



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 02:01 PM JST

PDB ID : 7CZT  
EMDB ID : EMD-30516  
Title : S protein of SARS-CoV-2 in complex bound with P5A-2G9  
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Zhou, Q.  
Deposited on : 2020-09-09  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

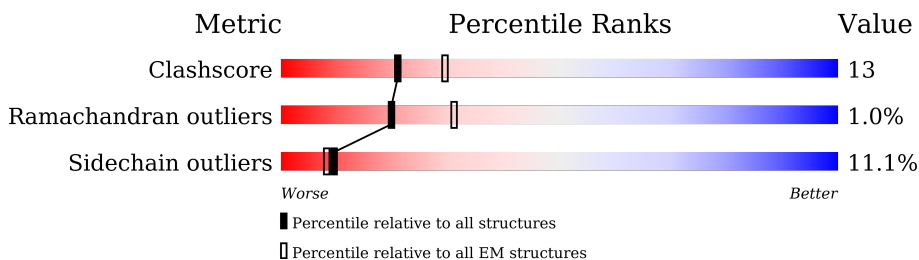
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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.



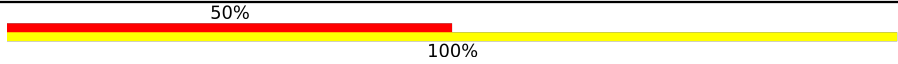














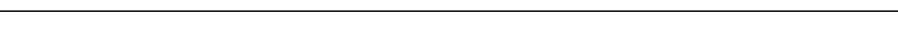
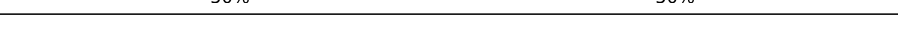
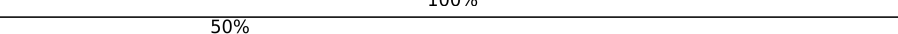

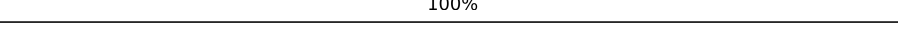
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	H	449	
2	I	449	
3	L	222	
3	M	222	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	
4	F	2	
4	G	2	
4	J	2	
4	K	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31060 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
			Total	C	N	O	S		
1	A	1006	7863	5019	1308	1500	36	0	0
1	B	982	7696	4920	1279	1462	35	0	0
1	C	1004	7853	5014	1307	1496	36	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	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
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	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

- Molecule 2 is a protein called Immunoglobulin heavy variable 3-33,chainH of P5A-2G9,Imm unoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	221	1677	1065	284	322	6	0	0
2	I	221	1677	1065	284	322	6	0	0

- Molecule 3 is a protein called IG c689\_light\_IGLV5-37\_IGLJ3,IGL@ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	219	1657	1046	269	337	5	0	0
3	M	219	1657	1046	269	337	5	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	31	SER	GLY	conflict	UNP A0A5C2GMM2
L	57	ASP	ASN	conflict	UNP A0A5C2GMM2
L	103	ALA	-	insertion	UNP A0A5C2GMM2
L	104	LEU	VAL	conflict	UNP A0A5C2GMM2
L	105	TYR	TRP	conflict	UNP A0A5C2GMM2
L	109	THR	GLY	conflict	UNP A0A5C2GMM2
L	113	VAL	LEU	conflict	UNP A0A5C2GMM2
M	31	SER	GLY	conflict	UNP A0A5C2GMM2
M	57	ASP	ASN	conflict	UNP A0A5C2GMM2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	103	ALA	-	insertion	UNP A0A5C2GMM2
M	104	LEU	VAL	conflict	UNP A0A5C2GMM2
M	105	TYR	TRP	conflict	UNP A0A5C2GMM2
M	109	THR	GLY	conflict	UNP A0A5C2GMM2
M	113	VAL	LEU	conflict	UNP A0A5C2GMM2

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



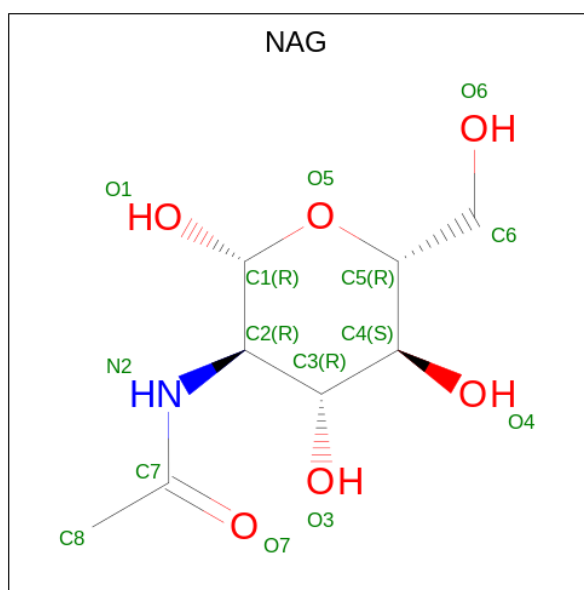
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0
4	G	2	28	16	2	10	0	0
4	J	2	28	16	2	10	0	0
4	K	2	28	16	2	10	0	0
4	N	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0
4	Q	2	28	16	2	10	0	0
4	R	2	28	16	2	10	0	0
4	S	2	28	16	2	10	0	0
4	T	2	28	16	2	10	0	0
4	U	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	V	2	Total 28	C 16	N 2	O 10	0	0
4	W	2	Total 28	C 16	N 2	O 10	0	0
4	X	2	Total 28	C 16	N 2	O 10	0	0
4	Y	2	Total 28	C 16	N 2	O 10	0	0
4	Z	2	Total 28	C 16	N 2	O 10	0	0
4	a	2	Total 28	C 16	N 2	O 10	0	0
4	b	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	B	1	Total 154	C 88	N 11	O 55	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0

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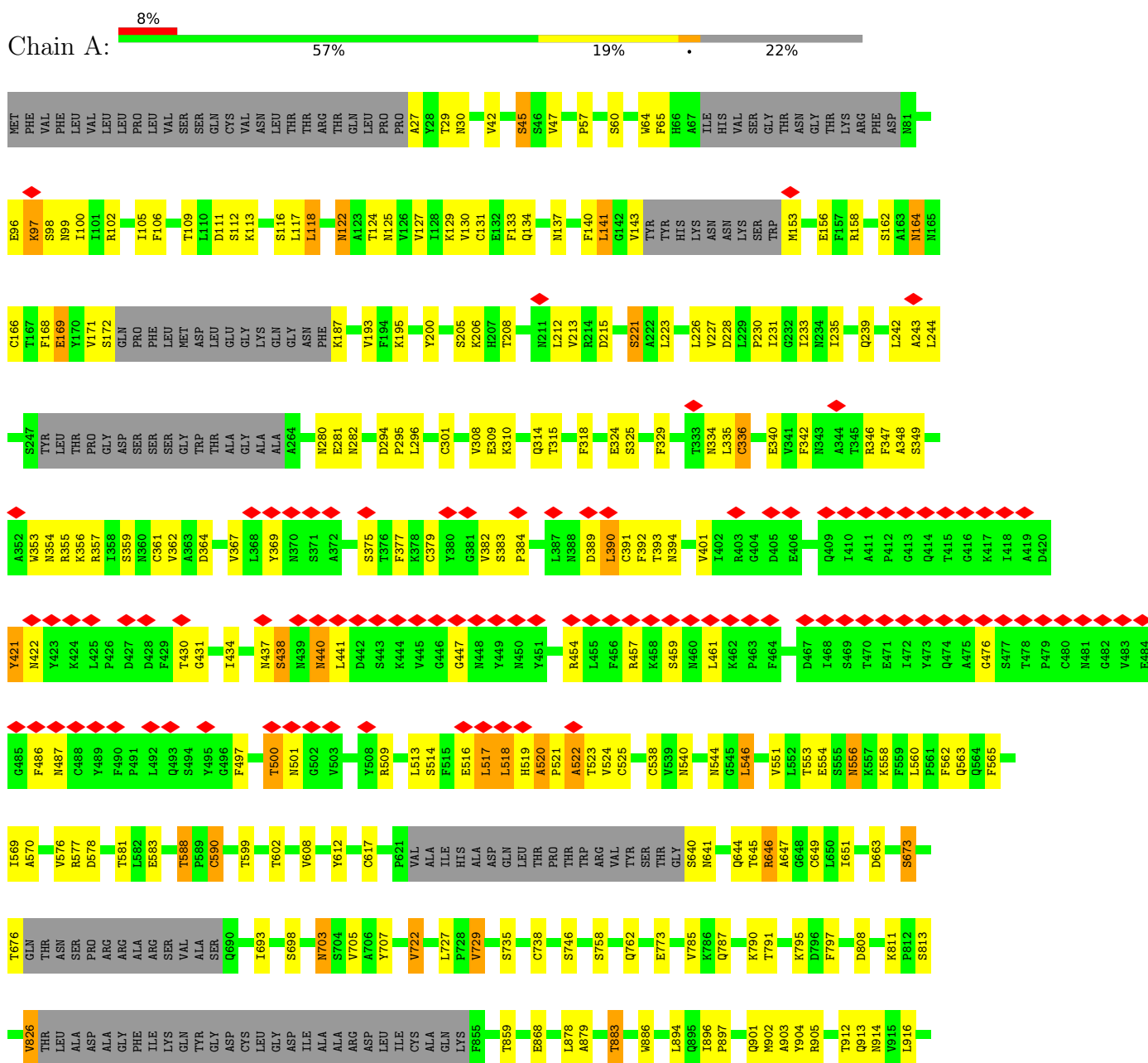
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0

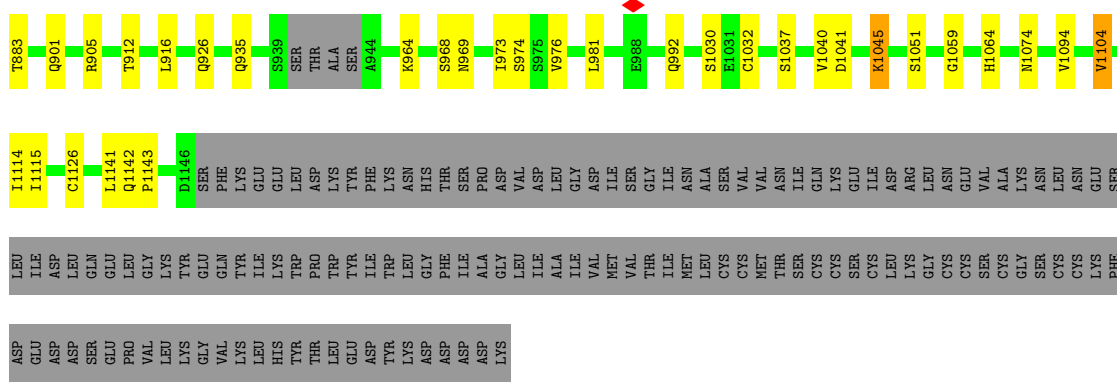
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

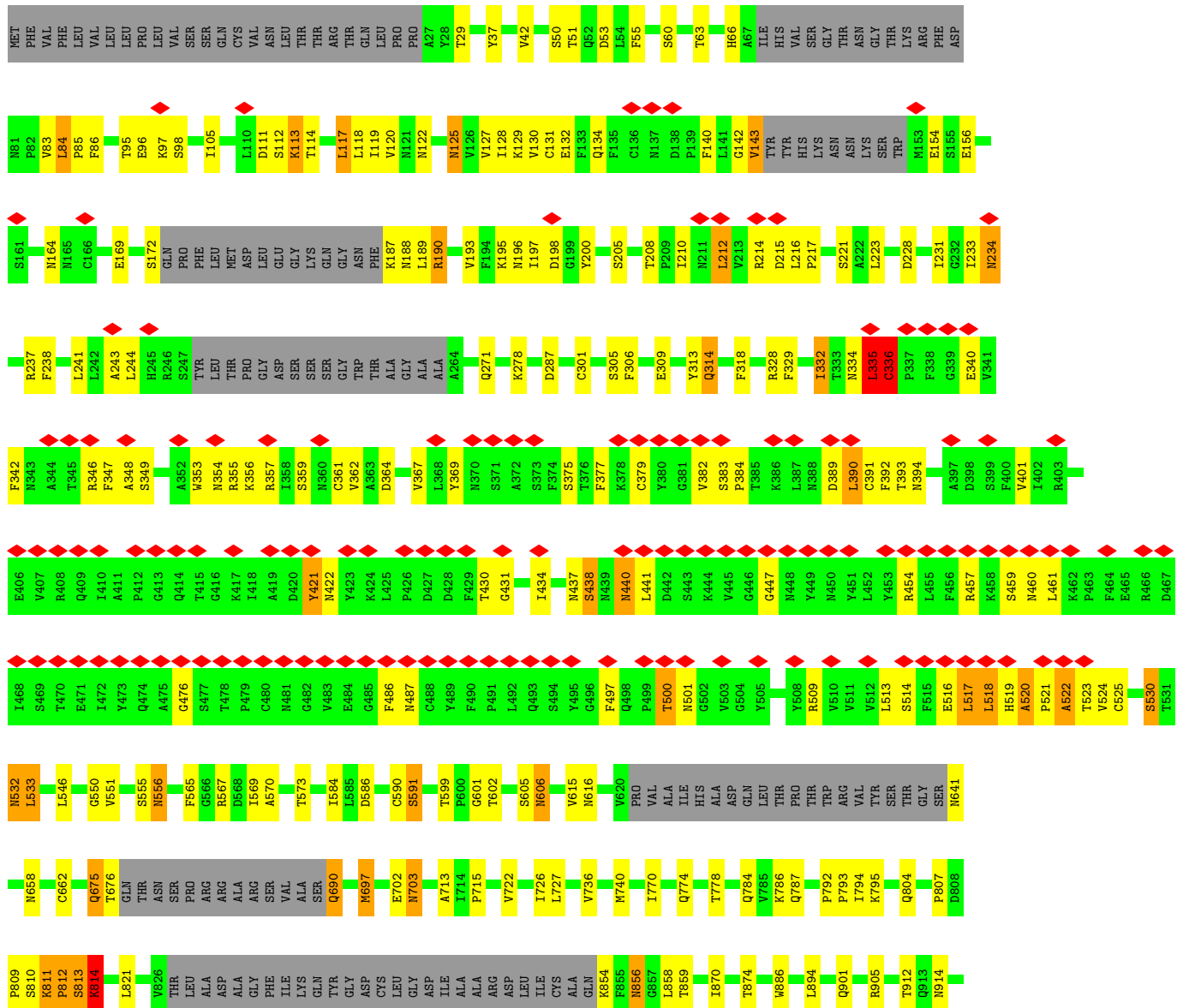
#### • Molecule 1: Spike glycoprotein







● Molecule 1: Spike glycoprotein





A61	D62	S63	V64	K65	G66	R67	F68	T69	I70	S71	R72	D73	N74	S75	K76	N77	T78	L79	Y80	L81	Q82	M83	N84	S85	L86	R87	A88	E89	D90	T91	A92	V93	Y94	Y95	C96	A97	R98	W99	F100	H101	T102	G103	G104	Y105	F106	D107	Y108	W109	G110	Q111	G112	T113	L114	V115	T116	V117	S118	S119	A120
S121	T122	K123	G124	P125	S126	V127	F128	F129	L130	A131	P132	S133	S134	K135	S136	T137	S138	G139	G140	T141	A142	A143	L144	G145	C146	L147	V148	K149	D150	Y151	F152	P153	A154	P155	V156	T157	V158	S159	W160	N161	S162	G163	A164	L165	T166	S167	G168	V169	H170	T171	F172	P173	A174	V175	L176	Q177	S178	S179	G180
L181	Y182	S183	L184	S185	S186	V187	V188	T189	V190	P191	S192	S193	S194	L195	G196	T197	Q198	T199	Y200	L201	C202	N203	V204	N205	H206	K207	P208	S209	N210	T211	K212	V213	D214	K215	K216	V217	E218	P219	K220	S221	CYS	ASP	LYS	THR	HIS	THR	CYS	PRO	PRO	CYS	PRO	ALA	PRO	GLU	LEU	LEU	GLY	GLY	PRO
SER	VAL	PHE	LEU	PHE	PRO	LYS	PRO	ASP	THR	MET	ILE	LEU	ASN	THR	PRO	GLY	THR	VAL	VAL	ASP	VAL	VAL	HIS	GLU	ASP	GLU	LYS	PHE	ASN	TRP	TYR	VAL	ASP	GLY	VAL	GLU	VAL	GLU	VAL	ASN	THR	LYS	PRO	PRO	PRO	GLY	PRO	GLU	GLN	ARG	ASP	TYR	ASN	SER					
THR	TYR	ARG	VAL	VAL	SER	LEU	THR	VAL	CYS	THR	TRP	LEU	ASN	GLY	LYS	GLU	LYS	VAL	VAL	ASN	GLY	GLN	PRO	ALA	LEU	PRO	ALA	PRO	ILE	LYS	LEU	ALA	GLY	GLN	ARG	GLU	VAL	TYR	VAL	LYS	THR	THR	LEU	THR	VAL	PRO	GLY	LEU	PRO	ARG	SER	GLN	THR	LEU					
THR	LYS	ASN	GLN	VAL	SER	LEU	CYS	VAL	HIS	VAL	TRP	LEU	LYS	GLY	PHE	LEU	HIS	TRP	PRO	ASN	ASP	THR	THR	ALA	GLU	ASN	TYR	THR	PRO	VAL	LEU	ASP	GLY	SER	PHE	ARG	VAL	LEU	TYR	SER	LYS	VAL	THR	THR	VAL	THR	THR	VAL	THR	VAL	VAL	GLN							
GLN	GLY	ASN	VAL	PHE	SER	CYS	VAL	VAL	HIS	HIS	ASN	HIS	THR	GLN	LYS	SER	LEU	SER	LEU	SER	PRO	GLY	LYS																																				

• Molecule 3: IG c689\_light\_IGLV5-37\_IGLJ3,IGL@ protein

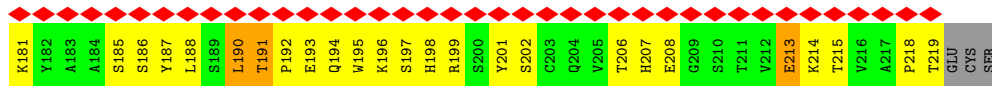


Q1	P2	V3	L4	T5	Q6	P7	P8	S9	S10	S11	A12	S13	P14	G15	E16	S17	A18	R19	L20	T21	C22	T23	L24	P25	S26	D27	I28	N29	V30	S31	S32	Y33	N34	I35	Y36	W37	Q38	Q39	Q40	K41	P42	G43	S44	P45	P46	R47	Y48	L49	L50	Y51	K112	V113	T114	V115	D55	S56	D57	K58	G59	Q60
G61	S62	G63	V64	P65	S66	R67	F68	S69	G70	S71	K72	D73	A74	S75	A76	N77	T78	G79	I80	L81	L82	I83	S84	G85	L86	Q87	S88	E89	D90	E91	A92	D93	Y94	Y95	C96	M97	I98	W99	P100	N102	A103	L104	Y105	V106	P107	F108	T109	G110	T111	K112	V113	T114	V115	L116	G117	Q118	P119	K120		
A121	A122	P123	S124	V125	T126	L127	F128	P129	P130	S131	S132	E133	E134	L135	Q136	A137	M138	K139	A140	T141	L142	V143	C144	L145	L146	S147	D148	F149	Y150	P151	G152	A153	V154	T155	V156	C96	M97	A158	K159	A160	D161	S162	S163	P164	V165	K166	A167	G168	V169	E170	E171	T172	T173	P174	S175	K176	Q177	S178	N179	N180
K181	Y182	A183	A184	S185	S186	Y187	L188	S189	L190	T191	P192	E193	Q194	W195	K196	S197	H198	R199	S200	Y201	S202	C203	Q204	V205	T206	H207	E208	G209	S210	T211	V212	E213	N34	I35	Y36	W37	A217	P218	T219	GLU	CYS	SER																		

• Molecule 3: IG c689\_light\_IGLV5-37\_IGLJ3,IGL@ protein



Q1	P2	V3	L4	T5	Q6	P7	P8	S9	S10	S11	A12	S13	P14	G15	E16	S17	A18	R19	L20	T21	C22	T23	L24	P25	S26	D27	I28	N29	V30	S31	S32	Y33	N34	I35	Y36	W37	Q38	Q39	Q40	K41	P42	G43	S44	P45	P46	R47	Y48	L49	L50	Y51	K112	V113	T114	V115	D55	S56	D57	K58	G59	Q60
G61	S62	G63	V64	P65	S66	R67	F68	S69	G70	S71	K72	D73	A74	S75	A76	N77	T78	G79	I80	L81	L82	I83	S84	G85	L86	Q87	S88	E89	D90	E91	A92	D93	Y94	Y95	C96	M97	I98	W99	P100	S101	N102	A103	L104	Y105	V106	F107	G108	T109	G110	L50	T111	K112	V113	T114	V115	L116	G117	Q118	P119	K120



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

Chain D: 100%



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

Chain E: 50%  
100%



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

Chain F: 50%  
50%



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

Chain G: 50%  
50%



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

Chain J: 50%  
50%



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

Chain K:  50% 50%



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

Chain N:  50% 50%



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

Chain O:  50% 50% 50%



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

Chain P:  50% 100%



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

Chain Q:  50% 50%



- 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:  100%



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

Chain T:

100%

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

Chain U:

50%

50%

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

Chain V:

50%

100%

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

Chain W:

50%

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

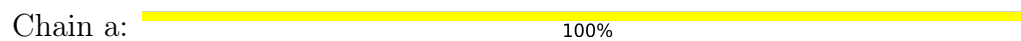
Chain Y:

100%

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



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	497874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0/8039	0.56	0/10936
1	B	0.49	0/7864	0.55	0/10691
1	C	0.59	0/8028	0.55	0/10919
2	H	0.52	0/1723	0.53	0/2347
2	I	0.52	0/1723	0.53	0/2347
3	L	0.53	0/1703	0.51	0/2331
3	M	0.53	0/1703	0.51	0/2331
All	All	0.55	0/30783	0.54	0/41902

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	7863	0	7659	197	0
1	B	7696	0	7514	140	0
1	C	7853	0	7653	195	0
2	H	1677	0	1629	64	0
2	I	1677	0	1629	55	0
3	L	1657	0	1600	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	1657	0	1600	92	0
4	D	28	0	25	0	0
4	E	28	0	25	3	0
4	F	28	0	25	0	0
4	G	28	0	25	1	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	4	0
4	W	28	0	25	1	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
5	A	126	0	117	5	0
5	B	154	0	142	10	0
5	C	112	0	104	2	0
All	All	31060	0	30172	812	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 13.

