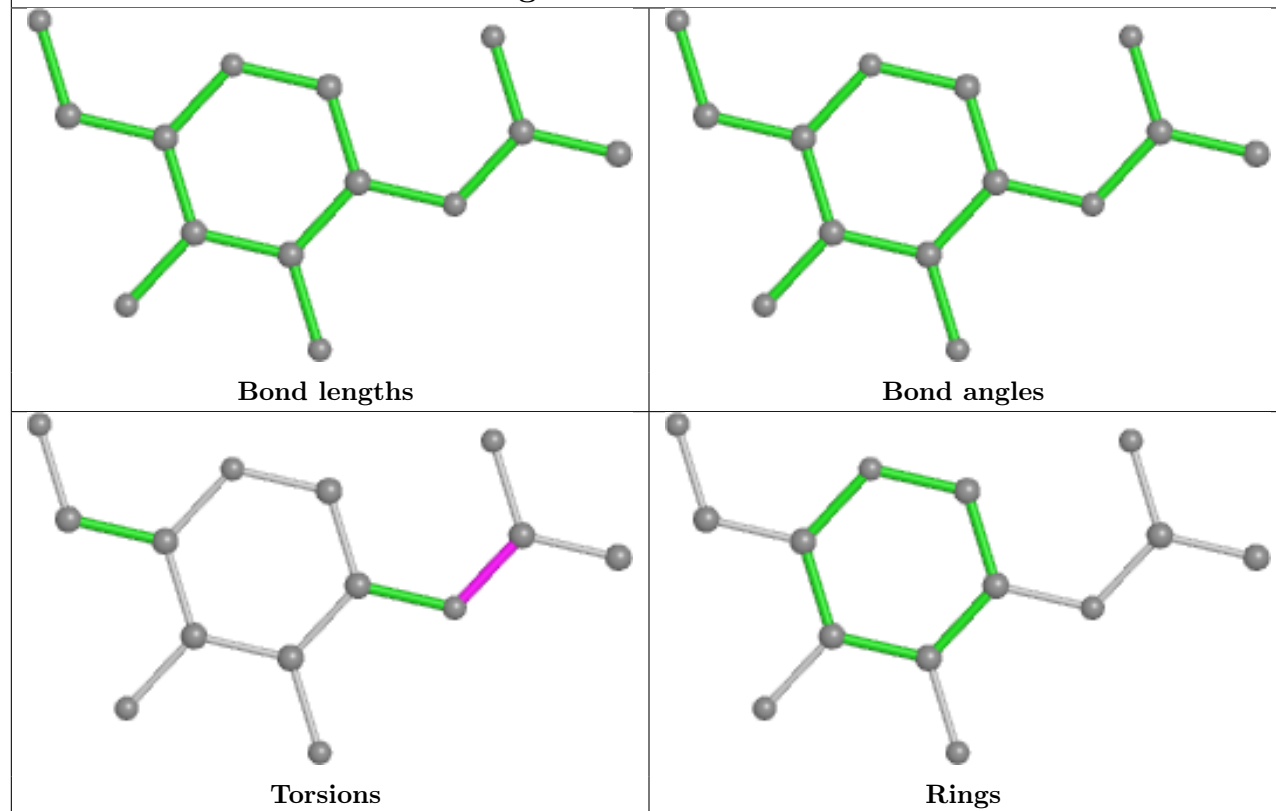
Ligand NAG C 1403



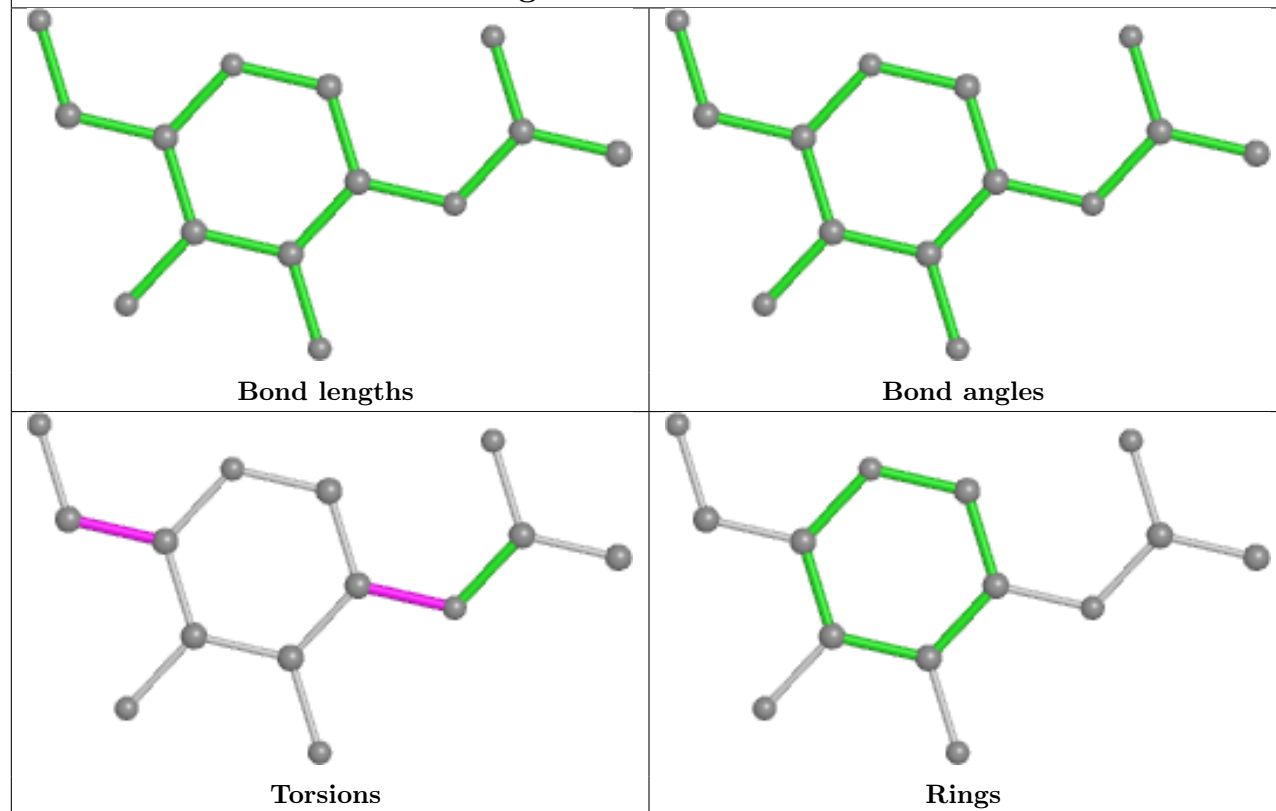
Ligand NAG C 1404



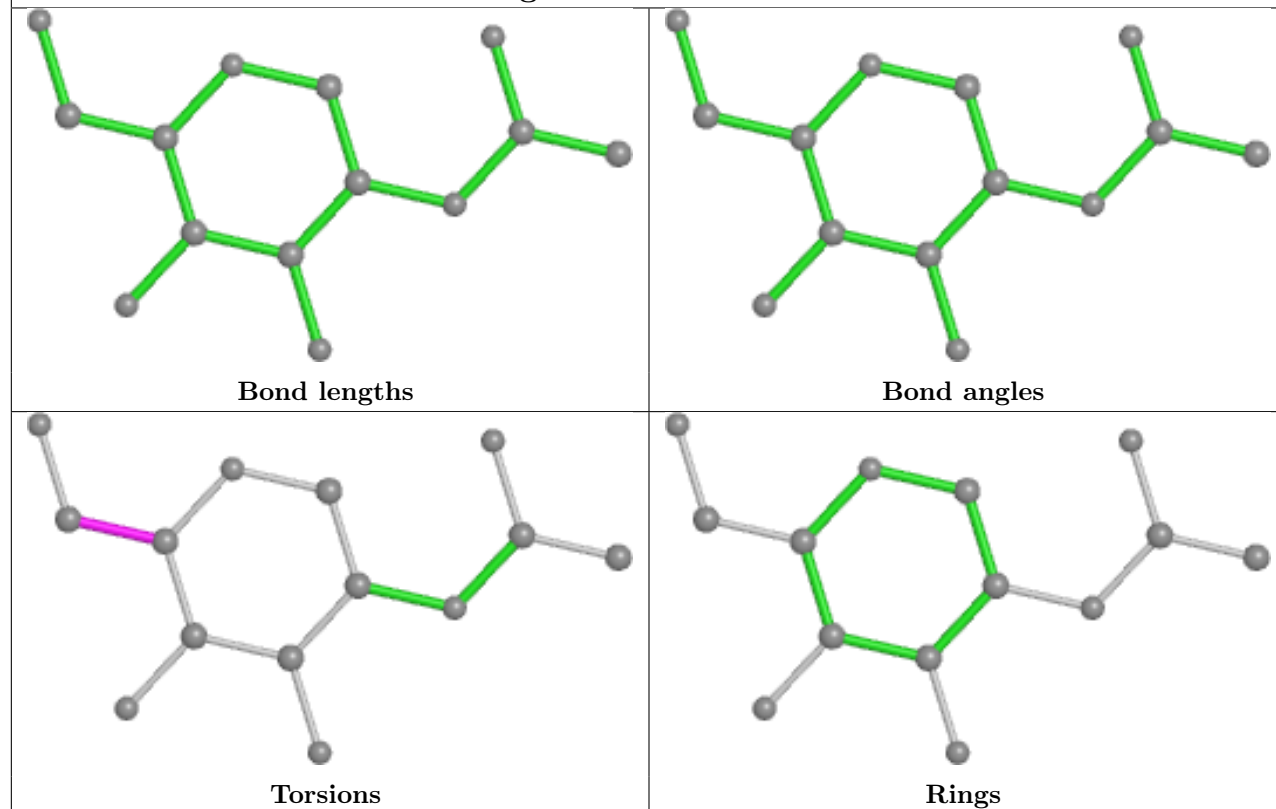
Ligand NAG A 1406



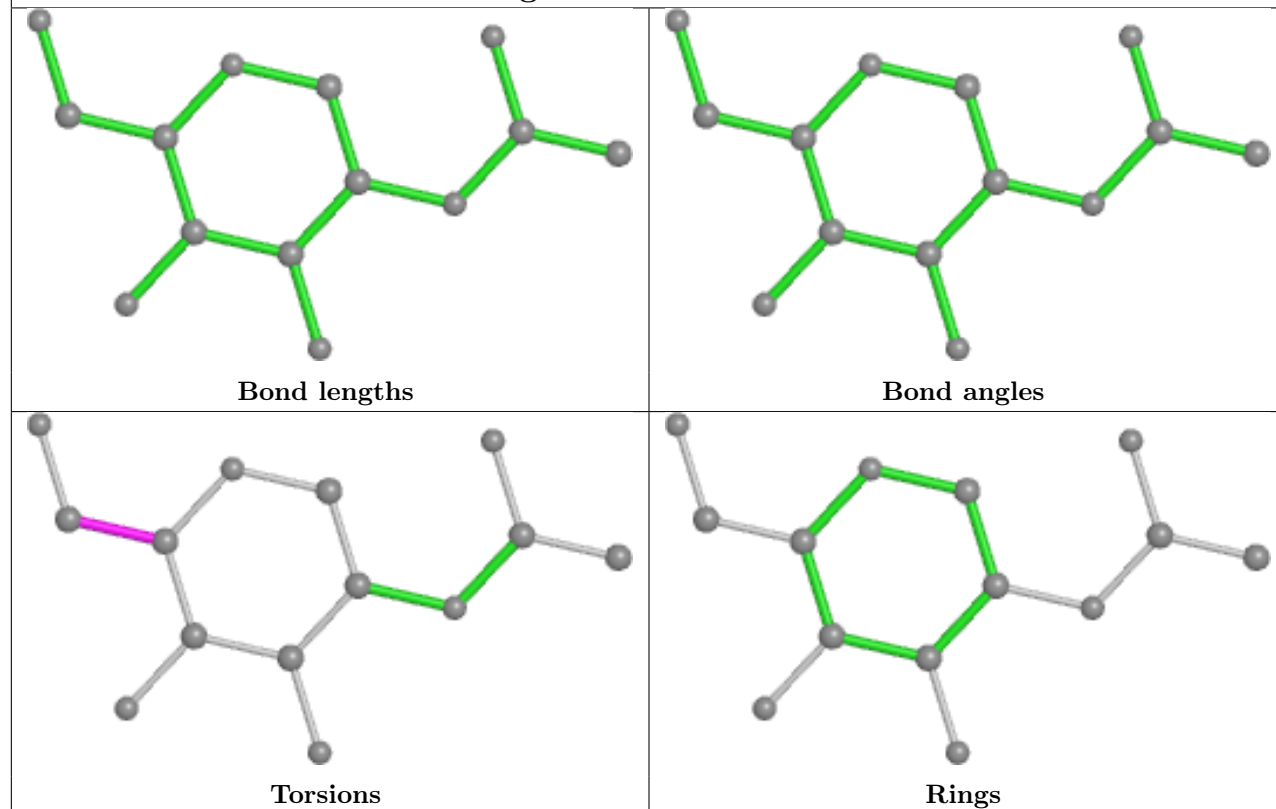