All (812) 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)
5:B:1410:NAG:O4	5:B:1411:NAG:C1	1.63	1.46
2:H:139:GLY:HA2	3:M:197:SER:CB	1.59	1.31
2:H:139:GLY:CA	3:M:197:SER:HB3	1.63	1.27
1:C:336:CYS:SG	1:C:361:CYS:CB	2.33	1.16
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.10
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.09
1:C:523:THR:HG22	1:C:524:VAL:H	0.97	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:THR:HG22	1:A:524:VAL:H	0.97	1.08
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.35	1.08
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.35	1.08
1:A:335:LEU:HA	1:A:362:VAL:CG1	1.85	1.06
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.05
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.04
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.88	1.01
1:B:422:ASN:HD21	1:B:455:LEU:H	1.08	1.01
5:B:1410:NAG:C4	5:B:1411:NAG:C1	2.38	1.00
1:C:523:THR:HG22	1:C:524:VAL:N	1.72	1.00
1:C:550:GLY:HA2	1:C:590:CYS:SG	2.01	1.00
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.91	1.00
1:A:335:LEU:CA	1:A:362:VAL:HG13	1.91	1.00
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.92	0.99
1:A:523:THR:HG22	1:A:524:VAL:N	1.72	0.99
1:A:334:ASN:O	1:A:362:VAL:HG12	1.61	0.98
1:C:676:THR:HA	1:C:690:GLN:HB3	1.46	0.98
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.98
1:C:336:CYS:SG	1:C:361:CYS:HB2	2.05	0.97
1:A:523:THR:CG2	1:A:524:VAL:H	1.77	0.97
1:C:675:GLN:HE21	1:C:675:GLN:HA	1.27	0.96
1:A:335:LEU:HA	1:A:362:VAL:HG13	0.97	0.96
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.95
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.95
1:C:523:THR:CG2	1:C:524:VAL:H	1.77	0.94
1:B:577:ARG:HH11	1:B:582:LEU:HD13	1.32	0.93
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.92
2:H:60:TYR:OH	2:H:69:THR:HA	1.71	0.91
2:I:60:TYR:OH	2:I:69:THR:HA	1.71	0.90
1:C:335:LEU:HA	1:C:362:VAL:HG13	1.53	0.90
3:M:100:PRO:HG2	3:M:104:LEU:HD21	1.56	0.87
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.11	0.86
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.86
1:C:393:THR:O	1:C:523:THR:HG21	1.76	0.86
3:L:100:PRO:HG2	3:L:104:LEU:HD21	1.56	0.86
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.85
1:A:393:THR:O	1:A:523:THR:HG21	1.76	0.85
1:C:336:CYS:HG	1:C:361:CYS:HG	1.22	0.85
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.85
1:B:577:ARG:HD3	1:B:582:LEU:CD1	2.07	0.85
3:M:25:PRO:HG2	3:M:28:ILE:HD12	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:CYS:SG	1:A:361:CYS:CB	2.65	0.85
3:L:25:PRO:HG2	3:L:28:ILE:HD12	1.58	0.84
1:C:520:ALA:HB1	1:C:521:PRO:CD	2.06	0.84
3:M:24:LEU:HB3	3:M:25:PRO:HD2	1.59	0.84
1:C:516:GLU:O	1:C:517:LEU:HD22	1.78	0.83
3:L:24:LEU:HB3	3:L:25:PRO:HD2	1.59	0.83
1:C:127:VAL:HG21	5:C:1402:NAG:H5	1.59	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.82
1:C:336:CYS:HG	1:C:361:CYS:CB	1.81	0.82
1:A:334:ASN:C	1:A:362:VAL:HG12	1.99	0.82
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.81
1:B:577:ARG:HD3	1:B:582:LEU:HD13	1.60	0.81
1:B:452:LEU:HG	1:B:492:LEU:HD22	1.63	0.81
1:C:334:ASN:O	1:C:362:VAL:HG12	1.81	0.81
1:B:214:ARG:H	1:B:214:ARG:HH21	1.30	0.80
1:C:392:PHE:O	1:C:523:THR:HB	1.83	0.79
3:L:104:LEU:HD23	3:L:104:LEU:O	1.83	0.79
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.78
1:C:676:THR:C	1:C:690:GLN:HE21	1.86	0.78
1:C:334:ASN:ND2	1:C:361:CYS:HA	1.97	0.78
1:C:390:LEU:HD23	1:C:391:CYS:H	1.48	0.78
1:C:336:CYS:SG	1:C:361:CYS:HB3	2.23	0.78
2:H:139:GLY:HA2	3:M:197:SER:HB3	0.81	0.78
3:M:104:LEU:O	3:M:104:LEU:HD23	1.83	0.77
1:C:332:ILE:H	1:C:332:ILE:HD12	1.49	0.77
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.77
3:L:28:ILE:HG22	3:L:33:TYR:CE1	2.20	0.77
1:A:390:LEU:HD23	1:A:391:CYS:H	1.48	0.76
3:M:28:ILE:HG22	3:M:33:TYR:CE1	2.20	0.76
3:M:28:ILE:CG2	3:M:33:TYR:CE1	2.69	0.76
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.76
3:L:24:LEU:HD23	3:L:24:LEU:N	2.01	0.76
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.76
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.75
1:C:675:GLN:HA	1:C:675:GLN:NE2	1.99	0.75
3:L:24:LEU:CB	3:L:25:PRO:HD2	2.16	0.75
3:M:24:LEU:CB	3:M:25:PRO:HD2	2.16	0.75
3:L:28:ILE:CG2	3:L:33:TYR:CE1	2.69	0.75
3:M:24:LEU:N	3:M:24:LEU:HD23	2.01	0.75
1:C:334:ASN:C	1:C:362:VAL:HG12	2.07	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:SER:OG	2:H:74:ASN:ND2	2.20	0.74
2:I:30:SER:OG	2:I:74:ASN:ND2	2.20	0.74
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.53	0.73
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.53	0.73
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.73
1:B:577:ARG:HH11	1:B:582:LEU:CD1	2.01	0.73
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.73
1:B:164:ASN:ND2	5:B:1403:NAG:O6	2.22	0.72
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.72
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.72
3:M:53:TYR:O	3:M:57:ASP:HB3	1.89	0.72
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.20	0.71
1:B:124:THR:OG1	5:B:1402:NAG:N2	2.22	0.71
2:H:74:ASN:OD1	2:H:74:ASN:N	2.22	0.71
2:H:60:TYR:CE2	2:H:68:PHE:O	2.44	0.71
3:L:53:TYR:O	3:L:57:ASP:HB3	1.89	0.71
5:B:1410:NAG:H4	5:B:1411:NAG:C1	2.21	0.71
3:L:25:PRO:HG2	3:L:28:ILE:CD1	2.20	0.71
3:M:25:PRO:HG2	3:M:28:ILE:CD1	2.20	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.70
3:L:101:SER:O	3:L:103:ALA:N	2.23	0.70
1:A:124:THR:HG21	5:A:1402:NAG:HN2	1.56	0.70
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.69
2:I:52:TRP:O	2:I:72:ARG:NH1	2.25	0.69
1:B:391:CYS:HA	1:B:525:CYS:HB2	1.73	0.69
1:C:676:THR:C	1:C:690:GLN:NE2	2.45	0.69
1:C:359:SER:O	1:C:524:VAL:CG1	2.39	0.69
2:I:60:TYR:CE2	2:I:68:PHE:O	2.44	0.69
1:A:359:SER:O	1:A:524:VAL:CG1	2.39	0.69
2:I:74:ASN:OD1	2:I:74:ASN:N	2.22	0.69
1:B:577:ARG:NH1	1:B:582:LEU:HD13	2.07	0.69
1:C:569:ILE:H	1:C:569:ILE:HD12	1.56	0.69
2:H:52:TRP:O	2:H:72:ARG:NH1	2.25	0.69
2:I:60:TYR:OH	2:I:70:ILE:N	2.25	0.69
1:C:233:ILE:HG12	1:C:234:ASN:H	1.58	0.69
1:A:334:ASN:O	1:A:362:VAL:CG1	2.39	0.68
3:M:24:LEU:CB	3:M:25:PRO:CD	2.71	0.68
2:H:60:TYR:OH	2:H:70:ILE:N	2.25	0.68
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.74	0.68
3:L:24:LEU:CB	3:L:25:PRO:CD	2.71	0.68
1:B:403:ARG:NH2	1:B:405:ASP:OD2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:101:SER:O	3:M:103:ALA:N	2.23	0.68
1:B:406:GLU:HG3	1:B:418:ILE:HG13	1.75	0.67
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.67
1:C:335:LEU:CA	1:C:362:VAL:HG13	2.24	0.67
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.67
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.29	0.67
2:I:94:TYR:O	2:I:112:GLY:HA2	1.95	0.67
1:A:310:LYS:NZ	1:A:663:ASP:OD1	2.27	0.66
1:B:97:LYS:HD3	1:B:97:LYS:H	1.60	0.66
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.66
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.77	0.66
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.09	0.66
1:C:85:PRO:HA	1:C:237:ARG:HA	1.78	0.66
1:B:83:VAL:HG11	1:B:237:ARG:HH21	1.59	0.66
1:B:577:ARG:NH1	1:B:582:LEU:CD1	2.58	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.66
1:C:486:PHE:HZ	2:I:62:ASP:OD2	1.79	0.66
2:H:94:TYR:O	2:H:112:GLY:HA2	1.95	0.66
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.78	0.66
1:C:392:PHE:HD2	1:C:517:LEU:CD2	2.09	0.65
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.65
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.28	0.65
1:C:332:ILE:HD12	1:C:332:ILE:N	2.09	0.65
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.65
1:A:486:PHE:HZ	2:H:62:ASP:OD2	1.79	0.65
3:L:27:ASP:O	3:L:28:ILE:HD12	1.96	0.65
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.65
1:C:523:THR:HG22	1:C:524:VAL:HG22	1.79	0.65
3:L:28:ILE:HG22	3:L:33:TYR:HE1	1.61	0.65
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.78	0.65
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.65
1:A:705:VAL:HB	1:B:883:THR:HG21	1.78	0.65
1:B:358:ILE:HB	1:B:395:VAL:HB	1.78	0.65
3:M:27:ASP:O	3:M:28:ILE:HD12	1.96	0.65
1:C:522:ALA:O	1:C:523:THR:OG1	2.14	0.65
1:A:523:THR:HG22	1:A:524:VAL:HG22	1.79	0.64
1:B:455:LEU:HD21	1:B:457:ARG:HG3	1.78	0.64
1:B:108:THR:HA	1:B:236:THR:HG22	1.79	0.64
3:L:29:ASN:O	3:L:31:SER:N	2.30	0.64
3:M:29:ASN:O	3:M:31:SER:N	2.30	0.64
2:H:205:ASN:HB3	2:H:212:LYS:HE2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:VAL:HG22	1:B:453:TYR:HB2	1.79	0.64
1:B:472:ILE:HD13	1:B:474:GLN:HB3	1.79	0.64
3:M:24:LEU:HB3	3:M:25:PRO:CD	2.27	0.64
1:C:676:THR:HA	1:C:690:GLN:CB	2.25	0.64
1:C:533:LEU:HG	1:C:533:LEU:O	1.98	0.64
3:M:28:ILE:HG22	3:M:33:TYR:HE1	1.61	0.64
3:L:24:LEU:HB3	3:L:25:PRO:CD	2.27	0.64
1:B:607:GLN:O	1:B:608:VAL:HG23	1.98	0.64
1:A:391:CYS:SG	1:A:523:THR:O	2.56	0.63
1:C:334:ASN:O	1:C:362:VAL:CG1	2.46	0.63
3:M:130:PRO:HD3	3:M:142:LEU:HD22	1.80	0.63
1:C:196:ASN:ND2	1:C:200:TYR:O	2.32	0.63
2:H:130:LEU:HD11	2:H:147:LEU:HB2	1.81	0.63
2:I:158:VAL:HG22	2:I:204:VAL:HG22	1.81	0.63
1:C:391:CYS:SG	1:C:523:THR:O	2.56	0.63
2:H:158:VAL:HG22	2:H:204:VAL:HG22	1.81	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
3:L:130:PRO:HD3	3:L:142:LEU:HD22	1.80	0.62
2:I:130:LEU:HD11	2:I:147:LEU:HB2	1.81	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:B:111:ASP:OD1	1:B:112:SER:N	2.31	0.62
3:L:151:PRO:HG2	3:L:207:HIS:CE1	2.35	0.62
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	0.62
1:C:811:LYS:HB2	1:C:812:PRO:HD3	1.80	0.62
3:M:151:PRO:HG2	3:M:207:HIS:CE1	2.34	0.62
1:C:334:ASN:C	1:C:362:VAL:CG1	2.68	0.62
1:C:813:SER:O	1:C:814:LYS:HE2	2.00	0.62
1:B:454:ARG:HH21	1:B:493:GLN:HG3	1.63	0.62
1:A:336:CYS:HG	1:A:361:CYS:CB	2.12	0.62
1:B:560:LEU:H	1:B:563:GLN:HE21	1.45	0.62
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.61
2:I:205:ASN:HB3	2:I:212:LYS:HE2	1.79	0.61
1:C:516:GLU:O	1:C:517:LEU:CD2	2.48	0.61
1:B:391:CYS:CA	1:B:525:CYS:HB2	2.30	0.61
1:A:334:ASN:C	1:A:362:VAL:CG1	2.69	0.61
1:C:457:ARG:NH1	1:C:459:SER:O	2.33	0.61
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
3:L:55:ASP:OD1	3:L:58:LYS:NZ	2.33	0.61
1:C:357:ARG:HH12	1:C:394:ASN:HD21	1.49	0.61
1:C:521:PRO:O	1:C:522:ALA:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:CYS:HG	1:A:361:CYS:HG	1.29	0.61
3:M:142:LEU:HB2	3:M:188:LEU:HB3	1.82	0.61
1:C:112:SER:HB2	1:C:113:LYS:HD3	1.83	0.60
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.60
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.60
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.60
1:B:409:GLN:NE2	1:B:416:GLY:HA3	2.16	0.60
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.84	0.60
3:L:142:LEU:HB2	3:L:188:LEU:HB3	1.82	0.60
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.60
1:A:336:CYS:SG	1:A:361:CYS:HB2	2.40	0.60
2:H:139:GLY:N	3:M:197:SER:HB3	2.15	0.60
1:A:556:ASN:HD22	1:A:556:ASN:H	1.50	0.60
3:M:55:ASP:OD1	3:M:58:LYS:NZ	2.33	0.60
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.84	0.60
1:B:206:LYS:HD2	1:B:207:HIS:H	1.68	0.59
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.82	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:C:95:THR:HG22	1:C:96:GLU:H	1.66	0.59
1:A:361:CYS:N	1:A:524:VAL:HG12	2.18	0.59
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.67	0.59
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.59
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.59
1:C:361:CYS:N	1:C:524:VAL:HG12	2.18	0.59
3:L:13:SER:N	3:L:16:GLU:OE1	2.21	0.58
3:L:159:LYS:HG2	3:L:160:ALA:O	2.03	0.58
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.58
1:C:336:CYS:CB	1:C:361:CYS:HB2	2.33	0.58
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.58
1:C:599:THR:HG22	1:C:601:GLY:H	1.66	0.58
3:L:62:SER:O	3:L:62:SER:OG	2.21	0.58
1:B:452:LEU:HD21	1:B:492:LEU:HD13	1.85	0.58
2:H:60:TYR:OH	2:H:69:THR:CA	2.50	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
3:L:93:ASP:N	3:L:93:ASP:OD1	2.36	0.58
4:Z:2:NAG:H3	4:Z:2:NAG:H83	1.86	0.58
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.58
3:M:159:LYS:HG2	3:M:160:ALA:O	2.03	0.58
3:M:93:ASP:OD1	3:M:93:ASP:N	2.36	0.58
1:B:214:ARG:HD3	1:B:214:ARG:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1405:NAG:H3	5:A:1405:NAG:H83	1.86	0.57
3:L:28:ILE:CG2	3:L:33:TYR:CZ	2.88	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
3:M:28:ILE:CG2	3:M:33:TYR:CZ	2.88	0.57
5:B:1405:NAG:H83	5:B:1405:NAG:H3	1.87	0.57
1:B:408:ARG:O	1:B:414:GLN:NE2	2.32	0.57
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.38	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:B:213:VAL:HB	1:B:214:ARG:HD3	1.87	0.56
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.56
3:L:123:PRO:HD3	3:L:207:HIS:HD2	1.69	0.56
2:I:67:ARG:NH2	2:I:90:ASP:OD2	2.39	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
1:B:105:ILE:HG13	1:B:110:LEU:HD11	1.87	0.56
3:M:213:GLU:OE1	3:M:215:THR:OG1	2.24	0.56
5:C:1405:NAG:H3	5:C:1405:NAG:H83	1.88	0.56
2:H:125:PRO:HB2	2:H:148:VAL:HG23	1.88	0.56
3:M:88:SER:OG	3:M:88:SER:O	2.24	0.56
1:B:187:LYS:NZ	1:B:213:VAL:HG13	2.21	0.56
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.85	0.56
3:M:123:PRO:HD3	3:M:207:HIS:HD2	1.69	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:A:391:CYS:SG	1:A:524:VAL:O	2.64	0.56
1:C:519:HIS:O	1:C:519:HIS:ND1	2.38	0.55
3:M:13:SER:N	3:M:16:GLU:OE1	2.21	0.55
3:M:34:ASN:HB3	3:M:53:TYR:HB2	1.87	0.55
4:J:2:NAG:H83	4:J:2:NAG:H3	1.87	0.55
1:B:577:ARG:CD	1:B:582:LEU:HD13	2.35	0.55
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.55
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
3:L:213:GLU:OE1	3:L:215:THR:OG1	2.24	0.55
2:I:60:TYR:OH	2:I:69:THR:CA	2.50	0.55
2:I:125:PRO:HB2	2:I:148:VAL:HG23	1.88	0.55
1:A:342:PHE:HB3	4:E:1:NAG:H82	1.88	0.55
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.55
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.55
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.55
1:C:113:LYS:HD2	1:C:164:ASN:HD21	1.71	0.55
3:M:169:VAL:HA	3:M:187:TYR:O	2.07	0.55
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:GLU:OE2	1:B:698:SER:OG	2.25	0.55
1:C:342:PHE:HB3	4:V:1:NAG:H82	1.87	0.55
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.55
1:C:391:CYS:SG	1:C:524:VAL:O	2.64	0.55
3:L:88:SER:O	3:L:88:SER:OG	2.24	0.55
4:V:1:NAG:H61	4:V:2:NAG:HN2	1.71	0.55
3:L:34:ASN:HB3	3:L:53:TYR:HB2	1.87	0.55
1:B:352:ALA:HB2	1:B:468:ILE:HD12	1.88	0.55
3:L:169:VAL:HA	3:L:187:TYR:O	2.07	0.55
1:C:129:LYS:HD3	1:C:131:CYS:SG	2.46	0.54
2:I:205:ASN:HD22	2:I:207:LYS:HE3	1.71	0.54
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.54
1:C:421:TYR:HA	1:C:461:LEU:HG	1.90	0.54
1:A:359:SER:O	1:A:524:VAL:HG11	2.06	0.54
1:A:551:VAL:HB	1:A:588:THR:HG23	1.88	0.54
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.90	0.54
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
1:B:166:CYS:SG	1:B:167:THR:N	2.81	0.54
2:H:185:SER:HB2	3:L:187:TYR:OH	2.08	0.54
3:L:28:ILE:CG2	3:L:33:TYR:OH	2.56	0.54
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:A:336:CYS:HB2	1:A:361:CYS:HB2	1.89	0.54
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.54
2:H:135:LYS:O	3:L:214:LYS:NZ	2.41	0.54
3:L:10:SER:OG	3:L:11:SER:N	2.41	0.54
2:I:118:SER:OG	2:I:119:SER:N	2.41	0.54
2:I:145:GLY:HA2	2:I:160:TRP:HZ2	1.73	0.54
3:M:56:SER:H	3:M:58:LYS:NZ	2.05	0.54
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.54
1:C:359:SER:O	1:C:524:VAL:HG11	2.06	0.54
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.89	0.54
2:H:205:ASN:HD22	2:H:207:LYS:HE3	1.71	0.54
3:M:62:SER:O	3:M:62:SER:OG	2.21	0.54
1:B:165:ASN:OD1	5:B:1403:NAG:N2	2.40	0.54
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.54
2:I:132:PRO:HG3	2:I:144:LEU:HD23	1.89	0.54
2:H:132:PRO:HG3	2:H:144:LEU:HD23	1.89	0.53
3:L:56:SER:H	3:L:58:LYS:NZ	2.05	0.53
2:I:61:ALA:O	2:I:64:VAL:HG22	2.08	0.53
2:I:73:ASP:OD1	2:I:76:LYS:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:THR:OG1	1:B:334:ASN:N	2.41	0.53
2:H:73:ASP:OD1	2:H:76:LYS:HG3	2.07	0.53
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.71	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:C:97:LYS:HB3	1:C:187:LYS:HA	1.89	0.53
2:I:185:SER:HB2	3:M:187:TYR:OH	2.08	0.53
3:M:28:ILE:CG2	3:M:33:TYR:OH	2.56	0.53
2:H:61:ALA:O	2:H:64:VAL:HG22	2.08	0.53
4:G:2:NAG:H83	4:G:2:NAG:H3	1.90	0.53
1:A:335:LEU:CA	1:A:362:VAL:CG1	2.68	0.53
1:C:476:GLY:H	1:C:487:ASN:HB3	1.74	0.53
2:I:60:TYR:HH	2:I:69:THR:HA	1.73	0.53
3:M:10:SER:OG	3:M:11:SER:N	2.41	0.53
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.53
1:C:105:ILE:HG23	1:C:241:LEU:HD11	1.91	0.53
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.86	0.53
2:H:154:GLU:CD	2:H:154:GLU:H	2.12	0.53
3:L:99:TRP:HE1	3:L:102:ASN:HA	1.73	0.53
1:B:402:ILE:O	1:B:507:PRO:HA	2.09	0.53
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.53
2:H:118:SER:OG	2:H:119:SER:N	2.41	0.53
2:I:135:LYS:O	3:M:214:LYS:NZ	2.41	0.53
3:M:99:TRP:HE1	3:M:102:ASN:HA	1.73	0.53
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.52
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.52
3:L:141:THR:HA	3:L:188:LEU:O	2.09	0.52
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.52
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.52
1:B:1045:LYS:HZ2	1:C:786:LYS:HE3	1.72	0.52
2:H:145:GLY:HA2	2:H:160:TRP:HZ2	1.73	0.52
1:B:424:LYS:HB3	1:B:463:PRO:HA	1.92	0.52
1:B:112:SER:O	1:B:113:LYS:HB2	2.10	0.52
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.82	0.52
1:B:403:ARG:HA	1:B:495:TYR:OH	2.10	0.52
1:B:457:ARG:NH2	1:B:469:SER:O	2.43	0.52
1:C:113:LYS:HD3	1:C:113:LYS:N	2.25	0.52
3:L:194:GLN:HA	3:L:197:SER:HB3	1.91	0.52
1:B:555:SER:OG	1:B:584:ILE:O	2.28	0.52
1:C:193:VAL:HG23	1:C:223:LEU:HD23	1.91	0.52
1:B:353:TRP:CZ2	1:B:466:ARG:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:154:GLU:CD	2:I:154:GLU:H	2.11	0.52
1:A:523:THR:CG2	1:A:524:VAL:N	2.45	0.51
1:B:380:TYR:O	1:B:430:THR:HA	2.11	0.51
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.08	0.51
1:B:560:LEU:H	1:B:563:GLN:NE2	2.08	0.51
1:C:83:VAL:HG22	1:C:237:ARG:HD2	1.92	0.51
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
3:M:141:THR:HA	3:M:188:LEU:O	2.09	0.51
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.51
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.51
3:M:101:SER:C	3:M:103:ALA:H	2.13	0.51
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.45	0.51
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.51
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.51
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.76	0.50
1:C:97:LYS:HD3	1:C:187:LYS:HA	1.93	0.50
1:C:113:LYS:H	1:C:132:GLU:HB3	1.76	0.50
3:L:101:SER:C	3:L:103:ALA:H	2.13	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.93	0.50
1:A:334:ASN:ND2	1:A:361:CYS:HA	2.27	0.50
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.50
1:A:336:CYS:CB	1:A:361:CYS:HB2	2.41	0.50
1:A:964:LYS:HE3	1:C:570:ALA:HA	1.93	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.50
1:B:616:ASN:HB3	1:B:618:THR:HG22	1.94	0.50
1:B:675:GLN:HA	1:B:690:GLN:HG3	1.93	0.50
1:C:332:ILE:H	1:C:332:ILE:CD1	2.17	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
3:L:25:PRO:O	3:L:27:ASP:N	2.45	0.50
1:C:336:CYS:HB2	1:C:361:CYS:HB2	1.94	0.50
4:S:1:NAG:H62	4:S:2:NAG:H2	1.93	0.50
1:B:112:SER:N	1:B:133:PHE:O	2.45	0.49
1:B:350:VAL:HG23	1:B:422:ASN:HD22	1.77	0.49
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.49
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.12	0.49
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
1:B:31:SER:O	1:B:59:PHE:HA	2.10	0.49
3:L:160:ALA:HB1	3:L:198:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:25:PRO:O	3:M:27:ASP:N	2.45	0.49
3:M:160:ALA:HB1	3:M:198:HIS:CD2	2.48	0.49
3:L:100:PRO:O	3:L:101:SER:HB3	2.13	0.49
2:I:125:PRO:HD3	2:I:206:HIS:HD1	1.78	0.49
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.49
2:H:61:ALA:O	2:H:64:VAL:CG2	2.61	0.49
3:M:34:ASN:OD1	3:M:34:ASN:N	2.39	0.49
1:B:331:ASN:HD22	4:O:1:NAG:H83	1.78	0.49
1:C:117:LEU:HB2	1:C:130:VAL:HG22	1.94	0.49
1:C:200:TYR:HB3	1:C:228:ASP:OD1	2.13	0.49
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.49
3:L:127:LEU:HD21	3:L:142:LEU:HD12	1.94	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.49
2:I:91:THR:HB	2:I:117:VAL:H	1.78	0.49
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.49
3:L:207:HIS:CE1	3:L:208:GLU:HG2	2.48	0.49
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.48
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.95	0.48
1:B:396:TYR:HB2	1:B:514:SER:HB2	1.95	0.48
3:M:199:ARG:O	3:M:218:PRO:HD2	2.13	0.48
1:C:431:GLY:HA3	1:C:513:LEU:O	2.13	0.48
2:I:61:ALA:O	2:I:64:VAL:CG2	2.61	0.48
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.48
1:B:457:ARG:NH1	1:B:467:ASP:HB3	2.28	0.48
2:H:91:THR:HB	2:H:117:VAL:H	1.78	0.48
3:M:127:LEU:HD21	3:M:142:LEU:HD12	1.94	0.48
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.94	0.48
1:B:327:VAL:HG22	1:B:542:ASN:HB3	1.96	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
2:H:125:PRO:HD3	2:H:206:HIS:HD1	1.78	0.48
3:M:207:HIS:CE1	3:M:208:GLU:HG2	2.48	0.48
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.48
1:B:281:GLU:OE2	5:B:1405:NAG:H81	2.14	0.48
1:C:550:GLY:CA	1:C:590:CYS:SG	2.90	0.48
1:C:675:GLN:NE2	1:C:675:GLN:CA	2.73	0.48
2:I:53:TYR:HA	2:I:72:ARG:NH1	2.28	0.48
3:M:100:PRO:O	3:M:101:SER:HB3	2.12	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
2:H:139:GLY:HA2	3:M:197:SER:OG	2.09	0.48
2:H:161:ASN:ND2	2:H:199:THR:O	2.45	0.48
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:CYS:CB	1:A:361:CYS:HG	2.26	0.48
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.77	0.48
1:C:118:LEU:O	1:C:128:ILE:HA	2.14	0.48
1:C:197:ILE:HG22	1:C:198:ASP:H	1.78	0.48
1:A:521:PRO:HB3	1:B:199:GLY:HA3	1.95	0.48
3:M:28:ILE:HG23	3:M:33:TYR:OH	2.14	0.48
1:B:557:LYS:NZ	1:B:575:ALA:HB2	2.29	0.47
2:H:156:VAL:HG22	2:H:206:HIS:CD2	2.49	0.47
3:L:196:LYS:NZ	3:L:219:THR:OG1	2.47	0.47
2:I:161:ASN:ND2	2:I:199:THR:O	2.45	0.47
1:B:576:VAL:O	1:B:584:ILE:HA	2.13	0.47
2:H:53:TYR:HA	2:H:72:ARG:NH1	2.28	0.47
2:H:137:THR:HG23	2:H:142:ALA:HB2	1.96	0.47
3:L:199:ARG:O	3:L:218:PRO:HD2	2.13	0.47
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.47
1:C:140:PHE:CE2	1:C:244:LEU:HB2	2.49	0.47
3:L:25:PRO:CG	3:L:28:ILE:CD1	2.92	0.47
3:L:28:ILE:HG21	3:L:33:TYR:CZ	2.49	0.47
3:L:39:GLN:NE2	3:L:41:LYS:HE3	2.30	0.47
1:A:45:SER:O	1:A:47:VAL:HG22	2.14	0.47
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.47
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.47
1:C:516:GLU:C	1:C:517:LEU:CD2	2.82	0.47
2:I:156:VAL:HG22	2:I:206:HIS:CD2	2.49	0.47
1:C:605:SER:OG	1:C:606:ASN:N	2.47	0.47
3:L:178:SER:O	3:L:180:ASN:ND2	2.47	0.47
2:H:153:PRO:HB2	2:H:206:HIS:NE2	2.29	0.47
3:L:28:ILE:HG23	3:L:33:TYR:OH	2.14	0.47
3:M:86:LEU:HD23	3:M:115:VAL:HG12	1.96	0.47
1:A:501:ASN:ND2	2:H:102:THR:HG21	2.29	0.47
1:C:66:HIS:CE1	1:C:214:ARG:HH22	2.32	0.47
1:C:278:LYS:HB2	1:C:306:PHE:CZ	2.50	0.47
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.96	0.47
3:L:29:ASN:O	3:L:32:SER:N	2.48	0.47
3:L:86:LEU:HD23	3:L:115:VAL:HG12	1.96	0.47
2:I:130:LEU:HB3	3:M:128:PHE:CD2	2.49	0.47
3:M:28:ILE:HG21	3:M:33:TYR:CZ	2.49	0.47
3:M:178:SER:O	3:M:180:ASN:ND2	2.47	0.47
3:M:196:LYS:NZ	3:M:219:THR:OG1	2.47	0.47
1:B:577:ARG:HD3	1:B:582:LEU:HD11	1.92	0.47
1:C:501:ASN:ND2	2:I:102:THR:HG21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.47
2:H:130:LEU:HB3	3:L:128:PHE:CD2	2.49	0.47
3:L:27:ASP:C	3:L:28:ILE:HG13	2.35	0.47
1:B:403:ARG:NH2	1:B:504:GLY:O	2.47	0.47
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.97	0.47
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	0.47
3:L:160:ALA:O	3:L:162:SER:N	2.48	0.47
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.47
2:I:153:PRO:HB2	2:I:206:HIS:NE2	2.29	0.47
3:M:24:LEU:N	3:M:24:LEU:CD2	2.73	0.47
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.46
1:A:393:THR:HA	1:A:523:THR:HB	1.97	0.46
2:H:13:GLN:HA	2:H:118:SER:O	2.15	0.46
2:H:107:ASP:N	2:H:107:ASP:OD1	2.47	0.46
2:I:137:THR:HG23	2:I:142:ALA:HB2	1.96	0.46
3:M:39:GLN:NE2	3:M:41:LYS:HE3	2.30	0.46
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.46
3:M:160:ALA:O	3:M:162:SER:N	2.48	0.46
3:M:170:GLU:O	3:M:186:SER:HA	2.15	0.46
1:A:985:ASP:OD1	1:A:985:ASP:N	2.46	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.46
1:C:66:HIS:HE1	1:C:214:ARG:HH22	1.62	0.46
3:L:31:SER:O	3:L:31:SER:OG	2.29	0.46
3:L:170:GLU:O	3:L:186:SER:HA	2.15	0.46
3:M:29:ASN:O	3:M:32:SER:N	2.48	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:B:603:ASN:OD1	5:B:1407:NAG:N2	2.49	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
2:I:13:GLN:HA	2:I:118:SER:O	2.15	0.46
1:C:393:THR:HA	1:C:523:THR:HB	1.97	0.46
2:H:206:HIS:CD2	2:H:208:PRO:HD2	2.51	0.46
3:L:129:PRO:HA	3:L:142:LEU:HD13	1.97	0.46
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
1:B:567:ARG:HE	1:B:567:ARG:HB3	1.48	0.46
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.51	0.46
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.46
2:I:25:SER:OG	2:I:26:GLY:N	2.49	0.46
1:A:127:VAL:HG11	5:A:1402:NAG:H61	1.98	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ASN:ND2	1:B:533:LEU:H	2.14	0.46
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.46
2:I:107:ASP:OD1	2:I:107:ASP:N	2.47	0.46
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.46
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	0.46
1:A:361:CYS:H	1:A:524:VAL:HG12	1.79	0.46
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.46
1:B:437:ASN:HD21	1:B:506:GLN:HE21	1.64	0.46
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.46
1:B:424:LYS:HG3	1:B:461:LEU:O	2.17	0.45
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.45
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.45
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.45
3:M:27:ASP:C	3:M:28:ILE:HG13	2.35	0.45
2:H:25:SER:OG	2:H:26:GLY:N	2.49	0.45
3:M:25:PRO:CG	3:M:28:ILE:CD1	2.92	0.45
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.45
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.99	0.45
1:B:130:VAL:HG21	1:B:231:ILE:HD12	1.99	0.45
2:H:177:GLN:OE1	2:H:183:SER:OG	2.31	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:C:37:TYR:HA	1:C:223:LEU:H	1.81	0.45
2:H:39:GLN:O	2:H:92:ALA:HB1	2.17	0.45
2:I:133:SER:HB3	2:I:135:LYS:HG2	1.98	0.45
2:I:206:HIS:CD2	2:I:208:PRO:HD2	2.51	0.45
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.45
2:H:133:SER:HB3	2:H:135:LYS:HG2	1.98	0.45
1:B:521:PRO:HG3	1:B:564:GLN:HE21	1.81	0.45
1:C:314:GLN:HE21	1:C:314:GLN:HB2	1.56	0.45
1:C:447:GLY:HA2	1:C:497:PHE:O	2.16	0.45
2:I:151:TYR:OH	2:I:184:LEU:HD23	2.17	0.45
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.45
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.45
1:B:364:ASP:OD1	1:B:364:ASP:N	2.50	0.45
1:C:676:THR:CA	1:C:690:GLN:HE21	2.29	0.45
3:M:1:GLN:H3	3:M:1:GLN:CD	2.21	0.45
3:M:129:PRO:HA	3:M:142:LEU:HD13	1.97	0.45
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.45
2:H:151:TYR:OH	2:H:184:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:39:GLN:O	2:I:92:ALA:HB1	2.17	0.45
3:M:202:SER:HB2	3:M:214:LYS:O	2.17	0.45
1:A:336:CYS:CB	1:A:361:CYS:SG	3.05	0.45
1:B:521:PRO:HG3	1:B:564:GLN:NE2	2.32	0.45
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.45
1:A:676:THR:HB	1:A:693:ILE:HG21	1.98	0.44
1:B:437:ASN:OD1	1:B:438:SER:N	2.51	0.44
3:L:202:SER:HB2	3:L:214:LYS:O	2.17	0.44
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.44
1:B:350:VAL:HG11	1:B:402:ILE:HG23	2.00	0.44
1:B:472:ILE:H	1:B:472:ILE:HG13	1.56	0.44
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.17	0.44
1:A:500:THR:O	1:A:500:THR:OG1	2.31	0.44
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.44
3:M:199:ARG:HA	3:M:199:ARG:HD2	1.67	0.44
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.44
1:B:376:THR:CG2	1:B:378:LYS:HG3	2.48	0.44
1:B:454:ARG:NH2	1:B:456:PHE:HZ	2.16	0.44
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.44
1:C:142:GLY:H	1:C:243:ALA:HA	1.83	0.44
3:L:151:PRO:HG2	3:L:207:HIS:HE1	1.80	0.44
1:B:453:TYR:HD1	1:B:453:TYR:H	1.64	0.44
1:C:329:PHE:HB2	1:C:530:SER:OG	2.18	0.44
1:C:335:LEU:HA	1:C:362:VAL:CG1	2.36	0.44
2:H:160:TRP:HD1	2:H:169:VAL:HG13	1.83	0.44
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.44
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.44
3:M:176:LYS:HE2	3:M:176:LYS:HB3	1.79	0.44
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.44
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.44
1:B:461:LEU:HD12	1:B:461:LEU:HA	1.85	0.44
2:I:160:TRP:HD1	2:I:169:VAL:HG13	1.83	0.44
4:V:1:NAG:H61	4:V:2:NAG:N2	2.33	0.44
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.00	0.43
1:C:361:CYS:H	1:C:524:VAL:HG12	1.79	0.43
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.33	0.43
2:H:60:TYR:HH	2:H:69:THR:HA	1.78	0.43
1:B:167:THR:HG22	1:B:168:PHE:H	1.82	0.43
1:C:84:LEU:HD13	1:C:238:PHE:CE1	2.52	0.43
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.84	0.43
3:L:199:ARG:HD2	3:L:199:ARG:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:196:LYS:HA	3:M:196:LYS:HD2	1.75	0.43
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.77	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.43
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.43
1:B:439:ASN:HB3	1:B:506:GLN:HB2	1.99	0.43
3:L:88:SER:HA	3:L:115:VAL:HG21	1.99	0.43
3:M:29:ASN:C	3:M:31:SER:N	2.71	0.43
1:A:1097:SER:HA	1:A:1101:HIS:O	2.19	0.43
1:C:119:ILE:HG13	1:C:128:ILE:HG23	2.01	0.43
3:L:29:ASN:C	3:L:31:SER:N	2.71	0.43
3:L:191:THR:HG23	3:L:194:GLN:HB2	2.01	0.43
3:M:29:ASN:O	3:M:30:VAL:C	2.56	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43
1:B:559:PHE:O	1:B:560:LEU:HD13	2.18	0.43
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.43
3:L:29:ASN:O	3:L:30:VAL:C	2.56	0.43
3:L:117:GLY:O	3:L:118:GLN:HG2	2.19	0.43
3:M:117:GLY:O	3:M:118:GLN:HG2	2.19	0.43
3:M:151:PRO:HG2	3:M:207:HIS:HE1	1.80	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.43
3:L:25:PRO:C	3:L:27:ASP:N	2.71	0.43
3:M:130:PRO:HG2	3:M:140:ALA:HB1	2.01	0.43
1:B:121:ASN:O	1:B:121:ASN:ND2	2.50	0.43
2:I:73:ASP:OD1	2:I:75:SER:OG	2.24	0.43
2:I:201:ILE:HG23	2:I:216:LYS:HD2	2.00	0.43
3:M:191:THR:HG23	3:M:194:GLN:HB2	2.01	0.43
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.43
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.43
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.43
1:B:91:TYR:OH	1:B:191:GLU:HG2	2.19	0.43
3:L:91:GLU:OE2	3:L:91:GLU:N	2.32	0.43
4:E:1:NAG:H61	4:E:2:NAG:N2	2.33	0.43
1:A:113:LYS:O	1:A:113:LYS:NZ	2.31	0.43
1:B:462:LYS:H	1:B:462:LYS:HD3	1.84	0.43
1:C:516:GLU:C	1:C:517:LEU:HD23	2.39	0.43
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.51	0.43
2:H:38:ARG:NE	2:H:46:GLU:OE2	2.47	0.43
2:H:138:SER:HG	3:M:198:HIS:CE1	2.37	0.43
3:L:27:ASP:C	3:L:28:ILE:CG1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:131:SER:O	3:L:135:LEU:HG	2.19	0.43
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.42
5:A:1404:NAG:HO3	5:A:1404:NAG:C7	2.32	0.42
1:B:459:SER:C	1:B:461:LEU:H	2.22	0.42
5:B:1410:NAG:O4	5:B:1411:NAG:O5	2.28	0.42
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
2:H:148:VAL:HG13	2:H:184:LEU:HG	2.01	0.42
3:M:161:ASP:OD1	3:M:199:ARG:N	2.52	0.42
1:B:600:PRO:HB3	1:B:674:TYR:HB2	2.00	0.42
1:B:748:GLU:CD	1:B:981:LEU:HD21	2.39	0.42
1:C:521:PRO:O	1:C:522:ALA:CB	2.66	0.42
1:C:784:GLN:HE21	1:C:784:GLN:HB3	1.63	0.42
3:M:27:ASP:C	3:M:28:ILE:CG1	2.86	0.42
3:M:148:ASP:HA	3:M:181:LYS:HG3	2.01	0.42
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.42
1:B:29:THR:OG1	1:B:30:ASN:N	2.50	0.42
2:H:161:ASN:OD1	2:H:201:ILE:HG13	2.19	0.42
3:L:192:PRO:HA	3:L:195:TRP:HB3	2.02	0.42
3:M:25:PRO:C	3:M:27:ASP:N	2.71	0.42
3:M:88:SER:HA	3:M:115:VAL:HG21	1.99	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:A:127:VAL:HG21	5:A:1402:NAG:H5	2.01	0.42
1:C:143:VAL:C	1:C:154:GLU:HA	2.39	0.42
3:M:192:PRO:HA	3:M:195:TRP:HB3	2.02	0.42
1:B:472:ILE:CD1	1:B:474:GLN:HB3	2.47	0.42
1:C:233:ILE:HG12	1:C:234:ASN:N	2.28	0.42
1:C:532:ASN:OD1	1:C:532:ASN:N	2.51	0.42
2:H:184:LEU:HD12	2:H:185:SER:N	2.34	0.42
2:I:148:VAL:HG13	2:I:184:LEU:HG	2.01	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.42
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.42
3:L:130:PRO:HG2	3:L:140:ALA:HB1	2.01	0.42
3:L:161:ASP:OD1	3:L:199:ARG:N	2.52	0.42
2:I:153:PRO:HD2	2:I:206:HIS:CE1	2.54	0.42
2:I:161:ASN:OD1	2:I:201:ILE:HG13	2.19	0.42
2:I:195:LEU:HB3	2:I:219:PRO:HG3	2.02	0.42
3:M:131:SER:O	3:M:135:LEU:HG	2.19	0.42
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.46	0.42
1:B:567:ARG:HG2	1:C:42:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:PRO:HD2	2:H:206:HIS:CE1	2.54	0.42
2:H:195:LEU:HB3	2:H:219:PRO:HG3	2.02	0.42
1:A:334:ASN:CG	1:A:361:CYS:HA	2.39	0.42
3:L:148:ASP:HA	3:L:181:LYS:HG3	2.01	0.42
2:I:13:GLN:H	2:I:13:GLN:HG2	1.61	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:B:341:VAL:HG23	1:B:342:PHE:HD1	1.84	0.42
1:B:495:TYR:CZ	1:B:507:PRO:HG3	2.55	0.42
1:C:129:LYS:HZ3	1:C:169:GLU:HG2	1.84	0.42
1:C:556:ASN:HD22	1:C:556:ASN:HA	1.53	0.42
2:H:201:ILE:HG23	2:H:216:LYS:HD2	2.00	0.42
3:M:127:LEU:HD23	3:M:128:PHE:N	2.34	0.42
3:M:139:LYS:HD2	3:M:139:LYS:HA	1.70	0.42
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.55	0.42
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.42
3:L:1:GLN:H3	3:L:1:GLN:CD	2.21	0.42
1:A:99:ASN:O	1:A:102:ARG:NE	2.35	0.41
1:A:393:THR:O	1:A:523:THR:CG2	2.58	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.41
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.41
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.71	0.41
1:B:379:CYS:HA	1:B:432:CYS:HA	2.02	0.41
1:C:393:THR:H	1:C:517:LEU:HD22	1.85	0.41
3:M:142:LEU:HD23	3:M:190:LEU:HD11	2.02	0.41
4:W:1:NAG:H83	4:W:1:NAG:H3	2.02	0.41
1:B:376:THR:O	1:B:434:ILE:HA	2.20	0.41
2:I:14:PRO:HB3	2:I:88:ALA:HB2	2.02	0.41
1:B:81:ASN:O	1:B:239:GLN:NE2	2.54	0.41
1:C:122:ASN:ND2	1:C:125:ASN:HB2	2.35	0.41
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.41
3:L:127:LEU:HD23	3:L:128:PHE:N	2.34	0.41
3:M:101:SER:C	3:M:103:ALA:N	2.73	0.41
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.87	0.41
1:B:506:GLN:HA	1:B:507:PRO:HD3	1.94	0.41
1:C:117:LEU:HD22	1:C:231:ILE:HD12	2.03	0.41
1:C:460:ASN:OD1	1:C:460:ASN:N	2.53	0.41
2:I:184:LEU:HD12	2:I:185:SER:N	2.34	0.41
3:M:138:ASN:OD1	3:M:138:ASN:N	2.54	0.41
1:A:280:ASN:OD1	1:A:281:GLU:N	2.51	0.41
1:A:295:PRO:HB2	1:A:608:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:H	1:A:309:GLU:HG2	1.71	0.41
1:B:142:GLY:O	1:B:156:GLU:HG3	2.21	0.41
3:M:196:LYS:NZ	3:M:218:PRO:HB2	2.36	0.41
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.41
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.41
2:H:14:PRO:HB3	2:H:88:ALA:HB2	2.02	0.41
2:I:57:ASN:HB3	2:I:59:TYR:CE2	2.55	0.41
1:A:226:LEU:HB3	1:A:227:VAL:HG23	2.03	0.41
1:B:187:LYS:HG2	1:B:212:LEU:O	2.21	0.41
1:B:541:PHE:O	1:B:547:THR:HA	2.20	0.41
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41
1:C:188:ASN:HB2	1:C:190:ARG:HH11	1.86	0.41
3:L:25:PRO:CG	3:L:28:ILE:HD12	2.40	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:B:403:ARG:NE	1:B:505:TYR:HD1	2.19	0.41
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.41
1:C:854:LYS:HE2	1:C:854:LYS:HB3	1.88	0.41
1:C:931:ILE:HD13	1:C:931:ILE:HA	1.86	0.41
2:H:57:ASN:HB3	2:H:59:TYR:CE2	2.55	0.41
2:H:206:HIS:HD2	2:H:208:PRO:HD2	1.86	0.41
3:L:134:GLU:OE2	3:L:141:THR:OG1	2.29	0.41
3:L:160:ALA:HA	3:L:201:TYR:CD1	2.55	0.41
1:A:392:PHE:CA	1:A:517:LEU:HD21	2.49	0.41
1:B:1040:VAL:O	1:B:1041:ASP:HB2	2.21	0.41
2:H:109:TRP:CD1	2:H:109:TRP:N	2.88	0.41
1:B:132:GLU:HG3	1:B:165:ASN:HB2	2.02	0.40
1:B:458:LYS:HE2	1:B:458:LYS:HB2	1.79	0.40
1:B:578:ASP:N	1:B:583:GLU:O	2.37	0.40
1:C:342:PHE:CB	4:V:1:NAG:H82	2.52	0.40
3:L:196:LYS:NZ	3:L:218:PRO:HB2	2.36	0.40
3:M:194:GLN:O	3:M:201:TYR:OH	2.39	0.40
1:A:166:CYS:HB3	1:A:169:GLU:OE1	2.21	0.40
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.78	0.40
1:B:646:ARG:O	1:B:646:ARG:HG3	2.22	0.40
1:C:334:ASN:O	1:C:336:CYS:N	2.53	0.40
1:C:334:ASN:C	1:C:336:CYS:N	2.73	0.40
1:C:334:ASN:CG	1:C:361:CYS:HA	2.39	0.40
1:C:501:ASN:HD21	2:I:102:THR:HG21	1.86	0.40
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.40
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204:VAL:O	2:H:212:LYS:HA	2.22	0.40
1:B:273:ARG:HA	1:B:273:ARG:HD3	1.70	0.40
1:B:794:ILE:H	1:B:794:ILE:HG13	1.69	0.40
2:I:215:LYS:HD2	2:I:215:LYS:HA	1.92	0.40
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.56	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:B:135:PHE:HE1	1:B:159:VAL:HG12	1.86	0.40
1:C:369:TYR:CZ	1:C:384:PRO:HB2	2.57	0.40
2:H:61:ALA:H	2:H:64:VAL:HG23	1.86	0.40
3:L:67:ARG:NH1	3:L:90:ASP:OD2	2.55	0.40
3:L:138:ASN:OD1	3:L:138:ASN:N	2.54	0.40
3:L:164:PRO:HB2	3:L:166:LYS:NZ	2.36	0.40
1:A:334:ASN:O	1:A:362:VAL:N	2.44	0.40
1:A:703:ASN:O	1:B:789:TYR:HA	2.22	0.40
1:A:879:ALA:O	1:A:883:THR:HB	2.22	0.40
1:B:122:ASN:OD1	1:B:122:ASN:N	2.48	0.40
1:C:309:GLU:O	1:C:313:TYR:OH	2.28	0.40
1:C:615:VAL:HG12	1:C:616:ASN:O	2.20	0.40
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.40
2:H:7:SER:OG	2:H:8:GLY:N	2.55	0.40
2:H:58:LYS:HA	2:H:58:LYS:HD2	1.77	0.40
3:L:142:LEU:HD23	3:L:190:LEU:HD11	2.02	0.40
2:I:109:TRP:CD1	2:I:109:TRP:N	2.88	0.40
3:M:67:ARG:NH1	3:M:90:ASP:OD2	2.55	0.40
3:M:89:GLU:OE2	3:M:89:GLU:N	2.54	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	988/1283 (77%)	895 (91%)	89 (9%)	4 (0%)	34 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	958/1283 (75%)	868 (91%)	89 (9%)	1 (0%)	51	78
1	C	986/1283 (77%)	892 (90%)	82 (8%)	12 (1%)	13	32
2	H	219/449 (49%)	186 (85%)	31 (14%)	2 (1%)	17	40
2	I	219/449 (49%)	186 (85%)	31 (14%)	2 (1%)	17	40
3	L	217/222 (98%)	182 (84%)	27 (12%)	8 (4%)	3	7
3	M	217/222 (98%)	182 (84%)	27 (12%)	8 (4%)	3	7
All	All	3804/5191 (73%)	3391 (89%)	376 (10%)	37 (1%)	20	37