Ligand NAG A 1407



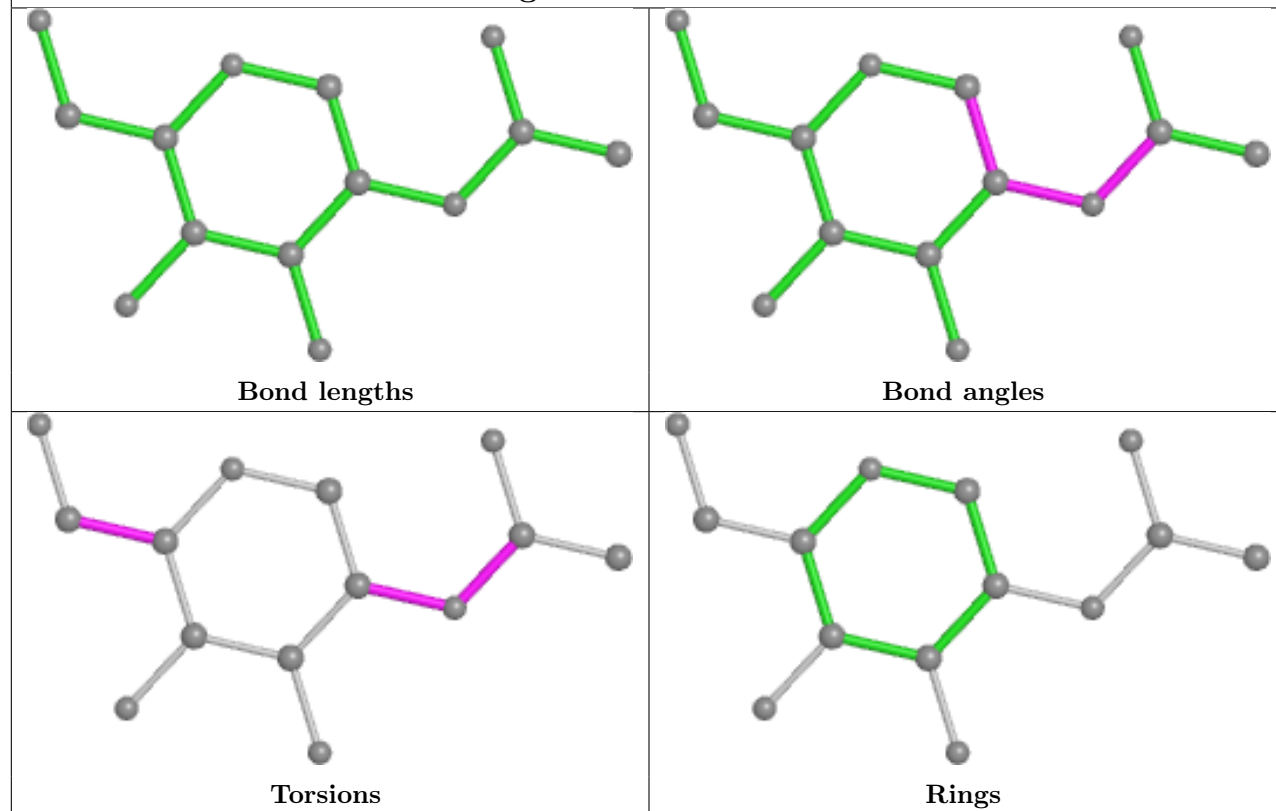
Ligand NAG B 1404



Ligand NAG B 1408



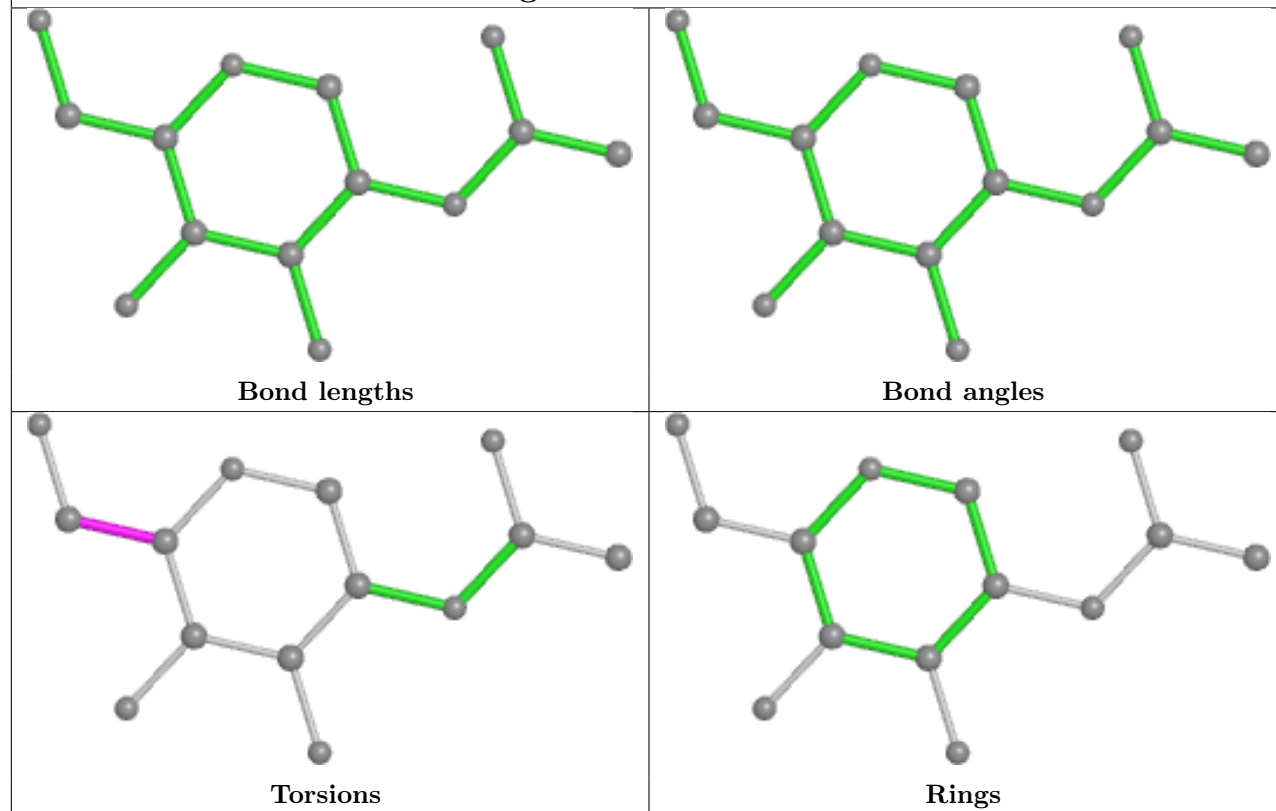
Ligand NAG C 1405



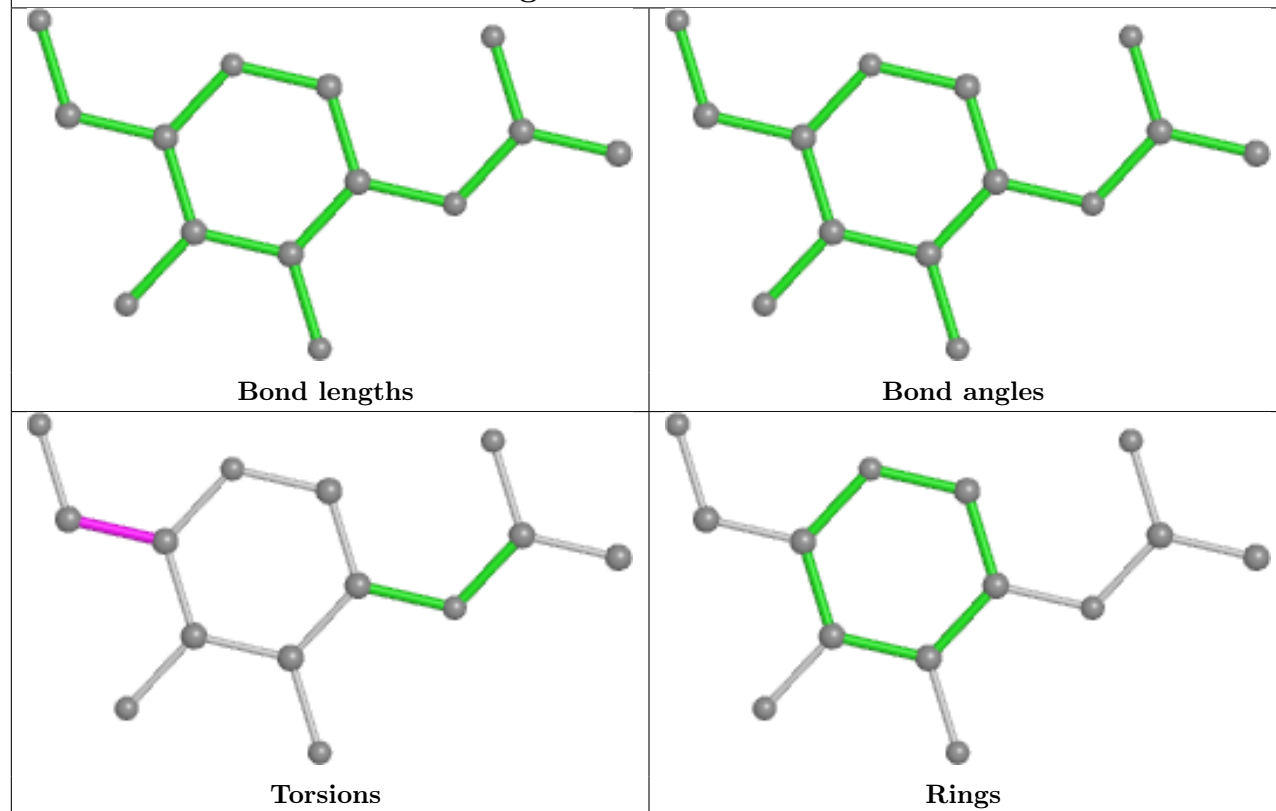
Ligand NAG A 1408



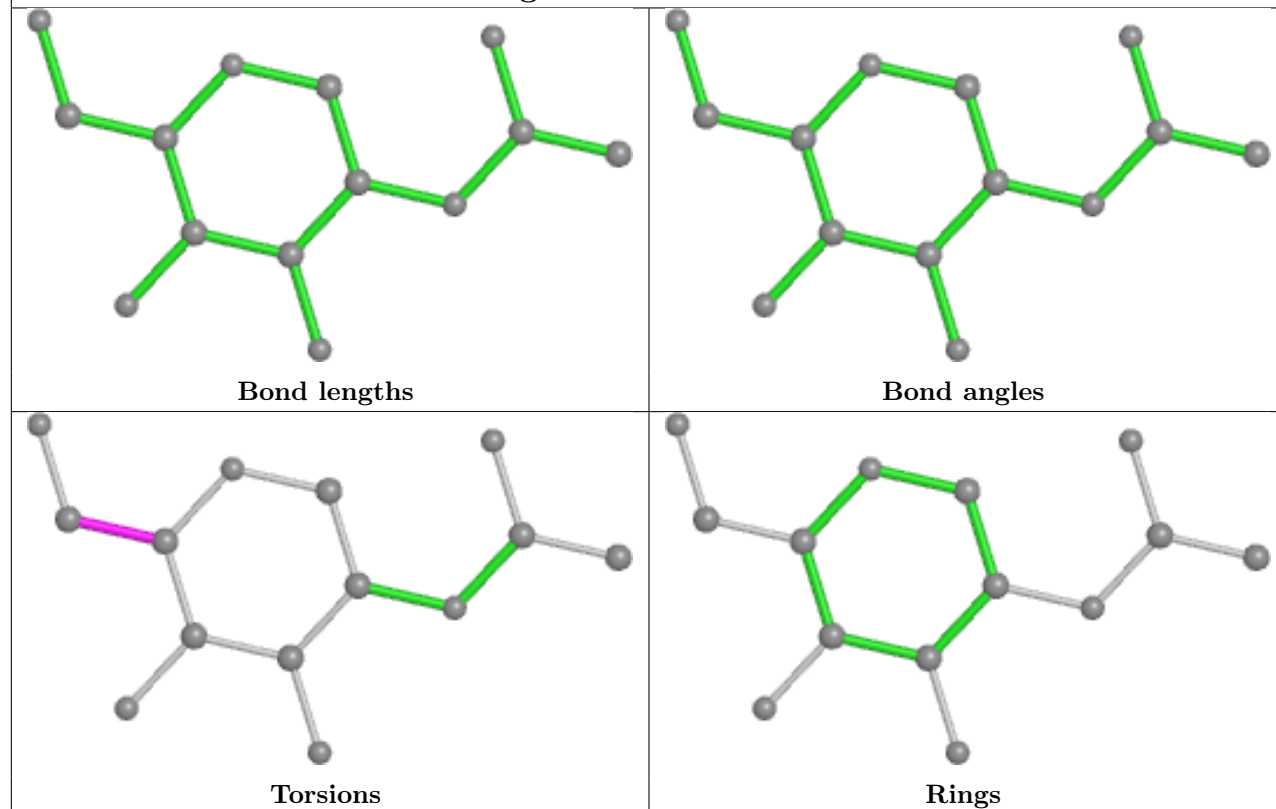
Ligand NAG B 1401



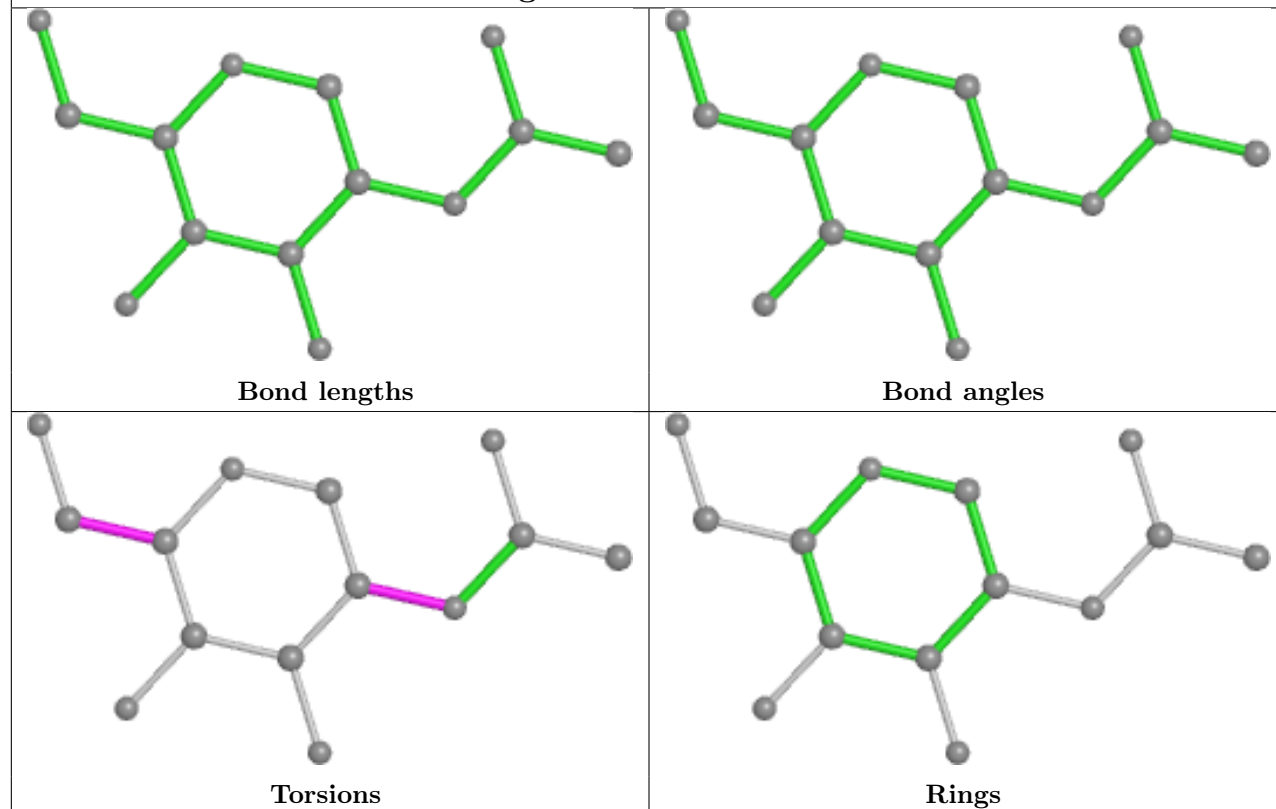
Ligand NAG B 1403



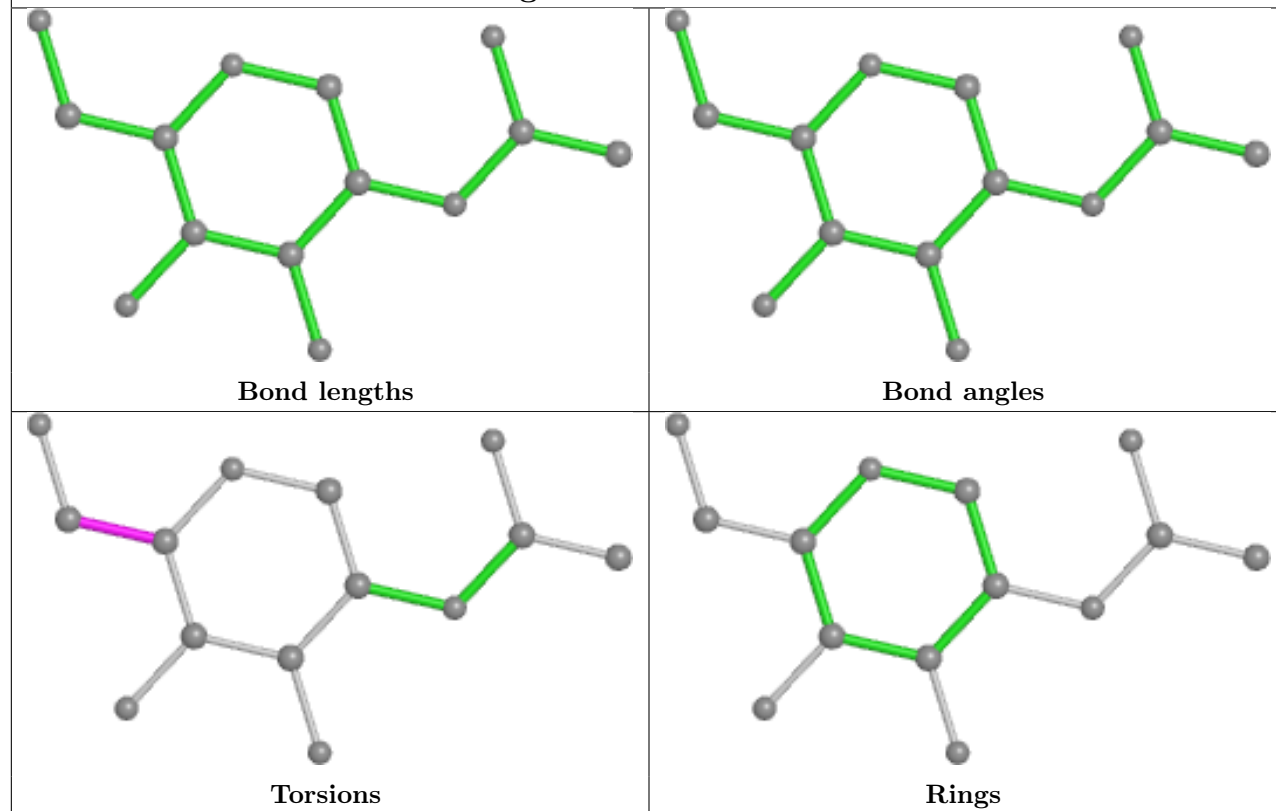
Ligand NAG B 1409