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	LEU
1	C	518	LEU
1	C	814	LYS
2	H	63	SER
3	L	102	ASN
2	I	63	SER
3	M	102	ASN
1	C	591	SER
1	C	810	SER
2	H	62	ASP
3	L	24	LEU
3	L	26	SER
3	L	30	VAL
2	I	62	ASP
3	M	24	LEU
3	M	26	SER
3	M	30	VAL
1	A	522	ALA
1	C	522	ALA
1	A	349	SER
1	A	520	ALA
1	C	349	SER
1	C	520	ALA
1	C	813	SER
3	L	28	ILE
3	L	100	PRO
3	L	101	SER
3	M	28	ILE
3	M	100	PRO

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Mol	Chain	Res	Type
3	M	101	SER
1	B	88	ASP
1	C	335	LEU
1	C	336	CYS
1	C	812	PRO
3	L	55	ASP
3	M	55	ASP
1	C	811	LYS

### 5.3.2 Protein sidechains [i](#)

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	881/1122 (78%)	788 (89%)	93 (11%)	6	15
1	B	862/1122 (77%)	762 (88%)	100 (12%)	5	12
1	C	879/1122 (78%)	789 (90%)	90 (10%)	7	17
2	H	185/396 (47%)	164 (89%)	21 (11%)	5	13
2	I	185/396 (47%)	164 (89%)	21 (11%)	5	13
3	L	188/191 (98%)	164 (87%)	24 (13%)	4	10
3	M	188/191 (98%)	163 (87%)	25 (13%)	4	9
All	All	3368/4540 (74%)	2994 (89%)	374 (11%)	9	14

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	141	LEU
1	A	143	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	282	ASN
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	318	PHE
1	A	324	GLU
1	A	325	SER
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
1	A	525	CYS
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	558	LYS
1	A	576	VAL
1	A	583	GLU
1	A	588	THR
1	A	590	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	599	THR
1	A	602	THR
1	A	646	ARG
1	A	673	SER
1	A	698	SER
1	A	703	ASN
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER
1	A	773	GLU
1	A	785	VAL
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	937	SER
1	A	939	SER
1	A	951	VAL
1	A	967	SER
1	A	982	SER
1	A	994	ASP
1	A	1005	GLN
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1141	LEU
1	A	1142	GLN
1	A	1144	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	45	SER
1	B	48	LEU
1	B	50	SER
1	B	51	THR
1	B	52	GLN
1	B	53	ASP
1	B	60	SER
1	B	87	ASN
1	B	88	ASP
1	B	95	THR
1	B	97	LYS
1	B	99	ASN
1	B	108	THR
1	B	109	THR
1	B	112	SER
1	B	113	LYS
1	B	116	SER
1	B	120	VAL
1	B	127	VAL
1	B	158	ARG
1	B	164	ASN
1	B	205	SER
1	B	207	HIS
1	B	208	THR
1	B	214	ARG
1	B	240	THR
1	B	278	LYS
1	B	307	THR
1	B	318	PHE
1	B	328	ARG
1	B	345	THR
1	B	359	SER
1	B	371	SER
1	B	382	VAL
1	B	385	THR
1	B	388	ASN
1	B	402	ILE
1	B	403	ARG
1	B	409	GLN
1	B	417	LYS
1	B	430	THR
1	B	453	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	462	LYS
1	B	464	PHE
1	B	467	ASP
1	B	473	TYR
1	B	487	ASN
1	B	490	PHE
1	B	494	SER
1	B	495	TYR
1	B	506	GLN
1	B	514	SER
1	B	525	CYS
1	B	531	THR
1	B	532	ASN
1	B	533	LEU
1	B	534	VAL
1	B	567	ARG
1	B	569	ILE
1	B	576	VAL
1	B	582	LEU
1	B	597	VAL
1	B	606	ASN
1	B	607	GLN
1	B	614	ASP
1	B	615	VAL
1	B	617	CYS
1	B	640	SER
1	B	649	CYS
1	B	676	THR
1	B	704	SER
1	B	710	ASN
1	B	746	SER
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	808	ASP
1	B	854	LYS
1	B	855	PHE
1	B	856	ASN
1	B	868	GLU
1	B	878	LEU
1	B	912	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	916	LEU
1	B	935	GLN
1	B	964	LYS
1	B	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1141	LEU
1	C	29	THR
1	C	50	SER
1	C	51	THR
1	C	60	SER
1	C	63	THR
1	C	84	LEU
1	C	86	PHE
1	C	98	SER
1	C	113	LYS
1	C	114	THR
1	C	117	LEU
1	C	120	VAL
1	C	125	ASN
1	C	143	VAL
1	C	156	GLU
1	C	172	SER
1	C	190	ARG
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	212	LEU
1	C	215	ASP
1	C	221	SER
1	C	234	ASN
1	C	271	GLN
1	C	287	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	301	CYS
1	C	305	SER
1	C	314	GLN
1	C	318	PHE
1	C	332	ILE
1	C	335	LEU
1	C	336	CYS
1	C	353	TRP
1	C	355	ARG
1	C	375	SER
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	421	TYR
1	C	430	THR
1	C	438	SER
1	C	440	ASN
1	C	500	THR
1	C	514	SER
1	C	517	LEU
1	C	518	LEU
1	C	525	CYS
1	C	530	SER
1	C	532	ASN
1	C	533	LEU
1	C	546	LEU
1	C	551	VAL
1	C	555	SER
1	C	556	ASN
1	C	567	ARG
1	C	573	THR
1	C	584	ILE
1	C	586	ASP
1	C	591	SER
1	C	602	THR
1	C	606	ASN
1	C	641	ASN
1	C	658	ASN
1	C	675	GLN
1	C	690	GLN
1	C	697	MET
1	C	703	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	727	LEU
1	C	740	MET
1	C	778	THR
1	C	787	GLN
1	C	814	LYS
1	C	856	ASN
1	C	859	THR
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1017	GLU
1	C	1077	THR
1	C	1094	VAL
1	C	1104	VAL
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	H	3	GLN
2	H	19	ARG
2	H	25	SER
2	H	28	THR
2	H	31	SER
2	H	52	TRP
2	H	63	SER
2	H	65	LYS
2	H	74	ASN
2	H	91	THR
2	H	118	SER
2	H	126	SER
2	H	138	SER
2	H	144	LEU
2	H	148	VAL
2	H	166	THR
2	H	179	SER
2	H	185	SER
2	H	203	ASN
2	H	207	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	214	ASP
3	L	9	SER
3	L	10	SER
3	L	21	THR
3	L	24	LEU
3	L	28	ILE
3	L	30	VAL
3	L	44	SER
3	L	56	SER
3	L	71	SER
3	L	73	ASP
3	L	93	ASP
3	L	104	LEU
3	L	124	SER
3	L	138	ASN
3	L	155	THR
3	L	175	SER
3	L	178	SER
3	L	185	SER
3	L	190	LEU
3	L	191	THR
3	L	193	GLU
3	L	197	SER
3	L	206	THR
3	L	213	GLU
2	I	3	GLN
2	I	19	ARG
2	I	25	SER
2	I	28	THR
2	I	31	SER
2	I	52	TRP
2	I	63	SER
2	I	65	LYS
2	I	74	ASN
2	I	91	THR
2	I	118	SER
2	I	126	SER
2	I	138	SER
2	I	144	LEU
2	I	148	VAL
2	I	166	THR
2	I	179	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	185	SER
2	I	203	ASN
2	I	207	LYS
2	I	214	ASP
3	M	5	THR
3	M	9	SER
3	M	10	SER
3	M	21	THR
3	M	24	LEU
3	M	28	ILE
3	M	30	VAL
3	M	44	SER
3	M	46	PRO
3	M	56	SER
3	M	71	SER
3	M	73	ASP
3	M	93	ASP
3	M	104	LEU
3	M	124	SER
3	M	138	ASN
3	M	155	THR
3	M	175	SER
3	M	178	SER
3	M	185	SER
3	M	190	LEU
3	M	191	THR
3	M	193	GLU
3	M	206	THR
3	M	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	354	ASN
1	A	360	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	498	GLN
1	A	540	ASN
1	A	556	ASN
1	A	644	GLN
1	A	658	ASN
1	A	690	GLN
1	A	703	ASN
1	A	762	GLN
1	A	787	GLN
1	A	856	ASN
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	955	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN
1	B	115	GLN
1	B	134	GLN
1	B	164	ASN
1	B	188	ASN
1	B	245	HIS
1	B	354	ASN
1	B	422	ASN
1	B	487	ASN
1	B	506	GLN
1	B	532	ASN
1	B	540	ASN
1	B	563	GLN
1	B	606	ASN
1	B	607	GLN
1	B	655	HIS
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1054	GLN
1	C	66	HIS
1	C	188	ASN
1	C	207	HIS
1	C	271	GLN
1	C	314	GLN
1	C	321	GLN
1	C	354	ASN
1	C	360	ASN
1	C	394	ASN
1	C	422	ASN
1	C	440	ASN
1	C	498	GLN
1	C	556	ASN
1	C	606	ASN
1	C	641	ASN
1	C	675	GLN
1	C	690	GLN
1	C	703	ASN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1106	GLN
2	H	111	GLN
3	L	6	GLN
3	L	40	GLN
3	L	60	GLN
3	L	118	GLN
3	L	198	HIS
3	L	204	GLN
2	I	111	GLN
3	M	6	GLN
3	M	40	GLN

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Mol	Chain	Res	Type
3	M	60	GLN
3	M	118	GLN
3	M	198	HIS
3	M	204	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

42 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	4,1	14,14,15	0.52	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.59	0
4	NAG	E	1	4,1	14,14,15	0.57	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	F	1	4,1	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
4	NAG	F	2	4	14,14,15	0.52	0	17,19,21	0.46	0
4	NAG	G	1	4,1	14,14,15	0.38	0	17,19,21	0.72	0
4	NAG	G	2	4	14,14,15	0.30	0	17,19,21	1.31	2 (11%)
4	NAG	J	1	4,1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
4	NAG	J	2	4	14,14,15	0.41	0	17,19,21	1.40	3 (17%)
4	NAG	K	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	K	2	4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	N	1	4,1	14,14,15	0.25	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	N	2	4	14,14,15	0.15	0	17,19,21	0.46	0
4	NAG	O	1	4,1	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	O	2	4	14,14,15	0.16	0	17,19,21	0.47	0
4	NAG	P	1	4,1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	P	2	4	14,14,15	0.37	0	17,19,21	0.37	0
4	NAG	Q	1	4,1	14,14,15	0.34	0	17,19,21	1.12	1 (5%)
4	NAG	Q	2	4	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	R	1	4,1	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
4	NAG	R	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	S	1	4,1	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	S	2	4	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
4	NAG	T	1	4,1	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	T	2	4	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	U	1	4,1	14,14,15	0.40	0	17,19,21	0.57	0
4	NAG	U	2	4	14,14,15	0.25	0	17,19,21	0.61	1 (5%)
4	NAG	V	1	4,1	14,14,15	0.56	0	17,19,21	0.56	0
4	NAG	V	2	4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	W	1	4,1	14,14,15	0.23	0	17,19,21	1.35	1 (5%)
4	NAG	W	2	4	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	X	1	4,1	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
4	NAG	X	2	4	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	Y	1	4,1	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	Y	2	4	14,14,15	0.20	0	17,19,21	0.73	0
4	NAG	Z	1	4,1	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	Z	2	4	14,14,15	0.56	0	17,19,21	1.32	1 (5%)
4	NAG	a	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.44	0
4	NAG	a	2	4	14,14,15	0.31	0	17,19,21	1.35	2 (11%)
4	NAG	b	1	4,1	14,14,15	0.42	0	17,19,21	0.43	0
4	NAG	b	2	4	14,14,15	0.24	0	17,19,21	0.48	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	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	5/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	3/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	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	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	4/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	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	4,1	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	b	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	O5-C1	-2.70	1.39	1.43
4	K	1	NAG	O5-C1	-2.55	1.39	1.43
4	J	1	NAG	O5-C1	-2.34	1.40	1.43
4	a	1	NAG	O5-C1	-2.18	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	1	NAG	C2-N2-C7	4.64	129.51	122.90
4	J	2	NAG	C2-N2-C7	4.38	129.14	122.90
4	Z	2	NAG	C2-N2-C7	4.36	129.11	122.90
4	a	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	G	2	NAG	C2-N2-C7	4.31	129.05	122.90
4	Q	1	NAG	C1-O5-C5	3.24	116.58	112.19
4	J	2	NAG	C1-C2-N2	2.40	114.58	110.49
4	S	1	NAG	O4-C4-C3	-2.39	104.82	110.35
4	X	1	NAG	C1-O5-C5	2.26	115.26	112.19
4	a	2	NAG	C1-C2-N2	2.26	114.35	110.49
4	G	2	NAG	C1-C2-N2	2.25	114.34	110.49
4	R	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	N	1	NAG	C1-O5-C5	2.16	115.11	112.19
4	J	2	NAG	C1-O5-C5	2.11	115.05	112.19
4	U	2	NAG	C1-O5-C5	2.08	115.01	112.19
4	F	1	NAG	C1-O5-C5	2.07	114.99	112.19
4	S	2	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	W	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	S	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	T	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6

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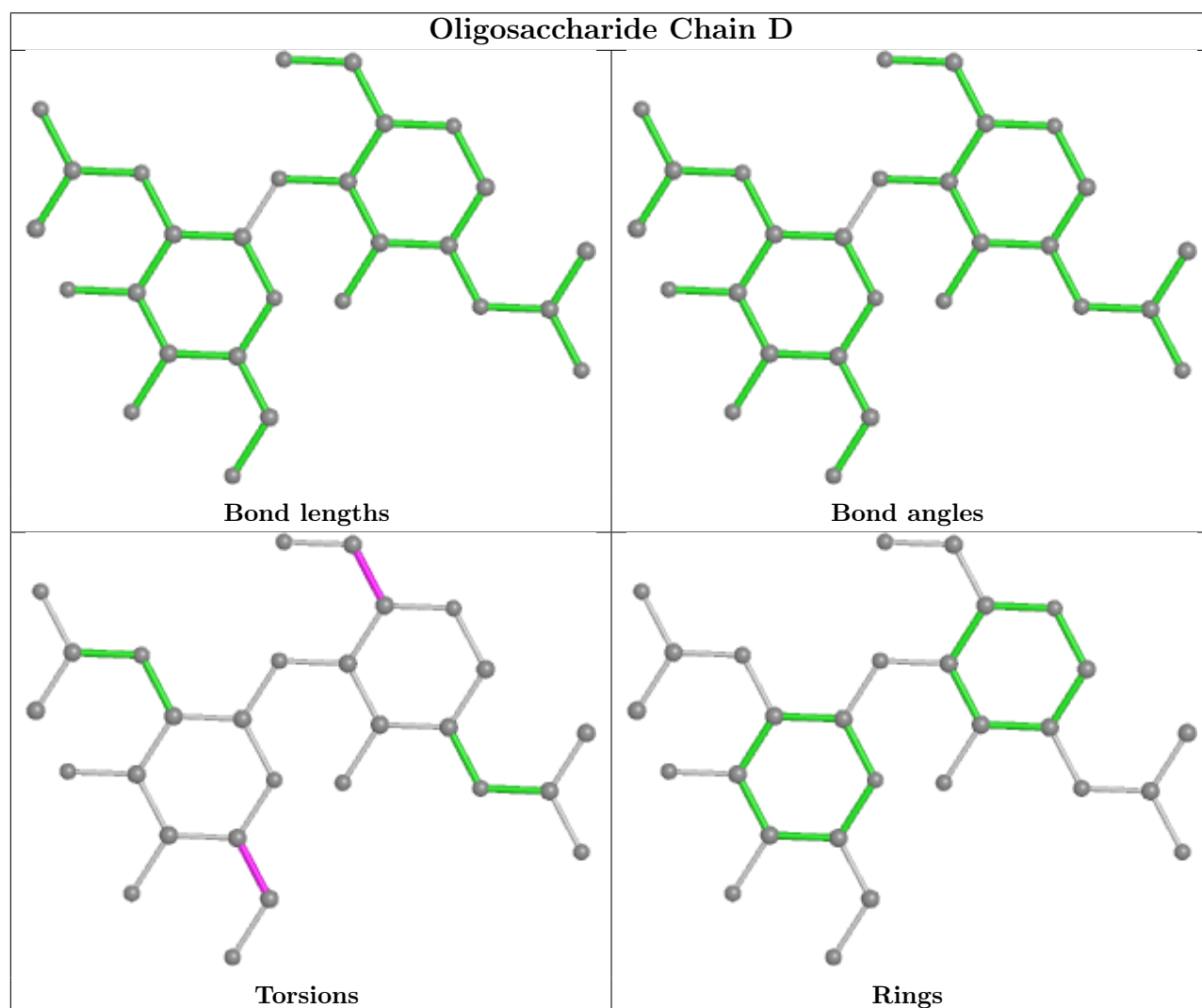
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	V	2	NAG	C1-C2-N2-C7
4	a	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	W	1	NAG	C1-C2-N2-C7
4	V	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	Z	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7
4	V	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

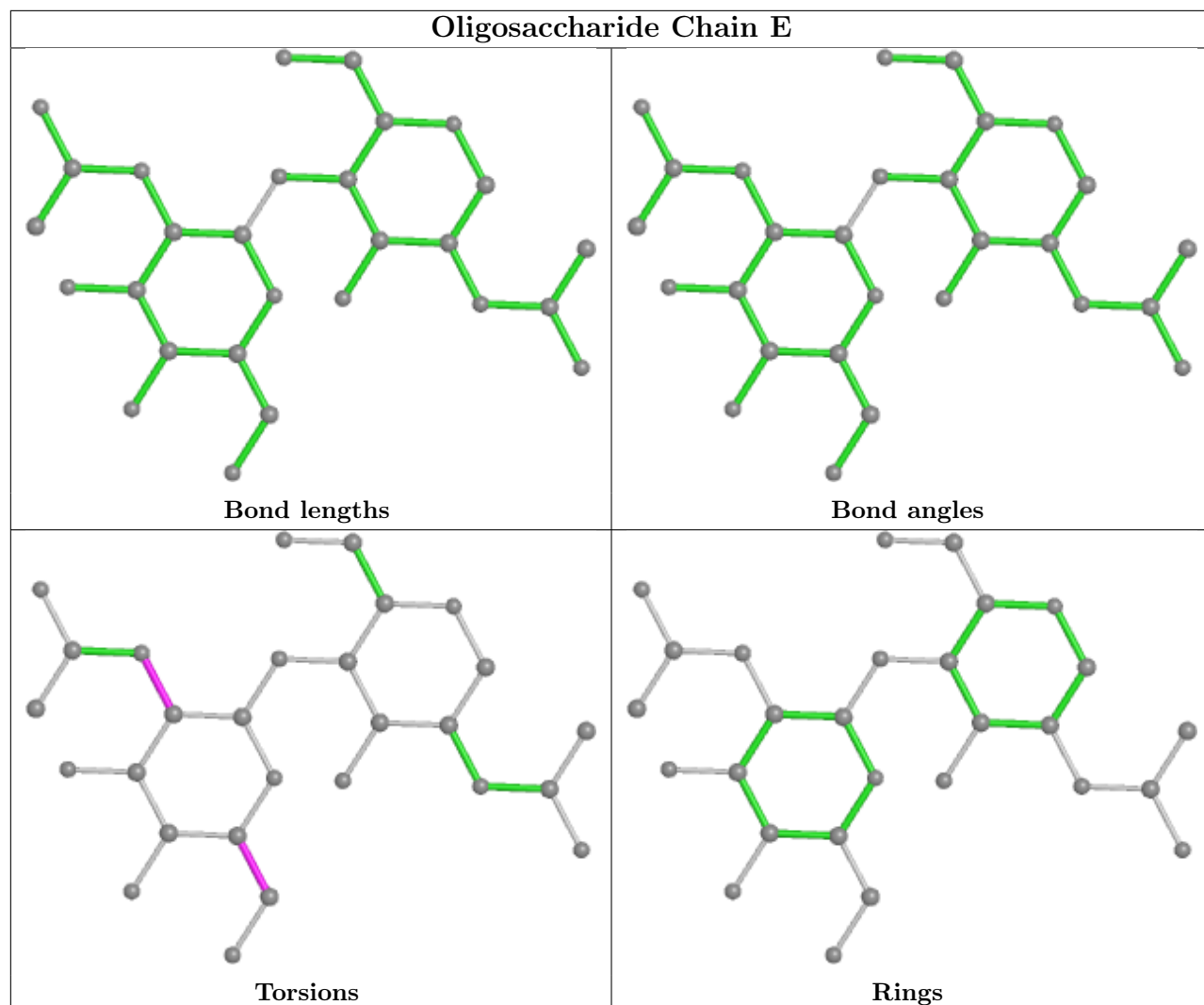
There are no ring outliers.

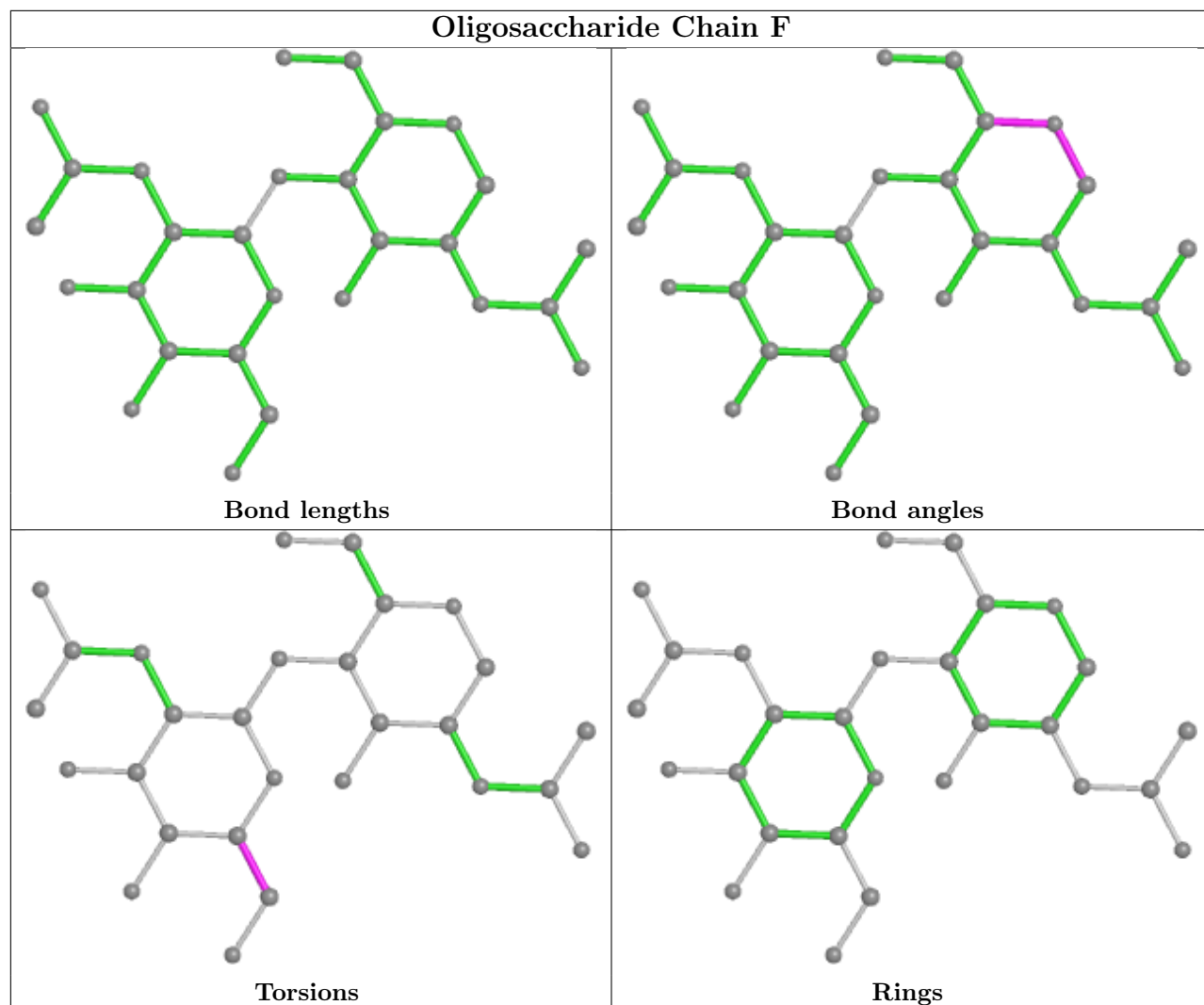
11 monomers are involved in 13 short contacts:

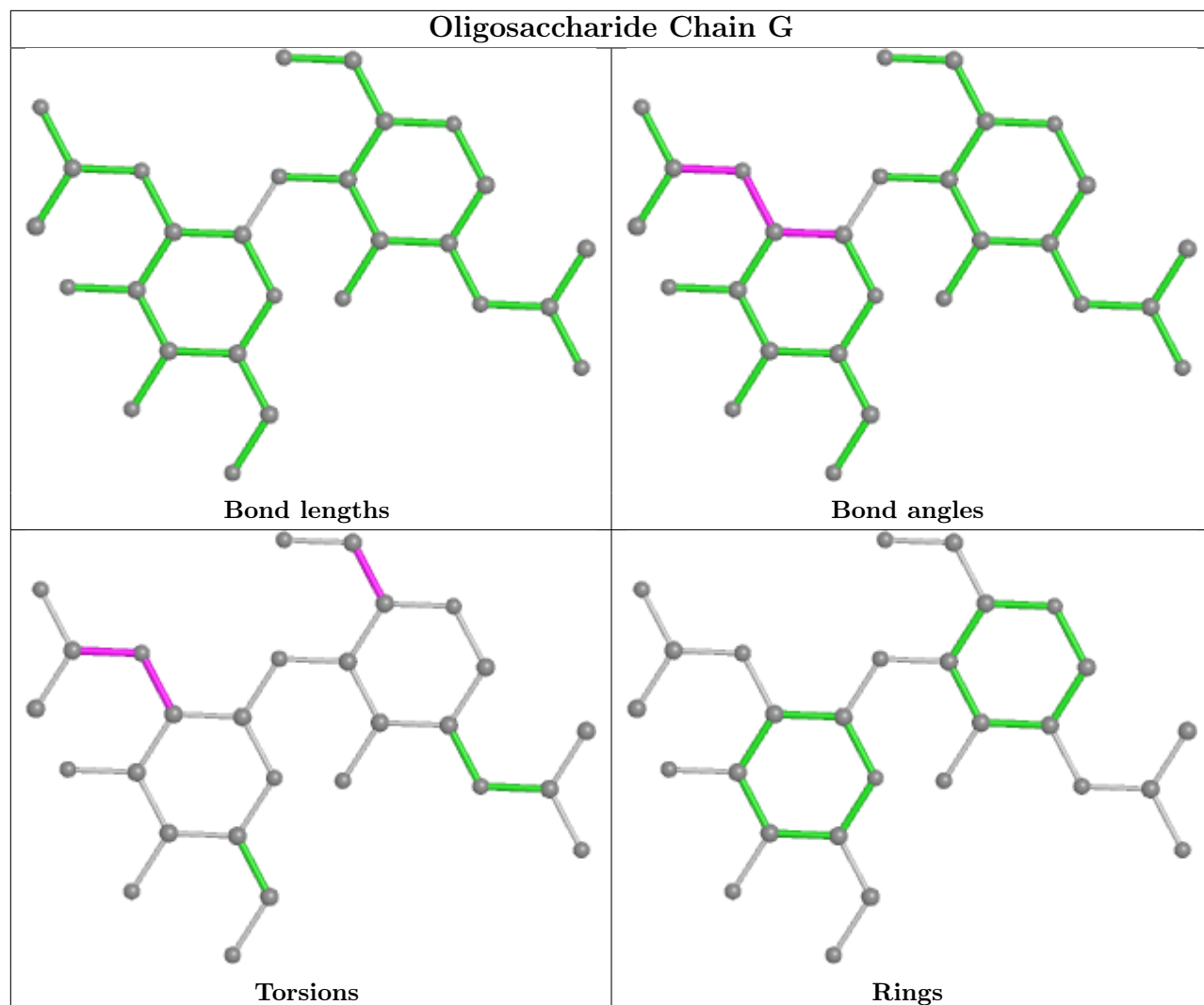
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	1	0
4	J	2	NAG	1	0
4	S	2	NAG	1	0
4	V	2	NAG	2	0
4	Z	2	NAG	1	0
4	G	2	NAG	1	0
4	O	1	NAG	1	0
4	W	1	NAG	1	0
4	E	2	NAG	2	0
4	V	1	NAG	4	0
4	E	1	NAG	3	0