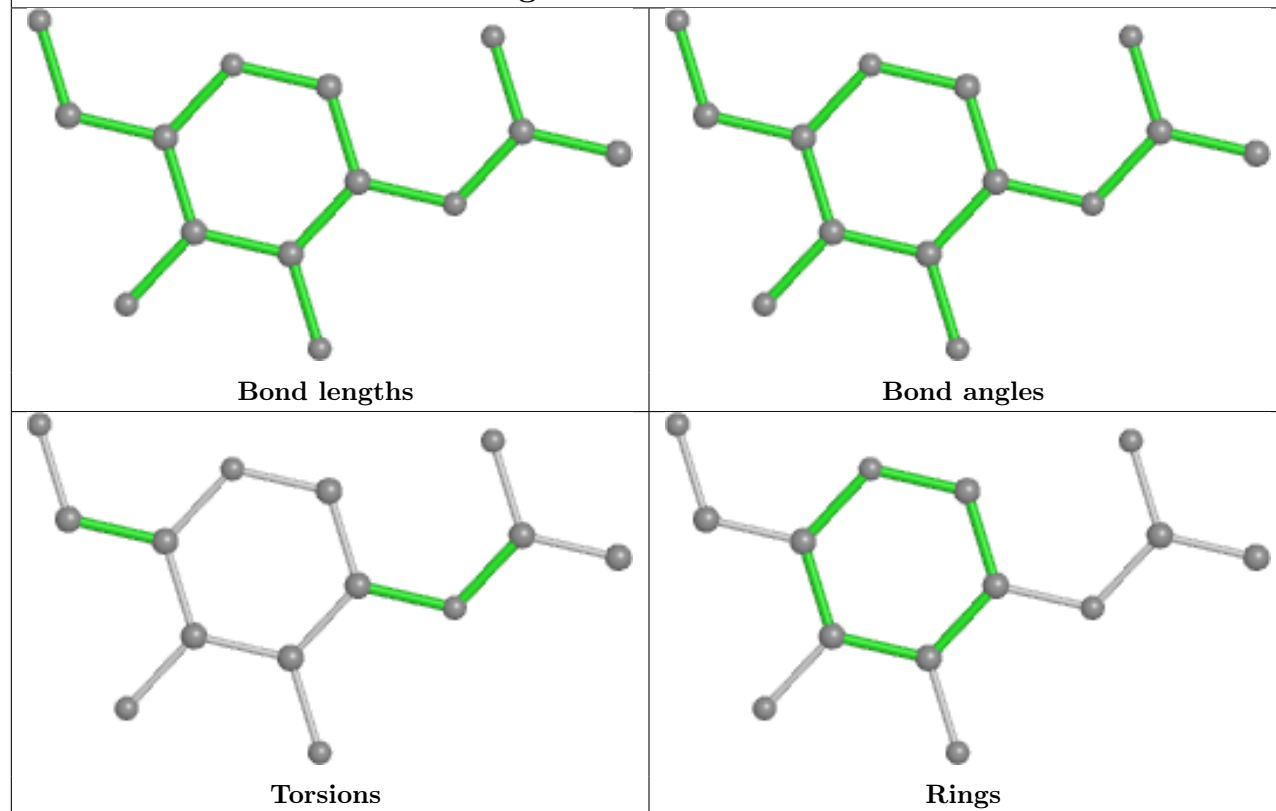
Ligand NAG A 1403



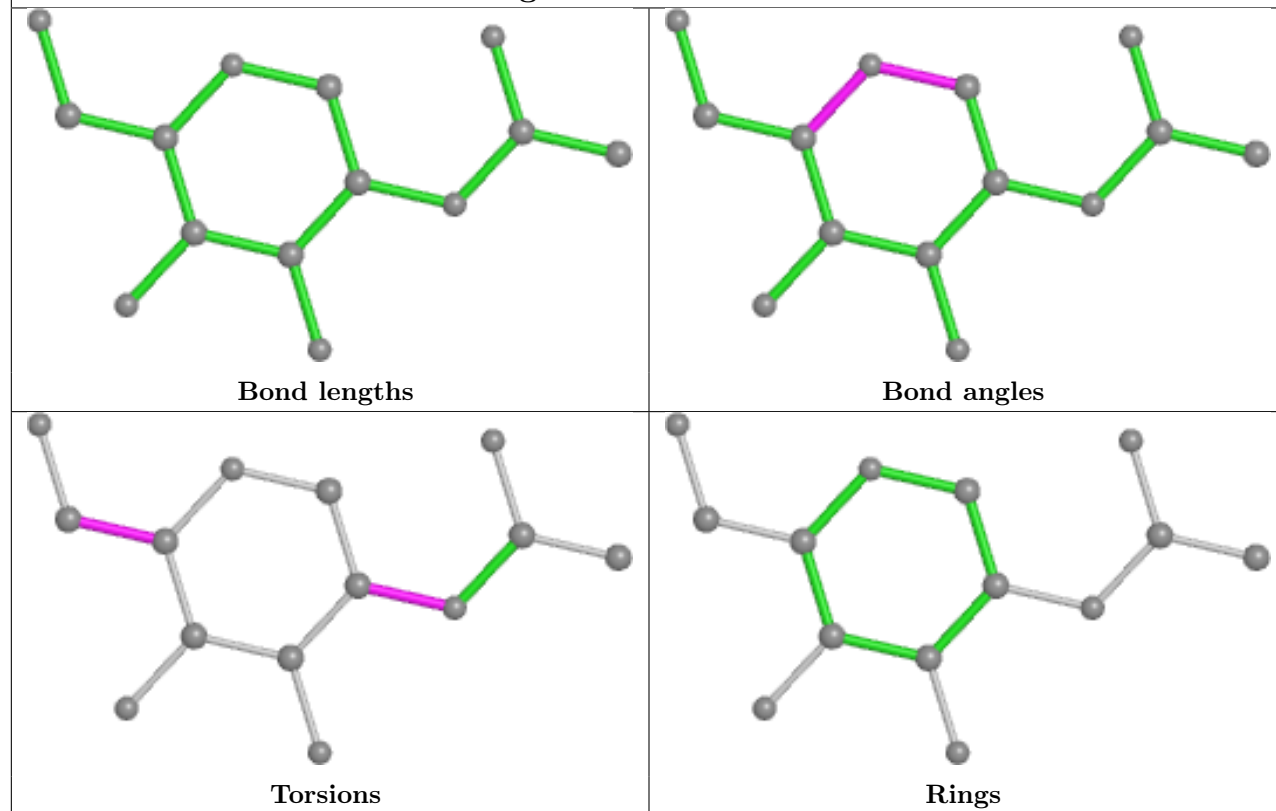
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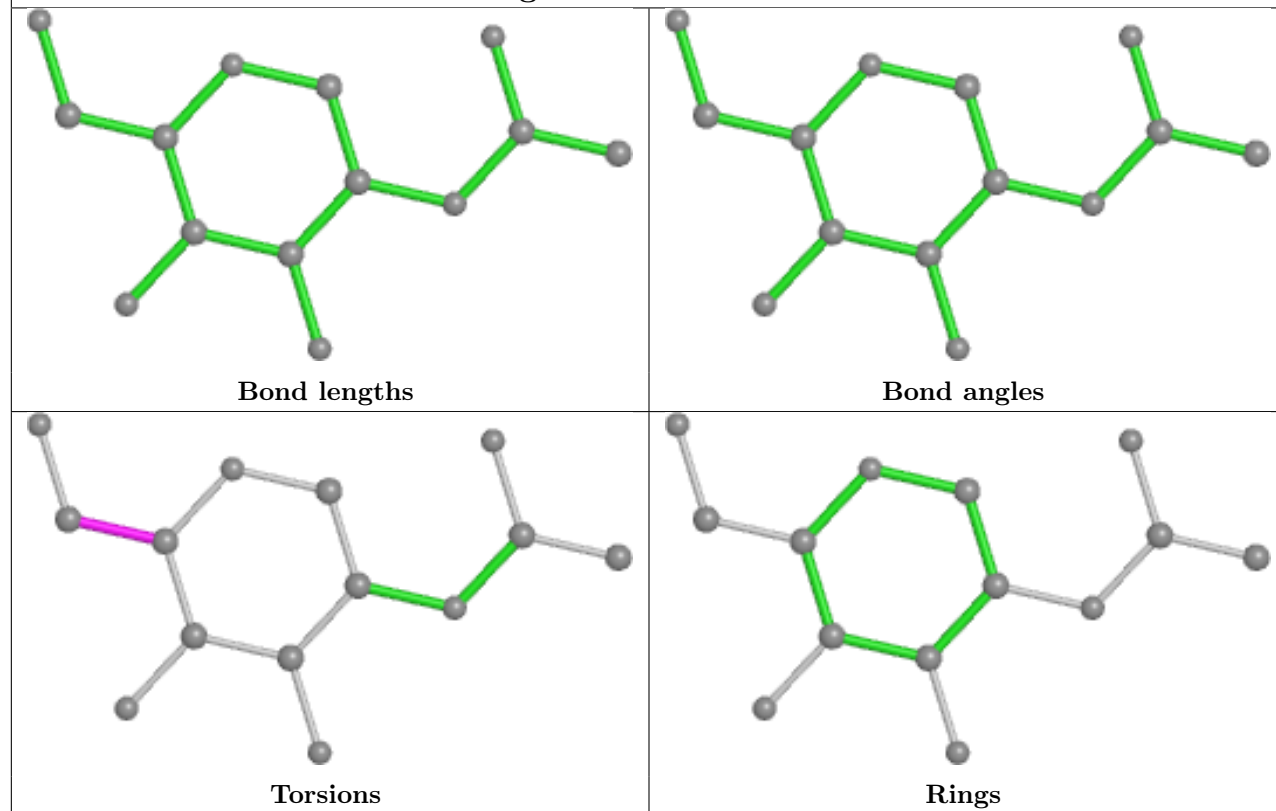
Ligand NAG A 1402



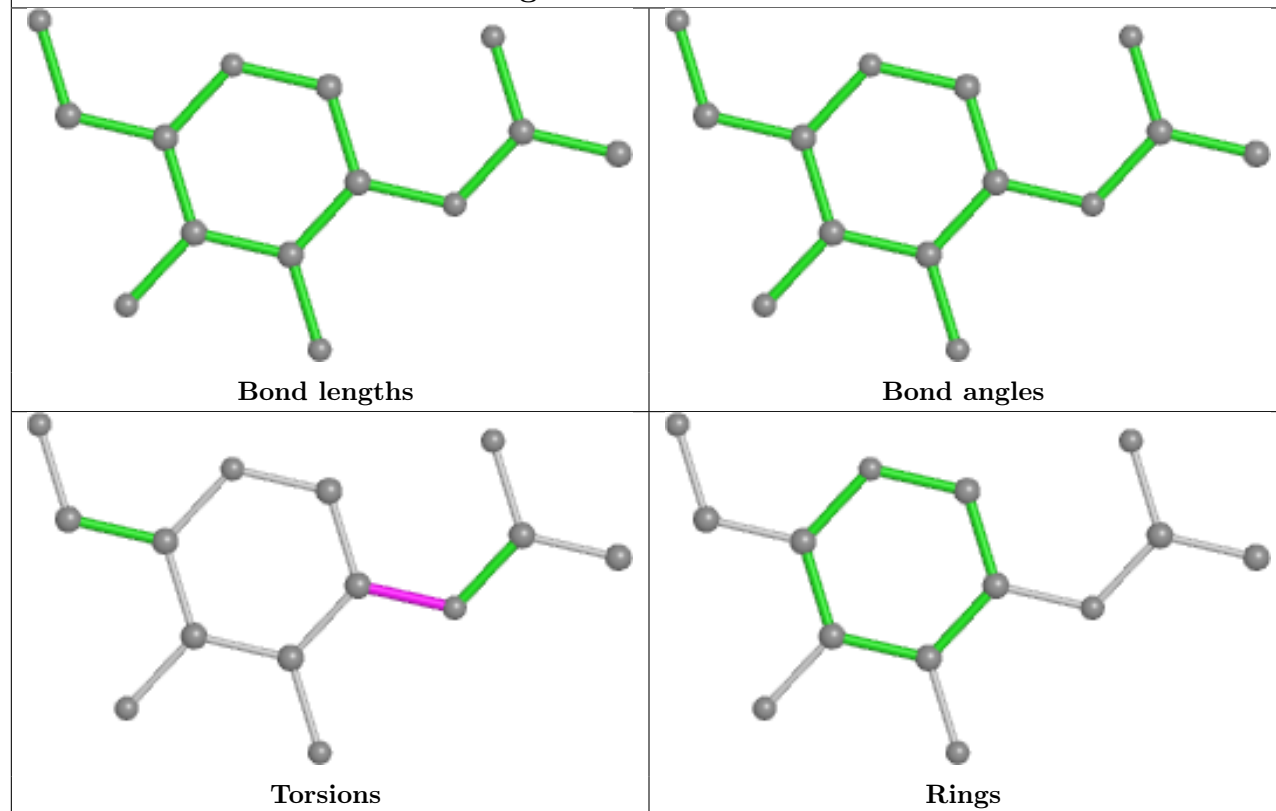
Ligand NAG C 1407



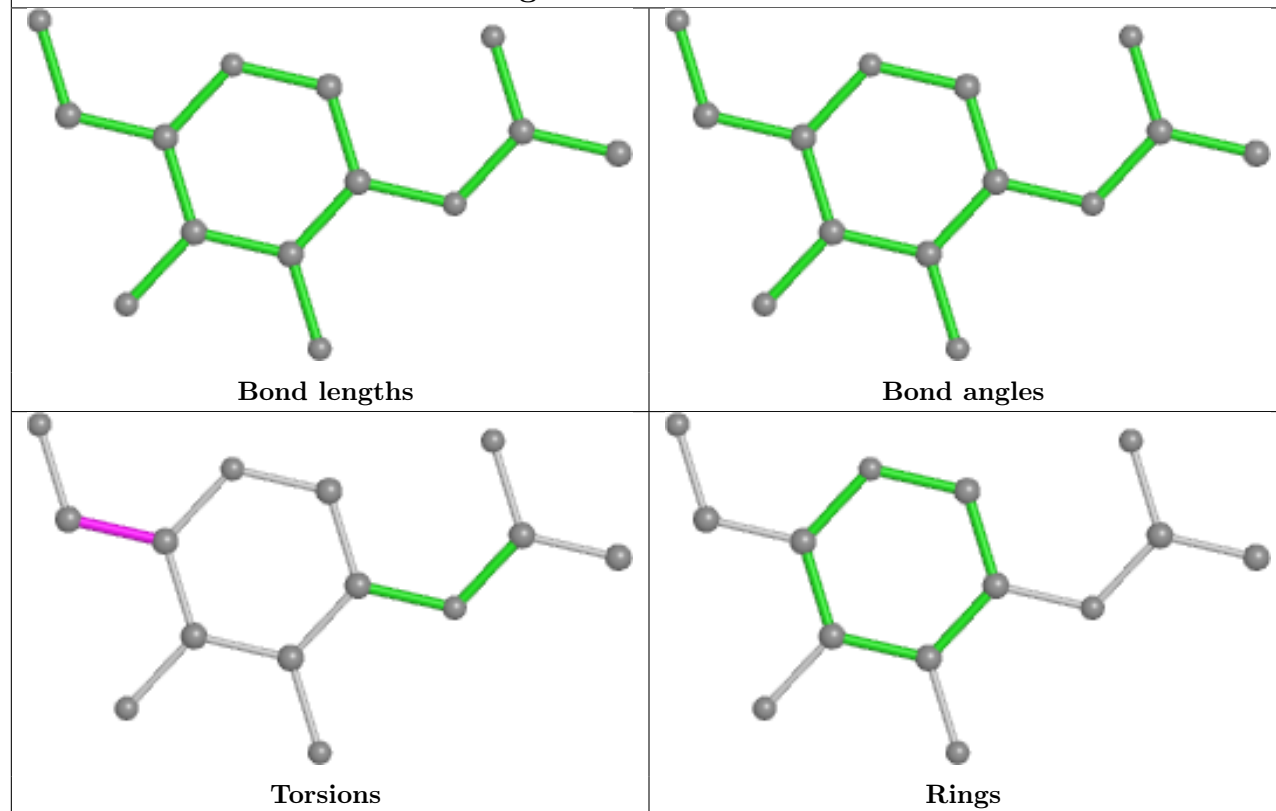
Ligand NAG C 1408



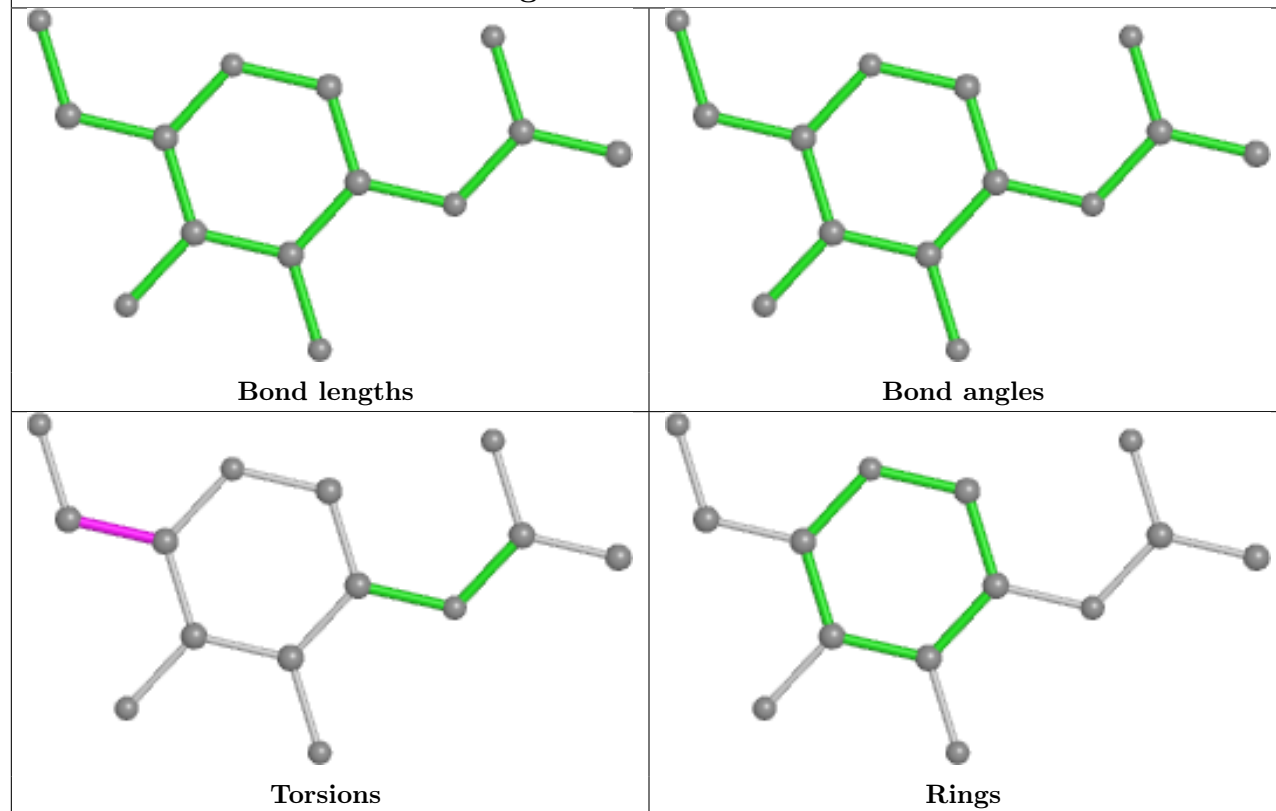
Ligand NAG B 1407



Ligand NAG C 1401



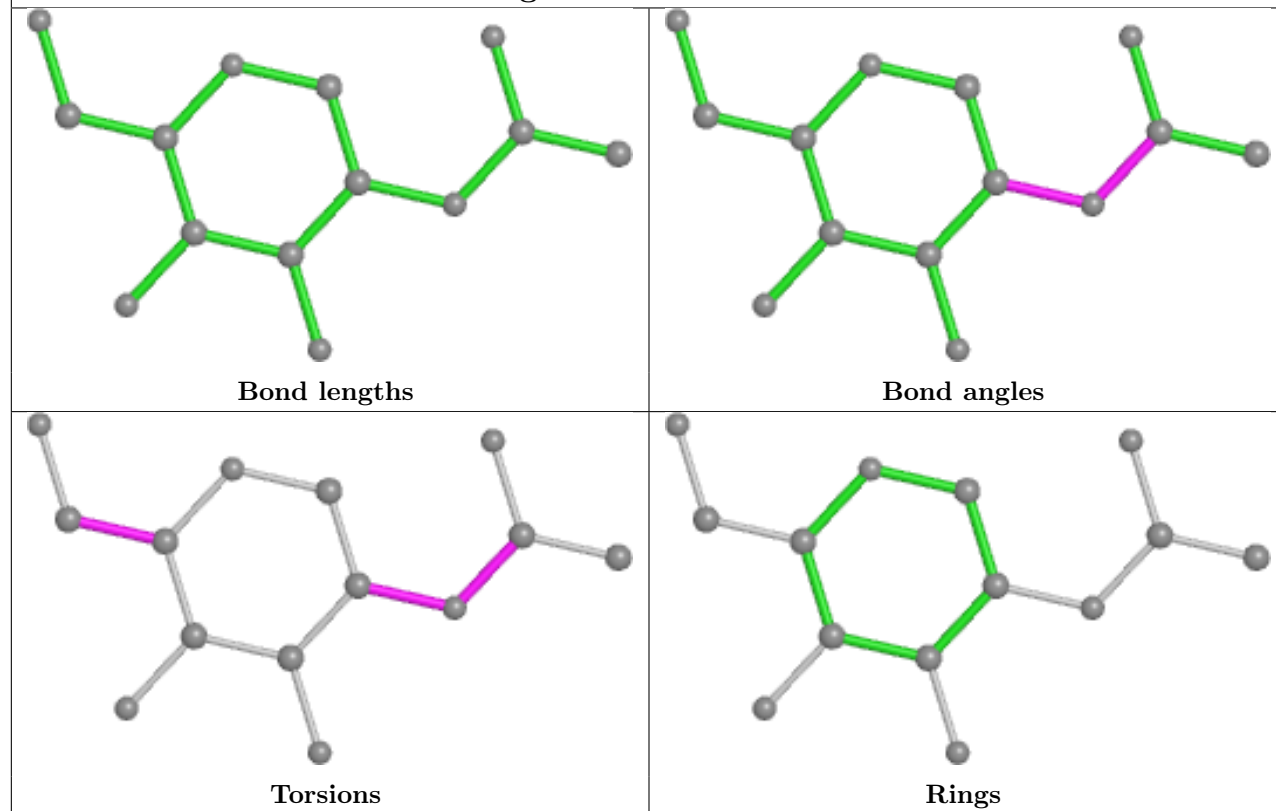
Ligand NAG B 1406



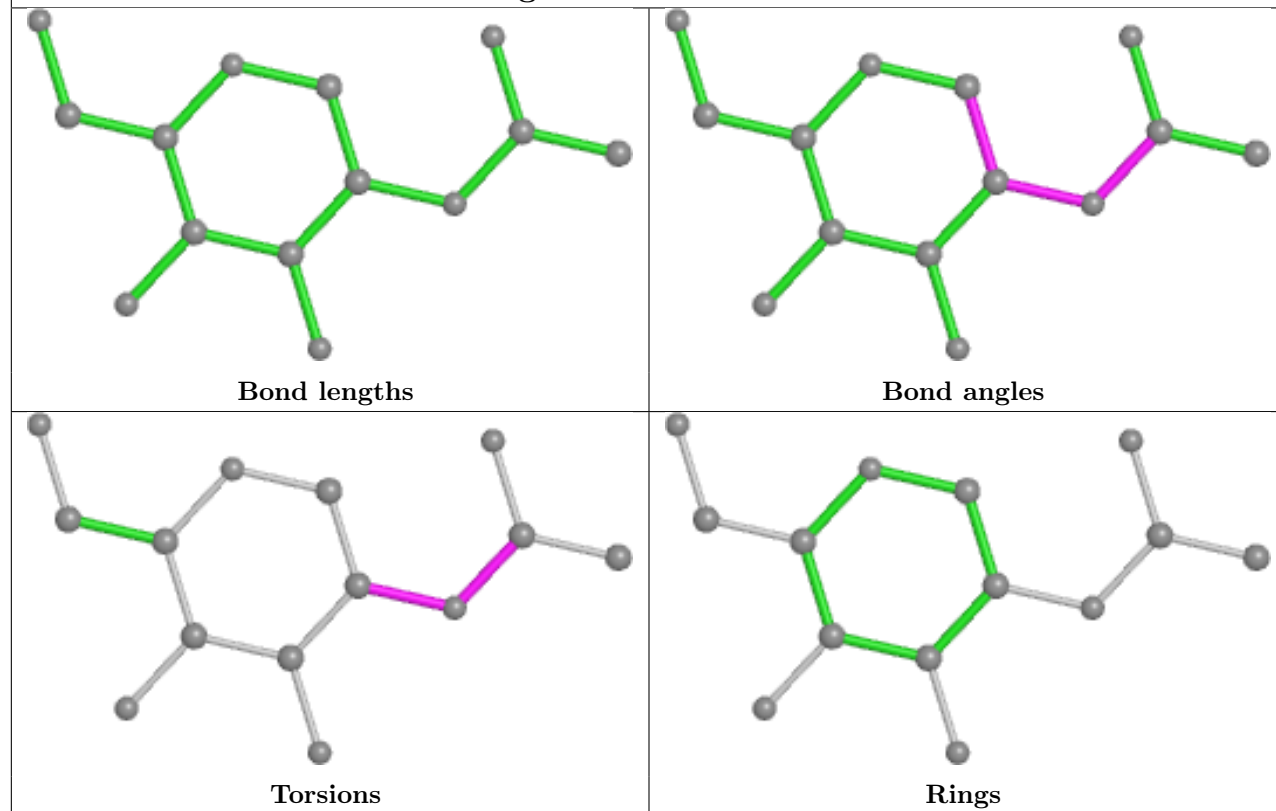
Ligand NAG C 1409



Ligand NAG B 1405



Ligand NAG A 1405



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.

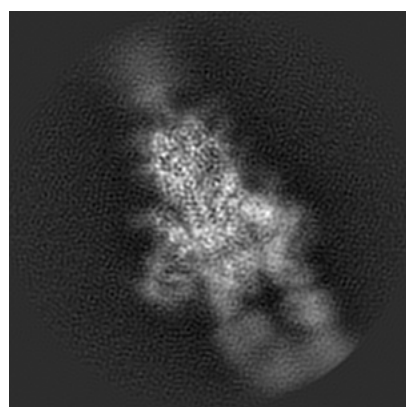
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30531. These allow visual inspection of the internal detail of the map and identification of artifacts.

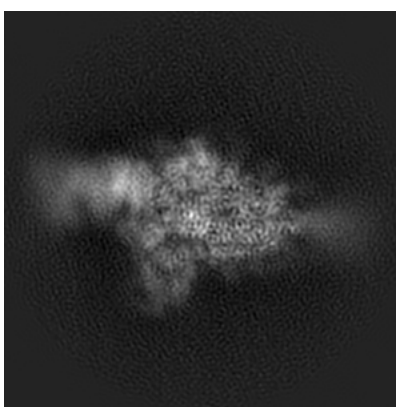
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