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

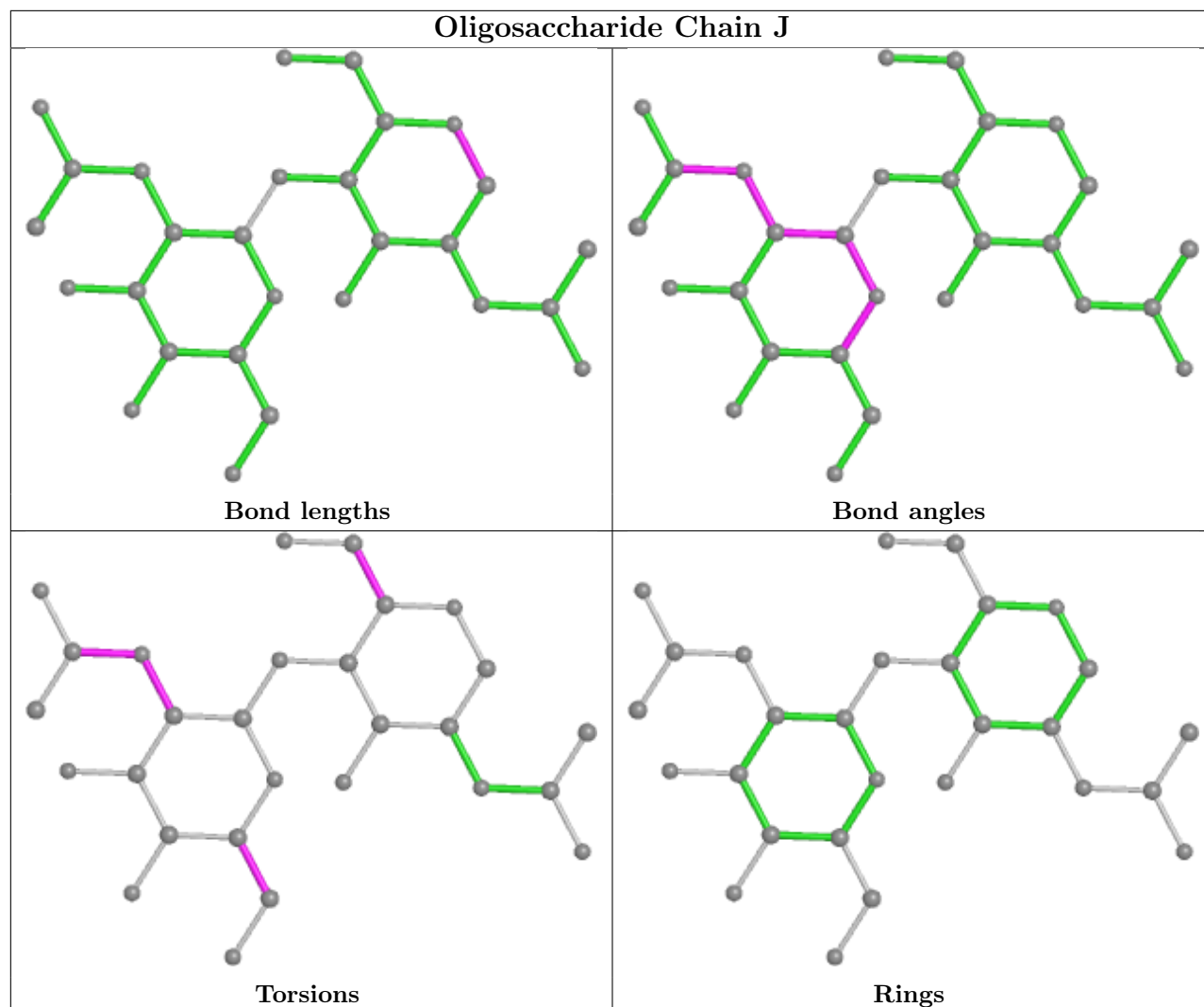


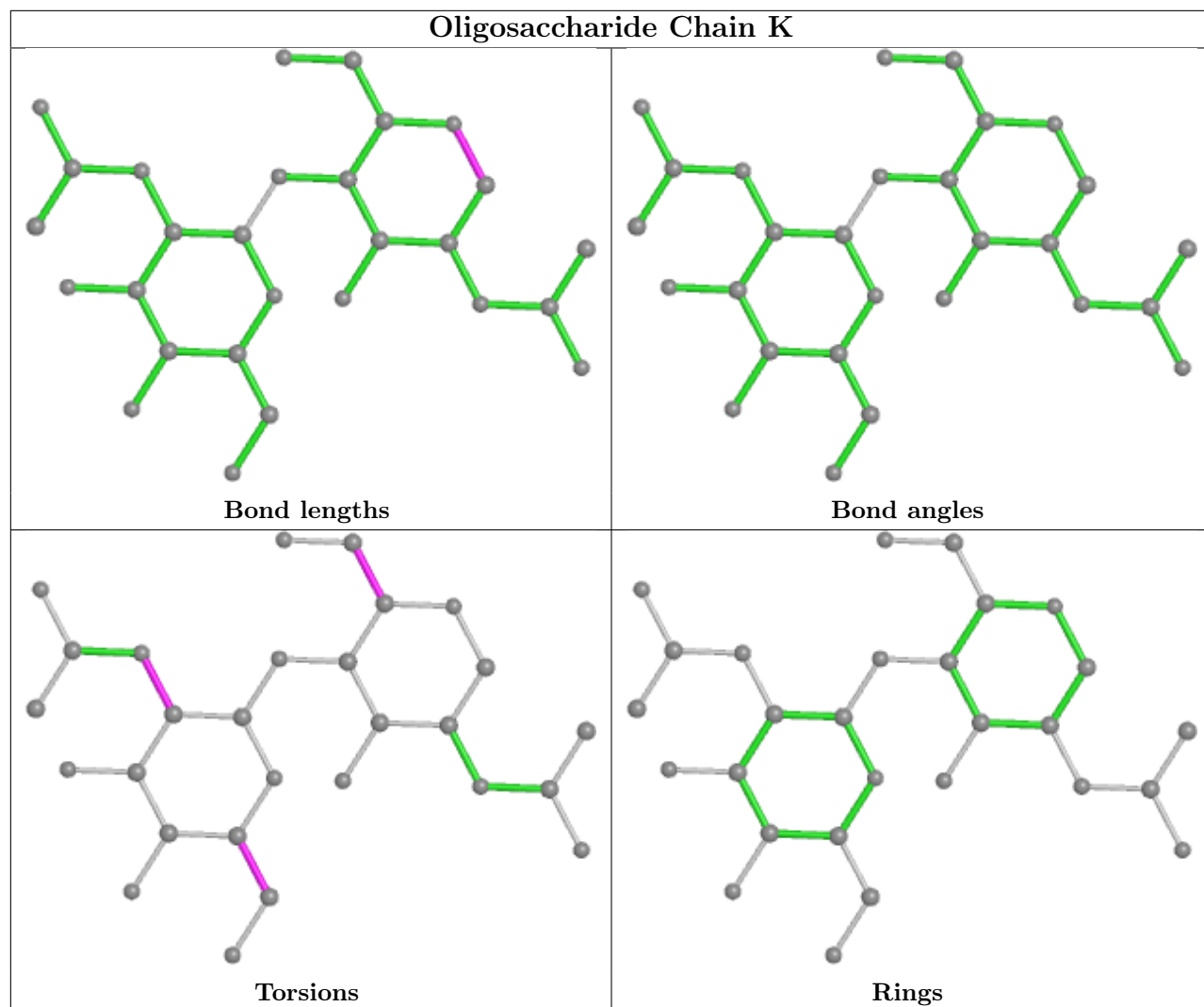


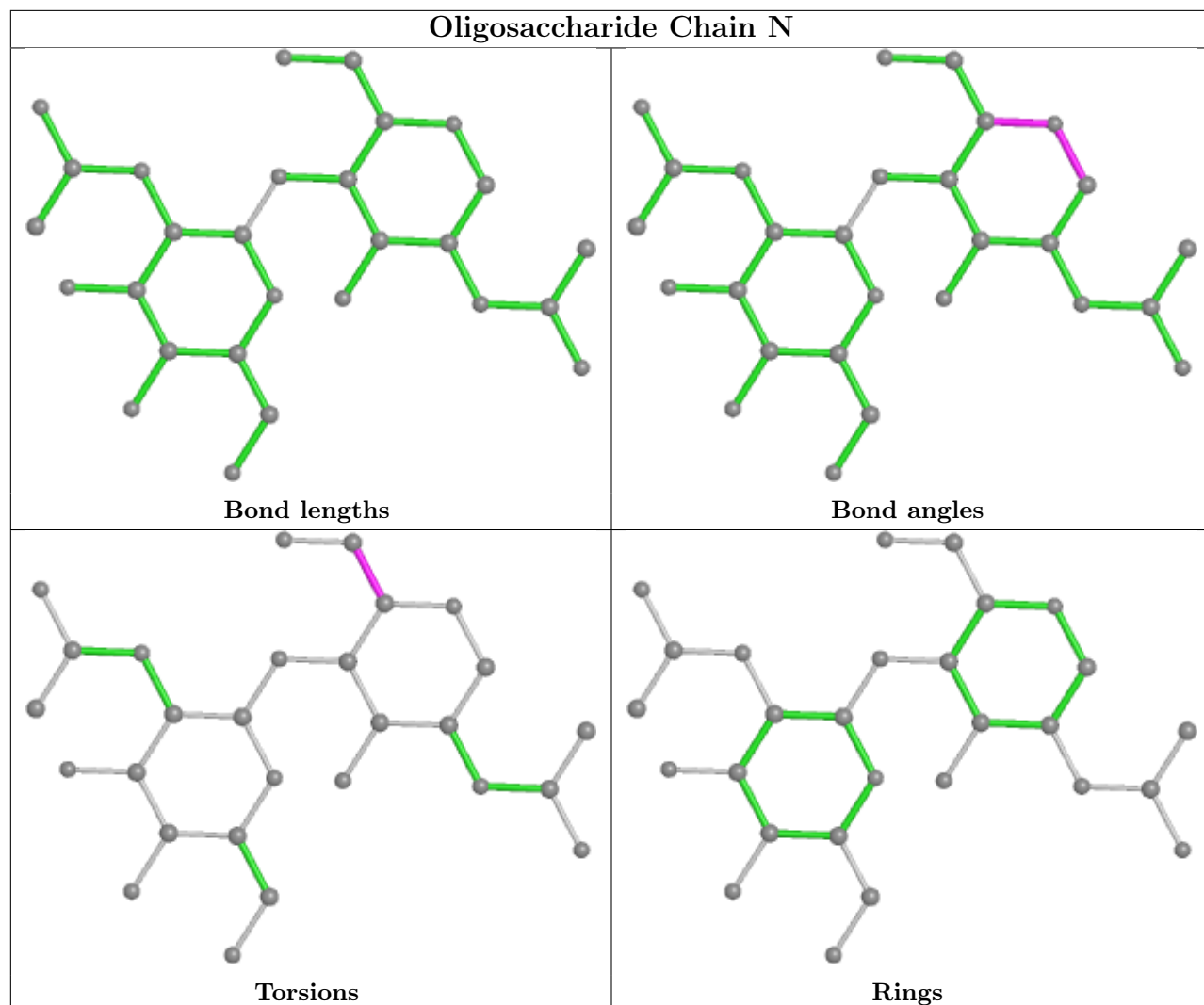


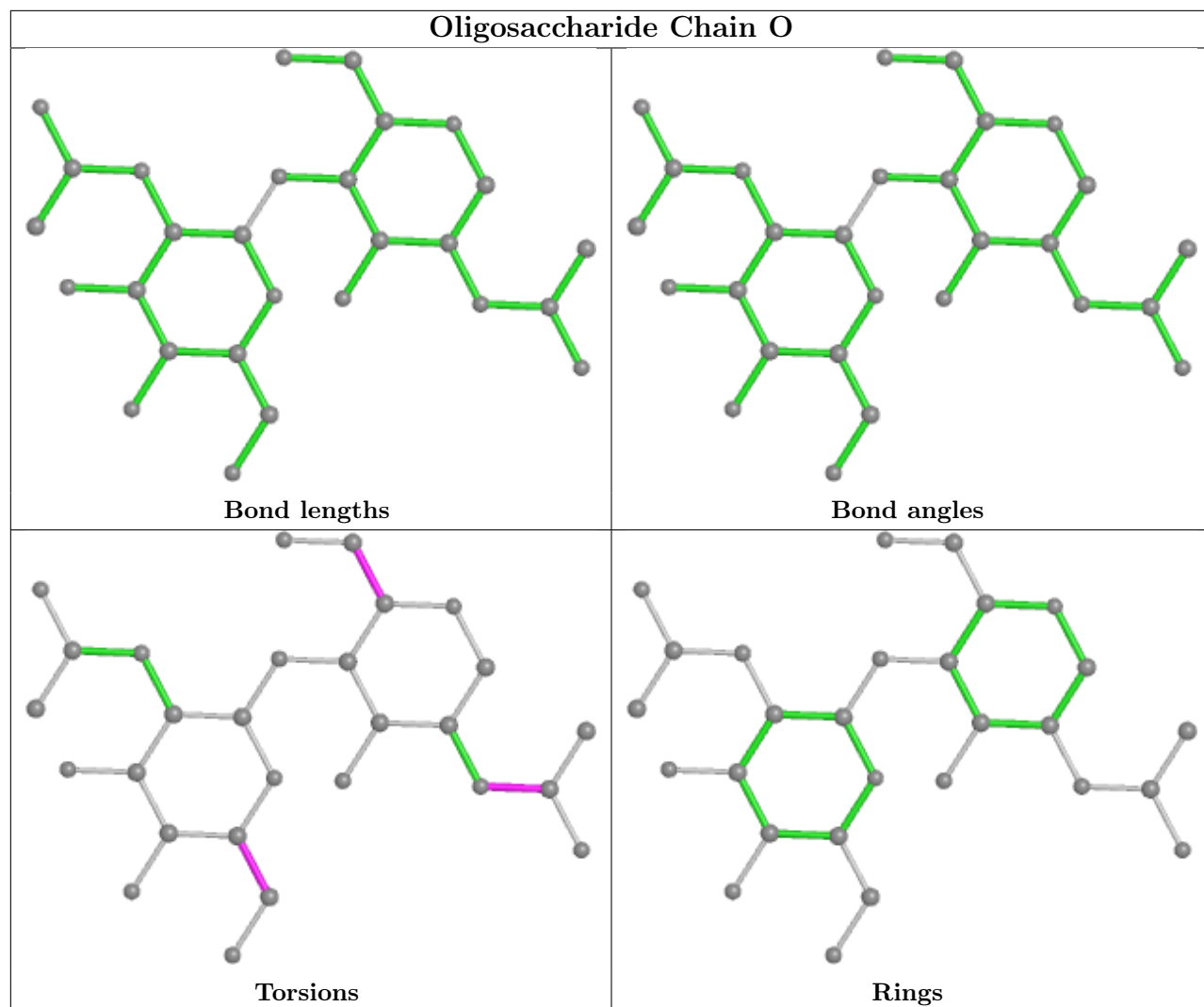


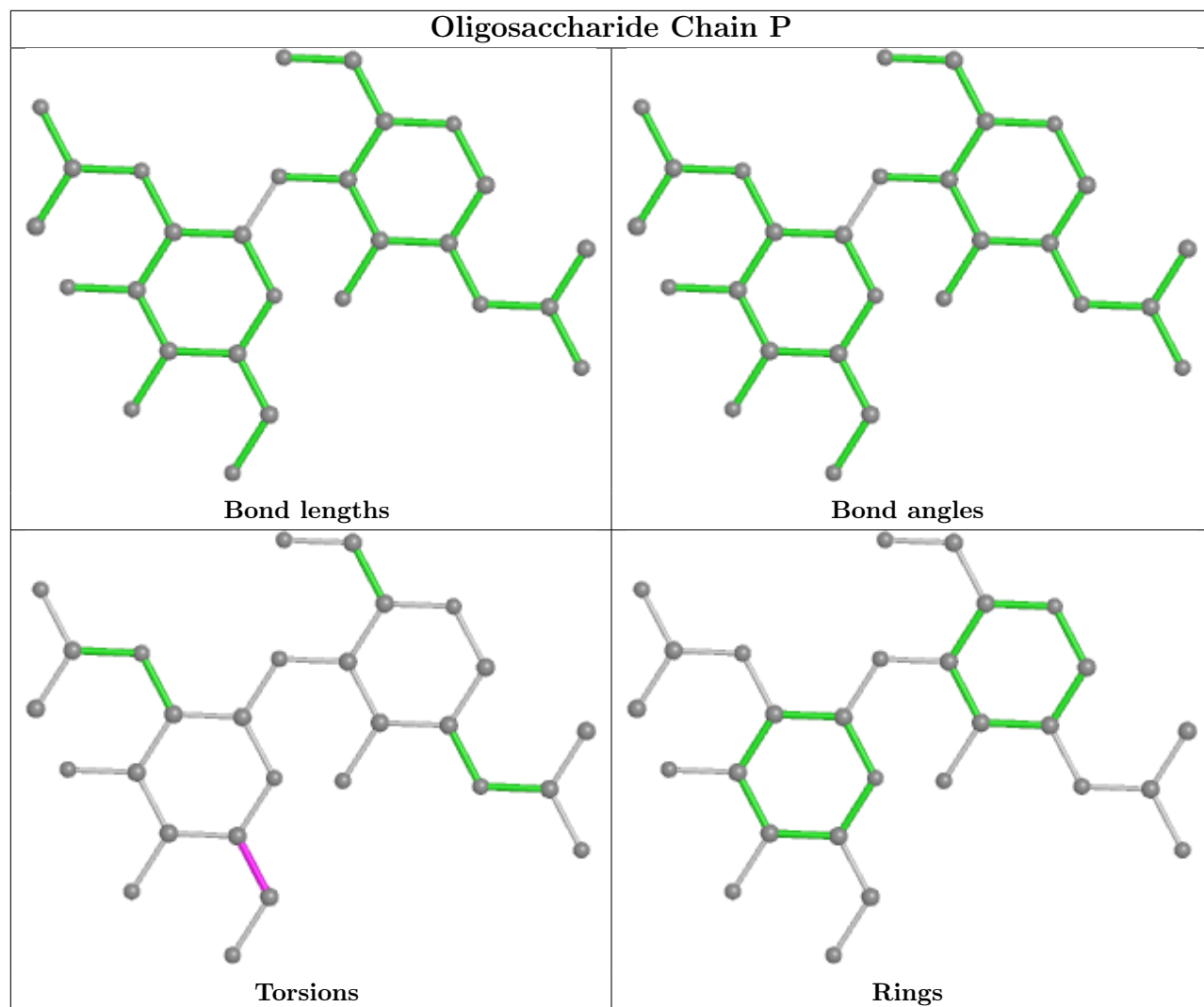


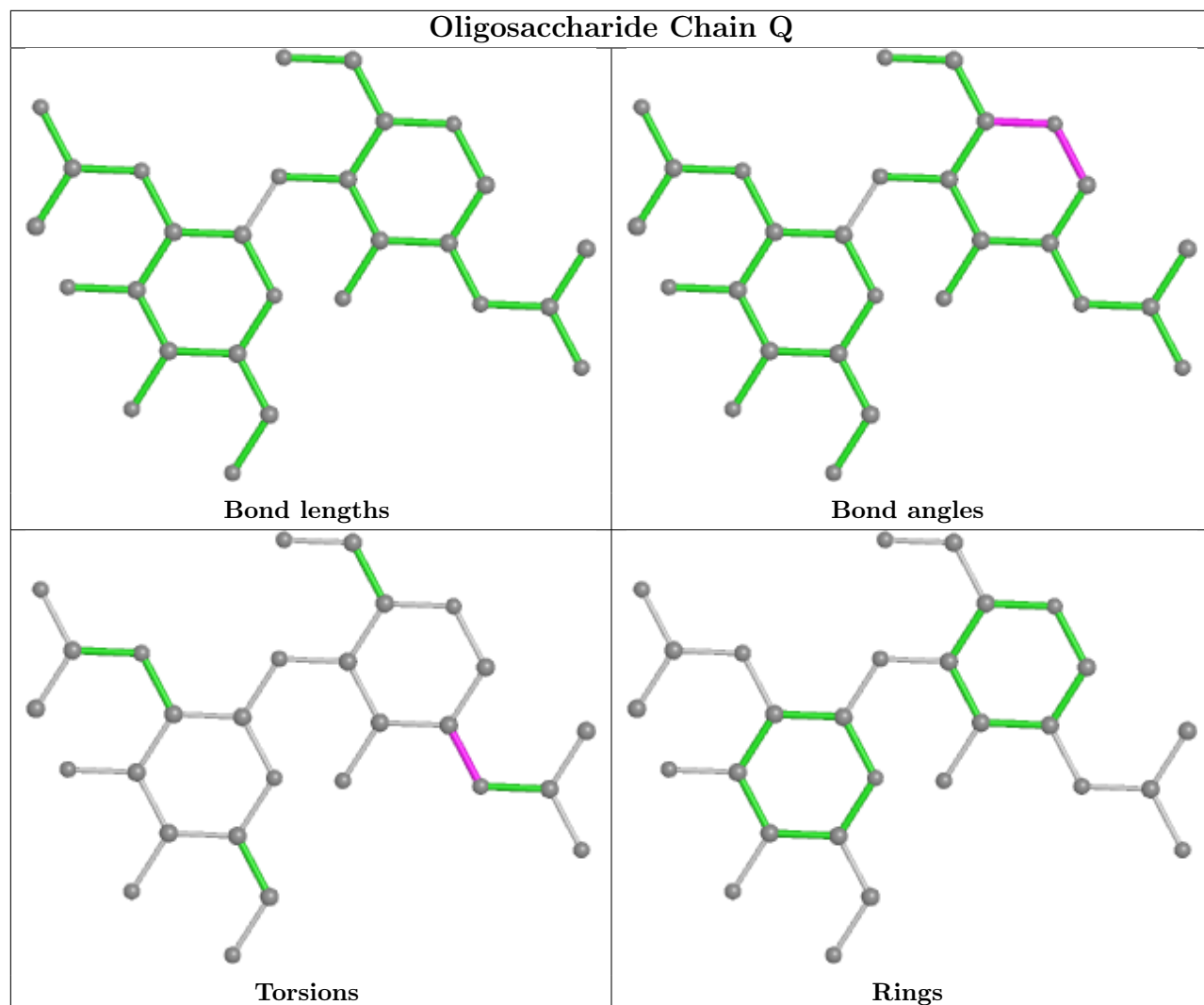


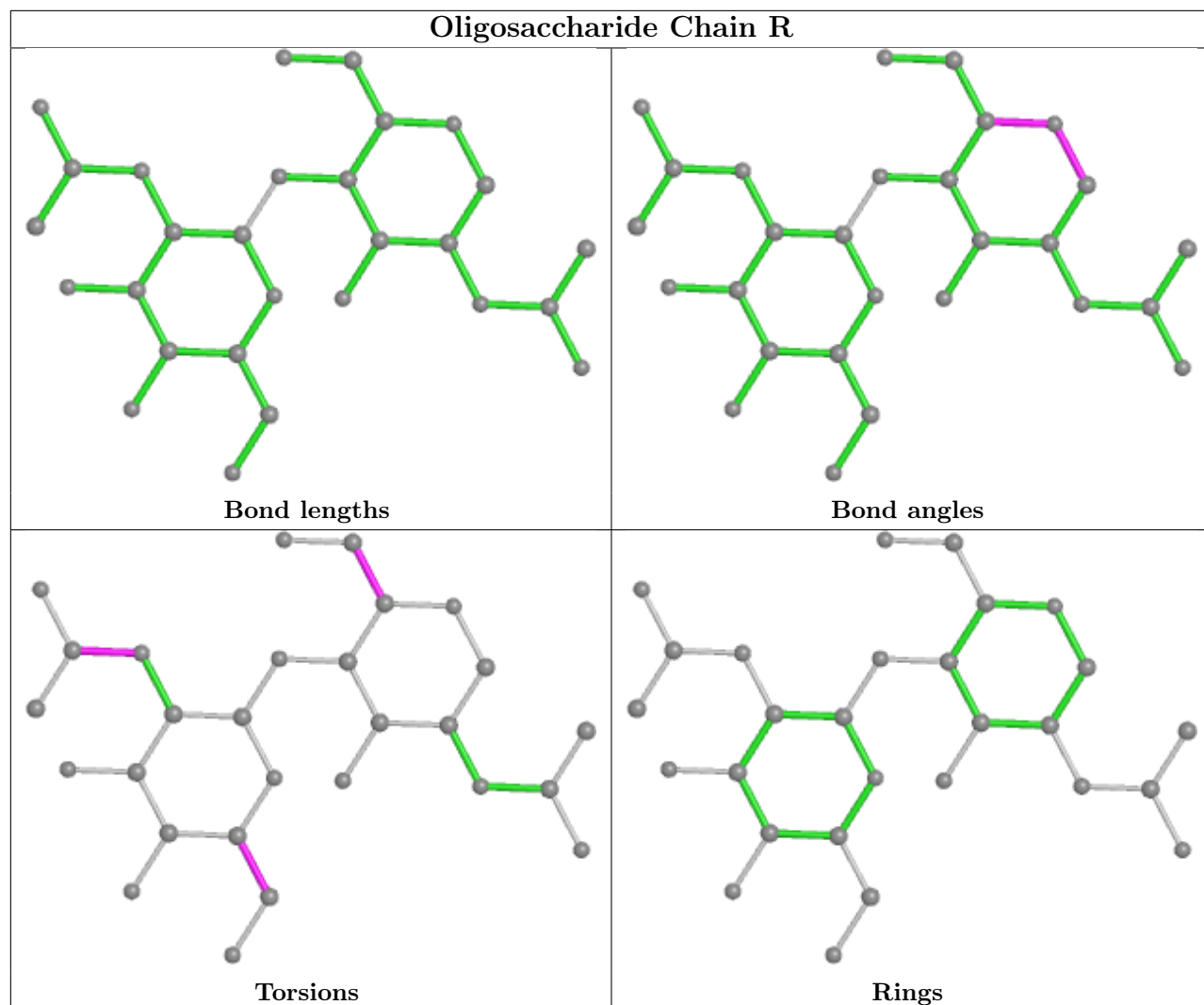


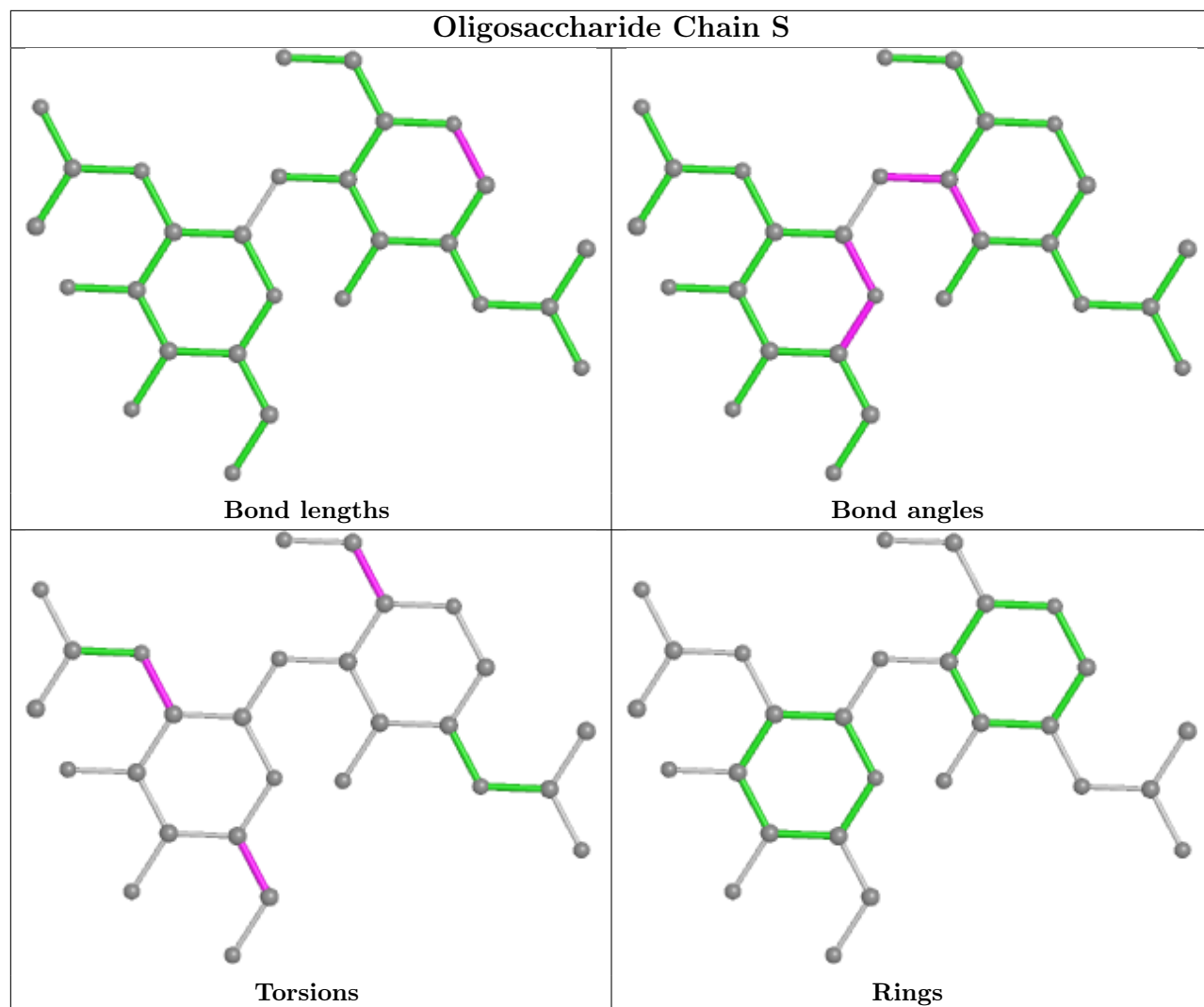




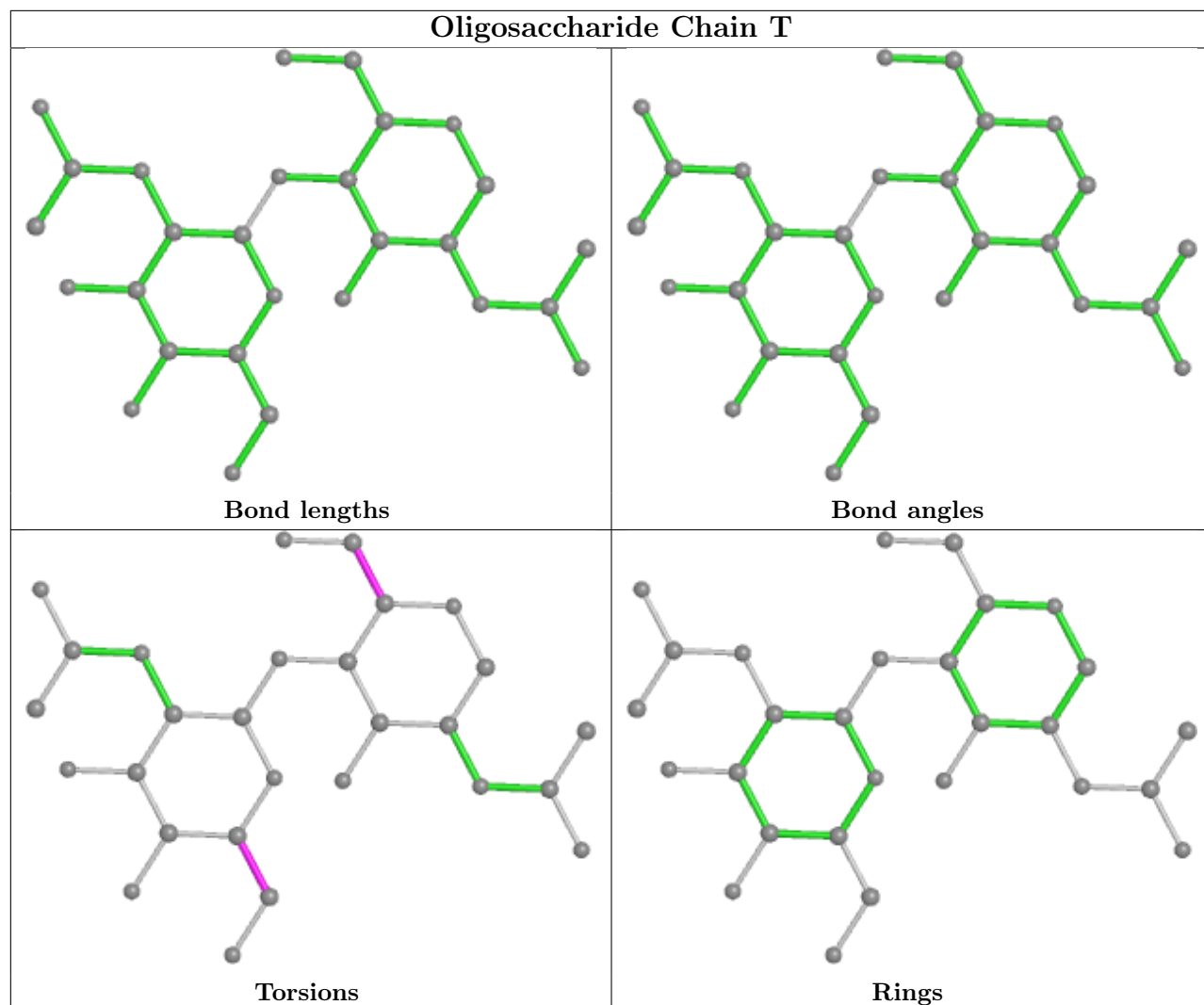


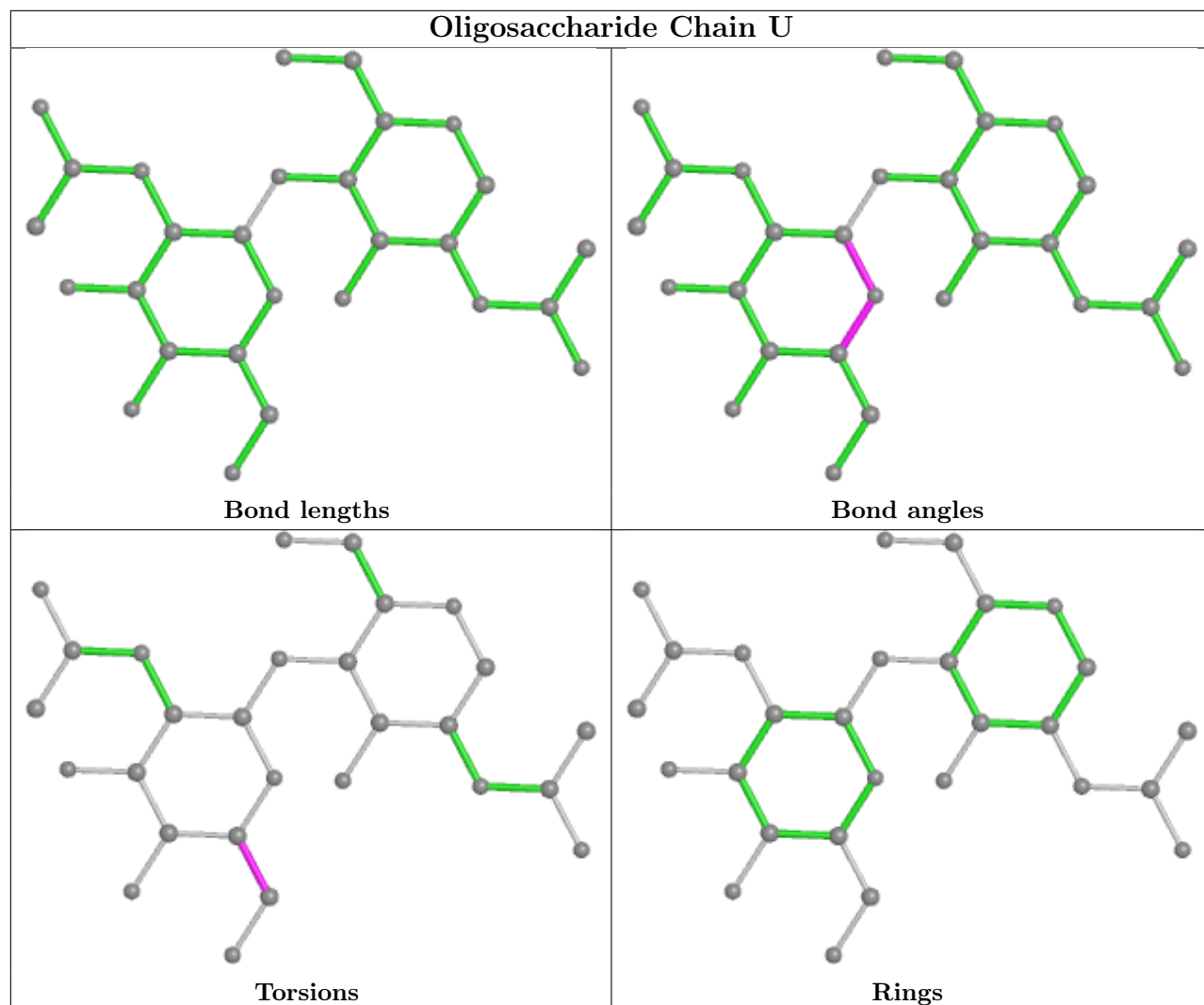


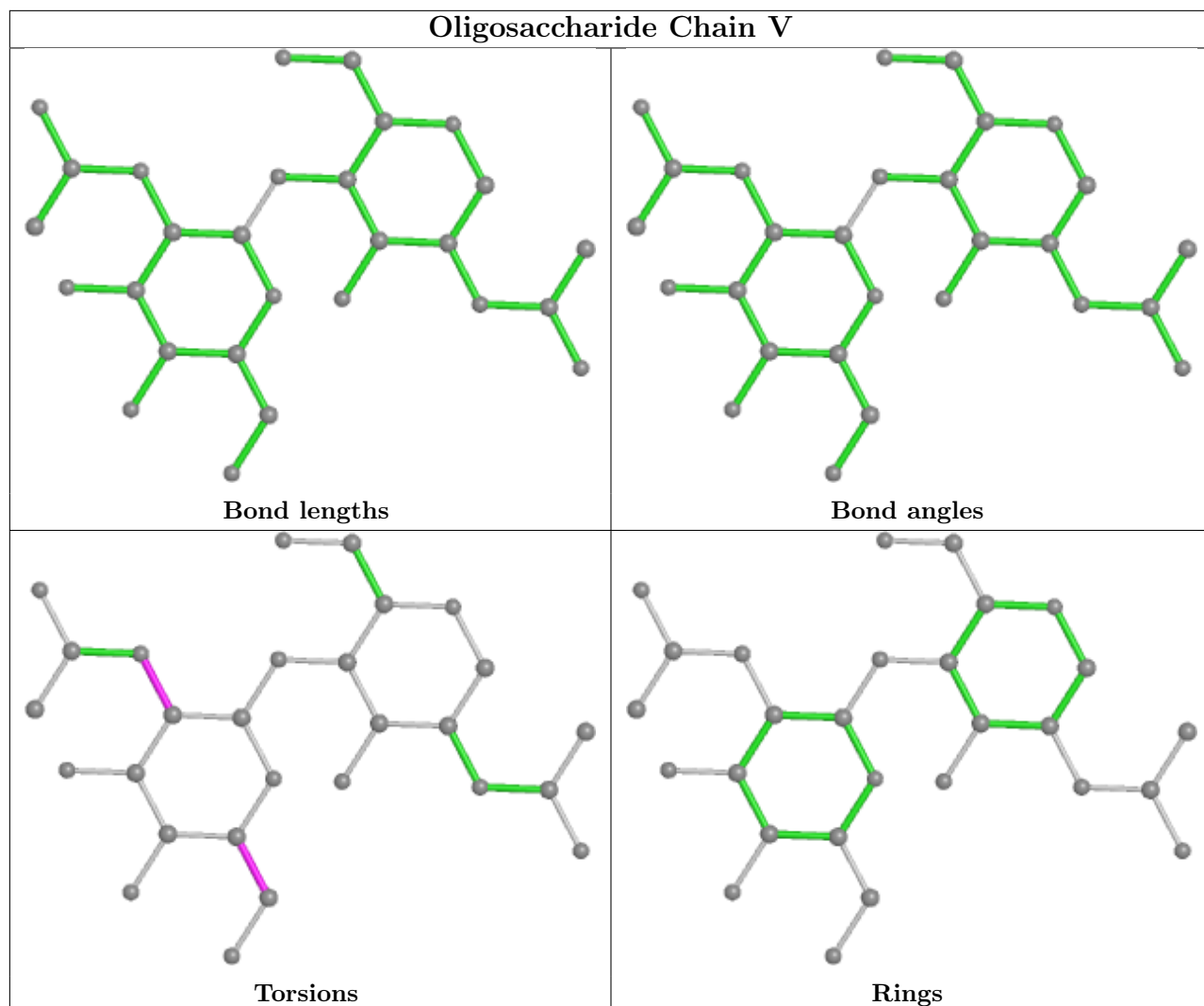


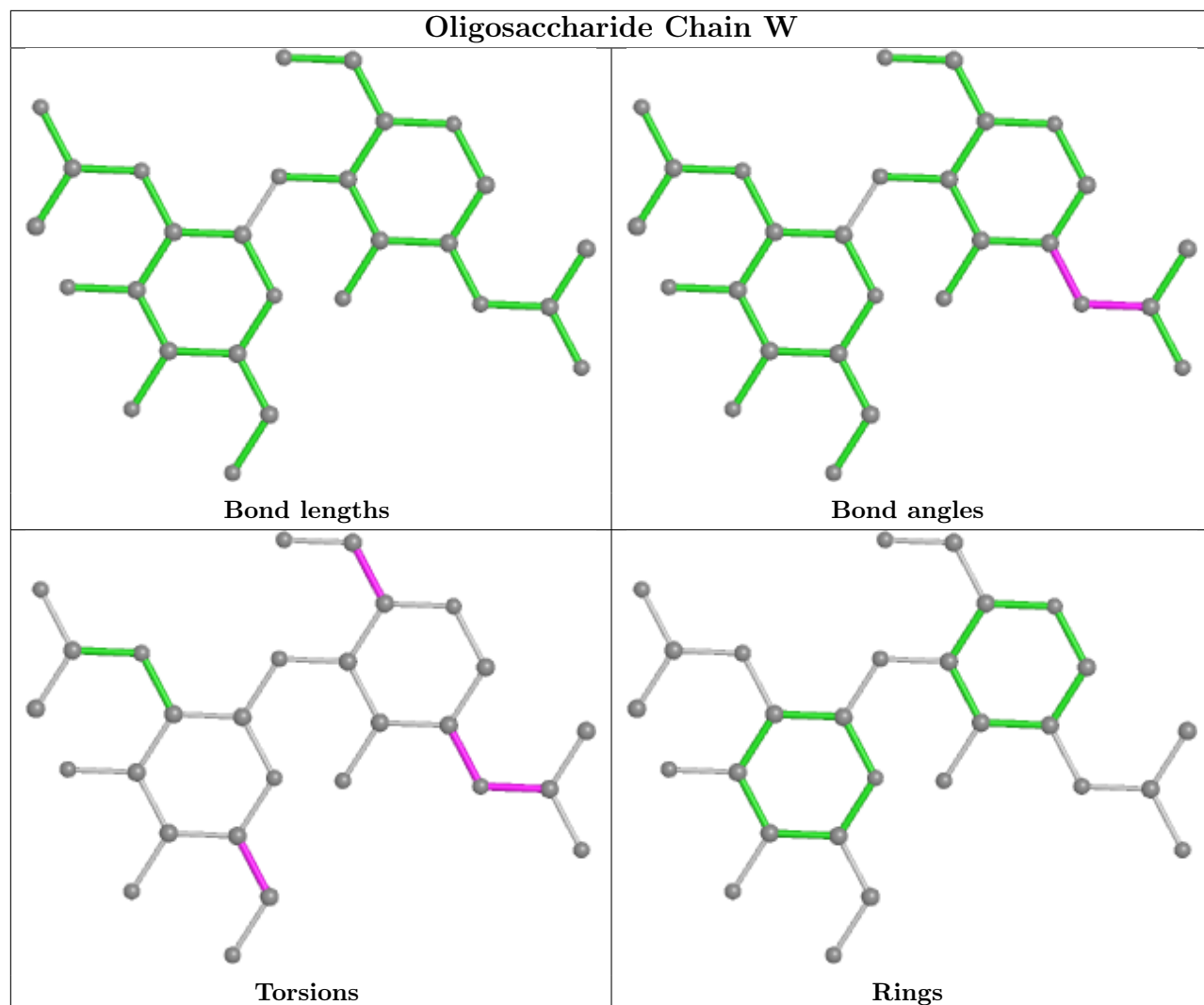


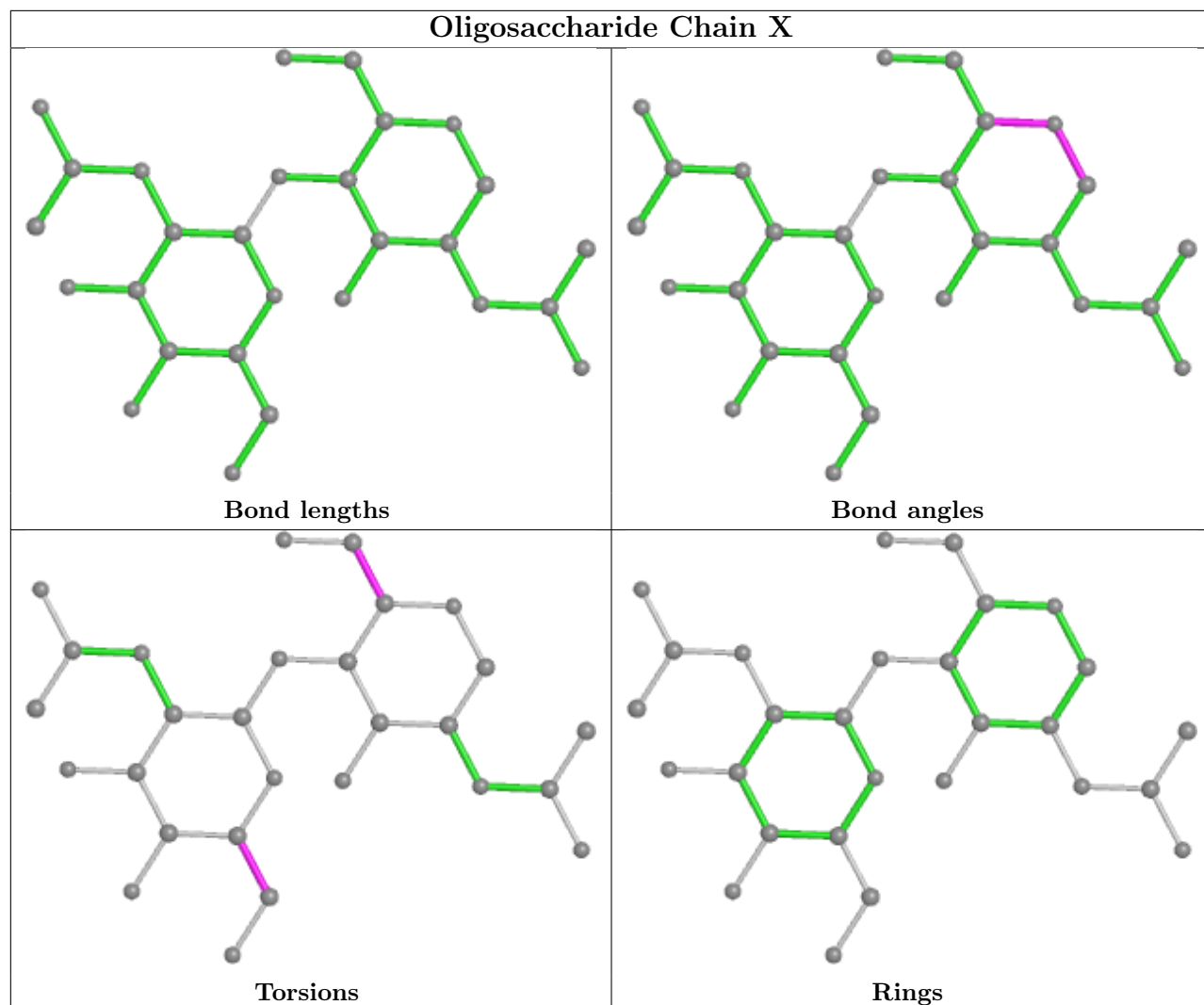


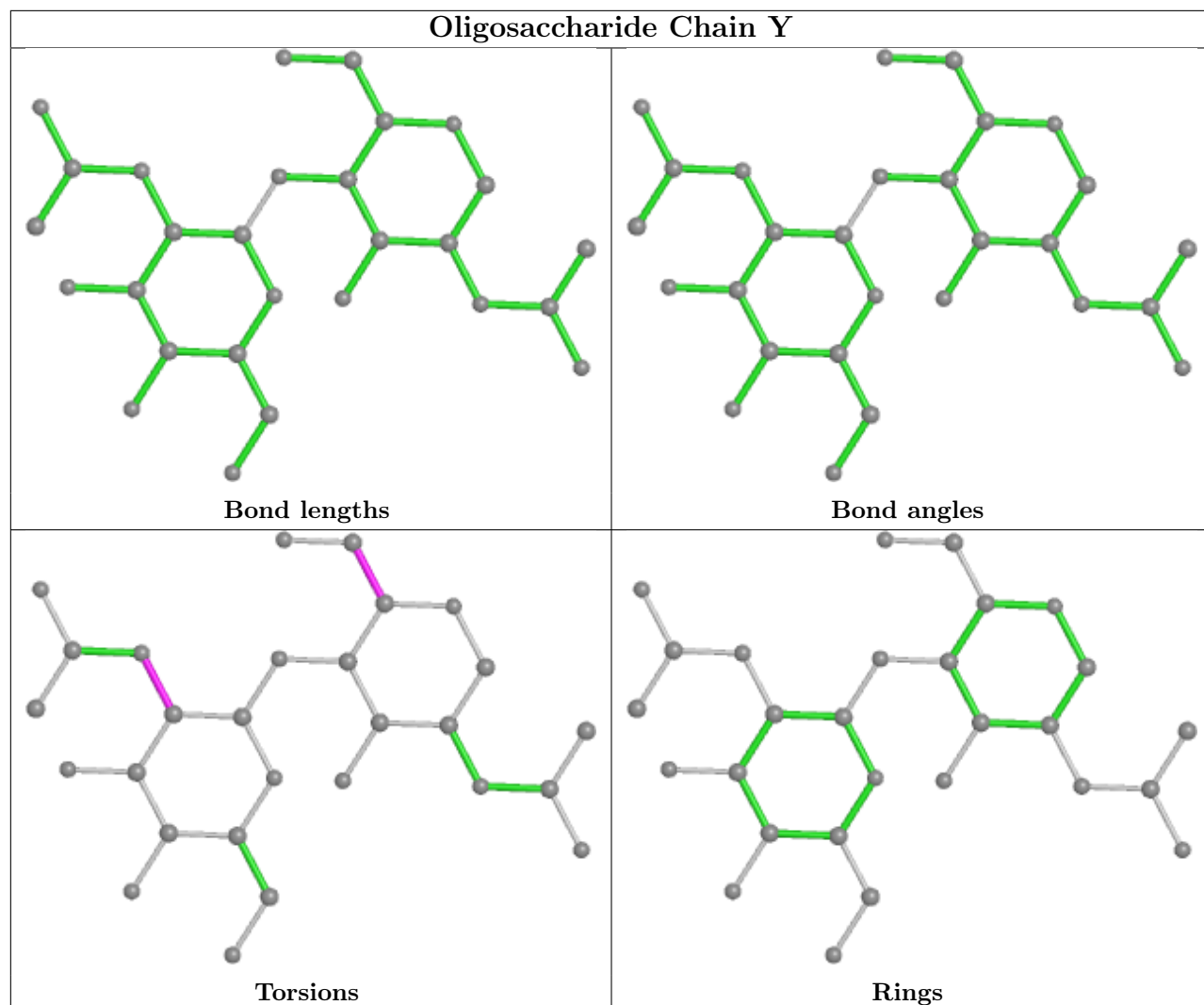


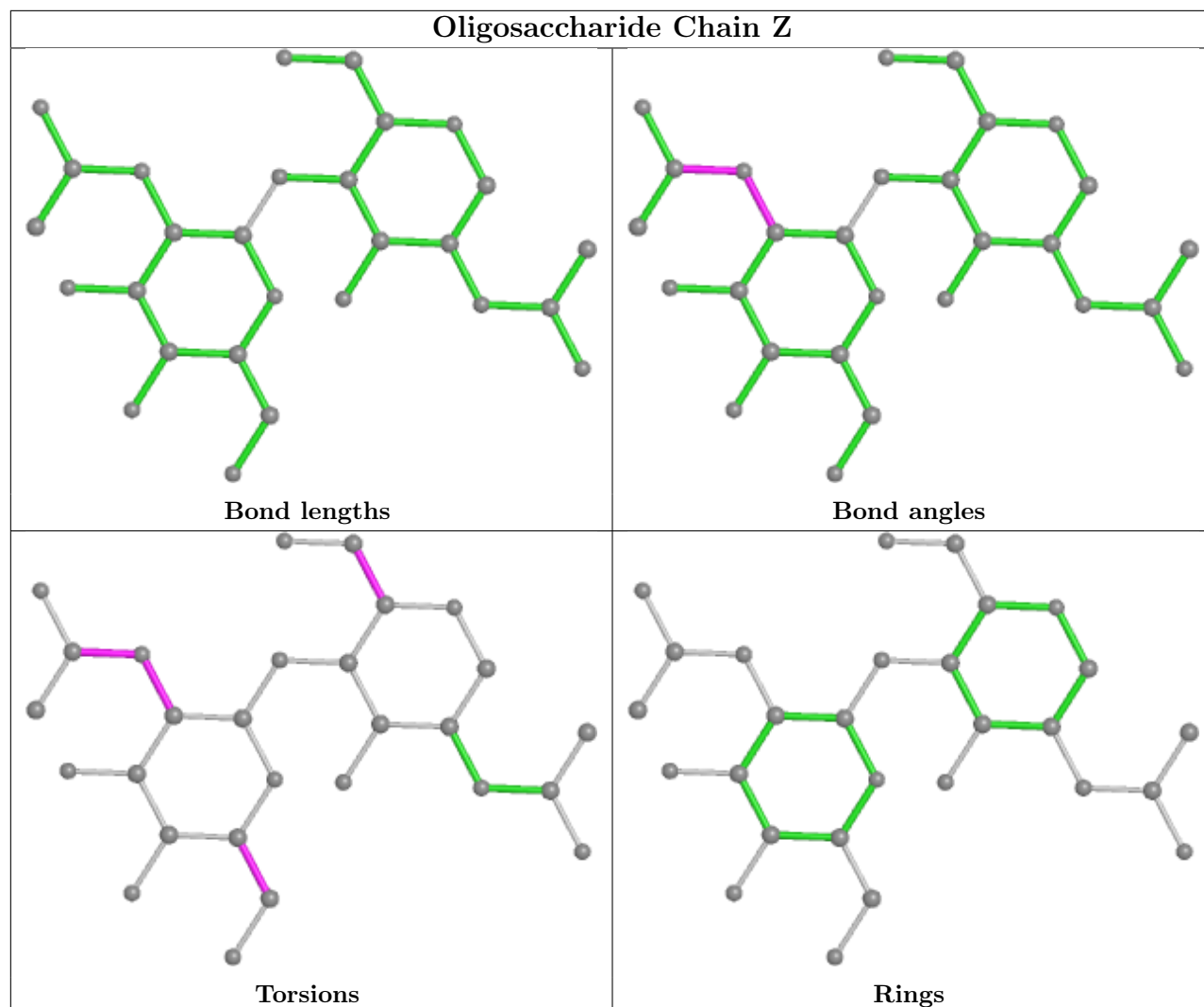


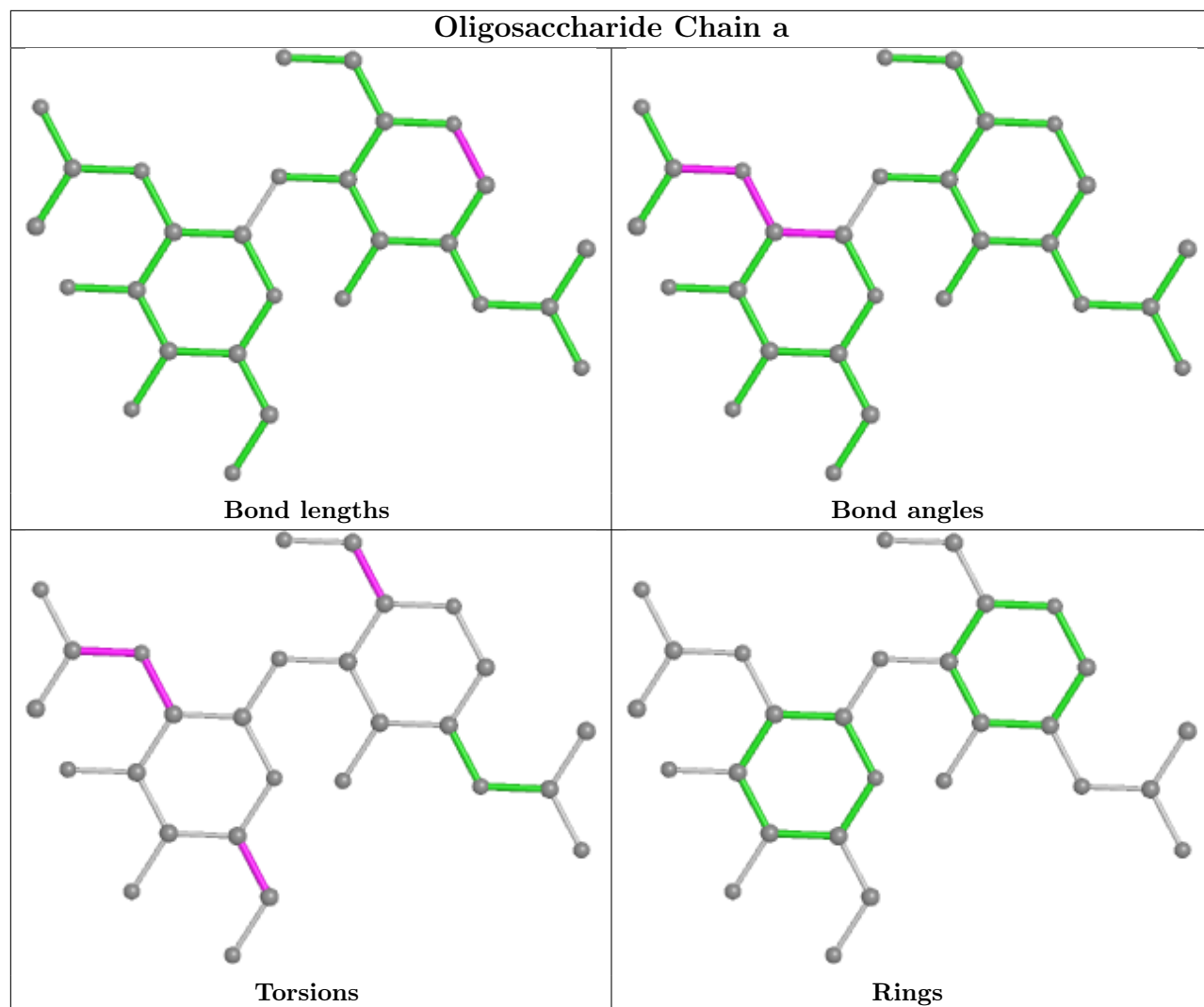




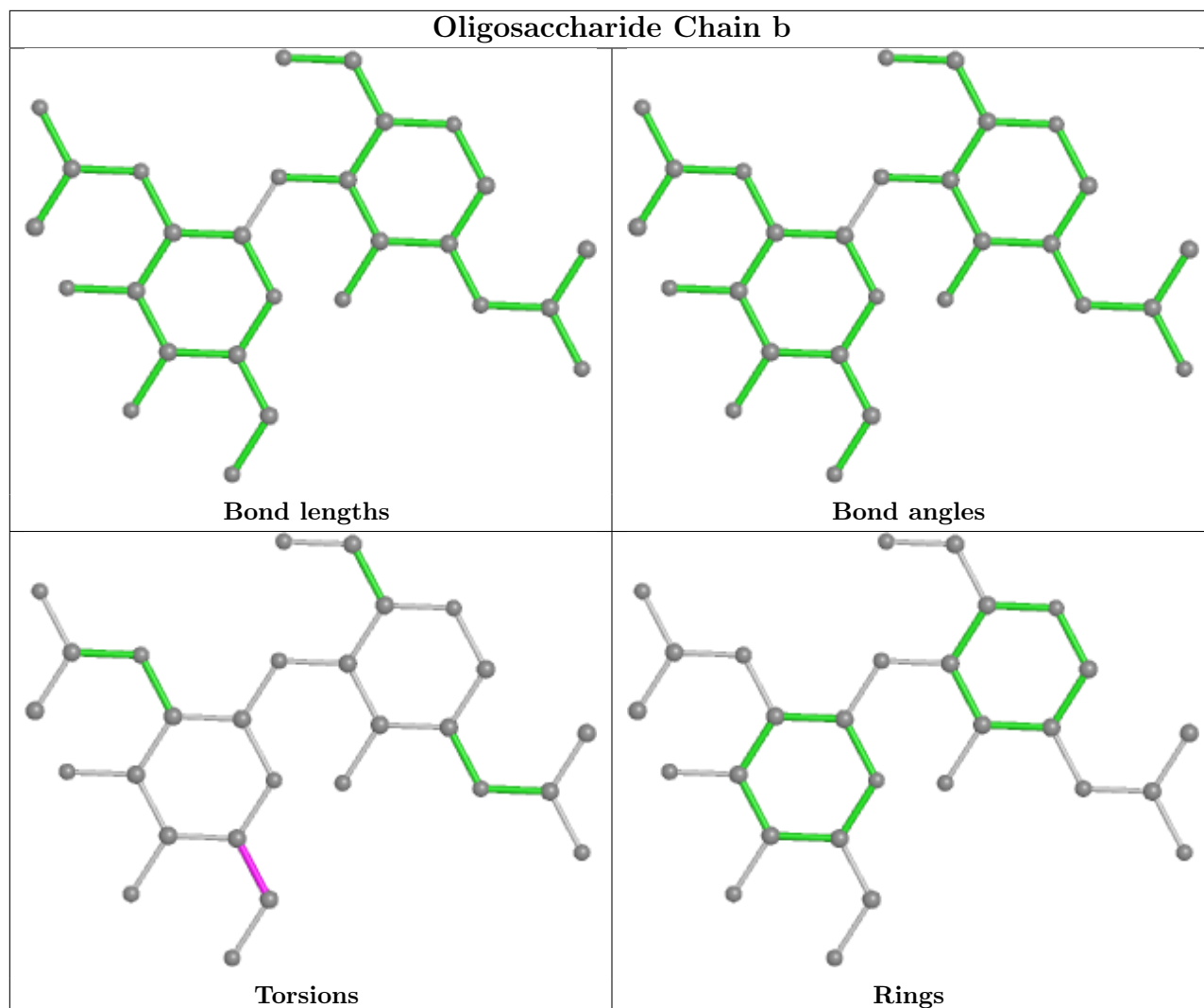












## 5.6 Ligand geometry [i](#)

28 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	1401	1	14,14,15	0.29	0	17,19,21	0.34	0
5	NAG	B	1408	1	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	A	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	1406	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
5	NAG	B	1409	1	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	B	1402	1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	A	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	B	1403	1	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	C	1403	1	14,14,15	0.54	0	17,19,21	0.45	0
5	NAG	A	1403	1	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.63	0
5	NAG	B	1401	1	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
5	NAG	C	1407	1	14,14,15	0.36	0	17,19,21	0.63	0
5	NAG	B	1404	1	14,14,15	0.33	0	17,19,21	0.59	0
5	NAG	A	1404	1	14,14,15	0.44	0	17,19,21	0.54	0
5	NAG	C	1405	1	14,14,15	0.36	0	17,19,21	1.29	2 (11%)
5	NAG	C	1404	1	14,14,15	0.29	0	17,19,21	0.37	0
5	NAG	A	1409	1	14,14,15	0.49	0	17,19,21	0.35	0
5	NAG	C	1402	1	14,14,15	0.46	0	17,19,21	0.56	0
5	NAG	B	1411	-	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	C	1408	1	14,14,15	0.16	0	17,19,21	0.56	0