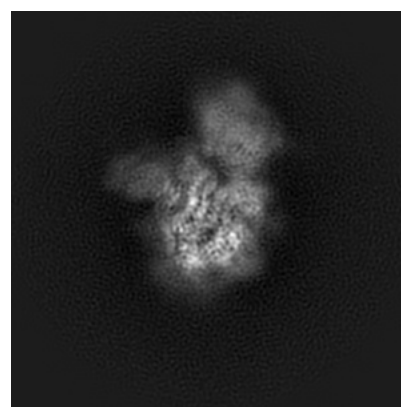
6.1.1 Primary map



X



Y

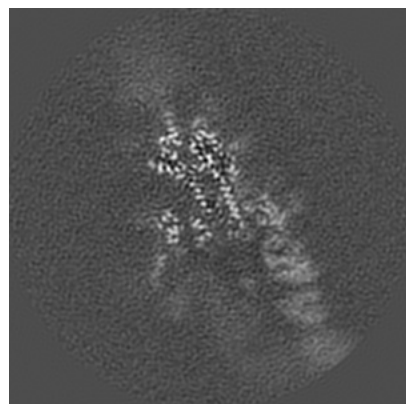


Z

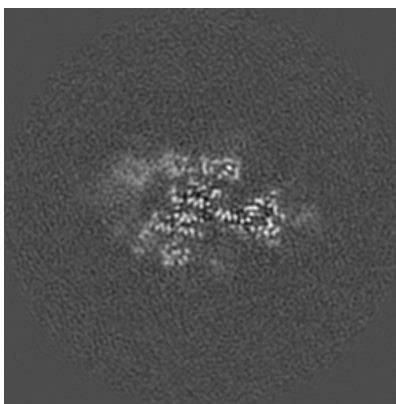
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

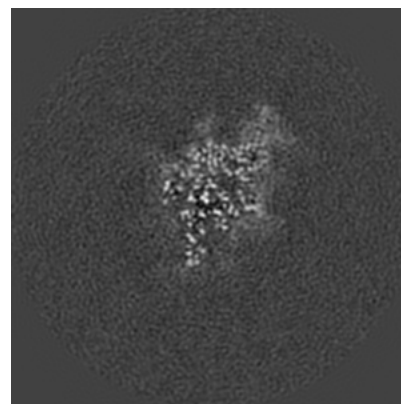
6.2.1 Primary map



X Index: 144



Y Index: 144

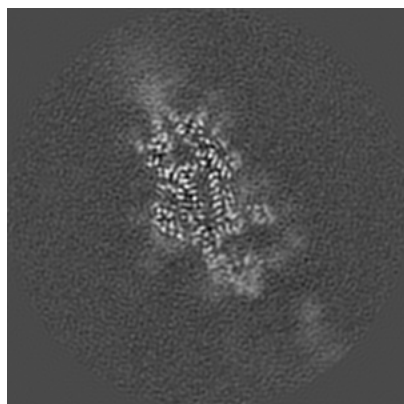


Z Index: 144

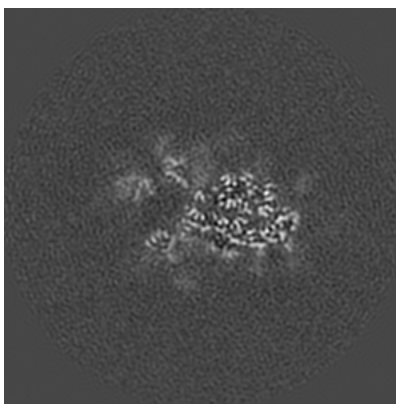
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

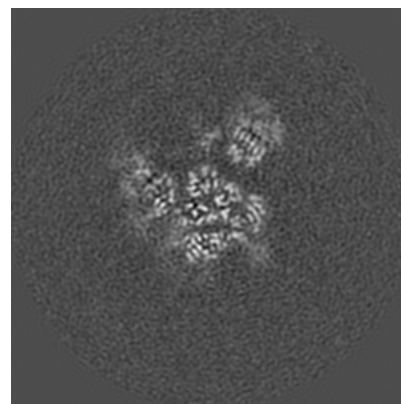
6.3.1 Primary map



X Index: 132



Y Index: 132

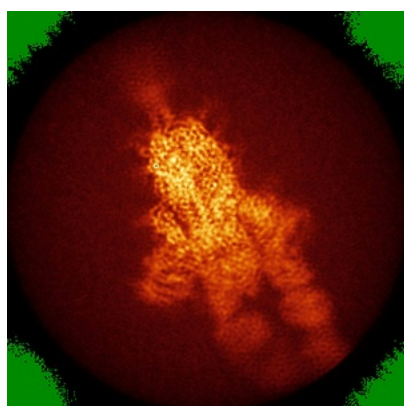


Z Index: 129

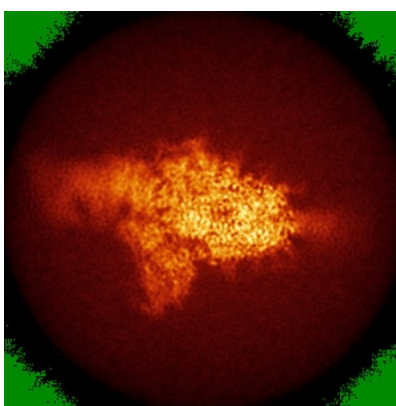
The images above show the largest variance slices of the map in three orthogonal directions.

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

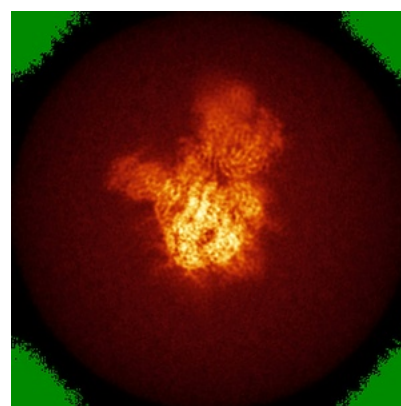
6.4.1 Primary map



X



Y

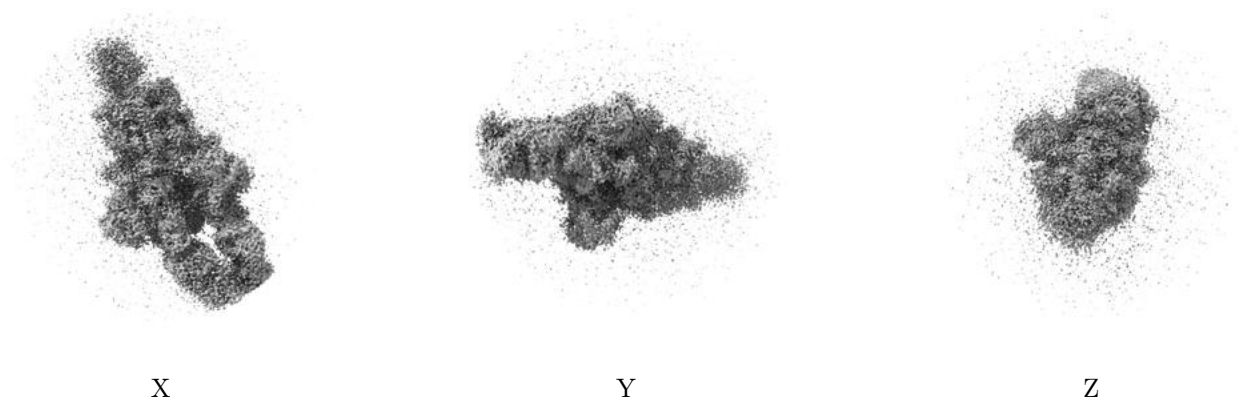


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0087. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

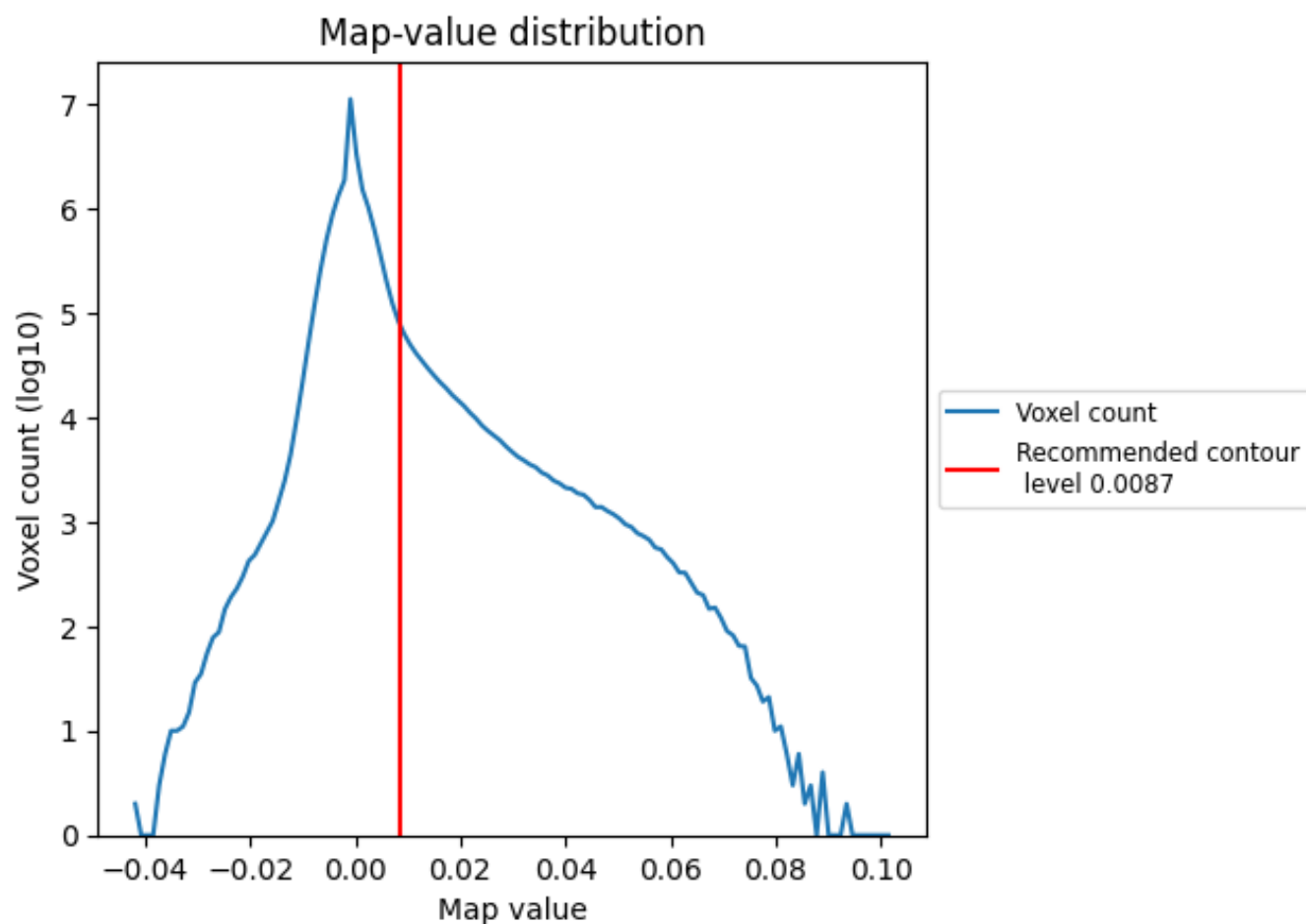
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

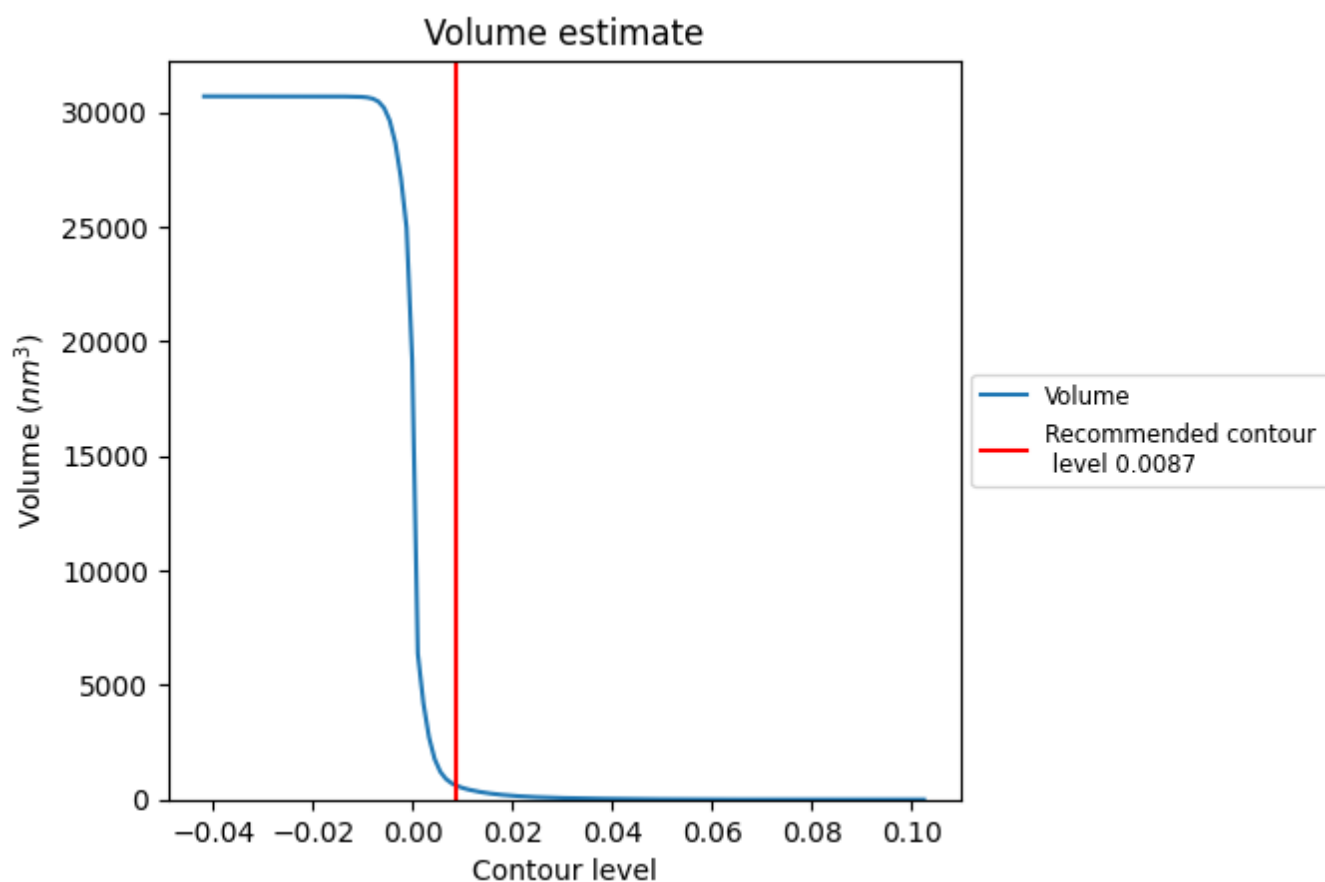
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

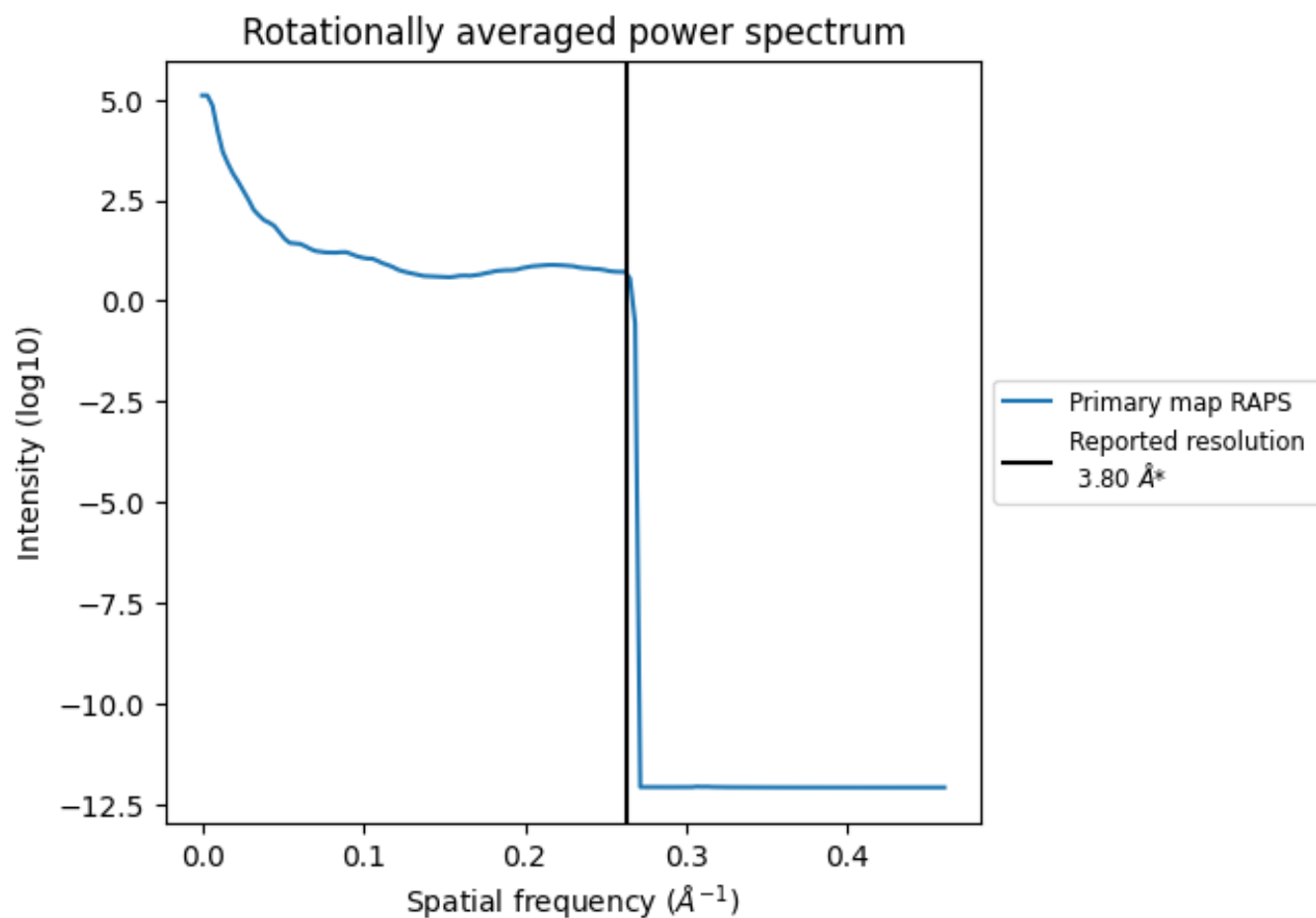
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm³; this corresponds to an approximate mass of 557 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 0.263 Å⁻¹