5	NAG	C	1406	1	14,14,15	0.21	0	17,19,21	0.37	0
5	NAG	B	1407	1	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
5	NAG	B	1405	1	14,14,15	0.38	0	17,19,21	1.28	2 (11%)
5	NAG	C	1401	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
5	NAG	B	1410	1	14,14,15	0.41	0	17,19,21	1.16	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	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	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	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1411	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1405	NAG	C2-N2-C7	4.32	129.05	122.90
5	C	1405	NAG	C2-N2-C7	4.31	129.04	122.90
5	B	1405	NAG	C2-N2-C7	4.13	128.79	122.90
5	C	1401	NAG	C1-O5-C5	2.87	116.08	112.19
5	B	1406	NAG	C1-O5-C5	2.57	115.67	112.19
5	B	1407	NAG	C1-O5-C5	2.41	115.46	112.19
5	B	1410	NAG	C8-C7-N2	2.31	120.01	116.10
5	C	1405	NAG	C1-C2-N2	2.24	114.31	110.49
5	B	1405	NAG	C1-C2-N2	2.11	114.09	110.49
5	B	1410	NAG	C2-N2-C7	-2.02	120.02	122.90

There are no chirality outliers.

All (59) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	B	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	C	1407	NAG	O5-C5-C6-O6
5	B	1409	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	B	1406	NAG	C3-C2-N2-C7
5	B	1407	NAG	C3-C2-N2-C7
5	C	1407	NAG	C3-C2-N2-C7
5	A	1407	NAG	C1-C2-N2-C7
5	A	1405	NAG	C3-C2-N2-C7
5	B	1405	NAG	C3-C2-N2-C7
5	C	1403	NAG	C3-C2-N2-C7
5	C	1405	NAG	C3-C2-N2-C7

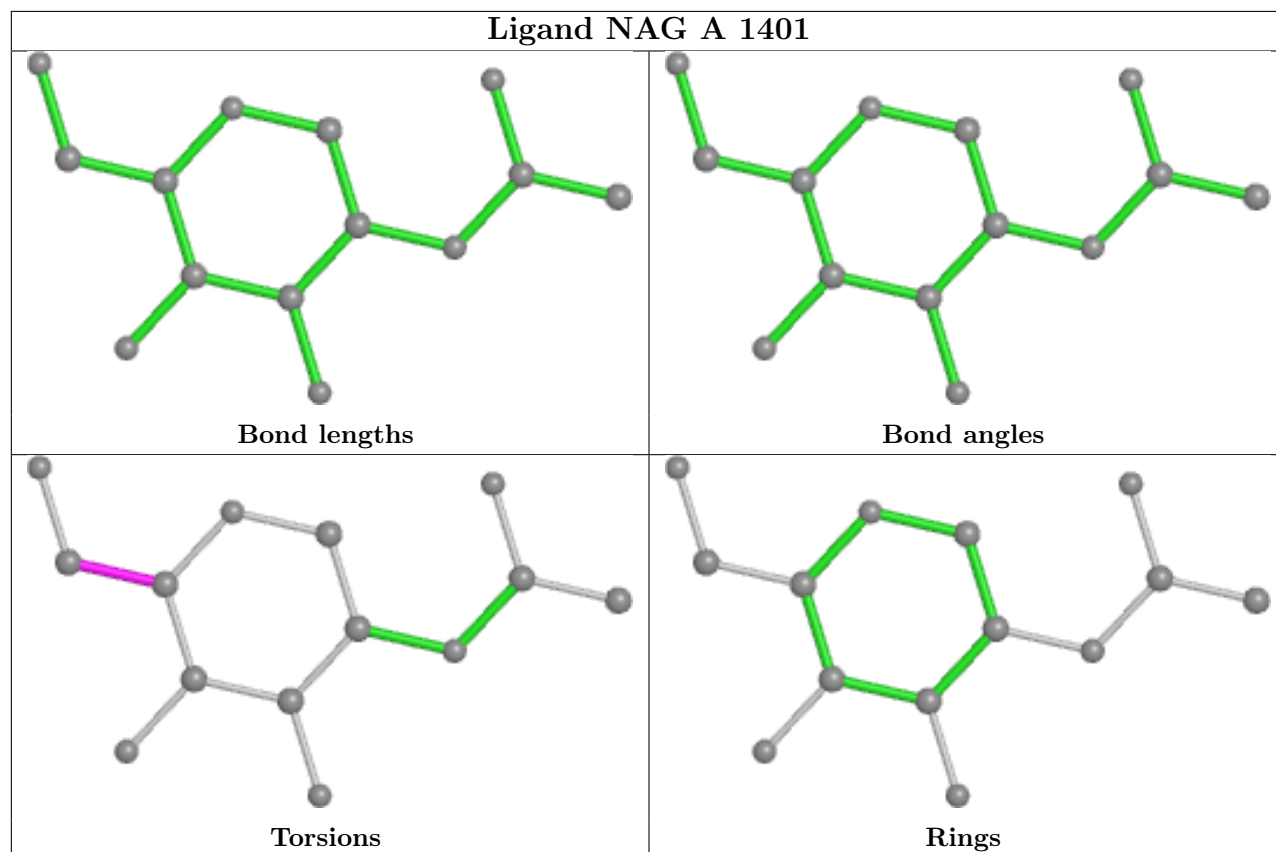
There are no ring outliers.

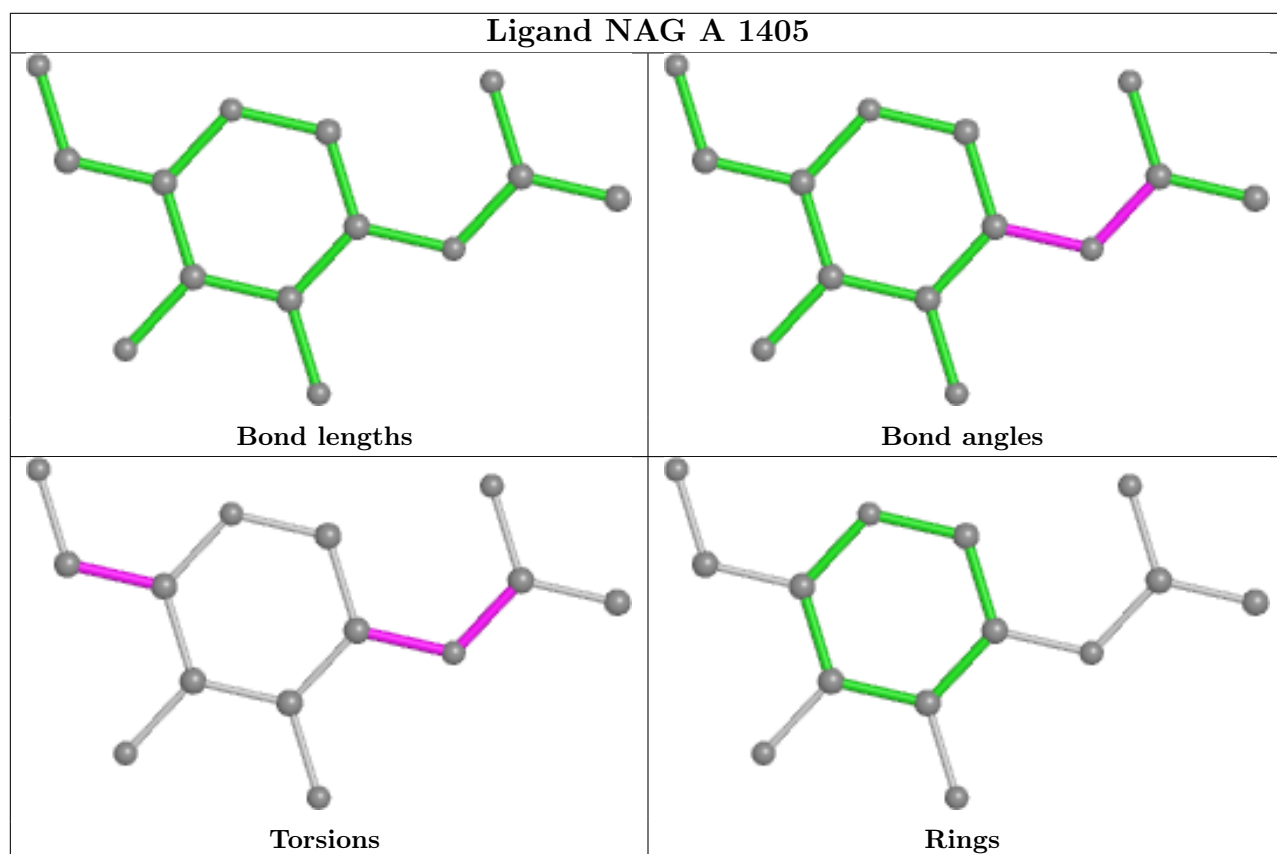
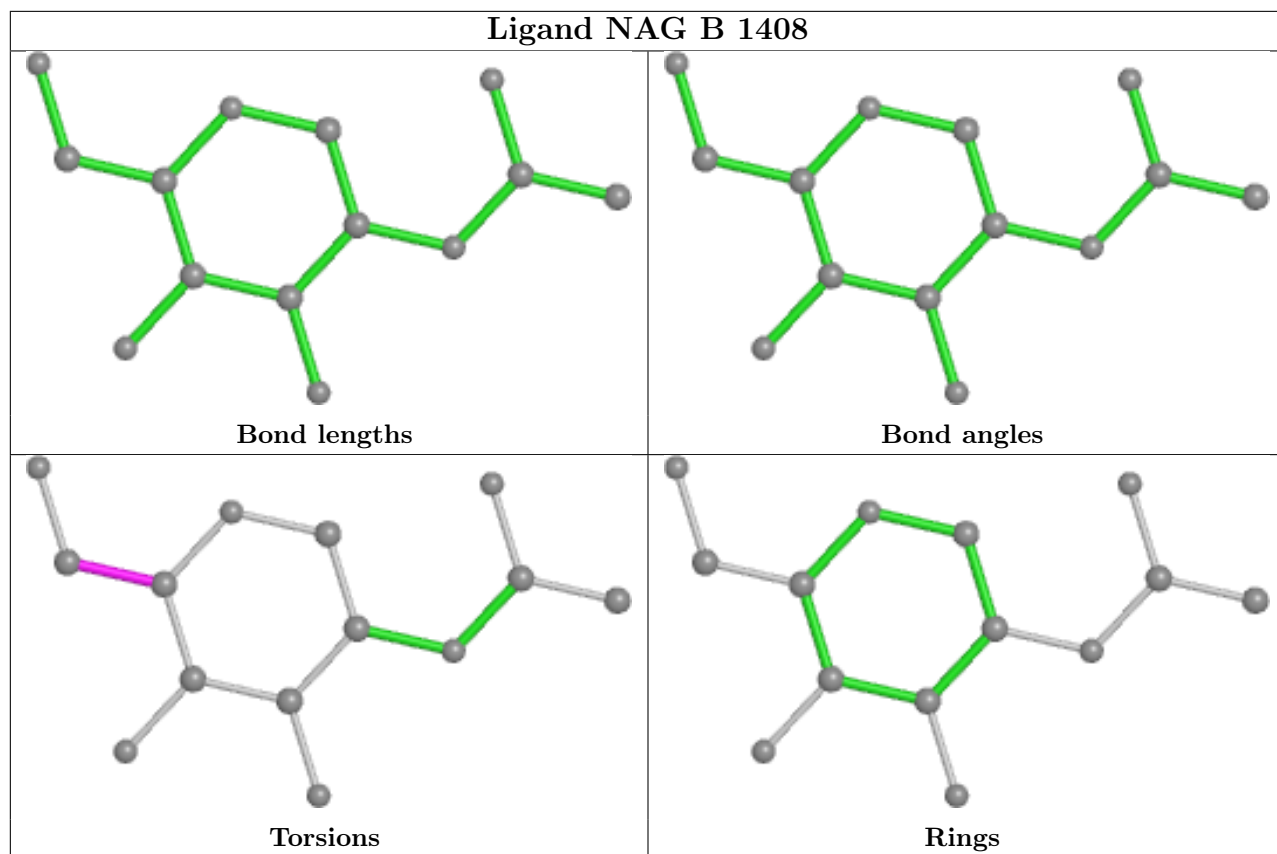
11 monomers are involved in 17 short contacts:

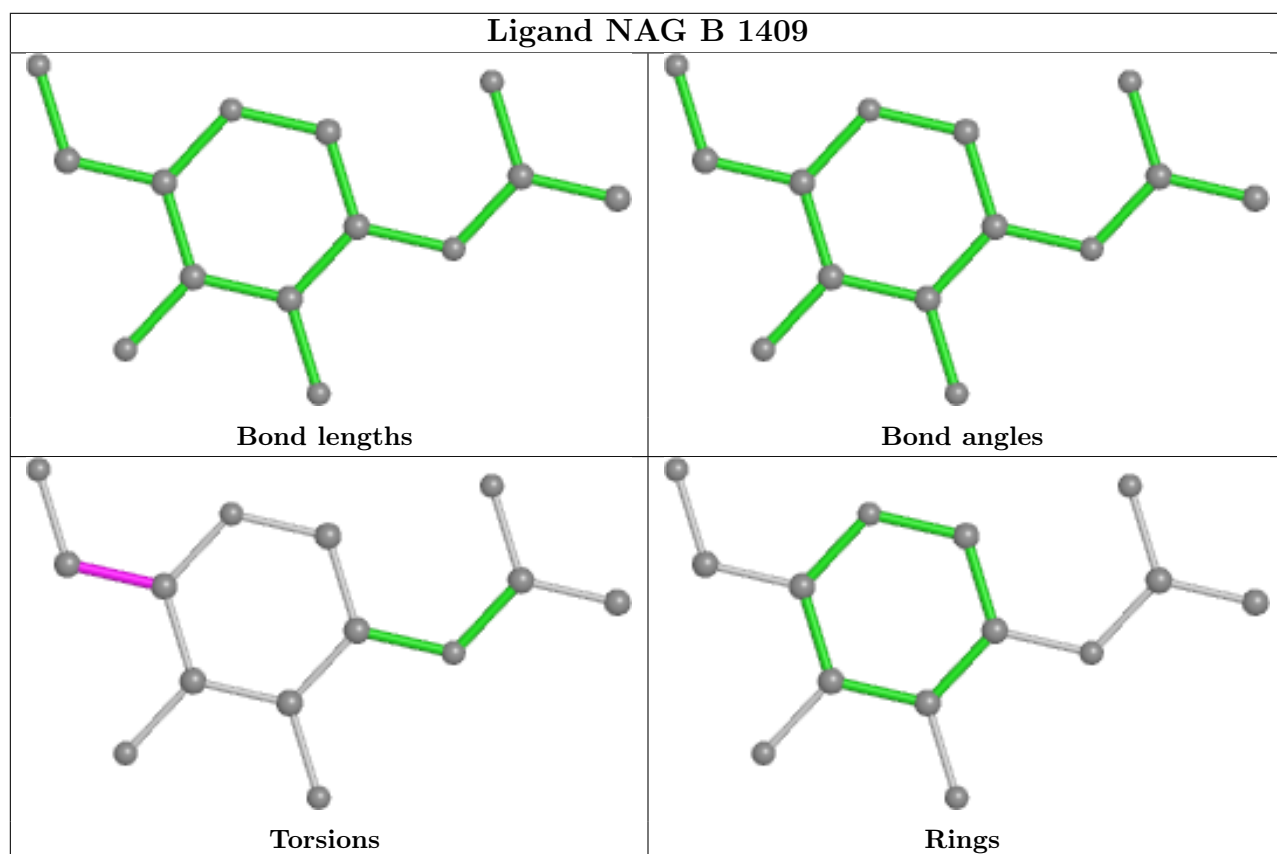
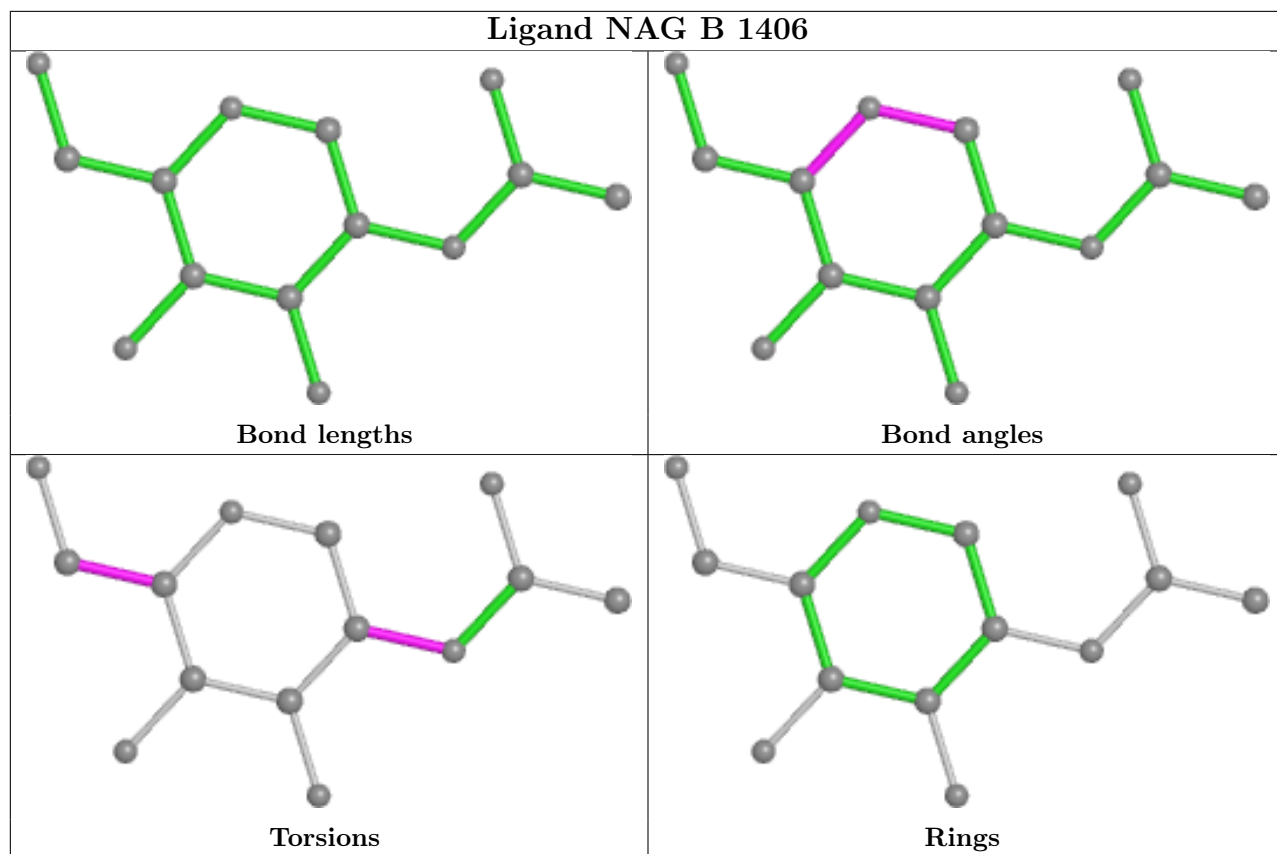
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1405	NAG	1	0
5	B	1402	NAG	1	0
5	B	1403	NAG	2	0
5	A	1402	NAG	3	0
5	A	1404	NAG	1	0
5	C	1405	NAG	1	0
5	C	1402	NAG	1	0
5	B	1411	NAG	4	0
5	B	1407	NAG	1	0
5	B	1405	NAG	2	0
5	B	1410	NAG	4	0