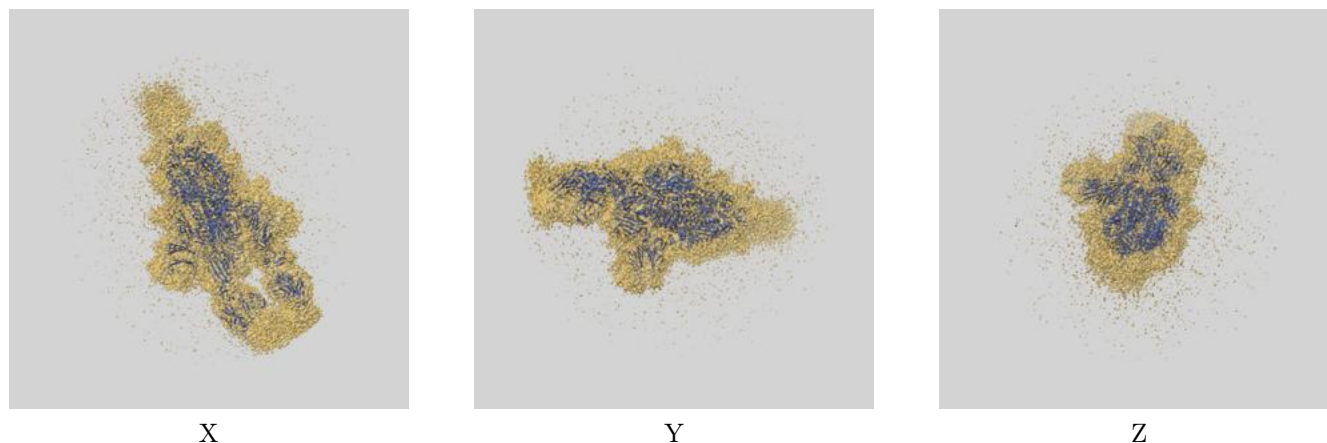
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

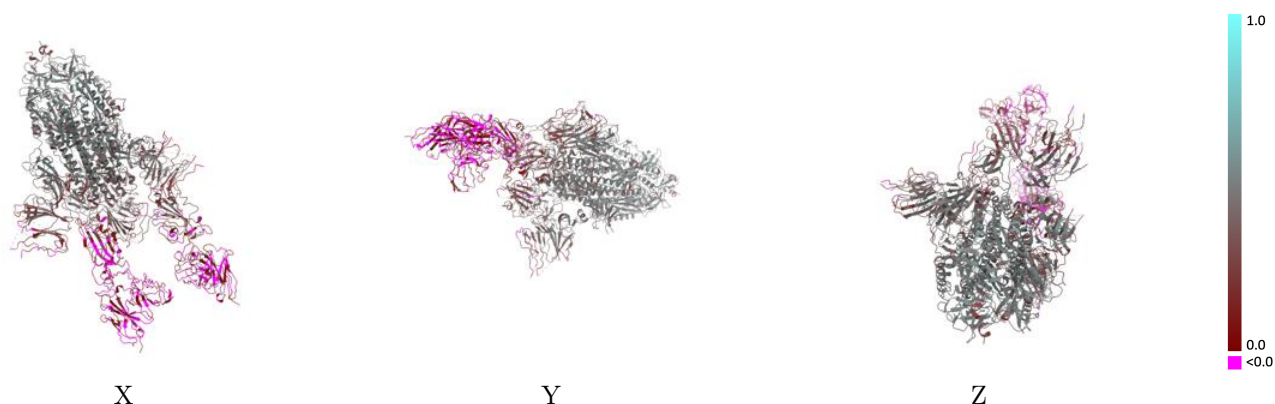
This section contains information regarding the fit between EMDB map EMD-30531 and PDB model 7D0D. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



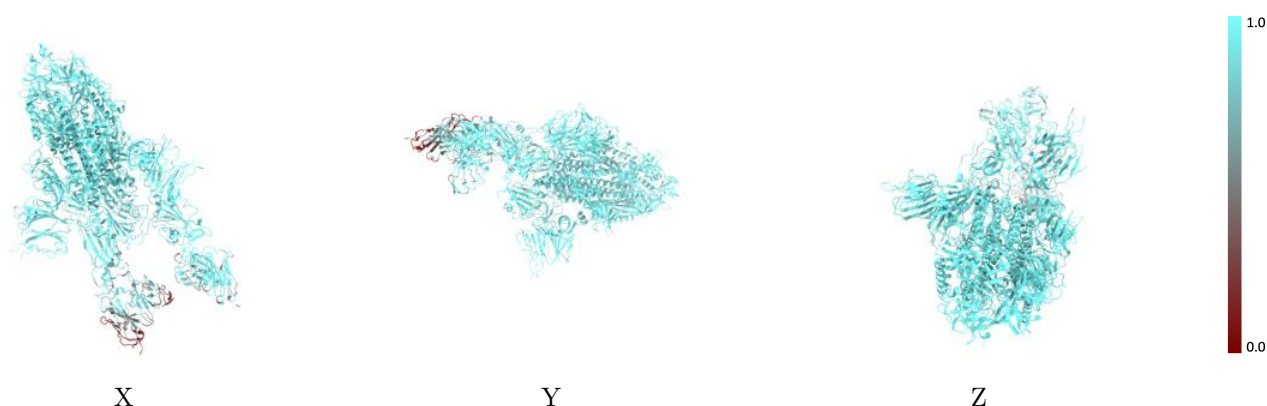
The images above show the 3D surface view of the map at the recommended contour level 0.0087 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



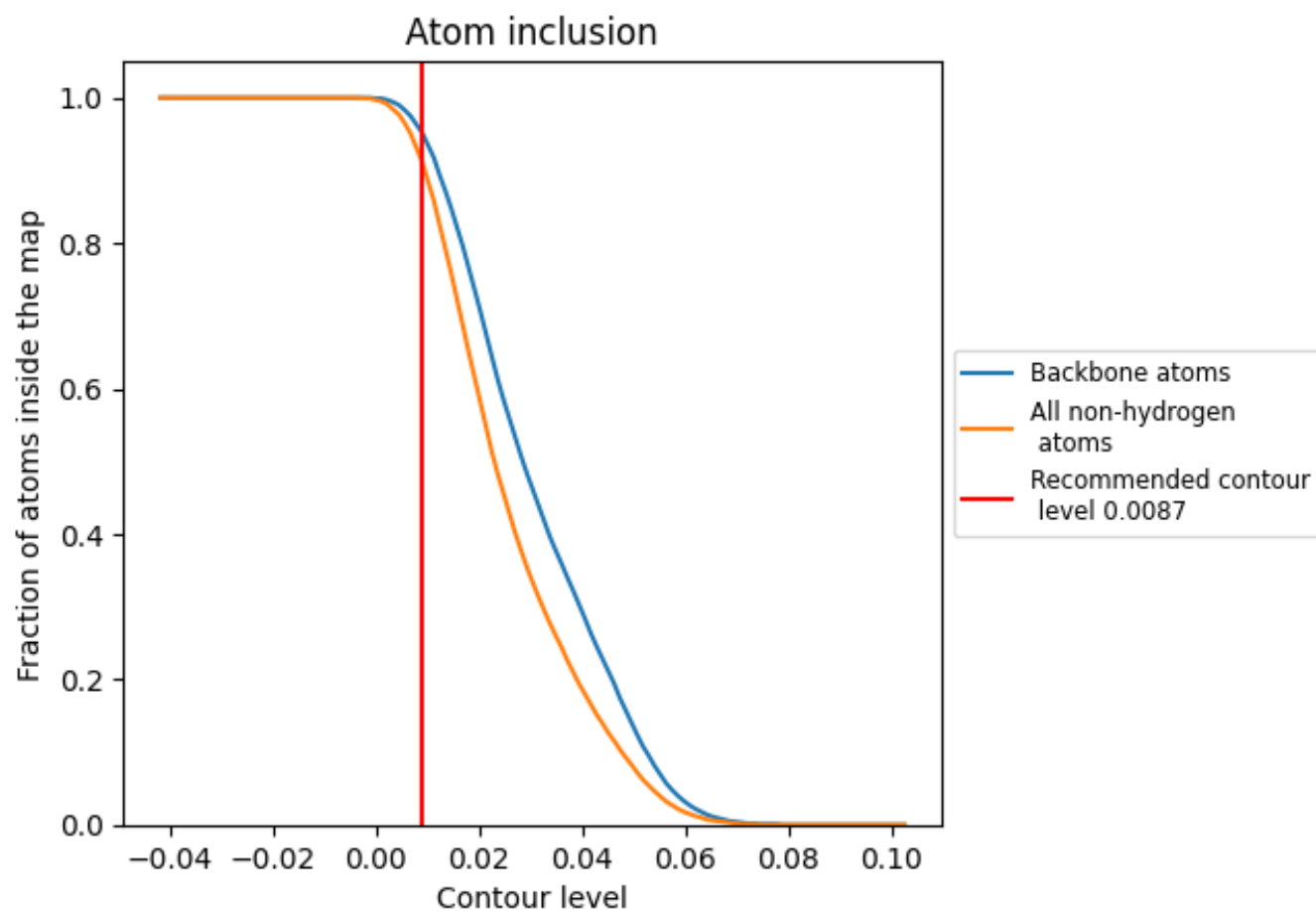
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0087).





























































9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.0087) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.3330
A	 0.9530	 0.3890
B	 0.9450	 0.3600
C	 0.9490	 0.3880
D	 0.9290	 0.3170
E	 0.8570	 0.1990
F	 0.6470	 0.0300
G	 0.4960	 0.0250
H	 0.8670	 0.0340
I	 0.8570	 0.2530
J	 0.9640	 0.4020
K	 0.9640	 0.3300
L	 0.8280	 0.0650
M	 0.8930	 0.2930
N	 1.0000	 0.4450
O	 1.0000	 0.3170
P	 0.5710	 0.1670
Q	 0.8210	 0.2180
R	 0.9290	 0.3960
S	 0.9290	 0.3260
T	 0.9640	 0.3430
U	 0.8930	 0.2410
V	 0.8570	 0.3370
W	 0.8210	 0.2260
X	 0.9290	 0.3700
Y	 0.9290	 0.3470
Z	 0.7500	 0.2840
a	 0.9290	 0.3930
b	 1.0000	 0.3010
c	 0.7500	 0.1650