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

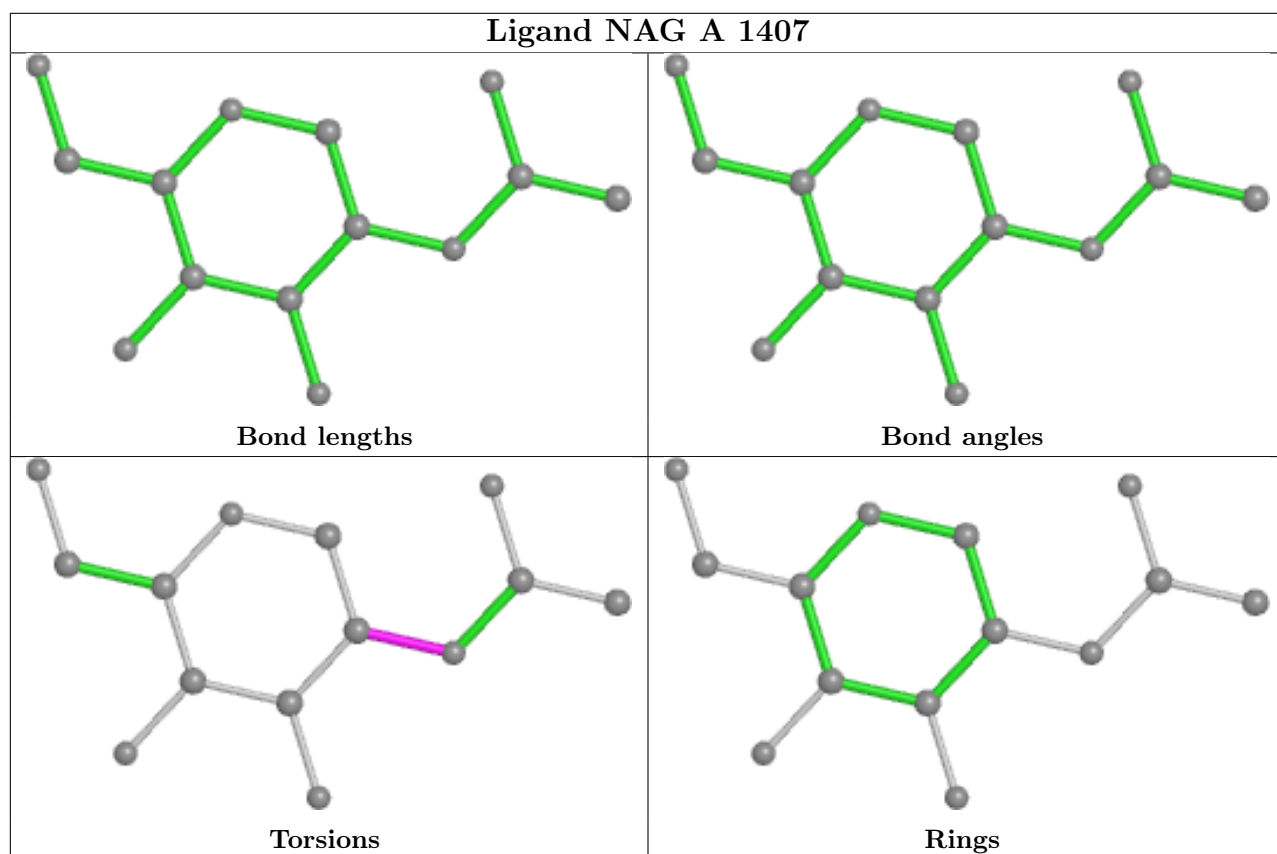
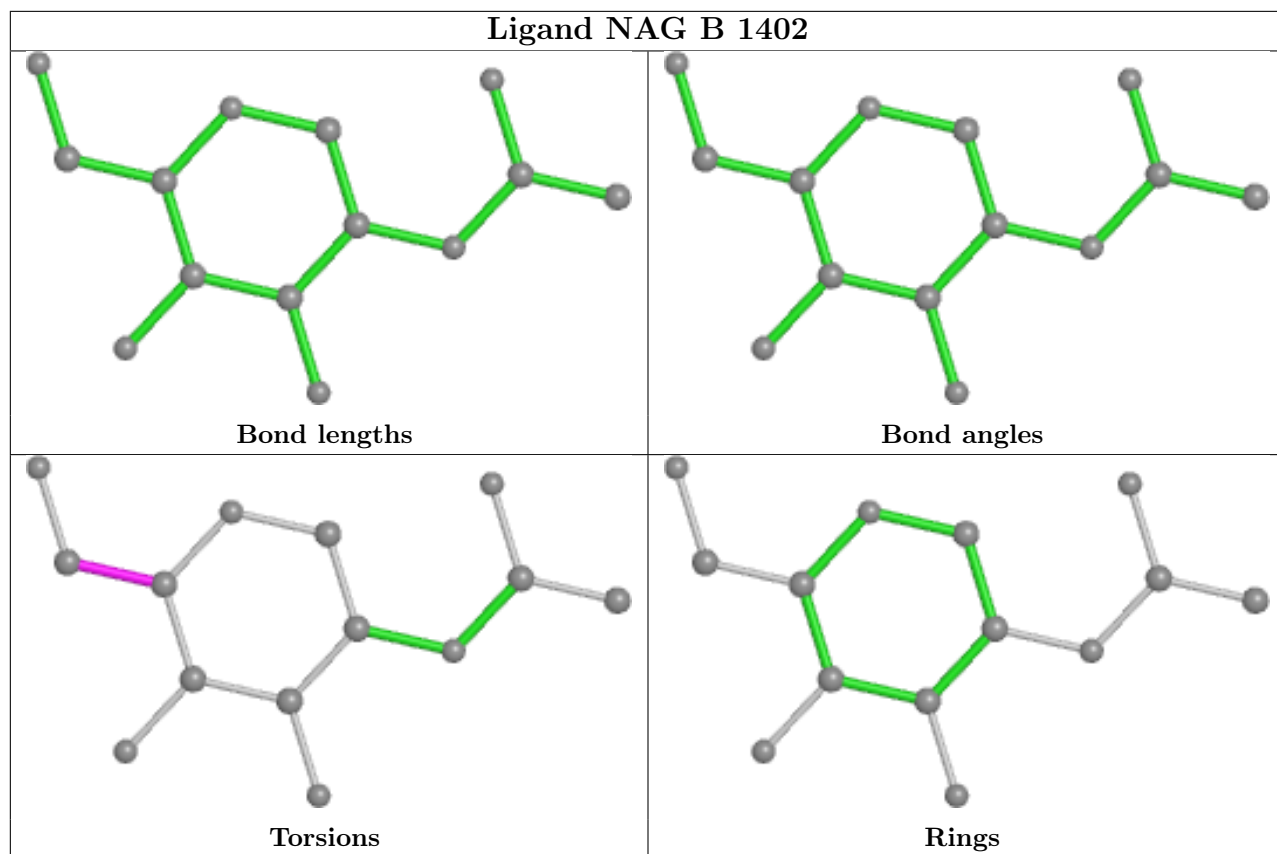
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

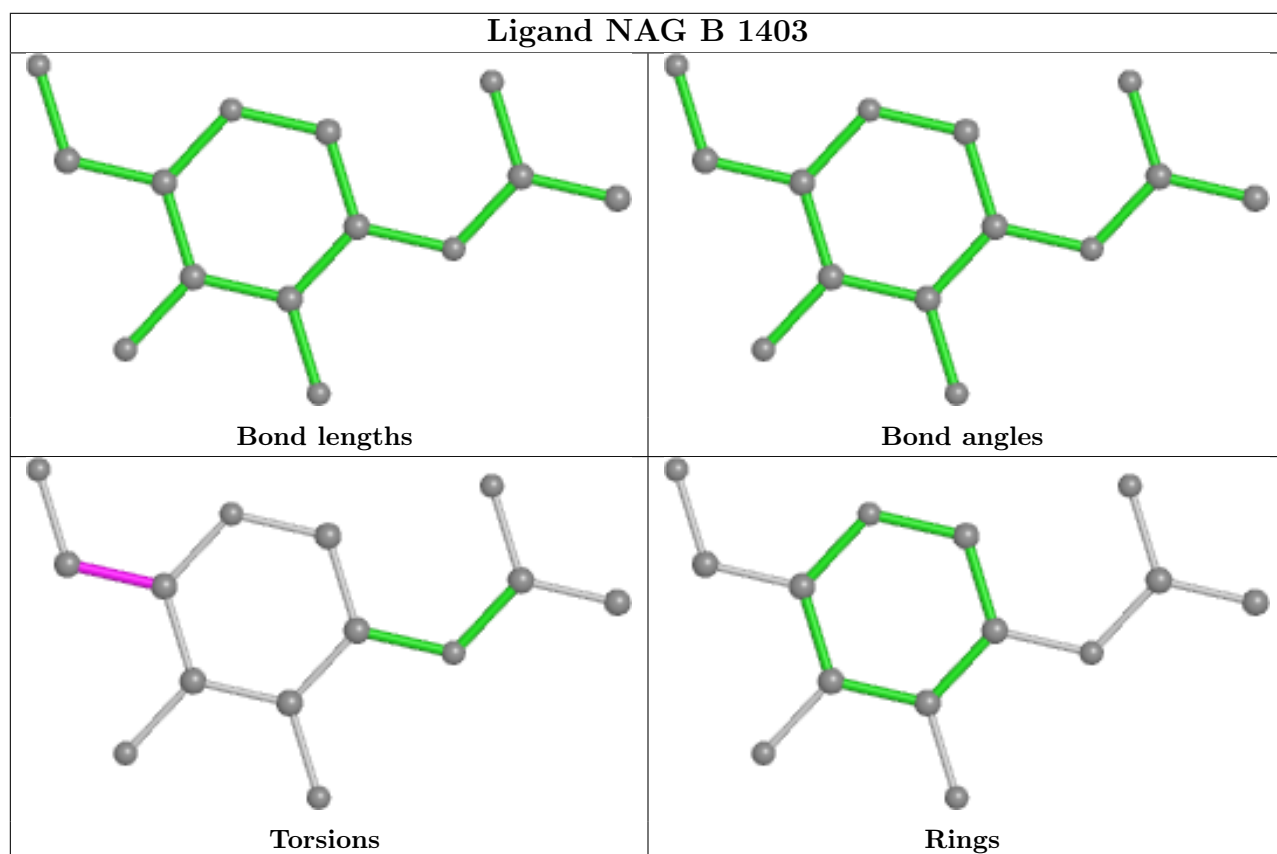
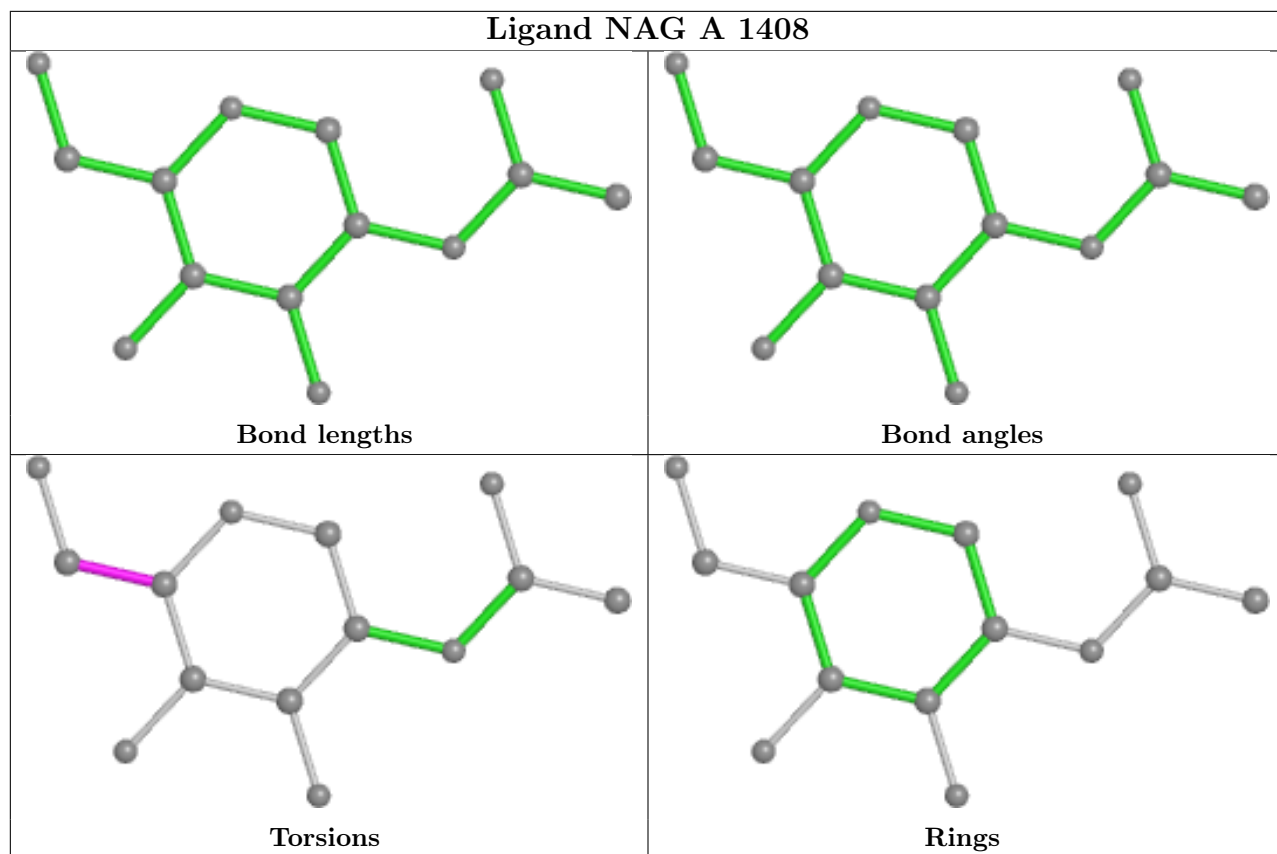


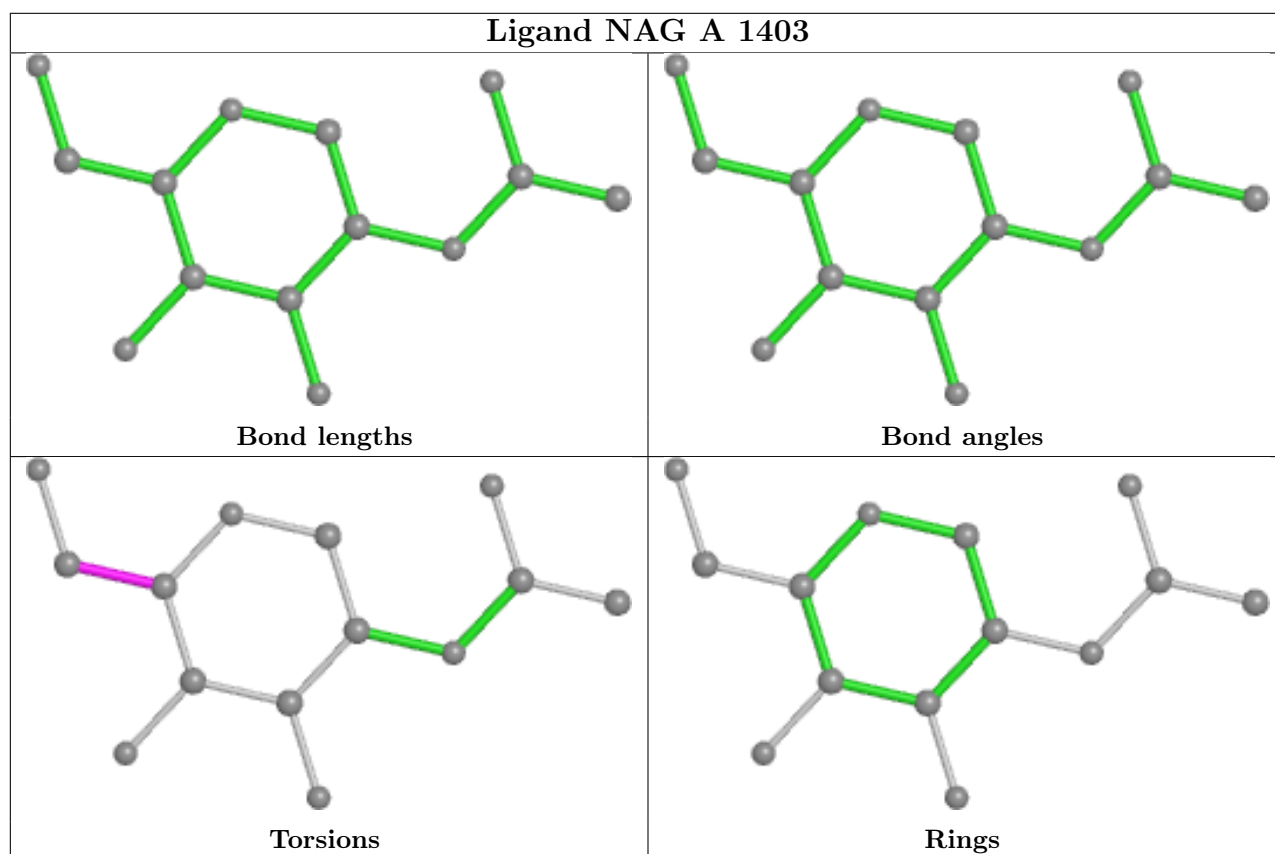
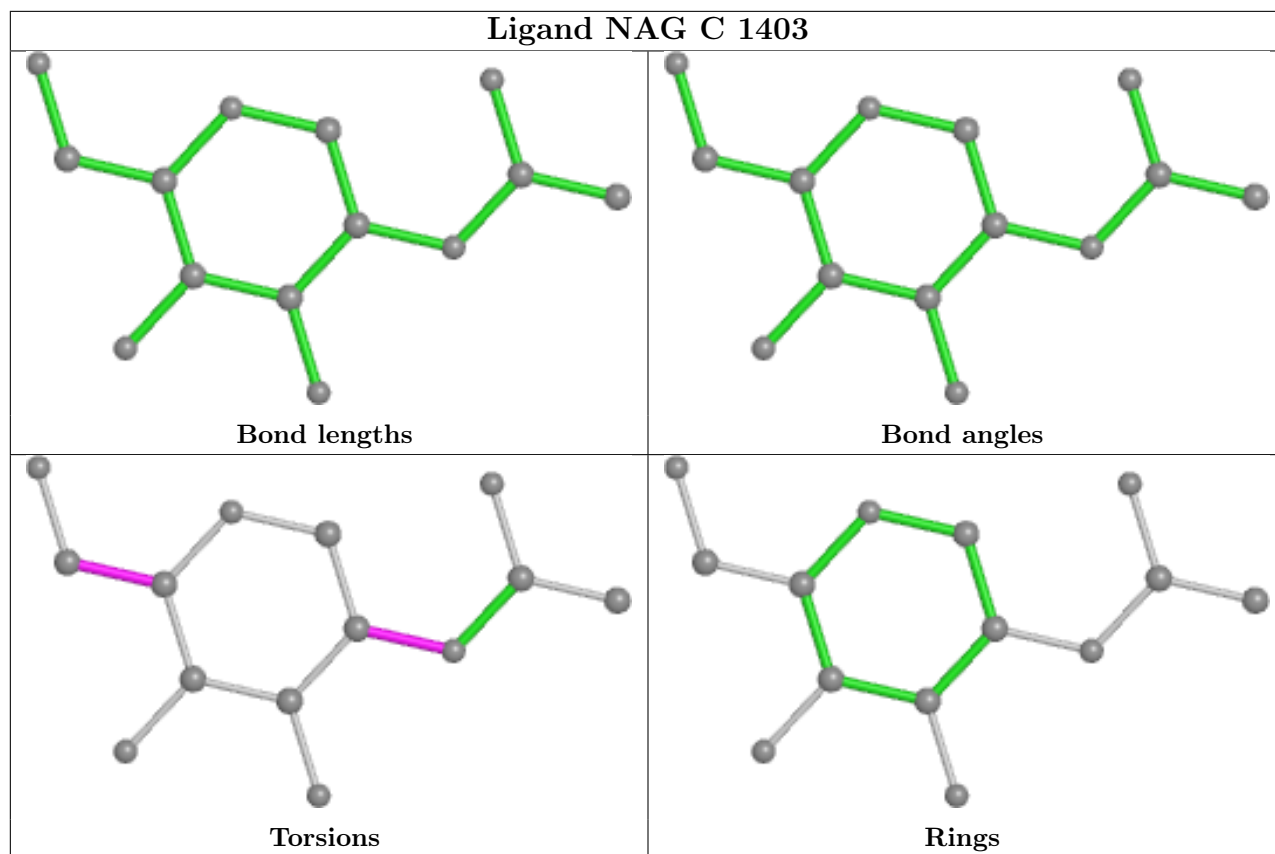


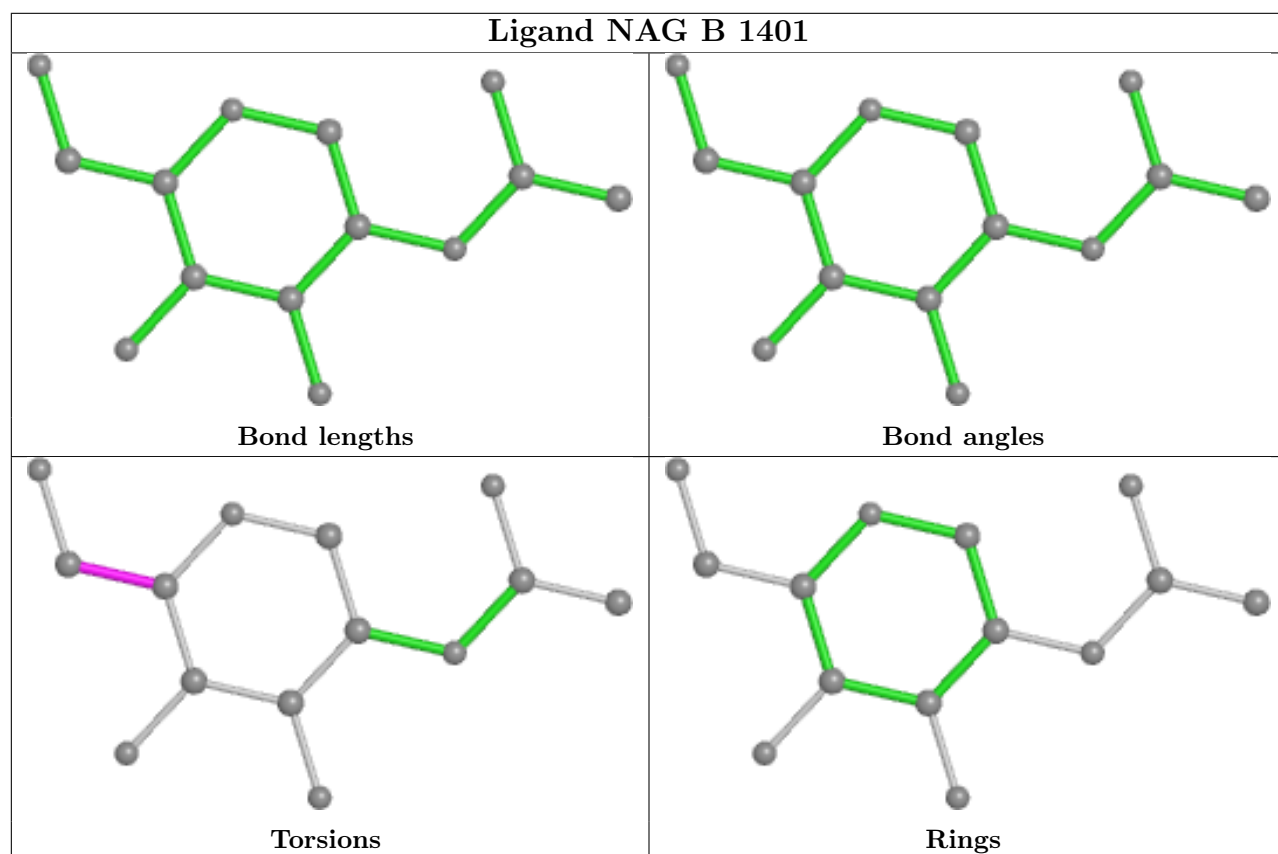
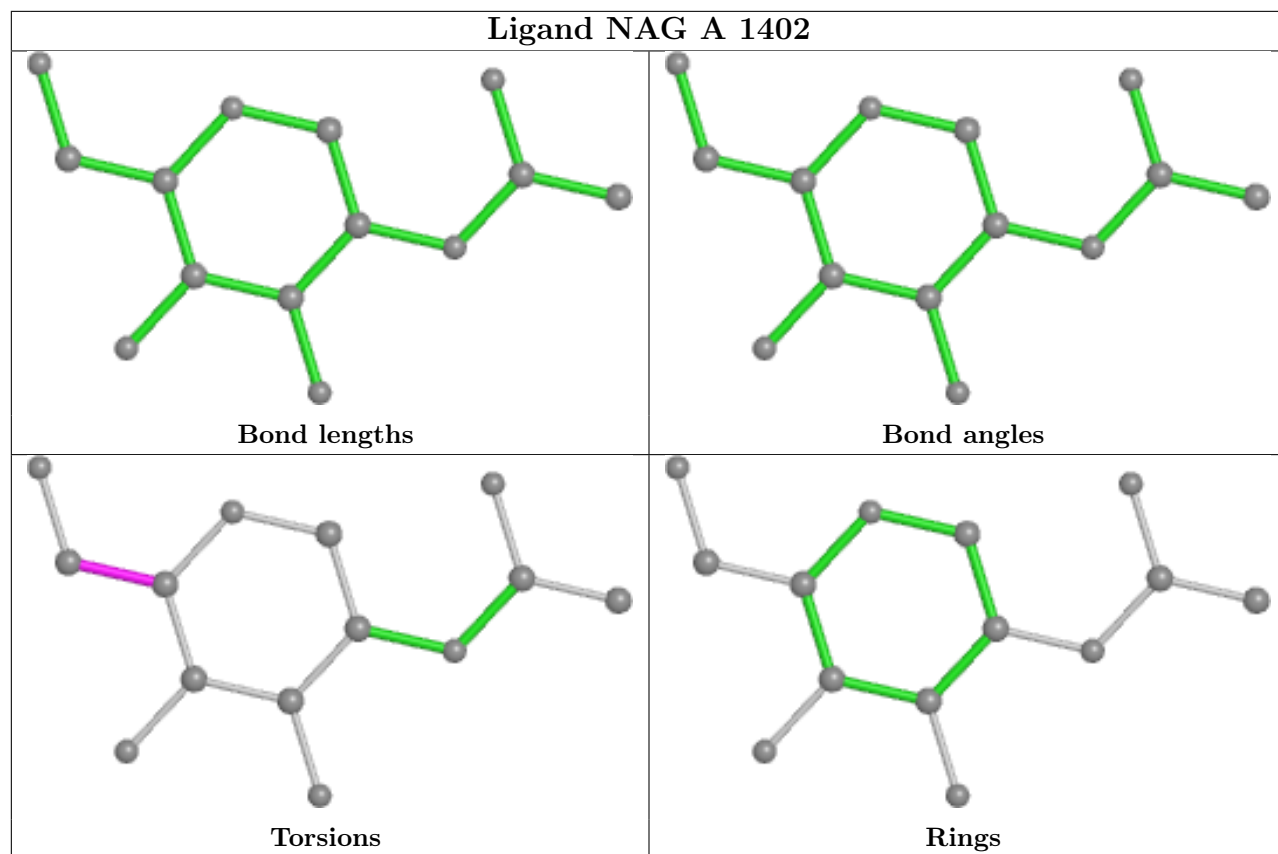


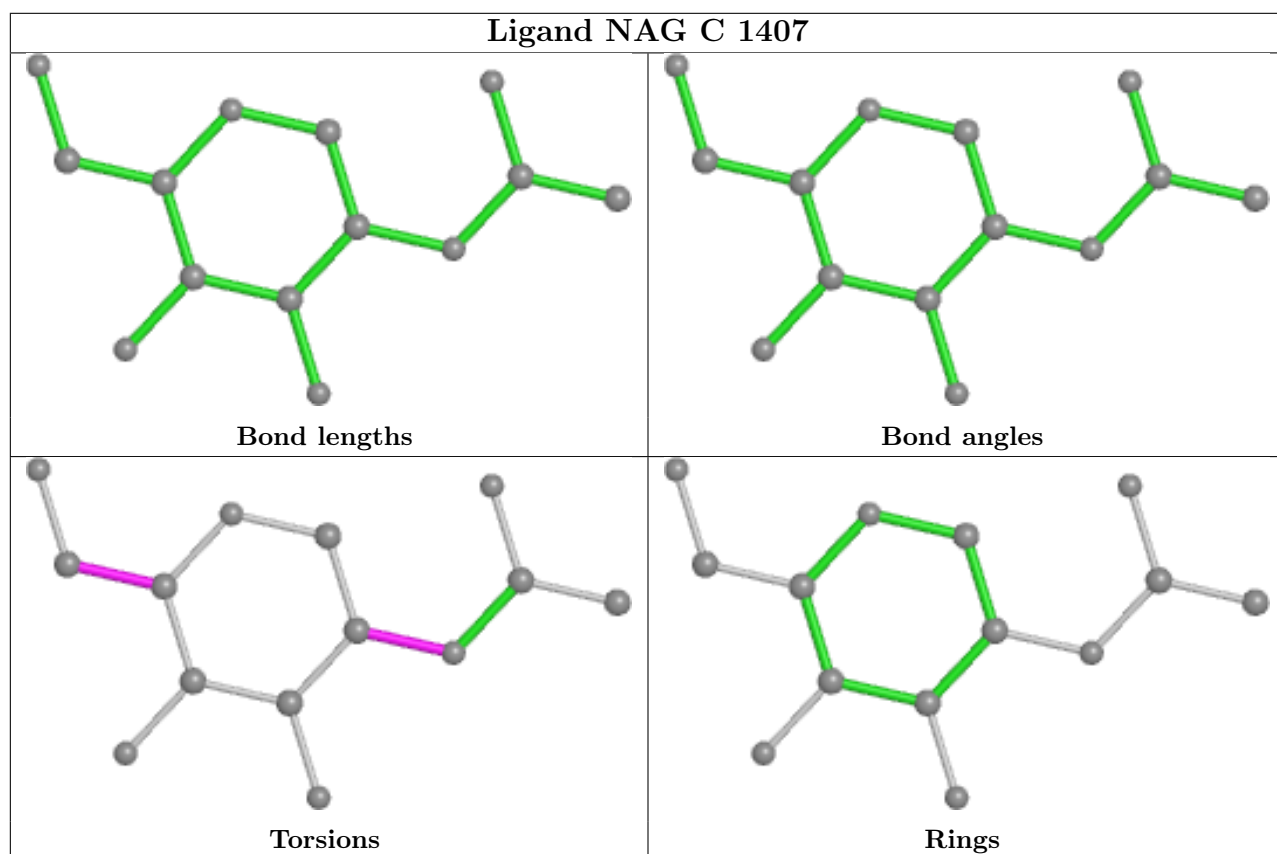
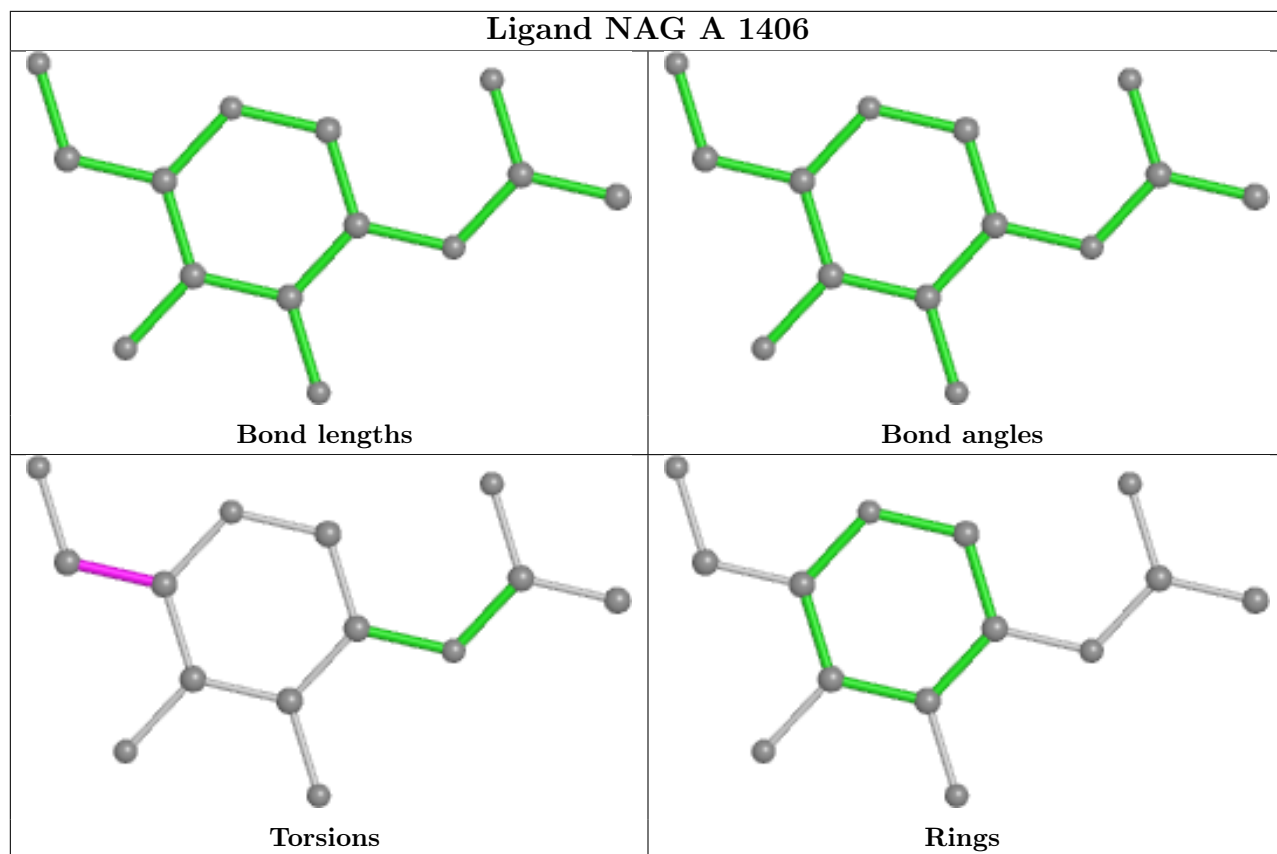


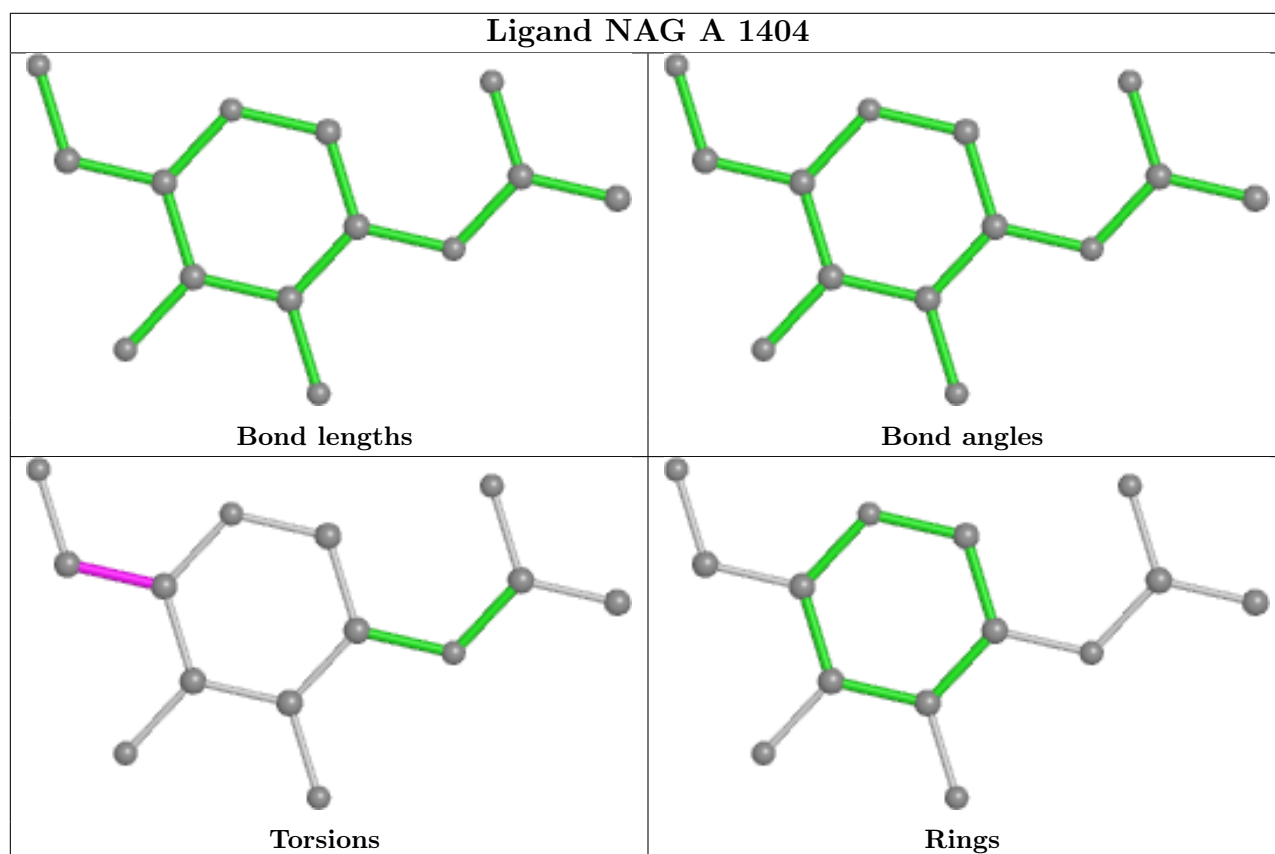
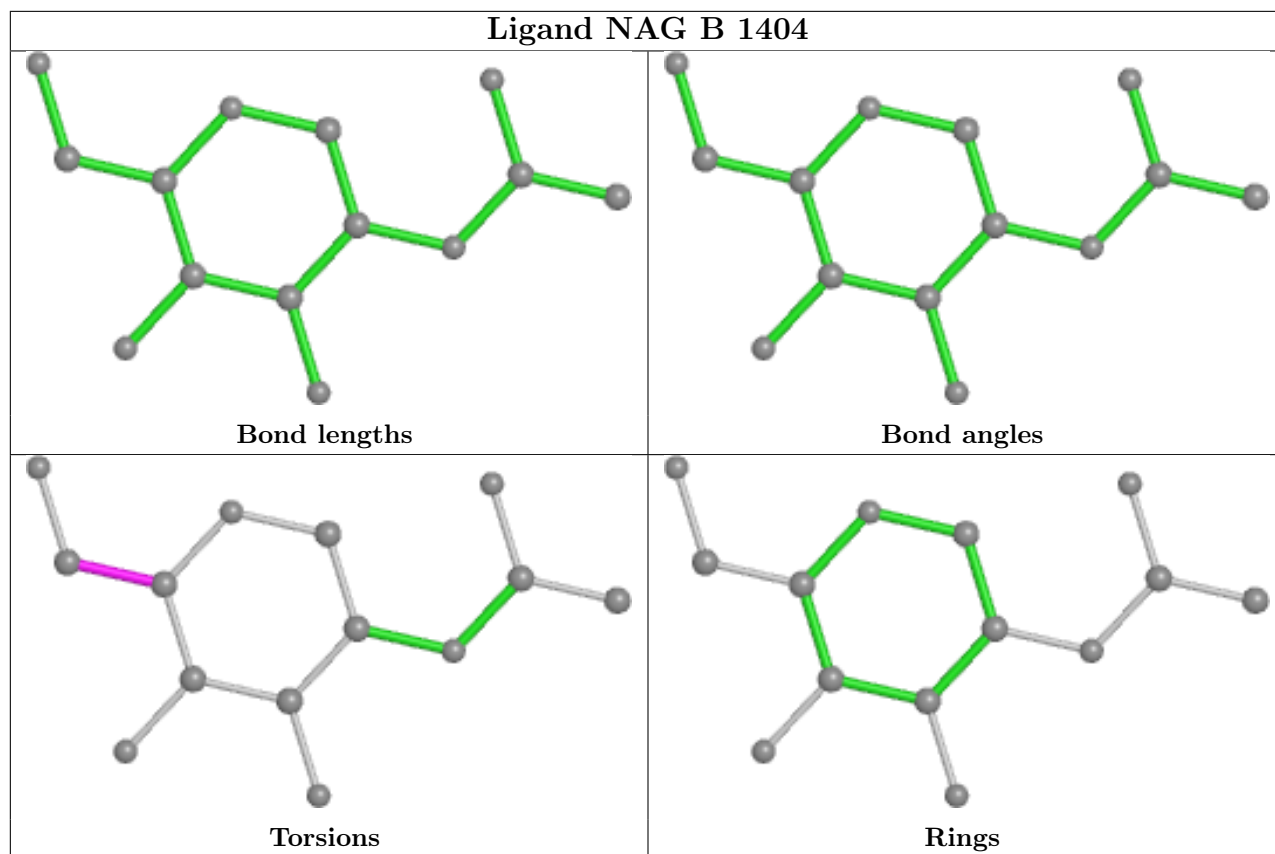


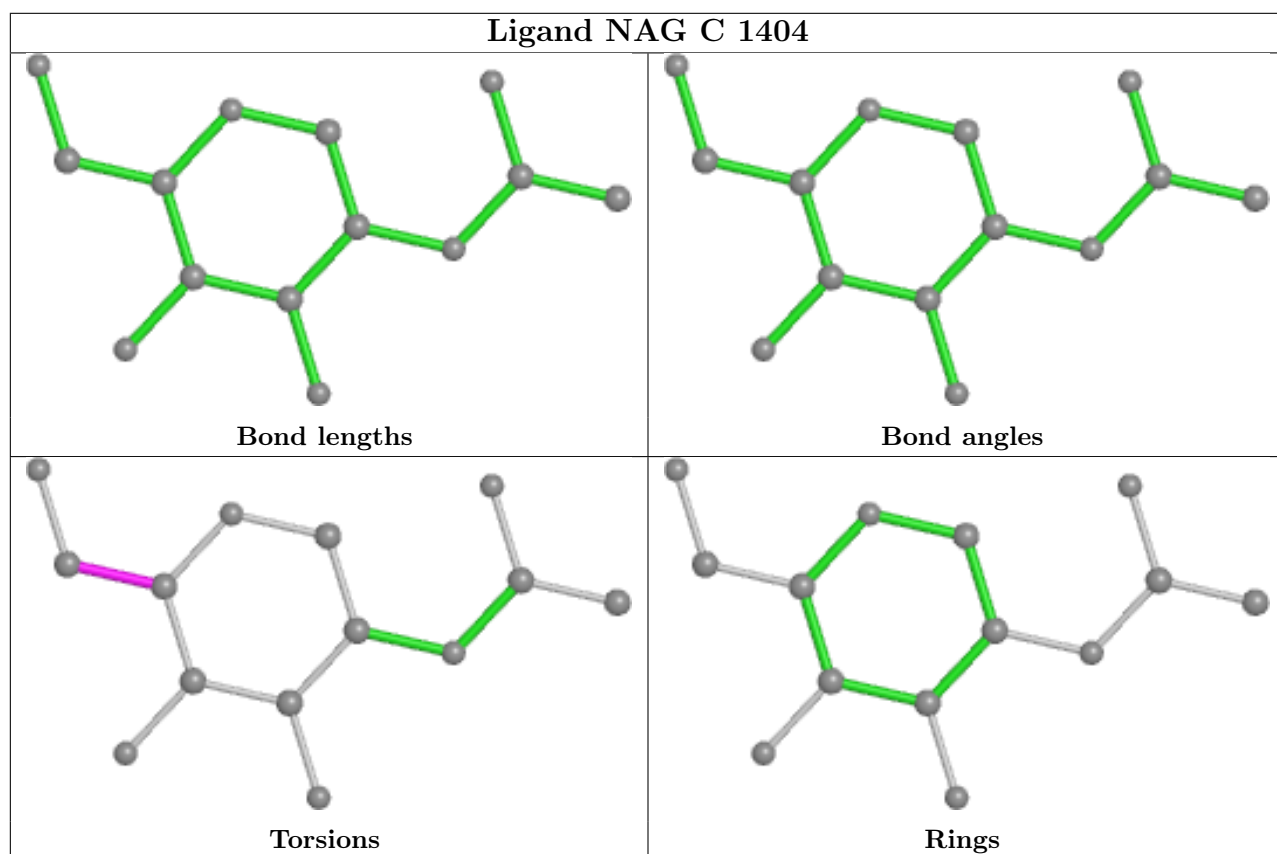
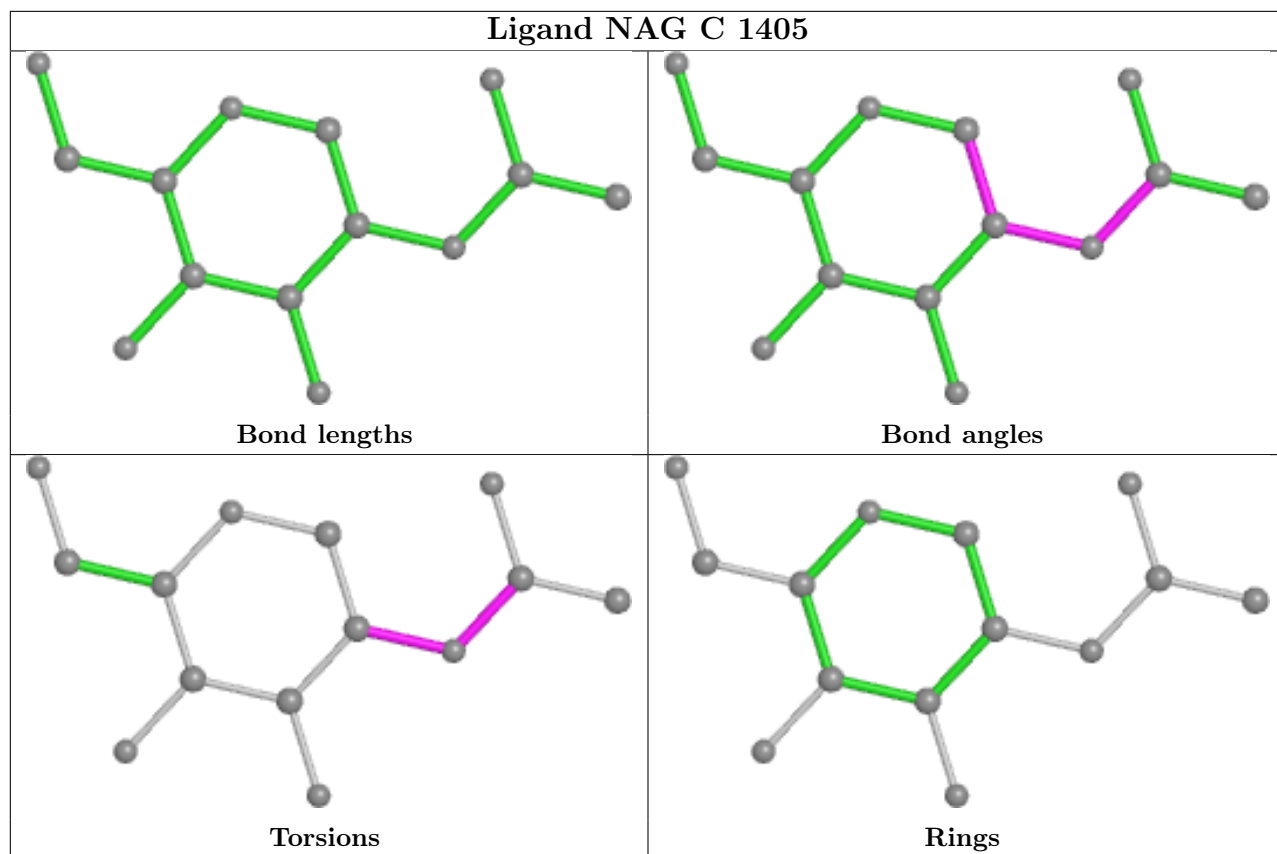


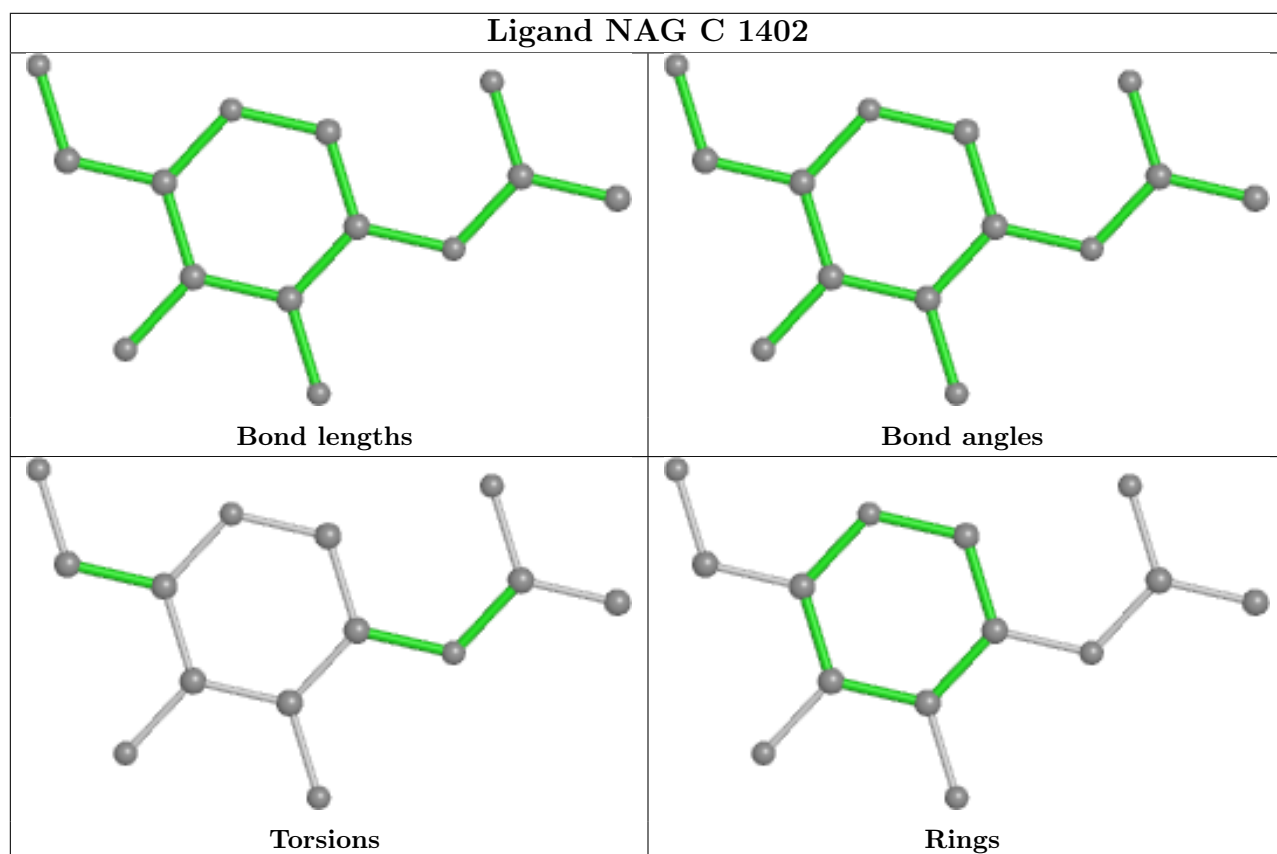
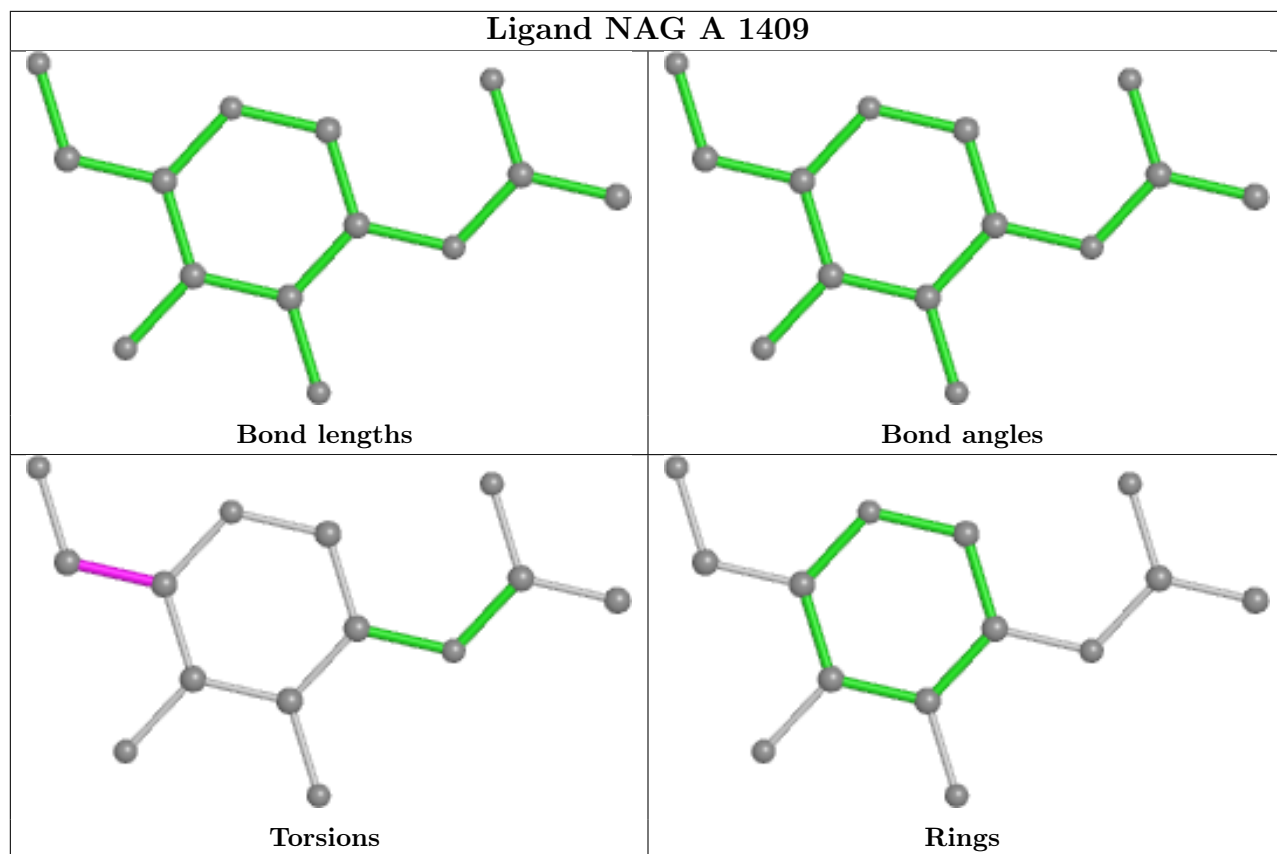




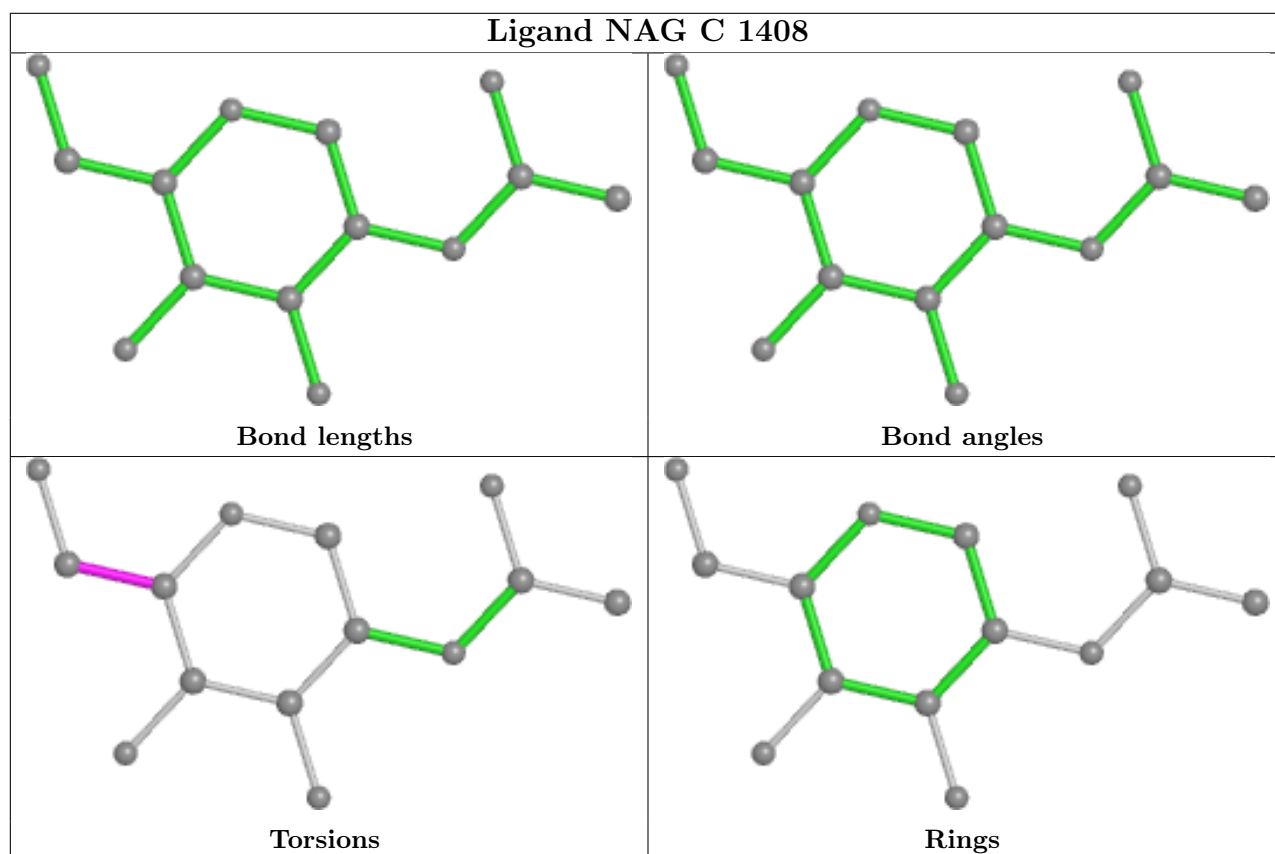
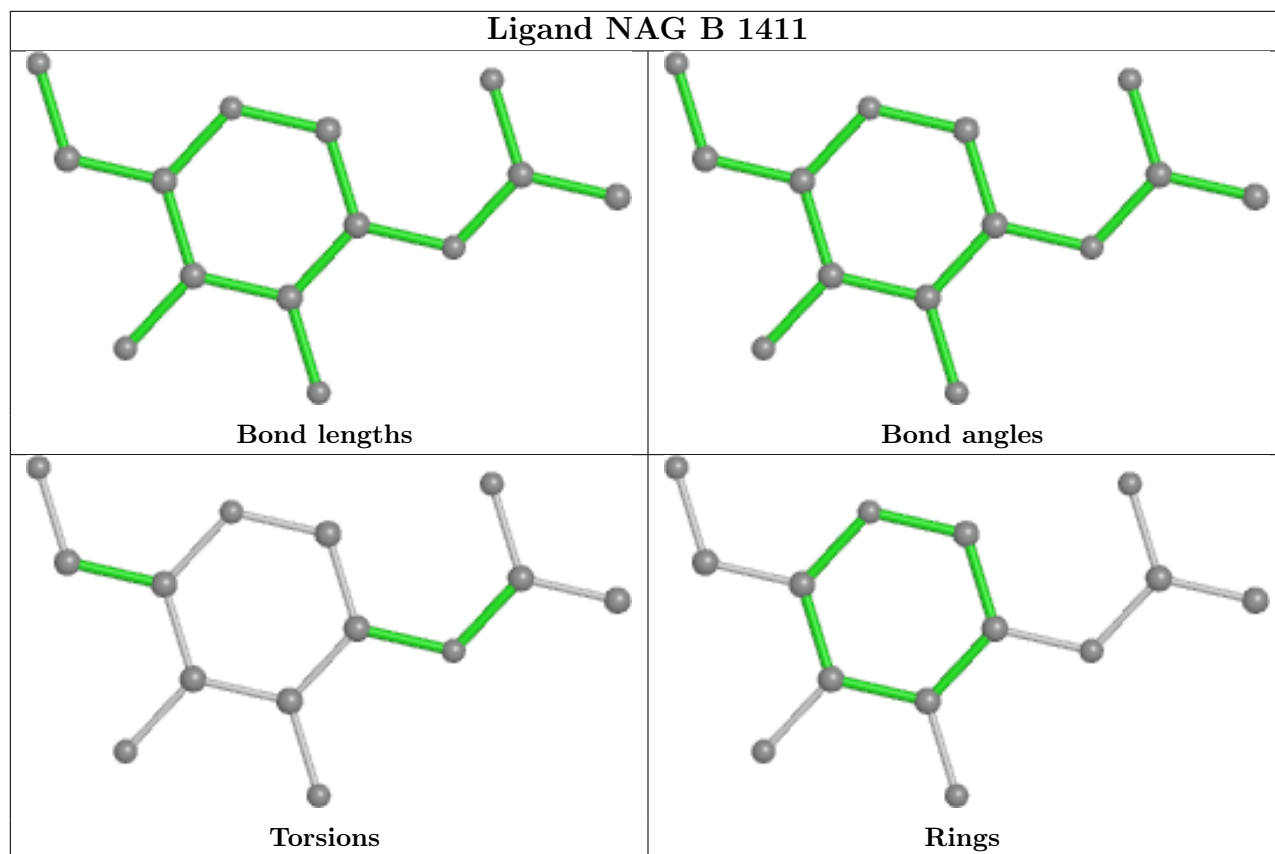


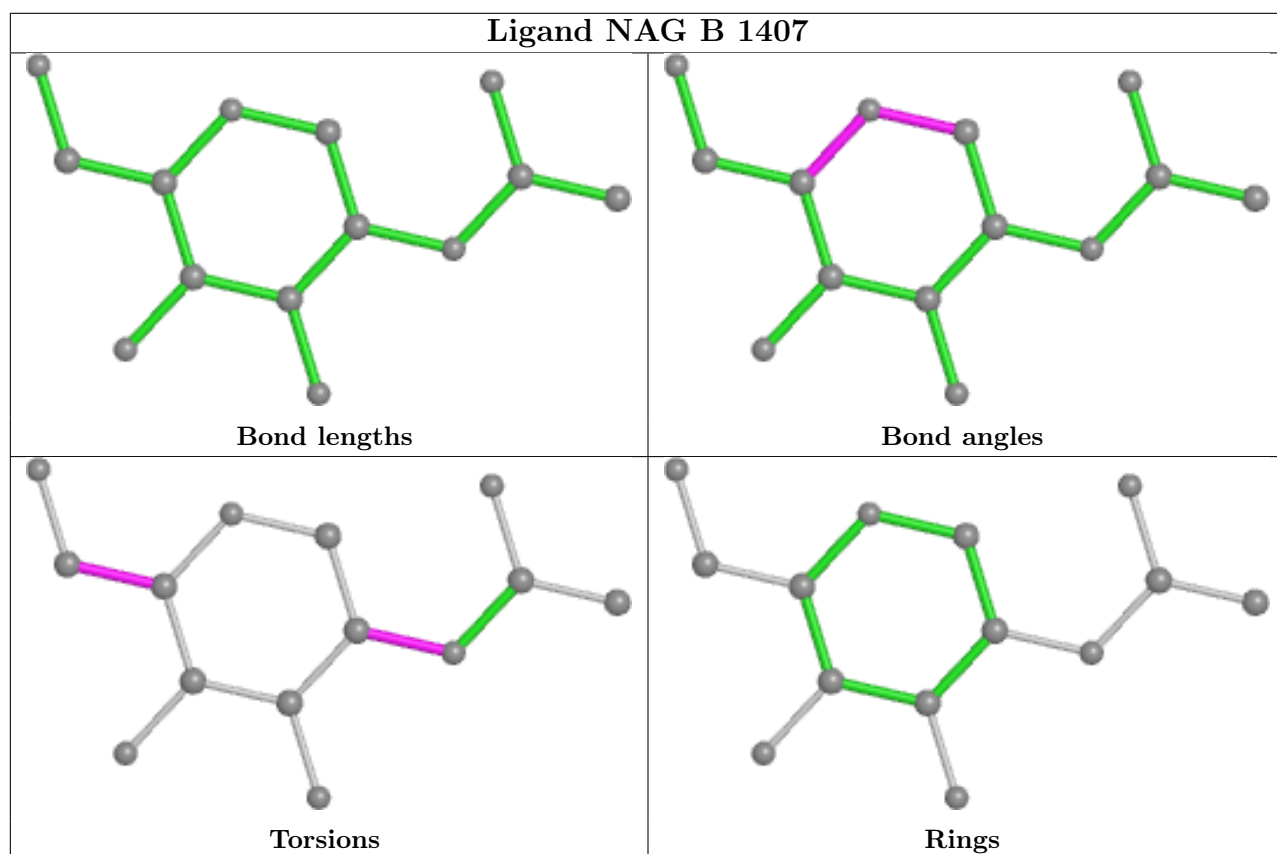
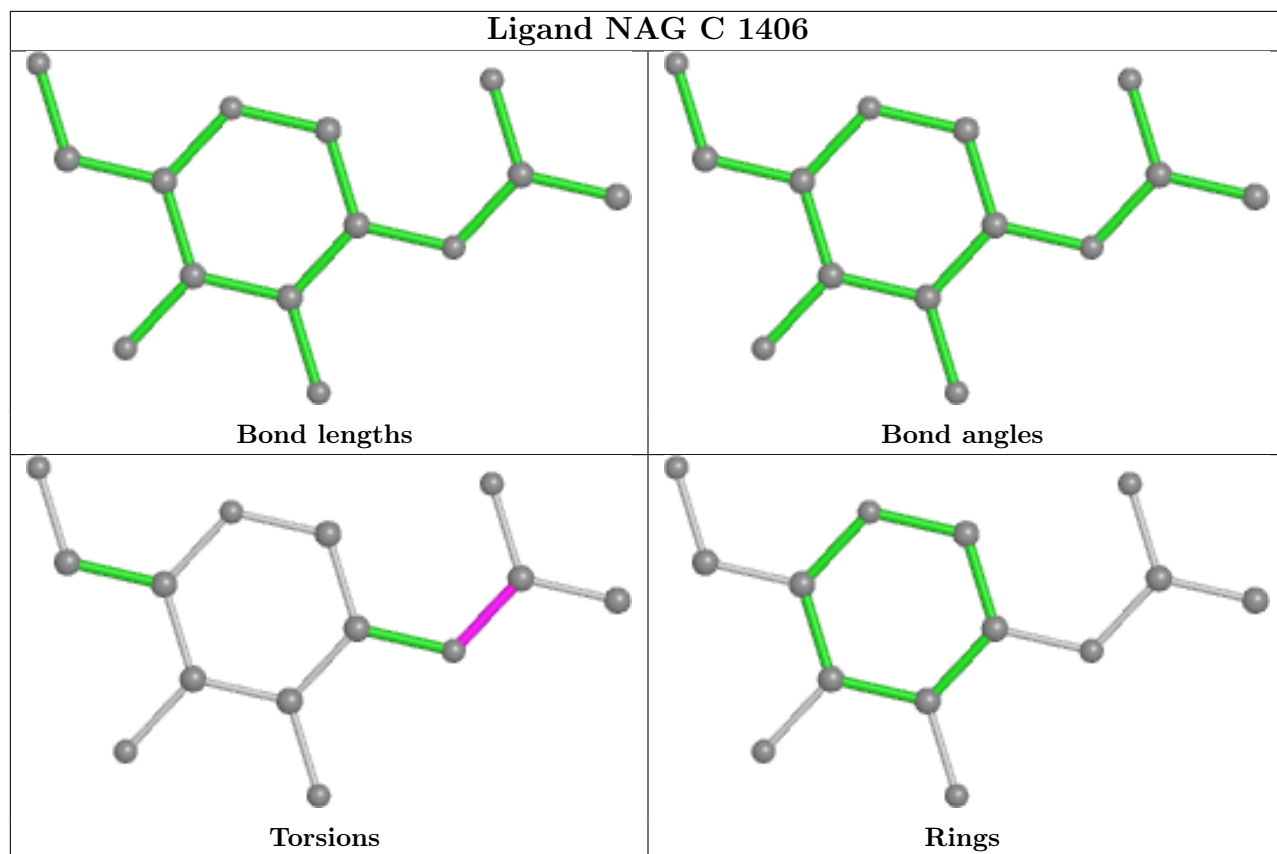


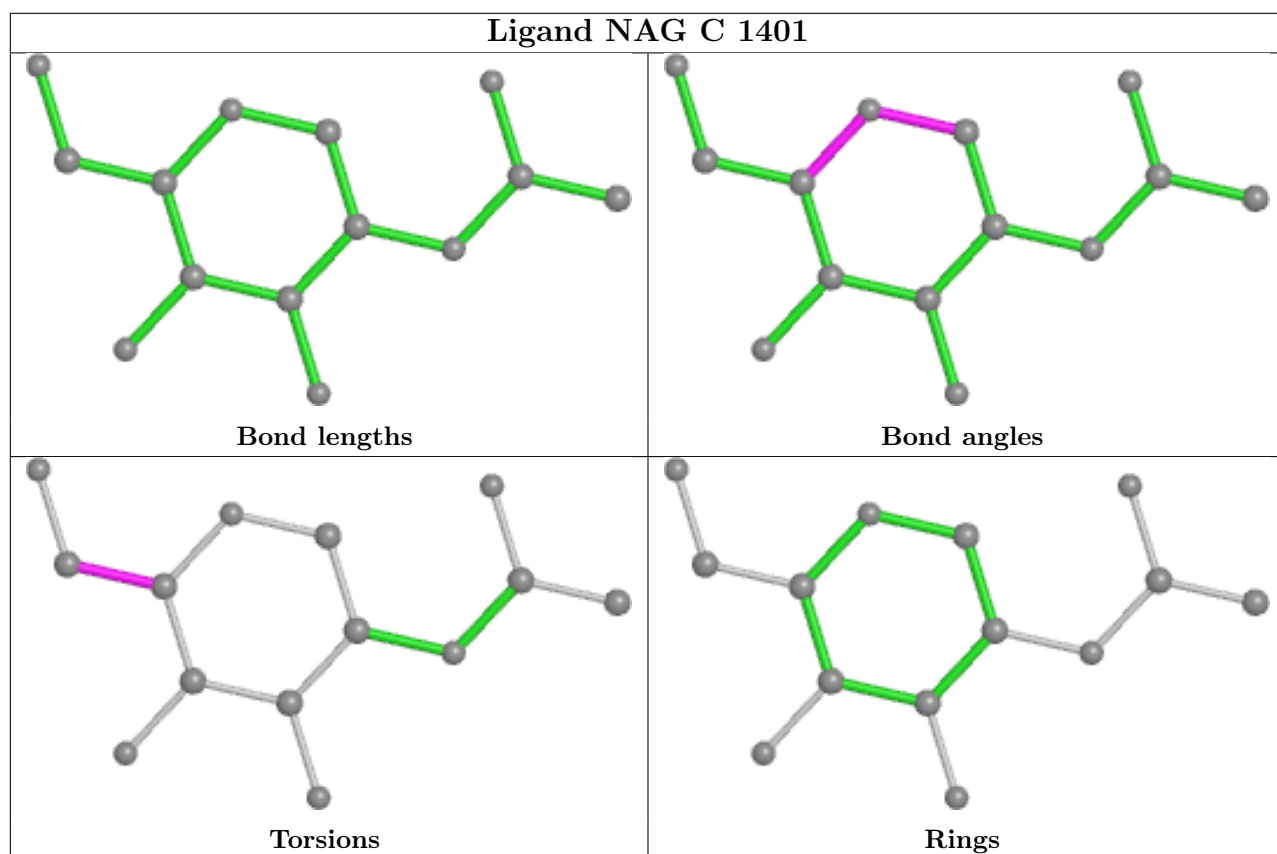
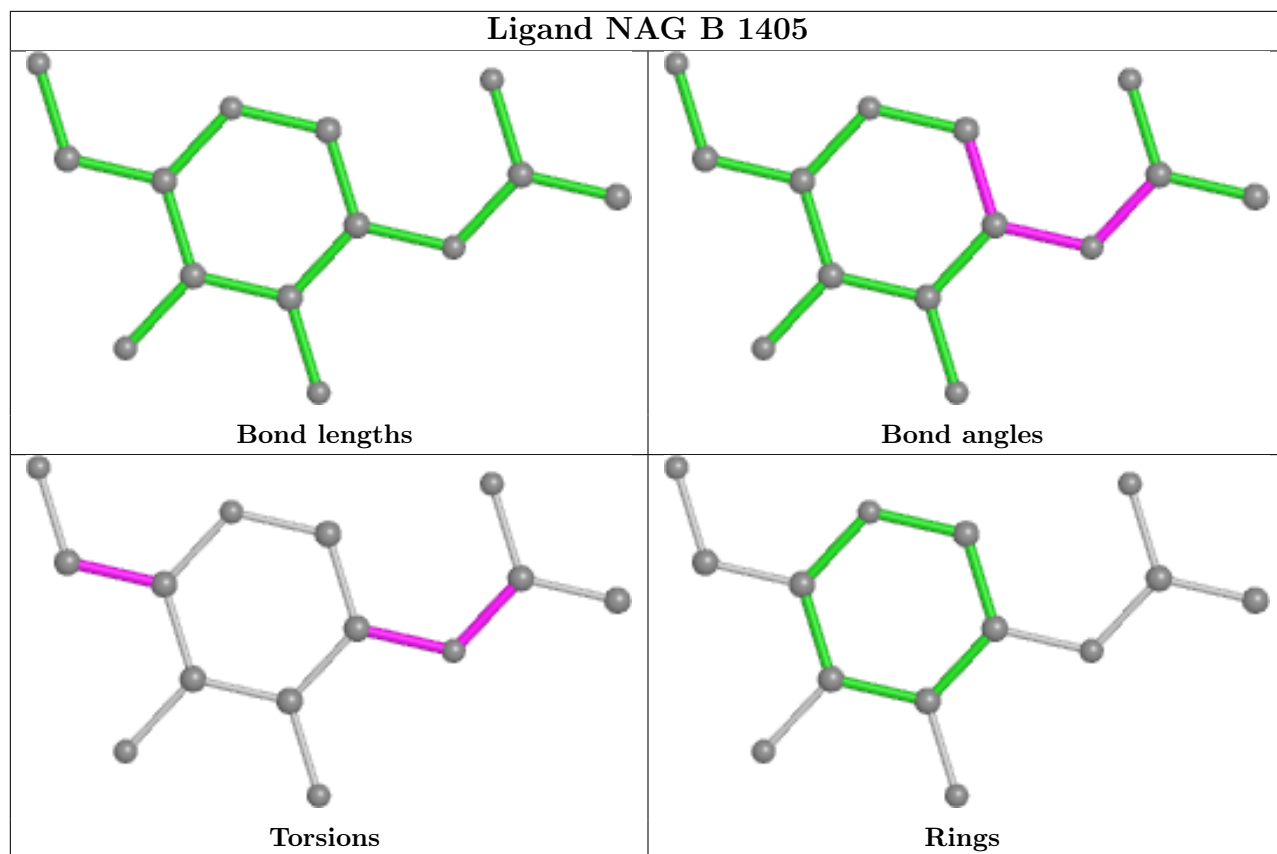


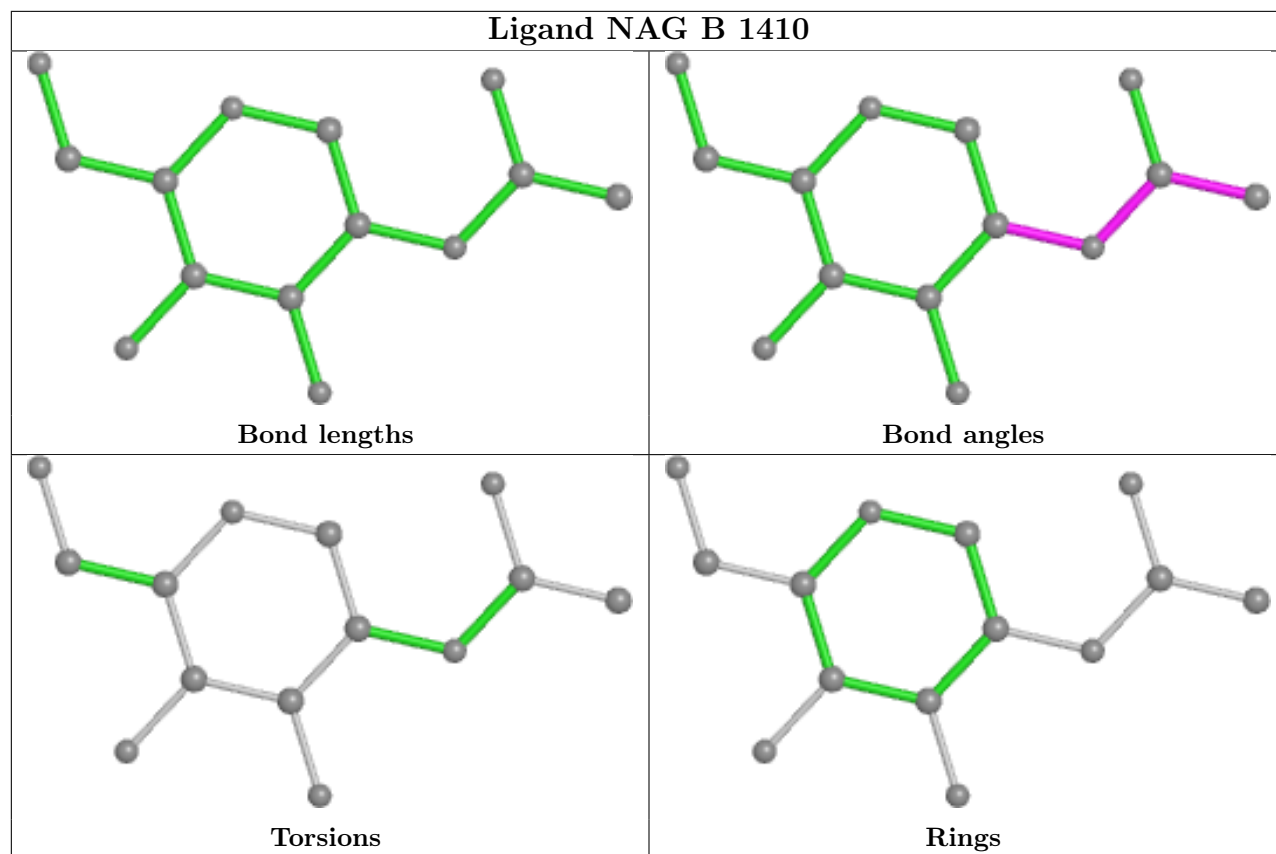












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

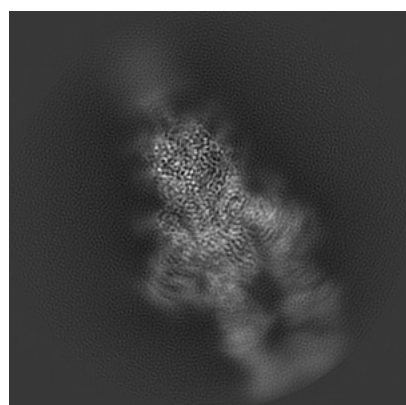
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30516. These allow visual inspection of the internal detail of the map and identification of artifacts.

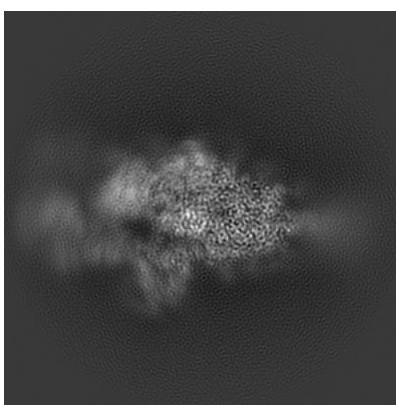
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

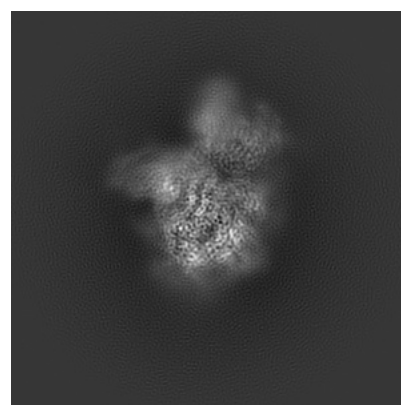
#### 6.1.1 Primary map



X



Y

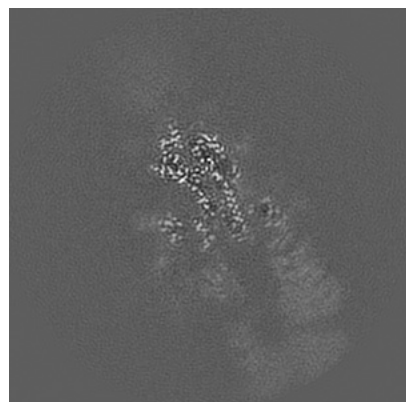


Z

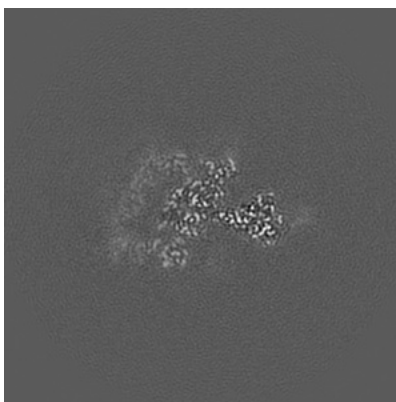
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

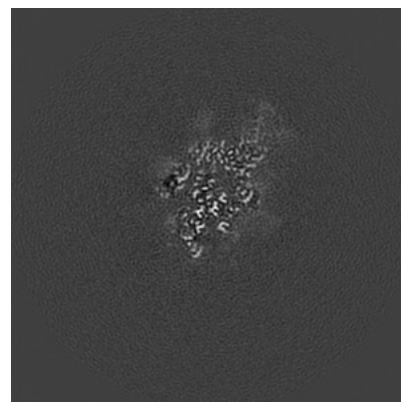
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

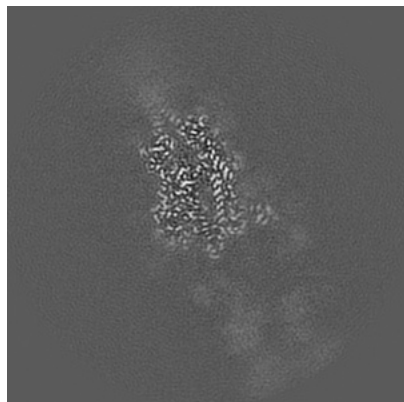


Z Index: 144

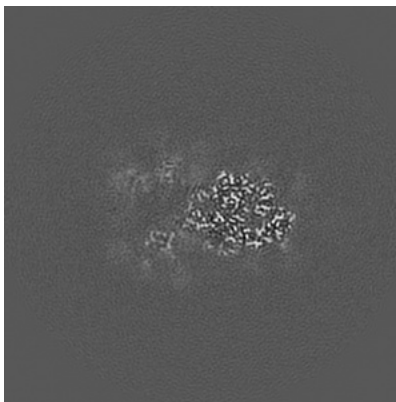
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

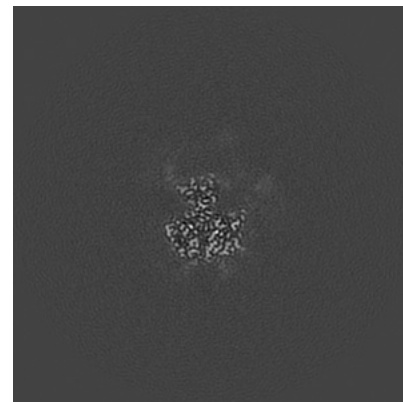
### 6.3.1 Primary map



X Index: 131



Y Index: 133



Z Index: 168

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

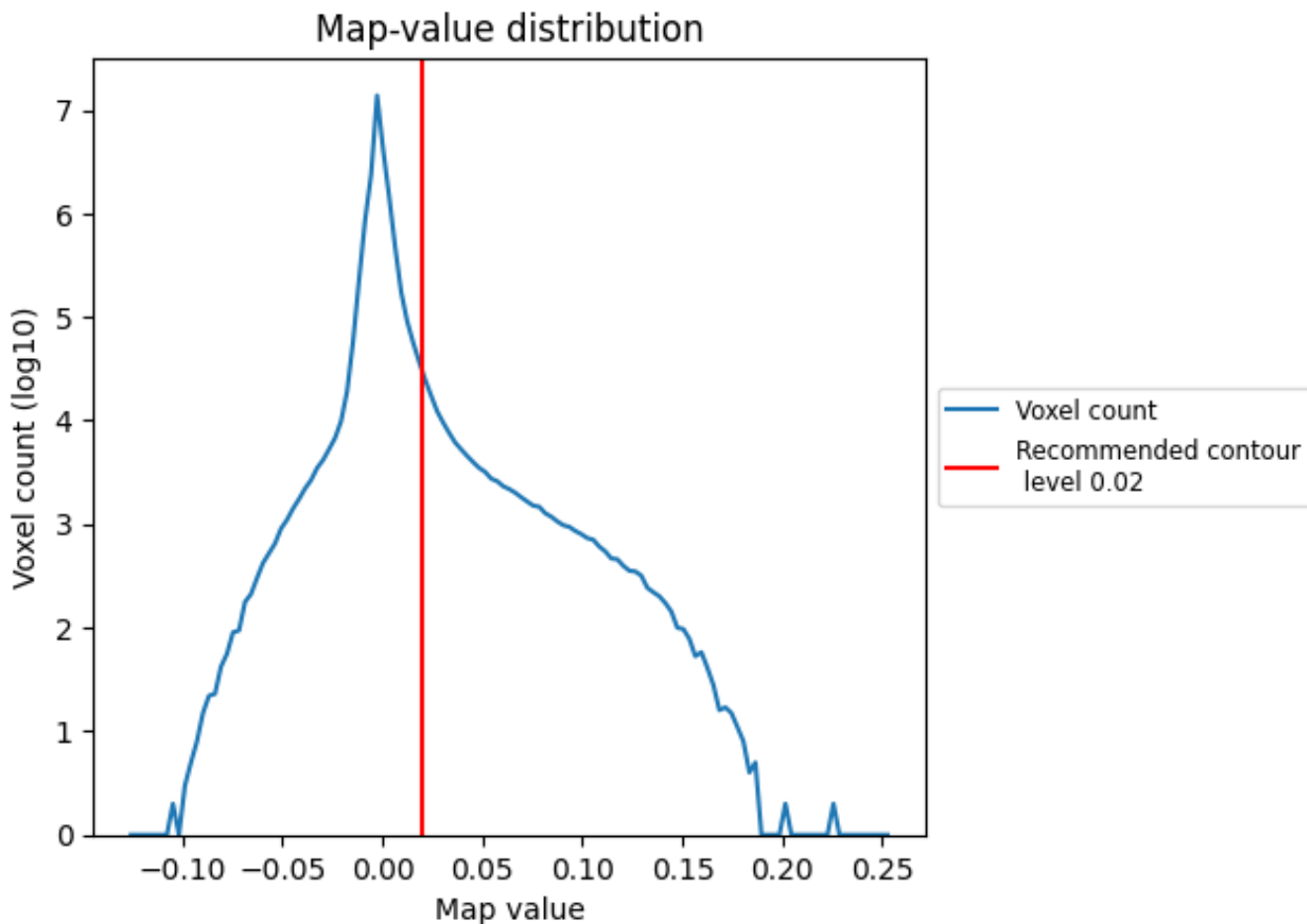
## 6.5 Mask visualisation

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.

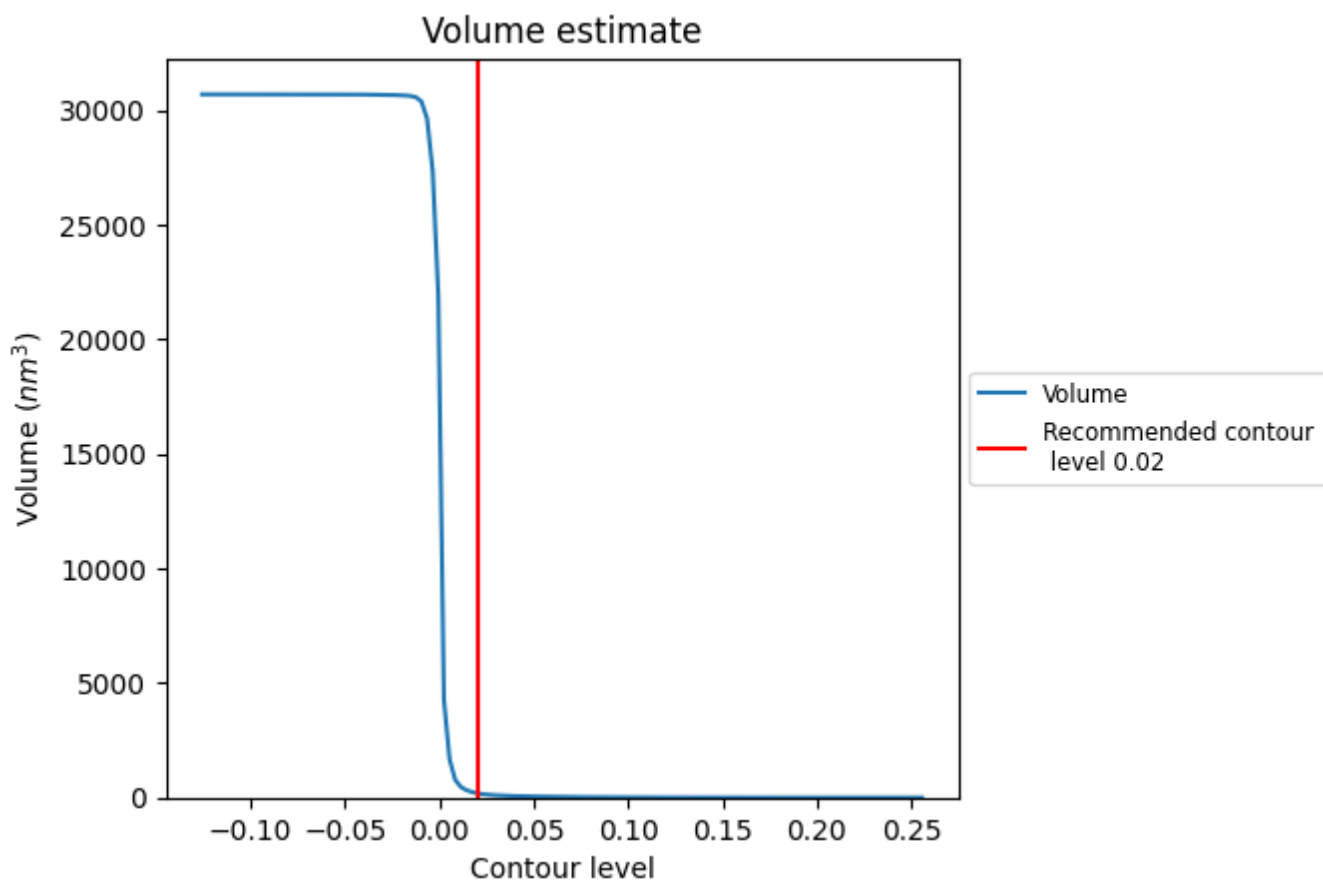
### 7.1 Map-value distribution [i](#)



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.



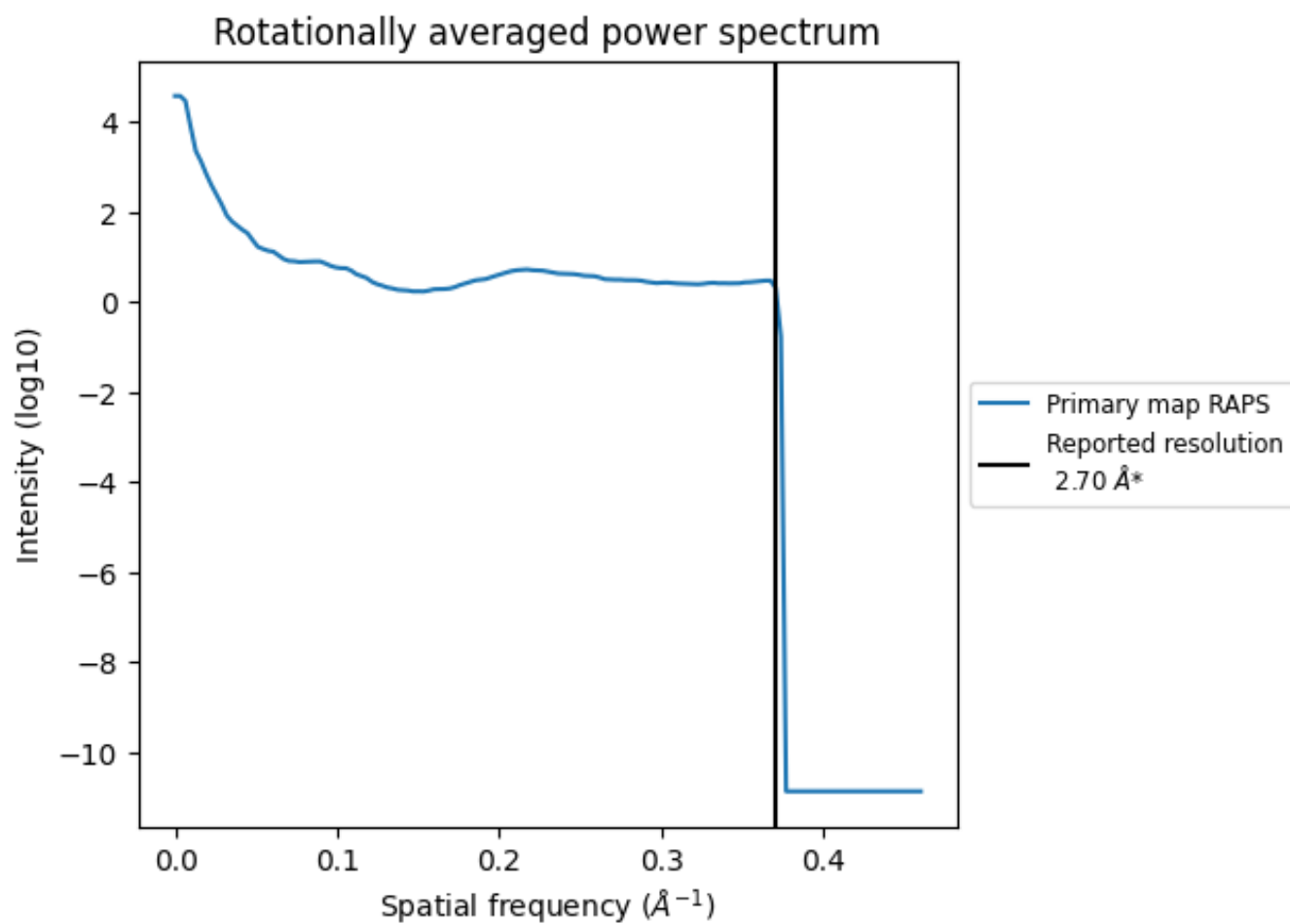
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm<sup>3</sup>; this corresponds to an approximate mass of 170 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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

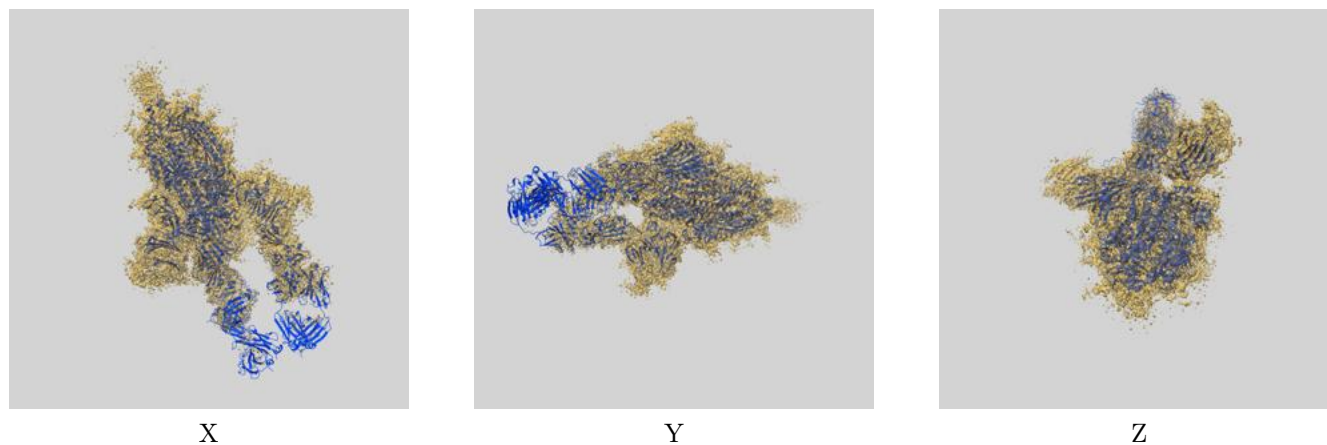
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

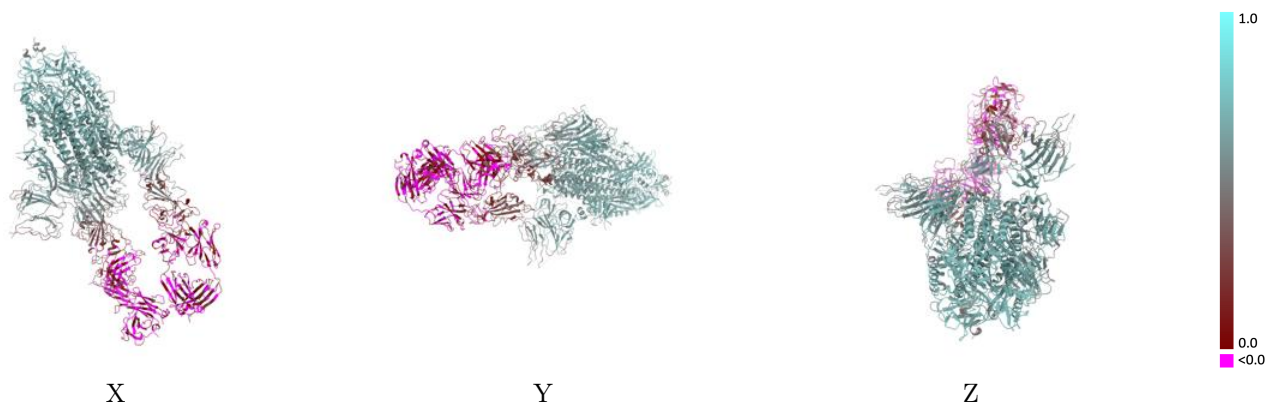
This section contains information regarding the fit between EMDB map EMD-30516 and PDB model 7CZT. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



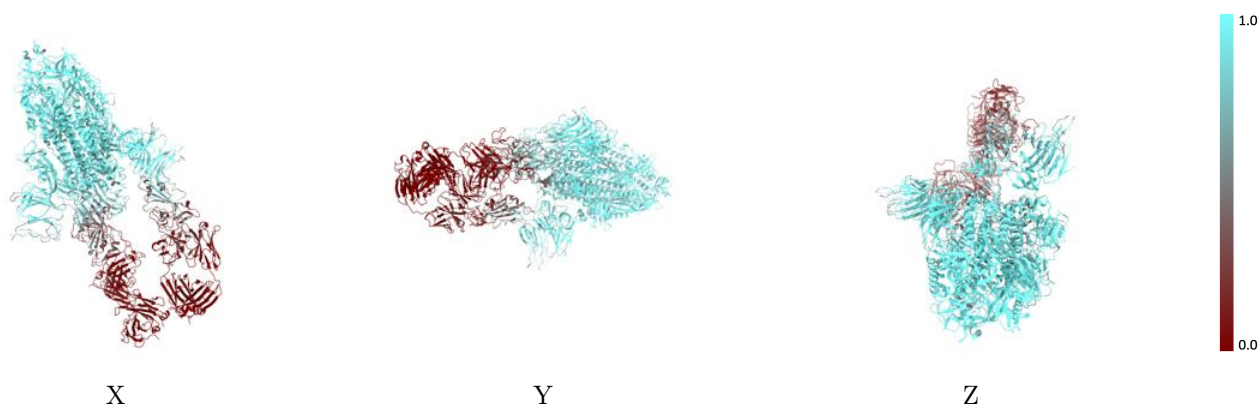
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



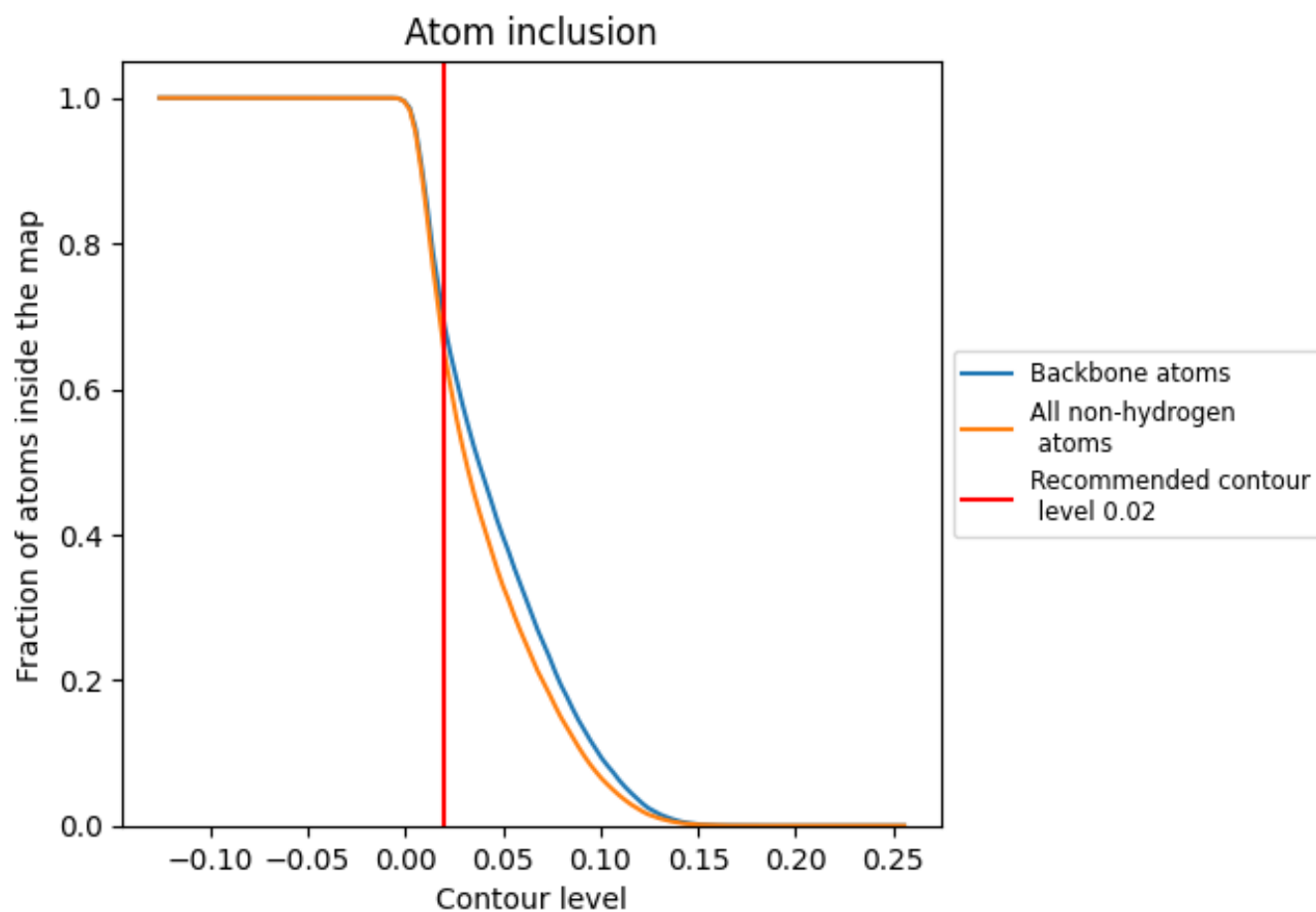
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 65% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6515	 0.4400
A	 0.8256	 0.5460
B	 0.8391	 0.5880
C	 0.7925	 0.5240
D	 0.6786	 0.4890
E	 0.3929	 0.3560
F	 0.9286	 0.5770
G	 0.7857	 0.4900
H	 0.0541	 0.0470
I	 0.0395	 0.0290
J	 0.7143	 0.5740
K	 0.8929	 0.5630
L	 0.0644	 0.0330
M	 0.0300	 0.0320
N	 0.8571	 0.5360
O	 0.3929	 0.3870
P	 0.5357	 0.3540
Q	 0.9286	 0.5360
R	 0.7857	 0.5840
S	 0.8929	 0.5210
T	 0.8214	 0.5270
U	 0.6429	 0.3350
V	 0.2500	 0.1940
W	 0.6071	 0.4110
X	 0.9643	 0.5840
Y	 0.7857	 0.4850
Z	 0.5357	 0.4190
a	 0.8571	 0.5480
b	 0.6429	 0.5090

